



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 6, 2025 – 01:29 pm BST

PDB ID : 9QEX / pdb\_00009qex  
Title : Structure of native leukocyte myeloperoxidase in complex with a truncated version of the Staphylococcal Peroxidase Inhibitor SPIN and thiocyanate at pH 7.5  
Authors : Leitgeb, U.; Pfanzagl, V.  
Deposited on : 2025-03-11  
Resolution : 1.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

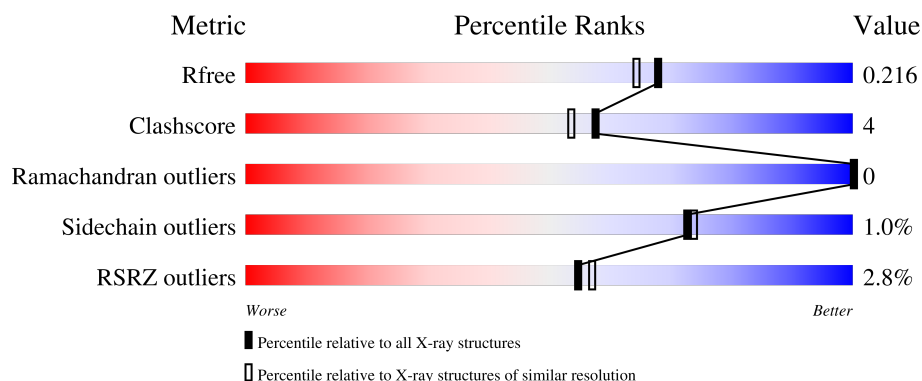
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

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








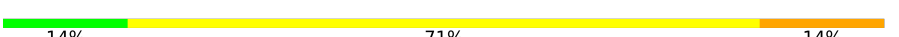
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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  $\geq 3$ , 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	B	467	<div> <div>0%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
1	D	467	<div> <div>0%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
2	E	60	<div> <div>2%</div> <div>85%</div> <div>8%</div> <div>7%</div> <div>.</div> </div>
2	F	60	<div> <div>42%</div> <div>65%</div> <div>32%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	A	114	
3	C	114	
4	G	2	
4	J	2	
5	I	6	
6	H	7	

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
9	SCN	B	806	-	-	X	-

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 21160 atoms, of which 9941 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 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	465	Total	C	H	N	O	S	0	0	0
			7380	2346	3654	686	667	27			
1	D	465	Total	C	H	N	O	S	0	0	0
			7388	2348	3660	686	667	27			

- Molecule 2 is a protein called Myeloperoxidase inhibitor SPIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	56	Total	C	H	N	O		0	0	0
			887	287	434	76	90				
2	F	58	Total	C	H	N	O		0	0	0
			918	298	446	80	94				

- Molecule 3 is a protein called Myeloperoxidase light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	105	Total	C	H	N	O	S	0	2	0
			1638	535	790	150	158	5			
3	C	105	Total	C	H	N	O	S	0	0	0
			1627	532	785	149	156	5			

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



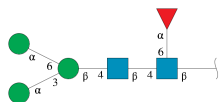
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	G	2	Total	C	H	N	O		0	0	0
			43	16	15	2	10				

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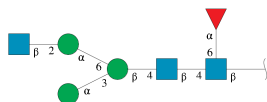
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	2	Total	C	H	N	O	0	0	0
			44	16	16	2	10			

- Molecule 5 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
5	I	6	Total	C	H	N	O	0	0	0
			114	40	43	2	29			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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	H	7	Total	C	H	N	O	0	0	0
			135	48	50	3	34			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

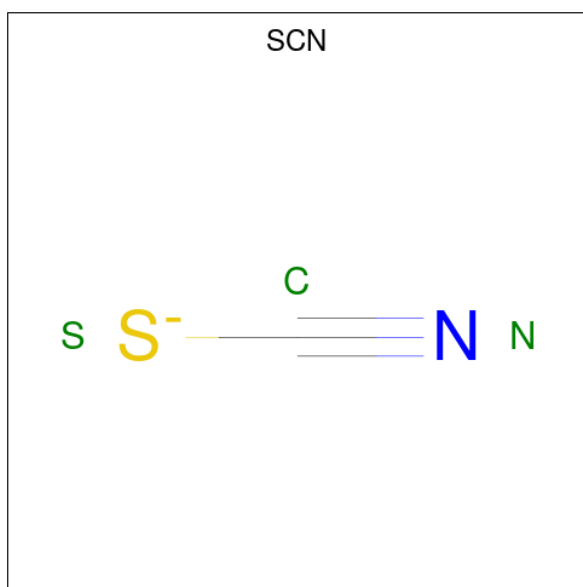


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	H	N	O	0	0
			22	8	8	1	5		
7	D	1	Total	C	H	N	O	0	0
			22	8	8	1	5		

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 9 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	S	0	0
			3	1	1	1		
9	B	1	Total	C	N	S	0	0
			3	1	1	1		
9	B	1	Total	C	N	S	0	0
			3	1	1	1		
9	B	1	Total	C	N	S	0	0
			3	1	1	1		
9	B	1	Total	C	N	S	0	0
			3	1	1	1		
9	B	1	Total	C	N	S	0	0
			3	1	1	1		
9	D	1	Total	C	N	S	0	0
			3	1	1	1		
9	D	1	Total	C	N	S	0	0
			3	1	1	1		
9	D	1	Total	C	N	S	0	0
			3	1	1	1		
9	A	1	Total	C	N	S	0	0
			3	1	1	1		
9	A	1	Total	C	N	S	0	0
			3	1	1	1		
9	C	1	Total	C	N	S	0	0
			3	1	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	N	S	0	0
			3	1	1	1		

- # HEM

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total 59	C 34	Fe 1	H 16	N 4	O 4	0	0
10	D	1	Total 59	C 34	Fe 1	H 16	N 4	O 4	0	0

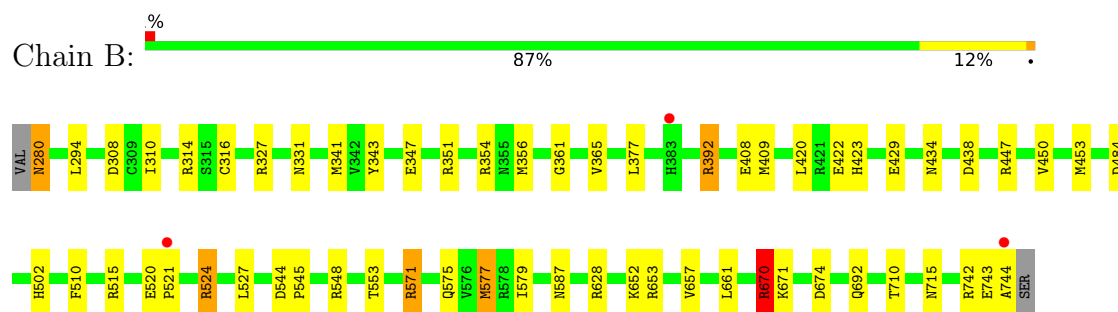
- | Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 11  | B     | 350      | Total O<br>352 352 | 0       | 2       |
| 11  | D     | 245      | Total O<br>245 245 | 0       | 0       |
| 11  | E     | 23       | Total O<br>23 23   | 0       | 0       |
| 11  | F     | 2        | Total O<br>2 2     | 0       | 0       |
| 11  | A     | 85       | Total O<br>85 85   | 0       | 0       |
| 11  | C     | 70       | Total O<br>70 70   | 0       | 0       |



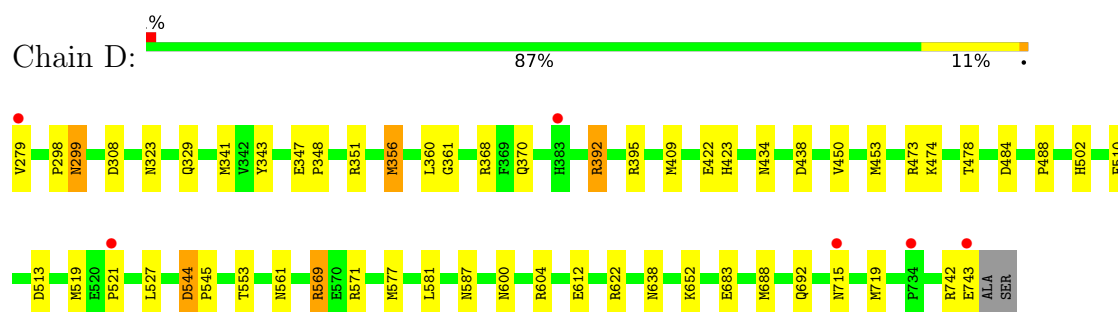
### 3 Residue-property plots [i](#)

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.

