



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2024 – 07:18 PM EST

PDB ID : 3F9P
Title : Crystal structure of myeloperoxidase from human leukocytes
Authors : Carpena, X.; Fita, I.; Obinger, C.
Deposited on : 2008-11-14
Resolution : 2.93 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

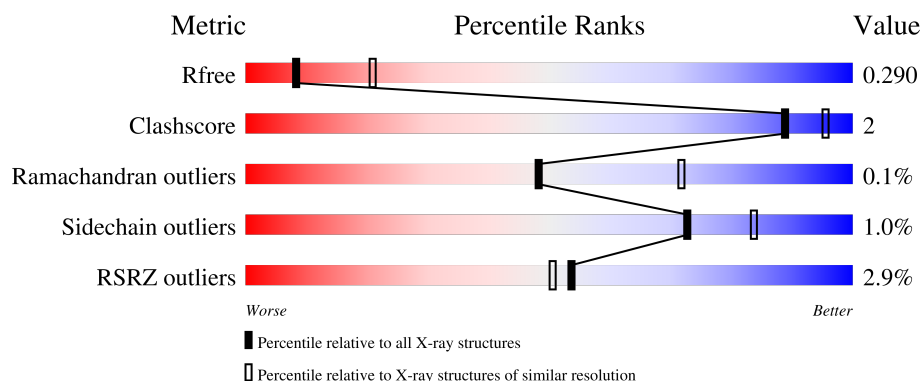
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 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	1067 (2.96-2.92)
Clashscore	180529	1122 (2.96-2.92)
Ramachandran outliers	177936	1075 (2.96-2.92)
Sidechain outliers	177891	1075 (2.96-2.92)
RSRZ outliers	164620	1067 (2.96-2.92)

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	<div> <div>3%</div> <div>92%</div> <div>6%</div> </div>
1	B	114	<div> <div>2%</div> <div>89%</div> <div>6%</div> <div>5%</div> </div>
2	C	467	<div> <div>3%</div> <div>94%</div> <div>6%</div> </div>
2	D	467	<div> <div>3%</div> <div>95%</div> <div>5%</div> </div>
3	E	6	<div> <div>67%</div> <div>33%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	6	 <div>67% 33%</div>

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
8	ACT	C	605	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9483 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.

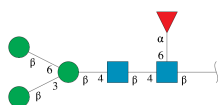
- Molecule 1 is a protein called Myeloperoxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	107	Total	C	N	O	S	0	0	0
			860	542	154	159	5			
1	B	108	Total	C	N	O	S	0	0	1
			861	542	155	159	5			

- Molecule 2 is a protein called Myeloperoxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	467	Total	C	N	O	S	0	0	1
			3733	2351	688	667	27			
2	D	467	Total	C	N	O	S	0	0	1
			3733	2351	688	667	27			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-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
3	E	6	Total	C	N	O	0	0	0
			71	40	2	29			
3	F	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

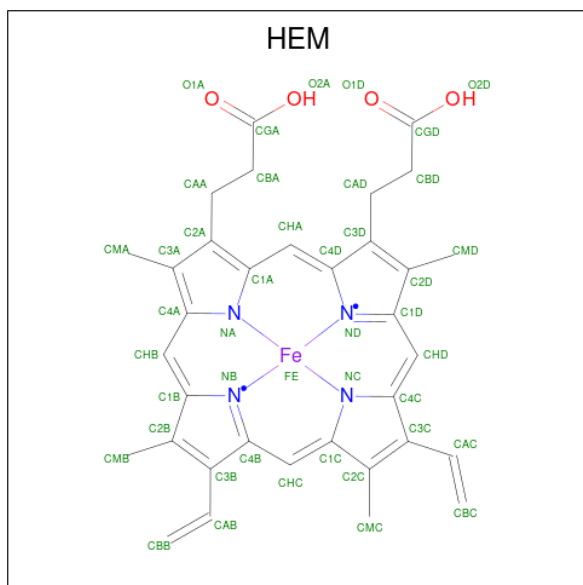
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Cl 1 1	0	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

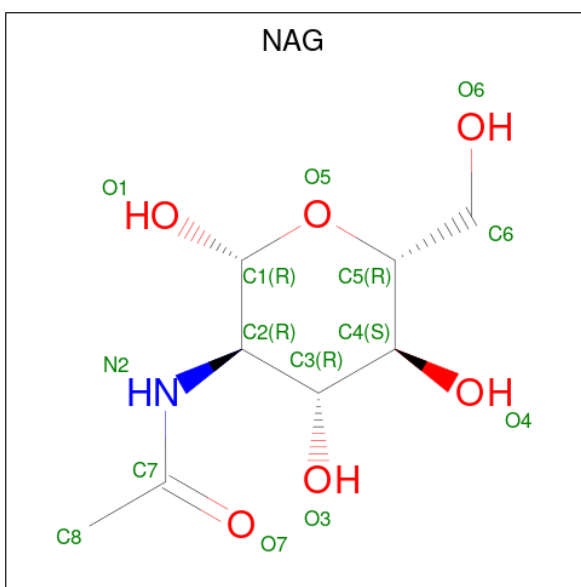


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

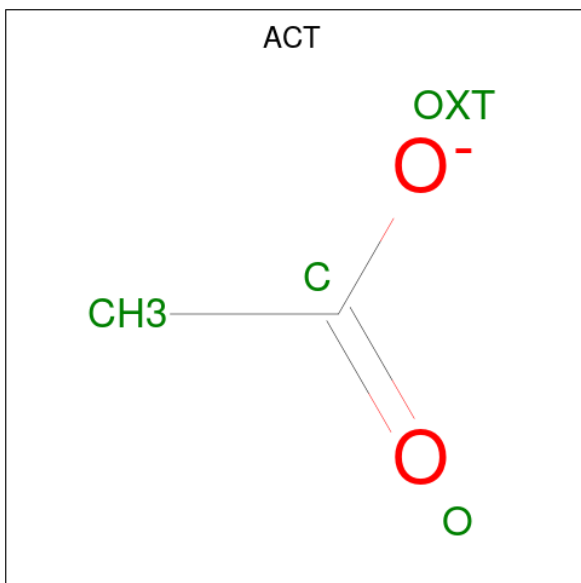
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total Ca 1 1	0	0
6	D	1	Total Ca 1 1	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $\text{C}_8\text{H}_{15}\text{NO}_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

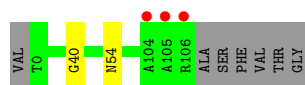


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total 4	C 2	O 2	0	0
8	D	1	Total 4	C 2	O 2	0	0

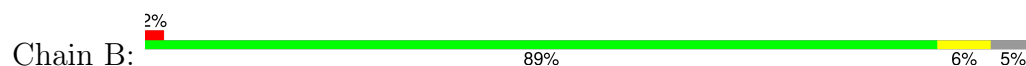
3 Residue-property plots [i](#)

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.

