



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:51 AM UTC

PDB ID : 6L5G / pdb_00006l5g
Title : Crystal structure of yak lactoperoxidase with disordered heme moiety at 2.50 Å resolution
Authors : Singh, P.K.; Rani, C.; Sharma, P.; Sharma, S.; Singh, T.P.
Deposited on : 2019-10-23
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

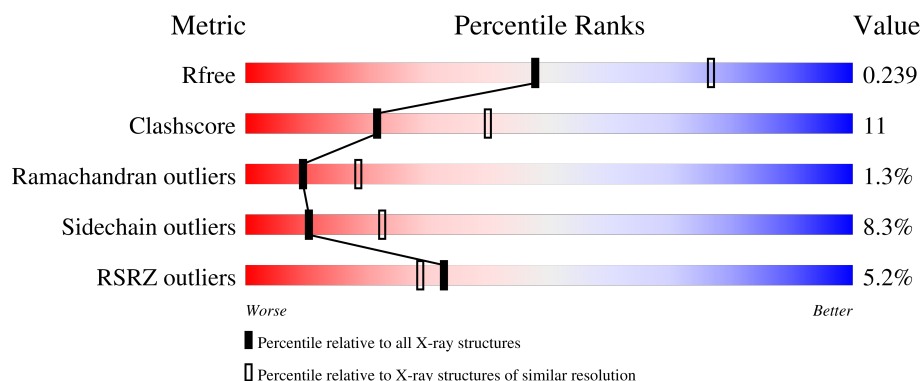
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	595	5% 79% 18% ..
2	B	2	50% 50%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5278 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 Lactoperoxidase.

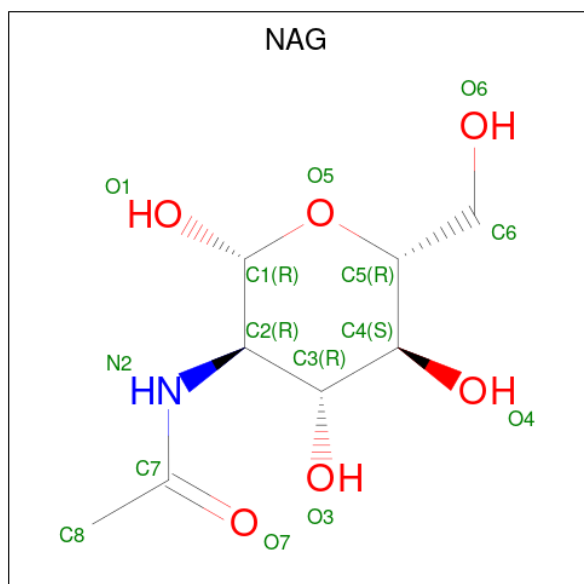
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	0	0
			4770	3037	847	860	26			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

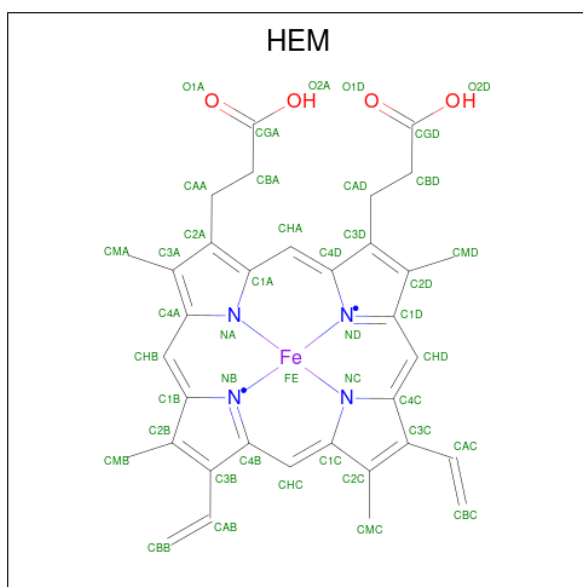


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	1
			50	38	1	5	6		

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	K	0	0
			2	2		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Zn	0	0
			1	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		

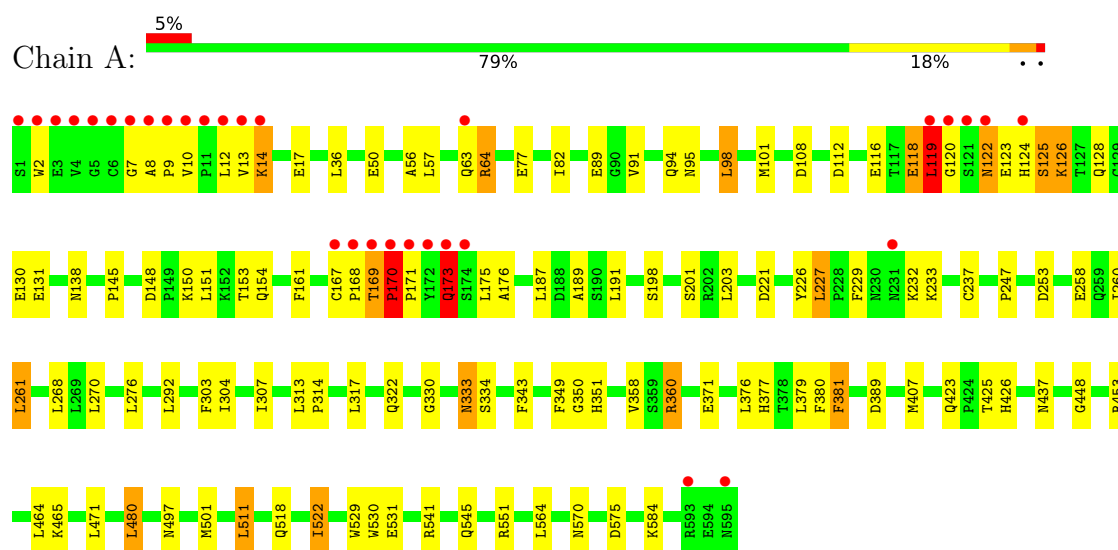
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	354	Total	O	0	0
			354	354		

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: Lactoperoxidase



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.82Å 84.71Å 99.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.38 – 2.50 64.38 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (64.38-2.50) 99.9 (64.38-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.185 , 0.239 0.191 , 0.239	Depositor DCC
R_{free} test set	1139 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.699	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.5	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	0.94	EDS
Total number of atoms	5278	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, HEM, NAG, CA, ZN, GOL

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	1.00	0/4898	1.41	12/6645 (0.2%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	PRO	N-CA-C	-6.92	99.40	112.33
1	A	168	PRO	CB-CA-C	6.33	121.70	113.09
1	A	170	PRO	N-CA-C	6.18	118.24	110.70
1	A	381	PHE	CA-CB-CG	-5.71	108.09	113.80
1	A	448	GLY	CA-C-N	5.55	128.03	120.54
1	A	448	GLY	C-N-CA	5.55	128.03	120.54
1	A	173	GLN	CB-CG-CD	5.50	121.96	112.60
1	A	453	ARG	CA-C-N	5.21	125.73	119.94
1	A	453	ARG	C-N-CA	5.21	125.73	119.94
1	A	122	ASN	CB-CA-C	5.16	120.70	110.42
1	A	176	ALA	CA-C-N	5.01	127.89	120.82
1	A	176	ALA	C-N-CA	5.01	127.89	120.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4770	0	4688	97	0
2	B	28	0	25	0	0
3	A	42	0	39	1	0
4	A	1	0	0	0	0
5	A	50	0	10	3	0
6	A	2	0	0	0	0
7	A	1	0	0	0	0
8	A	30	0	40	4	0
9	A	354	0	0	4	0
All	All	5278	0	4802	99	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 11.