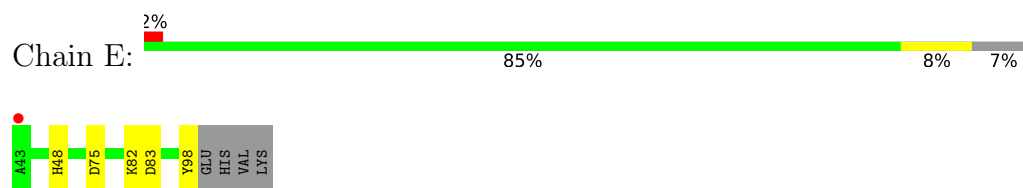
- Molecule 1: Myeloperoxidase heavy chain



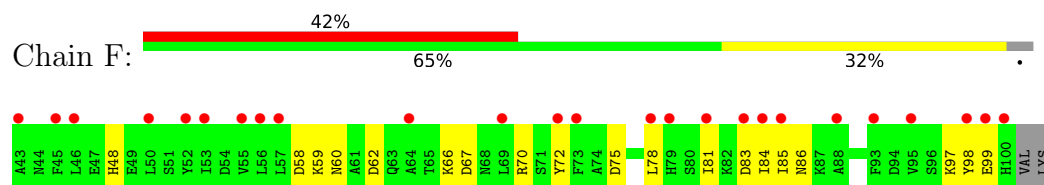
- Molecule 1: Myeloperoxidase heavy chain




- Molecule 2: Myeloperoxidase inhibitor SPIN

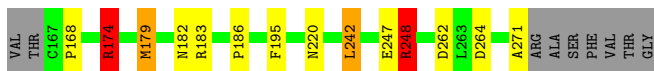


- Molecule 2: Myeloperoxidase inhibitor SPIN




- Molecule 3: Myeloperoxidase light chain

Chain A:  80% 9% 8%




- Molecule 3: Myeloperoxidase light chain

Chain C:  84% 8% 8%



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

Chain G:  50% 50%



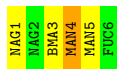
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%

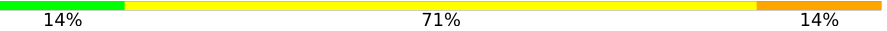


- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  33% 50% 17%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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 H:  14% 71% 14%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.33Å 111.33Å 242.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	101.19 – 1.90 101.19 – 1.90	Depositor EDS
% Data completeness (in resolution range)	72.1 (101.19-1.90) 72.1 (101.19-1.90)	Depositor EDS
$R_{merge}$	0.26	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.100)	Depositor
R, $R_{free}$	0.168 , 0.216 0.168 , 0.216	Depositor DCC
$R_{free}$ test set	4245 reflections (3.54%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 40.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	21160	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG, 2CO, CA, HEM, FUC, SCN, BMA

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	B	0.82	1/3803 (0.0%)	1.24	20/5158 (0.4%)
1	D	0.73	0/3805	1.21	18/5161 (0.3%)
2	E	0.76	0/460	1.34	4/617 (0.6%)
2	F	0.59	0/480	1.29	5/644 (0.8%)
3	A	0.83	0/881	1.36	10/1201 (0.8%)
3	C	0.74	0/867	1.24	3/1181 (0.3%)
All	All	0.77	1/10296 (0.0%)	1.25	60/13962 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	7
1	D	0	6
2	F	0	1
3	A	0	2
All	All	0	16

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	571	ARG	NE-CZ	5.09	1.38	1.33

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	174	ARG	NE-CZ-NH2	-10.33	109.90	119.20
3	A	174	ARG	CD-NE-CZ	9.47	137.66	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	577	MET	CG-SD-CE	-9.41	80.19	100.90
2	F	99	GLU	N-CA-CB	-8.44	100.23	110.53
1	D	308	ASP	CA-CB-CG	8.15	120.75	112.60

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	524	ARG	Sidechain
1	B	548	ARG	Sidechain
1	B	571	ARG	Sidechain
1	B	628	ARG	Sidechain
1	B	653	ARG	Sidechain

## 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	B	3726	3654	3715	34	0
1	D	3728	3660	3719	31	0
2	E	453	434	441	2	0
2	F	472	446	454	7	0
3	A	848	790	794	7	0
3	C	842	785	800	4	0
4	G	28	15	25	1	0
4	J	28	16	25	0	0
5	I	71	43	61	1	0
6	H	85	50	73	2	0
7	B	14	8	13	0	0
7	D	14	8	13	0	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	A	6	0	0	0	0
9	B	21	0	0	5	0
9	C	6	0	0	0	0
9	D	12	0	0	1	0
10	B	43	16	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	43	16	30	2	0
11	A	85	0	0	3	0
11	B	352	0	0	12	1
11	C	70	0	0	0	0
11	D	245	0	0	9	1
11	E	23	0	0	0	0
11	F	2	0	0	0	0
All	All	11219	9941	10193	90	1

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

The worst 5 of 90 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:719:MET:HE3	11:D:1099:HOH:O	1.82	0.80
1:B:280:ASN:OD1	1:B:280:ASN:N	2.11	0.78
3:A:174:ARG:HD2	11:A:474:HOH:O	1.83	0.77
2:F:59:LYS:HG3	2:F:60:ASN:HD22	1.50	0.75
1:B:502:HIS:HD1	1:B:587:ASN:HD21	1.36	0.74

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:969:HOH:O	11:D:1101:HOH:O[6_545]	2.19	0.01

## 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	B	462/467 (99%)	455 (98%)	7 (2%)	0	100	100
1	D	462/467 (99%)	455 (98%)	7 (2%)	0	100	100
2	E	54/60 (90%)	53 (98%)	1 (2%)	0	100	100
2	F	56/60 (93%)	56 (100%)	0	0	100	100
3	A	105/114 (92%)	100 (95%)	5 (5%)	0	100	100
3	C	103/114 (90%)	100 (97%)	3 (3%)	0	100	100
All	All	1242/1282 (97%)	1219 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	B	409/411 (100%)	406 (99%)	3 (1%)	81	83
1	D	410/411 (100%)	405 (99%)	5 (1%)	67	68
2	E	49/53 (92%)	49 (100%)	0	100	100
2	F	51/53 (96%)	49 (96%)	2 (4%)	27	20
3	A	92/97 (95%)	91 (99%)	1 (1%)	70	71
3	C	90/97 (93%)	90 (100%)	0	100	100
All	All	1101/1122 (98%)	1090 (99%)	11 (1%)	73	74

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	527	LEU
2	F	62	ASP
3	A	242	LEU
2	F	86	ASN
1	D	341	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	48	HIS
2	F	68	ASN
3	C	192	ASN
2	F	79	HIS
2	F	60	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	$\# Z  > 2$
1	2CO	D	316	1	3,7,8	0.51	0	1,7,9	0.24	0
1	2CO	B	316	1	3,7,8	0.51	0	1,7,9	0.28	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
1	2CO	D	316	1	-	0/1/6/8	-
1	2CO	B	316	1	-	0/1/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	316	2CO	1	0

