



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:10 PM UTC

PDB ID : 3ZBY / pdb_00003zby
Title : Ligand-free structure of CYP142 from Mycobacterium smegmatis
Authors : Garcia-Fernandez, E.; Frank, D.J.; Galan, B.; Kells, P.M.; Podust, L.M.; Garcia, J.L.; Ortiz de Montellano, P.R.
Deposited on : 2012-11-13
Resolution : 1.93 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

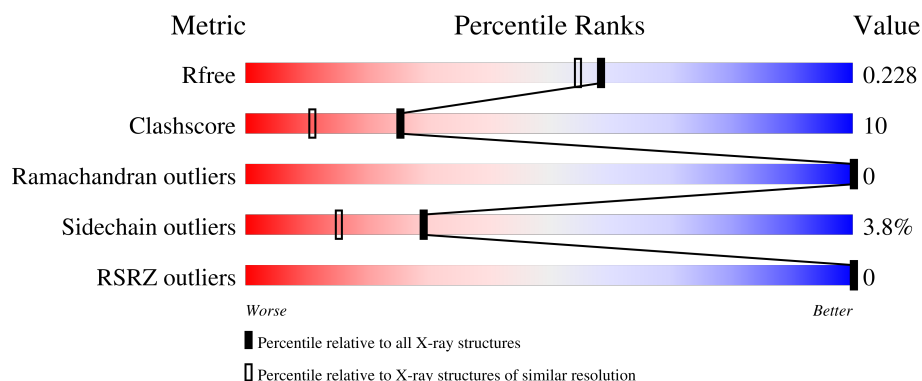
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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.



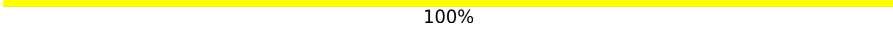
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	407	 82% 15% ..
1	B	407	 80% 17% ..
1	C	407	 83% 13% ..
1	D	407	 81% 15% ..
1	E	407	 83% 14% ..

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Mol	Chain	Length	Quality of chain
1	F	407	 80% 16% ..
2	G	7	 86% 14%
2	H	7	 71% 29%
2	I	7	 71% 29%
2	J	7	 86% 14%
2	K	7	 100%
2	L	7	 86% 14%

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
2	GLC	G	1	X	-	-	-
2	GLC	G	7	X	-	-	-
2	GLC	H	1	X	-	-	-
2	GLC	H	7	X	-	-	-
2	GLC	I	1	X	-	-	-
2	GLC	I	7	X	-	-	-
2	GLC	J	7	X	-	-	-
2	GLC	K	1	X	-	-	-
2	GLC	K	4	X	-	-	-
2	GLC	K	7	X	-	-	-
2	GLC	L	4	X	-	-	-
2	GLC	L	6	X	-	-	-
4	SO4	A	502	-	-	X	-
4	SO4	B	504	-	-	X	-
4	SO4	C	504	-	-	X	-
4	SO4	D	504	-	-	X	-
4	SO4	E	504	-	-	X	-
4	SO4	F	504	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22588 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 P450 HEME-THIOLATE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	5	0
			3171	1990	561	595	25			
1	B	404	Total	C	N	O	S	0	5	0
			3181	1994	559	604	24			
1	C	402	Total	C	N	O	S	0	7	0
			3180	1995	561	600	24			
1	D	402	Total	C	N	O	S	0	7	0
			3205	2005	569	606	25			
1	E	402	Total	C	N	O	S	0	6	0
			3199	1999	574	602	24			
1	F	402	Total	C	N	O	S	0	6	0
			3186	1996	563	603	24			

There are 36 discrepancies between the modelled and reference sequences:

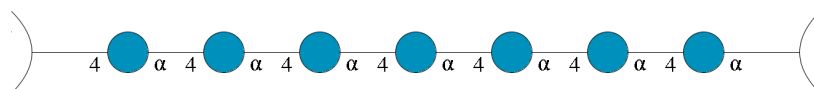
Chain	Residue	Modelled	Actual	Comment	Reference
A	402	HIS	-	expression tag	UNP A0R4Q6
A	403	HIS	-	expression tag	UNP A0R4Q6
A	404	HIS	-	expression tag	UNP A0R4Q6
A	405	HIS	-	expression tag	UNP A0R4Q6
A	406	HIS	-	expression tag	UNP A0R4Q6
A	407	HIS	-	expression tag	UNP A0R4Q6
B	402	HIS	-	expression tag	UNP A0R4Q6
B	403	HIS	-	expression tag	UNP A0R4Q6
B	404	HIS	-	expression tag	UNP A0R4Q6
B	405	HIS	-	expression tag	UNP A0R4Q6
B	406	HIS	-	expression tag	UNP A0R4Q6
B	407	HIS	-	expression tag	UNP A0R4Q6
C	402	HIS	-	expression tag	UNP A0R4Q6
C	403	HIS	-	expression tag	UNP A0R4Q6
C	404	HIS	-	expression tag	UNP A0R4Q6
C	405	HIS	-	expression tag	UNP A0R4Q6
C	406	HIS	-	expression tag	UNP A0R4Q6

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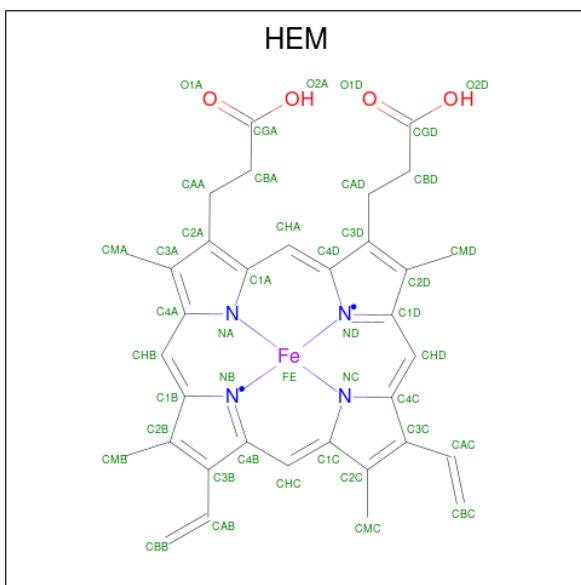
Chain	Residue	Modelled	Actual	Comment	Reference
C	407	HIS	-	expression tag	UNP A0R4Q6
D	402	HIS	-	expression tag	UNP A0R4Q6
D	403	HIS	-	expression tag	UNP A0R4Q6
D	404	HIS	-	expression tag	UNP A0R4Q6
D	405	HIS	-	expression tag	UNP A0R4Q6
D	406	HIS	-	expression tag	UNP A0R4Q6
D	407	HIS	-	expression tag	UNP A0R4Q6
E	402	HIS	-	expression tag	UNP A0R4Q6
E	403	HIS	-	expression tag	UNP A0R4Q6
E	404	HIS	-	expression tag	UNP A0R4Q6
E	405	HIS	-	expression tag	UNP A0R4Q6
E	406	HIS	-	expression tag	UNP A0R4Q6
E	407	HIS	-	expression tag	UNP A0R4Q6
F	402	HIS	-	expression tag	UNP A0R4Q6
F	403	HIS	-	expression tag	UNP A0R4Q6
F	404	HIS	-	expression tag	UNP A0R4Q6
F	405	HIS	-	expression tag	UNP A0R4Q6
F	406	HIS	-	expression tag	UNP A0R4Q6
F	407	HIS	-	expression tag	UNP A0R4Q6

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



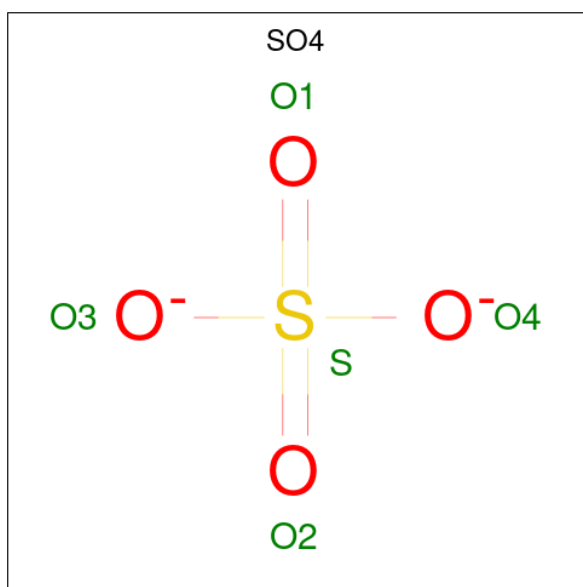
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	G	7	Total	C	O	0	0	0
			77	42	35			
2	H	7	Total	C	O	0	0	0
			77	42	35			
2	I	7	Total	C	O	0	0	0
			77	42	35			
2	J	7	Total	C	O	0	0	0
			77	42	35			
2	K	7	Total	C	O	0	0	0
			77	42	35			
2	L	7	Total	C	O	0	0	0
			77	42	35			

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



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



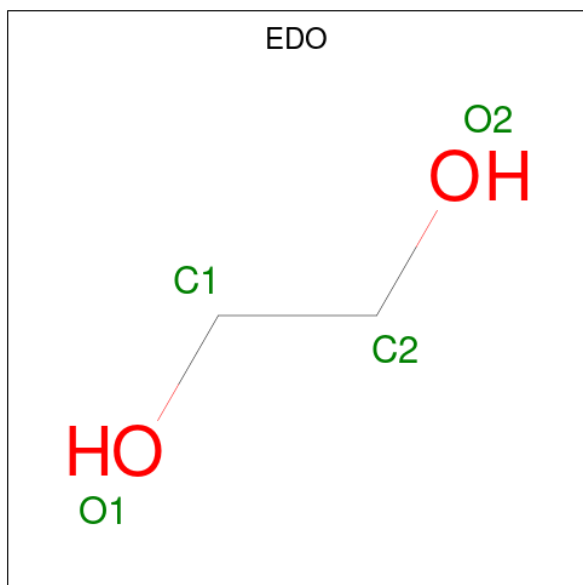
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).

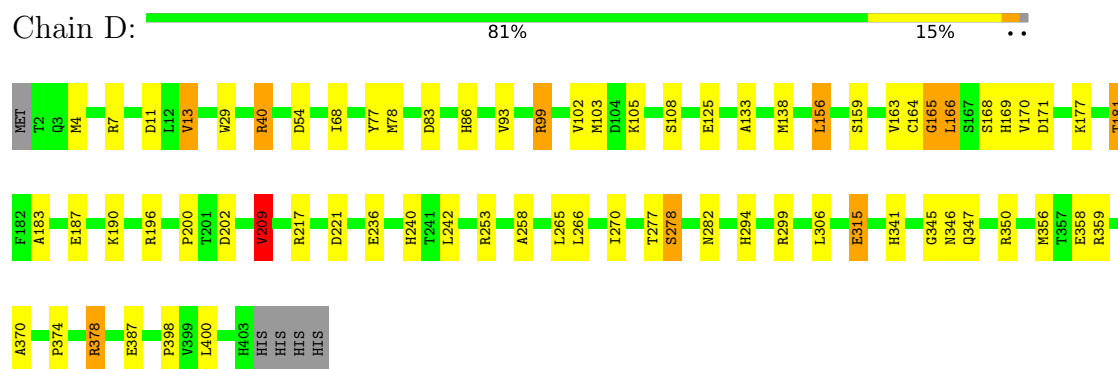


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		

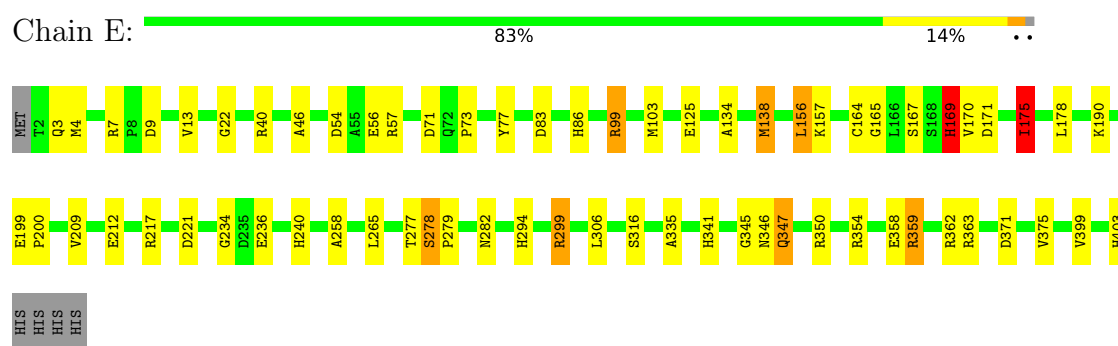
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	439	Total 439	O 439	0	0
6	B	432	Total 432	O 432	0	0
6	C	443	Total 443	O 443	0	0
6	D	432	Total 432	O 432	0	0
6	E	460	Total 460	O 460	0	0
6	F	431	Total 431	O 431	0	0

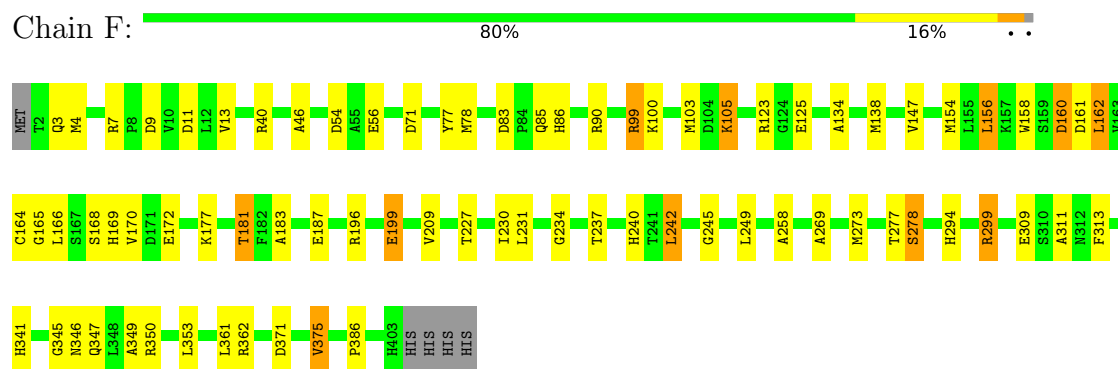
- Molecule 1: P450 HEME-THIOLATE PROTEIN



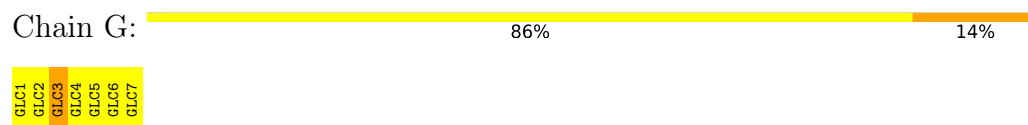
- Molecule 1: P450 HEME-THIOLATE PROTEIN



- Molecule 1: P450 HEME-THIOLATE PROTEIN



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

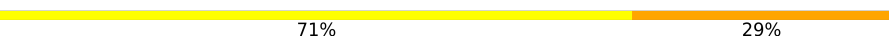


- Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)





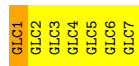
- Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)

Chain I:  71% 29%

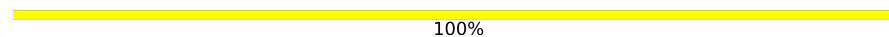


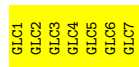
- Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)

Chain J:  86% 14%



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

Chain K:  100%



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

Chain L:  86% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	94.05Å 162.85Å 266.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	266.44 – 1.93 266.44 – 1.93	Depositor EDS
% Data completeness (in resolution range)	94.3 (266.44-1.93) 94.6 (266.44-1.93)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.190 , 0.230 0.189 , 0.228	Depositor DCC
R_{free} test set	14356 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.460 for -1/2*h+1/2*k,3/2*h+1/2*k,-l 0.467 for -1/2*h-1/2*k,-3/2*h+1/2*k,-l 0.467 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.467 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.467 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22588	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GLC, HEM, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.40	7/3237 (0.2%)	1.18	8/4391 (0.2%)
1	B	1.43	14/3251 (0.4%)	1.18	6/4414 (0.1%)
1	C	1.41	7/3255 (0.2%)	1.19	10/4416 (0.2%)
1	D	1.37	8/3274 (0.2%)	1.19	9/4439 (0.2%)
1	E	1.41	9/3265 (0.3%)	1.22	15/4427 (0.3%)
1	F	1.41	17/3258 (0.5%)	1.20	14/4420 (0.3%)
All	All	1.41	62/19540 (0.3%)	1.19	62/26507 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	278	SER	N-CA	9.88	1.53	1.46
1	F	278	SER	N-CA	9.43	1.53	1.46
1	D	278	SER	N-CA	7.09	1.51	1.46
1	F	278	SER	C-O	7.08	1.27	1.23
1	C	349	ALA	CA-CB	7.05	1.64	1.53
1	E	347	GLN	CA-C	6.98	1.61	1.52
1	B	156	LEU	CA-C	6.83	1.61	1.52
1	F	156	LEU	CA-C	6.76	1.61	1.52
1	E	46	ALA	CA-CB	6.46	1.61	1.53
1	D	159	SER	N-CA	-6.37	1.38	1.46
1	C	132	ILE	CA-CB	6.36	1.63	1.54
1	E	278	SER	C-O	-6.26	1.20	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	163	VAL	CA-C	6.26	1.60	1.52
1	A	159	SER	N-CA	-6.21	1.38	1.46
1	B	278	SER	C-O	-6.16	1.20	1.23
1	F	386	PRO	CA-C	6.13	1.59	1.52
1	F	46	ALA	CA-CB	6.05	1.61	1.53
1	B	311	ALA	CA-CB	5.92	1.62	1.53
1	C	163	VAL	CA-C	5.88	1.60	1.52
1	B	52	VAL	CA-CB	5.85	1.61	1.54
1	A	170	VAL	N-CA	5.78	1.53	1.46
1	A	336	PHE	N-CA	5.61	1.53	1.46
1	D	258	ALA	CA-CB	5.59	1.62	1.53
1	B	32	ALA	CA-CB	5.58	1.62	1.53
1	F	78	MET	C-O	-5.57	1.17	1.24
1	B	147	VAL	CA-C	5.57	1.57	1.52
1	C	75	MET	C-O	5.56	1.29	1.24
1	B	403	HIS	N-CA	5.54	1.53	1.46
1	C	236	GLU	CD-OE1	5.53	1.35	1.25
1	F	170	VAL	CA-CB	5.52	1.60	1.54
1	B	299	ARG	N-CA	-5.47	1.39	1.46
1	A	46	ALA	CA-CB	5.41	1.59	1.53
1	F	361	LEU	N-CA	5.38	1.52	1.46
1	B	258	ALA	CA-CB	5.36	1.61	1.53
1	F	258	ALA	CA-CB	5.36	1.61	1.53
1	E	258	ALA	CA-CB	5.34	1.61	1.53
1	F	231	LEU	N-CA	5.34	1.52	1.46
1	D	163	VAL	CA-C	5.33	1.59	1.52
1	E	175	ILE	CA-CB	5.29	1.60	1.54
1	A	51	ALA	CA-C	5.28	1.59	1.52
1	D	315	GLU	CD-OE1	5.27	1.35	1.25
1	F	353	LEU	C-O	-5.25	1.18	1.24
1	C	170	VAL	CA-CB	5.24	1.62	1.54
1	F	311	ALA	CA-CB	5.21	1.61	1.53
1	B	175	ILE	CA-CB	5.18	1.60	1.54
1	E	359	ARG	CZ-NH1	5.17	1.40	1.32
1	E	335	ALA	CA-C	5.13	1.59	1.52
1	C	164	CYS	N-CA	5.13	1.52	1.46
1	A	175	ILE	CA-CB	5.11	1.60	1.54
1	B	170	VAL	CA-CB	5.10	1.61	1.54
1	F	147	VAL	CA-C	5.08	1.57	1.52
1	F	313	PHE	N-CA	5.07	1.52	1.46
1	F	349	ALA	CA-CB	5.07	1.61	1.53
1	D	209	VAL	CA-CB	5.05	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	167	SER	CA-C	5.05	1.59	1.52
1	A	311	ALA	CA-CB	5.05	1.61	1.53
1	E	22	GLY	N-CA	5.05	1.52	1.45
1	D	13	VAL	CA-CB	5.04	1.60	1.54
1	B	401	ALA	CA-C	5.04	1.59	1.52
1	D	370	ALA	C-O	-5.02	1.18	1.24
1	F	299	ARG	N-CA	-5.01	1.39	1.45
1	F	375	VAL	CA-C	5.00	1.57	1.53

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	VAL	N-CA-C	10.41	120.92	110.82
1	F	162	LEU	N-CA-C	-8.46	101.28	111.69
1	B	156	LEU	CB-CA-C	7.86	124.22	110.85
1	E	170	VAL	N-CA-C	7.43	117.51	110.74
1	C	162	LEU	N-CA-C	-7.32	102.69	111.69
1	E	156	LEU	N-CA-C	-7.21	103.15	112.23
1	D	164[A]	CYS	CA-C-N	-7.19	111.57	122.28
1	D	164[A]	CYS	C-N-CA	-7.19	111.57	122.28
1	D	164[B]	CYS	CA-C-N	-7.19	111.57	122.28
1	D	164[B]	CYS	C-N-CA	-7.19	111.57	122.28
1	D	170	VAL	N-CA-C	7.16	117.26	110.53
1	D	166	LEU	N-CA-C	-6.98	103.60	111.14
1	A	156	LEU	N-CA-C	-6.82	103.63	112.23
1	F	156	LEU	CB-CA-C	6.56	123.27	110.67
1	F	375	VAL	N-CA-CB	-6.50	103.27	110.23
1	F	199	GLU	CA-C-N	6.47	126.50	119.90
1	F	199	GLU	C-N-CA	6.47	126.50	119.90
1	A	375	VAL	N-CA-CB	-6.29	103.50	110.23
1	C	65	THR	OG1-CB-CG2	6.21	121.72	109.30
1	C	156	LEU	N-CA-C	-6.14	104.50	112.23
1	A	372	ASP	N-CA-C	6.07	120.53	113.18
1	B	162	LEU	N-CA-C	-6.07	104.22	111.69
1	B	175	ILE	N-CA-C	-5.88	105.00	110.53
1	E	169	HIS	N-CA-C	5.84	120.56	113.38
1	C	287	LEU	CA-CB-CG	-5.79	96.04	116.30
1	C	199	GLU	CA-C-N	5.77	125.78	119.89
1	C	199	GLU	C-N-CA	5.77	125.78	119.89
1	D	13	VAL	N-CA-C	-5.71	107.42	112.90
1	C	169	HIS	N-CA-C	5.70	117.28	110.44
1	E	13	VAL	N-CA-C	-5.69	107.20	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	160	ASP	CA-C-N	-5.67	113.57	122.65
1	F	160	ASP	C-N-CA	-5.67	113.57	122.65
1	E	375	VAL	N-CA-CB	-5.67	104.81	110.08
1	B	375	VAL	CB-CA-C	5.52	116.08	110.94
1	F	170	VAL	N-CA-C	5.47	115.68	110.42
1	E	156	LEU	CB-CA-C	5.46	121.52	110.38
1	F	242	LEU	CB-CG-CD2	-5.44	94.39	110.70
1	D	156	LEU	CB-CA-C	5.41	121.06	110.67
1	E	157	LYS	N-CA-C	5.39	117.02	111.03
1	A	156	LEU	CB-CA-C	5.37	121.33	110.38
1	E	199	GLU	CA-C-N	5.34	125.34	119.89
1	E	199	GLU	C-N-CA	5.34	125.34	119.89
1	E	134	ALA	CA-C-N	-5.33	113.54	119.19
1	E	134	ALA	C-N-CA	-5.33	113.54	119.19
1	C	65	THR	N-CA-CB	-5.32	101.74	110.40
1	B	156	LEU	CD1-CG-CD2	-5.26	99.23	110.80
1	A	157	LYS	N-CA-C	5.22	116.78	111.14
1	F	90	ARG	N-CA-C	5.21	116.65	111.07
1	C	316	SER	N-CA-C	-5.19	106.20	112.54
1	E	156	LEU	CD1-CG-CD2	-5.18	99.39	110.80
1	E	73	PRO	CA-C-N	5.16	125.24	120.34
1	E	73	PRO	C-N-CA	5.16	125.24	120.34
1	C	141	ILE	N-CA-C	5.16	115.37	110.42
1	F	375	VAL	N-CA-C	-5.15	104.20	108.63
1	F	161	ASP	CB-CA-C	5.14	119.25	110.56
1	E	316	SER	N-CA-C	-5.13	106.28	112.54
1	A	199	GLU	CA-C-N	5.13	125.04	119.76
1	A	199	GLU	C-N-CA	5.13	125.04	119.76
1	F	227	THR	N-CA-C	-5.12	105.61	111.14
1	B	13	VAL	N-CA-C	-5.10	107.78	112.83
1	D	156	LEU	N-CA-C	-5.06	105.95	111.82
1	F	309	GLU	N-CA-C	-5.00	105.91	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	165	GLY	Peptide

