



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 03:12 AM UTC

PDB ID : 9PRU / pdb_00009pru
Title : Complex of the 3G8 Fab bound to Fc gamma receptor 3a / CD16a F158 allotype
Authors : Barb, A.W.; Lanzilotta, W.N.; Kremer, P.G.
Deposited on : 2025-07-24
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

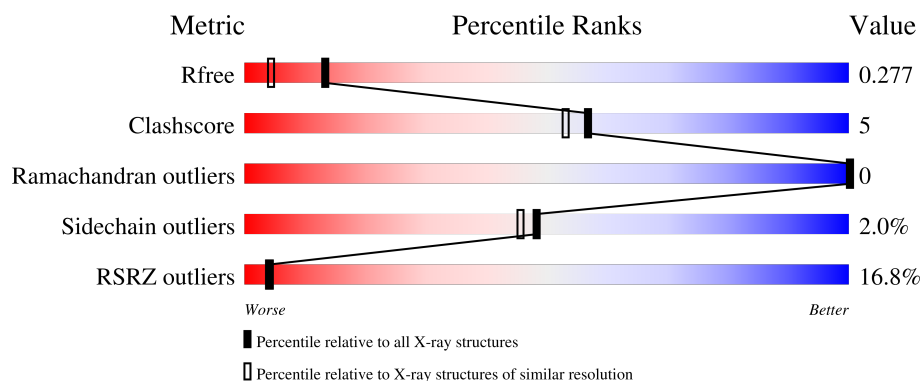
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	218	<div> <div>16%</div> <div>83%16%.</div> </div>
1	C	218	<div> <div>4%</div> <div>91%6%..</div> </div>
1	E	218	<div> <div>6%</div> <div>91%8%</div> </div>
1	G	218	<div> <div>25%</div> <div>85%13%. .</div> </div>
2	B	221	<div> <div>23%</div> <div>84%14%. .</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	221	
2	F	221	
2	H	221	
3	W	175	
3	X	175	
3	Y	175	
3	Z	175	
4	I	3	
4	J	3	
4	L	3	
5	K	2	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 19484 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 3G8 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1603	1003	267	327	6			
1	C	213	Total	C	N	O	S	0	0	0
			1632	1019	271	336	6			
1	E	217	Total	C	N	O	S	0	0	0
			1624	1015	270	333	6			
1	G	213	Total	C	N	O	S	0	0	0
			1576	982	261	327	6			

- Molecule 2 is a protein called 3G8 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1587	1016	256	309	6			
2	D	218	Total	C	N	O	S	0	0	0
			1617	1031	263	317	6			
2	F	217	Total	C	N	O	S	0	0	0
			1590	1020	257	307	6			
2	H	218	Total	C	N	O	S	0	0	0
			1616	1032	263	315	6			

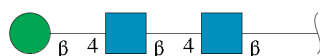
- Molecule 3 is a protein called Low affinity immunoglobulin gamma Fc region receptor III-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	W	171	Total	C	N	O	S	0	0	0
			1352	858	228	262	4			
3	X	165	Total	C	N	O	S	0	0	0
			1238	785	214	235	4			
3	Y	160	Total	C	N	O	S	0	0	0
			1241	796	209	232	4			
3	Z	171	Total	C	N	O	S	0	0	0
			1340	858	227	251	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	38	GLN	ASN	engineered mutation	UNP P08637
W	74	GLN	ASN	engineered mutation	UNP P08637
W	169	GLN	ASN	engineered mutation	UNP P08637
X	38	GLN	ASN	engineered mutation	UNP P08637
X	74	GLN	ASN	engineered mutation	UNP P08637
X	169	GLN	ASN	engineered mutation	UNP P08637
Y	38	GLN	ASN	engineered mutation	UNP P08637
Y	74	GLN	ASN	engineered mutation	UNP P08637
Y	169	GLN	ASN	engineered mutation	UNP P08637
Z	38	GLN	ASN	engineered mutation	UNP P08637
Z	74	GLN	ASN	engineered mutation	UNP P08637
Z	169	GLN	ASN	engineered mutation	UNP P08637

- Molecule 4 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
4	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	L	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 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
5	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	1	Total	Na	0	0
			1	1		
7	G	1	Total	Na	0	0
			1	1		
7	H	1	Total	Na	0	0
			1	1		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	1	Total	Cl	0	0
			1	1		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	W	1	Total	C	N	O	0	0
			14	8	1	5		
9	X	1	Total	C	N	O	0	0
			14	8	1	5		
9	Y	1	Total	C	N	O	0	0
			14	8	1	5		
9	Z	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	98	Total	O	0	0
			98	98		
10	B	56	Total	O	0	0
			56	56		
10	C	175	Total	O	0	0
			175	175		
10	D	141	Total	O	0	0
			141	141		
10	E	140	Total	O	0	0
			140	140		
10	F	114	Total	O	0	0
			114	114		
10	G	90	Total	O	0	0
			90	90		
10	H	82	Total	O	0	0
			82	82		

Continued on next page...

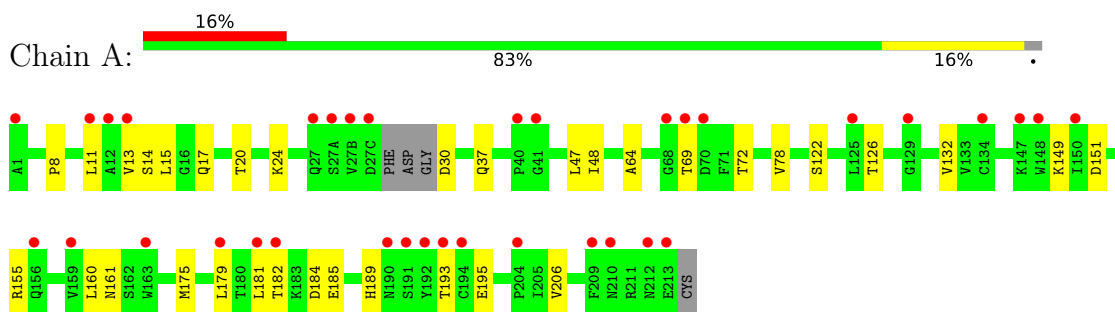
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	W	137	Total 137	O 137	0	0
10	X	39	Total 39	O 39	0	0
10	Y	54	Total 54	O 54	0	0
10	Z	119	Total 119	O 119	0	0

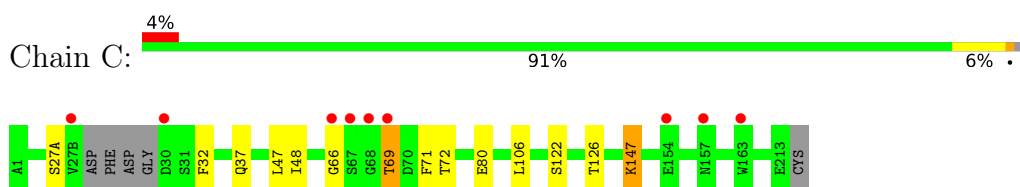
3 Residue-property plots [i](#)

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.

