Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 08:29 PM EDT

PDB ID	:	3LD6 / pdb_00003ld6
Title	:	Crystal structure of human lanosterol 14alpha-demethylase (CYP51) in complex with ketoconazole
Authors	:	Strushkevich, N.; Tempel, W.; MacKenzie, F.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Weigelt, J.; Park, H.; Structural Genomics Consortium (SGC)
Deposited on	:	2010-01-12
Resolution	:	2.80 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 (i)) were used in the production of this report:

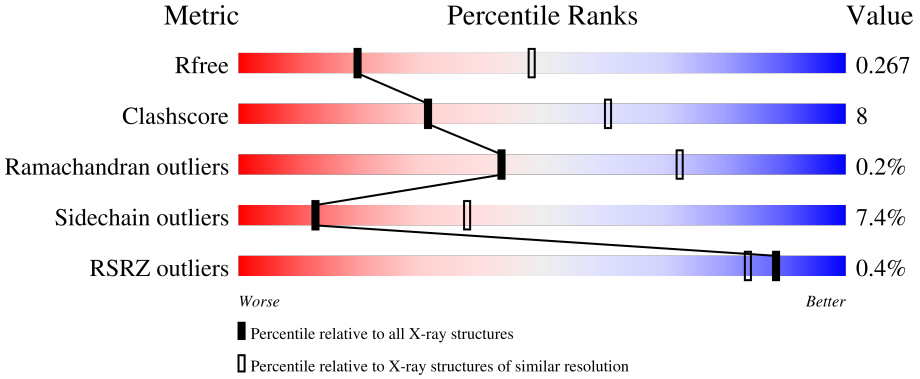
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	73% 21% • •
1	B	461	75% 19% • •
2	C	7	43% 43% 14%
2	D	7	14% 57% 29%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7522 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.

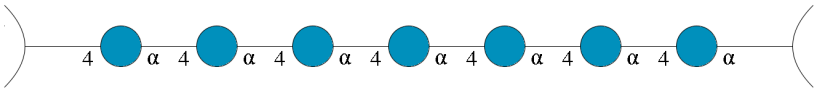
- Molecule 1 is a protein called Lanosterol 14-alpha demethylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	445	3589	2310	611	652	16	0	0	0
1	B	444	3583	2307	610	650	16	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

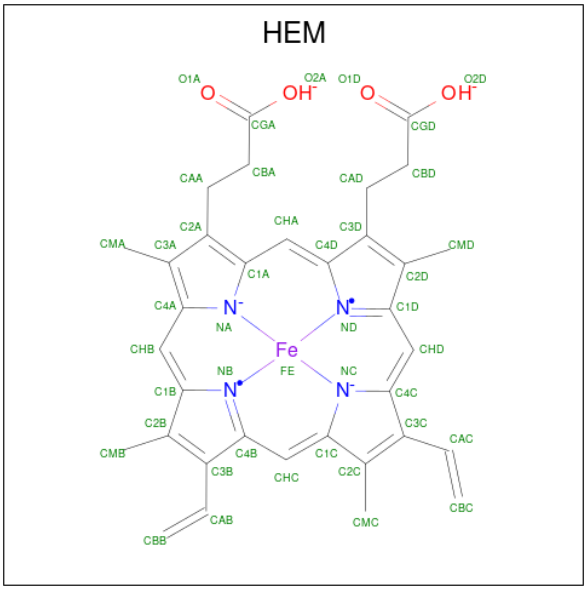
Chain	Residue	Modelled	Actual	Comment	Reference
A	49	MET	-	expression tag	UNP Q16850
A	50	ALA	-	expression tag	UNP Q16850
A	51	LYS	-	expression tag	UNP Q16850
A	52	LYS	-	expression tag	UNP Q16850
A	53	THR	-	expression tag	UNP Q16850
A	503	THR	-	expression tag	UNP Q16850
A	504	HIS	-	expression tag	UNP 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).



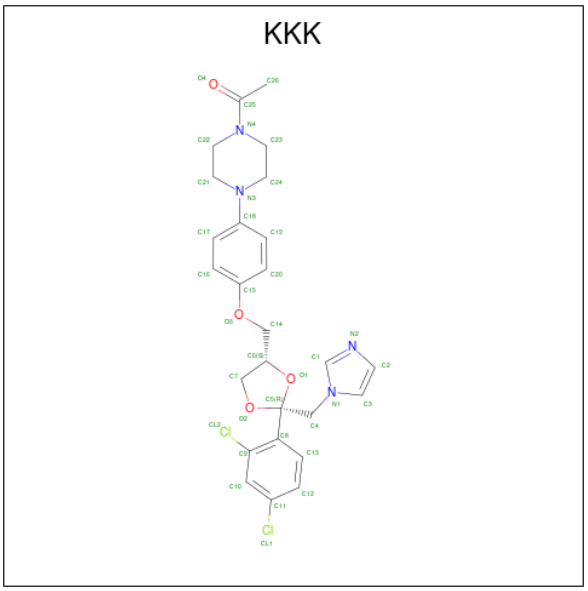
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	C	7	77	42	35	0	0	0
2	D	7	77	42	35	0	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is 1-acetyl-4-(4-{[(2R,4S)-2-(2,4-dichlorophenyl)-2-(1H-imidazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxy}phenyl)piperazine (CCD ID: KKK) (formula: $C_{26}H_{28}Cl_2N_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
4	A	1	36	26	2	4	4	0	0
			Total	C	Cl	N	O		
4	B	1	36	26	2	4	4	0	0

- Molecule 5 is water.

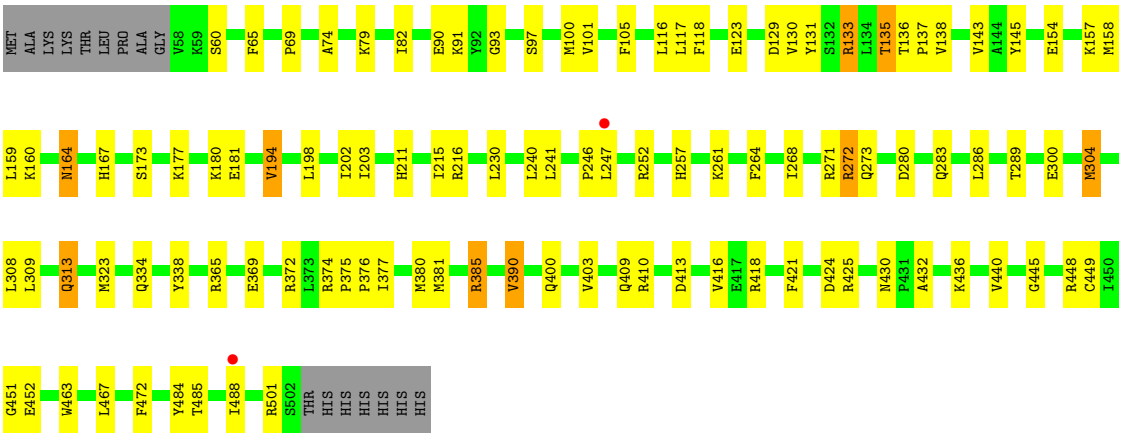
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	26	26	26	0	0
			Total	O		
5	B	12	12	12	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

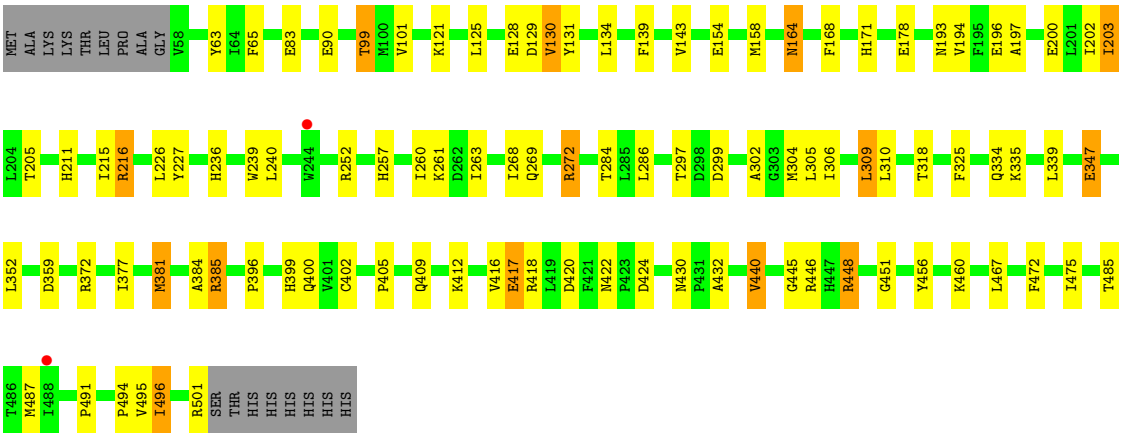
• Molecule 1: Lanosterol 14-alpha demethylase