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	3171	0	3105	59	0
1	B	3181	0	3091	76	0
1	C	3180	0	3116	51	0
1	D	3205	0	3134	64	0
1	E	3199	0	3132	53	0
1	F	3186	0	3126	65	0
2	G	77	0	63	1	0
2	H	77	0	63	4	0
2	I	77	0	63	3	0
2	J	77	0	63	2	0
2	K	77	0	60	0	0
2	L	77	0	61	1	0
3	A	43	0	30	6	0
3	B	43	0	30	6	0
3	C	43	0	30	5	0
3	D	43	0	30	6	0
3	E	43	0	30	6	0
3	F	43	0	30	10	0
4	A	10	0	0	8	0
4	B	15	0	0	5	0
4	C	15	0	0	3	0
4	D	15	0	0	5	0
4	E	15	0	0	7	0
4	F	15	0	0	5	0
5	A	4	0	5	0	0
5	B	4	0	5	1	0
5	C	4	0	5	1	0
5	D	4	0	5	0	0
5	E	4	0	5	0	0
5	F	4	0	5	0	0
6	A	439	0	0	17	0
6	B	432	0	0	15	0
6	C	443	0	0	13	0
6	D	432	0	0	12	0
6	E	460	0	0	14	1
6	F	431	0	0	18	1
All	All	22588	0	19287	378	1

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 (378) 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:E:169:HIS:O	1:E:175:ILE:HD11	1.28	1.29
1:E:4:MET:N	4:E:504:SO4:O4	1.69	1.24
1:D:40:ARG:HH11	1:D:40:ARG:CG	1.58	1.14
1:F:164:CYS:HB3	6:F:899:HOH:O	1.49	1.12
1:F:230:ILE:HG23	3:F:501:HEM:HBC1	1.27	1.12
1:F:99[A]:ARG:NE	1:F:99[A]:ARG:HA	1.64	1.08
1:C:7:ARG:HD2	4:C:504:SO4:O3	1.55	1.07
1:F:99[A]:ARG:HA	1:F:99[A]:ARG:HE	1.12	1.06
1:F:138:MET:HE1	6:F:786:HOH:O	1.55	1.06
1:E:299:ARG:HG3	1:E:299:ARG:HH11	1.18	1.04
1:E:7:ARG:HD2	4:E:504:SO4:O2	1.55	1.04
1:D:7:ARG:HD2	4:D:504:SO4:O3	1.59	1.00
1:D:99[B]:ARG:NH2	6:D:601:HOH:O	1.92	1.00
1:D:40:ARG:HG3	1:D:40:ARG:NH1	1.59	0.99
1:F:4:MET:N	4:F:504:SO4:O3	1.96	0.99
1:E:169:HIS:O	1:E:175:ILE:CD1	2.10	0.98
1:B:179:MET:HE2	2:H:5:GLC:H62	1.42	0.97
1:E:138:MET:HB3	1:E:156:LEU:HD13	1.47	0.97
1:F:7:ARG:HD2	4:F:504:SO4:O2	1.65	0.96
1:B:169:HIS:O	1:B:175:ILE:HD11	1.67	0.94
1:B:138:MET:HB3	1:B:156:LEU:HD13	1.50	0.93
1:C:138:MET:HB3	1:C:156:LEU:CD1	2.00	0.92
3:F:501:HEM:HMB1	3:F:501:HEM:HBB2	1.50	0.91
1:D:40:ARG:HH11	1:D:40:ARG:HG3	0.76	0.90
1:B:7:ARG:NH1	4:B:504:SO4:O1	2.07	0.88
1:F:99[A]:ARG:HE	1:F:99[A]:ARG:CA	1.67	0.86
1:E:138:MET:HB3	1:E:156:LEU:CD1	2.05	0.85
1:D:183:ALA:O	1:D:187[B]:GLU:HG3	1.76	0.85
1:D:138:MET:HB3	1:D:156:LEU:CD1	2.07	0.84
1:E:299:ARG:HG3	1:E:299:ARG:NH1	1.92	0.84
1:E:403:HIS:HD2	6:E:972:HOH:O	1.60	0.84
1:C:4:MET:N	4:C:504:SO4:O2	2.11	0.84
1:F:138:MET:HB3	1:F:156:LEU:HD13	1.57	0.84
1:F:230:ILE:HG23	3:F:501:HEM:CBC	2.07	0.83
1:D:138:MET:HB3	1:D:156:LEU:HD13	1.61	0.82
1:F:138:MET:HB3	1:F:156:LEU:CD1	2.10	0.81
1:A:99:ARG:HD3	1:A:347[A]:GLN:HE22	1.42	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:MET:HB3	1:C:156:LEU:HD13	1.62	0.81
1:E:99:ARG:HE	1:E:347:GLN:HE22	1.28	0.80
1:B:378:ARG:NH1	1:B:387[A]:GLU:OE1	2.15	0.78
1:B:86:HIS:HE1	3:B:501:HEM:O2D	1.64	0.78
1:A:144:MET:HE2	6:A:998:HOH:O	1.83	0.78
1:E:359:ARG:HG2	1:E:362[B]:ARG:HH21	1.48	0.78
1:B:81:MET:HE1	1:B:89:ARG:CB	2.13	0.77
1:A:7:ARG:HD2	4:A:502:SO4:O4	1.85	0.76
1:D:299:ARG:HD3	6:D:919:HOH:O	1.85	0.76
1:B:133:ALA:HA	1:B:242:LEU:HD23	1.66	0.75
1:A:3:GLN:HA	4:A:502:SO4:O1	1.86	0.75
1:B:81:MET:CE	1:B:86:HIS:HA	2.17	0.75
1:C:315:GLU:OE1	6:C:601:HOH:O	2.04	0.75
1:F:138:MET:HE2	6:F:820:HOH:O	1.86	0.75
1:B:81:MET:HE1	1:B:89:ARG:HB3	1.68	0.74
1:B:111:ARG:HH22	1:B:405:HIS:CD2	2.05	0.74
1:D:99[A]:ARG:H	1:D:99[A]:ARG:CD	1.99	0.74
1:E:358:GLU:OE1	6:E:601:HOH:O	2.06	0.74
1:F:160:ASP:OD2	6:F:603:HOH:O	2.06	0.73
1:F:86:HIS:HE1	3:F:501:HEM:O2D	1.70	0.73
1:B:99:ARG:CD	6:B:966:HOH:O	2.35	0.73
1:B:169:HIS:O	1:B:175:ILE:CD1	2.36	0.73
1:B:196:ARG:NH1	6:B:601:HOH:O	2.19	0.73
1:B:138:MET:HB3	1:B:156:LEU:CD1	2.19	0.72
1:A:362:ARG:NH2	6:A:603:HOH:O	2.21	0.72
1:D:165:GLY:O	1:D:169:HIS:HB3	1.90	0.71
1:F:249[B]:LEU:N	1:F:249[B]:LEU:HD12	2.04	0.71
1:E:86:HIS:HE1	3:E:501:HEM:O2D	1.73	0.71
1:C:65:THR:HG21	6:C:950:HOH:O	1.90	0.71
1:A:169:HIS:HD2	6:A:902:HOH:O	1.73	0.71
1:D:221:ASP:HB3	2:J:1:GLC:H62	1.72	0.71
1:B:81:MET:HE3	1:B:86:HIS:HA	1.71	0.70
1:D:86:HIS:HE1	3:D:501:HEM:O2D	1.73	0.70
1:C:86:HIS:HE1	3:C:501:HEM:O2D	1.74	0.70
1:A:86:HIS:HE1	3:A:501:HEM:O2D	1.76	0.69
1:D:240:HIS:HE1	6:D:617:HOH:O	1.74	0.69
1:B:88:LEU:HD12	1:B:213:VAL:HG21	1.75	0.68
1:D:99[A]:ARG:H	1:D:99[A]:ARG:HD2	1.59	0.68
1:C:341:HIS:HD2	3:C:501:HEM:O1D	1.77	0.68
1:D:29:TRP:HH2	4:D:504:SO4:O1	1.77	0.67
1:B:341:HIS:HE1	6:B:726:HOH:O	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:105:LYS:HG3	6:F:1002:HOH:O	1.94	0.67
1:E:341:HIS:HD2	3:E:501:HEM:O1D	1.78	0.66
1:A:144:MET:HE1	1:A:348:LEU:CD2	2.25	0.66
1:A:387[A]:GLU:OE1	6:A:601:HOH:O	2.13	0.66
1:B:179:MET:HE2	2:H:5:GLC:C6	2.21	0.66
1:A:83:ASP:OD1	1:A:86:HIS:HD2	1.78	0.66
1:A:176:GLN:HA	1:A:176:GLN:OE1	1.95	0.66
1:B:154:MET:HE2	1:B:158:TRP:CH2	2.30	0.66
1:B:172:GLU:CB	6:B:671:HOH:O	2.45	0.65
1:F:181:THR:HG22	6:F:896:HOH:O	1.96	0.65
1:D:29:TRP:CH2	4:D:504:SO4:O1	2.50	0.64
1:F:85:GLN:HB3	6:F:1023:HOH:O	1.97	0.64
1:A:4:MET:N	4:A:502:SO4:O1	2.30	0.64
1:D:315:GLU:OE1	6:D:602:HOH:O	2.15	0.64
1:A:341:HIS:HD2	3:A:501:HEM:O1D	1.81	0.63
1:A:346:ASN:HD22	1:A:350:ARG:HH11	1.46	0.63
1:F:341:HIS:HD2	3:F:501:HEM:O1D	1.82	0.63
1:B:374:PRO:HD3	6:B:969:HOH:O	1.97	0.63
1:A:11:ASP:OD1	1:A:13[B]:VAL:HG22	1.99	0.63
1:F:3:GLN:HA	4:F:504:SO4:O3	1.99	0.62
1:F:187[B]:GLU:HG3	6:F:724:HOH:O	1.98	0.62
1:F:245:GLY:O	1:F:249[B]:LEU:HD13	2.00	0.62
1:B:363:ARG:HD2	6:B:629:HOH:O	1.98	0.62
1:E:7:ARG:CD	4:E:504:SO4:O2	2.40	0.62
1:F:99[A]:ARG:NE	1:F:99[A]:ARG:CA	2.33	0.62
1:B:88:LEU:CD1	1:B:213:VAL:CG2	2.78	0.61
1:A:105:LYS:HG3	6:A:998:HOH:O	2.00	0.61
1:A:144:MET:HE1	1:A:348:LEU:HD21	1.83	0.61
1:F:154:MET:HE2	1:F:158:TRP:CH2	2.36	0.60
1:B:240:HIS:HE1	6:B:611:HOH:O	1.84	0.60
1:C:346:ASN:HD22	1:C:350:ARG:HH11	1.49	0.60
1:D:196:ARG:HD3	6:D:701:HOH:O	2.01	0.60
1:D:358:GLU:OE1	6:D:603:HOH:O	2.16	0.60
3:F:501:HEM:HBB2	3:F:501:HEM:CMB	2.26	0.60
1:A:133:ALA:HA	1:A:242:LEU:HD23	1.83	0.60
1:B:154:MET:CE	1:B:158:TRP:CH2	2.84	0.60
1:E:99:ARG:HD3	1:E:103:MET:HG2	1.84	0.60
1:A:103:MET:HE3	1:A:347[A]:GLN:NE2	2.17	0.60
1:D:341:HIS:HD2	3:D:501:HEM:O1D	1.84	0.59
1:E:341:HIS:HE1	6:E:662:HOH:O	1.84	0.59
1:F:240:HIS:HE1	6:F:614:HOH:O	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:MET:HE3	1:A:347[A]:GLN:HE21	1.66	0.59
1:F:341:HIS:HE1	6:F:662:HOH:O	1.85	0.59
1:D:166:LEU:O	1:D:169:HIS:CE1	2.56	0.58
1:D:177:LYS:O	1:D:181:THR:HG23	2.03	0.58
1:E:346:ASN:HD22	1:E:350:ARG:HH11	1.49	0.58
1:F:99[A]:ARG:HH22	1:F:347:GLN:CB	2.16	0.58
1:F:177:LYS:O	1:F:181:THR:HG23	2.04	0.58
1:B:105:LYS:HG3	6:B:875:HOH:O	2.04	0.58
1:B:88:LEU:HD12	1:B:213:VAL:CG2	2.33	0.58
1:B:225:PHE:CE2	2:H:2:GLC:H62	2.39	0.58
1:F:7:ARG:CD	4:F:504:SO4:O2	2.48	0.58
1:D:4:MET:N	4:D:504:SO4:O2	2.36	0.58
1:F:346:ASN:HD22	1:F:350:ARG:HH11	1.51	0.57
1:B:88:LEU:CD1	1:B:213:VAL:HG23	2.34	0.57
1:E:9:ASP:OD1	1:E:40:ARG:HD3	2.05	0.57
1:F:83:ASP:OD1	1:F:86:HIS:HD2	1.87	0.57
1:D:374:PRO:O	6:D:604:HOH:O	2.17	0.57
3:E:501:HEM:HMC1	3:E:501:HEM:HBC2	1.87	0.57
1:A:341:HIS:HE1	6:A:643:HOH:O	1.86	0.57
1:C:11:ASP:OD1	1:C:13[A]:VAL:HG22	2.05	0.57
1:E:240:HIS:HE1	6:E:604:HOH:O	1.87	0.57
1:D:99[B]:ARG:HG3	1:D:99[B]:ARG:HH11	1.70	0.56
1:D:341:HIS:HE1	6:D:664:HOH:O	1.87	0.56
1:F:99[A]:ARG:HH22	1:F:347:GLN:HB2	1.70	0.56
1:D:99[B]:ARG:HG3	1:D:99[B]:ARG:NH1	2.19	0.56
1:F:249[B]:LEU:H	1:F:249[B]:LEU:CD1	2.18	0.56
1:F:99[A]:ARG:HH11	1:F:103:MET:HE3	1.71	0.56
1:C:9:ASP:OD1	1:C:40:ARG:HD3	2.06	0.56
1:F:249[B]:LEU:HD12	1:F:249[B]:LEU:H	1.70	0.56
6:F:1031:HOH:O	2:L:2:GLC:O6	2.07	0.55
1:C:378:ARG:NH1	1:C:387:GLU:HG2	2.20	0.55
1:F:99[A]:ARG:HH12	1:F:347:GLN:HB3	1.71	0.55
1:B:346:ASN:HD22	1:B:350:ARG:HH11	1.51	0.55
1:C:341:HIS:HE1	6:C:656:HOH:O	1.89	0.55
1:A:83:ASP:OD1	1:A:86:HIS:CD2	2.59	0.55
1:B:341:HIS:HD2	3:B:501:HEM:O1D	1.90	0.55
1:A:171:ASP:CG	6:A:834:HOH:O	2.49	0.55
1:F:249[B]:LEU:N	1:F:249[B]:LEU:CD1	2.69	0.55
1:F:362:ARG:NH2	6:F:609:HOH:O	2.39	0.55
1:D:133:ALA:HA	1:D:242:LEU:HD23	1.87	0.55
1:B:86:HIS:CE1	3:B:501:HEM:O2D	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:VAL:HG23	1:B:213:VAL:O	2.07	0.54
1:A:3:GLN:HG2	1:A:7:ARG:HD2	1.88	0.54
1:D:177:LYS:O	1:D:181:THR:CG2	2.56	0.54
1:E:71:ASP:CB	6:E:659:HOH:O	2.56	0.54
1:C:54:ASP:OD2	1:C:294:HIS:HE1	1.91	0.54
1:C:221:ASP:OD2	2:I:3:GLC:O2	2.17	0.54
1:B:3:GLN:HA	4:B:504:SO4:O2	2.08	0.53
1:C:236:GLU:OE1	1:C:240:HIS:HE1	1.91	0.53
1:F:371:ASP:O	6:F:604:HOH:O	2.18	0.53
1:B:198:ALA:O	1:B:199[B]:GLU:OE1	2.25	0.53
1:D:102:VAL:HG11	1:D:347[A]:GLN:HG2	1.90	0.53
1:E:171:ASP:HB2	6:E:613:HOH:O	2.07	0.53
1:C:83:ASP:OD1	1:C:86:HIS:HD2	1.92	0.53
1:D:54:ASP:OD2	1:D:294:HIS:HE1	1.91	0.53
1:F:71:ASP:CB	6:F:812:HOH:O	2.55	0.53
1:B:54:ASP:OD2	1:B:294:HIS:HE1	1.92	0.53
1:A:378:ARG:HD3	1:A:387[B]:GLU:CD	2.34	0.53
1:C:7:ARG:CD	4:C:504:SO4:O3	2.45	0.53
1:D:221:ASP:CB	2:J:1:GLC:H62	2.38	0.53
1:A:359:ARG:HG2	6:A:605:HOH:O	2.09	0.52
1:B:88:LEU:HD11	1:B:213:VAL:HG23	1.91	0.52
1:B:225:PHE:HE2	2:H:2:GLC:H62	1.73	0.52
3:B:501:HEM:HMC1	3:B:501:HEM:HBC2	1.92	0.52
1:A:172:GLU:HA	1:A:175:ILE:HD12	1.91	0.52
1:E:54:ASP:OD2	1:E:294:HIS:HE1	1.92	0.52
1:F:11:ASP:OD1	1:F:13[A]:VAL:HG22	2.09	0.52
1:A:346:ASN:HD22	1:A:350:ARG:NH1	2.08	0.52
1:D:166:LEU:O	1:D:169:HIS:ND1	2.43	0.52
1:E:200:PRO:HG3	6:E:904:HOH:O	2.09	0.52
1:F:154:MET:CE	1:F:158:TRP:CH2	2.93	0.52
1:C:371:ASP:OD1	1:C:371:ASP:C	2.53	0.52
1:E:403:HIS:CD2	6:E:972:HOH:O	2.46	0.52
1:A:240:HIS:HE1	6:A:617:HOH:O	1.92	0.51
1:D:346:ASN:HD22	1:D:350:ARG:HH11	1.56	0.51
1:C:395:PRO:O	6:C:602:HOH:O	2.18	0.51
1:D:4:MET:HG3	4:D:504:SO4:O2	2.10	0.51
1:F:162:LEU:O	1:F:166:LEU:HG	2.10	0.51
1:A:3:GLN:CA	4:A:502:SO4:O1	2.59	0.51
1:C:165:GLY:HA3	1:C:178:LEU:HD13	1.93	0.51
1:D:190:LYS:NZ	1:D:221:ASP:OD1	2.44	0.51
1:F:83:ASP:OD1	1:F:86:HIS:CD2	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347[B]:GLN:HG3	6:C:680:HOH:O	2.10	0.51
1:B:4:MET:HB2	4:B:504:SO4:O4	2.11	0.51
1:E:3:GLN:HA	4:E:504:SO4:O4	2.11	0.51
1:A:102:VAL:HG12	1:A:103:MET:HE2	1.91	0.50
1:E:56:GLU:OE2	3:E:501:HEM:O2A	2.29	0.50
1:F:245:GLY:O	1:F:249[B]:LEU:CD1	2.60	0.50
1:D:102:VAL:HG12	1:D:103:MET:HE2	1.93	0.50
1:D:341:HIS:O	3:D:501:HEM:HBA2	2.11	0.50
1:A:134:ALA:O	1:A:138:MET:HG3	2.12	0.50
1:E:99:ARG:HD3	1:E:103:MET:CG	2.41	0.50
1:E:236:GLU:HG3	6:E:795:HOH:O	2.11	0.50
1:A:254:ASP:HB2	6:A:840:HOH:O	2.12	0.49
1:B:83:ASP:OD1	1:B:86:HIS:HD2	1.96	0.49
1:C:170:VAL:N	6:C:614:HOH:O	2.42	0.49
1:E:83:ASP:OD1	1:E:86:HIS:HD2	1.95	0.49
1:F:56:GLU:OE2	3:F:501:HEM:O2A	2.29	0.49
1:B:88:LEU:HD11	1:B:213:VAL:CG2	2.43	0.49
1:F:345:GLY:HA3	3:F:501:HEM:C3C	2.48	0.49
3:A:501:HEM:CMB	3:A:501:HEM:HBB2	2.43	0.49
3:A:501:HEM:HBB2	3:A:501:HEM:HMB2	1.95	0.49
1:F:346:ASN:HD22	1:F:350:ARG:NH1	2.10	0.49
1:A:402:HIS:O	6:A:602:HOH:O	2.20	0.49
1:B:166:LEU:O	1:B:169:HIS:ND1	2.45	0.48
1:D:11:ASP:OD1	1:D:13:VAL:HG22	2.13	0.48
1:D:83:ASP:OD1	1:D:86:HIS:HD2	1.96	0.48
1:D:190:LYS:CE	1:D:221:ASP:OD1	2.61	0.48
1:A:144:MET:HE1	1:A:348:LEU:HD22	1.94	0.48
1:A:4:MET:HB2	4:A:502:SO4:O2	2.13	0.48
1:A:378:ARG:HD3	1:A:387[B]:GLU:OE1	2.12	0.48
1:D:266:LEU:O	1:D:270:ILE:HG12	2.13	0.48
1:A:7:ARG:CD	4:A:502:SO4:O4	2.58	0.48
1:A:138:MET:HB3	1:A:156:LEU:HD13	1.96	0.48
1:B:3:GLN:CA	4:B:504:SO4:O2	2.61	0.48
1:B:254[A]:ASP:OD1	6:B:603:HOH:O	2.19	0.48
1:C:105[A]:LYS:HE2	6:C:760:HOH:O	2.12	0.48
1:E:57:ARG:NH1	6:E:602:HOH:O	2.18	0.48
1:A:242:LEU:HD21	1:A:356:MET:HG2	1.94	0.48
1:A:345:GLY:HA3	3:A:501:HEM:C3C	2.49	0.48
1:C:346:ASN:HD22	1:C:350:ARG:NH1	2.11	0.48
1:D:346:ASN:HD22	1:D:350:ARG:NH1	2.12	0.48
1:F:9:ASP:OD1	1:F:40:ARG:HD3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:ASP:OD2	1:B:294:HIS:CE1	2.66	0.48
1:B:179:MET:HE3	1:B:179:MET:HA	1.96	0.48
1:B:240:HIS:HD2	6:B:622:HOH:O	1.97	0.48
1:E:99:ARG:HE	1:E:347:GLN:NE2	2.03	0.48
1:F:165:GLY:O	1:F:169:HIS:HB3	2.14	0.48
1:B:166:LEU:O	1:B:169:HIS:CE1	2.67	0.47
1:B:378:ARG:HD3	1:B:387[A]:GLU:CD	2.39	0.47
1:C:56:GLU:OE2	3:C:501:HEM:O2A	2.32	0.47
1:C:13[B]:VAL:O	1:C:13[B]:VAL:HG12	2.13	0.47
1:A:234:GLY:HA2	3:A:501:HEM:C2C	2.49	0.47
1:B:217:ARG:NE	6:B:612:HOH:O	2.46	0.47
3:B:501:HEM:HBB2	3:B:501:HEM:CMB	2.45	0.47
1:D:105:LYS:HE3	1:D:108:SER:OG	2.15	0.47
1:D:378:ARG:HB2	1:D:387[A]:GLU:HG2	1.95	0.47
3:D:501:HEM:HBB2	3:D:501:HEM:CMB	2.45	0.47
1:C:54:ASP:OD2	1:C:294:HIS:CE1	2.67	0.47
1:D:40:ARG:CG	1:D:40:ARG:NH1	2.34	0.47
1:B:234:GLY:HA2	3:B:501:HEM:C2C	2.50	0.46
1:B:387[B]:GLU:OE2	6:B:602:HOH:O	2.19	0.46
1:F:172:GLU:CG	6:F:1026:HOH:O	2.63	0.46
1:E:165:GLY:HA3	1:E:178:LEU:HD13	1.98	0.46
1:F:234:GLY:HA2	3:F:501:HEM:C2C	2.50	0.46
1:B:3:GLN:CB	4:B:504:SO4:O2	2.63	0.46
1:C:378:ARG:NH1	1:C:387:GLU:OE2	2.48	0.46
1:E:277:THR:O	1:E:278:SER:C	2.57	0.46
1:A:282:ASN:HA	1:A:306:LEU:O	2.16	0.46
1:C:240:HIS:CG	1:C:385:GLY:HA3	2.51	0.46
1:E:190:LYS:NZ	1:E:221:ASP:OD1	2.48	0.46
1:B:198:ALA:C	1:B:199[B]:GLU:OE1	2.58	0.46
1:A:169:HIS:CD2	6:A:902:HOH:O	2.56	0.46
1:C:85[A]:GLN:HG3	6:C:604:HOH:O	2.15	0.46
1:F:54:ASP:OD2	1:F:294:HIS:HE1	1.98	0.46
1:D:345:GLY:HA3	3:D:501:HEM:C3C	2.51	0.46
1:F:240:HIS:HD2	6:F:661:HOH:O	1.98	0.46
1:B:9:ASP:OD1	1:B:40:ARG:HD3	2.16	0.45
1:A:196:ARG:HD3	6:A:891:HOH:O	2.16	0.45
1:E:190:LYS:CE	1:E:221:ASP:OD1	2.63	0.45
1:C:111:ARG:NH2	6:C:616:HOH:O	2.43	0.45
1:D:165:GLY:CA	1:D:168:SER:H	2.29	0.45
1:A:4:MET:SD	4:A:502:SO4:O2	2.75	0.45
1:D:242:LEU:HD21	1:D:356:MET:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:ASP:OD2	6:C:603:HOH:O	2.21	0.45
1:E:240:HIS:HD2	6:E:642:HOH:O	1.98	0.45
1:E:3:GLN:CA	4:E:504:SO4:O4	2.65	0.45
1:A:240:HIS:HD2	6:A:649:HOH:O	2.00	0.45
1:B:382:PHE:HB3	6:B:802:HOH:O	2.17	0.45
1:A:277:THR:O	1:A:278:SER:C	2.59	0.44
1:E:347:GLN:HG3	6:E:947:HOH:O	2.17	0.44
1:E:403:HIS:HB2	6:E:695:HOH:O	2.17	0.44
1:D:378:ARG:NH1	1:D:387[A]:GLU:OE1	2.49	0.44
1:F:237:THR:HG23	6:F:737:HOH:O	2.16	0.44
1:B:346:ASN:HD22	1:B:350:ARG:NH1	2.13	0.44
1:B:371:ASP:C	1:B:371:ASP:OD1	2.61	0.44
1:A:54:ASP:OD2	1:A:294:HIS:HE1	2.01	0.44
1:C:166:LEU:O	1:C:169:HIS:ND1	2.50	0.44
1:C:282:ASN:HA	1:C:306:LEU:O	2.18	0.44
3:D:501:HEM:HBB2	3:D:501:HEM:HMB2	2.00	0.44
1:D:359:ARG:HG2	6:D:605:HOH:O	2.18	0.44
1:E:3:GLN:C	4:E:504:SO4:O4	2.52	0.44
1:E:345:GLY:HA3	3:E:501:HEM:C3C	2.53	0.43
1:A:156:LEU:HB3	6:A:894:HOH:O	2.18	0.43
1:C:345:GLY:HA3	3:C:501:HEM:C3C	2.52	0.43
1:D:236:GLU:HG3	6:D:799:HOH:O	2.18	0.43
1:B:111:ARG:NH2	1:B:405:HIS:NE2	2.67	0.43
1:B:399:VAL:O	1:B:400:LEU:C	2.62	0.43
1:D:277:THR:O	1:D:278:SER:C	2.61	0.43
1:E:282:ASN:HA	1:E:306:LEU:O	2.19	0.43
1:F:99[A]:ARG:NH1	1:F:103:MET:HE3	2.32	0.43
1:B:81:MET:HE1	1:B:89:ARG:HB2	1.98	0.43
1:B:277:THR:O	1:B:278:SER:C	2.62	0.43
1:B:305:MET:HB3	1:B:305:MET:HE3	1.83	0.43
1:C:234:GLY:HA2	3:C:501:HEM:C2C	2.54	0.43
1:E:346:ASN:HD22	1:E:350:ARG:NH1	2.15	0.43
1:D:398:PRO:HB2	1:D:400:LEU:HG	1.99	0.43
1:E:359:ARG:HG2	1:E:362[B]:ARG:NH2	2.25	0.43
1:F:85:GLN:CB	6:F:1023:HOH:O	2.61	0.43
1:F:123:ARG:HG2	1:F:125:GLU:OE2	2.19	0.43
1:B:233:GLY:HA2	5:B:505:EDO:H22	2.00	0.43
1:E:234:GLY:HA2	3:E:501:HEM:C2C	2.54	0.43
1:F:277:THR:O	1:F:278:SER:C	2.61	0.43
1:C:141:ILE:HG21	1:C:231:LEU:HD23	2.00	0.43
1:C:233:GLY:HA2	5:C:505:EDO:H22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:MET:HB2	1:A:144:MET:HE3	1.54	0.42
1:B:81:MET:HE2	1:B:86:HIS:HA	1.99	0.42
1:B:177:LYS:O	1:B:181:THR:HG23	2.19	0.42
1:C:294:HIS:HD2	6:C:980:HOH:O	2.02	0.42
1:D:200:PRO:HG3	6:D:774:HOH:O	2.19	0.42
1:E:99:ARG:NE	1:E:347:GLN:HE22	2.05	0.42
1:F:183:ALA:O	1:F:187[B]:GLU:HG2	2.19	0.42
1:D:78:MET:HE1	1:D:93:VAL:HB	2.02	0.42
1:D:181:THR:HB	6:D:620:HOH:O	2.19	0.42
1:A:4:MET:CG	4:A:502:SO4:O2	2.68	0.42
1:A:211:SER:O	1:A:217:ARG:HG2	2.19	0.42
1:B:78:MET:HE1	1:B:93:VAL:HB	2.01	0.42
1:A:366:ASP:O	1:A:368[A]:ARG:HG3	2.19	0.42
1:C:240:HIS:HD2	6:C:651:HOH:O	2.01	0.42
1:E:299:ARG:HH11	1:E:299:ARG:CG	2.05	0.42
1:A:49:TYR:CD1	1:A:317:VAL:HG21	2.55	0.42
1:D:209:VAL:O	1:D:217:ARG:NH2	2.52	0.42
1:E:212:GLU:OE1	1:E:217[A]:ARG:CZ	2.68	0.42
1:B:105:LYS:HA	1:B:105:LYS:HD3	1.75	0.42
1:B:282:ASN:HA	1:B:306:LEU:O	2.20	0.41
1:C:162:LEU:O	1:C:166:LEU:HG	2.19	0.41
1:C:190:LYS:NZ	1:C:221:ASP:OD1	2.45	0.41
1:D:282:ASN:HA	1:D:306:LEU:O	2.20	0.41
1:E:362[B]:ARG:HG2	1:E:363:ARG:HG3	2.01	0.41
1:B:199[B]:GLU:OE1	1:B:199[B]:GLU:CA	2.66	0.41
1:B:213:VAL:CG2	1:B:213:VAL:O	2.69	0.41
1:E:278:SER:N	1:E:279:PRO:HD3	2.35	0.41
1:F:3:GLN:CA	4:F:504:SO4:O3	2.67	0.41
1:F:86:HIS:CE1	3:F:501:HEM:O2D	2.60	0.41
1:C:225:PHE:CE2	2:I:2:GLC:H62	2.54	0.41
1:D:103:MET:HE3	1:D:347[A]:GLN:HE21	1.85	0.41
1:C:221:ASP:CG	2:I:3:GLC:H5	2.45	0.41
1:E:294:HIS:HD2	6:E:988:HOH:O	2.03	0.41
1:A:187:GLU:OE1	6:A:604:HOH:O	2.22	0.41
1:A:99:ARG:HD2	1:A:103:MET:HG3	2.03	0.41
1:B:236:GLU:HG3	6:B:770:HOH:O	2.21	0.41
1:F:134:ALA:O	1:F:138:MET:HG3	2.21	0.41
1:A:114:ASP:OD1	6:A:605:HOH:O	2.22	0.41
1:C:83:ASP:OD1	1:C:86:HIS:CD2	2.71	0.41
1:C:166:LEU:O	1:C:169:HIS:CE1	2.74	0.41
1:D:253:ARG:HA	1:D:253:ARG:HD2	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:196:ARG:HD3	1:F:196:ARG:HA	1.95	0.40
1:F:269:ALA:O	1:F:273:MET:HG3	2.21	0.40
1:B:199[A]:GLU:OE1	6:B:604:HOH:O	2.22	0.40
1:B:78:MET:HA	1:B:81:MET:HE2	2.04	0.40
1:C:253:ARG:HA	1:C:253:ARG:HD2	1.81	0.40
1:D:103:MET:HE3	1:D:347[A]:GLN:NE2	2.36	0.40
1:E:7:ARG:NH1	4:E:504:SO4:O2	2.45	0.40
1:A:221:ASP:CG	2:G:3:GLC:O5	2.65	0.40
1:B:75:MET:HE3	1:B:75:MET:HB3	1.95	0.40
1:C:111:ARG:NE	6:C:616:HOH:O	2.46	0.40
1:C:111:ARG:O	1:C:115:THR:HG23	2.20	0.40
1:C:341:HIS:O	1:C:342:PHE:C	2.64	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:1046:HOH:O	6:F:601:HOH:O[3_545]	1.89	0.31