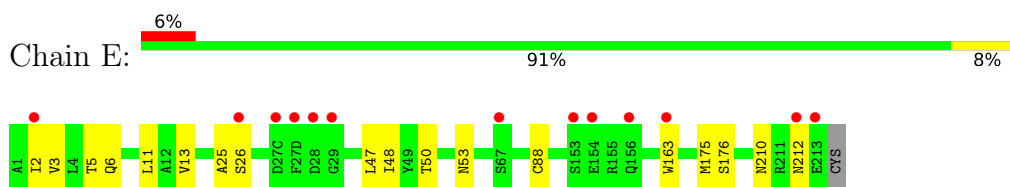
- Molecule 1: 3G8 Fab light chain



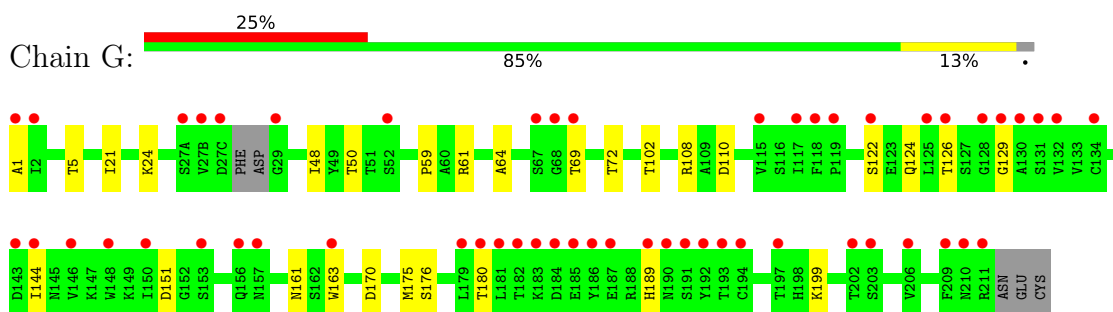
- Molecule 1: 3G8 Fab light chain



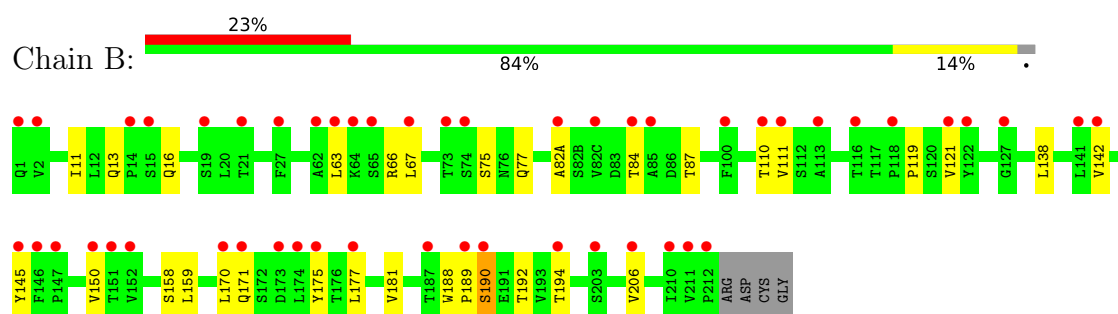
- Molecule 1: 3G8 Fab light chain



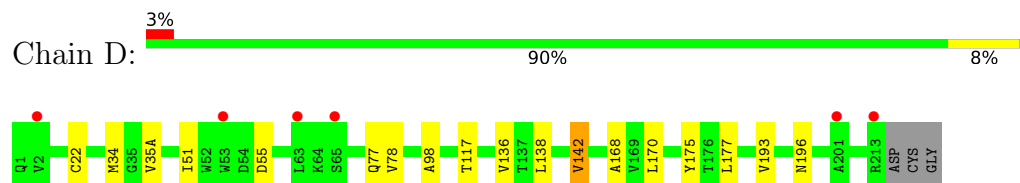
- Molecule 1: 3G8 Fab light chain



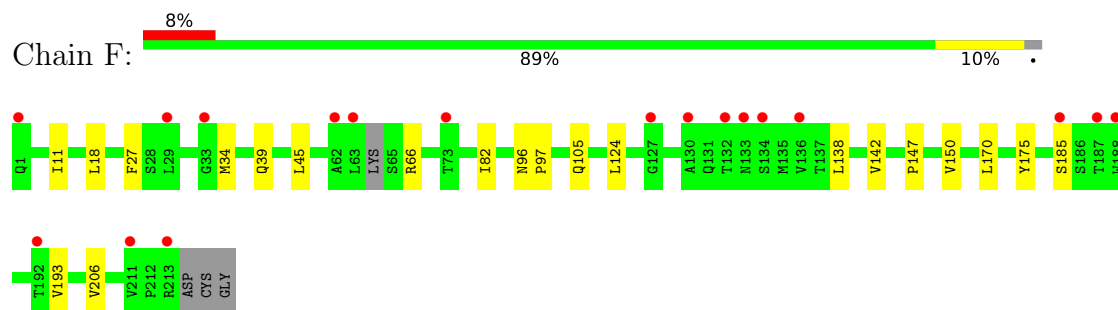
- Molecule 2: 3G8 Fab Heavy Chain



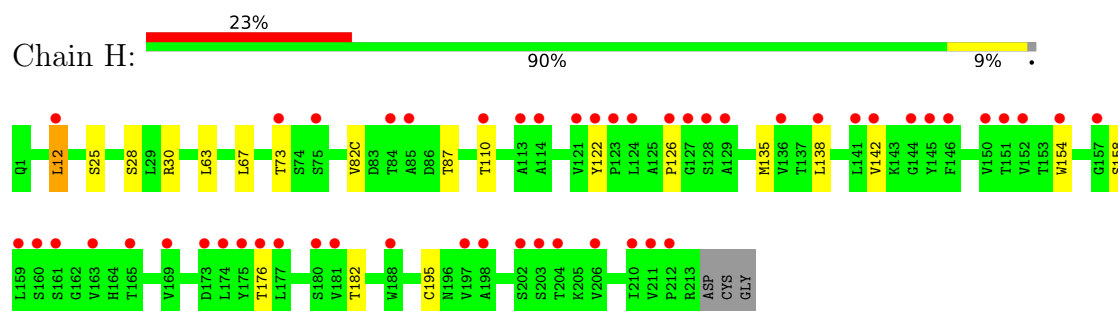
- Molecule 2: 3G8 Fab Heavy Chain



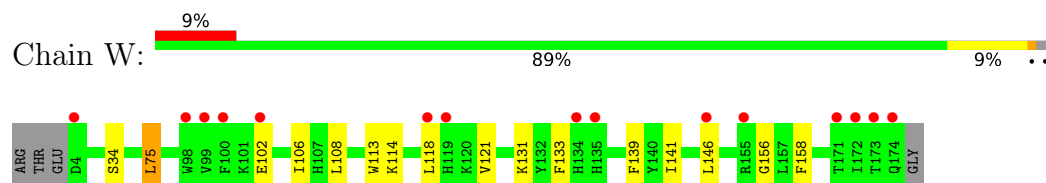
- Molecule 2: 3G8 Fab Heavy Chain



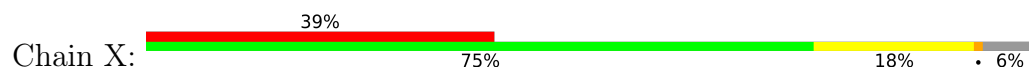
- Molecule 2: 3G8 Fab Heavy Chain

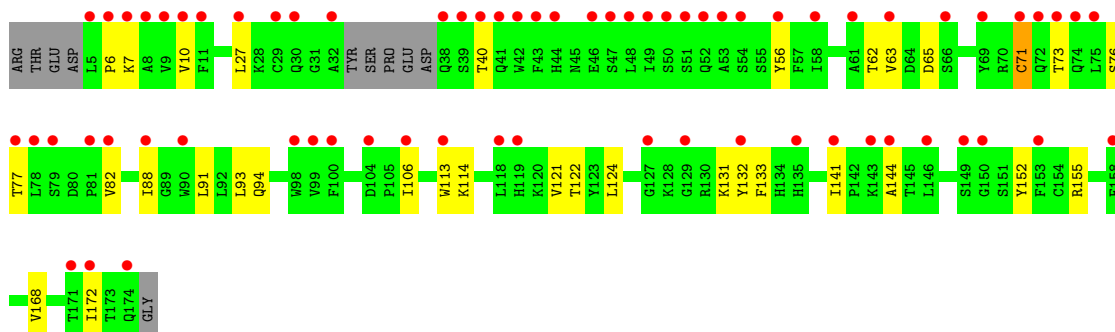


- Molecule 3: Low affinity immunoglobulin gamma Fc region receptor III-A

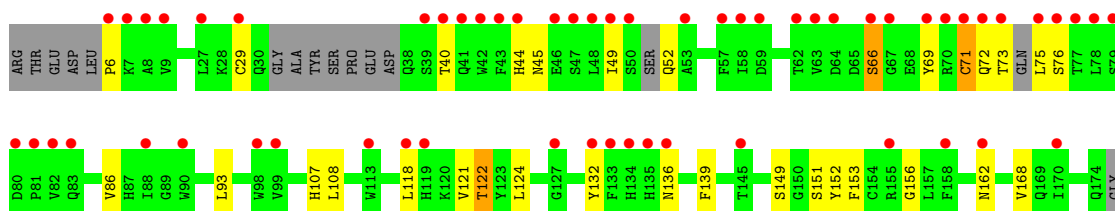


- Molecule 3: Low affinity immunoglobulin gamma Fc region receptor III-A

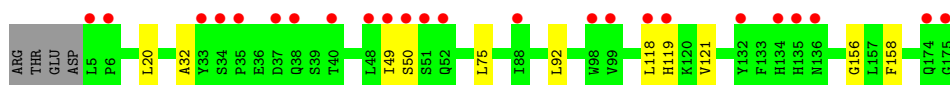
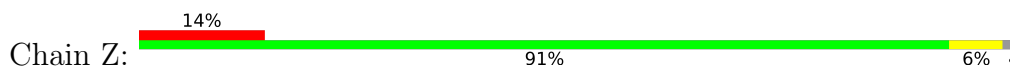




- Molecule 3: Low affinity immunoglobulin gamma Fc region receptor III-A



- Molecule 3: Low affinity immunoglobulin gamma Fc region receptor III-A



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



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



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



MAG1
MAG2
BMA3

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	130.06Å 130.59Å 170.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 1.90 48.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.00-1.90) 92.0 (48.00-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.230 , 0.280 0.231 , 0.277	Depositor DCC
R_{free} test set	2003 reflections (0.88%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.831	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19484	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.64 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.7170e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, CL, NA, GOL

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	0.37	0/1639	0.58	0/2236
1	C	0.40	0/1668	0.59	0/2268
1	E	0.33	0/1661	0.54	0/2266
1	G	0.35	0/1611	0.54	0/2200
2	B	0.29	0/1634	0.55	1/2254 (0.0%)
2	D	0.33	0/1664	0.57	0/2291
2	F	0.36	1/1636 (0.1%)	0.54	0/2255
2	H	0.30	0/1663	0.51	0/2290
3	W	0.35	0/1389	0.55	0/1893
3	X	0.31	0/1269	0.48	0/1733
3	Y	0.30	0/1273	0.52	0/1734
3	Z	0.34	0/1378	0.48	0/1878
All	All	0.34	1/18485 (0.0%)	0.54	1/25298 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	105	GLN	CD-OE1	-7.15	1.09	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	190	SER	N-CA-C	6.41	117.95	110.97

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	1603	0	1480	20	0
1	C	1632	0	1541	7	0
1	E	1624	0	1503	12	0
1	G	1576	0	1429	17	0
2	B	1587	0	1484	19	0
2	D	1617	0	1539	10	0
2	F	1590	0	1496	7	0
2	H	1616	0	1542	14	0
3	W	1352	0	1239	8	0
3	X	1238	0	1091	23	0
3	Y	1241	0	1129	21	0
3	Z	1340	0	1242	9	0
4	I	39	0	34	0	0
4	J	39	0	34	0	0
4	L	39	0	34	0	0
5	K	28	0	25	1	0
6	A	6	0	8	1	0
6	C	6	0	8	0	0
6	E	6	0	8	0	0
7	E	1	0	0	0	0
7	G	1	0	0	0	0
7	H	1	0	0	0	0
8	G	1	0	0	0	0
9	W	14	0	13	0	0
9	X	14	0	13	0	0
9	Y	14	0	13	1	0
9	Z	14	0	13	0	0
10	A	98	0	0	0	0
10	B	56	0	0	0	0
10	C	175	0	0	0	0
10	D	141	0	0	1	0
10	E	140	0	0	1	0
10	F	114	0	0	0	0
10	G	90	0	0	2	0
10	H	82	0	0	2	0
10	W	137	0	0	0	0
10	X	39	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	Y	54	0	0	0	0
10	Z	119	0	0	0	0
All	All	19484	0	16918	160	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.

