



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 14, 2021 – 01:40 PM EDT

PDB ID : 7MLM  
Title : Crystal structure of mouse TLR4/MD-2 in complex with sulfatides  
Authors : Su, L.; Beutler, B.  
Deposited on : 2021-04-28  
Resolution : 2.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.1  
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) : 2.23.1

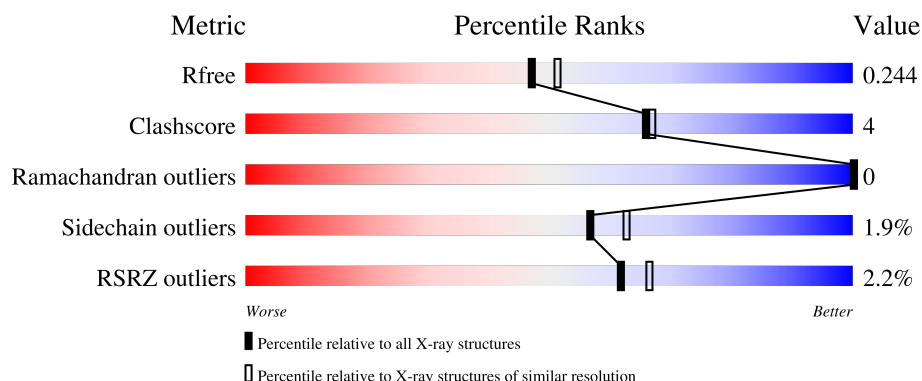
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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	
2	C	188	
3	B	2	
4	D	3	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6361 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, Variable lymphocyte receptor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	590	Total	C	N	O	S	0	1	0
			4711	3014	784	888	25			

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP Q9QUK6
A	-14	LEU	-	expression tag	UNP Q9QUK6
A	-13	LEU	-	expression tag	UNP Q9QUK6
A	-12	VAL	-	expression tag	UNP Q9QUK6
A	-11	ASN	-	expression tag	UNP Q9QUK6
A	-10	GLN	-	expression tag	UNP Q9QUK6
A	-9	SER	-	expression tag	UNP Q9QUK6
A	-8	HIS	-	expression tag	UNP Q9QUK6
A	-7	GLN	-	expression tag	UNP Q9QUK6
A	-6	GLY	-	expression tag	UNP Q9QUK6
A	-5	PHE	-	expression tag	UNP Q9QUK6
A	-4	ASN	-	expression tag	UNP Q9QUK6
A	-3	LYS	-	expression tag	UNP Q9QUK6
A	-2	GLU	-	expression tag	UNP Q9QUK6
A	-1	HIS	-	expression tag	UNP Q9QUK6
A	0	THR	-	expression tag	UNP Q9QUK6
A	1	SER	-	expression tag	UNP Q9QUK6
A	2	LYS	-	expression tag	UNP Q9QUK6
A	3	MET	-	expression tag	UNP Q9QUK6
A	4	VAL	-	expression tag	UNP Q9QUK6
A	5	SER	-	expression tag	UNP Q9QUK6
A	6	ALA	-	expression tag	UNP Q9QUK6
A	7	ILE	-	expression tag	UNP Q9QUK6
A	8	VAL	-	expression tag	UNP Q9QUK6
A	9	LEU	-	expression tag	UNP Q9QUK6
A	10	TYR	-	expression tag	UNP Q9QUK6
A	11	VAL	-	expression tag	UNP Q9QUK6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	12	LEU	-	expression tag	UNP Q9QUK6
A	13	LEU	-	expression tag	UNP Q9QUK6
A	14	ALA	-	expression tag	UNP Q9QUK6
A	15	ALA	-	expression tag	UNP Q9QUK6
A	16	ALA	-	expression tag	UNP Q9QUK6
A	17	ALA	-	expression tag	UNP Q9QUK6
A	18	HIS	-	expression tag	UNP Q9QUK6
A	19	SER	-	expression tag	UNP Q9QUK6
A	20	ALA	-	expression tag	UNP Q9QUK6
A	21	PHE	-	expression tag	UNP Q9QUK6
A	22	ALA	-	expression tag	UNP Q9QUK6
A	23	ALA	-	expression tag	UNP Q9QUK6
A	24	ASP	-	expression tag	UNP Q9QUK6
A	25	PRO	-	expression tag	UNP Q9QUK6

- Molecule 2 is a protein called Lymphocyte antigen 96.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	136	Total	C	N	O	S	0	0	0
			1103	712	186	198	7			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-22	MET	-	initiating methionine	UNP Q9JHF9
C	-21	LEU	-	expression tag	UNP Q9JHF9
C	-20	LEU	-	expression tag	UNP Q9JHF9
C	-19	VAL	-	expression tag	UNP Q9JHF9
C	-18	ASN	-	expression tag	UNP Q9JHF9
C	-17	GLN	-	expression tag	UNP Q9JHF9
C	-16	SER	-	expression tag	UNP Q9JHF9
C	-15	HIS	-	expression tag	UNP Q9JHF9
C	-14	GLN	-	expression tag	UNP Q9JHF9
C	-13	GLY	-	expression tag	UNP Q9JHF9
C	-12	PHE	-	expression tag	UNP Q9JHF9
C	-11	ASN	-	expression tag	UNP Q9JHF9
C	-10	LYS	-	expression tag	UNP Q9JHF9
C	-9	GLU	-	expression tag	UNP Q9JHF9
C	-8	HIS	-	expression tag	UNP Q9JHF9
C	-7	THR	-	expression tag	UNP Q9JHF9
C	-6	SER	-	expression tag	UNP Q9JHF9
C	-5	LYS	-	expression tag	UNP Q9JHF9

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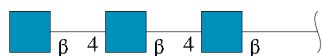
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	MET	-	expression tag	UNP Q9JHF9
C	-3	VAL	-	expression tag	UNP Q9JHF9
C	-2	SER	-	expression tag	UNP Q9JHF9
C	-1	ALA	-	expression tag	UNP Q9JHF9
C	0	ILE	-	expression tag	UNP Q9JHF9
C	1	VAL	-	expression tag	UNP Q9JHF9
C	2	LEU	-	expression tag	UNP Q9JHF9
C	3	TYR	-	expression tag	UNP Q9JHF9
C	4	VAL	-	expression tag	UNP Q9JHF9
C	5	LEU	-	expression tag	UNP Q9JHF9
C	6	LEU	-	expression tag	UNP Q9JHF9
C	7	ALA	-	expression tag	UNP Q9JHF9
C	8	ALA	-	expression tag	UNP Q9JHF9
C	9	ALA	-	expression tag	UNP Q9JHF9
C	10	ALA	-	expression tag	UNP Q9JHF9
C	11	HIS	-	expression tag	UNP Q9JHF9
C	12	SER	-	expression tag	UNP Q9JHF9
C	13	ALA	-	expression tag	UNP Q9JHF9
C	14	PHE	-	expression tag	UNP Q9JHF9
C	15	ALA	-	expression tag	UNP Q9JHF9
C	16	ALA	-	expression tag	UNP Q9JHF9
C	17	ASP	-	expression tag	UNP Q9JHF9
C	18	PRO	-	expression tag	UNP Q9JHF9
C	161	LEU	-	expression tag	UNP Q9JHF9
C	162	VAL	-	expression tag	UNP Q9JHF9
C	163	PRO	-	expression tag	UNP Q9JHF9
C	164	ARG	-	expression tag	UNP Q9JHF9
C	165	GLY	-	expression tag	UNP Q9JHF9

