



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 19, 2024 – 07:03 AM EDT

PDB ID : 4G8A
Title : Crystal structure of human TLR4 polymorphic variant D299G and T399I in complex with MD-2 and LPS
Authors : Ohto, U.; Shimizu, T.
Deposited on : 2012-07-23
Resolution : 2.40 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

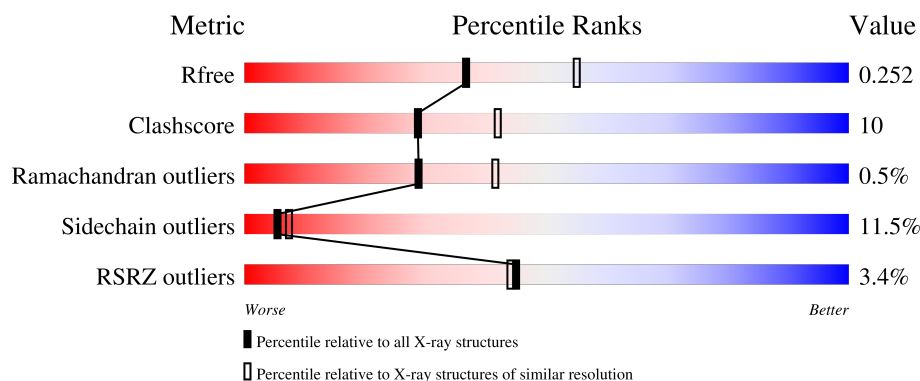
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




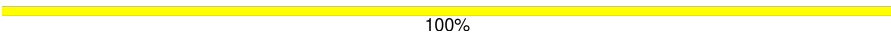

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	635	 4% 69% 21% 5% 5%
1	B	635	 2% 68% 23% 5% 5%
2	C	144	 6% 68% 27% 5% 5%
2	D	144	 3% 63% 30% 5% 5%
3	E	2	 50% 50%

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Mol	Chain	Length	Quality of chain
3	F	2	 50%50%
3	G	2	 100%
3	H	2	 50%50%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12381 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 Toll-like receptor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	0	0
			4800	3075	790	908	27			
1	B	605	Total	C	N	O	S	0	0	0
			4836	3099	795	915	27			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ARG	-	expression tag	UNP O00206
A	4	SER	-	expression tag	UNP O00206
A	5	PRO	-	expression tag	UNP O00206
A	6	TRP	-	expression tag	UNP O00206
A	7	ASP	-	expression tag	UNP O00206
A	8	TYR	-	expression tag	UNP O00206
A	9	LYS	-	expression tag	UNP O00206
A	10	ASP	-	expression tag	UNP O00206
A	11	ASP	-	expression tag	UNP O00206
A	12	ASP	-	expression tag	UNP O00206
A	13	ASP	-	expression tag	UNP O00206
A	14	LYS	-	expression tag	UNP O00206
A	15	LEU	-	expression tag	UNP O00206
A	16	ALA	-	expression tag	UNP O00206
A	17	ALA	-	expression tag	UNP O00206
A	18	ALA	-	expression tag	UNP O00206
A	19	ASN	-	expression tag	UNP O00206
A	20	SER	-	expression tag	UNP O00206
A	21	SER	-	expression tag	UNP O00206
A	22	ILE	-	expression tag	UNP O00206
A	299	GLY	ASP	engineered mutation	UNP O00206
A	399	ILE	THR	engineered mutation	UNP O00206
A	630	THR	-	expression tag	UNP O00206
A	631	GLY	-	expression tag	UNP O00206
A	632	HIS	-	expression tag	UNP O00206

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Chain	Residue	Modelled	Actual	Comment	Reference
A	633	HIS	-	expression tag	UNP O00206
A	634	HIS	-	expression tag	UNP O00206
A	635	HIS	-	expression tag	UNP O00206
A	636	HIS	-	expression tag	UNP O00206
A	637	HIS	-	expression tag	UNP O00206
B	3	ARG	-	expression tag	UNP O00206
B	4	SER	-	expression tag	UNP O00206
B	5	PRO	-	expression tag	UNP O00206
B	6	TRP	-	expression tag	UNP O00206
B	7	ASP	-	expression tag	UNP O00206
B	8	TYR	-	expression tag	UNP O00206
B	9	LYS	-	expression tag	UNP O00206
B	10	ASP	-	expression tag	UNP O00206
B	11	ASP	-	expression tag	UNP O00206
B	12	ASP	-	expression tag	UNP O00206
B	13	ASP	-	expression tag	UNP O00206
B	14	LYS	-	expression tag	UNP O00206
B	15	LEU	-	expression tag	UNP O00206
B	16	ALA	-	expression tag	UNP O00206
B	17	ALA	-	expression tag	UNP O00206
B	18	ALA	-	expression tag	UNP O00206
B	19	ASN	-	expression tag	UNP O00206
B	20	SER	-	expression tag	UNP O00206
B	21	SER	-	expression tag	UNP O00206
B	22	ILE	-	expression tag	UNP O00206
B	299	GLY	ASP	engineered mutation	UNP O00206
B	399	ILE	THR	engineered mutation	UNP O00206
B	630	THR	-	expression tag	UNP O00206
B	631	GLY	-	expression tag	UNP O00206
B	632	HIS	-	expression tag	UNP O00206
B	633	HIS	-	expression tag	UNP O00206
B	634	HIS	-	expression tag	UNP O00206
B	635	HIS	-	expression tag	UNP O00206
B	636	HIS	-	expression tag	UNP O00206
B	637	HIS	-	expression tag	UNP O00206

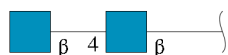
- Molecule 2 is a protein called Lymphocyte antigen 96.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	140	Total	C	N	O	S	0	0	0
			1133	730	186	207	10			
2	D	140	Total	C	N	O	S	0	0	0
			1133	730	186	207	10			

There are 2 discrepancies between the modelled and reference sequences:

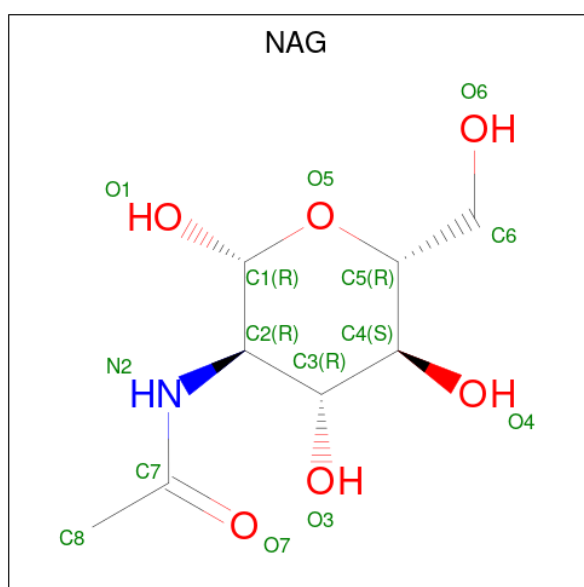
Chain	Residue	Modelled	Actual	Comment	Reference
C	56	GLY	ARG	engineered mutation	UNP Q9Y6Y9
D	56	GLY	ARG	engineered mutation	UNP Q9Y6Y9

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



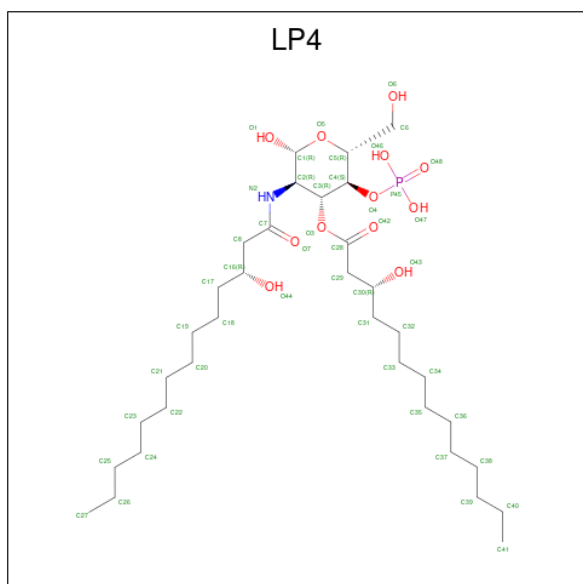
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



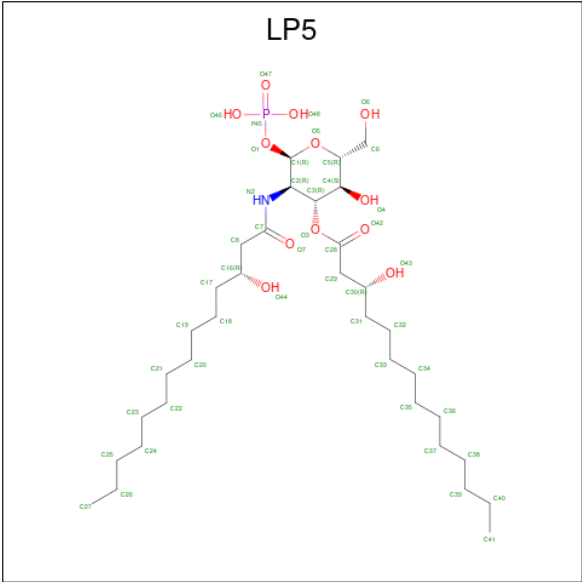
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	B	1	Total 14	C 8	N 1	O 5	0	0
4	C	1	Total 14	C 8	N 1	O 5	0	0
4	D	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 5 is 2-deoxy-3-O-[(3R)-3-hydroxytetradecanoyl]-2-[(3R)-3-hydroxytetradecanoylamino]-4-O-phosphono-beta-D-glucopyranose (three-letter code: LP4) (formula: C₃₄H₆₆NO₁₂P).



