Full wwPDB X-ray Structure Validation Report (i)

Aug 28, 2023 – 02:21 AM EDT

PDB ID	:	3JUS
Title	:	Crystal structure of human lanosterol 14alpha-demethylase (CYP51) in complex with econazole
Authors	:	Strushkevich, N.; MacKenzie, F.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Weigelt, J.; Usanov, S.A.; Park, H.; Structural Genomics Consortium (SGC)
Deposited on	:	2009-09-15
Resolution	:	2.90 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 (i) 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 (1)) were used in the production of this report:

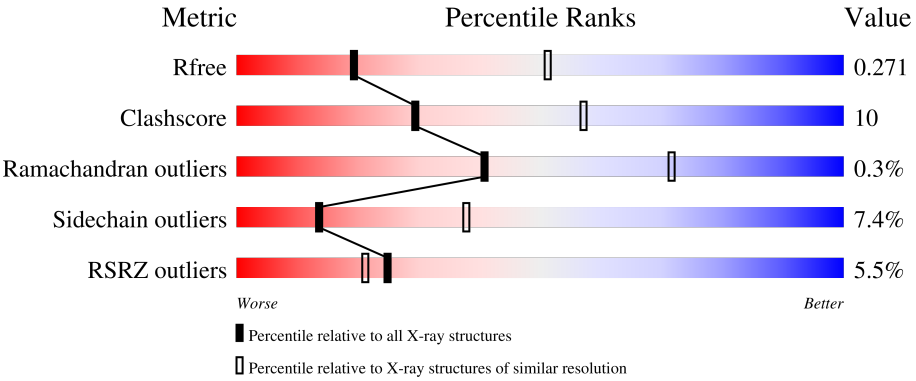
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	461	4% 76% 18%
1	B	461	7% 73% 21%
2	C	7	71% 29%
2	D	7	100%

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	ECN	A	602[A]	-	-	X	-
5	ECN	B	602[A]	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7553 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.

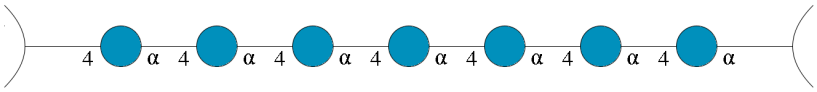
- Molecule 1 is a protein called Lanosterol 14-alpha demethylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3589	2310	611	652	16			
1	B	445	Total	C	N	O	S	0	0	0
			3589	2310	611	652	16			

There are 24 discrepancies between the modelled and reference sequences:

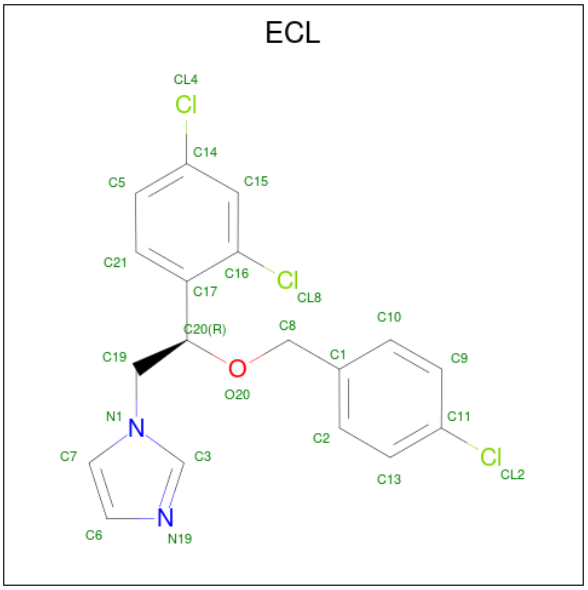
Chain	Residue	Modelled	Actual	Comment	Reference
A	49	MET	-	expression tag	UNP Q16850
A	50	ALA	-	expression tag	UNP Q16850
A	51	LYS	-	expression tag	UNP Q16850
A	52	LYS	-	expression tag	UNP Q16850
A	53	THR	-	expression tag	UNP Q16850
A	503	THR	-	expression tag	UNP Q16850
A	504	HIS	-	expression tag	UNP Q16850
A	505	HIS	-	expression tag	UNP Q16850
A	506	HIS	-	expression tag	UNP Q16850
A	507	HIS	-	expression tag	UNP Q16850
A	508	HIS	-	expression tag	UNP Q16850
A	509	HIS	-	expression tag	UNP Q16850
B	49	MET	-	expression tag	UNP Q16850
B	50	ALA	-	expression tag	UNP Q16850
B	51	LYS	-	expression tag	UNP Q16850
B	52	LYS	-	expression tag	UNP Q16850
B	53	THR	-	expression tag	UNP Q16850
B	503	THR	-	expression tag	UNP Q16850
B	504	HIS	-	expression tag	UNP Q16850
B	505	HIS	-	expression tag	UNP Q16850
B	506	HIS	-	expression tag	UNP Q16850
B	507	HIS	-	expression tag	UNP Q16850
B	508	HIS	-	expression tag	UNP Q16850
B	509	HIS	-	expression tag	UNP Q16850

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



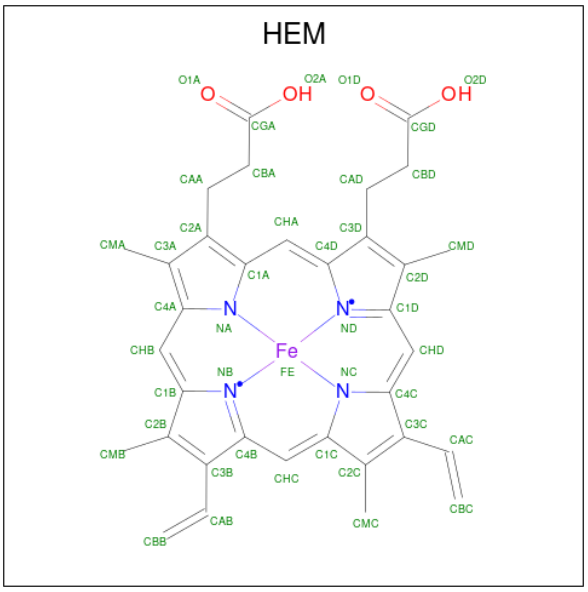
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	C	7	Total C O 77 42 35	0	0	0
2	D	7	Total C O 77 42 35	0	0	0

- Molecule 3 is 1-[(2R)-2-[(4-chlorobenzyl)oxy]-2-(2,4-dichlorophenyl)ethyl]-1H-imidazole (three-letter code: ECL) (formula: $C_{18}H_{15}Cl_3N_2O$).



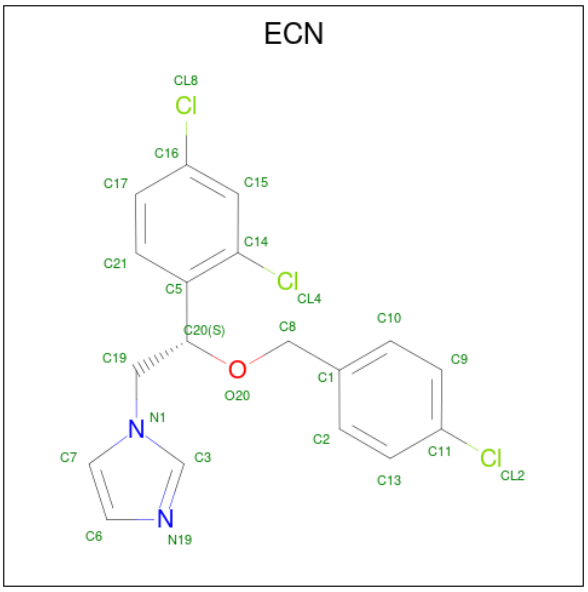
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C Cl N O 24 18 3 2 1	0	1
3	B	1	Total C Cl N O 24 18 3 2 1	0	1

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 5 is 1-[(2S)-2-[(4-CHLOROBENZYL)OXY]-2-(2,4-DICHLOROPHENYL)ETHYL]-1H-IMIDAZOLE (three-letter code: ECN) (formula: $C_{18}H_{15}Cl_3N_2O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	0	1
			24	18	3	2	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	Cl	N	O	0	1
			24	18	3	2	1		

- Molecule 6 is water.

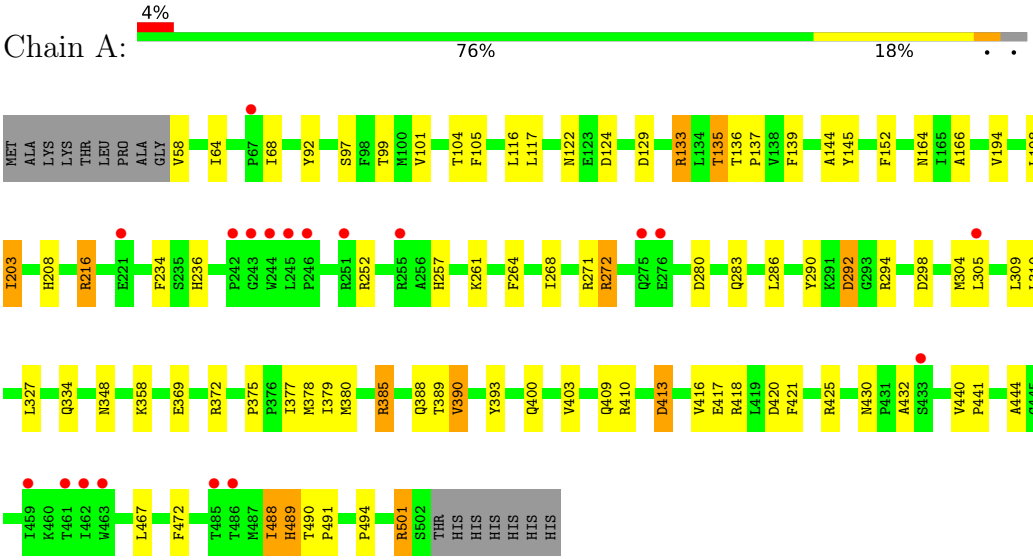
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	29	Total	O	0	0
			29	29		
6	B	10	Total	O	0	0
			10	10		

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.

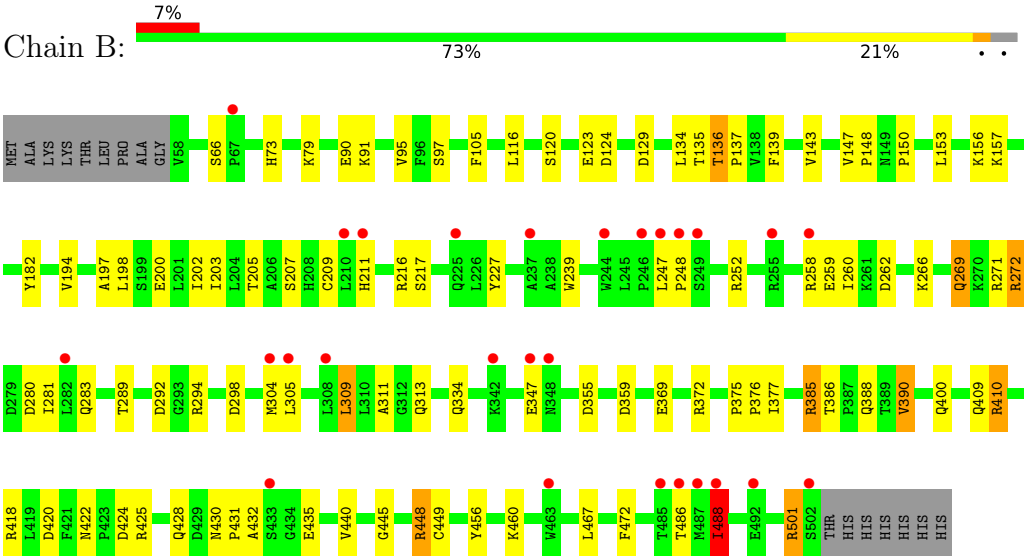
• Molecule 1: Lanosterol 14-alpha demethylase

Chain A:



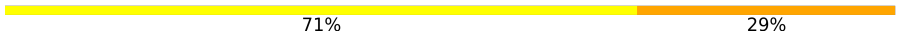
• Molecule 1: Lanosterol 14-alpha demethylase

Chain B:



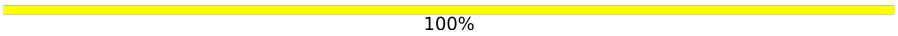
• Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)

Chain C:



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

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	146.63Å 146.63Å 110.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.52 – 2.90 24.50 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.2 (24.52-2.90) 99.2 (24.50-2.89)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	4.17 (at 2.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.203 , 0.272 0.203 , 0.271	Depositor DCC
R_{free} test set	1373 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	66.4	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7553	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ECL, HEM, ECN, GLC

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	0.48	0/3682	0.59	0/4988
1	B	0.45	0/3682	0.58	0/4988
All	All	0.47	0/7364	0.59	0/9976

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3589	0	3581	66	0
1	B	3589	0	3581	58	0
2	C	77	0	63	1	0
2	D	77	0	63	0	0
3	A	24	0	15	0	0
3	B	24	0	15	1	0
4	A	43	0	30	7	0
4	B	43	0	30	6	0
5	A	24	0	15	8	0
5	B	24	0	15	7	0
6	A	29	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	10	0	0	2	0
All	All	7553	0	7408	142	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 10.

