wwPDB X-ray Structure Validation Summary Report (i)

Aug 9, 2020 – 03:12 PM BST

PDB ID	:	1D2V
Title	:	CRYSTAL STRUCTURE OF BROMIDE-BOUND HUMAN MYELOPER-OXIDASE ISOFORM C AT PH 5.5
Authors	:	Fiedler, T.J.; Davey, C.A.; Fenna, R.E.
Deposited on	:	1999-09-28
Resolution	:	1.75 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 (i) symbol.

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

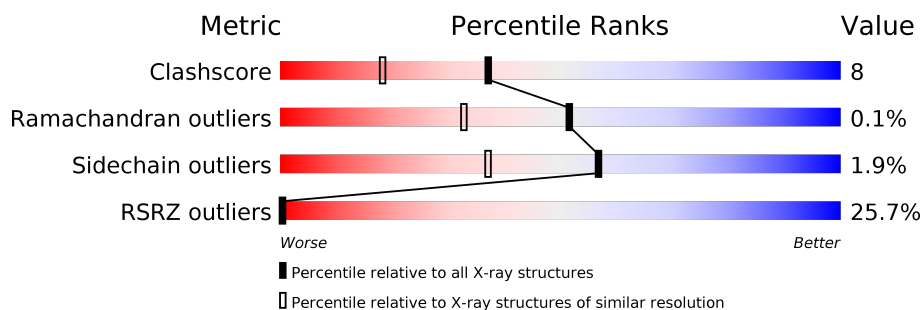|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 1.75 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	Percentile Ranks	Value
Clashscore		8
Ramachandran outliers		0.1%
Sidechain outliers		1.9%
RSRZ outliers		25.7%

Worse .... *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	104	18% / 80% / 20%
1	B	104	26% / 90% / 10%
2	C	466	23% / 79% / 20% •
2	D	466	30% / 82% / 18% •
3	E	6	100%
3	F	6	50% / 50%

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
5	BR	A	843	-	-	X	-
9	ACT	C	1606	-	-	X	-
9	ACT	D	2604	-	-	X	X

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 10306 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 838	C 529	N 148	O 156	S 5	0	0	0
1	B	104	Total 838	C 529	N 148	O 156	S 5	0	0	0

- Molecule 2 is a protein called MYELOPEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	466	Total 3733	C 2351	N 687	O 668	S 27	0	0	0
2	D	466	Total 3733	C 2351	N 687	O 668	S 27	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	150	CSO	CYS	modified residue	UNP P05164
D	150	CSO	CYS	modified residue	UNP P05164

- Molecule 3 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.
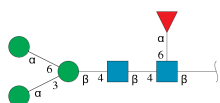
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	6	Total 71	C 40	N 2	O 29	0	0	0
3	F	6	Total 71	C 40	N 2	O 29	0	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Ca 1	0	0
4	A	1	Total 1	Ca 1	0	0

- Molecule 5 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	4	Total 4	Br 4	0	0
5	A	4	Total 4	Br 4	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
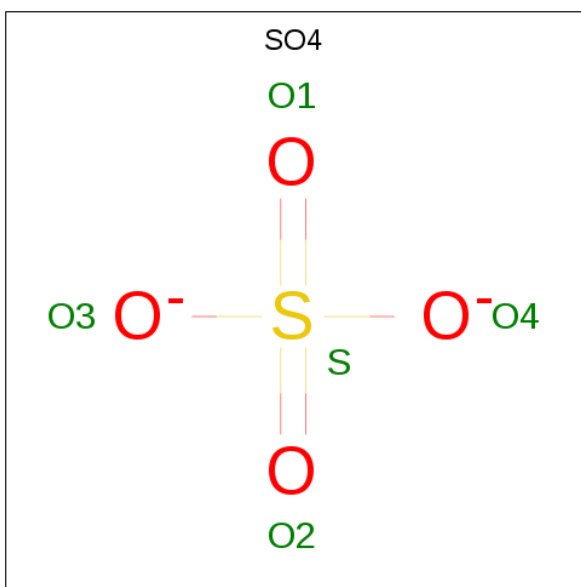
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 5	O 4	S 1	0	0
6	C	1	Total 5	O 4	S 1	0	0
6	B	1	Total 5	O 4	S 1	0	0

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

HEM
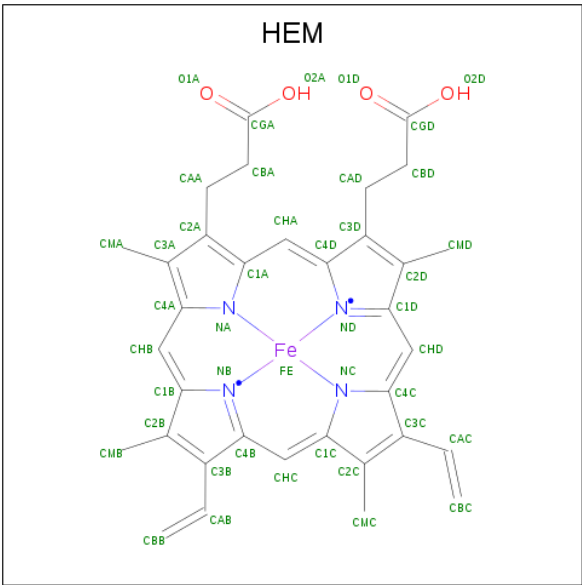
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

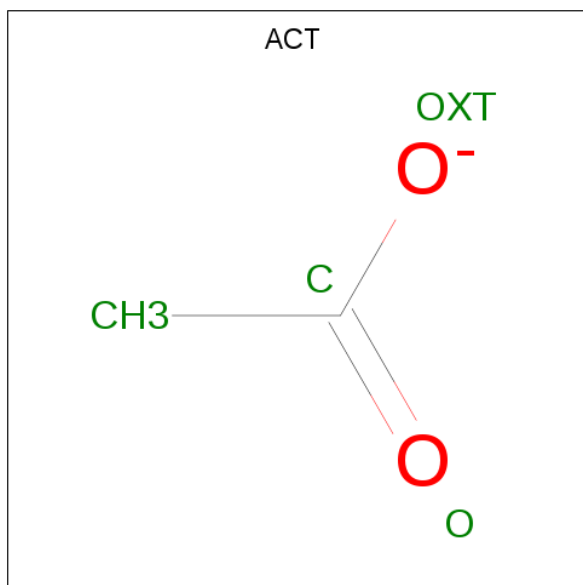- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