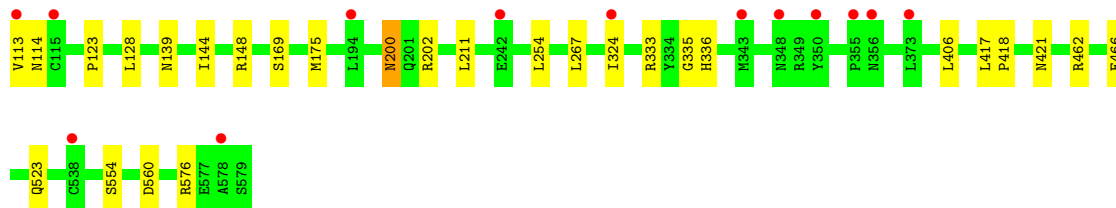
- Molecule 1: Myeloperoxidase



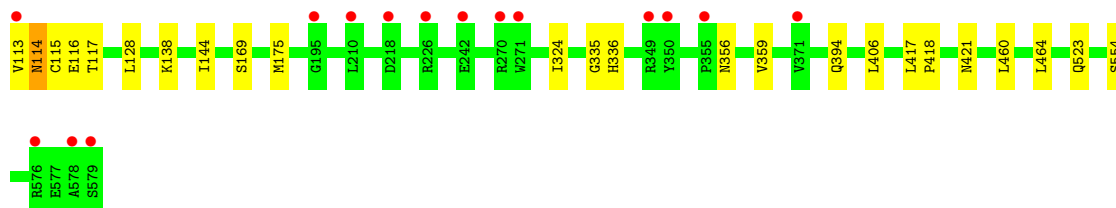
- Molecule 1: Myeloperoxidase



- Molecule 2: Myeloperoxidase



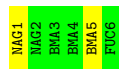
- Molecule 2: Myeloperoxidase



- Molecule 3: beta-D-mannopyranose-(1-3)-[beta-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-

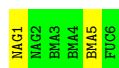
2-deoxy-beta-D-glucopyranose

Chain E:  67% 33%



- Molecule 3: beta-D-mannopyranose-(1-3)-[beta-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 F:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	110.74Å 110.74Å 255.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.93 20.00 – 2.93	Depositor EDS
% Data completeness (in resolution range)	96.2 (20.00-2.93) 95.8 (20.00-2.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.236 , 0.257 0.273 , 0.290	Depositor DCC
R_{free} test set	1707 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	63.0	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 1.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9483	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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: FUC, CL, HEM, CA, BMA, CSO, NAG, ACT

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	0.33	0/885	0.48	0/1205
1	B	0.35	0/886	0.51	0/1207
2	C	0.32	0/3811	0.46	0/5170
2	D	0.32	0/3811	0.47	0/5170
All	All	0.33	0/9393	0.47	0/12752

There are no bond length outliers.

There are no bond angle outliers.

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	860	0	823	1	0
1	B	861	0	823	6	0
2	C	3733	0	3725	15	0
2	D	3733	0	3725	17	0
3	E	71	0	61	0	0
3	F	71	0	61	0	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	C	43	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	43	0	30	1	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	C	28	0	26	0	0
7	D	28	0	26	0	0
8	C	4	0	3	2	0
8	D	4	0	3	0	0
All	All	9483	0	9336	34	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 2.

All (34) 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)
2:D:113:VAL:HA	2:D:114:ASN:HB2	1.11	1.09
2:D:113:VAL:HA	2:D:114:ASN:CB	1.97	0.95
2:D:113:VAL:CA	2:D:114:ASN:HB2	1.98	0.93
2:C:336:HIS:HD1	2:C:421:ASN:HD21	1.21	0.86
2:C:335:GLY:HA3	5:C:601:HEM:HBC2	1.68	0.74
2:D:336:HIS:HD1	2:D:421:ASN:HD21	1.35	0.74
1:B:106:ARG:H	2:D:113:VAL:HG22	1.63	0.63
2:C:113:VAL:N	2:C:114:ASN:HA	2.14	0.61
2:C:211:LEU:HD23	2:C:254:LEU:HD13	1.87	0.56
2:C:128:LEU:HB2	2:C:144:ILE:HB	1.88	0.54
2:C:148:ARG:HD3	8:C:605:ACT:H1	1.92	0.51
2:C:462:ARG:O	2:C:466:GLU:HG2	2.10	0.51
2:D:169:SER:HB2	2:D:324:ILE:HG12	1.95	0.49
1:A:40:GLY:HA2	1:B:20:PRO:HD2	1.93	0.49
2:C:333:ARG:HH21	5:C:601:HEM:HAD1	1.77	0.49
2:D:116:GLU:HG2	2:D:117:THR:HG23	1.95	0.48
2:C:406:LEU:HD22	2:C:417:LEU:HB2	1.96	0.48
1:B:64:VAL:HG13	1:B:68:ILE:HD12	1.98	0.46
2:C:267:LEU:HD12	2:C:576:ARG:HB2	1.96	0.46
2:C:169:SER:HB2	2:C:324:ILE:HG12	1.97	0.45
2:C:200:ASN:HD22	2:C:202:ARG:H	1.63	0.45
2:D:128:LEU:HB2	2:D:144:ILE:HB	1.99	0.45
2:D:113:VAL:HB	2:D:115:CYS:H	1.82	0.45
2:C:554:SER:HB3	2:C:560:ASP:HB3	1.99	0.44
2:C:417:LEU:HB3	2:C:418:PRO:HD3	2.01	0.43
2:D:335:GLY:HA3	5:D:601:HEM:HBC2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:356:ASN:HB3	2:D:359:VAL:HG22	2.00	0.43
2:D:394:GLN:HB3	2:D:460:LEU:HD22	2.01	0.42
2:D:406:LEU:HD22	2:D:417:LEU:HB2	2.01	0.42
1:B:83:SER:HB3	2:D:554:SER:O	2.19	0.42
1:B:68:ILE:HD13	2:D:464:LEU:HD23	2.02	0.41
1:B:106:ARG:N	2:D:113:VAL:HG22	2.33	0.41
2:C:123:PRO:HB3	8:C:605:ACT:H3	2.04	0.40
2:D:417:LEU:HB3	2:D:418:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/114 (92%)	102 (97%)	3 (3%)	0	100	100
1	B	106/114 (93%)	102 (96%)	4 (4%)	0	100	100
2	C	464/467 (99%)	452 (97%)	12 (3%)	0	100	100
2	D	464/467 (99%)	450 (97%)	13 (3%)	1 (0%)	44	66
All	All	1139/1162 (98%)	1106 (97%)	32 (3%)	1 (0%)	48	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	114	ASN

