



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 09:39 AM BST

PDB ID : 6Q6L  
Title : Crystal structure of recombinant human beta-glucocerebrosidase in complex with adamantyl-cyclophellitol inhibitor (ME656)  
Authors : Rowland, R.J.; Davies, G.J.  
Deposited on : 2018-12-11  
Resolution : 1.81 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 : 2.13.1  
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) : 2.13.1

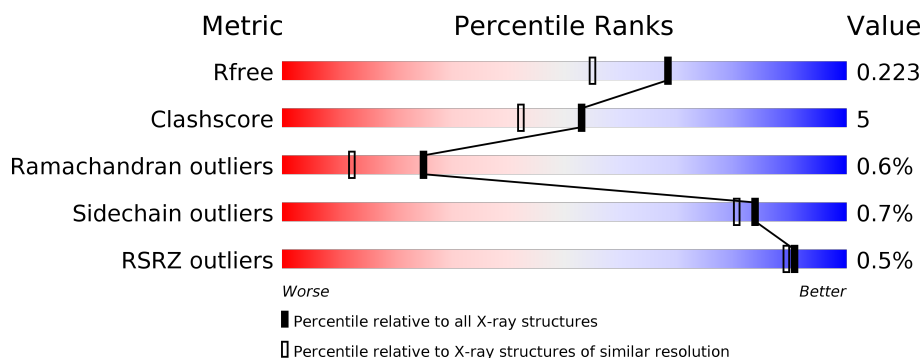
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



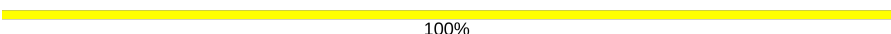
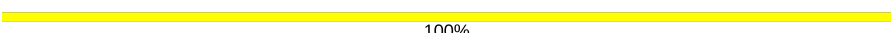
The reported resolution of this entry is 1.81 Å.

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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	497	 92% 8%
1	B	497	 88% 11%
2	C	2	 100%
3	D	3	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ACT	A	509	-	-	X	-
5	ACT	A	526	-	-	X	-
5	ACT	B	517	-	-	X	-
5	ACT	B	518	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9230 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 Glucosylceramidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	6	0
			3965	2553	678	718	16			
1	B	495	Total	C	N	O	S	0	9	0
			3995	2578	682	719	16			

There are 2 discrepancies between the modelled and reference sequences:

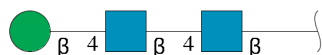
Chain	Residue	Modelled	Actual	Comment	Reference
A	495	HIS	ARG	variant	UNP P04062
B	495	HIS	ARG	variant	UNP P04062

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

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(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
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



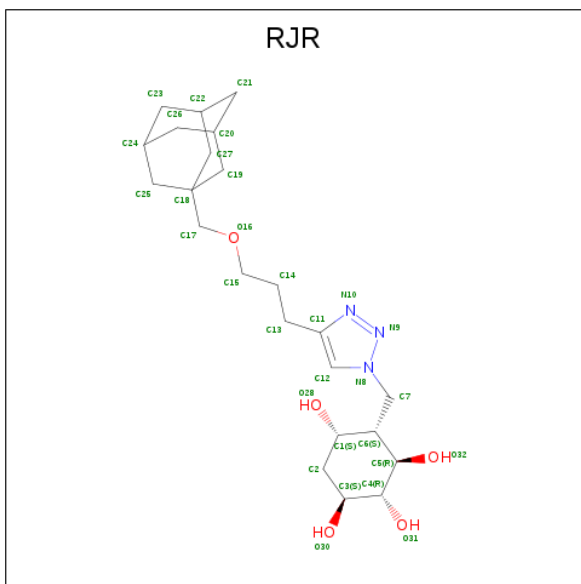
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0

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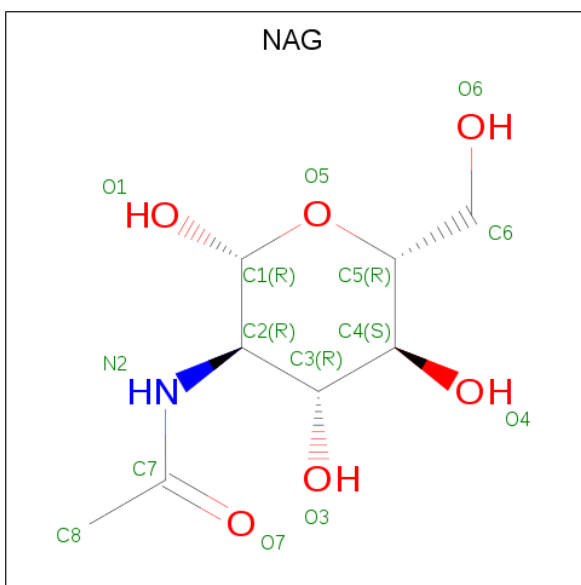
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0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

- Molecule 6 is (1 {S},2 {R},3 {R},4 {S},5 {S})-4-[[4-[3-(1-adamantylmethoxy)propyl]-1,2,3-triazol-1-yl]methyl]cyclohexane-1,2,3,5-tetrol (three-letter code: RJR) (formula:  $C_{23}H_{37}N_3O_5$ ) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			31	23	3	5		
6	B	1	Total	C	N	O	0	0
			31	23	3	5		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).





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

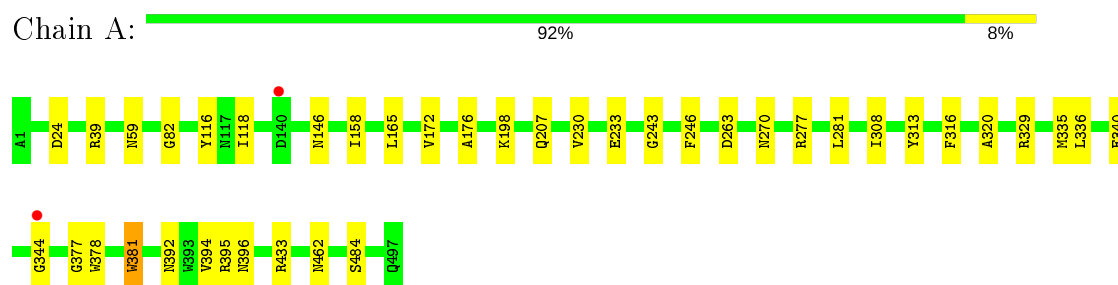
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	497	Total	O	0	0
			497	497		
8	B	439	Total	O	0	0
			439	439		

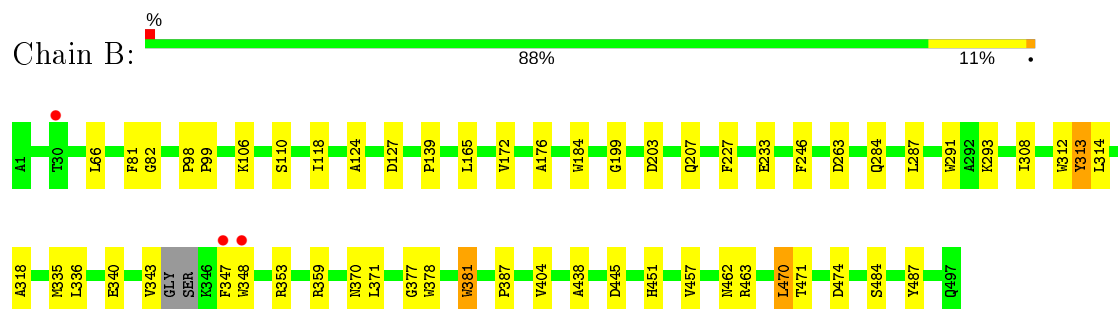
### 3 Residue-property plots [i](#)

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.