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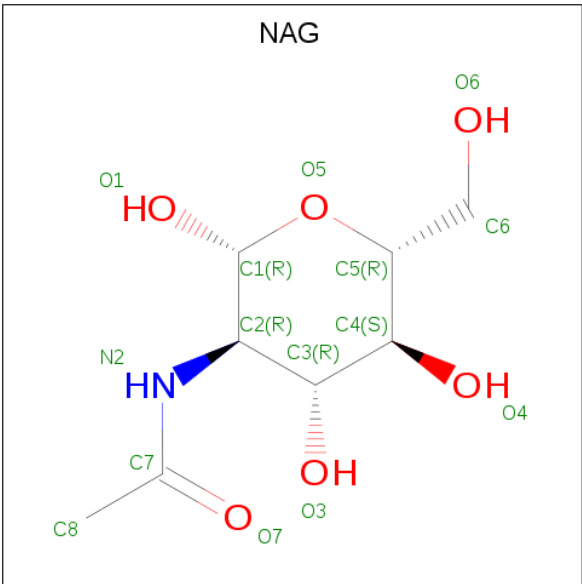
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O		0	0
			14	8	1	5			

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

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

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

- Molecule 10 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	98	Total 98	O 98	0	0
10	C	319	Total 319	O 319	0	0
10	B	100	Total 100	O 100	0	0
10	D	314	Total 314	O 314	0	0

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.
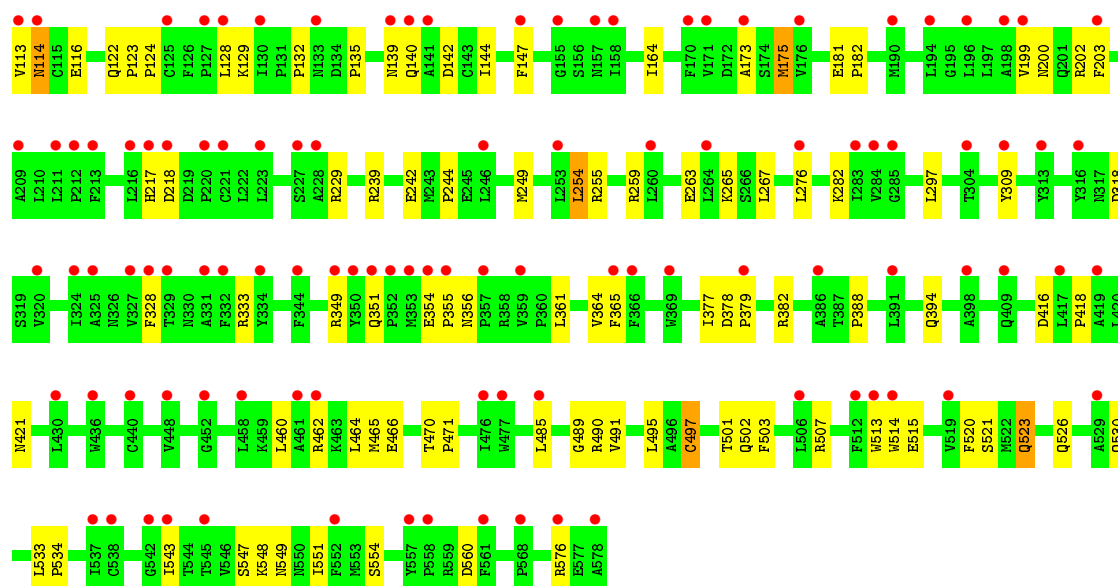
- Molecule 1: MYELOPEROXIDASE
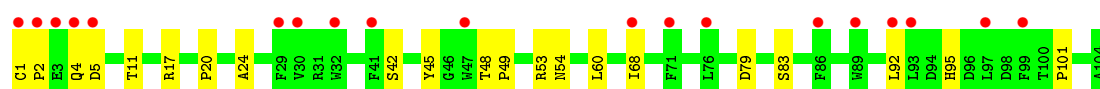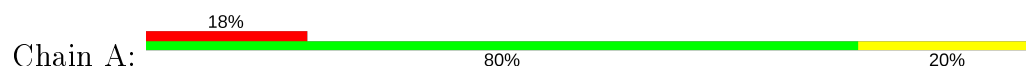
- Molecule 1: MYELOPEROXIDASE
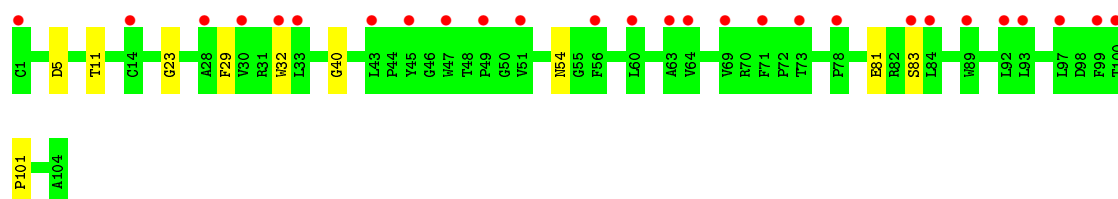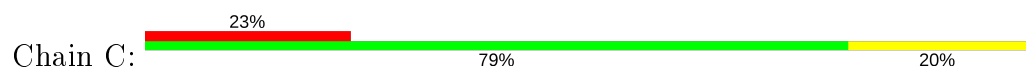
- Molecule 2: MYELOPEROXIDASE

● Molecule 2: MYELOPEROXIDASE

Chain D:

● Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyrano se-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamid o-2-deoxy-beta-D-glucopyranose

Chain E:

● Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyrano se-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamid o-2-deoxy-beta-D-glucopyranose

Chain F:
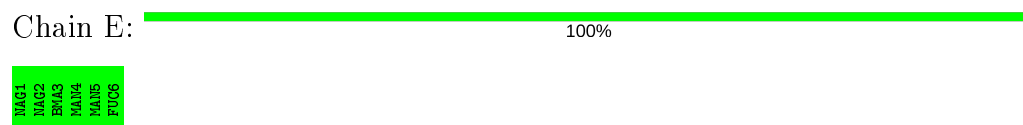
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	111.16Å 63.49Å 92.48Å 90.00° 97.36° 90.00°	Depositor
Resolution (Å)	30.00 – 1.75 44.41 – 1.76	Depositor EDS
% Data completeness (in resolution range)	87.3 (30.00-1.75) 90.4 (44.41-1.76)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.37 (at 1.76Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.243 , 0.296 0.237 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	12.2	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 56.0	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	10306	wwPDB-VP
Average B, all atoms (Å^2)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CSO, BMA, NAG, CA, FUC, BR, ACT, HEM, MAN, SO4