Chain A: 73% 21%



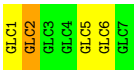
• Molecule 1: Lanosterol 14-alpha demethylase

Chain B: 75% 19%



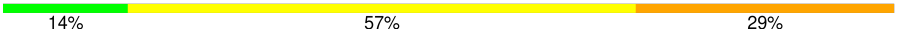
• Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)

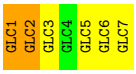
Chain C: 43% 43% 14%



• 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	145.73Å 145.73Å 110.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.29 – 2.80 24.29 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (24.29-2.80) 98.7 (24.29-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.95 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.212 , 0.275 0.210 , 0.267	Depositor DCC
R_{free} test set	1491 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	59.8	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 34.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7522	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: KKK, HEM, 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	0.54	0/3682	0.88	7/4988 (0.1%)
1	B	0.51	0/3676	0.84	0/4980
All	All	0.53	0/7358	0.86	7/9968 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	93	GLY	CA-C-N	5.71	125.33	119.56
1	A	93	GLY	C-N-CA	5.71	125.33	119.56
1	A	374	ARG	CA-C-N	-5.47	114.75	120.38
1	A	374	ARG	C-N-CA	-5.47	114.75	120.38
1	A	194	VAL	CB-CA-C	-5.25	105.16	111.88
1	A	241	LEU	CA-C-N	5.00	125.00	119.89
1	A	241	LEU	C-N-CA	5.00	125.00	119.89

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	3589	0	3581	62	0
1	B	3583	0	3576	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	77	0	63	1	0
2	D	77	0	63	2	0
3	A	43	0	30	6	0
3	B	43	0	30	4	0
4	A	36	0	28	2	0
4	B	36	0	28	5	0
5	A	26	0	0	2	0
5	B	12	0	0	1	0
All	All	7522	0	7399	122	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (122) 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:135:THR:HG22	5:A:20:HOH:O	1.63	0.98
1:A:116:LEU:HB2	1:A:390:VAL:HG21	1.51	0.92
1:B:381:MET:HE2	4:B:602:KKK:H21	1.55	0.87
1:A:334:GLN:HE22	1:A:472:PHE:H	1.26	0.83
1:B:467:LEU:O	1:B:501:ARG:HD3	1.80	0.82
1:B:334:GLN:HE22	1:B:472:PHE:H	1.26	0.79
1:B:129:ASP:OD2	1:B:385:ARG:HD3	1.87	0.75
1:A:409:GLN:HE21	1:A:440:VAL:H	1.33	0.74
1:B:372:ARG:NH2	1:B:418:ARG:O	2.20	0.74
1:A:309:LEU:O	1:A:313:GLN:HB2	1.87	0.73
1:B:456:TYR:O	1:B:460:LYS:HB2	1.88	0.73
1:A:116:LEU:HB2	1:A:390:VAL:CG2	2.18	0.72
1:B:381:MET:CE	4:B:602:KKK:H21	2.20	0.71
1:A:101:VAL:HG12	1:A:101:VAL:O	1.91	0.69
1:A:131:TYR:CZ	4:A:602:KKK:H14	2.28	0.68
3:B:601:HEM:HBB2	3:B:601:HEM:HMB2	1.76	0.67
1:A:135:THR:HG21	1:A:145:TYR:HD1	1.60	0.66
1:B:130:VAL:HG11	1:B:381:MET:HB3	1.78	0.65
1:A:130:VAL:HB	1:A:381:MET:HE3	1.77	0.65
1:B:297:THR:HG22	1:B:299:ASP:H	1.62	0.65
1:B:101:VAL:HG12	1:B:101:VAL:O	1.95	0.64
1:A:198:LEU:O	1:A:202:ILE:HG12	1.97	0.64
1:A:133:ARG:HG3	5:A:21:HOH:O	1.97	0.64
1:B:226:LEU:HB3	1:B:260:ILE:HD11	1.81	0.62
1:A:430:ASN:ND2	1:A:432:ALA:HB3	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:VAL:HG13	1:A:230:LEU:HD22	1.83	0.61
1:A:129:ASP:OD2	1:A:385:ARG:HD3	1.99	0.60
1:B:193:ASN:HB3	1:B:196:GLU:HG2	1.83	0.59
1:B:131:TYR:CE2	4:B:602:KKK:H14	2.37	0.58
1:B:65:PHE:HD1	2:D:2:GLC:H3	1.68	0.58
1:B:154:GLU:O	1:B:158:MET:HG3	2.04	0.57
1:B:194:VAL:HB	1:B:496:ILE:CG1	2.35	0.57
1:B:131:TYR:CZ	4:B:602:KKK:H14	2.40	0.57
1:B:409:GLN:NE2	1:B:440:VAL:H	2.03	0.57
1:A:410:ARG:HG2	1:A:418:ARG:NH1	2.21	0.56
1:B:335:LYS:O	1:B:339:LEU:HG	2.05	0.56
1:A:323:MET:HE2	1:A:463:TRP:CD1	2.41	0.56
1:A:177:LYS:O	1:A:181:GLU:HG3	2.05	0.56
1:A:369:GLU:OE1	1:A:372:ARG:HD3	2.05	0.56
1:A:416:VAL:O	1:A:425:ARG:NH2	2.39	0.56
1:A:159:LEU:HD22	1:A:308:LEU:HD21	1.87	0.55
1:A:272:ARG:NH1	1:A:286:LEU:HD22	2.21	0.55
1:B:211:HIS:HB3	1:B:215:ILE:HD12	1.88	0.55
1:B:257:HIS:CE1	1:B:261:LYS:HE3	2.41	0.55
1:A:272:ARG:HH11	1:A:286:LEU:HD22	1.72	0.55
1:B:302:ALA:HA	1:B:305:LEU:HD12	1.90	0.54
1:B:63:TYR:OH	1:B:99:THR:OG1	2.25	0.54
1:B:430:ASN:ND2	1:B:432:ALA:HB3	2.23	0.53
1:B:325:PHE:CE2	1:B:496:ILE:HG23	2.44	0.53
1:A:154:GLU:O	1:A:158:MET:HG3	2.08	0.52
1:A:271:ARG:C	1:A:273:GLN:H	2.17	0.52
1:A:300:GLU:O	1:A:304:MET:HG2	2.10	0.52
1:B:416:VAL:HG12	1:B:417:GLU:HG2	1.90	0.52
1:B:440:VAL:O	1:B:440:VAL:HG13	2.09	0.52
1:B:164:ASN:HD22	1:B:164:ASN:C	2.18	0.52
1:A:467:LEU:O	1:A:501:ARG:HD2	2.09	0.52
3:B:601:HEM:HBB2	3:B:601:HEM:CMB	2.39	0.51
3:B:601:HEM:C1A	4:B:602:KKK:H1	2.46	0.50
1:B:268:ILE:O	1:B:272:ARG:HB2	2.12	0.50
1:A:74:ALA:HA	1:A:100:MET:HE3	1.94	0.50
1:B:200:GLU:O	1:B:203:ILE:HG22	2.12	0.50
1:A:118:PHE:HE2	1:A:380:MET:CE	2.26	0.48
1:B:430:ASN:HD22	1:B:432:ALA:HB3	1.78	0.48
1:B:377:ILE:HD12	1:B:377:ILE:N	2.28	0.48
1:B:196:GLU:HG3	1:B:197:ALA:N	2.30	0.47
1:B:422:ASN:HD21	1:B:424:ASP:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:GLY:HA3	3:B:601:HEM:C2C	2.49	0.47
1:B:202:ILE:HA	1:B:205:THR:OG1	2.15	0.47
1:A:117:LEU:HD13	1:A:403:VAL:HG23	1.96	0.47
1:B:318:THR:HG22	5:B:9:HOH:O	2.14	0.47
1:A:97:SER:HA	1:A:105:PHE:O	2.15	0.46
1:A:211:HIS:HB3	1:A:215:ILE:HD12	1.98	0.46
1:B:194:VAL:HB	1:B:496:ILE:HG13	1.97	0.46
1:B:125:LEU:HD23	1:B:384:ALA:HA	1.98	0.46
1:A:101:VAL:HG11	1:A:240:LEU:HD22	1.98	0.46
1:B:121:LYS:HD2	1:B:446:ARG:NH2	2.31	0.46
1:B:260:ILE:HA	1:B:263:ILE:HD12	1.97	0.46
1:B:381:MET:HG2	1:B:402:CYS:SG	2.56	0.45
1:A:449:CYS:HB2	3:A:601:HEM:NA	2.31	0.45
1:A:449:CYS:HA	3:A:601:HEM:C4D	2.52	0.45
1:B:445:GLY:O	1:B:448:ARG:HB3	2.17	0.45
1:A:271:ARG:HD3	1:A:283:GLN:OE1	2.16	0.45
1:A:271:ARG:C	1:A:273:GLN:N	2.73	0.45
1:B:491:PRO:HB2	1:B:494:PRO:HB3	1.98	0.45
1:A:377:ILE:HD12	3:A:601:HEM:C4A	2.51	0.44
1:B:396:PRO:HG2	1:B:399:HIS:CD2	2.53	0.44
1:B:178:GLU:OE2	1:B:216:ARG:HD2	2.18	0.44
1:A:334:GLN:HE22	1:A:472:PHE:N	2.05	0.44
1:B:168:PHE:HD1	1:B:171:HIS:HD2	1.65	0.44
1:B:134:LEU:HD22	1:B:239:TRP:HD1	1.81	0.44
1:A:65:PHE:HD1	2:C:2:GLC:H3	1.83	0.44
1:A:118:PHE:HE2	1:A:380:MET:HE1	1.82	0.44
1:A:211:HIS:CE1	1:A:309:LEU:HB2	2.53	0.44
1:A:369:GLU:HG3	1:A:421:PHE:CD1	2.53	0.44
1:A:375:PRO:HA	1:A:376:PRO:HD3	1.85	0.43
1:A:304:MET:HG2	1:A:304:MET:H	1.67	0.43
1:B:272:ARG:HH11	1:B:286:LEU:HD22	1.83	0.43
1:A:79:LYS:HD3	1:A:79:LYS:HA	1.77	0.42
1:B:101:VAL:HG11	1:B:240:LEU:HD22	2.00	0.42
1:B:347:GLU:H	1:B:347:GLU:HG2	1.63	0.42
1:A:338:TYR:CD1	1:A:501:ARG:HD3	2.55	0.42
1:A:365:ARG:NH1	1:A:424:ASP:OD1	2.49	0.42
1:B:139:PHE:HD2	1:B:306:ILE:HG22	1.85	0.41
1:A:448:ARG:NH2	1:A:452:GLU:OE1	2.51	0.41
2:D:1:GLC:H62	2:D:2:GLC:H5	2.02	0.41
1:A:257:HIS:CE1	1:A:261:LYS:HE3	2.55	0.41
1:A:164:ASN:ND2	1:A:167:HIS:H	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:TYR:CD2	1:B:309:LEU:HD21	2.55	0.41
1:B:475:ILE:HD11	1:B:495:VAL:HG12	2.02	0.41
1:A:82:ILE:HD12	1:A:484:TYR:OH	2.20	0.41
1:A:136:THR:HB	1:A:137:PRO:HD3	2.03	0.41
1:A:451:GLY:HA3	3:A:601:HEM:C2C	2.55	0.41
1:B:405:PRO:HB3	1:B:409:GLN:HE22	1.86	0.41
1:A:377:ILE:HD12	3:A:601:HEM:CHB	2.51	0.41
1:A:413:ASP:OD1	1:A:413:ASP:N	2.54	0.41
1:A:449:CYS:HB2	3:A:601:HEM:C1A	2.54	0.41
4:A:602:KKK:CL2	4:A:602:KKK:O2	2.75	0.41
1:A:101:VAL:O	1:A:101:VAL:CG1	2.63	0.40
1:A:271:ARG:HH12	1:A:280:ASP:CG	2.27	0.40
1:A:445:GLY:O	1:A:448:ARG:HB2	2.20	0.40
1:A:264:PHE:O	1:A:268:ILE:HG13	2.20	0.40
1:A:448:ARG:HD3	1:A:449:CYS:N	2.36	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%)	425 (96%)	16 (4%)	2 (0%)	24 55
1	B	442/461 (96%)	415 (94%)	27 (6%)	0	100 100
All	All	885/922 (96%)	840 (95%)	43 (5%)	2 (0%)	43 72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	246	PRO
1	A	69	PRO

