



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 30, 2025 – 10:14 AM EDT

PDB ID : 9C22 / pdb_00009c22
Title : Crystal structure of chimeric hemagglutinin cH11/1 in complex with broad protective antibody 3E1
Authors : Nguyen, T.K.Y.; Wilson, I.A.
Deposited on : 2024-05-30
Resolution : 4.60 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

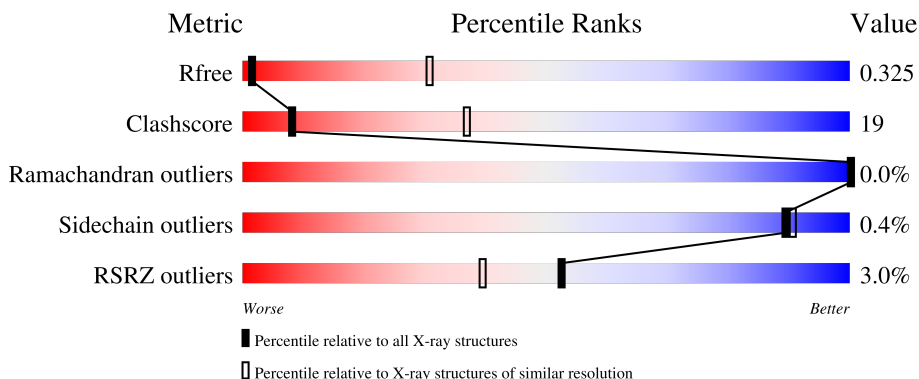
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.60 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.




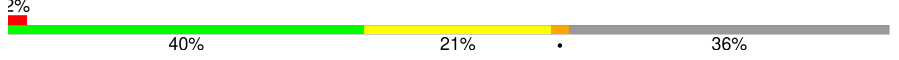

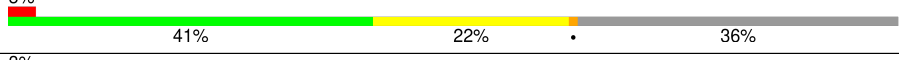
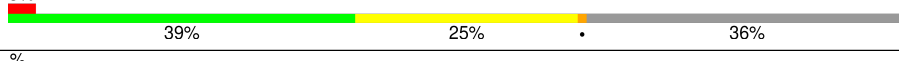
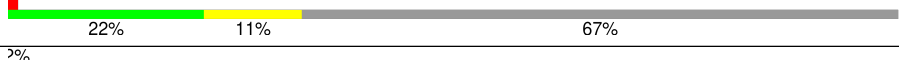
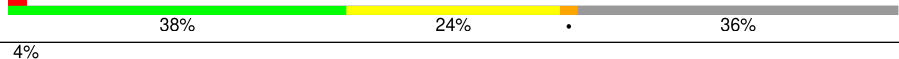
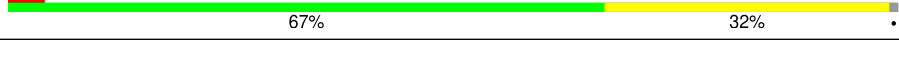

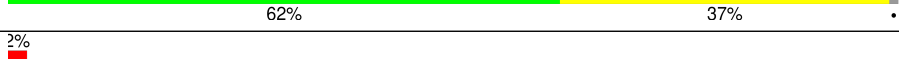
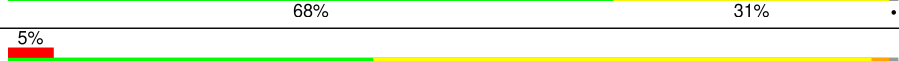
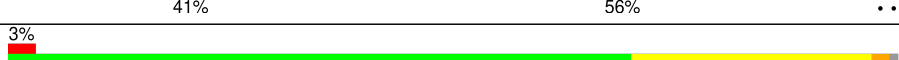
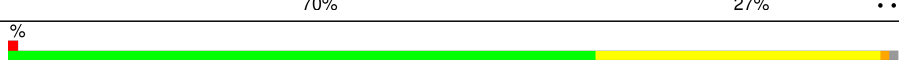
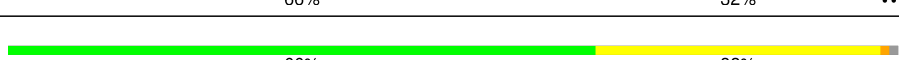
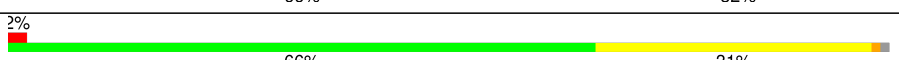
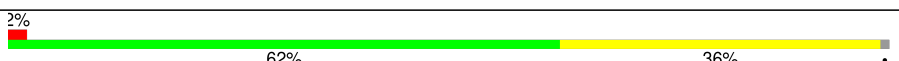
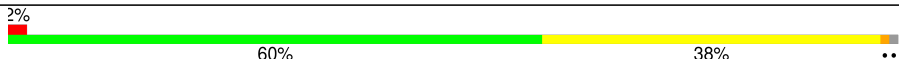
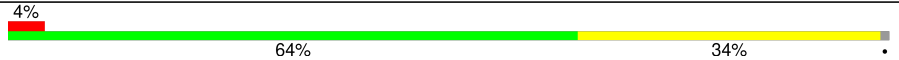

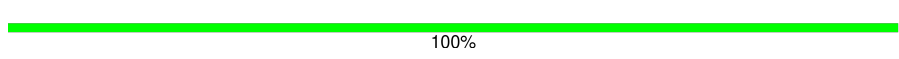
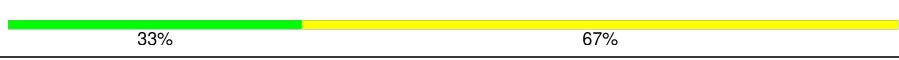
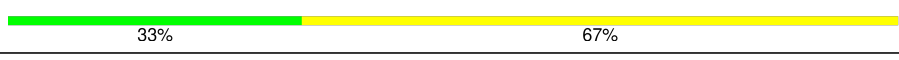

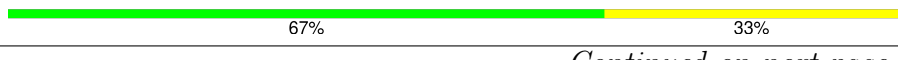

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1068 (5.30-3.90)
Clashscore	180529	1123 (5.30-3.90)
Ramachandran outliers	177936	1015 (5.30-3.90)
Sidechain outliers	177891	1016 (5.32-3.88)
RSRZ outliers	164620	1064 (5.30-3.90)

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	B	504	
1	C	504	
1	H	504	
1	I	504	
1	L	504	

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Mol	Chain	Length	Quality of chain
1	P	504	
1	Q	504	
1	U	504	
1	V	504	
1	Y	504	
1	a	504	
1	b	504	
2	D	214	
2	J	214	
2	M	214	
2	R	214	
2	W	214	
2	c	214	
3	E	224	
3	K	224	
3	N	224	
3	S	224	
3	X	224	
3	d	224	
4	A	2	
4	Z	2	
5	F	3	
5	G	3	
5	O	3	
5	T	3	