All (142) 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)
5:A:602[A]:ECN:H8C1	5:A:602[A]:ECN:C3	1.49	1.40
5:B:602[A]:ECN:H8C1	5:B:602[A]:ECN:C3	1.65	1.25
5:A:602[A]:ECN:C3	5:A:602[A]:ECN:C8	2.39	1.01
5:A:602[A]:ECN:H8C1	5:A:602[A]:ECN:N1	1.71	0.93
1:B:334:GLN:HE22	1:B:472:PHE:H	1.23	0.86
1:A:409:GLN:HE21	1:A:440:VAL:H	1.24	0.85
5:B:602[A]:ECN:H8C1	5:B:602[A]:ECN:H3	1.57	0.83
5:A:602[A]:ECN:H8C1	5:A:602[A]:ECN:H3	1.63	0.81
5:B:602[A]:ECN:C3	5:B:602[A]:ECN:C8	2.56	0.79
1:B:409:GLN:HE21	1:B:440:VAL:H	1.32	0.77
1:A:198:LEU:O	1:A:202:ILE:HG12	1.86	0.76
5:B:602[A]:ECN:CL4	5:B:602[A]:ECN:H191	2.24	0.74
1:B:124:ASP:HB3	1:B:388:GLN:NE2	2.03	0.73
1:B:200:GLU:O	1:B:203:ILE:HG22	1.89	0.73
1:A:124:ASP:HB3	1:A:388:GLN:HE21	1.53	0.71
1:A:416:VAL:O	1:A:425:ARG:NH2	2.24	0.70
1:A:372:ARG:NH2	1:A:418:ARG:O	2.20	0.69
1:B:309:LEU:O	1:B:313:GLN:HB2	1.93	0.69
5:B:602[A]:ECN:H8C1	5:B:602[A]:ECN:N1	2.05	0.66
1:B:271:ARG:HD3	1:B:283:GLN:OE1	1.96	0.66
4:B:601:HEM:HBB2	4:B:601:HEM:HMB2	1.79	0.64
1:A:430:ASN:ND2	1:A:432:ALA:HB3	2.12	0.64
1:B:372:ARG:NH2	1:B:418:ARG:O	2.27	0.64
1:A:334:GLN:HE22	1:A:472:PHE:H	1.46	0.64
1:A:467:LEU:O	1:A:501:ARG:HD2	1.98	0.63
5:B:602[A]:ECN:H3	5:B:602[A]:ECN:C8	2.22	0.63
1:B:116:LEU:HB2	1:B:390:VAL:HG21	1.81	0.63
1:A:271:ARG:HD3	1:A:283:GLN:OE1	1.99	0.62
1:A:257:HIS:CE1	1:A:261:LYS:HE3	2.34	0.62
1:B:269:GLN:HA	1:B:272:ARG:HB2	1.80	0.62
1:A:124:ASP:HB3	1:A:388:GLN:NE2	2.16	0.60
1:A:292:ASP:HB3	1:A:294:ARG:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:ARG:O	1:B:410:ARG:HG2	2.00	0.60
1:B:292:ASP:HB3	1:B:294:ARG:H	1.66	0.60
1:B:430:ASN:ND2	1:B:432:ALA:HB3	2.18	0.59
1:B:456:TYR:O	1:B:460:LYS:HB2	2.03	0.59
1:A:117:LEU:HD13	1:A:403:VAL:HG23	1.85	0.58
5:A:602[A]:ECN:C8	5:A:602[A]:ECN:H3	2.23	0.58
1:B:422:ASN:HD21	1:B:424:ASP:HB2	1.69	0.58
1:A:272:ARG:NH1	1:A:298:ASP:OD1	2.37	0.58
1:A:309:LEU:O	1:A:313:GLN:HB2	2.04	0.58
1:B:449:CYS:HA	4:B:601:HEM:C4D	2.40	0.57
1:B:416:VAL:O	1:B:425:ARG:NH2	2.38	0.57
1:A:116:LEU:HB2	1:A:390:VAL:HG21	1.87	0.56
1:A:234:PHE:CE2	5:A:602[A]:ECN:H17	2.40	0.56
1:B:135:THR:HG23	1:B:139:PHE:CD1	2.41	0.56
1:B:334:GLN:NE2	1:B:472:PHE:H	1.99	0.56
1:A:99:THR:HG22	1:A:104:THR:OG1	2.06	0.56
1:B:409:GLN:NE2	1:B:440:VAL:H	2.02	0.56
1:A:135:THR:HG21	1:A:145:TYR:HD1	1.70	0.55
1:A:271:ARG:HH12	1:A:280:ASP:CG	2.09	0.55
1:A:264:PHE:HE2	1:A:305:LEU:HB3	1.71	0.55
1:A:271:ARG:NH1	1:A:280:ASP:OD1	2.38	0.55
1:B:377:ILE:HD12	4:B:601:HEM:C4A	2.42	0.55
1:A:116:LEU:HB2	1:A:390:VAL:CG2	2.36	0.55
5:B:602[A]:ECN:CL4	5:B:602[A]:ECN:O20	2.62	0.55
1:B:227:TYR:CE2	1:B:309:LEU:HD22	2.43	0.54
1:B:430:ASN:HD22	1:B:432:ALA:HB3	1.72	0.54
1:B:150:PRO:HA	1:B:153:LEU:HD12	1.90	0.54
1:B:135:THR:HG22	6:B:2:HOH:O	2.08	0.54
1:B:129:ASP:OD2	1:B:385:ARG:HD3	2.08	0.54
1:A:290:TYR:HB2	1:A:292:ASP:HB2	1.90	0.53
1:B:278:ILE:O	1:B:283:GLN:HG2	2.08	0.53
1:A:416:VAL:HG12	1:A:417:GLU:HG3	1.90	0.53
1:A:444:ALA:HA	1:A:448:ARG:HG2	1.91	0.53
1:A:369:GLU:OE1	1:A:372:ARG:HD3	2.09	0.53
1:A:449:CYS:HB2	4:A:601:HEM:NA	2.24	0.52
1:B:281:ILE:HD12	1:B:281:ILE:N	2.25	0.52
1:B:415:TRP:CE2	1:B:431:PRO:HG2	2.44	0.52
1:A:369:GLU:OE1	1:A:369:GLU:HA	2.09	0.52
2:C:2:GLC:H5	2:C:3:GLC:O5	2.09	0.52
1:A:283:GLN:HA	1:A:286:LEU:HD12	1.91	0.51
1:A:410:ARG:HG2	1:A:418:ARG:NH1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ALA:HA	1:A:152:PHE:CD2	2.46	0.51
1:A:208:HIS:CA	1:A:216:ARG:HG3	2.41	0.51
1:A:491:PRO:HB2	1:A:494:PRO:HB3	1.93	0.50
1:B:116:LEU:HB2	1:B:390:VAL:CG2	2.42	0.49
1:A:348:ASN:OD1	1:A:348:ASN:N	2.45	0.49
1:B:175:ILE:HG12	1:B:205:THR:HB	1.95	0.49
4:B:601:HEM:HBB2	4:B:601:HEM:CMB	2.42	0.48
1:A:144:ALA:HA	1:A:152:PHE:CE2	2.48	0.48
1:A:380:MET:HG2	4:A:601:HEM:CGA	2.43	0.48
1:B:369:GLU:HA	1:B:369:GLU:OE1	2.13	0.48
4:A:601:HEM:HBB2	4:A:601:HEM:HMB2	1.94	0.48
1:B:211:HIS:CD2	1:B:305:LEU:HD22	2.48	0.48
1:B:271:ARG:NH1	1:B:280:ASP:OD1	2.43	0.48
1:A:122:ASN:H	1:A:446:ARG:NH2	2.12	0.47
1:A:97:SER:HA	1:A:105:PHE:O	2.14	0.47
1:A:389:THR:HA	1:A:393:TYR:O	2.14	0.47
1:B:271:ARG:HH12	1:B:280:ASP:CG	2.18	0.47
1:A:409:GLN:NE2	1:A:440:VAL:H	2.04	0.46
1:B:269:GLN:HA	1:B:272:ARG:CB	2.45	0.46
1:B:136:THR:HB	1:B:137:PRO:HD3	1.96	0.46
5:A:602[A]:ECN:C8	5:A:602[A]:ECN:N1	2.59	0.46
1:B:97:SER:HA	1:B:105:PHE:O	2.16	0.46
1:B:79:LYS:HD3	1:B:79:LYS:HA	1.75	0.46
1:B:182:TYR:OH	1:B:197:ALA:HA	2.15	0.45
1:A:200:GLU:O	1:A:203:ILE:HG22	2.17	0.45
1:A:488:ILE:H	1:A:488:ILE:HG13	1.46	0.45
1:A:101:VAL:HG12	1:A:101:VAL:O	2.17	0.45
1:A:449:CYS:HB2	4:A:601:HEM:C1A	2.51	0.45
1:B:445:GLY:O	1:B:448:ARG:HB2	2.17	0.45
1:A:448:ARG:HD2	1:A:449:CYS:O	2.17	0.44
1:B:486:THR:HB	1:B:488:ILE:HG13	1.99	0.44
1:A:64:ILE:HG12	1:A:92:TYR:CE1	2.52	0.44
1:A:377:ILE:HD12	4:A:601:HEM:C4A	2.52	0.44
1:B:147:VAL:HG23	1:B:148:PRO:O	2.18	0.44
1:B:467:LEU:O	1:B:501:ARG:CD	2.65	0.44
1:A:375:PRO:O	1:A:489:HIS:HD2	2.00	0.44
1:B:66:SER:HB2	1:B:73:HIS:NE2	2.32	0.44
1:B:209:CYS:O	1:B:281:ILE:HD13	2.18	0.44
1:A:377:ILE:HD12	4:A:601:HEM:C3A	2.53	0.43
1:B:431:PRO:HB3	1:B:435:GLU:OE2	2.18	0.43
1:A:129:ASP:OD2	1:A:385:ARG:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:LEU:HD11	1:B:239:TRP:CD1	2.53	0.43
1:A:133:ARG:HG3	6:A:3:HOH:O	2.19	0.43
1:A:208:HIS:HA	1:A:216:ARG:HG3	2.01	0.43
1:B:211:HIS:CE1	1:B:309:LEU:HB2	2.53	0.43
1:A:409:GLN:NE2	1:A:441:PRO:HD3	2.34	0.42
5:A:602[A]:ECN:O20	5:A:602[A]:ECN:CL4	2.74	0.42
1:A:136:THR:N	1:A:137:PRO:CD	2.83	0.42
1:A:139:PHE:HE2	1:A:310:LEU:HD12	1.84	0.42
1:B:156:LYS:HE3	4:B:601:HEM:HAD2	2.02	0.42
1:A:164:ASN:HD22	1:A:166:ALA:H	1.67	0.42
1:A:413:ASP:OD1	1:A:413:ASP:N	2.53	0.42
1:B:120:SER:HB2	6:B:22:HOH:O	2.20	0.42
1:B:248:PRO:HB2	1:B:252:ARG:NH2	2.35	0.42
1:A:268:ILE:HG23	1:A:286:LEU:HD21	2.02	0.41
1:A:327:LEU:HB3	1:A:334:GLN:HG3	2.00	0.41
1:A:449:CYS:HA	4:A:601:HEM:C4D	2.56	0.41
1:A:133:ARG:HG3	1:A:133:ARG:H	1.58	0.41
1:A:309:LEU:O	1:A:309:LEU:HG	2.20	0.41
1:B:449:CYS:HA	4:B:601:HEM:CHA	2.50	0.41
1:B:198:LEU:O	1:B:202:ILE:HG12	2.21	0.41
1:B:375:PRO:HA	1:B:376:PRO:HD3	1.98	0.41
1:A:369:GLU:HG3	1:A:421:PHE:CD1	2.56	0.41
1:A:430:ASN:HD22	1:A:432:ALA:HB3	1.82	0.40
1:B:95:VAL:HG21	1:B:390:VAL:HG12	2.02	0.40
1:B:164:ASN:HD22	1:B:164:ASN:C	2.23	0.40
1:B:258:ARG:O	1:B:262:ASP:HB2	2.20	0.40
1:B:311:ALA:HB2	3:B:600[B]:ECL:H9	2.03	0.40
1:A:378:MET:O	1:A:379:ILE:HG13	2.22	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	443/461 (96%)	424 (96%)	17 (4%)	2 (0%)	29 61
1	B	443/461 (96%)	416 (94%)	26 (6%)	1 (0%)	47 78
All	All	886/922 (96%)	840 (95%)	43 (5%)	3 (0%)	41 71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	ASP
1	A	489	HIS
1	B	488	ILE