## 5.5 Carbohydrates [i](#)

17 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	$\# Z  > 2$
4	NAG	G	1	4,1	14,14,15	0.48	0	17,19,21	0.79	1 (5%)
4	NAG	G	2	4	14,14,15	0.46	0	17,19,21	0.90	1 (5%)
6	NAG	H	1	6,1	14,14,15	0.38	0	17,19,21	1.03	1 (5%)
6	NAG	H	2	6	14,14,15	0.46	0	17,19,21	1.02	1 (5%)
6	BMA	H	3	6	11,11,12	0.82	0	15,15,17	0.80	0
6	MAN	H	4	6	11,11,12	0.96	0	15,15,17	1.11	2 (13%)
6	NAG	H	5	6	14,14,15	0.39	0	17,19,21	1.82	4 (23%)
6	MAN	H	6	6	11,11,12	0.51	0	15,15,17	1.54	2 (13%)
6	FUC	H	7	6	10,10,11	0.80	0	14,14,16	0.82	0
5	NAG	I	1	5,1	14,14,15	0.26	0	17,19,21	1.29	2 (11%)
5	NAG	I	2	5	14,14,15	0.35	0	17,19,21	0.84	0
5	BMA	I	3	5	11,11,12	0.48	0	15,15,17	0.94	1 (6%)
5	MAN	I	4	5	11,11,12	0.92	1 (9%)	15,15,17	0.80	0
5	MAN	I	5	5	11,11,12	0.84	1 (9%)	15,15,17	1.08	2 (13%)
5	FUC	I	6	5	10,10,11	0.63	0	14,14,16	0.77	0
4	NAG	J	1	4,1	14,14,15	0.29	0	17,19,21	0.57	0
4	NAG	J	2	4	14,14,15	0.49	0	17,19,21	1.38	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	3/6/23/26	0/1/1/1
6	NAG	H	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	H	2	6	-	0/6/23/26	0/1/1/1
6	BMA	H	3	6	-	0/2/19/22	0/1/1/1
6	MAN	H	4	6	-	0/2/19/22	0/1/1/1
6	NAG	H	5	6	-	4/6/23/26	0/1/1/1
6	MAN	H	6	6	-	1/2/19/22	0/1/1/1
6	FUC	H	7	6	-	-	0/1/1/1
5	NAG	I	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
5	MAN	I	4	5	-	0/2/19/22	0/1/1/1
5	MAN	I	5	5	-	0/2/19/22	0/1/1/1
5	FUC	I	6	5	-	-	0/1/1/1
4	NAG	J	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	4	MAN	O5-C5	2.55	1.48	1.43
5	I	5	MAN	C4-C5	-2.16	1.48	1.53

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	5	NAG	C2-N2-C7	4.15	128.81	122.90
6	H	6	MAN	C1-O5-C5	3.87	117.43	112.19
6	H	5	NAG	C1-C2-N2	3.83	117.04	110.49
6	H	5	NAG	O5-C1-C2	-3.78	105.32	111.29
4	J	2	NAG	C1-O5-C5	3.30	116.67	112.19

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
6	H	5	NAG	C8-C7-N2-C2
6	H	5	NAG	O7-C7-N2-C2

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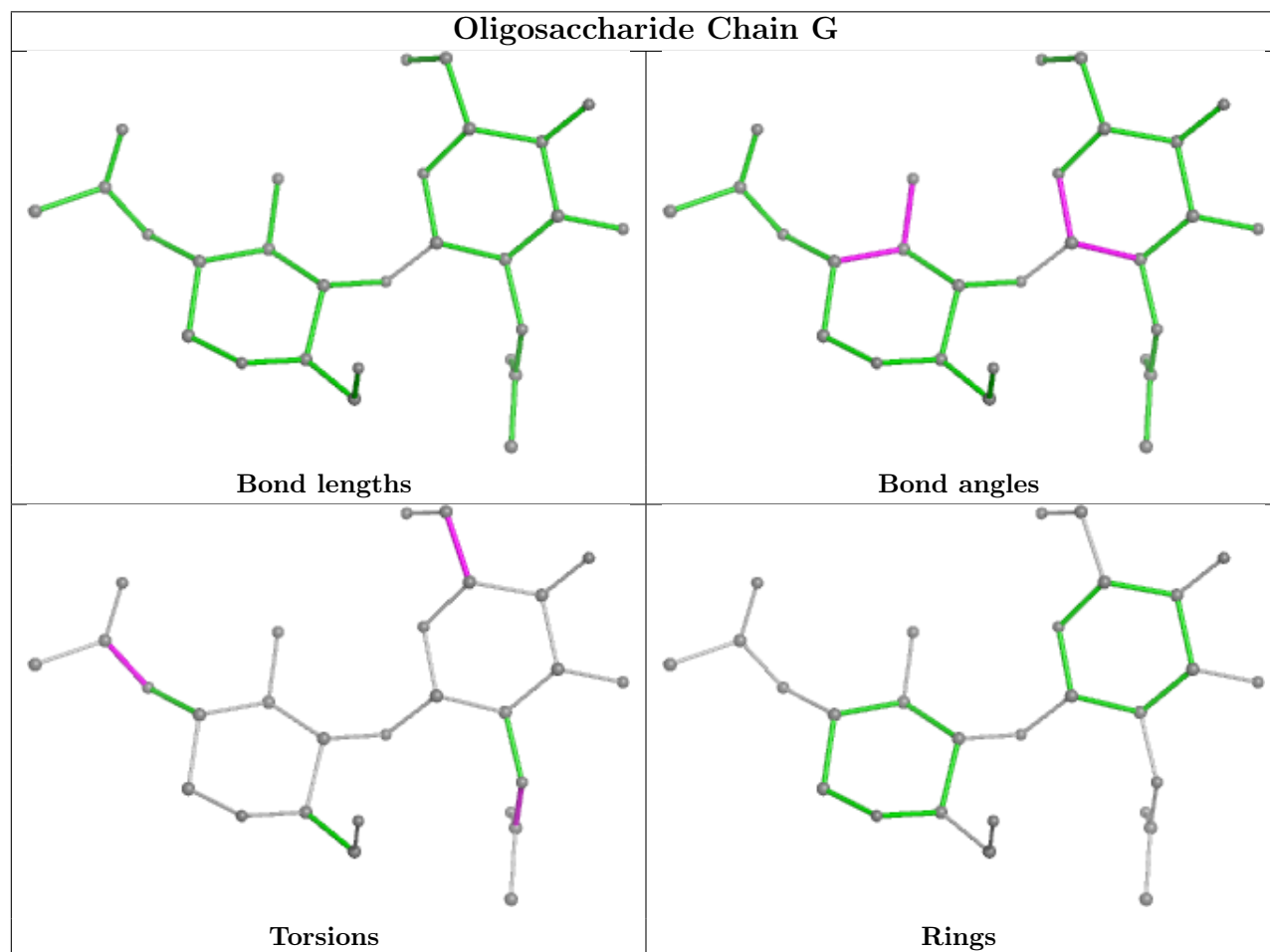
Mol	Chain	Res	Type	Atoms
4	J	2	NAG	O5-C5-C6-O6

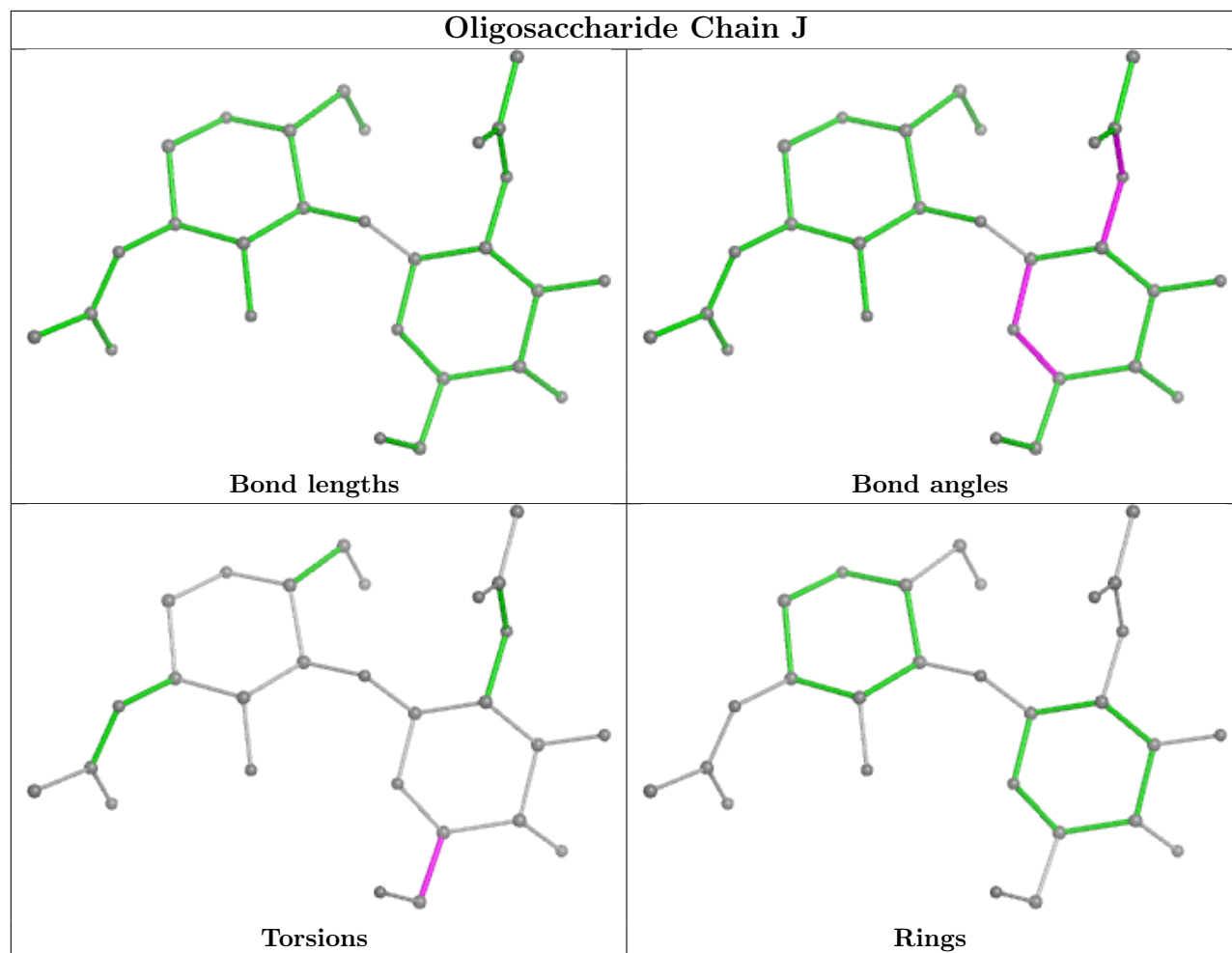
There are no ring outliers.