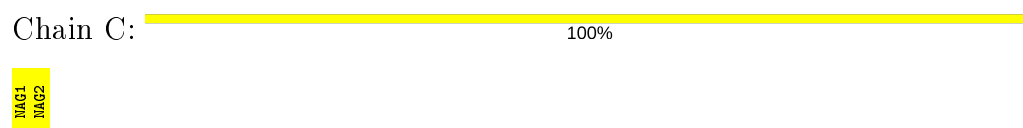
- Molecule 1: Glucosylceramidase



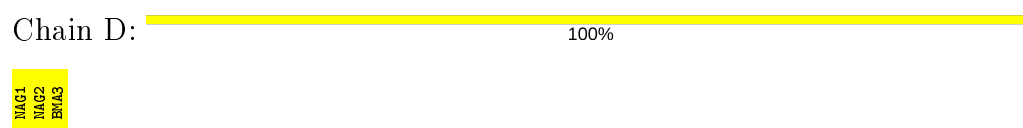
- Molecule 1: Glucosylceramidase



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



- Molecule 3: beta-D-mannopyranose-(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, $\alpha$ , $\beta$ , $\gamma$	110.21Å 285.13Å 92.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.08 – 1.81 71.98 – 1.81	Depositor EDS
% Data completeness (in resolution range)	99.9 (72.08-1.81) 99.9 (71.98-1.81)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.176 , 0.210 0.191 , 0.223	Depositor DCC
$R_{free}$ test set	6547 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.8	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9230	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, BMA, NAG, RJR, SO4

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	0.77	2/4086 (0.0%)	0.84	2/5572 (0.0%)
1	B	0.74	1/4119 (0.0%)	0.82	1/5617 (0.0%)
All	All	0.76	3/8205 (0.0%)	0.83	3/11189 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	340	GLU	CD-OE2	17.61	1.45	1.25
1	B	340	GLU	CD-OE2	14.38	1.41	1.25
1	A	340	GLU	CD-OE1	7.13	1.33	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	284	GLN	CB-CA-C	7.05	124.50	110.40
1	A	433	ARG	NE-CZ-NH1	-6.47	117.06	120.30
1	A	433	ARG	NE-CZ-NH2	5.46	123.03	120.30

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	A	3965	0	3860	31	0
1	B	3995	0	3887	52	0
2	C	28	0	25	0	0
3	D	39	0	34	0	0
4	A	60	0	0	1	0
4	B	35	0	0	1	0
5	A	44	0	33	9	0
5	B	52	0	39	7	0
6	A	31	0	0	0	0
6	B	31	0	0	0	0
7	B	14	0	13	0	0
8	A	497	0	0	9	0
8	B	439	0	0	5	0
All	All	9230	0	7891	88	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 5.