All (99) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:CYS:CB	1:A:170:PRO:HA	1.69	1.23
1:A:167:CYS:HB3	1:A:170:PRO:CA	1.75	1.15
1:A:167:CYS:HB3	1:A:170:PRO:HA	0.93	0.92
1:A:116:GLU:OE2	8:A:612:GOL:O2	1.88	0.91
1:A:120:GLY:HA3	1:A:126:LYS:NZ	1.88	0.88
1:A:123:GLU:HB3	1:A:126:LYS:HG2	1.56	0.88
1:A:360:ARG:NH1	1:A:371:GLU:O	2.08	0.87
1:A:351:HIS:HD1	1:A:437:ASN:HD21	1.26	0.83
1:A:227:LEU:HD22	1:A:270:LEU:HD22	1.65	0.79
1:A:82:ILE:HD13	1:A:480:LEU:HD13	1.68	0.76
1:A:167:CYS:CB	1:A:170:PRO:CA	2.48	0.75
1:A:170:PRO:HB2	1:A:171:PRO:CD	2.18	0.72
1:A:150:LYS:HZ2	1:A:154:GLN:HE22	1.38	0.70
1:A:170:PRO:HB2	1:A:171:PRO:HD2	1.73	0.69
1:A:150:LYS:NZ	1:A:154:GLN:HE22	1.90	0.68
1:A:120:GLY:HA3	1:A:126:LYS:HZ3	1.55	0.68
1:A:119:LEU:HD11	1:A:138:ASN:HD22	1.60	0.66
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.31	0.66
1:A:360:ARG:NH2	1:A:389:ASP:OD2	2.30	0.65
1:A:77:GLU:HG2	1:A:145:PRO:HB3	1.78	0.64
1:A:123:GLU:HB3	1:A:126:LYS:CG	2.29	0.62
1:A:130:GLU:CD	1:A:426:HIS:HD1	2.08	0.62
1:A:118:GLU:OE1	1:A:118:GLU:HA	2.01	0.61
1:A:570:ASN:HD22	1:A:575:ASP:HB3	1.65	0.61
1:A:119:LEU:O	1:A:123:GLU:OE1	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLU:OE1	1:A:426:HIS:ND1	2.34	0.61
1:A:423:GLN:OE1	8:A:612:GOL:H32	2.00	0.60
1:A:333:ASN:C	1:A:333:ASN:HD22	2.09	0.59
1:A:126:LYS:HE2	1:A:161:PHE:CE2	2.38	0.59
1:A:120:GLY:HA2	1:A:123:GLU:HB2	1.84	0.58
1:A:333:ASN:HD22	1:A:334:SER:N	2.01	0.57
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.86	0.57
1:A:120:GLY:HA3	1:A:126:LYS:HZ2	1.70	0.57
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.71	0.56
1:A:63:GLN:O	1:A:64:ARG:HB2	2.05	0.56
1:A:330:GLY:HA3	9:A:1002:HOH:O	2.05	0.56
1:A:82:ILE:HD13	1:A:480:LEU:CD1	2.35	0.56
1:A:94:GLN:H	8:A:614:GOL:H32	1.70	0.55
1:A:8:ALA:HB3	1:A:9:PRO:HD3	1.89	0.54
1:A:13:VAL:HG22	1:A:14:LYS:O	2.06	0.54
1:A:118:GLU:C	1:A:119:LEU:HG	2.32	0.54
1:A:63:GLN:O	1:A:64:ARG:CB	2.57	0.53
1:A:120:GLY:CA	1:A:126:LYS:NZ	2.68	0.52
1:A:545:GLN:HB2	9:A:845:HOH:O	2.10	0.52
1:A:189:ALA:HB2	1:A:304:ILE:HD12	1.93	0.51
1:A:167:CYS:SG	1:A:170:PRO:HA	2.49	0.51
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.44	0.51
1:A:95:ASN:ND2	3:A:601:NAG:H83	2.26	0.51
1:A:170:PRO:CB	1:A:171:PRO:CD	2.89	0.50
1:A:120:GLY:HA2	1:A:123:GLU:CB	2.41	0.50
1:A:82:ILE:CD1	1:A:480:LEU:HD13	2.38	0.49
1:A:118:GLU:O	1:A:120:GLY:N	2.35	0.49
1:A:123:GLU:HG3	1:A:125:SER:H	1.77	0.48
1:A:112:ASP:OD2	5:A:607[B]:HEM:O1D	2.31	0.48
1:A:118:GLU:C	1:A:120:GLY:H	2.19	0.48
1:A:77:GLU:HG2	1:A:145:PRO:CB	2.44	0.47
1:A:541:ARG:O	1:A:545:GLN:HG3	2.14	0.47
1:A:407:MET:HB3	1:A:501:MET:HE3	1.96	0.47
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.49	0.47
1:A:425:THR:HG21	9:A:1007:HOH:O	2.15	0.47
1:A:130:GLU:OE1	1:A:426:HIS:CE1	2.69	0.46
1:A:167:CYS:HB3	1:A:170:PRO:N	2.25	0.46
1:A:169:THR:HG22	1:A:169:THR:O	2.16	0.46
1:A:313:LEU:N	1:A:314:PRO:CD	2.79	0.46
1:A:63:GLN:H	1:A:63:GLN:CD	2.23	0.45
1:A:150:LYS:NZ	1:A:154:GLN:NE2	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLU:CD	1:A:426:HIS:ND1	2.72	0.45
1:A:303:PHE:O	1:A:307:ILE:HG12	2.16	0.45
1:A:138:ASN:O	1:A:161:PHE:HA	2.17	0.45
1:A:120:GLY:CA	1:A:126:LYS:HZ2	2.30	0.45
1:A:237:CYS:HA	1:A:381:PHE:O	2.18	0.44
1:A:118:GLU:C	1:A:120:GLY:N	2.76	0.44
1:A:511:LEU:HD12	1:A:511:LEU:HA	1.90	0.43
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.53	0.43
5:A:607[A]:HEM:HBD1	9:A:701:HOH:O	2.19	0.42
1:A:50:GLU:OE2	8:A:615:GOL:H32	2.19	0.42
1:A:98:LEU:HD23	1:A:98:LEU:HA	1.89	0.42
1:A:148:ASP:O	1:A:151:LEU:HB2	2.20	0.42
1:A:518:GLN:O	1:A:522:ILE:HG23	2.20	0.42
1:A:333:ASN:C	1:A:333:ASN:ND2	2.76	0.42
1:A:169:THR:O	1:A:170:PRO:O	2.38	0.41
1:A:260:ILE:HG23	1:A:261:LEU:HD13	2.02	0.41
1:A:358:VAL:HB	1:A:379:LEU:CD1	2.51	0.41
1:A:191:LEU:HA	1:A:253:ASP:HB2	2.03	0.41
1:A:522:ILE:C	1:A:522:ILE:HD12	2.46	0.41
1:A:529:TRP:CD1	1:A:531:GLU:HB2	2.55	0.41
1:A:229:PHE:HB3	1:A:247:PRO:HG2	2.03	0.40
1:A:423:GLN:HE21	1:A:423:GLN:HA	1.86	0.40
1:A:98:LEU:HD22	1:A:101:MET:HE3	2.02	0.40
1:A:313:LEU:HD23	1:A:313:LEU:HA	1.96	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	593/595 (100%)	558 (94%)	27 (5%)	8 (1%)	9 18

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	ARG
1	A	169	THR
1	A	170	PRO
1	A	118	GLU
1	A	119	LEU
1	A	173	GLN
1	A	56	ALA
1	A	7	GLY

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	518/518 (100%)	475 (92%)	43 (8%)	10	22

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TRP
1	A	10	VAL
1	A	12	LEU
1	A	14	LYS
1	A	17	GLU
1	A	36	LEU
1	A	57	LEU
1	A	89	GLU
1	A	91	VAL
1	A	98	LEU
1	A	119	LEU
1	A	122	ASN
1	A	124	HIS
1	A	125	SER
1	A	126	LYS
1	A	128	GLN
1	A	131	GLU

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Mol	Chain	Res	Type
1	A	153	THR
1	A	173	GLN
1	A	175	LEU
1	A	187	LEU
1	A	198	SER
1	A	201	SER
1	A	203	LEU
1	A	227	LEU
1	A	232	LYS
1	A	233	LYS
1	A	261	LEU
1	A	268	LEU
1	A	276	LEU
1	A	292	LEU
1	A	317	LEU
1	A	322	GLN
1	A	333	ASN
1	A	360	ARG
1	A	376	LEU
1	A	464	LEU
1	A	465	LYS
1	A	471	LEU
1	A	480	LEU
1	A	511	LEU
1	A	522	ILE
1	A	564	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	138	ASN
1	A	147	ASN
1	A	154	GLN
1	A	231	ASN
1	A	329	GLN
1	A	333	ASN
1	A	341	ASN
1	A	468	GLN
1	A	497	ASN
1	A	520	GLN
1	A	570	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

2 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	$\# Z > 2$
2	NAG	B	1	1,2	14,14,15	0.57	0	17,19,21	0.94	0
2	NAG	B	2	2	14,14,15	0.65	0	17,19,21	1.53	5 (29%)

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	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	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(°)
2	B	2	NAG	O4-C4-C5	3.32	117.51	109.32
2	B	2	NAG	C1-O5-C5	2.48	115.51	112.19
2	B	2	NAG	O5-C1-C2	-2.33	107.69	111.29
2	B	2	NAG	C3-C4-C5	-2.30	106.06	110.23
2	B	2	NAG	C4-C3-C2	-2.09	107.95	111.02

There are no chirality outliers.

