



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 11:58 PM EDT

PDB ID : 3DL9
Title : Crystal structure of CYP2R1 in complex with 1-alpha-hydroxy-vitamin D2
Authors : Strushkevich, N.V.; Tempel, W.; Gilep, A.A.; Loppnau, P.; Arrowsmith, C.H.;
Edwards, A.M.; Bountra, C.; Wilkstrom, M.; Bochkarev, A.; Park, H.; Structural Genomics Consortium (SGC)
Deposited on : 2008-06-26
Resolution : 2.72 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

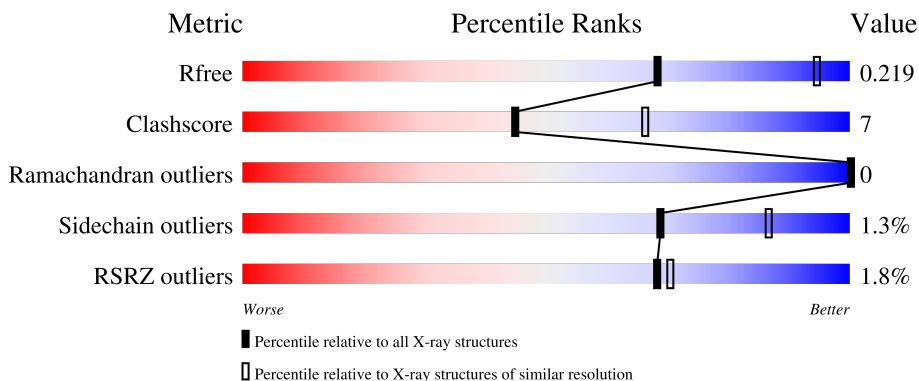
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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}	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	479	 2% 86% 11%
1	B	479	 1% 85% 12%
2	C	7	 14% 86%
2	D	7	 100%

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 7959 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.

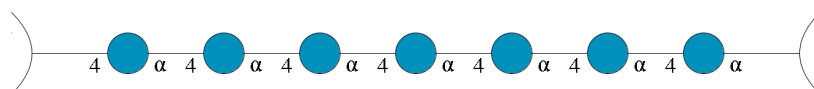
- Molecule 1 is a protein called Cytochrome P450 2R1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	465	3720	2421	612	669	18	0	0	0
1	B	467	3733	2432	622	661	18	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	expression tag	UNP Q6V VX0
A	28	ALA	-	expression tag	UNP Q6V VX0
A	29	LYS	-	expression tag	UNP Q6V VX0
A	30	LYS	-	expression tag	UNP Q6V VX0
A	31	THR	-	expression tag	UNP Q6V VX0
A	502	HIS	-	expression tag	UNP Q6V VX0
A	503	HIS	-	expression tag	UNP Q6V VX0
A	504	HIS	-	expression tag	UNP Q6V VX0
A	505	HIS	-	expression tag	UNP Q6V VX0
B	27	MET	-	expression tag	UNP Q6V VX0
B	28	ALA	-	expression tag	UNP Q6V VX0
B	29	LYS	-	expression tag	UNP Q6V VX0
B	30	LYS	-	expression tag	UNP Q6V VX0
B	31	THR	-	expression tag	UNP Q6V VX0
B	502	HIS	-	expression tag	UNP Q6V VX0
B	503	HIS	-	expression tag	UNP Q6V VX0
B	504	HIS	-	expression tag	UNP Q6V VX0
B	505	HIS	-	expression tag	UNP Q6V VX0

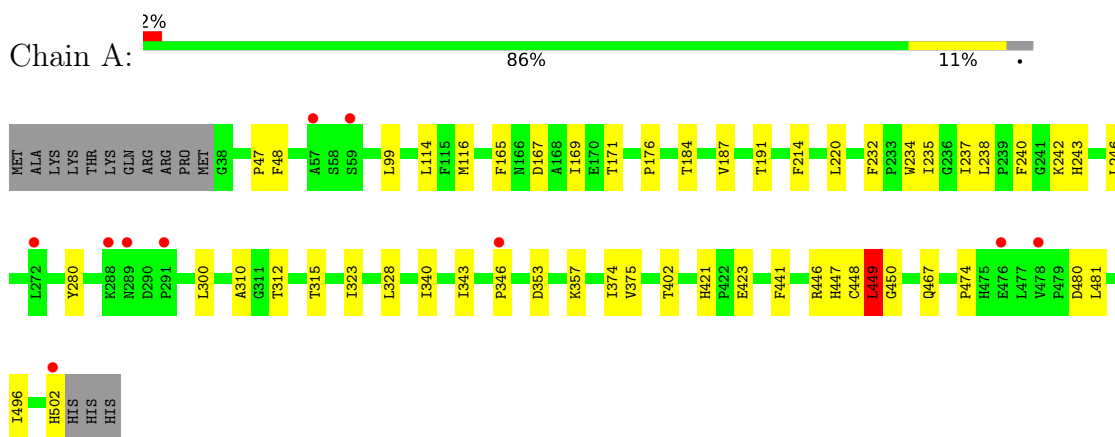
- Molecule 2 is an oligosaccharide called Cycloheptakis-(1-4)-(alpha-D-glucopyranose).



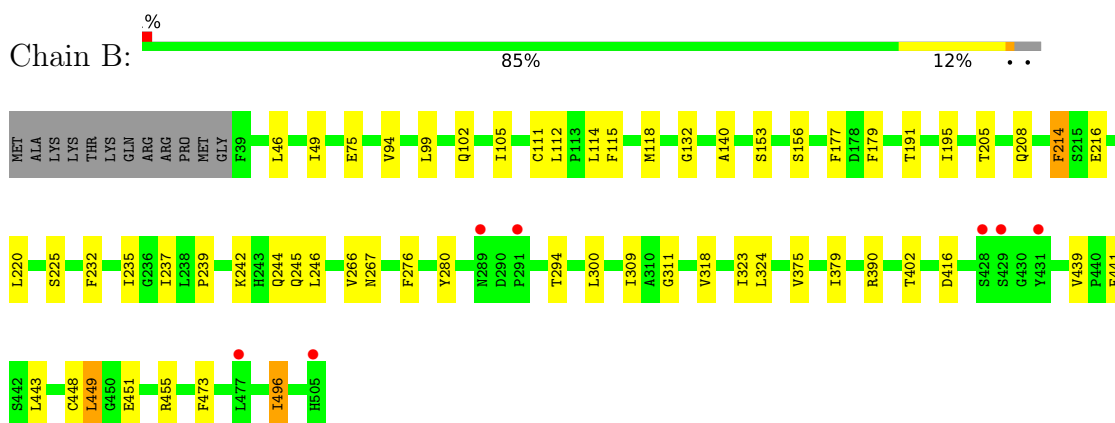
3 Residue-property plots [i](#)

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: Cytochrome P450 2R1



- Molecule 1: Cytochrome P450 2R1



- Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)



- Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)



GLC1
GLC2
GLC3
GLC4
GLC5
GLC6
GLC7

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	137.30Å 163.04Å 152.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.72 29.31 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.00-2.72) 99.2 (29.31-2.72)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 2.72Å)	Xtrriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.183 , 0.218 0.189 , 0.219	Depositor DCC
R_{free} test set	1369 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtrriage
Anisotropy	0.103	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7959	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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: HEM, GLC, V2H

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	0.66	0/3829	0.63	3/5199 (0.1%)
1	B	0.64	1/3845 (0.0%)	0.61	0/5224
All	All	0.65	1/7674 (0.0%)	0.62	3/10423 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111	CYS	CB-SG	-5.23	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	446	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	446	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	449	LEU	CA-CB-CG	5.14	127.12	115.30

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	3720	0	3592	42	0
1	B	3733	0	3597	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	77	0	63	0	0
2	D	77	0	63	0	0
3	A	86	0	60	16	0
3	B	86	0	60	13	0
4	A	30	0	44	1	0
4	B	30	0	44	1	0
5	A	74	0	0	1	0
5	B	46	0	0	0	0
All	All	7959	0	7523	100	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 7.