All (88) 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:277:ARG:NH1	4:A:518:SO4:O4	2.06	0.88
1:A:207:GLN:NE2	1:A:263:ASP:OD1	2.07	0.87
5:A:526:ACT:H3	8:A:914:HOH:O	1.76	0.86
1:A:392[A]:ASN:ND2	1:A:396:ASN:OD1	2.12	0.82
4:B:516:SO4:O3	8:B:601:HOH:O	1.97	0.81
1:A:243:GLY:O	1:B:348:TRP:CZ3	2.33	0.81
1:B:371:LEU:CD2	1:B:378[B]:TRP:CZ2	2.68	0.77
1:B:378[B]:TRP:N	1:B:378[B]:TRP:CE3	2.58	0.71
1:B:81:PHE:CE2	1:B:378[B]:TRP:CE3	2.79	0.70
1:B:377:GLY:HA2	1:B:378[B]:TRP:CE3	2.26	0.70
1:B:371:LEU:HD21	1:B:378[B]:TRP:CH2	2.26	0.70
1:B:377:GLY:HA2	1:B:378[B]:TRP:CZ3	2.26	0.70
1:B:371:LEU:HD21	1:B:378[B]:TRP:CZ2	2.26	0.69
1:A:59:ASN:HB3	8:A:1009:HOH:O	1.91	0.69
1:B:377:GLY:C	1:B:378[B]:TRP:CD2	2.68	0.66
5:A:524:ACT:H3	8:A:832:HOH:O	1.95	0.66
1:B:451:HIS:NE2	1:B:457[B]:VAL:CG2	2.58	0.66
1:B:378[B]:TRP:CD2	1:B:378[B]:TRP:N	2.65	0.64
1:A:270:ASN:ND2	8:A:603:HOH:O	2.32	0.62
1:B:312:TRP:CZ2	1:B:318:ALA:HB2	2.35	0.61
1:B:371:LEU:HD23	1:B:378[B]:TRP:HZ2	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:HIS:NE2	1:B:457[B]:VAL:HG21	2.16	0.61
1:A:320:ALA:H	5:A:525:ACT:H1	1.64	0.61
1:B:438:ALA:HB2	5:B:522:ACT:H3	1.81	0.60
5:A:526:ACT:H1	8:A:698:HOH:O	2.01	0.60
1:B:371:LEU:HD23	1:B:378[B]:TRP:CZ2	2.36	0.60
1:B:377:GLY:CA	1:B:378[B]:TRP:CE3	2.85	0.60
1:B:377:GLY:C	1:B:378[B]:TRP:CE3	2.76	0.59
1:A:165:LEU:HD22	1:A:172:VAL:HB	1.84	0.58
1:A:158:ILE:HG22	5:A:526:ACT:H2	1.86	0.57
1:B:313:TYR:CD2	1:B:313:TYR:N	2.73	0.56
1:B:207:GLN:OE1	1:B:263:ASP:OD1	2.27	0.53
5:B:518:ACT:CH3	8:B:799:HOH:O	2.56	0.53
1:A:24:ASP:OD2	5:A:520:ACT:H1	2.09	0.52
1:A:329:ARG:HH12	5:A:509:ACT:H2	1.74	0.52
5:B:509:ACT:H2	8:B:864:HOH:O	2.09	0.52
1:A:392[A]:ASN:CG	1:A:396:ASN:OD1	2.49	0.51
1:A:39[C]:ARG:CZ	8:A:620:HOH:O	2.58	0.51
1:B:312:TRP:CH2	1:B:318:ALA:HB2	2.45	0.51
1:B:81:PHE:CZ	1:B:378[B]:TRP:CZ3	2.99	0.51
1:B:165:LEU:HD22	1:B:172:VAL:HB	1.92	0.50
1:B:381:TRP:CE3	1:B:381:TRP:HA	2.47	0.50
1:B:98:PRO:HB2	1:B:99:PRO:HD3	1.94	0.49
5:B:517:ACT:H1	8:B:921:HOH:O	2.13	0.48
1:A:207:GLN:HE22	1:A:263:ASP:HA	1.79	0.48
1:B:308:ILE:HB	1:B:336:LEU:HD23	1.97	0.47
1:A:316:PHE:O	8:A:601:HOH:O	2.20	0.47
1:B:66:LEU:HD12	1:B:471:THR:HB	1.97	0.47
1:A:243:GLY:C	1:B:348:TRP:CZ3	2.89	0.46
1:A:82:GLY:HA2	1:A:116:TYR:CD2	2.51	0.46
1:B:314:LEU:HB2	1:B:343:VAL:HG13	1.97	0.45
1:B:387:PRO:HD3	1:B:404:VAL:O	2.17	0.45
1:B:462:ASN:HB2	1:B:484:SER:OG	2.16	0.45
1:B:445:ASP:OD2	1:B:463[A]:ARG:NH1	2.50	0.45
1:B:470:LEU:N	1:B:470:LEU:CD1	2.79	0.45
1:B:81:PHE:CZ	1:B:378[B]:TRP:CE3	3.04	0.45
1:B:381:TRP:HE3	1:B:381:TRP:HA	1.81	0.45
1:B:127:ASP:HB3	1:B:246:PHE:CG	2.52	0.44
5:B:518:ACT:H2	8:B:799:HOH:O	2.17	0.44
1:A:246:PHE:HB3	1:A:394[A]:VAL:HG21	2.00	0.43
1:A:308:ILE:HB	1:A:336:LEU:HD23	2.01	0.43
1:B:353:ARG:HG3	1:B:359:ARG:CZ	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:LYS:O	1:B:110:SER:HB3	2.18	0.43
1:A:39[C]:ARG:NE	8:A:620:HOH:O	2.51	0.43
1:B:176:ALA:HB2	1:B:227:PHE:CE2	2.54	0.43
1:B:313:TYR:N	1:B:313:TYR:HD2	2.16	0.43
1:A:146:ASN:ND2	8:A:612:HOH:O	2.45	0.42
1:A:381:TRP:HA	1:A:381:TRP:CE3	2.55	0.42
1:A:243:GLY:HA3	1:B:348:TRP:HZ3	1.85	0.42
1:B:199:GLY:HA3	1:B:203:ASP:OD2	2.20	0.42
1:B:287:LEU:HB3	1:B:291:TRP:CD1	2.55	0.41
1:B:463[A]:ARG:O	1:B:487[A]:TYR:HE1	2.03	0.41
1:B:82:GLY:HA3	1:B:118[B]:ILE:O	2.20	0.41
1:A:462:ASN:HB2	1:A:484:SER:OG	2.21	0.41
1:A:377:GLY:HA2	1:A:378:TRP:CE3	2.56	0.41
1:B:139:PRO:HA	1:B:184:TRP:CD1	2.56	0.41
1:B:313:TYR:HB3	5:B:523:ACT:H3	2.02	0.41
1:B:377:GLY:CA	1:B:378[B]:TRP:CZ3	2.99	0.41
1:B:314:LEU:HB2	1:B:343:VAL:CG1	2.51	0.41
1:B:293:LYS:HE2	5:B:517:ACT:H3	2.03	0.41
1:A:198:LYS:HG2	5:A:523:ACT:H3	2.02	0.40
1:A:313:TYR:CE1	1:A:344:GLY:HA2	2.57	0.40
1:A:329:ARG:HH12	5:A:509:ACT:CH3	2.34	0.40
1:B:370:ASN:HB3	1:B:378[B]:TRP:HE1	1.87	0.40
1:A:82:GLY:HA3	1:A:118:ILE:O	2.22	0.40
1:B:474:ASP:C	1:B:474:ASP:OD1	2.60	0.40
1:A:176:ALA:O	1:A:230:VAL:HA	2.21	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	501/497 (101%)	478 (95%)	20 (4%)	3 (1%)	25 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	500/497 (101%)	481 (96%)	16 (3%)	3 (1%)	25	12
All	All	1001/994 (101%)	959 (96%)	36 (4%)	6 (1%)	25	12

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	GLU
1	B	347	PHE
1	A	395	ARG
1	B	233	GLU
1	A	281	LEU
1	B	124	ALA

### 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	425/424 (100%)	423 (100%)	2 (0%)	88	87
1	B	429/424 (101%)	425 (99%)	4 (1%)	78	74
All	All	854/848 (101%)	848 (99%)	6 (1%)	84	80

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	335	MET
1	A	381	TRP
1	B	313	TYR
1	B	335	MET
1	B	381	TRP
1	B	470	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:



Mol	Chain	Res	Type
1	B	70	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 ⓘ

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	$\# Z  > 2$
2	NAG	C	1	1,2	14,14,15	0.74	0	17,19,21	1.63	5 (29%)
2	NAG	C	2	2	14,14,15	0.63	0	17,19,21	1.23	2 (11%)
3	NAG	D	1	1,3	14,14,15	0.63	0	17,19,21	1.36	3 (17%)
3	NAG	D	2	3	14,14,15	0.58	0	17,19,21	1.52	3 (17%)
3	BMA	D	3	3	11,11,12	0.47	0	15,15,17	0.95	1 (6%)

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	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	O5-C1-C2	-4.38	104.37	111.29
3	D	1	NAG	O5-C5-C6	3.64	112.91	107.20
3	D	2	NAG	O5-C1-C2	-3.42	105.88	111.29
3	D	2	NAG	C2-N2-C7	-3.21	118.33	122.90
3	D	2	NAG	C1-C2-N2	2.56	114.87	110.49
3	D	3	BMA	O5-C5-C6	2.55	111.20	107.20
3	D	1	NAG	O4-C4-C5	-2.45	103.21	109.30
3	D	1	NAG	O5-C1-C2	-2.45	107.42	111.29
2	C	2	NAG	C1-C2-N2	2.43	114.64	110.49
2	C	1	NAG	O5-C5-C6	2.35	110.88	107.20
2	C	2	NAG	O4-C4-C5	2.24	114.86	109.30
2	C	1	NAG	C3-C4-C5	2.23	114.21	110.24
2	C	1	NAG	C6-C5-C4	-2.16	107.95	113.00
2	C	1	NAG	C1-C2-N2	2.16	114.17	110.49

There are no chirality outliers.