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	0.75	0/863	0.73	0/1174
1	B	0.76	0/863	0.72	0/1174
2	C	0.73	1/3811 (0.0%)	0.65	0/5168
2	D	0.70	0/3811	0.63	0/5168
All	All	0.72	1/9348 (0.0%)	0.66	0/12684

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	114	ASN	C-N	-6.21	1.19	1.34

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	838	0	798	17	0
1	B	838	0	798	8	0
2	C	3733	0	3723	65	0
2	D	3733	0	3725	65	0
3	E	71	0	61	0	0
3	F	71	0	61	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	4	0	0	3	0
5	B	4	0	0	1	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
7	A	43	0	30	3	0
7	B	43	0	30	2	0
8	C	28	0	26	1	0
8	D	28	0	26	0	0
9	C	12	0	9	4	0
9	D	12	0	9	3	0
10	A	98	0	0	4	0
10	B	100	0	0	1	0
10	C	319	0	0	10	0
10	D	314	0	0	4	0
All	All	10306	0	9296	147	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 8.

The worst 5 of 147 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:C:355:PRO:HG2	2:C:356:ASN:HD22	1.44	0.82
2:D:333:ARG:HH11	2:D:421:ASN:HD22	1.31	0.78
2:C:132:PRO:HG3	2:C:140:GLN:NE2	2.04	0.72
2:C:355:PRO:HG2	2:C:356:ASN:ND2	2.05	0.71
2:C:200:ASN:HD22	2:C:203:PHE:H	1.36	0.70

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	102/104 (98%)	100 (98%)	1 (1%)	1 (1%)	15	4
1	B	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
2	C	463/466 (99%)	445 (96%)	18 (4%)	0	100	100
2	D	463/466 (99%)	449 (97%)	14 (3%)	0	100	100
All	All	1130/1140 (99%)	1094 (97%)	35 (3%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	90/90 (100%)	89 (99%)	1 (1%)	73	60
1	B	90/90 (100%)	88 (98%)	2 (2%)	52	29
2	C	410/410 (100%)	401 (98%)	9 (2%)	52	29
2	D	410/410 (100%)	403 (98%)	7 (2%)	60	42
All	All	1000/1000 (100%)	981 (98%)	19 (2%)	57	37

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

Mol	Chain	Res	Type
2	C	497	CYS
1	B	54	ASN
2	D	267	LEU
2	C	470	THR
2	D	318	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such

sidechains are listed below:

Mol	Chain	Res	Type
2	C	526	GLN
2	C	530	GLN
2	D	421	ASN
2	C	356	ASN
2	D	122	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	0.93	0	0,6,8	0.00	-
2	CSO	C	150	2	3,6,7	0.75	0	0,6,8	0.00	-

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	-	0/1/5/7	-
2	CSO	C	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)

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	0.85	0	17,19,21	0.93	0
3	NAG	E	2	3	14,14,15	0.75	0	17,19,21	0.79	0
3	BMA	E	3	3	11,11,12	0.70	0	15,15,17	0.62	0
3	MAN	E	4	3	11,11,12	0.67	0	15,15,17	0.85	0
3	MAN	E	5	3	11,11,12	0.57	0	15,15,17	0.72	0
3	FUC	E	6	3	10,10,11	0.69	0	14,14,16	0.61	0
3	NAG	F	1	3,2	14,14,15	0.71	0	17,19,21	1.15	1 (5%)
3	NAG	F	2	3	14,14,15	0.87	0	17,19,21	0.92	1 (5%)
3	BMA	F	3	3	11,11,12	0.85	0	15,15,17	0.62	0
3	MAN	F	4	3	11,11,12	0.80	0	15,15,17	0.98	1 (6%)
3	MAN	F	5	3	11,11,12	0.77	0	15,15,17	0.76	0
3	FUC	F	6	3	10,10,11	0.94	0	14,14,16	0.68	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	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	MAN	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	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	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 (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	1	NAG	C2-N2-C7	-3.11	118.48	122.90
3	F	4	MAN	C1-O5-C5	3.02	116.28	112.19
3	F	2	NAG	C2-N2-C7	-2.68	119.09	122.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	5	MAN	O5-C5-C6-O6
3	F	5	MAN	C4-C5-C6-O6

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.