- 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	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



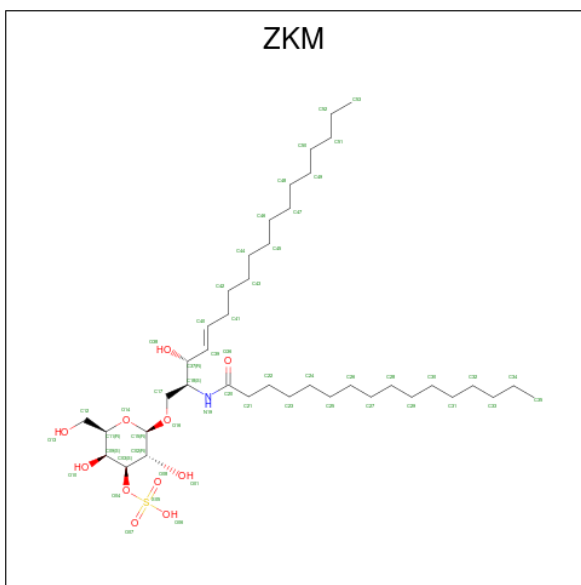
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O	0	0	0
			42	24	3	15			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 6 is N-[(1S,2R,3E)-2-hydroxy-1-[(3-O-sulfo-beta-D-galactopyranosyl)oxy]methyl]heptadec-3-en-1-yl]-hexadecanamide (three-letter code: ZKM) (formula:  $C_{40}H_{77}NO_{11}S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 53	C 40	N 1	O 11	S 1	0	0
6	A	1	Total 53	C 40	N 1	O 11	S 1	0	0
6	C	1	Total 53	C 40	N 1	O 11	S 1	0	0

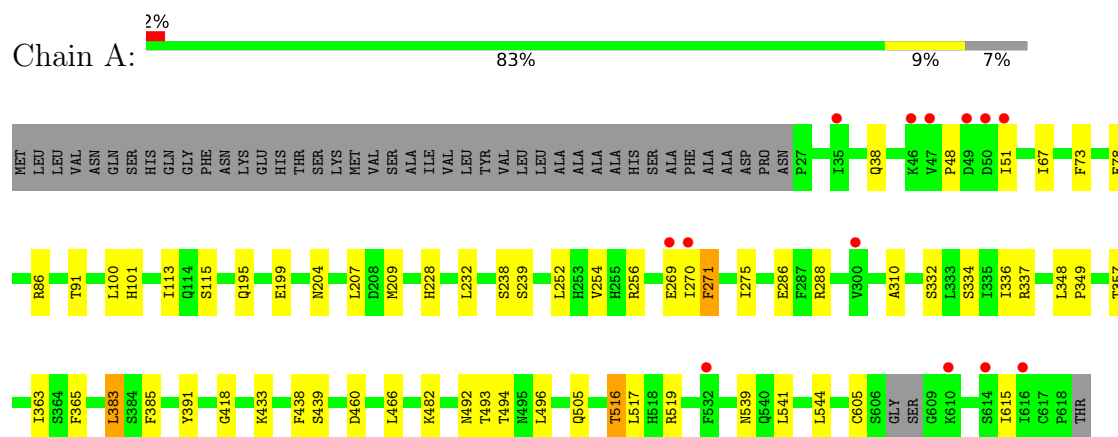
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	209	Total O 209 209	0	0
7	C	53	Total O 53 53	0	0

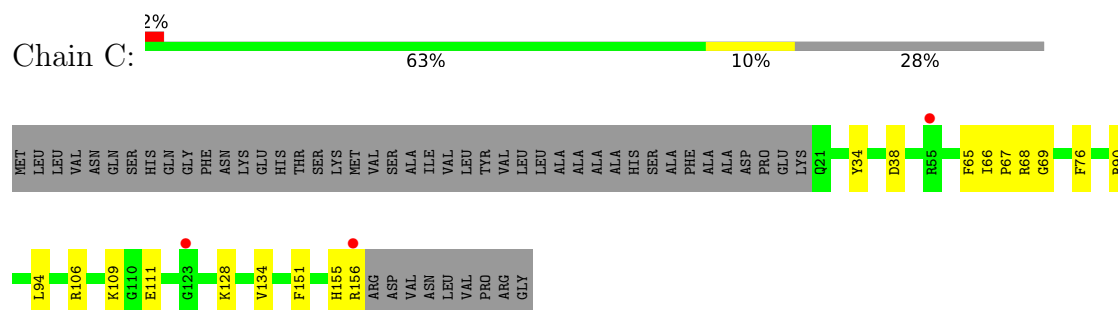
### 3 Residue-property plots [i](#)

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: Toll-like receptor 4, Variable lymphocyte receptor B



- Molecule 2: Lymphocyte antigen 96



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



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







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.09Å 164.29Å 89.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.40 – 2.10 46.40 – 2.10	Depositor EDS
% Data completeness (in resolution range)	75.1 (46.40-2.10) 75.1 (46.40-2.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.73 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.210 , 0.244 0.210 , 0.244	Depositor DCC
$R_{free}$ test set	2000 reflections (4.28%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6361	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NAG, ZKM

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	0.26	0/4814	0.46	1/6522 (0.0%)
2	C	0.27	0/1134	0.51	0/1533
All	All	0.26	0/5948	0.47	1/8055 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	383	LEU	CA-CB-CG	5.53	128.01	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4711	0	4695	35	0
2	C	1103	0	1062	13	0
3	B	28	0	25	0	0
4	D	42	0	37	1	0
5	A	28	0	26	0	0
5	C	28	0	26	2	0
6	A	106	0	0	0	0
6	C	53	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	209	0	0	3	0
7	C	53	0	0	1	0
All	All	6361	0	5871	48	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 4.