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%)	363 (93%)	27 (7%)	14	41
1	B	389/403 (96%)	358 (92%)	31 (8%)	11	34
All	All	779/806 (97%)	721 (93%)	58 (7%)	13	37

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

Mol	Chain	Res	Type
1	A	60	SER
1	A	90	GLU
1	A	91	LYS
1	A	123	GLU
1	A	133	ARG
1	A	135	THR
1	A	143	VAL
1	A	157	LYS
1	A	160	LYS
1	A	164	ASN
1	A	173	SER
1	A	180	LYS
1	A	194	VAL
1	A	203	ILE
1	A	216	ARG
1	A	247	LEU
1	A	252	ARG
1	A	272	ARG
1	A	289	THR
1	A	304	MET
1	A	313	GLN
1	A	385	ARG
1	A	390	VAL
1	A	400	GLN
1	A	436	LYS
1	A	485	THR
1	A	488	ILE

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Mol	Chain	Res	Type
1	B	83	GLU
1	B	90	GLU
1	B	99	THR
1	B	128	GLU
1	B	130	VAL
1	B	143	VAL
1	B	164	ASN
1	B	203	ILE
1	B	216	ARG
1	B	236	HIS
1	B	252	ARG
1	B	269	GLN
1	B	272	ARG
1	B	284	THR
1	B	304	MET
1	B	309	LEU
1	B	310	LEU
1	B	347	GLU
1	B	352	LEU
1	B	359	ASP
1	B	381	MET
1	B	385	ARG
1	B	400	GLN
1	B	412	LYS
1	B	417	GLU
1	B	420	ASP
1	B	440	VAL
1	B	448	ARG
1	B	485	THR
1	B	487	MET
1	B	496	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	ASN
1	A	164	ASN
1	A	170	GLN
1	A	334	GLN
1	A	388	GLN
1	A	409	GLN
1	A	422	ASN

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Mol	Chain	Res	Type
1	A	430	ASN
1	A	489	HIS
1	A	493	ASN
1	B	164	ASN
1	B	334	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	0.36	0	15,15,17	0.91	1 (6%)
2	GLC	C	2	2	11,11,12	0.37	0	15,15,17	2.47	3 (20%)
2	GLC	C	3	2	11,11,12	0.32	0	15,15,17	0.82	0
2	GLC	C	4	2	11,11,12	0.56	0	15,15,17	1.06	0
2	GLC	C	5	2	11,11,12	0.51	0	15,15,17	1.50	2 (13%)
2	GLC	C	6	2	11,11,12	0.43	0	15,15,17	2.23	3 (20%)
2	GLC	C	7	2	11,11,12	0.41	0	15,15,17	0.74	0
2	GLC	D	1	2	11,11,12	0.34	0	15,15,17	1.27	1 (6%)
2	GLC	D	2	2	11,11,12	0.24	0	15,15,17	0.98	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GLC	D	3	2	11,11,12	0.34	0	15,15,17	0.95	1 (6%)
2	GLC	D	4	2	11,11,12	0.44	0	15,15,17	0.65	0
2	GLC	D	5	2	11,11,12	0.51	0	15,15,17	0.89	1 (6%)
2	GLC	D	6	2	11,11,12	0.61	0	15,15,17	1.87	4 (26%)
2	GLC	D	7	2	11,11,12	0.70	0	15,15,17	1.33	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	-	0/2/19/22	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	-	2/2/19/22	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	-	2/2/19/22	0/1/1/1
2	GLC	D	1	2	-	0/2/19/22	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
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 (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	GLC	C1-O5-C5	8.19	123.16	112.19
2	C	6	GLC	C1-O5-C5	7.18	121.81	112.19
2	D	6	GLC	C1-O5-C5	4.70	118.49	112.19
2	D	1	GLC	C1-O5-C5	3.48	116.85	112.19
2	D	7	GLC	C1-C2-C3	3.33	114.49	109.64
2	D	7	GLC	C2-C3-C4	3.31	116.68	110.86
2	C	5	GLC	C3-C4-C5	-3.20	104.43	110.23
2	C	6	GLC	O5-C5-C4	3.02	118.17	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	6	GLC	C2-C3-C4	2.80	115.79	110.86
2	C	5	GLC	O5-C5-C6	2.75	113.02	107.66
2	C	1	GLC	O4-C4-C3	-2.53	104.42	110.38
2	D	6	GLC	C1-C2-C3	2.48	113.25	109.64
2	C	6	GLC	C3-C4-C5	2.46	114.70	110.23
2	C	2	GLC	O4-C4-C3	-2.45	104.61	110.38
2	D	3	GLC	O4-C4-C3	-2.43	104.64	110.38
2	D	6	GLC	C3-C4-C5	2.19	114.20	110.23
2	C	2	GLC	O5-C5-C4	2.17	116.10	110.83
2	D	5	GLC	C1-C2-C3	2.15	112.77	109.64
2	D	2	GLC	O4-C4-C3	-2.08	105.48	110.38

There are no chirality outliers.