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths   Bond angles

Torsions   Rings
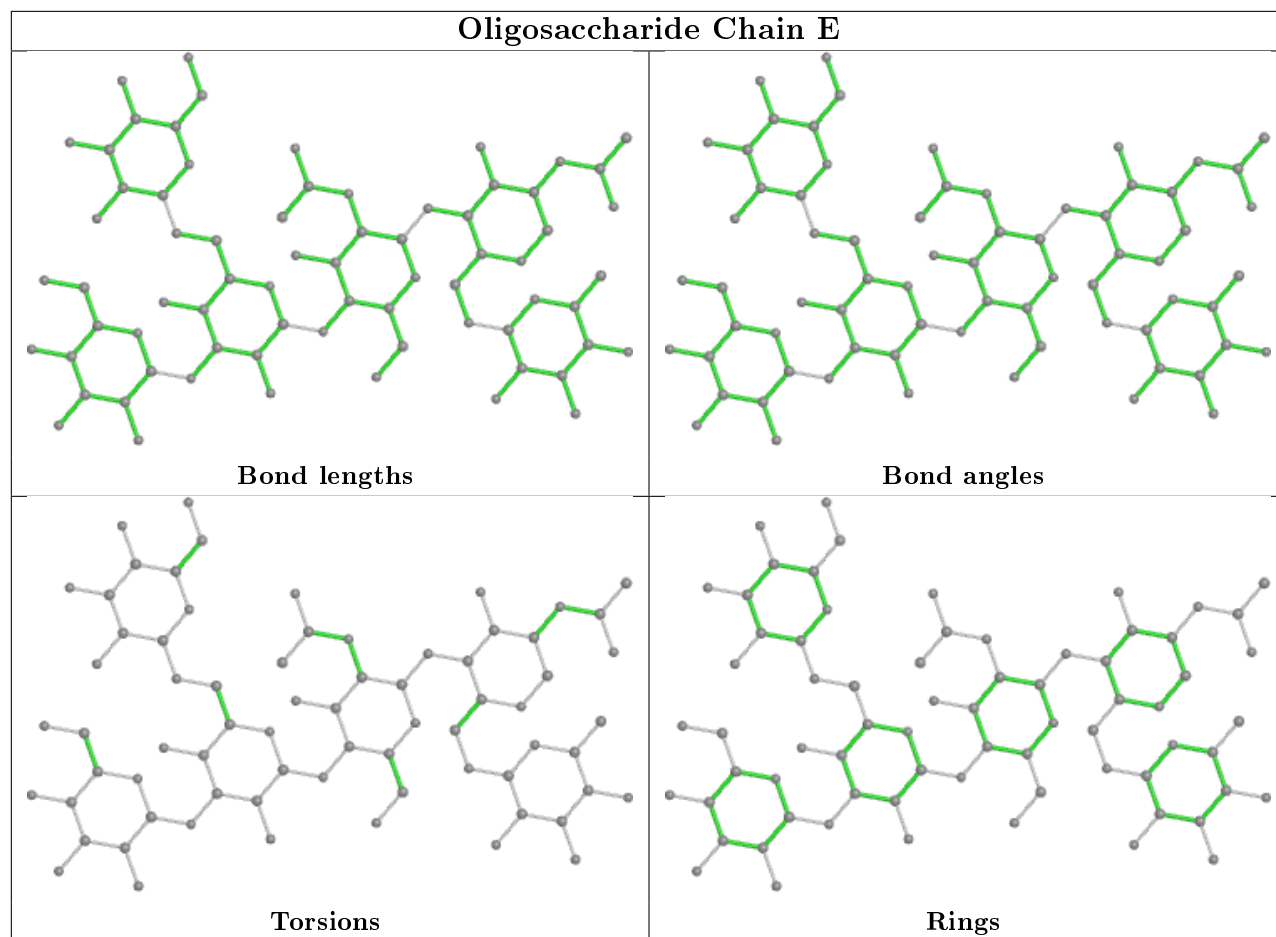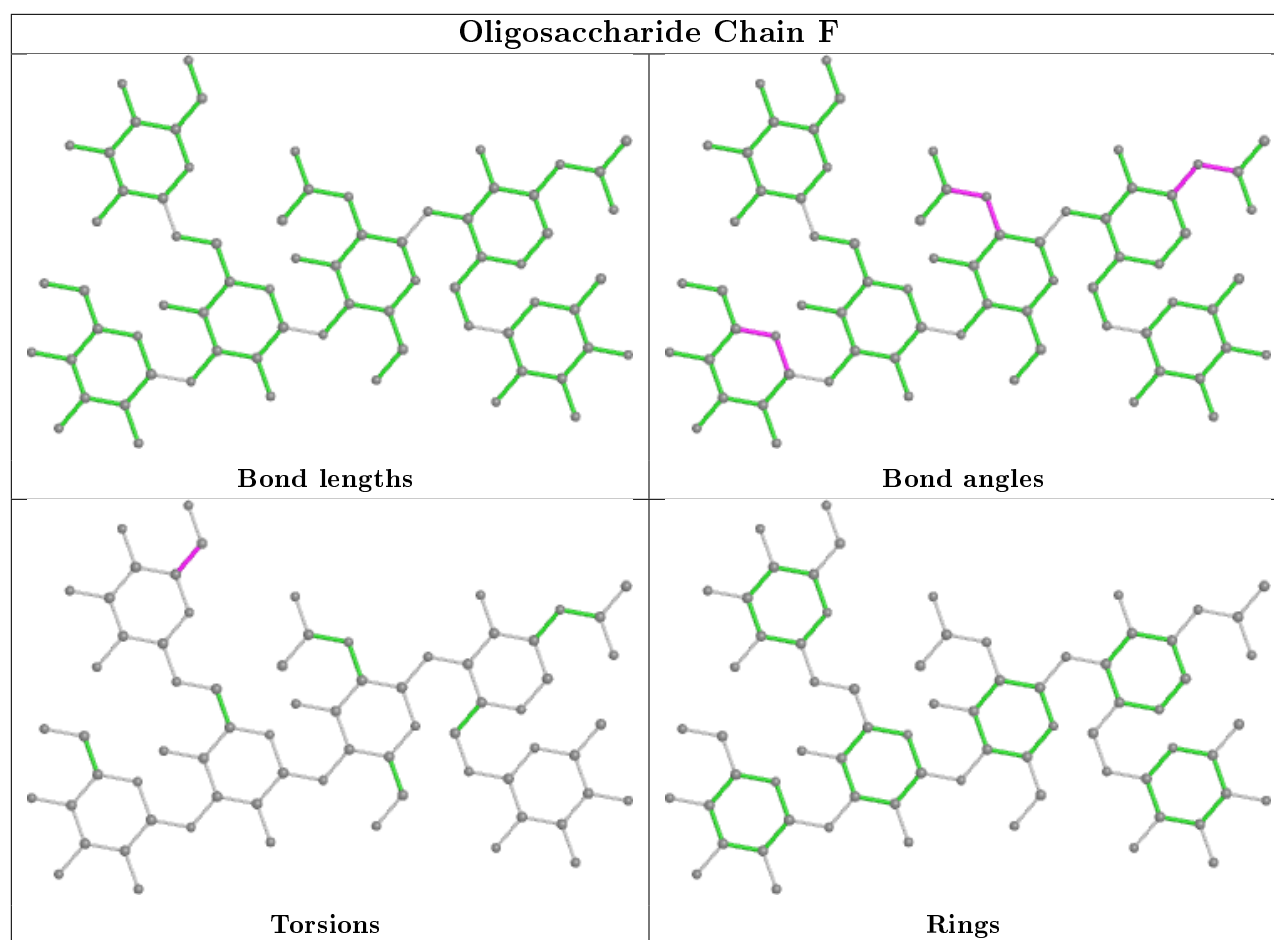
5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 10 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
8	NAG	C	1630	2	14,14,15	0.53	0	17,19,21	0.81	0
9	ACT	C	1604	-	1,3,3	3.48	1 (100%)	0,3,3	0.00	-
9	ACT	D	2607	-	1,3,3	3.46	1 (100%)	0,3,3	0.00	-
7	HEM	B	605	1,10,2	27,50,50	1.65	7 (25%)	17,82,82	1.17	1 (5%)
6	SO4	B	2602	-	4,4,4	0.29	0	6,6,6	0.06	0
6	SO4	C	1603	-	4,4,4	0.25	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
9	ACT	C	1606	-	1,3,3	2.72	1 (100%)	0,3,3	0.00	-
9	ACT	D	2604	-	1,3,3	3.42	1 (100%)	0,3,3	0.00	-
8	NAG	D	2620	2	14,14,15	0.53	0	17,19,21	0.74	0
8	NAG	D	2630	2	14,14,15	0.81	0	17,19,21	1.06	2 (11%)
6	SO4	A	1602	-	4,4,4	0.14	0	6,6,6	0.16	0
9	ACT	C	1607	-	1,3,3	3.91	1 (100%)	0,3,3	0.00	-
8	NAG	C	1620	2	14,14,15	0.67	0	17,19,21	1.12	2 (11%)
7	HEM	A	605	1,10,2	27,50,50	1.69	5 (18%)	17,82,82	1.20	1 (5%)
9	ACT	D	2606	-	1,3,3	2.30	1 (100%)	0,3,3	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	C	1630	2	-	0/6/23/26	0/1/1/1
7	HEM	B	605	1,10,2	-	0/6/54/54	-
8	NAG	D	2620	2	-	0/6/23/26	0/1/1/1
8	NAG	D	2630	2	-	1/6/23/26	0/1/1/1
8	NAG	C	1620	2	-	2/6/23/26	0/1/1/1
7	HEM	A	605	1,10,2	-	0/6/54/54	-

