



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 01:22 PM UTC

PDB ID : 5WDJ / pdb_00005wdj
Title : CRYSTAL STRUCTURE OF MYELOPEROXIDASE SUBFORM C (MPO)
COMPLEX WITH COMPOUND-6 AKA 7-(BENZYLOXY)-1H-[1,2, 3]TRIA
ZOLO[4,5-D]PYRIMIDIN-5-AMINE
Authors : Khan, J.A.
Deposited on : 2017-07-05
Resolution : 2.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

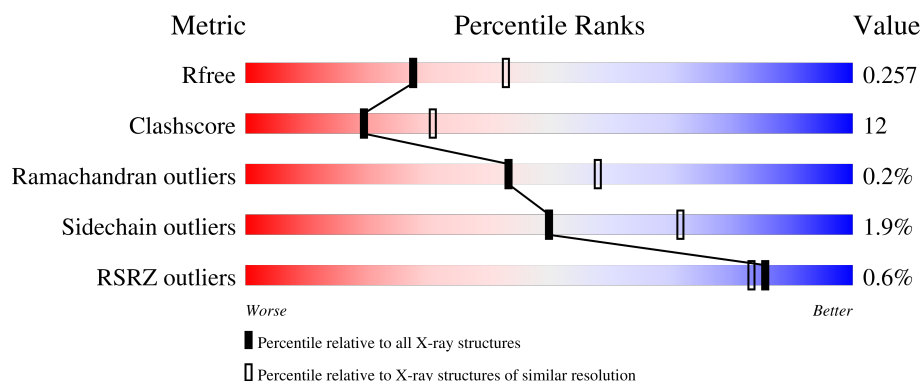
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.



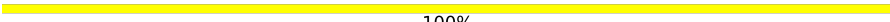
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	105	77% 22% .
1	D	105	% 73% 24% ..
2	B	467	80% 18% .
2	E	467	% 82% 17% .

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Mol	Chain	Length	Quality of chain
3	C	3	 100%
4	F	3	 33% 67%

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 9895 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Myeloperoxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	0	0
			825	522	146	152	5			
1	D	103	Total	C	N	O	S	0	0	0
			824	521	146	152	5			

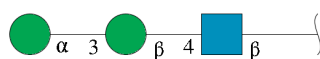
- Molecule 2 is a protein called Myeloperoxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	466	Total	C	N	O	S	0	0	0
			3696	2338	669	662	27			
2	E	465	Total	C	N	O	S	0	0	0
			3702	2338	675	662	27			

There are 2 discrepancies between the modelled and reference sequences:

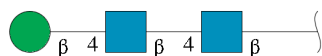
Chain	Residue	Modelled	Actual	Comment	Reference
B	112	ALA	-	expression tag	UNP P05164
E	112	ALA	-	expression tag	UNP P05164

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



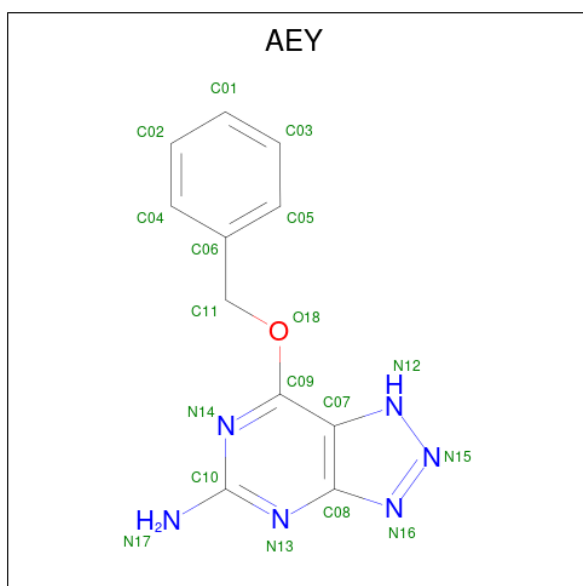
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			36	20	1	15			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

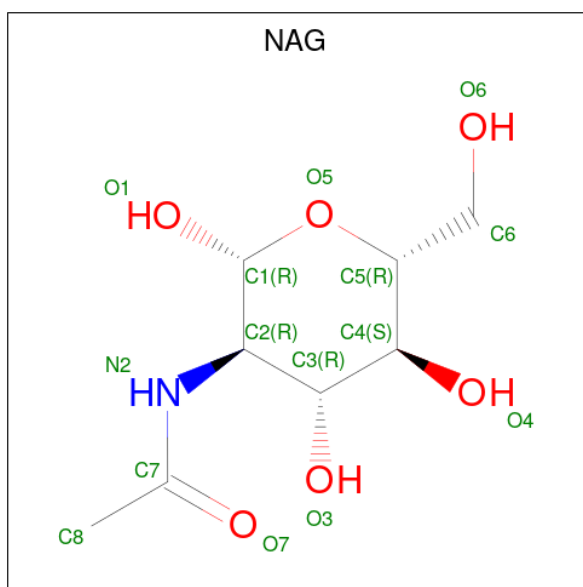
- Molecule 5 is 7-(benzyloxy)-1H-[1,2,3]triazolo[4,5-d]pyrimidin-5-amine (CCD ID: AEY) (formula: C₁₁H₁₀N₆O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			18	11	6	1		
5	E	1	Total	C	N	O	0	0
			18	11	6	1		

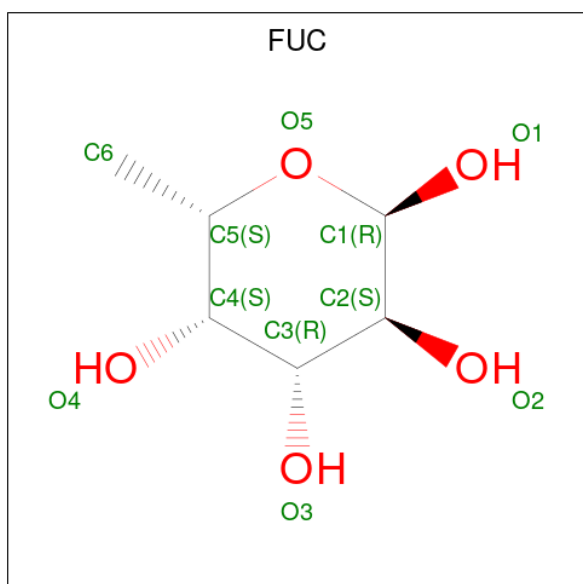
- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		
6	B	1	Total	Cl	0	0
			1	1		
6	D	1	Total	Cl	0	0
			1	1		
6	E	1	Total	Cl	0	0
			1	1		