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Mol	Chain	Length	Quality of chain
5	e	3	<div><div></div><div>67%</div><div>33%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 43211 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	168	Total	C	N	O	S	0	0	0
			1360	850	231	273	6			
1	C	323	Total	C	N	O	S	0	0	0
			2505	1585	432	475	13			
1	H	168	Total	C	N	O	S	0	0	0
			1360	850	231	273	6			
1	I	168	Total	C	N	O	S	0	0	0
			1360	850	231	273	6			
1	L	323	Total	C	N	O	S	0	0	0
			2505	1585	432	475	13			
1	P	168	Total	C	N	O	S	0	0	0
			1360	850	231	273	6			
1	Q	323	Total	C	N	O	S	0	0	0
			2505	1585	432	475	13			
1	U	168	Total	C	N	O	S	0	0	0
			1360	850	231	273	6			
1	V	323	Total	C	N	O	S	0	0	0
			2505	1585	432	475	13			
1	Y	323	Total	C	N	O	S	0	0	0
			2505	1585	432	475	13			
1	a	168	Total	C	N	O	S	0	0	0
			1360	850	231	273	6			
1	b	323	Total	C	N	O	S	0	0	0
			2505	1585	432	475	13			

- Molecule 2 is a protein called Antibody 3E1 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	212	Total	C	N	O	S	0	0	0
			1636	1029	273	329	5			
2	J	212	Total	C	N	O	S	0	0	0
			1636	1029	273	329	5			

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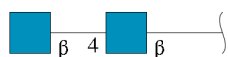
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	212	Total	C	N	O	S	0	0	0
			1636	1029	273	329	5			
2	R	212	Total	C	N	O	S	0	0	0
			1636	1029	273	329	5			
2	W	211	Total	C	N	O	S	0	0	0
			1628	1025	272	326	5			
2	c	212	Total	C	N	O	S	0	0	0
			1636	1029	273	329	5			

- Molecule 3 is a protein called Antibody 3E1 Fab heavy chain.

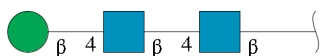
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	221	Total	C	N	O	S	0	0	0
			1658	1050	278	325	5			
3	K	221	Total	C	N	O	S	0	0	0
			1658	1050	278	325	5			
3	N	221	Total	C	N	O	S	0	0	0
			1658	1050	278	325	5			
3	S	221	Total	C	N	O	S	0	0	0
			1658	1050	278	325	5			
3	X	221	Total	C	N	O	S	0	0	0
			1658	1050	278	325	5			
3	d	221	Total	C	N	O	S	0	0	0
			1658	1050	278	325	5			

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



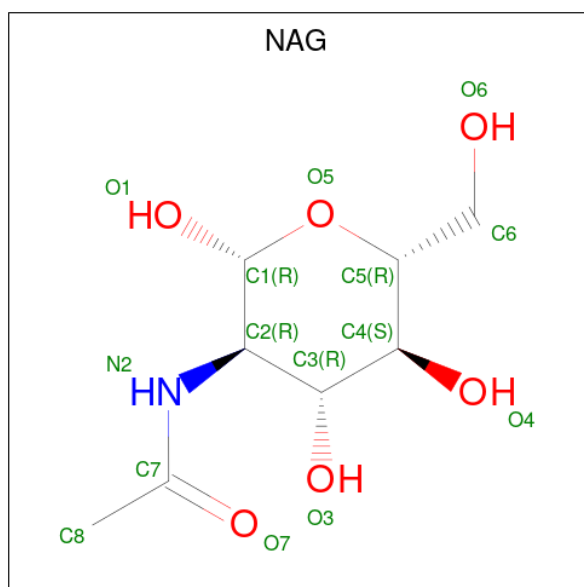
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	A	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 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
5	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	O	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	T	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	e	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

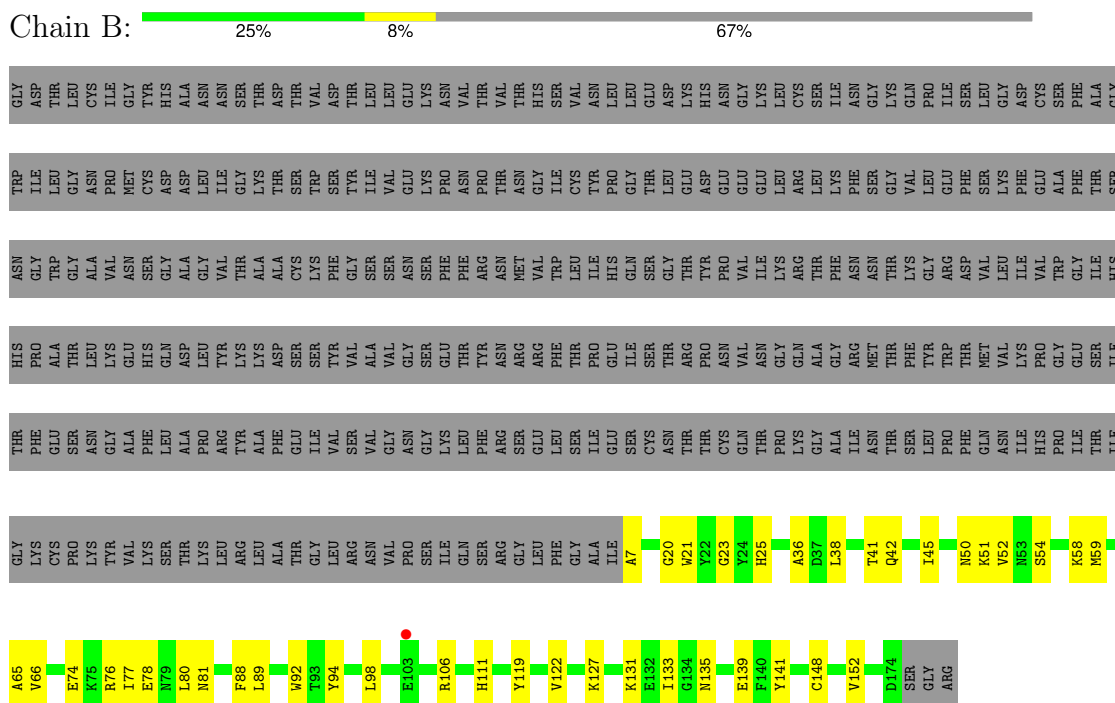


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	V	1	Total	C	N	O	0	0
			14	8	1	5		