All (100) 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)
3:B:601[A]:HEM:HMB2	3:B:601[A]:HEM:HBB2	1.52	0.92
3:B:601[B]:HEM:HBC2	3:B:601[B]:HEM:HMC1	1.60	0.83
3:A:601[A]:HEM:HMB2	3:A:601[A]:HEM:HBB2	1.60	0.82
3:B:601[B]:HEM:HBB2	3:B:601[B]:HEM:HMB2	1.62	0.81
3:A:601[A]:HEM:HBC2	3:A:601[A]:HEM:HMC2	1.64	0.78
3:B:601[A]:HEM:HBC2	3:B:601[A]:HEM:HMC2	1.66	0.77
3:A:601[B]:HEM:HMC1	3:A:601[B]:HEM:HBC2	1.68	0.75
1:A:237:ILE:HD11	1:B:237:ILE:HD11	1.68	0.75
1:A:323:ILE:CG2	1:A:496:ILE:HD12	2.20	0.71
3:A:601[B]:HEM:HBB2	3:A:601[B]:HEM:HMB2	1.73	0.70
3:B:601[A]:HEM:HBB2	3:B:601[A]:HEM:CMB	2.22	0.70
1:B:239:PRO:HA	1:B:244:GLN:HE21	1.57	0.69
1:B:323:ILE:CG2	1:B:496:ILE:HD12	2.24	0.68
1:B:46:LEU:HD12	1:B:49:ILE:HD11	1.75	0.67
1:A:48:PHE:CE1	1:A:232:PHE:CE2	2.85	0.64
1:B:451:GLU:O	1:B:455:ARG:HG3	1.97	0.64
1:A:280:TYR:CG	1:A:300:LEU:HD13	2.34	0.63
1:B:323:ILE:HG22	1:B:496:ILE:HD12	1.79	0.62
1:A:450:GLY:HA3	3:A:601[B]:HEM:C2B	2.35	0.62
3:B:601[B]:HEM:HBC2	3:B:601[B]:HEM:CMC	2.29	0.62
3:B:601[B]:HEM:HBB2	3:B:601[B]:HEM:CMB	2.31	0.61
3:A:601[A]:HEM:HBB2	3:A:601[A]:HEM:CMB	2.30	0.60
1:A:449:LEU:C	1:A:449:LEU:HD23	2.22	0.59
1:B:191:THR:HG22	1:B:195:ILE:HD12	1.85	0.59
1:B:75:GLU:HB3	1:B:94:VAL:HG21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:601[A]:HEM:HBC2	3:A:601[A]:HEM:CMC	2.33	0.58
1:A:191:THR:HG23	5:A:638:HOH:O	2.03	0.58
1:A:421:HIS:CE1	1:A:423:GLU:HB3	2.39	0.58
1:B:99:LEU:HD11	1:B:402:THR:HG21	1.85	0.56
3:B:601[A]:HEM:HHA	3:B:601[A]:HEM:HBA2	1.87	0.56
1:B:439:VAL:HG12	1:B:443:LEU:HD21	1.87	0.56
3:A:601[A]:HEM:HHA	3:A:601[A]:HEM:HBA2	1.88	0.56
3:B:601[A]:HEM:HBC2	3:B:601[A]:HEM:CMC	2.36	0.55
1:A:449:LEU:HD13	3:A:601[B]:HEM:CMA	2.36	0.55
1:B:112:LEU:HD12	1:B:115:PHE:CE1	2.42	0.55
1:B:323:ILE:HG22	1:B:496:ILE:CD1	2.36	0.54
1:A:99:LEU:HD11	1:A:402:THR:HG21	1.89	0.54
1:B:220:LEU:HD22	1:B:242:LYS:HB3	1.89	0.54
1:B:232:PHE:O	1:B:235:ILE:HG23	2.08	0.54
1:A:449:LEU:HD13	3:A:601[B]:HEM:HMA1	1.90	0.54
1:A:114:LEU:HD11	1:A:246:LEU:HD22	1.89	0.53
1:B:379:ILE:HD12	3:B:601[B]:HEM:HAD1	1.89	0.53
1:A:237:ILE:HD11	1:B:237:ILE:CD1	2.37	0.53
3:A:601[B]:HEM:HBC2	3:A:601[B]:HEM:CMC	2.38	0.53
1:A:449:LEU:HD22	3:A:601[B]:HEM:HMA2	1.91	0.52
4:B:602:V2H:HAEA	4:B:602:V2H:HAR	1.91	0.51
1:B:75:GLU:OE2	1:B:94:VAL:HG23	2.09	0.51
1:B:153:SER:O	1:B:156:SER:OG	2.27	0.50
1:A:343:ILE:HD12	1:A:357:LYS:HB3	1.92	0.50
1:A:187:VAL:HG11	1:A:315:THR:HB	1.94	0.49
1:A:323:ILE:HG22	1:A:496:ILE:HD12	1.93	0.49
1:B:449:LEU:HD23	1:B:449:LEU:C	2.32	0.49
1:B:195:ILE:HA	1:B:276:PHE:HB3	1.95	0.48
1:B:280:TYR:CG	1:B:300:LEU:HD13	2.49	0.48
1:A:232:PHE:HB3	1:A:234:TRP:CE2	2.49	0.48
3:A:601[B]:HEM:HBB2	3:A:601[B]:HEM:CMB	2.42	0.48
1:B:46:LEU:CD1	1:B:49:ILE:HD11	2.44	0.47
1:A:176:PRO:HB3	1:A:474:PRO:HG3	1.96	0.47
1:A:323:ILE:CG2	1:A:496:ILE:CD1	2.91	0.47
1:B:266:VAL:HG12	1:B:267:ASN:OD1	2.15	0.47
1:B:311:GLY:HA2	3:B:601[A]:HEM:CMC	2.45	0.46
1:A:323:ILE:HG22	1:A:496:ILE:CD1	2.45	0.46
1:B:216:GLU:OE1	1:B:245:GLN:NE2	2.48	0.46
1:A:480:ASP:C	1:A:481:LEU:HD23	2.36	0.46
1:A:235:ILE:HG23	1:A:238:LEU:HD12	1.97	0.46
1:B:214:PHE:HB3	1:B:309:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:THR:CG2	1:B:195:ILE:HD12	2.45	0.45
1:A:340:ILE:HG21	1:A:467:GLN:HB2	1.97	0.45
1:B:114:LEU:O	1:B:118:MET:HG2	2.17	0.45
1:A:167:ASP:O	1:A:171:THR:HG23	2.16	0.45
1:B:75:GLU:CB	1:B:94:VAL:HG21	2.45	0.45
1:B:441:PHE:HB3	1:B:448:CYS:HB3	1.98	0.45
1:A:240:PHE:O	1:A:243:HIS:HE1	1.99	0.45
1:A:375:VAL:HB	3:A:601[A]:HEM:HMA2	1.99	0.45
1:A:220:LEU:HD22	1:A:242:LYS:HB3	1.99	0.44
1:A:310:ALA:HB1	3:A:601[A]:HEM:CHD	2.47	0.44
1:B:324:LEU:HD12	1:B:473:PHE:CZ	2.51	0.44
1:A:48:PHE:CZ	1:A:232:PHE:CE2	3.05	0.43
1:A:328:LEU:HD22	1:A:481:LEU:HD11	2.00	0.43
1:A:441:PHE:HB3	1:A:448:CYS:HB3	1.99	0.43
1:B:177:PHE:CZ	1:B:179:PHE:CE2	3.06	0.43
1:A:346:PRO:HB3	1:A:502:HIS:NE2	2.33	0.43
1:A:47:PRO:O	1:A:48:PHE:HB3	2.18	0.43
1:B:140:ALA:CB	1:B:449:LEU:HD11	2.49	0.42
1:A:310:ALA:CB	3:A:601[A]:HEM:CHD	2.97	0.42
1:B:205:THR:HA	1:B:208:GLN:CG	2.49	0.42
1:B:323:ILE:CG2	1:B:496:ILE:CD1	2.92	0.42
1:B:102:GLN:HB3	1:B:105:ILE:HD12	2.01	0.42
1:A:165:PHE:CZ	1:A:169:ILE:HD11	2.55	0.41
1:A:374:ILE:HD12	1:A:374:ILE:N	2.35	0.41
4:A:602:V2H:HAR	4:A:602:V2H:HAEA	2.02	0.41
1:B:132:GLY:HA2	1:B:294:THR:HG21	2.02	0.41
1:B:375:VAL:HG11	3:B:601[B]:HEM:HMD3	2.02	0.41
1:B:318:VAL:HG21	3:B:601[A]:HEM:HBB1	2.01	0.41
1:A:184:THR:HG23	1:A:312:THR:CG2	2.51	0.41
1:A:481:LEU:HD23	1:A:481:LEU:N	2.36	0.41
1:A:447:HIS:O	1:A:448:CYS:C	2.60	0.40
1:B:114:LEU:HD11	1:B:246:LEU:HD22	2.02	0.40
1:A:346:PRO:HB3	1:A:502:HIS:CE1	2.56	0.40
1:A:323:ILE:HG21	1:A:496:ILE:HD12	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	463/479 (97%)	447 (96%)	16 (4%)	0	100	100
1	B	465/479 (97%)	449 (97%)	16 (3%)	0	100	100
All	All	928/958 (97%)	896 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	395/422 (94%)	391 (99%)	4 (1%)	76	90
1	B	393/422 (93%)	387 (98%)	6 (2%)	65	85
All	All	788/844 (93%)	778 (99%)	10 (1%)	69	86

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

Mol	Chain	Res	Type
1	A	116	MET
1	A	214	PHE
1	A	353	ASP
1	A	449	LEU
1	B	214	PHE
1	B	225	SER
1	B	390	ARG
1	B	416	ASP

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Mol	Chain	Res	Type
1	B	449	LEU
1	B	496	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	244	GLN
1	B	245	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](#)

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

5.5 Carbohydrates [i](#)

14 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	GLC	C	1	2	11,11,12	0.71	0	15,15,17	1.60	2 (13%)
2	GLC	C	2	2	11,11,12	0.82	0	15,15,17	1.06	2 (13%)
2	GLC	C	3	2	11,11,12	0.78	0	15,15,17	1.33	3 (20%)
2	GLC	C	4	2	11,11,12	0.37	0	15,15,17	1.63	2 (13%)
2	GLC	C	5	2	11,11,12	0.61	0	15,15,17	2.13	3 (20%)
2	GLC	C	6	2	11,11,12	0.76	0	15,15,17	0.93	0
2	GLC	C	7	2	11,11,12	0.60	0	15,15,17	1.82	4 (26%)
2	GLC	D	1	2	11,11,12	0.70	0	15,15,17	1.80	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	D	2	2	11,11,12	0.73	0	15,15,17	1.44	3 (20%)
2	GLC	D	3	2	11,11,12	0.96	1 (9%)	15,15,17	1.47	2 (13%)
2	GLC	D	4	2	11,11,12	0.54	0	15,15,17	2.16	4 (26%)
2	GLC	D	5	2	11,11,12	0.93	1 (9%)	15,15,17	1.42	1 (6%)
2	GLC	D	6	2	11,11,12	0.95	0	15,15,17	1.83	3 (20%)
2	GLC	D	7	2	11,11,12	0.54	0	15,15,17	1.27	2 (13%)

