



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 20, 2026 – 10:57 am BST

PDB ID : 30EW / pdb_000030ew
Title : XN-IL lectin from Xenorhabdus nematophila in complex with lactose
Authors : Korsak, M.; Wimmerova, M.
Deposited on : 2026-04-22
Resolution : 1.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.8.4, CSD as541be (2020)
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

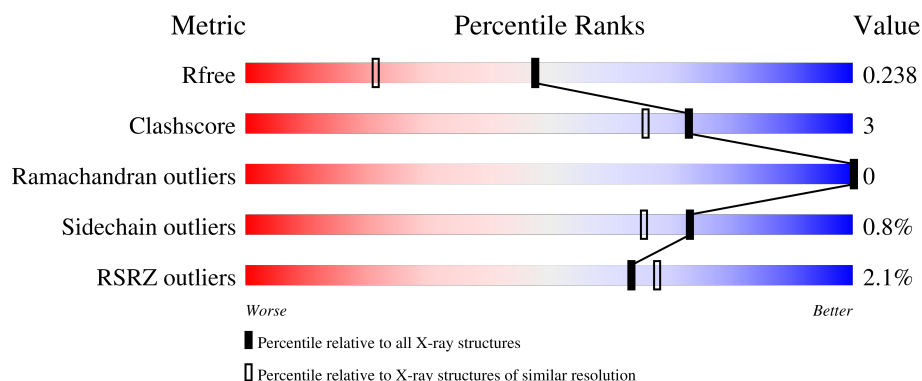
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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

Mol	Chain	Length	Quality of chain
1	AAA	125	<div> <div>2%</div> <div>95% 5%</div> </div>
1	BBB	125	<div> <div>2%</div> <div>94% 6%</div> </div>
1	CCC	125	<div> <div>3%</div> <div>91% 8%</div> </div>
1	DDD	125	<div> <div>2%</div> <div>92% 7%</div> </div>
1	EEE	125	<div> <div>2%</div> <div>90% 8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	FFF	125	
1	GGG	125	
1	HHH	125	
1	III	125	
1	JJJ	125	
1	KKK	125	
1	LLL	125	
1	MMM	125	
1	NNN	125	
1	OOO	125	
1	PPP	125	
2	WWW	2	
2	XXX	2	
2	YYY	2	
2	ZZZ	2	
2	aaa	2	
2	ccc	2	
2	ddd	2	
2	eee	2	
2	ggg	2	
3	bbb	2	
3	fff	2	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 17293 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 PA-I galactophilic lectin (PA-IL) (Galactose-binding lectin).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	125	Total	C	N	O	S	0	2	0
			979	636	156	185	2			
1	BBB	124	Total	C	N	O		0	0	0
			952	618	152	182				
1	CCC	125	Total	C	N	O		0	0	0
			955	621	152	182				
1	DDD	124	Total	C	N	O	S	0	0	0
			958	624	153	180	1			
1	EEE	124	Total	C	N	O	S	0	1	0
			960	624	153	182	1			
1	FFF	125	Total	C	N	O	S	0	1	0
			976	635	153	187	1			
1	GGG	124	Total	C	N	O		0	0	0
			951	617	152	182				
1	HHH	123	Total	C	N	O		0	0	0
			944	614	151	179				
1	III	124	Total	C	N	O		0	0	0
			956	621	153	182				
1	JJJ	125	Total	C	N	O	S	0	0	0
			955	622	151	181	1			
1	KKK	125	Total	C	N	O		0	0	0
			961	625	154	182				
1	LLL	124	Total	C	N	O	S	0	1	0
			963	627	153	182	1			
1	MMM	124	Total	C	N	O		0	1	0
			954	619	153	182				
1	NNN	125	Total	C	N	O		0	0	0
			958	623	153	182				
1	OOO	125	Total	C	N	O	S	0	1	0
			970	629	153	187	1			
1	PPP	124	Total	C	N	O		0	1	0
			959	621	153	185				

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	11	LYS	ARG	conflict	UNP D3VE08
BBB	11	LYS	ARG	conflict	UNP D3VE08
CCC	11	LYS	ARG	conflict	UNP D3VE08
DDD	11	LYS	ARG	conflict	UNP D3VE08
EEE	11	LYS	ARG	conflict	UNP D3VE08
FFF	11	LYS	ARG	conflict	UNP D3VE08
GGG	11	LYS	ARG	conflict	UNP D3VE08
HHH	11	LYS	ARG	conflict	UNP D3VE08
III	11	LYS	ARG	conflict	UNP D3VE08
JJJ	11	LYS	ARG	conflict	UNP D3VE08
KKK	11	LYS	ARG	conflict	UNP D3VE08
LLL	11	LYS	ARG	conflict	UNP D3VE08
MMM	11	LYS	ARG	conflict	UNP D3VE08
NNN	11	LYS	ARG	conflict	UNP D3VE08
OOO	11	LYS	ARG	conflict	UNP D3VE08
PPP	11	LYS	ARG	conflict	UNP D3VE08

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



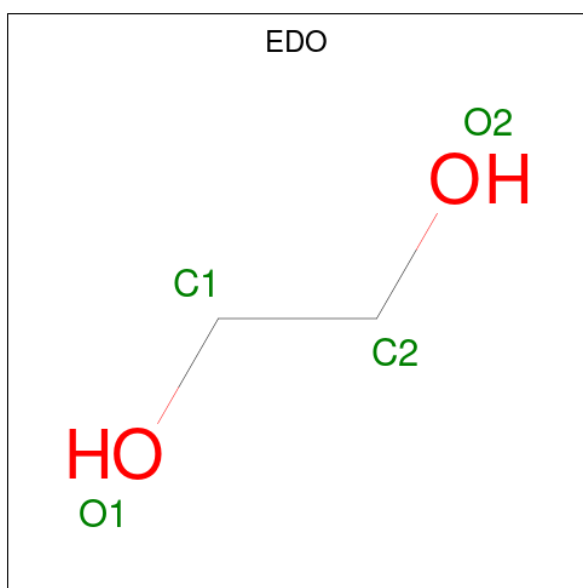
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	WWW	2	Total	C	O	0	0	0
			23	12	11			
2	XXX	2	Total	C	O	0	0	0
			23	12	11			
2	YYY	2	Total	C	O	0	0	0
			23	12	11			
2	ZZZ	2	Total	C	O	0	0	0
			23	12	11			
2	aaa	2	Total	C	O	0	0	0
			23	12	11			
2	ccc	2	Total	C	O	0	0	0
			23	12	11			
2	ddd	2	Total	C	O	0	0	0
			23	12	11			
2	eee	2	Total	C	O	0	0	0
			23	12	11			
2	ggg	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-alpha-D-glucopyranoside.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	bbb	2	Total	C	O	0	0	0
			23	12	11			
3	fff	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			4	2	2		
4	CCC	1	Total	C	O	0	0
			4	2	2		
4	CCC	1	Total	C	O	0	0
			4	2	2		
4	DDD	1	Total	C	O	0	0
			4	2	2		
4	III	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	3	Total Ca 3 3	0	0
5	BBB	1	Total Ca 1 1	0	0
5	CCC	1	Total Ca 1 1	0	0
5	DDD	1	Total Ca 1 1	0	0
5	EEE	1	Total Ca 1 1	0	0
5	FFF	2	Total Ca 2 2	0	0
5	GGG	1	Total Ca 1 1	0	0
5	HHH	3	Total Ca 3 3	0	0
5	III	2	Total Ca 2 2	0	0
5	JJJ	2	Total Ca 2 2	0	0
5	KKK	2	Total Ca 2 2	0	0
5	LLL	1	Total Ca 1 1	0	0
5	MMM	1	Total Ca 1 1	0	0
5	NNN	1	Total Ca 1 1	0	0
5	OOO	3	Total Ca 3 3	0	0
5	PPP	1	Total Ca 1 1	0	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

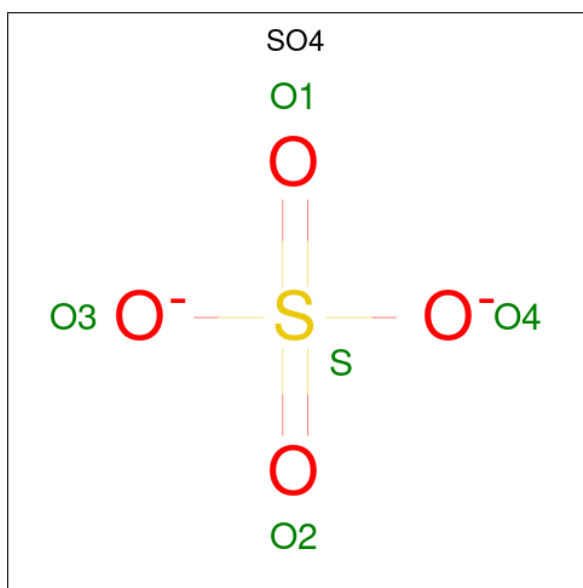
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	1	Total Mg 1 1	0	0
6	BBB	1	Total Mg 1 1	0	0
6	CCC	1	Total Mg 1 1	0	0
6	DDD	1	Total Mg 1 1	0	0

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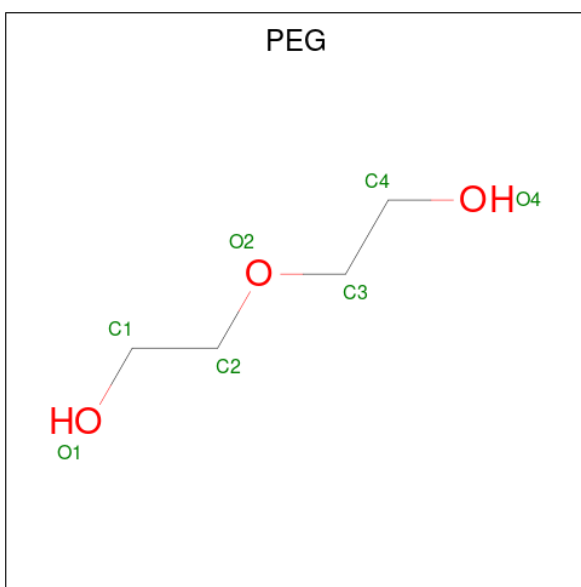
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	EEE	1	Total 1	Mg 1	0	0
6	FFF	3	Total 3	Mg 3	0	0
6	GGG	1	Total 1	Mg 1	0	0
6	HHH	1	Total 1	Mg 1	0	0
6	III	1	Total 1	Mg 1	0	0
6	JJJ	1	Total 1	Mg 1	0	0
6	KKK	1	Total 1	Mg 1	0	0
6	LLL	1	Total 1	Mg 1	0	0
6	MMM	1	Total 1	Mg 1	0	0
6	NNN	1	Total 1	Mg 1	0	0
6	OOO	1	Total 1	Mg 1	0	0
6	PPP	1	Total 1	Mg 1	0	0

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



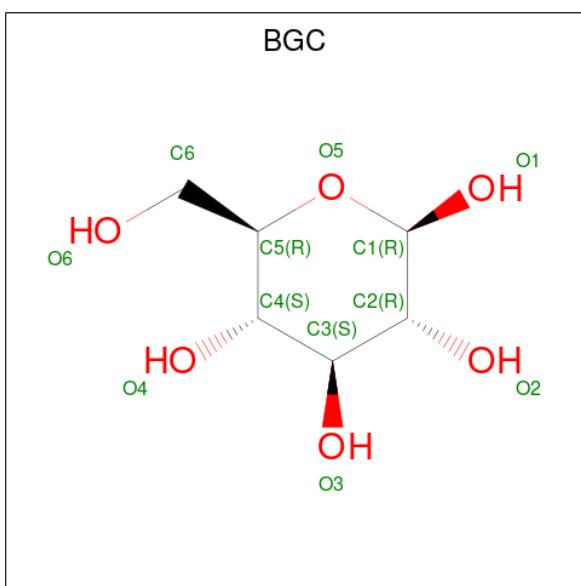
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	1	Total O S 5 4 1	0	0
7	AAA	1	Total O S 5 4 1	0	0
7	AAA	1	Total O S 5 4 1	0	0
7	BBB	1	Total O S 5 4 1	0	0
7	BBB	1	Total O S 5 4 1	0	0
7	CCC	1	Total O S 5 4 1	0	0
7	EEE	1	Total O S 5 4 1	0	0
7	EEE	1	Total O S 5 4 1	0	0
7	GGG	1	Total O S 5 4 1	0	0
7	GGG	1	Total O S 5 4 1	0	0
7	GGG	1	Total O S 5 4 1	0	0
7	HHH	1	Total O S 5 4 1	0	0
7	III	1	Total O S 5 4 1	0	0
7	JJJ	1	Total O S 5 4 1	0	0
7	KKK	1	Total O S 5 4 1	0	0
7	KKK	1	Total O S 5 4 1	0	0
7	LLL	1	Total O S 5 4 1	0	0
7	NNN	1	Total O S 5 4 1	0	0
7	OOO	1	Total O S 5 4 1	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



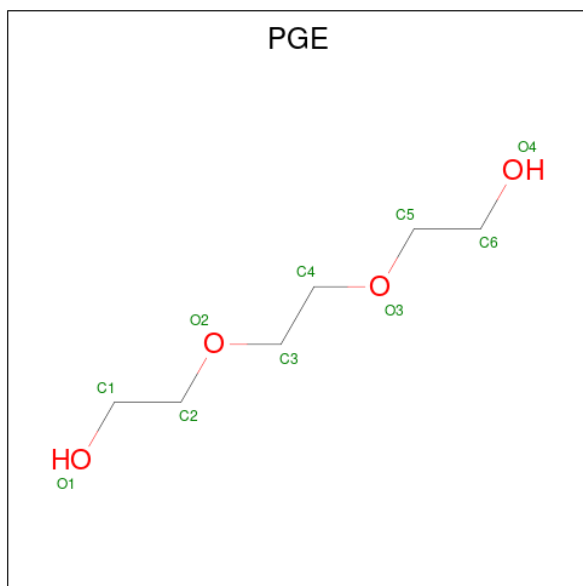
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	BBB	1	Total	C	O	0	0
			7	4	3		
8	GGG	1	Total	C	O	0	0
			7	4	3		
8	LLL	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is beta-D-glucopyranose (CCD ID: BGC) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	BBB	1	Total	C	O	0	0
			12	6	6		
9	GGG	1	Total	C	O	0	0
			12	6	6		
9	NNN	1	Total	C	O	0	0
			12	6	6		

- Molecule 10 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	CCC	1	Total	C	O	0	0
			10	6	4		

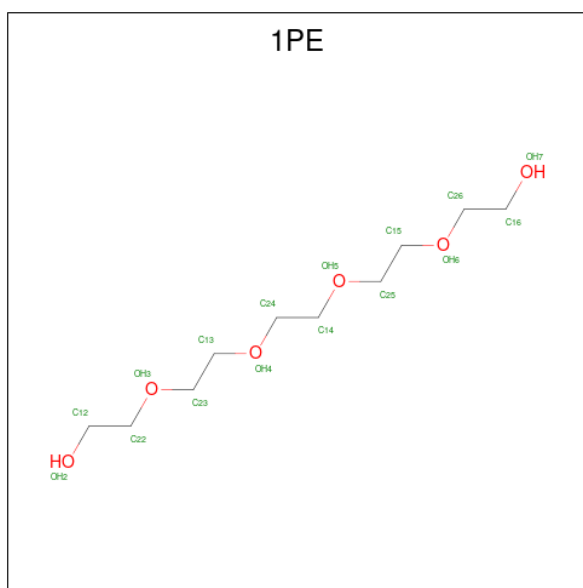
- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	GGG	1	Total	Cl	0	0
			1	1		
11	OOO	1	Total	Cl	0	0
			1	1		

- Molecule 12 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	GGG	1	Total	Na	0	0
			1	1		

- Molecule 13 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	LLL	1	Total	C O	0	0
			16	10 6		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	AAA	88	Total	O	0	0
			88	88		
14	BBB	73	Total	O	0	0
			73	73		
14	CCC	97	Total	O	0	0
			97	97		
14	DDD	70	Total	O	0	0
			70	70		
14	EEE	95	Total	O	0	0
			95	95		
14	FFF	127	Total	O	0	0
			127	127		
14	GGG	112	Total	O	0	0
			112	112		
14	HHH	75	Total	O	0	0
			75	75		
14	III	106	Total	O	0	0
			106	106		
14	JJJ	101	Total	O	0	0
			101	101		

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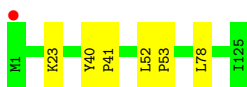
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	KKK	105	Total 105	O 105	0	0
14	LLL	93	Total 93	O 93	0	0
14	MMM	70	Total 70	O 70	0	0
14	NNN	69	Total 69	O 69	0	0
14	OOO	72	Total 72	O 72	0	0
14	PPP	91	Total 91	O 91	0	0

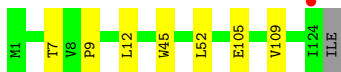
3 Residue-property plots [i](#)

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.

