



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 10:08 AM UTC

PDB ID : 7QZR / pdb_00007qzr
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

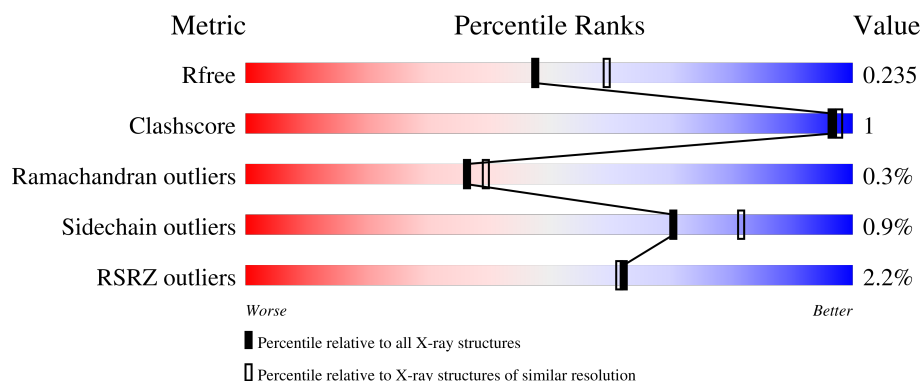
1 Overall quality at a glance

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.



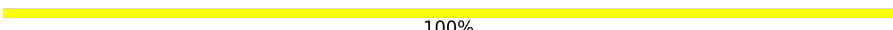
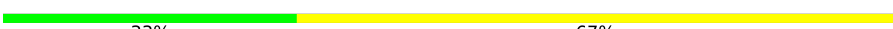
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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 $\leq 5\%$. 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	0% (Poor fit) 88% (Green) • 8% (Grey)
1	C	114	2% (Red) 87% (Green) 5% (Yellow) 8% (Grey)
2	B	467	2% (Red) 95% (Green) • (Yellow)
3	D	467	0% (Poor fit) 95% (Green) • • (Yellow)
4	E	102	6% (Red) 68% (Green) • 31% (Grey)

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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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	PO4	B	804	-	X	-	-

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.

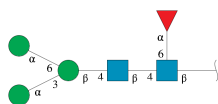
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	70	Total	C	H	N	O	546	0	0
			1112	357	546	95	114			
4	F	69	Total	C	H	N	O	531	0	0
			1091	352	531	95	113			

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



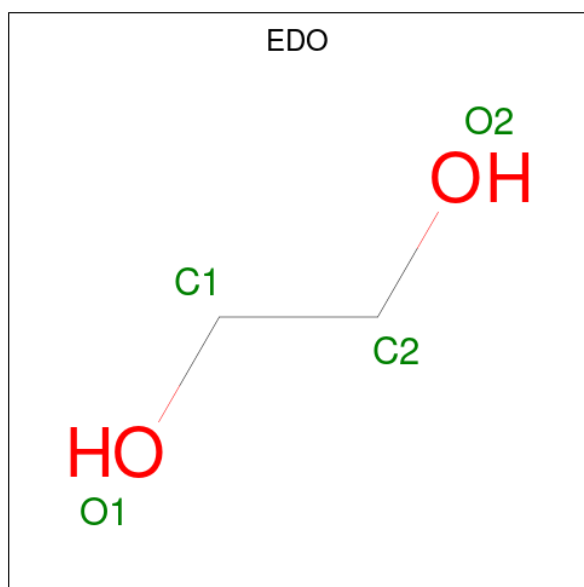
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	2	Total	C	H	N	O	25	0	0
			53	16	25	2	10			
5	H	2	Total	C	H	N	O	25	0	0
			53	16	25	2	10			
5	J	2	Total	C	H	N	O	25	0	0
			53	16	25	2	10			
5	K	2	Total	C	H	N	O	25	0	0
			53	16	25	2	10			

- 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.



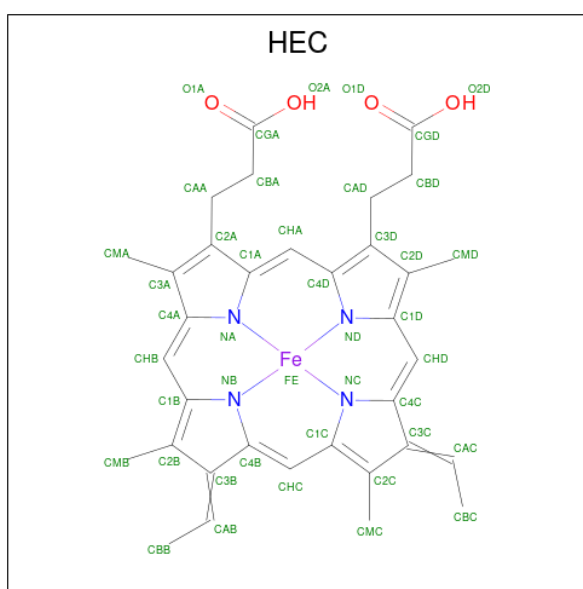
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	I	6	Total	C	H	N	O	61	0	0
			132	40	61	2	29			
6	L	6	Total	C	H	N	O	61	0	0
			132	40	61	2	29			

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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 (CCD ID: 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 (CCD ID: CL) (formula: Cl).

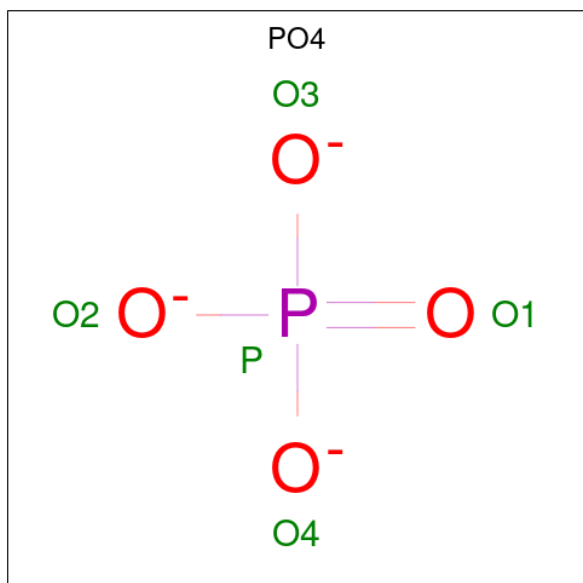
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Cl 1 1	0	0
9	C	1	Total Cl 1 1	0	0

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest"

by depositor).

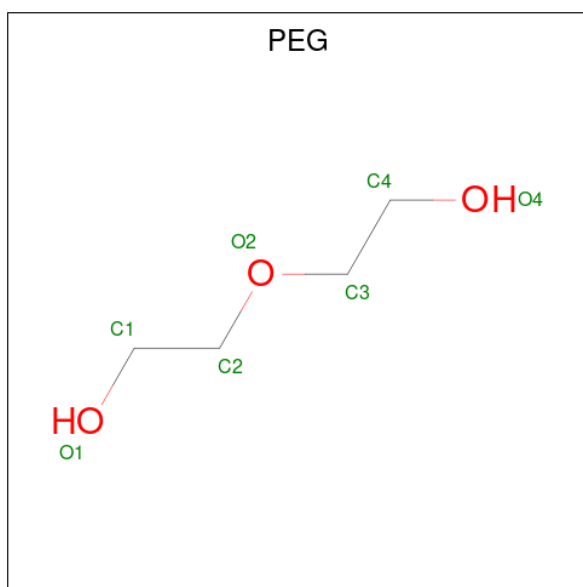
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	Ca	0	0
			1	1		
10	D	1	Total	Ca	0	0
			1	1		

- Molecule 11 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 12 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

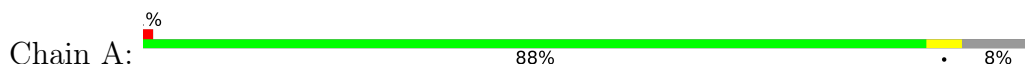
- Molecule 13 is water.

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

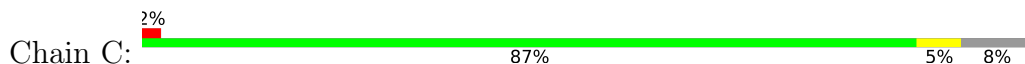
3 Residue-property plots [i](#)

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.

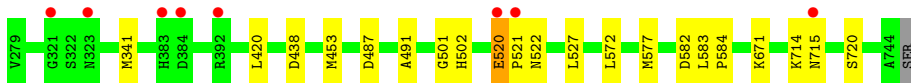
- Molecule 1: Myeloperoxidase light chain



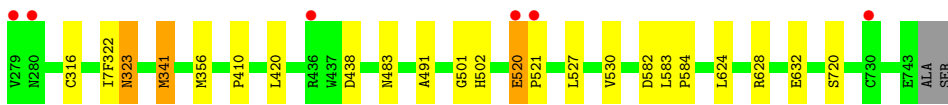
- Molecule 1: Myeloperoxidase light chain



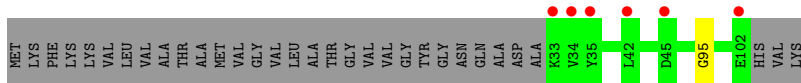
- Molecule 2: Myeloperoxidase heavy chain



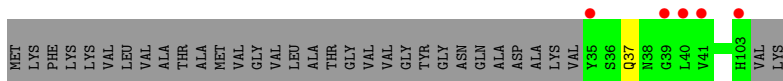
- Molecule 3: Myeloperoxidase heavy chain



- Molecule 4: Exported protein



- Molecule 4: Exported protein



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



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



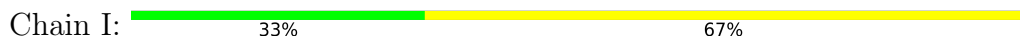
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- 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



- 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



MAG1
MAG2
BM/A3
MAN4
MAN5
ENC6

4 Data and refinement statistics

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) 82.3 (19.81-2.18)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 2CO, CA, HEC, MAN, PO4, PEG, I7F, CL, BMA, NAG, CSO, FUC, EDO

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	0.77	0/867	1.06	1/1181 (0.1%)
1	C	0.76	0/867	1.01	0/1181
2	B	0.79	1/3810 (0.0%)	1.00	4/5168 (0.1%)
3	D	0.80	1/3798 (0.0%)	1.01	3/5150 (0.1%)
4	E	0.73	0/575	0.98	1/773 (0.1%)
4	F	0.69	0/570	1.02	0/767
All	All	0.78	2/10487 (0.0%)	1.01	9/14220 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	453	MET	SD-CE	-5.13	1.66	1.79
3	D	323	ASN	CA-C	5.07	1.63	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	323	ASN	N-CA-CB	7.35	122.99	110.50
2	B	438	ASP	CA-CB-CG	6.17	118.77	112.60
1	A	186	PRO	N-CA-C	5.22	120.72	113.98
4	E	95	GLY	N-CA-C	5.21	121.99	115.21
3	D	483	ASN	OD1-CG-ND2	-5.18	117.42	122.60
2	B	487	ASP	CA-CB-CG	5.11	117.71	112.60
3	D	438	ASP	CA-CB-CG	5.06	117.66	112.60
2	B	714	LYS	CA-C-N	5.01	131.11	121.54
2	B	714	LYS	C-N-CA	5.01	131.11	121.54