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	92/97 (95%)	91 (99%)	1 (1%)	70	82
1	B	92/97 (95%)	90 (98%)	2 (2%)	47	70
2	C	410/411 (100%)	406 (99%)	4 (1%)	73	84
2	D	410/411 (100%)	407 (99%)	3 (1%)	81	89
All	All	1004/1016 (99%)	994 (99%)	10 (1%)	73	84

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

Mol	Chain	Res	Type
1	A	54	ASN
2	C	139	ASN
2	C	175	MET
2	C	200	ASN
2	C	523	GLN
1	B	3	GLU
1	B	54	ASN
2	D	138	LYS
2	D	175	MET
2	D	523	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
2	C	139	ASN
2	C	200	ASN
2	C	421	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	D	150	2	3,6,7	0.68	0	1,6,8	0.55	0
2	CSO	C	150	2	3,6,7	0.65	0	1,6,8	0.55	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	D	150	2	-	1/1/5/7	-
2	CSO	C	150	2	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	150	CSO	N-CA-CB-SG
2	C	150	CSO	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

12 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	E	1	3,2	14,14,15	0.53	0	17,19,21	1.09	1 (5%)
3	NAG	E	2	3	14,14,15	0.46	0	17,19,21	0.65	0
3	BMA	E	3	3	11,11,12	0.48	0	15,15,17	0.81	0
3	BMA	E	4	3	11,11,12	0.58	0	15,15,17	0.62	0
3	BMA	E	5	3	11,11,12	0.61	0	15,15,17	1.16	2 (13%)
3	FUC	E	6	3	10,10,11	0.64	0	14,14,16	0.54	0
3	NAG	F	1	3,2	14,14,15	0.52	0	17,19,21	1.04	1 (5%)
3	NAG	F	2	3	14,14,15	0.49	0	17,19,21	0.61	0
3	BMA	F	3	3	11,11,12	0.48	0	15,15,17	0.91	0
3	BMA	F	4	3	11,11,12	0.54	0	15,15,17	0.51	0
3	BMA	F	5	3	11,11,12	0.55	0	15,15,17	0.93	1 (6%)
3	FUC	F	6	3	10,10,11	0.64	0	14,14,16	0.57	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	E	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	2/2/19/22	0/1/1/1
3	BMA	E	4	3	-	0/2/19/22	0/1/1/1
3	BMA	E	5	3	-	0/2/19/22	0/1/1/1
3	FUC	E	6	3	-	-	0/1/1/1
3	NAG	F	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
3	BMA	F	4	3	-	2/2/19/22	0/1/1/1
3	BMA	F	5	3	-	2/2/19/22	0/1/1/1
3	FUC	F	6	3	-	-	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	5	BMA	C3-C4-C5	2.48	114.73	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5	BMA	C3-C4-C5	2.48	114.73	110.23
3	F	1	NAG	C1-O5-C5	2.31	115.29	112.19
3	E	5	BMA	C1-O5-C5	-2.30	109.10	112.19
3	E	1	NAG	C4-C3-C2	2.13	114.13	111.02

There are no chirality outliers.

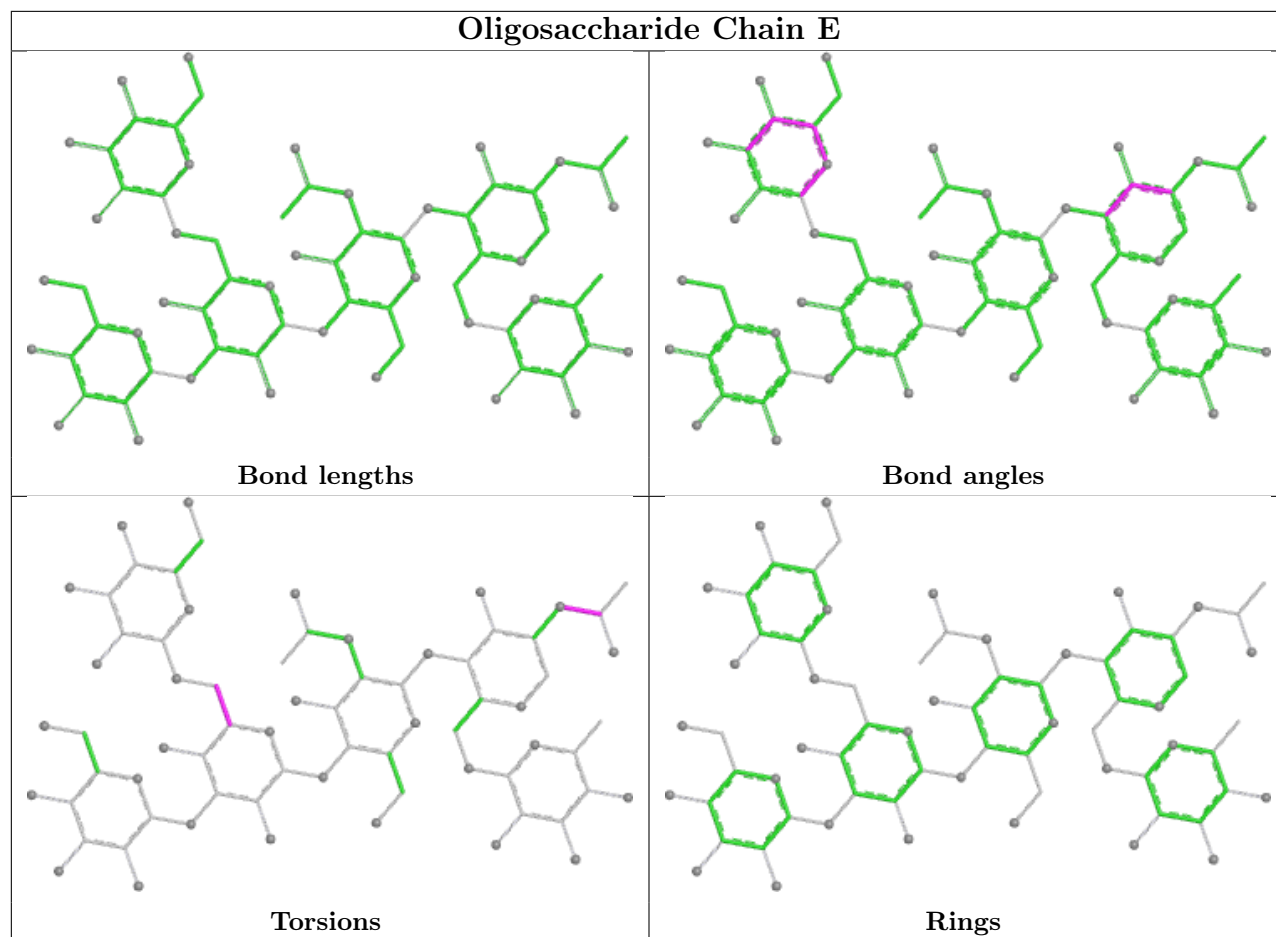
All (12) torsion outliers are listed below:

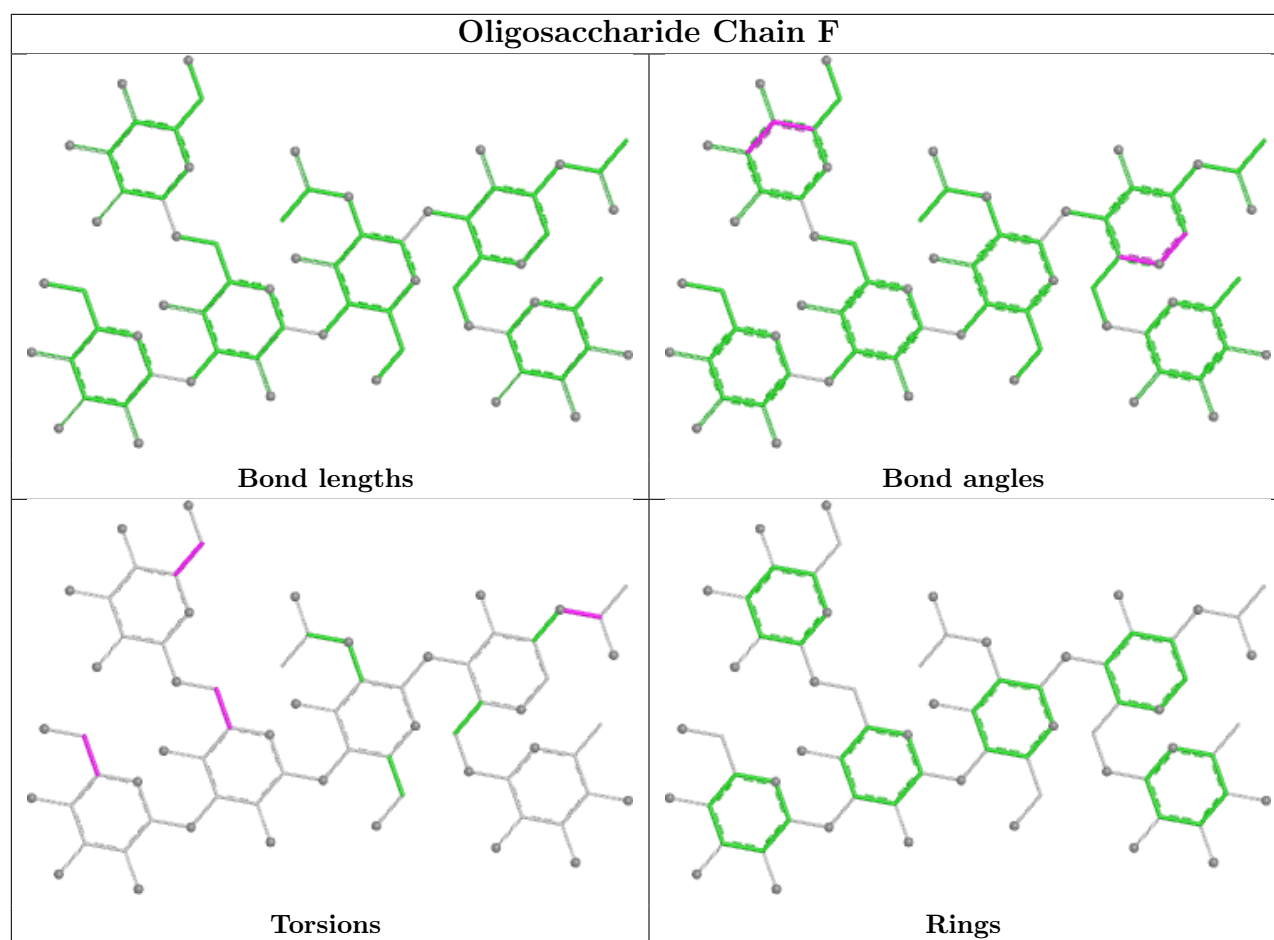
Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	E	3	BMA	C4-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
3	F	5	BMA	O5-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
3	F	5	BMA	C4-C5-C6-O6
3	F	4	BMA	C4-C5-C6-O6
3	F	4	BMA	O5-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2

There are no ring outliers.