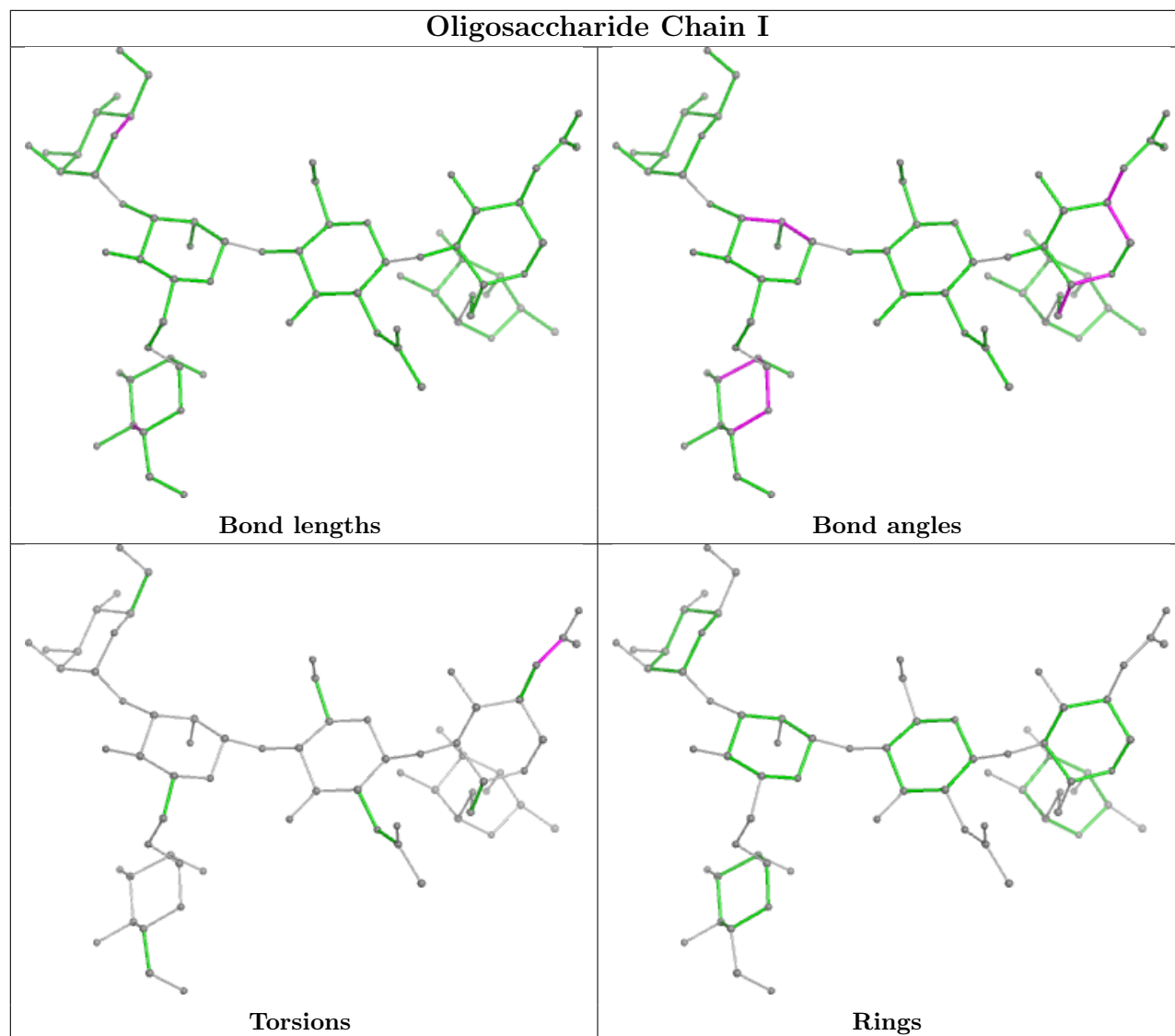
4 monomers are involved in 4 short contacts:

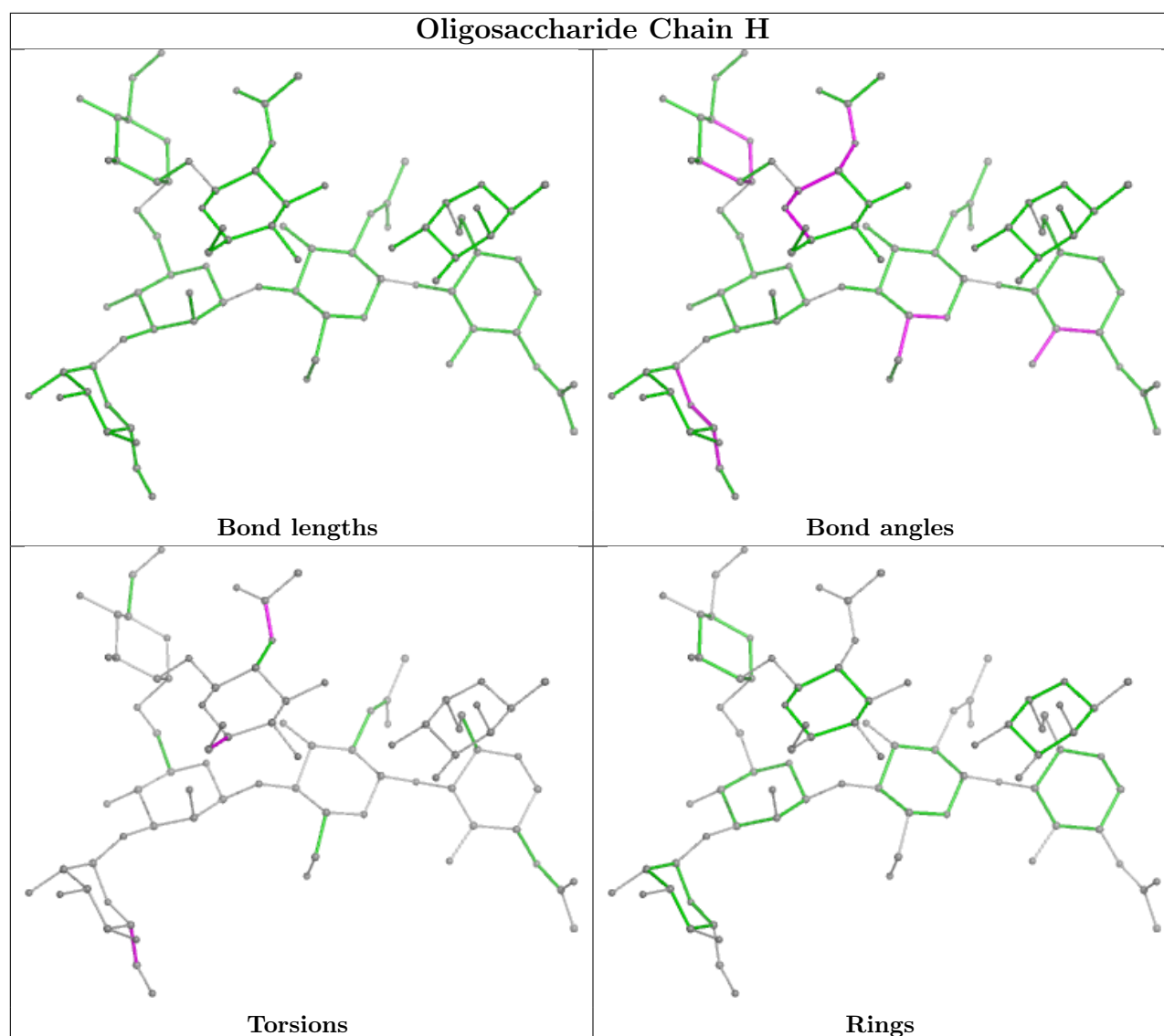
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	4	MAN	1	0
6	H	3	BMA	1	0
4	G	1	NAG	1	0
6	H	5	NAG	2	0