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	5	0
2	B	3733	3728	3724	8	0
3	D	3728	3723	3715	10	0
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	1	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	22	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 (22) 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:356:MET:HE2	3:D:356:MET:HA	1.93	0.49
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
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
1:C:262:ASP:HB2	3:D:341:MET:HE3	2.03	0.41
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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	30	31
3	D	461/467 (99%)	445 (96%)	14 (3%)	2 (0%)	30	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	36	39

All (4) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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%)	405 (99%)	5 (1%)	63	75
3	D	409/410 (100%)	405 (99%)	4 (1%)	68	79
4	E	62/85 (73%)	62 (100%)	0	100	100
4	F	61/85 (72%)	60 (98%)	1 (2%)	55	68
All	All	1122/1185 (95%)	1112 (99%)	10 (1%)	70	81

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	341	MET
2	B	420	LEU
2	B	522	ASN
2	B	527	LEU
2	B	577	MET
3	D	341	MET

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Mol	Chain	Res	Type
3	D	420	LEU
3	D	527	LEU
3	D	632	GLU
4	F	37	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
2	B	517	GLN
2	B	575	GLN
2	B	639	ASN
2	B	682	ASN
2	B	692	GLN
2	B	696	GLN
1	C	192	ASN
3	D	367	GLN
3	D	383	HIS
3	D	514	ASN
3	D	562	GLN
3	D	589	GLN
3	D	682	ASN
3	D	706	ASN
3	D	737	ASN
4	E	38	ASN
4	F	93	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	CSO	D	316	3	3,6,7	0.78	0	1,6,8	3.08	1 (100%)
3	I7F	D	322	3	5,6,7	1.50	1 (20%)	0,6,8	-	-
2	2CO	B	316	2	3,7,8	0.55	0	1,7,9	1.21	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	CSO	D	316	3	-	0/1/5/7	-
3	I7F	D	322	3	-	1/1/5/7	-
2	2CO	B	316	2	-	0/1/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	322	I7F	O1-OG	-2.77	1.42	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	316	CSO	CB-CA-C	-3.08	102.42	110.80

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	322	I7F	C-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

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	0.27	0	17,19,21	0.88	1 (5%)
5	NAG	G	2	5	14,14,15	0.28	0	17,19,21	0.57	0
5	NAG	H	1	5,2	14,14,15	0.26	0	17,19,21	0.78	1 (5%)
5	NAG	H	2	5	14,14,15	0.29	0	17,19,21	0.57	0
6	NAG	I	1	6,2	14,14,15	0.29	0	17,19,21	1.10	1 (5%)
6	NAG	I	2	6	14,14,15	0.29	0	17,19,21	0.84	1 (5%)
6	BMA	I	3	6	11,11,12	0.24	0	15,15,17	0.62	0
6	MAN	I	4	6	11,11,12	0.70	0	15,15,17	1.26	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	0.31	0
5	NAG	J	1	3,5	14,14,15	0.29	0	17,19,21	0.91	1 (5%)
5	NAG	J	2	5	14,14,15	0.27	0	17,19,21	0.54	0
5	NAG	K	1	3,5	14,14,15	0.31	0	17,19,21	0.90	1 (5%)
5	NAG	K	2	5	14,14,15	0.28	0	17,19,21	0.62	1 (5%)
6	NAG	L	1	3,6	14,14,15	0.31	0	17,19,21	1.04	1 (5%)
6	NAG	L	2	6	14,14,15	0.26	0	17,19,21	0.80	1 (5%)
6	BMA	L	3	6	11,11,12	0.25	0	15,15,17	0.74	0
6	MAN	L	4	6	11,11,12	0.65	0	15,15,17	1.10	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	0.45	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
5	NAG	G	2	5	-	1/6/23/26	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	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	1	NAG	O5-C1-C2	-4.19	104.81	111.29
6	L	1	NAG	O5-C1-C2	-3.80	105.42	111.29
6	I	4	MAN	C1-O5-C5	3.78	117.26	112.19
5	J	1	NAG	C1-O5-C5	3.34	116.66	112.19
5	K	1	NAG	O5-C1-C2	-3.21	106.32	111.29
5	G	1	NAG	C1-O5-C5	2.92	116.10	112.19
6	L	4	MAN	C1-O5-C5	2.78	115.91	112.19
6	L	4	MAN	C1-C2-C3	2.48	113.26	109.64
5	H	1	NAG	O5-C1-C2	-2.46	107.48	111.29
6	I	4	MAN	C1-C2-C3	2.43	113.18	109.64
6	L	2	NAG	C1-O5-C5	2.38	115.37	112.19
6	I	5	MAN	C1-O5-C5	2.35	115.34	112.19
6	I	2	NAG	C1-O5-C5	2.23	115.18	112.19
6	L	5	MAN	C1-O5-C5	2.12	115.03	112.19
5	K	2	NAG	O5-C1-C2	-2.10	108.03	111.29

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	2	NAG	O5-C5-C6-O6

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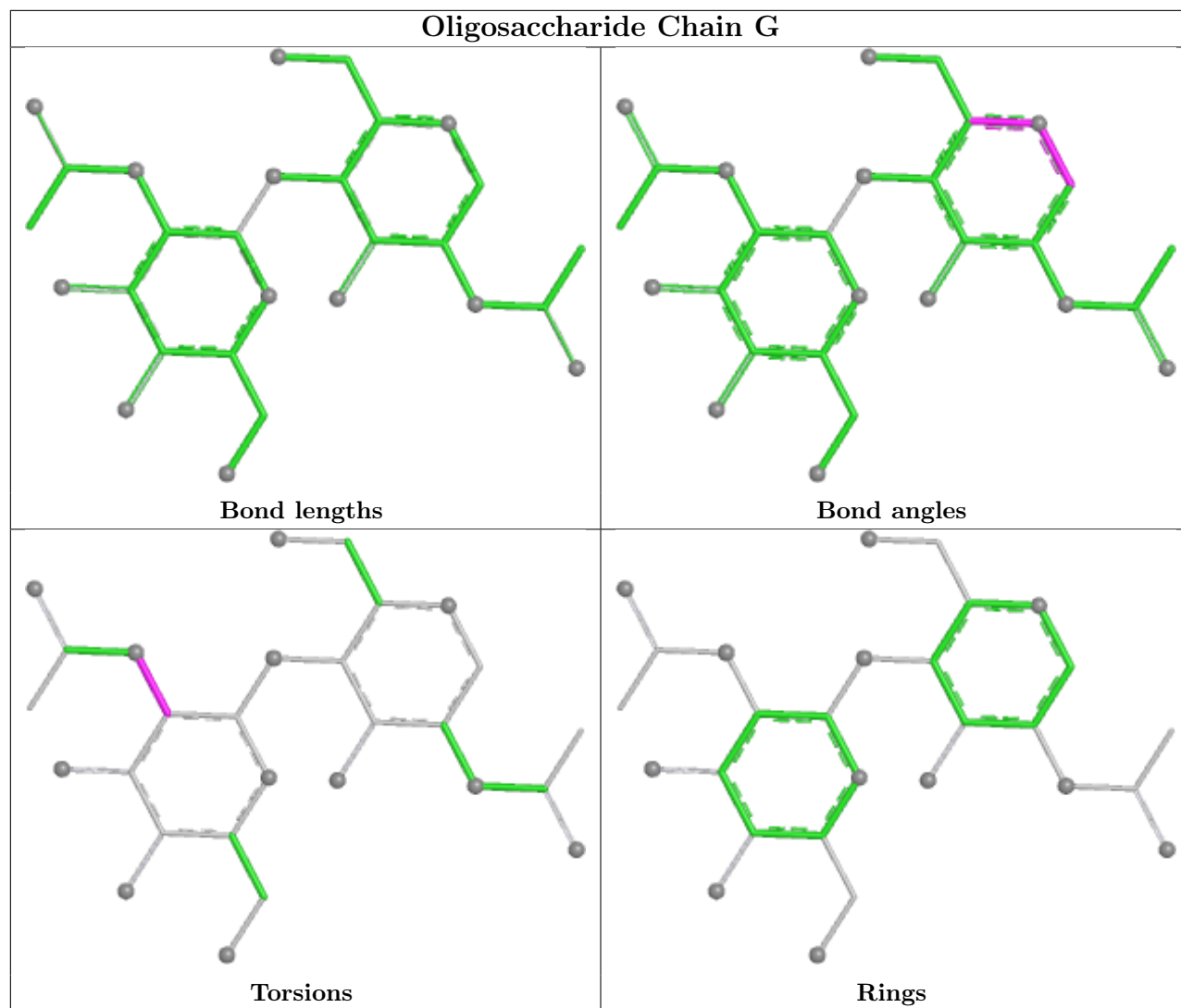
Mol	Chain	Res	Type	Atoms
5	K	1	NAG	O5-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
5	G	2	NAG	C1-C2-N2-C7
6	I	1	NAG	C1-C2-N2-C7
6	L	4	MAN	O5-C5-C6-O6