All (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:THR:HG22	1:A:519:ARG:HH21	1.66	0.60
1:A:539:ASN:ND2	7:A:801:HOH:O	2.36	0.58
1:A:86:ARG:HD3	2:C:66:ILE:HG21	1.85	0.57
1:A:336:ILE:HG22	1:A:337:ARG:HG3	1.87	0.57
2:C:69:GLY:HA2	2:C:109:LYS:HB2	1.88	0.56
2:C:106:ARG:NH1	2:C:111:GLU:OE1	2.31	0.56
2:C:128:LYS:HG3	2:C:156:ARG:HB2	1.87	0.55
1:A:363:ILE:HG13	1:A:383:LEU:HD23	1.88	0.54
2:C:38:ASP:H	5:C:202:NAG:C8	2.22	0.53
1:A:48:PRO:HD2	1:A:51:ILE:HD11	1.90	0.53
1:A:254:VAL:HG12	1:A:256:ARG:N	2.24	0.52
1:A:494:THR:HG22	1:A:519:ARG:NH2	2.24	0.52
1:A:466:LEU:HD23	1:A:492:ASN:OD1	2.10	0.52
1:A:516:THR:HG22	1:A:517:LEU:HD23	1.91	0.52
1:A:493:THR:HB	1:A:496:LEU:HG	1.92	0.51
2:C:67:PRO:HD2	2:C:111:GLU:O	2.10	0.51
1:A:204:ASN:OD1	1:A:228:HIS:HB2	2.11	0.51
2:C:38:ASP:H	5:C:202:NAG:H81	1.76	0.50
1:A:271:PHE:HA	1:A:275:ILE:HD12	1.92	0.50
1:A:541:LEU:HB3	1:A:544:LEU:HB2	1.95	0.48
1:A:269:GLU:HG2	1:A:270:ILE:HG13	1.95	0.48
1:A:252:LEU:HG	1:A:254:VAL:HG23	1.97	0.47
1:A:391:TYR:HB2	1:A:418:GLY:HA3	1.96	0.47
1:A:113:ILE:O	1:A:115:SER:N	2.48	0.47
1:A:207:LEU:HD13	1:A:209:MET:HE2	1.98	0.46
1:A:239:SER:HB3	1:A:275:ILE:HD11	1.97	0.45
1:A:209:MET:HB2	1:A:232:LEU:HD23	1.99	0.45
1:A:38:GLN:NE2	7:A:809:HOH:O	2.42	0.44
1:A:460:ASP:OD1	1:A:482:LYS:HD2	2.17	0.44
1:A:365:PHE:HB2	1:A:383:LEU:HD11	1.99	0.44
4:D:3:NAG:O7	4:D:3:NAG:O3	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:CYS:SG	1:A:615:ILE:HD11	2.57	0.43
1:A:254:VAL:HG12	1:A:256:ARG:H	1.82	0.43
2:C:76:PHE:HE1	2:C:94:LEU:HD12	1.83	0.43
2:C:128:LYS:NZ	2:C:156:ARG:HB2	2.33	0.43
1:A:336:ILE:HG12	1:A:357:THR:HG22	2.00	0.43
1:A:439:SER:OG	1:A:466:LEU:HD12	2.18	0.43
2:C:34:TYR:HB3	2:C:151:PHE:CD1	2.54	0.43
2:C:155:HIS:O	2:C:156:ARG:HB3	2.20	0.42
2:C:90:ARG:HD2	7:C:301:HOH:O	2.19	0.42
1:A:541:LEU:HD13	1:A:544:LEU:HD22	2.02	0.41
1:A:73:PHE:HB3	1:A:100:LEU:HD21	2.01	0.41
1:A:286:GLU:HG2	1:A:310:ALA:HB3	2.02	0.41
1:A:67:ILE:HG13	1:A:91:THR:HB	2.01	0.41
2:C:68:ARG:O	2:C:109:LYS:HD3	2.21	0.41
1:A:195:GLN:O	1:A:199:GLU:HG2	2.22	0.40
1:A:348:LEU:HA	1:A:349:PRO:HD3	1.94	0.40
1:A:505:GLN:NE2	7:A:820:HOH:O	2.47	0.40

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	A	587/635 (92%)	570 (97%)	17 (3%)	0	100	100
2	C	134/188 (71%)	132 (98%)	2 (2%)	0	100	100
All	All	721/823 (88%)	702 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	549/583 (94%)	538 (98%)	11 (2%)	55	60
2	C	123/165 (74%)	121 (98%)	2 (2%)	62	69
All	All	672/748 (90%)	659 (98%)	13 (2%)	57	63

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	GLU
1	A	101	HIS
1	A	238	SER
1	A	271	PHE
1	A	288	ARG
1	A	332	SER
1	A	334	SER
1	A	385	PHE
1	A	433	LYS
1	A	438	PHE
1	A	516	THR
2	C	65	PHE
2	C	134	VAL

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

5 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	B	1	3,1	14,14,15	0.50	0	17,19,21	1.23	1 (5%)
3	NAG	B	2	3	14,14,15	0.18	0	17,19,21	0.62	0
4	NAG	D	1	4,1	14,14,15	0.66	0	17,19,21	1.19	1 (5%)
4	NAG	D	2	4	14,14,15	0.25	0	17,19,21	0.54	0
4	NAG	D	3	4	14,14,15	0.37	0	17,19,21	0.53	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
3	NAG	B	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	B	2	3	-	2/6/23/26	0/1/1/1
4	NAG	D	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	D	3	4	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	NAG	C1-O5-C5	3.92	117.51	112.19
4	D	1	NAG	C1-O5-C5	3.53	116.97	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2	NAG	O5-C5-C6-O6
3	B	2	NAG	C4-C5-C6-O6
3	B	1	NAG	C8-C7-N2-C2
3	B	1	NAG	O7-C7-N2-C2
3	B	1	NAG	O5-C5-C6-O6
4	D	3	NAG	C1-C2-N2-C7
4	D	1	NAG	C4-C5-C6-O6
4	D	3	NAG	C4-C5-C6-O6
4	D	3	NAG	C3-C2-N2-C7

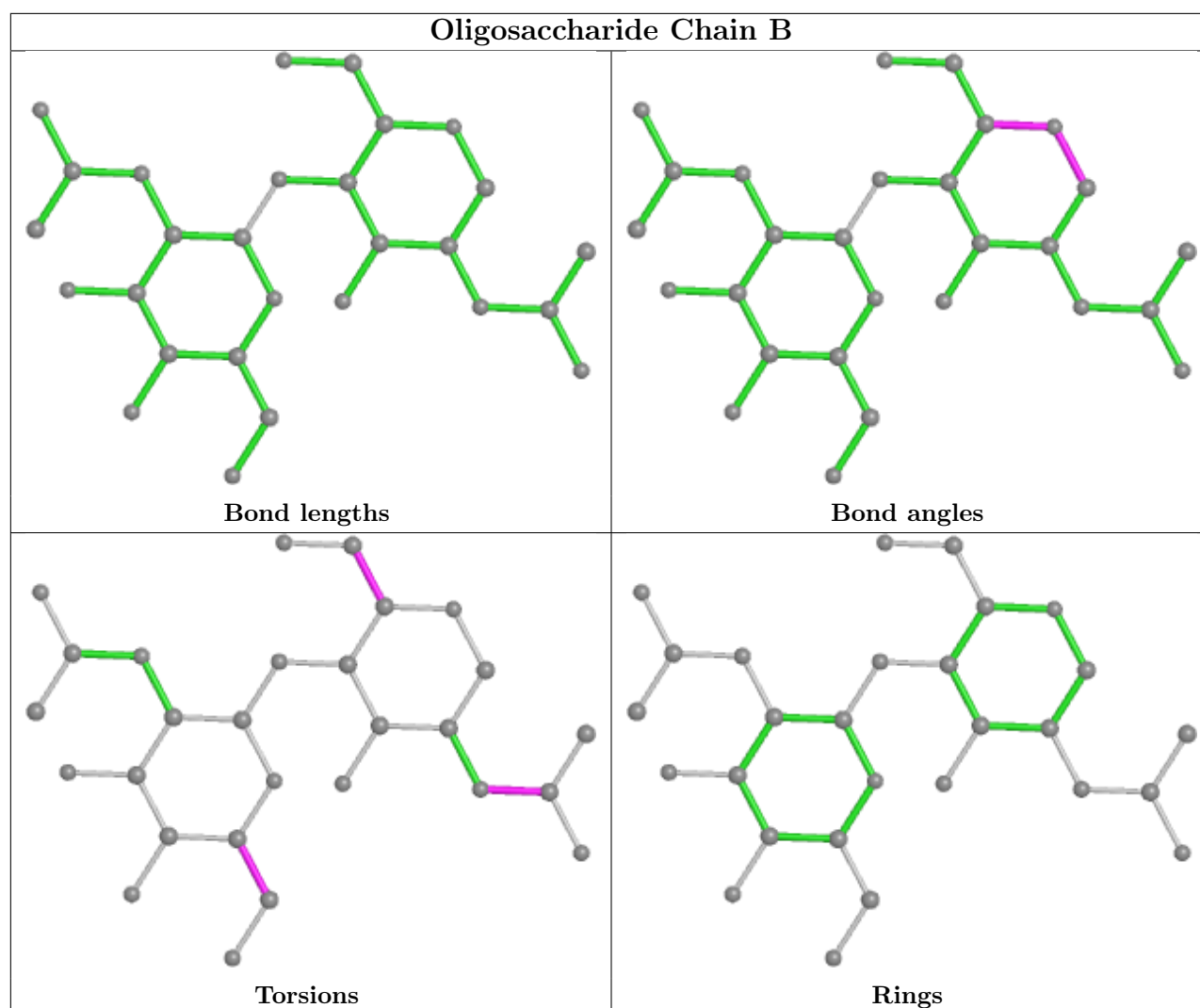
There are no ring outliers.