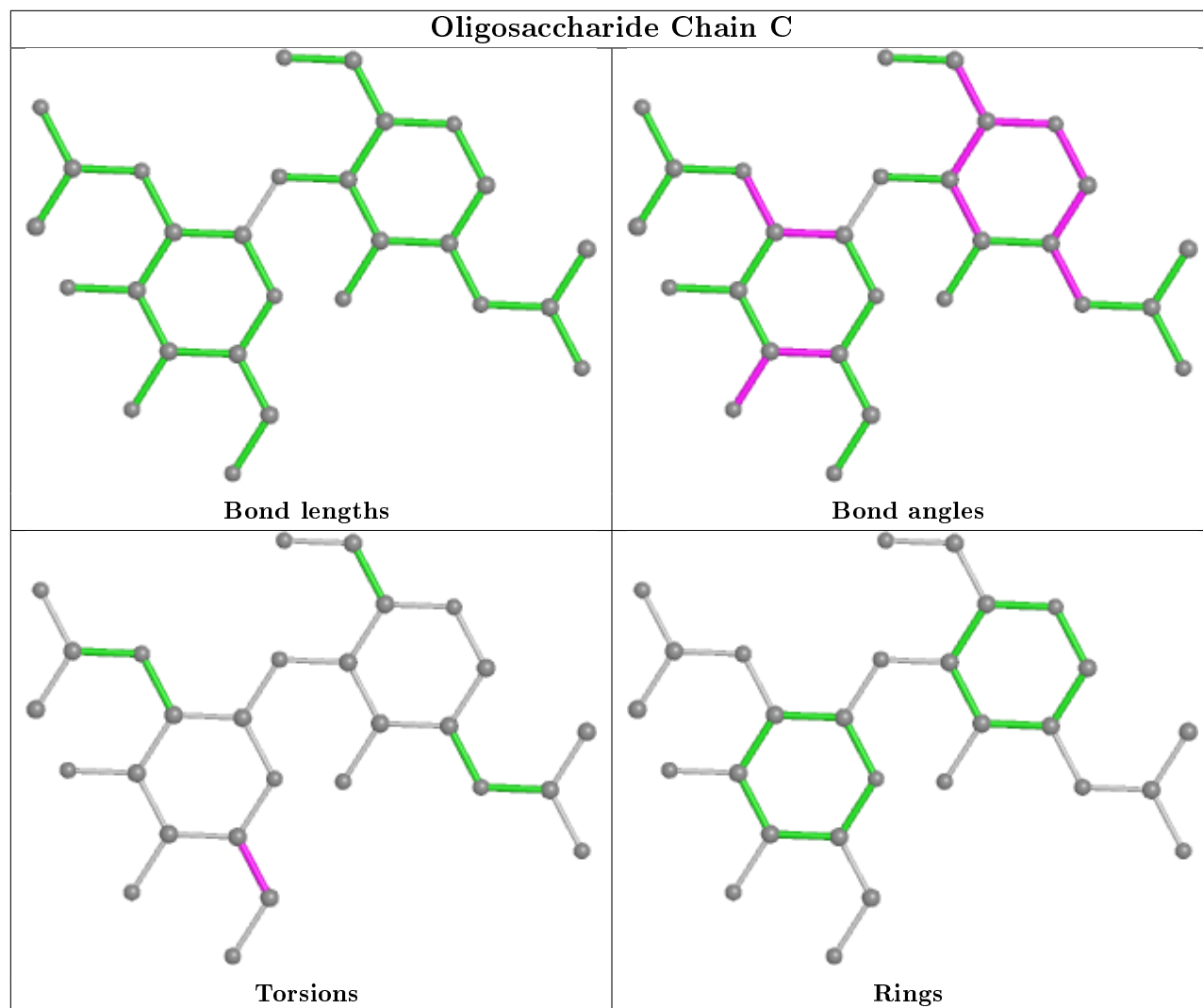
All (4) torsion outliers are listed below:

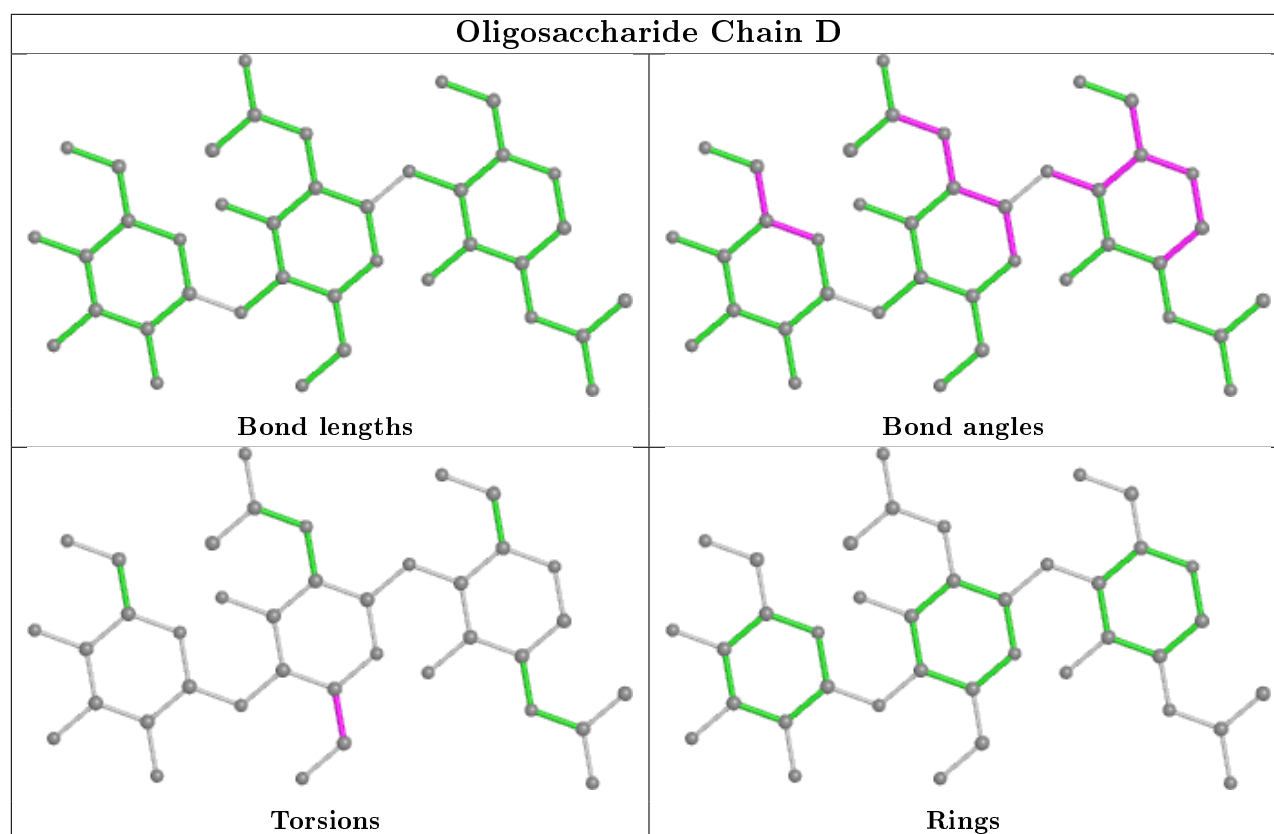
Mol	Chain	Res	Type	Atoms
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6

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](#)