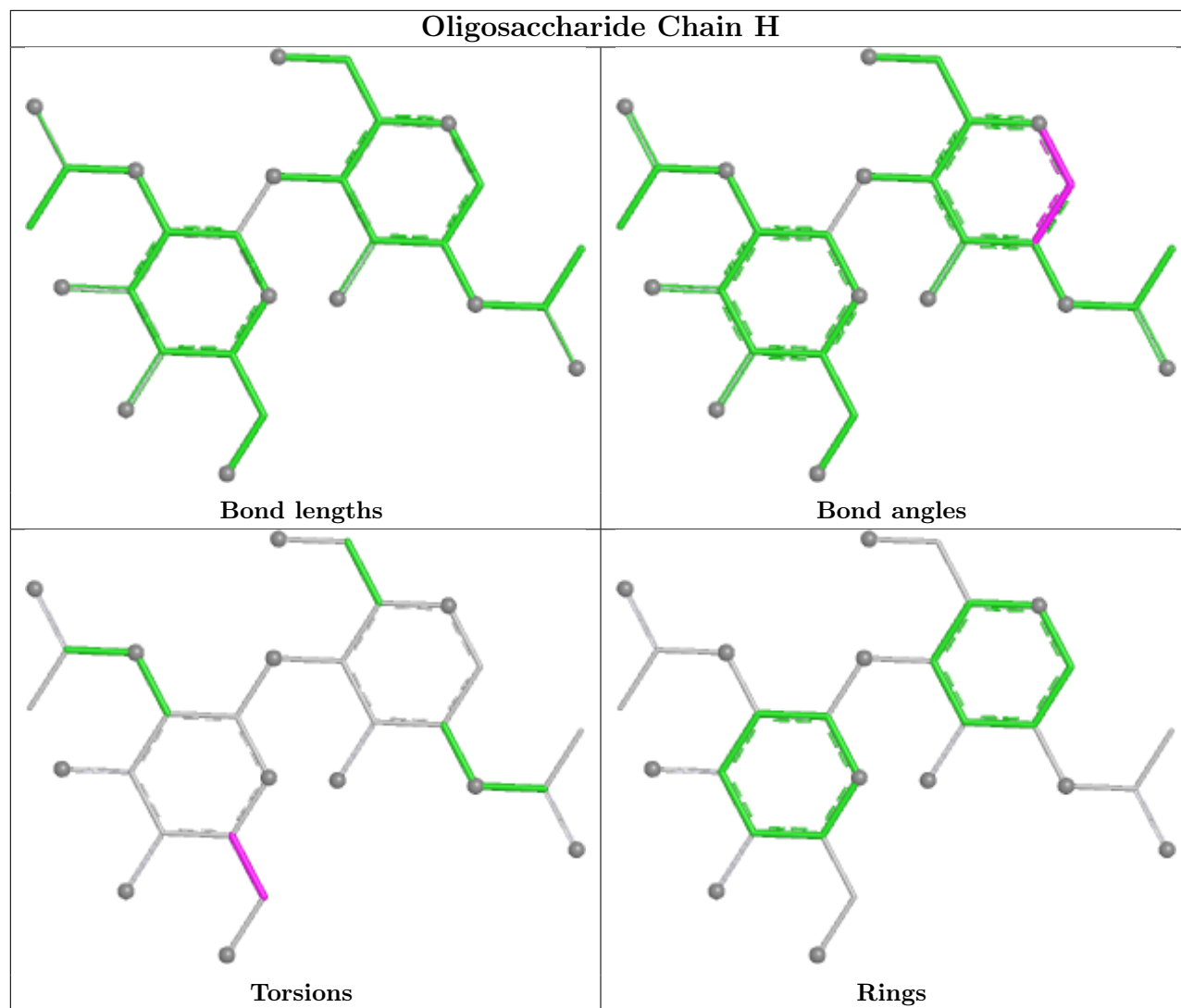
All (1) ring outliers are listed below:

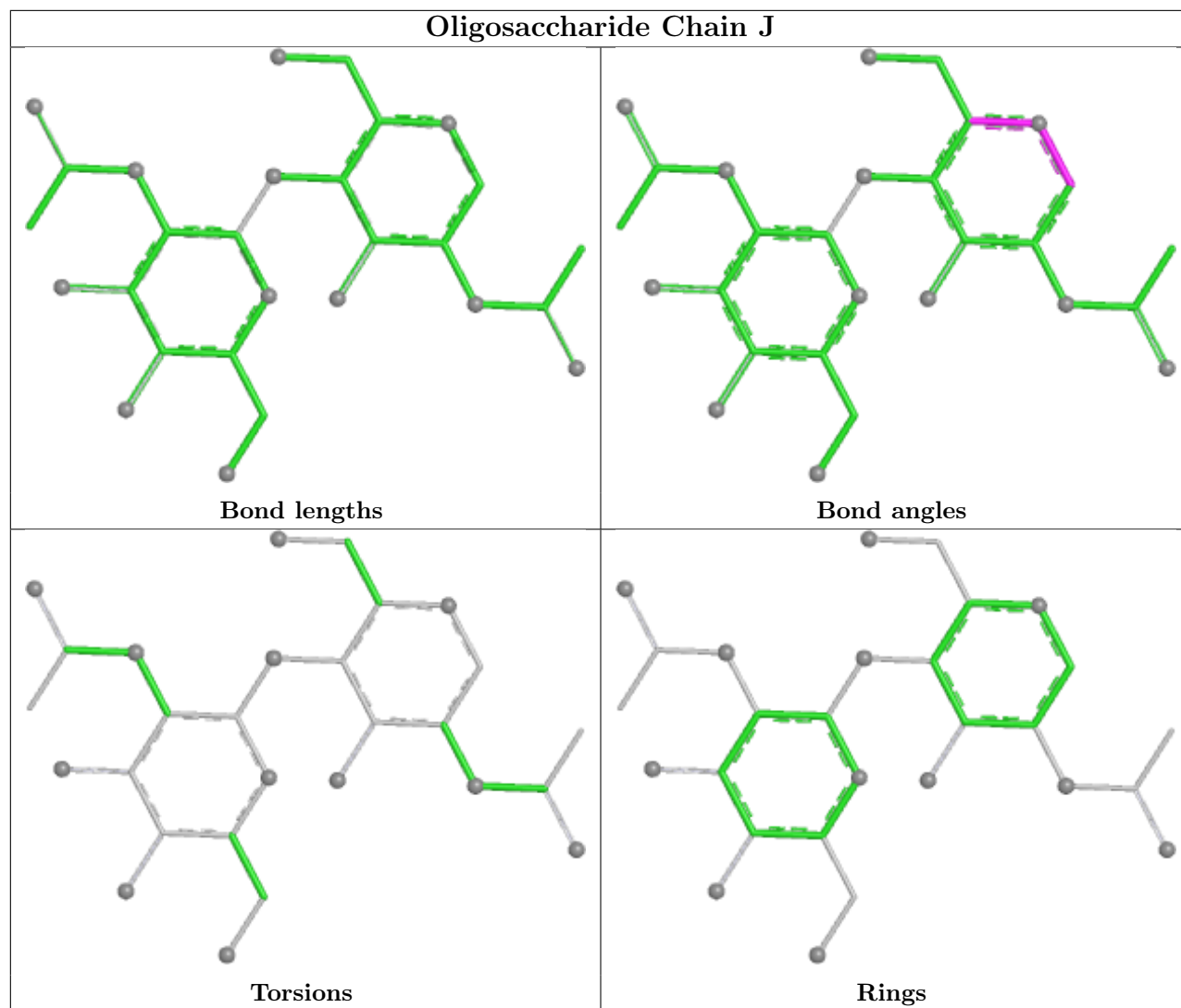
Mol	Chain	Res	Type	Atoms
6	I	4	MAN	C1-C2-C3-C4-C5-O5

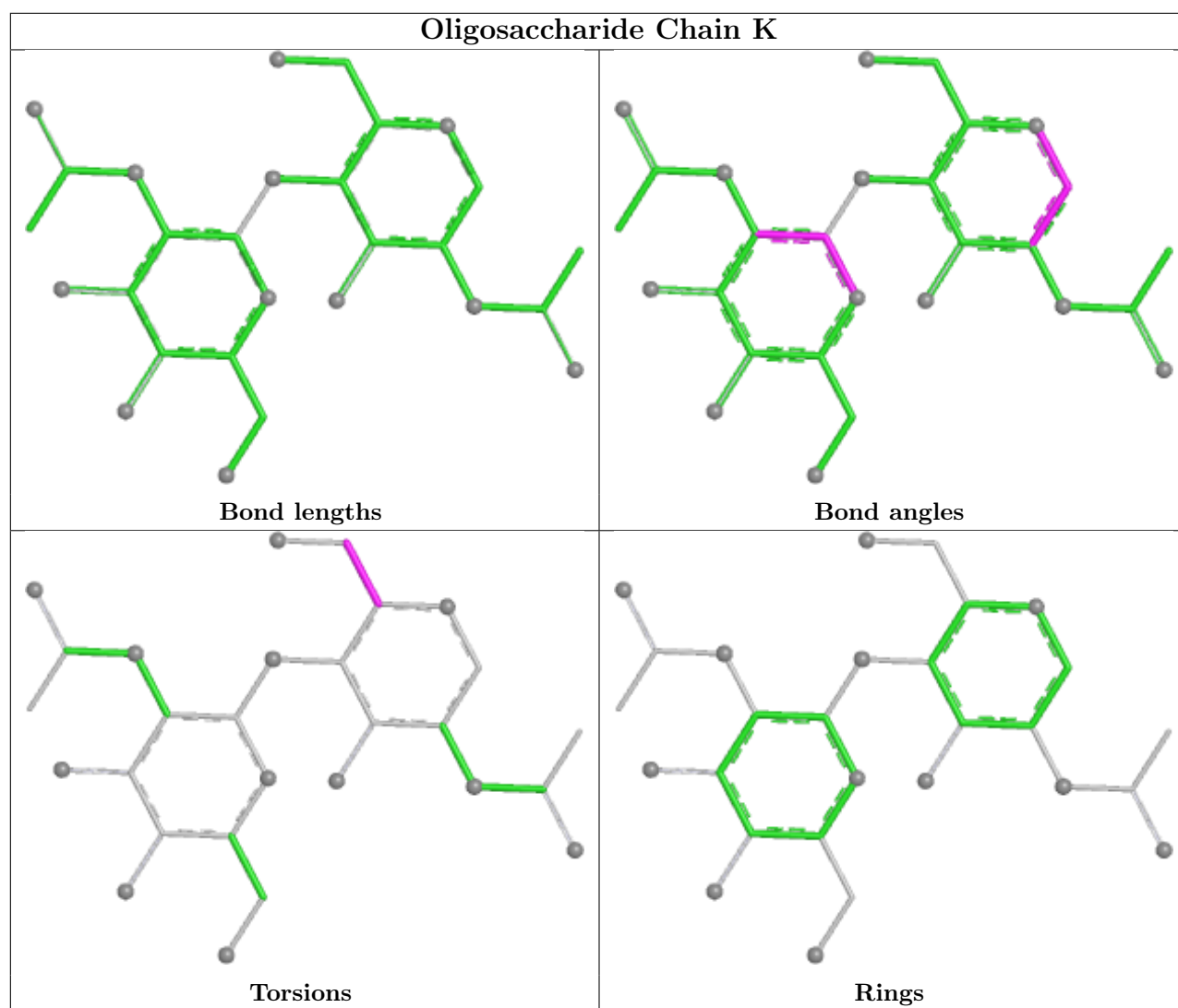
No monomer is involved in short contacts.