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	605	HEM	C3C-CAC	-4.13	1.39	1.47
7	B	605	HEM	C3B-C2B	-3.93	1.34	1.40
9	C	1607	ACT	CH3-C	3.91	1.53	1.48
7	A	605	HEM	C3B-CAB	-3.72	1.40	1.47
9	C	1604	ACT	CH3-C	3.48	1.53	1.48

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	2630	NAG	C1-C2-N2	-2.56	106.12	110.49
8	C	1620	NAG	C2-N2-C7	-2.46	119.39	122.90
7	A	605	HEM	C3B-C4B-NB	2.46	112.38	109.21
8	D	2630	NAG	C1-O5-C5	-2.28	109.10	112.19
7	B	605	HEM	C3B-C4B-NB	2.19	112.03	109.21

There are no chirality outliers.

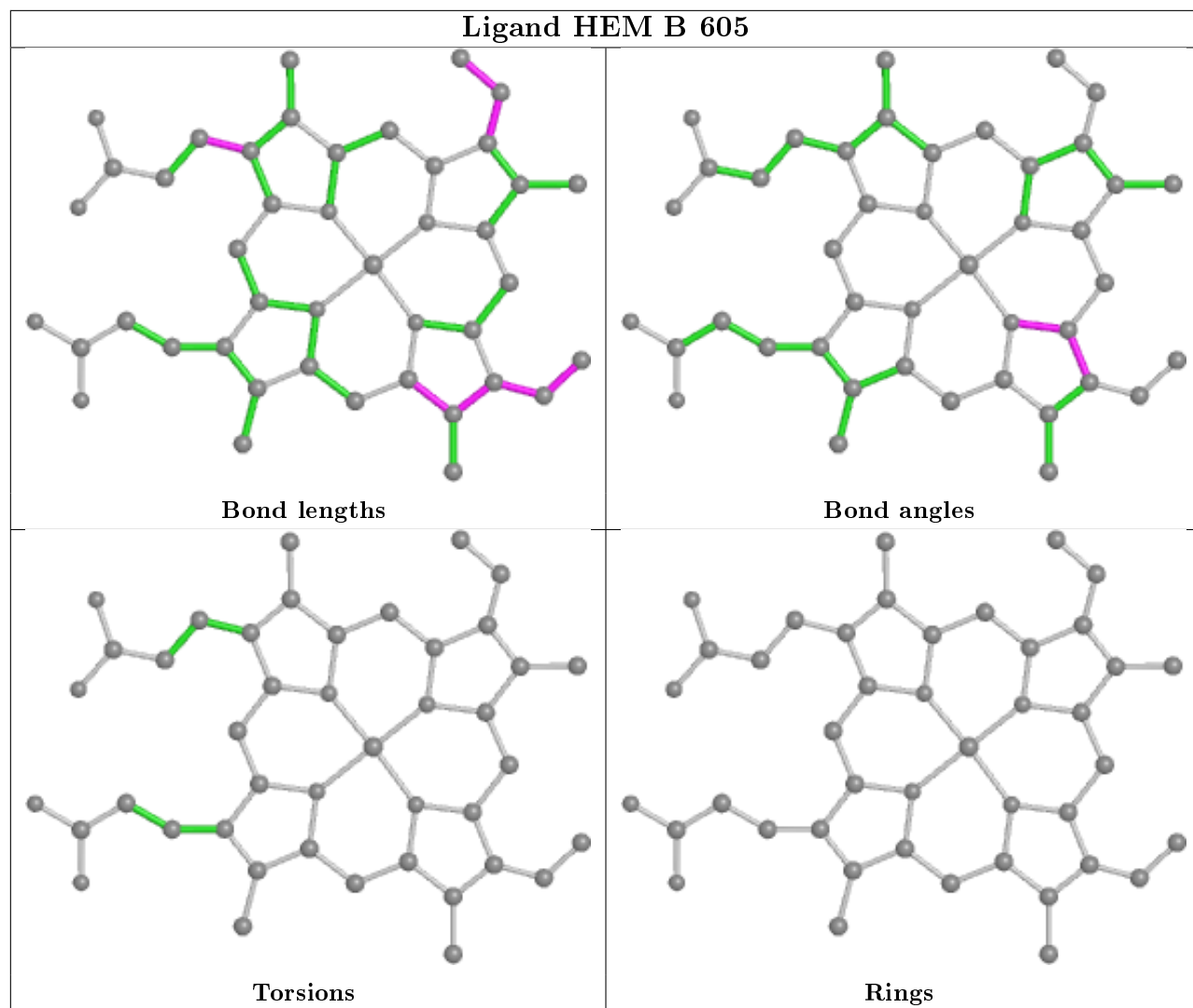All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	1620	NAG	O5-C5-C6-O6
8	C	1620	NAG	C4-C5-C6-O6
8	D	2630	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	605	HEM	2	0
9	C	1606	ACT	4	0
9	D	2604	ACT	3	0
8	C	1620	NAG	1	0
7	A	605	HEM	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand HEM B 605