The worst 5 of 160 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)
2:B:87:THR:HG22	2:B:111:VAL:H	1.38	0.89
3:X:122:THR:HG22	3:X:132:TYR:HD1	1.53	0.74
1:A:8:PRO:HG3	1:A:11:LEU:HD13	1.71	0.72
2:H:30:ARG:HG2	2:H:73:THR:HG21	1.75	0.68
1:A:195:GLU:HG3	1:A:206:VAL:HG22	1.77	0.67

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	210/218 (96%)	204 (97%)	6 (3%)	0	100	100
1	C	209/218 (96%)	201 (96%)	8 (4%)	0	100	100
1	E	215/218 (99%)	210 (98%)	5 (2%)	0	100	100
1	G	209/218 (96%)	200 (96%)	9 (4%)	0	100	100
2	B	215/221 (97%)	205 (95%)	10 (5%)	0	100	100
2	D	216/221 (98%)	211 (98%)	5 (2%)	0	100	100
2	F	213/221 (96%)	207 (97%)	6 (3%)	0	100	100
2	H	216/221 (98%)	207 (96%)	9 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	W	169/175 (97%)	163 (96%)	6 (4%)	0	100	100
3	X	161/175 (92%)	152 (94%)	9 (6%)	0	100	100
3	Y	152/175 (87%)	143 (94%)	9 (6%)	0	100	100
3	Z	169/175 (97%)	165 (98%)	4 (2%)	0	100	100
All	All	2354/2456 (96%)	2268 (96%)	86 (4%)	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	171/192 (89%)	169 (99%)	2 (1%)	63	63
1	C	181/192 (94%)	177 (98%)	4 (2%)	45	42
1	E	174/192 (91%)	173 (99%)	1 (1%)	78	81
1	G	166/192 (86%)	163 (98%)	3 (2%)	51	50
2	B	167/189 (88%)	163 (98%)	4 (2%)	43	38
2	D	176/189 (93%)	173 (98%)	3 (2%)	53	52
2	F	168/189 (89%)	162 (96%)	6 (4%)	31	23
2	H	176/189 (93%)	173 (98%)	3 (2%)	53	52
3	W	144/158 (91%)	141 (98%)	3 (2%)	47	44
3	X	119/158 (75%)	117 (98%)	2 (2%)	53	52
3	Y	127/158 (80%)	120 (94%)	7 (6%)	19	11
3	Z	140/158 (89%)	140 (100%)	0	100	100
All	All	1909/2156 (88%)	1871 (98%)	38 (2%)	48	46

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	W	146	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Y	136	ASN
3	X	71	CYS
3	Y	66	SER
3	Y	151	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	17	GLN
3	W	119	HIS
1	E	53	ASN
3	X	83	GLN
2	H	39	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 ⓘ

11 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	$\# Z > 2$
4	NAG	I	1	3,4	14,14,15	1.03	1 (7%)	17,19,21	1.33	2 (11%)
4	NAG	I	2	4	14,14,15	0.85	0	17,19,21	1.39	3 (17%)
4	BMA	I	3	4	11,11,12	0.89	0	15,15,17	1.90	3 (20%)
4	NAG	J	1	3,4	14,14,15	0.63	0	17,19,21	1.40	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	J	2	4	14,14,15	0.71	0	17,19,21	1.57	2 (11%)
4	BMA	J	3	4	11,11,12	1.18	1 (9%)	15,15,17	2.35	5 (33%)
5	NAG	K	1	5,3	14,14,15	0.87	1 (7%)	17,19,21	1.34	3 (17%)
5	NAG	K	2	5	14,14,15	0.70	0	17,19,21	1.43	2 (11%)
4	NAG	L	1	3,4	14,14,15	0.65	0	17,19,21	1.57	3 (17%)
4	NAG	L	2	4	14,14,15	0.77	0	17,19,21	1.65	2 (11%)
4	BMA	L	3	4	11,11,12	1.05	1 (9%)	15,15,17	1.86	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	BMA	I	3	4	-	0/2/19/22	0/1/1/1
4	NAG	J	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	3/6/23/26	0/1/1/1
4	BMA	J	3	4	-	2/2/19/22	0/1/1/1
5	NAG	K	1	5,3	-	3/6/23/26	0/1/1/1
5	NAG	K	2	5	-	4/6/23/26	0/1/1/1
4	NAG	L	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
4	BMA	L	3	4	-	1/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	3	BMA	C2-C3	3.11	1.57	1.52
4	I	1	NAG	O5-C1	-2.98	1.38	1.43
5	K	1	NAG	O5-C1	-2.73	1.39	1.43
4	L	3	BMA	C2-C3	2.47	1.56	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	3	BMA	C1-O5-C5	6.34	120.68	112.19
4	I	3	BMA	C1-O5-C5	5.19	119.14	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	3	BMA	C1-O5-C5	4.71	118.49	112.19
4	L	1	NAG	C1-O5-C5	4.37	118.04	112.19
4	L	2	NAG	O5-C1-C2	-3.82	105.37	111.29