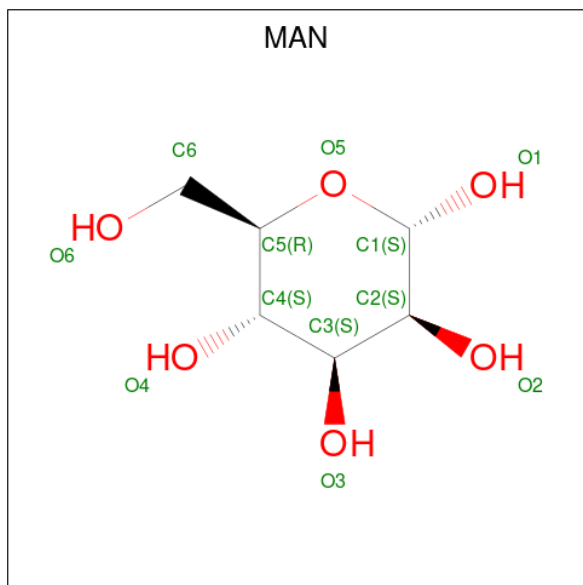
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	E	1	Total	C	N	O	0	0
			14	8	1	5		
9	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 10 is alpha-L-fucopyranose (CCD ID: FUC) (formula: $C_6H_{12}O_5$).



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

- Molecule 11 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			11	6	5		
11	B	1	Total	C	O	0	0
			11	6	5		
11	E	1	Total	C	O	0	0
			11	6	5		

- Molecule 12 is water.

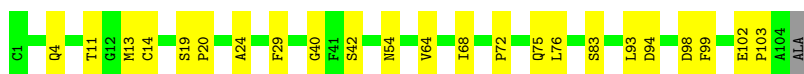
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	55	Total	O	0	0
			55	55		
12	B	203	Total	O	0	0
			203	203		
12	D	55	Total	O	0	0
			55	55		
12	E	209	Total	O	0	0
			209	209		

3 Residue-property plots

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.

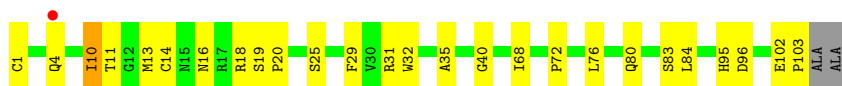
- Molecule 1: Myeloperoxidase

Chain A: 



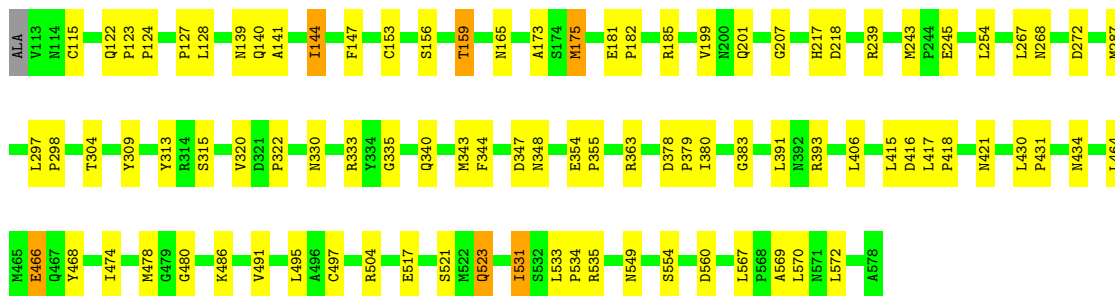
- Molecule 1: Myeloperoxidase

Chain D: 



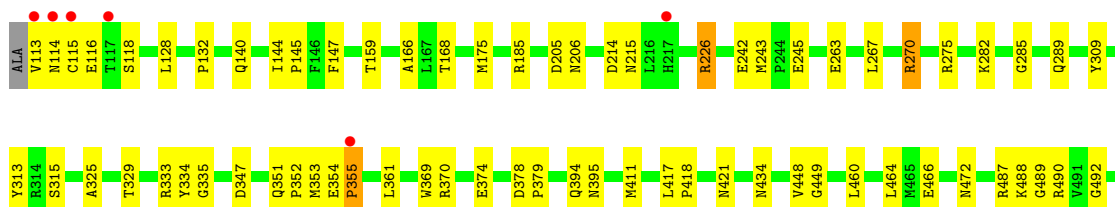
- Molecule 2: Myeloperoxidase

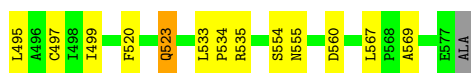
Chain B: 



- Molecule 2: Myeloperoxidase

Chain E: 





- Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  100%



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

Chain F:  33%  67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.92Å 103.92Å 242.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.51 – 2.40 95.51 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (95.51-2.40) 99.6 (95.51-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 2.39Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.194 , 0.248 0.212 , 0.257	Depositor DCC
R_{free} test set	2676 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 23.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9895	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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: AEY, MAN, CA, CSO, NAG, FUC, BMA, HEM, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.42	0/850	0.82	2/1160 (0.2%)
1	D	0.44	0/849	0.82	3/1158 (0.3%)
2	B	0.44	0/3774	0.76	3/5120 (0.1%)
2	E	0.44	0/3780	0.76	2/5129 (0.0%)
All	All	0.44	0/9253	0.77	10/12567 (0.1%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	SER	CA-C-N	6.20	127.58	119.84
1	A	19	SER	C-N-CA	6.20	127.58	119.84
1	D	19	SER	CA-C-N	5.99	126.77	120.12
1	D	19	SER	C-N-CA	5.99	126.77	120.12
2	B	434	ASN	N-CA-C	5.51	117.29	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	825	0	777	20	0
1	D	824	0	778	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3696	0	3666	87	0
2	E	3702	0	3678	80	0
3	C	36	0	29	3	0
4	F	39	0	32	3	0
5	A	18	0	0	0	0
5	E	18	0	0	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
7	A	43	0	30	13	0
7	D	43	0	30	14	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0
9	B	42	0	39	7	0
9	E	28	0	26	0	0
10	B	10	0	9	2	0
10	E	10	0	9	0	0
11	B	22	0	18	3	0
11	E	11	0	10	1	0
12	A	55	0	0	4	0
12	B	203	0	0	25	0
12	D	55	0	0	5	0
12	E	209	0	0	16	0
All	All	9895	0	9131	215	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 12.