46 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	SO4	A	506	-	4,4,4	0.43	0	6,6,6	0.30	0
4	SO4	A	516	-	4,4,4	0.42	0	6,6,6	0.18	0
4	SO4	B	504	-	4,4,4	0.46	0	6,6,6	0.21	0
5	ACT	A	508	-	1,3,3	0.93	0	0,3,3	0.00	-
5	ACT	B	508	-	1,3,3	5.62	1 (100%)	0,3,3	0.00	-
4	SO4	B	507	-	4,4,4	0.47	0	6,6,6	0.25	0
5	ACT	B	521	-	1,3,3	5.31	1 (100%)	0,3,3	0.00	-
4	SO4	A	518	-	4,4,4	0.45	0	6,6,6	0.20	0
4	SO4	A	512	-	4,4,4	0.33	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	ACT	A	520	-	1,3,3	4.59	1 (100%)	0,3,3	0.00	-
5	ACT	B	524	-	1,3,3	2.41	1 (100%)	0,3,3	0.00	-
5	ACT	B	517	-	1,3,3	3.53	1 (100%)	0,3,3	0.00	-
5	ACT	A	519	-	1,3,3	2.30	1 (100%)	0,3,3	0.00	-
4	SO4	A	515	-	4,4,4	0.57	0	6,6,6	0.27	0
5	ACT	B	520	-	1,3,3	3.72	1 (100%)	0,3,3	0.00	-
5	ACT	B	509	-	1,3,3	4.39	1 (100%)	0,3,3	0.00	-
5	ACT	B	511	-	1,3,3	3.98	1 (100%)	0,3,3	0.00	-
5	ACT	A	522	-	1,3,3	4.70	1 (100%)	0,3,3	0.00	-
4	SO4	A	514	-	4,4,4	0.35	0	6,6,6	0.08	0
7	NAG	B	512	1	14,14,15	0.98	0	17,19,21	1.29	1 (5%)
5	ACT	B	522	-	1,3,3	4.73	1 (100%)	0,3,3	0.00	-
4	SO4	A	507	-	4,4,4	0.39	0	6,6,6	0.27	0
4	SO4	B	506	-	4,4,4	0.40	0	6,6,6	0.15	0
4	SO4	A	517	-	4,4,4	0.37	0	6,6,6	0.14	0
5	ACT	B	525	-	1,3,3	4.09	1 (100%)	0,3,3	0.00	-
6	RJR	B	513	1	34,35,35	1.36	4 (11%)	42,52,52	1.18	3 (7%)
4	SO4	B	516	-	4,4,4	0.67	0	6,6,6	0.11	0
5	ACT	B	510	-	1,3,3	3.62	1 (100%)	0,3,3	0.00	-
5	ACT	A	510	-	1,3,3	3.26	1 (100%)	0,3,3	0.00	-
5	ACT	A	523	-	1,3,3	5.18	1 (100%)	0,3,3	0.00	-
5	ACT	A	521	-	1,3,3	5.75	1 (100%)	0,3,3	0.00	-
5	ACT	B	523	-	1,3,3	4.69	1 (100%)	0,3,3	0.00	-
4	SO4	A	511	-	4,4,4	0.27	0	6,6,6	0.20	0
5	ACT	A	525	-	1,3,3	1.91	0	0,3,3	0.00	-
4	SO4	B	514	-	4,4,4	0.37	0	6,6,6	0.08	0
5	ACT	A	526	-	1,3,3	0.30	0	0,3,3	0.00	-
4	SO4	A	505	-	4,4,4	0.39	0	6,6,6	0.23	0
5	ACT	B	519	-	1,3,3	3.55	1 (100%)	0,3,3	0.00	-
5	ACT	A	524	-	1,3,3	6.13	1 (100%)	0,3,3	0.00	-
4	SO4	B	515	-	4,4,4	0.42	0	6,6,6	0.09	0
6	RJR	A	513	1	34,35,35	0.94	2 (5%)	42,52,52	1.05	2 (4%)
4	SO4	A	503	-	4,4,4	0.50	0	6,6,6	0.34	0
5	ACT	A	509	-	1,3,3	1.45	0	0,3,3	0.00	-
5	ACT	B	518	-	1,3,3	0.39	0	0,3,3	0.00	-
4	SO4	A	504	-	4,4,4	0.42	0	6,6,6	0.28	0
4	SO4	B	505	-	4,4,4	0.38	0	6,6,6	0.24	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
7	NAG	B	512	1	-	1/6/23/26	0/1/1/1
6	RJR	A	513	1	-	7/13/60/60	0/6/5/5
6	RJR	B	513	1	-	5/13/60/60	0/6/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	524	ACT	CH3-C	6.13	1.56	1.48
5	A	521	ACT	CH3-C	5.75	1.56	1.48
5	B	508	ACT	CH3-C	5.62	1.55	1.48
5	B	521	ACT	CH3-C	5.31	1.55	1.48
5	A	523	ACT	CH3-C	5.18	1.55	1.48
5	B	522	ACT	CH3-C	4.73	1.54	1.48
5	A	522	ACT	CH3-C	4.70	1.54	1.48
5	B	523	ACT	CH3-C	4.69	1.54	1.48
5	A	520	ACT	CH3-C	4.59	1.54	1.48
5	B	509	ACT	CH3-C	4.39	1.54	1.48
6	B	513	RJR	C12-C11	4.23	1.42	1.36
5	B	525	ACT	CH3-C	4.09	1.53	1.48
5	B	511	ACT	CH3-C	3.98	1.53	1.48
6	B	513	RJR	N10-N9	3.79	1.41	1.34
5	B	520	ACT	CH3-C	3.72	1.53	1.48
5	B	510	ACT	CH3-C	3.62	1.53	1.48
6	B	513	RJR	N9-N8	3.61	1.41	1.34
5	B	519	ACT	CH3-C	3.55	1.53	1.48
5	B	517	ACT	CH3-C	3.53	1.53	1.48
5	A	510	ACT	CH3-C	3.26	1.52	1.48
5	B	524	ACT	CH3-C	2.41	1.51	1.48
6	A	513	RJR	N9-N8	2.38	1.39	1.34
5	A	519	ACT	CH3-C	2.30	1.51	1.48
6	A	513	RJR	C12-N8	-2.14	1.33	1.35
6	B	513	RJR	C11-N10	2.04	1.36	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	513	RJR	C7-N8-C12	4.46	140.31	129.82
6	B	513	RJR	C27-C18-C25	-3.47	105.71	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	512	NAG	O7-C7-C8	-2.57	117.28	122.06
6	B	513	RJR	C14-C13-C11	2.54	121.09	113.11
6	B	513	RJR	C7-N8-C12	2.53	135.76	129.82
6	A	513	RJR	N10-N9-N8	-2.11	105.73	107.31

There are no chirality outliers.

All (13) torsion outliers are listed below:

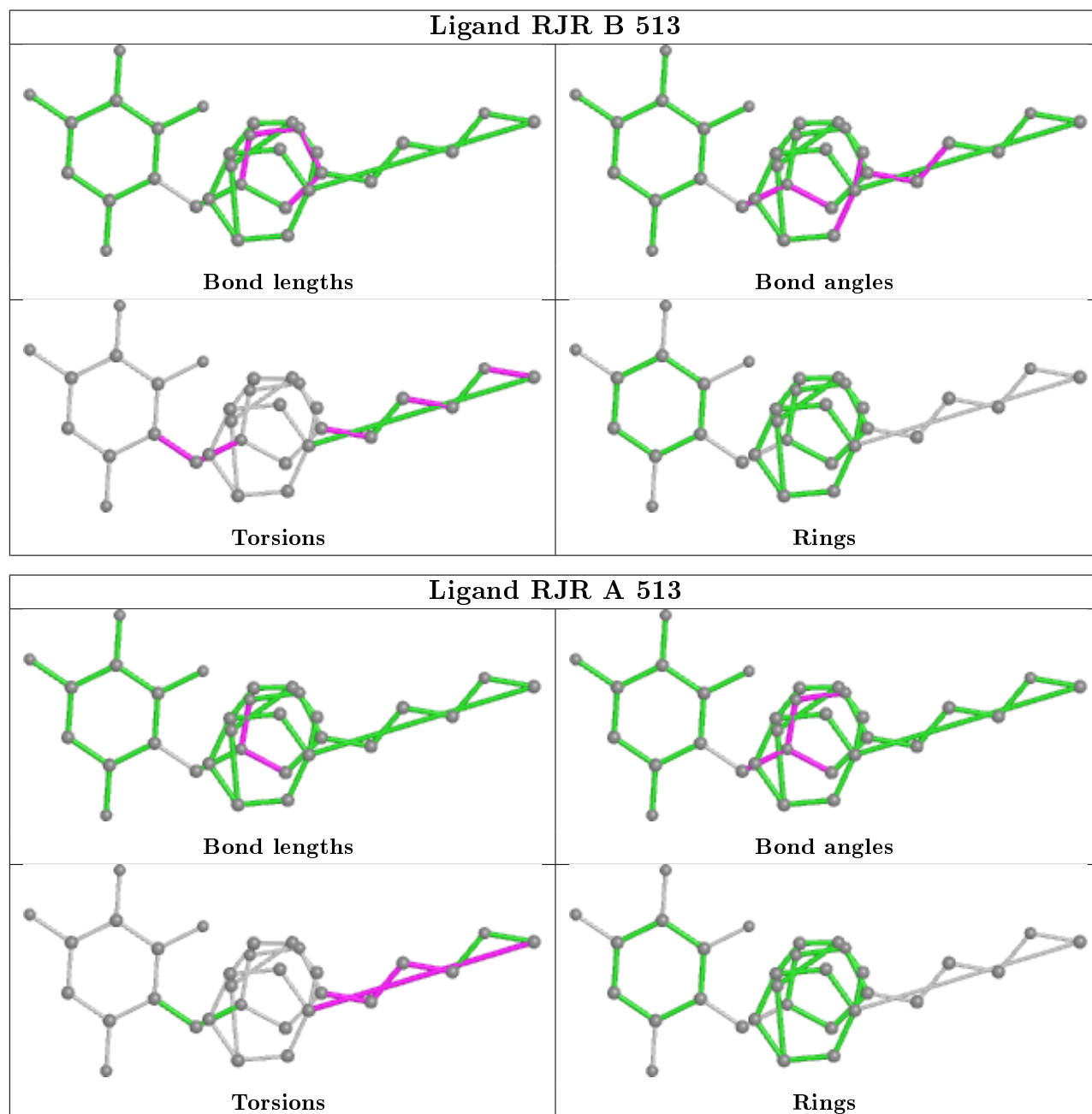
Mol	Chain	Res	Type	Atoms
6	B	513	RJR	N10-C11-C13-C14
6	A	513	RJR	N10-C11-C13-C14
6	A	513	RJR	C12-C11-C13-C14
6	A	513	RJR	O16-C17-C18-C27
6	B	513	RJR	C13-C14-C15-O16
6	A	513	RJR	C13-C14-C15-O16
6	A	513	RJR	O16-C17-C18-C25
6	B	513	RJR	C6-C7-N8-C12
6	B	513	RJR	C18-C17-O16-C15
6	A	513	RJR	O16-C17-C18-C19
6	A	513	RJR	C11-C13-C14-C15
6	B	513	RJR	C1-C6-C7-N8
7	B	512	NAG	C4-C5-C6-O6

There are no ring outliers.

13 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	518	SO4	1	0
5	A	520	ACT	1	0
5	B	517	ACT	2	0
5	B	509	ACT	1	0
5	B	522	ACT	1	0
4	B	516	SO4	1	0
5	A	523	ACT	1	0
5	B	523	ACT	1	0
5	A	525	ACT	1	0
5	A	526	ACT	3	0
5	A	524	ACT	1	0
5	A	509	ACT	2	0
5	B	518	ACT	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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 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	497/497 (100%)	-0.50	2 (0%) 92 91	18, 25, 41, 63	6 (1%)
1	B	495/497 (99%)	-0.45	3 (0%) 89 88	18, 26, 47, 91	7 (1%)
All	All	992/994 (99%)	-0.48	5 (0%) 91 89	18, 25, 44, 91	13 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	ASP	3.7
1	B	347	PHE	2.6
1	A	344	GLY	2.4
1	B	348	TRP	2.4
1	B	30	THR	2.0

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

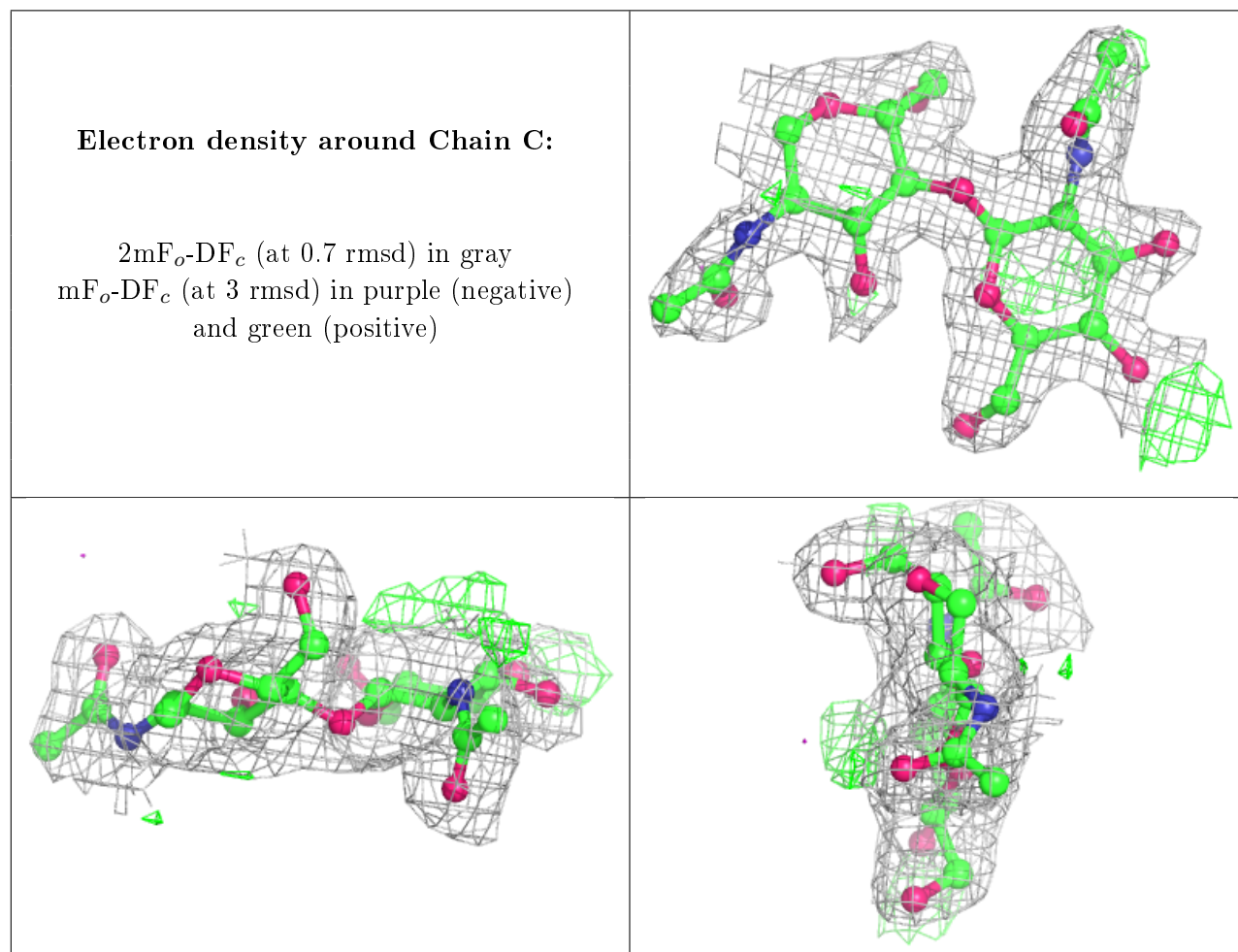
There are no non-standard protein/DNA/RNA residues in this entry.