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

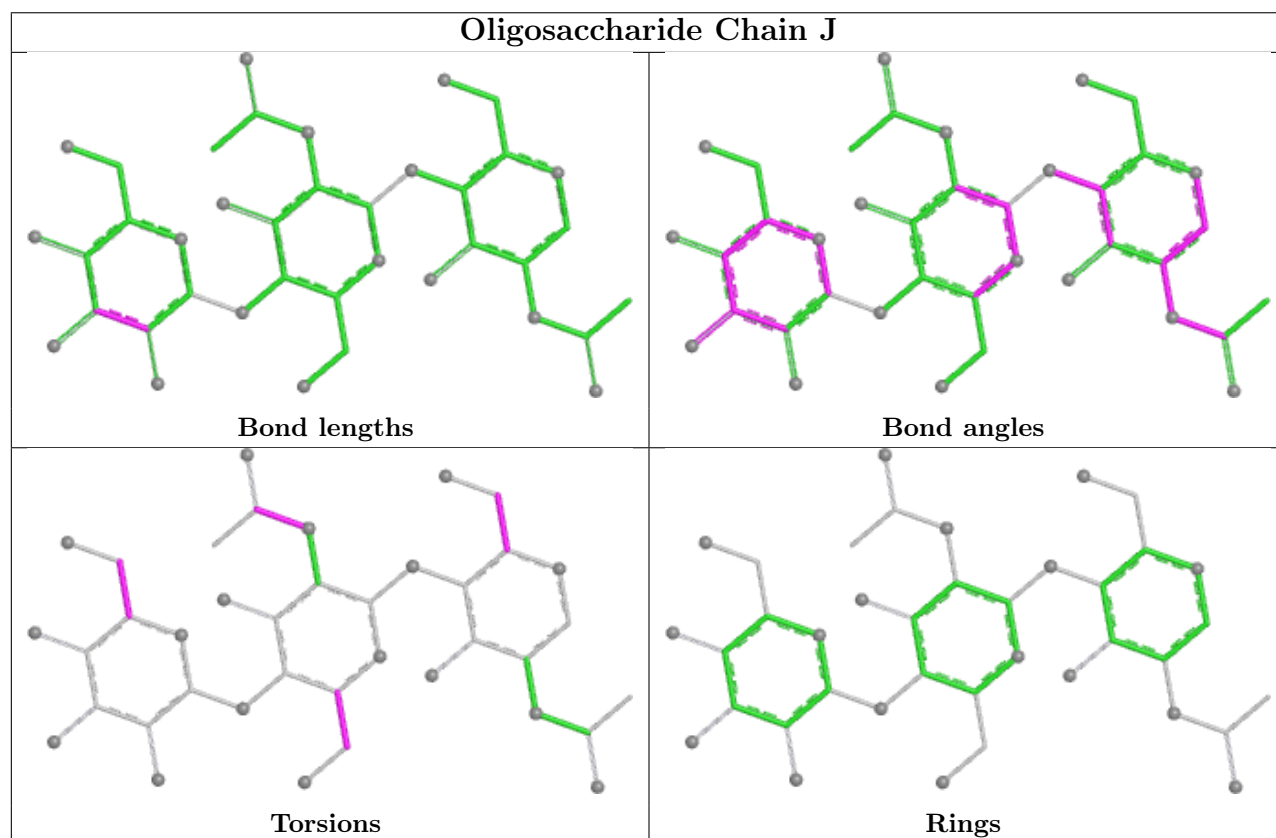
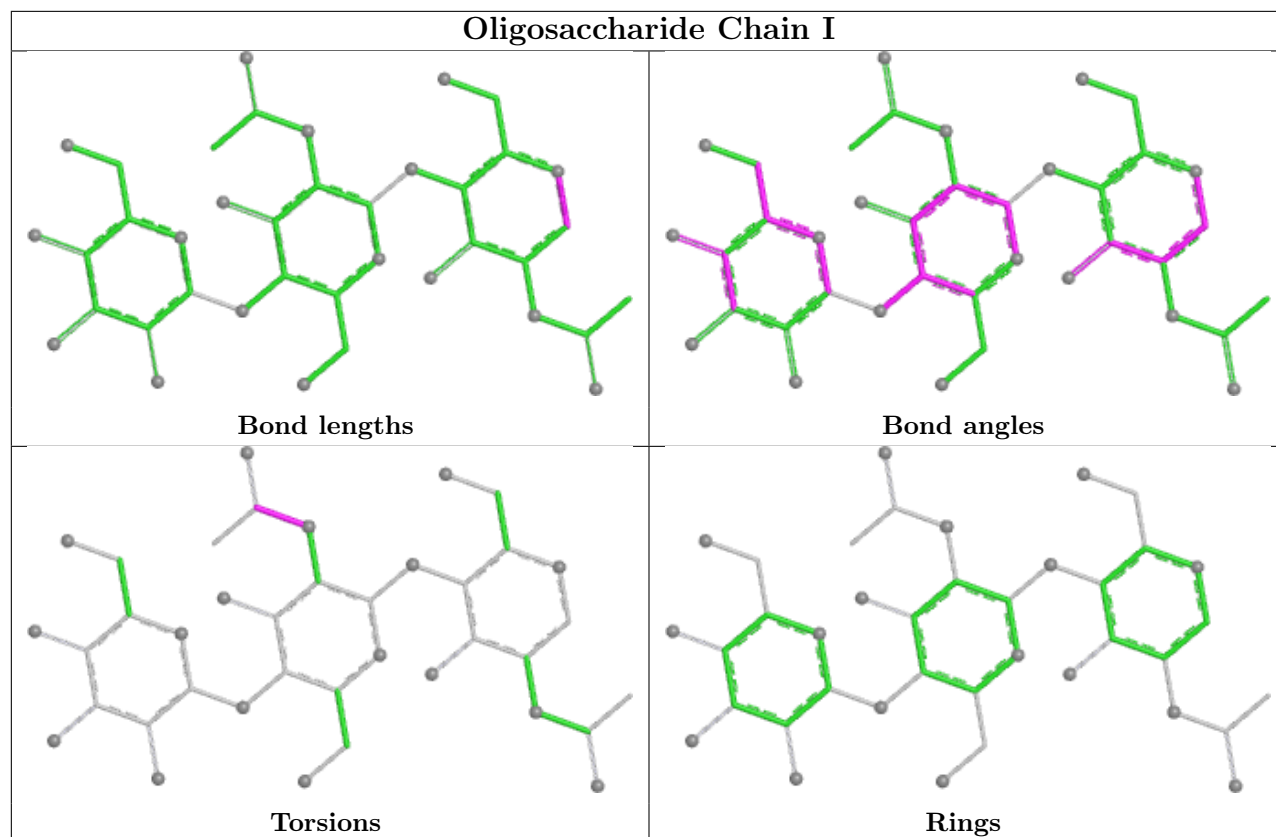
Mol	Chain	Res	Type	Atoms
4	L	2	NAG	O5-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
4	J	3	BMA	C4-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6

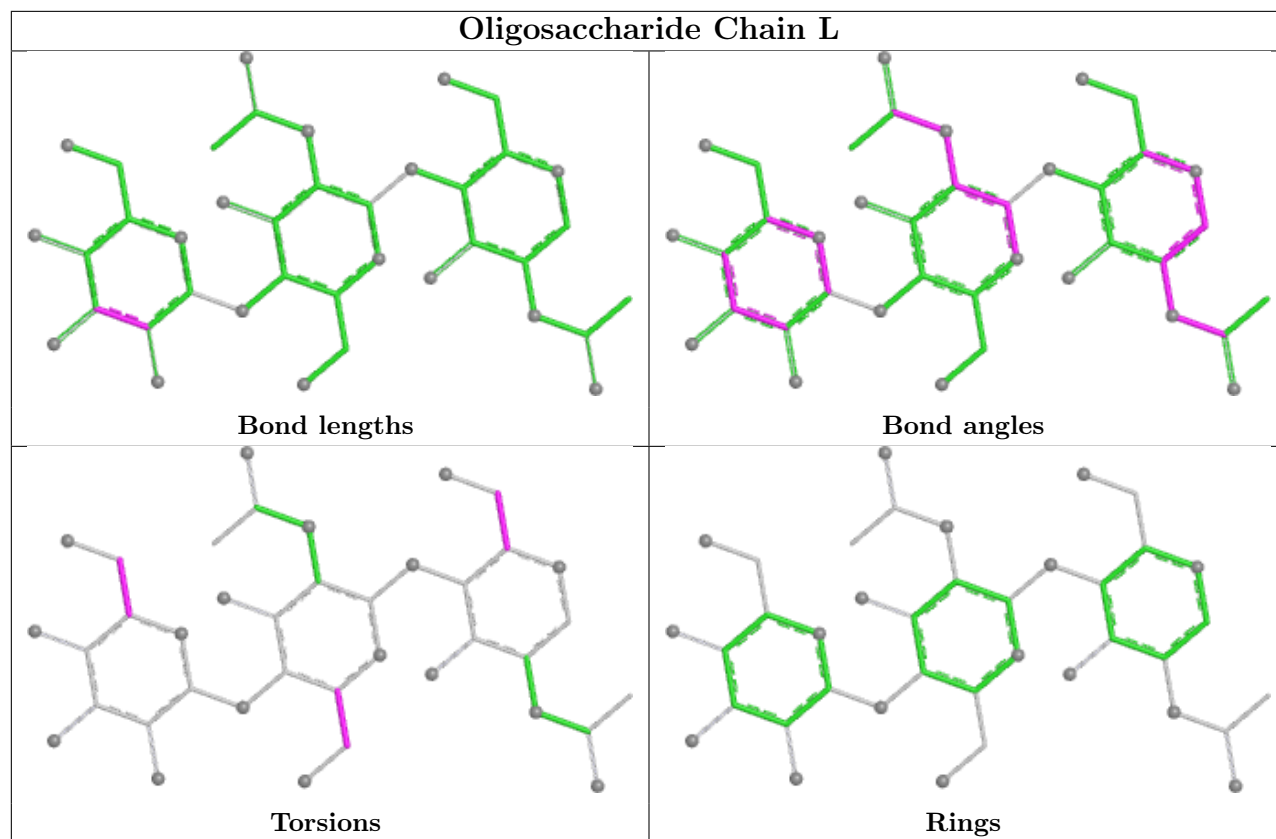
There are no ring outliers.