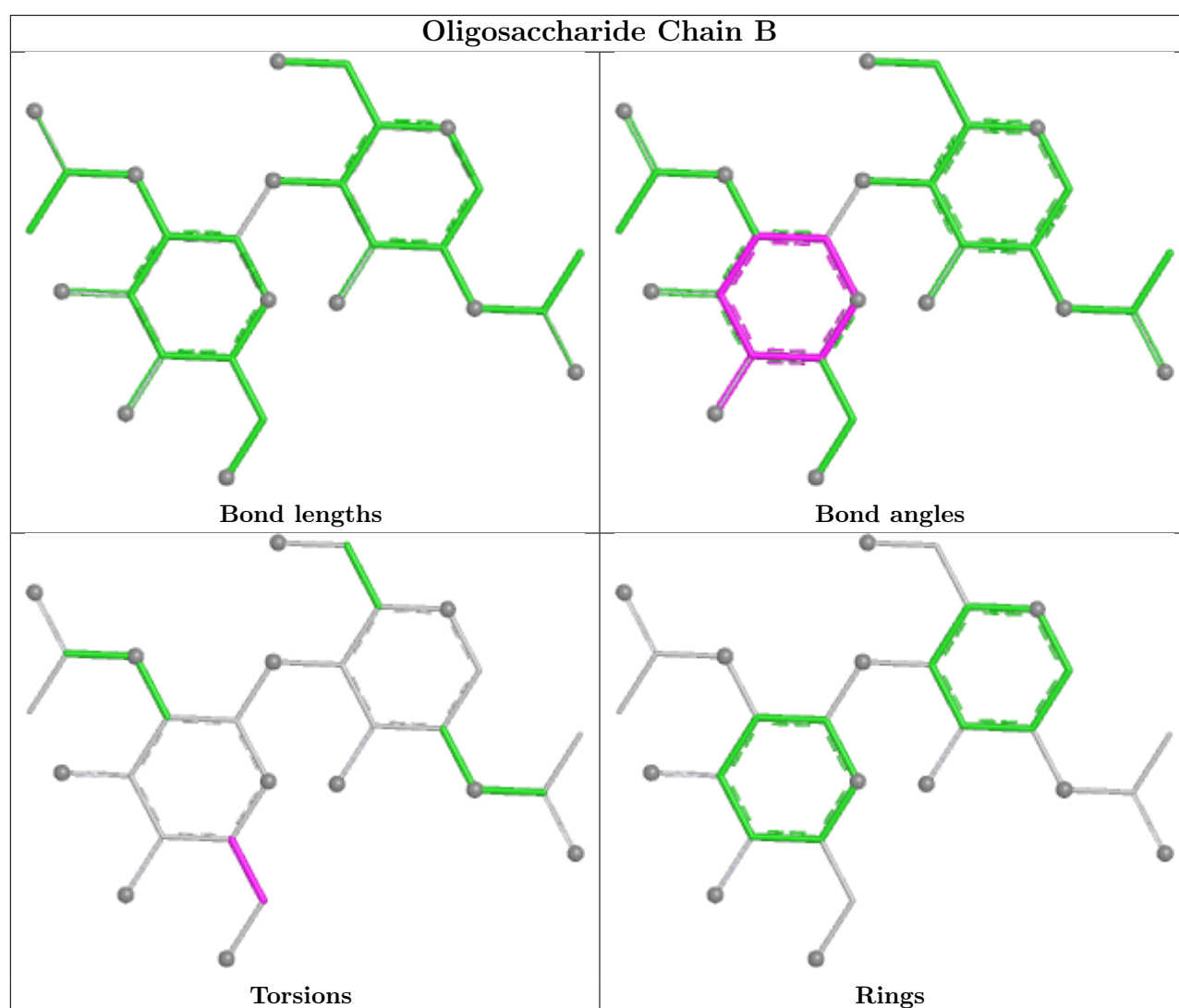
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-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.



5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	$\# Z > 2$
3	NAG	A	601	1	14,14,15	0.57	0	17,19,21	1.45	2 (11%)
5	HEM	A	607[B]	-	50,50,50	1.70	11 (22%)	67,82,82	1.71	15 (22%)
8	GOL	A	613	-	5,5,5	0.17	0	5,5,5	0.46	0
3	NAG	A	604	1	14,14,15	0.70	0	17,19,21	1.61	3 (17%)
3	NAG	A	605	1	14,14,15	0.62	0	17,19,21	1.50	3 (17%)
8	GOL	A	615	-	5,5,5	0.15	0	5,5,5	0.35	0
5	HEM	A	607[A]	6	50,50,50	1.69	11 (22%)	67,82,82	1.74	16 (23%)
8	GOL	A	612	-	5,5,5	0.19	0	5,5,5	0.46	0
8	GOL	A	614	-	5,5,5	0.19	0	5,5,5	0.49	0
8	GOL	A	611	-	5,5,5	0.17	0	5,5,5	0.47	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	A	601	1	-	3/6/23/26	0/1/1/1
5	HEM	A	607[B]	-	-	4/14/54/54	-
8	GOL	A	613	-	-	4/4/4/4	-
3	NAG	A	604	1	-	0/6/23/26	0/1/1/1
3	NAG	A	605	1	-	0/6/23/26	0/1/1/1
8	GOL	A	615	-	-	2/4/4/4	-
5	HEM	A	607[A]	6	-	5/14/54/54	-
8	GOL	A	612	-	-	3/4/4/4	-
8	GOL	A	614	-	-	4/4/4/4	-
8	GOL	A	611	-	-	4/4/4/4	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	607[A]	HEM	FE-NB	5.54	2.12	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	607[B]	HEM	FE-NB	5.54	2.12	1.94
5	A	607[A]	HEM	FE-NC	4.41	2.09	1.95
5	A	607[B]	HEM	FE-NC	4.41	2.09	1.95
5	A	607[A]	HEM	C4D-ND	-3.09	1.34	1.40
5	A	607[B]	HEM	C4D-ND	-3.09	1.34	1.40
5	A	607[A]	HEM	C1C-C2C	-2.79	1.39	1.45
5	A	607[B]	HEM	C1C-C2C	-2.79	1.39	1.45
5	A	607[A]	HEM	C1B-NB	-2.75	1.35	1.40
5	A	607[B]	HEM	C1B-NB	-2.75	1.35	1.40
5	A	607[A]	HEM	C3C-C4C	-2.68	1.41	1.46
5	A	607[B]	HEM	C3C-C4C	-2.68	1.41	1.46
5	A	607[A]	HEM	FE-ND	-2.60	1.86	1.94
5	A	607[B]	HEM	FE-ND	-2.60	1.86	1.94
5	A	607[A]	HEM	C4C-NC	-2.28	1.35	1.39
5	A	607[B]	HEM	C4C-NC	-2.28	1.35	1.39
5	A	607[A]	HEM	C3B-C4B	2.27	1.49	1.44
5	A	607[B]	HEM	C3B-C4B	2.27	1.49	1.44
5	A	607[A]	HEM	C1D-ND	-2.25	1.34	1.38
5	A	607[B]	HEM	C1D-ND	-2.25	1.34	1.38
5	A	607[A]	HEM	C4B-NB	-2.11	1.34	1.38
5	A	607[B]	HEM	C4B-NB	-2.11	1.34	1.38