All (16) torsion outliers are listed below:

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

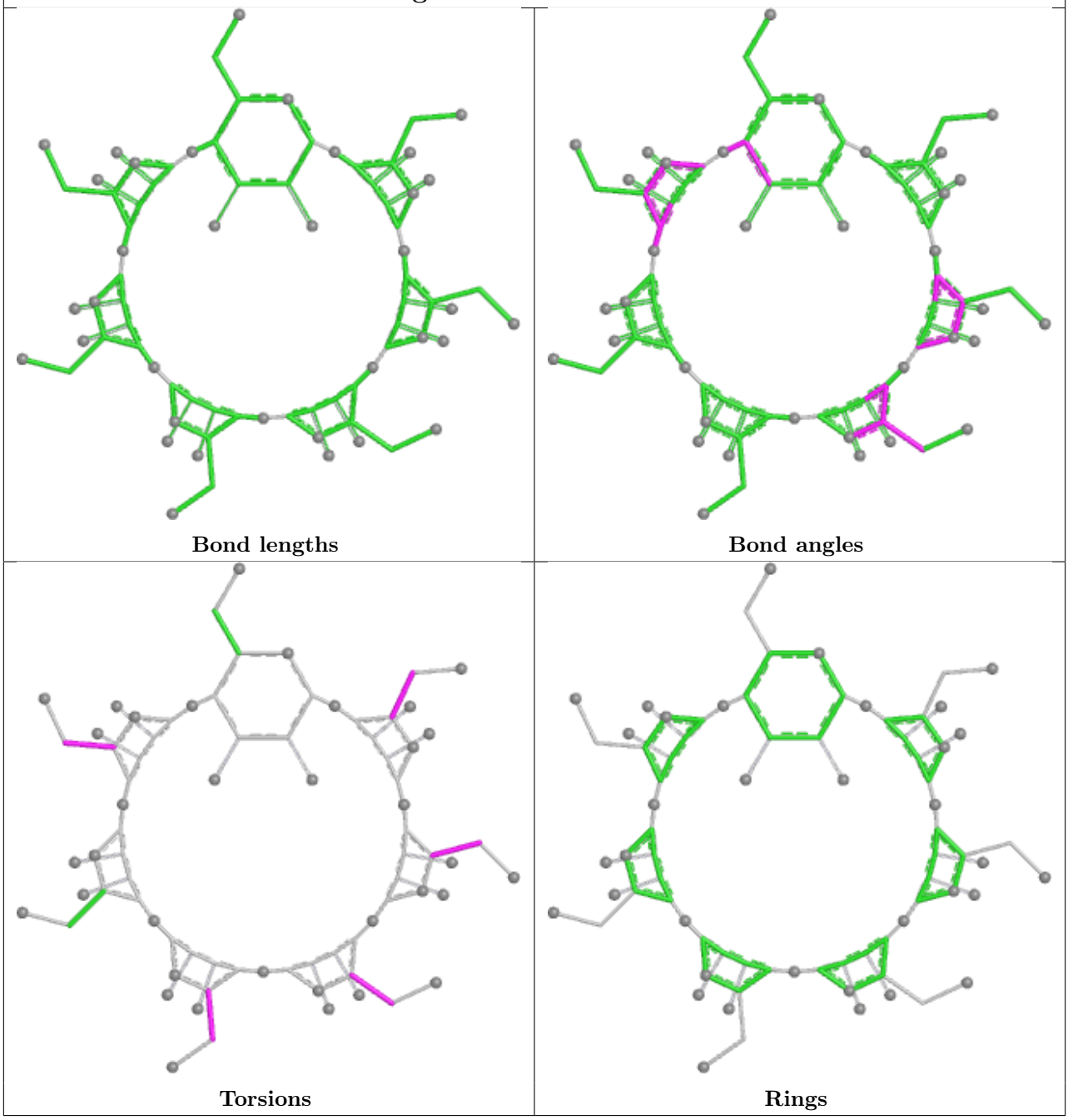
There are no ring outliers.

3 monomers are involved in 3 short contacts:

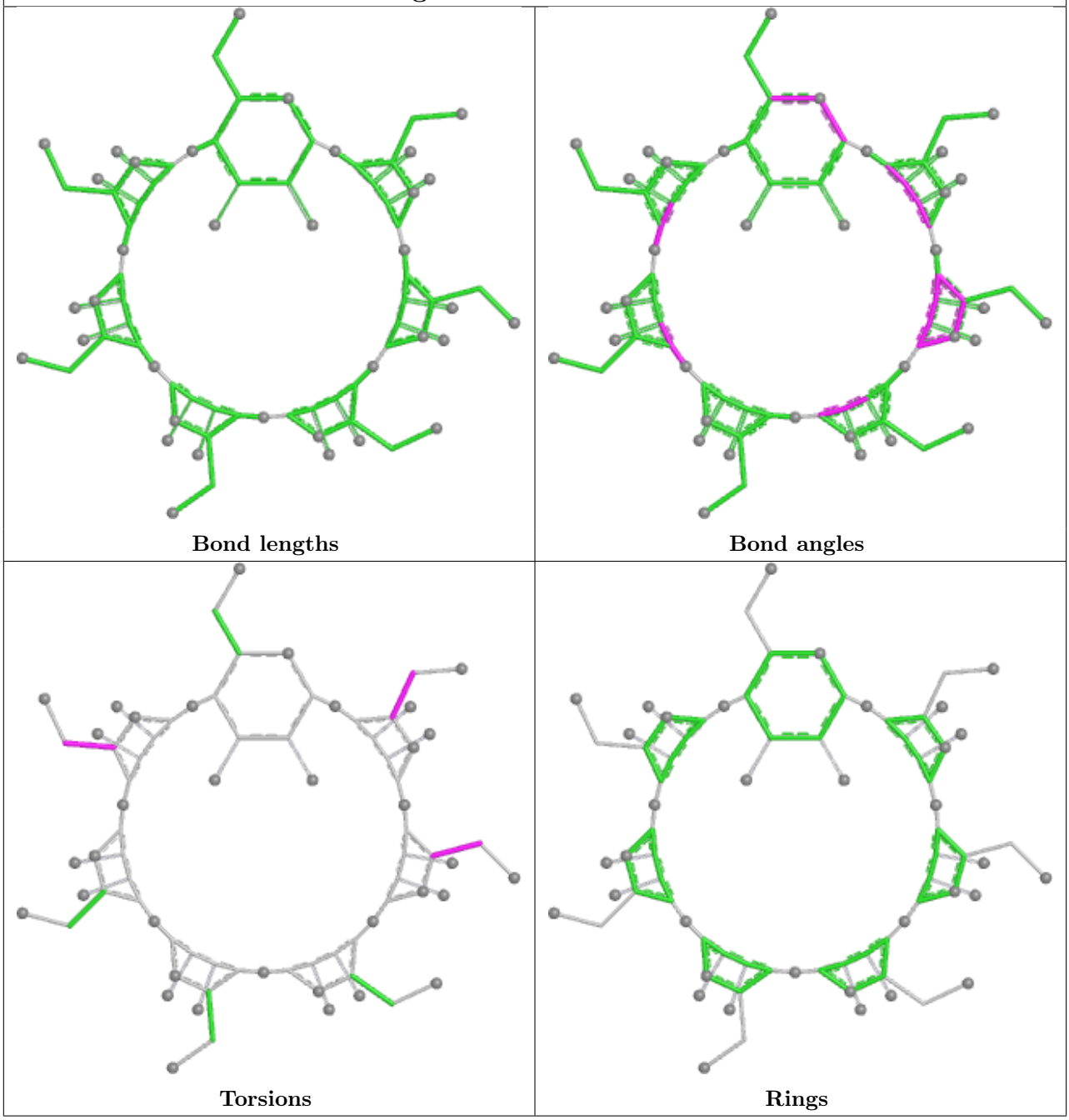
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	GLC	1	0
2	D	1	GLC	1	0
2	D	2	GLC	2	0

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

Oligosaccharide Chain C



Oligosaccharide Chain D



5.6 Ligand geometry (i)

4 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	$\#\|Z\|>2$
4	KKK	A	602	3	40,40,40	0.93	3 (7%)	57,57,57	1.66	8 (14%)
3	HEM	A	601	4,1	50,50,50	1.80	9 (18%)	67,82,82	1.20	6 (8%)
3	HEM	B	601	4,1	50,50,50	1.94	9 (18%)	67,82,82	1.27	6 (8%)
4	KKK	B	602	3	40,40,40	0.81	2 (5%)	57,57,57	1.48	9 (15%)