The worst 5 of 215 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)
7:A:203:HEM:HBB1	2:B:243:MET:SD	1.39	1.59
7:D:201:HEM:HBB1	2:E:243:MET:SD	1.44	1.55
2:E:113:VAL:CB	2:E:114:ASN:HA	1.20	1.50
7:D:201:HEM:CMB	2:E:242:GLU:OE2	1.63	1.42
9:B:601:NAG:O6	10:B:602:FUC:C1	1.69	1.38

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	102/105 (97%)	95 (93%)	6 (6%)	1 (1%)	12	20
1	D	101/105 (96%)	97 (96%)	4 (4%)	0	100	100
2	B	463/467 (99%)	444 (96%)	19 (4%)	0	100	100
2	E	462/467 (99%)	444 (96%)	17 (4%)	1 (0%)	43	58
All	All	1128/1144 (99%)	1080 (96%)	46 (4%)	2 (0%)	43	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	SER
2	E	355	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	87/90 (97%)	87 (100%)	0	100	100
1	D	88/90 (98%)	84 (96%)	4 (4%)	24	42
2	B	399/410 (97%)	391 (98%)	8 (2%)	48	70
2	E	403/410 (98%)	396 (98%)	7 (2%)	53	74
All	All	977/1000 (98%)	958 (98%)	19 (2%)	50	71

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	226	ARG
2	E	466	GLU
2	E	523	GLN
2	E	361	LEU
1	D	4	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	409	GLN
2	E	540	ASN
2	E	563	ASN
2	E	549	ASN
2	B	434	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	$\# Z > 2$
2	CSO	E	150	2	3,6,7	0.91	0	1,6,8	1.42	0
2	CSO	B	150	2	3,6,7	0.58	0	1,6,8	0.72	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSO	E	150	2	-	0/1/5/7	-
2	CSO	B	150	2	-	0/1/5/7	-

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.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

6 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$
3	NAG	C	1	3	14,14,15	0.55	0	17,19,21	0.82	0
3	BMA	C	2	3	11,11,12	1.20	0	15,15,17	3.19	5 (33%)
3	MAN	C	3	3	11,11,12	4.05	4 (36%)	15,15,17	2.66	5 (33%)
4	NAG	F	1	2,4	14,14,15	1.27	1 (7%)	17,19,21	1.99	4 (23%)
4	NAG	F	2	4	14,14,15	0.65	0	17,19,21	0.90	0
4	BMA	F	3	4	11,11,12	0.28	0	15,15,17	0.91	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	NAG	C	1	3	-	0/6/23/26	0/1/1/1
3	BMA	C	2	3	-	2/2/19/22	0/1/1/1
3	MAN	C	3	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	MAN	O6-C6	-8.35	1.07	1.42
3	C	3	MAN	C4-C5	6.91	1.67	1.53
3	C	3	MAN	C4-C3	-6.19	1.36	1.52
3	C	3	MAN	C2-C3	4.15	1.58	1.52
4	F	1	NAG	O7-C7	-2.32	1.18	1.23

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	BMA	C1-O5-C5	7.03	121.61	112.19
3	C	2	BMA	C1-C2-C3	6.67	119.36	109.64
3	C	2	BMA	C3-C4-C5	5.39	120.00	110.23
3	C	3	MAN	C1-O5-C5	5.10	119.02	112.19
3	C	3	MAN	O5-C5-C4	-5.08	98.46	110.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