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









## 5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 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	$\# Z  > 2$
9	SCN	C	301	-	1,2,2	3.18	1 (100%)	0,1,1	-	-
9	SCN	B	803	-	1,2,2	2.76	1 (100%)	0,1,1	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	B	801	1	14,14,15	0.62	0	17,19,21	1.17	1 (5%)
9	SCN	B	808	-	1,2,2	2.62	1 (100%)	0,1,1	-	-
9	SCN	B	809	-	1,2,2	0.44	0	0,1,1	-	-
9	SCN	B	807	-	1,2,2	0.19	0	0,1,1	-	-
9	SCN	D	803	-	1,2,2	0.93	0	0,1,1	-	-
9	SCN	D	804	-	1,2,2	1.18	0	0,1,1	-	-
9	SCN	B	806	-	1,2,2	1.12	0	0,1,1	-	-
9	SCN	D	806	-	1,2,2	1.26	0	0,1,1	-	-
10	HEM	B	810	3,1	41,50,50	1.54	8 (19%)	45,82,82	1.52	4 (8%)
7	NAG	D	801	1	14,14,15	0.40	0	17,19,21	1.04	1 (5%)
9	SCN	B	805	-	1,2,2	0.40	0	0,1,1	-	-
9	SCN	C	302	-	1,2,2	0.87	0	0,1,1	-	-
10	HEM	D	807	3,1,11	41,50,50	1.84	11 (26%)	45,82,82	1.84	10 (22%)
9	SCN	D	805	-	1,2,2	1.78	0	0,1,1	-	-
9	SCN	A	302	-	1,2,2	2.91	1 (100%)	0,1,1	-	-
9	SCN	B	804	-	1,2,2	0.75	0	0,1,1	-	-
9	SCN	A	301	-	1,2,2	3.49	1 (100%)	0,1,1	-	-

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
10	HEM	D	807	3,1,11	-	4/12/54/54	-
10	HEM	B	810	3,1	-	4/12/54/54	-
7	NAG	B	801	1	-	0/6/23/26	0/1/1/1
7	NAG	D	801	1	-	0/6/23/26	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	807	HEM	FE-ND	4.17	2.17	1.96
10	B	810	HEM	C1B-C2B	-3.91	1.37	1.44
10	D	807	HEM	C4D-ND	-3.90	1.33	1.40
10	D	807	HEM	FE-NB	3.87	2.16	1.96
10	B	810	HEM	FE-ND	3.57	2.14	1.96

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	807	HEM	C4C-CHD-C1D	7.14	131.97	122.56
10	B	810	HEM	C4C-CHD-C1D	6.06	130.55	122.56
10	B	810	HEM	C4B-CHC-C1C	5.14	129.34	122.56
10	D	807	HEM	C4B-CHC-C1C	4.42	128.39	122.56
10	D	807	HEM	C4D-ND-C1D	3.81	109.01	105.07

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	D	807	HEM	CAD-CBD-CGD-O2D
10	B	810	HEM	CAD-CBD-CGD-O2D
10	D	807	HEM	CAD-CBD-CGD-O1D
10	B	810	HEM	CAD-CBD-CGD-O1D
10	D	807	HEM	CAA-CBA-CGA-O1A

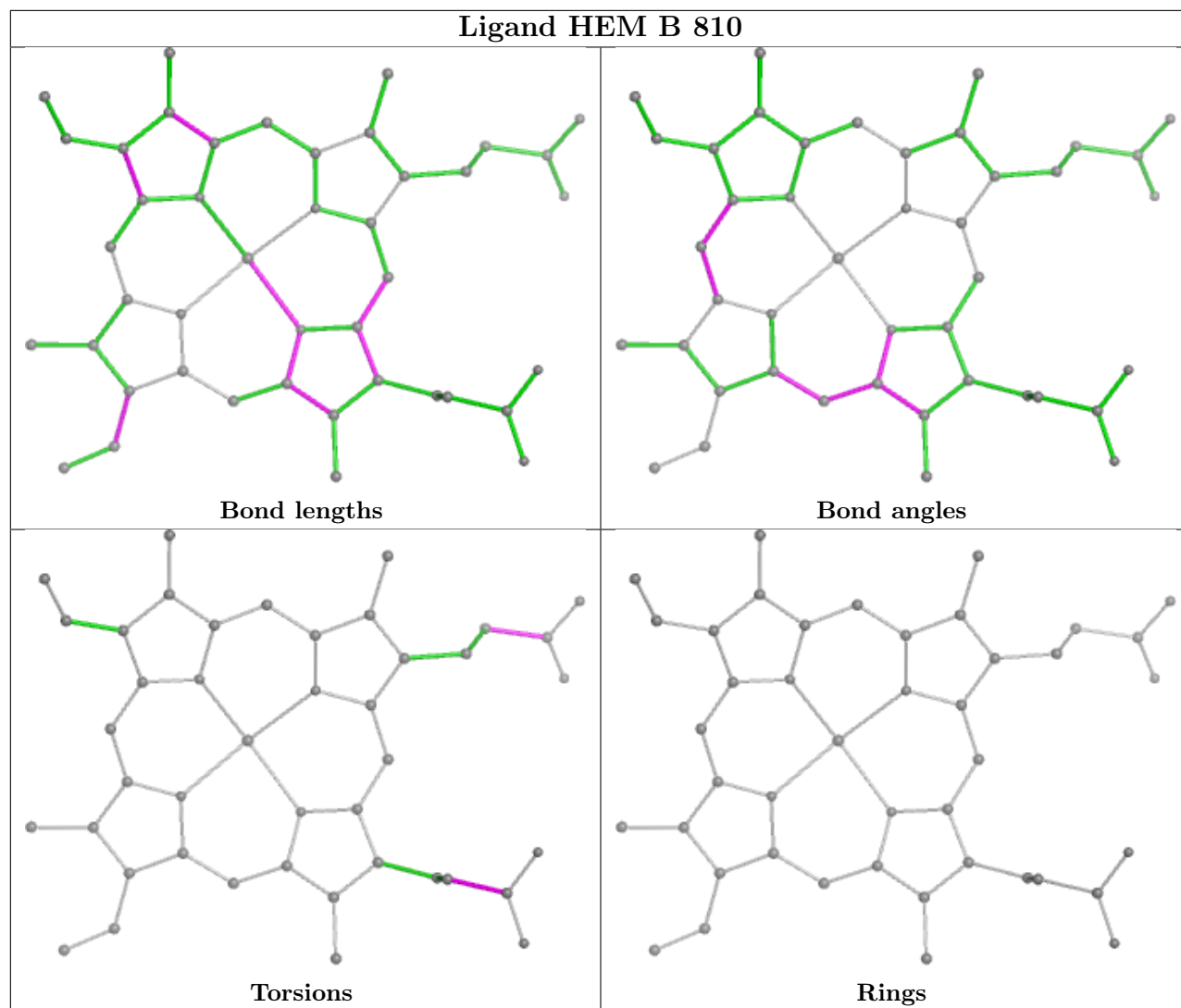
There are no ring outliers.