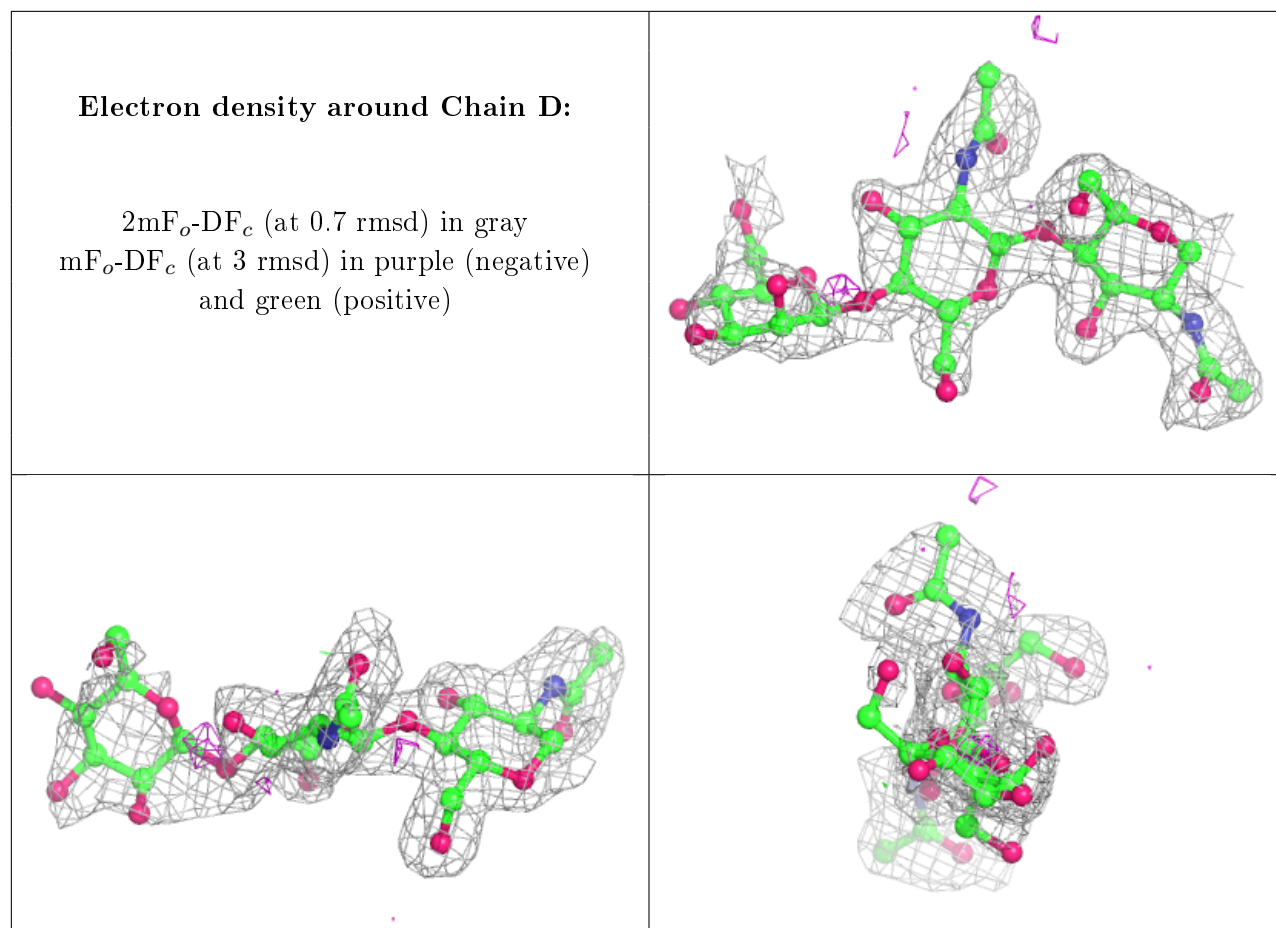
### 6.3 Carbohydrates ⓘ

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, 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	BMA	D	3	11/12	0.64	0.20	102,107,114,115	0
2	NAG	C	2	14/15	0.78	0.13	49,60,67,69	0
3	NAG	D	2	14/15	0.88	0.15	45,62,74,93	0
2	NAG	C	1	14/15	0.90	0.12	32,43,48,50	0
3	NAG	D	1	14/15	0.94	0.07	32,36,47,47	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 ⓘ

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
4	SO4	A	512	5/5	0.69	0.16	86,89,94,108	0
5	ACT	B	524	4/4	0.69	0.19	33,44,48,60	0
7	NAG	B	512	14/15	0.75	0.20	54,64,81,82	0
5	ACT	B	523	4/4	0.75	0.18	53,58,62,66	0
5	ACT	A	519	4/4	0.76	0.13	66,67,70,70	0
5	ACT	B	508	4/4	0.78	0.17	40,49,52,53	0
5	ACT	B	525	4/4	0.78	0.15	59,65,67,73	0
5	ACT	A	522	4/4	0.78	0.14	64,67,68,70	0
5	ACT	A	525	4/4	0.78	0.14	38,49,56,63	0
5	ACT	B	510	4/4	0.80	0.13	48,56,57,64	0
5	ACT	A	526	4/4	0.80	0.23	35,42,56,61	0
5	ACT	A	524	4/4	0.80	0.21	46,47,48,57	0