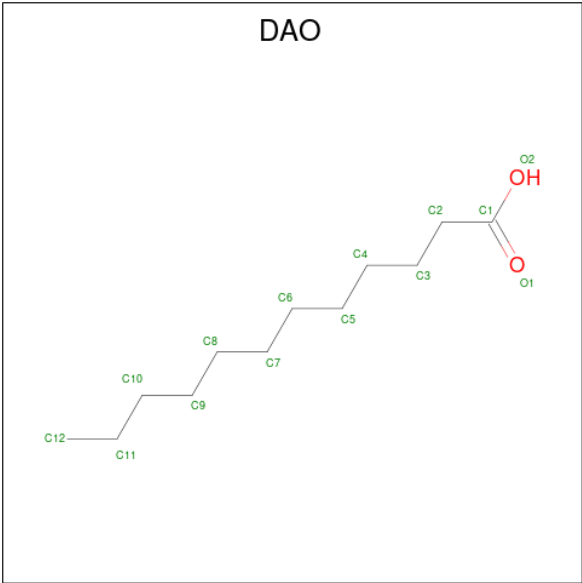
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total 45	C 32	N 1	O 11	P 1	0	0
5	D	1	Total 45	C 32	N 1	O 11	P 1	0	0

- Molecule 6 is (R)-((2R,3S,4R,5R,6R)-3-HYDROXY-2-(HYDROXYMETHYL)-5-((R)-3-HYDROXYTETRADECANAMIDO)-6-(PHOSPHONOOXY)TETRAHYDRO-2H-PYRAN-4-YL) 3-HYDROXYTETRADECANOATE (three-letter code: LP5) (formula: C₃₄H₆₆NO₁₂P).



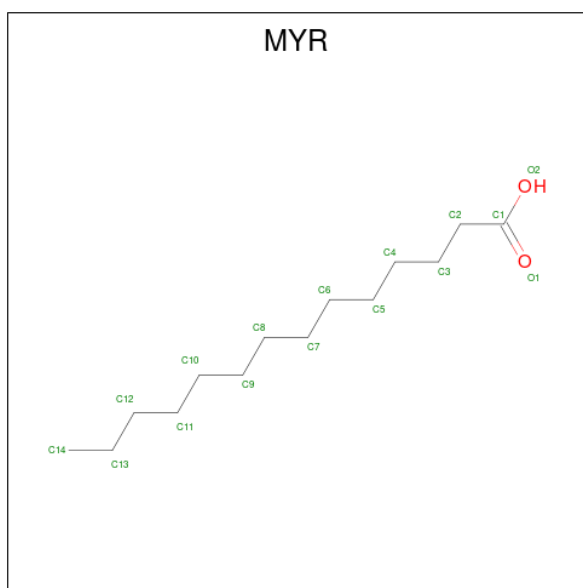
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total 48	C 34	N 1	O 12	P 1	0	0
6	D	1	Total 48	C 34	N 1	O 12	P 1	0	0

- Molecule 7 is LAURIC ACID (three-letter code: DAO) (formula: C₁₂H₂₄O₂).



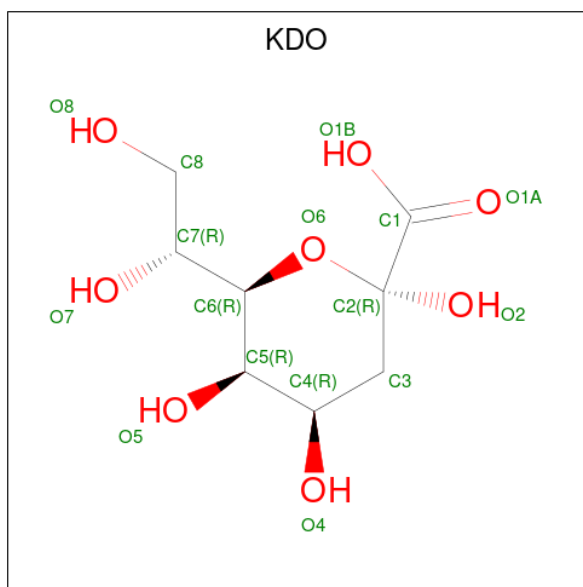
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			13	12	1		
7	D	1	Total	C	O	0	0
			13	12	1		

- Molecule 8 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			15	14	1		
8	D	1	Total	C	O	0	0
			15	14	1		

- Molecule 9 is 3-deoxy- α -D-manno-oct-2-ulopyranosonic acid (three-letter code: KDO) (formula: $C_8H_{14}O_8$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			15	8	7		
9	D	1	Total	C	O	0	0
			15	8	7		

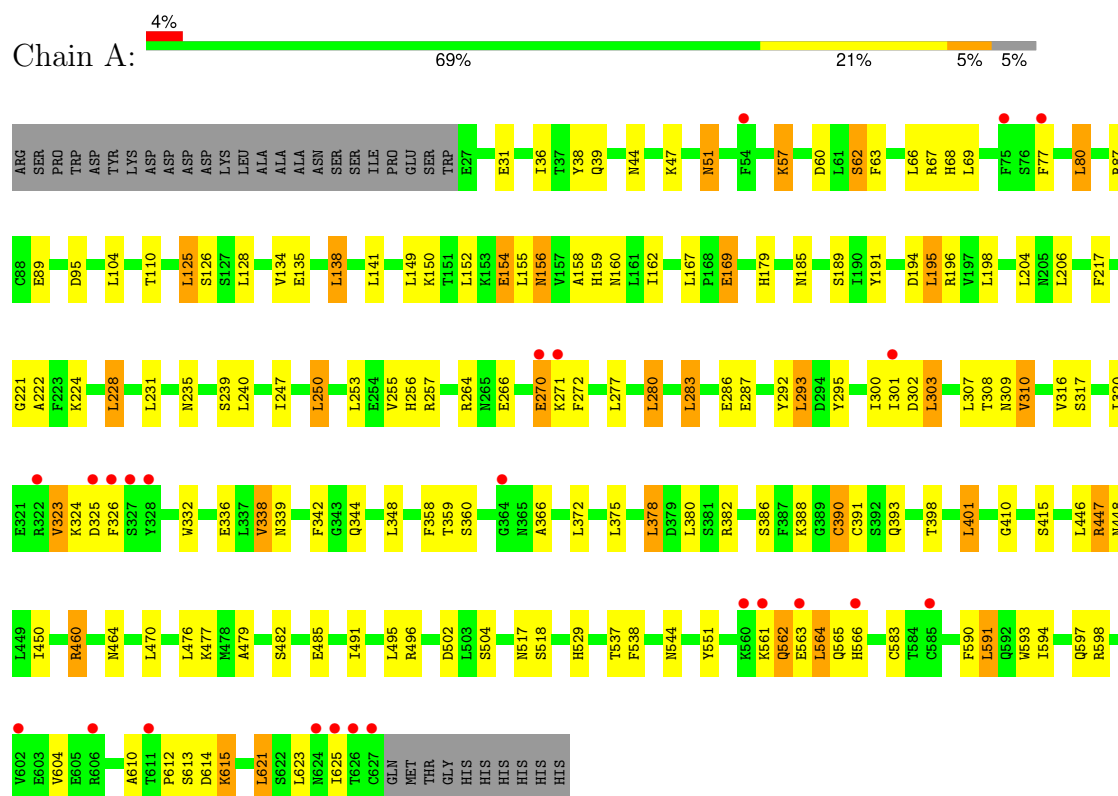
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	15	Total	O	0	0
			15	15		
10	B	21	Total	O	0	0
			21	21		
10	D	3	Total	O	0	0
			3	3		

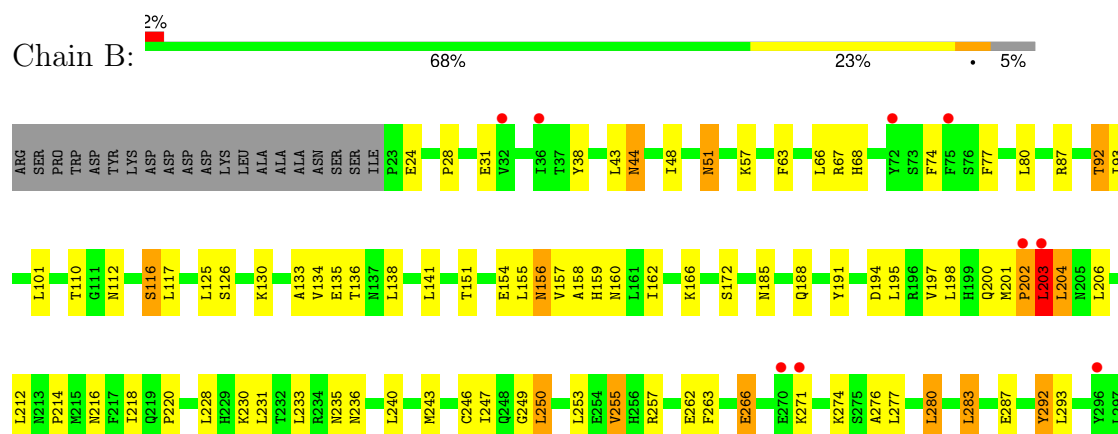
3 Residue-property plots [i](#)

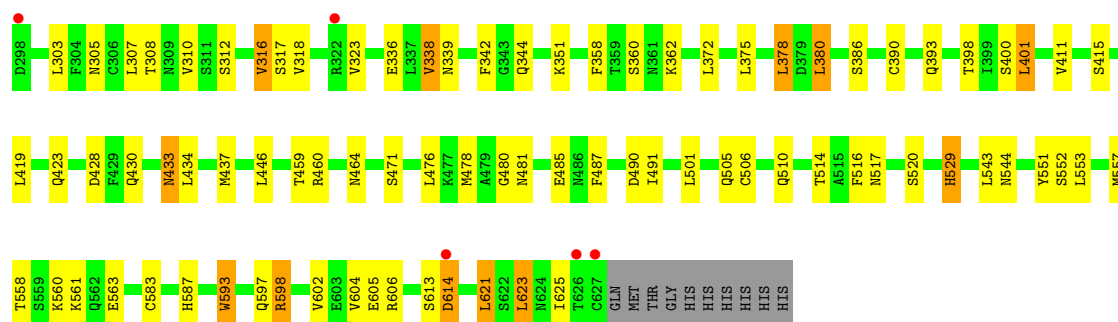
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Toll-like receptor 4