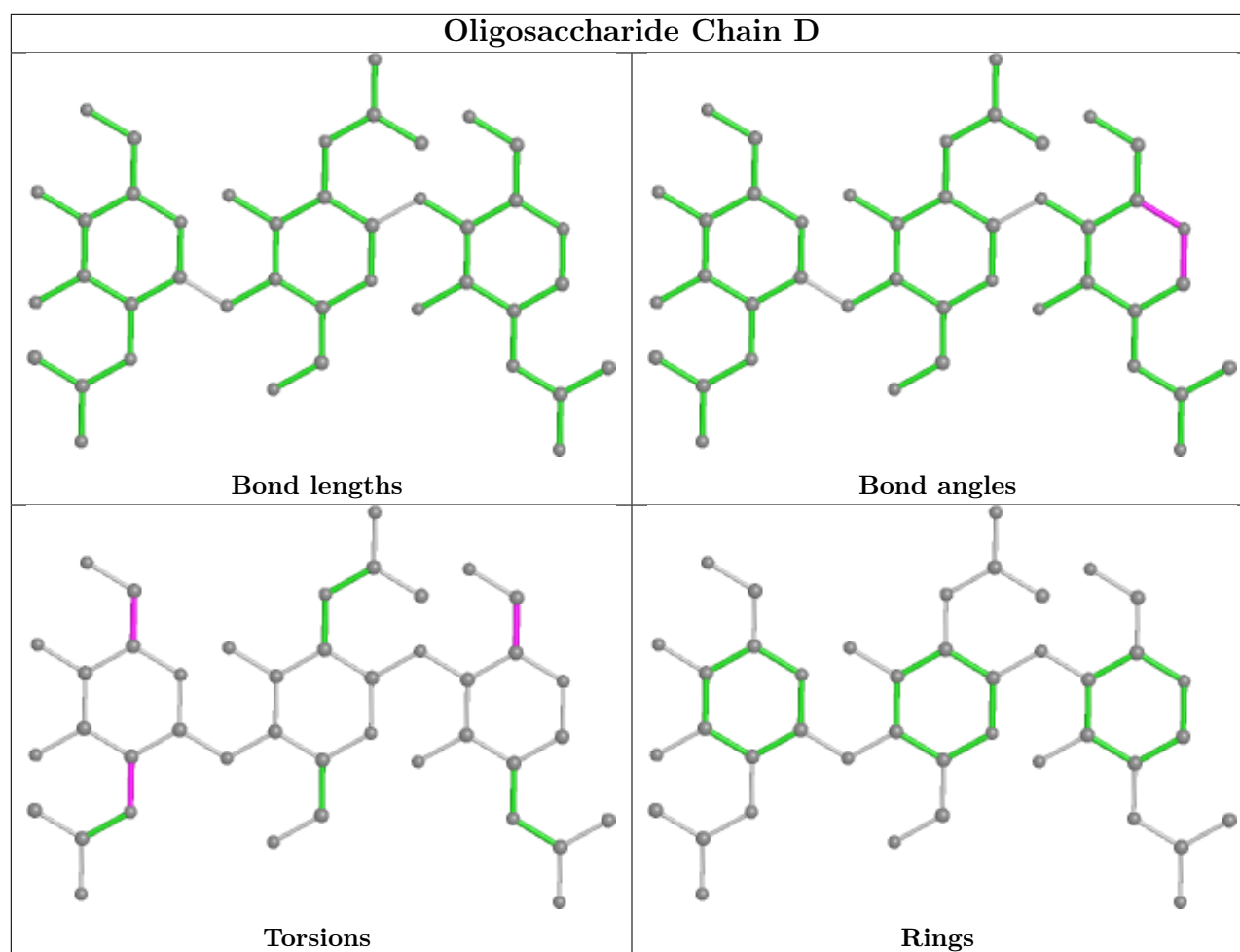
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3	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](#)

7 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	ZKM	A	703	-	52,53,53	1.36	6 (11%)	57,64,64	0.98	4 (7%)
5	NAG	C	201	2	14,14,15	0.37	0	17,19,21	0.38	0
5	NAG	A	701	1	14,14,15	0.45	0	17,19,21	0.65	0
5	NAG	A	702	1	14,14,15	0.33	0	17,19,21	0.39	0
6	ZKM	C	203	-	52,53,53	1.39	6 (11%)	57,64,64	1.37	9 (15%)
5	NAG	C	202	2	14,14,15	0.45	0	17,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	ZKM	A	704	-	52,53,53	1.43	6 (11%)	57,64,64	1.24	6 (10%)

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	ZKM	A	703	-	-	34/50/70/70	0/1/1/1
5	NAG	C	201	2	-	4/6/23/26	0/1/1/1
5	NAG	A	701	1	-	2/6/23/26	0/1/1/1
5	NAG	A	702	1	-	3/6/23/26	0/1/1/1
6	ZKM	C	203	-	-	27/50/70/70	0/1/1/1
5	NAG	C	202	2	-	2/6/23/26	0/1/1/1
6	ZKM	A	704	-	-	35/50/70/70	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	704	ZKM	C20-N19	6.86	1.48	1.34
6	A	703	ZKM	C20-N19	6.17	1.47	1.34
6	C	203	ZKM	C20-N19	5.97	1.46	1.34
6	C	203	ZKM	O14-C11	2.98	1.51	1.44
6	C	203	ZKM	O04-S05	2.81	1.65	1.57
6	A	703	ZKM	O04-S05	2.77	1.65	1.57
6	A	704	ZKM	O04-S05	2.75	1.65	1.57
6	C	203	ZKM	C37-C39	2.61	1.54	1.50
6	A	703	ZKM	C37-C39	2.56	1.54	1.50
6	A	703	ZKM	O14-C11	2.53	1.50	1.44
6	A	704	ZKM	C37-C39	2.51	1.54	1.50
6	C	203	ZKM	O36-C20	-2.51	1.18	1.23
6	C	203	ZKM	O14-C15	2.41	1.48	1.41
6	A	704	ZKM	O14-C11	2.27	1.49	1.44
6	A	703	ZKM	O14-C15	2.27	1.47	1.41
6	A	704	ZKM	O36-C20	-2.19	1.18	1.23
6	A	703	ZKM	O36-C20	-2.14	1.18	1.23
6	A	704	ZKM	O14-C15	2.02	1.47	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	704	ZKM	C21-C20-N19	4.80	124.15	115.83
6	C	203	ZKM	O14-C11-C09	4.30	117.50	109.69
6	C	203	ZKM	C18-N19-C20	-3.73	117.20	123.48
6	C	203	ZKM	C15-O14-C11	3.48	120.52	113.69
6	A	703	ZKM	C03-O04-S05	-2.96	113.15	118.88
6	A	704	ZKM	O36-C20-N19	-2.88	118.08	122.95
6	C	203	ZKM	O36-C20-N19	-2.83	118.18	122.95
6	C	203	ZKM	O08-S05-O07	-2.75	101.20	112.22
6	A	703	ZKM	O08-S05-O07	-2.73	101.25	112.22
6	A	704	ZKM	O08-S05-O07	-2.73	101.25	112.22
6	C	203	ZKM	C37-C39-C40	-2.71	118.74	124.79
6	C	203	ZKM	C37-C18-N19	-2.52	105.44	110.01
6	A	704	ZKM	C18-N19-C20	2.48	127.67	123.48
6	A	704	ZKM	C37-C39-C40	-2.40	119.44	124.79
6	A	704	ZKM	O36-C20-C21	-2.32	117.77	122.02
6	A	703	ZKM	C18-N19-C20	-2.32	119.57	123.48
6	A	703	ZKM	C22-C21-C20	-2.07	107.45	113.26
6	C	203	ZKM	C21-C20-N19	2.05	119.38	115.83
6	C	203	ZKM	O14-C15-C02	2.03	114.64	110.35

There are no chirality outliers.