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	405/407 (100%)	393 (97%)	12 (3%)	0	100	100
1	B	407/407 (100%)	394 (97%)	13 (3%)	0	100	100
1	C	407/407 (100%)	391 (96%)	16 (4%)	0	100	100
1	D	407/407 (100%)	395 (97%)	12 (3%)	0	100	100
1	E	406/407 (100%)	395 (97%)	11 (3%)	0	100	100
1	F	406/407 (100%)	397 (98%)	9 (2%)	0	100	100
All	All	2438/2442 (100%)	2365 (97%)	73 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	340/349 (97%)	327 (96%)	13 (4%)	29	15
1	B	341/349 (98%)	324 (95%)	17 (5%)	22	9
1	C	343/349 (98%)	328 (96%)	15 (4%)	25	12
1	D	346/349 (99%)	334 (96%)	12 (4%)	32	18
1	E	345/349 (99%)	332 (96%)	13 (4%)	29	15
1	F	346/349 (99%)	334 (96%)	12 (4%)	32	18
All	All	2061/2094 (98%)	1979 (96%)	82 (4%)	29	14

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	68	ILE
1	A	77	TYR
1	A	99	ARG
1	A	105	LYS
1	A	112	LEU
1	A	125	GLU
1	A	138	MET
1	A	169	HIS
1	A	199	GLU
1	A	209	VAL
1	A	230	ILE
1	A	378	ARG
1	B	77	TYR
1	B	104	ASP
1	B	125	GLU
1	B	138	MET
1	B	164	CYS
1	B	179	MET

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Mol	Chain	Res	Type
1	B	181	THR
1	B	199[A]	GLU
1	B	199[B]	GLU
1	B	214	GLU
1	B	216	GLN
1	B	230	ILE
1	B	265	LEU
1	B	305	MET
1	B	378	ARG
1	B	399	VAL
1	B	405	HIS
1	C	65	THR
1	C	77	TYR
1	C	108	SER
1	C	138	MET
1	C	170	VAL
1	C	202	ASP
1	C	253	ARG
1	C	265	LEU
1	C	368[A]	ARG
1	C	368[B]	ARG
1	C	371	ASP
1	C	372[A]	ASP
1	C	372[B]	ASP
1	C	378	ARG
1	C	399	VAL
1	D	40	ARG
1	D	68	ILE
1	D	77	TYR
1	D	99[A]	ARG
1	D	99[B]	ARG
1	D	125	GLU
1	D	171	ASP
1	D	181	THR
1	D	202	ASP
1	D	209	VAL
1	D	265	LEU
1	D	378	ARG
1	E	77	TYR
1	E	99	ARG
1	E	125	GLU
1	E	138	MET

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Mol	Chain	Res	Type
1	E	164	CYS
1	E	169	HIS
1	E	175	ILE
1	E	209	VAL
1	E	265	LEU
1	E	299	ARG
1	E	354	ARG
1	E	371	ASP
1	E	399	VAL
1	F	77	TYR
1	F	99[A]	ARG
1	F	99[B]	ARG
1	F	100	LYS
1	F	105	LYS
1	F	168	SER
1	F	181	THR
1	F	199	GLU
1	F	209	VAL
1	F	242	LEU
1	F	299	ARG
1	F	375	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	85	GLN
1	A	86	HIS
1	A	94	ASN
1	A	169	HIS
1	A	216	GLN
1	A	240	HIS
1	A	294	HIS
1	A	323	ASN
1	A	341	HIS
1	A	346	ASN
1	A	402	HIS
1	B	3	GLN
1	B	50	GLN
1	B	72	GLN
1	B	86	HIS
1	B	240	HIS

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Mol	Chain	Res	Type
1	B	294	HIS
1	B	323	ASN
1	B	341	HIS
1	B	346	ASN
1	C	58	ASN
1	C	86	HIS
1	C	94	ASN
1	C	216	GLN
1	C	240	HIS
1	C	294	HIS
1	C	323	ASN
1	C	341	HIS
1	C	346	ASN
1	D	41	ASN
1	D	50	GLN
1	D	86	HIS
1	D	240	HIS
1	D	294	HIS
1	D	323	ASN
1	D	341	HIS
1	D	346	ASN
1	E	86	HIS
1	E	94	ASN
1	E	210	ASN
1	E	240	HIS
1	E	294	HIS
1	E	323	ASN
1	E	341	HIS
1	E	346	ASN
1	E	347	GLN
1	E	402	HIS
1	F	86	HIS
1	F	94	ASN
1	F	216	GLN
1	F	240	HIS
1	F	294	HIS
1	F	323	ASN
1	F	341	HIS
1	F	346	ASN
1	F	347	GLN
1	F	403	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

42 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	G	1	2	11,11,12	0.79	0	15,15,17	2.22	5 (33%)
2	GLC	G	2	2	11,11,12	1.12	1 (9%)	15,15,17	2.35	9 (60%)
2	GLC	G	3	2	11,11,12	1.08	0	15,15,17	2.33	7 (46%)
2	GLC	G	4	2	11,11,12	0.57	0	15,15,17	2.52	4 (26%)
2	GLC	G	5	2	11,11,12	0.74	0	15,15,17	2.35	5 (33%)
2	GLC	G	6	2	11,11,12	0.65	0	15,15,17	3.59	9 (60%)
2	GLC	G	7	2	11,11,12	0.67	0	15,15,17	2.29	6 (40%)
2	GLC	H	1	2	11,11,12	0.77	0	15,15,17	2.04	7 (46%)
2	GLC	H	2	2	11,11,12	1.56	1 (9%)	15,15,17	3.22	8 (53%)
2	GLC	H	3	2	11,11,12	0.92	1 (9%)	15,15,17	4.08	8 (53%)
2	GLC	H	4	2	11,11,12	0.73	0	15,15,17	2.35	10 (66%)
2	GLC	H	5	2	11,11,12	1.25	2 (18%)	15,15,17	2.33	6 (40%)
2	GLC	H	6	2	11,11,12	0.86	1 (9%)	15,15,17	3.41	9 (60%)
2	GLC	H	7	2	11,11,12	0.85	0	15,15,17	2.28	5 (33%)
2	GLC	I	1	2	11,11,12	1.29	1 (9%)	15,15,17	1.93	6 (40%)
2	GLC	I	2	2	11,11,12	1.74	1 (9%)	15,15,17	2.67	9 (60%)
2	GLC	I	3	2	11,11,12	1.63	2 (18%)	15,15,17	3.28	8 (53%)
2	GLC	I	4	2	11,11,12	0.75	0	15,15,17	2.73	8 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	I	5	2	11,11,12	0.87	1 (9%)	15,15,17	1.84	5 (33%)
2	GLC	I	6	2	11,11,12	0.80	0	15,15,17	2.16	5 (33%)
2	GLC	I	7	2	11,11,12	0.88	0	15,15,17	2.50	6 (40%)
2	GLC	J	1	2	11,11,12	0.71	0	15,15,17	1.69	3 (20%)
2	GLC	J	2	2	11,11,12	0.89	0	15,15,17	2.67	7 (46%)
2	GLC	J	3	2	11,11,12	1.04	0	15,15,17	2.96	9 (60%)
2	GLC	J	4	2	11,11,12	0.52	0	15,15,17	2.33	7 (46%)
2	GLC	J	5	2	11,11,12	0.57	0	15,15,17	1.69	5 (33%)
2	GLC	J	6	2	11,11,12	0.86	0	15,15,17	2.86	4 (26%)
2	GLC	J	7	2	11,11,12	0.59	0	15,15,17	2.67	4 (26%)
2	GLC	K	1	2	11,11,12	0.72	0	15,15,17	1.91	6 (40%)
2	GLC	K	2	2	11,11,12	0.98	0	15,15,17	2.27	5 (33%)
2	GLC	K	3	2	11,11,12	1.27	2 (18%)	15,15,17	2.85	10 (66%)
2	GLC	K	4	2	11,11,12	1.38	1 (9%)	15,15,17	3.23	8 (53%)
2	GLC	K	5	2	11,11,12	0.80	0	15,15,17	4.01	10 (66%)
2	GLC	K	6	2	11,11,12	0.83	0	15,15,17	2.52	8 (53%)
2	GLC	K	7	2	11,11,12	1.33	1 (9%)	15,15,17	3.39	6 (40%)
2	GLC	L	1	2	11,11,12	1.08	1 (9%)	15,15,17	2.55	6 (40%)
2	GLC	L	2	2	11,11,12	0.73	0	15,15,17	2.17	5 (33%)
2	GLC	L	3	2	11,11,12	0.57	0	15,15,17	1.66	5 (33%)
2	GLC	L	4	2	11,11,12	0.55	0	15,15,17	2.01	5 (33%)
2	GLC	L	5	2	11,11,12	0.62	0	15,15,17	2.08	9 (60%)
2	GLC	L	6	2	11,11,12	0.61	0	15,15,17	3.25	7 (46%)
2	GLC	L	7	2	11,11,12	0.84	0	15,15,17	3.83	10 (66%)

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	G	1	2	1/1/4/5	2/2/19/22	0/1/1/1
2	GLC	G	2	2	-	1/2/19/22	0/1/1/1
2	GLC	G	3	2	-	0/2/19/22	0/1/1/1
2	GLC	G	4	2	-	2/2/19/22	0/1/1/1
2	GLC	G	5	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	G	6	2	-	1/2/19/22	0/1/1/1
2	GLC	G	7	2	1/1/4/5	2/2/19/22	0/1/1/1
2	GLC	H	1	2	1/1/4/5	1/2/19/22	0/1/1/1
2	GLC	H	2	2	-	2/2/19/22	0/1/1/1
2	GLC	H	3	2	-	2/2/19/22	0/1/1/1
2	GLC	H	4	2	-	2/2/19/22	0/1/1/1
2	GLC	H	5	2	-	0/2/19/22	0/1/1/1
2	GLC	H	6	2	-	0/2/19/22	0/1/1/1
2	GLC	H	7	2	1/1/4/5	2/2/19/22	0/1/1/1
2	GLC	I	1	2	1/1/4/5	2/2/19/22	0/1/1/1
2	GLC	I	2	2	-	1/2/19/22	0/1/1/1
2	GLC	I	3	2	-	0/2/19/22	0/1/1/1
2	GLC	I	4	2	-	1/2/19/22	0/1/1/1
2	GLC	I	5	2	-	0/2/19/22	0/1/1/1
2	GLC	I	6	2	-	1/2/19/22	0/1/1/1
2	GLC	I	7	2	1/1/4/5	0/2/19/22	0/1/1/1
2	GLC	J	1	2	-	0/2/19/22	0/1/1/1
2	GLC	J	2	2	-	2/2/19/22	0/1/1/1
2	GLC	J	3	2	-	0/2/19/22	0/1/1/1
2	GLC	J	4	2	-	1/2/19/22	0/1/1/1
2	GLC	J	5	2	-	2/2/19/22	0/1/1/1
2	GLC	J	6	2	-	1/2/19/22	0/1/1/1
2	GLC	J	7	2	1/1/4/5	1/2/19/22	0/1/1/1
2	GLC	K	1	2	1/1/4/5	2/2/19/22	0/1/1/1
2	GLC	K	2	2	-	1/2/19/22	0/1/1/1
2	GLC	K	3	2	-	2/2/19/22	0/1/1/1
2	GLC	K	4	2	1/1/4/5	1/2/19/22	0/1/1/1
2	GLC	K	5	2	-	2/2/19/22	0/1/1/1
2	GLC	K	6	2	-	2/2/19/22	0/1/1/1
2	GLC	K	7	2	1/1/4/5	0/2/19/22	0/1/1/1
2	GLC	L	1	2	-	2/2/19/22	0/1/1/1
2	GLC	L	2	2	-	2/2/19/22	0/1/1/1
2	GLC	L	3	2	-	0/2/19/22	0/1/1/1
2	GLC	L	4	2	1/1/4/5	0/2/19/22	0/1/1/1
2	GLC	L	5	2	-	2/2/19/22	0/1/1/1
2	GLC	L	6	2	1/1/4/5	0/2/19/22	1/1/1/1
2	GLC	L	7	2	-	0/2/19/22	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	GLC	O5-C1	4.89	1.51	1.43
2	H	2	GLC	O5-C1	4.62	1.51	1.43
2	I	3	GLC	C2-C3	3.92	1.58	1.52
2	K	7	GLC	C2-C3	2.98	1.57	1.52
2	K	3	GLC	O5-C5	2.80	1.48	1.43
2	H	5	GLC	O2-C2	2.41	1.48	1.43
2	H	6	GLC	O5-C1	2.39	1.47	1.43
2	I	3	GLC	C1-C2	2.34	1.57	1.52
2	G	2	GLC	O5-C1	2.34	1.47	1.43
2	H	3	GLC	C2-C3	2.31	1.56	1.52
2	H	5	GLC	C2-C3	2.31	1.56	1.52
2	K	4	GLC	C1-C2	2.27	1.57	1.52
2	L	1	GLC	O5-C1	2.17	1.47	1.43
2	I	1	GLC	O5-C5	2.14	1.47	1.43
2	I	5	GLC	O5-C5	2.12	1.47	1.43
2	K	3	GLC	O4-C4	2.00	1.47	1.43