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
4	KKK	A	602	3	-	8/24/45/45	0/5/5/5
3	HEM	A	601	4,1	-	1/14/54/54	-
3	HEM	B	601	4,1	-	3/14/54/54	-
4	KKK	B	602	3	-	10/24/45/45	0/5/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	HEM	C3D-C2D	7.98	1.54	1.36
3	A	601	HEM	C3D-C2D	7.59	1.53	1.36
3	B	601	HEM	FE-ND	6.04	2.13	1.94
3	A	601	HEM	FE-NB	4.08	2.07	1.94
3	A	601	HEM	FE-NA	3.89	2.08	1.95
3	A	601	HEM	FE-ND	3.45	2.05	1.94
3	B	601	HEM	FE-NB	3.44	2.05	1.94
4	A	602	KKK	C5-C8	-3.29	1.50	1.53
3	A	601	HEM	CAB-C3B	3.13	1.55	1.47
3	B	601	HEM	CAB-C3B	3.00	1.55	1.47
3	B	601	HEM	CAC-C3C	2.84	1.55	1.47
3	B	601	HEM	FE-NA	2.74	2.04	1.95
4	B	602	KKK	C9-CL2	2.74	1.80	1.73
4	A	602	KKK	C9-CL2	2.71	1.80	1.73
3	A	601	HEM	CAC-C3C	2.71	1.54	1.47
3	B	601	HEM	FE-NC	2.34	2.02	1.95
3	B	601	HEM	CMA-C3A	2.25	1.55	1.50
4	B	602	KKK	C11-CL1	2.18	1.79	1.74
3	A	601	HEM	CMB-C2B	2.14	1.55	1.50
3	A	601	HEM	CMC-C2C	2.12	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	KKK	C11-CL1	2.10	1.79	1.74
3	A	601	HEM	CMA-C3A	2.01	1.54	1.50
3	B	601	HEM	CMC-C2C	2.01	1.54	1.50

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	602	KKK	C5-C4-N1	7.17	119.00	112.76
3	B	601	HEM	C4D-ND-C1D	5.13	111.29	105.21
3	A	601	HEM	C4D-ND-C1D	4.84	110.94	105.21
4	B	602	KKK	C5-C4-N1	4.12	116.34	112.76
4	B	602	KKK	C4-C5-C8	3.93	115.11	109.59
4	A	602	KKK	C14-O3-C15	3.66	125.90	117.85
4	B	602	KKK	C5-C8-C9	-3.39	121.32	123.72
4	A	602	KKK	C5-C8-C9	-3.28	121.40	123.72
4	A	602	KKK	C4-C5-C8	3.25	114.16	109.59
4	A	602	KKK	C13-C8-C9	3.03	119.74	116.51
4	A	602	KKK	C24-C23-N4	-3.02	104.41	110.42
4	A	602	KKK	C23-C24-N3	-2.84	104.81	110.78
3	B	601	HEM	CAD-C3D-C4D	2.81	129.60	124.70
3	A	601	HEM	C1B-NB-C4B	2.57	108.25	105.21
3	A	601	HEM	CAD-CBD-CGD	-2.43	107.22	113.67
4	B	602	KKK	O1-C5-C4	-2.38	105.85	109.00
3	B	601	HEM	CHD-C4C-NC	2.36	127.03	124.45
4	B	602	KKK	C24-C23-N4	-2.28	105.87	110.42
3	A	601	HEM	CHA-C4D-ND	2.28	127.19	124.37
4	B	602	KKK	C12-C11-CL1	2.27	122.71	119.36
3	B	601	HEM	C3B-C2B-C1B	2.19	108.05	106.41
3	A	601	HEM	C3B-C4B-NB	-2.15	107.92	109.47
4	B	602	KKK	C10-C9-CL2	-2.12	114.98	118.45
3	B	601	HEM	C2A-C1A-NA	-2.09	107.83	110.15
3	A	601	HEM	CMD-C2D-C1D	2.08	128.28	125.03
4	B	602	KKK	C23-C24-N3	-2.07	106.43	110.78
4	B	602	KKK	C8-C9-CL2	2.05	124.17	121.70
3	B	601	HEM	C1B-NB-C4B	2.03	107.61	105.21
4	A	602	KKK	C14-C6-C7	-2.02	106.77	112.95

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	HEM	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
4	A	602	KKK	N1-C4-C5-O1
4	A	602	KKK	N1-C4-C5-O2
4	A	602	KKK	N1-C4-C5-C8
4	A	602	KKK	O3-C14-C6-O1
4	A	602	KKK	O3-C14-C6-C7
4	B	602	KKK	N1-C4-C5-O1
4	B	602	KKK	N1-C4-C5-O2
4	B	602	KKK	N1-C4-C5-C8
4	B	602	KKK	O3-C14-C6-O1
4	B	602	KKK	O3-C14-C6-C7
4	B	602	KKK	C16-C15-O3-C14
4	B	602	KKK	C20-C15-O3-C14
4	A	602	KKK	C16-C15-O3-C14
4	A	602	KKK	C20-C15-O3-C14
3	B	601	HEM	C4C-C3C-CAC-CBC
4	A	602	KKK	C6-C14-O3-C15
4	B	602	KKK	C6-C14-O3-C15
4	B	602	KKK	C19-C18-N3-C21
4	B	602	KKK	C17-C18-N3-C21
3	B	601	HEM	CAA-CBA-CGA-O2A
3	A	601	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

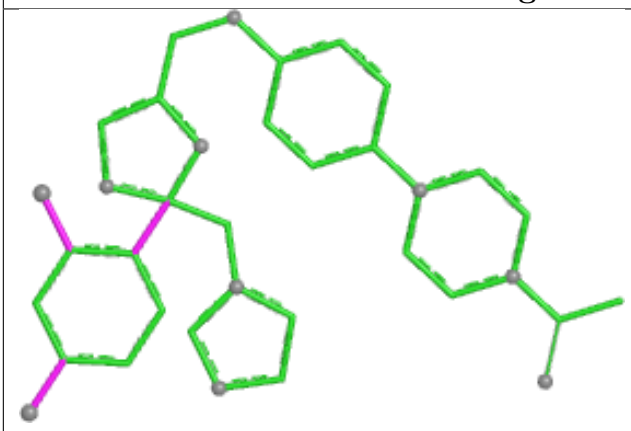
4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	KKK	2	0
3	A	601	HEM	6	0
3	B	601	HEM	4	0
4	B	602	KKK	5	0

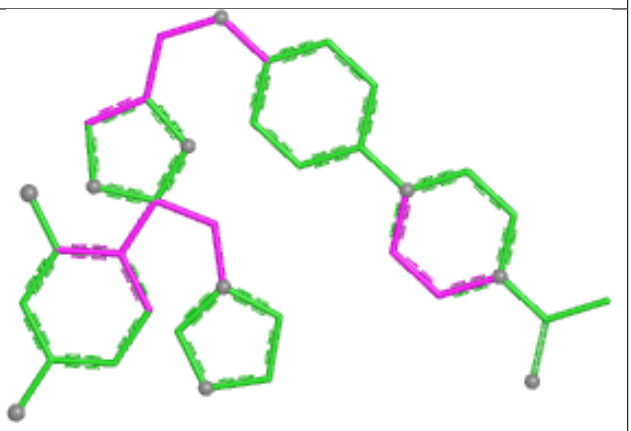
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