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	607[A]	HEM	CHA-C4D-ND	4.66	130.14	124.37
5	A	607[B]	HEM	CHA-C4D-ND	4.66	130.14	124.37
5	A	607[A]	HEM	CHD-C1D-ND	4.66	129.44	124.42
5	A	607[B]	HEM	CHD-C1D-ND	4.66	129.44	124.42
5	A	607[A]	HEM	CMD-C2D-C1D	4.24	131.66	125.03
5	A	607[B]	HEM	CMD-C2D-C1D	4.24	131.66	125.03
5	A	607[A]	HEM	CHC-C4B-NB	3.98	128.71	124.42
5	A	607[B]	HEM	CHC-C4B-NB	3.98	128.71	124.42
5	A	607[A]	HEM	O2A-CGA-CBA	3.08	123.73	114.00
5	A	607[B]	HEM	O2A-CGA-CBA	3.08	123.73	114.00
3	A	601	NAG	C8-C7-N2	3.07	121.22	116.12
3	A	605	NAG	C1-O5-C5	3.06	116.28	112.19
3	A	605	NAG	C3-C4-C5	-3.04	104.71	110.23
5	A	607[A]	HEM	C1B-NB-C4B	2.99	108.75	105.21
5	A	607[B]	HEM	C1B-NB-C4B	2.99	108.75	105.21
5	A	607[A]	HEM	CBD-CAD-C3D	-2.92	104.45	112.53
5	A	607[A]	HEM	CHA-C4D-C3D	-2.84	119.98	125.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	607[B]	HEM	CHA-C4D-C3D	-2.84	119.98	125.23
3	A	601	NAG	O5-C5-C6	-2.79	102.23	107.66
3	A	604	NAG	O3-C3-C2	-2.68	103.83	109.40
5	A	607[A]	HEM	O2A-CGA-O1A	-2.66	116.49	123.33
5	A	607[B]	HEM	O2A-CGA-O1A	-2.66	116.49	123.33
3	A	604	NAG	O7-C7-N2	2.54	126.47	121.98
5	A	607[A]	HEM	CHD-C1D-C2D	-2.52	121.05	125.03
5	A	607[B]	HEM	CHD-C1D-C2D	-2.52	121.05	125.03
5	A	607[A]	HEM	O2D-CGD-CBD	2.46	121.76	114.00
5	A	607[A]	HEM	CHB-C1B-NB	2.36	127.29	124.37
5	A	607[B]	HEM	CHB-C1B-NB	2.36	127.29	124.37
3	A	605	NAG	C1-C2-N2	-2.23	106.92	110.43
5	A	607[A]	HEM	C4C-CHD-C1D	-2.11	121.54	126.02
5	A	607[B]	HEM	C4C-CHD-C1D	-2.11	121.54	126.02
5	A	607[A]	HEM	C4B-C3B-C2B	-2.11	105.34	107.28
5	A	607[B]	HEM	C4B-C3B-C2B	-2.11	105.34	107.28
5	A	607[B]	HEM	CBD-CAD-C3D	-2.10	106.72	112.53
5	A	607[A]	HEM	C1A-CHA-C4D	-2.09	121.34	126.25
5	A	607[A]	HEM	C3B-C2B-C1B	2.07	107.96	106.41
5	A	607[B]	HEM	C3B-C2B-C1B	2.07	107.96	106.41
5	A	607[B]	HEM	O2D-CGD-CBD	2.05	120.49	114.00
3	A	604	NAG	C1-C2-N2	-2.03	107.23	110.43

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	611	GOL	O1-C1-C2-C3
8	A	612	GOL	O1-C1-C2-C3
8	A	613	GOL	O1-C1-C2-C3
8	A	614	GOL	O1-C1-C2-C3
8	A	614	GOL	C1-C2-C3-O3
3	A	601	NAG	C8-C7-N2-C2
3	A	601	NAG	O7-C7-N2-C2
8	A	613	GOL	O1-C1-C2-O2
3	A	601	NAG	O5-C5-C6-O6
8	A	611	GOL	C1-C2-C3-O3
8	A	613	GOL	C1-C2-C3-O3
8	A	615	GOL	O1-C1-C2-C3
8	A	611	GOL	O1-C1-C2-O2
8	A	612	GOL	O1-C1-C2-O2
8	A	614	GOL	O1-C1-C2-O2

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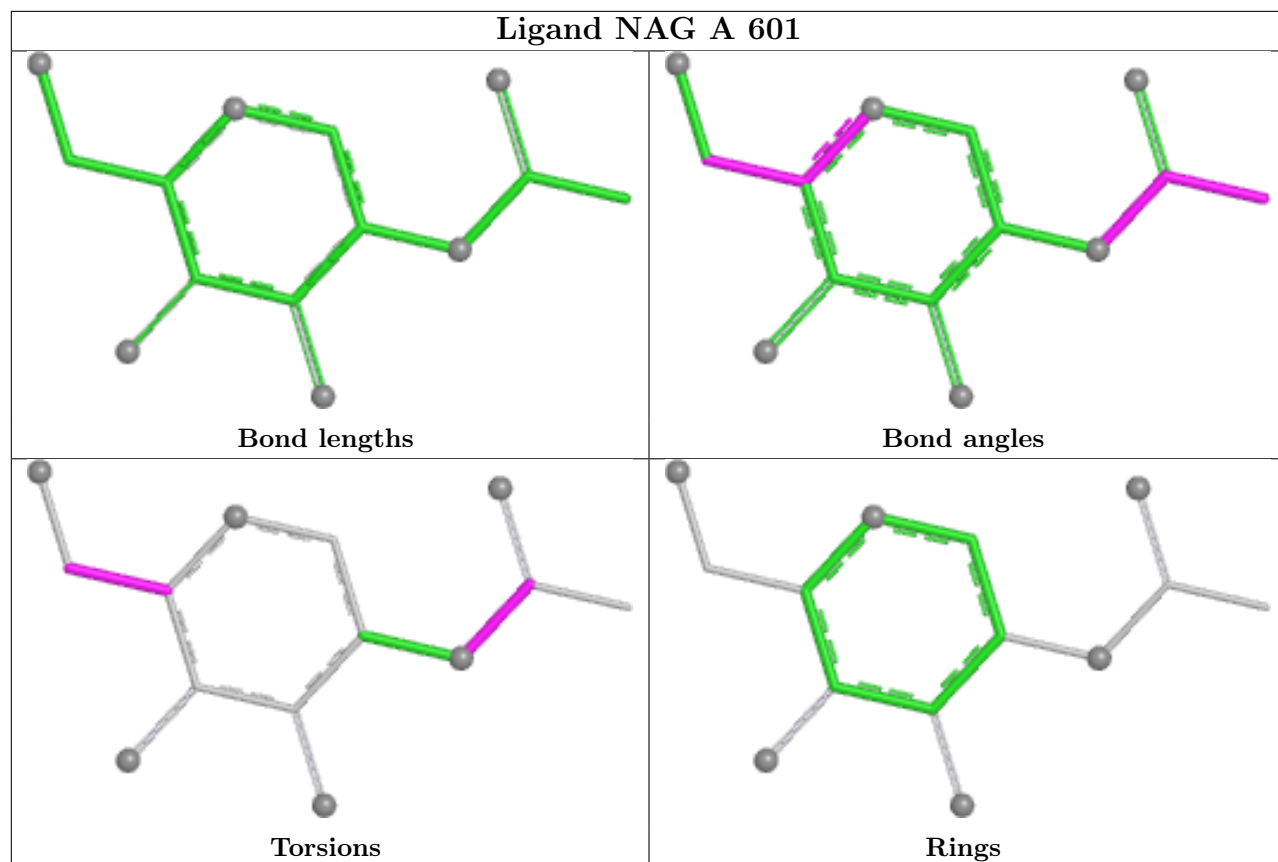
Mol	Chain	Res	Type	Atoms
8	A	614	GOL	O2-C2-C3-O3
8	A	613	GOL	O2-C2-C3-O3
8	A	615	GOL	O1-C1-C2-O2
5	A	607[A]	HEM	CAA-CBA-CGA-O1A
5	A	607[B]	HEM	CAA-CBA-CGA-O1A
5	A	607[A]	HEM	CAD-CBD-CGD-O1D
5	A	607[A]	HEM	CAD-CBD-CGD-O2D
5	A	607[A]	HEM	C3D-CAD-CBD-CGD
5	A	607[A]	HEM	CAA-CBA-CGA-O2A
5	A	607[B]	HEM	CAA-CBA-CGA-O2A
5	A	607[B]	HEM	CAD-CBD-CGD-O2D
8	A	611	GOL	O2-C2-C3-O3
8	A	612	GOL	O2-C2-C3-O3
5	A	607[B]	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