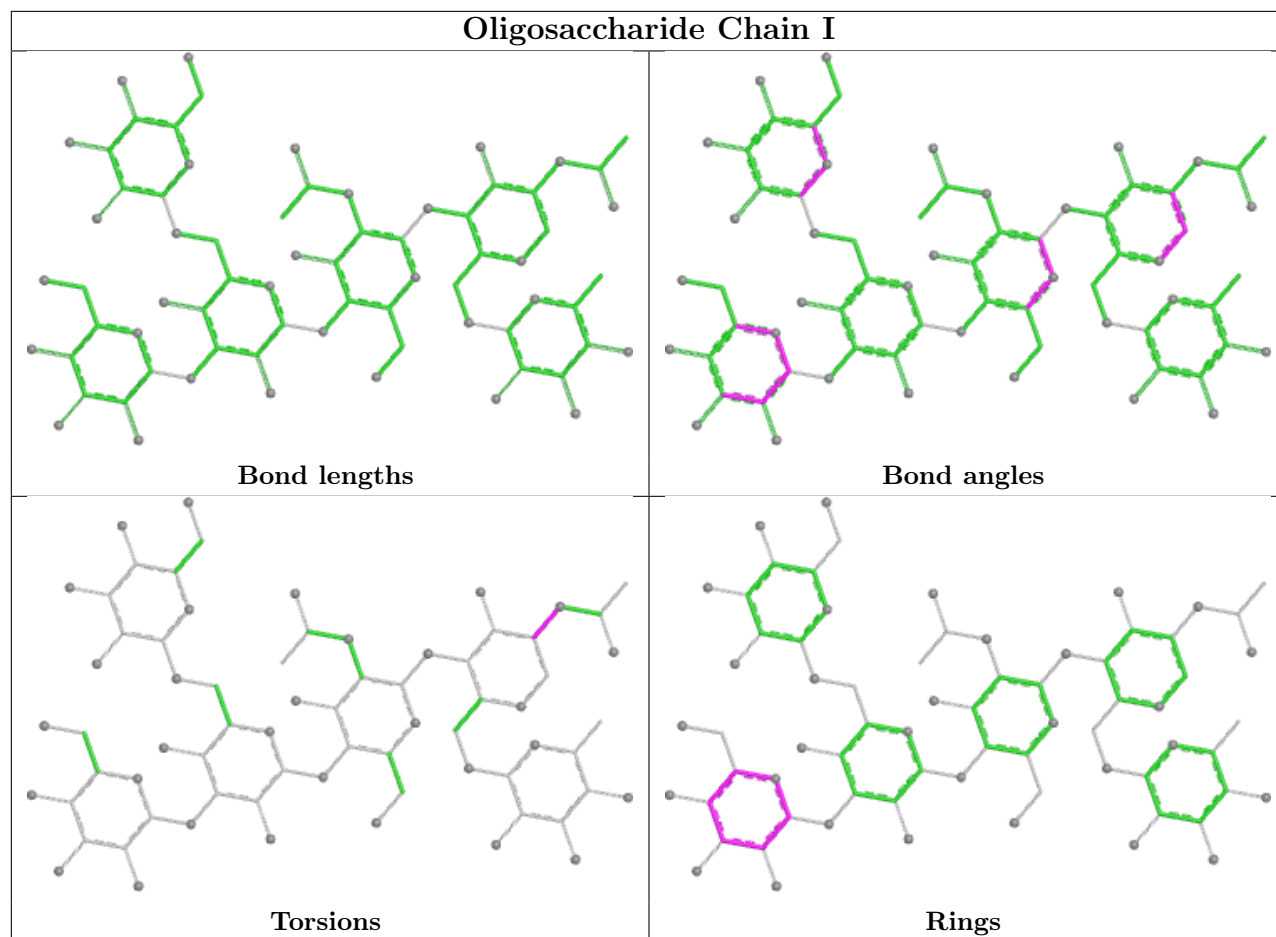
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

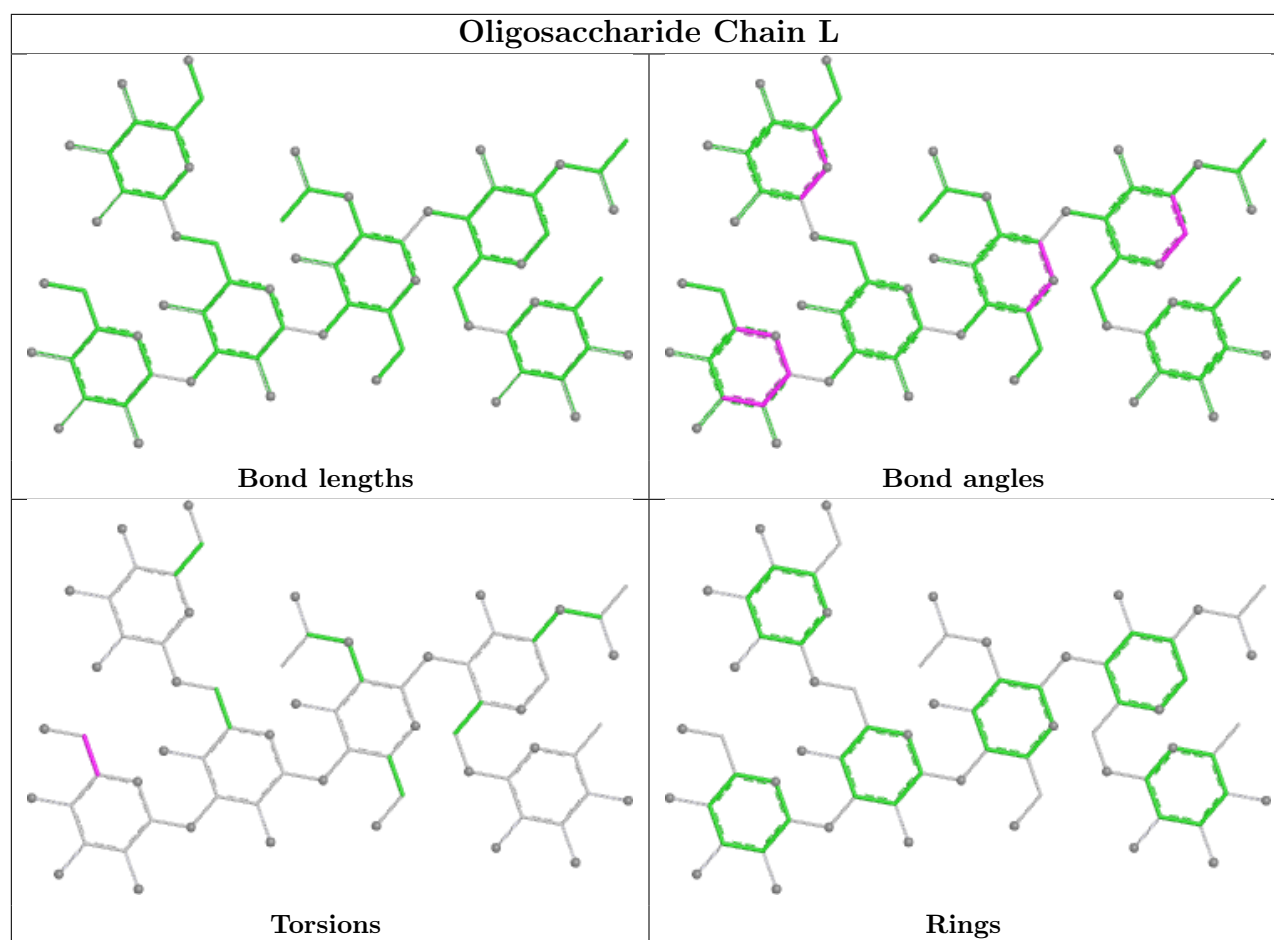












5.6 Ligand geometry [i](#)

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
8	HEC	C	301	3	46,50,50	2.72	28 (60%)	58,82,82	2.48	26 (44%)
7	EDO	B	802	-	3,3,3	0.67	0	2,2,2	0.46	0
11	PO4	B	804	-	4,4,4	2.04	4 (100%)	6,6,6	0.50	0
8	HEC	A	302	2	46,50,50	2.66	24 (52%)	58,82,82	2.36	24 (41%)
7	EDO	A	301	-	3,3,3	0.50	0	2,2,2	0.33	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
7	EDO	B	806	-	3,3,3	0.50	0	2,2,2	0.37	0
7	EDO	B	803	-	3,3,3	0.64	0	2,2,2	0.36	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
8	HEC	C	301	3	-	8/14/54/54	-
7	EDO	B	802	-	-	0/1/1/1	-
8	HEC	A	302	2	-	8/14/54/54	-
7	EDO	A	301	-	-	0/1/1/1	-
12	PEG	B	805	-	-	3/4/4/4	-
7	EDO	B	806	-	-	0/1/1/1	-
7	EDO	B	803	-	-	1/1/1/1	-

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	301	HEC	CAC-C3C	5.49	1.52	1.35
8	C	301	HEC	CHC-C4B	5.49	1.49	1.38
8	A	302	HEC	CAC-C3C	5.41	1.52	1.35
8	A	302	HEC	CAB-C3B	5.39	1.52	1.35
8	C	301	HEC	C2A-C3A	5.33	1.48	1.36
8	C	301	HEC	CAB-C3B	5.12	1.51	1.35
8	C	301	HEC	CHB-C4A	4.85	1.47	1.38
8	A	302	HEC	C2A-C3A	4.81	1.47	1.36
8	A	302	HEC	CHC-C4B	4.81	1.47	1.38
8	A	302	HEC	CHD-C4C	4.43	1.47	1.38
8	C	301	HEC	CHD-C4C	4.35	1.46	1.38
8	A	302	HEC	CHA-C1A	4.34	1.46	1.38
8	A	302	HEC	CHB-C4A	4.14	1.46	1.38
8	C	301	HEC	CHA-C1A	4.10	1.46	1.38
8	C	301	HEC	CHB-C1B	4.08	1.48	1.39
8	A	302	HEC	CHC-C1C	3.98	1.48	1.39
8	C	301	HEC	CHC-C1C	3.95	1.48	1.39
8	A	302	HEC	CHB-C1B	3.81	1.48	1.39
8	C	301	HEC	CHA-C4D	3.69	1.47	1.39
8	A	302	HEC	CHA-C4D	3.66	1.47	1.39
8	A	302	HEC	CHD-C1D	3.55	1.47	1.39
8	C	301	HEC	CHD-C1D	3.43	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	302	HEC	C3D-C2D	3.29	1.47	1.38
8	C	301	HEC	C3D-C2D	3.19	1.47	1.38
8	A	302	HEC	C1D-C2D	2.85	1.49	1.43
8	A	302	HEC	C4A-NA	-2.85	1.34	1.39
8	C	301	HEC	C1C-C2C	2.81	1.49	1.43
8	C	301	HEC	C4D-ND	-2.68	1.34	1.39
8	C	301	HEC	C1D-ND	-2.58	1.34	1.39
8	A	302	HEC	C4D-ND	-2.53	1.34	1.39
8	C	301	HEC	C1B-C2B	2.46	1.48	1.43
8	A	302	HEC	C3B-C4B	2.45	1.50	1.46
8	C	301	HEC	C1D-C2D	2.42	1.48	1.43
8	A	302	HEC	C4C-NC	-2.37	1.35	1.39
8	A	302	HEC	C3C-C2C	2.36	1.49	1.41
8	A	302	HEC	C1C-C2C	2.35	1.48	1.43
8	A	302	HEC	C1A-NA	-2.31	1.35	1.39
8	C	301	HEC	C3C-C2C	2.25	1.48	1.41
8	C	301	HEC	C4C-NC	-2.24	1.35	1.39
8	C	301	HEC	C1C-NC	-2.21	1.35	1.39
8	A	302	HEC	C1B-C2B	2.17	1.48	1.43
8	C	301	HEC	C1B-NB	-2.16	1.35	1.39
8	A	302	HEC	C4D-C3D	2.16	1.48	1.44
8	C	301	HEC	C1A-NA	-2.15	1.35	1.39
8	A	302	HEC	C1C-NC	-2.09	1.35	1.39
8	C	301	HEC	C4B-NB	-2.09	1.35	1.39
8	C	301	HEC	C3B-C4B	2.08	1.49	1.46
8	C	301	HEC	C4A-C3A	2.07	1.49	1.45
8	C	301	HEC	C3B-C2B	2.07	1.48	1.41
8	C	301	HEC	C4A-NA	-2.06	1.35	1.39
11	B	804	PO4	P-O3	2.05	1.60	1.54
11	B	804	PO4	P-O2	2.04	1.60	1.54
11	B	804	PO4	P-O4	2.04	1.60	1.54
11	B	804	PO4	P-O1	2.02	1.55	1.50
8	A	302	HEC	C3B-C2B	2.01	1.48	1.41
8	C	301	HEC	C1A-C2A	2.01	1.48	1.45