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	390/403 (97%)	368 (94%)	22 (6%)	21 52
1	B	390/403 (97%)	354 (91%)	36 (9%)	9 27
All	All	780/806 (97%)	722 (93%)	58 (7%)	13 38

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	VAL
1	A	68	ILE
1	A	133	ARG
1	A	135	THR
1	A	194	VAL
1	A	203	ILE
1	A	216	ARG
1	A	236	HIS
1	A	252	ARG
1	A	272	ARG
1	A	304	MET
1	A	323	MET
1	A	358	LYS

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Mol	Chain	Res	Type
1	A	385	ARG
1	A	390	VAL
1	A	400	GLN
1	A	413	ASP
1	A	420	ASP
1	A	448	ARG
1	A	488	ILE
1	A	490	THR
1	A	501	ARG
1	B	90	GLU
1	B	91	LYS
1	B	123	GLU
1	B	136	THR
1	B	143	VAL
1	B	157	LYS
1	B	160	LYS
1	B	164	ASN
1	B	194	VAL
1	B	207	SER
1	B	216	ARG
1	B	217	SER
1	B	247	LEU
1	B	259	GLU
1	B	260	ILE
1	B	266	LYS
1	B	269	GLN
1	B	272	ARG
1	B	289	THR
1	B	298	ASP
1	B	304	MET
1	B	309	LEU
1	B	347	GLU
1	B	355	ASP
1	B	359	ASP
1	B	385	ARG
1	B	386	THR
1	B	390	VAL
1	B	400	GLN
1	B	410	ARG
1	B	413	ASP
1	B	420	ASP
1	B	428	GLN

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Mol	Chain	Res	Type
1	B	448	ARG
1	B	488	ILE
1	B	501	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
1	A	149	ASN
1	A	164	ASN
1	A	170	GLN
1	A	257	HIS
1	A	275	GLN
1	A	334	GLN
1	A	388	GLN
1	A	409	GLN
1	A	422	ASN
1	A	430	ASN
1	A	489	HIS
1	B	164	ASN
1	B	334	GLN
1	B	388	GLN
1	B	409	GLN
1	B	422	ASN
1	B	430	ASN

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	0.53	0	15,15,17	1.70	4 (26%)
2	GLC	C	2	2	11,11,12	0.49	0	15,15,17	2.13	3 (20%)
2	GLC	C	3	2	11,11,12	0.40	0	15,15,17	0.99	1 (6%)
2	GLC	C	4	2	11,11,12	0.37	0	15,15,17	1.03	2 (13%)
2	GLC	C	5	2	11,11,12	0.53	0	15,15,17	1.47	2 (13%)
2	GLC	C	6	2	11,11,12	0.38	0	15,15,17	1.79	2 (13%)
2	GLC	C	7	2	11,11,12	0.52	0	15,15,17	1.50	2 (13%)
2	GLC	D	1	2	11,11,12	0.43	0	15,15,17	2.30	3 (20%)
2	GLC	D	2	2	11,11,12	0.33	0	15,15,17	2.11	3 (20%)
2	GLC	D	3	2	11,11,12	0.44	0	15,15,17	1.23	2 (13%)
2	GLC	D	4	2	11,11,12	0.40	0	15,15,17	0.87	1 (6%)
2	GLC	D	5	2	11,11,12	0.41	0	15,15,17	1.38	1 (6%)
2	GLC	D	6	2	11,11,12	0.51	0	15,15,17	1.68	5 (33%)
2	GLC	D	7	2	11,11,12	0.74	0	15,15,17	1.99	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	-	1/2/19/22	0/1/1/1
2	GLC	C	2	2	-	2/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	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	-	2/2/19/22	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	-	0/2/19/22	0/1/1/1
2	GLC	D	4	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	D	5	2	-	0/2/19/22	0/1/1/1
2	GLC	D	6	2	-	2/2/19/22	0/1/1/1
2	GLC	D	7	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	GLC	C1-O5-C5	7.10	121.81	112.19
2	C	2	GLC	C1-O5-C5	6.71	121.28	112.19
2	D	2	GLC	C1-O5-C5	6.23	120.64	112.19
2	C	6	GLC	C1-O5-C5	5.58	119.76	112.19
2	D	7	GLC	C1-C2-C3	5.44	116.35	109.67
2	D	7	GLC	C2-C3-C4	4.59	118.85	110.89
2	D	5	GLC	C1-C2-C3	4.09	114.70	109.67
2	C	5	GLC	C1-O5-C5	3.91	117.48	112.19
2	C	7	GLC	C2-C3-C4	3.16	116.37	110.89
2	C	1	GLC	O4-C4-C3	-3.14	103.08	110.35
2	D	6	GLC	O4-C4-C3	-3.10	103.18	110.35
2	D	1	GLC	C6-C5-C4	-3.01	105.94	113.00
2	D	2	GLC	O4-C4-C3	-3.00	103.40	110.35
2	C	1	GLC	C1-C2-C3	2.91	113.24	109.67
2	D	2	GLC	C3-C4-C5	2.89	115.40	110.24
2	C	7	GLC	C1-C2-C3	2.87	113.20	109.67
2	C	1	GLC	O5-C5-C6	2.87	111.70	107.20
2	D	6	GLC	C1-O5-C5	2.86	116.07	112.19
2	D	3	GLC	O4-C4-C3	-2.63	104.26	110.35
2	C	2	GLC	O5-C1-C2	2.63	114.83	110.77
2	C	5	GLC	C1-C2-C3	2.61	112.87	109.67
2	C	4	GLC	O4-C4-C3	-2.45	104.68	110.35
2	D	4	GLC	O4-C4-C3	-2.36	104.88	110.35
2	C	4	GLC	C1-O5-C5	2.35	115.37	112.19
2	D	6	GLC	O3-C3-C4	-2.34	104.93	110.35
2	C	1	GLC	C2-C3-C4	2.29	114.86	110.89
2	D	1	GLC	C3-C4-C5	2.29	114.32	110.24
2	C	2	GLC	O5-C5-C4	2.27	116.36	110.83
2	C	3	GLC	C1-O5-C5	2.26	115.25	112.19
2	C	6	GLC	O5-C5-C4	2.17	116.11	110.83
2	D	6	GLC	C2-C3-C4	2.16	114.63	110.89
2	D	6	GLC	C1-C2-C3	2.15	112.31	109.67
2	D	3	GLC	C1-C2-C3	2.05	112.19	109.67

There are no chirality outliers.

All (17) torsion outliers are listed below:

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

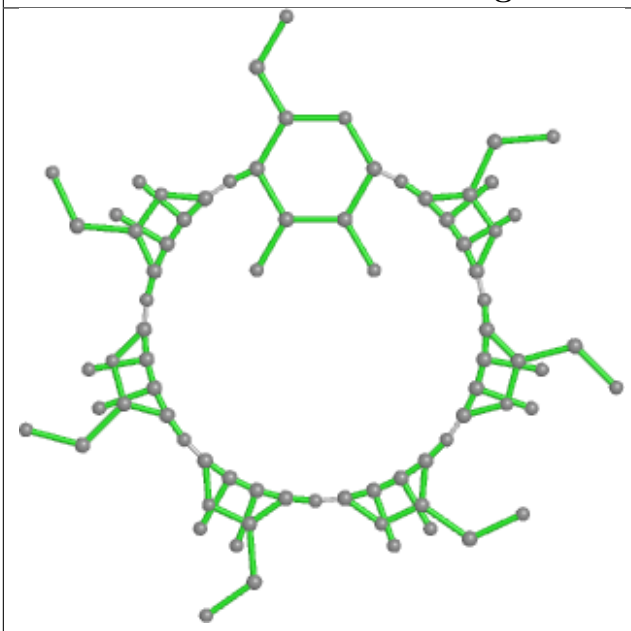
There are no ring outliers.

2 monomers are involved in 1 short contact:

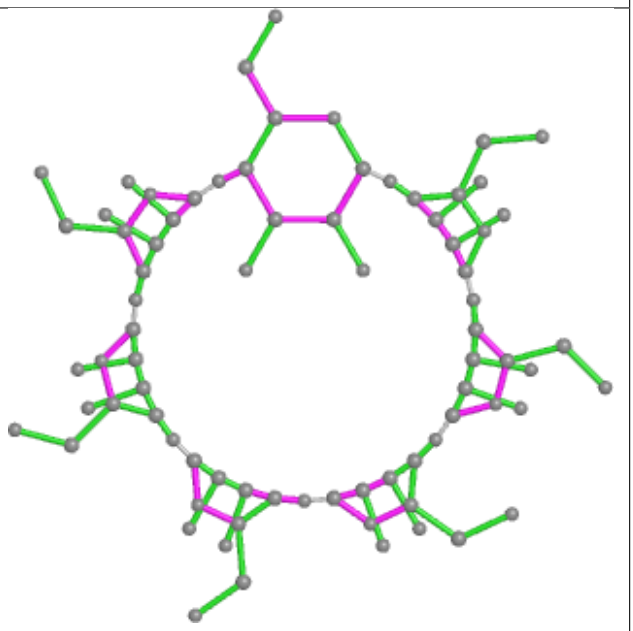
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	GLC	1	0
2	C	3	GLC	1	0