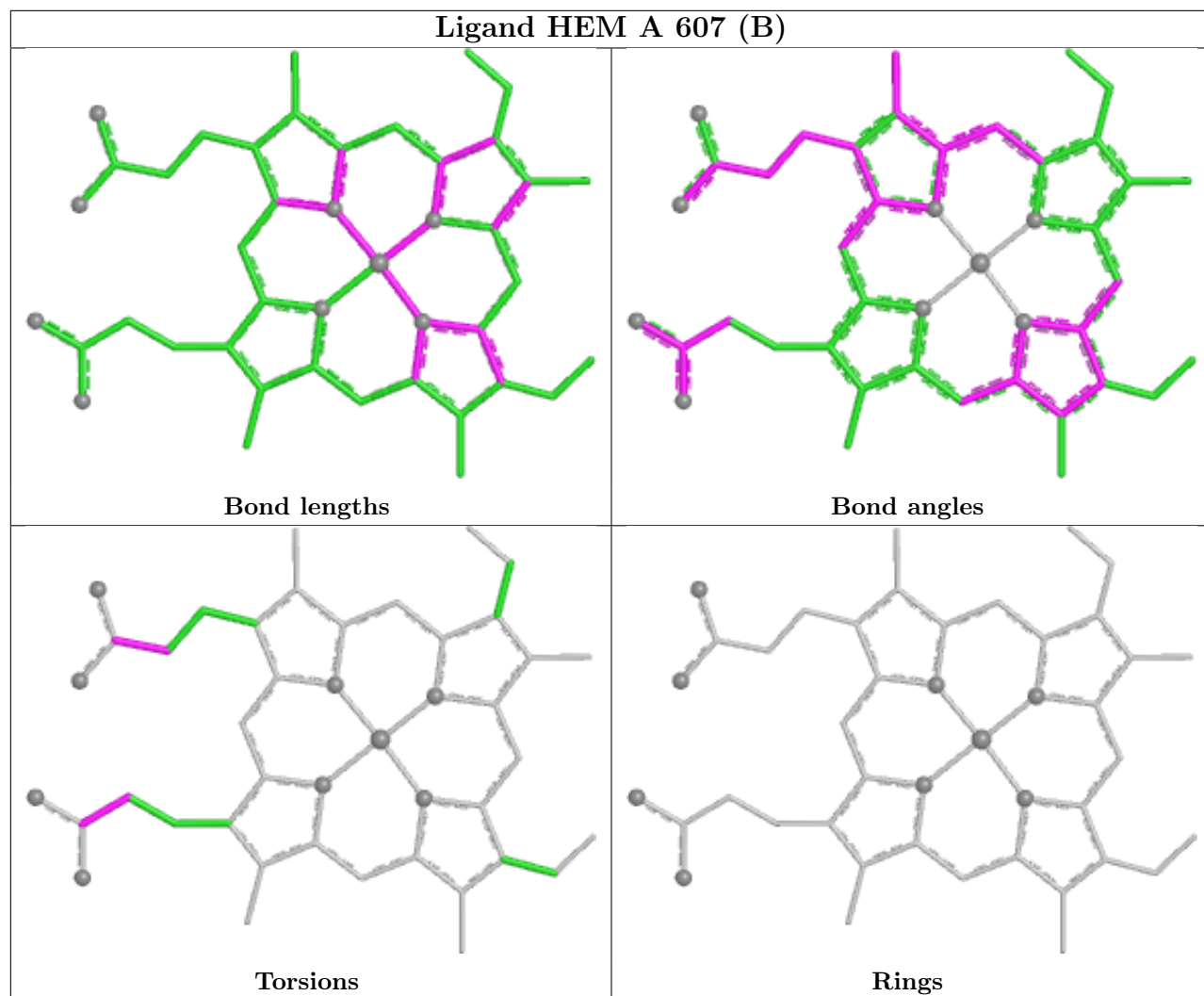
6 monomers are involved in 8 short contacts:

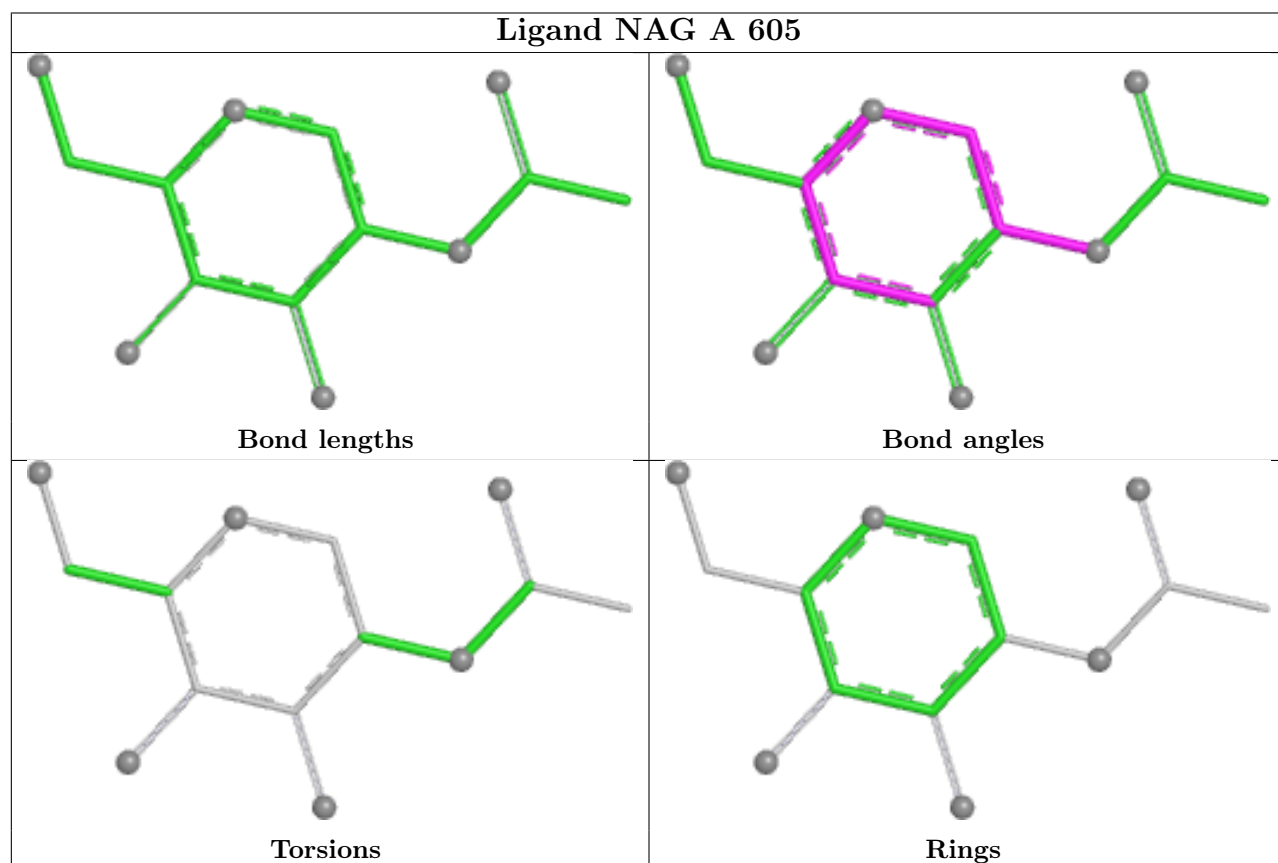
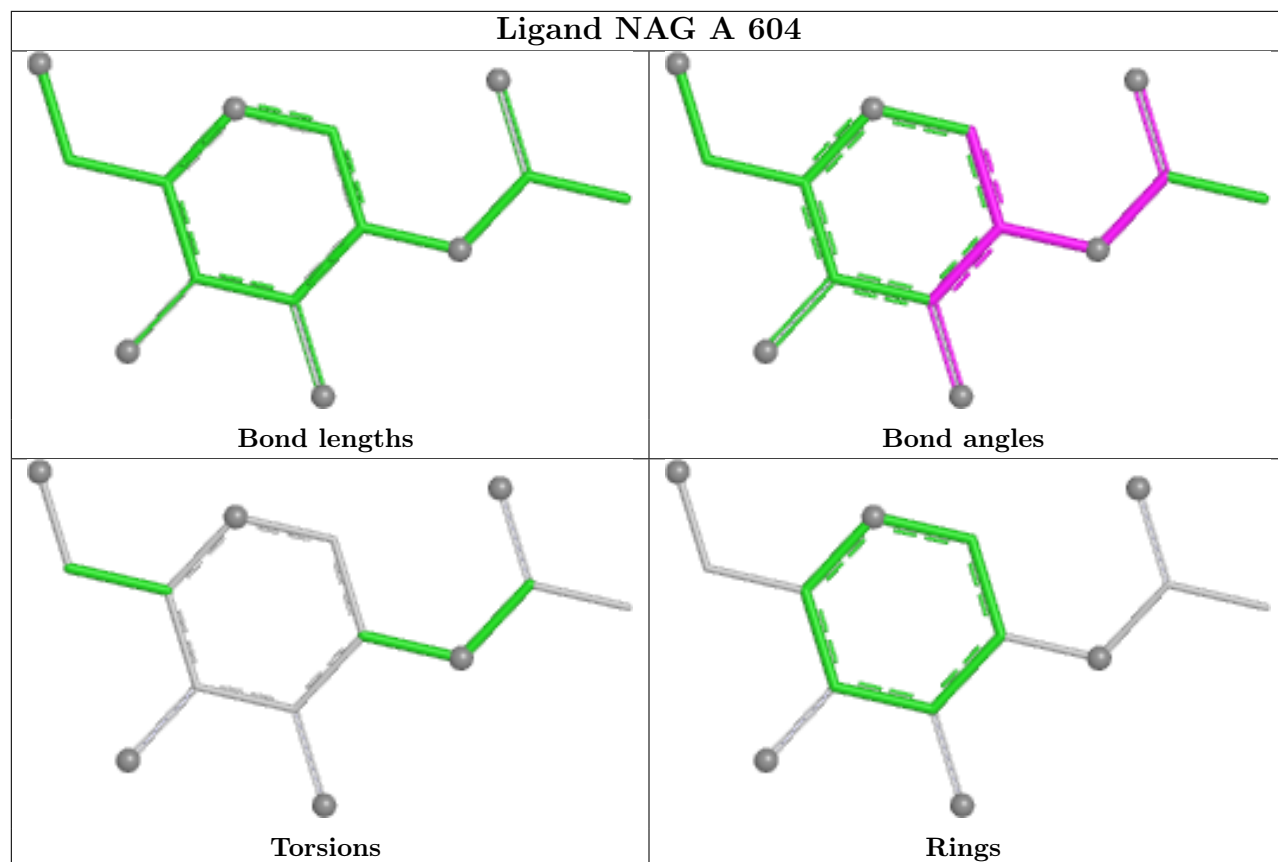
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	NAG	1	0
5	A	607[B]	HEM	1	0
8	A	615	GOL	1	0
5	A	607[A]	HEM	2	0
8	A	612	GOL	2	0
8	A	614	GOL	1	0