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	301	HEC	CBB-CAB-C3B	-8.46	110.52	127.43
8	A	302	HEC	CBB-CAB-C3B	-7.11	113.23	127.43
8	C	301	HEC	CBC-CAC-C3C	-5.60	116.23	127.43
8	A	302	HEC	CBC-CAC-C3C	-4.82	117.80	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	302	HEC	CHD-C4C-C3C	-4.38	117.82	125.21
8	C	301	HEC	CHD-C4C-C3C	-4.19	118.15	125.21
8	A	302	HEC	C2A-C1A-NA	4.18	114.36	110.32
8	A	302	HEC	CHA-C1A-C2A	-4.15	118.31	124.86
8	C	301	HEC	C1D-C2D-C3D	-4.04	102.19	106.82
8	C	301	HEC	CBD-CAD-C3D	-4.03	101.38	112.53
8	C	301	HEC	CHA-C1A-C2A	-4.00	118.54	124.86
8	A	302	HEC	C1D-C2D-C3D	-3.88	102.37	106.82
8	A	302	HEC	CHD-C4C-NC	3.79	128.58	124.45
8	A	302	HEC	CBD-CAD-C3D	-3.63	102.51	112.53
8	C	301	HEC	C2A-C1A-NA	3.48	113.68	110.32
8	A	302	HEC	C1A-C2A-C3A	-3.47	102.54	107.11
8	C	301	HEC	CBA-CAA-C2A	-3.24	103.58	112.53
8	A	302	HEC	CHB-C1B-C2B	-3.13	118.33	127.43
8	C	301	HEC	CHC-C4B-C3B	-2.99	120.16	125.21
8	C	301	HEC	CHD-C1D-C2D	-2.93	118.91	127.43
8	C	301	HEC	C1A-C2A-C3A	-2.92	103.26	107.11
8	C	301	HEC	CHB-C1B-C2B	-2.86	119.13	127.43
8	A	302	HEC	CMD-C2D-C1D	2.85	129.76	125.42
8	A	302	HEC	CBA-CAA-C2A	-2.80	104.80	112.53
8	C	301	HEC	CHC-C4B-NB	2.76	127.46	124.45
8	C	301	HEC	CMD-C2D-C1D	2.71	129.55	125.42
8	A	302	HEC	CHB-C4A-C3A	-2.70	119.86	125.49
8	A	302	HEC	CHB-C1B-NB	2.68	128.72	123.86
8	A	302	HEC	CHD-C1D-C2D	-2.68	119.66	127.43
8	C	301	HEC	CHA-C4D-C3D	-2.65	119.50	125.30
8	A	302	HEC	C3D-C4D-ND	2.64	113.09	110.15
8	C	301	HEC	CHB-C4A-C3A	-2.63	120.01	125.49
8	C	301	HEC	CHA-C1A-NA	2.63	127.32	124.45
8	A	302	HEC	CHC-C1C-C2C	-2.54	120.05	127.43
8	A	302	HEC	CHA-C4D-C3D	-2.51	119.80	125.30
8	C	301	HEC	CHD-C4C-NC	2.49	127.17	124.45
8	C	301	HEC	CMA-C3A-C4A	2.46	129.06	124.73
8	C	301	HEC	C2D-C1D-ND	2.40	113.99	110.14
8	C	301	HEC	CHC-C1C-C2C	-2.39	120.47	127.43
8	C	301	HEC	C4A-C3A-C2A	-2.36	103.47	106.97
8	C	301	HEC	C3D-C4D-ND	2.33	112.73	110.15
8	A	302	HEC	C2D-C1D-ND	2.20	113.67	110.14
8	A	302	HEC	CHA-C1A-NA	2.18	126.83	124.45
8	C	301	HEC	CHB-C4A-NA	2.18	126.82	124.45
8	A	302	HEC	C4A-C3A-C2A	-2.16	103.77	106.97
8	A	302	HEC	CHC-C1C-NC	2.15	127.75	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	301	HEC	CHB-C1B-NB	2.12	127.71	123.86
8	A	302	HEC	C3A-C4A-NA	2.10	113.52	109.64
8	C	301	HEC	O2A-CGA-CBA	2.05	120.48	114.00
8	A	302	HEC	CHC-C4B-C3B	-2.05	121.76	125.21

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	302	HEC	C2B-C3B-CAB-CBB
8	A	302	HEC	C4B-C3B-CAB-CBB
8	A	302	HEC	C2C-C3C-CAC-CBC
8	A	302	HEC	C4C-C3C-CAC-CBC
8	C	301	HEC	C2B-C3B-CAB-CBB
8	C	301	HEC	C4B-C3B-CAB-CBB
8	C	301	HEC	C2C-C3C-CAC-CBC
8	C	301	HEC	C4C-C3C-CAC-CBC
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	A	302	HEC	CAD-CBD-CGD-O1D
8	C	301	HEC	CAD-CBD-CGD-O1D
8	C	301	HEC	CAD-CBD-CGD-O2D
8	A	302	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

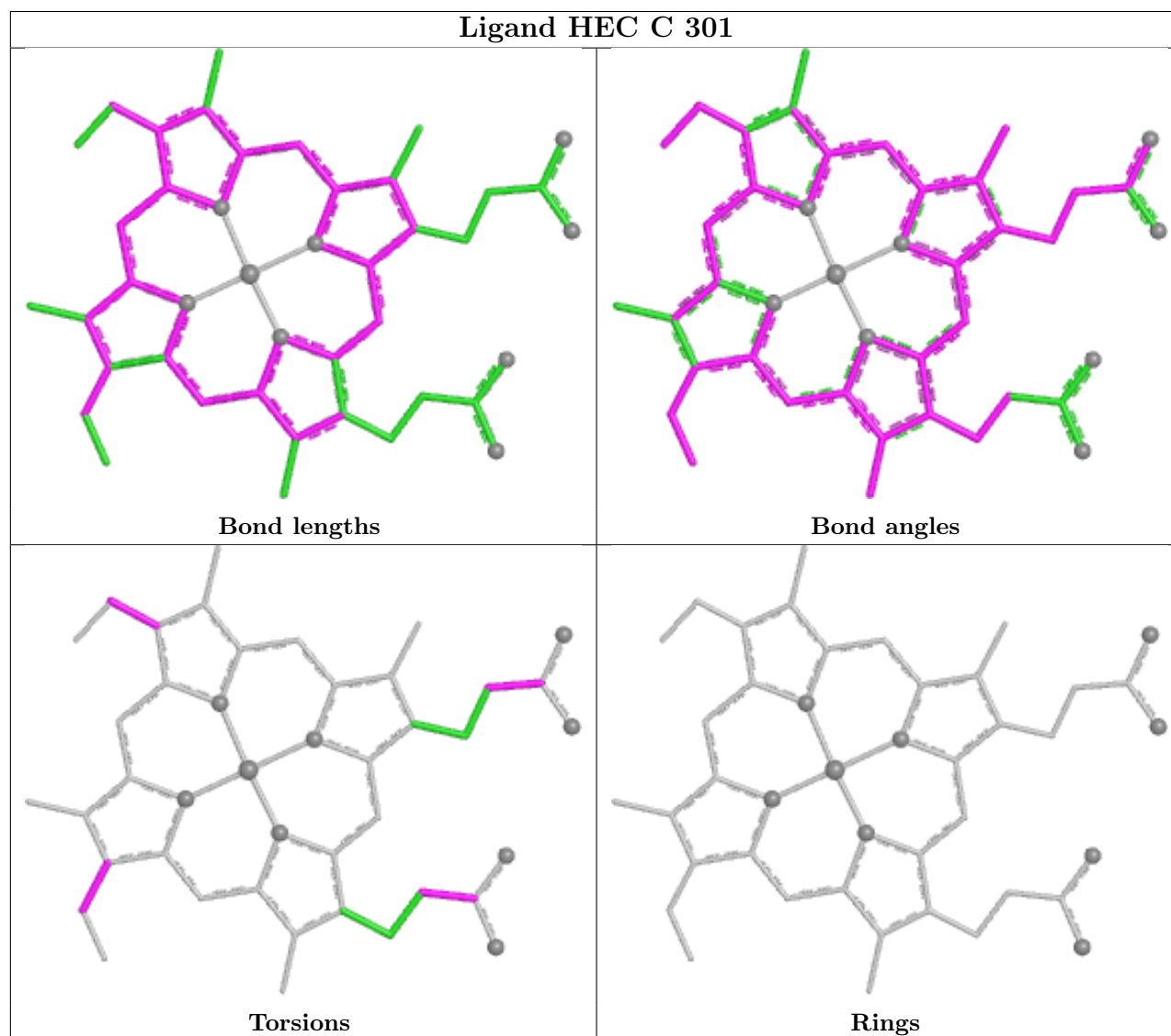
There are no ring outliers.