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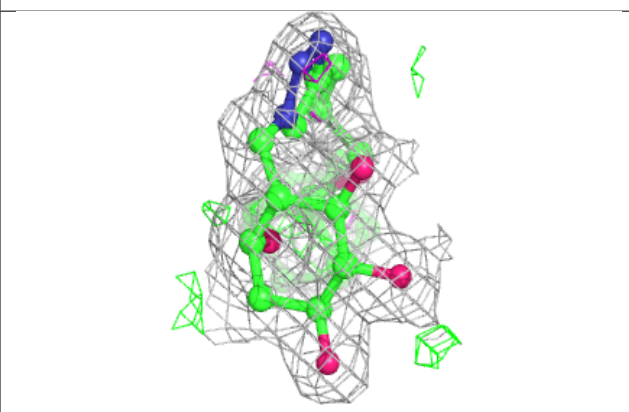
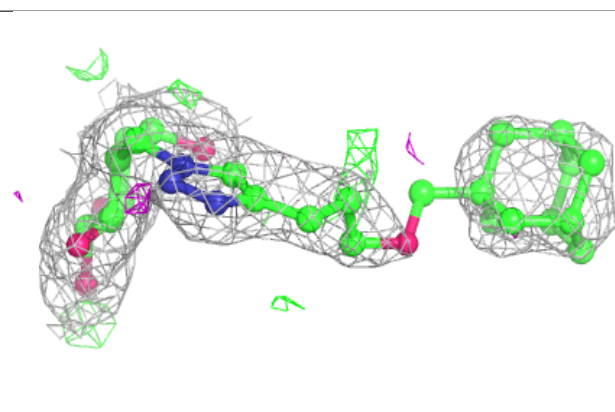
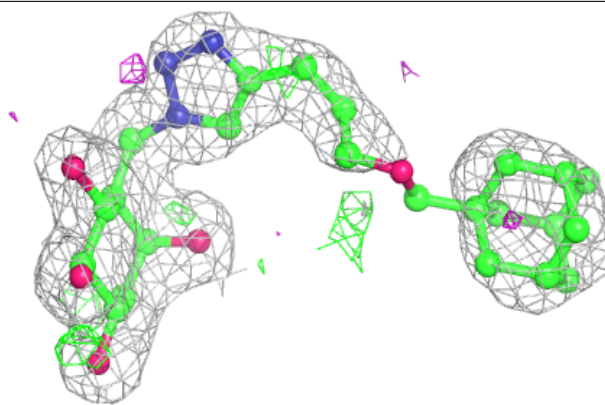
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ACT	B	522	4/4	0.82	0.14	63,64,67,71	0
5	ACT	A	523	4/4	0.82	0.16	49,50,53,61	0
4	SO4	A	517	5/5	0.84	0.21	42,44,48,52	5
4	SO4	A	514	5/5	0.85	0.21	104,105,110,111	0
5	ACT	A	520	4/4	0.86	0.24	39,44,46,53	0
5	ACT	B	520	4/4	0.88	0.14	67,70,70,71	0
5	ACT	A	521	4/4	0.89	0.14	33,34,36,36	0
5	ACT	B	518	4/4	0.89	0.14	44,49,49,56	0
5	ACT	B	511	4/4	0.90	0.18	43,46,52,53	0
5	ACT	B	521	4/4	0.91	0.13	46,53,54,58	0
4	SO4	B	514	5/5	0.91	0.14	44,45,46,51	5
5	ACT	A	509	4/4	0.91	0.15	38,40,40,54	0
5	ACT	B	519	4/4	0.92	0.11	54,54,56,62	0
5	ACT	A	510	4/4	0.92	0.16	54,54,56,57	0
4	SO4	A	511	5/5	0.93	0.11	64,67,73,74	0
5	ACT	B	517	4/4	0.94	0.09	48,50,51,53	0
5	ACT	B	509	4/4	0.95	0.13	36,39,42,46	0
4	SO4	A	516	5/5	0.95	0.12	29,31,34,38	5
4	SO4	B	515	5/5	0.95	0.14	47,49,51,51	5
6	RJR	A	513	31/31	0.95	0.11	22,45,90,94	0
6	RJR	B	513	31/31	0.95	0.12	19,41,96,98	0
4	SO4	A	518	5/5	0.95	0.11	35,36,39,40	5
5	ACT	A	508	4/4	0.96	0.14	34,38,41,42	0
4	SO4	A	515	5/5	0.96	0.15	31,32,35,36	5
4	SO4	B	516	5/5	0.96	0.26	24,32,36,37	5
4	SO4	A	507	5/5	0.97	0.10	45,46,52,58	0
4	SO4	B	505	5/5	0.97	0.13	42,54,59,65	0
4	SO4	A	506	5/5	0.98	0.10	41,53,56,57	0
4	SO4	B	504	5/5	0.98	0.09	30,32,33,38	0
4	SO4	A	504	5/5	0.98	0.09	41,42,48,52	0
4	SO4	B	507	5/5	0.98	0.07	44,47,51,51	0
4	SO4	A	505	5/5	0.99	0.06	39,41,43,46	0
4	SO4	A	503	5/5	0.99	0.06	25,27,29,32	0
4	SO4	B	506	5/5	0.99	0.07	38,44,51,53	0

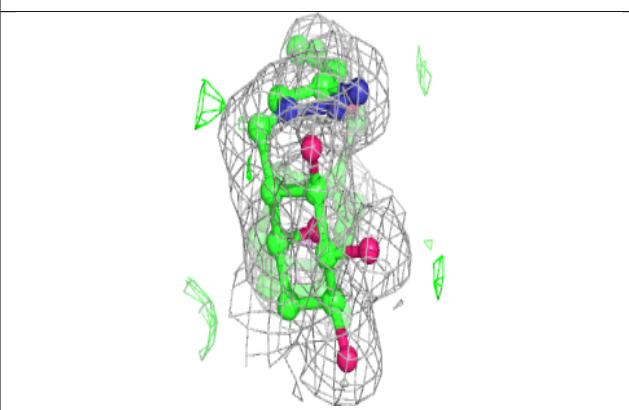
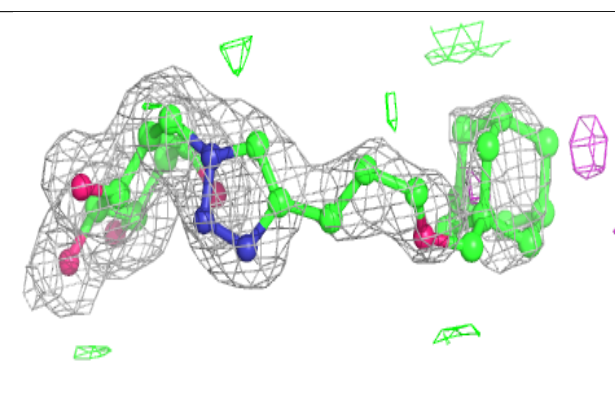
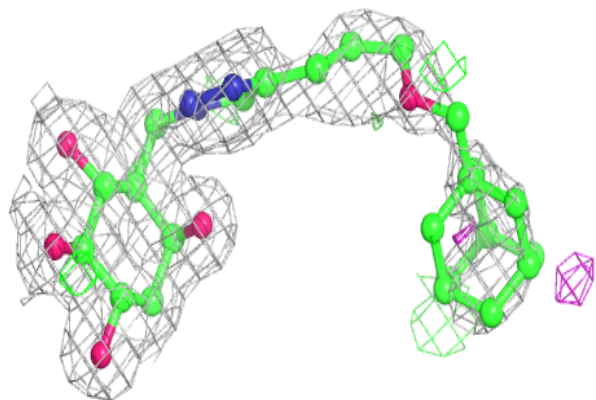
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around RJR A 513:**

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

**Electron density around RJR B 513:**

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



## 6.5 Other polymers

There are no such residues in this entry.