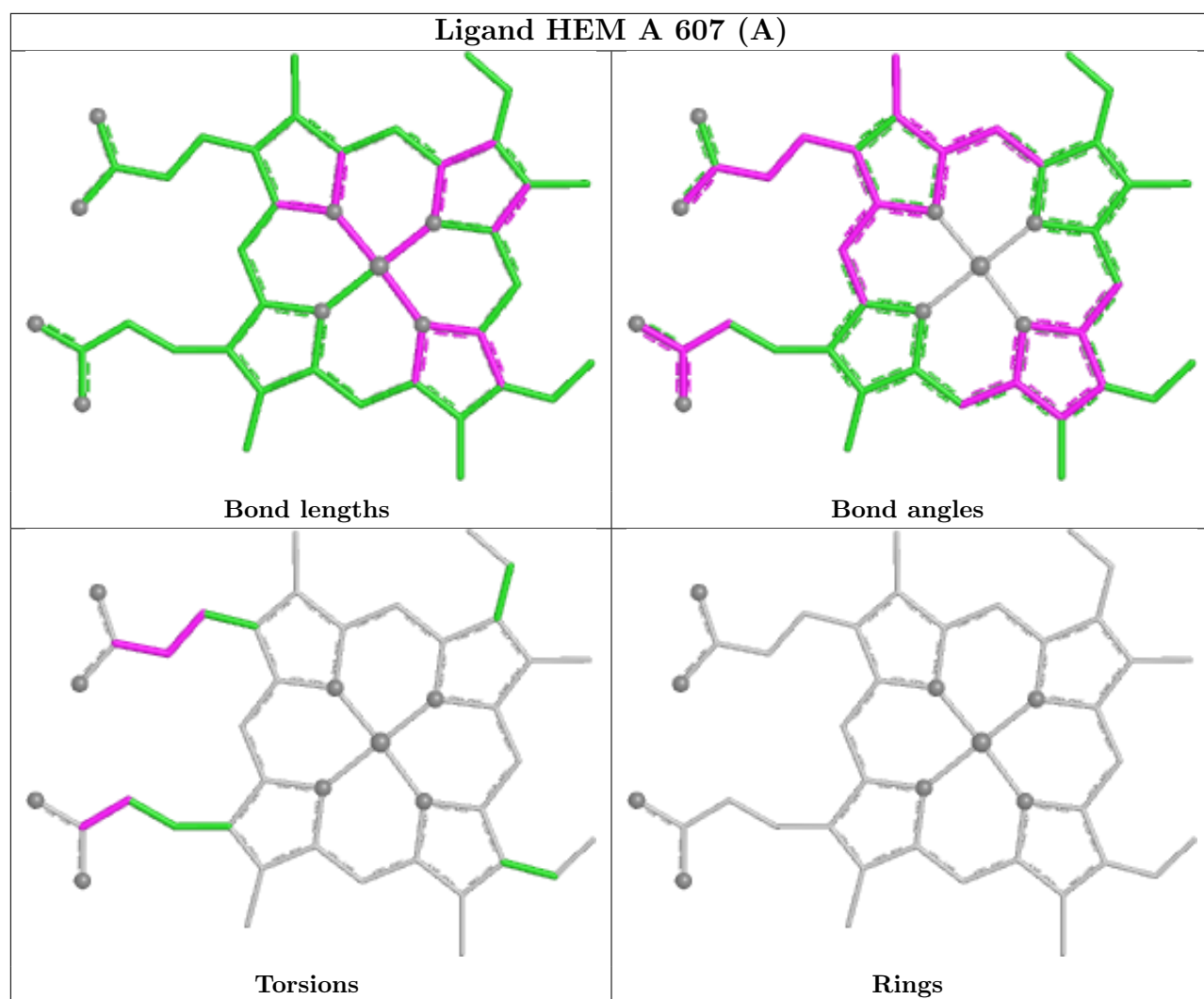
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand HEM A 607 (B)







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	595/595 (100%)	0.05	31 (5%)	33 29	18, 29, 75, 163	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	168	PRO	8.5
1	A	9	PRO	7.2
1	A	169	THR	6.7
1	A	4	VAL	6.2
1	A	6	CYS	5.5
1	A	119	LEU	5.4
1	A	167	CYS	5.4
1	A	7	GLY	5.0
1	A	13	VAL	4.9
1	A	171	PRO	4.9
1	A	122	ASN	4.6
1	A	8	ALA	4.6
1	A	11	PRO	4.3
1	A	2	TRP	4.3
1	A	172	TYR	3.9
1	A	5	GLY	3.9
1	A	12	LEU	3.8
1	A	170	PRO	3.8
1	A	10	VAL	3.4
1	A	595	ASN	3.1
1	A	124	HIS	3.1
1	A	3	GLU	2.9
1	A	1	SER	2.8
1	A	173	GLN	2.5
1	A	120	GLY	2.5
1	A	231	ASN	2.5
1	A	121	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	593	ARG	2.3
1	A	63	GLN	2.1
1	A	174	SER	2.1
1	A	14	LYS	2.1