All (107) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	703	ZKM	O14-C15-O16-C17
6	A	703	ZKM	C17-C18-C37-C39
6	A	703	ZKM	C17-C18-C37-O38
6	A	703	ZKM	N19-C18-C37-O38
6	A	703	ZKM	C18-C37-C39-C40
6	A	703	ZKM	C03-O04-S05-O06
6	A	703	ZKM	C03-O04-S05-O07
6	A	704	ZKM	C18-C37-C39-C40
6	C	203	ZKM	O14-C15-O16-C17
6	C	203	ZKM	C03-O04-S05-O06
6	A	704	ZKM	C21-C20-N19-C18
6	C	203	ZKM	C21-C20-N19-C18
5	A	701	NAG	O5-C5-C6-O6
6	A	703	ZKM	C09-C11-C12-O13
5	A	701	NAG	C4-C5-C6-O6
6	A	704	ZKM	C26-C27-C28-C29
6	A	704	ZKM	O36-C20-N19-C18
6	C	203	ZKM	O36-C20-N19-C18
6	A	704	ZKM	O14-C11-C12-O13

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Mol	Chain	Res	Type	Atoms
6	A	703	ZKM	O14-C11-C12-O13
6	A	704	ZKM	C28-C29-C30-C31
5	C	201	NAG	C4-C5-C6-O6
6	A	704	ZKM	C24-C25-C26-C27
6	A	704	ZKM	C42-C43-C44-C45
6	A	704	ZKM	C09-C11-C12-O13
5	A	702	NAG	C8-C7-N2-C2
5	A	702	NAG	O7-C7-N2-C2
5	C	201	NAG	C8-C7-N2-C2
5	C	201	NAG	O7-C7-N2-C2
5	C	202	NAG	C8-C7-N2-C2
5	C	202	NAG	O7-C7-N2-C2
6	C	203	ZKM	C02-C15-O16-C17
5	C	201	NAG	O5-C5-C6-O6
6	A	703	ZKM	C25-C26-C27-C28
6	A	704	ZKM	C44-C45-C46-C47
6	A	703	ZKM	C45-C46-C47-C48
6	A	704	ZKM	O38-C37-C39-C40
6	A	703	ZKM	C02-C15-O16-C17
6	A	703	ZKM	C27-C28-C29-C30
6	C	203	ZKM	C22-C23-C24-C25
6	A	704	ZKM	C23-C24-C25-C26
6	A	703	ZKM	C28-C29-C30-C31
6	A	703	ZKM	C29-C30-C31-C32
6	C	203	ZKM	C46-C47-C48-C49
6	A	704	ZKM	C41-C42-C43-C44
6	C	203	ZKM	C42-C43-C44-C45
6	A	704	ZKM	C30-C31-C32-C33
6	C	203	ZKM	C31-C32-C33-C34
6	A	704	ZKM	C17-C18-N19-C20
6	A	704	ZKM	C20-C21-C22-C23
6	A	703	ZKM	C21-C22-C23-C24
6	A	704	ZKM	C29-C30-C31-C32
6	A	704	ZKM	C40-C41-C42-C43
6	A	703	ZKM	C47-C48-C49-C50
6	C	203	ZKM	C21-C22-C23-C24
6	C	203	ZKM	C45-C46-C47-C48
6	A	704	ZKM	C03-O04-S05-O07
6	C	203	ZKM	C03-O04-S05-O07
6	C	203	ZKM	C03-O04-S05-O08
6	A	703	ZKM	N19-C20-C21-C22
6	A	703	ZKM	C46-C47-C48-C49

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Mol	Chain	Res	Type	Atoms
6	A	704	ZKM	C21-C22-C23-C24
6	A	704	ZKM	C47-C48-C49-C50
6	A	703	ZKM	O36-C20-C21-C22
6	A	703	ZKM	C49-C50-C51-C52
6	A	704	ZKM	C22-C23-C24-C25
6	A	704	ZKM	C32-C33-C34-C35
6	A	703	ZKM	O38-C37-C39-C40
6	C	203	ZKM	C50-C51-C52-C53
6	A	703	ZKM	C48-C49-C50-C51
6	A	703	ZKM	C32-C33-C34-C35
6	A	704	ZKM	C27-C28-C29-C30
6	A	703	ZKM	C50-C51-C52-C53
6	A	704	ZKM	C46-C47-C48-C49
6	A	704	ZKM	C48-C49-C50-C51
6	C	203	ZKM	C41-C42-C43-C44
6	A	704	ZKM	C03-O04-S05-O06
6	A	704	ZKM	N19-C18-C37-O38
6	A	703	ZKM	C40-C41-C42-C43
6	C	203	ZKM	C28-C29-C30-C31
6	C	203	ZKM	C29-C30-C31-C32
6	A	704	ZKM	C37-C18-N19-C20
6	C	203	ZKM	C09-C11-C12-O13
6	A	703	ZKM	O16-C17-C18-N19
6	A	704	ZKM	O16-C17-C18-N19
6	C	203	ZKM	O16-C17-C18-N19
6	A	703	ZKM	O16-C17-C18-C37
6	C	203	ZKM	C17-C18-C37-O38
6	A	703	ZKM	C23-C24-C25-C26
6	C	203	ZKM	O38-C37-C39-C40
6	C	203	ZKM	C48-C49-C50-C51
6	A	703	ZKM	C03-O04-S05-O08
5	A	702	NAG	C4-C5-C6-O6
6	A	704	ZKM	C43-C44-C45-C46
6	C	203	ZKM	C44-C45-C46-C47
6	A	703	ZKM	C44-C45-C46-C47
6	A	703	ZKM	C43-C44-C45-C46
6	A	704	ZKM	C18-C17-O16-C15
6	C	203	ZKM	C18-C37-C39-C40
6	A	704	ZKM	C39-C40-C41-C42
6	A	703	ZKM	N19-C18-C37-C39
6	A	704	ZKM	N19-C18-C37-C39
6	A	704	ZKM	C03-O04-S05-O08