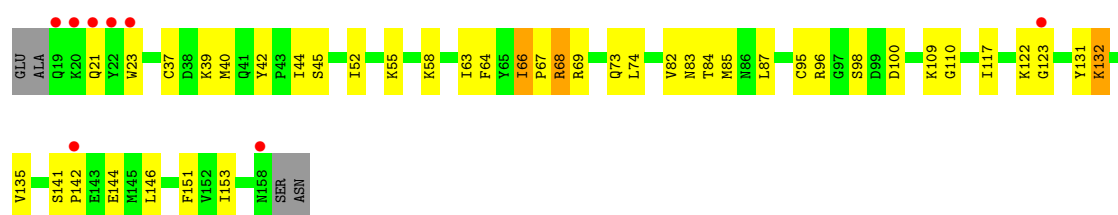


• Molecule 1: Toll-like receptor 4

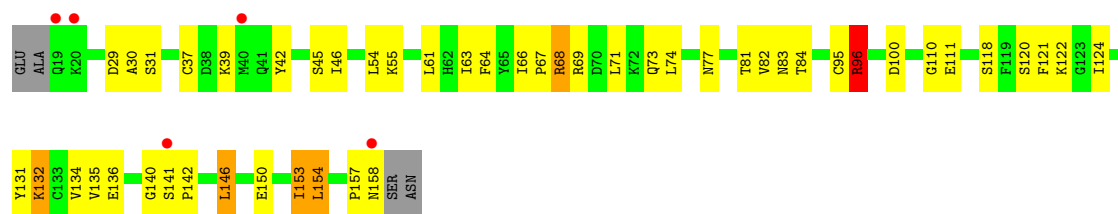




• Molecule 2: Lymphocyte antigen 96



• Molecule 2: Lymphocyte antigen 96




• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

MAG1
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  50%  50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.04Å 124.68Å 109.14Å 90.00° 115.72° 90.00°	Depositor
Resolution (Å)	39.18 – 2.40 39.18 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.18-2.40) 99.6 (39.18-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.199 , 0.249 0.201 , 0.252	Depositor DCC
R_{free} test set	3753 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12381	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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: LP5, MYR, NAG, KDO, DAO, LP4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	1/4900 (0.0%)	0.68	1/6634 (0.0%)
1	B	0.51	1/4939 (0.0%)	0.68	2/6688 (0.0%)
2	C	0.53	1/1159 (0.1%)	0.75	0/1562
2	D	0.52	0/1159	0.75	1/1562 (0.1%)
All	All	0.51	3/12157 (0.0%)	0.69	4/16446 (0.0%)

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	A	0	1
2	C	0	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	593	TRP	CD2-CE2	5.31	1.47	1.41
2	C	23	TRP	CD2-CE2	5.25	1.47	1.41
1	A	332	TRP	CD2-CE2	5.18	1.47	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	LEU	CA-CB-CG	5.87	128.81	115.30
1	A	283	LEU	CA-CB-CG	5.25	127.38	115.30
2	D	96	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	B	283	LEU	CA-CB-CG	5.17	127.20	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	610	ALA	Peptide
2	C	122	LYS	Peptide
2	C	141	SER	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	4800	0	4750	92	0
1	B	4836	0	4779	97	0
2	C	1133	0	1129	23	0
2	D	1133	0	1129	29	0
3	E	28	0	25	1	0
3	F	28	0	25	1	0
3	G	28	0	25	0	0
3	H	28	0	25	2	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
5	C	45	0	52	5	0
5	D	45	0	52	3	0
6	C	48	0	63	4	0
6	D	48	0	63	4	0
7	C	13	0	23	1	0
7	D	13	0	23	0	0
8	C	15	0	27	0	0
8	D	15	0	27	0	0
9	C	15	0	12	0	0
9	D	15	0	12	0	0
10	A	15	0	0	1	0
10	B	21	0	0	0	0
10	D	3	0	0	0	0
All	All	12381	0	12293	238	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 238 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:B:604:VAL:HG11	1:B:621:LEU:HG	1.50	0.94
2:D:81:THR:HB	2:D:132:LYS:HG3	1.49	0.93
2:C:42:TYR:CE1	2:C:68:ARG:HG3	2.04	0.93
2:D:96:ARG:HG2	2:D:96:ARG:HH21	1.38	0.84
1:B:287:GLU:HG2	1:B:312:SER:HB3	1.62	0.82

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	599/635 (94%)	559 (93%)	37 (6%)	3 (0%)	29	41
1	B	603/635 (95%)	562 (93%)	37 (6%)	4 (1%)	22	32
2	C	138/144 (96%)	131 (95%)	6 (4%)	1 (1%)	22	32
2	D	138/144 (96%)	133 (96%)	5 (4%)	0	100	100
All	All	1478/1558 (95%)	1385 (94%)	85 (6%)	8 (0%)	29	41

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	142	PRO
1	A	564	LEU
1	B	202	PRO
1	B	292	TYR
1	A	292	TYR

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	558/588 (95%)	493 (88%)	65 (12%)	5	7
1	B	562/588 (96%)	500 (89%)	62 (11%)	6	8
2	C	130/133 (98%)	115 (88%)	15 (12%)	5	7
2	D	130/133 (98%)	113 (87%)	17 (13%)	4	4
All	All	1380/1442 (96%)	1221 (88%)	159 (12%)	5	7

5 of 159 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	517	ASN
2	D	37	CYS
1	B	561	LYS
2	C	55	LYS
2	D	84	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	456	HIS
2	C	26	ASN
1	B	458	HIS
1	B	565	GLN
2	D	73	GLN

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 ⓘ

8 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
3	NAG	E	1	3,1	14,14,15	0.67	0	17,19,21	1.00	1 (5%)
3	NAG	E	2	3	14,14,15	0.47	0	17,19,21	1.78	4 (23%)
3	NAG	F	1	3,1	14,14,15	0.49	0	17,19,21	1.54	3 (17%)
3	NAG	F	2	3	14,14,15	0.42	0	17,19,21	1.90	3 (17%)
3	NAG	G	1	3,1	14,14,15	0.65	0	17,19,21	1.23	1 (5%)
3	NAG	G	2	3	14,14,15	0.43	0	17,19,21	2.10	5 (29%)
3	NAG	H	1	3,1	14,14,15	0.72	1 (7%)	17,19,21	2.12	2 (11%)
3	NAG	H	2	3	14,14,15	0.53	0	17,19,21	1.24	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1	NAG	O5-C1	-2.13	1.40	1.43

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	NAG	C1-O5-C5	6.75	121.23	112.19
3	G	2	NAG	C1-O5-C5	6.32	120.65	112.19
3	F	2	NAG	C1-O5-C5	5.73	119.87	112.19
3	E	2	NAG	C1-O5-C5	4.75	118.55	112.19
3	F	1	NAG	C2-N2-C7	3.93	128.17	122.90

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

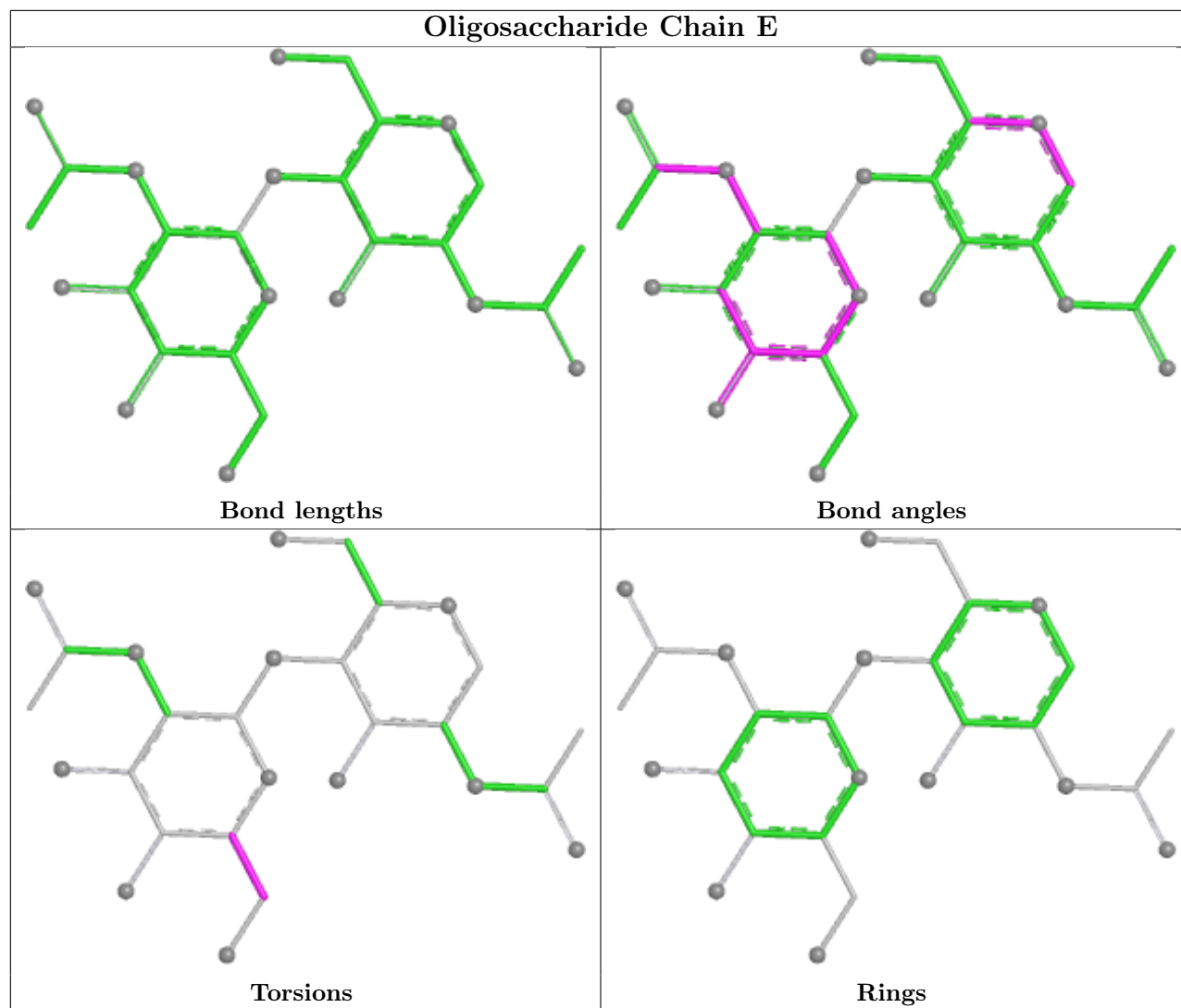
Mol	Chain	Res	Type	Atoms
3	H	2	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6