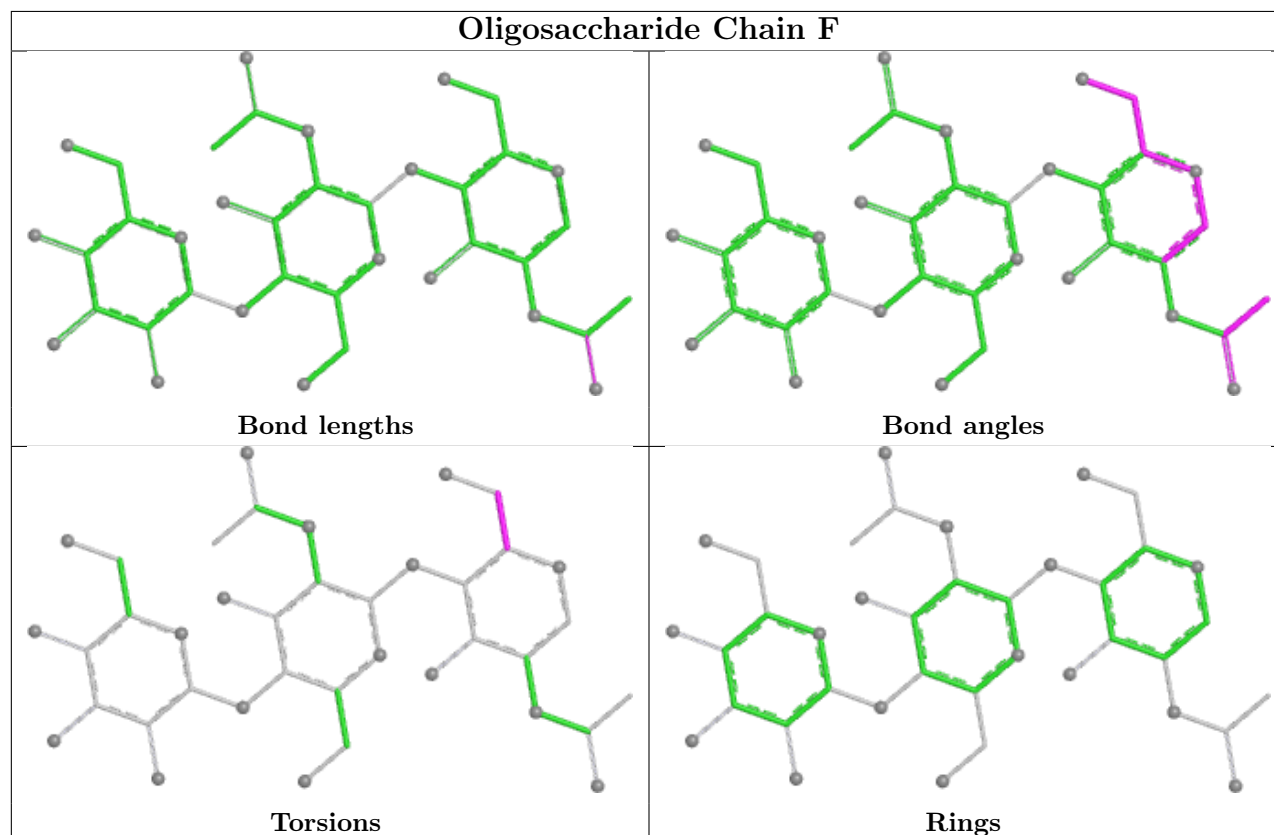
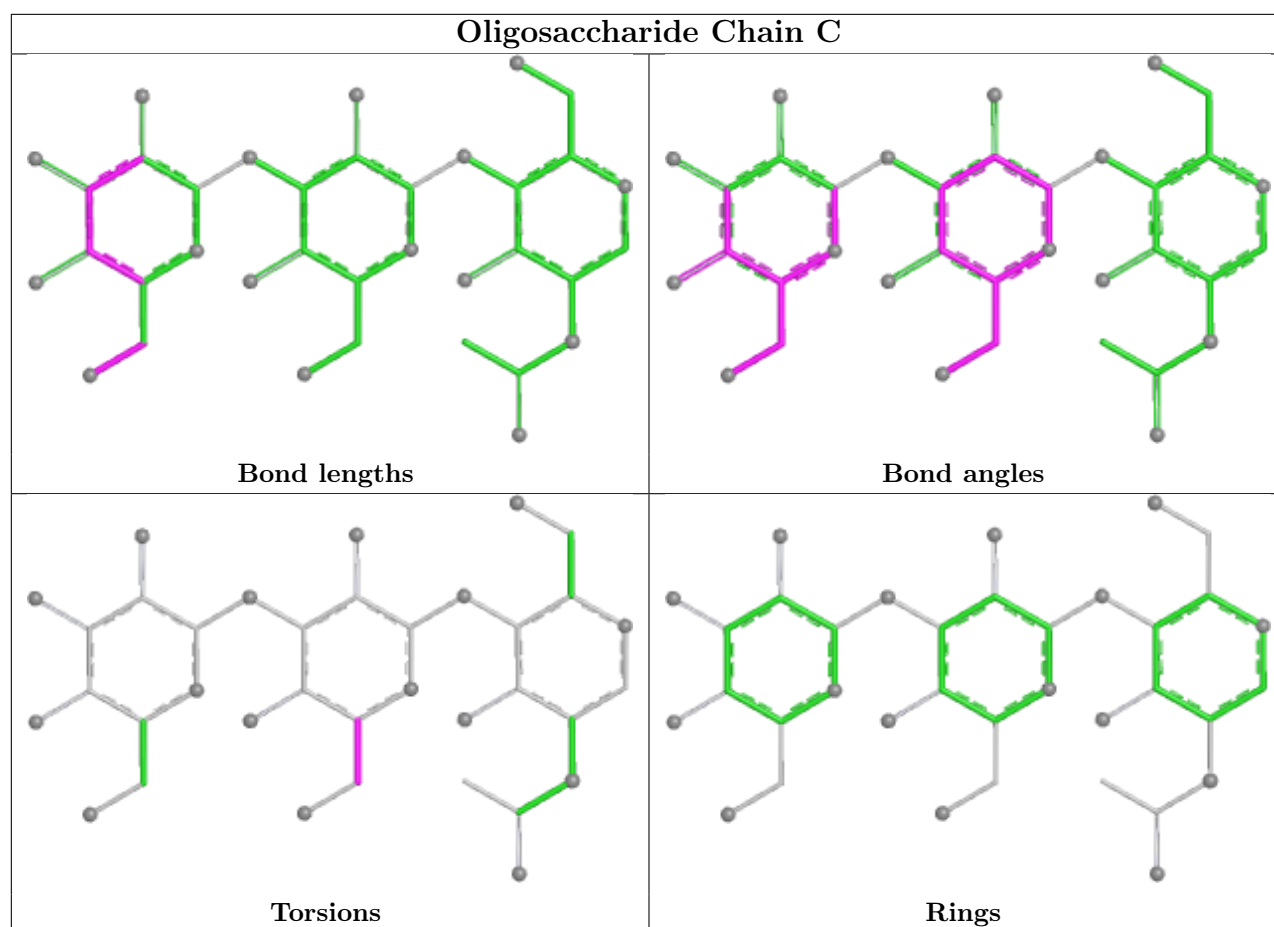
Mol	Chain	Res	Type	Atoms
3	C	2	BMA	O5-C5-C6-O6
3	C	2	BMA	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	3	BMA	3	0
3	C	1	NAG	3	0

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



5.6 Ligand geometry

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 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	NAG	E	609	2	14,14,15	0.45	0	17,19,21	0.92	0
9	NAG	B	604	2	14,14,15	1.23	2 (14%)	17,19,21	1.69	3 (17%)
11	MAN	E	604	-	11,11,12	3.56	6 (54%)	15,15,17	2.47	8 (53%)
9	NAG	E	610	2	14,14,15	0.57	0	17,19,21	0.74	0
10	FUC	B	602	-	10,10,11	3.51	7 (70%)	14,14,16	2.30	8 (57%)
5	AEY	E	611	-	19,20,20	1.36	1 (5%)	19,27,27	1.77	5 (26%)
11	MAN	B	606	-	11,11,12	1.28	1 (9%)	15,15,17	1.55	3 (20%)
5	AEY	A	201	-	19,20,20	1.32	2 (10%)	19,27,27	1.59	4 (21%)
7	HEM	A	203	2,1	50,50,50	2.05	9 (18%)	67,82,82	1.25	6 (8%)
11	MAN	B	605	-	11,11,12	4.03	6 (54%)	15,15,17	2.52	6 (40%)
10	FUC	E	608	-	10,10,11	2.57	7 (70%)	14,14,16	1.78	4 (28%)
9	NAG	B	601	2	14,14,15	1.35	2 (14%)	17,19,21	2.14	4 (23%)
9	NAG	B	603	2	14,14,15	0.50	0	17,19,21	0.81	0
7	HEM	D	201	2,1	50,50,50	2.00	7 (14%)	67,82,82	1.26	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
9	NAG	E	609	2	-	0/6/23/26	0/1/1/1
9	NAG	B	604	2	-	0/6/23/26	0/1/1/1
11	MAN	E	604	-	-	1/2/19/22	0/1/1/1
9	NAG	E	610	2	-	1/6/23/26	0/1/1/1
10	FUC	B	602	-	-	-	0/1/1/1
5	AEY	E	611	-	-	0/5/5/5	0/3/3/3
11	MAN	B	606	-	-	2/2/19/22	0/1/1/1
5	AEY	A	201	-	-	0/5/5/5	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	HEM	A	203	2,1	-	4/14/54/54	-
11	MAN	B	605	-	-	0/2/19/22	0/1/1/1
10	FUC	E	608	-	-	-	0/1/1/1
9	NAG	B	601	2	-	0/6/23/26	0/1/1/1
9	NAG	B	603	2	-	0/6/23/26	0/1/1/1
7	HEM	D	201	2,1	-	4/14/54/54	-