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 605

Bond lengths

Bond angles

Torsions

Rings
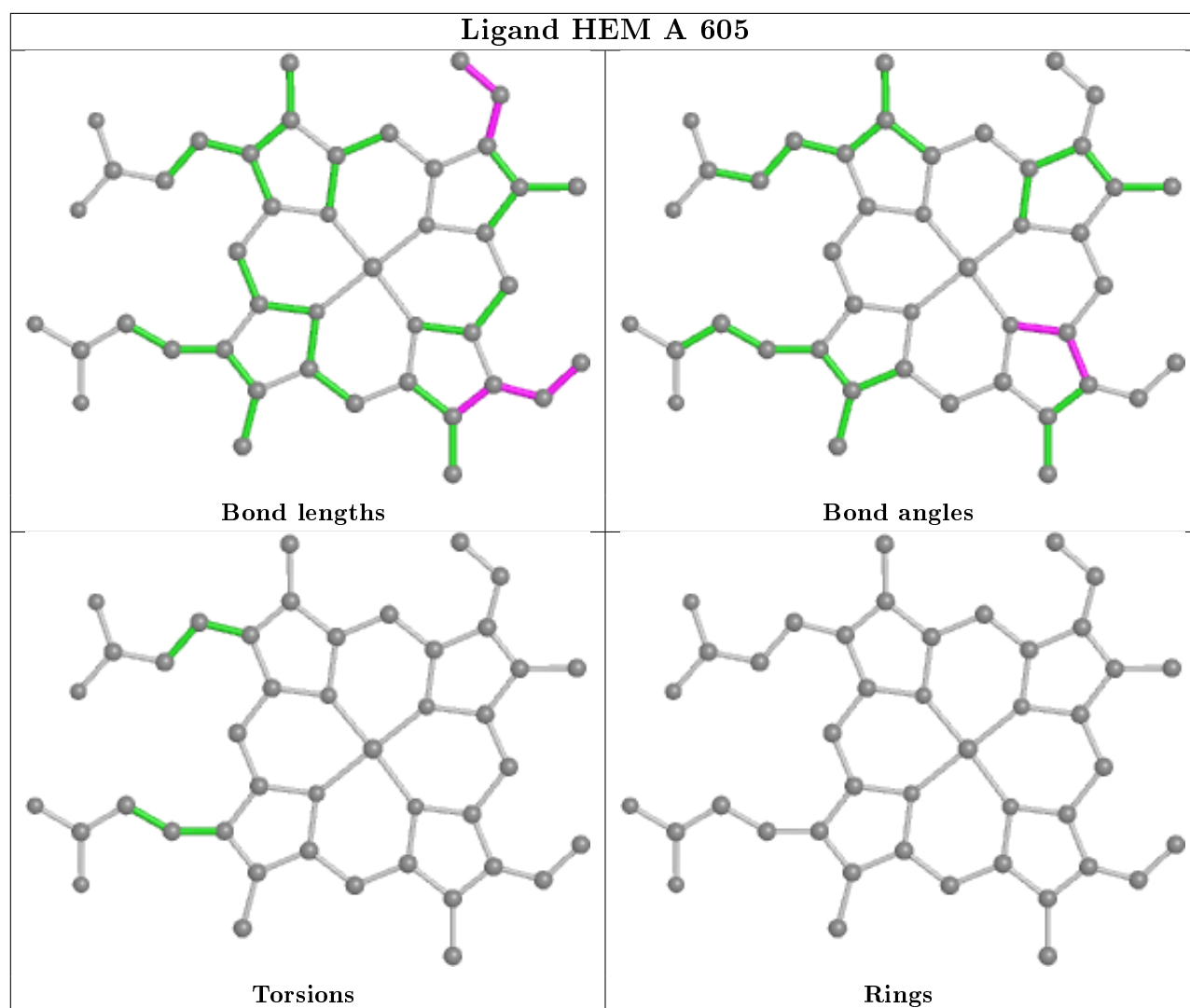
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	114:ASN	C	115:CYS	N	1.19

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	104/104 (100%)	1.39	19 (18%)	1	1	2, 6, 17, 43	0
1	B	104/104 (100%)	1.44	27 (25%)	0	0	3, 7, 15, 23	0
2	C	465/466 (99%)	1.48	106 (22%)	0	0	2, 7, 19, 35	0
2	D	465/466 (99%)	1.64	141 (30%)	0	0	3, 9, 24, 41	0
All	All	1138/1140 (99%)	1.53	293 (25%)	0	0	2, 8, 22, 43	0

The worst 5 of 293 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	113	VAL	14.8
2	D	355	PRO	8.9
2	D	568	PRO	6.2
1	A	4	GLN	5.8
2	D	578	ALA	5.2