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
7	NAG	C	604	2	14,14,15	0.49	0	17,19,21	0.64	0
5	HEM	C	601	2	42,50,50	2.02	9 (21%)	46,82,82	1.52	5 (10%)
5	HEM	D	601	2	42,50,50	1.99	9 (21%)	46,82,82	1.53	5 (10%)
8	ACT	D	606	-	3,3,3	0.81	0	3,3,3	1.39	0
7	NAG	D	605	2	14,14,15	0.50	0	17,19,21	0.66	0
7	NAG	C	603	2	14,14,15	0.51	0	17,19,21	0.73	0
7	NAG	D	604	2	14,14,15	0.55	0	17,19,21	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	ACT	C	605	-	3,3,3	0.81	0	3,3,3	1.37	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
7	NAG	C	604	2	-	3/6/23/26	0/1/1/1
5	HEM	C	601	2	-	6/12/54/54	-
5	HEM	D	601	2	-	6/12/54/54	-
7	NAG	D	605	2	-	4/6/23/26	0/1/1/1
7	NAG	C	603	2	-	2/6/23/26	0/1/1/1
7	NAG	D	604	2	-	2/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	601	HEM	C3D-C2D	7.94	1.53	1.36
5	D	601	HEM	C3D-C2D	7.92	1.53	1.36
5	C	601	HEM	C3C-C2C	-4.49	1.34	1.40
5	D	601	HEM	C3C-C2C	-4.01	1.34	1.40
5	D	601	HEM	C3C-CAC	3.55	1.55	1.47
5	C	601	HEM	C3C-CAC	3.43	1.55	1.47
5	C	601	HEM	CAB-C3B	2.92	1.55	1.47
5	C	601	HEM	FE-ND	2.88	2.14	1.98
5	D	601	HEM	CAB-C3B	2.88	1.55	1.47
5	D	601	HEM	C3C-C4C	2.86	1.45	1.41
5	C	601	HEM	C3C-C4C	2.80	1.45	1.41
5	D	601	HEM	FE-ND	2.80	2.13	1.98
5	C	601	HEM	FE-NB	2.63	2.12	1.98
5	D	601	HEM	FE-NB	2.30	2.10	1.98
5	C	601	HEM	CMB-C2B	2.28	1.55	1.50
5	D	601	HEM	CMB-C2B	2.15	1.55	1.50
5	D	601	HEM	CMD-C2D	2.12	1.55	1.50
5	C	601	HEM	CMD-C2D	2.10	1.55	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	601	HEM	C4D-ND-C1D	5.16	111.32	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	601	HEM	C4D-ND-C1D	5.15	111.30	105.21
5	D	601	HEM	C4C-CHD-C1D	3.51	127.19	122.56
5	C	601	HEM	C4C-CHD-C1D	3.33	126.95	122.56
5	C	601	HEM	CBA-CAA-C2A	-2.81	107.82	112.54
5	D	601	HEM	C4B-CHC-C1C	2.57	125.95	122.56
5	C	601	HEM	C4B-CHC-C1C	2.32	125.62	122.56
5	C	601	HEM	C1B-NB-C4B	2.10	107.69	105.21
5	D	601	HEM	CBA-CAA-C2A	-2.03	109.13	112.54
5	D	601	HEM	CMA-C3A-C4A	-2.01	125.51	128.46

There are no chirality outliers.

All (23) torsion outliers are listed below:

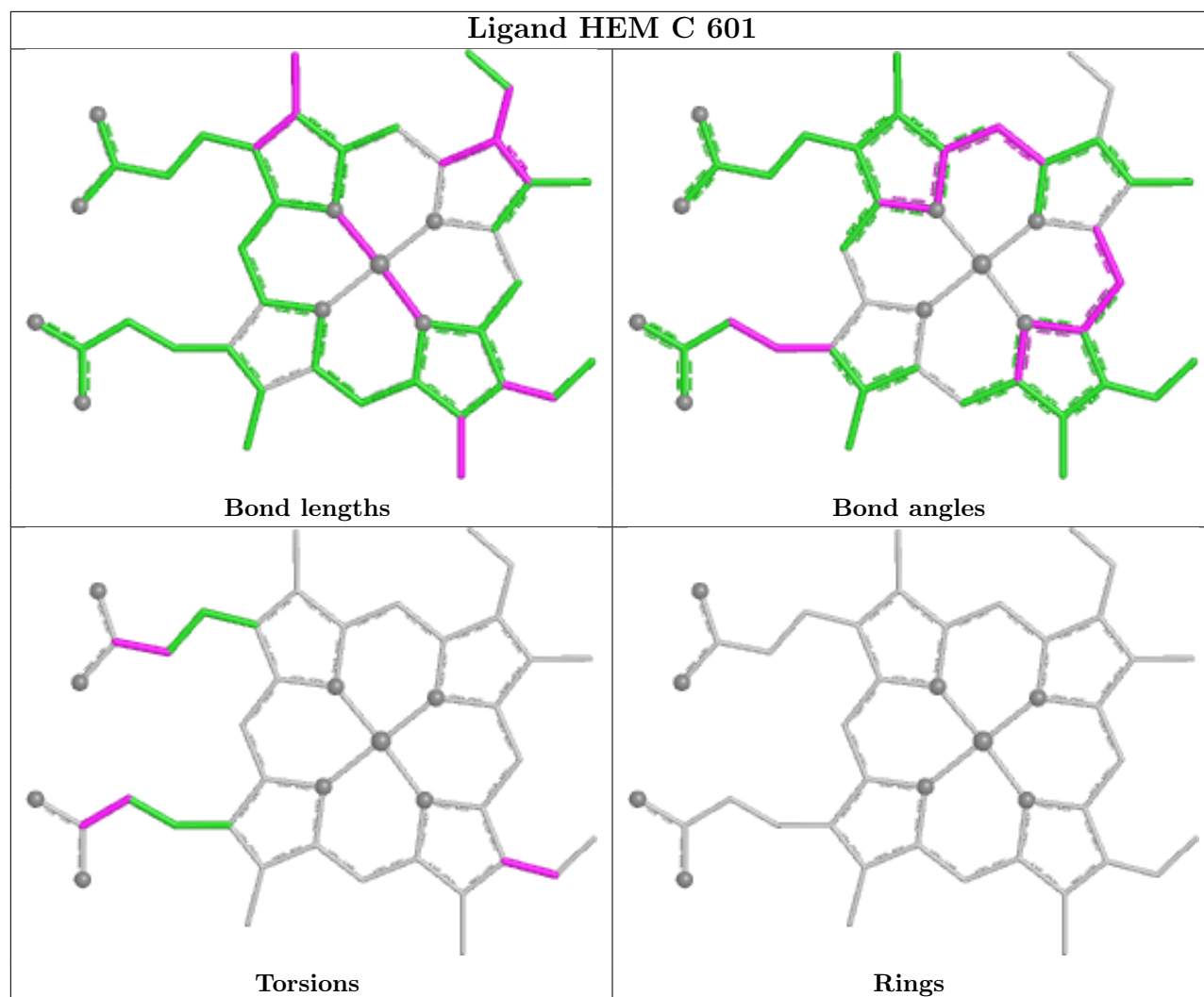
Mol	Chain	Res	Type	Atoms
5	C	601	HEM	C2B-C3B-CAB-CBB
5	C	601	HEM	C4B-C3B-CAB-CBB
5	D	601	HEM	C2B-C3B-CAB-CBB
5	D	601	HEM	C4B-C3B-CAB-CBB
7	C	604	NAG	C8-C7-N2-C2
7	C	604	NAG	O7-C7-N2-C2
7	D	605	NAG	C8-C7-N2-C2
7	D	605	NAG	O7-C7-N2-C2
7	D	604	NAG	C8-C7-N2-C2
7	D	604	NAG	O7-C7-N2-C2
7	D	605	NAG	C4-C5-C6-O6
7	D	605	NAG	O5-C5-C6-O6
7	C	604	NAG	C4-C5-C6-O6
7	C	603	NAG	C4-C5-C6-O6
5	C	601	HEM	CAD-CBD-CGD-O2D
5	C	601	HEM	CAD-CBD-CGD-O1D
5	D	601	HEM	CAD-CBD-CGD-O2D
5	C	601	HEM	CAA-CBA-CGA-O2A
5	C	601	HEM	CAA-CBA-CGA-O1A
5	D	601	HEM	CAA-CBA-CGA-O2A
5	D	601	HEM	CAD-CBD-CGD-O1D
5	D	601	HEM	CAA-CBA-CGA-O1A
7	C	603	NAG	O5-C5-C6-O6