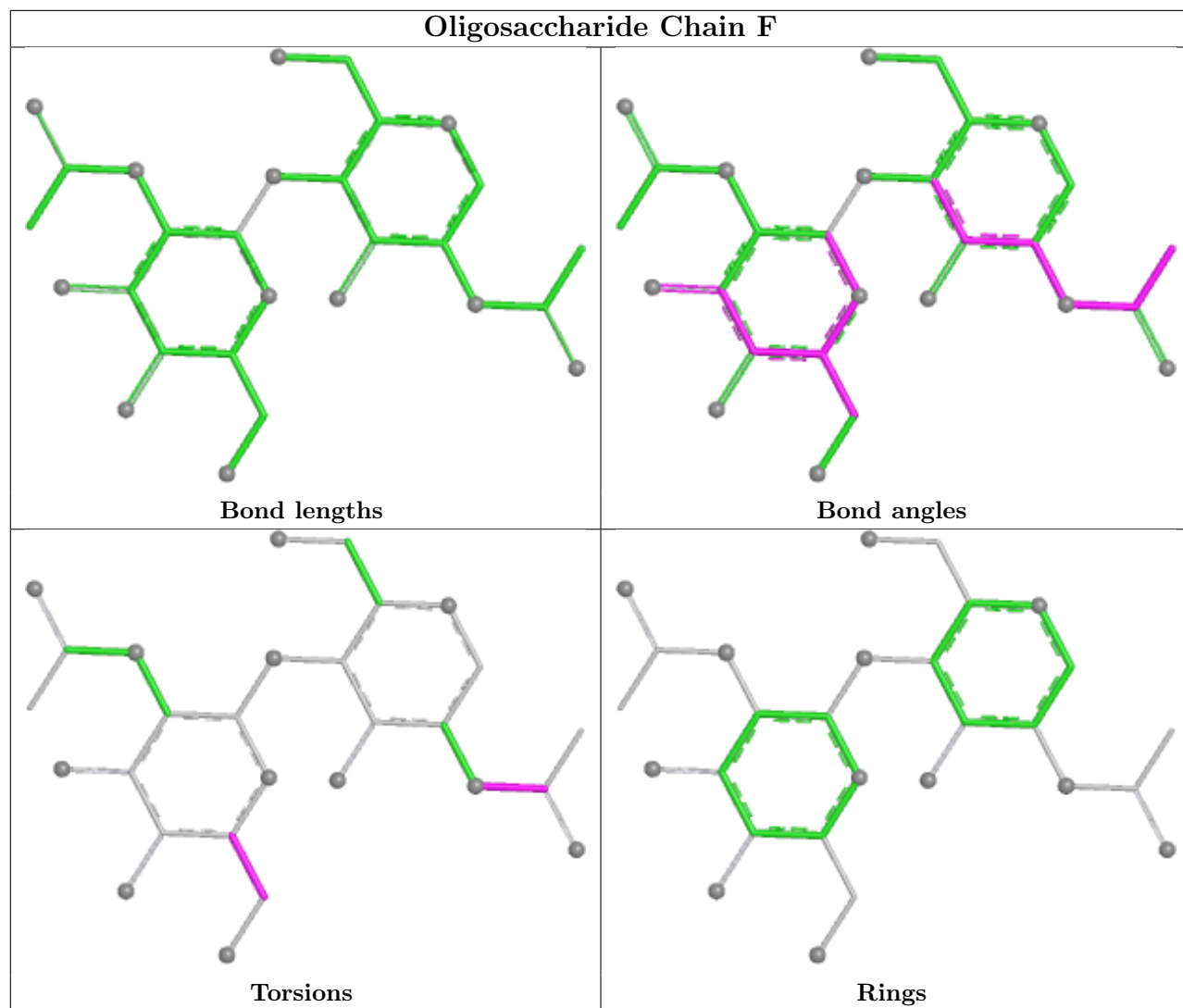
There are no ring outliers.

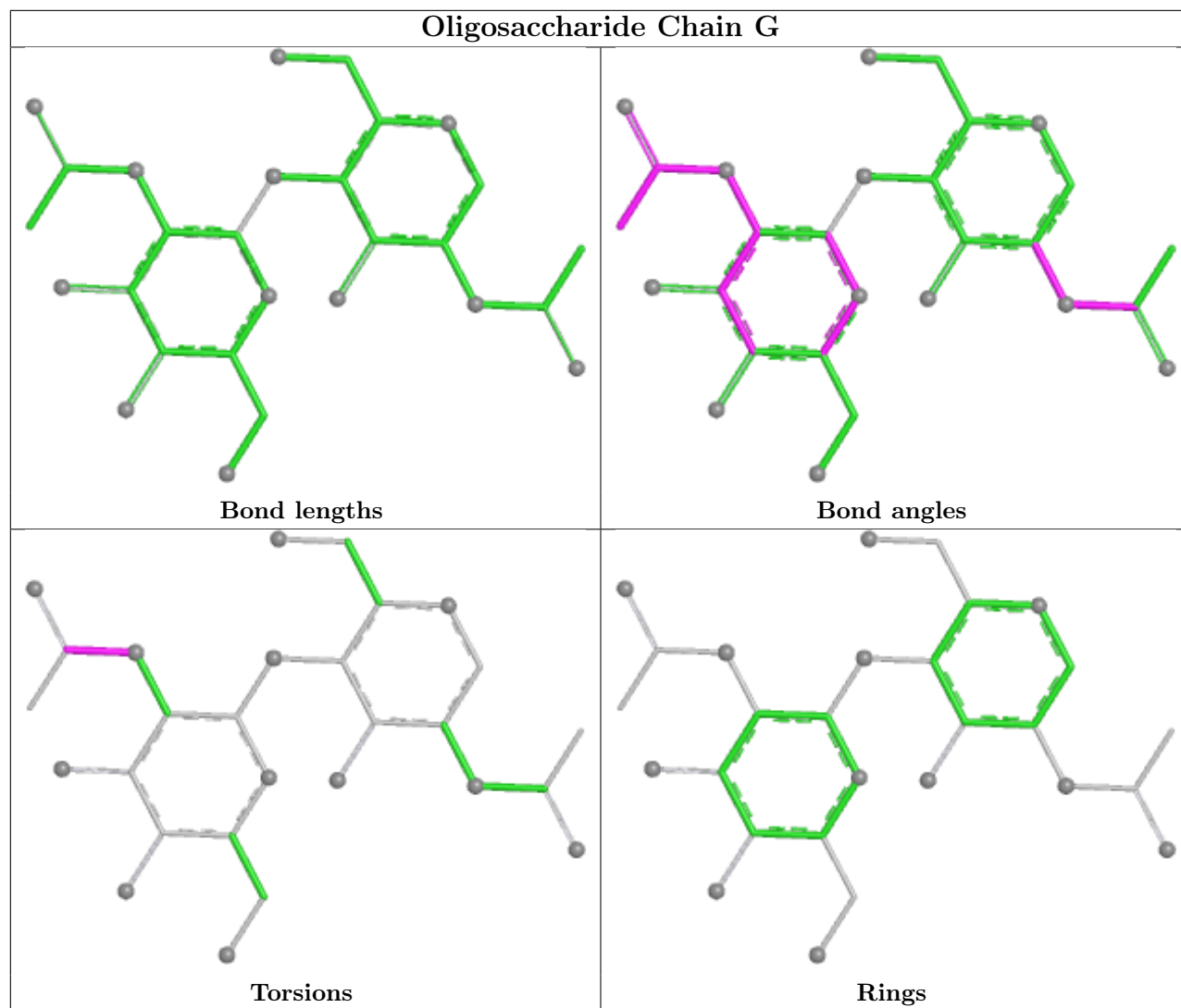
3 monomers are involved in 3 short contacts:

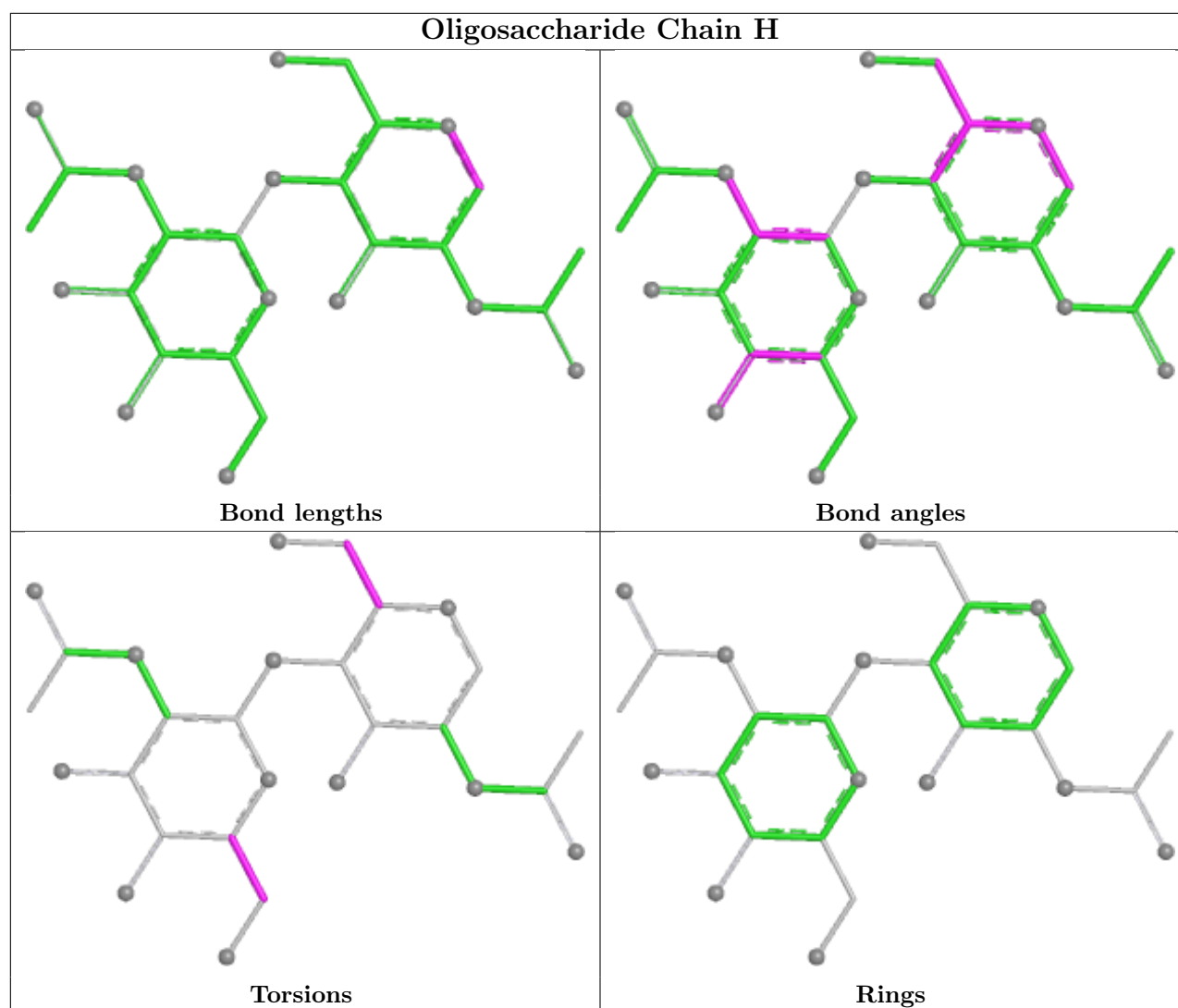
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	NAG	1	0
3	H	1	NAG	2	0
3	F	1	NAG	1	0