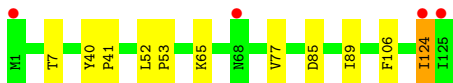
- Molecule 1: PA-I galactophilic lectin (PA-IL) (Galactose-binding lectin)



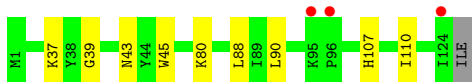
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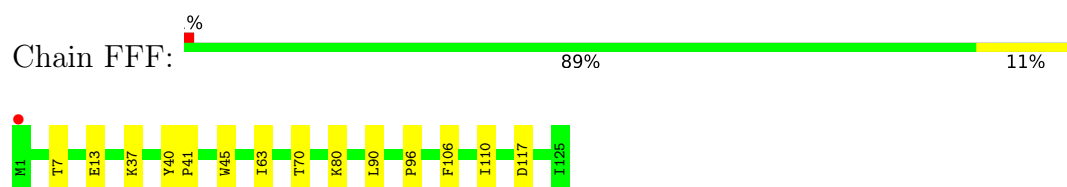
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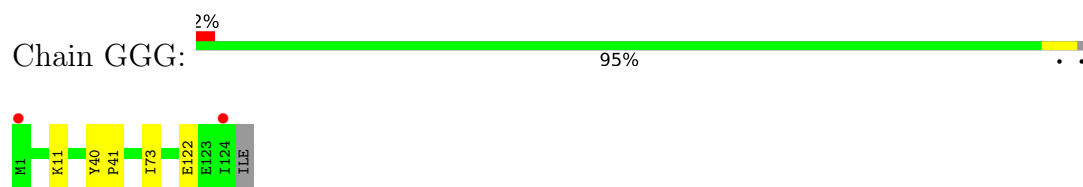
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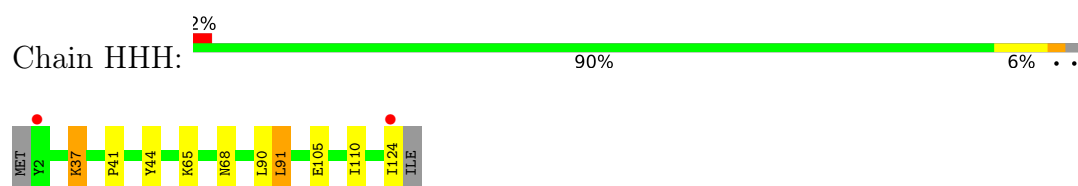
- Molecule 1: PA-I galactophilic lectin (PA-IL) (Galactose-binding lectin)



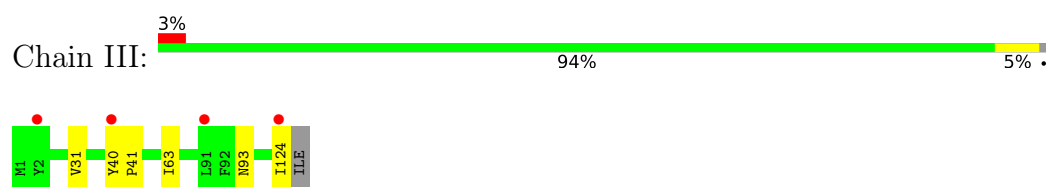
- Molecule 1: PA-I galactophilic lectin (PA-IL) (Galactose-binding lectin)



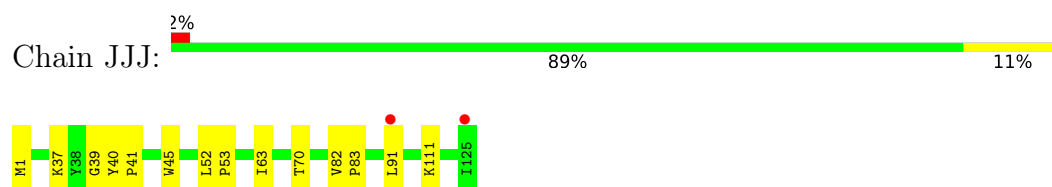
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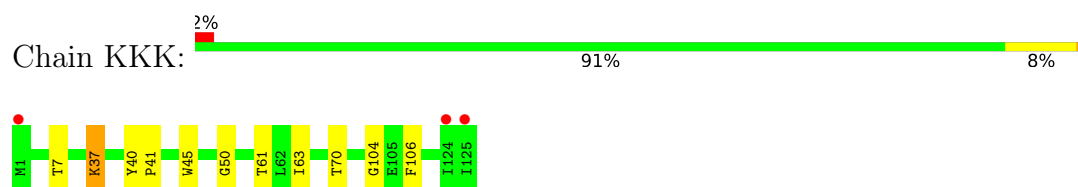
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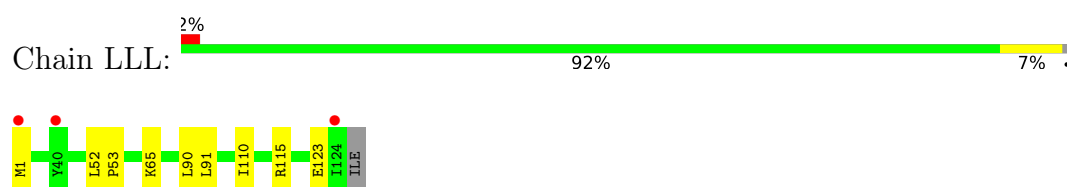
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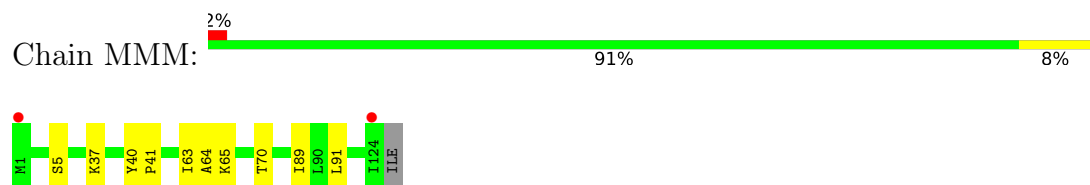
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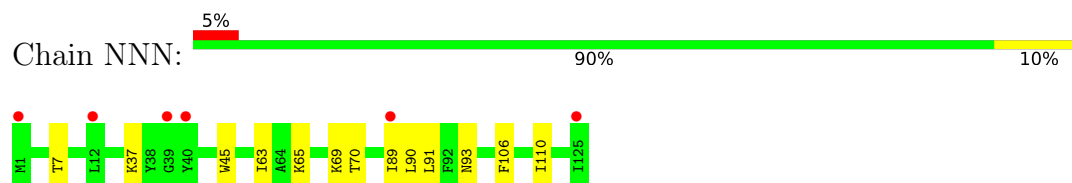
- Molecule 1: PA-I galactophilic lectin (PA-IL) (Galactose-binding lectin)



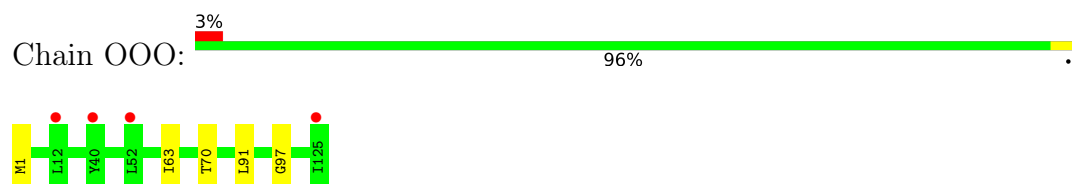
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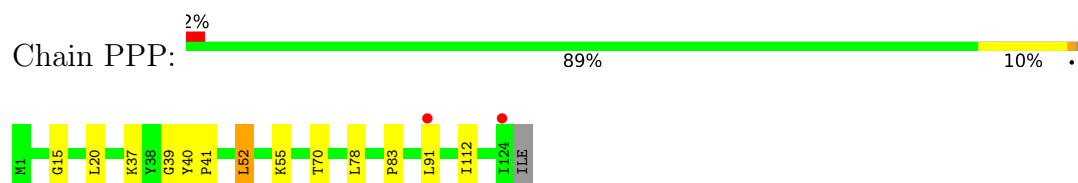
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- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



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Chain ZZZ:  100%

BGC1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain aaa:  100%

BGC1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain ccc:  100%

BGC1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain ddd:  100%


BGC1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain eee:  100%

BGC1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain ggg:  100%

BGC1
GAL2

- Molecule 3: beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose

Chain bbb:  100%

GLC1
GAL2

- Molecule 3: beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose

Chain fff:  100%

GLC1
GAL2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.61Å 140.32Å 94.63Å 90.00° 113.97° 90.00°	Depositor
Resolution (Å)	48.44 – 1.70 48.44 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.44-1.70) 98.6 (48.44-1.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.193 , 0.231 0.201 , 0.238	Depositor DCC
R_{free} test set	12294 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 27.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.036 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17293	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.01 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4375e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PEG, 1PE, SO4, EDO, GAL, PGE, GLC, CL, CA, BGC, MG, NA

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	AAA	1.06	0/1005	1.12	0/1368
1	BBB	1.01	0/978	1.17	0/1335
1	CCC	1.02	0/981	1.19	1/1338 (0.1%)
1	DDD	1.07	0/984	1.18	0/1340
1	EEE	1.06	0/990	1.12	0/1351
1	FFF	1.06	0/1002	1.12	1/1364 (0.1%)
1	GGG	1.05	0/977	1.19	1/1334 (0.1%)
1	HHH	1.00	0/970	1.16	0/1324
1	III	1.03	0/982	1.17	0/1339
1	JJJ	1.04	0/981	1.16	0/1338
1	KKK	1.06	1/987 (0.1%)	1.20	1/1345 (0.1%)
1	LLL	1.03	0/992	1.20	0/1352
1	MMM	1.00	0/980	1.21	0/1339
1	NNN	1.08	0/984	1.20	1/1343 (0.1%)
1	OOO	1.07	0/996	1.18	0/1358
1	PPP	1.02	1/985 (0.1%)	1.21	0/1344
All	All	1.04	2/15774 (0.0%)	1.17	5/21512 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	PPP	83	PRO	C-O	-5.42	1.17	1.24
1	KKK	37	LYS	C-O	5.29	1.30	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	GGG	73	ILE	N-CA-C	-5.79	107.05	111.62
1	FFF	117	ASP	CA-CB-CG	5.38	117.98	112.60
1	NNN	93	ASN	CA-CB-CG	5.19	117.79	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	85	ASP	CA-CB-CG	5.10	117.70	112.60
1	KKK	104	GLY	CA-C-O	-5.01	118.23	122.29

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	979	0	967	3	0
1	BBB	952	0	932	4	0
1	CCC	955	0	929	8	0
1	DDD	958	0	952	9	0
1	EEE	960	0	939	7	0
1	FFF	976	0	958	7	0
1	GGG	951	0	929	3	0
1	HHH	944	0	925	7	0
1	III	956	0	943	5	0
1	JJJ	955	0	935	9	0
1	KKK	961	0	950	5	0
1	LLL	963	0	959	6	0
1	MMM	954	0	932	8	0
1	NNN	958	0	944	9	0
1	OOO	970	0	946	3	0
1	PPP	959	0	930	7	0
2	WWW	23	0	19	0	0
2	XXX	23	0	19	0	0
2	YYY	23	0	19	0	0
2	ZZZ	23	0	19	0	0
2	aaa	23	0	19	0	0
2	ccc	23	0	19	0	0
2	ddd	23	0	19	0	0
2	eee	23	0	19	0	0
2	ggg	23	0	19	0	0
3	bbb	23	0	19	0	0
3	fff	23	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AAA	4	0	6	3	0
4	CCC	8	0	12	2	0
4	DDD	4	0	6	2	0
4	III	4	0	6	0	0
5	AAA	3	0	0	0	0
5	BBB	1	0	0	0	0
5	CCC	1	0	0	0	0
5	DDD	1	0	0	0	0
5	EEE	1	0	0	0	0
5	FFF	2	0	0	0	0
5	GGG	1	0	0	0	0
5	HHH	3	0	0	0	0
5	III	2	0	0	0	0
5	JJJ	2	0	0	0	0
5	KKK	2	0	0	0	0
5	LLL	1	0	0	0	0
5	MMM	1	0	0	0	0
5	NNN	1	0	0	0	0
5	OOO	3	0	0	0	0
5	PPP	1	0	0	0	0
6	AAA	1	0	0	0	0
6	BBB	1	0	0	0	0
6	CCC	1	0	0	0	0
6	DDD	1	0	0	0	0
6	EEE	1	0	0	0	0
6	FFF	3	0	0	0	0
6	GGG	1	0	0	0	0
6	HHH	1	0	0	0	0
6	III	1	0	0	0	0
6	JJJ	1	0	0	0	0
6	KKK	1	0	0	0	0
6	LLL	1	0	0	0	0
6	MMM	1	0	0	0	0
6	NNN	1	0	0	0	0
6	OOO	1	0	0	0	0
6	PPP	1	0	0	0	0
7	AAA	15	0	0	0	0
7	BBB	10	0	0	0	0
7	CCC	5	0	0	0	0
7	EEE	10	0	0	0	0
7	GGG	15	0	0	0	0
7	HHH	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	III	5	0	0	0	0
7	JJJ	5	0	0	0	0
7	KKK	10	0	0	0	0
7	LLL	5	0	0	0	0
7	NNN	5	0	0	0	0
7	OOO	5	0	0	0	0
8	BBB	7	0	10	0	0
8	GGG	7	0	10	3	0
8	LLL	7	0	10	1	0
9	BBB	12	0	10	0	0
9	GGG	12	0	10	0	0
9	NNN	12	0	10	0	0
10	CCC	10	0	14	3	0
11	GGG	1	0	0	0	0
11	OOO	1	0	0	1	0
12	GGG	1	0	0	0	0
13	LLL	16	0	22	0	0
14	AAA	88	0	0	3	0
14	BBB	73	0	0	0	0
14	CCC	97	0	0	2	0
14	DDD	70	0	0	0	0
14	EEE	95	0	0	0	0
14	FFF	127	0	0	0	0
14	GGG	112	0	0	0	0
14	HHH	75	0	0	1	0
14	III	106	0	0	2	0
14	JJJ	101	0	0	1	0
14	KKK	105	0	0	0	0
14	LLL	93	0	0	1	0
14	MMM	70	0	0	0	0
14	NNN	69	0	0	0	0
14	OOO	72	0	0	2	0
14	PPP	91	0	0	0	0
All	All	17293	0	15405	101	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 3.

The worst 5 of 101 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:NNN:63:ILE:HD11	1:NNN:91:LEU:HD23	1.50	0.91
1:MMM:63:ILE:HD11	1:MMM:91:LEU:HD23	1.61	0.82
1:LLL:115:ARG:H	8:LLL:201:PEG:H22	1.60	0.66
1:CCC:77:VAL:HG11	4:CCC:201:EDO:H11	1.78	0.65
1:CCC:65:LYS:CE	14:CCC:395:HOH:O	2.47	0.62

There are no symmetry-related clashes.

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	AAA	124/125 (99%)	123 (99%)	1 (1%)	0	100	100
1	BBB	122/125 (98%)	122 (100%)	0	0	100	100
1	CCC	123/125 (98%)	123 (100%)	0	0	100	100
1	DDD	122/125 (98%)	120 (98%)	2 (2%)	0	100	100
1	EEE	123/125 (98%)	122 (99%)	1 (1%)	0	100	100
1	FFF	124/125 (99%)	124 (100%)	0	0	100	100
1	GGG	122/125 (98%)	120 (98%)	2 (2%)	0	100	100
1	HHH	121/125 (97%)	121 (100%)	0	0	100	100
1	III	122/125 (98%)	120 (98%)	2 (2%)	0	100	100
1	JJJ	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	KKK	123/125 (98%)	122 (99%)	1 (1%)	0	100	100
1	LLL	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	MMM	123/125 (98%)	123 (100%)	0	0	100	100
1	NNN	123/125 (98%)	122 (99%)	1 (1%)	0	100	100
1	OOO	124/125 (99%)	123 (99%)	1 (1%)	0	100	100
1	PPP	123/125 (98%)	119 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1965/2000 (98%)	1946 (99%)	19 (1%)	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	AAA	103/104 (99%)	102 (99%)	1 (1%)	68	58
1	BBB	100/104 (96%)	100 (100%)	0	100	100
1	CCC	98/104 (94%)	97 (99%)	1 (1%)	68	58
1	DDD	101/104 (97%)	101 (100%)	0	100	100
1	EEE	101/104 (97%)	99 (98%)	2 (2%)	48	32
1	FFF	102/104 (98%)	102 (100%)	0	100	100
1	GGG	100/104 (96%)	99 (99%)	1 (1%)	68	58
1	HHH	99/104 (95%)	96 (97%)	3 (3%)	36	19
1	III	101/104 (97%)	100 (99%)	1 (1%)	68	58
1	JJJ	99/104 (95%)	99 (100%)	0	100	100
1	KKK	101/104 (97%)	101 (100%)	0	100	100
1	LLL	103/104 (99%)	103 (100%)	0	100	100
1	MMM	100/104 (96%)	98 (98%)	2 (2%)	48	32
1	NNN	101/104 (97%)	101 (100%)	0	100	100
1	OOO	102/104 (98%)	101 (99%)	1 (1%)	68	58
1	PPP	100/104 (96%)	99 (99%)	1 (1%)	68	58
All	All	1611/1664 (97%)	1598 (99%)	13 (1%)	73	65

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	HHH	105	GLU

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Mol	Chain	Res	Type
1	III	124	ILE
1	PPP	52	LEU
1	MMM	37	LYS
1	OOO	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