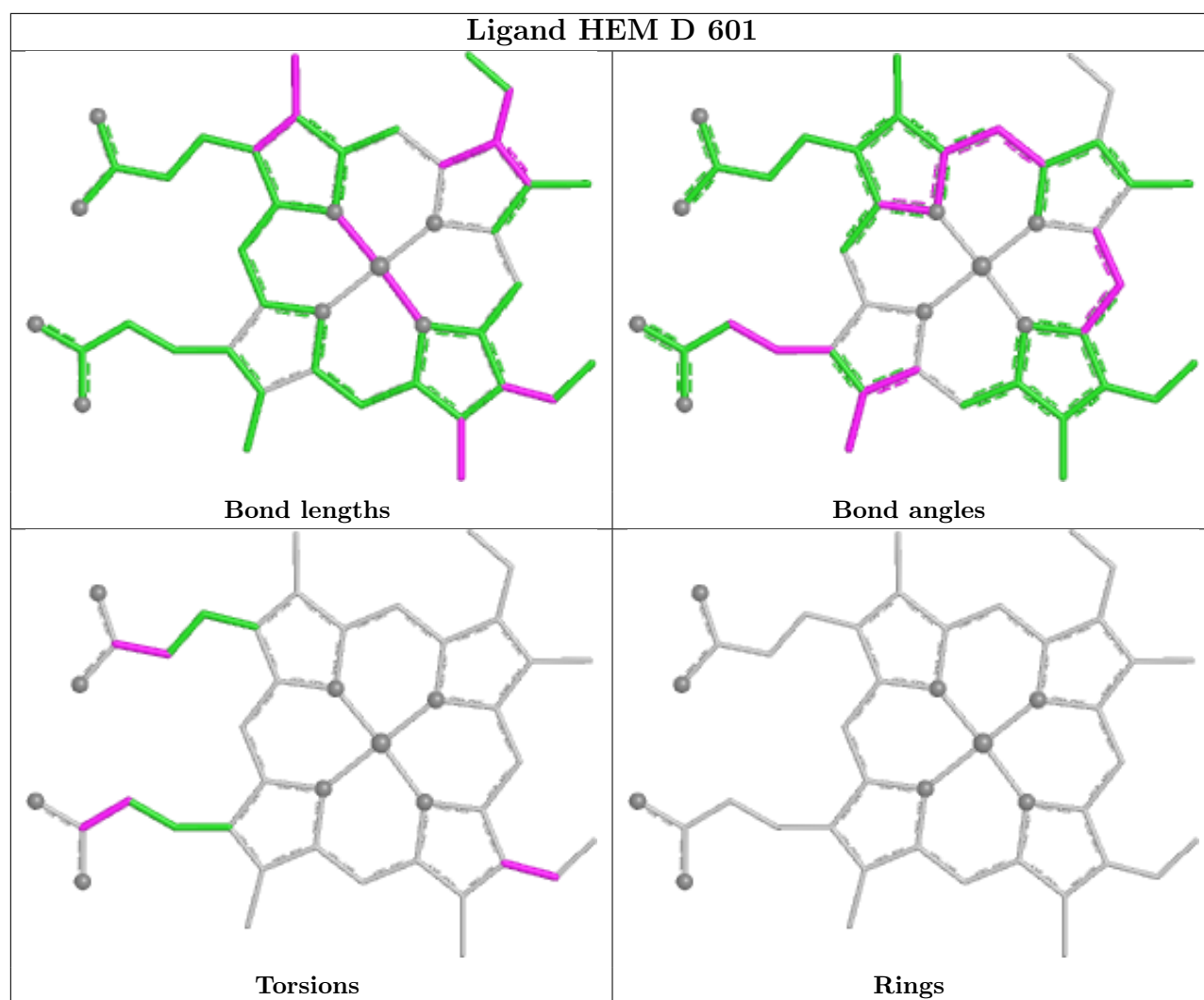
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	601	HEM	2	0
5	D	601	HEM	1	0
8	C	605	ACT	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, 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	107/114 (93%)	0.48	3 (2%) 55 51	66, 67, 69, 70	0
1	B	108/114 (94%)	0.58	2 (1%) 66 64	66, 67, 69, 70	0
2	C	466/467 (99%)	0.57	13 (2%) 55 51	66, 67, 68, 69	0
2	D	466/467 (99%)	0.54	15 (3%) 50 47	66, 67, 68, 69	0
All	All	1147/1162 (98%)	0.55	33 (2%) 54 50	66, 67, 68, 70	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	579	SER	7.6
2	D	578	ALA	7.1
2	C	113	VAL	5.1
2	D	242	GLU	3.8
2	C	355	PRO	3.4
2	C	242	GLU	3.4
2	D	113	VAL	3.2
1	A	106	ARG	3.2
2	D	195	GLY	3.2
2	D	576	ARG	3.0
2	C	373	LEU	2.9
1	B	0	THR	2.8
2	C	194	LEU	2.6
2	C	538	CYS	2.6
2	C	578	ALA	2.5
2	C	350	TYR	2.5
2	D	349	ARG	2.4
1	A	105	ALA	2.4
2	C	356	ASN	2.3
2	C	343	MET	2.3
2	C	324	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	104	ALA	2.2
2	C	115	CYS	2.2
2	D	270	ARG	2.2
2	D	210	LEU	2.2
2	D	271	TRP	2.2
2	D	218	ASP	2.1
1	B	106	ARG	2.1
2	C	348	ASN	2.1
2	D	226	ARG	2.1
2	D	350	TYR	2.1
2	D	355	PRO	2.1
2	D	371	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	D	150	7/8	0.74	0.17	67,67,68,68	0
2	CSO	C	150	7/8	0.82	0.13	67,68,68,68	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(Å ²)	Q<0.9
3	BMA	E	4	11/12	0.60	0.16	69,69,69,70	0
3	BMA	F	4	11/12	0.73	0.15	68,68,68,69	0
3	BMA	F	5	11/12	0.77	0.17	67,67,68,68	0
3	BMA	E	5	11/12	0.81	0.14	66,67,67,67	0
3	NAG	E	1	14/15	0.89	0.13	64,65,65,65	0
3	NAG	F	1	14/15	0.89	0.14	62,63,64,64	0
3	BMA	E	3	11/12	0.92	0.12	67,67,68,68	0
3	BMA	F	3	11/12	0.92	0.12	66,66,67,67	0
3	FUC	E	6	10/11	0.93	0.10	63,63,64,64	0