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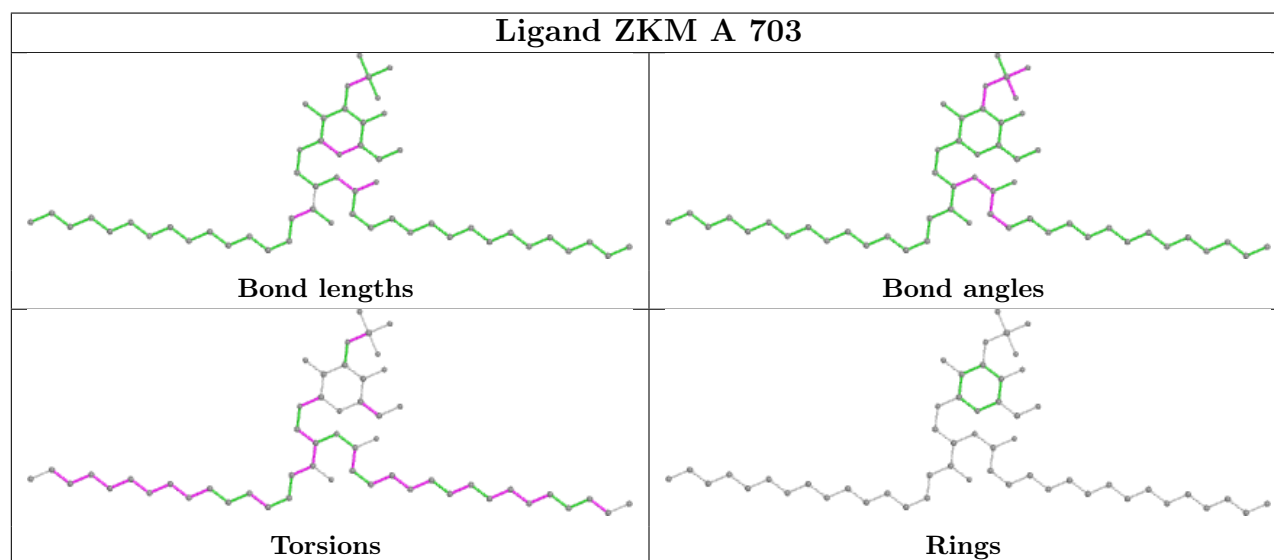
Mol	Chain	Res	Type	Atoms
6	C	203	ZKM	N19-C18-C37-C39
6	C	203	ZKM	C47-C48-C49-C50
6	A	703	ZKM	C22-C23-C24-C25
6	C	203	ZKM	C43-C44-C45-C46

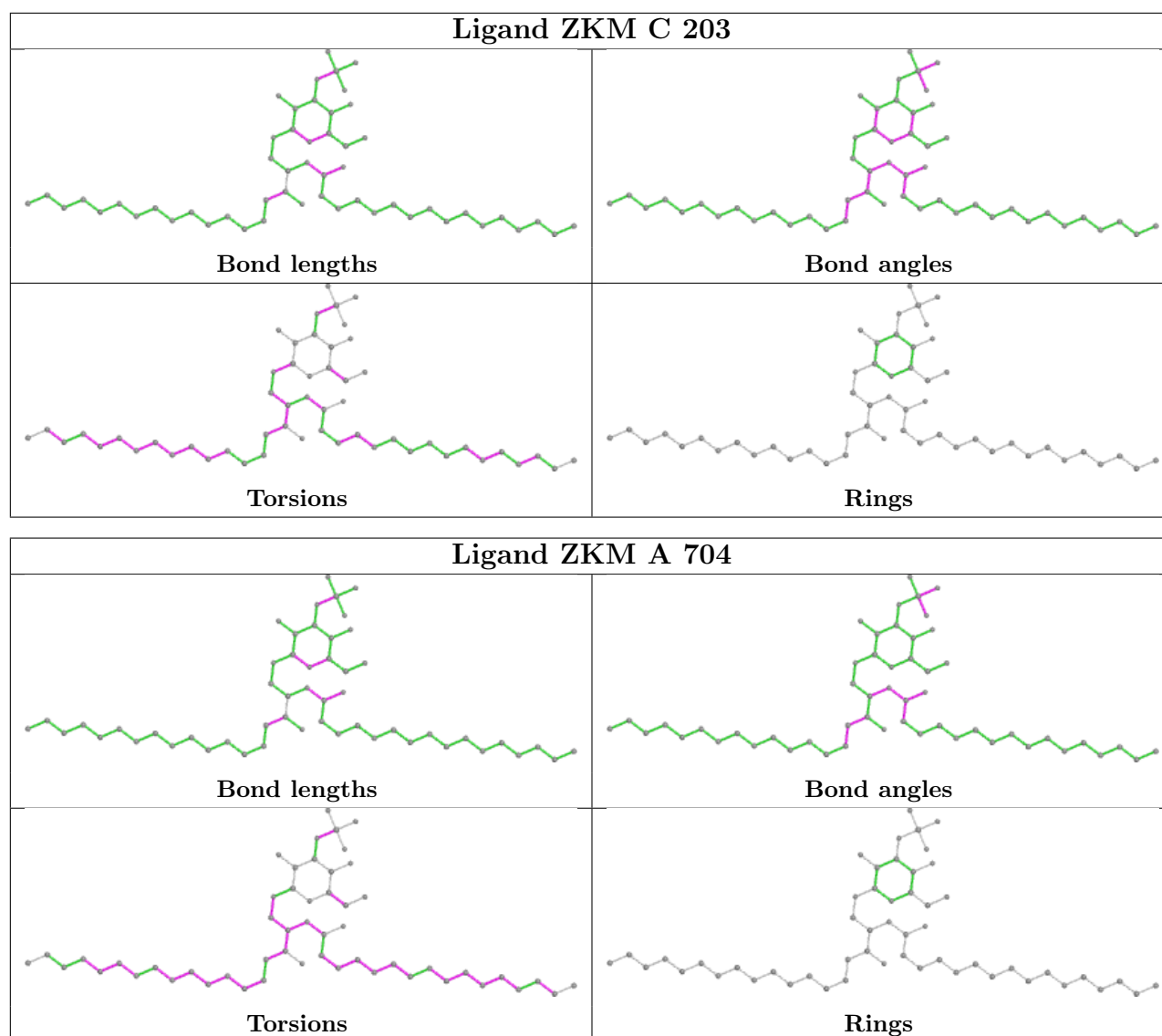
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	202	NAG	2	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	590/635 (92%)	-0.04	13 (2%) 62 66	17, 32, 60, 80	0
2	C	136/188 (72%)	-0.12	3 (2%) 62 66	18, 34, 55, 79	0
All	All	726/823 (88%)	-0.06	16 (2%) 62 66	17, 33, 59, 80	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	269	GLU	4.1
1	A	49	ASP	4.0
1	A	270	ILE	3.6
1	A	50	ASP	3.2
1	A	51	ILE	3.1
2	C	156	ARG	3.1
1	A	616	ILE	2.9
1	A	610	LYS	2.9
1	A	300	VAL	2.6
1	A	532	PHE	2.3
1	A	614	SER	2.3
1	A	47	VAL	2.3
2	C	123	GLY	2.3
1	A	35	ILE	2.2
1	A	46	LYS	2.1
2	C	55	ARG	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