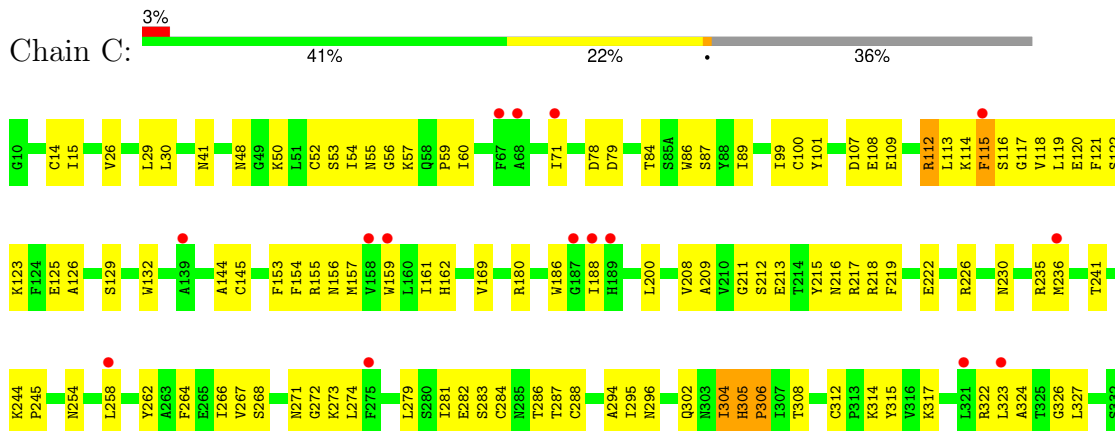
3 Residue-property plots

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: Hemagglutinin



• Molecule 1: Hemagglutinin



ARG	ASN	GLU	ILE
	TYR	LYS	GLN
	LEU	MET	SER
	GLU	ASN	ARG
	LYS	THR	GLY
	VAL	GLN	LEU
	ARG	PHE	THR
	SER	THR	GLY
	GLN	ALA	ALA
	LEU	VAL	ILE
	LYS	GLY	ALA
	ASN	LYS	GLY
	ASN	GLU	PHE
	ALA	PHE	ILE
	LYS	ASN	GLU
	GLU	HIS	GLY
	ILE	LEU	GLY
	GLY	GLU	TRP
	ASN	LYS	THR
	GLY	ARG	GLY
	CYS	ILE	MET
	PHE	GLU	VAL
	GLU	ASN	ASP
	PHE	LEU	GLY
	TYR	ASN	TRP
	HIS	LYS	TYR
	CYS	LYS	GLY
	CYS	VAL	TYR
	ASN	ASP	HIS
	ASN	ASP	HIS
	THR	GLY	GLN
	CYS	PHE	ASN
	MET	LEU	GLU
	GLU	ASP	GLN
	SER	ILE	GLY
	VAL	TRP	SER
	LYS	THR	GLY
	ASN	TYR	TYR
	GLY	ASN	ALA
	THR	ALA	ALA
	ASP	GLU	ASP
	TYR	LEU	LEU
	GLU	LEU	LYS
	GLU	VAL	SER
	ALA	ARG	THR
	LYS	THR	GLY
	LEU	LEU	ILE
	ASN	ASP	THR
	ARG	TYR	ASN
	GLU	HIS	LYS
	GLU	ASP	VAL
	ILE	SER	ASN
	ASP	ASN	SER
	SER	VAL	THR
	GLY	LYS	ILE

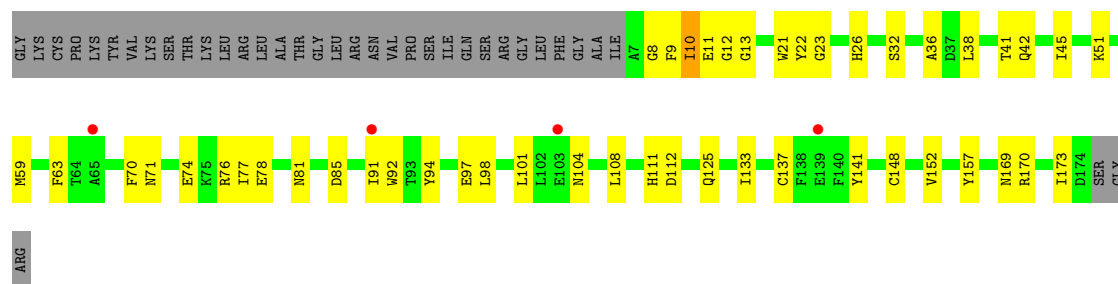
- Molecule 1: Hemagglutinin

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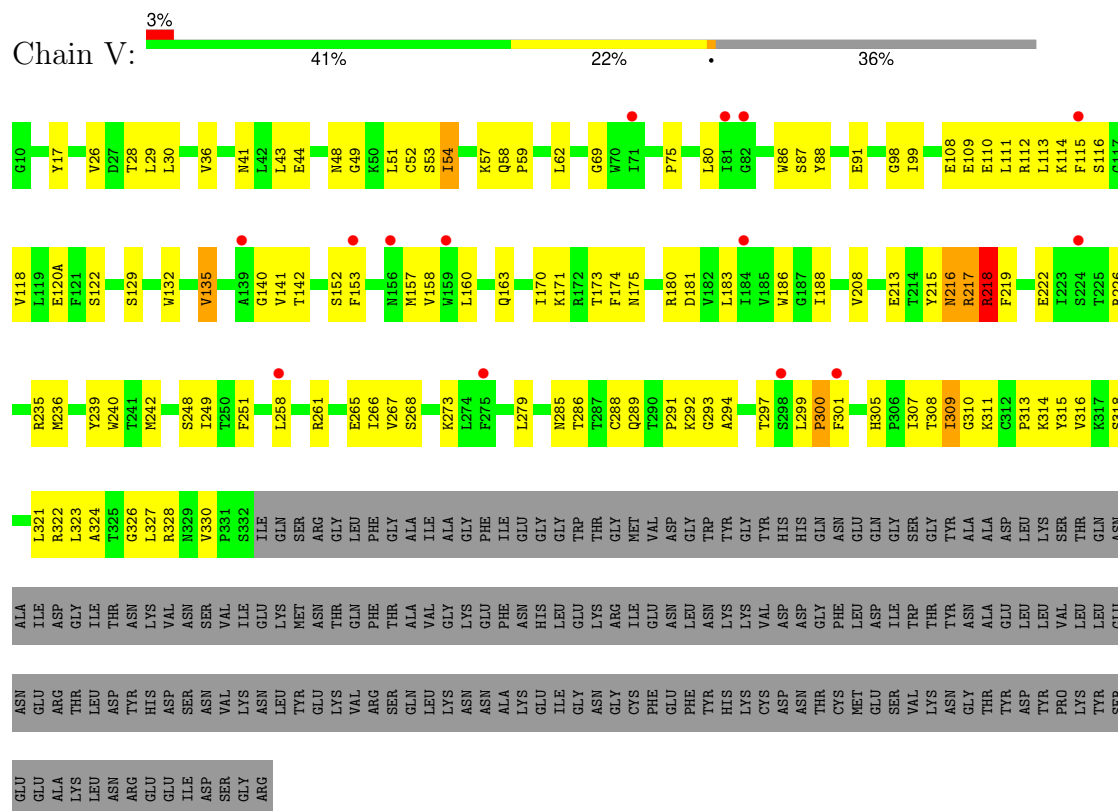
- Molecule 1: Hemagglutinin