All (284) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	7	GLC	C3-C4-C5	-9.81	92.44	110.23
2	K	4	GLC	O5-C5-C4	-9.47	87.79	110.83
2	G	6	GLC	C3-C4-C5	-9.33	93.32	110.23
2	K	5	GLC	O5-C5-C4	-8.57	89.97	110.83
2	H	6	GLC	C3-C4-C5	-8.39	95.01	110.23
2	H	3	GLC	C1-C2-C3	-7.81	98.28	109.64
2	J	3	GLC	C1-O5-C5	7.80	122.64	112.19
2	I	3	GLC	O5-C5-C4	-7.78	91.90	110.83
2	J	6	GLC	C1-O5-C5	7.57	122.33	112.19
2	H	3	GLC	C3-C4-C5	-7.45	96.72	110.23
2	L	1	GLC	O5-C5-C6	-7.44	93.17	107.66
2	J	7	GLC	C2-C3-C4	-7.16	98.27	110.86
2	K	5	GLC	O4-C4-C5	6.66	125.74	109.32
2	K	7	GLC	C1-O5-C5	-6.66	103.26	112.19
2	I	7	GLC	C1-O5-C5	-6.53	103.43	112.19
2	G	4	GLC	O4-C4-C3	-6.27	95.59	110.38
2	H	2	GLC	O5-C5-C6	6.21	119.76	107.66
2	L	6	GLC	C2-C3-C4	-6.11	100.11	110.86
2	K	5	GLC	C3-C4-C5	-5.84	99.65	110.23
2	L	6	GLC	C1-C2-C3	-5.81	101.19	109.64
2	L	4	GLC	C1-O5-C5	-5.76	104.47	112.19
2	H	7	GLC	O2-C2-C3	-5.63	98.49	110.15
2	H	5	GLC	C1-C2-C3	-5.58	101.53	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	7	GLC	C1-C2-C3	5.55	117.72	109.64
2	J	7	GLC	C1-C2-C3	-5.53	101.60	109.64
2	G	6	GLC	O4-C4-C5	5.52	122.91	109.32
2	J	6	GLC	C2-C3-C4	-5.46	101.25	110.86
2	H	2	GLC	C3-C4-C5	-5.45	100.36	110.23
2	I	2	GLC	O4-C4-C5	5.44	122.72	109.32
2	K	7	GLC	C3-C4-C5	-5.43	100.39	110.23
2	H	3	GLC	O5-C5-C4	-5.36	97.79	110.83
2	H	6	GLC	C1-C2-C3	5.29	117.34	109.64
2	J	2	GLC	O5-C5-C6	-5.27	97.40	107.66
2	K	7	GLC	C1-C2-C3	5.19	117.20	109.64
2	G	7	GLC	O4-C4-C3	-5.16	98.22	110.38
2	I	4	GLC	O5-C5-C4	-5.08	98.47	110.83
2	L	2	GLC	O2-C2-C1	5.06	120.80	109.22
2	K	7	GLC	O5-C5-C6	5.04	117.47	107.66
2	K	5	GLC	C6-C5-C4	5.04	125.39	113.02
2	L	7	GLC	C2-C3-C4	-4.99	102.08	110.86
2	H	3	GLC	C1-O5-C5	4.89	118.74	112.19
2	H	3	GLC	O3-C3-C2	4.83	119.92	110.05
2	G	4	GLC	O5-C1-C2	4.81	122.27	110.79
2	K	2	GLC	C3-C4-C5	-4.80	101.52	110.23
2	K	7	GLC	O4-C4-C3	4.80	121.68	110.38
2	I	3	GLC	O5-C5-C6	4.79	116.98	107.66
2	I	3	GLC	O4-C4-C3	4.75	121.58	110.38
2	K	3	GLC	O5-C1-C2	-4.72	99.52	110.79
2	H	3	GLC	C6-C5-C4	4.67	124.48	113.02
2	H	2	GLC	O5-C1-C2	4.57	121.70	110.79
2	J	4	GLC	O5-C5-C6	-4.57	98.78	107.66
2	L	6	GLC	O5-C5-C4	-4.57	99.72	110.83
2	L	6	GLC	C1-O5-C5	-4.53	106.12	112.19
2	G	3	GLC	C6-C5-C4	4.52	124.13	113.02
2	G	2	GLC	O2-C2-C3	-4.50	100.83	110.15
2	G	1	GLC	O5-C5-C6	4.48	116.38	107.66
2	J	2	GLC	C6-C5-C4	4.43	123.90	113.02
2	H	2	GLC	C2-C3-C4	-4.42	103.09	110.86
2	K	4	GLC	C2-C3-C4	-4.29	103.32	110.86
2	K	3	GLC	C1-C2-C3	4.26	115.85	109.64
2	J	2	GLC	O4-C4-C5	4.25	119.79	109.32
2	L	7	GLC	O2-C2-C1	4.24	118.92	109.22
2	I	4	GLC	C1-C2-C3	4.22	115.79	109.64
2	H	2	GLC	O5-C5-C4	-4.22	100.57	110.83
2	G	1	GLC	C1-C2-C3	4.21	115.78	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	3	GLC	O5-C1-C2	-4.20	100.78	110.79
2	J	4	GLC	C1-O5-C5	-4.18	106.58	112.19
2	K	5	GLC	O5-C1-C2	4.17	120.75	110.79
2	I	6	GLC	C1-C2-C3	-4.17	103.58	109.64
2	K	2	GLC	O5-C5-C6	4.14	115.73	107.66
2	K	3	GLC	O5-C5-C4	4.14	120.90	110.83
2	G	5	GLC	C1-O5-C5	4.12	117.71	112.19
2	G	6	GLC	C6-C5-C4	4.09	123.07	113.02
2	G	6	GLC	C1-O5-C5	4.09	117.67	112.19
2	K	6	GLC	C1-C2-C3	-4.08	103.70	109.64
2	G	5	GLC	O3-C3-C4	-4.06	100.81	110.38
2	J	3	GLC	O2-C2-C1	4.03	118.44	109.22
2	I	4	GLC	O4-C4-C5	4.00	119.19	109.32
2	H	1	GLC	O4-C4-C3	4.00	119.81	110.38
2	G	3	GLC	C1-O5-C5	3.96	117.49	112.19
2	K	5	GLC	C2-C3-C4	-3.92	103.97	110.86
2	G	7	GLC	C3-C4-C5	-3.90	103.15	110.23
2	K	6	GLC	O2-C2-C3	3.86	118.15	110.15
2	K	3	GLC	O2-C2-C1	-3.86	100.39	109.22
2	H	6	GLC	O6-C6-C5	-3.85	98.21	111.33
2	H	7	GLC	C6-C5-C4	-3.85	103.56	113.02
2	H	4	GLC	C2-C3-C4	-3.83	104.12	110.86
2	H	6	GLC	C6-C5-C4	3.81	122.36	113.02
2	K	7	GLC	O5-C5-C4	-3.80	101.57	110.83
2	I	1	GLC	C1-C2-C3	3.79	115.17	109.64
2	I	6	GLC	C3-C4-C5	-3.76	103.42	110.23
2	G	5	GLC	O2-C2-C1	3.76	117.82	109.22
2	L	5	GLC	C2-C3-C4	-3.74	104.29	110.86
2	K	2	GLC	C1-O5-C5	3.72	117.18	112.19
2	L	6	GLC	O2-C2-C3	3.72	117.86	110.15
2	H	2	GLC	O4-C4-C3	3.70	119.11	110.38
2	I	4	GLC	O3-C3-C4	-3.70	101.65	110.38
2	K	2	GLC	O4-C4-C3	3.68	119.06	110.38
2	I	5	GLC	O5-C5-C6	3.67	114.81	107.66
2	I	4	GLC	C1-O5-C5	3.64	117.07	112.19
2	G	5	GLC	O4-C4-C3	-3.63	101.82	110.38
2	K	5	GLC	C1-O5-C5	-3.61	107.35	112.19
2	G	4	GLC	C3-C4-C5	-3.60	103.70	110.23
2	J	2	GLC	C3-C4-C5	-3.60	103.70	110.23
2	I	3	GLC	C1-C2-C3	3.60	114.88	109.64
2	K	4	GLC	C6-C5-C4	3.58	121.80	113.02
2	K	3	GLC	C3-C4-C5	-3.58	103.75	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	7	GLC	O5-C1-C2	-3.56	102.31	110.79
2	G	6	GLC	O3-C3-C2	3.55	117.30	110.05
2	K	4	GLC	C1-C2-C3	3.51	114.75	109.64
2	K	1	GLC	O4-C4-C3	3.47	118.56	110.38
2	I	5	GLC	C3-C4-C5	-3.47	103.94	110.23
2	I	1	GLC	O4-C4-C3	3.46	118.54	110.38
2	K	6	GLC	O4-C4-C5	3.46	117.85	109.32
2	I	2	GLC	O5-C1-C2	3.46	119.04	110.79
2	H	7	GLC	C2-C3-C4	-3.45	104.80	110.86
2	I	7	GLC	C6-C5-C4	3.42	121.42	113.02
2	G	1	GLC	C3-C4-C5	-3.41	104.05	110.23
2	K	6	GLC	C3-C4-C5	-3.40	104.07	110.23
2	H	4	GLC	O3-C3-C2	3.36	116.92	110.05
2	K	1	GLC	C2-C3-C4	-3.36	104.95	110.86
2	L	6	GLC	C3-C4-C5	-3.35	104.15	110.23
2	H	5	GLC	O2-C2-C1	3.35	116.88	109.22
2	H	4	GLC	O3-C3-C4	-3.34	102.50	110.38
2	L	7	GLC	O6-C6-C5	-3.33	100.01	111.33
2	L	7	GLC	O5-C5-C6	-3.31	101.22	107.66
2	I	2	GLC	C3-C4-C5	-3.30	104.24	110.23
2	H	6	GLC	O4-C4-C3	3.27	118.08	110.38
2	I	2	GLC	C1-C2-C3	3.25	114.38	109.64
2	G	2	GLC	C1-C2-C3	3.22	114.33	109.64
2	I	2	GLC	O2-C2-C1	3.20	116.54	109.22
2	J	4	GLC	C2-C3-C4	-3.13	105.36	110.86
2	G	3	GLC	O5-C5-C4	-3.12	103.23	110.83
2	G	7	GLC	C1-C2-C3	-3.12	105.10	109.64
2	G	2	GLC	O4-C4-C3	-3.12	103.02	110.38
2	G	6	GLC	C2-C3-C4	-3.12	105.37	110.86
2	I	6	GLC	O2-C2-C3	3.09	116.54	110.15
2	J	1	GLC	O3-C3-C2	-3.08	103.76	110.05
2	J	3	GLC	C2-C3-C4	-3.07	105.46	110.86
2	I	4	GLC	O5-C1-C2	3.06	118.09	110.79
2	H	3	GLC	O4-C4-C5	3.06	116.86	109.32
2	J	5	GLC	O4-C4-C5	3.06	116.86	109.32
2	H	6	GLC	O5-C1-C2	3.03	118.00	110.79
2	J	6	GLC	O2-C2-C1	3.02	116.13	109.22
2	G	2	GLC	O6-C6-C5	3.02	121.61	111.33
2	J	1	GLC	C1-C2-C3	-3.00	105.28	109.64
2	H	4	GLC	O5-C1-C2	2.98	117.90	110.79
2	L	3	GLC	O2-C2-C1	2.98	116.05	109.22
2	H	5	GLC	O5-C5-C6	2.98	113.46	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	2	GLC	O4-C4-C3	-2.97	103.38	110.38
2	L	6	GLC	O3-C3-C2	2.96	116.09	110.05
2	I	6	GLC	O5-C1-C2	-2.95	103.75	110.79
2	G	2	GLC	C6-C5-C4	2.94	120.25	113.02
2	L	1	GLC	O6-C6-C5	-2.92	101.38	111.33
2	K	3	GLC	O4-C4-C3	-2.92	103.50	110.38
2	I	3	GLC	C6-C5-C4	2.90	120.14	113.02
2	L	5	GLC	O3-C3-C2	2.90	115.97	110.05
2	H	5	GLC	O5-C5-C4	-2.90	103.78	110.83
2	L	7	GLC	O4-C4-C5	2.89	116.44	109.32
2	K	6	GLC	O4-C4-C3	2.85	117.10	110.38
2	L	2	GLC	O6-C6-C5	-2.83	101.70	111.33
2	G	3	GLC	C1-C2-C3	-2.82	105.53	109.64
2	I	3	GLC	C3-C4-C5	-2.82	105.11	110.23
2	J	6	GLC	O4-C4-C3	-2.82	103.74	110.38
2	G	1	GLC	C1-O5-C5	-2.81	108.42	112.19
2	J	3	GLC	C1-C2-C3	2.79	113.71	109.64
2	K	6	GLC	O5-C1-C2	-2.78	104.16	110.79
2	J	4	GLC	O4-C4-C5	2.77	116.15	109.32
2	J	4	GLC	C1-C2-C3	-2.76	105.63	109.64
2	J	5	GLC	O2-C2-C1	2.76	115.53	109.22
2	L	1	GLC	O3-C3-C2	2.75	115.67	110.05
2	L	5	GLC	O5-C1-C2	-2.74	104.25	110.79
2	L	3	GLC	O3-C3-C4	2.74	116.83	110.38
2	L	5	GLC	O5-C5-C6	2.73	112.97	107.66
2	J	7	GLC	O4-C4-C3	2.70	116.75	110.38
2	H	6	GLC	C1-O5-C5	-2.68	108.59	112.19
2	I	6	GLC	O5-C5-C4	-2.68	104.31	110.83
2	L	2	GLC	C1-C2-C3	-2.67	105.75	109.64
2	G	2	GLC	O3-C3-C4	2.67	116.68	110.38
2	G	3	GLC	O2-C2-C1	2.67	115.34	109.22
2	K	1	GLC	C1-O5-C5	-2.67	108.61	112.19
2	J	4	GLC	O3-C3-C2	2.66	115.47	110.05
2	L	4	GLC	O5-C1-C2	-2.65	104.47	110.79
2	J	1	GLC	O3-C3-C4	-2.65	104.14	110.38
2	G	6	GLC	O5-C1-C2	2.63	117.07	110.79
2	I	5	GLC	C1-O5-C5	2.63	115.70	112.19
2	K	1	GLC	O6-C6-C5	-2.62	102.40	111.33
2	H	1	GLC	O2-C2-C1	-2.62	103.23	109.22
2	I	2	GLC	O5-C5-C4	-2.61	104.47	110.83
2	J	2	GLC	O2-C2-C1	2.61	115.20	109.22
2	I	2	GLC	C6-C5-C4	2.60	119.41	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	4	GLC	C2-C3-C4	-2.58	106.32	110.86
2	J	3	GLC	C3-C4-C5	-2.57	105.57	110.23
2	I	7	GLC	O2-C2-C1	2.55	115.06	109.22
2	I	7	GLC	C3-C4-C5	-2.54	105.62	110.23
2	I	3	GLC	O2-C2-C3	2.52	115.37	110.15
2	H	4	GLC	O4-C4-C3	-2.50	104.47	110.38
2	L	5	GLC	O2-C2-C3	2.49	115.31	110.15
2	L	3	GLC	C3-C4-C5	-2.48	105.73	110.23
2	H	1	GLC	O5-C5-C4	-2.47	104.81	110.83
2	J	5	GLC	C3-C4-C5	-2.46	105.77	110.23
2	L	4	GLC	O3-C3-C4	-2.45	104.61	110.38
2	L	7	GLC	C6-C5-C4	2.44	119.00	113.02
2	K	5	GLC	O6-C6-C5	-2.44	103.04	111.33
2	H	5	GLC	O5-C1-C2	-2.43	104.98	110.79
2	J	3	GLC	O4-C4-C5	2.41	115.26	109.32
2	G	4	GLC	O4-C4-C5	2.41	115.25	109.32
2	H	4	GLC	O5-C5-C6	2.39	112.32	107.66
2	H	1	GLC	C1-O5-C5	-2.38	108.99	112.19
2	J	2	GLC	O3-C3-C4	2.36	115.93	110.38
2	L	3	GLC	O3-C3-C2	-2.35	105.26	110.05
2	H	6	GLC	C2-C3-C4	-2.35	106.73	110.86
2	H	7	GLC	O6-C6-C5	-2.34	103.36	111.33
2	I	2	GLC	O4-C4-C3	-2.34	104.86	110.38
2	G	2	GLC	O5-C5-C4	-2.34	105.14	110.83
2	L	1	GLC	O2-C2-C3	-2.33	105.31	110.15
2	K	3	GLC	C1-O5-C5	2.33	115.31	112.19
2	H	4	GLC	O5-C5-C4	-2.33	105.16	110.83
2	L	2	GLC	C6-C5-C4	2.32	118.70	113.02
2	I	2	GLC	C2-C3-C4	-2.31	106.80	110.86
2	I	1	GLC	O5-C5-C6	2.31	112.16	107.66
2	L	5	GLC	O6-C6-C5	2.30	119.18	111.33
2	G	7	GLC	O4-C4-C5	2.30	114.99	109.32
2	H	7	GLC	O4-C4-C5	-2.30	103.66	109.32
2	I	4	GLC	O5-C5-C6	2.30	112.13	107.66
2	K	1	GLC	O2-C2-C3	2.27	114.86	110.15
2	J	3	GLC	O5-C1-C2	2.26	116.18	110.79
2	J	2	GLC	C1-C2-C3	-2.26	106.35	109.64
2	K	5	GLC	O3-C3-C2	2.26	114.66	110.05
2	K	6	GLC	O5-C5-C4	-2.25	105.34	110.83
2	L	1	GLC	O4-C4-C5	2.25	114.87	109.32
2	L	7	GLC	O2-C2-C3	-2.25	105.49	110.15
2	H	4	GLC	C1-O5-C5	2.24	115.19	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	6	GLC	C6-C5-C4	-2.22	107.56	113.02
2	L	5	GLC	C3-C4-C5	-2.22	106.20	110.23
2	I	1	GLC	C1-O5-C5	2.22	115.16	112.19
2	I	1	GLC	O2-C2-C3	2.21	114.73	110.15
2	G	7	GLC	O5-C5-C6	2.20	111.94	107.66
2	H	1	GLC	C2-C3-C4	-2.20	107.00	110.86
2	G	6	GLC	O5-C5-C4	-2.19	105.51	110.83
2	J	3	GLC	O3-C3-C2	2.18	114.50	110.05
2	K	3	GLC	O3-C3-C2	2.18	114.50	110.05
2	I	5	GLC	C1-C2-C3	-2.17	106.48	109.64
2	G	3	GLC	O4-C4-C5	-2.17	103.98	109.32
2	L	3	GLC	C2-C3-C4	-2.17	107.05	110.86
2	H	5	GLC	O2-C2-C3	2.16	114.64	110.15
2	K	3	GLC	O4-C4-C5	2.15	114.62	109.32
2	I	1	GLC	O3-C3-C2	-2.15	105.67	110.05
2	G	7	GLC	O2-C2-C1	2.15	114.14	109.22
2	K	4	GLC	O3-C3-C2	2.14	114.43	110.05
2	H	2	GLC	O3-C3-C4	2.14	115.43	110.38
2	H	4	GLC	C1-C2-C3	2.14	112.75	109.64
2	G	3	GLC	O3-C3-C4	2.13	115.41	110.38
2	G	5	GLC	C6-C5-C4	2.13	118.25	113.02
2	L	1	GLC	C1-O5-C5	-2.13	109.33	112.19
2	H	1	GLC	O4-C4-C5	-2.11	104.13	109.32
2	J	5	GLC	C1-C2-C3	-2.10	106.58	109.64
2	L	7	GLC	O4-C4-C3	2.09	115.31	110.38
2	G	6	GLC	O5-C5-C6	2.09	111.74	107.66
2	G	2	GLC	O5-C1-C2	2.09	115.78	110.79
2	K	4	GLC	O2-C2-C3	-2.09	105.82	110.15
2	H	4	GLC	O4-C4-C5	2.09	114.46	109.32
2	H	1	GLC	O5-C5-C6	2.07	111.70	107.66
2	J	5	GLC	C2-C3-C4	-2.07	107.22	110.86
2	I	7	GLC	O6-C6-C5	-2.07	104.28	111.33
2	J	7	GLC	O4-C4-C5	2.07	114.41	109.32
2	K	3	GLC	O3-C3-C4	2.06	115.24	110.38
2	L	4	GLC	O4-C4-C5	2.06	114.40	109.32
2	L	4	GLC	O5-C5-C4	-2.06	105.82	110.83
2	K	2	GLC	O2-C2-C3	2.06	114.41	110.15
2	K	1	GLC	O5-C1-C2	-2.05	105.90	110.79
2	K	4	GLC	C3-C4-C5	2.04	113.93	110.23
2	I	3	GLC	O3-C3-C2	2.04	114.22	110.05
2	K	4	GLC	O5-C1-C2	2.04	115.65	110.79
2	L	5	GLC	C6-C5-C4	2.03	118.02	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	5	GLC	O3-C3-C4	2.02	115.13	110.38
2	L	5	GLC	O5-C5-C4	-2.02	105.92	110.83
2	H	2	GLC	O4-C4-C5	2.02	114.29	109.32
2	J	4	GLC	O5-C5-C4	-2.01	105.94	110.83
2	G	1	GLC	O3-C3-C2	2.00	114.14	110.05
2	H	6	GLC	O3-C3-C4	2.00	115.10	110.38
2	G	2	GLC	O2-C2-C1	2.00	113.81	109.22
2	J	3	GLC	O6-C6-C5	2.00	118.15	111.33
2	K	5	GLC	O4-C4-C3	2.00	115.09	110.38

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	1	GLC	C1
2	G	7	GLC	C1
2	H	1	GLC	C1
2	H	7	GLC	C1
2	I	1	GLC	C1
2	I	7	GLC	C1
2	J	7	GLC	C1
2	K	1	GLC	C1
2	K	4	GLC	C1
2	K	7	GLC	C1
2	L	4	GLC	C1
2	L	6	GLC	C2

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	7	GLC	C4-C5-C6-O6
2	K	3	GLC	O5-C5-C6-O6
2	L	2	GLC	O5-C5-C6-O6
2	H	7	GLC	O5-C5-C6-O6
2	I	1	GLC	O5-C5-C6-O6
2	I	1	GLC	C4-C5-C6-O6
2	L	2	GLC	C4-C5-C6-O6
2	J	5	GLC	O5-C5-C6-O6
2	G	1	GLC	O5-C5-C6-O6
2	H	2	GLC	O5-C5-C6-O6
2	J	5	GLC	C4-C5-C6-O6
2	K	6	GLC	C4-C5-C6-O6
2	K	6	GLC	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	G	7	GLC	C4-C5-C6-O6
2	K	1	GLC	C4-C5-C6-O6
2	G	4	GLC	C4-C5-C6-O6
2	K	3	GLC	C4-C5-C6-O6
2	L	5	GLC	C4-C5-C6-O6
2	G	1	GLC	C4-C5-C6-O6
2	H	3	GLC	O5-C5-C6-O6
2	J	2	GLC	O5-C5-C6-O6
2	H	4	GLC	O5-C5-C6-O6
2	K	1	GLC	O5-C5-C6-O6
2	L	5	GLC	O5-C5-C6-O6
2	G	7	GLC	O5-C5-C6-O6
2	H	2	GLC	C4-C5-C6-O6
2	H	3	GLC	C4-C5-C6-O6
2	G	4	GLC	O5-C5-C6-O6
2	L	1	GLC	C4-C5-C6-O6
2	L	1	GLC	O5-C5-C6-O6
2	K	5	GLC	C4-C5-C6-O6
2	G	2	GLC	O5-C5-C6-O6
2	I	4	GLC	O5-C5-C6-O6
2	J	2	GLC	C4-C5-C6-O6
2	H	4	GLC	C4-C5-C6-O6
2	H	1	GLC	O5-C5-C6-O6
2	K	2	GLC	O5-C5-C6-O6
2	I	2	GLC	O5-C5-C6-O6
2	J	6	GLC	O5-C5-C6-O6
2	J	7	GLC	C4-C5-C6-O6
2	K	4	GLC	O5-C5-C6-O6
2	K	5	GLC	O5-C5-C6-O6
2	G	5	GLC	C4-C5-C6-O6
2	G	5	GLC	O5-C5-C6-O6
2	I	6	GLC	O5-C5-C6-O6
2	G	6	GLC	C4-C5-C6-O6
2	J	4	GLC	C4-C5-C6-O6

All (1) ring outliers are listed below:

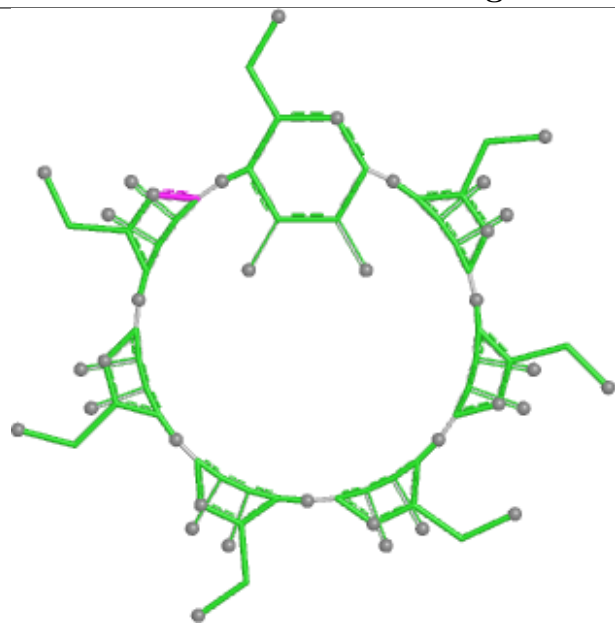
Mol	Chain	Res	Type	Atoms
2	L	6	GLC	C1-C2-C3-C4-C5-O5

7 monomers are involved in 11 short contacts:

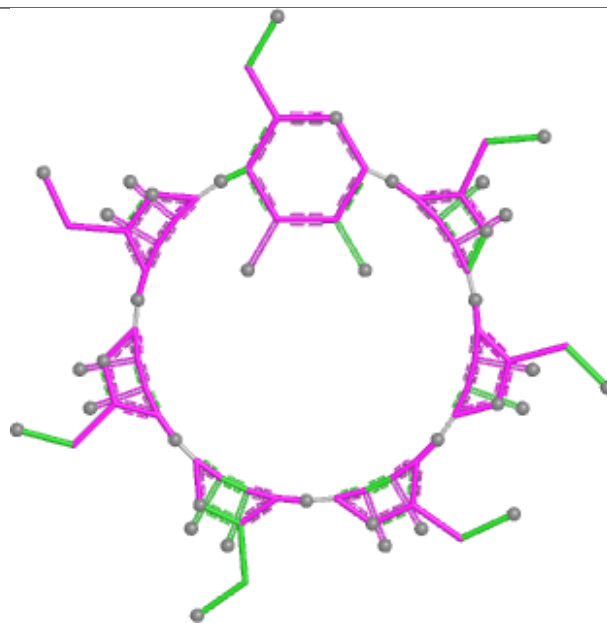
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	3	GLC	2	0
2	G	3	GLC	1	0
2	I	2	GLC	1	0
2	H	5	GLC	2	0
2	H	2	GLC	2	0
2	L	2	GLC	1	0
2	J	1	GLC	2	0