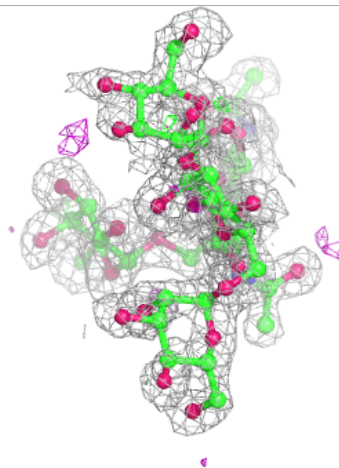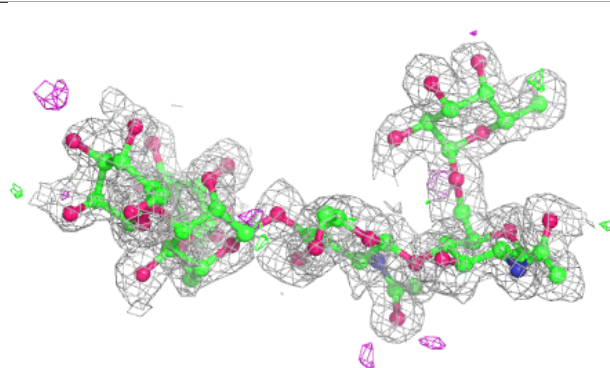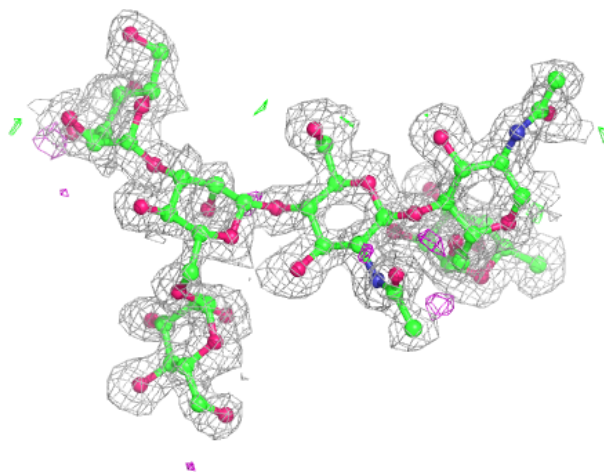## 6.2 Non-standard residues in protein, DNA, RNA chains (i)

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	D	150	7/8	0.91	0.13	5,6,8,10	0
2	CSO	C	150	7/8	0.94	0.10	2,5,7,9	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	MAN	F	4	11/12	0.68	0.26	17,20,22,23	0
3	FUC	F	6	10/11	0.79	0.22	10,14,16,19	0
3	MAN	E	4	11/12	0.80	0.23	21,25,26,28	0
3	MAN	F	5	11/12	0.82	0.22	9,14,18,23	0
3	BMA	E	3	11/12	0.84	0.22	9,14,15,18	0
3	FUC	E	6	10/11	0.85	0.14	9,13,15,17	0
3	MAN	E	5	11/12	0.86	0.18	13,15,17,18	0
3	BMA	F	3	11/12	0.87	0.17	9,12,14,18	0
3	NAG	E	2	14/15	0.88	0.17	5,8,11,12	0
3	NAG	F	1	14/15	0.88	0.15	9,10,15,16	0
3	NAG	E	1	14/15	0.89	0.14	6,8,11,13	0
3	NAG	F	2	14/15	0.91	0.13	6,8,10,11	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)

Electron density around Chain F:

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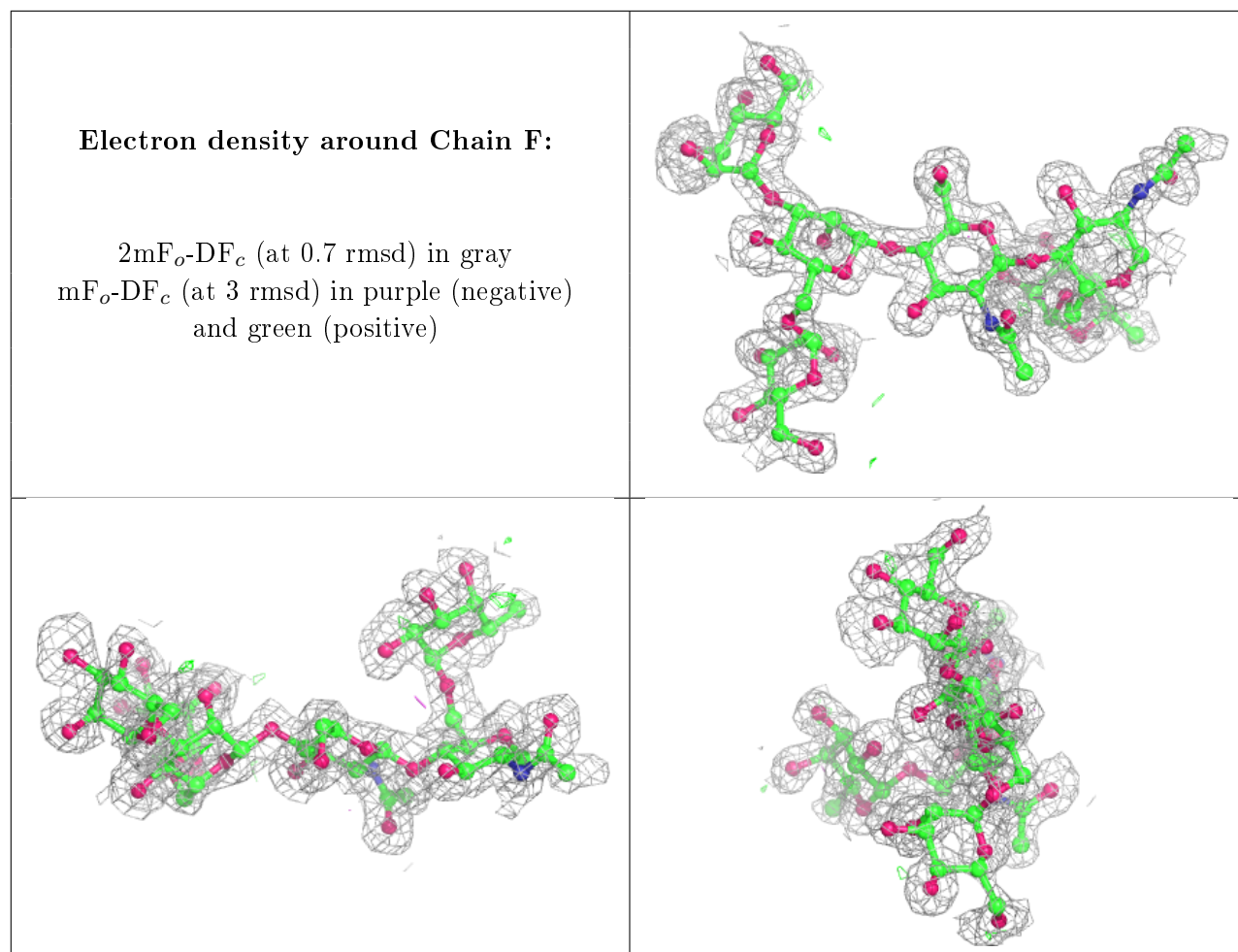
6.4 Ligands (i)