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









5.6 Ligand geometry [i](#)

14 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$
6	LP5	C	203	5	47,48,48	1.02	2 (4%)	58,60,60	1.26	6 (10%)
8	MYR	D	205	5	14,14,15	0.86	1 (7%)	13,13,15	0.81	0
4	NAG	A	701	1	14,14,15	0.51	0	17,19,21	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	701	1	14,14,15	0.66	0	17,19,21	1.93	3 (17%)
7	DAO	D	204	5	12,12,13	0.99	1 (8%)	11,11,13	0.77	0
9	KDO	D	206	5	15,15,16	0.84	0	17,21,24	1.36	2 (11%)
6	LP5	D	203	5	47,48,48	0.86	2 (4%)	58,60,60	1.31	6 (10%)
8	MYR	C	205	5	14,14,15	0.89	1 (7%)	13,13,15	0.87	0
9	KDO	C	206	5	15,15,16	0.67	0	17,21,24	1.09	1 (5%)
4	NAG	D	201	2	14,14,15	0.52	0	17,19,21	1.33	1 (5%)
4	NAG	C	201	2	14,14,15	0.49	0	17,19,21	1.18	1 (5%)
5	LP4	C	202	9,8,6,7	45,45,48	0.66	0	54,56,60	1.15	3 (5%)
5	LP4	D	202	9,8,6,7	45,45,48	0.80	2 (4%)	54,56,60	1.42	8 (14%)
7	DAO	C	204	5	12,12,13	0.96	1 (8%)	11,11,13	0.68	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
6	LP5	C	203	5	-	14/44/65/65	0/1/1/1
8	MYR	D	205	5	-	11/12/12/13	-
4	NAG	A	701	1	-	1/6/23/26	0/1/1/1
4	NAG	B	701	1	-	3/6/23/26	0/1/1/1
7	DAO	D	204	5	-	8/10/10/11	-
9	KDO	D	206	5	-	2/10/26/30	0/1/1/1
6	LP5	D	203	5	-	16/44/65/65	0/1/1/1
8	MYR	C	205	5	-	10/12/12/13	-
9	KDO	C	206	5	-	6/10/26/30	0/1/1/1
4	NAG	D	201	2	-	0/6/23/26	0/1/1/1
4	NAG	C	201	2	-	0/6/23/26	0/1/1/1
5	LP4	C	202	9,8,6,7	-	11/43/60/65	0/1/1/1
5	LP4	D	202	9,8,6,7	-	17/43/60/65	0/1/1/1
7	DAO	C	204	5	-	5/10/10/11	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	203	LP5	P45-O47	4.70	1.65	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	204	DAO	O2-C1	-3.38	1.24	1.42
6	D	203	LP5	P45-O47	3.38	1.61	1.50
7	C	204	DAO	O2-C1	-3.29	1.25	1.42
8	C	205	MYR	O2-C1	-3.24	1.25	1.42

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	202	LP4	C1-O5-C5	-5.08	105.38	112.19
4	B	701	NAG	C2-N2-C7	4.82	129.36	122.90
4	C	201	NAG	C1-O5-C5	4.11	117.70	112.19
4	D	201	NAG	C1-O5-C5	4.06	117.62	112.19
6	D	203	LP5	O5-C1-O1	-3.85	106.33	111.36

There are no chirality outliers.

5 of 104 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	202	LP4	C17-C16-C8-C7
5	C	202	LP4	O44-C16-C8-C7
5	C	202	LP4	C8-C16-C17-C18
5	D	202	LP4	C17-C16-C8-C7
5	D	202	LP4	O44-C16-C8-C7

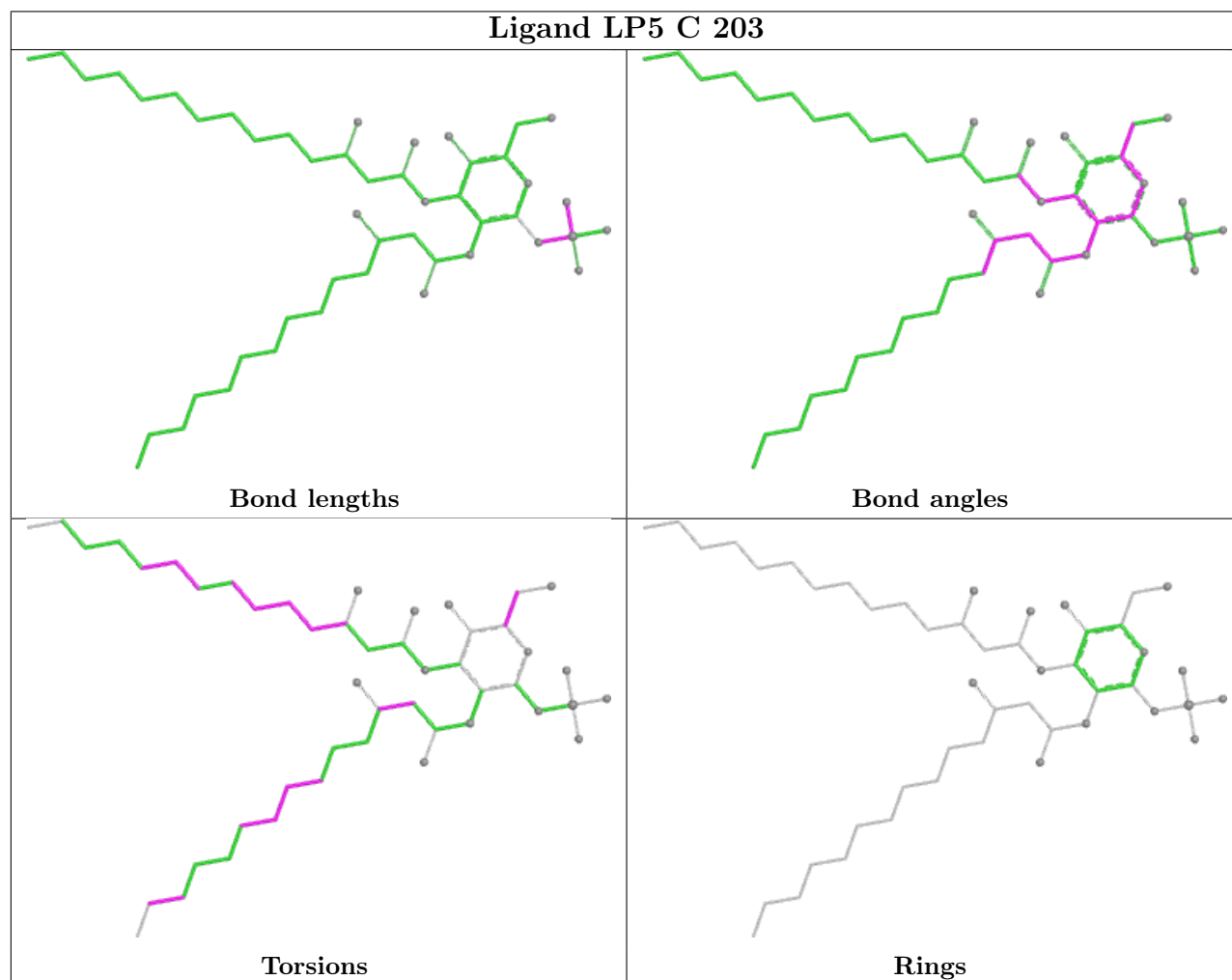
There are no ring outliers.