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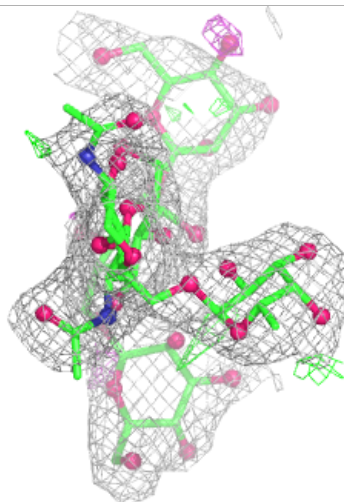
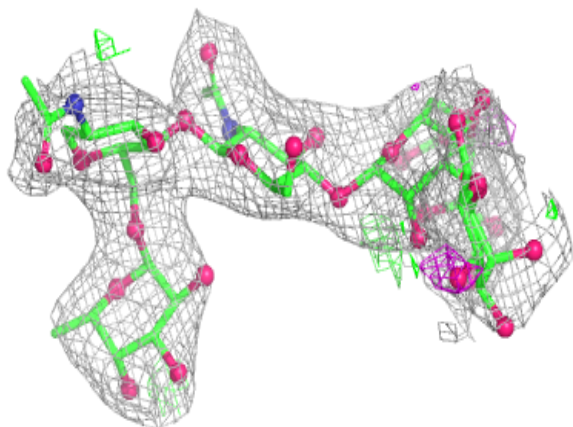
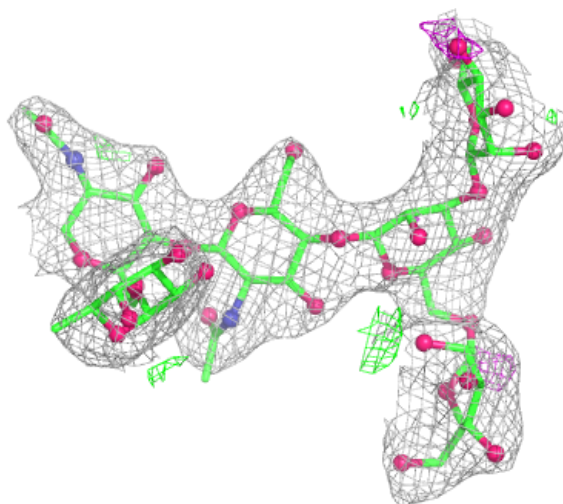
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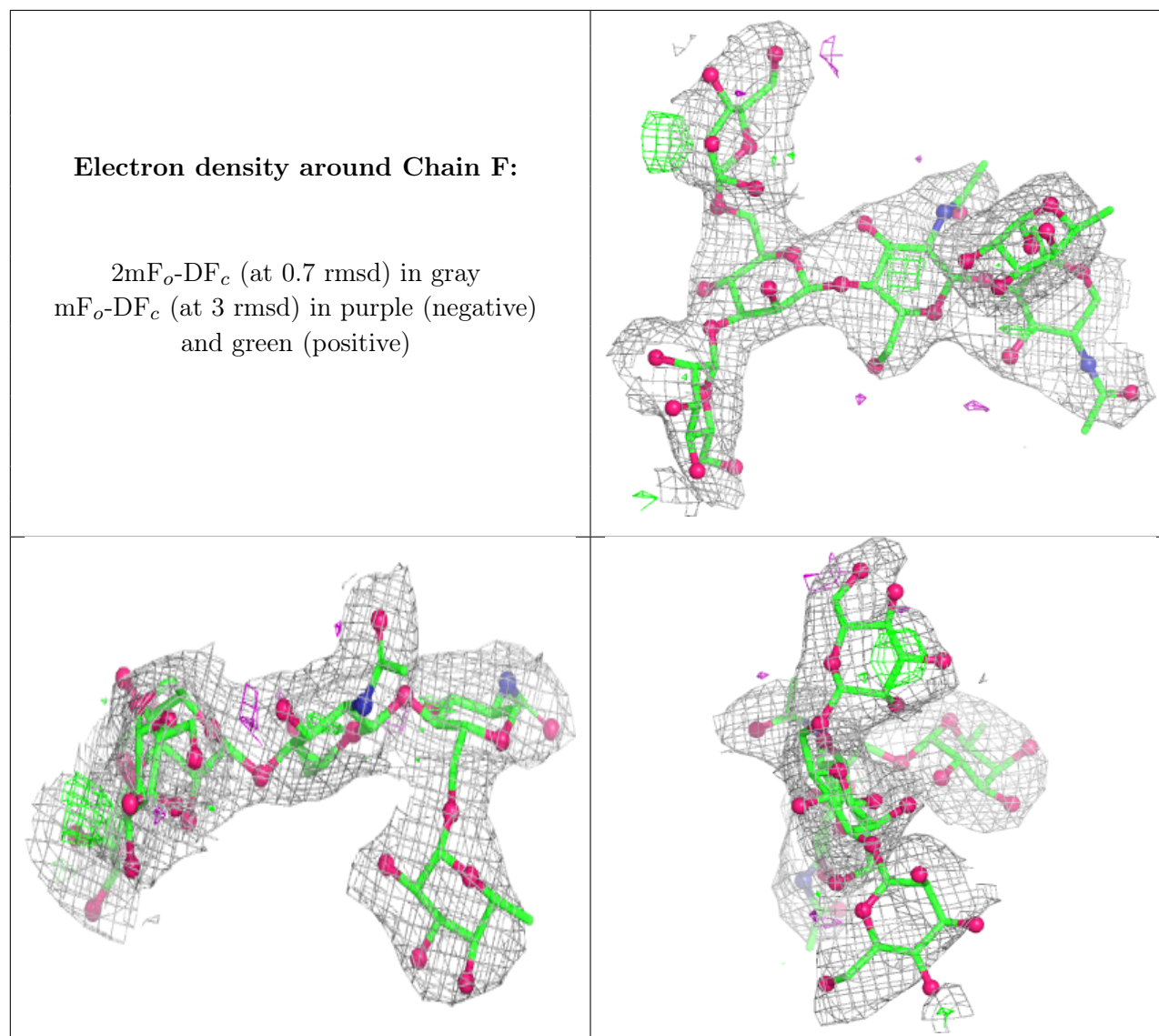
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	E	2	14/15	0.93	0.10	65,66,66,66	0
3	NAG	F	2	14/15	0.93	0.14	63,64,64,65	0
3	FUC	F	6	10/11	0.93	0.12	62,62,62,62	0