22 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	BGC	WWW	1	2,5	12,12,12	0.86	0	17,17,17	1.69	5 (29%)
2	GAL	WWW	2	2	11,11,12	0.45	0	15,15,17	0.70	0
2	BGC	XXX	1	2,5	12,12,12	0.49	0	17,17,17	1.34	3 (17%)
2	GAL	XXX	2	2	11,11,12	0.66	0	15,15,17	1.98	5 (33%)
2	BGC	YYY	1	2,5	12,12,12	0.88	0	17,17,17	1.54	3 (17%)
2	GAL	YYY	2	2	11,11,12	0.71	0	15,15,17	1.33	1 (6%)
2	BGC	ZZZ	1	2,5	12,12,12	0.78	0	17,17,17	1.87	6 (35%)
2	GAL	ZZZ	2	2	11,11,12	0.44	0	15,15,17	1.21	1 (6%)
2	BGC	aaa	1	2,5	12,12,12	0.70	0	17,17,17	1.57	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GAL	aaa	2	2	11,11,12	0.65	0	15,15,17	1.63	2 (13%)
3	GLC	bbb	1	5,3	12,12,12	1.05	1 (8%)	17,17,17	1.49	3 (17%)
3	GAL	bbb	2	3	11,11,12	0.92	0	15,15,17	1.44	4 (26%)
2	BGC	ccc	1	2,5	12,12,12	1.09	1 (8%)	17,17,17	1.41	2 (11%)
2	GAL	ccc	2	2	11,11,12	0.87	0	15,15,17	2.04	4 (26%)
2	BGC	ddd	1	2,5	12,12,12	0.73	0	17,17,17	1.88	5 (29%)
2	GAL	ddd	2	2	11,11,12	0.84	0	15,15,17	1.46	2 (13%)
2	BGC	eee	1	2,5	12,12,12	0.69	0	17,17,17	1.19	1 (5%)
2	GAL	eee	2	2	11,11,12	0.66	0	15,15,17	1.32	1 (6%)
3	GLC	fff	1	5,3	12,12,12	1.14	0	17,17,17	1.81	3 (17%)
3	GAL	fff	2	3	11,11,12	0.71	0	15,15,17	1.92	3 (20%)
2	BGC	ggg	1	2,5	12,12,12	0.62	0	17,17,17	1.40	3 (17%)
2	GAL	ggg	2	2	11,11,12	0.25	0	15,15,17	1.29	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	BGC	WWW	1	2,5	-	1/2/22/22	0/1/1/1
2	GAL	WWW	2	2	-	1/2/19/22	0/1/1/1
2	BGC	XXX	1	2,5	-	0/2/22/22	0/1/1/1
2	GAL	XXX	2	2	-	2/2/19/22	0/1/1/1
2	BGC	YYY	1	2,5	-	1/2/22/22	0/1/1/1
2	GAL	YYY	2	2	-	1/2/19/22	0/1/1/1
2	BGC	ZZZ	1	2,5	-	0/2/22/22	0/1/1/1
2	GAL	ZZZ	2	2	-	0/2/19/22	0/1/1/1
2	BGC	aaa	1	2,5	-	2/2/22/22	0/1/1/1
2	GAL	aaa	2	2	-	2/2/19/22	0/1/1/1
3	GLC	bbb	1	5,3	-	2/2/22/22	0/1/1/1
3	GAL	bbb	2	3	-	2/2/19/22	0/1/1/1
2	BGC	ccc	1	2,5	-	0/2/22/22	0/1/1/1
2	GAL	ccc	2	2	-	2/2/19/22	0/1/1/1
2	BGC	ddd	1	2,5	-	0/2/22/22	0/1/1/1
2	GAL	ddd	2	2	-	1/2/19/22	0/1/1/1
2	BGC	eee	1	2,5	-	2/2/22/22	0/1/1/1
2	GAL	eee	2	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	fff	1	5,3	-	0/2/22/22	0/1/1/1
3	GAL	fff	2	3	-	2/2/19/22	0/1/1/1
2	BGC	ggg	1	2,5	-	1/2/22/22	0/1/1/1
2	GAL	ggg	2	2	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	bbb	1	GLC	O1-C1	2.04	1.46	1.39
2	ccc	1	BGC	O4-C4	2.03	1.47	1.43

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	fff	2	GAL	C1-O5-C5	5.72	119.95	112.19
2	ccc	2	GAL	C1-C2-C3	5.00	115.81	109.67
2	ddd	1	BGC	O3-C3-C2	-4.47	100.00	110.35
2	aaa	2	GAL	O5-C5-C6	4.13	113.69	107.20
3	fff	1	GLC	O3-C3-C2	-4.12	100.83	110.35

There are no chirality outliers.

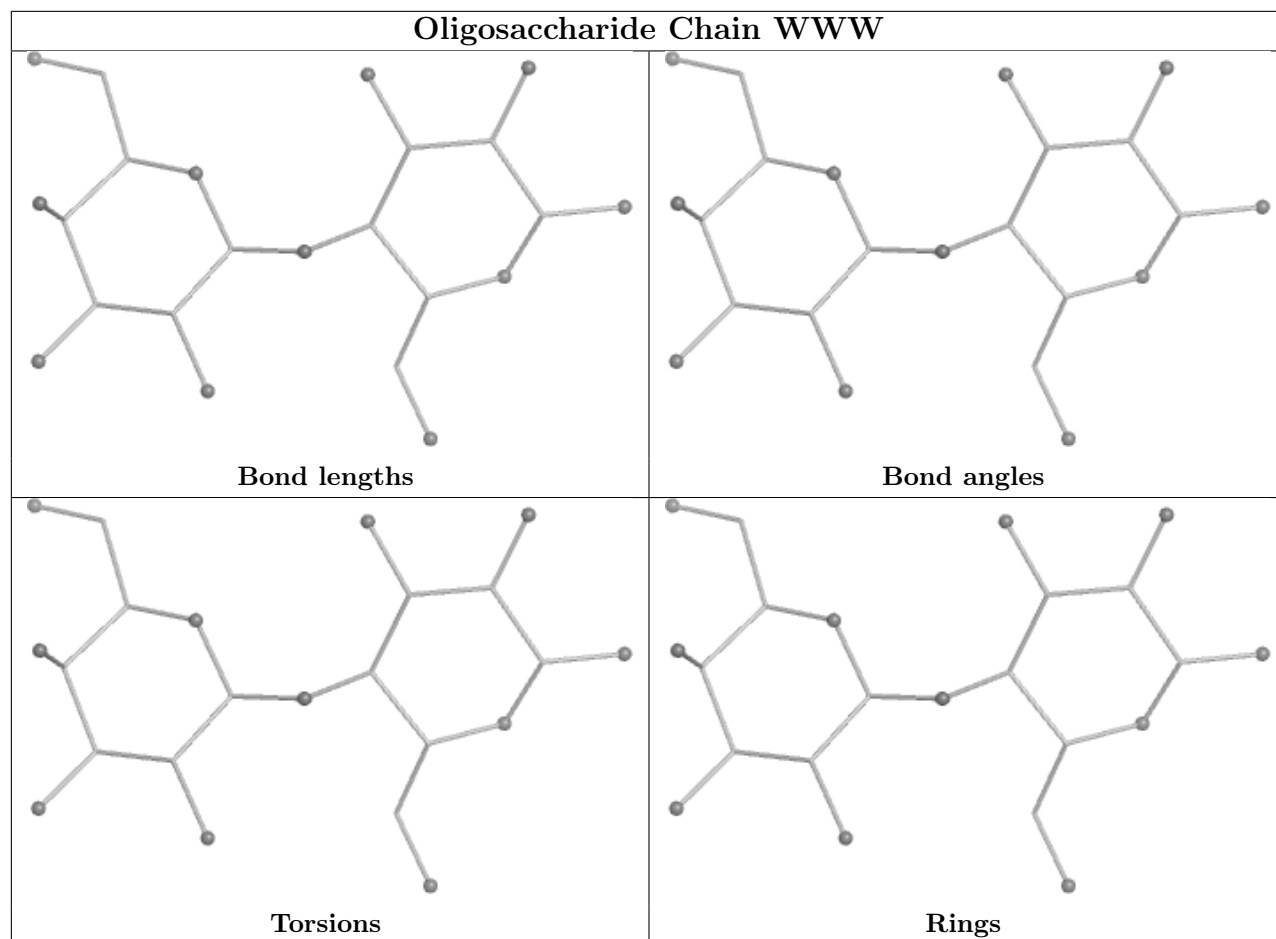
5 of 24 torsion outliers are listed below:

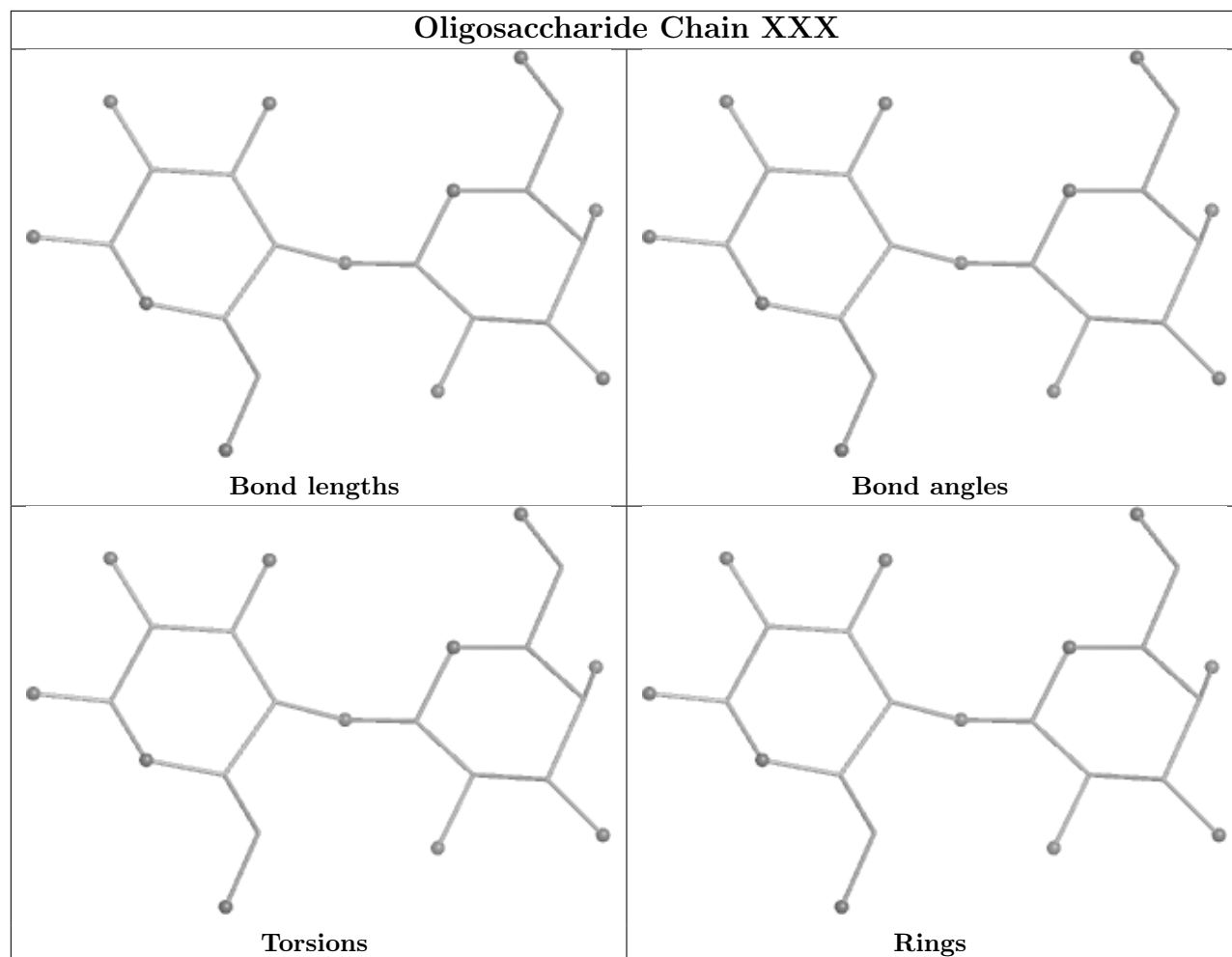
Mol	Chain	Res	Type	Atoms
2	aaa	1	BGC	O5-C5-C6-O6
3	fff	2	GAL	O5-C5-C6-O6
2	XXX	2	GAL	O5-C5-C6-O6
3	bbb	2	GAL	C4-C5-C6-O6
3	bbb	2	GAL	O5-C5-C6-O6

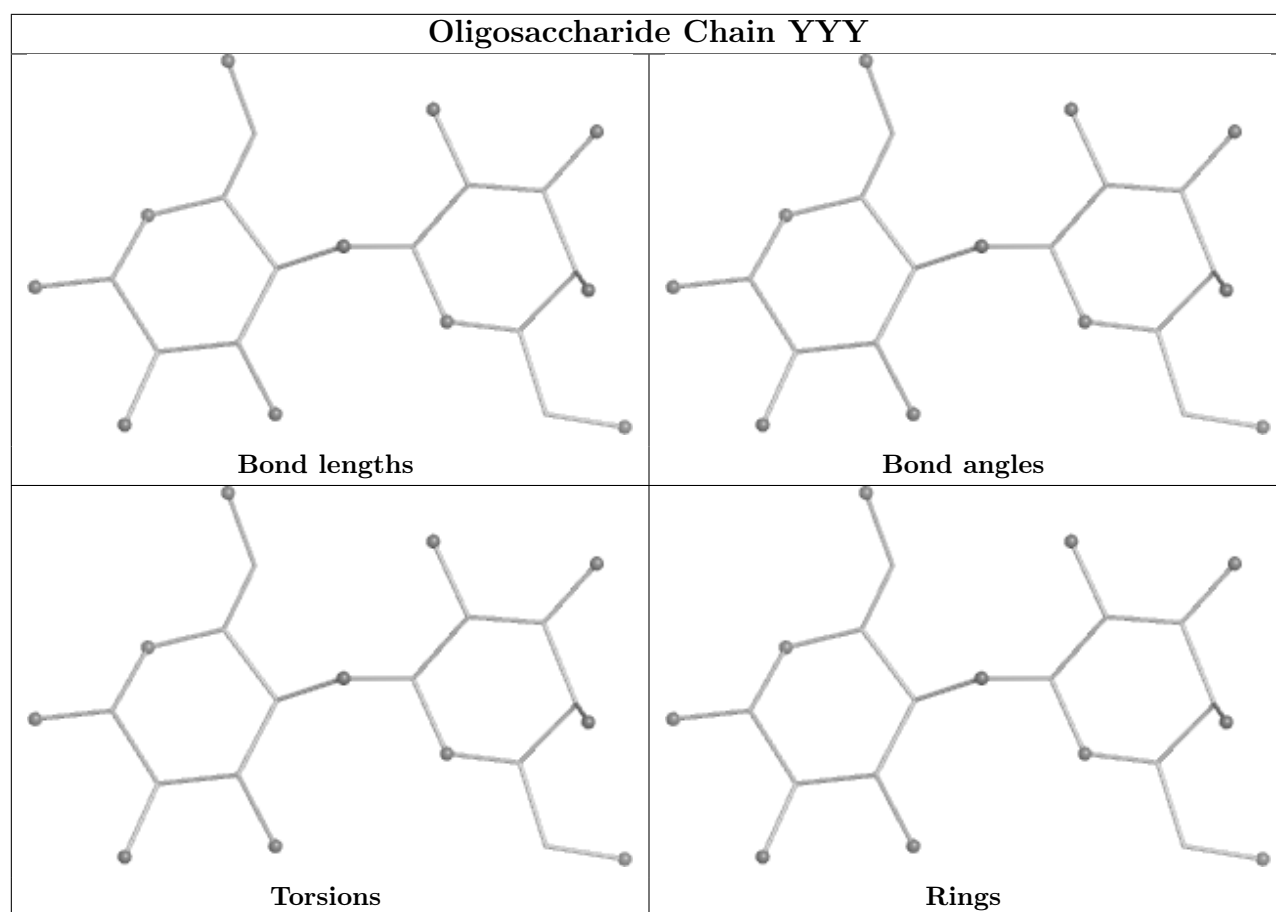
There are no ring outliers.