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	605	MAN	C2-C3	9.03	1.66	1.52
7	D	201	HEM	C3D-C2D	7.74	1.53	1.36
7	A	203	HEM	C3D-C2D	7.58	1.53	1.36
10	B	602	FUC	O5-C5	-7.19	1.29	1.43
11	E	604	MAN	C1-C2	-6.88	1.35	1.52

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	605	MAN	C1-O5-C5	6.49	120.89	112.19
9	B	601	NAG	O5-C1-C2	-5.43	102.90	111.29
9	B	601	NAG	C1-O5-C5	5.18	119.13	112.19
7	A	203	HEM	C4D-ND-C1D	4.94	111.06	105.21
7	D	201	HEM	C4D-ND-C1D	4.84	110.94	105.21

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	B	606	MAN	C4-C5-C6-O6
11	B	606	MAN	O5-C5-C6-O6
7	D	201	HEM	CAA-CBA-CGA-O1A
9	E	610	NAG	C4-C5-C6-O6
7	D	201	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

8 monomers are involved in 39 short contacts:

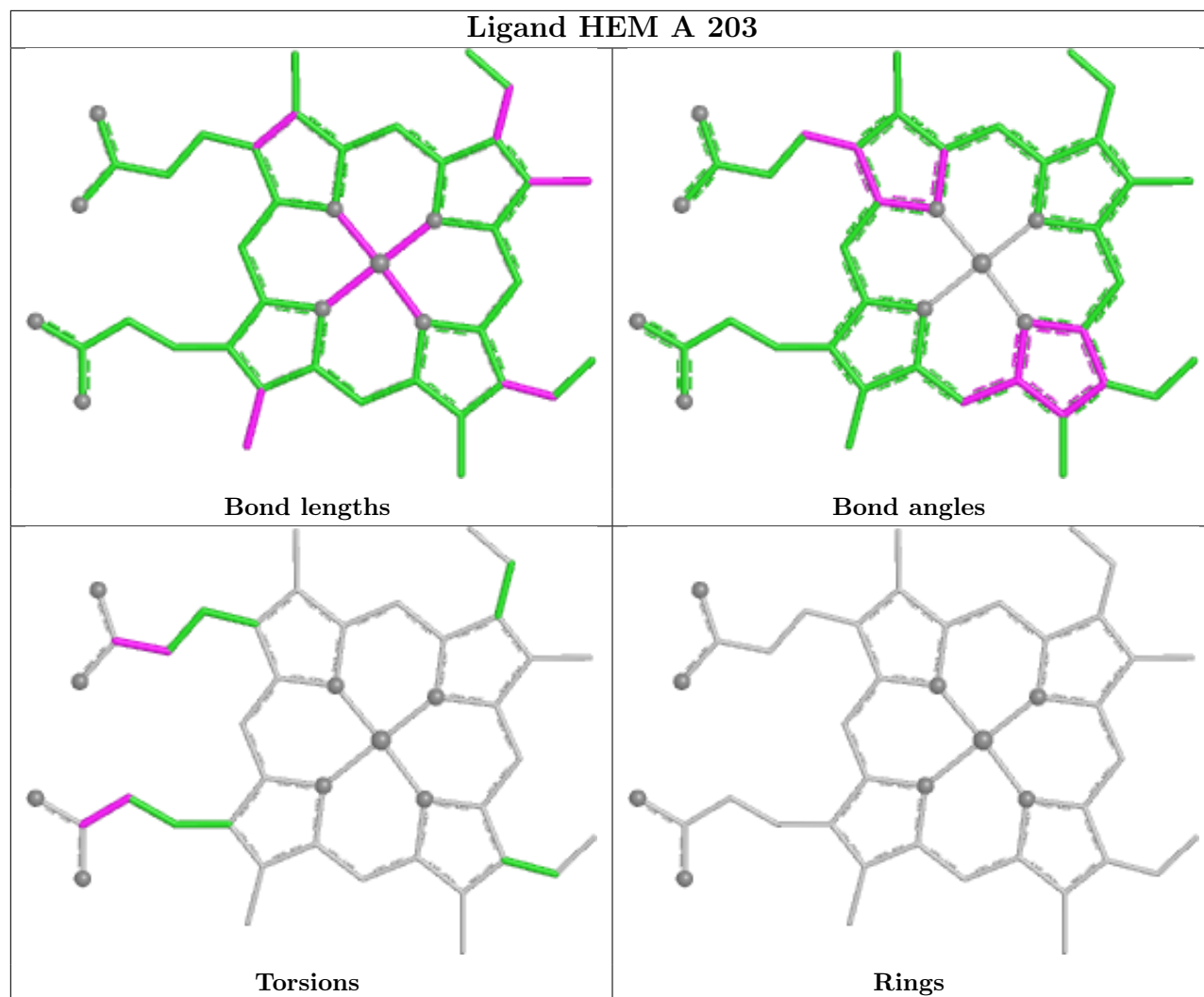
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	E	604	MAN	1	0