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

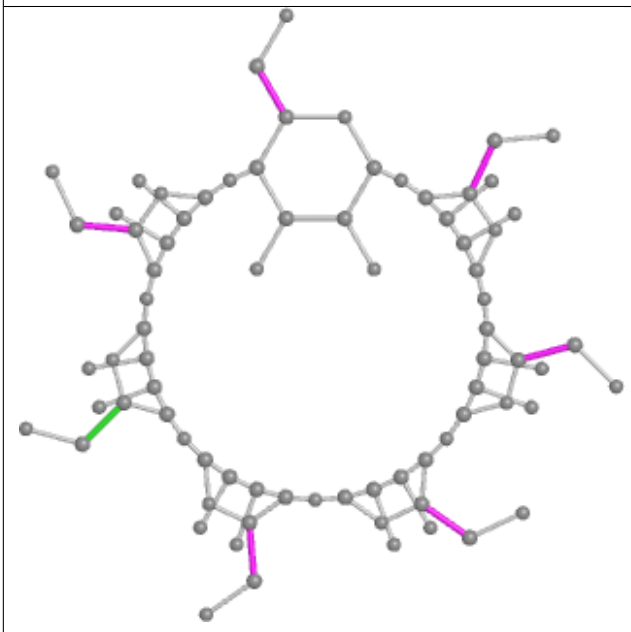
Oligosaccharide Chain C



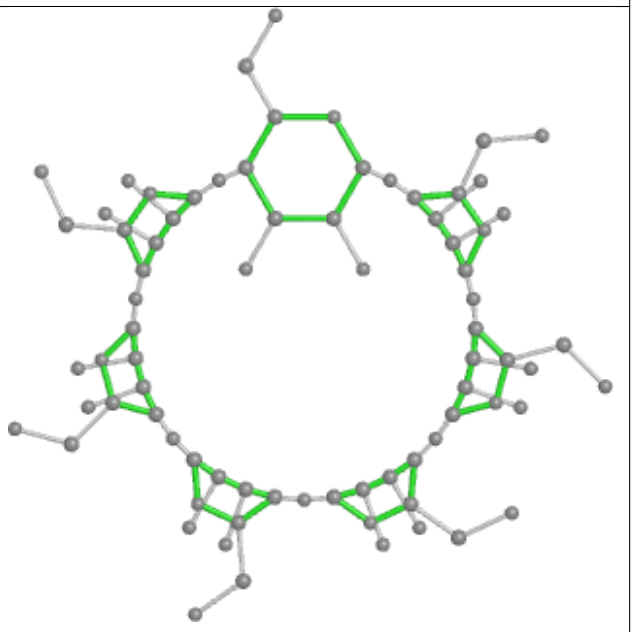
Bond lengths



Bond angles

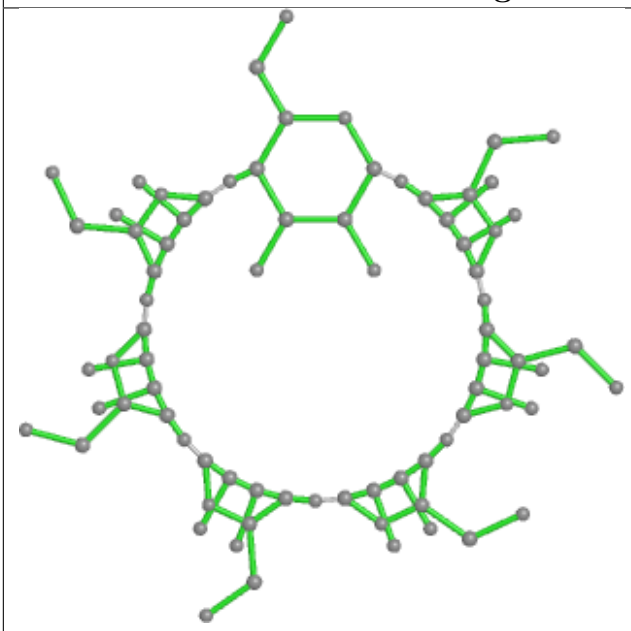


Torsions

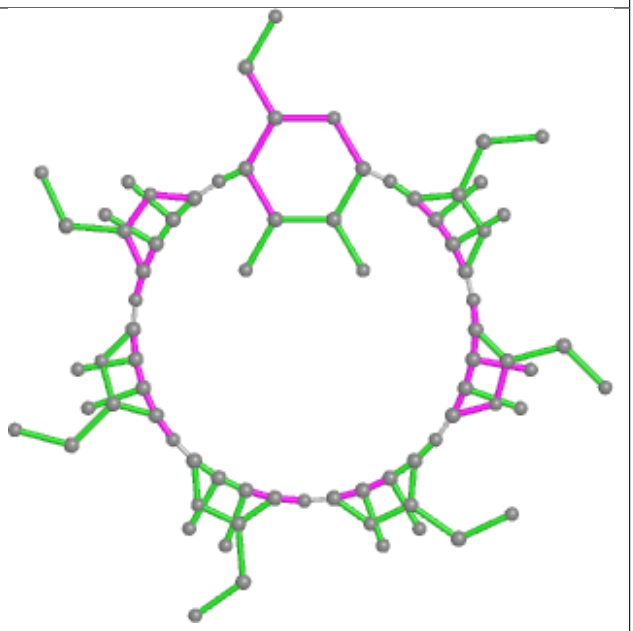


Rings

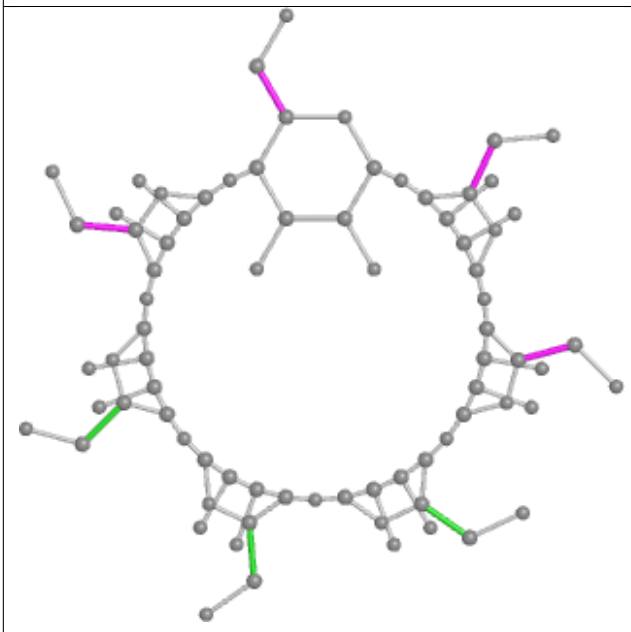
Oligosaccharide Chain D



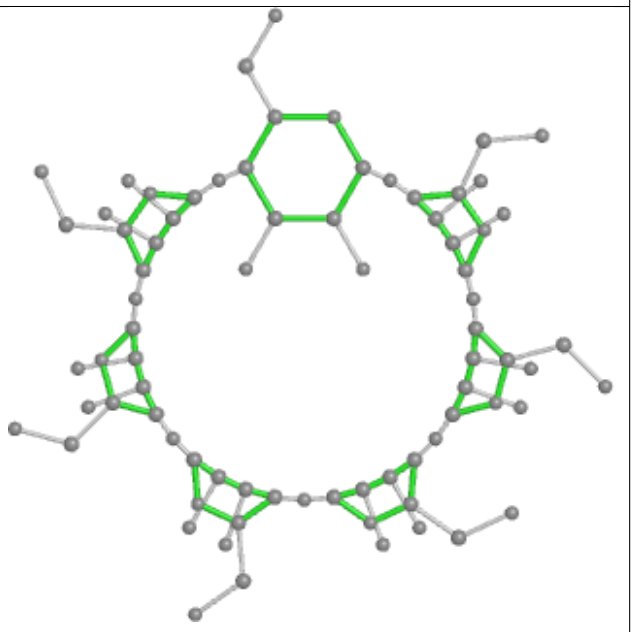
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

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	$\#\|Z\|>2$
5	ECN	A	602[A]	4	24,26,26	1.02	3 (12%)	32,35,35	1.47	4 (12%)
4	HEM	B	601	3,1,5	41,50,50	1.97	7 (17%)	45,82,82	1.55	5 (11%)
3	ECL	A	600[B]	4	24,26,26	1.12	3 (12%)	32,35,35	1.27	4 (12%)
4	HEM	A	601	3,1,5	41,50,50	1.92	7 (17%)	45,82,82	1.73	9 (20%)
5	ECN	B	602[A]	4	24,26,26	1.20	4 (16%)	32,35,35	1.66	5 (15%)
3	ECL	B	600[B]	4	24,26,26	1.39	6 (25%)	32,35,35	1.40	4 (12%)

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
5	ECN	A	602[A]	4	-	5/13/13/13	0/3/3/3
4	HEM	B	601	3,1,5	-	2/12/54/54	-
3	ECL	A	600[B]	4	-	2/13/13/13	0/3/3/3
4	HEM	A	601	3,1,5	-	0/12/54/54	-
5	ECN	B	602[A]	4	-	5/13/13/13	0/3/3/3
3	ECL	B	600[B]	4	-	2/13/13/13	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	HEM	C3D-C2D	8.23	1.54	1.36
4	A	601	HEM	C3D-C2D	7.43	1.52	1.36
4	A	601	HEM	C3C-C2C	-4.05	1.34	1.40
4	B	601	HEM	C3C-C2C	-4.00	1.34	1.40
4	B	601	HEM	C3C-CAC	3.44	1.54	1.47
4	A	601	HEM	CAB-C3B	3.32	1.56	1.47
4	B	601	HEM	CAB-C3B	3.18	1.56	1.47
4	A	601	HEM	C3C-CAC	3.14	1.54	1.47
4	A	601	HEM	FE-ND	3.10	2.12	1.96
3	B	600[B]	ECL	O20-C8	2.96	1.50	1.42
5	B	602[A]	ECN	C19-N1	-2.89	1.45	1.48
3	B	600[B]	ECL	C16-CL8	2.77	1.80	1.73
3	A	600[B]	ECL	C11-CL2	2.76	1.80	1.74
3	B	600[B]	ECL	C11-CL2	2.69	1.80	1.74
4	A	601	HEM	CAA-C2A	2.55	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	602[A]	ECN	C14-CL4	2.54	1.79	1.73
3	A	600[B]	ECL	C16-CL8	2.53	1.79	1.73
4	B	601	HEM	FE-ND	2.49	2.09	1.96
5	A	602[A]	ECN	C16-CL8	2.49	1.79	1.74
3	A	600[B]	ECL	C14-CL4	2.42	1.79	1.74
3	B	600[B]	ECL	C19-N1	-2.37	1.45	1.48
5	B	602[A]	ECN	C11-CL2	2.33	1.79	1.74
3	B	600[B]	ECL	C14-CL4	2.28	1.79	1.74
5	A	602[A]	ECN	C11-CL2	2.28	1.79	1.74
5	A	602[A]	ECN	C7-N1	2.10	1.41	1.37
4	A	601	HEM	CMB-C2B	2.10	1.55	1.50
3	B	600[B]	ECL	C7-N1	-2.09	1.33	1.37
4	B	601	HEM	CMD-C2D	2.06	1.55	1.50
5	B	602[A]	ECN	C16-CL8	2.06	1.79	1.74
4	B	601	HEM	CAA-C2A	2.01	1.55	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	601	HEM	C4D-ND-C1D	6.21	111.49	105.07
4	B	601	HEM	C4D-ND-C1D	6.04	111.31	105.07
5	A	602[A]	ECN	O20-C20-C5	-4.98	104.55	112.08
5	B	602[A]	ECN	C14-C5-C20	-4.87	117.30	122.16
5	B	602[A]	ECN	C21-C5-C14	4.39	121.18	116.81
3	B	600[B]	ECL	C21-C17-C16	4.17	120.96	116.81
5	B	602[A]	ECN	O20-C20-C5	-4.16	105.80	112.08
3	B	600[B]	ECL	O20-C8-C1	-3.69	101.40	109.91
4	A	601	HEM	C4B-CHC-C1C	3.49	127.16	122.56
3	A	600[B]	ECL	O20-C8-C1	-3.33	102.25	109.91
4	A	601	HEM	C4C-CHD-C1D	3.24	126.84	122.56
4	B	601	HEM	C4B-CHC-C1C	3.06	126.60	122.56
4	A	601	HEM	CAD-CBD-CGD	-2.92	107.31	113.60
4	A	601	HEM	CMD-C2D-C1D	2.87	129.40	125.04
3	A	600[B]	ECL	C21-C17-C16	2.73	119.53	116.81
3	A	600[B]	ECL	C17-C16-CL8	2.66	123.17	120.41
4	B	601	HEM	C4C-CHD-C1D	2.54	125.91	122.56
5	A	602[A]	ECN	C21-C5-C14	2.53	119.32	116.81
5	B	602[A]	ECN	C19-C20-C5	-2.46	104.67	110.45
5	A	602[A]	ECN	C7-N1-C3	-2.41	105.84	108.21
4	B	601	HEM	C1B-NB-C4B	2.39	107.54	105.07
4	A	601	HEM	C1B-NB-C4B	2.38	107.53	105.07
3	B	600[B]	ECL	C15-C16-C17	-2.34	119.62	122.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	601	HEM	CAD-C3D-C4D	2.28	128.64	124.66
4	A	601	HEM	C2C-C3C-C4C	2.26	108.47	106.90
4	B	601	HEM	CAD-CBD-CGD	-2.24	108.78	113.60
5	A	602[A]	ECN	O20-C20-C19	2.15	110.61	106.33
3	B	600[B]	ECL	C16-C17-C20	-2.06	120.11	122.16
3	A	600[B]	ECL	O20-C20-C17	-2.06	108.97	112.08
4	A	601	HEM	C3B-C2B-C1B	2.03	108.00	106.49
5	B	602[A]	ECN	O20-C20-C19	2.03	110.37	106.33