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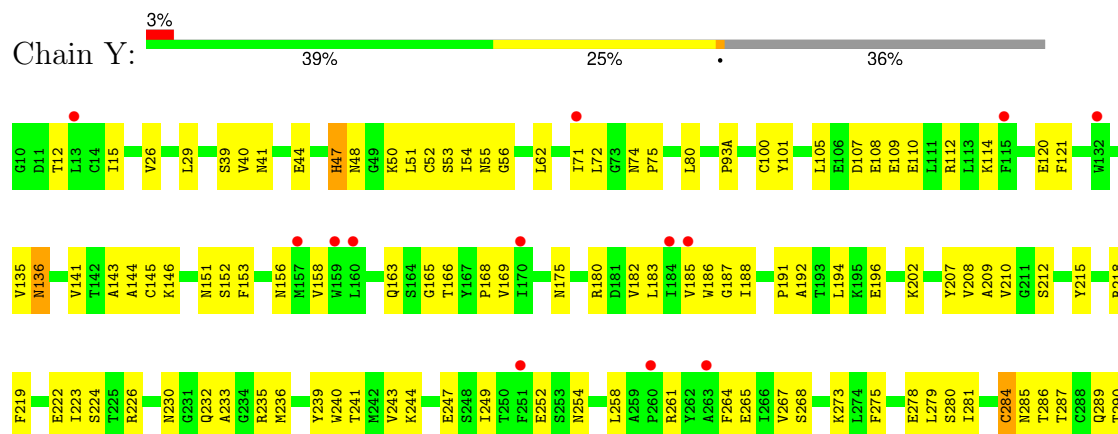


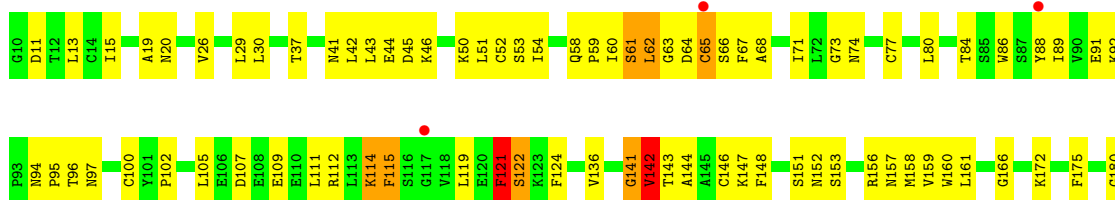


• Molecule 1: Hemagglutinin

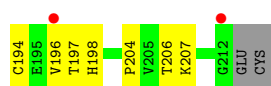


• Molecule 1: Hemagglutinin

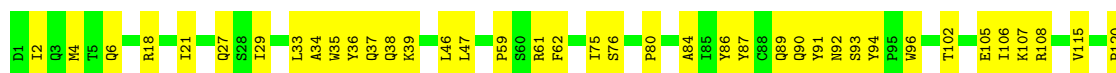




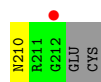
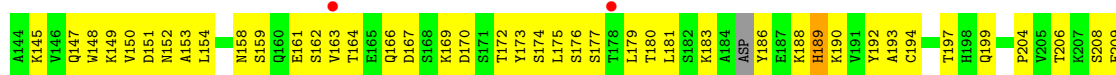
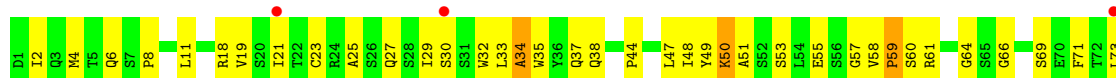
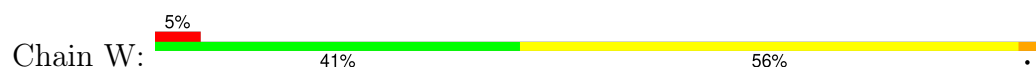




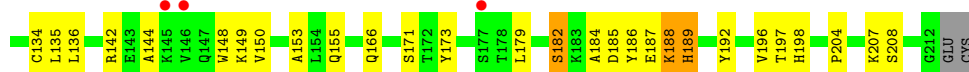
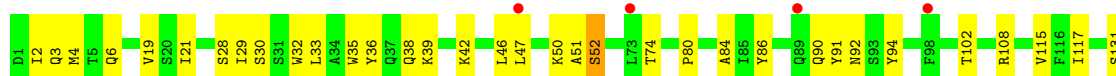
• Molecule 2: Antibody 3E1 Fab light chain



• Molecule 2: Antibody 3E1 Fab light chain

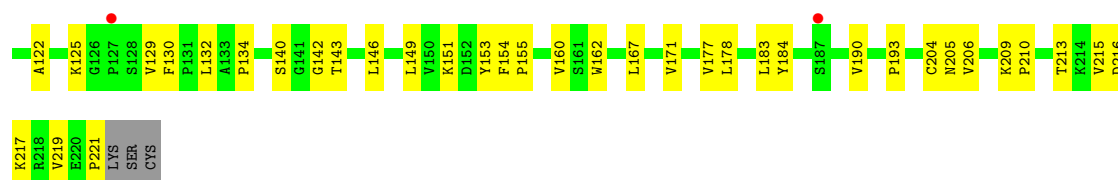


• Molecule 2: Antibody 3E1 Fab light chain



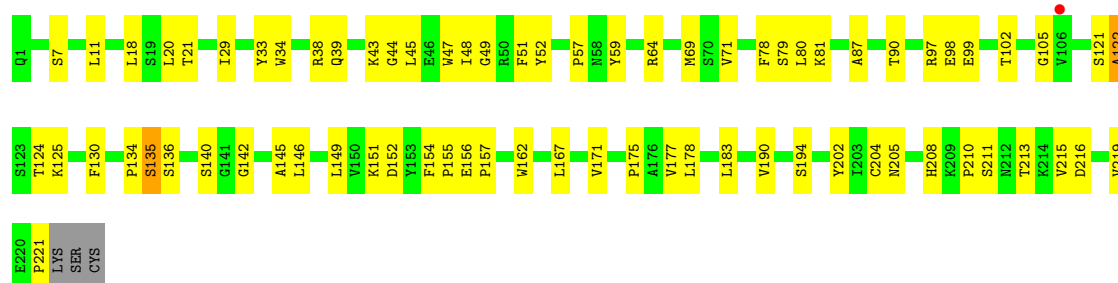
• Molecule 3: Antibody 3E1 Fab heavy chain





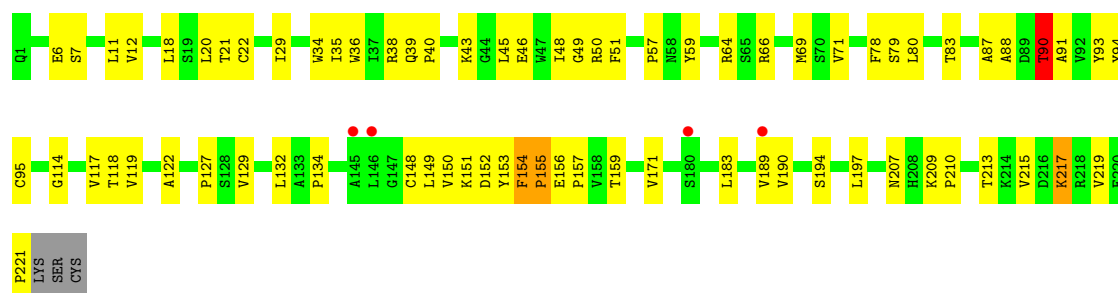
• Molecule 3: Antibody 3E1 Fab heavy chain

Chain K: 66% 32% ..