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
9	ACT	C	1606	4/4	0.46	0.28	22,23,24,25	0
6	SO4	B	2602	5/5	0.48	0.33	42,42,43,44	5
9	ACT	D	2607	4/4	0.49	0.29	29,30,30,31	0
9	ACT	D	2604	4/4	0.64	0.43	32,34,34,34	0
9	ACT	C	1604	4/4	0.73	0.23	17,17,20,22	0
8	NAG	C	1630	14/15	0.74	0.23	18,22,27,28	0
8	NAG	D	2630	14/15	0.75	0.26	26,30,34,35	0
9	ACT	C	1607	4/4	0.79	0.25	22,23,23,25	0
8	NAG	D	2620	14/15	0.79	0.24	16,21,26,28	0
8	NAG	C	1620	14/15	0.86	0.21	9,14,20,24	0
9	ACT	D	2606	4/4	0.91	0.13	13,14,14,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
7	HEM	B	605	43/43	0.93	0.16	2,5,8,9	0
6	SO4	C	1603	5/5	0.93	0.12	20,21,23,25	0
7	HEM	A	605	43/43	0.94	0.17	2,5,8,8	0
5	BR	B	758	1/1	0.94	0.12	18,18,18,18	1
6	SO4	A	1602	5/5	0.96	0.10	19,19,21,22	0
5	BR	A	843	1/1	0.97	0.14	12,12,12,12	1
5	BR	A	758	1/1	0.98	0.07	16,16,16,16	1
5	BR	B	889	1/1	0.98	0.06	23,23,23,23	1
5	BR	A	889	1/1	0.99	0.06	24,24,24,24	1
5	BR	B	843	1/1	0.99	0.06	12,12,12,12	1
4	CA	A	600	1/1	1.00	0.10	5,5,5,5	0
4	CA	B	600	1/1	1.00	0.13	7,7,7,7	0
5	BR	A	601	1/1	1.00	0.09	6,6,6,6	0
5	BR	B	601	1/1	1.00	0.10	6,6,6,6	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.
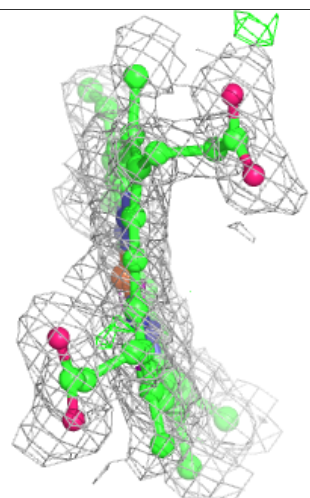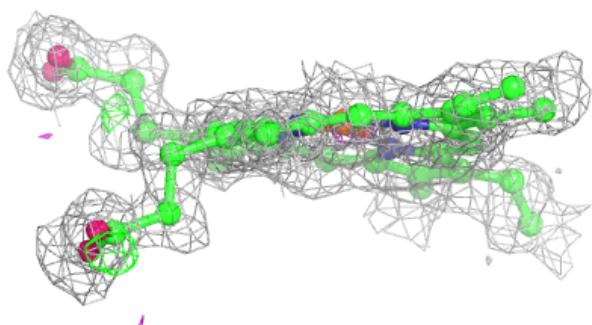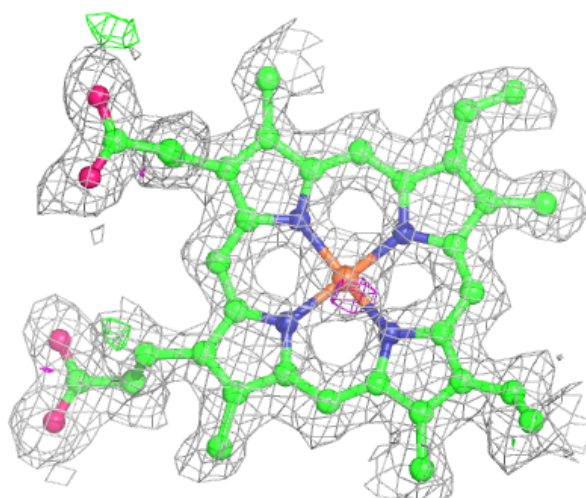
Electron density around HEM B 605:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
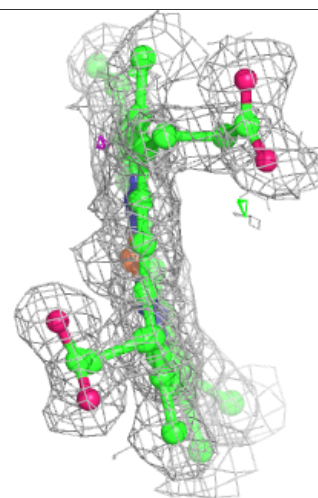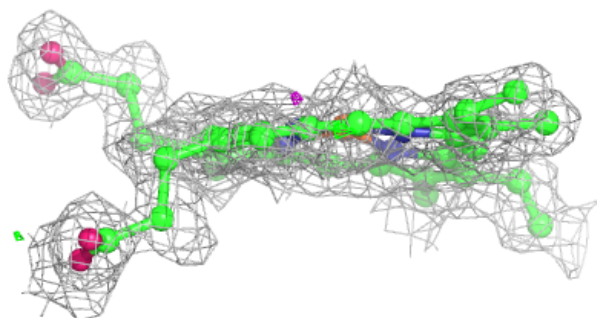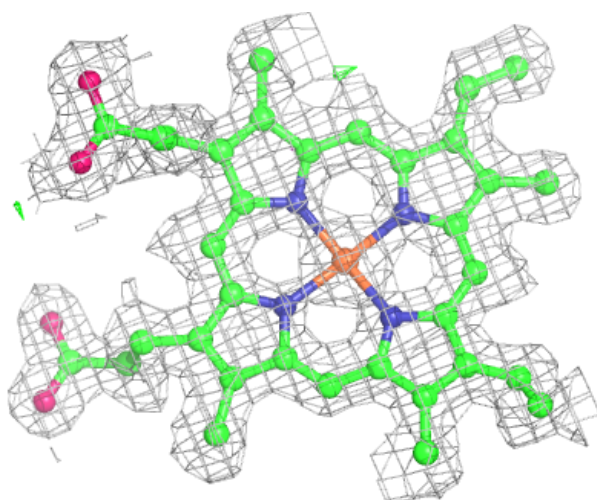
Electron density around HEM A 605:

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

6.5 Other polymers (i)

There are no such residues in this entry.