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	600[B]	ECL	C20-C19-N1-C3
3	A	600[B]	ECL	C20-C19-N1-C7
3	B	600[B]	ECL	C20-C19-N1-C3
5	A	602[A]	ECN	C19-C20-O20-C8
5	A	602[A]	ECN	C5-C20-O20-C8
5	B	602[A]	ECN	C19-C20-O20-C8
5	B	602[A]	ECN	C5-C20-O20-C8
5	B	602[A]	ECN	O20-C20-C5-C14
5	A	602[A]	ECN	O20-C20-C5-C21
5	B	602[A]	ECN	O20-C20-C5-C21
5	A	602[A]	ECN	C1-C8-O20-C20
5	A	602[A]	ECN	O20-C20-C5-C14
5	B	602[A]	ECN	C1-C8-O20-C20
4	B	601	HEM	CAA-CBA-CGA-O2A
4	B	601	HEM	CAA-CBA-CGA-O1A
3	B	600[B]	ECL	C20-C19-N1-C7

There are no ring outliers.

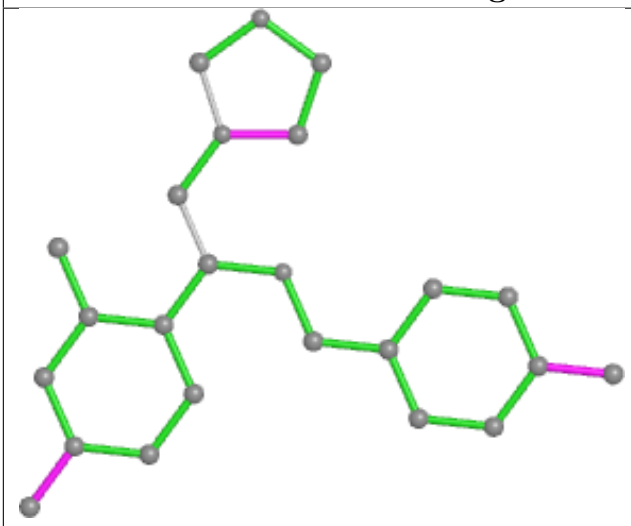
5 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	602[A]	ECN	8	0
4	B	601	HEM	6	0
4	A	601	HEM	7	0
5	B	602[A]	ECN	7	0
3	B	600[B]	ECL	1	0

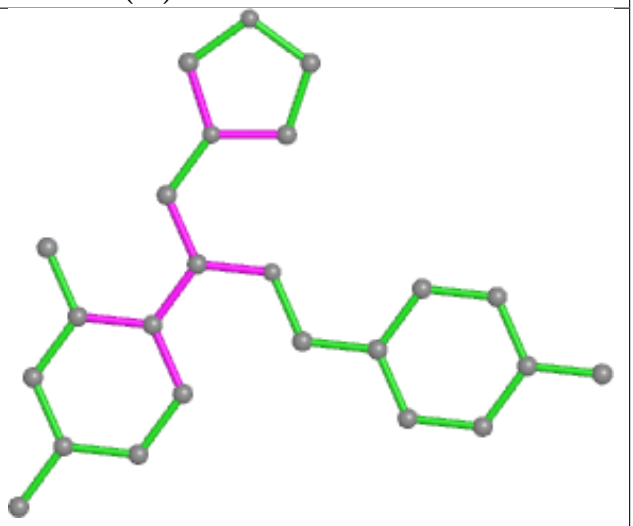
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 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.

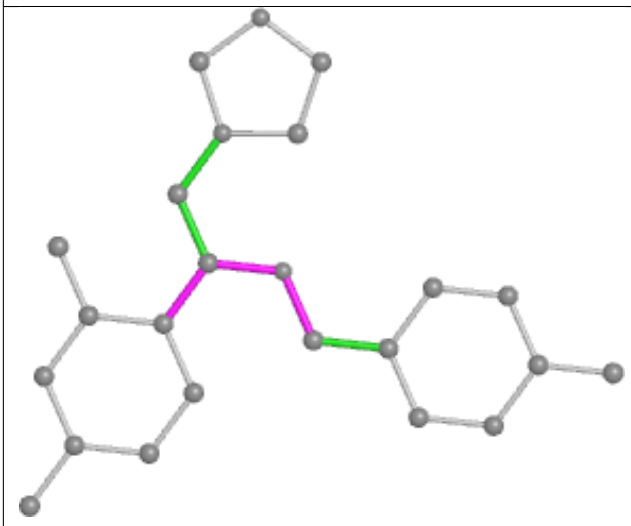
Ligand ECN A 602 (A)



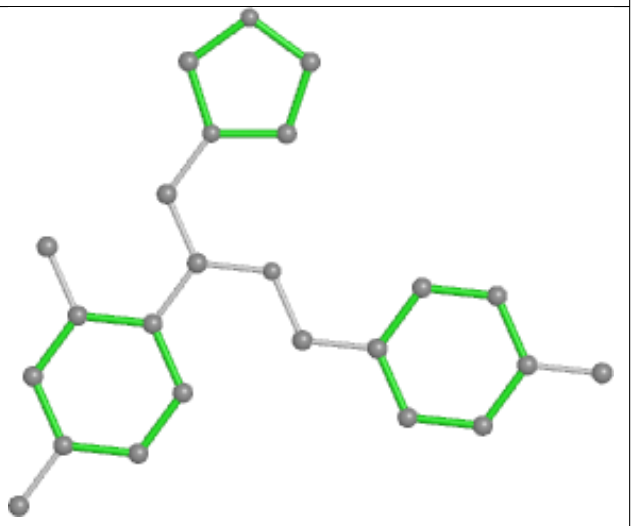
Bond lengths



Bond angles

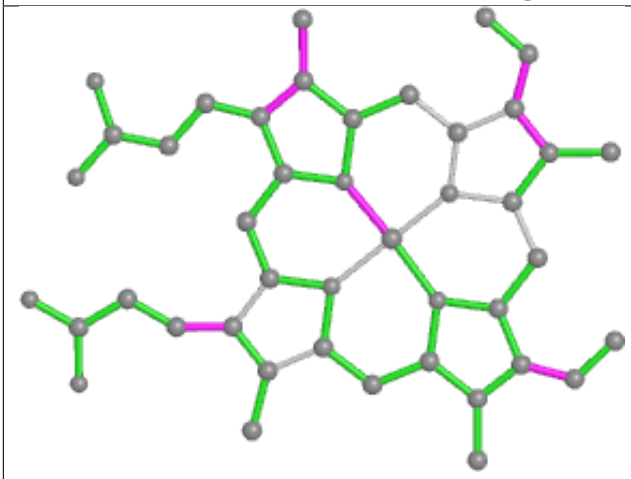


Torsions



Rings

Ligand HEM B 601



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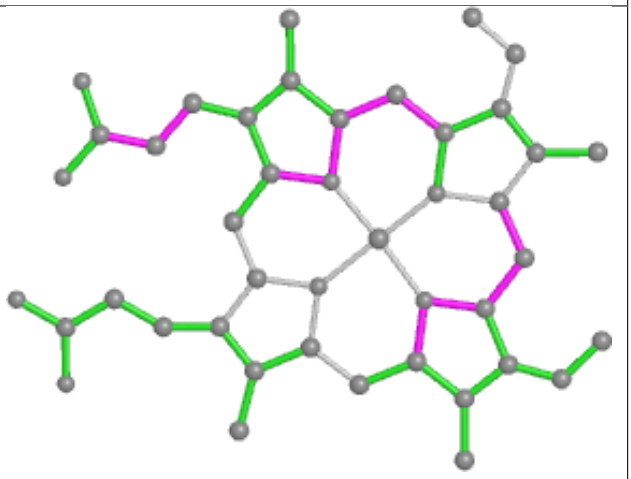
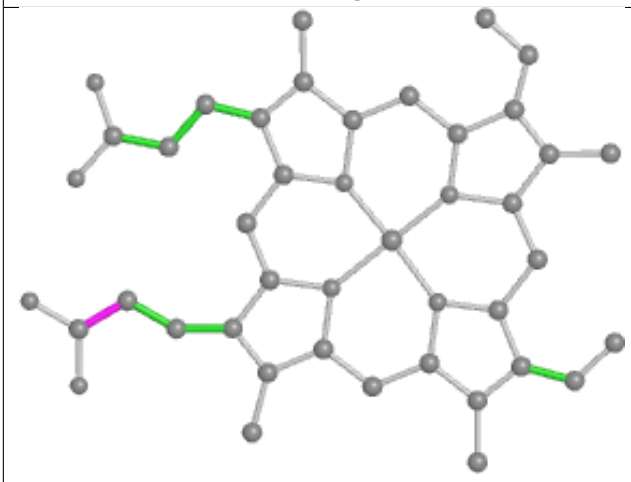
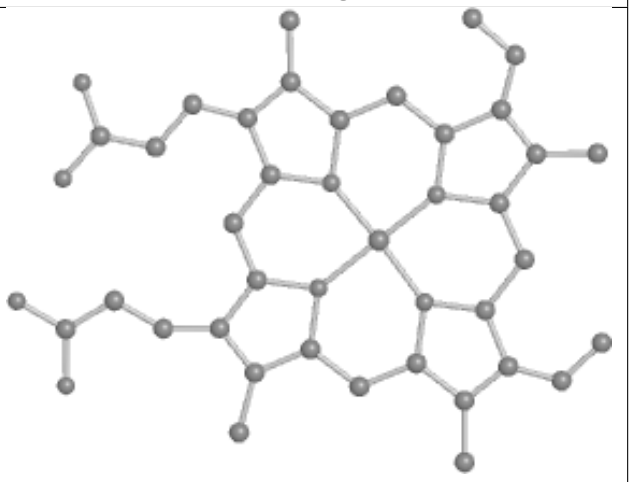