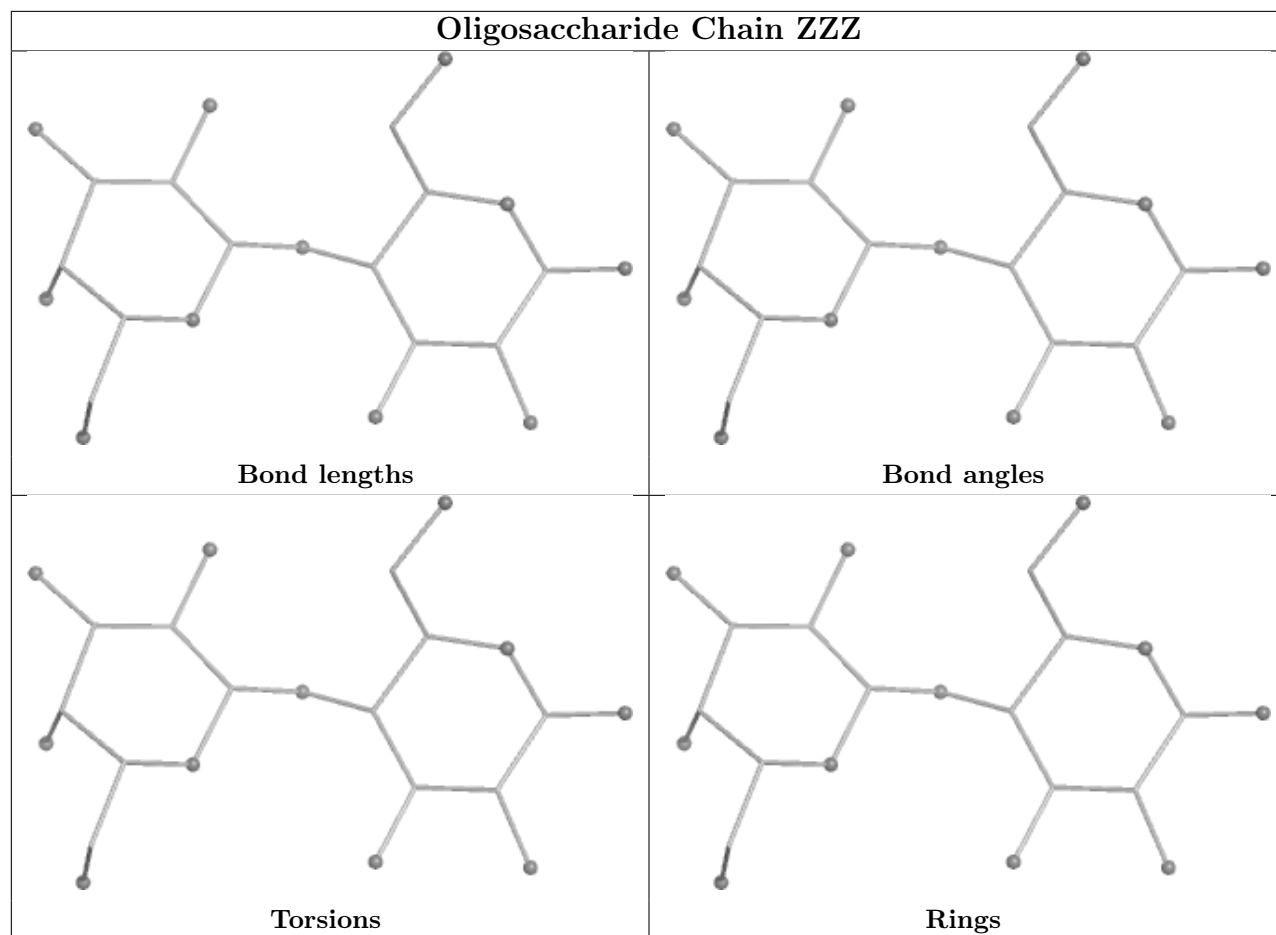
No monomer is involved in short contacts.

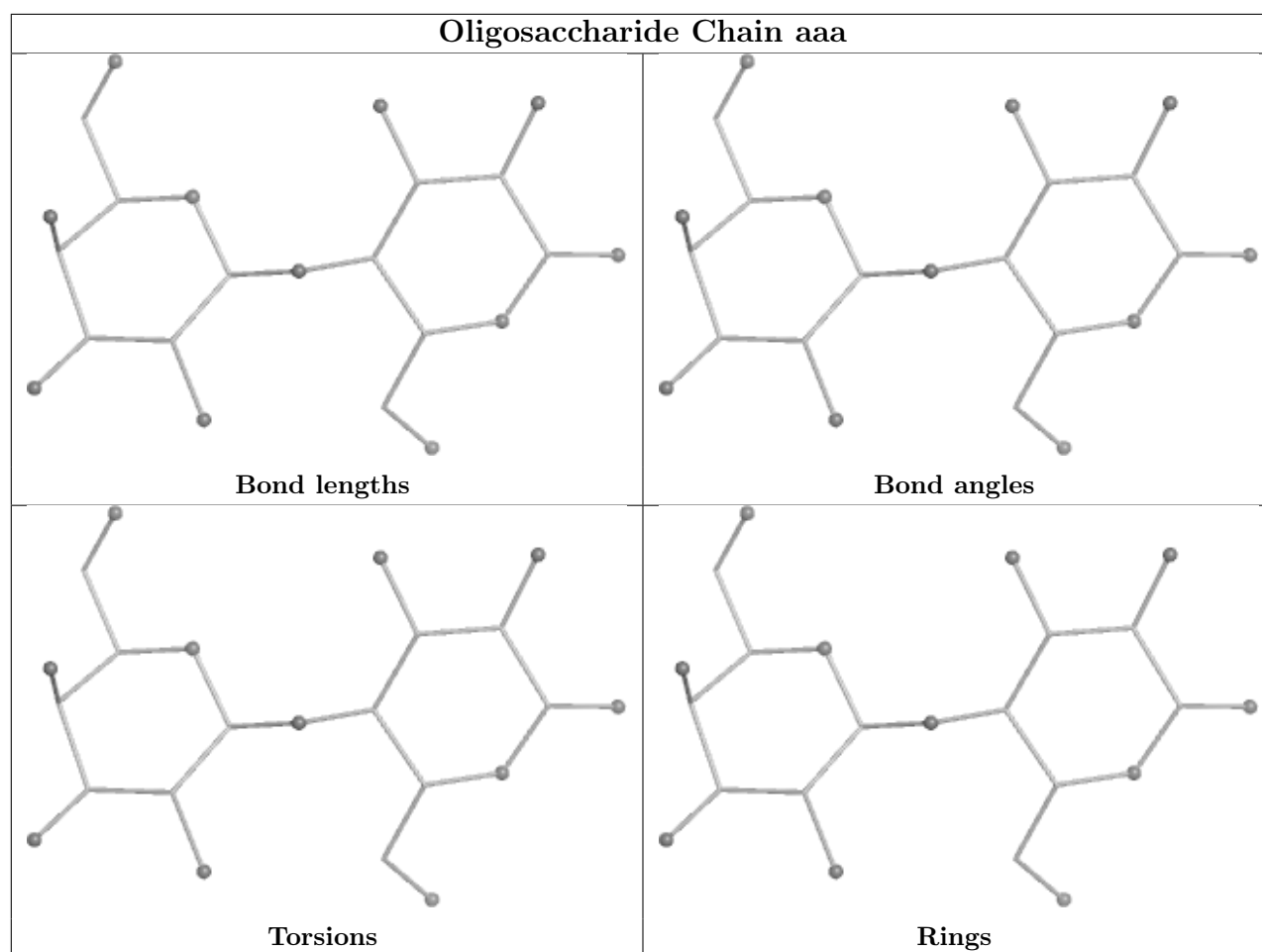
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