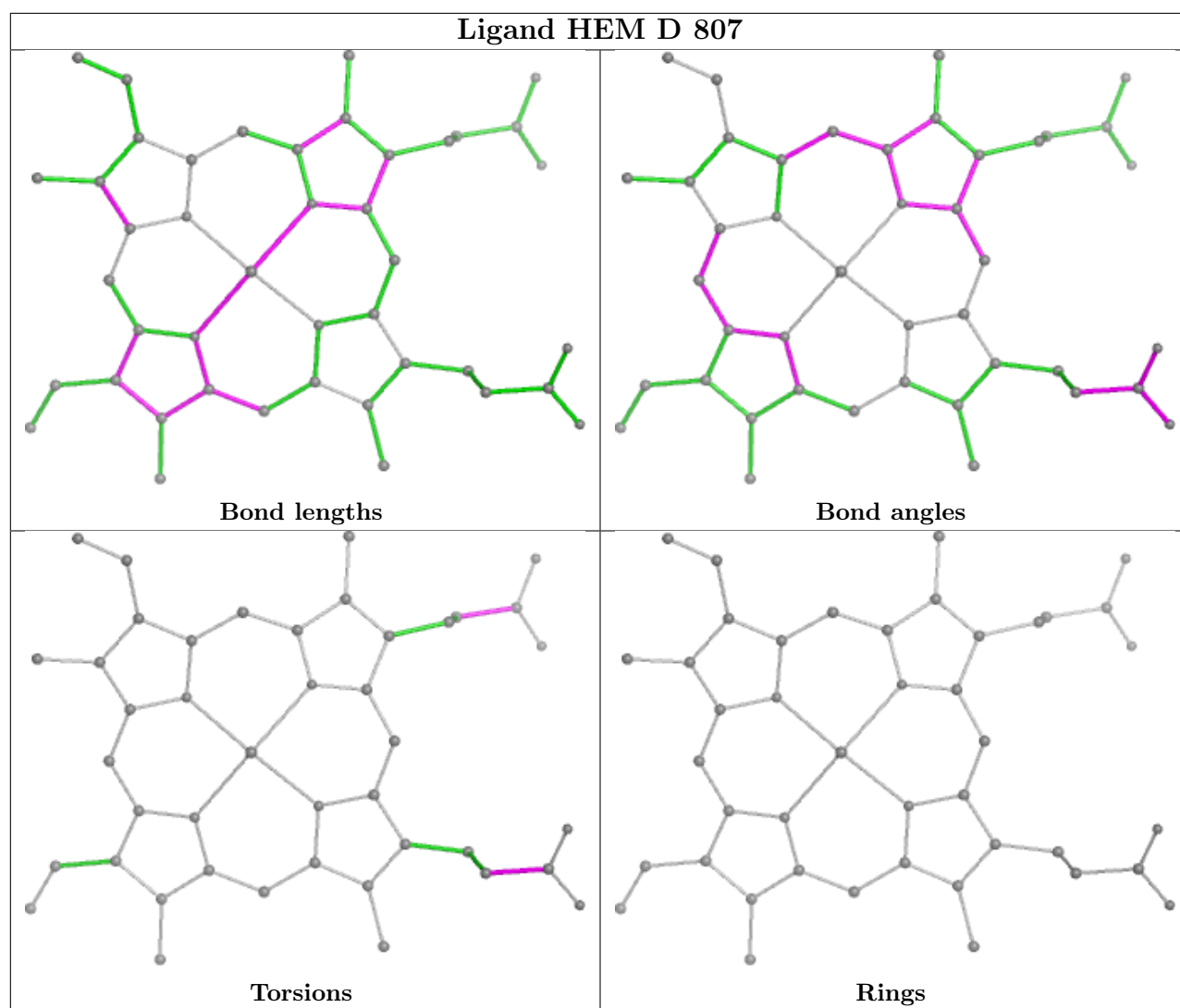
7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	803	SCN	1	0
9	B	809	SCN	1	0
9	B	807	SCN	1	0
9	B	806	SCN	2	0
9	D	806	SCN	1	0
10	B	810	HEM	2	0
10	D	807	HEM	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	B	464/467 (99%)	-0.65	3 (0%) 85 87	19, 29, 48, 82	0
1	D	464/467 (99%)	-0.22	6 (1%) 74 76	20, 39, 64, 92	0
2	E	56/60 (93%)	-0.03	1 (1%) 67 70	30, 41, 63, 82	0
2	F	58/60 (96%)	1.97	25 (43%) 1 0	82, 103, 117, 126	0
3	A	105/114 (92%)	-0.71	0 100 100	12, 26, 46, 83	1 (0%)
3	C	105/114 (92%)	-0.45	0 100 100	22, 32, 59, 89	0
All	All	1252/1282 (97%)	-0.33	35 (2%) 55 57	12, 33, 82, 126	1 (0%)

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	93	PHE	4.2
2	F	81	ILE	4.0
2	F	100	HIS	4.0
1	D	279	VAL	3.8
2	F	95	VAL	3.7

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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	2CO	D	316	8/9	0.96	0.06	25,26,34,39	0
1	2CO	B	316	8/9	0.97	0.05	21,23,28,39	0

### 6.3 Carbohydrates

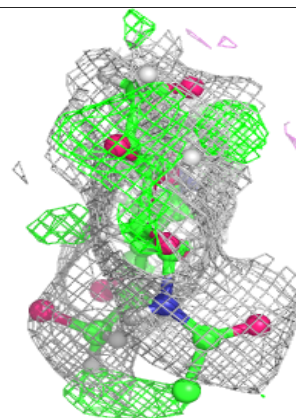
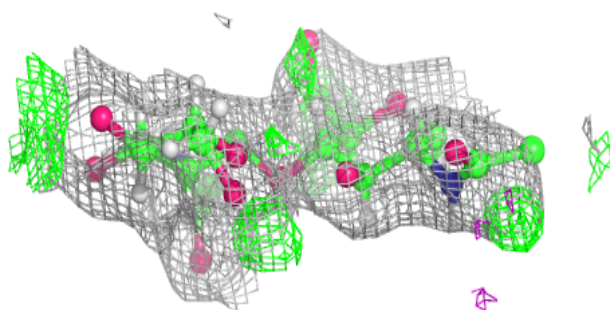
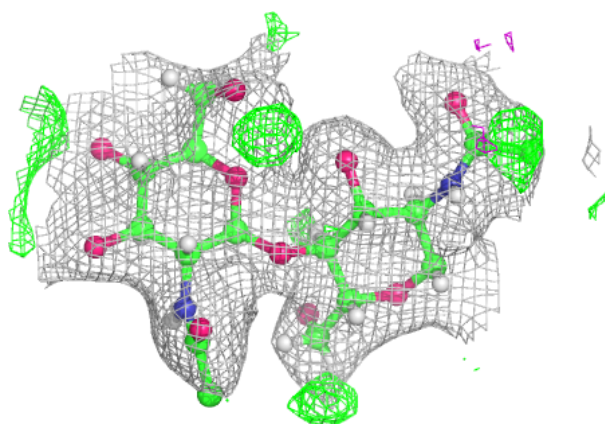
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	J	2	14/15	0.76	0.14	41,79,87,91	0
4	NAG	G	2	14/15	0.83	0.12	62,72,78,81	0
4	NAG	J	1	14/15	0.87	0.12	46,57,71,80	0
6	MAN	H	4	11/12	0.89	0.09	27,33,35,35	0
4	NAG	G	1	14/15	0.90	0.10	41,48,53,58	0
5	MAN	I	4	11/12	0.95	0.06	47,50,56,58	0
6	BMA	H	3	11/12	0.96	0.05	28,32,43,55	0
6	NAG	H	1	14/15	0.97	0.05	23,27,31,37	0
5	MAN	I	5	11/12	-	-	28,31,34,35	0
5	FUC	I	6	10/11	-	-	33,41,44,45	0
6	NAG	H	2	14/15	0.97	0.05	23,27,30,32	0
5	BMA	I	3	11/12	0.97	0.05	27,30,35,43	0
5	NAG	I	1	14/15	0.97	0.04	22,27,35,39	0
5	NAG	I	2	14/15	0.98	0.05	17,27,29,32	0
6	NAG	H	5	14/15	-	-	40,72,81,87	0
6	MAN	H	6	11/12	-	-	66,74,80,81	0
6	FUC	H	7	10/11	-	-	30,39,42,42	0

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.