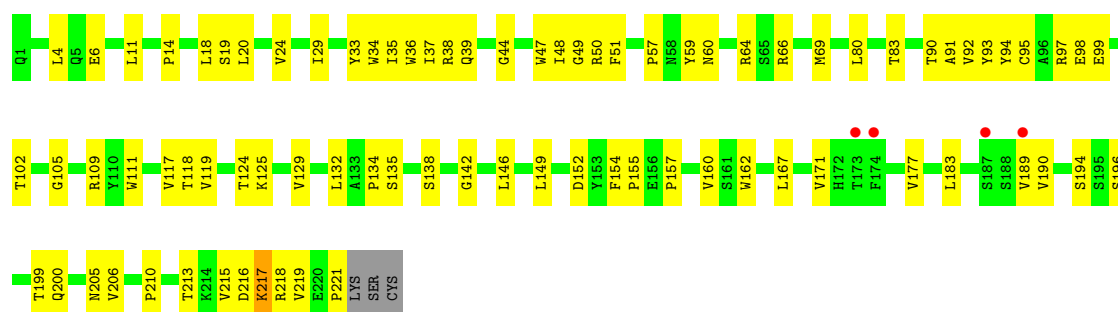
• Molecule 3: Antibody 3E1 Fab heavy chain

Chain N: 2% 66% 31% ..



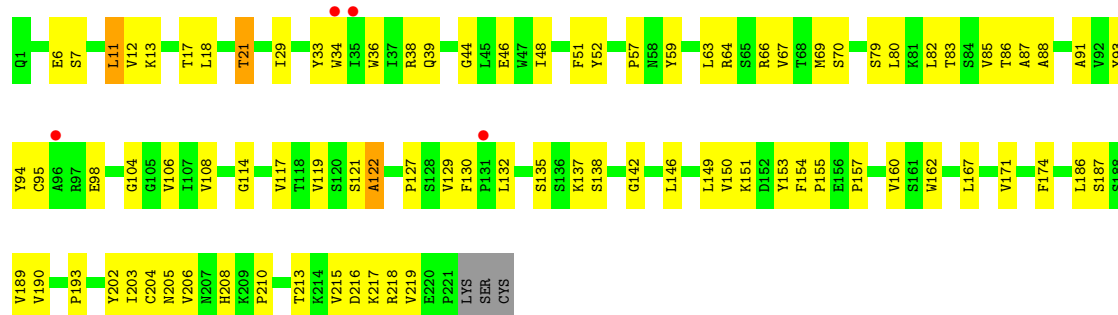
• Molecule 3: Antibody 3E1 Fab heavy chain

Chain S: 2% 62% 36% .

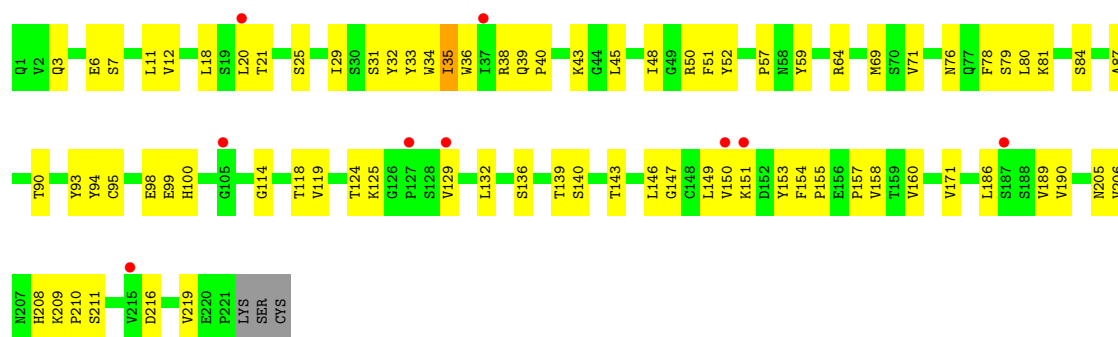


• Molecule 3: Antibody 3E1 Fab heavy chain

Chain X: 2% 60% 38% ..



● Molecule 3: Antibody 3E1 Fab heavy chain



● Molecule 4: 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



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



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

Chain G:  33% 67%

MAG1
MAG2
BMA3

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

Chain O:  33% 67%

MAG1
MAG2
BMA3

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

Chain T:  67% 33%

MAG1
MAG2
BMA3

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

Chain e:  67% 33%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	182.43Å 194.50Å 214.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.05 – 4.60 48.05 – 4.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.05-4.60) 99.4 (48.05-4.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 4.64Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.293 , 0.325 0.301 , 0.325	Depositor DCC
R_{free} test set	2056 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	133.6	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 423.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	43211	wwPDB-VP
Average B, all atoms (Å ²)	208.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	B	0.22	0/1387	0.57	4/1869 (0.2%)
1	C	0.30	1/2566 (0.0%)	0.61	7/3482 (0.2%)
1	H	0.23	0/1387	0.57	2/1869 (0.1%)
1	I	0.32	1/1387 (0.1%)	0.60	4/1869 (0.2%)
1	L	0.37	2/2566 (0.1%)	0.77	10/3482 (0.3%)
1	P	0.17	0/1387	0.37	0/1869
1	Q	0.42	1/2566 (0.0%)	1.04	20/3482 (0.6%)
1	U	0.20	0/1387	0.47	1/1869 (0.1%)
1	V	0.33	0/2566	0.64	4/3482 (0.1%)
1	Y	0.27	0/2566	0.64	8/3482 (0.2%)
1	a	0.23	0/1387	0.54	2/1869 (0.1%)
1	b	0.38	1/2566 (0.0%)	0.97	16/3482 (0.5%)
2	D	0.20	0/1674	0.53	2/2273 (0.1%)
2	J	0.28	0/1674	0.72	8/2273 (0.4%)
2	M	0.25	0/1674	0.52	1/2273 (0.0%)
2	R	0.24	0/1674	0.50	0/2273
2	W	0.47	0/1665	0.82	4/2259 (0.2%)
2	c	0.26	0/1674	0.66	6/2273 (0.3%)
3	E	0.26	0/1700	0.61	4/2323 (0.2%)
3	K	0.24	0/1700	0.63	5/2323 (0.2%)
3	N	0.31	0/1700	0.72	8/2323 (0.3%)
3	S	0.25	0/1700	0.57	3/2323 (0.1%)
3	X	0.28	1/1700 (0.1%)	0.59	4/2323 (0.2%)
3	d	0.30	0/1700	0.60	1/2323 (0.0%)
All	All	0.30	7/43953 (0.0%)	0.68	124/59668 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	I	0	1
1	Q	0	1
1	V	0	1
1	b	0	1
2	W	0	1
3	E	0	1
All	All	0	7

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	59	PRO	N-CD	9.64	1.61	1.47
1	I	77	ILE	CA-C	7.95	1.62	1.52
1	L	54	ILE	N-CA	7.89	1.56	1.46
1	b	121	PHE	C-N	-7.03	1.24	1.33
1	L	55	ASN	N-CA	6.32	1.54	1.45