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

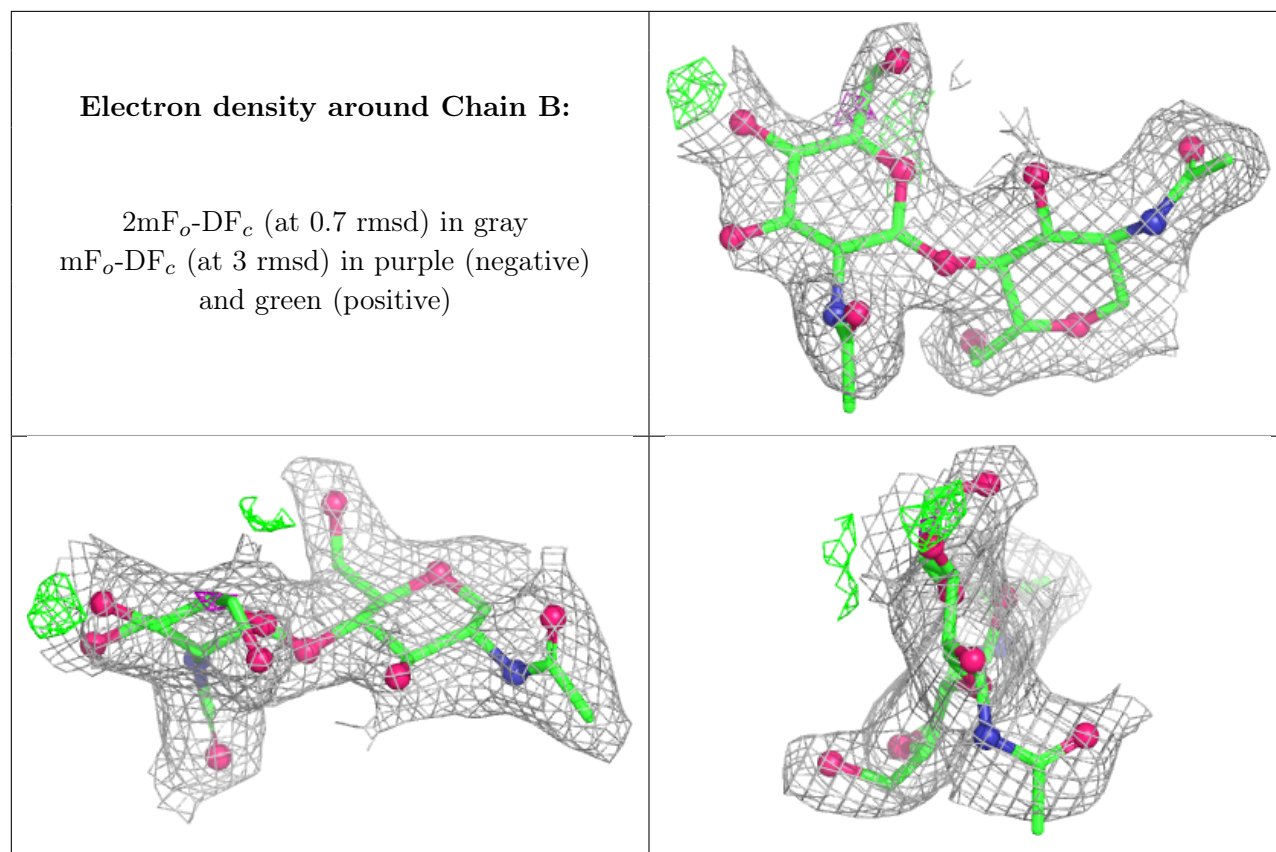
There are no non-standard protein/DNA/RNA residues in this entry.

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
2	NAG	B	2	14/15	0.79	0.13	53,58,66,67	0
2	NAG	B	1	14/15	0.91	0.08	31,37,42,45	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.

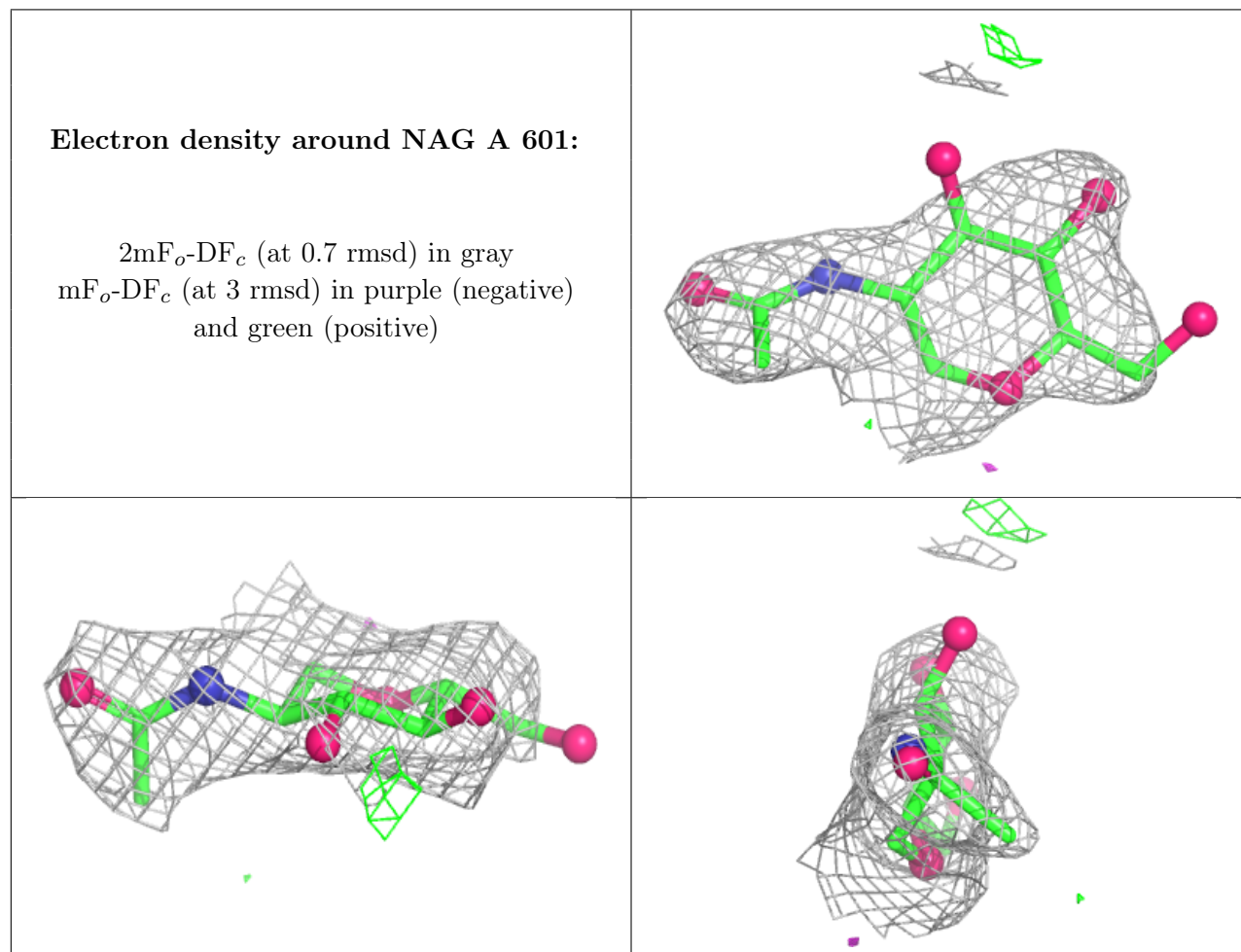


6.4 Ligands [i](#)

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.