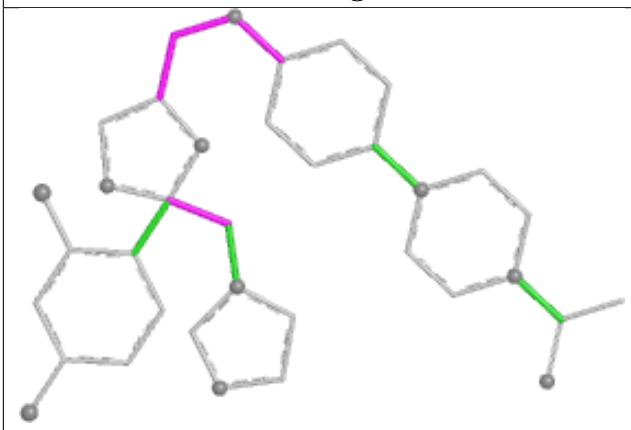
Ligand KKK A 602



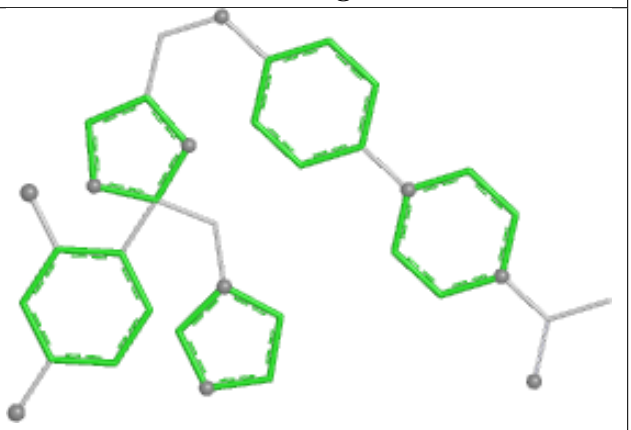
Bond lengths



Bond angles

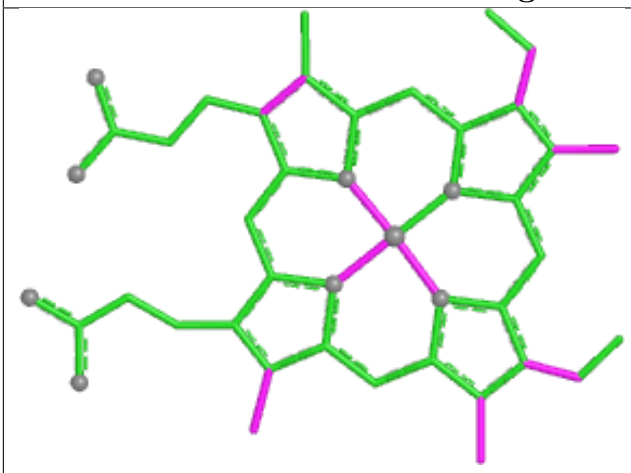


Torsions

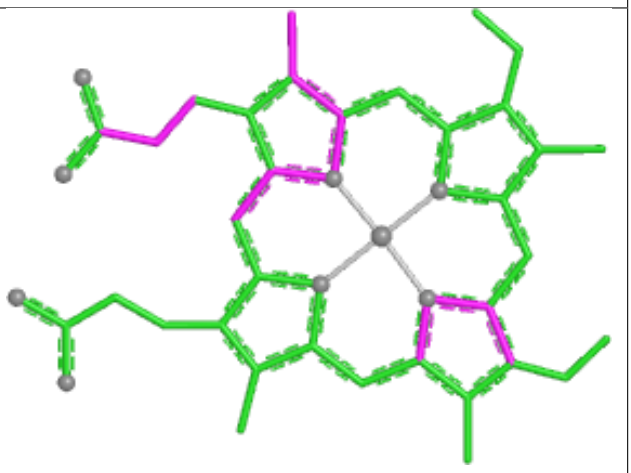


Rings

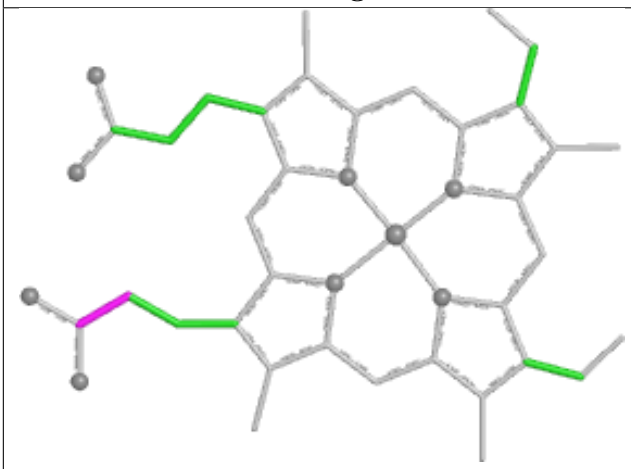
Ligand HEM A 601



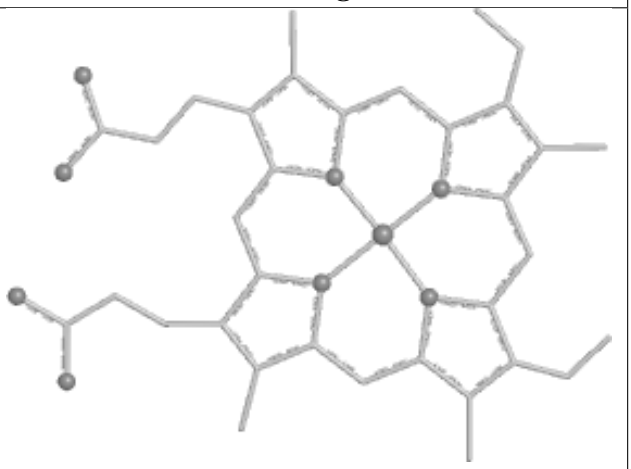
Bond lengths



Bond angles

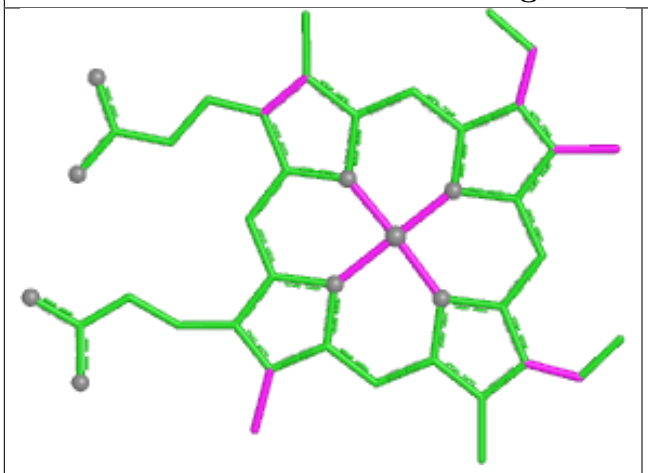


Torsions

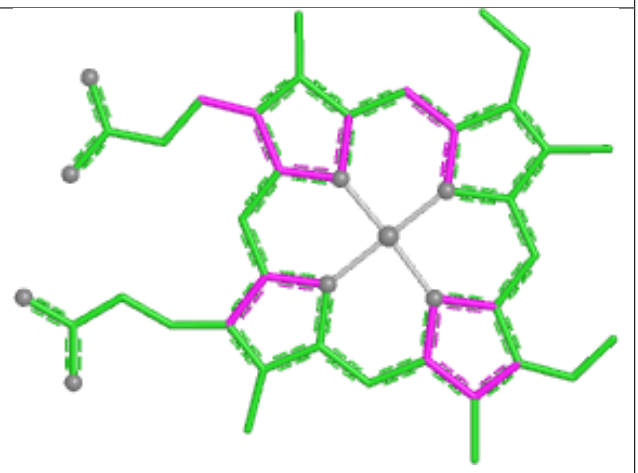


Rings

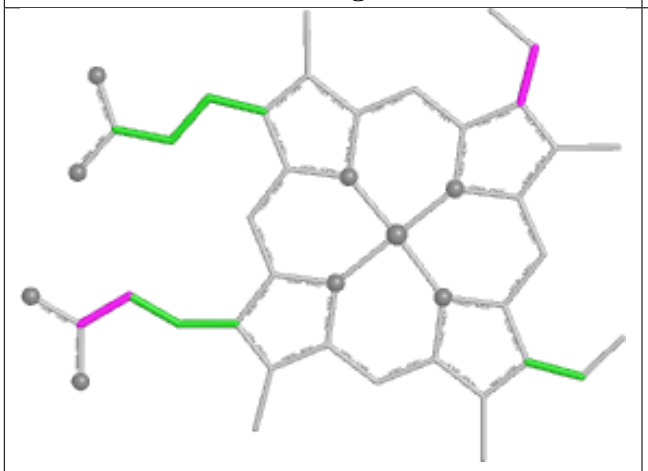
Ligand HEM B 601



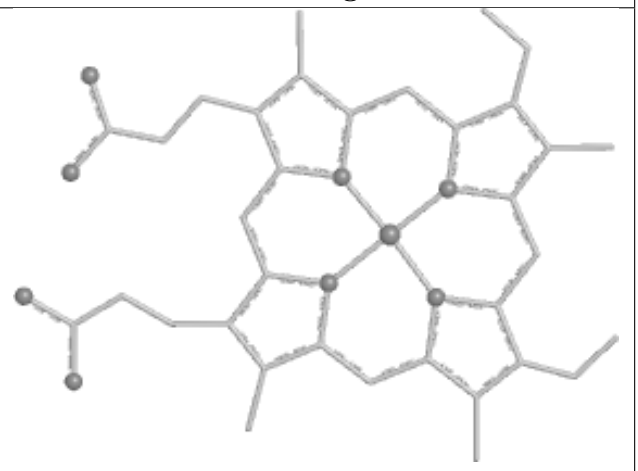
Bond lengths



Bond angles

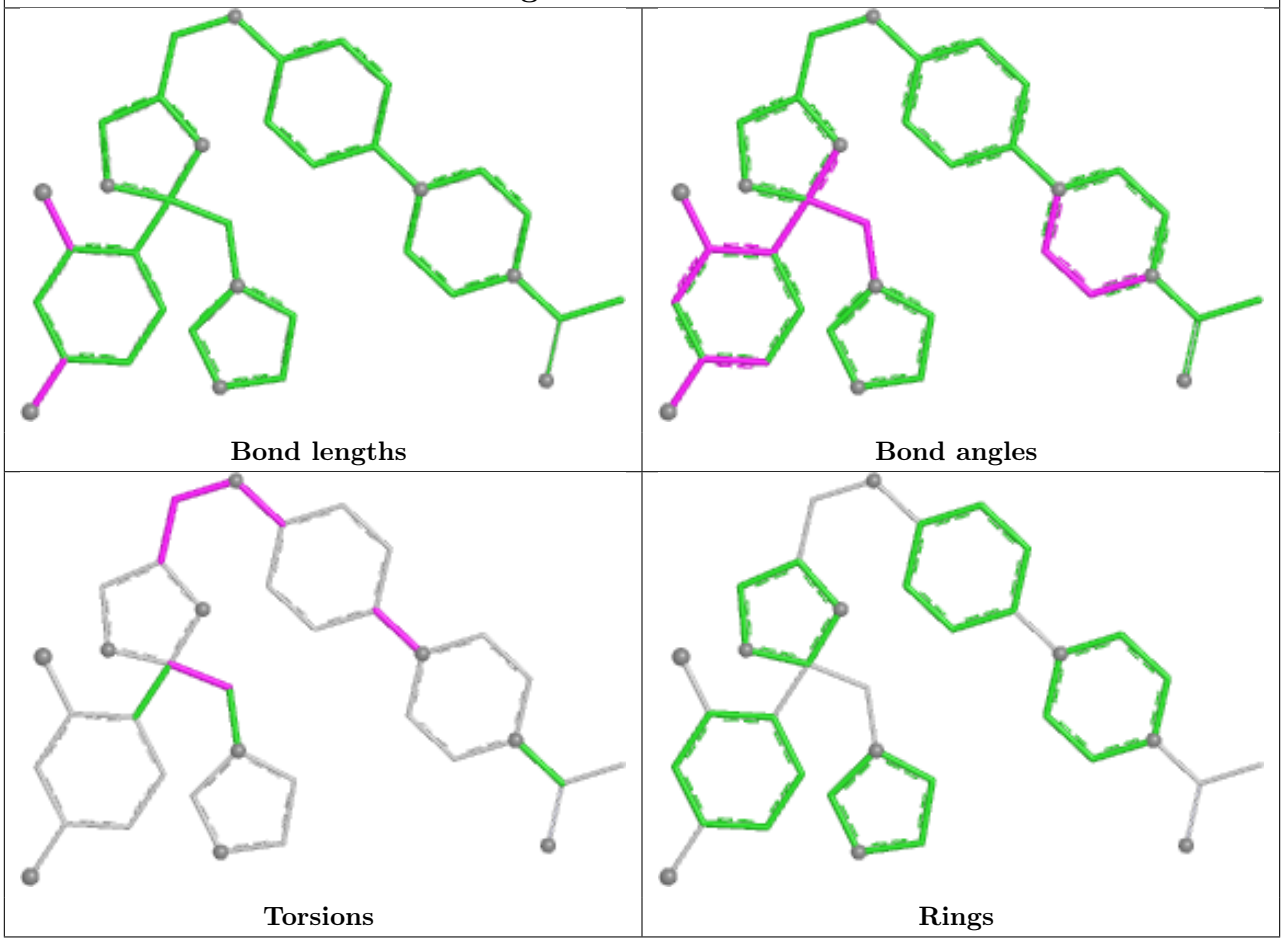


Torsions



Rings

Ligand KKK B 602



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	445/461 (96%)	-0.30	2 (0%)	88	84	32, 45, 70, 85	0
1	B	444/461 (96%)	0.05	2 (0%)	87	82	40, 61, 88, 98	0
All	All	889/922 (96%)	-0.13	4 (0%)	88	84	32, 52, 84, 98	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	488	ILE	3.1
1	A	247	LEU	2.9