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	GLC	C	1	2	-	2/2/19/22	0/1/1/1
2	GLC	C	2	2	-	1/2/19/22	0/1/1/1
2	GLC	C	3	2	-	2/2/19/22	0/1/1/1
2	GLC	C	4	2	-	1/2/19/22	0/1/1/1
2	GLC	C	5	2	-	2/2/19/22	0/1/1/1
2	GLC	C	6	2	-	1/2/19/22	0/1/1/1
2	GLC	C	7	2	-	1/2/19/22	0/1/1/1
2	GLC	D	1	2	-	2/2/19/22	0/1/1/1
2	GLC	D	2	2	-	2/2/19/22	0/1/1/1
2	GLC	D	3	2	-	2/2/19/22	0/1/1/1
2	GLC	D	4	2	-	0/2/19/22	0/1/1/1
2	GLC	D	5	2	-	2/2/19/22	0/1/1/1
2	GLC	D	6	2	-	2/2/19/22	0/1/1/1
2	GLC	D	7	2	-	1/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	GLC	C2-C3	2.04	1.55	1.52
2	D	5	GLC	C2-C3	2.01	1.55	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4	GLC	C1-C2-C3	5.83	116.84	109.67
2	C	5	GLC	C1-C2-C3	5.71	116.68	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	GLC	C1-O5-C5	4.04	117.67	112.19
2	C	7	GLC	C3-C4-C5	3.96	117.30	110.24
2	C	4	GLC	C1-O5-C5	3.96	117.56	112.19
2	C	5	GLC	C2-C3-C4	3.83	117.52	110.89
2	D	1	GLC	C3-C4-C5	3.82	117.06	110.24
2	D	2	GLC	C1-C2-C3	3.74	114.27	109.67
2	D	6	GLC	C1-C2-C3	3.74	114.26	109.67
2	D	1	GLC	O4-C4-C3	-3.67	101.86	110.35
2	C	7	GLC	C1-O5-C5	3.49	116.92	112.19
2	D	4	GLC	O5-C5-C6	3.48	112.65	107.20
2	C	4	GLC	C1-C2-C3	3.36	113.79	109.67
2	D	6	GLC	O5-C5-C6	3.29	112.36	107.20
2	C	1	GLC	O4-C4-C3	-3.24	102.85	110.35
2	D	1	GLC	O5-C1-C2	3.18	115.68	110.77
2	C	3	GLC	C1-C2-C3	3.17	113.56	109.67
2	D	4	GLC	O4-C4-C3	-2.84	103.78	110.35
2	D	4	GLC	C2-C3-C4	2.82	115.77	110.89
2	D	7	GLC	C1-O5-C5	2.76	115.93	112.19
2	D	7	GLC	O4-C4-C3	-2.71	104.08	110.35
2	D	5	GLC	C1-O5-C5	2.68	115.82	112.19
2	C	2	GLC	C1-C2-C3	2.58	112.84	109.67
2	C	5	GLC	O5-C5-C6	2.51	111.14	107.20
2	D	2	GLC	O5-C5-C6	2.49	111.11	107.20
2	C	7	GLC	C2-C3-C4	2.46	115.16	110.89
2	C	1	GLC	C3-C4-C5	2.42	114.56	110.24
2	D	2	GLC	C2-C3-C4	2.35	114.95	110.89
2	D	3	GLC	O2-C2-C3	2.30	114.75	110.14
2	C	3	GLC	C2-C3-C4	2.27	114.82	110.89
2	D	6	GLC	C2-C3-C4	2.26	114.81	110.89
2	C	7	GLC	O4-C4-C5	-2.03	104.25	109.30
2	C	3	GLC	C1-O5-C5	2.01	114.92	112.19
2	C	2	GLC	O5-C5-C6	2.00	110.34	107.20

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	GLC	O5-C5-C6-O6
2	D	3	GLC	O5-C5-C6-O6
2	D	5	GLC	O5-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6
2	D	5	GLC	C4-C5-C6-O6

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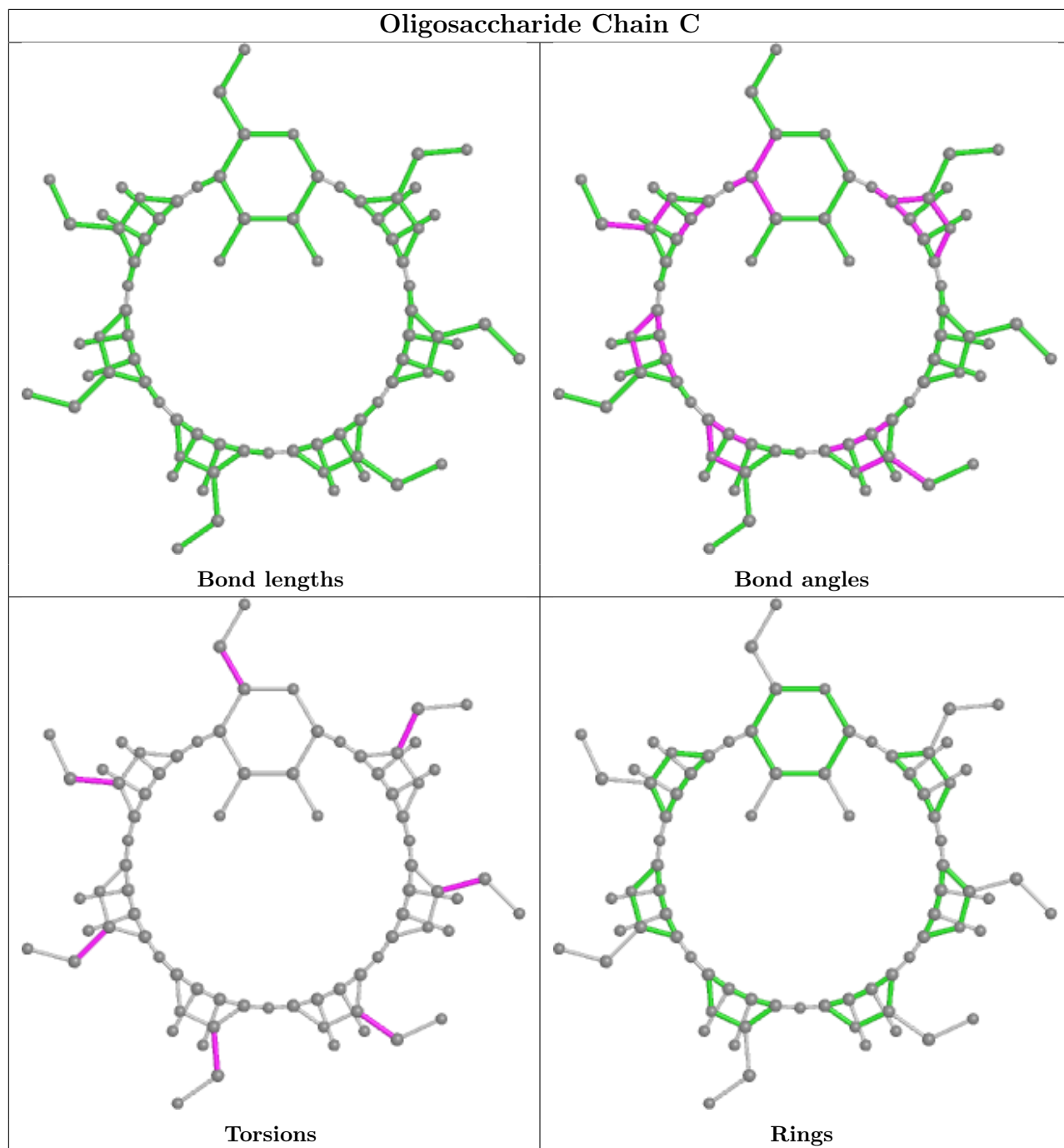
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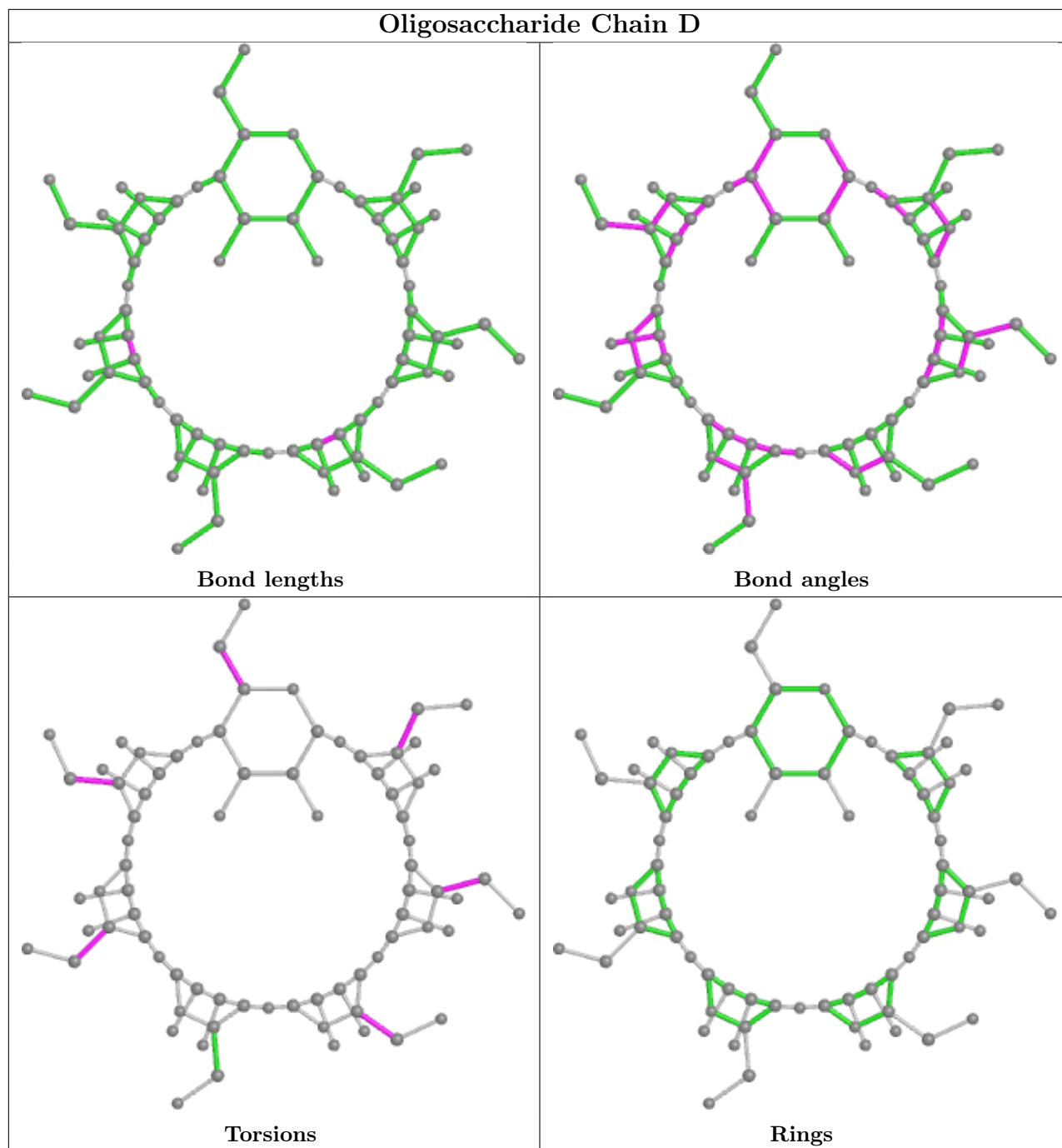
Mol	Chain	Res	Type	Atoms
2	C	3	GLC	O5-C5-C6-O6
2	D	3	GLC	C4-C5-C6-O6
2	D	2	GLC	C4-C5-C6-O6
2	D	1	GLC	C4-C5-C6-O6
2	D	6	GLC	O5-C5-C6-O6
2	C	1	GLC	C4-C5-C6-O6
2	C	6	GLC	O5-C5-C6-O6
2	D	6	GLC	C4-C5-C6-O6
2	D	7	GLC	O5-C5-C6-O6
2	C	7	GLC	O5-C5-C6-O6
2	C	4	GLC	C4-C5-C6-O6
2	D	1	GLC	O5-C5-C6-O6
2	C	2	GLC	O5-C5-C6-O6
2	C	3	GLC	C4-C5-C6-O6
2	C	5	GLC	C4-C5-C6-O6
2	C	5	GLC	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](#)