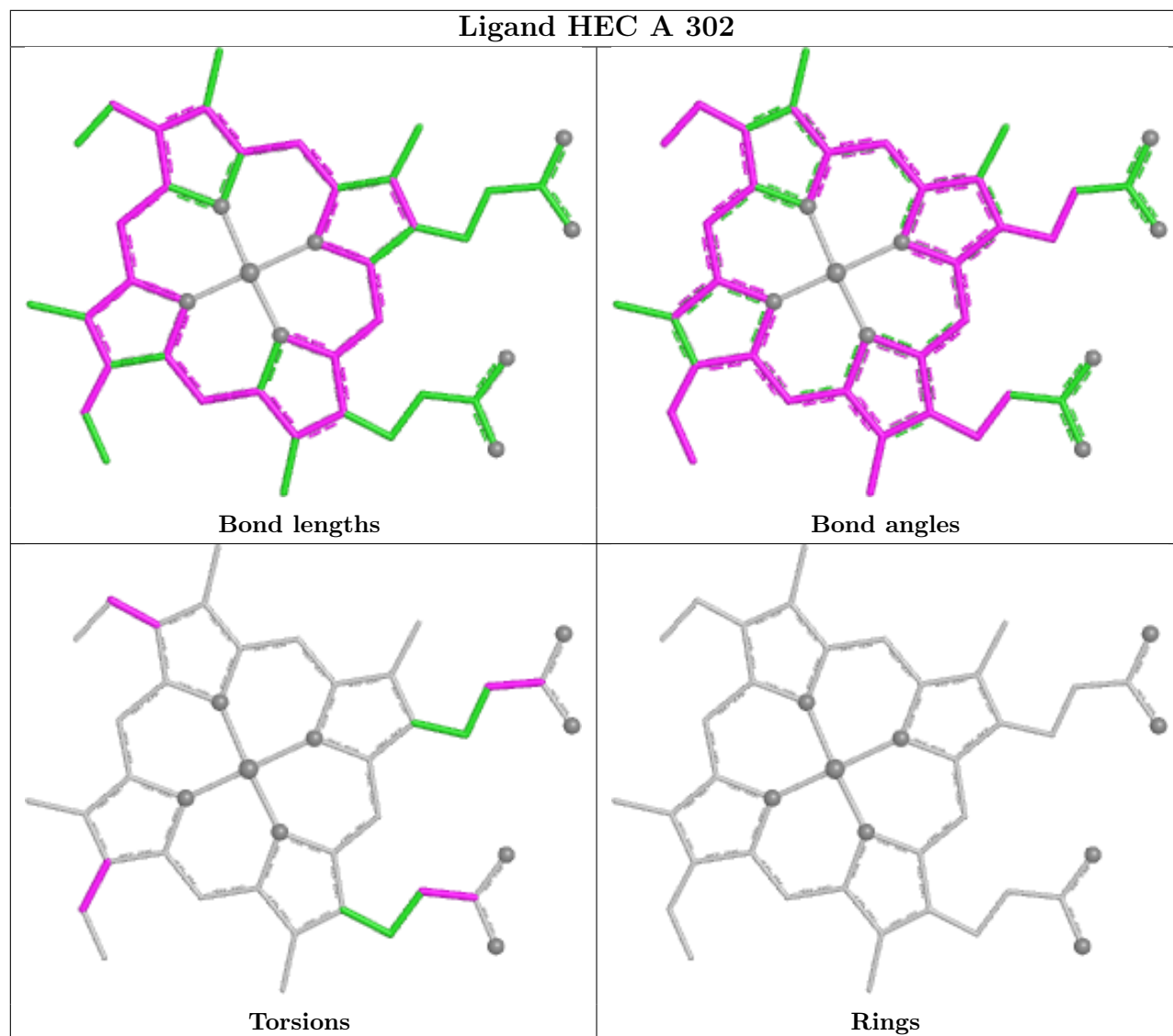
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	301	HEC	1	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 than 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.





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, 95th 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%)	-0.28	1 (0%) 79 79	9, 14, 22, 37	0
1	C	105/114 (92%)	-0.15	2 (1%) 66 65	8, 15, 25, 36	0
2	B	465/467 (99%)	-0.28	8 (1%) 69 68	8, 14, 23, 38	3 (0%)
3	D	463/467 (99%)	-0.20	6 (1%) 75 75	9, 15, 25, 38	2 (0%)
4	E	70/102 (68%)	0.32	6 (8%) 16 15	12, 22, 36, 41	0
4	F	69/102 (67%)	0.74	5 (7%) 21 21	16, 27, 42, 45	0
All	All	1277/1366 (93%)	-0.16	28 (2%) 62 61	8, 15, 29, 45	5 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	520	GLU	4.6
3	D	279	VAL	4.0
2	B	715	ASN	4.0
2	B	521	PRO	3.8
3	D	520	GLU	3.7
2	B	384	ASP	3.3
2	B	321	GLY	2.9
4	E	102	GLU	2.8
2	B	323	ASN	2.6
4	F	35	TYR	2.6
4	E	35	TYR	2.6
4	E	33	LYS	2.6
4	E	42	LEU	2.6
4	F	40	LEU	2.6
4	E	34	VAL	2.4
1	C	271	ALA	2.4
4	F	41	VAL	2.4
2	B	392	ARG	2.4
3	D	521	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	271	ALA	2.3
3	D	280	ASN	2.3
4	E	45	ASP	2.3
3	D	436	ARG	2.2
2	B	383	HIS	2.2
4	F	39	GLY	2.2
4	F	103	HIS	2.1
3	D	730	CYS	2.1
1	C	167	CYS	2.1

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, 95th 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	0.74	0.13	42,44,45,46	5
2	2CO	B	316	8/9	0.96	0.07	23,27,32,33	5
3	CSO	D	316	7/8	0.98	0.06	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, 95th 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.

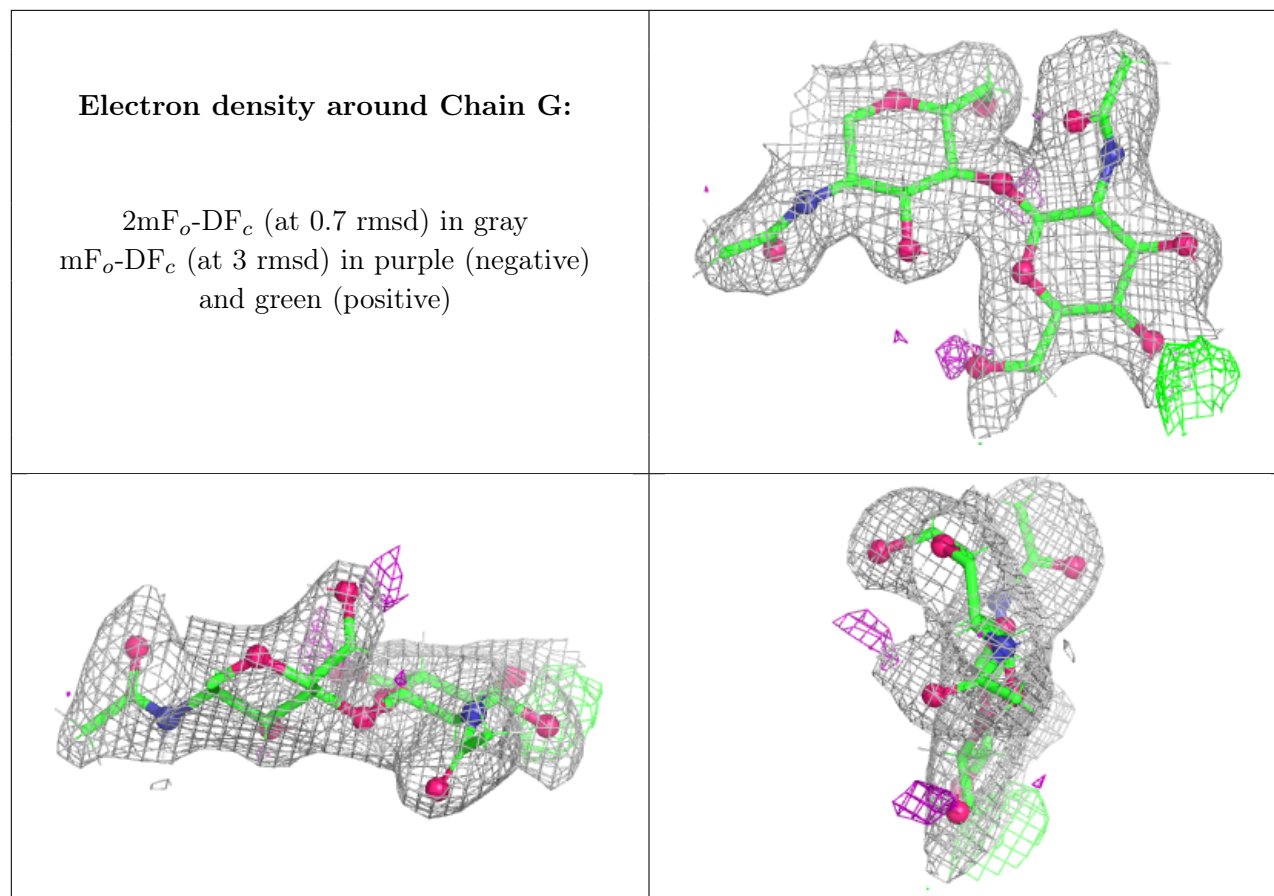
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	H	2	14/15	0.68	0.14	53,56,60,60	13
6	MAN	I	4	11/12	0.72	0.16	44,48,51,52	10
6	MAN	L	4	11/12	0.72	0.14	44,47,50,51	10
5	NAG	K	2	14/15	0.74	0.13	60,62,68,69	13
5	NAG	J	2	14/15	0.83	0.12	47,50,54,55	13
5	NAG	G	2	14/15	0.83	0.11	42,46,48,48	13
5	NAG	K	1	14/15	0.85	0.12	55,57,61,62	12
5	NAG	H	1	14/15	0.89	0.11	48,50,52,52	12
6	MAN	I	5	11/12	0.89	0.08	35,36,38,38	10
6	BMA	I	3	11/12	0.89	0.09	34,37,41,41	8
6	MAN	L	5	11/12	0.90	0.09	36,38,39,39	10

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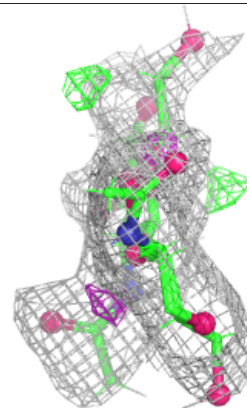
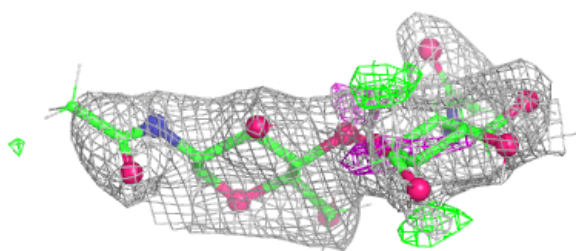
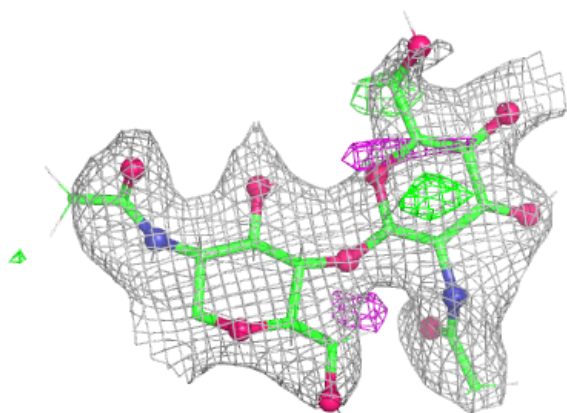
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	BMA	L	3	11/12	0.92	0.08	35,38,41,42	8
5	NAG	G	1	14/15	0.93	0.08	34,38,40,41	12
5	NAG	J	1	14/15	0.94	0.08	42,43,46,47	12
6	FUC	L	6	10/11	0.94	0.06	29,31,32,32	10
6	NAG	L	1	14/15	0.95	0.05	26,28,28,30	11
6	NAG	L	2	14/15	0.95	0.06	25,28,30,33	12
6	NAG	I	1	14/15	0.96	0.06	29,30,33,33	11
6	FUC	I	6	10/11	0.96	0.05	32,33,34,34	10
6	NAG	I	2	14/15	0.97	0.05	26,29,31,32	12

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.