The worst 5 of 124 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	54	ILE	N-CA-C	31.70	143.19	110.23
1	b	62	LEU	N-CA-C	-24.22	74.68	110.52
1	L	139	ALA	N-CA-C	-20.65	80.06	107.73
1	Q	55	ASN	N-CA-C	-18.13	89.06	113.18
1	b	114	LYS	N-CA-C	-13.15	94.09	111.71

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	115	PHE	Peptide
3	E	38	ARG	Sidechain
1	I	76	ARG	Sidechain
1	Q	52	CYS	Mainchain
1	V	218	ARG	Sidechain

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	B	1360	0	1276	37	0
1	C	2505	0	2455	110	0
1	H	1360	0	1276	55	0
1	I	1360	0	1276	63	0
1	L	2505	0	2453	117	0
1	P	1360	0	1276	45	0
1	Q	2505	0	2455	108	0
1	U	1360	0	1276	60	0
1	V	2505	0	2455	116	0
1	Y	2505	0	2453	135	0
1	a	1360	0	1276	59	0
1	b	2505	0	2459	133	0
2	D	1636	0	1591	58	0
2	J	1636	0	1591	69	0
2	M	1636	0	1591	62	1
2	R	1636	0	1591	59	0
2	W	1628	0	1586	136	0
2	c	1636	0	1591	57	2
3	E	1658	0	1642	61	0
3	K	1658	0	1642	55	0
3	N	1658	0	1642	53	0
3	S	1658	0	1642	78	2
3	X	1658	0	1642	76	0
3	d	1658	0	1640	63	1
4	A	28	0	25	0	0
4	Z	28	0	25	0	0
5	F	39	0	34	1	0
5	G	39	0	34	1	0
5	O	39	0	34	2	0
5	T	39	0	34	0	0
5	e	39	0	34	0	0
6	V	14	0	13	0	0
All	All	43211	0	42010	1628	3

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 19.

The worst 5 of 1628 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:W:6:GLN:CD	2:W:99:GLY:HA3	1.54	1.31
2:R:166:GLN:HE21	2:R:171:SER:CB	1.44	1.30
2:R:166:GLN:NE2	2:R:171:SER:HB3	1.49	1.24
1:C:304:ILE:O	1:C:305:HIS:CD2	1.98	1.17
1:b:54:ILE:HG23	1:b:285:CYS:O	1.48	1.14

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:199:THR:CA	2:c:182:SER:OG[3_654]	1.70	0.50
3:S:199:THR:C	2:c:182:SER:OG[3_654]	1.70	0.50
2:M:3:GLN:CD	3:d:84:SER:OG[3_554]	2.13	0.07

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	B	166/504 (33%)	162 (98%)	4 (2%)	0	100	100
1	C	321/504 (64%)	290 (90%)	31 (10%)	0	100	100
1	H	166/504 (33%)	157 (95%)	9 (5%)	0	100	100
1	I	166/504 (33%)	157 (95%)	9 (5%)	0	100	100
1	L	321/504 (64%)	295 (92%)	26 (8%)	0	100	100
1	P	166/504 (33%)	158 (95%)	8 (5%)	0	100	100
1	Q	321/504 (64%)	299 (93%)	22 (7%)	0	100	100
1	U	166/504 (33%)	157 (95%)	9 (5%)	0	100	100
1	V	321/504 (64%)	287 (89%)	33 (10%)	1 (0%)	37	72
1	Y	321/504 (64%)	293 (91%)	28 (9%)	0	100	100
1	a	166/504 (33%)	157 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	321/504 (64%)	288 (90%)	33 (10%)	0	100	100
2	D	210/214 (98%)	200 (95%)	10 (5%)	0	100	100
2	J	210/214 (98%)	197 (94%)	13 (6%)	0	100	100
2	M	210/214 (98%)	195 (93%)	15 (7%)	0	100	100
2	R	210/214 (98%)	197 (94%)	13 (6%)	0	100	100
2	W	207/214 (97%)	176 (85%)	31 (15%)	0	100	100
2	c	210/214 (98%)	194 (92%)	16 (8%)	0	100	100
3	E	219/224 (98%)	195 (89%)	24 (11%)	0	100	100
3	K	219/224 (98%)	207 (94%)	12 (6%)	0	100	100
3	N	219/224 (98%)	203 (93%)	16 (7%)	0	100	100
3	S	219/224 (98%)	198 (90%)	21 (10%)	0	100	100
3	X	219/224 (98%)	204 (93%)	15 (7%)	0	100	100
3	d	219/224 (98%)	205 (94%)	14 (6%)	0	100	100
All	All	5493/8676 (63%)	5071 (92%)	421 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	V	300	PRO

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	B	146/434 (34%)	146 (100%)	0	100	100
1	C	279/434 (64%)	279 (100%)	0	100	100
1	H	146/434 (34%)	146 (100%)	0	100	100
1	I	146/434 (34%)	146 (100%)	0	100	100
1	L	279/434 (64%)	278 (100%)	1 (0%)	89	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	146/434 (34%)	146 (100%)	0	100	100
1	Q	279/434 (64%)	275 (99%)	4 (1%)	62	75
1	U	146/434 (34%)	146 (100%)	0	100	100
1	V	279/434 (64%)	276 (99%)	3 (1%)	70	80
1	Y	279/434 (64%)	278 (100%)	1 (0%)	89	90
1	a	146/434 (34%)	145 (99%)	1 (1%)	81	87
1	b	279/434 (64%)	276 (99%)	3 (1%)	70	80
2	D	186/188 (99%)	186 (100%)	0	100	100
2	J	186/188 (99%)	186 (100%)	0	100	100
2	M	186/188 (99%)	186 (100%)	0	100	100
2	R	186/188 (99%)	186 (100%)	0	100	100
2	W	185/188 (98%)	183 (99%)	2 (1%)	70	80
2	c	186/188 (99%)	186 (100%)	0	100	100
3	E	190/193 (98%)	190 (100%)	0	100	100
3	K	190/193 (98%)	190 (100%)	0	100	100
3	N	190/193 (98%)	189 (100%)	1 (0%)	86	89
3	S	190/193 (98%)	190 (100%)	0	100	100
3	X	190/193 (98%)	189 (100%)	1 (0%)	86	89
3	d	190/193 (98%)	190 (100%)	0	100	100
All	All	4805/7494 (64%)	4788 (100%)	17 (0%)	89	90

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	b	142	VAL
1	b	286	ASN
1	V	216	ASN
1	V	309	ILE
2	W	50	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	Y	302	GLN

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Mol	Chain	Res	Type
2	c	158	ASN
1	a	26	HIS
1	b	290	GLN
1	Q	285	ASN