6 ligands 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	HEM	A	601[B]	1	41,50,50	1.87	7 (17%)	45,82,82	1.65	8 (17%)
3	HEM	A	601[A]	1	41,50,50	1.92	6 (14%)	45,82,82	1.52	7 (15%)
3	HEM	B	601[B]	-	41,50,50	1.90	5 (12%)	45,82,82	1.57	6 (13%)
3	HEM	B	601[A]	1	41,50,50	1.95	6 (14%)	45,82,82	1.58	6 (13%)
4	V2H	B	602	-	31,32,32	0.84	1 (3%)	43,47,47	1.53	7 (16%)
4	V2H	A	602	-	31,32,32	0.75	0	43,47,47	1.38	7 (16%)

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	HEM	A	601[B]	1	-	4/12/54/54	-
3	HEM	A	601[A]	1	-	6/12/54/54	-
3	HEM	B	601[B]	-	-	4/12/54/54	-
3	HEM	B	601[A]	1	-	4/12/54/54	-
4	V2H	B	602	-	-	1/18/62/62	0/3/3/3
4	V2H	A	602	-	-	2/18/62/62	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601[A]	HEM	C3D-C2D	7.76	1.53	1.36
3	B	601[B]	HEM	C3D-C2D	7.56	1.52	1.36
3	B	601[A]	HEM	C3D-C2D	7.39	1.52	1.36
3	A	601[B]	HEM	C3D-C2D	7.27	1.52	1.36
3	B	601[B]	HEM	C3C-C2C	-4.58	1.34	1.40
3	A	601[A]	HEM	C3C-C2C	-4.41	1.34	1.40
3	B	601[A]	HEM	C3C-C2C	-4.37	1.34	1.40
3	B	601[A]	HEM	FE-NB	4.32	2.18	1.96
3	A	601[B]	HEM	C3C-C2C	-4.28	1.34	1.40
3	A	601[B]	HEM	C3C-CAC	3.59	1.55	1.47
3	B	601[A]	HEM	C3C-CAC	3.54	1.55	1.47
3	B	601[B]	HEM	C3C-CAC	3.43	1.54	1.47
3	A	601[A]	HEM	C3C-CAC	3.42	1.54	1.47
3	B	601[B]	HEM	FE-ND	3.00	2.11	1.96
3	A	601[B]	HEM	CAB-C3B	2.97	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601[A]	HEM	CAB-C3B	2.86	1.55	1.47
3	B	601[B]	HEM	CAB-C3B	2.81	1.55	1.47
3	B	601[A]	HEM	CAB-C3B	2.63	1.54	1.47
4	B	602	V2H	CBC-CBA	-2.56	1.51	1.56
3	B	601[A]	HEM	CAA-C2A	2.50	1.55	1.52
3	A	601[A]	HEM	CAA-C2A	2.36	1.55	1.52
3	A	601[B]	HEM	FE-ND	2.35	2.08	1.96
3	A	601[B]	HEM	CMB-C2B	2.20	1.55	1.50
3	A	601[B]	HEM	CMD-C2D	2.12	1.55	1.50
3	A	601[A]	HEM	CMD-C2D	2.02	1.55	1.50

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601[B]	HEM	C4D-ND-C1D	5.83	111.10	105.07
3	A	601[A]	HEM	C4D-ND-C1D	5.74	111.00	105.07
3	A	601[B]	HEM	C4D-ND-C1D	5.52	110.78	105.07
3	B	601[A]	HEM	C4D-ND-C1D	5.52	110.77	105.07
4	A	602	V2H	CAZ-CAO-CAN	4.45	115.82	111.12
4	B	602	V2H	CAH-CAI-CAV	-3.74	120.56	126.20
4	B	602	V2H	CAM-CAV-CAI	-3.68	121.08	125.26
4	B	602	V2H	CAR-CBC-CBB	-3.16	111.84	116.57
3	A	601[B]	HEM	C4C-CHD-C1D	3.11	126.66	122.56
3	A	601[B]	HEM	CAD-CBD-CGD	-3.09	106.96	113.60
3	A	601[B]	HEM	CBA-CAA-C2A	-3.05	107.42	112.62
3	B	601[A]	HEM	CHA-C4D-ND	2.90	127.97	124.38
4	B	602	V2H	CAZ-CAO-CAN	2.83	114.11	111.12
4	B	602	V2H	CAR-CAL-CAM	2.83	117.69	111.38
4	B	602	V2H	CAP-CBA-CAV	-2.64	117.45	120.63
3	B	601[B]	HEM	C4B-CHC-C1C	2.61	126.00	122.56
4	B	602	V2H	CAL-CAM-CAV	2.58	117.74	111.83
3	B	601[B]	HEM	CAD-CBD-CGD	-2.57	108.07	113.60
3	A	601[B]	HEM	C4B-CHC-C1C	2.53	125.89	122.56
3	B	601[A]	HEM	CBD-CAD-C3D	-2.52	105.62	112.63
3	B	601[A]	HEM	C1D-C2D-C3D	-2.46	104.37	106.96
4	A	602	V2H	CAH-CAI-CAV	-2.43	122.53	126.20
4	A	602	V2H	CAM-CAV-CAI	-2.40	122.54	125.26
3	B	601[A]	HEM	C4B-CHC-C1C	2.35	125.66	122.56
3	A	601[A]	HEM	C4C-CHD-C1D	2.31	125.61	122.56
3	B	601[B]	HEM	C1B-NB-C4B	2.28	107.43	105.07
3	A	601[B]	HEM	CAD-C3D-C4D	2.27	128.62	124.66
4	A	602	V2H	CAR-CBC-CBB	-2.26	113.19	116.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	V2H	CAP-CBA-CBC	-2.23	102.22	104.21
3	A	601[A]	HEM	C4A-C3A-C2A	2.23	108.55	107.00
4	A	602	V2H	CAL-CAR-CBC	-2.17	110.47	113.17
3	A	601[A]	HEM	C1D-C2D-C3D	-2.16	104.69	106.96
3	A	601[A]	HEM	C1B-NB-C4B	2.15	107.29	105.07
3	A	601[A]	HEM	CAA-CBA-CGA	-2.10	107.86	113.76
3	A	601[B]	HEM	CHD-C1D-ND	2.10	126.71	124.43
3	B	601[B]	HEM	CAD-C3D-C4D	2.07	128.27	124.66
3	A	601[A]	HEM	C4B-CHC-C1C	2.06	125.28	122.56
3	A	601[B]	HEM	CMD-C2D-C1D	2.04	128.15	125.04
3	B	601[B]	HEM	CMD-C2D-C1D	2.04	128.14	125.04
4	A	602	V2H	CAR-CAL-CAM	2.04	115.93	111.38
3	B	601[A]	HEM	C4A-C3A-C2A	2.02	108.40	107.00

There are no chirality outliers.

All (21) torsion outliers are listed below:

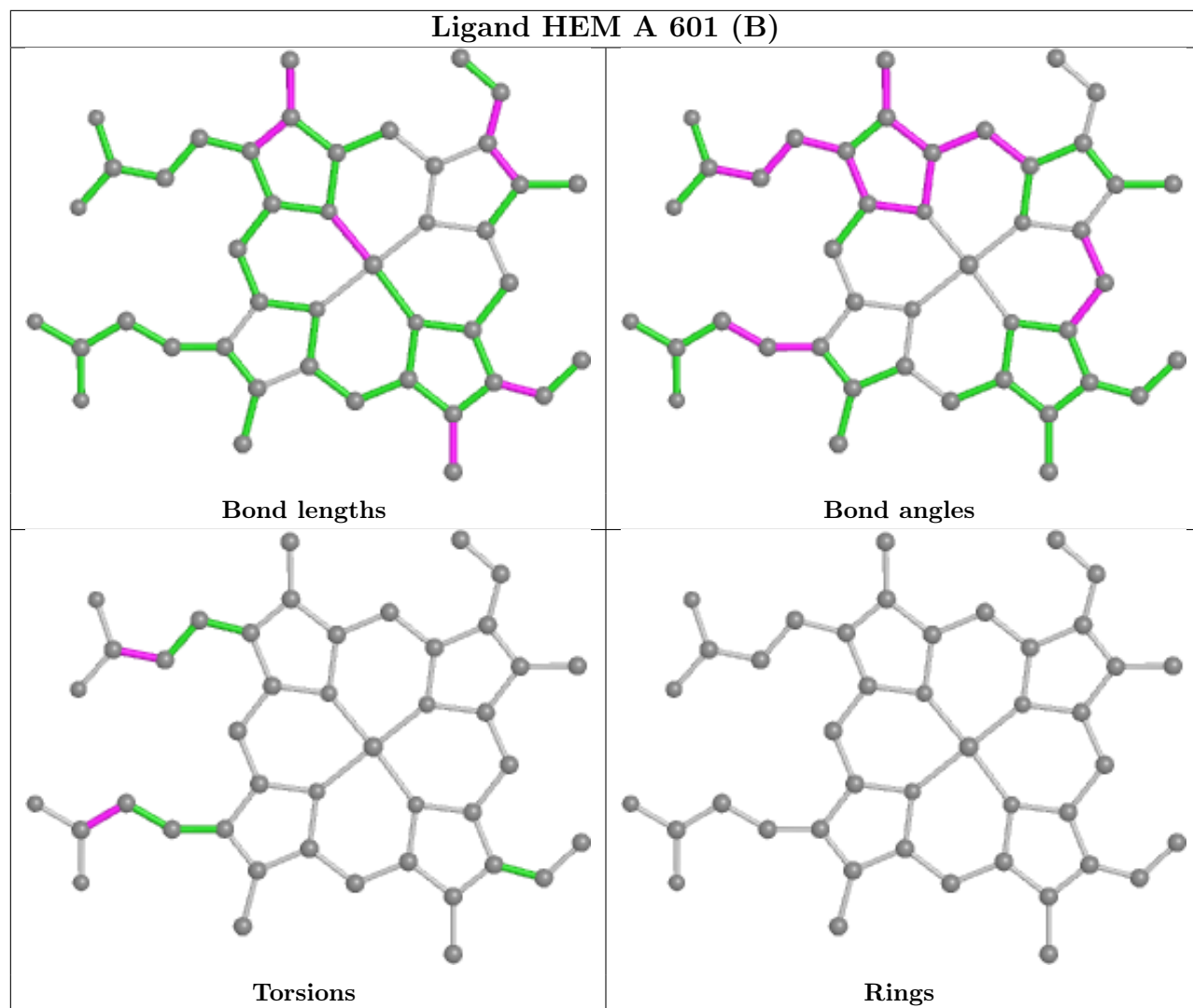
Mol	Chain	Res	Type	Atoms
3	A	601[A]	HEM	C1A-C2A-CAA-CBA
3	A	601[A]	HEM	C3A-C2A-CAA-CBA
3	B	601[A]	HEM	C1A-C2A-CAA-CBA
3	B	601[A]	HEM	C3A-C2A-CAA-CBA
4	A	602	V2H	CAJ-CAK-CAY-CBB
4	B	602	V2H	CAJ-CAK-CAY-CBB
3	A	601[A]	HEM	CAA-CBA-CGA-O2A
3	A	601[A]	HEM	CAA-CBA-CGA-O1A
3	B	601[A]	HEM	CAA-CBA-CGA-O1A
3	A	601[A]	HEM	CAD-CBD-CGD-O2D
3	B	601[A]	HEM	CAA-CBA-CGA-O2A
3	A	601[B]	HEM	CAD-CBD-CGD-O2D
3	A	601[A]	HEM	CAD-CBD-CGD-O1D
3	B	601[B]	HEM	CAD-CBD-CGD-O2D
3	B	601[B]	HEM	CAD-CBD-CGD-O1D
3	A	601[B]	HEM	CAA-CBA-CGA-O1A
3	A	601[B]	HEM	CAD-CBD-CGD-O1D
3	B	601[B]	HEM	CAA-CBA-CGA-O2A
3	A	601[B]	HEM	CAA-CBA-CGA-O2A
3	B	601[B]	HEM	CAA-CBA-CGA-O1A
4	A	602	V2H	CAJ-CAK-CAY-CAE

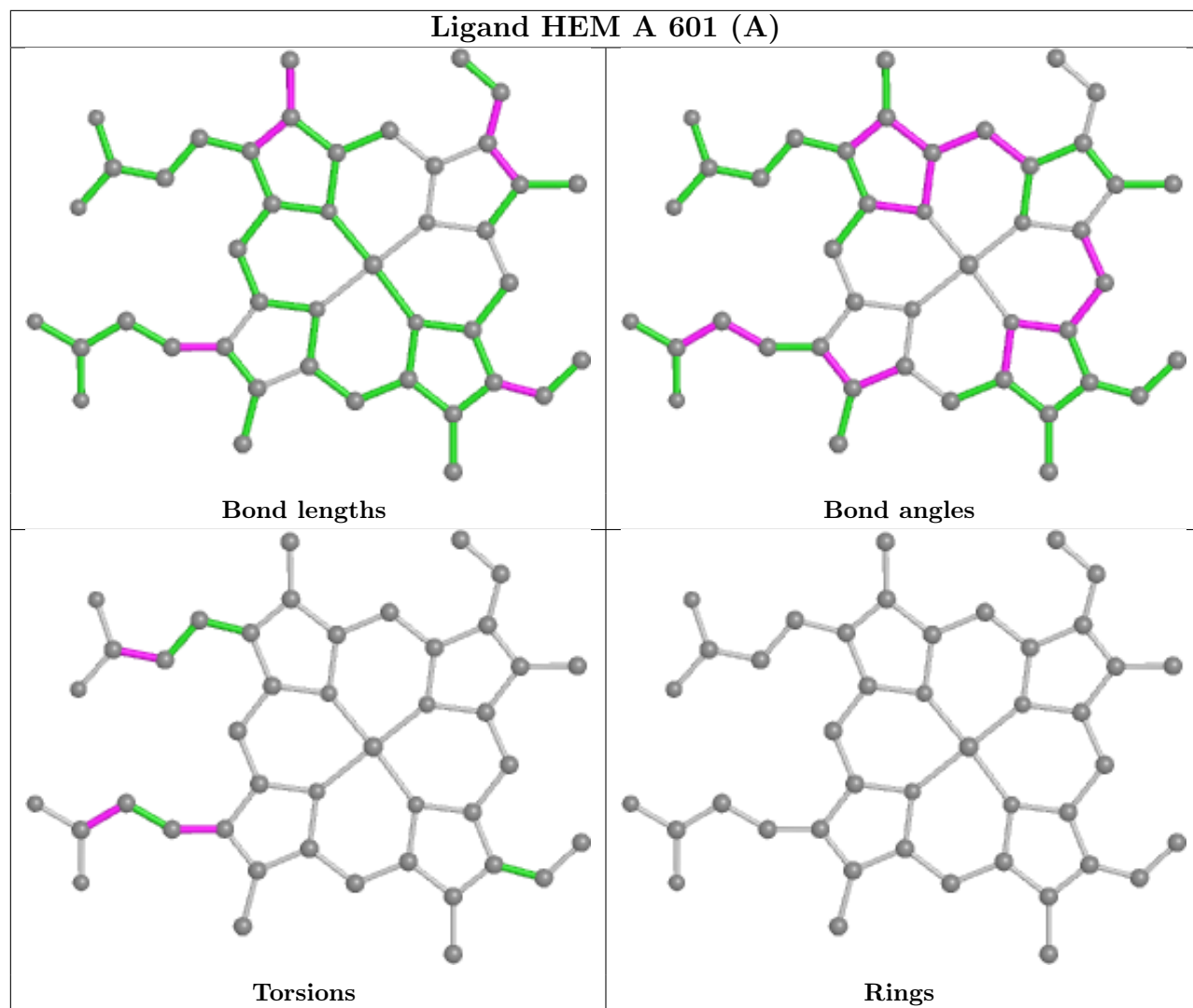
There are no ring outliers.

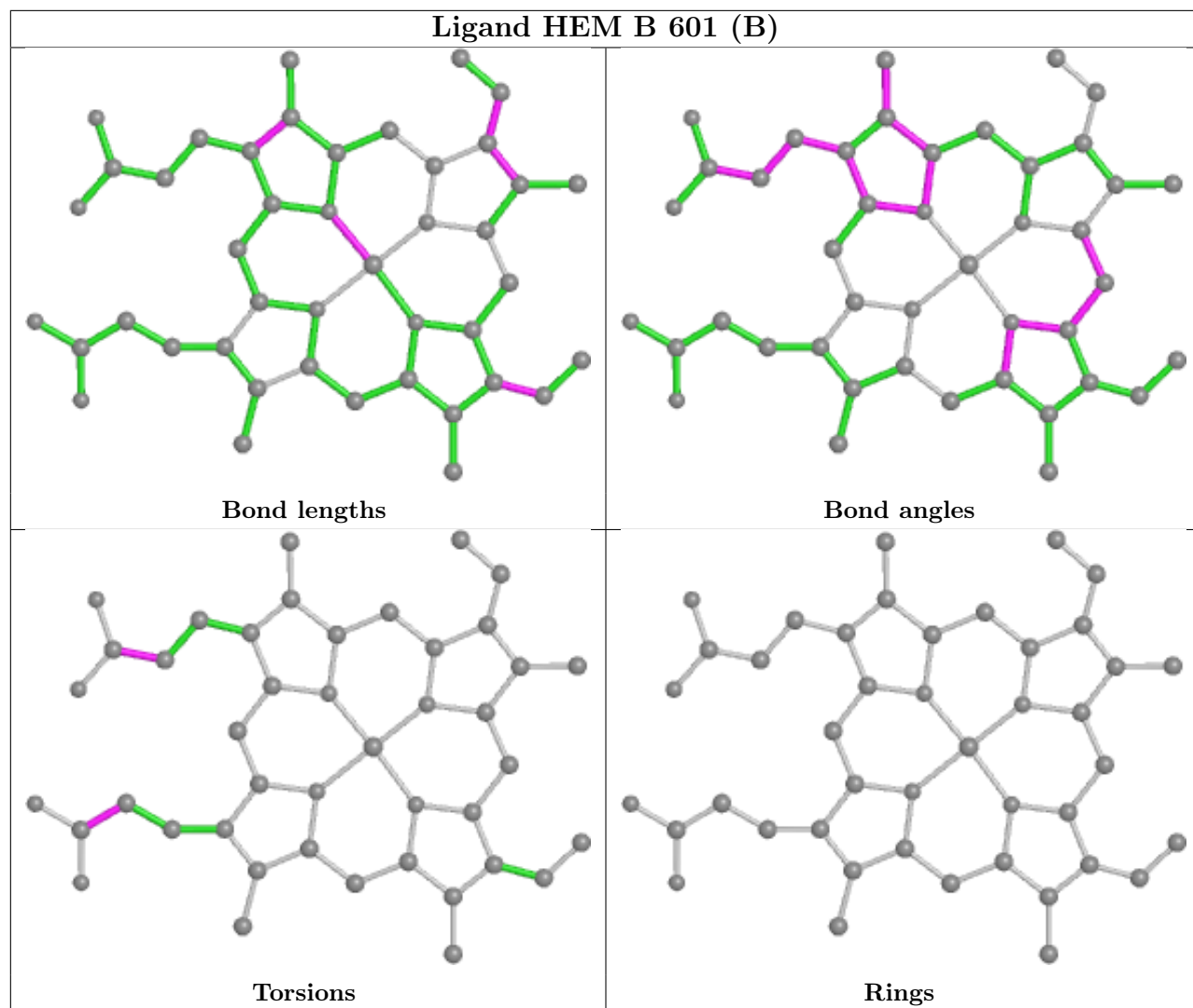
6 monomers are involved in 31 short contacts:

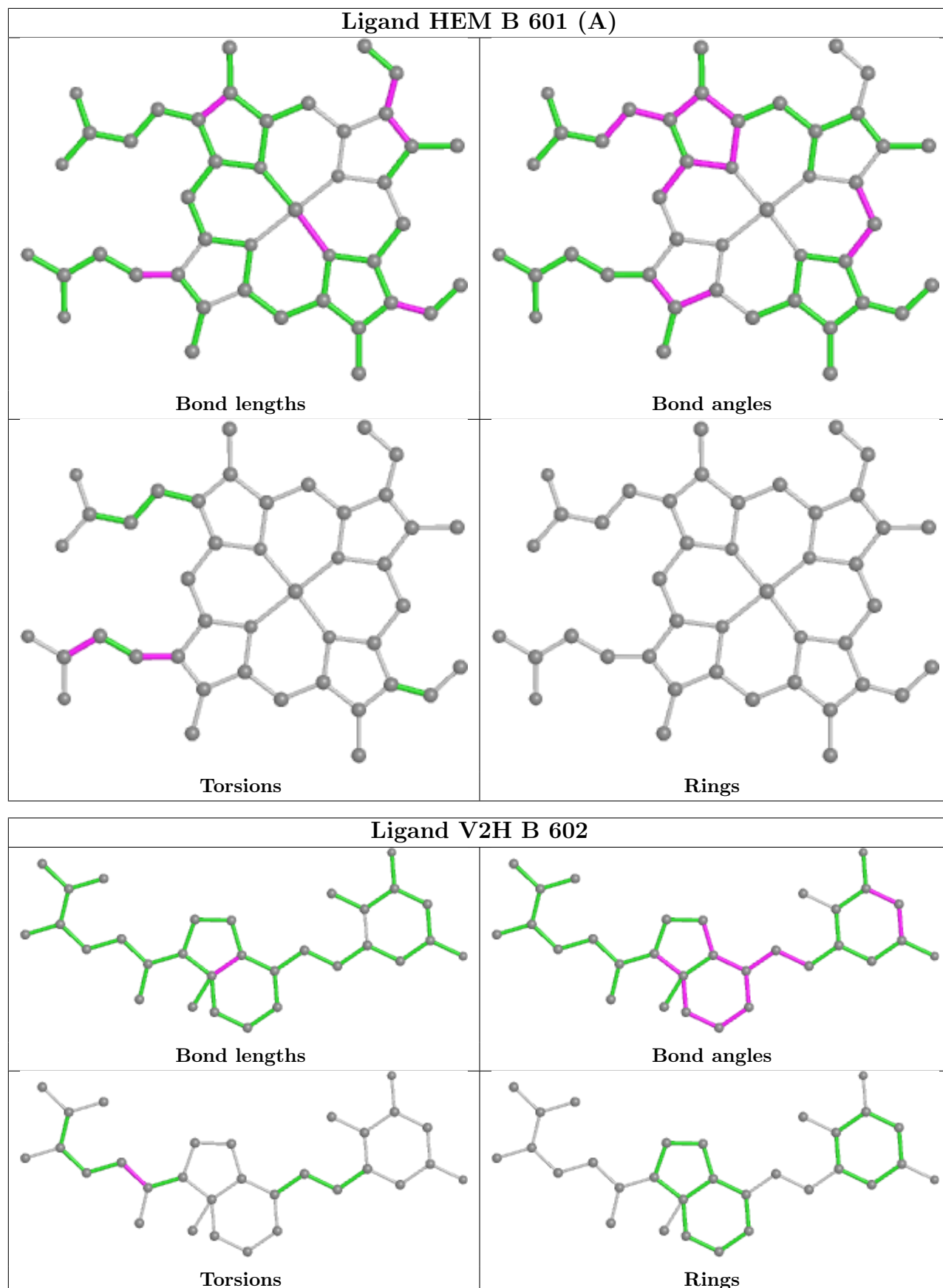
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601[B]	HEM	8	0
3	A	601[A]	HEM	8	0
3	B	601[B]	HEM	6	0
3	B	601[A]	HEM	7	0
4	B	602	V2H	1	0
4	A	602	V2H	1	0

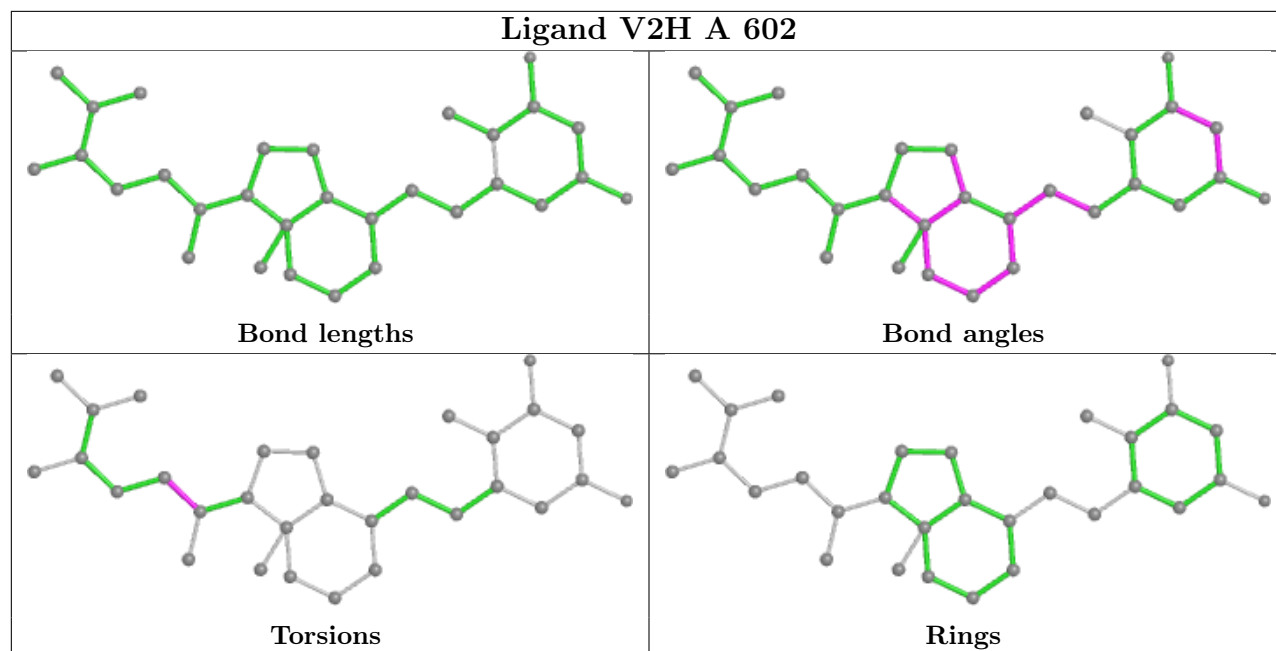
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.











5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	465/479 (97%)	-0.30	10 (2%) 62 63	24, 38, 59, 81	0
1	B	467/479 (97%)	-0.16	7 (1%) 73 76	30, 45, 65, 80	0
All	All	932/958 (97%)	-0.23	17 (1%) 68 70	24, 41, 64, 81	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	502	HIS	5.5
1	B	289	ASN	4.5
1	B	505	HIS	4.4
1	A	291	PRO	4.3
1	B	428	SER	3.2
1	A	289	ASN	3.1
1	B	429	SER	3.0
1	A	346	PRO	2.8
1	A	476	GLU	2.5
1	B	291	PRO	2.4
1	A	59	SER	2.4
1	A	288	LYS	2.4
1	A	478	VAL	2.3
1	B	431	TYR	2.3
1	B	477	LEU	2.2
1	A	57	ALA	2.2
1	A	272	LEU	2.0

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

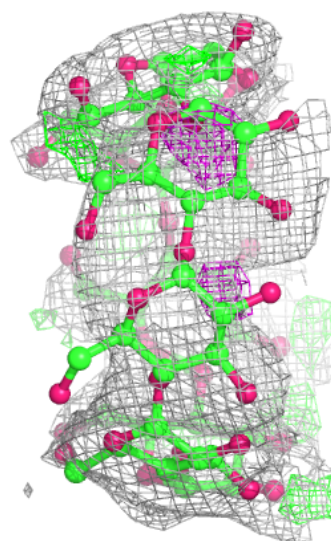
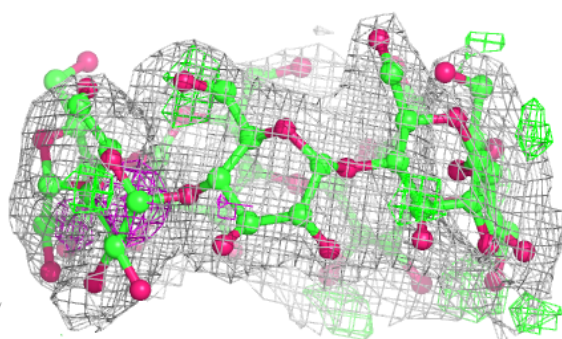
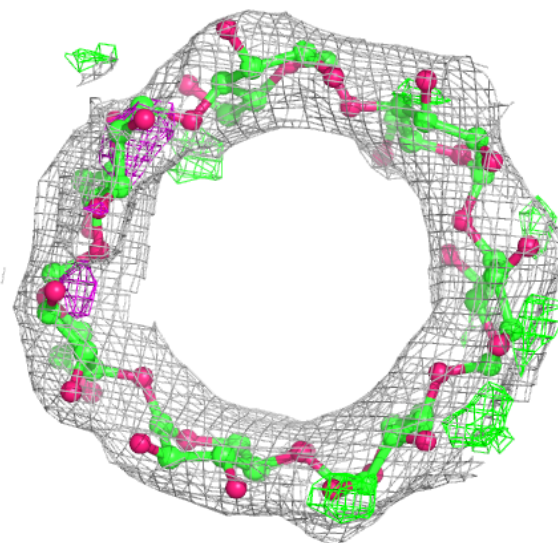
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