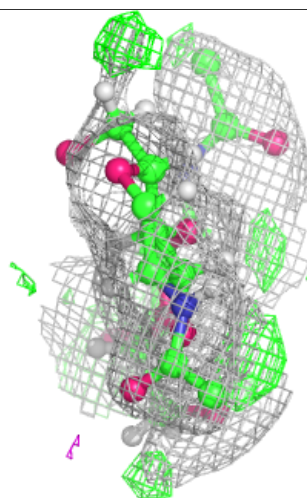
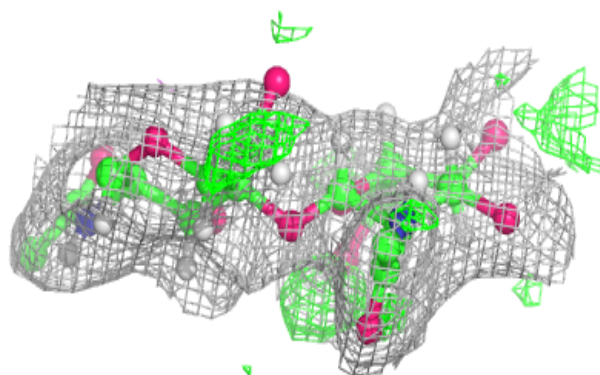
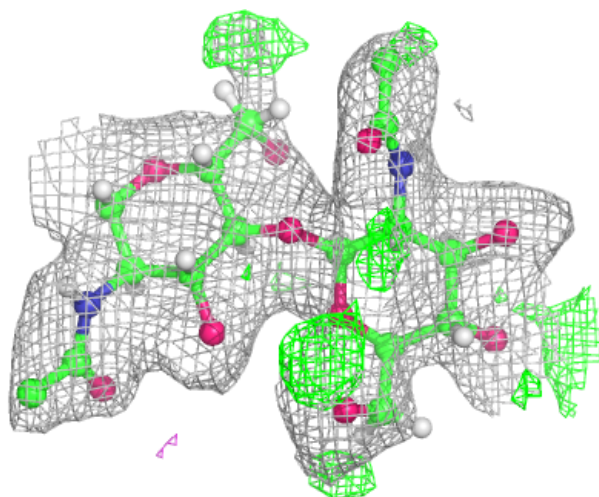
**Electron density around Chain G:**

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



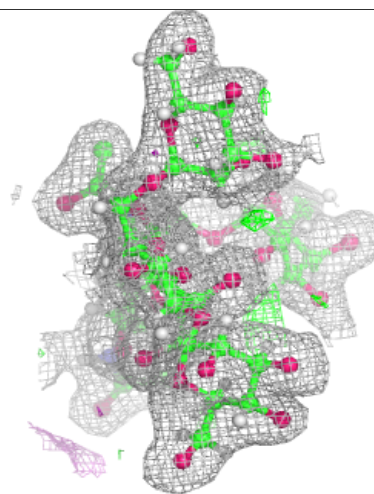
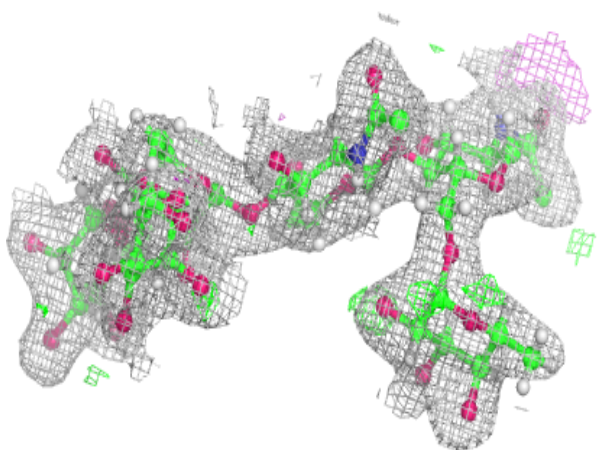
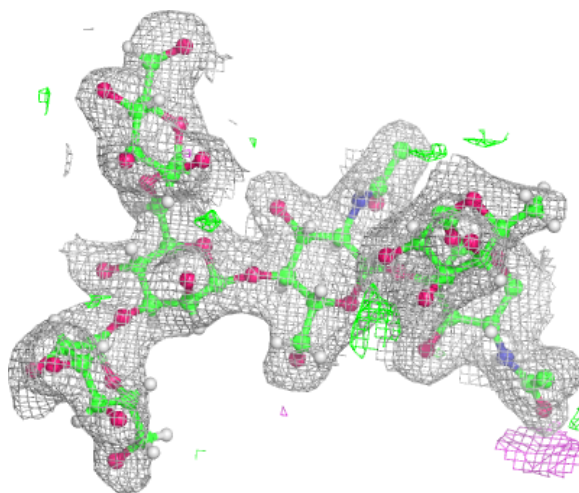
**Electron density around Chain J:**

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

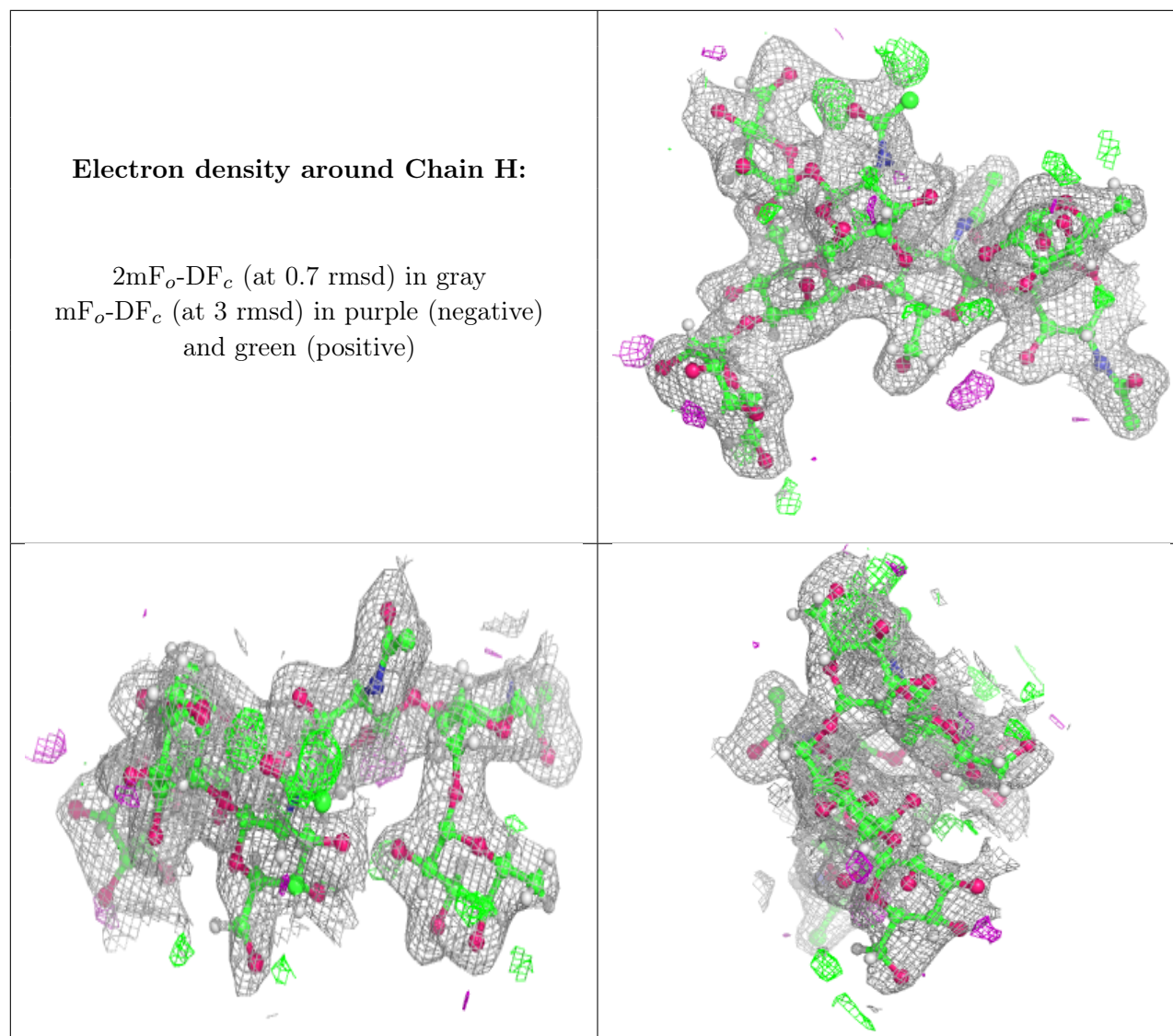


**Electron density around Chain I:**

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







## 6.4 Ligands [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	NAG	D	801	14/15	0.88	0.09	48,56,60,62	0
9	SCN	B	805	3/3	0.88	0.13	40,40,58,70	0
9	SCN	C	302	3/3	0.90	0.17	53,53,54,60	0
9	SCN	B	808	3/3	0.91	0.13	38,38,43,46	0
9	SCN	B	806	3/3	0.91	0.22	34,34,47,50	0
7	NAG	B	801	14/15	0.93	0.07	25,34,43,45	0
9	SCN	B	809	3/3	0.94	0.20	38,38,45,51	0