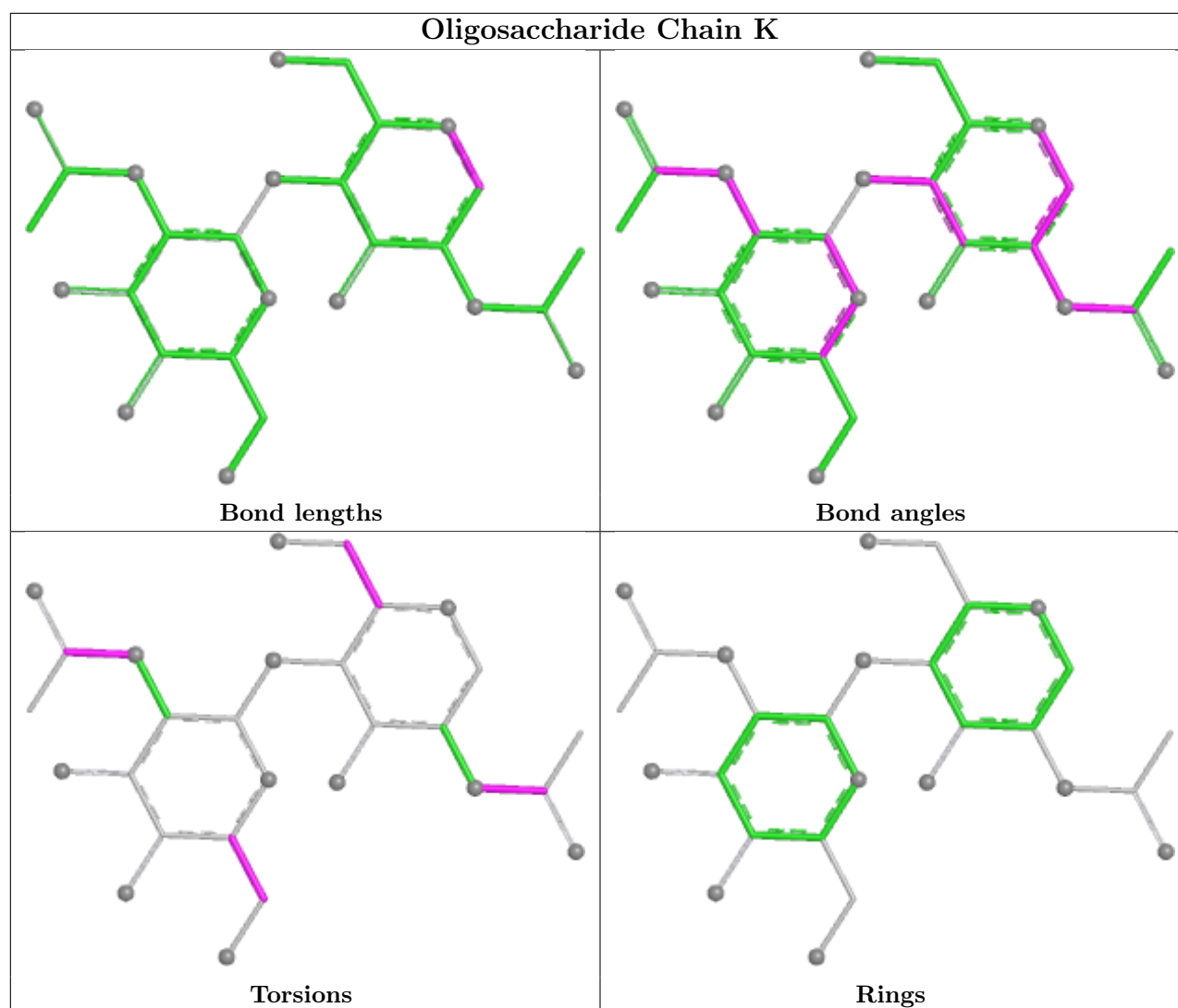
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	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](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	GOL	E	302	-	5,5,5	0.46	0	5,5,5	1.01	0
9	NAG	Y	201	3	14,14,15	0.76	0	17,19,21	2.12	6 (35%)
6	GOL	A	301	-	5,5,5	0.34	0	5,5,5	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	W	201	3	14,14,15	0.64	0	17,19,21	1.64	5 (29%)
9	NAG	Z	201	3	14,14,15	0.73	0	17,19,21	1.36	1 (5%)
6	GOL	C	301	-	5,5,5	0.71	0	5,5,5	1.48	1 (20%)
9	NAG	X	201	3	14,14,15	0.50	0	17,19,21	1.88	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
6	GOL	E	302	-	-	3/4/4/4	-
9	NAG	Y	201	3	-	0/6/23/26	0/1/1/1
6	GOL	A	301	-	-	2/4/4/4	-
9	NAG	W	201	3	-	4/6/23/26	0/1/1/1
9	NAG	Z	201	3	-	2/6/23/26	0/1/1/1
6	GOL	C	301	-	-	2/4/4/4	-
9	NAG	X	201	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	X	201	NAG	C1-O5-C5	6.61	121.04	112.19
9	Y	201	NAG	C1-C2-N2	4.62	117.71	110.43
9	Y	201	NAG	O5-C1-C2	-4.05	105.02	111.29
9	Y	201	NAG	C2-N2-C7	3.90	128.12	122.90
9	W	201	NAG	C3-C4-C5	3.16	115.96	110.23

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

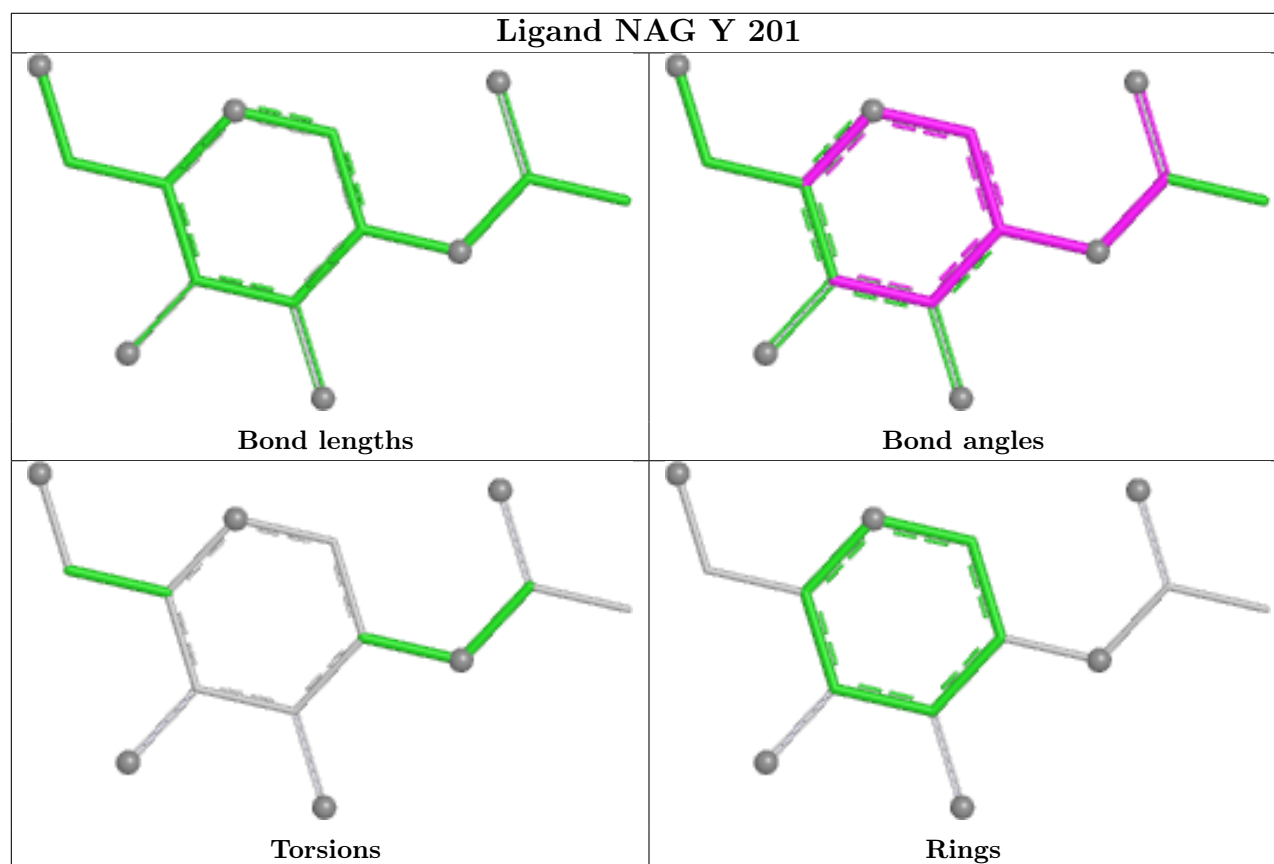
Mol	Chain	Res	Type	Atoms
6	A	301	GOL	C1-C2-C3-O3
6	E	302	GOL	O1-C1-C2-C3
9	Z	201	NAG	C4-C5-C6-O6
9	Z	201	NAG	O5-C5-C6-O6
6	C	301	GOL	C1-C2-C3-O3

There are no ring outliers.

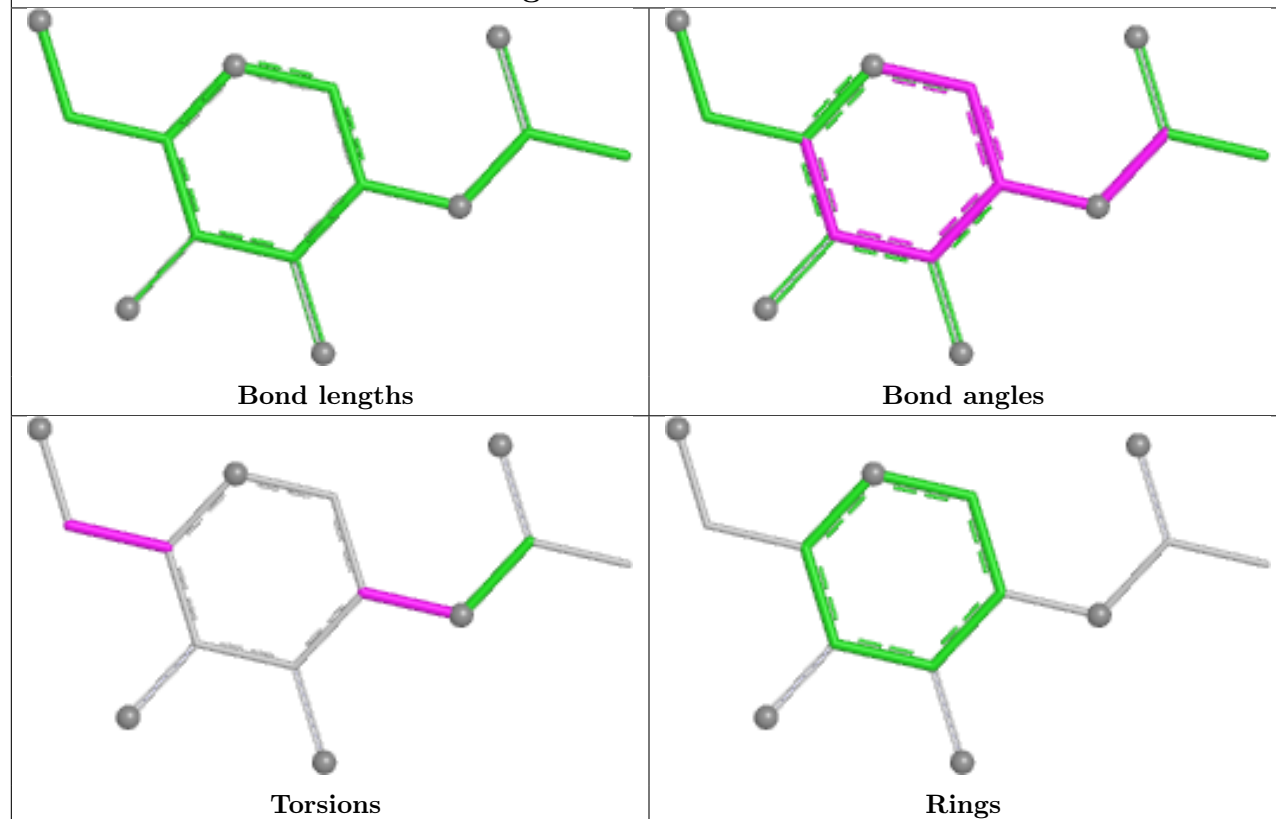
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	Y	201	NAG	1	0
6	A	301	GOL	1	0