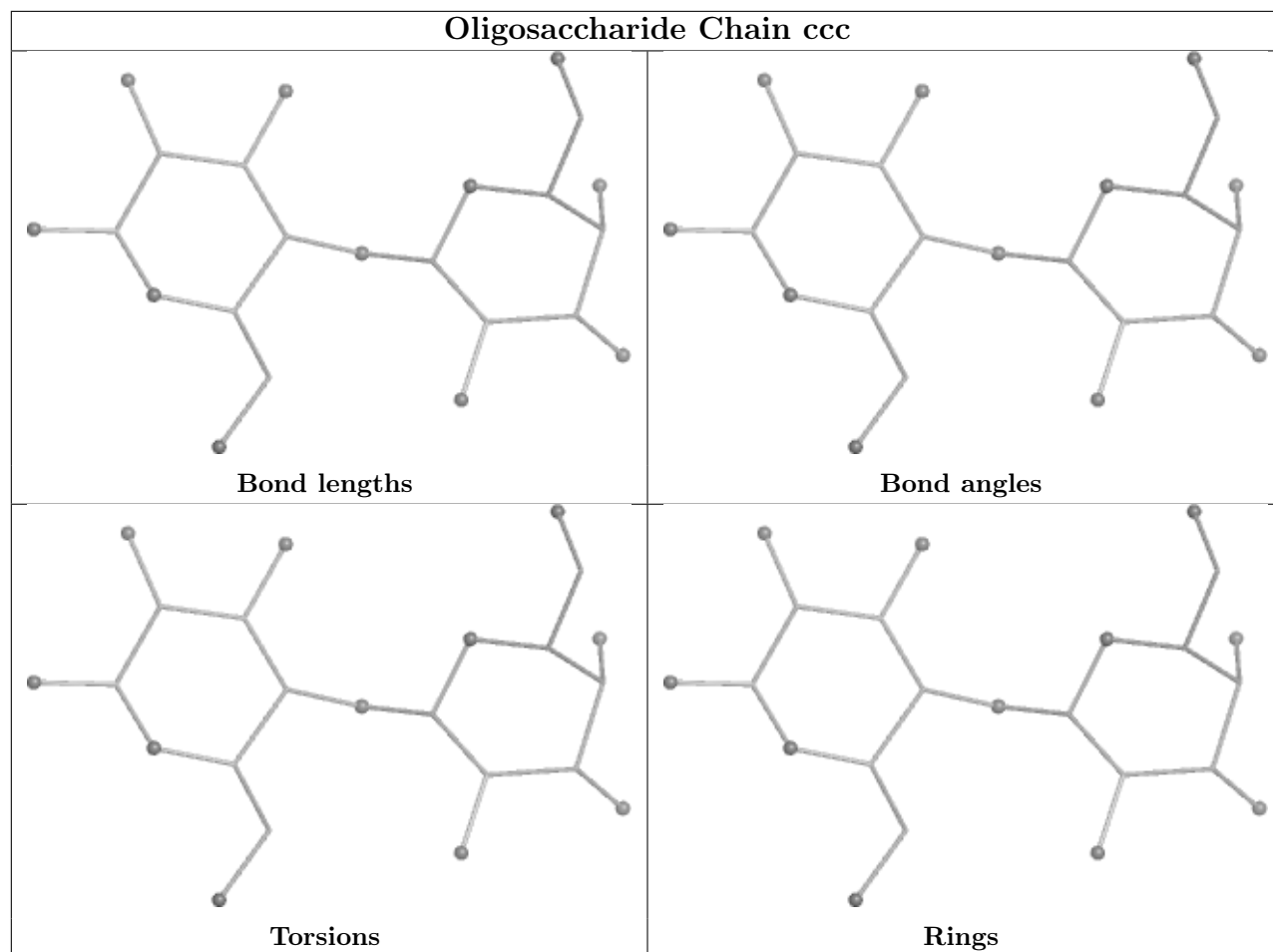


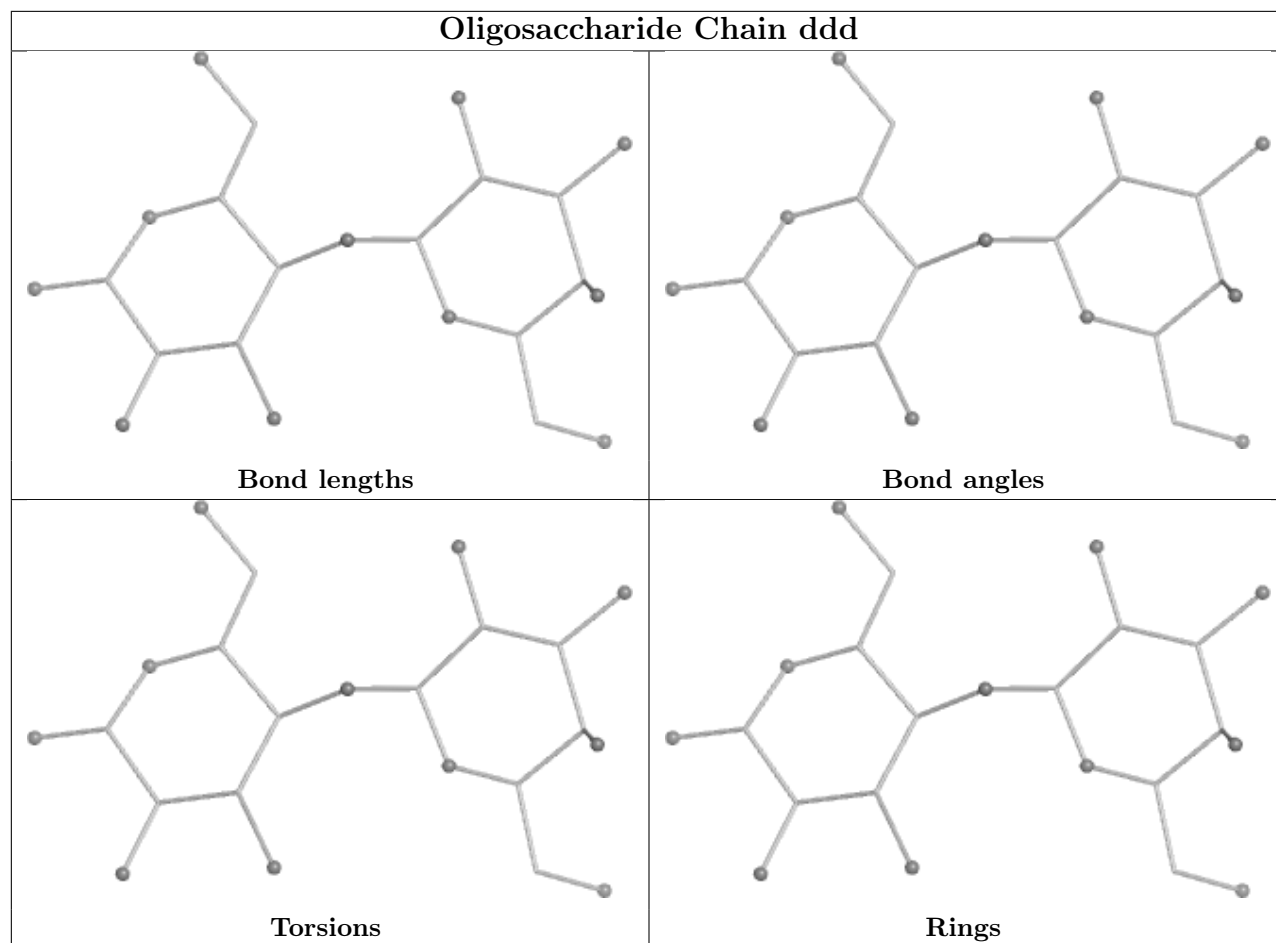


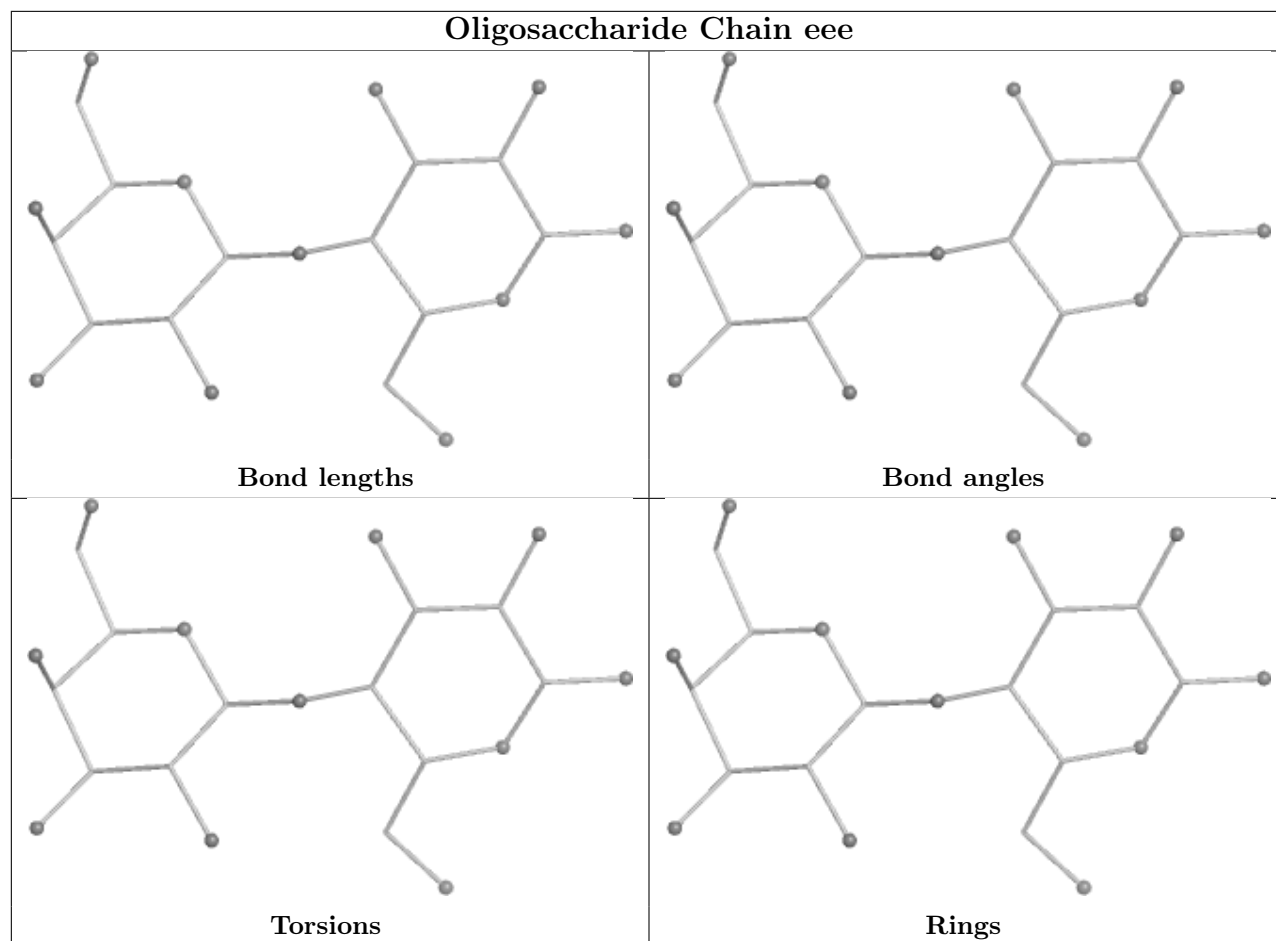


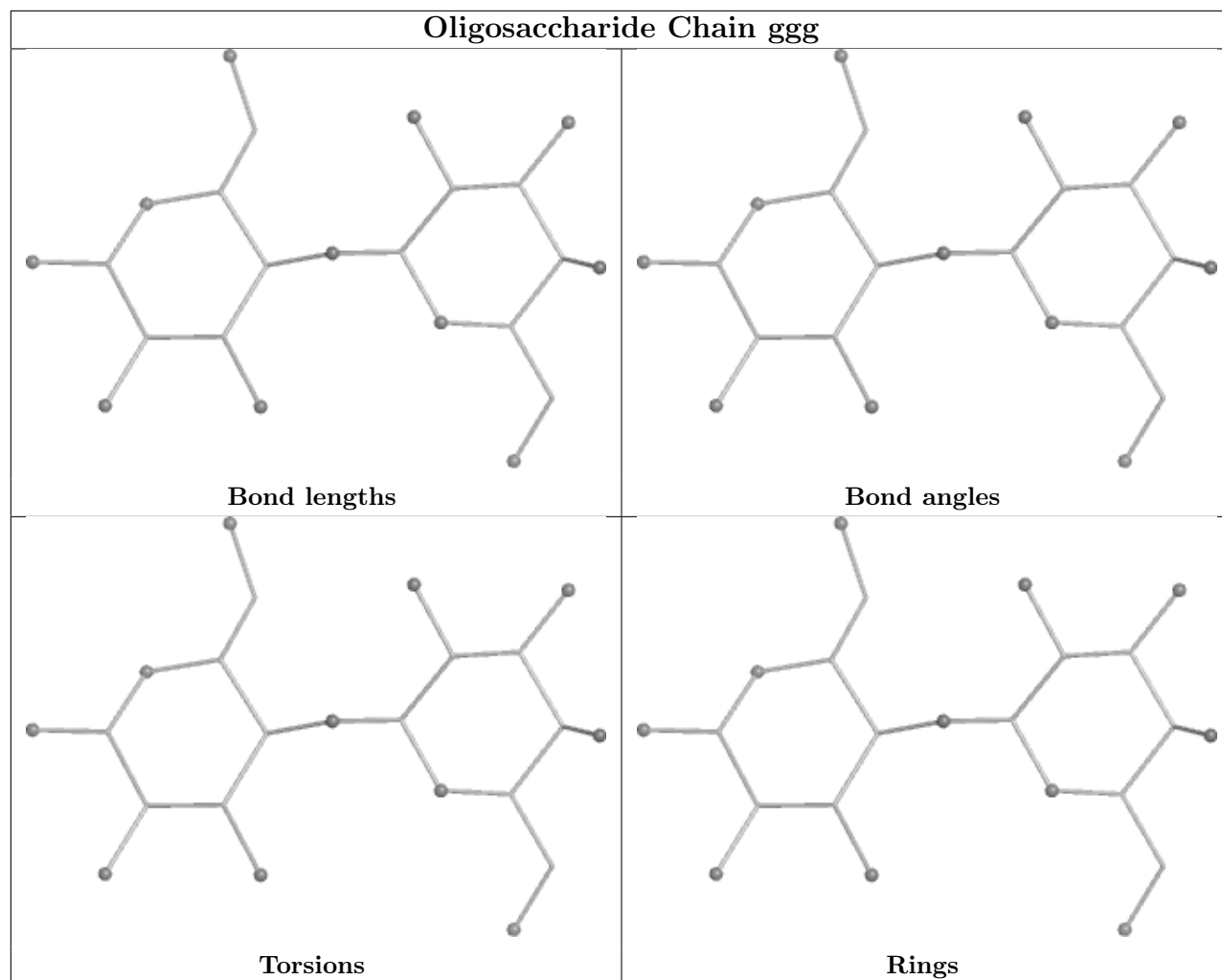


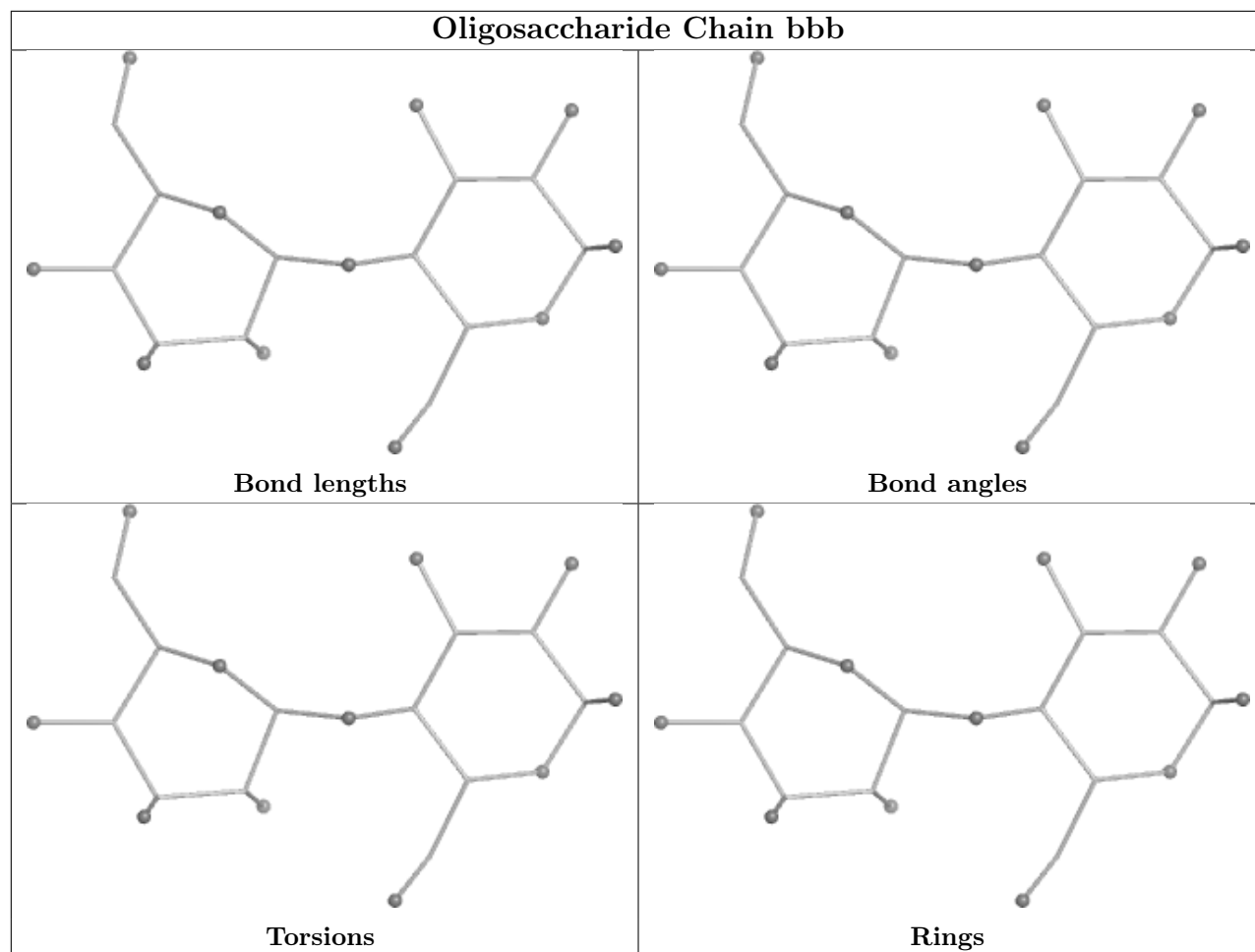


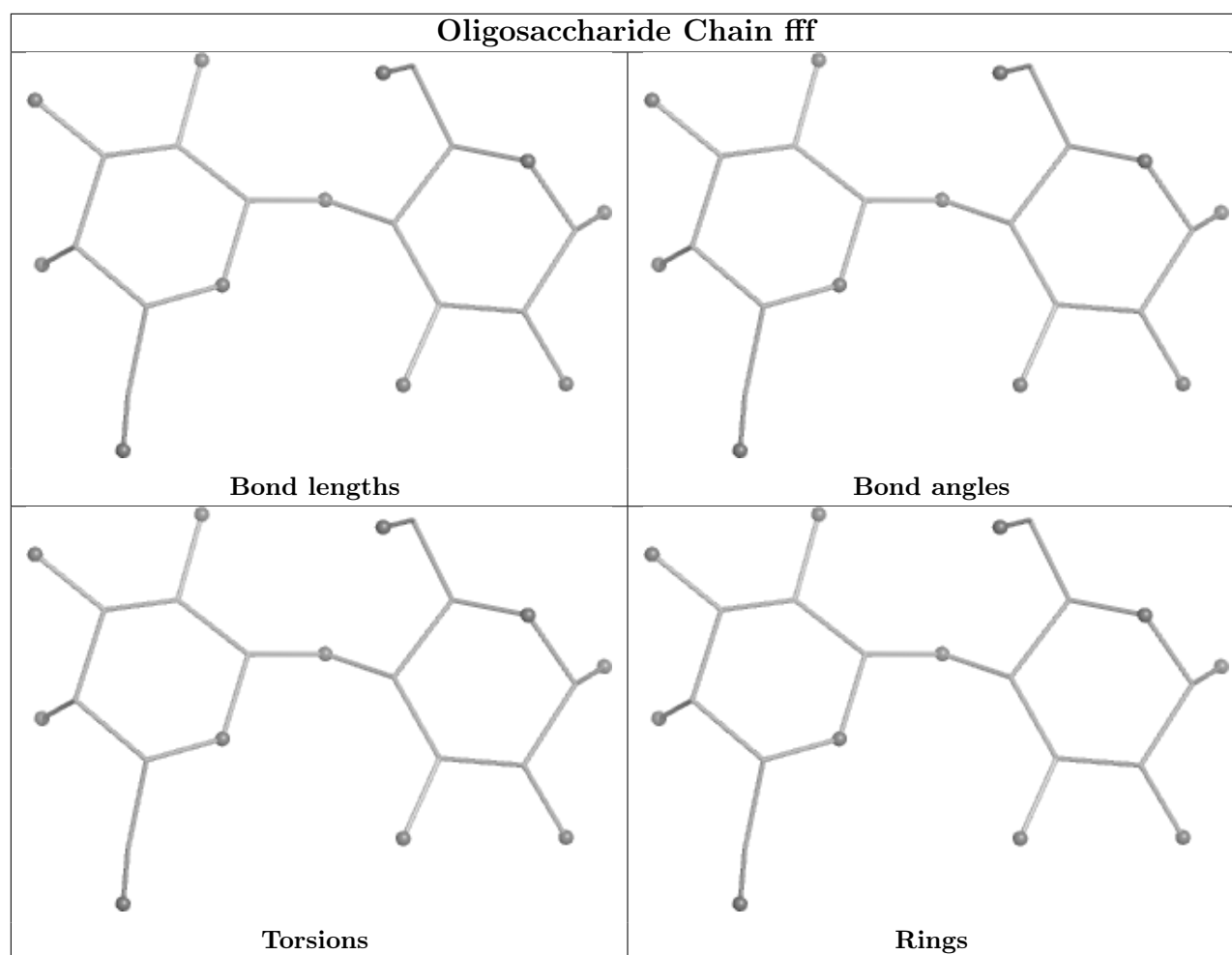












5.6 Ligand geometry [i](#)

Of 79 ligands modelled in this entry, 47 are monoatomic - leaving 32 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	PEG	GGG	201	-	6,6,6	0.38	0	5,5,5	0.26	0
4	EDO	AAA	201	-	3,3,3	0.21	0	2,2,2	0.40	0
7	SO4	BBB	206	-	4,4,4	0.25	0	6,6,6	0.06	0
7	SO4	GGG	205	-	4,4,4	0.35	0	6,6,6	0.10	0
7	SO4	CCC	206	-	4,4,4	0.22	0	6,6,6	0.07	0
13	1PE	LLL	202	-	15,15,15	0.35	0	14,14,14	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SO4	HHH	205	-	4,4,4	0.32	0	6,6,6	0.05	0
4	EDO	CCC	201	-	3,3,3	0.24	0	2,2,2	0.22	0
8	PEG	LLL	201	-	6,6,6	0.16	0	5,5,5	0.13	0
7	SO4	AAA	207	-	4,4,4	0.35	0	6,6,6	0.10	0
7	SO4	OOO	205	-	4,4,4	0.28	0	6,6,6	0.11	0
4	EDO	DDD	201	-	3,3,3	0.18	0	2,2,2	0.45	0
7	SO4	GGG	207	6	4,4,4	0.34	0	6,6,6	0.11	0
7	SO4	JJJ	204	-	4,4,4	0.35	0	6,6,6	0.17	0
9	BGC	BBB	202	5	12,12,12	1.10	0	17,17,17	1.72	3 (17%)
9	BGC	NNN	201	5	12,12,12	0.85	1 (8%)	17,17,17	1.97	5 (29%)
8	PEG	BBB	201	-	6,6,6	0.17	0	5,5,5	0.09	0
4	EDO	III	201	-	3,3,3	0.23	0	2,2,2	0.23	0
7	SO4	KKK	204	-	4,4,4	0.32	0	6,6,6	0.07	0
7	SO4	III	205	-	4,4,4	0.35	0	6,6,6	0.07	0
4	EDO	CCC	203	-	3,3,3	0.40	0	2,2,2	0.18	0
10	PGE	CCC	202	-	9,9,9	0.41	0	8,8,8	0.22	0
7	SO4	AAA	206	-	4,4,4	0.33	0	6,6,6	0.08	0
7	SO4	BBB	205	-	4,4,4	0.34	0	6,6,6	0.07	0
7	SO4	KKK	205	-	4,4,4	0.27	0	6,6,6	0.07	0
7	SO4	EEE	204	-	4,4,4	0.34	0	6,6,6	0.11	0
7	SO4	NNN	204	-	4,4,4	0.33	0	6,6,6	0.07	0
7	SO4	AAA	208	-	4,4,4	0.33	0	6,6,6	0.11	0
9	BGC	GGG	202	5	12,12,12	1.10	0	17,17,17	1.44	3 (17%)
7	SO4	EEE	203	-	4,4,4	0.37	0	6,6,6	0.07	0
7	SO4	LLL	205	-	4,4,4	0.34	0	6,6,6	0.05	0
7	SO4	GGG	206	-	4,4,4	0.23	0	6,6,6	0.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PEG	GGG	201	-	-	3/4/4/4	-
4	EDO	AAA	201	-	-	1/1/1/1	-
4	EDO	DDD	201	-	-	1/1/1/1	-
9	BGC	NNN	201	5	-	1/2/22/22	0/1/1/1
9	BGC	BBB	202	5	-	0/2/22/22	0/1/1/1
4	EDO	CCC	203	-	-	1/1/1/1	-
8	PEG	BBB	201	-	-	1/4/4/4	-
10	PGE	CCC	202	-	-	4/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BGC	GGG	202	5	-	0/2/22/22	0/1/1/1
13	1PE	LLL	202	-	-	8/13/13/13	-
4	EDO	CCC	201	-	-	1/1/1/1	-
4	EDO	III	201	-	-	0/1/1/1	-
8	PEG	LLL	201	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	NNN	201	BGC	O1-C1	2.06	1.46	1.39

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	NNN	201	BGC	O2-C2-C3	-4.12	100.83	110.35
9	NNN	201	BGC	O3-C3-C4	3.63	118.75	110.35
9	NNN	201	BGC	C4-C3-C2	-3.47	104.76	110.82
9	BBB	202	BGC	O2-C2-C1	3.44	117.14	109.16
9	GGG	202	BGC	O3-C3-C4	3.01	117.31	110.35