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

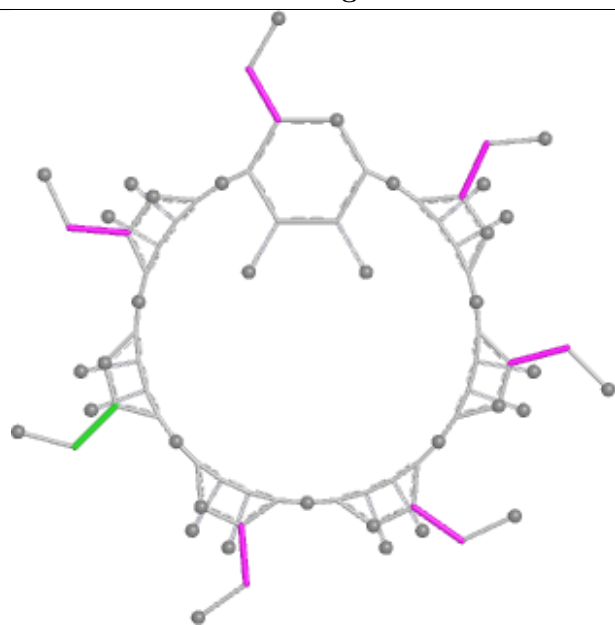
Oligosaccharide Chain G



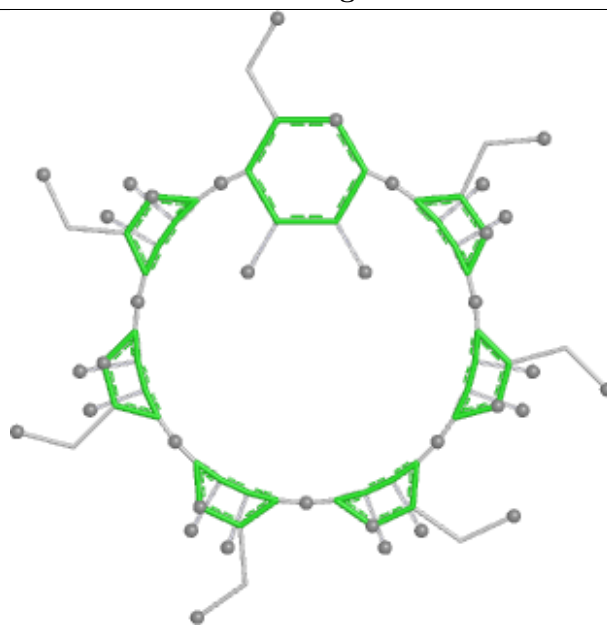
Bond lengths



Bond angles

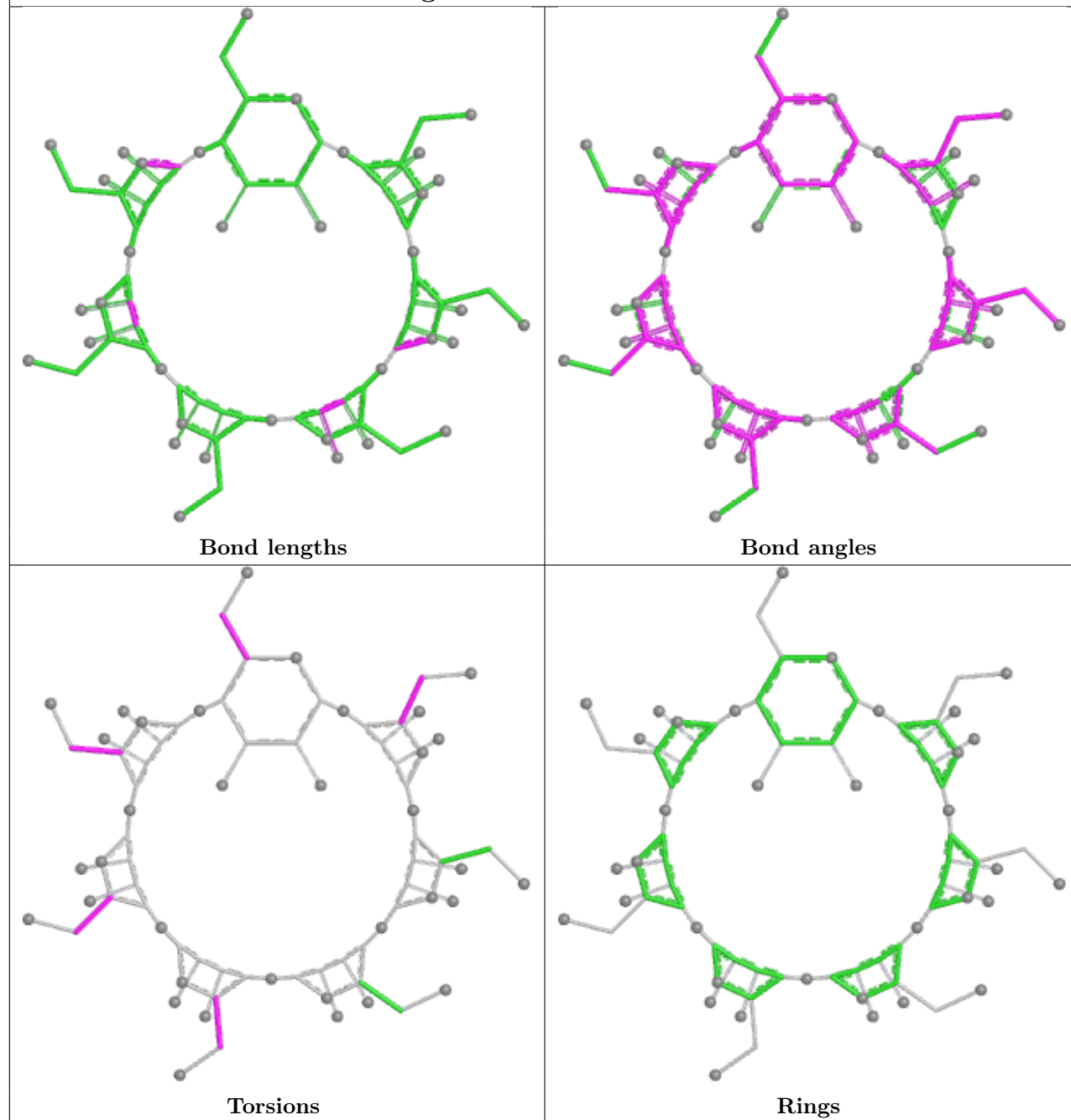


Torsions

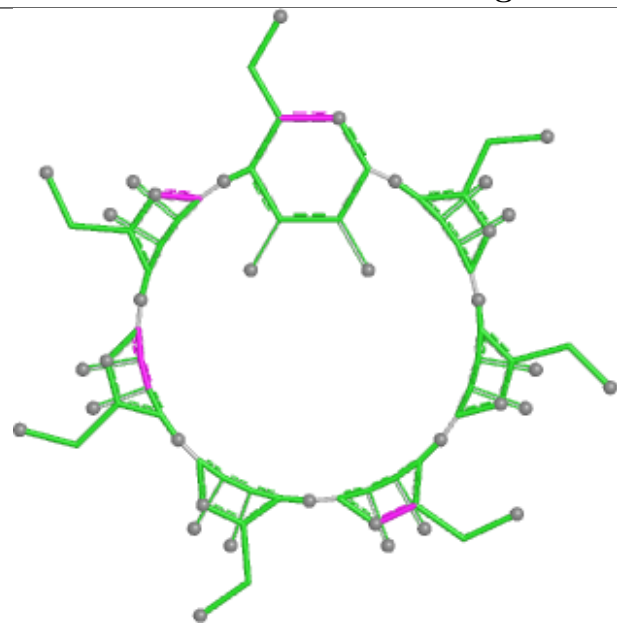


Rings

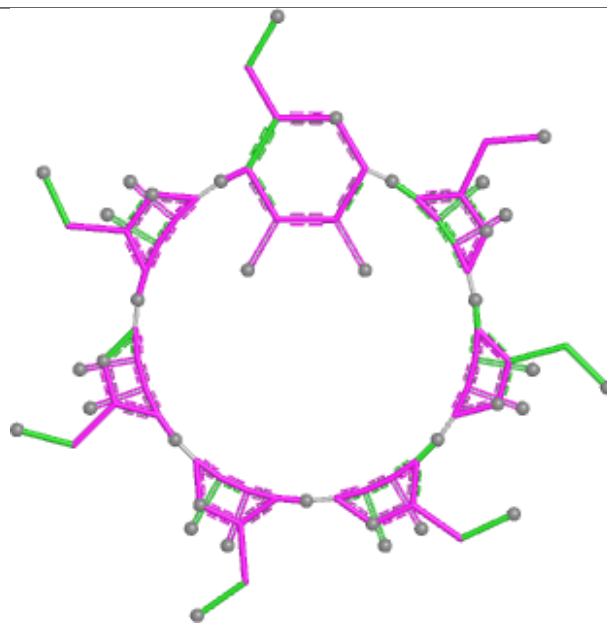
Oligosaccharide Chain H



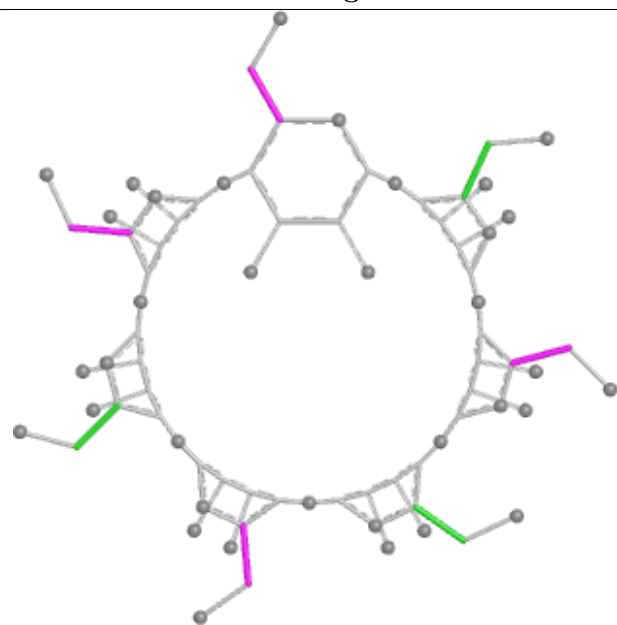
Oligosaccharide Chain I



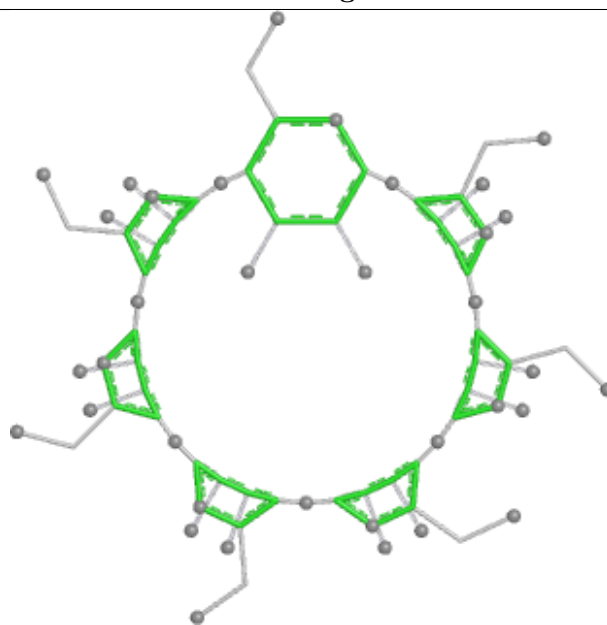
Bond lengths



Bond angles

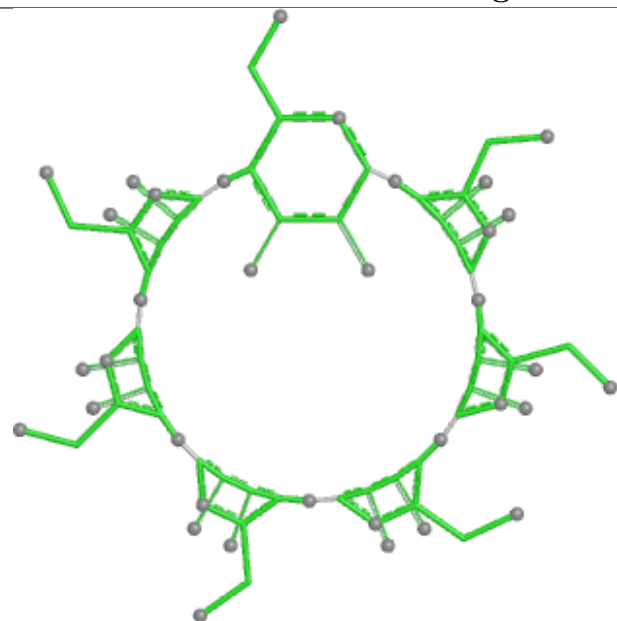


Torsions

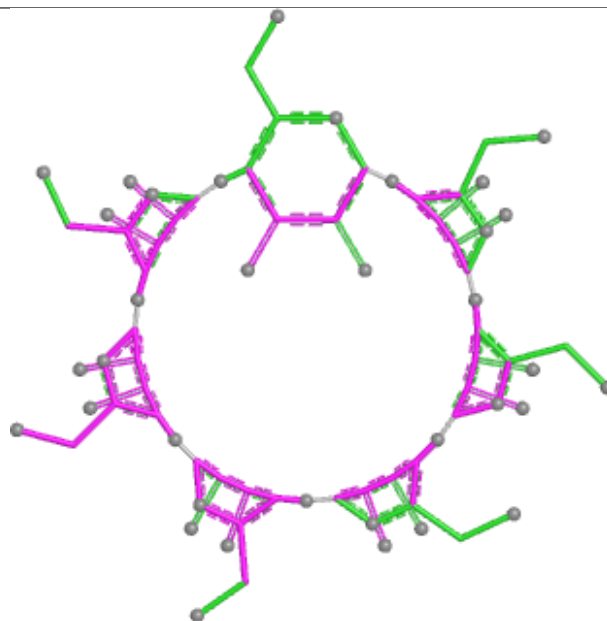


Rings

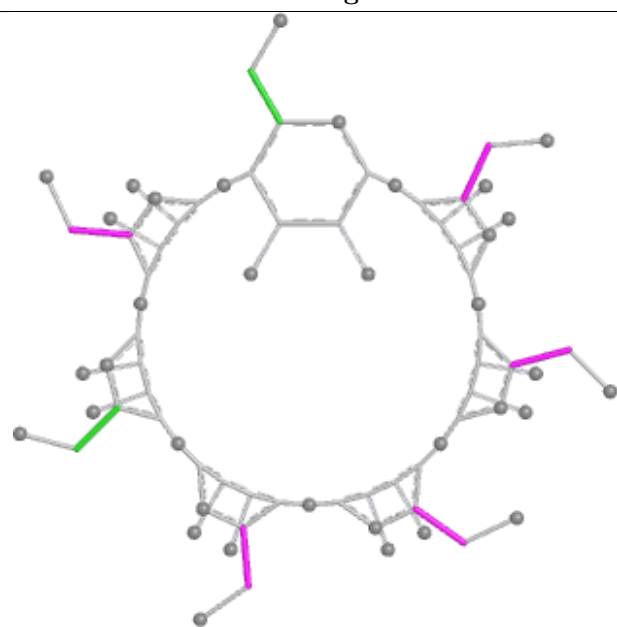
Oligosaccharide Chain J



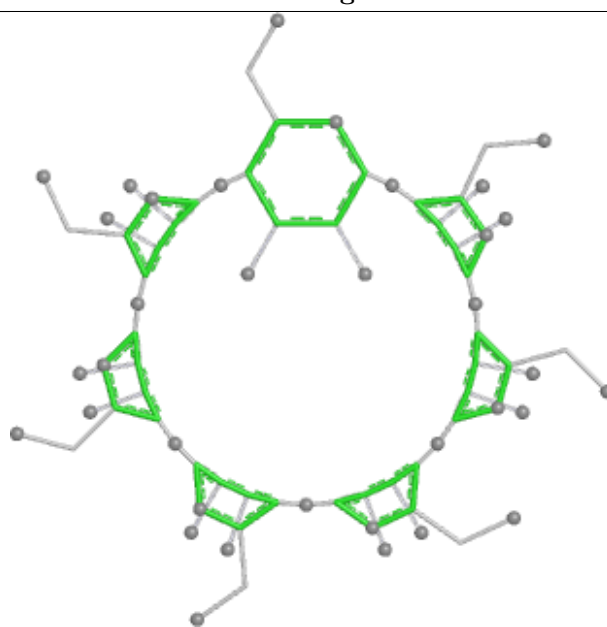
Bond lengths



Bond angles

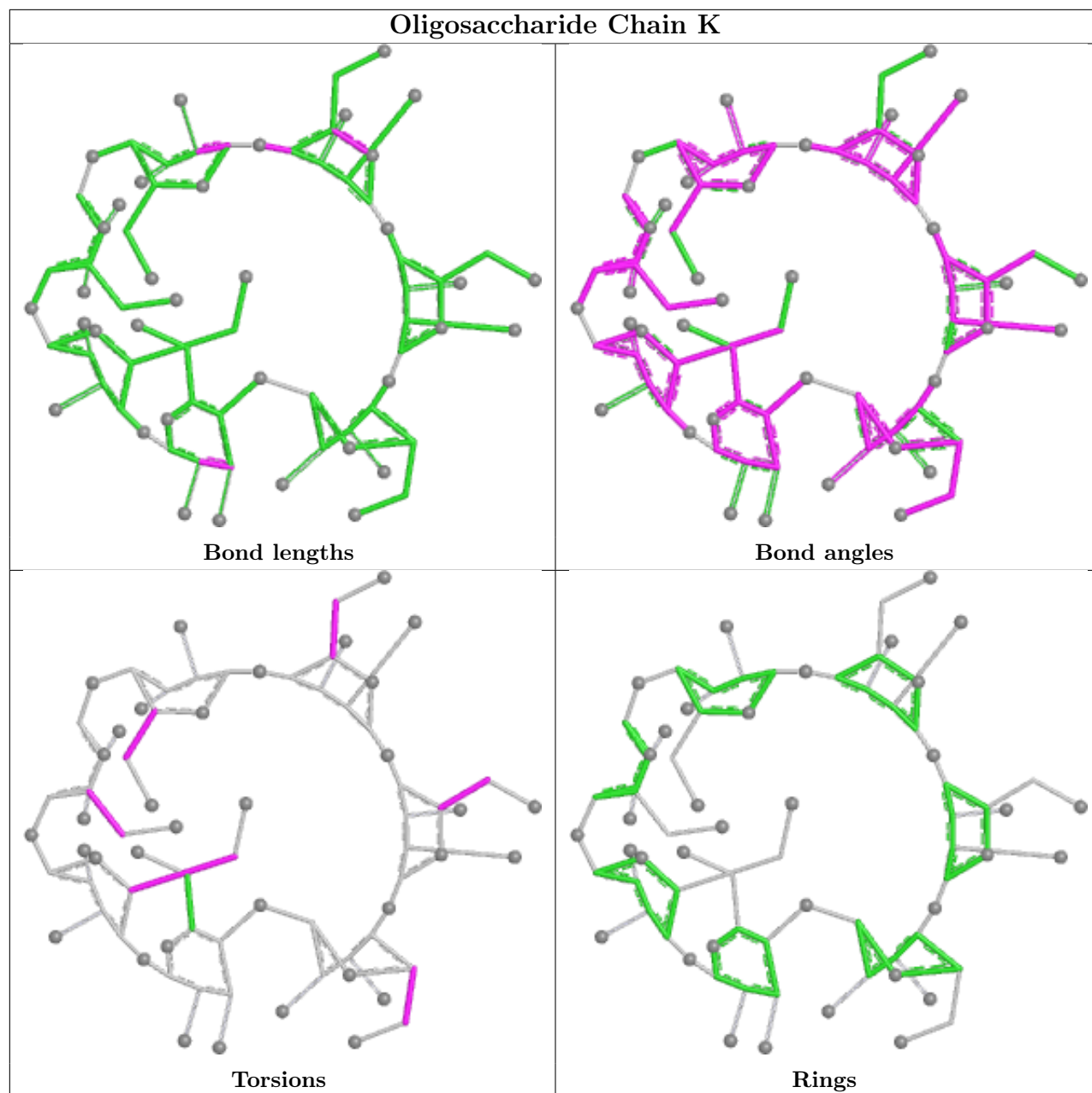


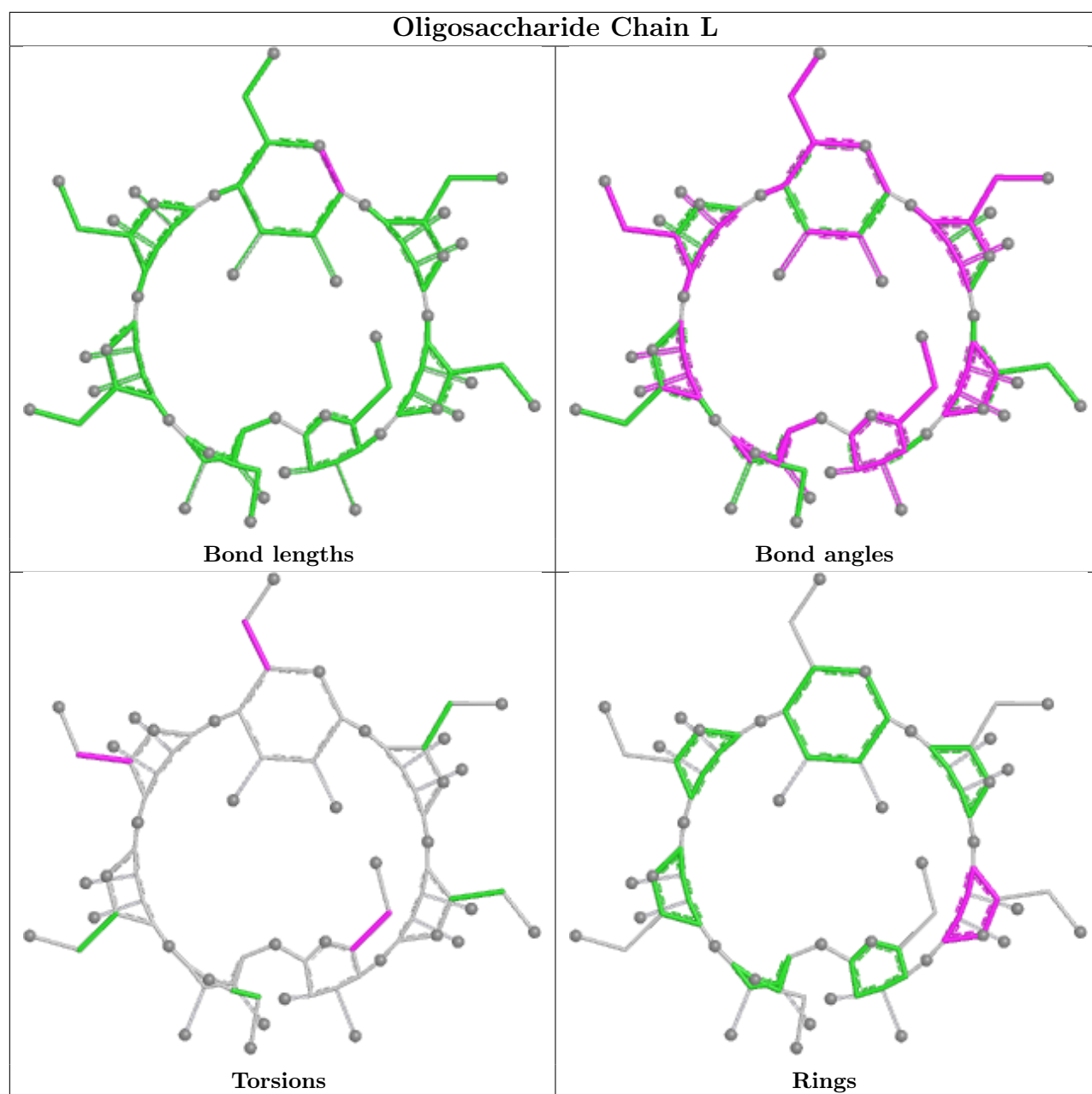
Torsions



Rings

Oligosaccharide Chain K





5.6 Ligand geometry [i](#)

29 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	EDO	D	505	3	3,3,3	1.16	0	2,2,2	0.79	0
4	SO4	C	504	-	4,4,4	0.61	0	6,6,6	0.84	0
4	SO4	E	502	-	4,4,4	0.65	0	6,6,6	0.59	0
4	SO4	C	502	-	4,4,4	0.72	0	6,6,6	0.85	0
4	SO4	D	502	-	4,4,4	0.78	0	6,6,6	0.48	0
4	SO4	E	504	-	4,4,4	0.55	0	6,6,6	0.69	0
4	SO4	F	503	-	4,4,4	0.89	0	6,6,6	0.67	0
5	EDO	C	505	3	3,3,3	0.81	0	2,2,2	0.05	0
3	HEM	B	501	1,5	50,50,50	2.14	14 (28%)	67,82,82	1.49	11 (16%)
4	SO4	F	504	-	4,4,4	0.45	0	6,6,6	0.60	0
4	SO4	A	502	-	4,4,4	0.73	0	6,6,6	1.10	0
4	SO4	B	504	-	4,4,4	0.75	0	6,6,6	0.87	0
3	HEM	C	501	1,5	50,50,50	2.24	14 (28%)	67,82,82	1.80	12 (17%)
3	HEM	E	501	1,5	50,50,50	2.23	13 (26%)	67,82,82	1.53	14 (20%)
5	EDO	B	505	3	3,3,3	1.38	0	2,2,2	0.93	0
4	SO4	E	503	-	4,4,4	0.82	0	6,6,6	0.53	0
5	EDO	F	505	3	3,3,3	1.28	0	2,2,2	0.69	0
4	SO4	C	503	-	4,4,4	0.76	0	6,6,6	0.57	0
4	SO4	F	502	-	4,4,4	0.72	0	6,6,6	0.61	0
5	EDO	A	504	3	3,3,3	1.34	0	2,2,2	0.88	0
3	HEM	D	501	1,5	50,50,50	2.05	14 (28%)	67,82,82	1.50	15 (22%)
5	EDO	E	505	3	3,3,3	1.37	0	2,2,2	0.86	0
3	HEM	A	501	1,5	50,50,50	2.24	12 (24%)	67,82,82	1.68	18 (26%)
4	SO4	B	503	-	4,4,4	0.60	0	6,6,6	0.63	0
4	SO4	A	503	-	4,4,4	0.65	0	6,6,6	0.81	0
4	SO4	D	504	-	4,4,4	0.80	0	6,6,6	1.07	0
4	SO4	B	502	-	4,4,4	0.75	0	6,6,6	0.68	0
4	SO4	D	503	-	4,4,4	0.97	0	6,6,6	0.59	0
3	HEM	F	501	1,5	50,50,50	1.94	11 (22%)	67,82,82	1.45	12 (17%)