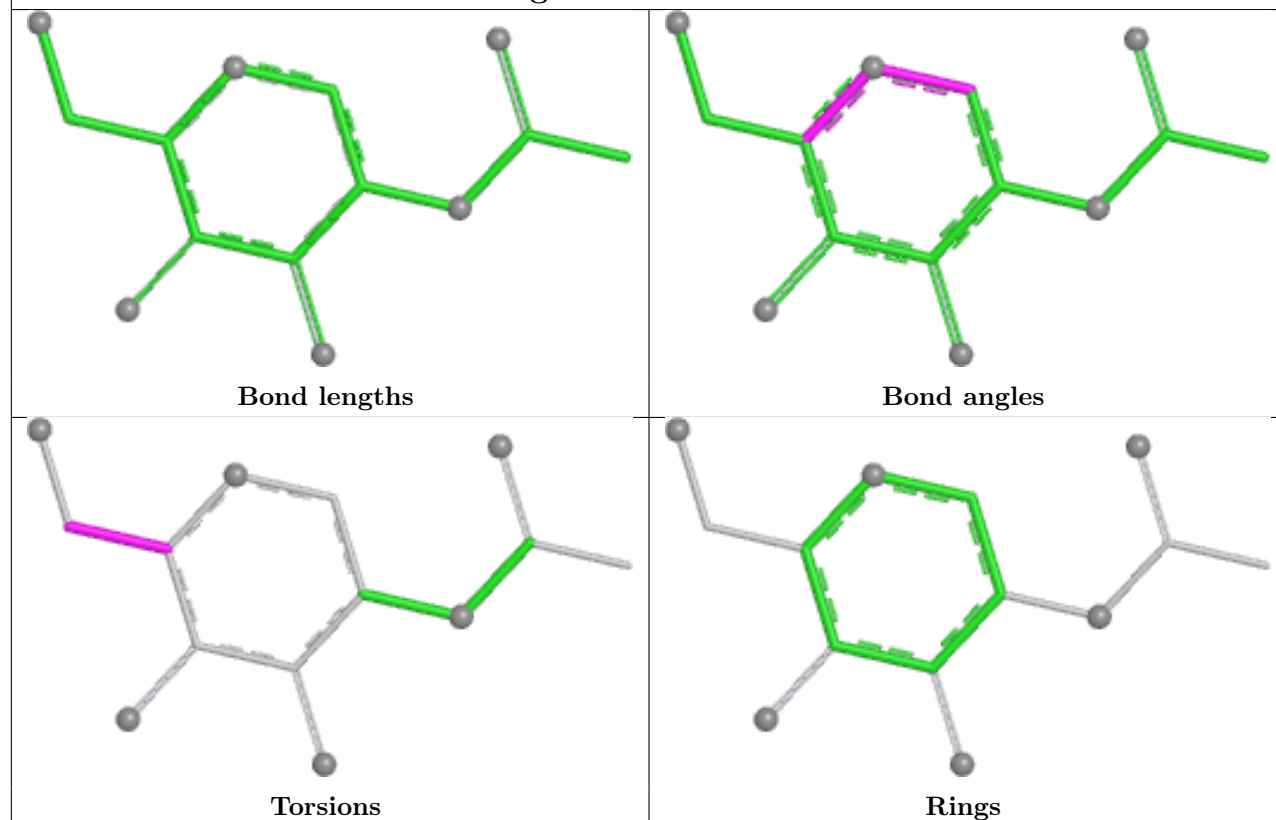
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

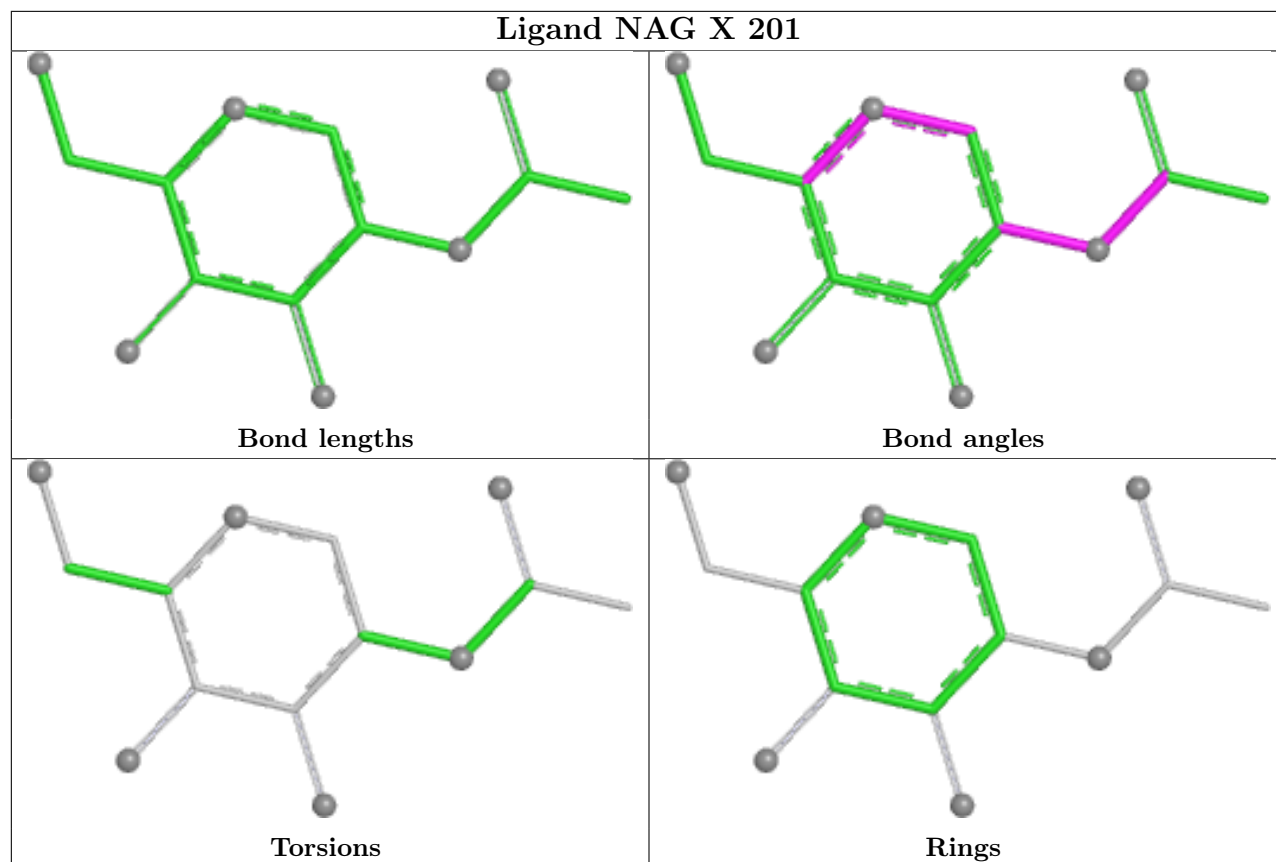


Ligand NAG W 201



Ligand NAG Z 201





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	214/218 (98%)	1.10	35 (16%) 4 4	26, 36, 62, 76	0
1	C	213/218 (97%)	0.46	9 (4%) 40 43	19, 29, 46, 61	0
1	E	217/218 (99%)	0.65	13 (5%) 27 29	22, 34, 52, 67	0
1	G	213/218 (97%)	1.27	54 (25%) 1 1	22, 38, 66, 74	0
2	B	217/221 (98%)	1.44	50 (23%) 2 2	28, 46, 59, 63	0
2	D	218/221 (98%)	0.62	6 (2%) 55 59	22, 33, 48, 59	0
2	F	217/221 (98%)	0.82	18 (8%) 17 18	25, 36, 57, 62	0
2	H	218/221 (98%)	1.27	51 (23%) 2 1	23, 43, 63, 73	0
3	W	171/175 (97%)	0.76	15 (8%) 15 16	21, 32, 50, 63	0
3	X	165/175 (94%)	1.92	68 (41%) 0 0	29, 48, 97, 102	0
3	Y	160/175 (91%)	1.79	58 (36%) 1 0	28, 46, 102, 109	0
3	Z	171/175 (97%)	0.80	24 (14%) 6 6	19, 33, 57, 81	0
All	All	2394/2456 (97%)	1.05	401 (16%) 4 4	19, 37, 65, 109	0

The worst 5 of 401 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Y	78	LEU	6.4
3	X	78	LEU	6.1
3	Y	75	LEU	5.5
3	X	32	ALA	5.4
3	X	98	TRP	5.2