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

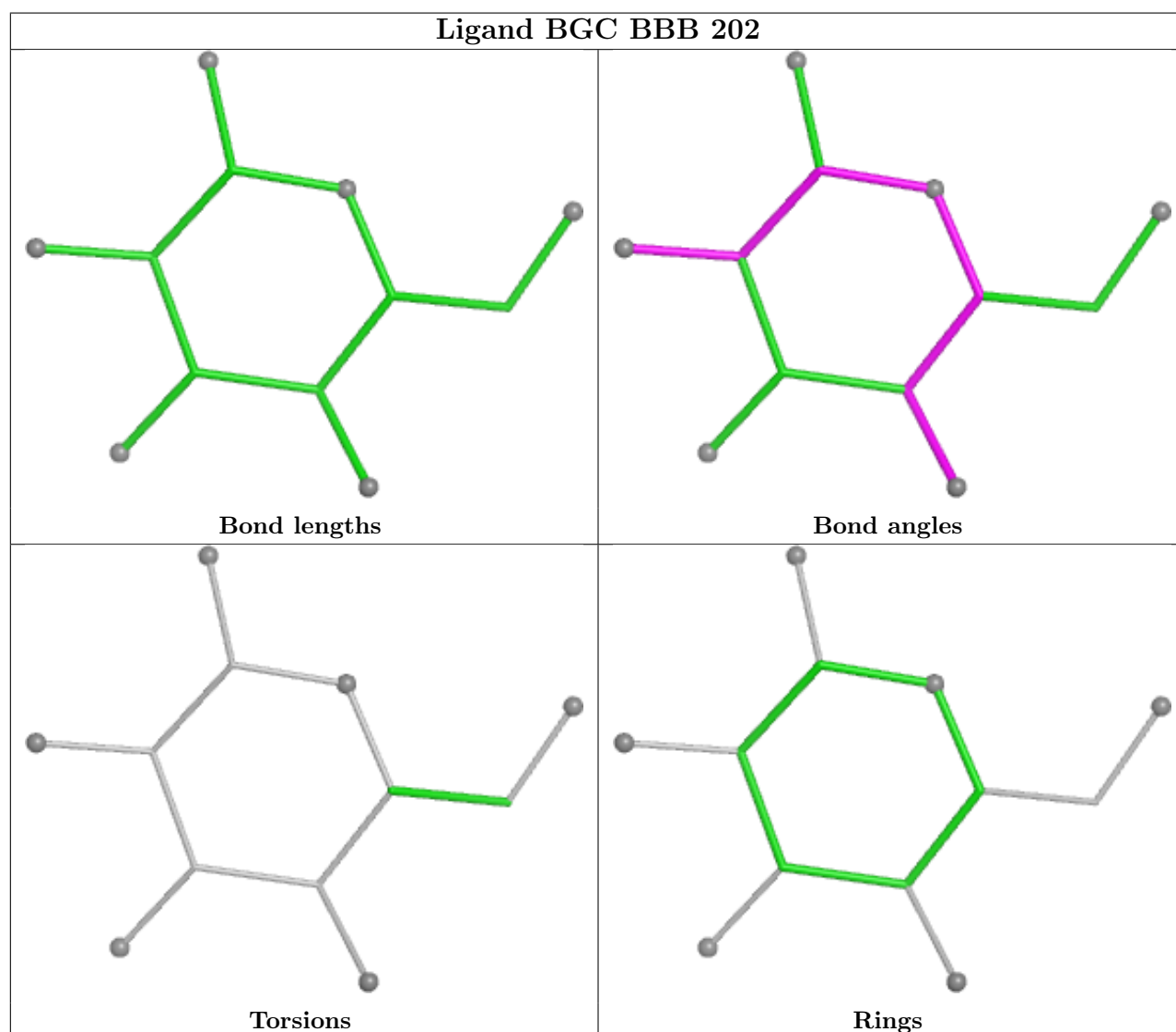
Mol	Chain	Res	Type	Atoms
8	GGG	201	PEG	C1-C2-O2-C3
13	LLL	202	1PE	OH2-C12-C22-OH3
8	GGG	201	PEG	O2-C3-C4-O4
8	LLL	201	PEG	O2-C3-C4-O4
4	CCC	203	EDO	O1-C1-C2-O2

There are no ring outliers.

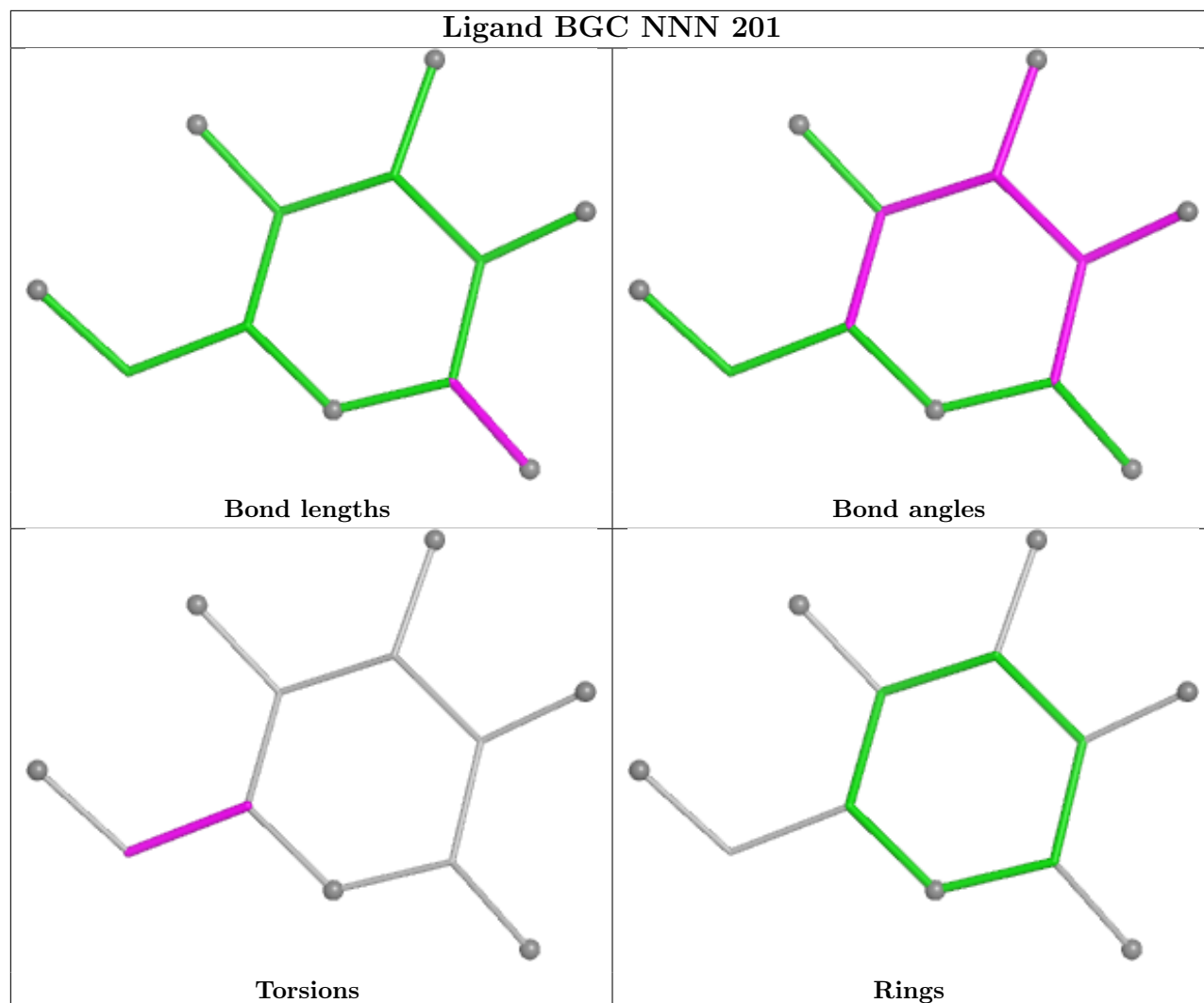
6 monomers are involved in 14 short contacts:

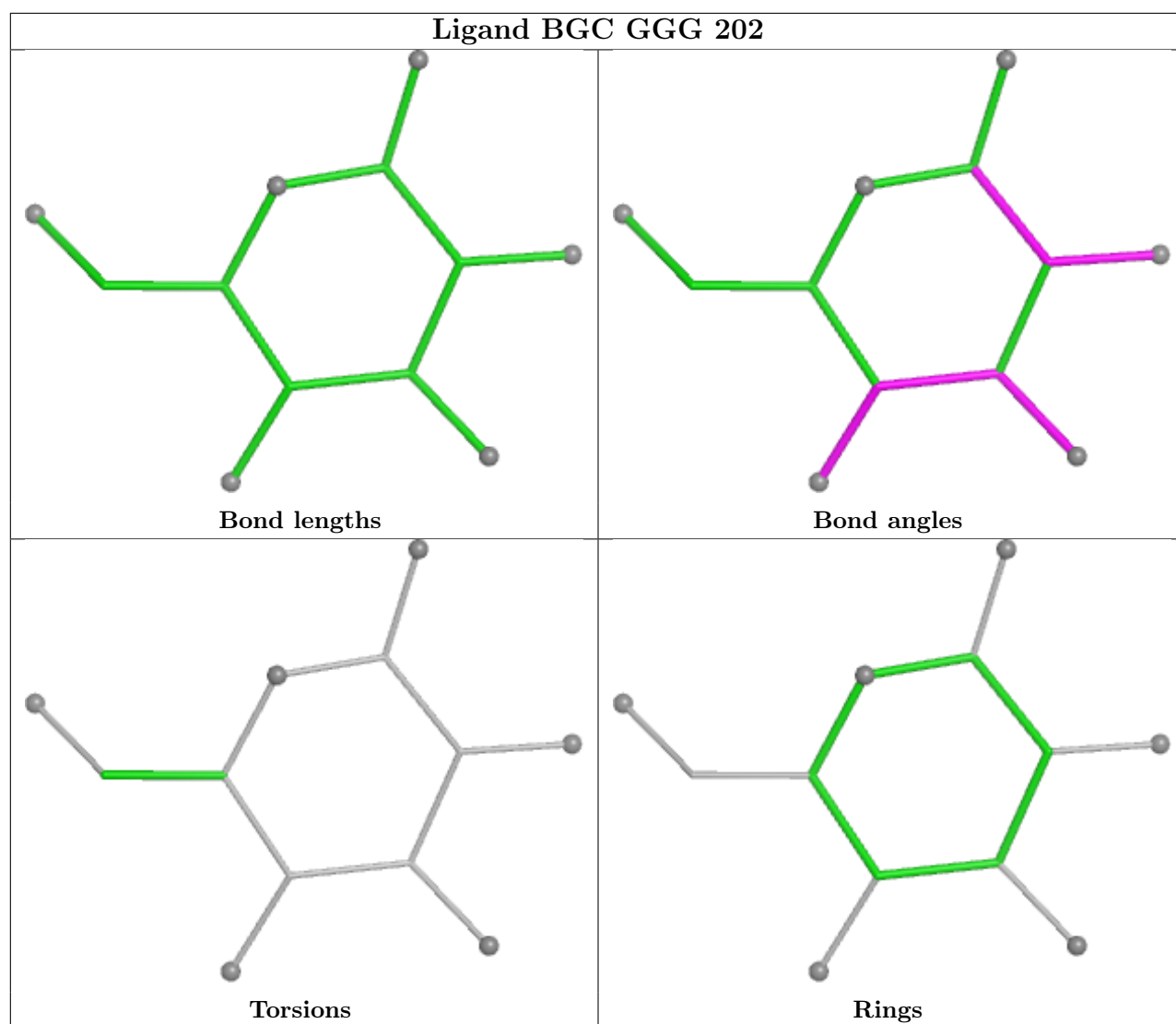
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	GGG	201	PEG	3	0
4	AAA	201	EDO	3	0
4	CCC	201	EDO	2	0
8	LLL	201	PEG	1	0
4	DDD	201	EDO	2	0
10	CCC	202	PGE	3	0

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



Ligand BGC NNN 201





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	125/125 (100%)	-0.02	1 (0%) 82 85	17, 26, 37, 44	2 (1%)
1	BBB	124/125 (99%)	-0.01	1 (0%) 82 85	20, 28, 39, 48	0
1	CCC	125/125 (100%)	-0.09	4 (3%) 50 54	19, 25, 40, 63	0
1	DDD	124/125 (99%)	0.01	3 (2%) 59 64	19, 27, 46, 57	0
1	EEE	124/125 (99%)	-0.14	2 (1%) 70 75	15, 25, 39, 57	1 (0%)
1	FFF	125/125 (100%)	-0.17	1 (0%) 82 85	11, 24, 35, 66	1 (0%)
1	GGG	124/125 (99%)	-0.04	2 (1%) 70 75	21, 28, 41, 54	0
1	HHH	123/125 (98%)	0.06	2 (1%) 70 75	22, 30, 40, 57	0
1	III	124/125 (99%)	0.01	4 (3%) 50 54	20, 26, 40, 56	0
1	JJJ	125/125 (100%)	0.19	2 (1%) 70 75	21, 29, 41, 47	0
1	KKK	125/125 (100%)	0.06	3 (2%) 59 64	19, 28, 40, 56	0
1	LLL	124/125 (99%)	0.15	3 (2%) 59 64	17, 28, 41, 61	1 (0%)
1	MMM	124/125 (99%)	0.27	2 (1%) 70 75	17, 34, 46, 51	1 (0%)
1	NNN	125/125 (100%)	0.56	6 (4%) 35 39	24, 34, 47, 60	0
1	OOO	125/125 (100%)	0.36	4 (3%) 50 54	16, 31, 47, 54	1 (0%)
1	PPP	124/125 (99%)	0.23	2 (1%) 70 75	15, 29, 42, 49	1 (0%)
All	All	1990/2000 (99%)	0.09	42 (2%) 63 68	11, 28, 43, 66	8 (0%)

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	PPP	124	ILE	5.2
1	EEE	124	ILE	4.6
1	LLL	124	ILE	4.3
1	AAA	1[A]	MET	4.2
1	DDD	124	ILE	4.1

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

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

6.3 Carbohydrates ⓘ

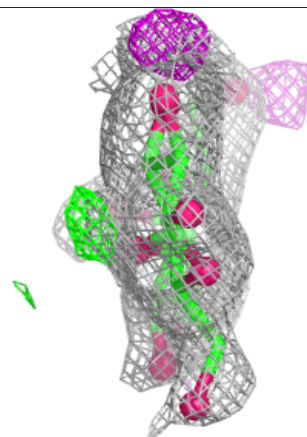
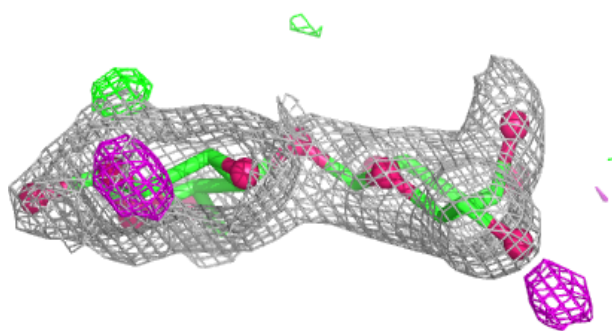
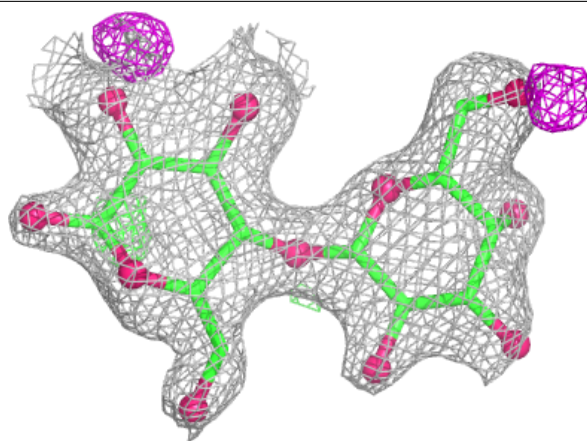
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BGC	WWW	1	12/12	-	-	33,44,54,56	0
2	GAL	WWW	2	11/12	-	-	42,53,63,64	0
2	BGC	XXX	1	12/12	-	-	30,40,49,55	0
2	GAL	XXX	2	11/12	-	-	50,52,60,66	0
2	BGC	YYY	1	12/12	-	-	30,49,55,58	0
2	GAL	YYY	2	11/12	-	-	49,54,62,64	0
2	BGC	ZZZ	1	12/12	-	-	27,36,47,55	0
2	GAL	ZZZ	2	11/12	-	-	48,50,57,57	0
2	BGC	aaa	1	12/12	-	-	32,46,54,59	0
2	GAL	aaa	2	11/12	-	-	54,63,71,74	0
2	BGC	ccc	1	12/12	-	-	29,40,48,48	0
2	GAL	ccc	2	11/12	-	-	47,53,57,64	0
2	BGC	ddd	1	12/12	-	-	39,49,59,67	0
2	GAL	ddd	2	11/12	-	-	50,52,56,60	0
2	BGC	eee	1	12/12	-	-	30,43,49,52	0
2	GAL	eee	2	11/12	-	-	52,54,60,66	0
2	BGC	ggg	1	12/12	-	-	36,50,57,58	0
2	GAL	ggg	2	11/12	-	-	60,64,73,74	0
3	GLC	bbb	1	12/12	-	-	33,52,69,73	0
3	GAL	bbb	2	11/12	-	-	61,68,73,74	0
3	GLC	fff	1	12/12	-	-	39,48,56,57	0
3	GAL	fff	2	11/12	-	-	59,63,70,71	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.