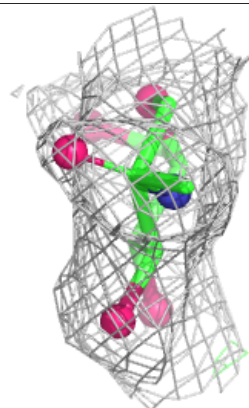
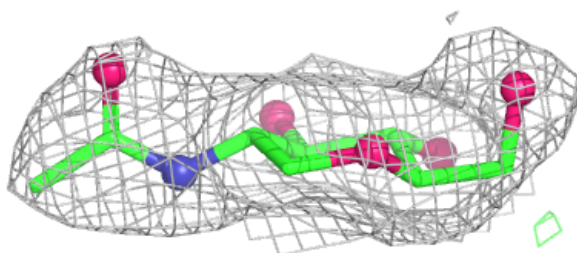
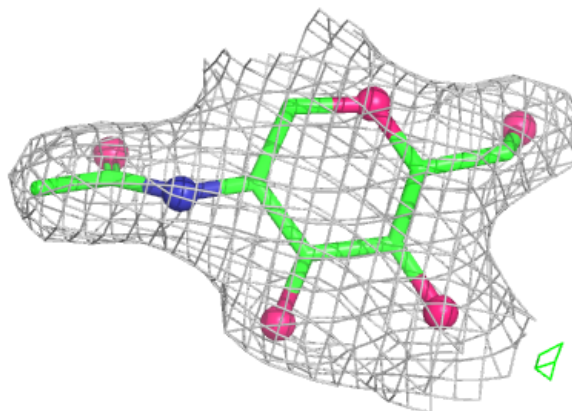
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	A	601	14/15	0.81	0.13	56,61,70,81	0
3	NAG	A	605	14/15	0.84	0.11	41,43,48,48	0
8	GOL	A	613	6/6	0.85	0.15	40,46,46,48	0
8	GOL	A	614	6/6	0.86	0.14	43,46,48,48	0
8	GOL	A	615	6/6	0.88	0.13	44,46,47,47	0
8	GOL	A	612	6/6	0.89	0.14	51,53,54,55	0
3	NAG	A	604	14/15	0.89	0.12	36,43,57,61	0
8	GOL	A	611	6/6	0.91	0.10	46,47,49,50	0
5	HEM	A	607[B]	43/43	0.97	0.07	19,21,22,22	7
5	HEM	A	607[A]	43/43	0.97	0.07	19,21,24,26	7
6	K	A	608	1/1	0.99	0.03	25,25,25,25	0
6	K	A	609	1/1	0.99	0.03	22,22,22,22	1
7	ZN	A	610	1/1	0.99	0.02	35,35,35,35	0
4	CA	A	606	1/1	0.99	0.03	19,19,19,19	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.



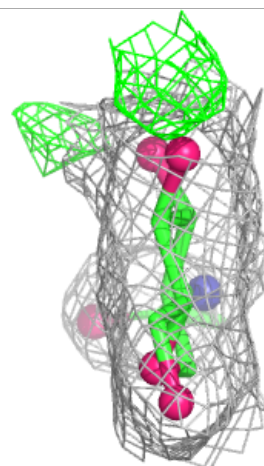
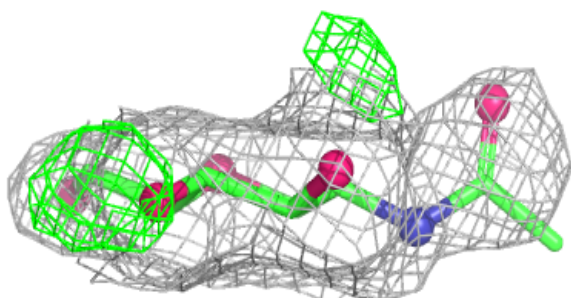
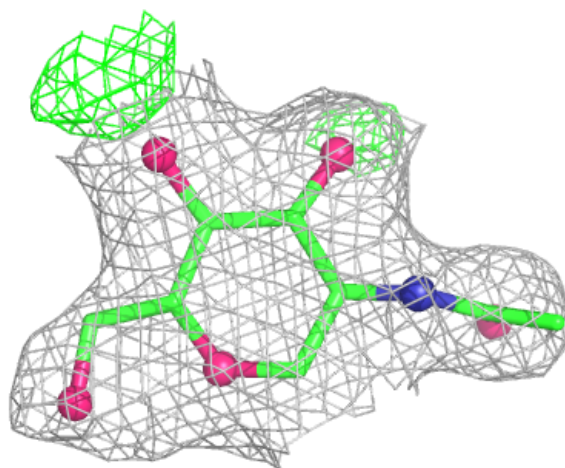
Electron density around NAG A 605:

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



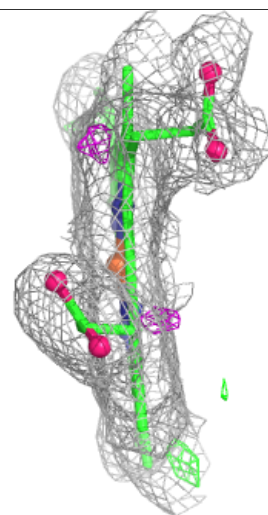
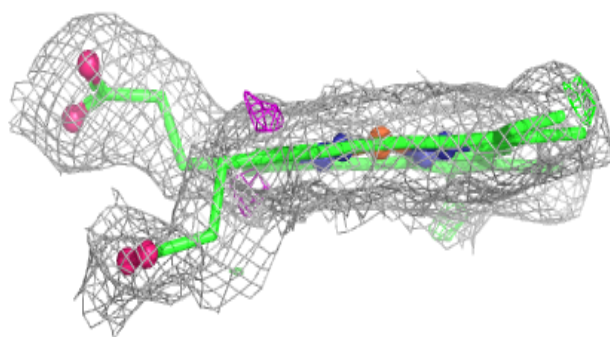
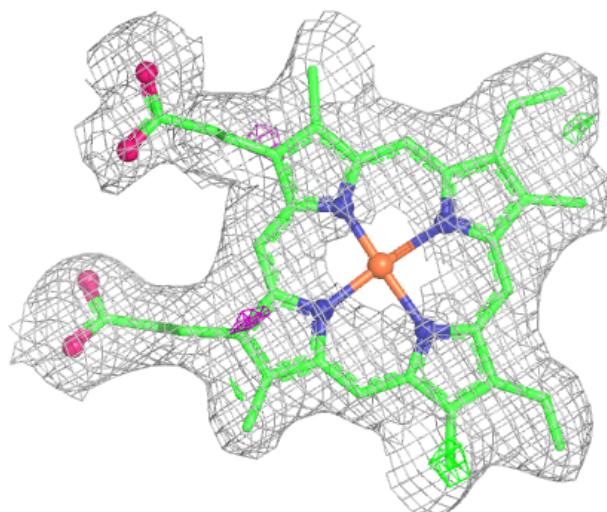
Electron density around NAG A 604:

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



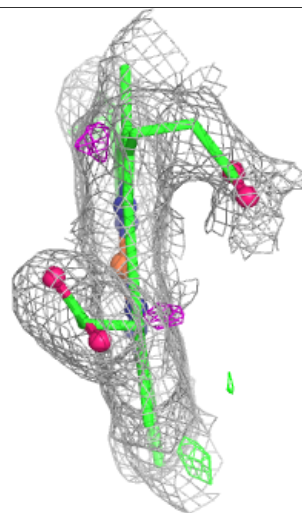
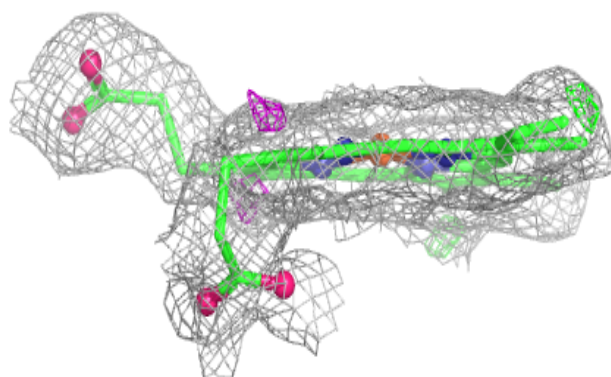
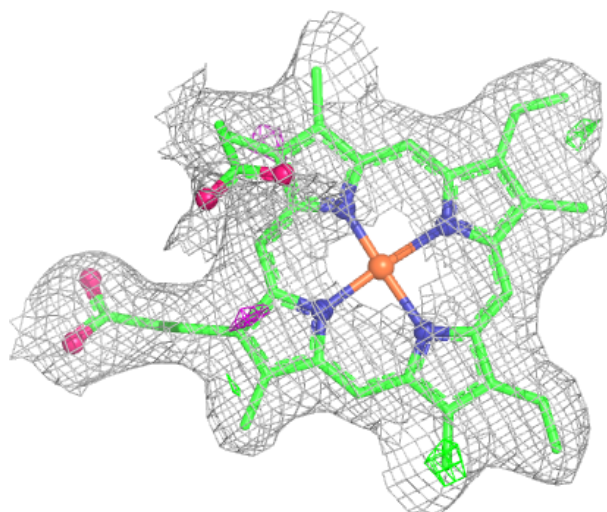
Electron density around HEM A 607 (B):

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



Electron density around HEM A 607 (A):

$2mF_o-DF_c$ (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.