Bond angles

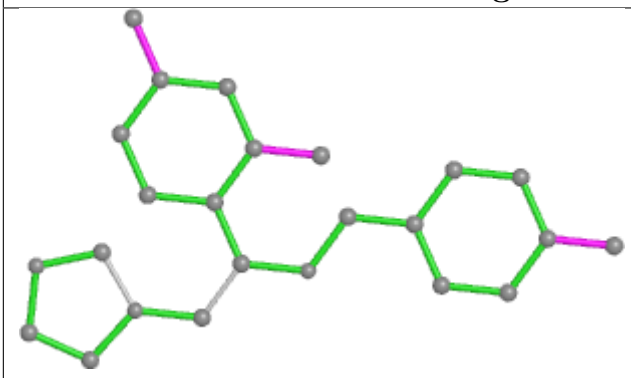


Torsions

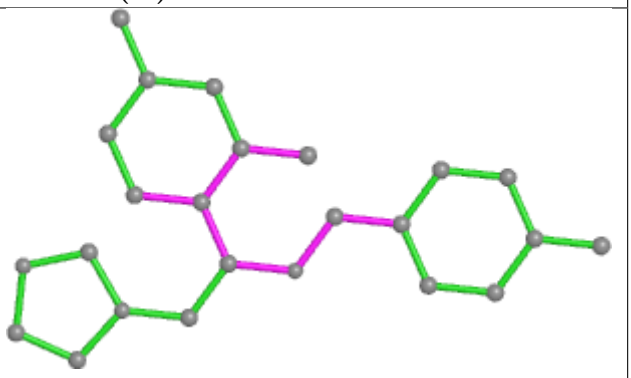


Rings

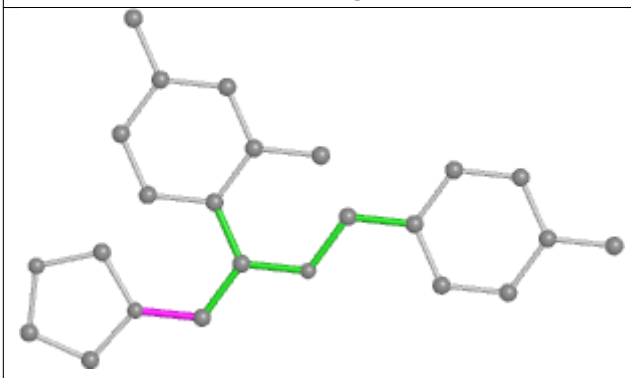
Ligand ECL A 600 (B)



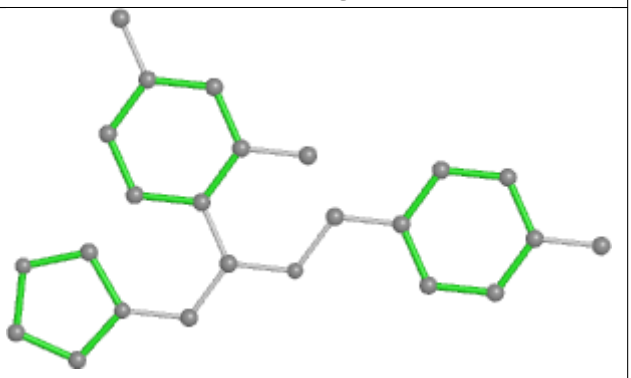
Bond lengths



Bond angles

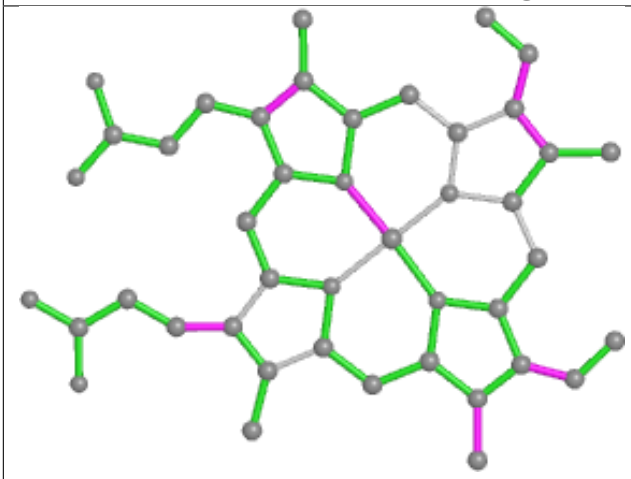


Torsions

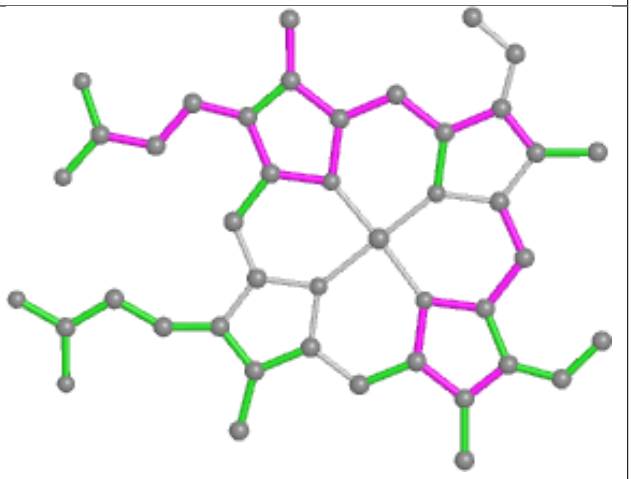


Rings

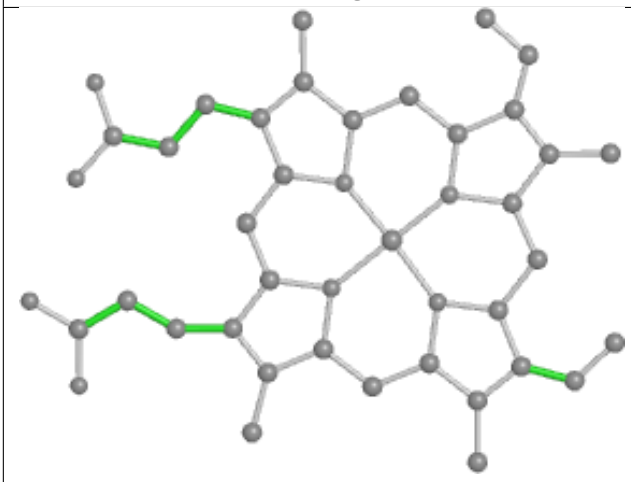
Ligand HEM A 601



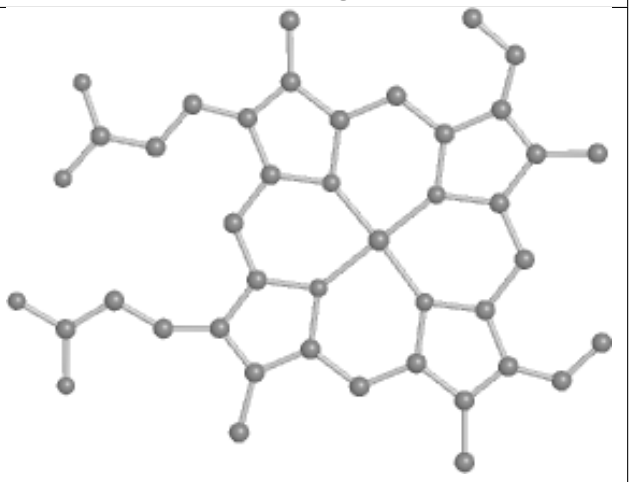
Bond lengths



Bond angles

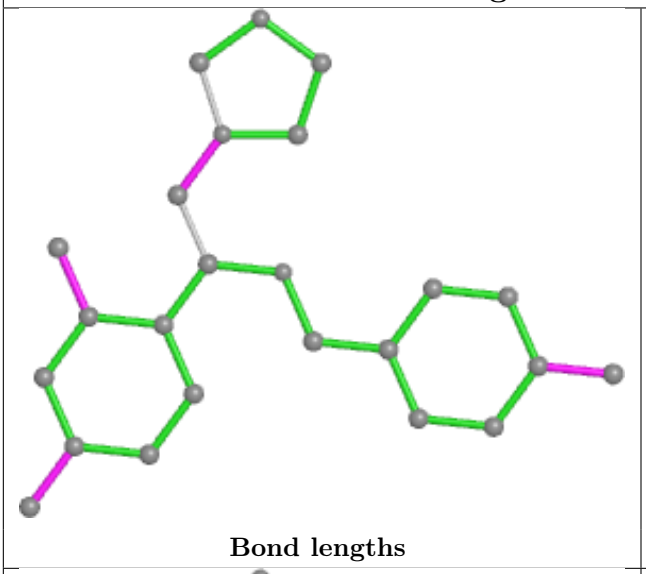


Torsions

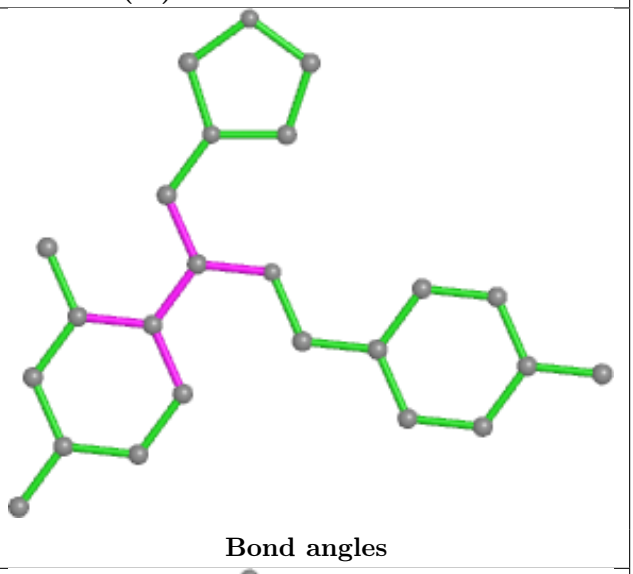


Rings

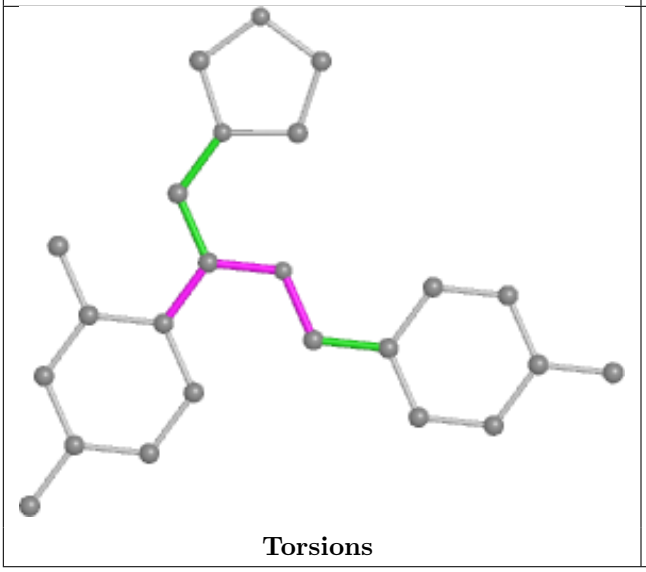
Ligand ECN B 602 (A)