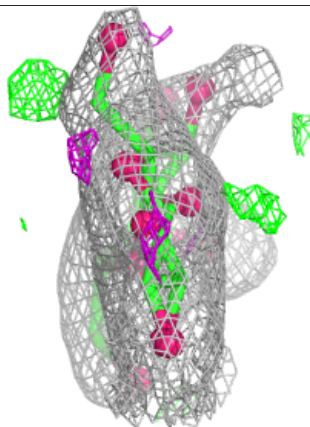
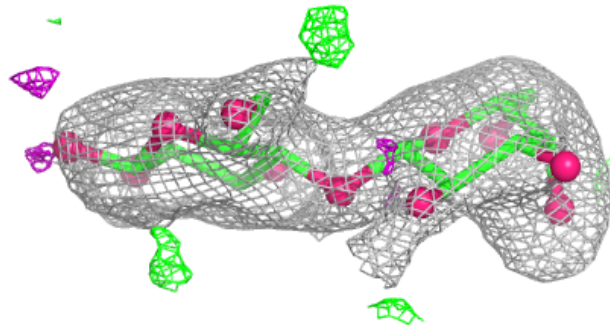
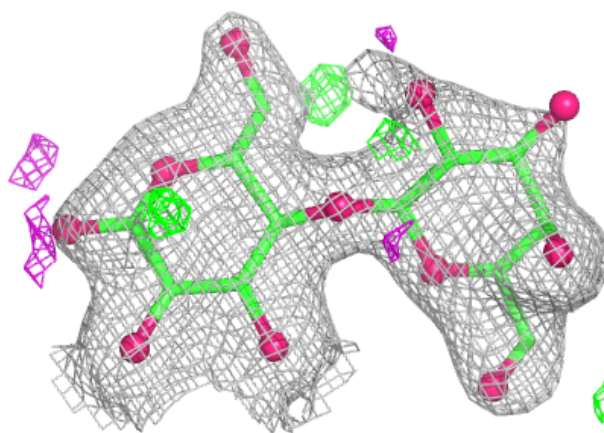
Electron density around Chain WWW:

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



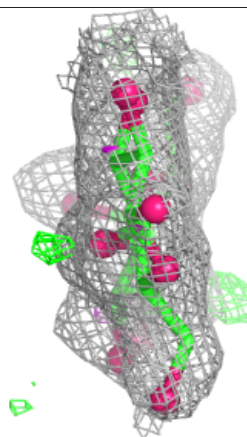
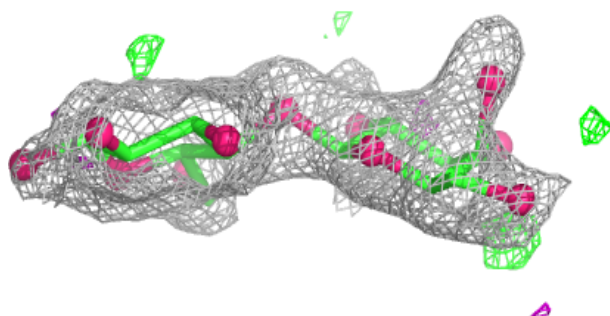
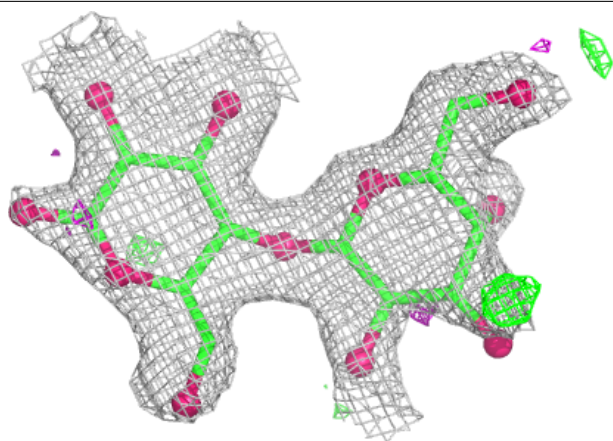
Electron density around Chain XXX:

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

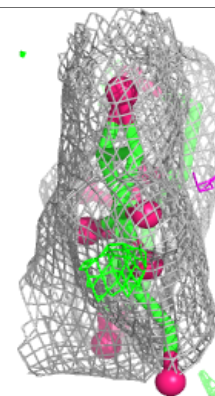
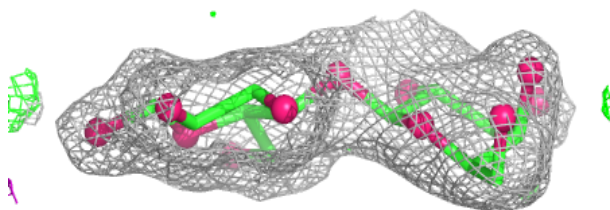
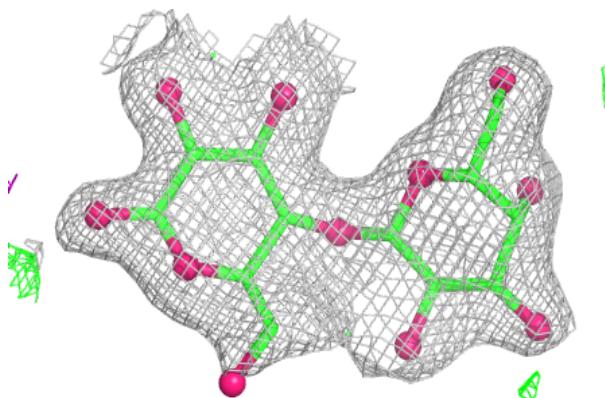


Electron density around Chain YYY:

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

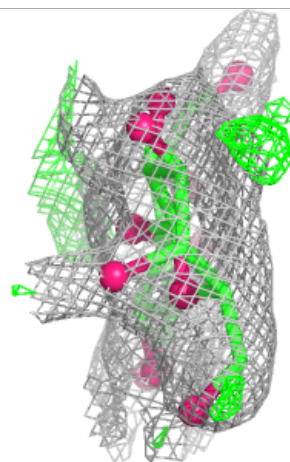
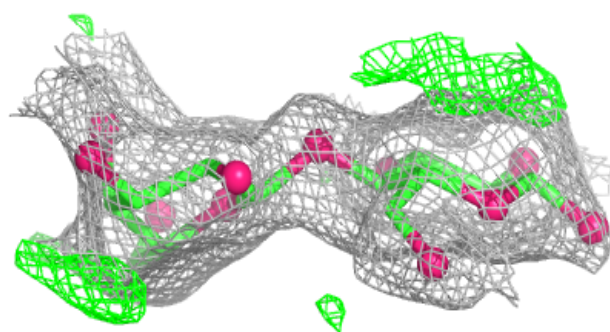
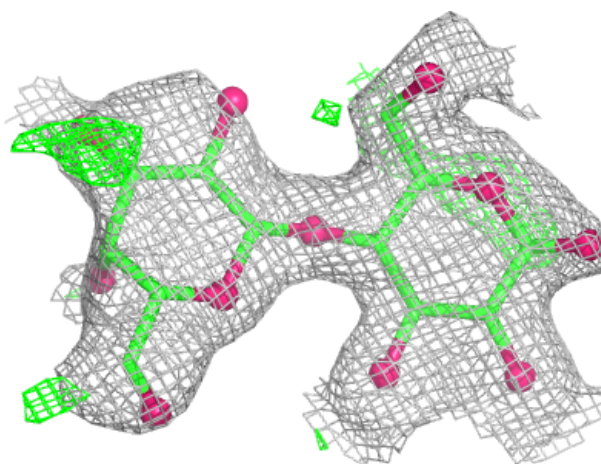
**Electron density around Chain ZZZ:**

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



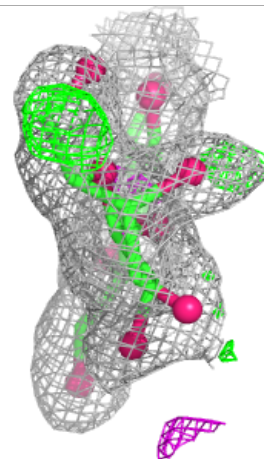
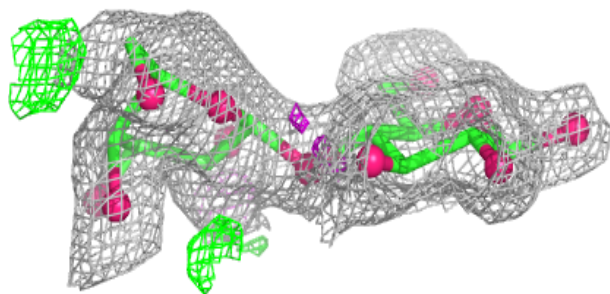
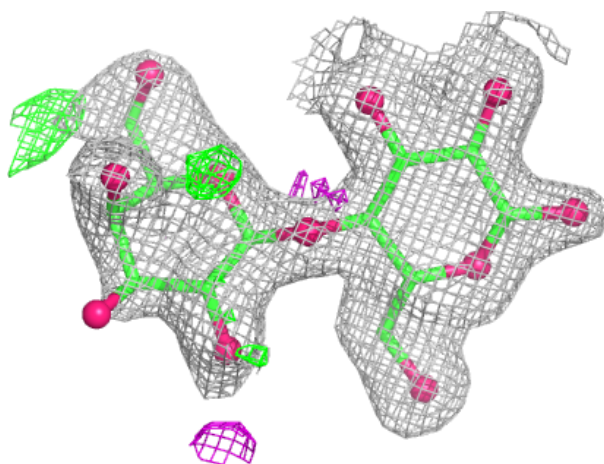
Electron density around Chain aaa:

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



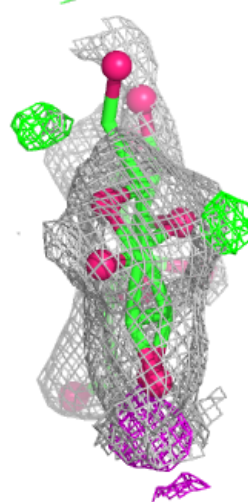
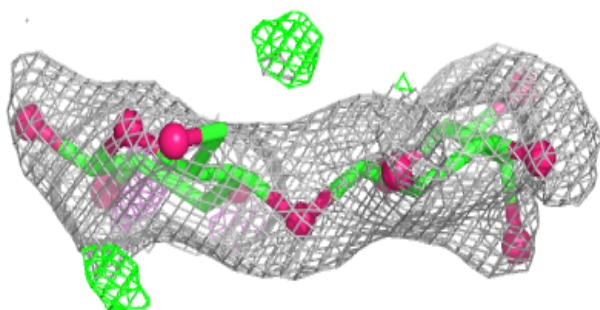
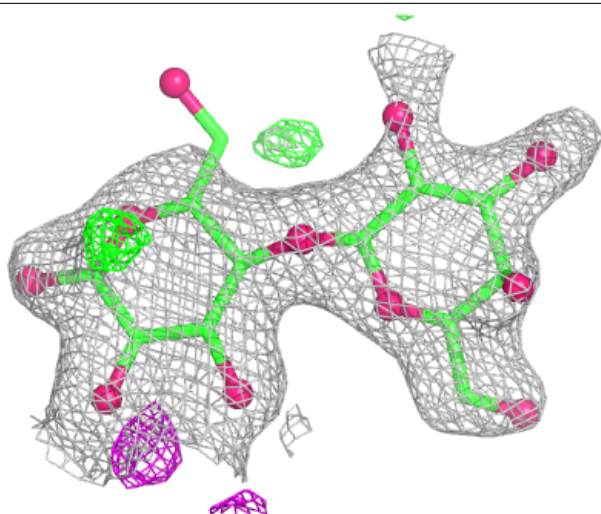
Electron density around Chain ccc:

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



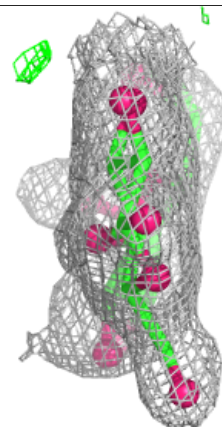
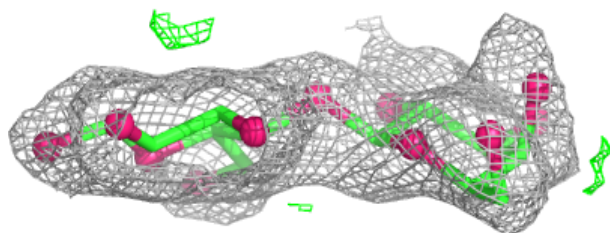
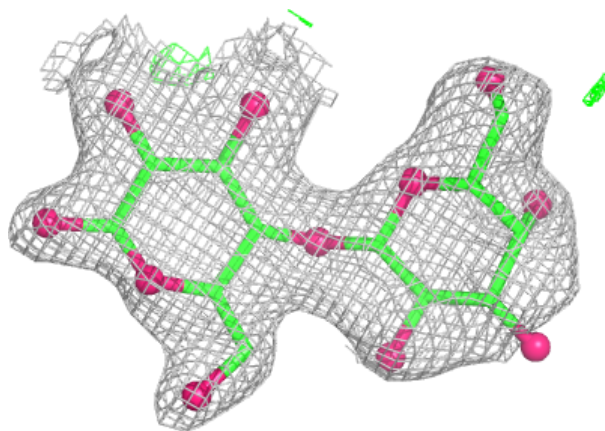
Electron density around Chain ddd:

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

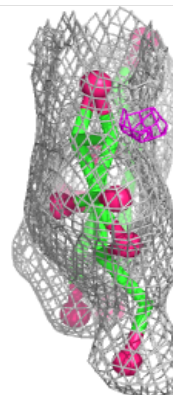
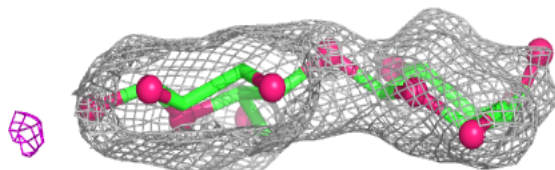
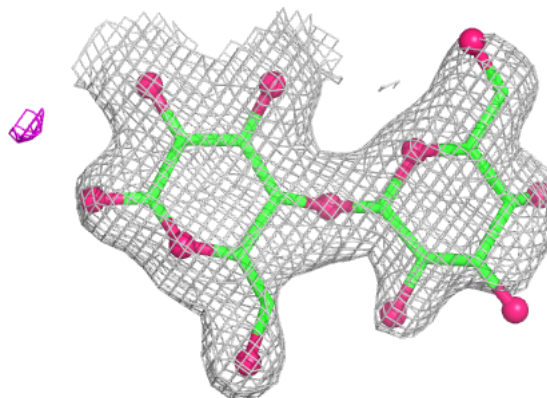


Electron density around Chain eee:

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

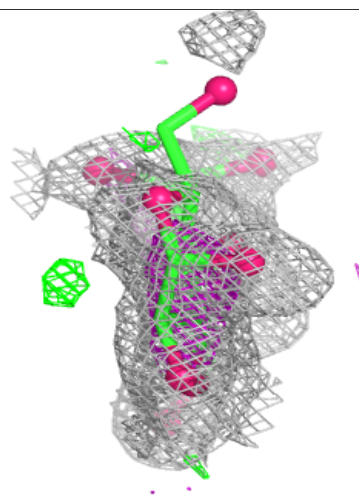
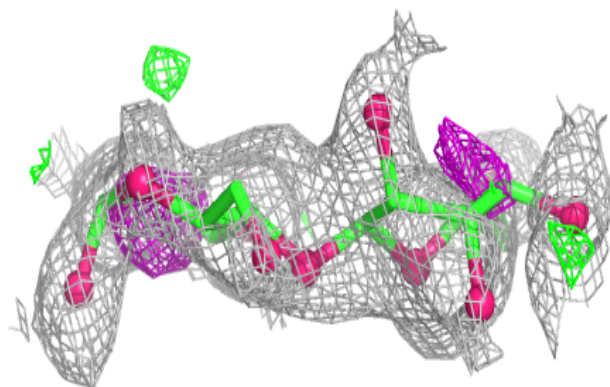
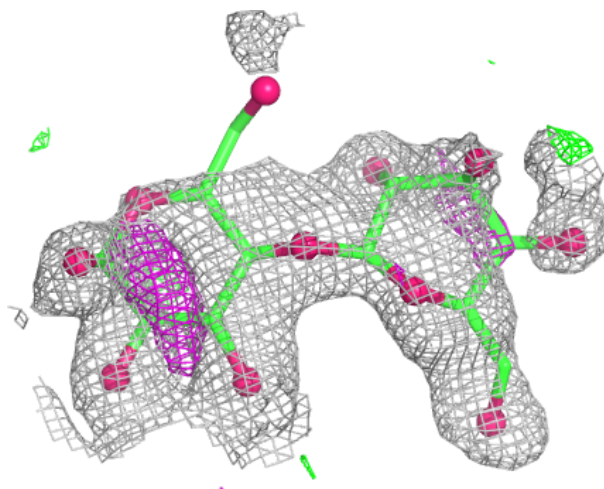
**Electron density around Chain ggg:**