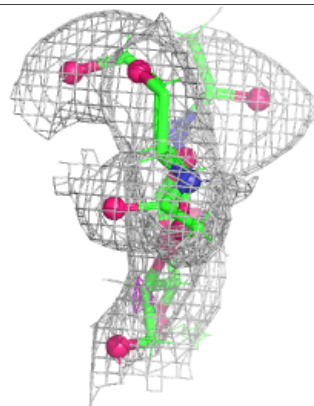
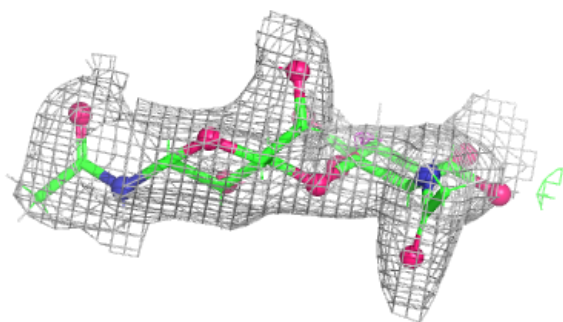
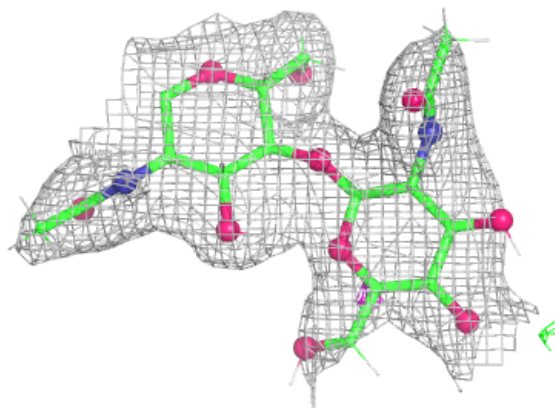


Electron density around Chain H:

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

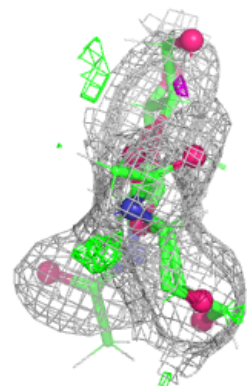
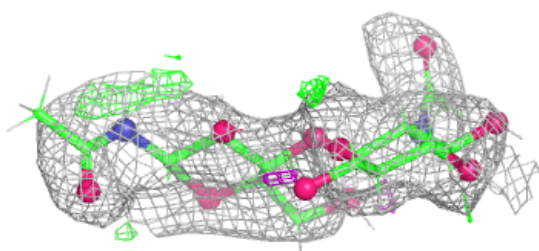
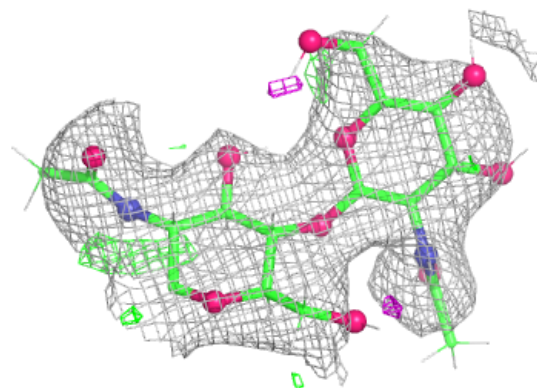
**Electron density around Chain J:**

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



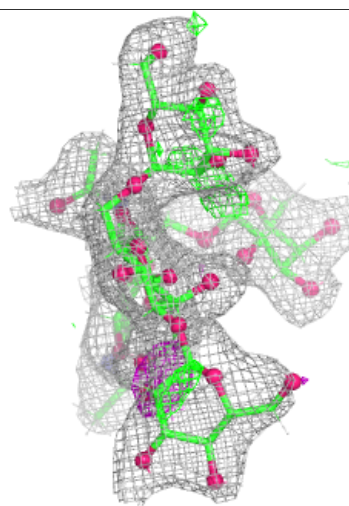
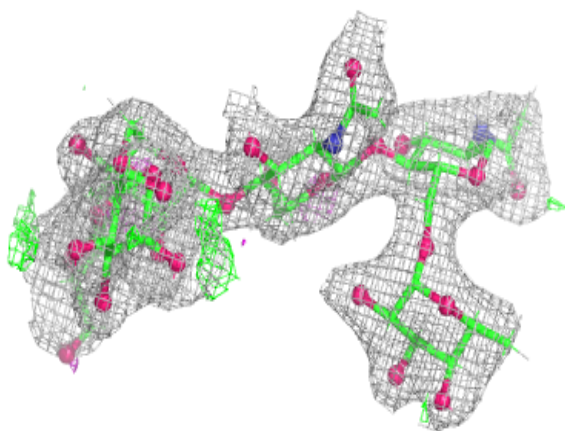
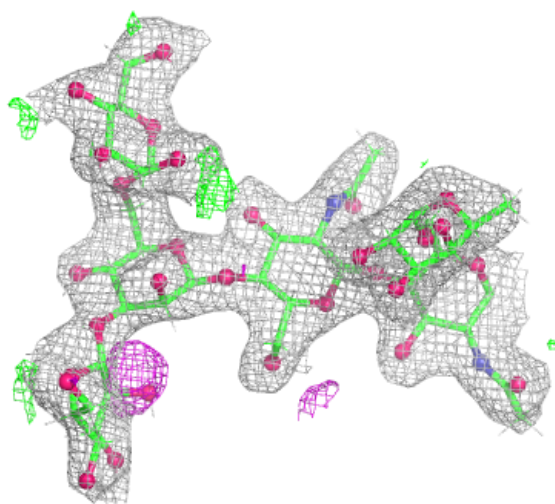
Electron density around Chain K:

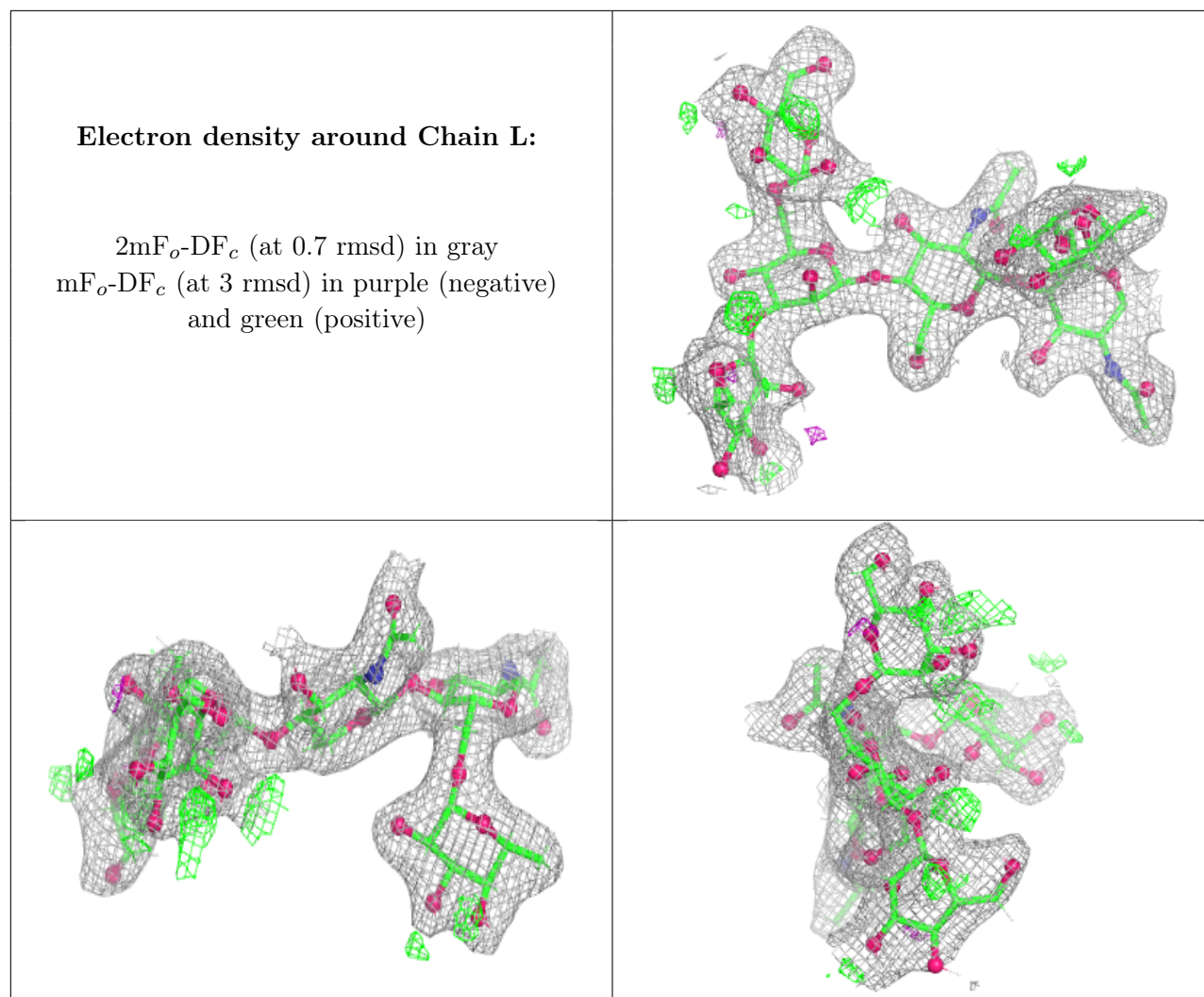
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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)





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, 95th 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	0.76	0.17	40,41,42,42	6
11	PO4	B	804	5/5	0.81	0.25	76,76,76,76	0
7	EDO	B	802	4/4	0.84	0.14	39,39,41,41	6
12	PEG	B	805	7/7	0.84	0.14	48,50,52,52	10
7	EDO	B	806	4/4	0.85	0.11	43,44,46,46	6
7	EDO	A	301	4/4	0.92	0.08	40,41,42,42	6
8	HEC	A	302	43/43	0.96	0.09	18,24,29,33	28
8	HEC	C	301	43/43	0.96	0.08	24,29,33,36	28
10	CA	D	801	1/1	0.98	0.02	25,25,25,25	0

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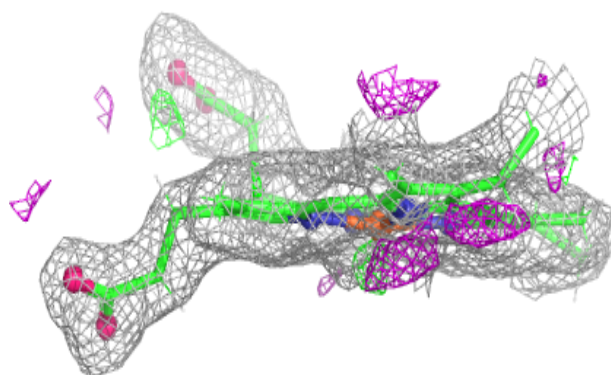
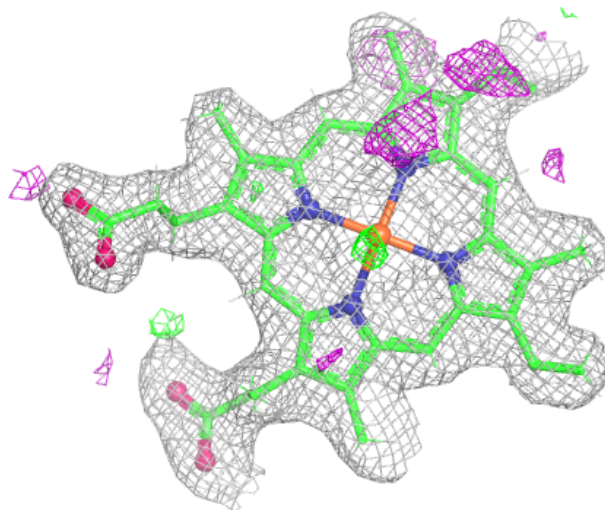
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	CL	C	302	1/1	0.99	0.04	20,20,20,20	0
10	CA	B	801	1/1	1.00	0.02	26,26,26,26	0
9	CL	A	303	1/1	1.00	0.01	21,21,21,21	0

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.