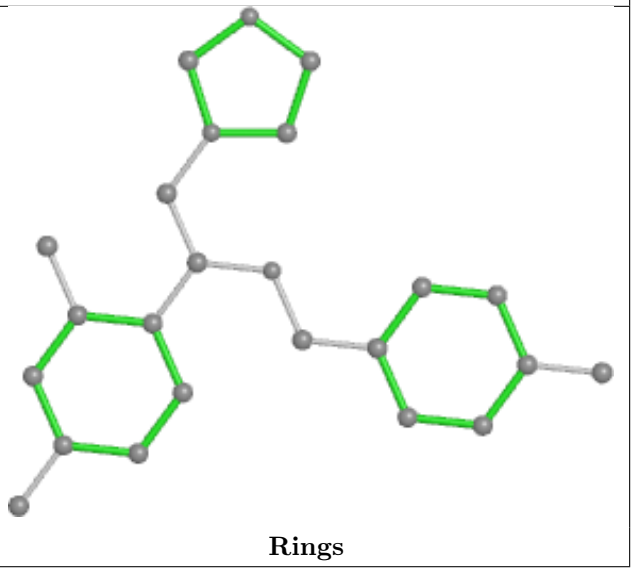
Bond lengths



Bond angles

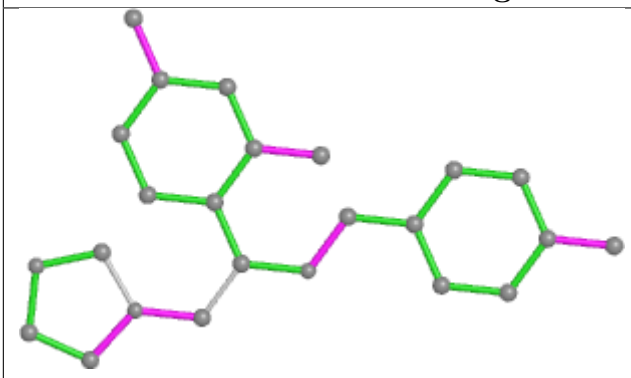


Torsions

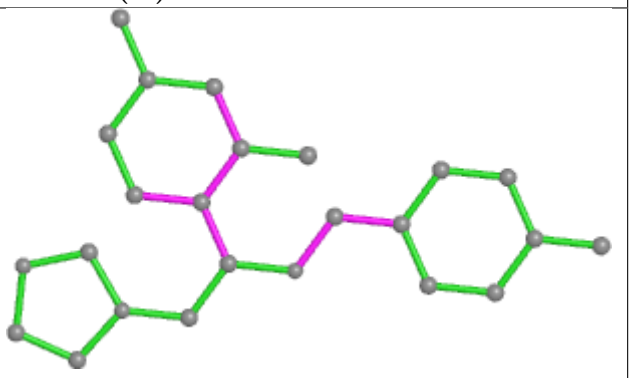


Rings

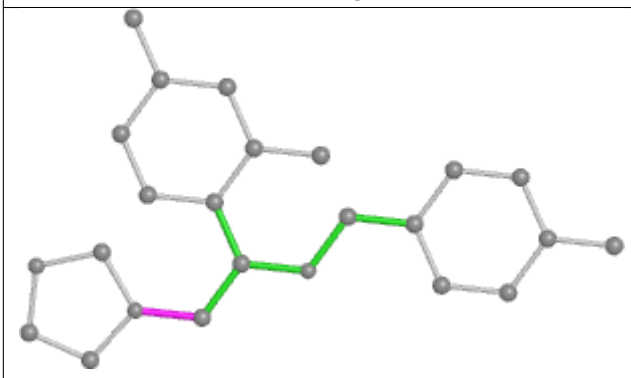
Ligand ECL B 600 (B)



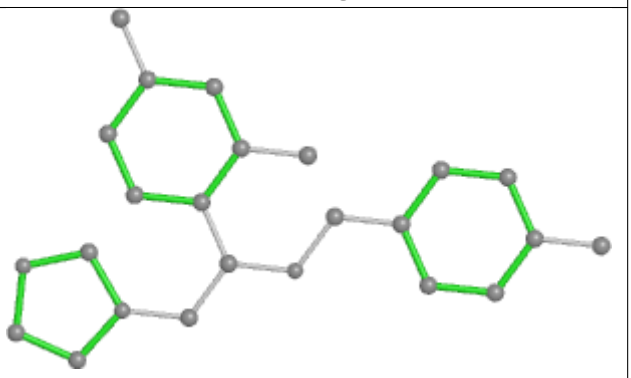
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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, 95^{th} 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	445/461 (96%)	0.08	19 (4%)	35	31	39, 56, 82, 98	0
1	B	445/461 (96%)	0.27	30 (6%)	17	13	47, 71, 95, 106	0
All	All	890/922 (96%)	0.17	49 (5%)	25	21	39, 62, 92, 106	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	276	GLU	4.7
1	B	485	THR	4.2
1	A	244	TRP	4.2
1	B	277	LYS	3.9
1	B	275	GLN	3.6
1	B	308	LEU	3.4
1	A	463	TRP	3.4
1	B	305	LEU	3.2
1	A	275	GLN	3.1
1	B	246	PRO	3.1
1	B	249	SER	3.0
1	B	488	ILE	2.9
1	B	304	MET	2.9
1	B	348	ASN	2.7
1	B	248	PRO	2.7
1	A	221	GLU	2.7
1	A	276	GLU	2.7
1	A	486	THR	2.7
1	B	67	PRO	2.7
1	A	433	SER	2.6
1	B	347	GLU	2.6
1	B	282	LEU	2.6
1	B	255	ARG	2.6
1	B	211	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	502	SER	2.4
1	B	210	LEU	2.4
1	B	244	TRP	2.3
1	B	433	SER	2.3
1	B	492	GLU	2.3
1	A	243	GLY	2.3
1	A	245	LEU	2.3
1	A	255	ARG	2.2
1	A	242	PRO	2.2
1	A	461	THR	2.2
1	A	462	ILE	2.2
1	B	486	THR	2.2
1	A	67	PRO	2.2
1	B	258	ARG	2.2
1	B	342	LYS	2.2
1	B	237	ALA	2.1
1	B	247	LEU	2.1
1	A	246	PRO	2.1
1	A	485	THR	2.1
1	A	251	ARG	2.1
1	B	487	MET	2.1
1	B	225	GLN	2.0
1	A	305	LEU	2.0
1	B	463	TRP	2.0
1	A	459	ILE	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 (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, 95^{th} 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	D	1	11/12	0.90	0.14	64,66,67,68	0
2	GLC	C	2	11/12	0.92	0.15	74,75,75,75	0
2	GLC	D	3	11/12	0.92	0.17	67,70,71,72	0

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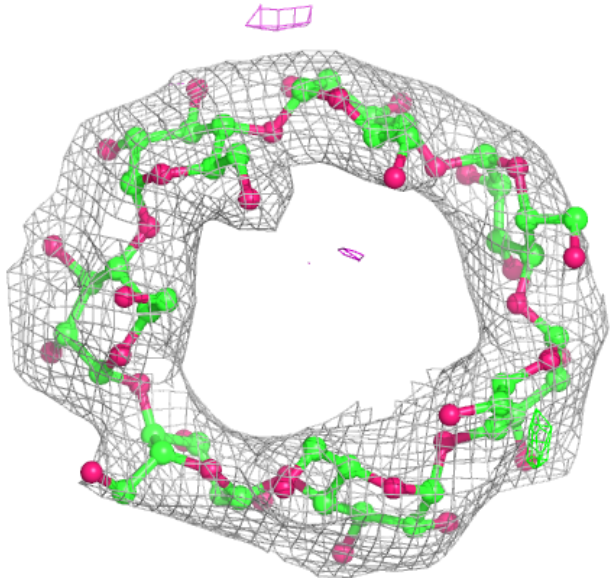
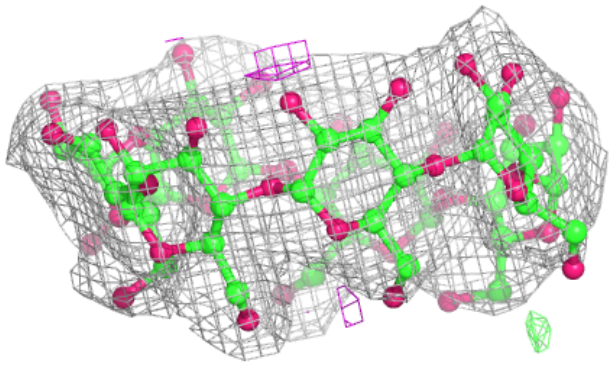
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	D	4	11/12	0.92	0.15	60,63,65,66	0
2	GLC	C	6	11/12	0.93	0.14	76,79,81,82	0
2	GLC	D	2	11/12	0.93	0.20	70,71,72,72	0
2	GLC	D	6	11/12	0.93	0.12	67,68,70,71	0
2	GLC	C	7	11/12	0.94	0.14	80,82,83,83	0
2	GLC	C	4	11/12	0.94	0.13	69,73,73,73	0
2	GLC	C	1	11/12	0.95	0.15	74,76,79,79	0
2	GLC	C	3	11/12	0.95	0.12	74,74,75,75	0
2	GLC	D	7	11/12	0.95	0.15	67,68,70,70	0
2	GLC	C	5	11/12	0.96	0.14	72,74,75,76	0
2	GLC	D	5	11/12	0.96	0.15	58,62,63,66	0

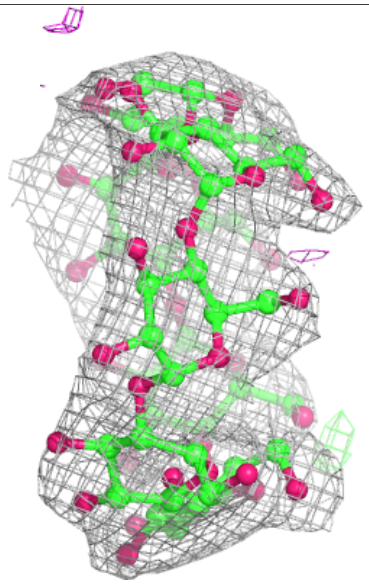
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

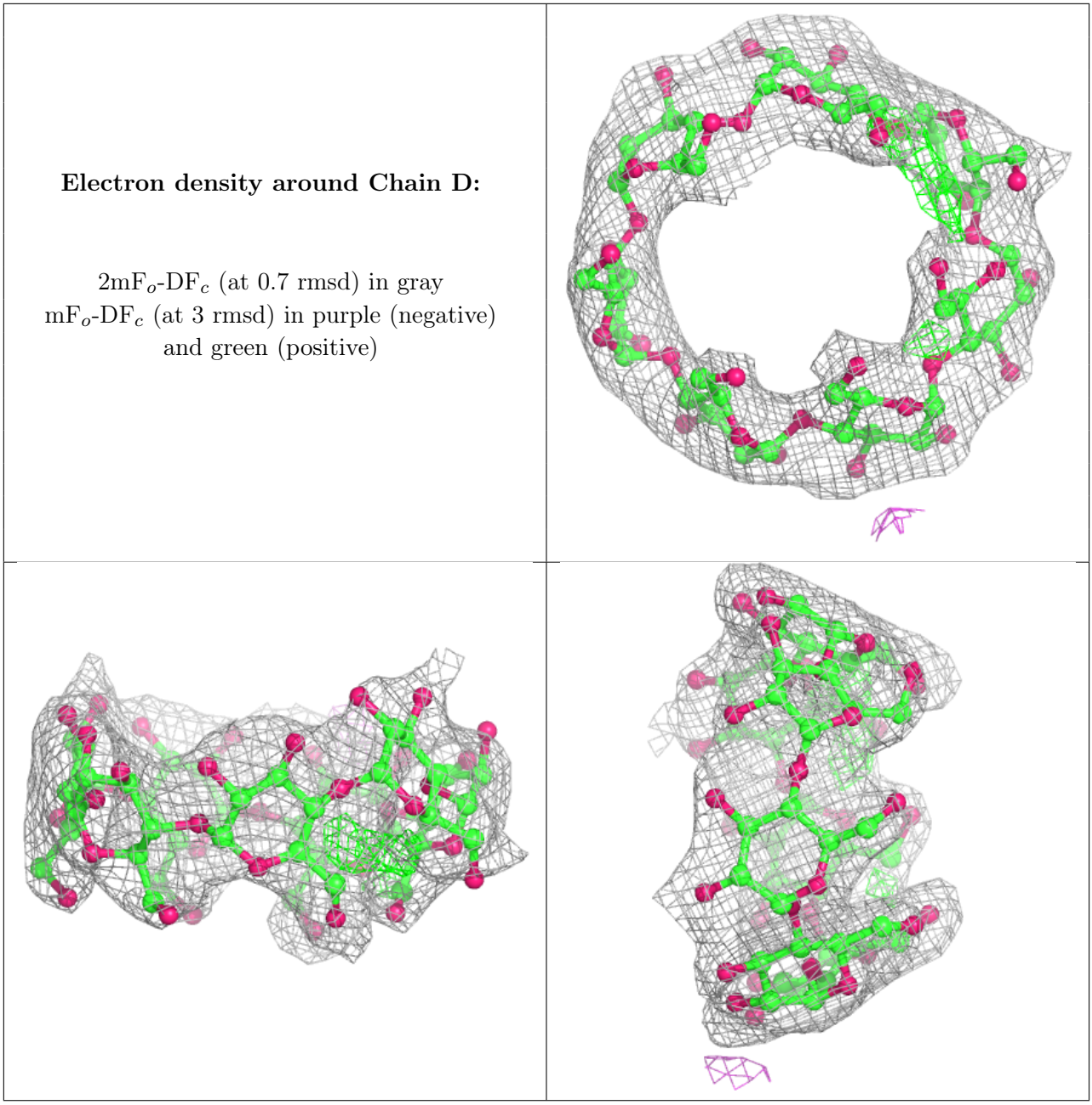






Electron density around Chain D:

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



6.4 Ligands

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, 95^{th} 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	ECL	B	600[B]	24/24	0.89	0.22	66,69,72,73	24
5	ECN	B	602[A]	24/24	0.89	0.24	74,78,81,82	24
5	ECN	A	602[A]	24/24	0.94	0.20	54,59,62,65	24

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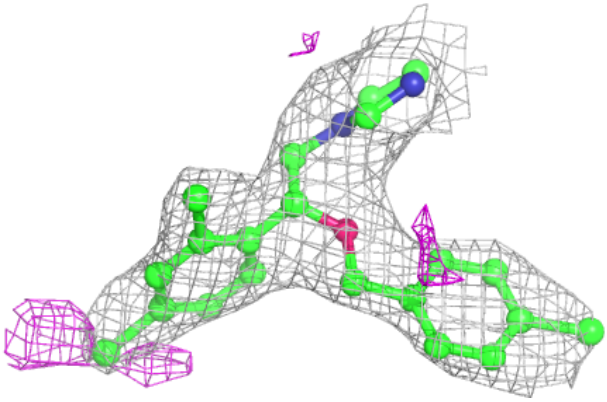
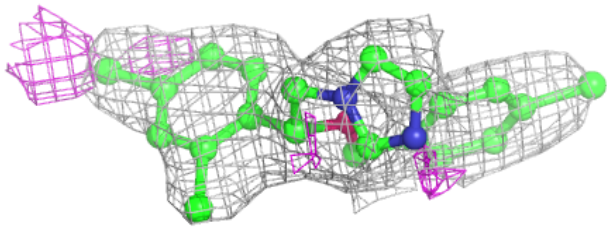
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ECL	A	600[B]	24/24	0.94	0.19	60,63,69,72	24
4	HEM	A	601	43/43	0.98	0.13	42,47,52,54	0
4	HEM	B	601	43/43	0.98	0.15	47,51,52,54	0

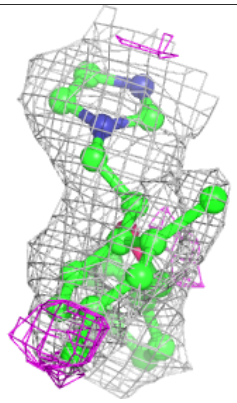
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ECL B 600 (B):

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

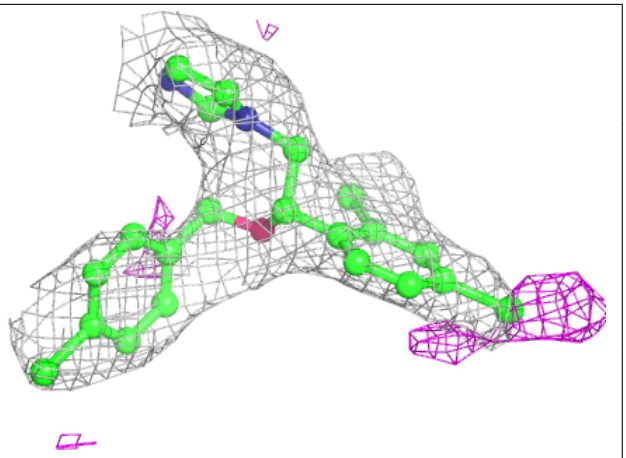


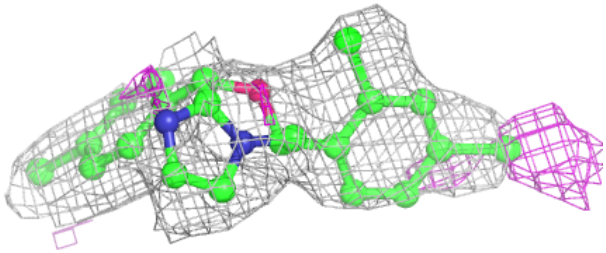


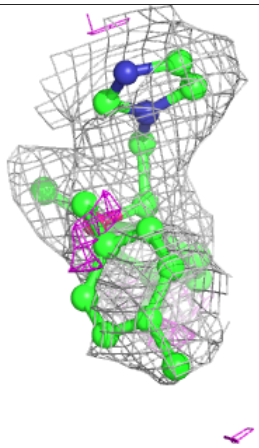


Electron density around ECN B 602 (A):

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

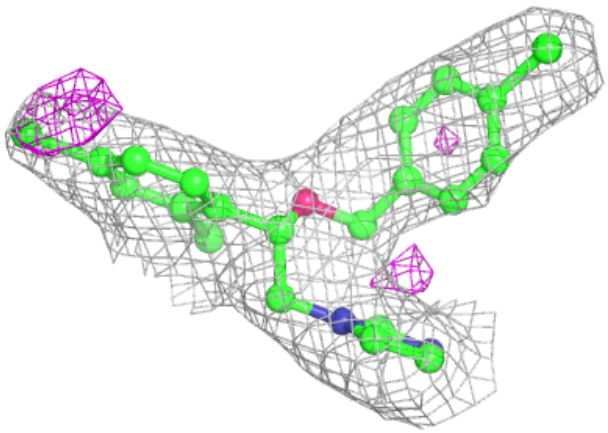


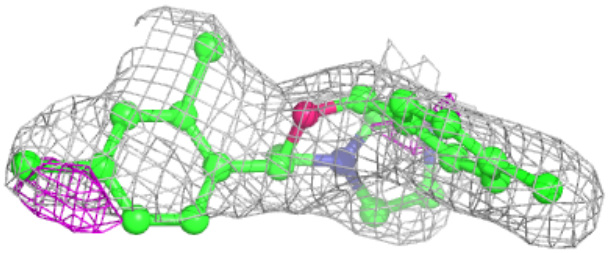


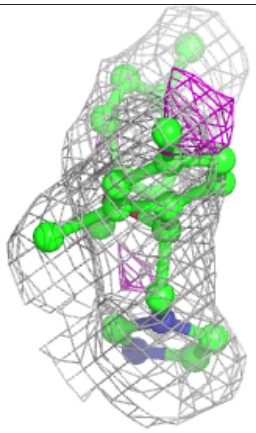


Electron density around ECN A 602 (A):

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

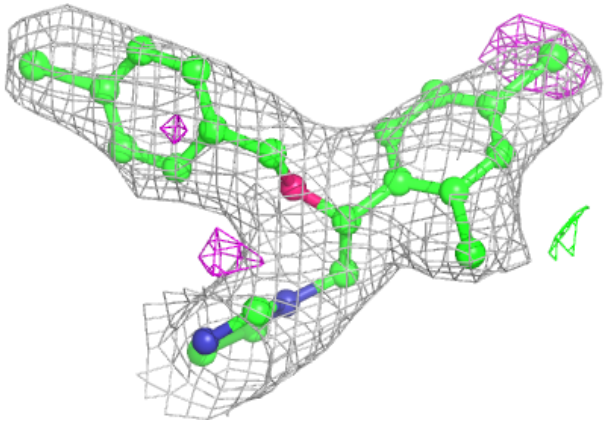


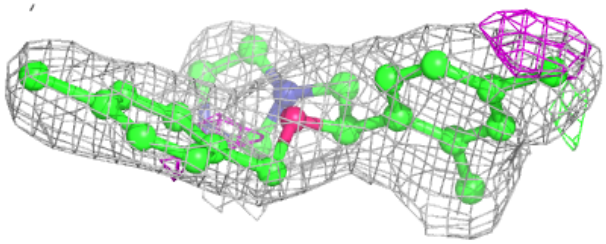


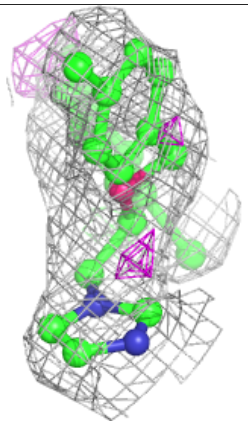


Electron density around ECL A 600 (B):

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

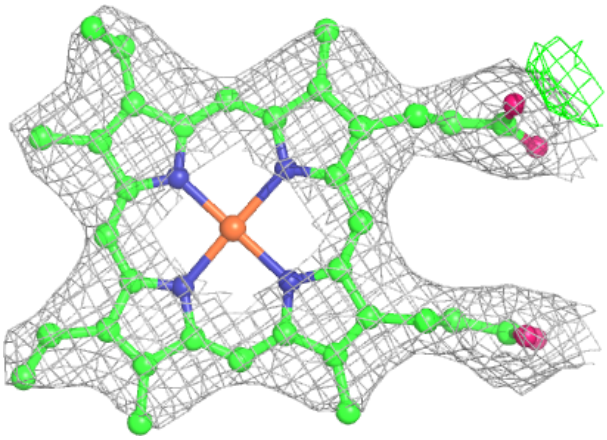


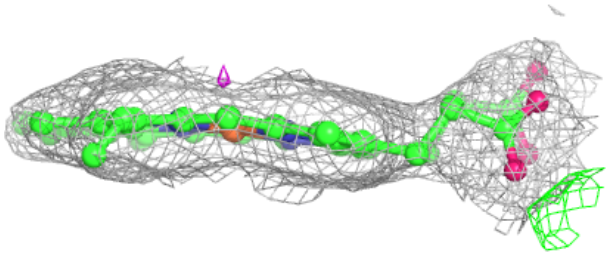


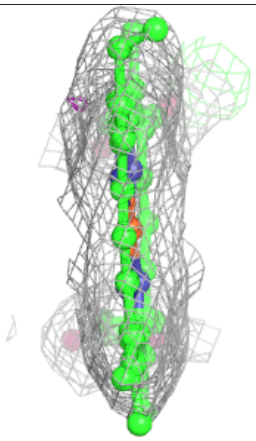


Electron density around HEM A 601:

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

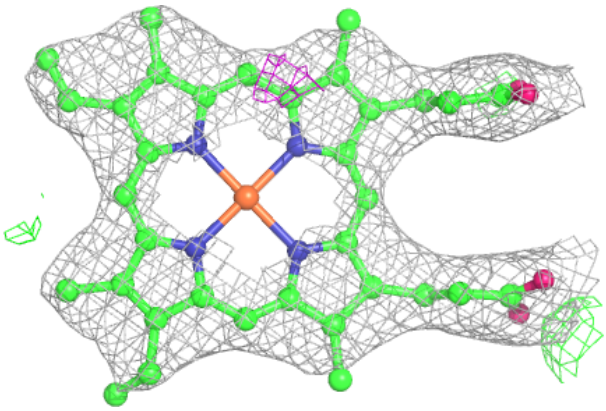


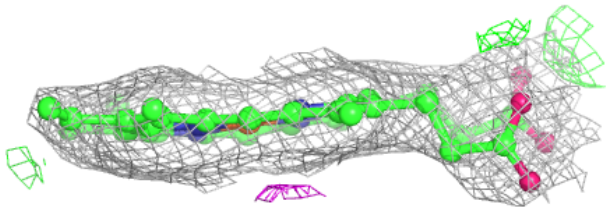


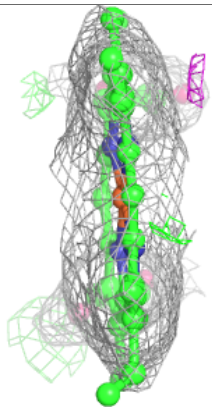


Electron density around HEM B 601:

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







6.5 Other polymers (i)

There are no such residues in this entry.