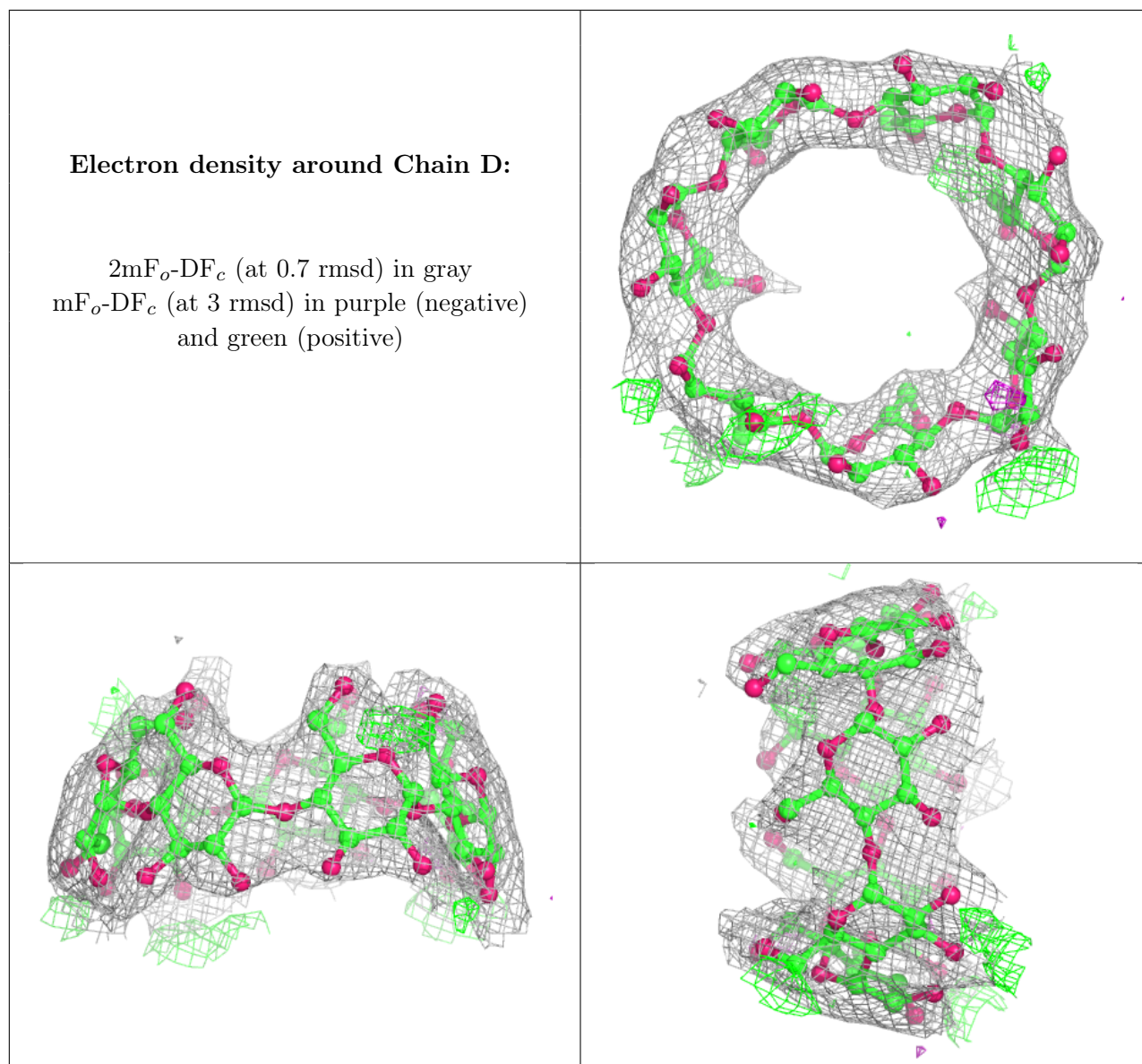
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	C	7	11/12	0.76	0.35	91,93,94,94	0
2	GLC	C	2	11/12	0.78	0.20	87,89,89,90	0
2	GLC	C	6	11/12	0.81	0.41	93,94,94,94	0
2	GLC	C	3	11/12	0.82	0.25	87,88,90,90	0
2	GLC	D	6	11/12	0.82	0.28	69,71,73,73	0
2	GLC	D	3	11/12	0.85	0.17	65,67,68,69	0
2	GLC	D	5	11/12	0.87	0.27	68,69,69,70	0
2	GLC	C	4	11/12	0.87	0.21	83,85,86,86	0
2	GLC	C	5	11/12	0.88	0.20	87,87,89,92	0
2	GLC	C	1	11/12	0.89	0.25	89,89,90,90	0
2	GLC	D	2	11/12	0.91	0.23	70,71,72,72	0
2	GLC	D	1	11/12	0.91	0.28	72,73,73,74	0
2	GLC	D	4	11/12	0.92	0.16	64,67,68,68	0
2	GLC	D	7	11/12	0.93	0.25	71,72,73,73	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 C:

$2mF_o-DF_c$ (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.

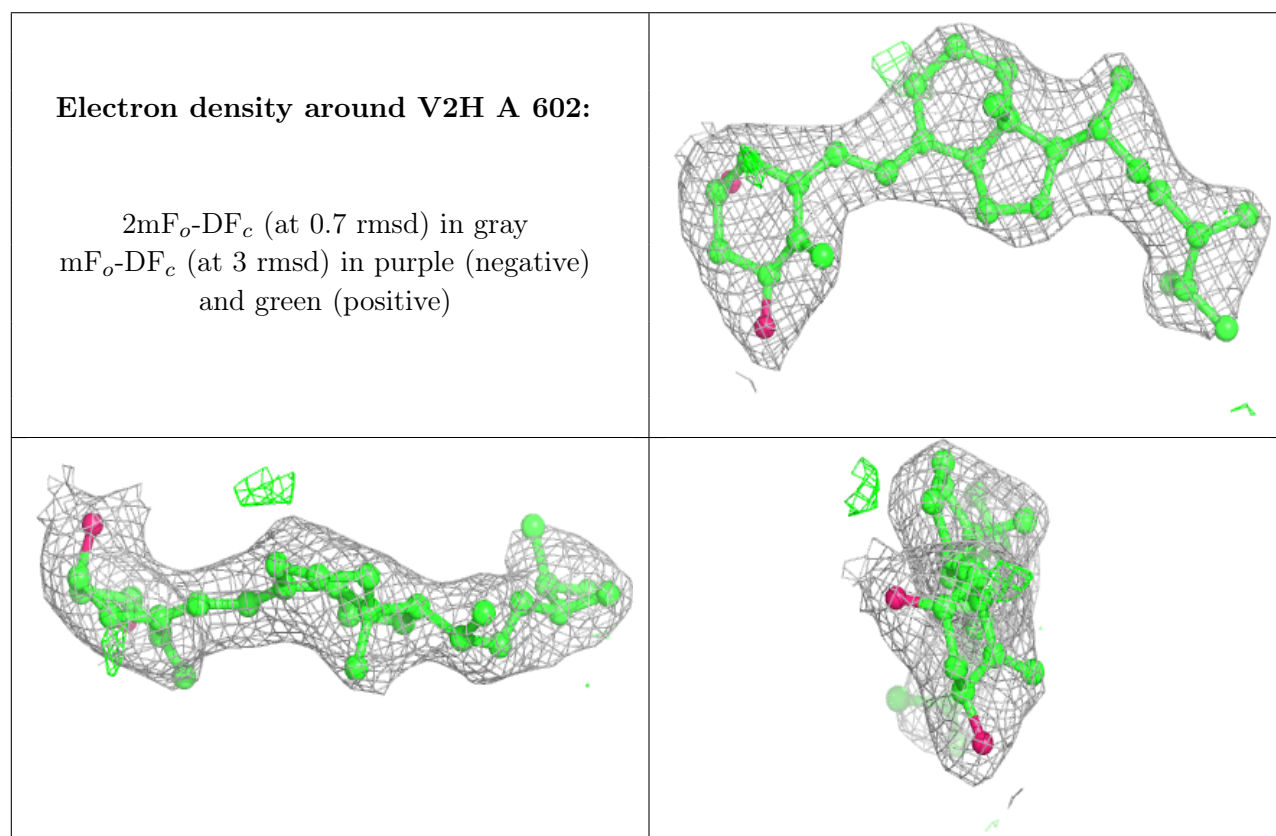
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	V2H	A	602	30/30	0.97	0.20	36,39,41,41	0
3	HEM	B	601[B]	43/43	0.98	0.20	29,31,33,33	43
3	HEM	B	601[A]	43/43	0.98	0.20	24,26,29,30	43
4	V2H	B	602	30/30	0.98	0.17	34,36,41,42	0
3	HEM	A	601[A]	43/43	0.99	0.15	27,30,30,31	43

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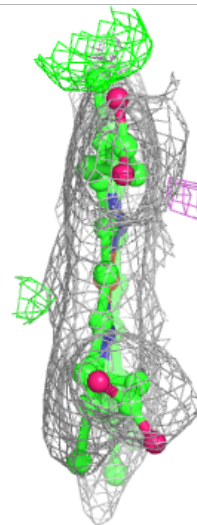
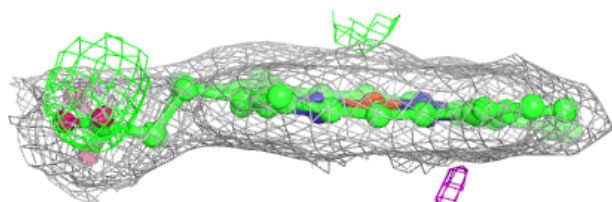
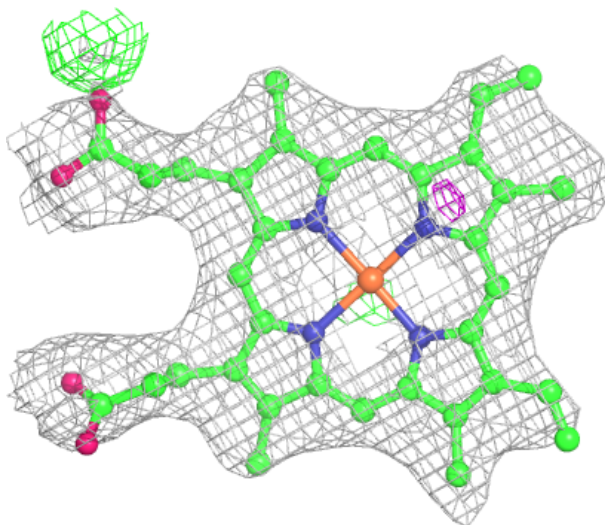
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	HEM	A	601[B]	43/43	0.99	0.15	23,27,29,31	43

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.