*Continued on next page...*



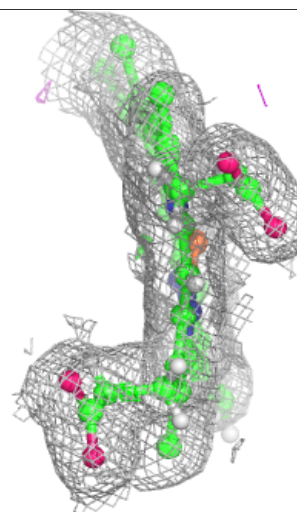
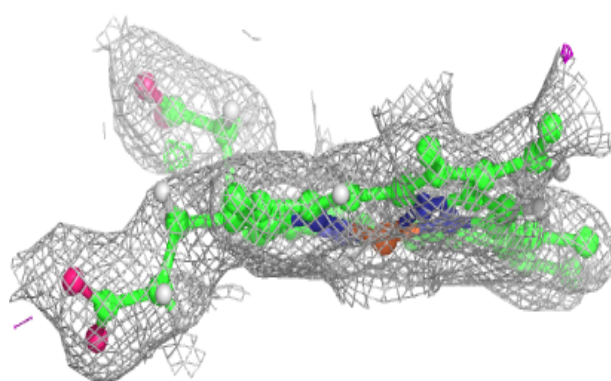
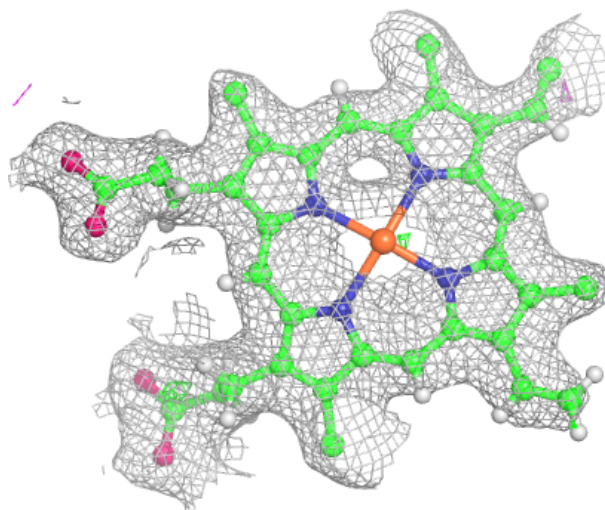
*Continued from previous page...*

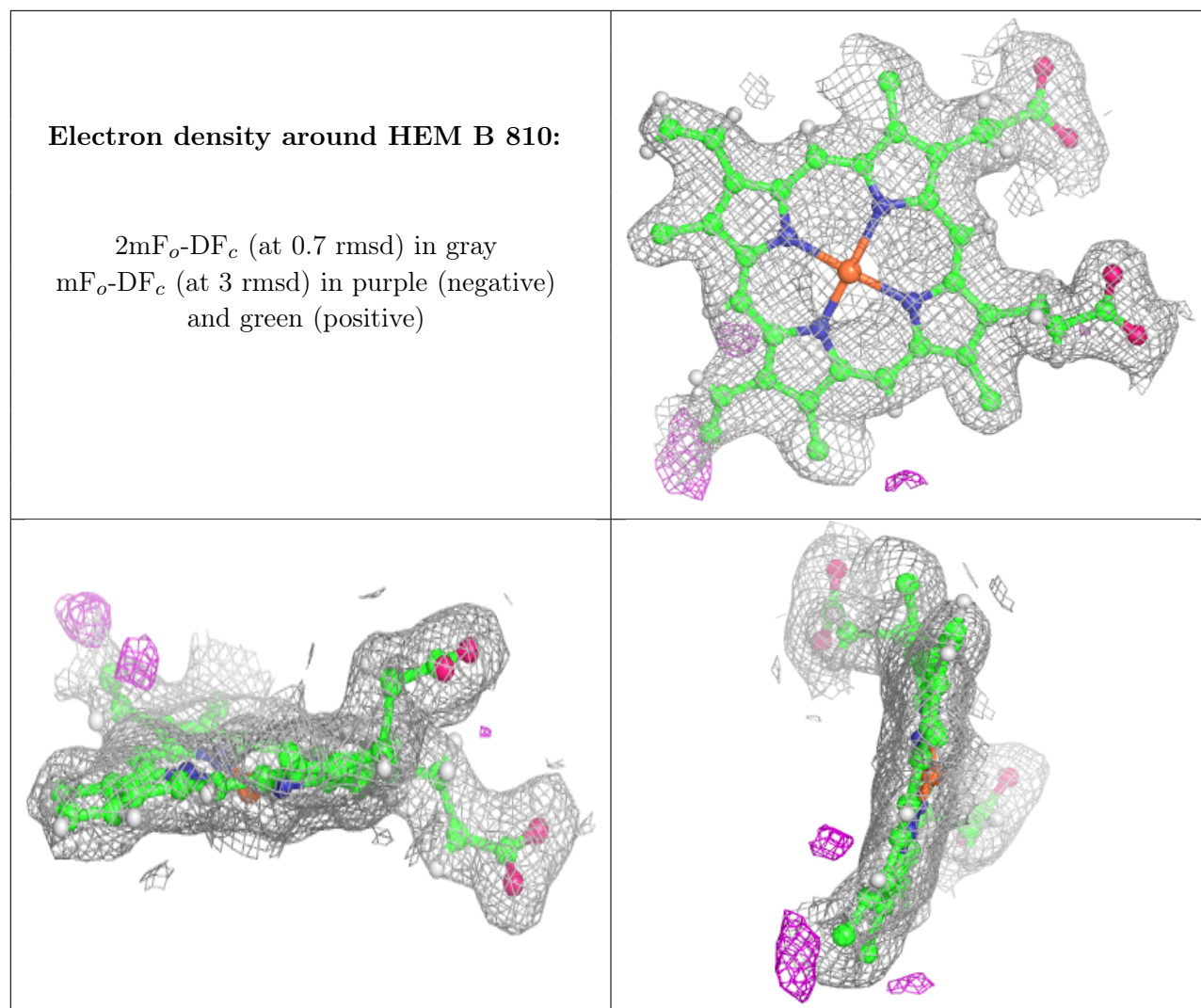
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	SCN	D	806	3/3	0.94	0.13	35,35,51,59	0
9	SCN	B	803	3/3	0.94	0.13	33,33,43,46	0
9	SCN	D	804	3/3	0.95	0.12	50,50,51,58	0
9	SCN	A	302	3/3	0.95	0.09	30,30,43,49	0
9	SCN	D	805	3/3	0.95	0.10	43,43,45,48	0
9	SCN	D	803	3/3	0.97	0.07	29,29,41,43	0
9	SCN	B	807	3/3	0.98	0.09	37,37,45,46	0
9	SCN	C	301	3/3	0.98	0.05	17,17,26,27	0
9	SCN	A	301	3/3	0.98	0.07	17,17,22,24	0
10	HEM	D	807	43/43	0.98	0.05	22,29,36,40	0
9	SCN	B	804	3/3	0.99	0.06	32,32,37,42	0
8	CA	D	802	1/1	0.99	0.03	30,30,30,30	0
10	HEM	B	810	43/43	0.99	0.04	18,21,25,30	0
8	CA	B	802	1/1	0.99	0.03	23,23,23,23	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 HEM D 807:**

$2mF_o-DF_c$  (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.