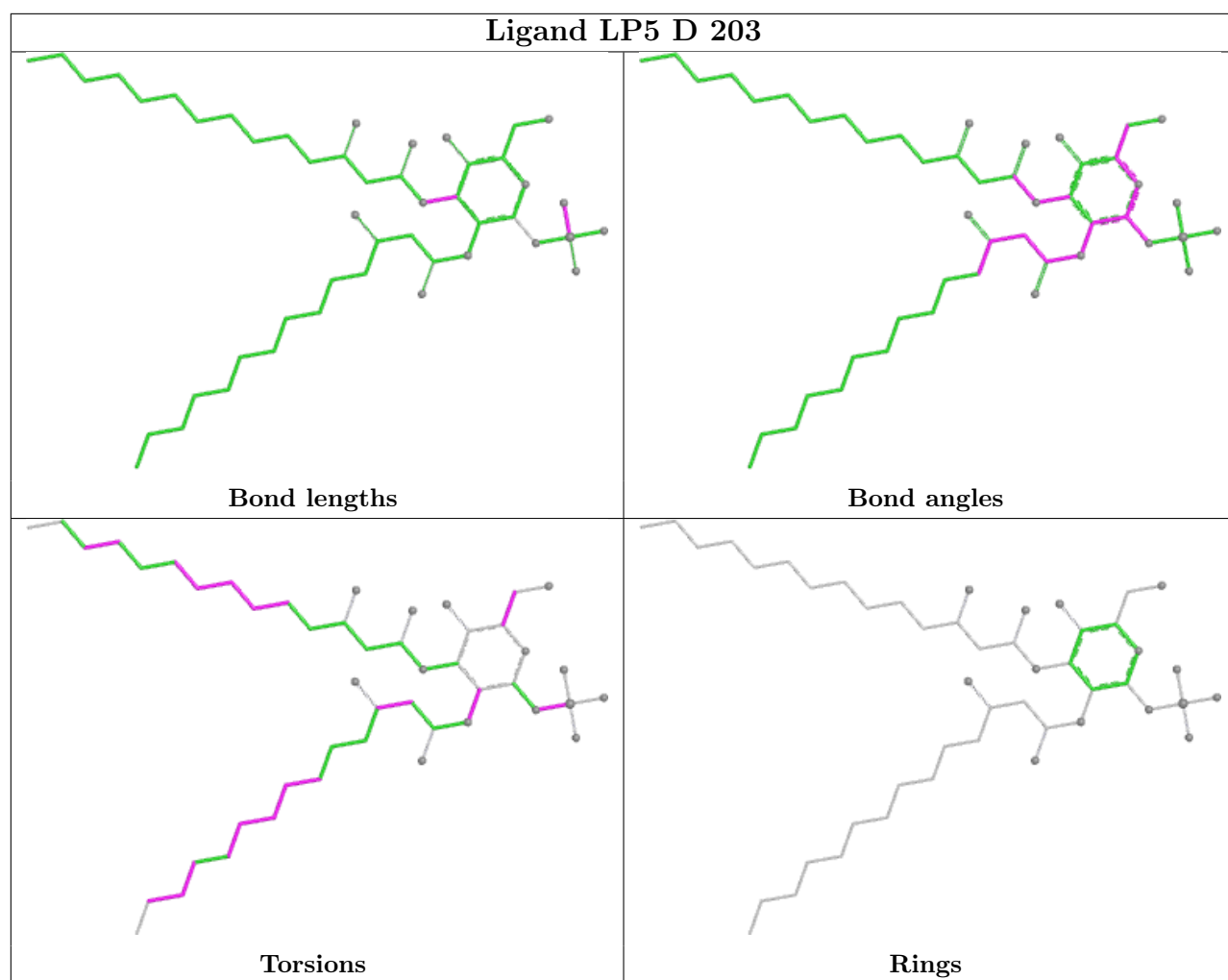
5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	203	LP5	4	0
6	D	203	LP5	4	0
5	C	202	LP4	5	0
5	D	202	LP4	3	0
7	C	204	DAO	1	0

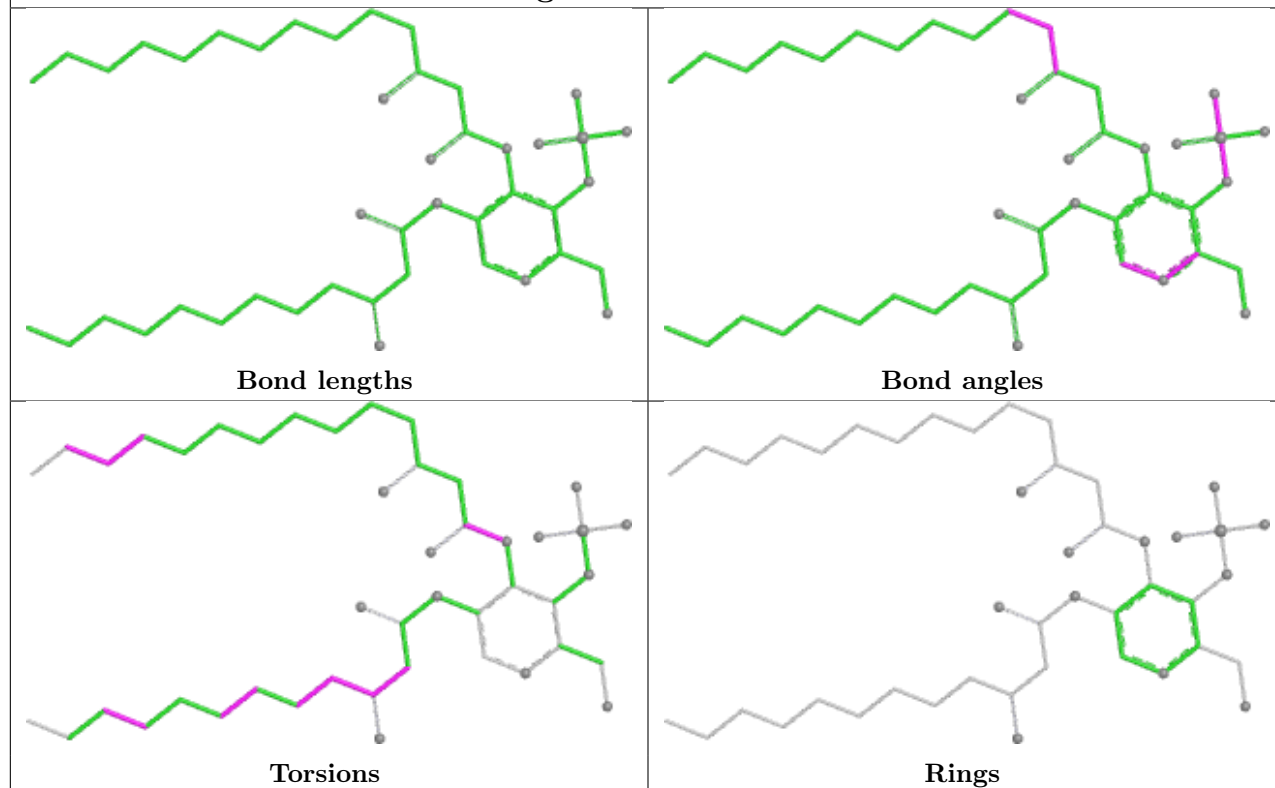
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

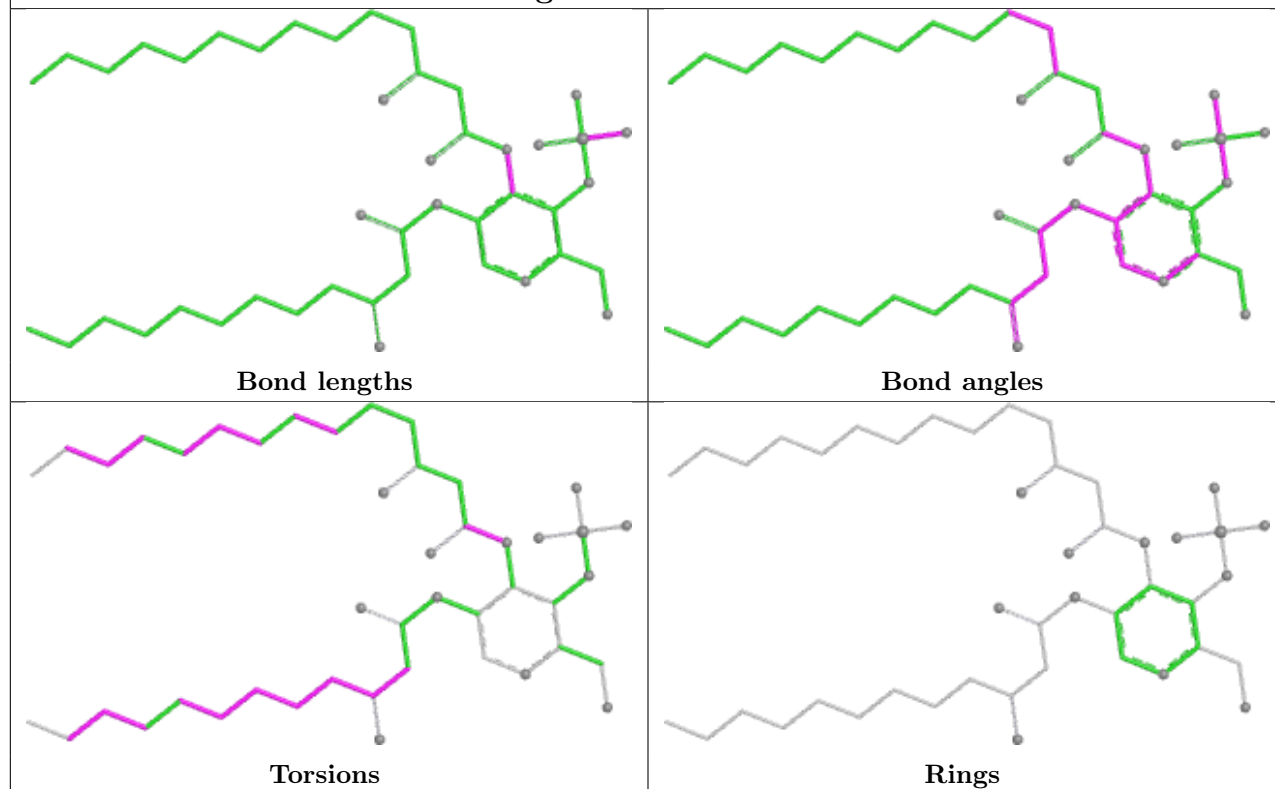




Ligand LP4 C 202



Ligand LP4 D 202



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	601/635 (94%)	0.06	24 (3%) 38 37	26, 44, 79, 120	0
1	B	605/635 (95%)	0.00	14 (2%) 60 58	27, 44, 69, 106	0
2	C	140/144 (97%)	0.21	8 (5%) 23 22	32, 49, 83, 103	0
2	D	140/144 (97%)	0.06	5 (3%) 42 42	33, 44, 76, 102	0
All	All	1486/1558 (95%)	0.05	51 (3%) 45 44	26, 44, 74, 120	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	203	LEU	10.9
2	D	19	GLN	6.2
1	A	625	ILE	6.0
1	A	75	PHE	6.0
1	A	301	ILE	5.6

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.