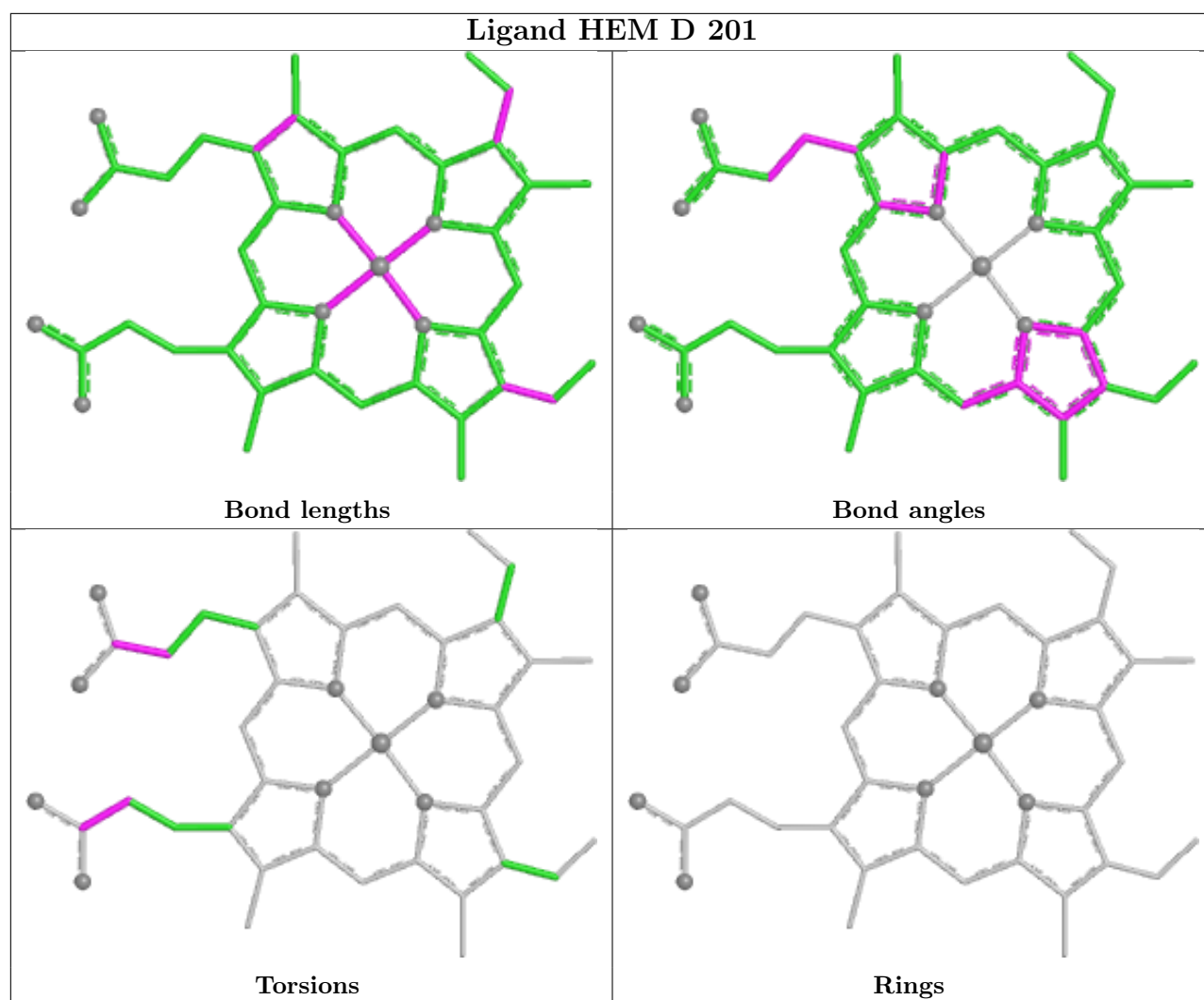
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	602	FUC	2	0
5	E	611	AEY	1	0
7	A	203	HEM	13	0
11	B	605	MAN	3	0
9	B	601	NAG	6	0
9	B	603	NAG	1	0
7	D	201	HEM	14	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	104/105 (99%)	-0.30	0 100 100	19, 22, 30, 39	0
1	D	103/105 (98%)	-0.29	1 (0%) 79 76	18, 22, 30, 39	0
2	B	465/467 (99%)	-0.28	0 100 100	17, 24, 33, 42	0
2	E	464/467 (99%)	-0.17	6 (1%) 75 71	17, 24, 33, 42	0
All	All	1136/1144 (99%)	-0.24	7 (0%) 85 83	17, 23, 34, 42	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	115	CYS	4.1
2	E	355	PRO	3.7
1	D	4	GLN	3.2
2	E	113	VAL	3.0
2	E	114	ASN	2.2

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.

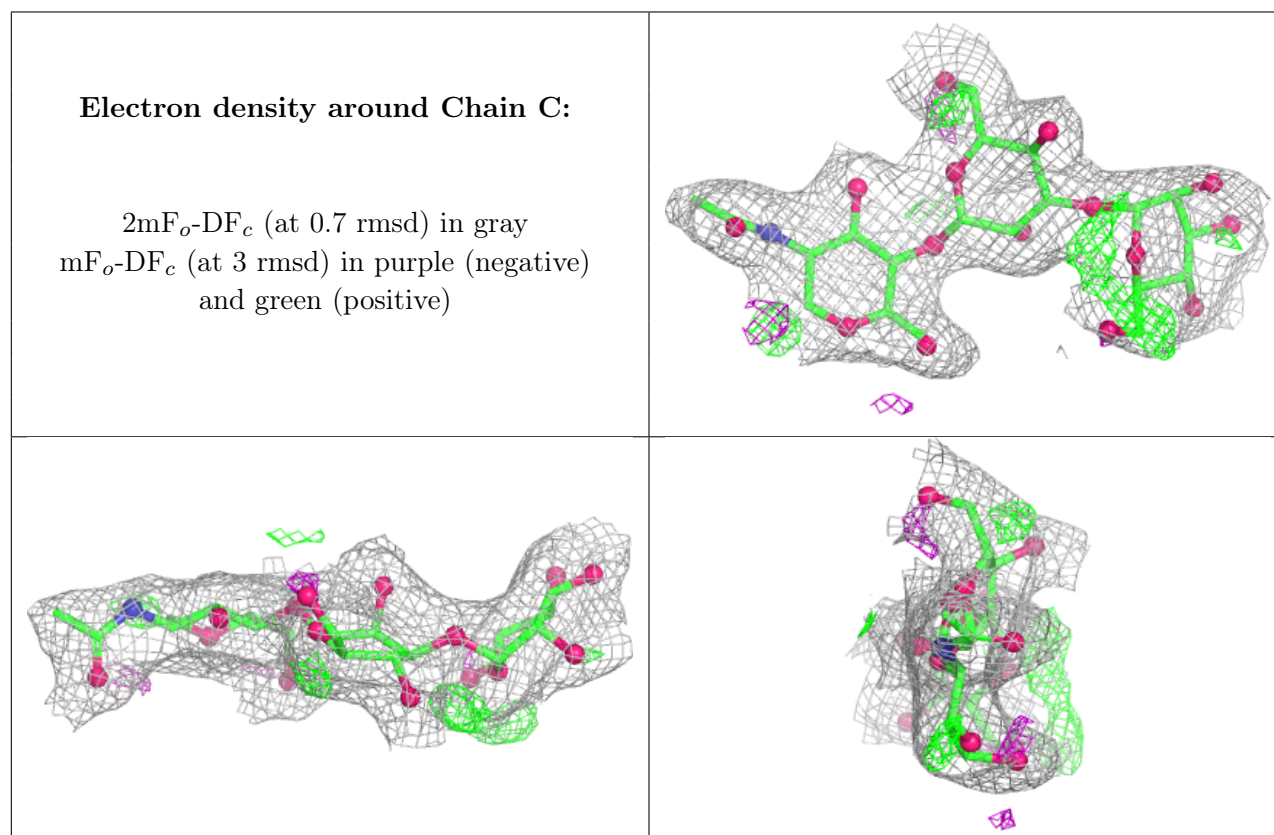
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CSO	B	150	7/8	0.94	0.08	22,23,24,25	0
2	CSO	E	150	7/8	0.95	0.07	22,23,24,25	0