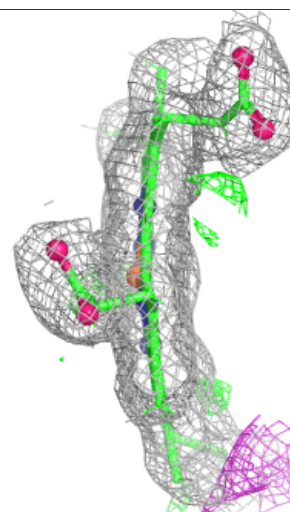
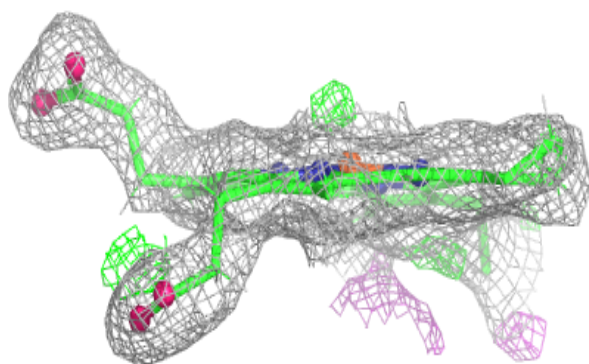
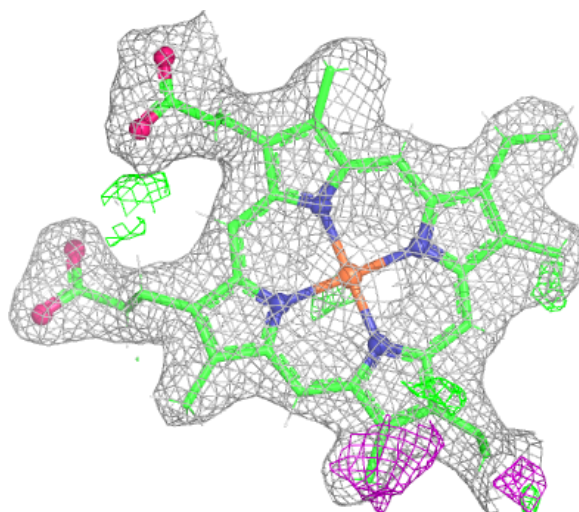
Electron density around HEC A 302:

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



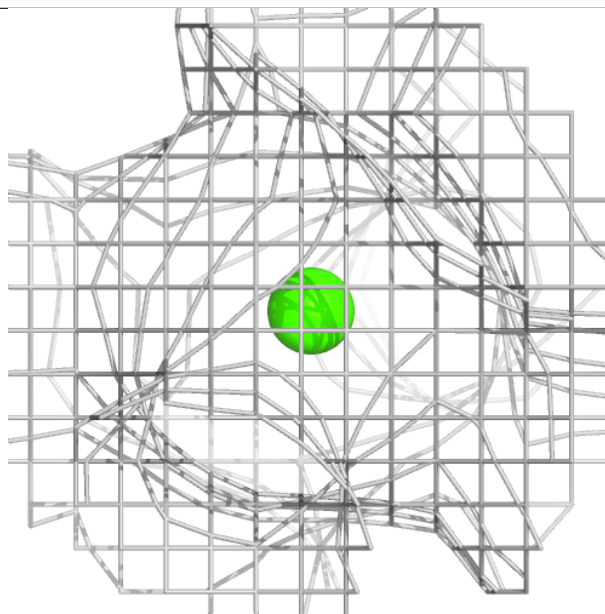
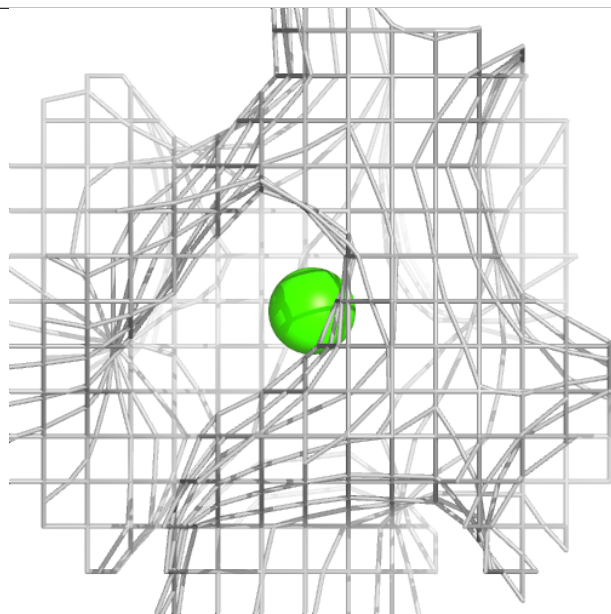
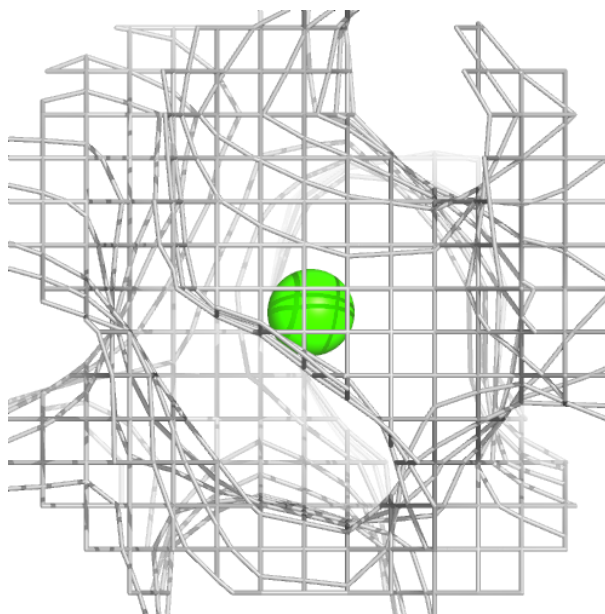
Electron density around HEC C 301:

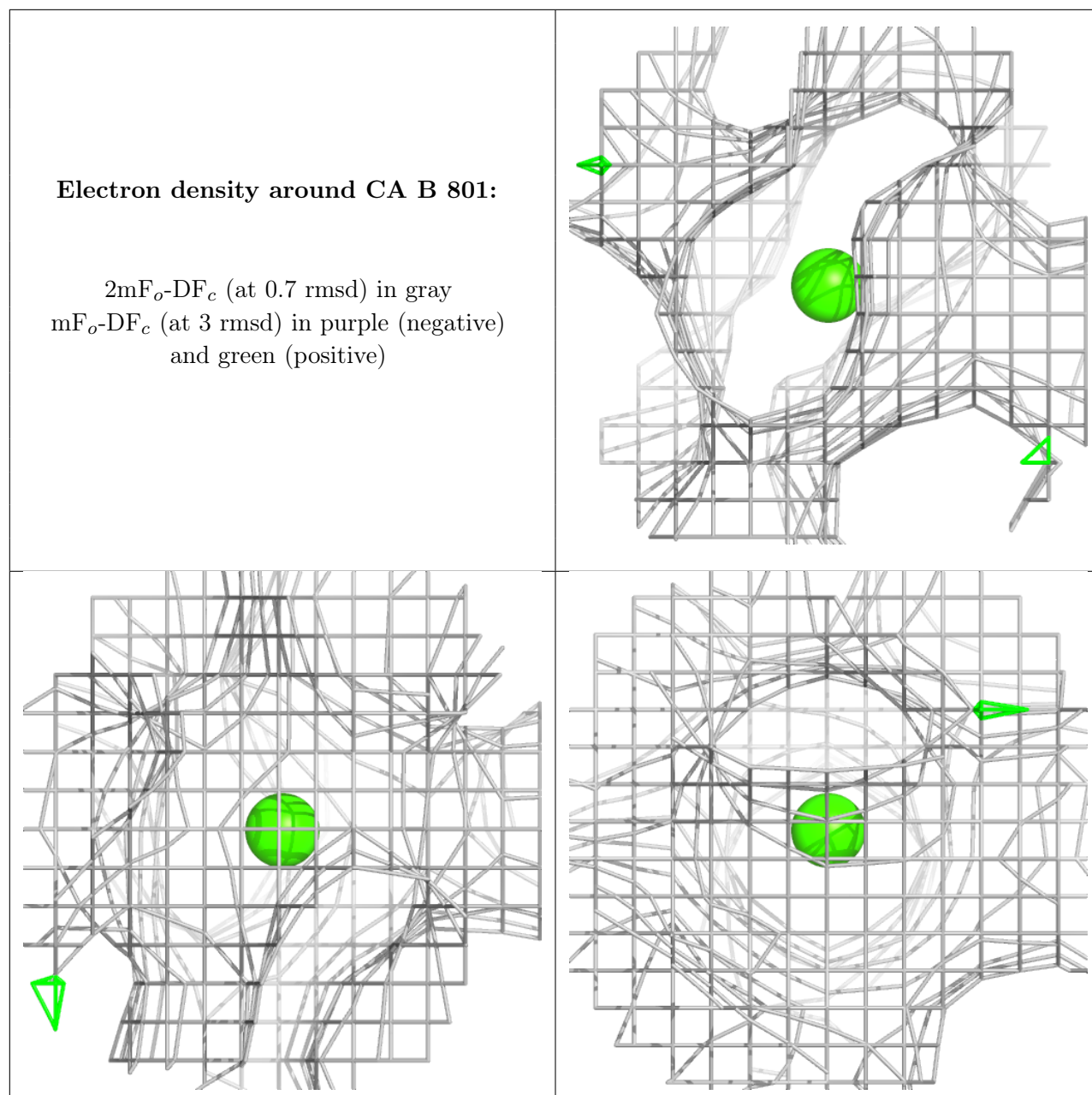
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.