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	EDO	D	505	3	-	1/1/1/1	-
3	HEM	E	501	1,5	-	1/14/54/54	-
3	HEM	D	501	1,5	-	1/14/54/54	-
3	HEM	F	501	1,5	-	2/14/54/54	-
5	EDO	B	505	3	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	E	505	3	-	1/1/1/1	-
5	EDO	A	504	3	-	1/1/1/1	-
3	HEM	A	501	1,5	-	0/14/54/54	-
5	EDO	F	505	3	-	1/1/1/1	-
5	EDO	C	505	3	-	1/1/1/1	-
3	HEM	C	501	1,5	-	0/14/54/54	-
3	HEM	B	501	1,5	-	0/14/54/54	-

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	HEM	C3D-C2D	8.21	1.54	1.36
3	E	501	HEM	C3D-C2D	8.09	1.54	1.36
3	C	501	HEM	C3D-C2D	7.93	1.53	1.36
3	F	501	HEM	C3D-C2D	7.30	1.52	1.36
3	B	501	HEM	C3D-C2D	7.22	1.52	1.36
3	D	501	HEM	C3D-C2D	7.08	1.52	1.36
3	C	501	HEM	FE-ND	7.01	2.16	1.94
3	A	501	HEM	FE-ND	6.25	2.14	1.94
3	E	501	HEM	FE-ND	5.94	2.13	1.94
3	C	501	HEM	FE-NB	4.64	2.09	1.94
3	D	501	HEM	FE-NA	4.63	2.10	1.95
3	A	501	HEM	CMB-C2B	4.37	1.59	1.50
3	B	501	HEM	FE-ND	4.27	2.08	1.94
3	F	501	HEM	FE-ND	4.18	2.07	1.94
3	E	501	HEM	CAC-C3C	4.09	1.58	1.47
3	D	501	HEM	CMB-C2B	4.07	1.59	1.50
3	B	501	HEM	CMB-C2B	3.99	1.58	1.50
3	A	501	HEM	CMC-C2C	3.92	1.58	1.50
3	A	501	HEM	FE-NA	3.91	2.08	1.95
3	D	501	HEM	CMD-C2D	3.86	1.58	1.50
3	A	501	HEM	FE-NB	3.85	2.06	1.94
3	B	501	HEM	CAC-C3C	3.83	1.57	1.47
3	E	501	HEM	CMB-C2B	3.75	1.58	1.50
3	D	501	HEM	CMC-C2C	3.71	1.58	1.50
3	A	501	HEM	CAC-C3C	3.68	1.57	1.47
3	F	501	HEM	FE-NB	3.62	2.06	1.94
3	C	501	HEM	FE-NA	3.60	2.07	1.95
3	B	501	HEM	CMC-C2C	3.59	1.58	1.50
3	B	501	HEM	CMD-C2D	3.55	1.58	1.50
3	C	501	HEM	FE-NC	3.51	2.06	1.95
3	C	501	HEM	CAC-C3C	3.48	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	501	HEM	CMB-C2B	3.48	1.57	1.50
3	E	501	HEM	CMD-C2D	3.45	1.57	1.50
3	B	501	HEM	FE-NB	3.42	2.05	1.94
3	F	501	HEM	CAC-C3C	3.40	1.56	1.47
3	F	501	HEM	FE-NA	3.39	2.06	1.95
3	B	501	HEM	FE-NA	3.38	2.06	1.95
3	E	501	HEM	FE-NA	3.27	2.05	1.95
3	A	501	HEM	FE-NC	3.25	2.05	1.95
3	B	501	HEM	FE-NC	3.19	2.05	1.95
3	F	501	HEM	CMD-C2D	3.05	1.57	1.50
3	A	501	HEM	CMD-C2D	3.05	1.57	1.50
3	D	501	HEM	CAB-C3B	3.04	1.55	1.47
3	E	501	HEM	FE-NC	3.00	2.05	1.95
3	D	501	HEM	CAC-C3C	2.98	1.55	1.47
3	E	501	HEM	CMC-C2C	2.96	1.56	1.50
3	E	501	HEM	FE-NB	2.93	2.03	1.94
3	D	501	HEM	FE-ND	2.89	2.03	1.94
3	E	501	HEM	CAB-C3B	2.82	1.54	1.47
3	B	501	HEM	CAB-C3B	2.78	1.54	1.47
3	B	501	HEM	CMA-C3A	2.77	1.56	1.50
3	B	501	HEM	O1D-CGD	2.76	1.31	1.22
3	C	501	HEM	CMB-C2B	2.75	1.56	1.50
3	F	501	HEM	CAB-C3B	2.73	1.54	1.47
3	C	501	HEM	CMD-C2D	2.71	1.56	1.50
3	D	501	HEM	FE-NC	2.66	2.03	1.95
3	A	501	HEM	CAB-C3B	2.61	1.54	1.47
3	E	501	HEM	C4B-NB	-2.57	1.33	1.38
3	E	501	HEM	CMA-C3A	2.54	1.56	1.50
3	C	501	HEM	O1D-CGD	2.42	1.30	1.22
3	F	501	HEM	O1D-CGD	2.38	1.29	1.22
3	D	501	HEM	O1D-CGD	2.37	1.29	1.22
3	E	501	HEM	O1D-CGD	2.36	1.29	1.22
3	C	501	HEM	CMC-C2C	2.28	1.55	1.50
3	B	501	HEM	CAA-C2A	2.28	1.57	1.51
3	C	501	HEM	CAB-C3B	2.26	1.53	1.47
3	C	501	HEM	CMA-C3A	2.26	1.55	1.50
3	B	501	HEM	CBD-CGD	2.25	1.55	1.50
3	D	501	HEM	CAA-C2A	2.19	1.57	1.51
3	D	501	HEM	FE-NB	2.12	2.01	1.94
3	F	501	HEM	FE-NC	2.12	2.02	1.95
3	F	501	HEM	CMC-C2C	2.09	1.55	1.50
3	C	501	HEM	C1A-C2A	2.08	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	HEM	CAD-C3D	2.07	1.56	1.51
3	A	501	HEM	O2A-CGA	-2.02	1.24	1.30
3	D	501	HEM	O2A-CGA	-2.02	1.24	1.30
3	A	501	HEM	CHA-C4D	-2.01	1.34	1.38
3	C	501	HEM	C4C-NC	-2.01	1.35	1.39

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	HEM	C4D-ND-C1D	6.91	113.39	105.21
3	A	501	HEM	C4D-ND-C1D	5.37	111.57	105.21
3	E	501	HEM	C4D-ND-C1D	5.10	111.24	105.21
3	F	501	HEM	C4D-ND-C1D	4.85	110.95	105.21
3	B	501	HEM	C4D-ND-C1D	4.58	110.63	105.21
3	D	501	HEM	CHC-C4B-NB	4.53	129.30	124.42
3	A	501	HEM	CHC-C4B-NB	4.31	129.06	124.42
3	C	501	HEM	C2A-C1A-NA	-4.12	105.58	110.15
3	C	501	HEM	CHD-C4C-NC	3.82	128.61	124.45
3	B	501	HEM	C4B-C3B-C2B	3.59	110.58	107.28
3	C	501	HEM	C3D-C4D-ND	-3.55	106.28	110.17
3	A	501	HEM	C1D-C2D-C3D	-3.33	103.48	106.98
3	F	501	HEM	C4C-C3C-C2C	3.32	109.69	106.81
3	D	501	HEM	CHD-C4C-NC	3.16	127.90	124.45
3	A	501	HEM	C3B-C4B-NB	-3.16	107.20	109.47
3	C	501	HEM	CHC-C4B-NB	3.15	127.81	124.42
3	E	501	HEM	CAD-CBD-CGD	-3.09	105.46	113.67
3	A	501	HEM	C4C-C3C-C2C	3.09	109.49	106.81
3	C	501	HEM	C1D-C2D-C3D	-3.05	103.78	106.98
3	F	501	HEM	C2A-C1A-NA	-3.04	106.78	110.15
3	F	501	HEM	CBC-CAC-C3C	-3.04	112.36	127.53
3	D	501	HEM	C2A-C1A-NA	-3.01	106.81	110.15
3	D	501	HEM	C4A-NA-C1A	2.99	110.69	105.82
3	C	501	HEM	CMD-C2D-C1D	2.97	129.68	125.03
3	E	501	HEM	C2A-C1A-NA	-2.95	106.88	110.15
3	A	501	HEM	C2A-C1A-NA	-2.93	106.90	110.15
3	C	501	HEM	C4C-C3C-C2C	2.91	109.34	106.81
3	D	501	HEM	C4D-ND-C1D	2.88	108.62	105.21
3	B	501	HEM	CHC-C4B-NB	2.84	127.48	124.42
3	E	501	HEM	C4B-C3B-C2B	2.84	109.89	107.28
3	B	501	HEM	CBA-CAA-C2A	-2.78	104.85	112.53
3	B	501	HEM	C3B-C2B-C1B	-2.75	104.34	106.41
3	A	501	HEM	C3D-C4D-ND	-2.74	107.17	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	HEM	CHD-C4C-NC	2.65	127.34	124.45
3	E	501	HEM	CHC-C4B-NB	2.65	127.27	124.42
3	F	501	HEM	CMC-C2C-C1C	2.64	129.38	124.73
3	D	501	HEM	CBD-CAD-C3D	-2.63	105.25	112.53
3	A	501	HEM	C4B-C3B-C2B	2.62	109.69	107.28
3	B	501	HEM	C1D-C2D-C3D	-2.59	104.25	106.98
3	C	501	HEM	C4A-NA-C1A	2.59	110.04	105.82
3	A	501	HEM	C4A-NA-C1A	2.59	110.04	105.82
3	C	501	HEM	CAC-C3C-C4C	-2.55	118.74	124.82
3	C	501	HEM	C4C-NC-C1C	2.54	109.95	105.82
3	A	501	HEM	CBD-CAD-C3D	-2.51	105.60	112.53
3	E	501	HEM	C3B-C4B-NB	-2.51	107.67	109.47
3	D	501	HEM	CAD-CBD-CGD	-2.50	107.03	113.67
3	F	501	HEM	CAA-CBA-CGA	-2.50	107.05	113.67
3	B	501	HEM	C3B-C4B-NB	-2.48	107.69	109.47
3	D	501	HEM	CBB-CAB-C3B	-2.45	115.31	127.53
3	D	501	HEM	CAC-C3C-C4C	-2.41	119.06	124.82
3	B	501	HEM	CAC-C3C-C4C	-2.41	119.07	124.82
3	D	501	HEM	CHC-C1C-NC	-2.41	121.83	124.45
3	D	501	HEM	C4C-C3C-C2C	2.38	108.88	106.81
3	E	501	HEM	CHA-C1A-NA	2.36	128.13	123.86
3	C	501	HEM	C4B-C3B-C2B	2.34	109.43	107.28
3	A	501	HEM	CBA-CAA-C2A	-2.34	106.07	112.53
3	A	501	HEM	C1B-NB-C4B	2.31	107.95	105.21
3	F	501	HEM	CHA-C1A-NA	2.30	128.04	123.86
3	F	501	HEM	CBB-CAB-C3B	-2.27	116.17	127.53
3	B	501	HEM	C4C-C3C-C2C	2.27	108.78	106.81
3	F	501	HEM	CBD-CAD-C3D	-2.27	106.26	112.53
3	F	501	HEM	C1D-C2D-C3D	-2.26	104.60	106.98
3	E	501	HEM	C1B-NB-C4B	2.25	107.87	105.21
3	B	501	HEM	C2A-C1A-NA	-2.23	107.67	110.15
3	E	501	HEM	C1D-C2D-C3D	-2.22	104.64	106.98
3	E	501	HEM	C3B-C2B-C1B	-2.18	104.77	106.41
3	F	501	HEM	C4A-NA-C1A	2.18	109.38	105.82
3	E	501	HEM	CHD-C1D-ND	2.18	126.77	124.42
3	D	501	HEM	CAA-CBA-CGA	-2.16	107.95	113.67
3	E	501	HEM	CBD-CAD-C3D	-2.15	106.59	112.53
3	F	501	HEM	CHB-C4A-NA	2.15	127.75	123.86
3	D	501	HEM	C1D-C2D-C3D	-2.10	104.77	106.98
3	A	501	HEM	CBB-CAB-C3B	-2.09	117.08	127.53
3	D	501	HEM	C3C-C2C-C1C	-2.08	105.08	107.05
3	A	501	HEM	CHA-C1A-NA	2.08	127.63	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	HEM	C3C-C2C-C1C	-2.08	105.08	107.05
3	A	501	HEM	CAD-CBD-CGD	-2.07	108.17	113.67
3	E	501	HEM	CMA-C3A-C4A	2.06	128.56	125.42
3	A	501	HEM	CHA-C4D-ND	2.06	126.91	124.37
3	E	501	HEM	CBB-CAB-C3B	-2.04	117.32	127.53
3	D	501	HEM	CHB-C4A-NA	2.01	127.50	123.86
3	A	501	HEM	C3C-C2C-C1C	-2.00	105.15	107.05

There are no chirality outliers.

All (10) torsion outliers are listed below:

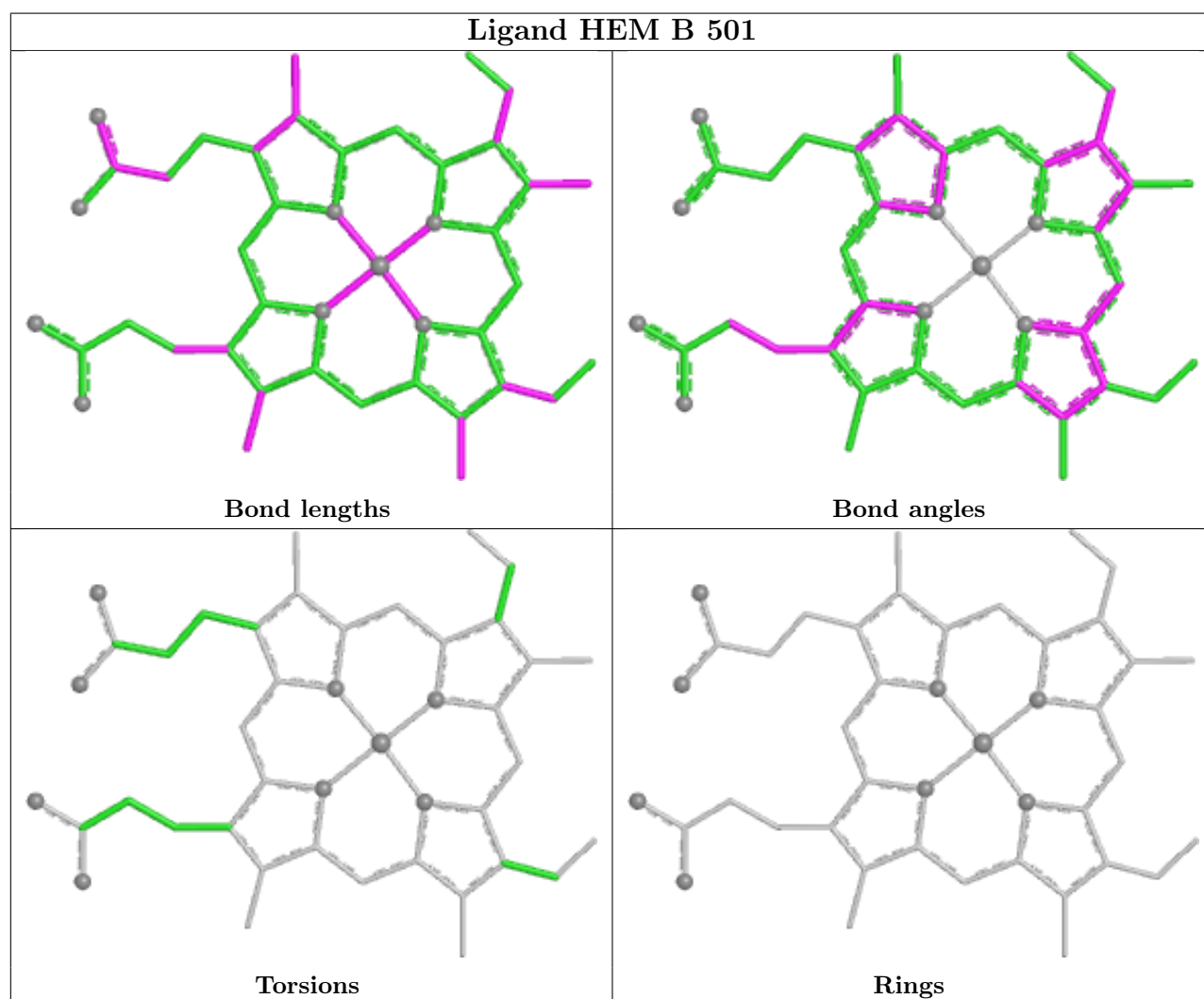
Mol	Chain	Res	Type	Atoms
3	F	501	HEM	C2C-C3C-CAC-CBC
3	F	501	HEM	C4C-C3C-CAC-CBC
5	B	505	EDO	O1-C1-C2-O2
5	D	505	EDO	O1-C1-C2-O2
5	A	504	EDO	O1-C1-C2-O2
5	F	505	EDO	O1-C1-C2-O2
5	C	505	EDO	O1-C1-C2-O2
5	E	505	EDO	O1-C1-C2-O2
3	D	501	HEM	C2A-CAA-CBA-CGA
3	E	501	HEM	C2A-CAA-CBA-CGA

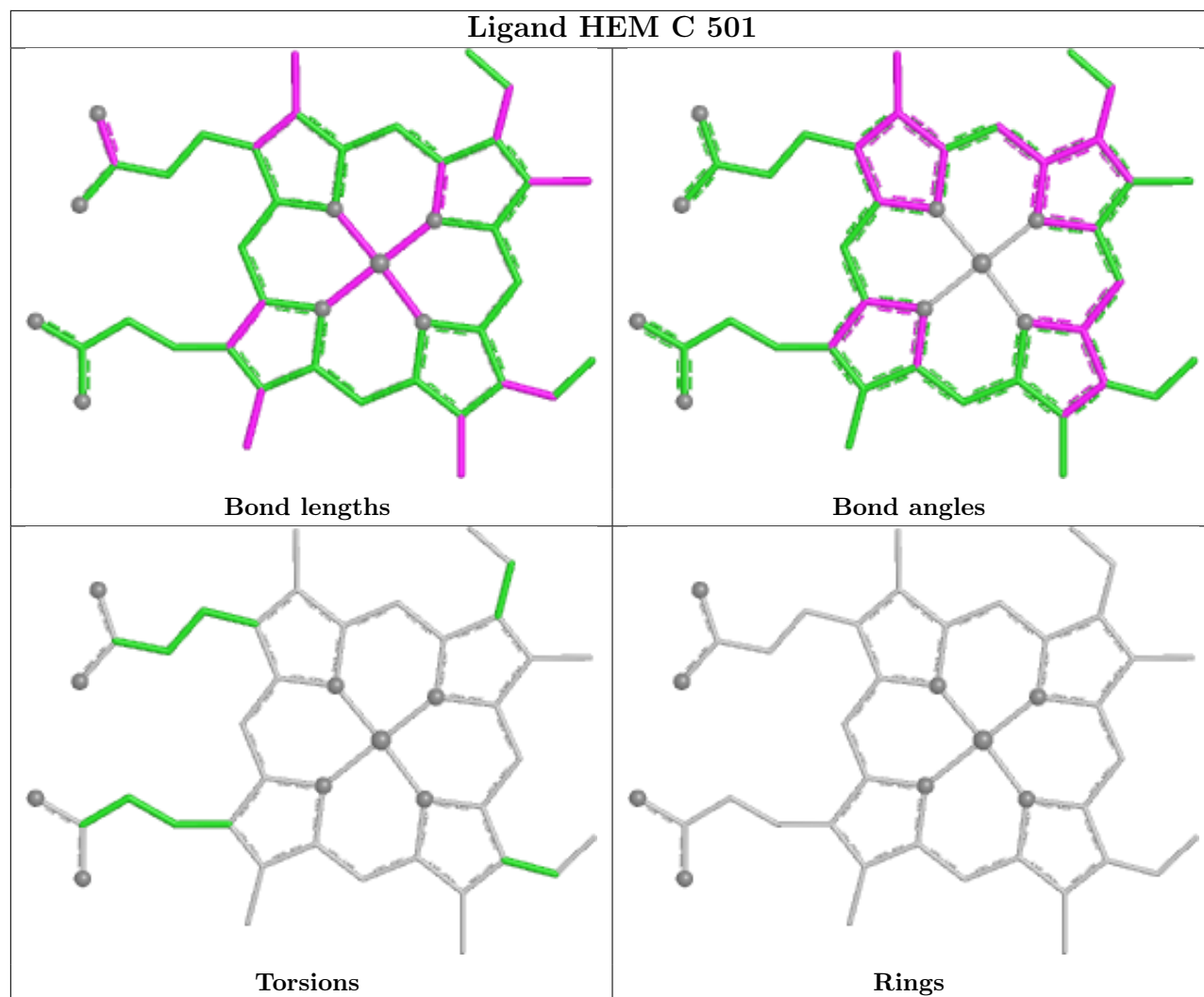
There are no ring outliers.