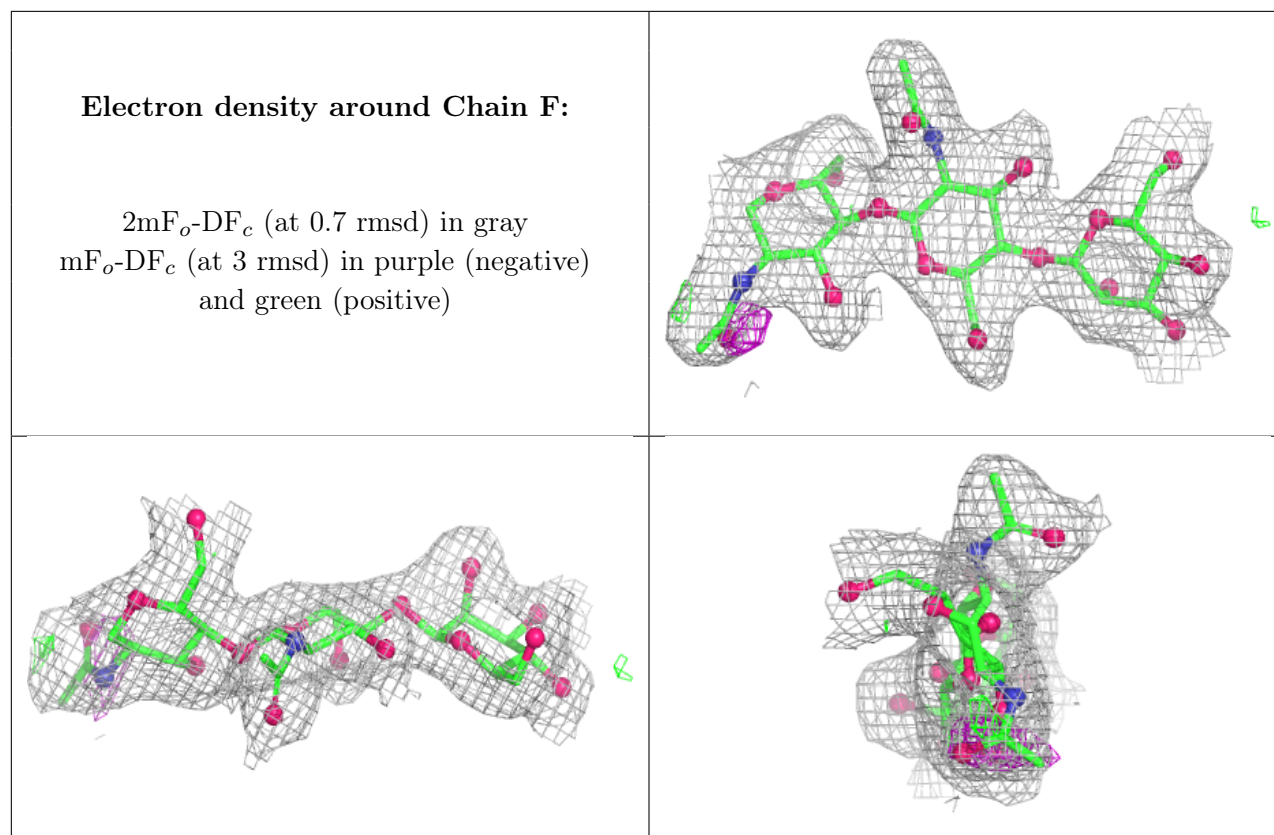
6.3 Carbohydrates [i](#)

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($\text{\AA}^2$)	Q<0.9
3	NAG	C	1	14/15	-	-	15,19,20,23	0
3	BMA	C	2	11/12	-	-	23,25,27,30	0
3	MAN	C	3	11/12	-	-	38,40,41,41	0
4	NAG	F	1	14/15	0.85	0.12	16,20,23,25	0
4	BMA	F	3	11/12	0.92	0.07	20,21,23,24	0
4	NAG	F	2	14/15	0.95	0.06	16,18,20,20	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.