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

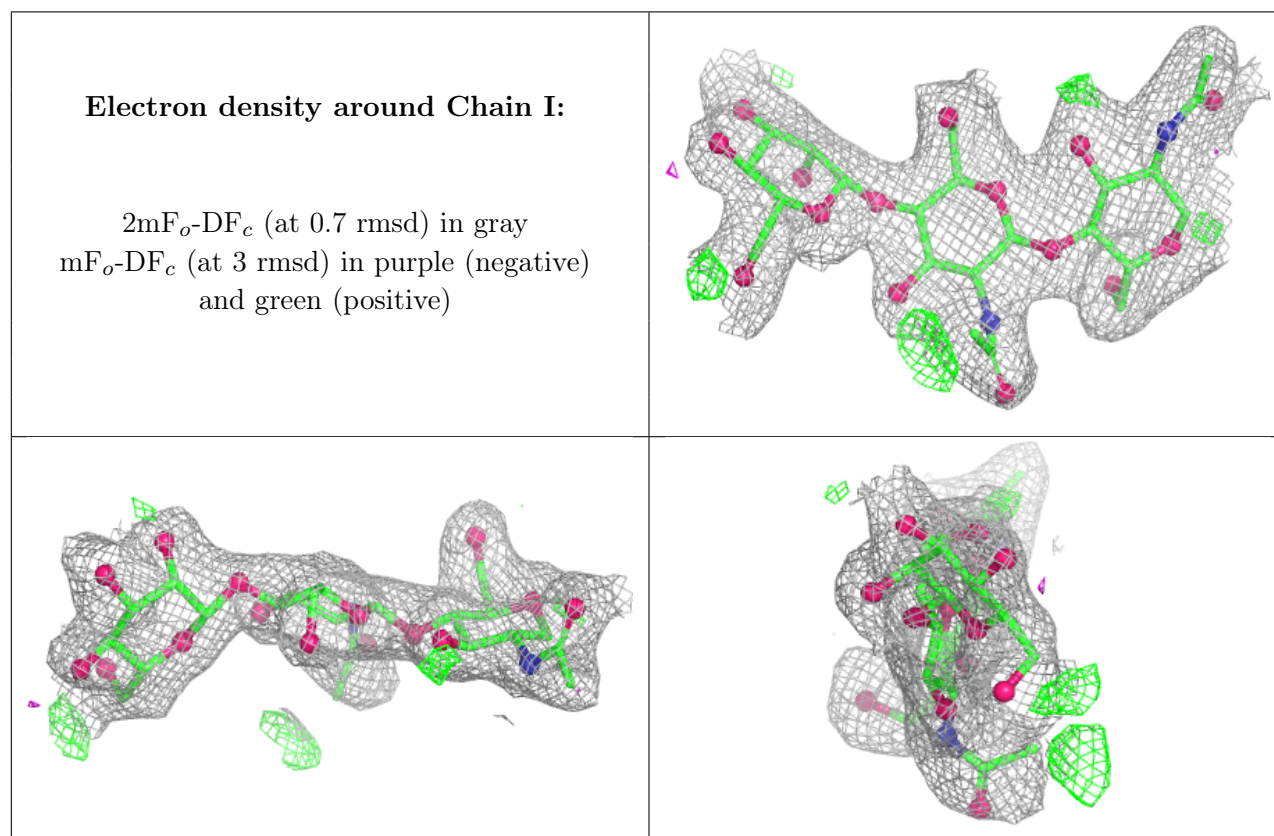
There are no non-standard protein/DNA/RNA residues in this entry.

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.

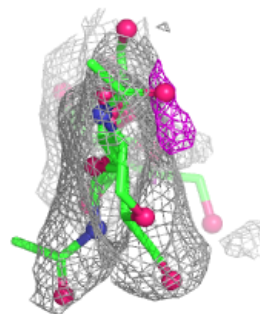
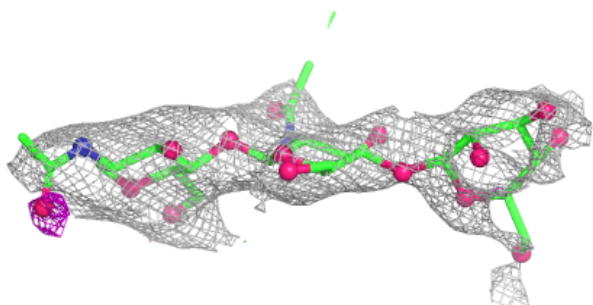
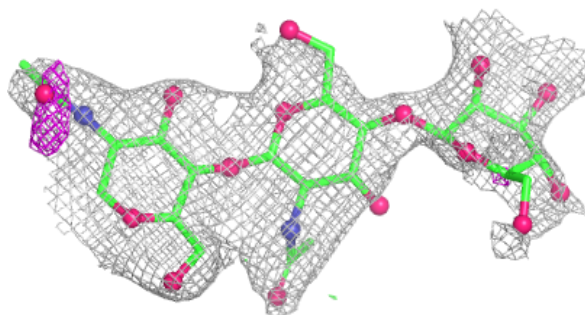
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	I	1	14/15	-	-	30,36,42,43	0
4	NAG	I	2	14/15	-	-	41,48,52,54	0
4	BMA	I	3	11/12	-	-	51,53,59,59	0
4	NAG	J	1	14/15	-	-	67,70,74,77	0
4	NAG	J	2	14/15	-	-	69,75,81,87	0
4	BMA	J	3	11/12	-	-	88,91,93,94	0
4	NAG	L	1	14/15	-	-	41,45,54,55	0
4	NAG	L	2	14/15	-	-	52,57,64,70	0
4	BMA	L	3	11/12	-	-	71,78,81,84	0
5	NAG	K	1	14/15	-	-	67,69,74,75	0
5	NAG	K	2	14/15	-	-	69,71,76,76	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.

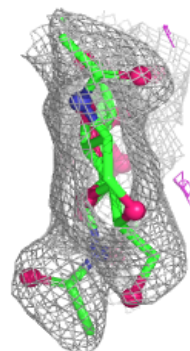
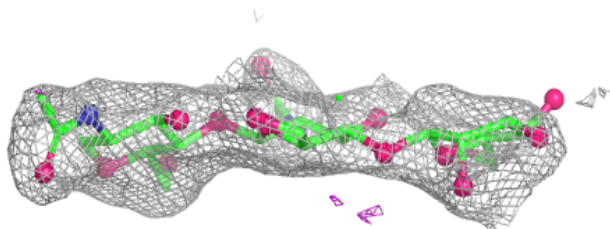
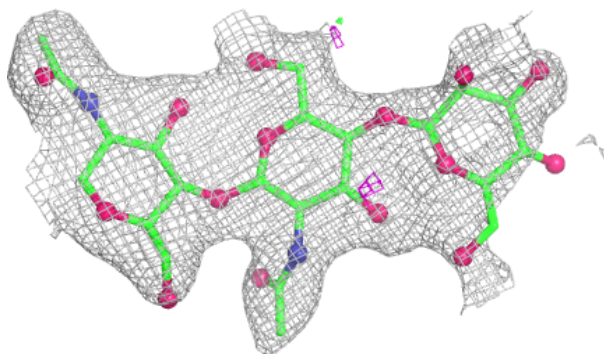


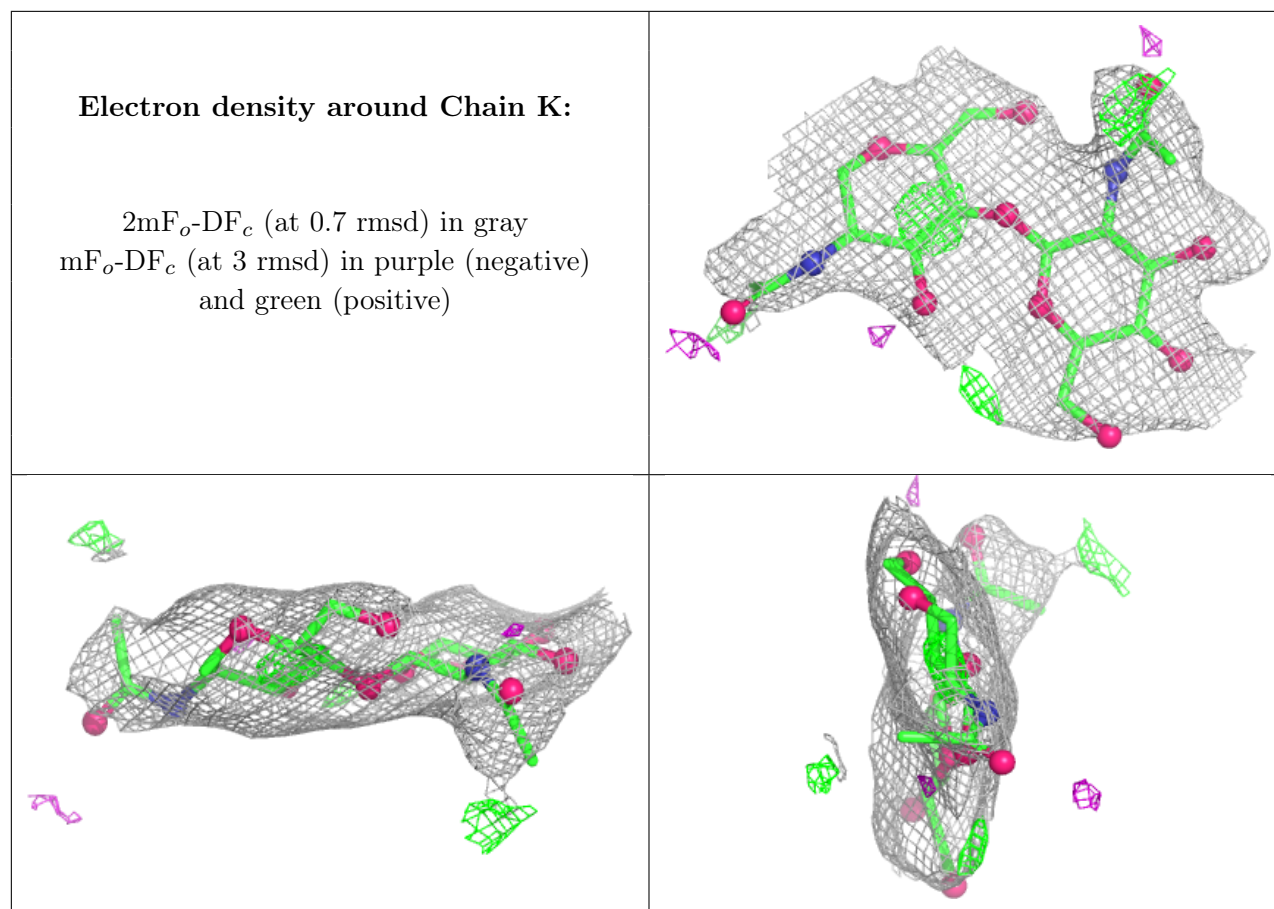
Electron density around Chain J:

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

**Electron density around Chain L:**

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





6.4 Ligands [i](#)

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

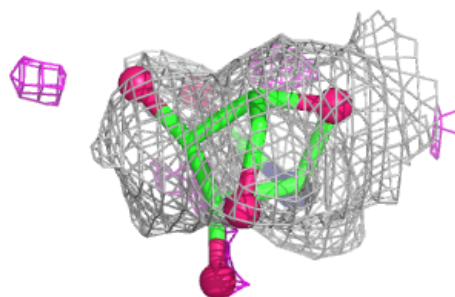
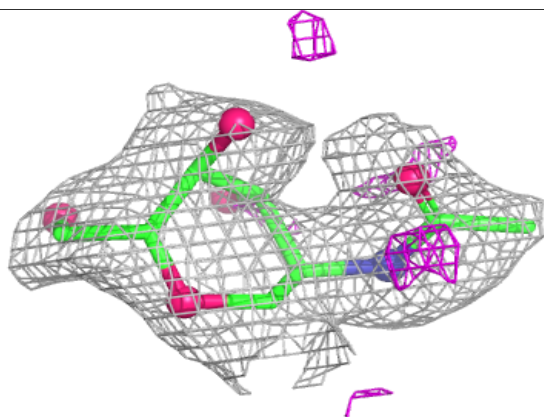
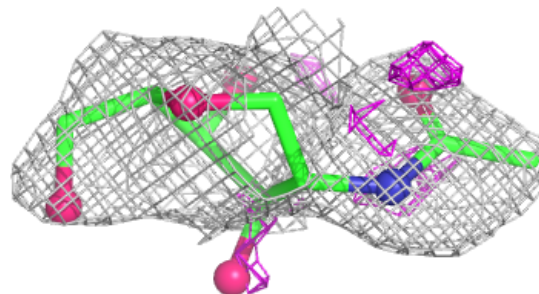
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	NA	G	301	1/1	0.66	0.19	50,50,50,50	0
9	NAG	W	201	14/15	0.67	0.16	47,57,65,68	0
9	NAG	Z	201	14/15	0.76	0.14	33,40,52,58	0
9	NAG	Y	201	14/15	0.77	0.14	44,56,60,60	0
7	NA	H	301	1/1	0.81	0.16	51,51,51,51	0
6	GOL	A	301	6/6	0.83	0.13	33,34,34,35	0
6	GOL	E	302	6/6	0.84	0.24	35,45,60,142	0
9	NAG	X	201	14/15	0.84	0.11	40,49,61,61	0
7	NA	E	301	1/1	0.85	0.13	61,61,61,61	0
6	GOL	C	301	6/6	0.88	0.27	38,42,60,142	0
8	CL	G	302	1/1	0.92	0.33	59,59,59,59	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.

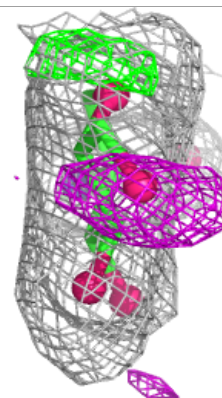
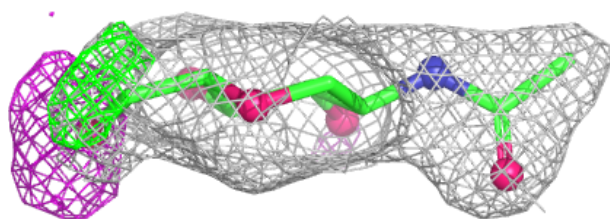
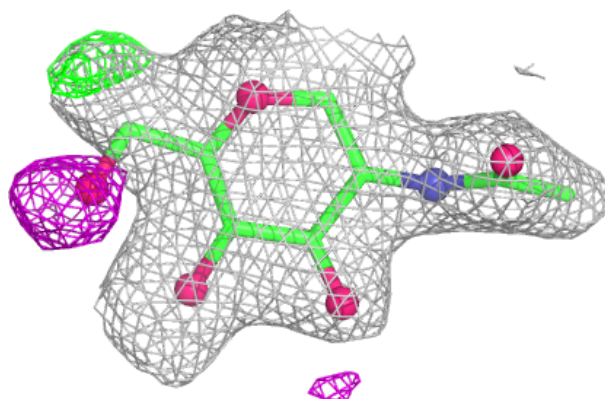
Electron density around NAG W 201:

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

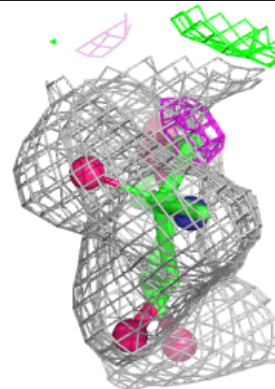
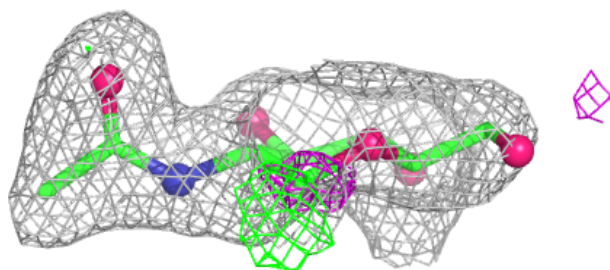
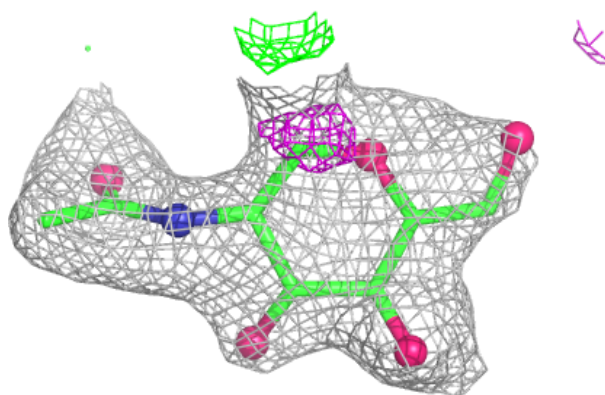


Electron density around NAG Z 201:

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

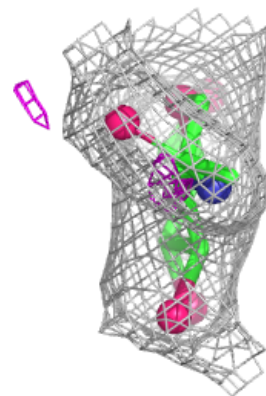
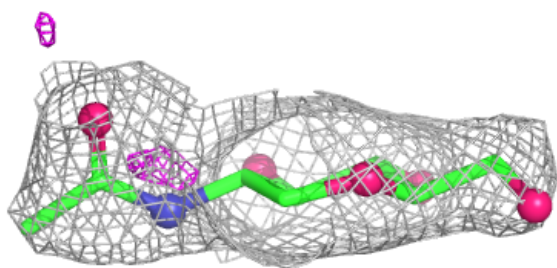
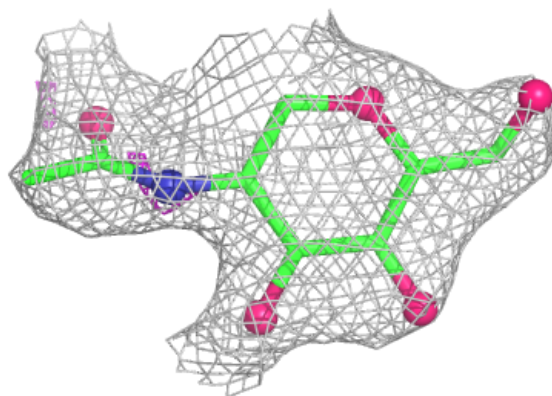
**Electron density around NAG Y 201:**

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



Electron density around NAG X 201:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.