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 ⓘ

19 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	A	1	4	14,14,15	0.32	0	17,19,21	0.39	0
4	NAG	A	2	4	14,14,15	0.35	0	17,19,21	0.67	1 (5%)
5	NAG	F	1	5	14,14,15	0.39	0	17,19,21	0.42	0
5	NAG	F	2	5	14,14,15	0.58	0	17,19,21	0.54	0
5	BMA	F	3	5	11,11,12	0.74	0	15,15,17	0.74	0
5	NAG	G	1	5	14,14,15	0.24	0	17,19,21	0.46	0
5	NAG	G	2	5	14,14,15	0.35	0	17,19,21	0.51	0
5	BMA	G	3	5	11,11,12	0.76	0	15,15,17	0.66	0
5	NAG	O	1	5	14,14,15	0.54	0	17,19,21	1.38	3 (17%)
5	NAG	O	2	5	14,14,15	2.19	2 (14%)	17,19,21	1.15	2 (11%)
5	BMA	O	3	5	11,11,12	1.99	5 (45%)	15,15,17	0.94	1 (6%)
5	NAG	T	1	5	14,14,15	0.37	0	17,19,21	0.50	0
5	NAG	T	2	5	14,14,15	0.33	0	17,19,21	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	T	3	5	11,11,12	1.25	1 (9%)	15,15,17	0.81	1 (6%)
4	NAG	Z	1	4	14,14,15	0.19	0	17,19,21	0.42	0
4	NAG	Z	2	4	14,14,15	0.43	0	17,19,21	0.42	0
5	NAG	e	1	5	14,14,15	0.23	0	17,19,21	0.67	0
5	NAG	e	2	5	14,14,15	0.27	0	17,19,21	0.81	0
5	BMA	e	3	5	11,11,12	0.72	0	15,15,17	0.83	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
4	NAG	A	1	4	-	0/6/23/26	0/1/1/1
4	NAG	A	2	4	-	2/6/23/26	0/1/1/1
5	NAG	F	1	5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	1/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
5	NAG	G	1	5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	BMA	G	3	5	-	1/2/19/22	0/1/1/1
5	NAG	O	1	5	-	4/6/23/26	0/1/1/1
5	NAG	O	2	5	-	1/6/23/26	0/1/1/1
5	BMA	O	3	5	-	2/2/19/22	0/1/1/1
5	NAG	T	1	5	-	0/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
5	BMA	T	3	5	-	1/2/19/22	0/1/1/1
4	NAG	Z	1	4	-	0/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	1/6/23/26	0/1/1/1
5	NAG	e	1	5	-	2/6/23/26	0/1/1/1
5	NAG	e	2	5	-	2/6/23/26	0/1/1/1
5	BMA	e	3	5	-	1/2/19/22	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	2	NAG	C1-C2	6.68	1.61	1.52
5	O	2	NAG	O5-C1	-4.15	1.36	1.43
5	O	3	BMA	C2-C3	3.88	1.58	1.52
5	O	3	BMA	C1-C2	2.50	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	T	3	BMA	C4-C5	2.49	1.58	1.53

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	1	NAG	C4-C3-C2	2.99	115.40	111.02
5	O	1	NAG	O4-C4-C3	-2.72	103.96	110.38
5	O	2	NAG	C4-C3-C2	2.36	114.48	111.02
5	T	3	BMA	O2-C2-C3	-2.22	105.55	110.15
5	O	2	NAG	O5-C5-C4	-2.20	105.47	110.83

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

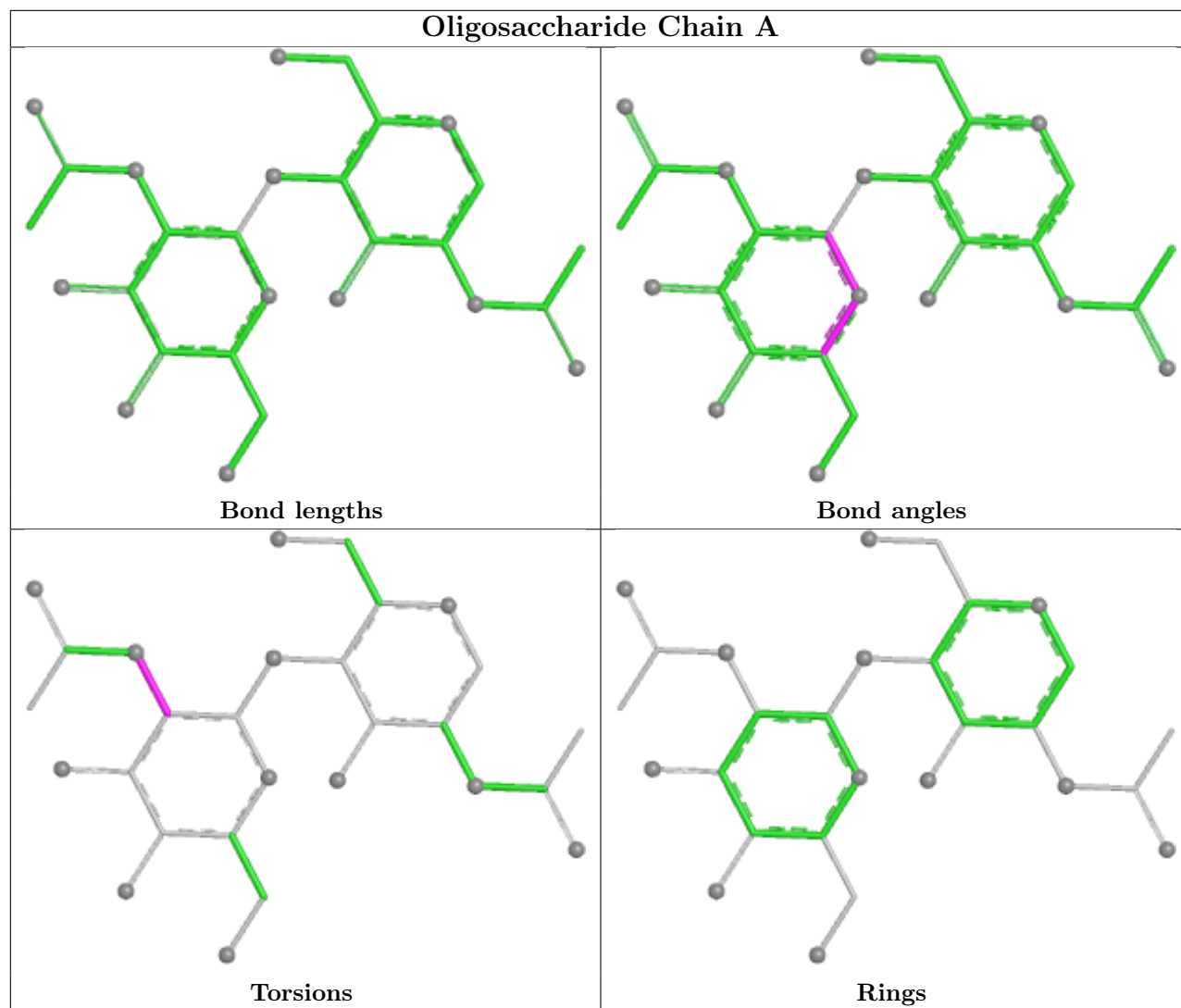
Mol	Chain	Res	Type	Atoms
5	e	2	NAG	C1-C2-N2-C7
5	O	3	BMA	C4-C5-C6-O6
5	O	3	BMA	O5-C5-C6-O6
5	O	1	NAG	O5-C5-C6-O6
5	O	1	NAG	C4-C5-C6-O6