1	A	488	ILE	2.7
1	B	244	TRP	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, 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	D	6	11/12	0.81	0.13	64,64,66,67	0
2	GLC	D	7	11/12	0.82	0.11	62,63,64,65	0
2	GLC	C	7	11/12	0.85	0.12	66,68,69,70	0
2	GLC	D	2	11/12	0.85	0.14	65,67,68,69	0
2	GLC	D	4	11/12	0.86	0.13	61,63,66,66	0

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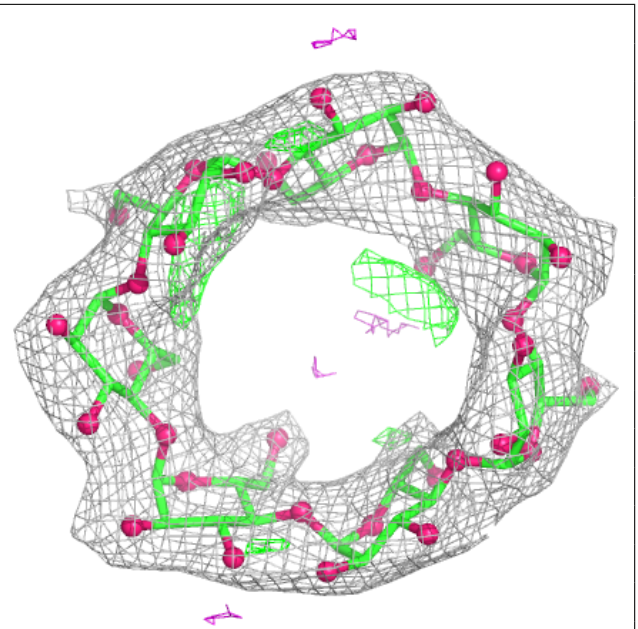
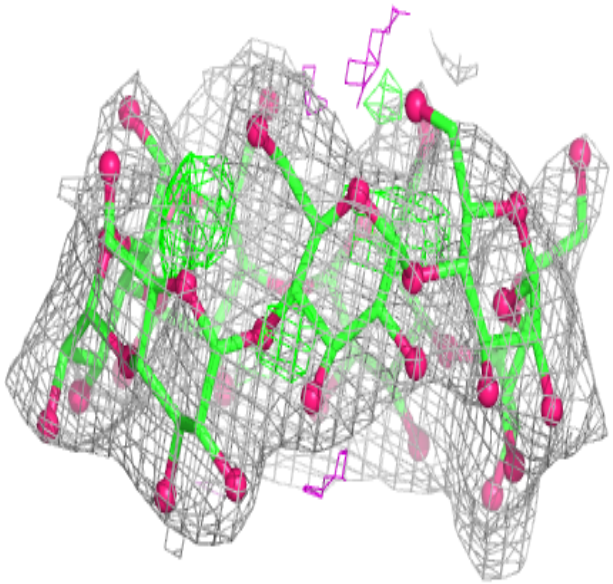
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	D	1	11/12	0.86	0.12	61,62,62,63	0
2	GLC	C	1	11/12	0.86	0.13	64,64,66,66	0
2	GLC	C	2	11/12	0.88	0.11	62,63,64,64	0
2	GLC	C	6	11/12	0.91	0.09	63,65,66,67	0
2	GLC	C	4	11/12	0.91	0.10	58,60,61,61	0
2	GLC	D	3	11/12	0.91	0.10	67,69,70,72	0
2	GLC	C	3	11/12	0.92	0.09	61,62,64,65	0
2	GLC	C	5	11/12	0.92	0.11	59,60,61,62	0
2	GLC	D	5	11/12	0.93	0.10	59,61,63,64	0

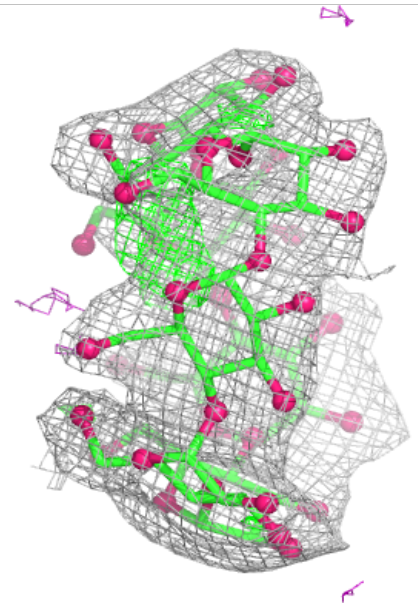
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