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, 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($\text{\AA}^2$)	Q<0.9
11	MAN	B	605	11/12	0.67	0.15	42,42,43,44	0
9	NAG	B	604	14/15	0.78	0.12	34,36,38,39	0
10	FUC	B	602	10/11	0.80	0.12	24,27,27,28	0
5	AEY	A	201	18/18	0.80	0.17	44,46,47,47	0
9	NAG	E	610	14/15	0.81	0.10	33,35,37,37	0
11	MAN	E	604	11/12	0.81	0.11	28,29,29,30	0
9	NAG	B	601	14/15	0.82	0.12	18,21,23,23	0
5	AEY	E	611	18/18	0.86	0.14	41,43,47,47	0
9	NAG	E	609	14/15	0.87	0.10	28,31,32,32	0
9	NAG	B	603	14/15	0.88	0.08	28,30,31,31	0
10	FUC	E	608	10/11	0.92	0.08	24,25,26,27	0
11	MAN	B	606	11/12	0.95	0.06	25,26,27,28	0
6	CL	B	607	1/1	0.96	0.36	47,47,47,47	0
6	CL	E	612	1/1	0.96	0.33	45,45,45,45	0

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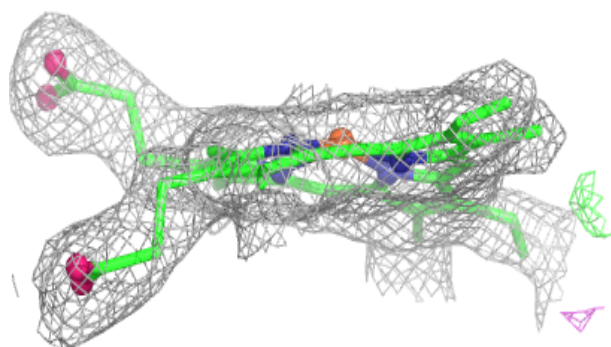
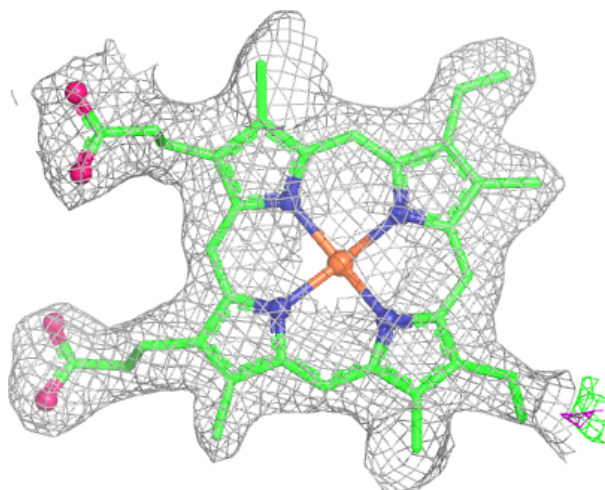
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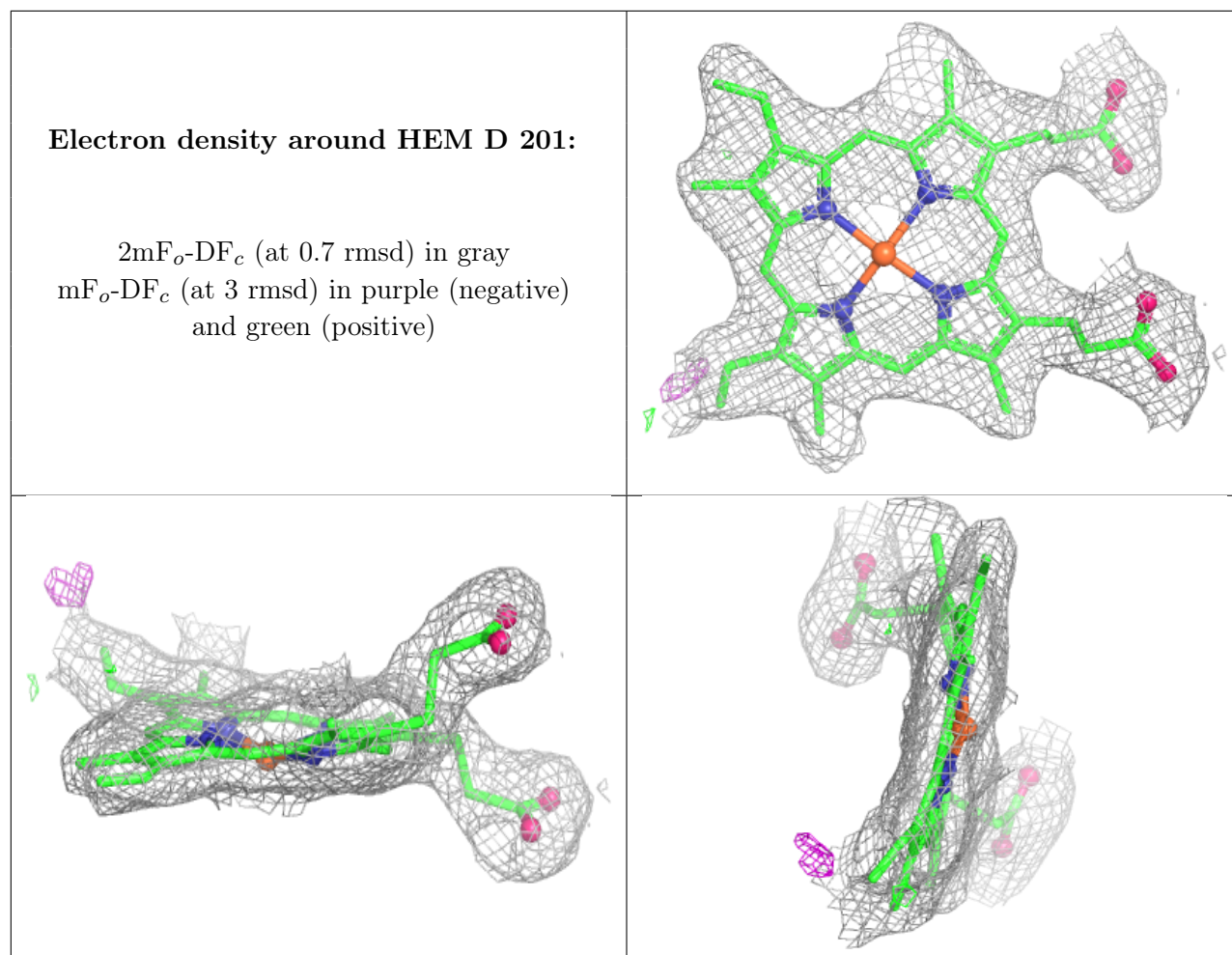
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	HEM	A	203	43/43	0.97	0.08	17,21,22,22	0
8	CA	D	203	1/1	0.97	0.10	28,28,28,28	0
7	HEM	D	201	43/43	0.98	0.07	13,18,20,21	0
6	CL	A	202	1/1	0.98	0.09	29,29,29,29	0
8	CA	A	204	1/1	0.99	0.14	31,31,31,31	0
6	CL	D	202	1/1	0.99	0.10	26,26,26,26	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 A 203:

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.