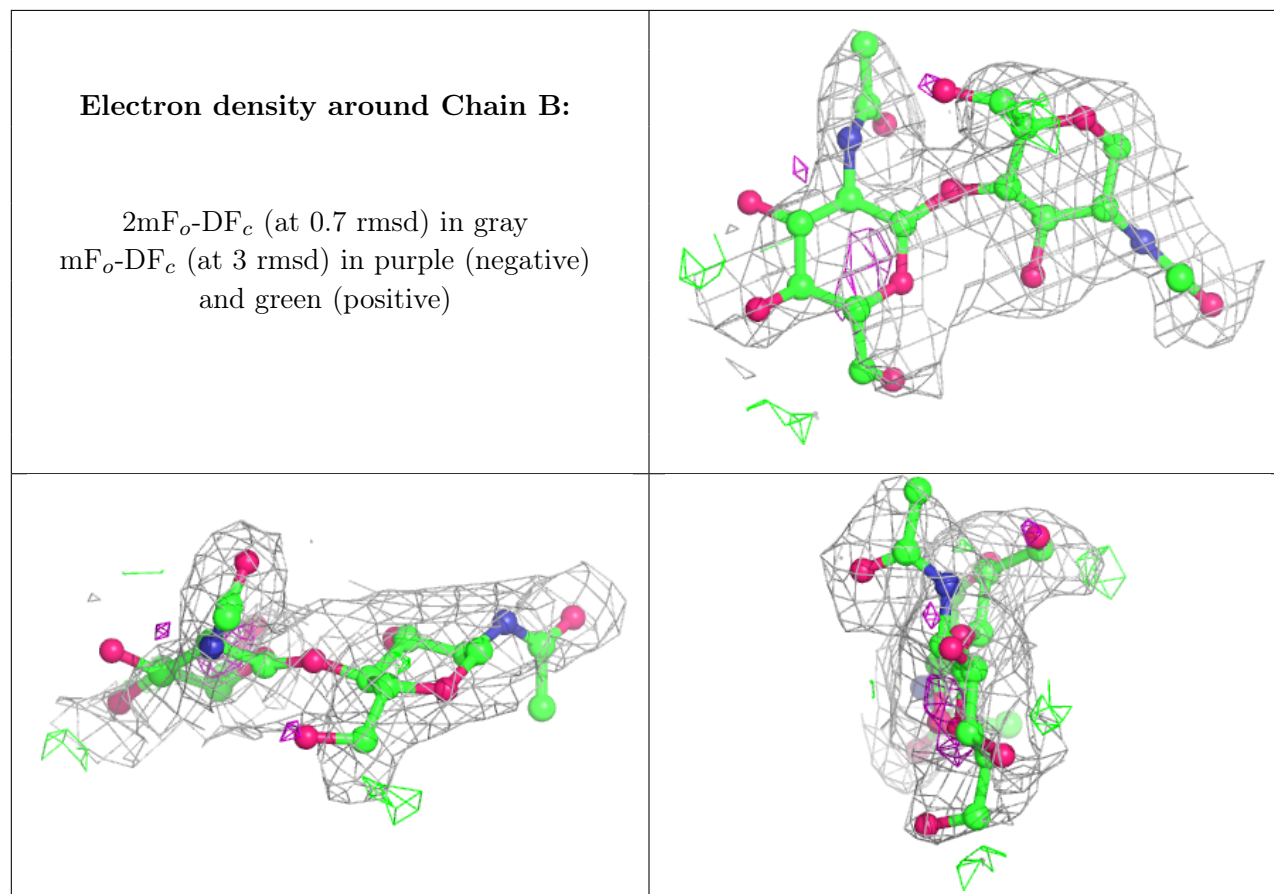
There are no non-standard protein/DNA/RNA residues in this entry.

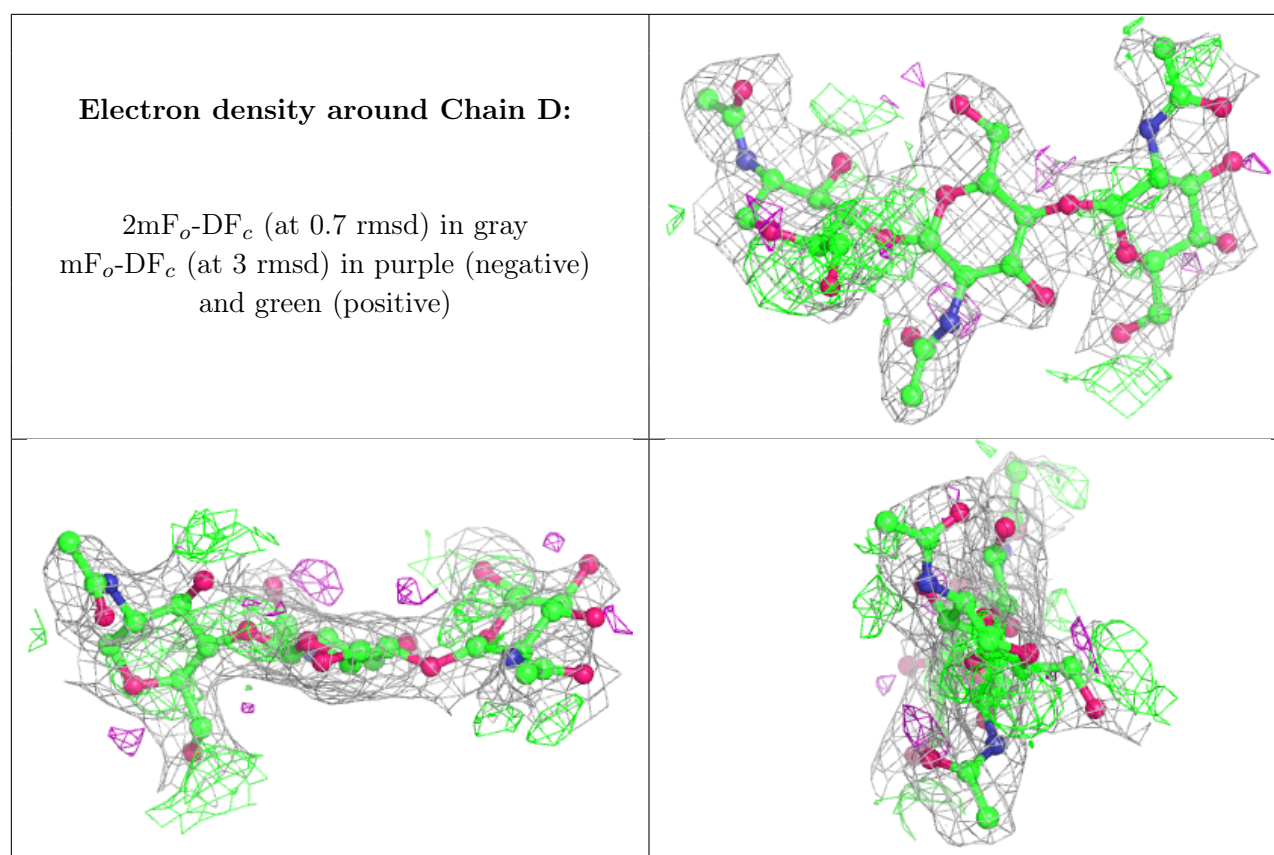
### 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NAG	B	2	14/15	0.72	0.25	40,75,82,83	0
4	NAG	D	1	14/15	0.73	0.22	49,54,59,66	0
4	NAG	D	3	14/15	0.80	0.19	52,66,72,75	0
4	NAG	D	2	14/15	0.86	0.17	48,57,61,66	0
3	NAG	B	1	14/15	0.87	0.18	44,56,75,79	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.