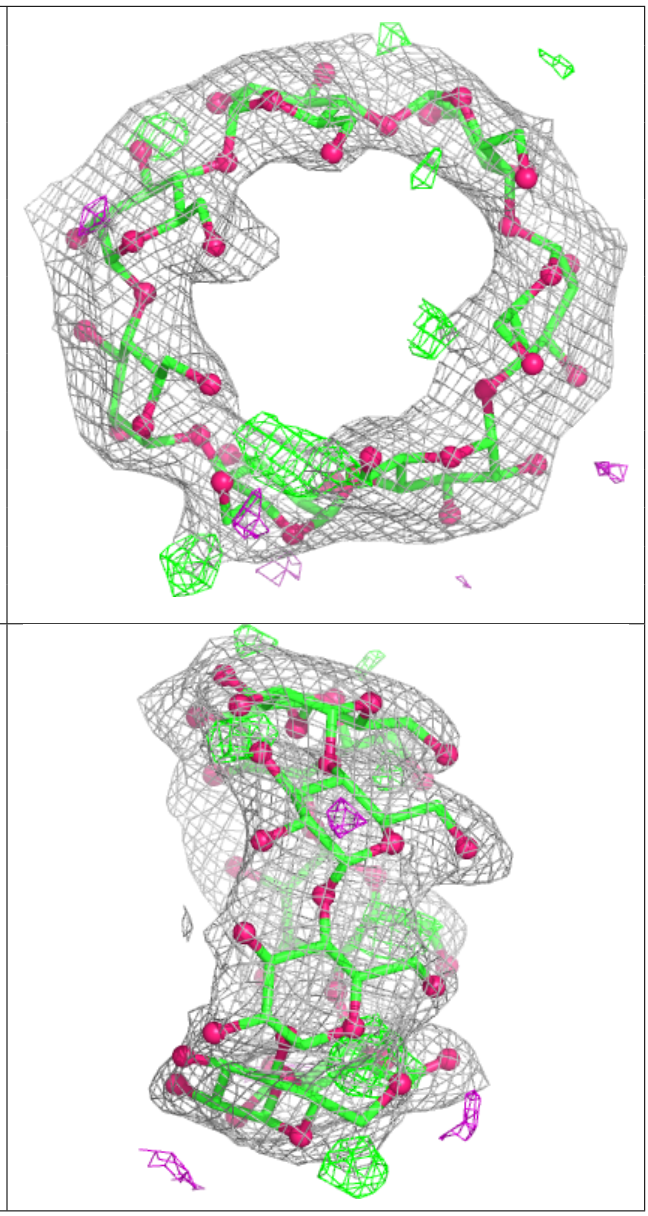






Electron density around Chain D:

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

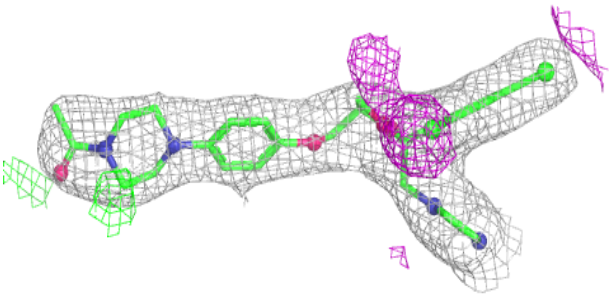
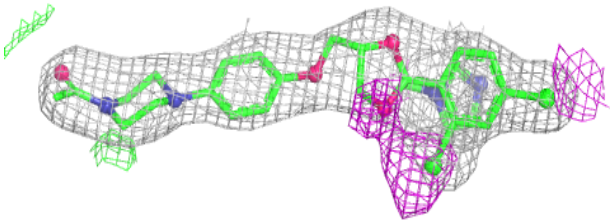
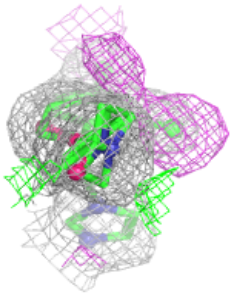


6.4 Ligands (i)

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.

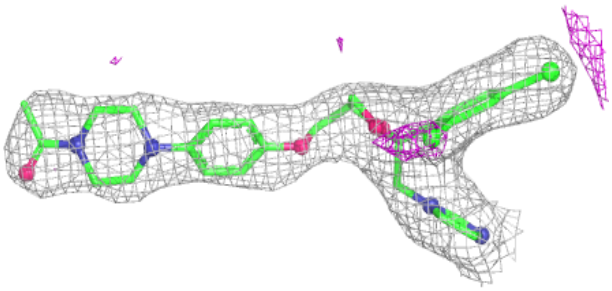
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	KKK	A	602	36/36	0.88	0.12	39,50,57,58	0
4	KKK	B	602	36/36	0.90	0.10	53,63,66,67	0
3	HEM	A	601	43/43	0.98	0.05	27,32,35,38	0
3	HEM	B	601	43/43	0.98	0.07	39,43,46,49	0

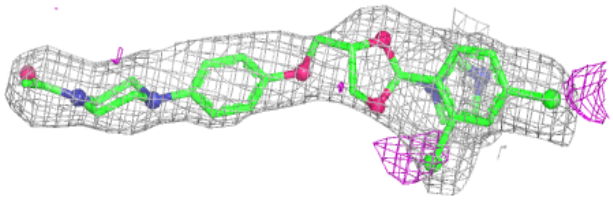
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

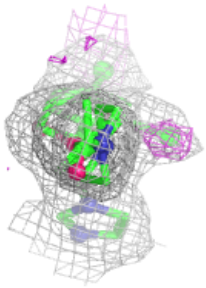
Electron density around KKK A 602: $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around KKK 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)

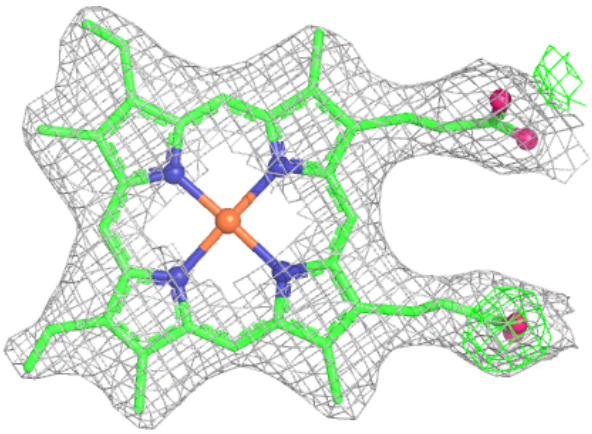


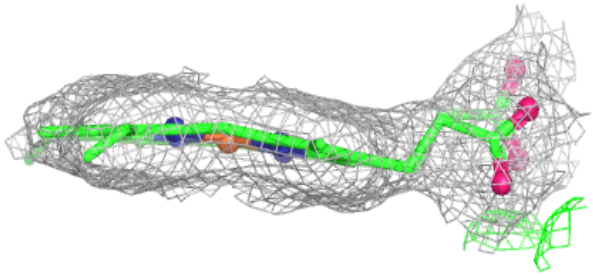


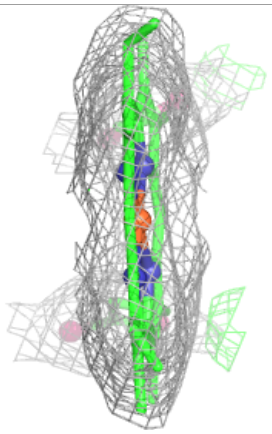


Electron density around HEM A 601:

$2mF_o$-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:

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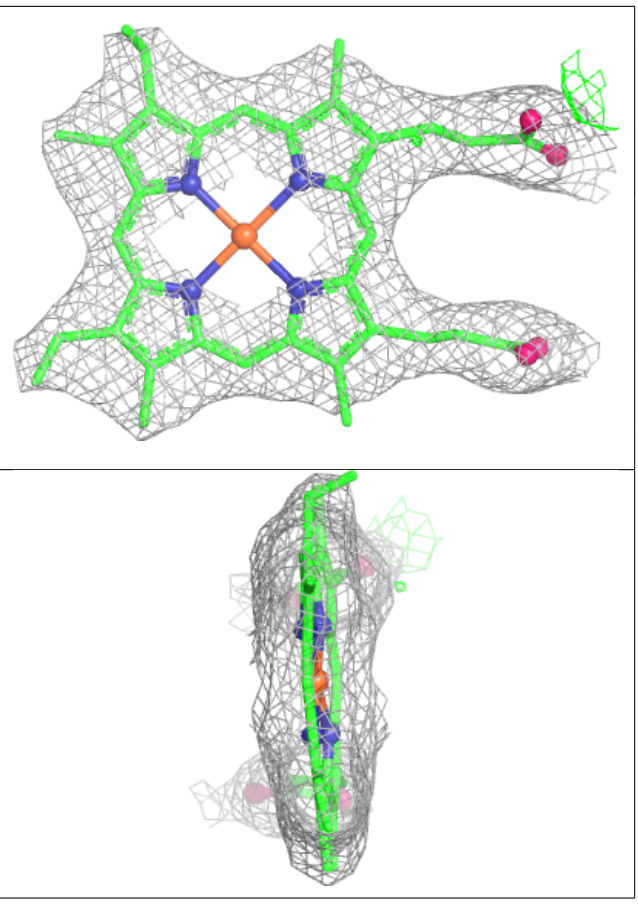
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.