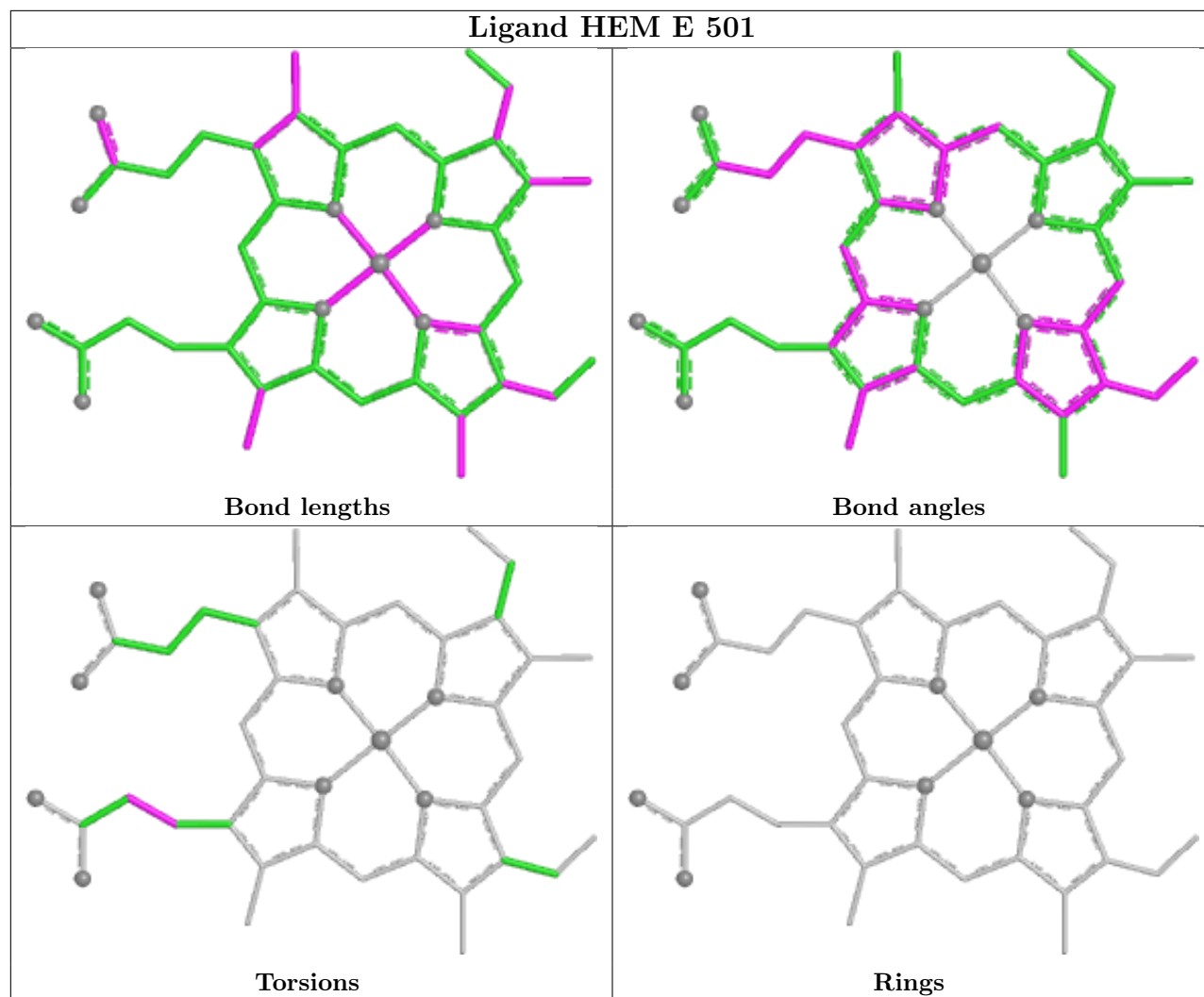
14 monomers are involved in 74 short contacts:

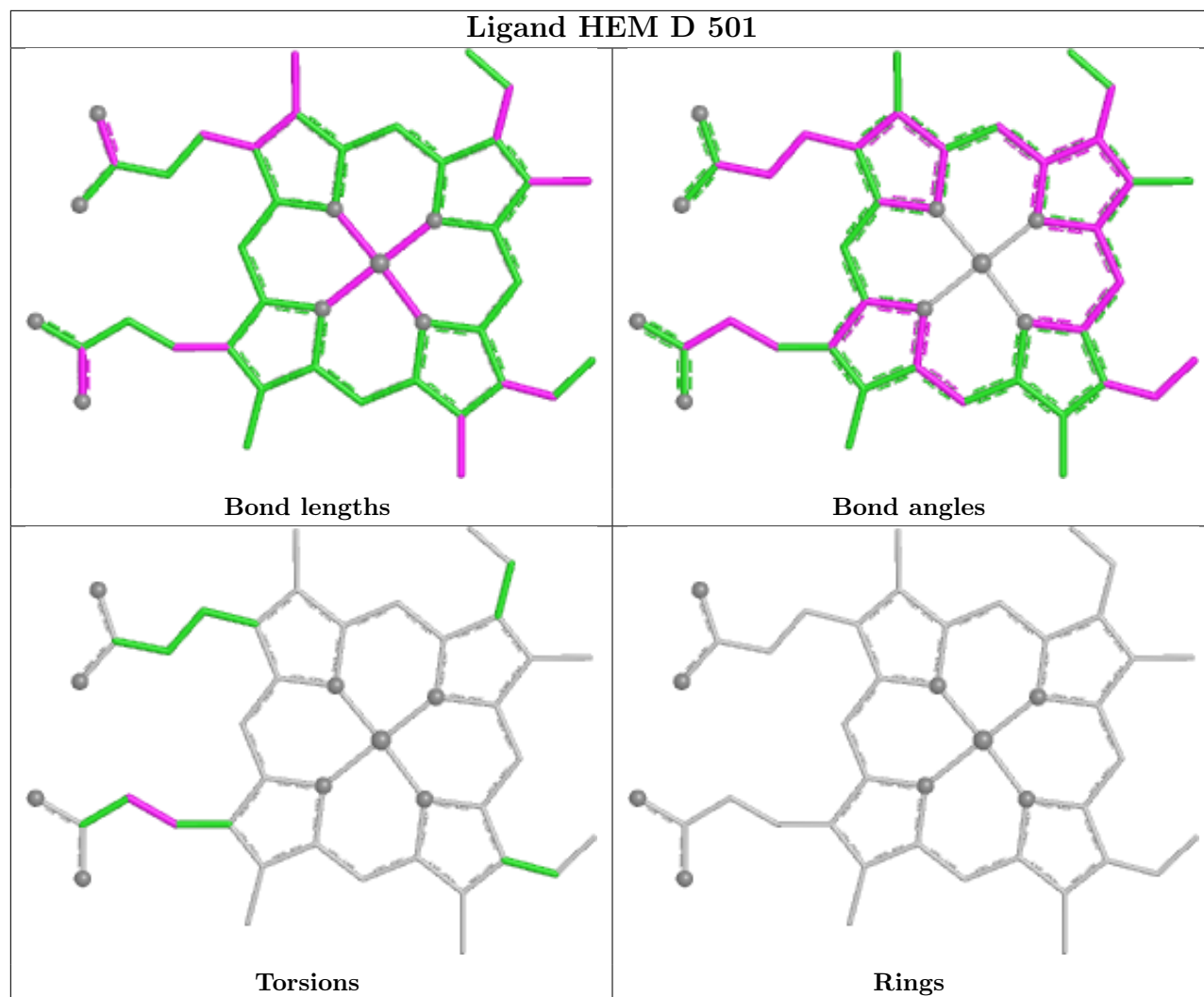
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	504	SO4	3	0
4	E	504	SO4	7	0
5	C	505	EDO	1	0
3	B	501	HEM	6	0
4	F	504	SO4	5	0
4	A	502	SO4	8	0
4	B	504	SO4	5	0
3	C	501	HEM	5	0
3	E	501	HEM	6	0
5	B	505	EDO	1	0
3	D	501	HEM	6	0
3	A	501	HEM	6	0
4	D	504	SO4	5	0
3	F	501	HEM	10	0

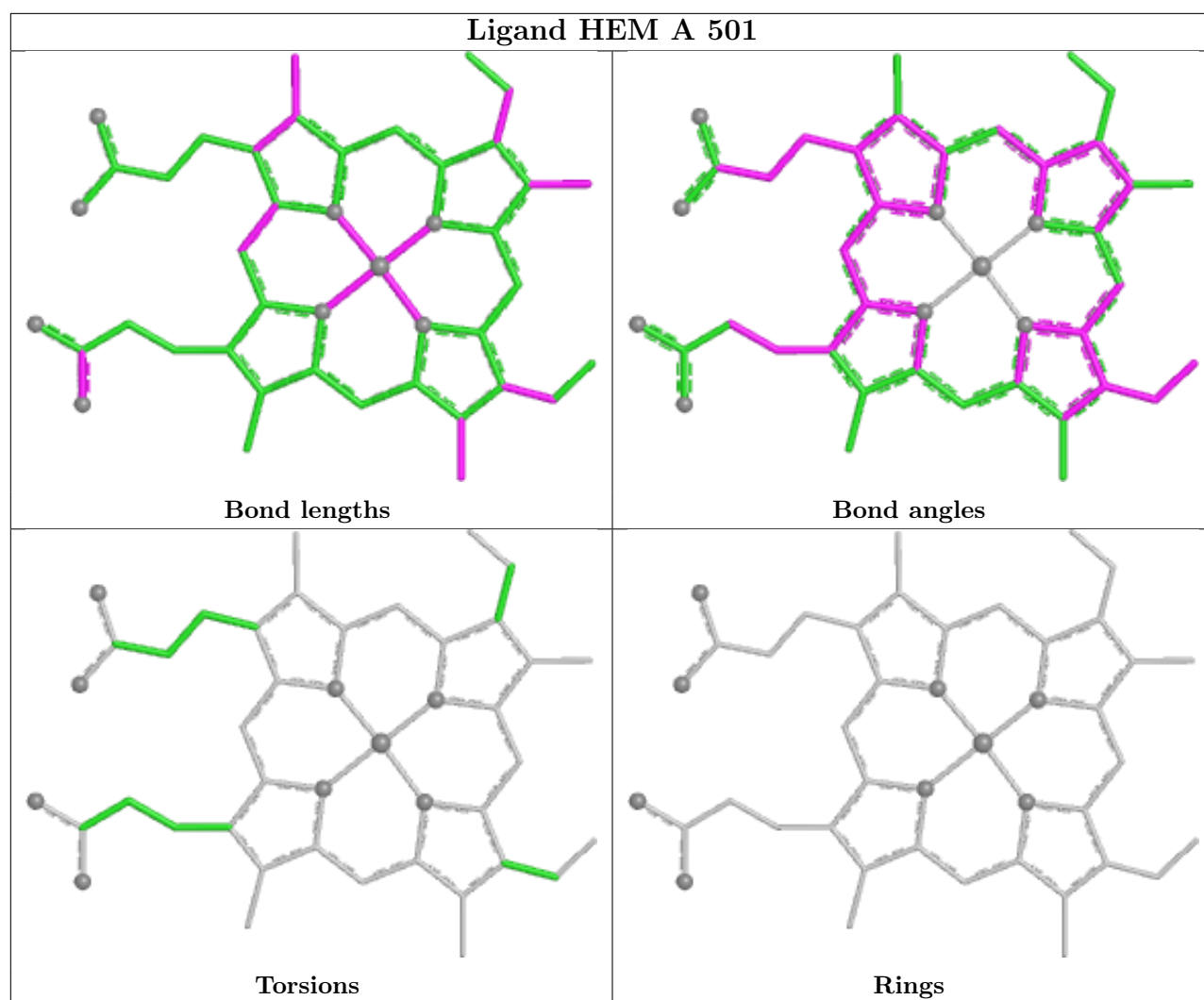
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

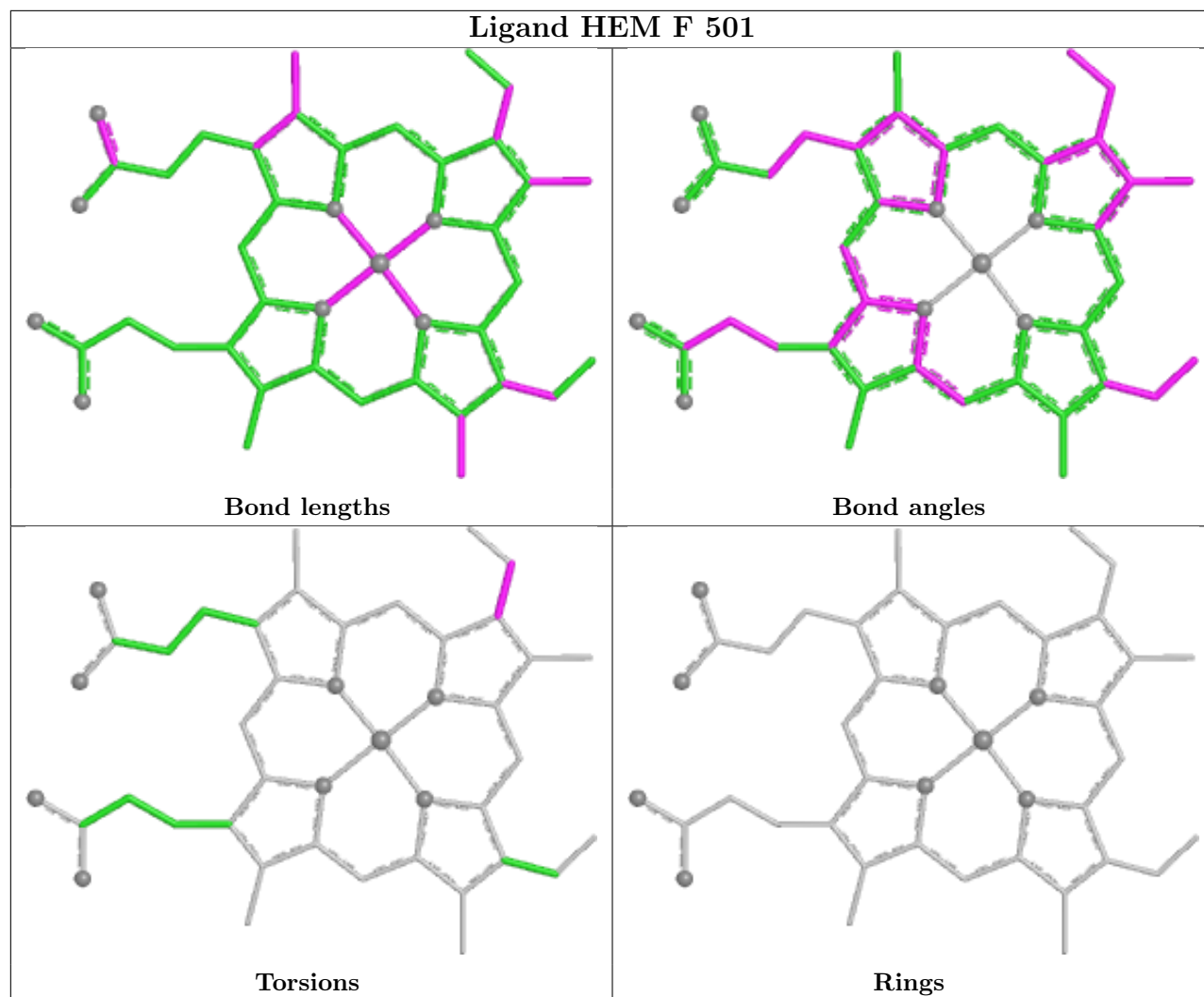












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	402/407 (98%)	-1.37	0 100 100	9, 22, 44, 60	5 (1%)
1	B	404/407 (99%)	-1.37	0 100 100	10, 22, 44, 64	5 (1%)
1	C	402/407 (98%)	-1.36	0 100 100	9, 22, 43, 56	7 (1%)
1	D	402/407 (98%)	-1.36	0 100 100	9, 22, 43, 61	7 (1%)
1	E	402/407 (98%)	-1.36	0 100 100	11, 22, 43, 56	6 (1%)
1	F	402/407 (98%)	-1.36	0 100 100	9, 22, 44, 55	6 (1%)
All	All	2414/2442 (98%)	-1.36	0 100 100	9, 22, 44, 64	36 (1%)

There are no RSRZ outliers to report.

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	J	7	11/12	0.98	0.06	33,42,44,44	11
2	GLC	G	2	11/12	0.99	0.05	30,37,40,44	11
2	GLC	G	3	11/12	0.99	0.05	21,38,44,45	11
2	GLC	G	4	11/12	0.99	0.04	34,41,46,48	11
2	GLC	G	5	11/12	0.99	0.06	38,41,45,49	11
2	GLC	G	6	11/12	0.99	0.04	33,39,43,43	11

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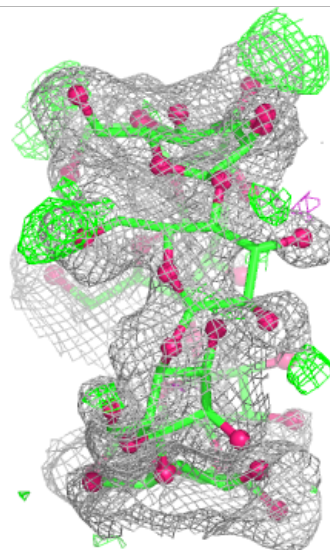
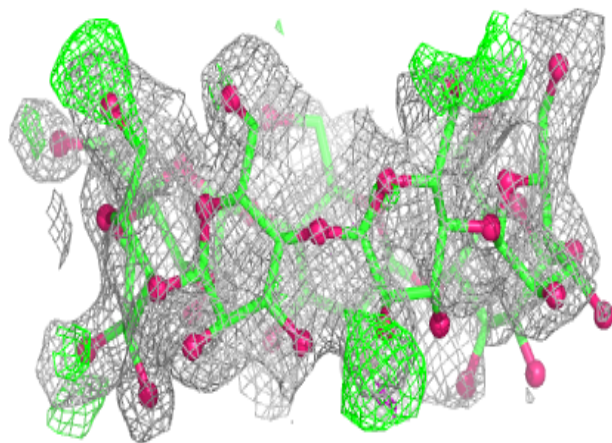
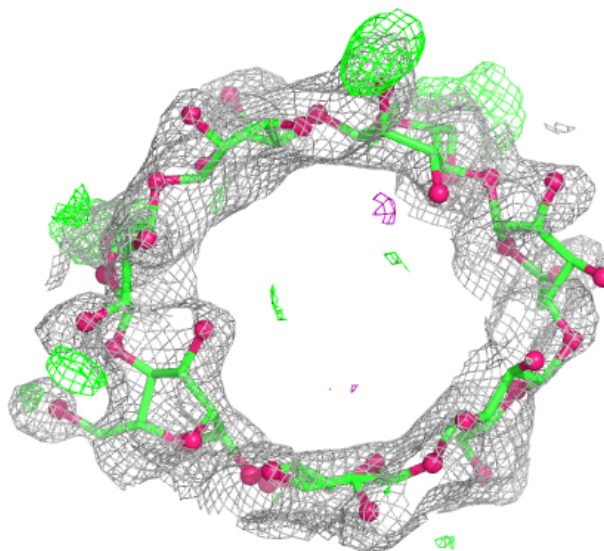
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	G	7	11/12	0.99	0.04	36,40,43,46	11
2	GLC	H	1	11/12	0.99	0.04	34,39,45,46	11
2	GLC	H	2	11/12	0.99	0.04	24,33,35,39	11
2	GLC	H	3	11/12	0.99	0.04	21,36,41,43	11
2	GLC	H	4	11/12	0.99	0.04	34,37,40,41	11
2	GLC	H	5	11/12	0.99	0.04	36,38,40,41	11
2	GLC	H	6	11/12	0.99	0.04	36,39,45,45	11
2	GLC	H	7	11/12	0.99	0.04	34,38,42,43	11
2	GLC	I	1	11/12	0.99	0.04	32,36,38,41	11
2	GLC	I	2	11/12	0.99	0.04	24,34,37,42	11
2	GLC	I	3	11/12	0.99	0.04	22,32,39,40	11
2	GLC	I	6	11/12	0.99	0.05	33,39,42,44	11
2	GLC	I	7	11/12	0.99	0.03	32,37,39,43	11
2	GLC	J	1	11/12	0.99	0.05	34,39,42,42	11
2	GLC	J	2	11/12	0.99	0.03	24,34,38,40	11
2	GLC	J	3	11/12	0.99	0.04	32,35,37,37	11
2	GLC	J	4	11/12	0.99	0.04	37,39,42,44	11
2	GLC	J	5	11/12	0.99	0.04	38,43,47,51	11
2	GLC	J	6	11/12	0.99	0.04	36,40,42,43	11
2	GLC	G	1	11/12	0.99	0.04	37,38,41,42	11
2	GLC	K	1	11/12	0.99	0.04	33,36,39,40	11
2	GLC	K	2	11/12	0.99	0.04	36,39,42,42	11
2	GLC	K	3	11/12	0.99	0.03	35,38,40,42	11
2	GLC	K	4	11/12	0.99	0.04	25,36,39,39	11
2	GLC	K	5	11/12	0.99	0.03	28,35,37,39	11
2	GLC	K	6	11/12	0.99	0.05	37,40,41,49	11
2	GLC	K	7	11/12	0.99	0.04	35,38,42,43	11
2	GLC	L	1	11/12	0.99	0.04	32,34,38,39	11
2	GLC	L	2	11/12	0.99	0.04	35,39,40,44	11
2	GLC	L	3	11/12	0.99	0.04	38,42,44,46	11
2	GLC	L	4	11/12	0.99	0.05	38,44,45,48	11
2	GLC	L	5	11/12	0.99	0.04	33,40,44,45	11
2	GLC	L	7	11/12	0.99	0.03	32,35,37,39	11
2	GLC	I	4	11/12	1.00	0.03	30,34,37,40	11
2	GLC	L	6	11/12	1.00	0.03	26,39,40,41	11
2	GLC	I	5	11/12	1.00	0.03	40,45,46,50	11

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.

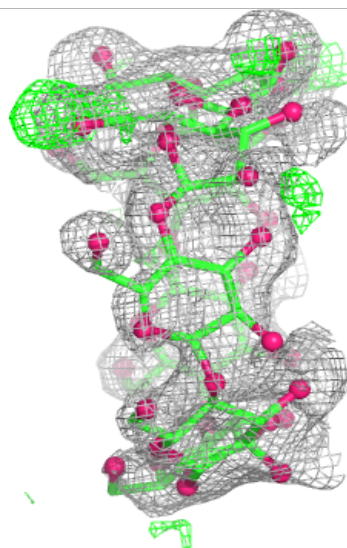
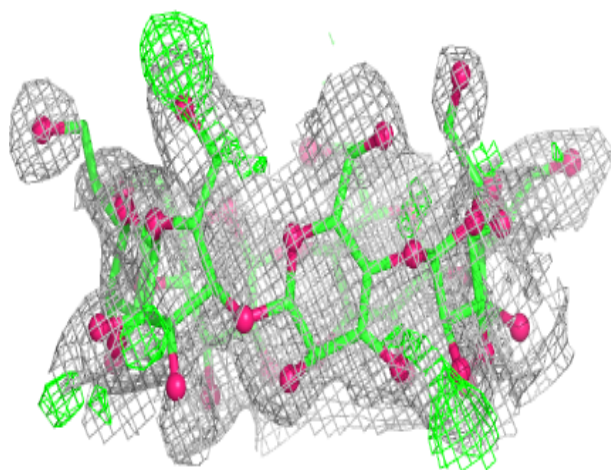
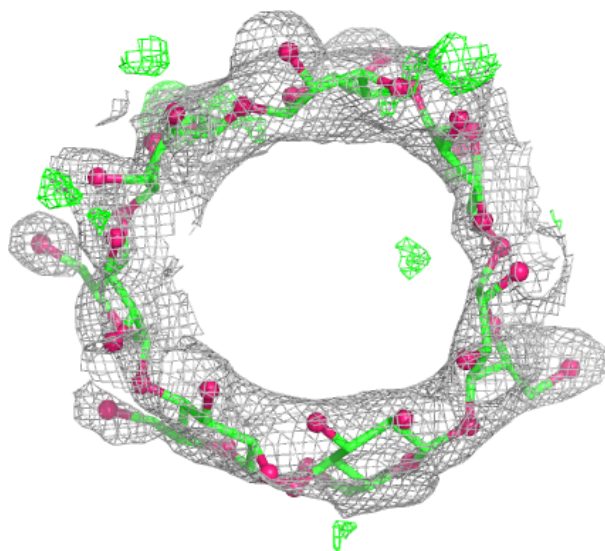
Electron density around Chain G:

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



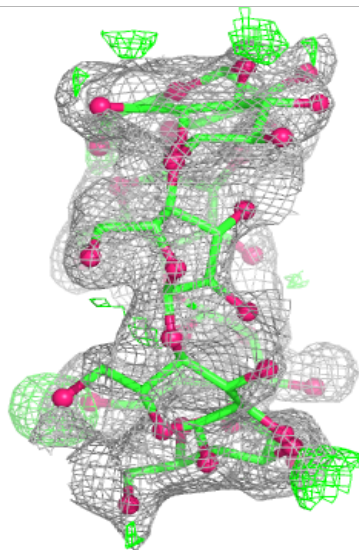
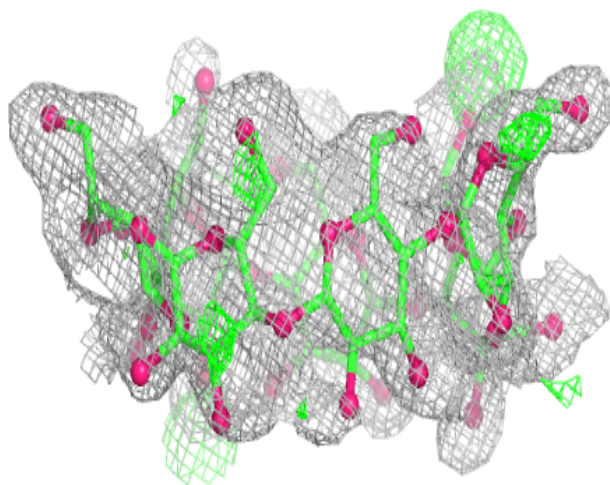
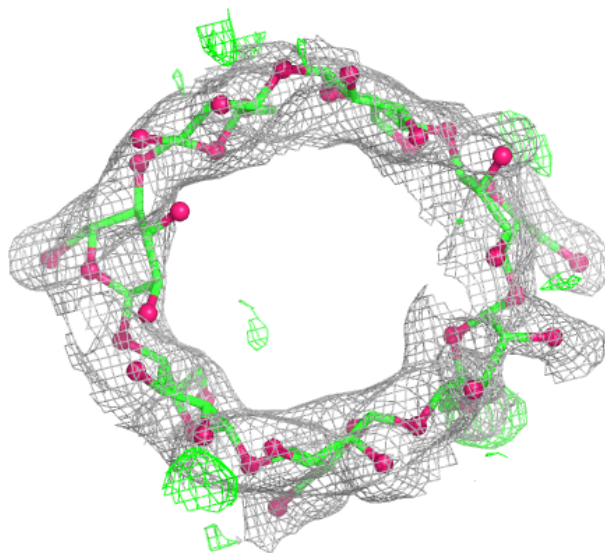
Electron density around Chain H:

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



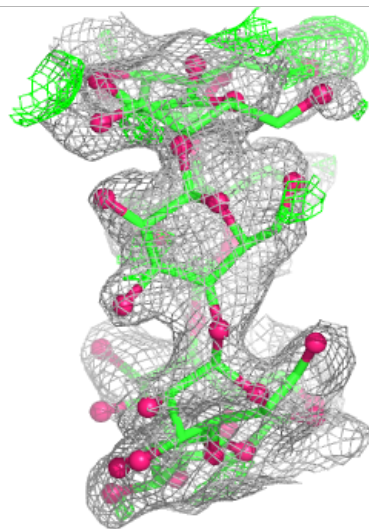
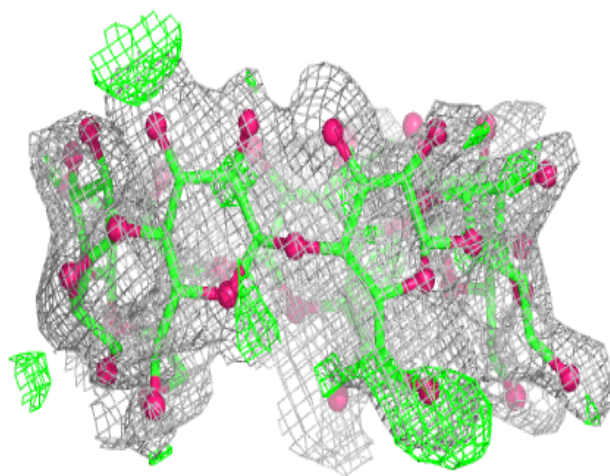
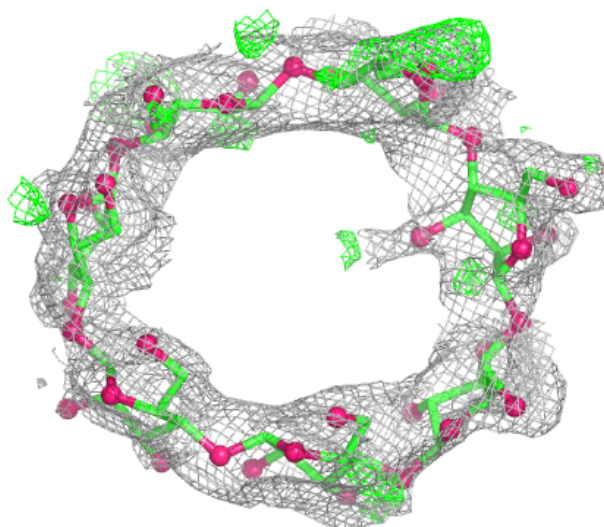
Electron density around Chain I:

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



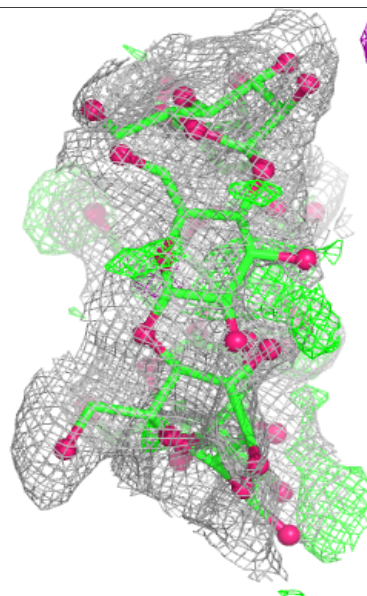
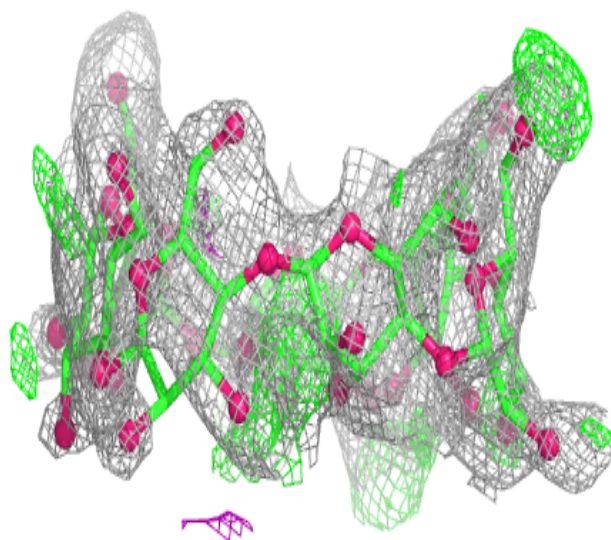
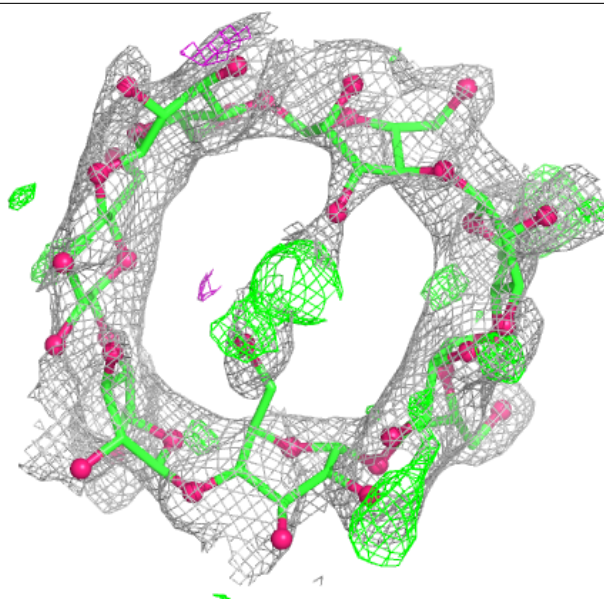
Electron density around Chain J:

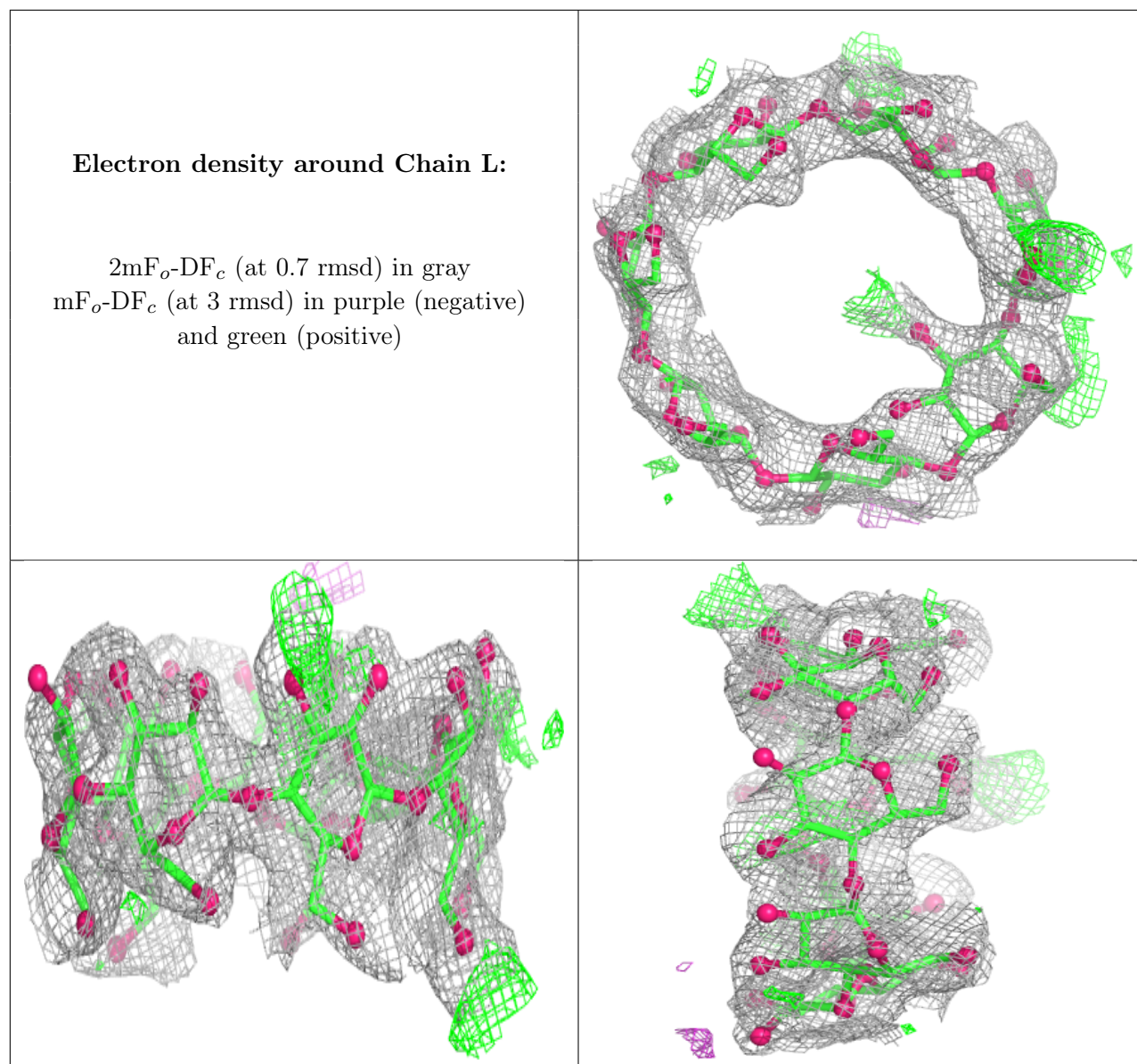
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain K:

$2mF_o-DF_c$ (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, 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	SO4	C	504	5/5	0.97	0.27	32,42,45,47	0
5	EDO	B	505	4/4	0.97	0.06	19,20,22,32	0
4	SO4	A	502	5/5	0.98	0.25	27,42,43,44	0
4	SO4	D	504	5/5	0.98	0.27	29,44,46,47	0
4	SO4	E	504	5/5	0.98	0.24	29,41,44,49	0

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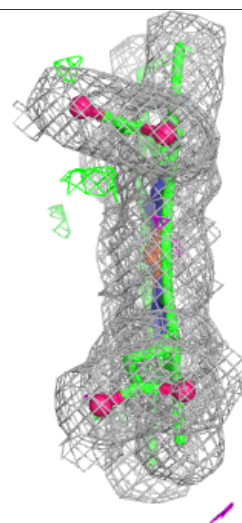
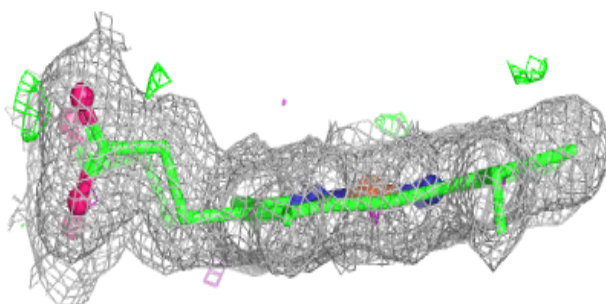
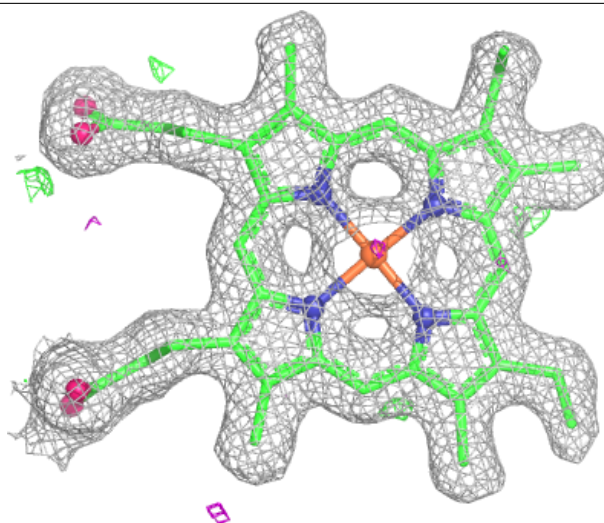
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	F	504	5/5	0.98	0.27	27,41,41,48	0
5	EDO	A	504	4/4	0.98	0.05	19,22,23,30	0
4	SO4	B	504	5/5	0.98	0.26	30,43,45,49	0
5	EDO	D	505	4/4	0.98	0.05	19,20,21,34	0
5	EDO	F	505	4/4	0.98	0.04	18,21,22,27	0
4	SO4	B	503	5/5	0.99	0.08	23,29,30,31	0
4	SO4	E	502	5/5	0.99	0.08	27,28,31,32	0
4	SO4	E	503	5/5	0.99	0.10	34,34,35,38	0
4	SO4	A	503	5/5	0.99	0.10	27,30,31,33	0
4	SO4	F	502	5/5	0.99	0.09	25,25,31,32	0
4	SO4	F	503	5/5	0.99	0.10	33,34,36,37	0
4	SO4	C	502	5/5	0.99	0.08	26,28,29,32	0
4	SO4	C	503	5/5	0.99	0.10	33,33,35,36	0
4	SO4	B	502	5/5	0.99	0.08	30,30,35,36	0
5	EDO	C	505	4/4	0.99	0.04	21,23,26,30	0
4	SO4	D	502	5/5	0.99	0.09	25,26,31,31	0
5	EDO	E	505	4/4	0.99	0.04	22,23,23,31	0
4	SO4	D	503	5/5	0.99	0.09	30,31,35,35	0
3	HEM	F	501	43/43	1.00	0.02	10,14,19,28	0
3	HEM	A	501	43/43	1.00	0.02	11,14,17,22	0
3	HEM	B	501	43/43	1.00	0.02	10,13,16,24	0
3	HEM	C	501	43/43	1.00	0.02	9,14,17,24	0
3	HEM	D	501	43/43	1.00	0.02	8,14,16,22	0
3	HEM	E	501	43/43	1.00	0.02	9,14,17,22	0

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

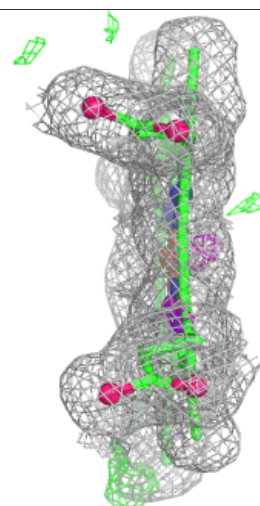
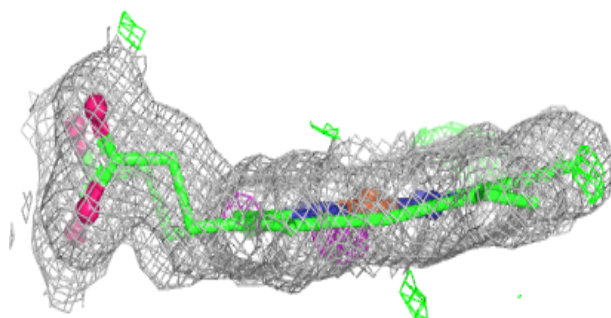
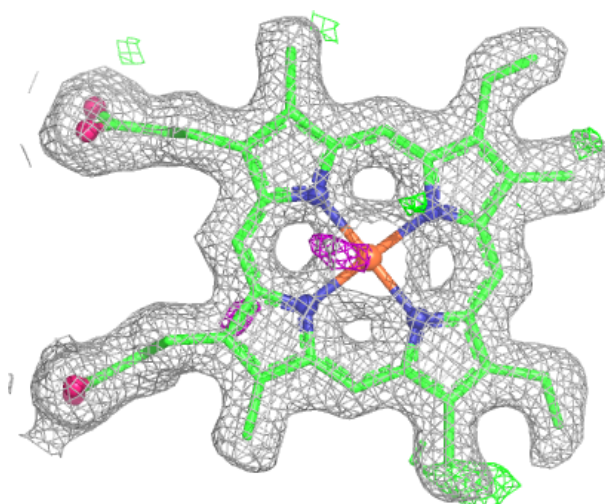
Electron density around HEM F 501:

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



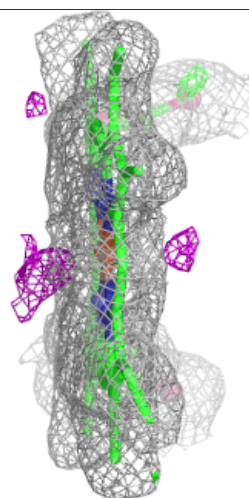
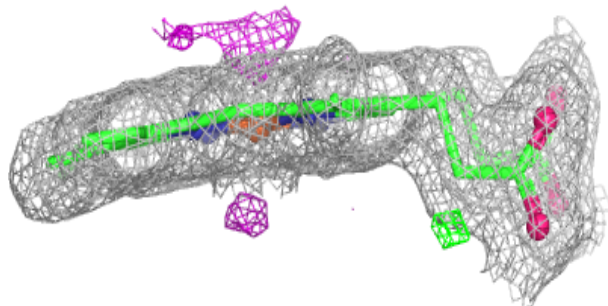
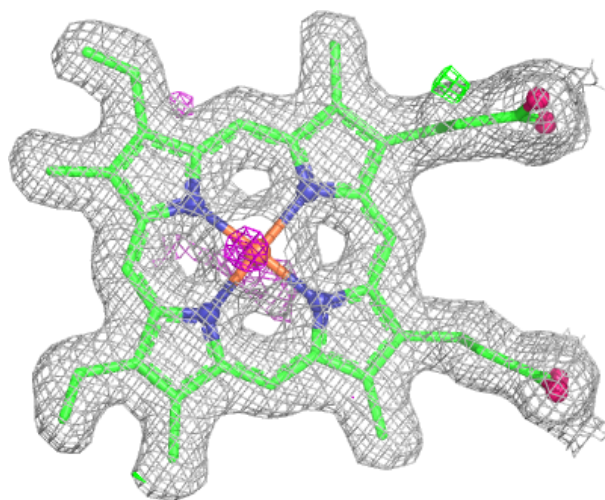
Electron density around HEM A 501:

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



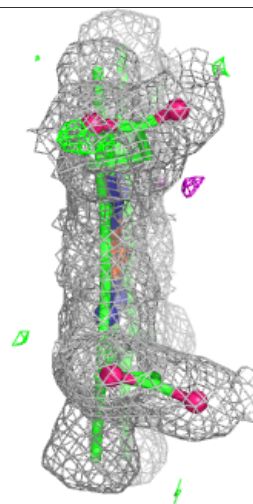
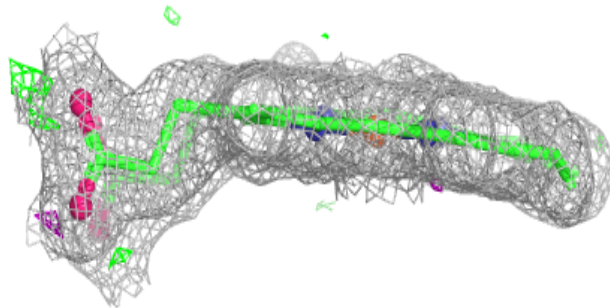
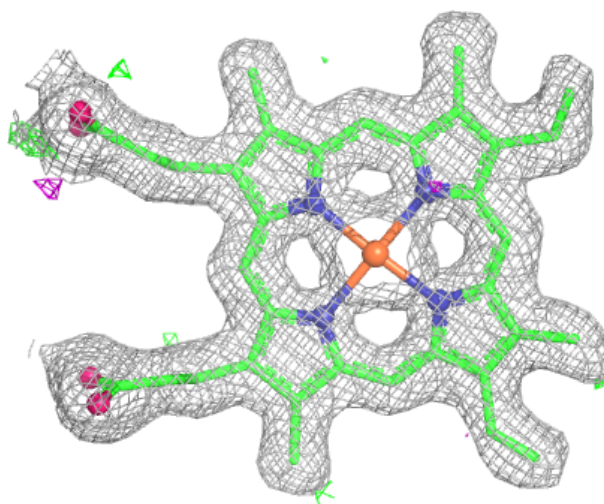
Electron density around HEM B 501:

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



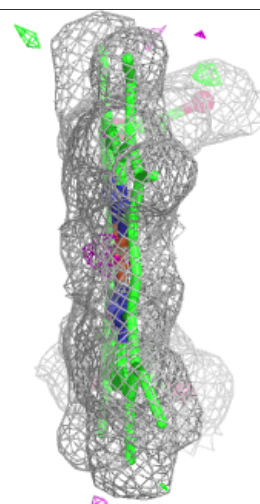
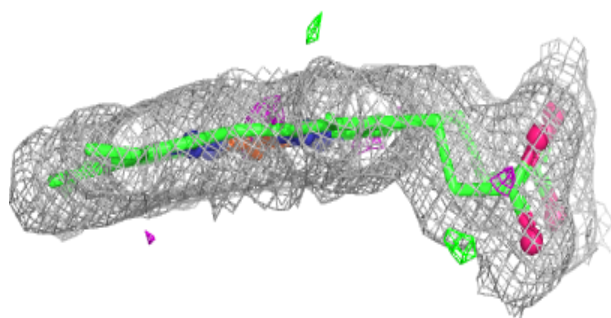
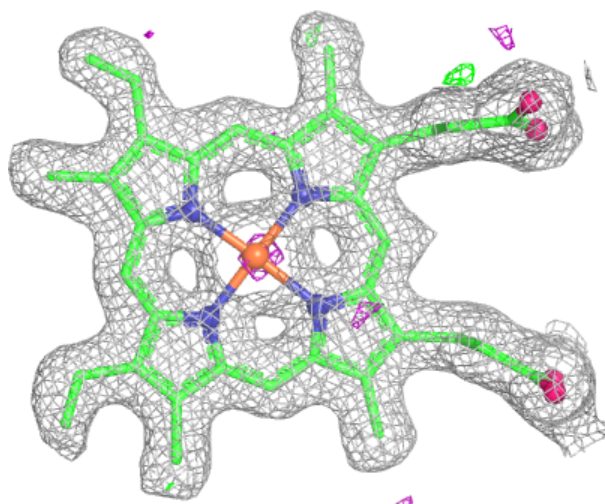
Electron density around HEM C 501:

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



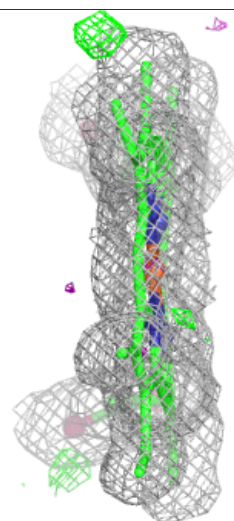
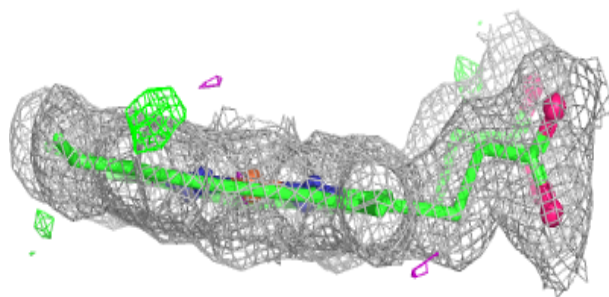
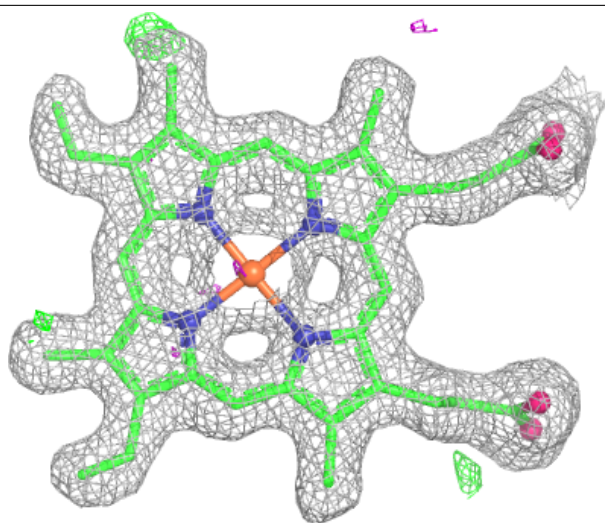
Electron density around HEM D 501:

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



Electron density around HEM E 501:

$2mF_o-DF_c$ (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.