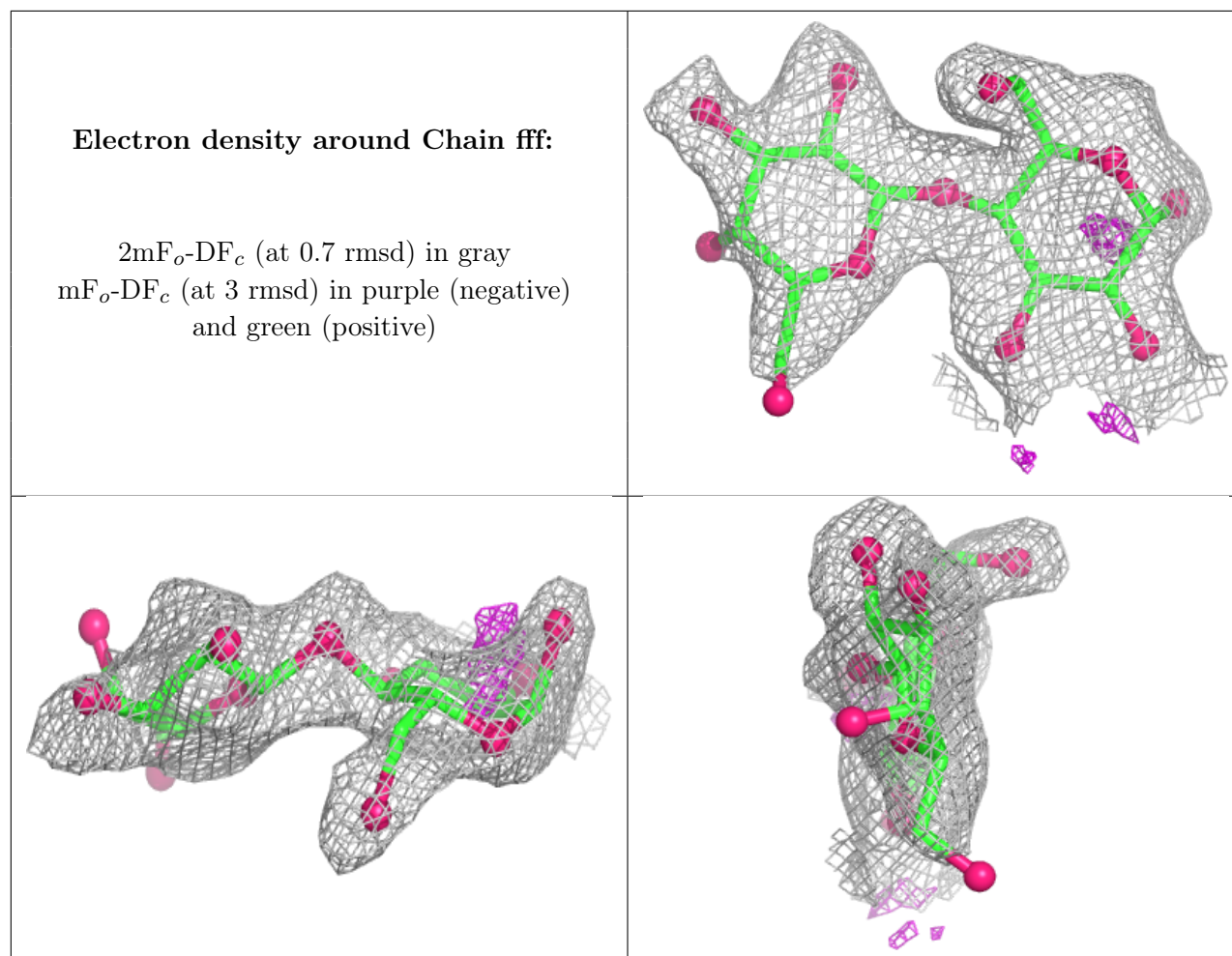
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain bbb:

$2mF_o-DF_c$ (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(\AA^2)	Q<0.9
7	SO4	GGG	207	5/5	0.30	0.18	98,120,124,124	0
7	SO4	JJJ	204	5/5	0.66	0.13	77,77,84,88	0
7	SO4	AAA	208	5/5	0.67	0.14	83,87,90,97	0
7	SO4	HHH	205	5/5	0.68	0.13	85,86,90,96	0
7	SO4	GGG	205	5/5	0.69	0.15	85,91,103,108	0
7	SO4	KKK	204	5/5	0.69	0.13	85,87,88,96	0
10	PGE	CCC	202	10/10	0.69	0.18	34,43,52,56	0
7	SO4	BBB	206	5/5	0.70	0.14	65,68,74,84	0
7	SO4	GGG	206	5/5	0.71	0.14	63,70,72,76	0
8	PEG	GGG	201	7/7	0.71	0.19	46,57,61,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	SO4	BBB	205	5/5	0.71	0.14	97,101,106,110	0
7	SO4	LLL	205	5/5	0.72	0.14	96,98,102,105	0
7	SO4	KKK	205	5/5	0.73	0.12	67,70,71,79	0
7	SO4	CCC	206	5/5	0.73	0.12	59,64,77,84	0
13	1PE	LLL	202	16/16	0.73	0.19	47,61,66,67	0
8	PEG	BBB	201	7/7	0.76	0.20	45,57,68,68	0
9	BGC	GGG	202	12/12	0.76	0.16	32,54,63,67	0
9	BGC	BBB	202	12/12	0.77	0.16	33,56,66,72	0
8	PEG	LLL	201	7/7	0.77	0.16	49,52,57,59	0
7	SO4	AAA	206	5/5	0.79	0.09	63,77,80,82	0
7	SO4	OOO	205	5/5	0.80	0.11	65,65,71,73	0
7	SO4	EEE	204	5/5	0.81	0.10	63,68,75,77	0
7	SO4	EEE	203	5/5	0.83	0.10	67,79,89,90	0
4	EDO	CCC	203	4/4	0.83	0.15	39,43,48,50	0
4	EDO	AAA	201	4/4	0.83	0.14	40,42,43,47	0
7	SO4	III	205	5/5	0.83	0.09	59,69,78,78	0
9	BGC	NNN	201	12/12	0.84	0.12	42,49,64,66	0
7	SO4	NNN	204	5/5	0.85	0.09	60,70,78,79	0
7	SO4	AAA	207	5/5	0.86	0.10	75,76,80,83	0
11	CL	GGG	208	1/1	0.86	0.14	53,53,53,53	0
4	EDO	III	201	4/4	0.86	0.14	41,48,50,54	0
5	CA	HHH	203	1/1	0.88	0.27	62,62,62,62	0
6	MG	FFF	204	1/1	0.88	0.09	55,55,55,55	0
4	EDO	CCC	201	4/4	0.88	0.13	39,44,46,50	0
6	MG	GGG	204	1/1	0.90	0.10	50,50,50,50	0
12	NA	GGG	209	1/1	0.90	0.26	53,53,53,53	0
6	MG	NNN	203	1/1	0.90	0.08	46,46,46,46	0
5	CA	OOO	203	1/1	0.91	0.09	61,61,61,61	0
4	EDO	DDD	201	4/4	0.92	0.10	44,45,46,49	0
5	CA	OOO	202	1/1	0.93	0.33	71,71,71,71	0
6	MG	PPP	202	1/1	0.94	0.08	52,52,52,52	0
6	MG	CCC	205	1/1	0.94	0.07	50,50,50,50	0
6	MG	HHH	204	1/1	0.94	0.17	39,39,39,39	0
5	CA	JJJ	202	1/1	0.94	0.09	65,65,65,65	0
6	MG	OOO	204	1/1	0.94	0.07	45,45,45,45	0
5	CA	III	203	1/1	0.95	0.13	62,62,62,62	0
5	CA	OOO	201	1/1	0.96	0.08	36,36,36,36	0
6	MG	FFF	205	1/1	0.96	0.10	42,42,42,42	0
5	CA	NNN	202	1/1	0.96	0.08	36,36,36,36	0
5	CA	HHH	202	1/1	0.97	0.26	55,55,55,55	0
5	CA	AAA	203	1/1	0.97	0.26	55,55,55,55	0
6	MG	KKK	203	1/1	0.97	0.09	44,44,44,44	0

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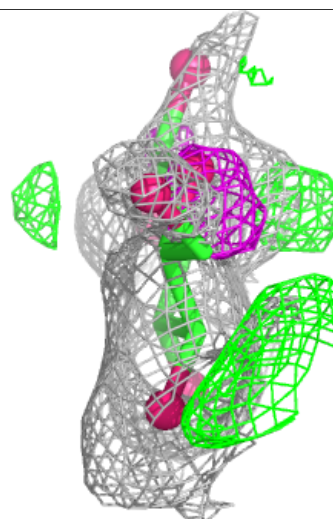
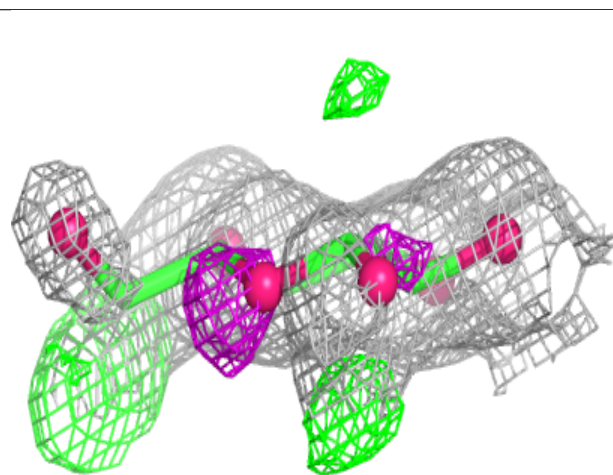
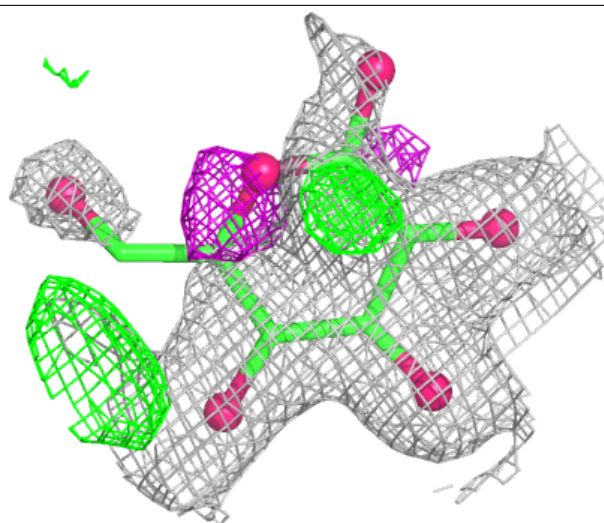
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	CL	OOO	206	1/1	0.97	0.13	52,52,52,52	0
5	CA	FFF	202	1/1	0.97	0.33	47,47,47,47	0
5	CA	JJJ	201	1/1	0.97	0.08	34,34,34,34	0
6	MG	BBB	204	1/1	0.98	0.08	40,40,40,40	0
5	CA	MMM	201	1/1	0.98	0.06	37,37,37,37	0
5	CA	AAA	202	1/1	0.98	0.06	30,30,30,30	0
5	CA	AAA	204	1/1	0.98	0.23	51,51,51,51	0
5	CA	KKK	202	1/1	0.98	0.27	46,46,46,46	0
5	CA	LLL	203	1/1	0.98	0.05	30,30,30,30	0
6	MG	III	204	1/1	0.98	0.09	36,36,36,36	0
6	MG	JJJ	203	1/1	0.98	0.05	42,42,42,42	0
6	MG	AAA	205	1/1	0.98	0.04	45,45,45,45	0
6	MG	LLL	204	1/1	0.98	0.10	44,44,44,44	0
6	MG	MMM	202	1/1	0.98	0.05	44,44,44,44	0
5	CA	BBB	203	1/1	0.99	0.04	25,25,25,25	0
5	CA	GGG	203	1/1	0.99	0.04	26,26,26,26	0
5	CA	HHH	201	1/1	0.99	0.04	28,28,28,28	0
6	MG	DDD	203	1/1	0.99	0.03	29,29,29,29	0
6	MG	EEE	202	1/1	0.99	0.06	29,29,29,29	0
6	MG	FFF	203	1/1	0.99	0.04	31,31,31,31	0
5	CA	CCC	204	1/1	0.99	0.02	27,27,27,27	0
5	CA	DDD	202	1/1	0.99	0.04	29,29,29,29	0
5	CA	III	202	1/1	0.99	0.03	26,26,26,26	0
5	CA	EEE	201	1/1	0.99	0.03	28,28,28,28	0
5	CA	FFF	201	1/1	0.99	0.03	27,27,27,27	0
5	CA	PPP	201	1/1	0.99	0.05	34,34,34,34	0
5	CA	KKK	201	1/1	1.00	0.04	27,27,27,27	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.

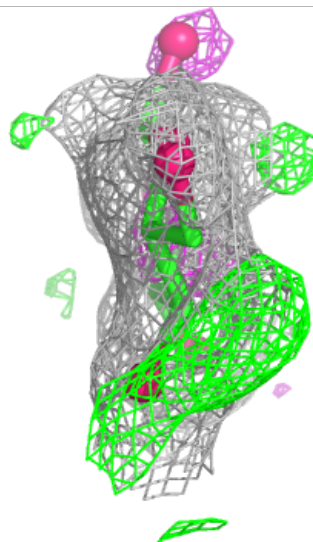
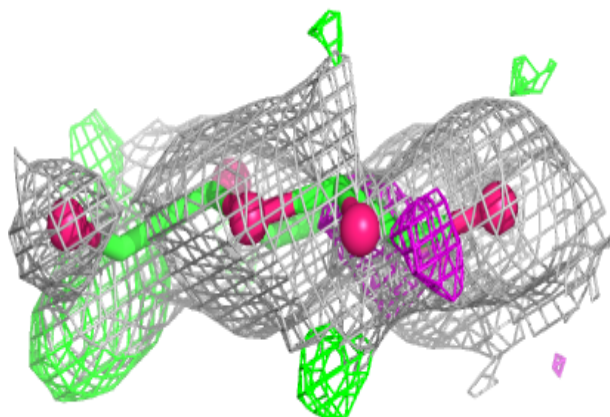
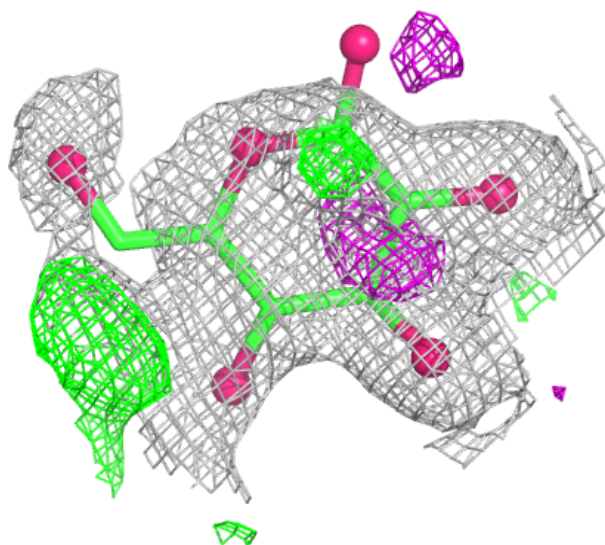
Electron density around BGC GGG 202:

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



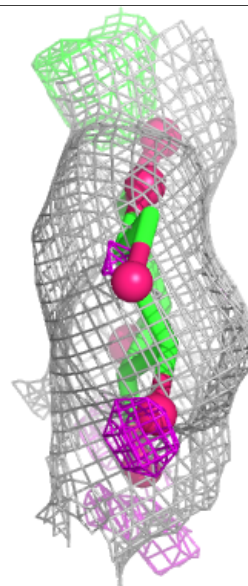
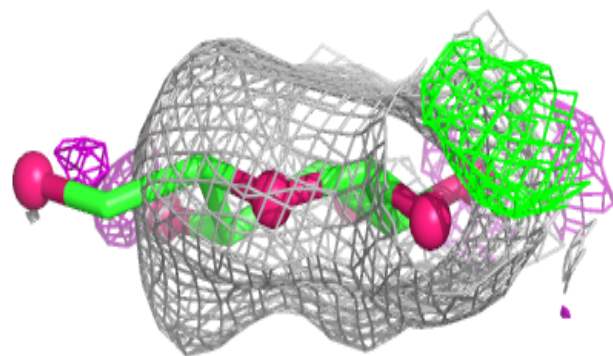
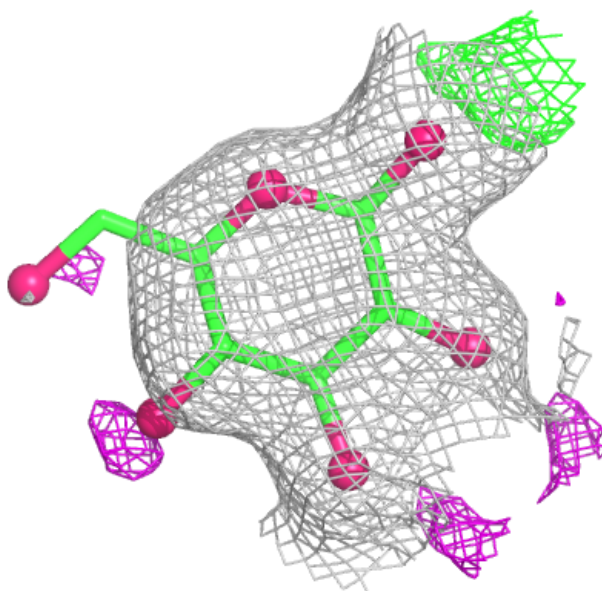
Electron density around BGC BBB 202:

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



Electron density around BGC NNN 201:

$2mF_o-DF_c$ (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.