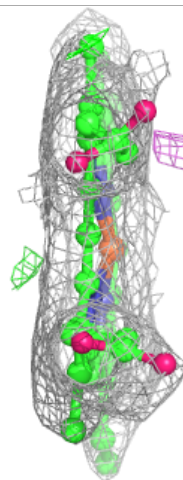
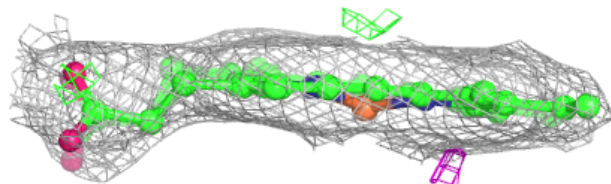
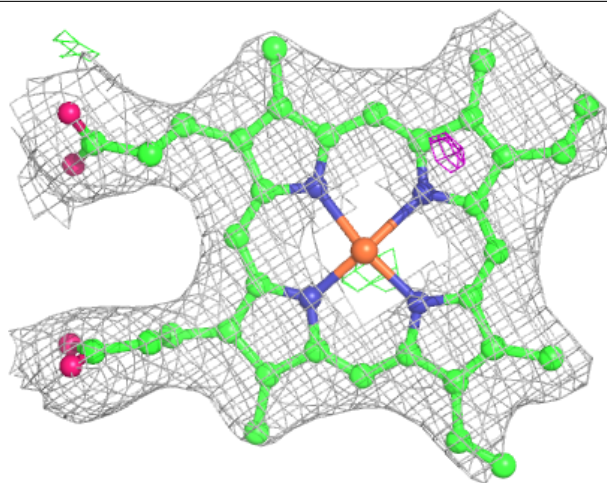
Electron density around HEM B 601 (B):

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



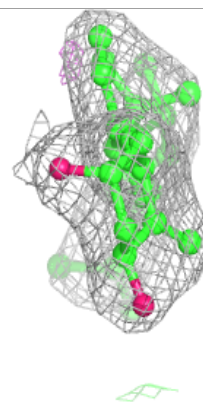
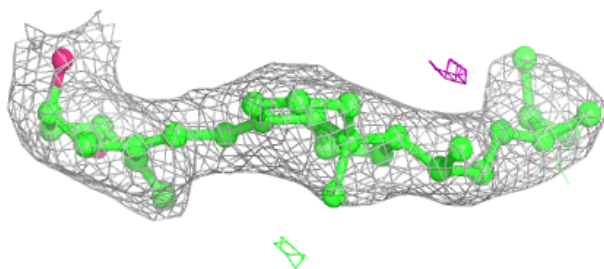
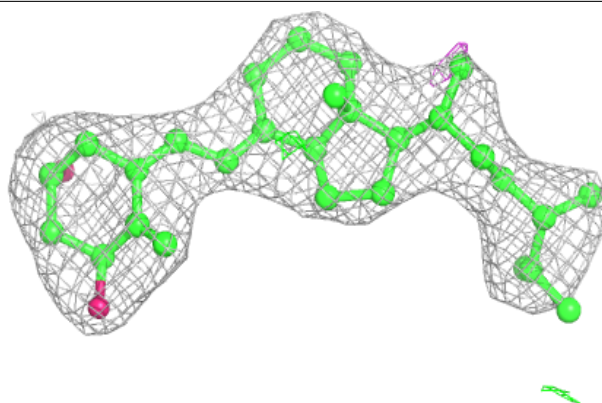
Electron density around HEM B 601 (A):

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

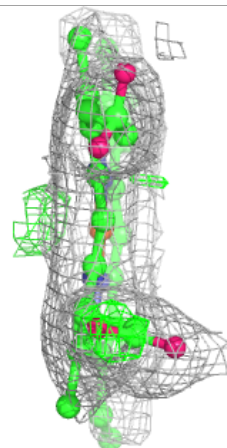
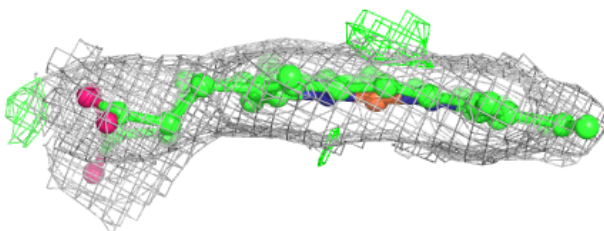
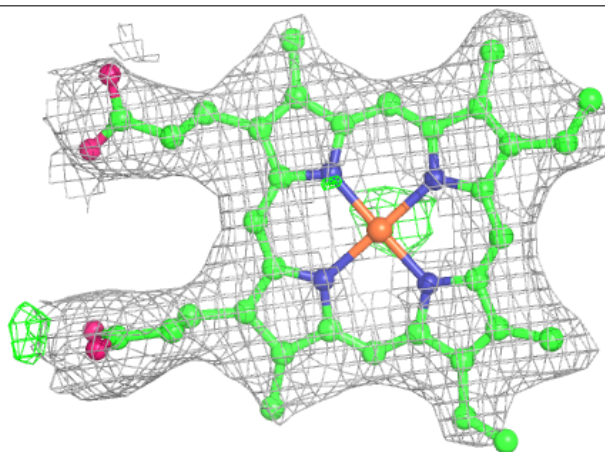


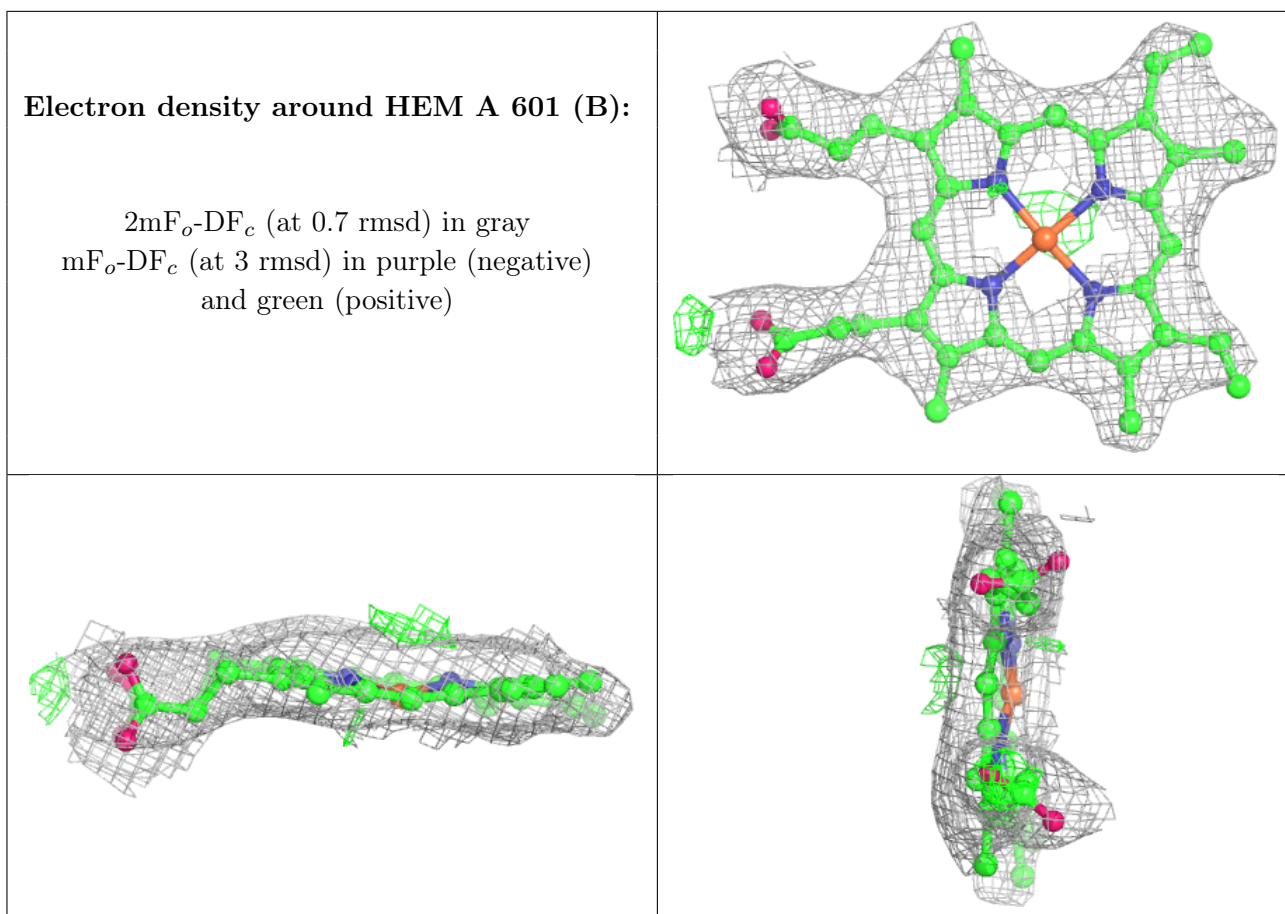
Electron density around V2H B 602:

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

**Electron density around HEM A 601 (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.