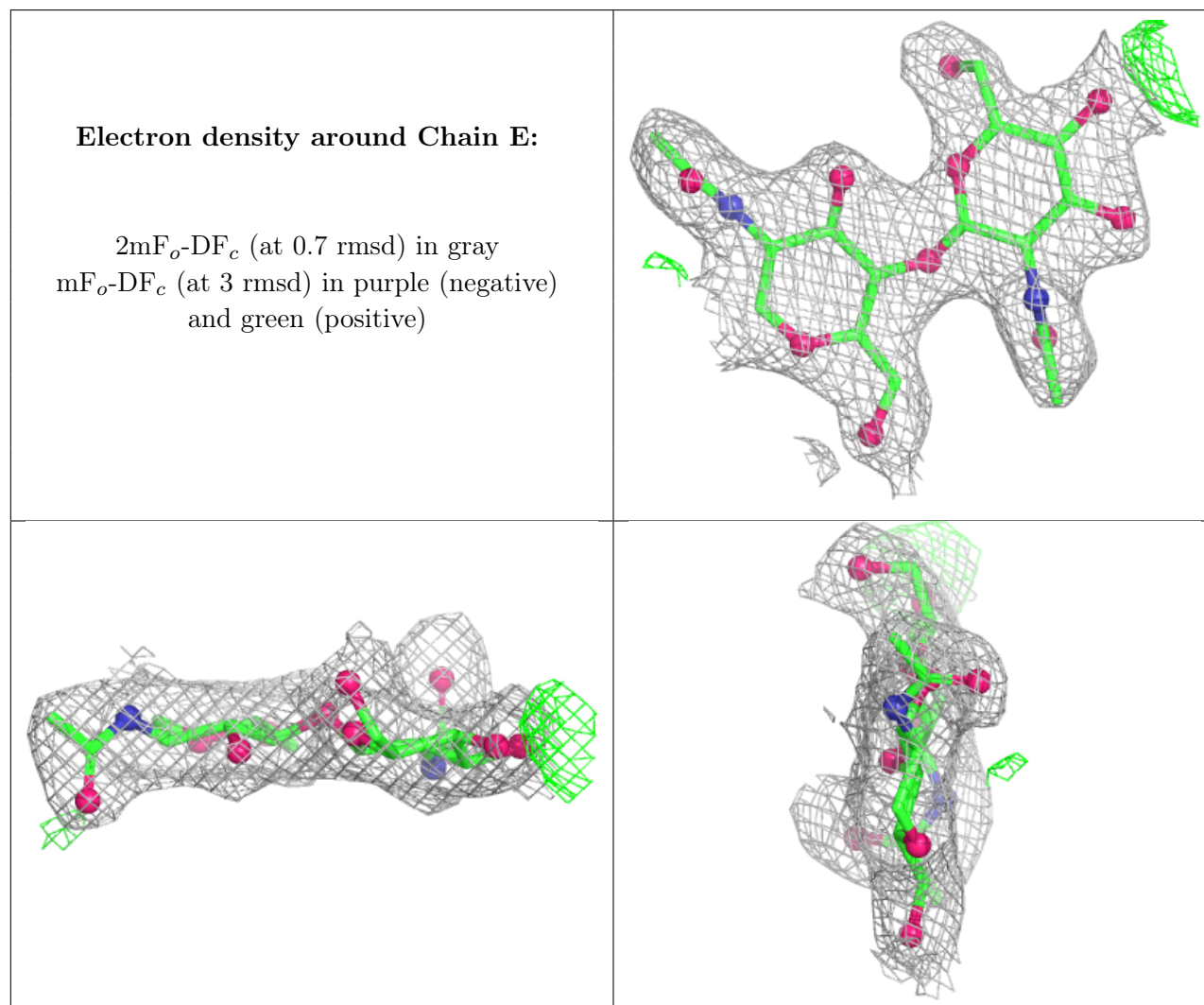
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	E	2	14/15	0.83	0.33	53,59,64,66	0
3	NAG	H	2	14/15	0.90	0.19	41,49,59,60	0

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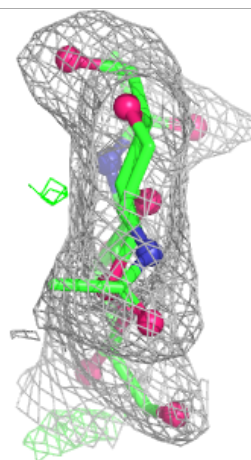
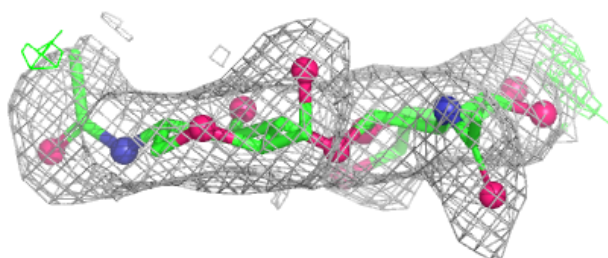
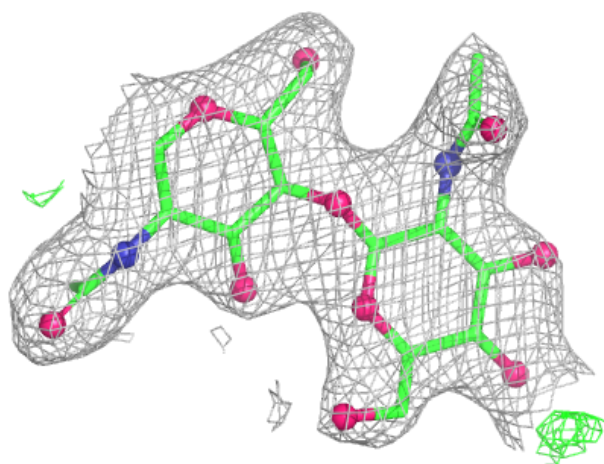
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	G	2	14/15	0.91	0.20	51,55,59,64	0
3	NAG	F	2	14/15	0.91	0.25	57,58,61,63	0
3	NAG	F	1	14/15	0.95	0.20	46,49,50,55	0
3	NAG	G	1	14/15	0.95	0.11	34,37,45,47	0
3	NAG	H	1	14/15	0.96	0.13	35,36,44,51	0
3	NAG	E	1	14/15	0.96	0.17	37,43,47,51	0

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.



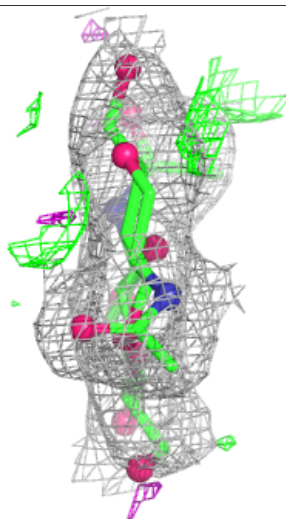
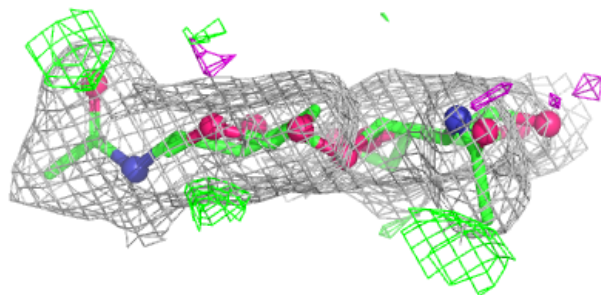
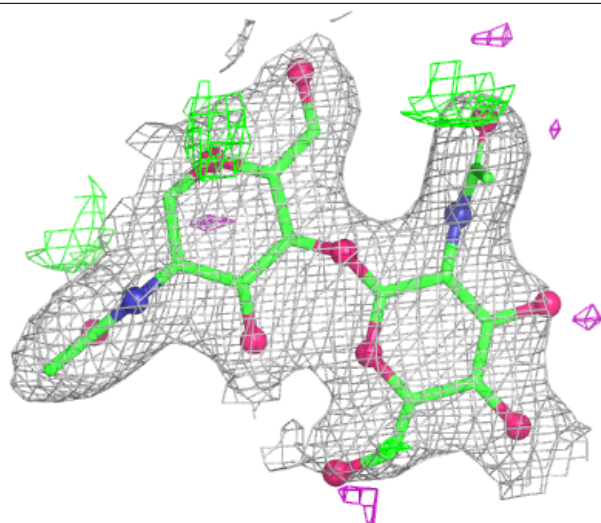
Electron density around Chain F:

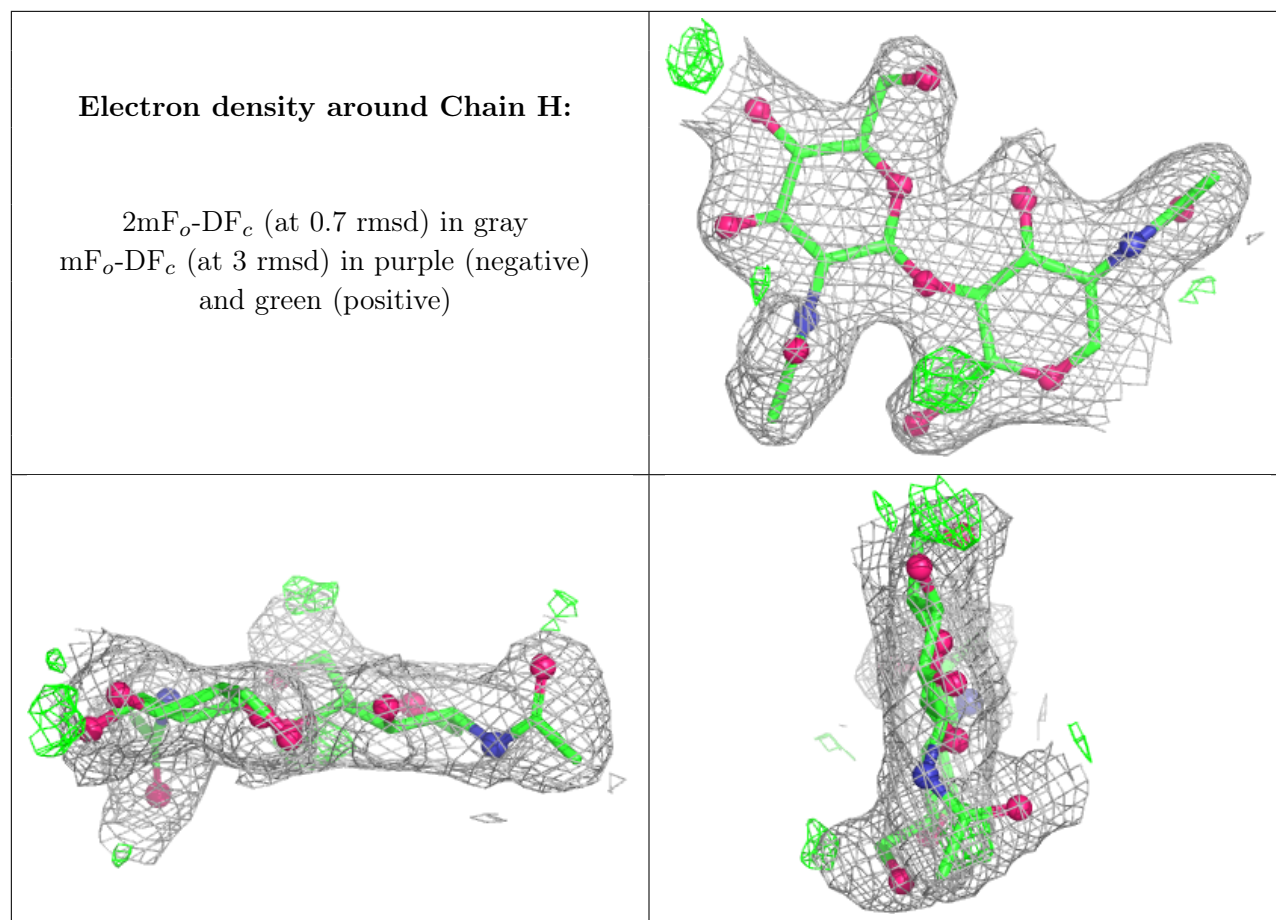
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

$2mF_o-DF_c$ (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
4	NAG	B	701	14/15	0.65	0.39	95,105,111,112	0
4	NAG	A	701	14/15	0.66	0.27	90,101,105,108	0
9	KDO	D	206	15/16	0.71	0.18	62,66,78,82	0
4	NAG	C	201	14/15	0.87	0.26	66,73,81,81	0
4	NAG	D	201	14/15	0.88	0.26	61,69,72,73	0
6	LP5	C	203	48/48	0.89	0.19	49,54,64,70	0
8	MYR	C	205	15/16	0.91	0.24	51,54,60,66	0
6	LP5	D	203	48/48	0.92	0.17	40,52,58,65	0
7	DAO	C	204	13/14	0.92	0.20	50,52,54,58	0
7	DAO	D	204	13/14	0.93	0.20	48,51,53,56	0
9	KDO	C	206	15/16	0.94	0.14	62,67,71,73	0
5	LP4	C	202	45/48	0.94	0.17	36,45,53,56	0

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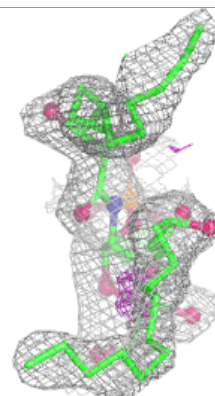
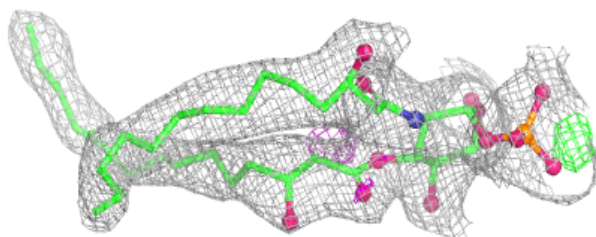
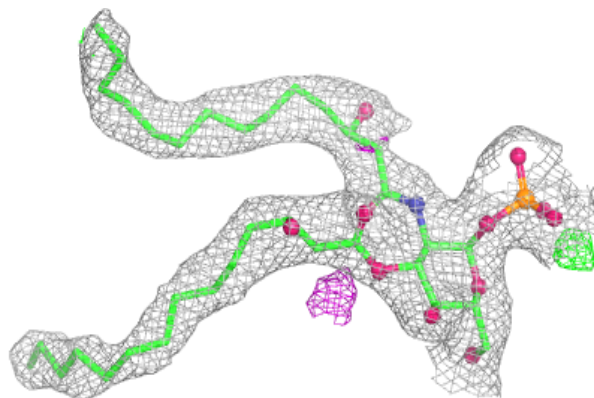
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	LP4	D	202	45/48	0.95	0.15	37,45,52,57	0
8	MYR	D	205	15/16	0.96	0.19	41,50,55,55	0

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.

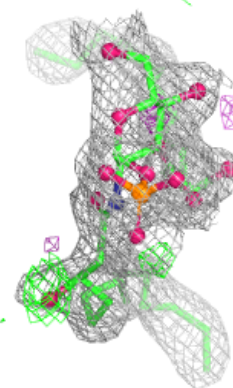
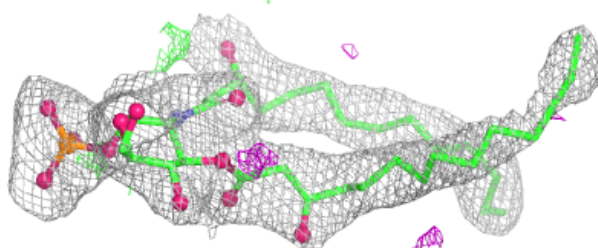
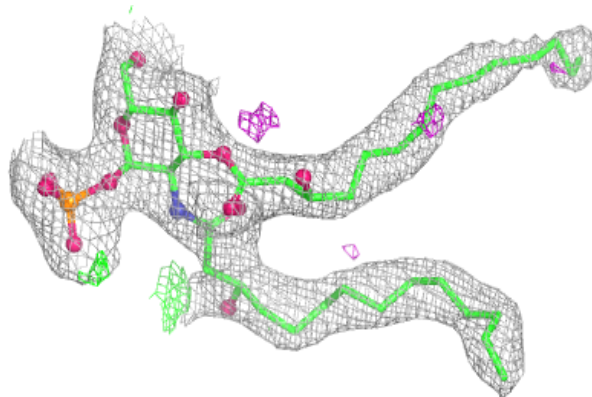
Electron density around LP5 C 203:

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

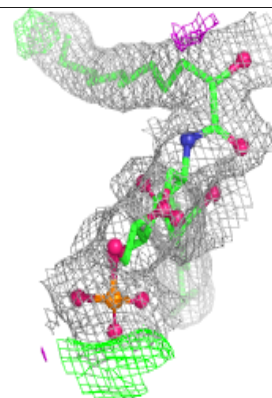
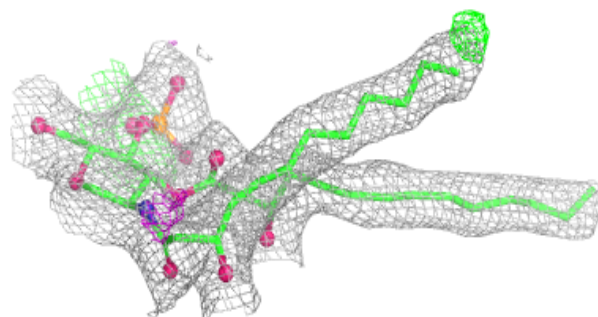
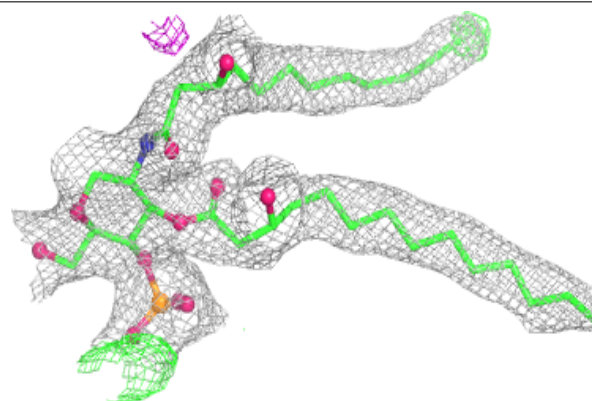


Electron density around LP5 D 203:

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

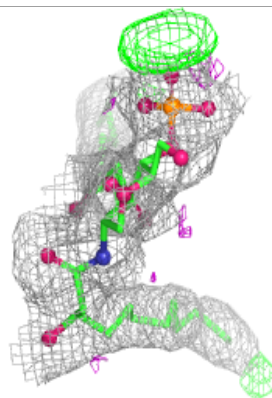
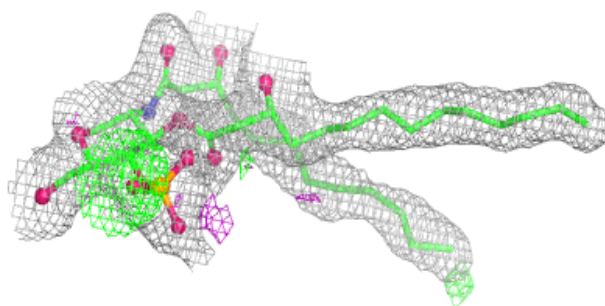
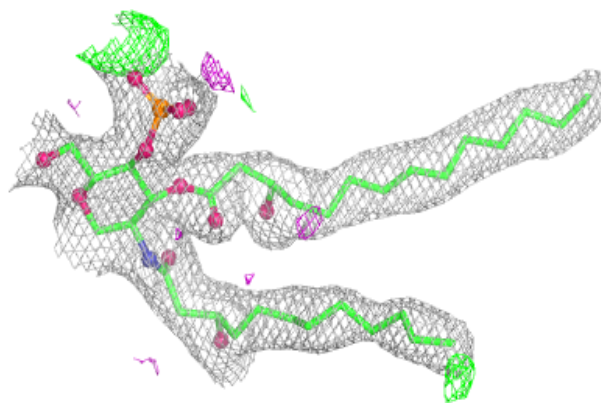
**Electron density around LP4 C 202:**

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



Electron density around LP4 D 202:

$2mF_o-DF_c$ (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.