## 6.4 Ligands [i](#)

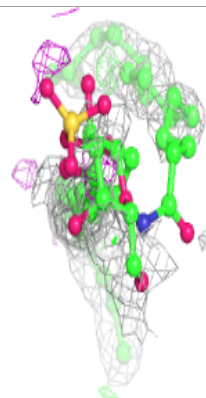
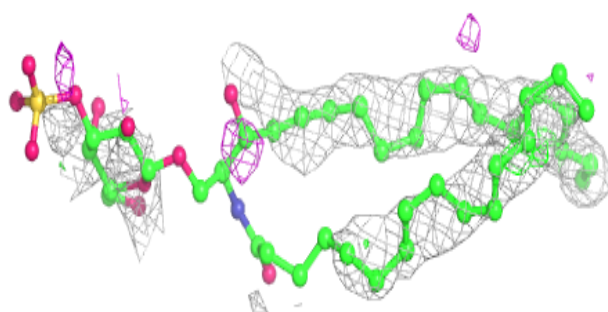
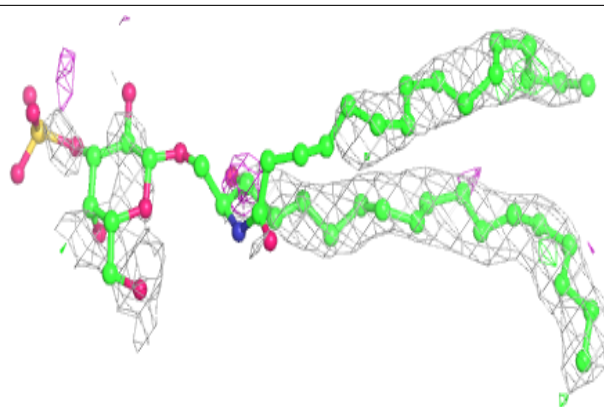
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	ZKM	A	704	53/53	0.65	0.39	38,81,147,150	0
6	ZKM	A	703	53/53	0.67	0.27	40,87,151,153	0
5	NAG	A	701	14/15	0.67	0.28	56,66,79,81	0
6	ZKM	C	203	53/53	0.76	0.22	37,67,142,144	0
5	NAG	C	201	14/15	0.78	0.24	56,67,69,74	0
5	NAG	C	202	14/15	0.85	0.15	42,50,57,59	0
5	NAG	A	702	14/15	0.87	0.14	43,51,57,60	0

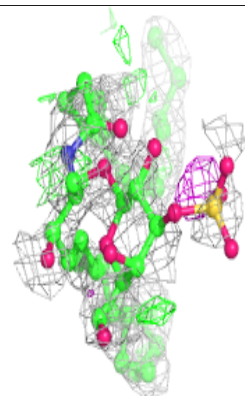
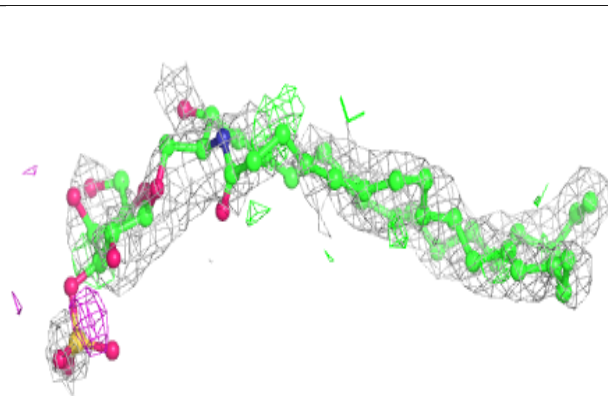
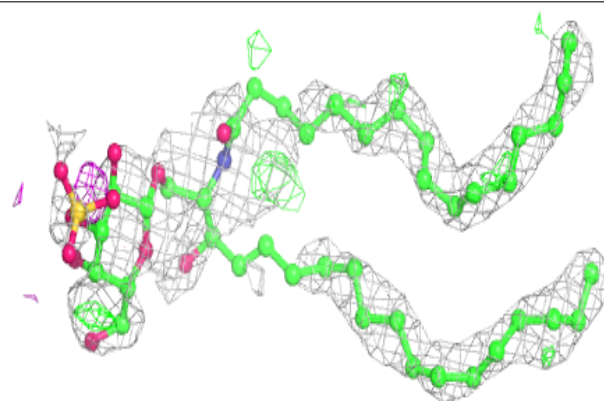
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

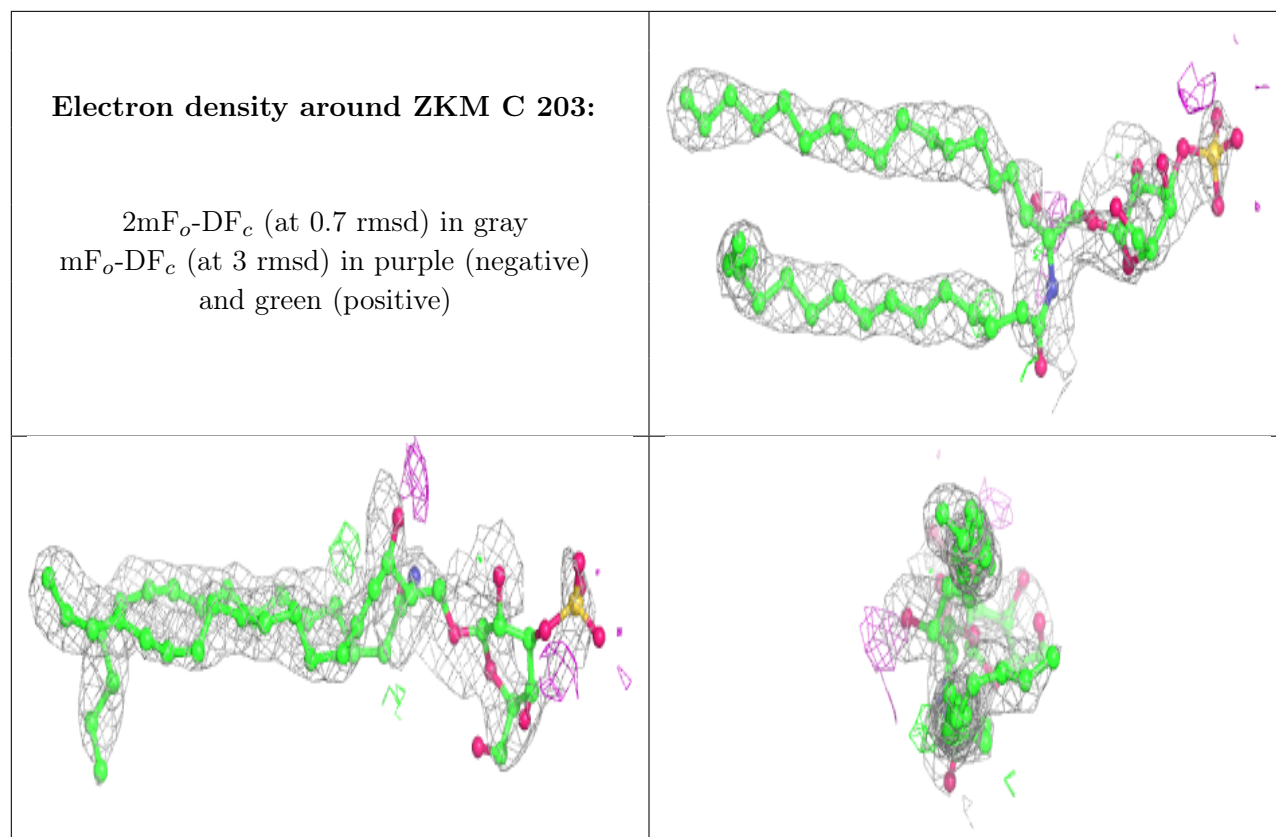
**Electron density around ZKM A 704:**

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

**Electron density around ZKM A 703:**

$2mF_o-DF_c$  (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.