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 E:

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, 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	NAG	C	604	14/15	0.49	0.17	65,66,66,66	0
7	NAG	D	605	14/15	0.72	0.13	65,65,65,66	0
7	NAG	C	603	14/15	0.75	0.12	65,65,66,66	0
7	NAG	D	604	14/15	0.77	0.13	65,65,65,65	0
8	ACT	D	606	4/4	0.77	0.22	68,68,68,68	0
8	ACT	C	605	4/4	0.79	0.16	69,69,69,69	0
5	HEM	C	601	43/43	0.92	0.13	67,67,68,68	0

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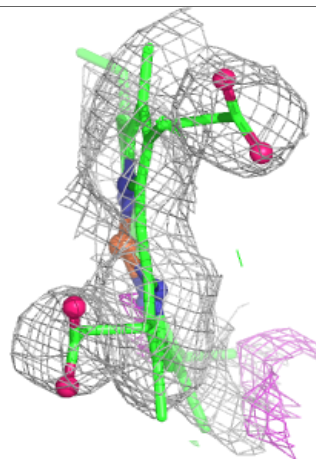
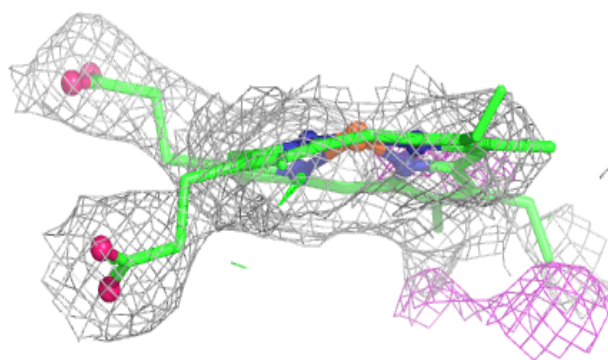
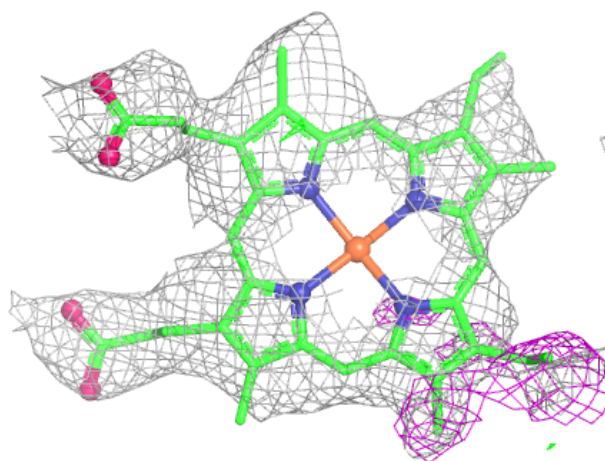
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	HEM	D	601	43/43	0.94	0.14	66,67,67,68	0
6	CA	C	602	1/1	0.94	0.07	67,67,67,67	0
4	CL	A	201	1/1	0.96	0.04	48,48,48,48	0
4	CL	D	603	1/1	0.97	0.12	53,53,53,53	0
6	CA	D	602	1/1	0.98	0.03	67,67,67,67	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.

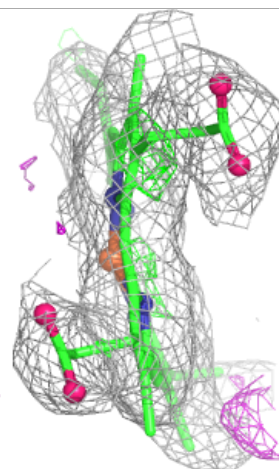
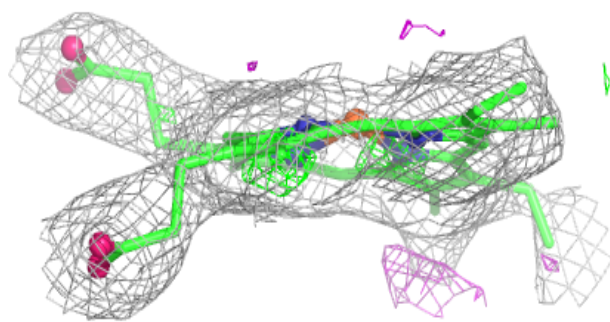
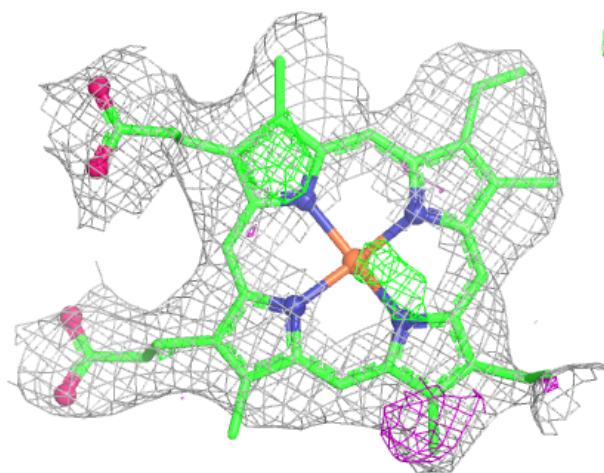
Electron density around HEM C 601:

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 HEM D 601:

$2mF_o-DF_c$ (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.