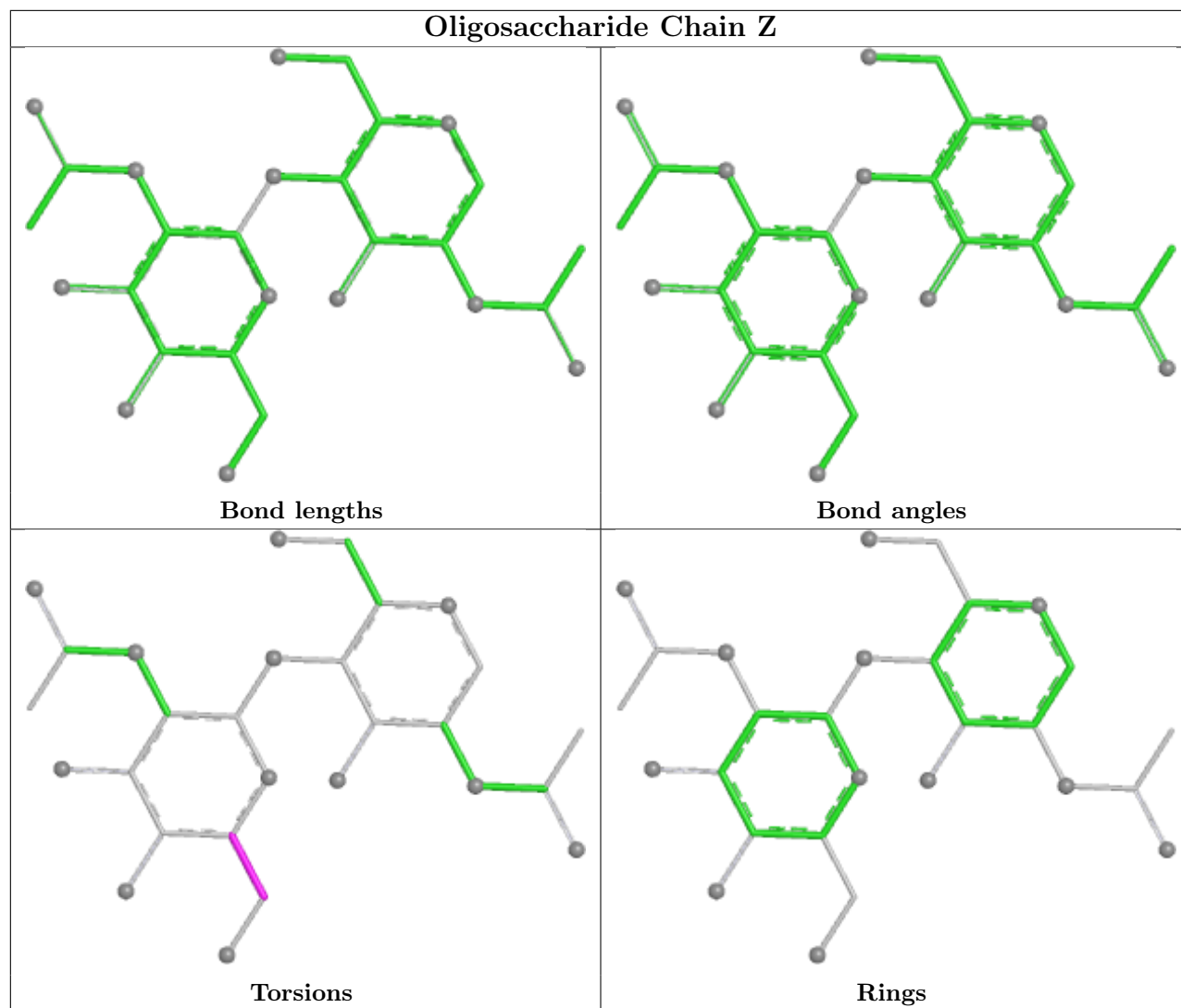
There are no ring outliers.

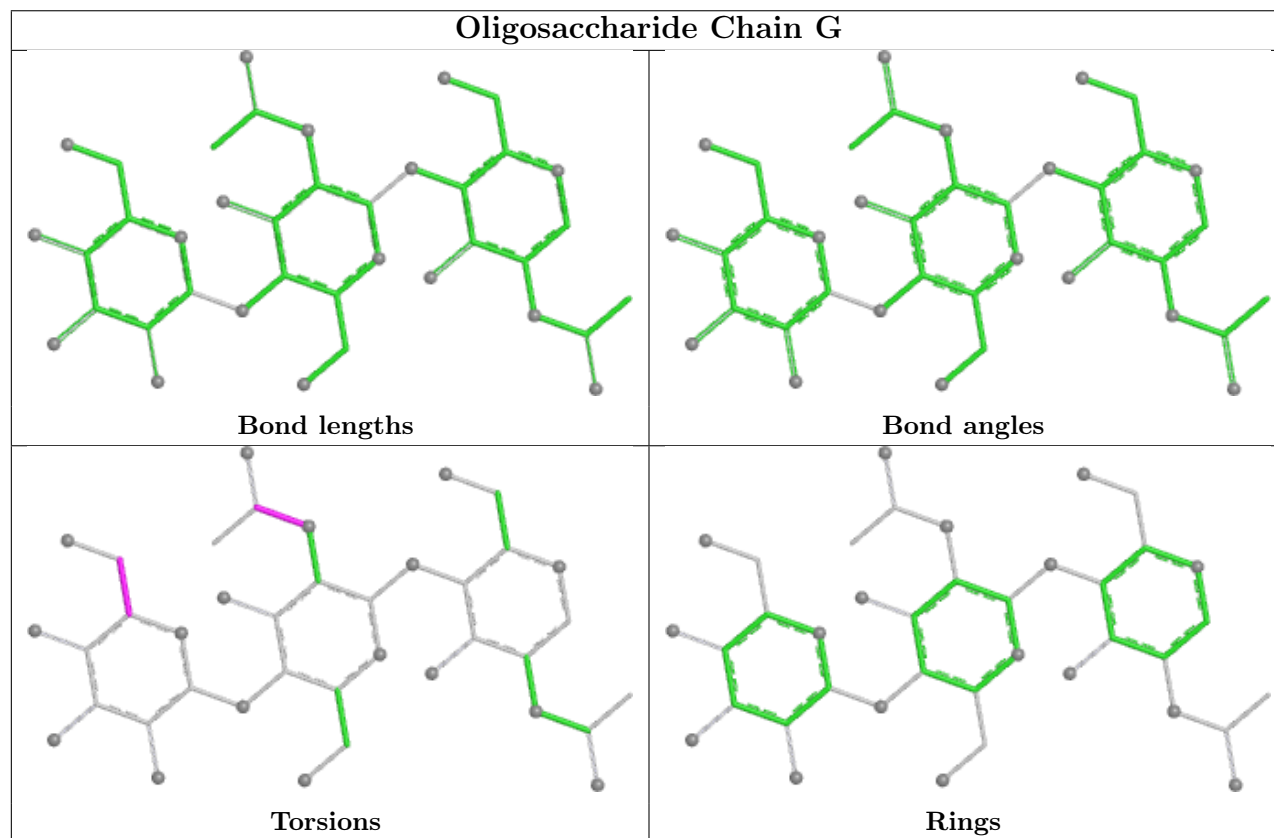
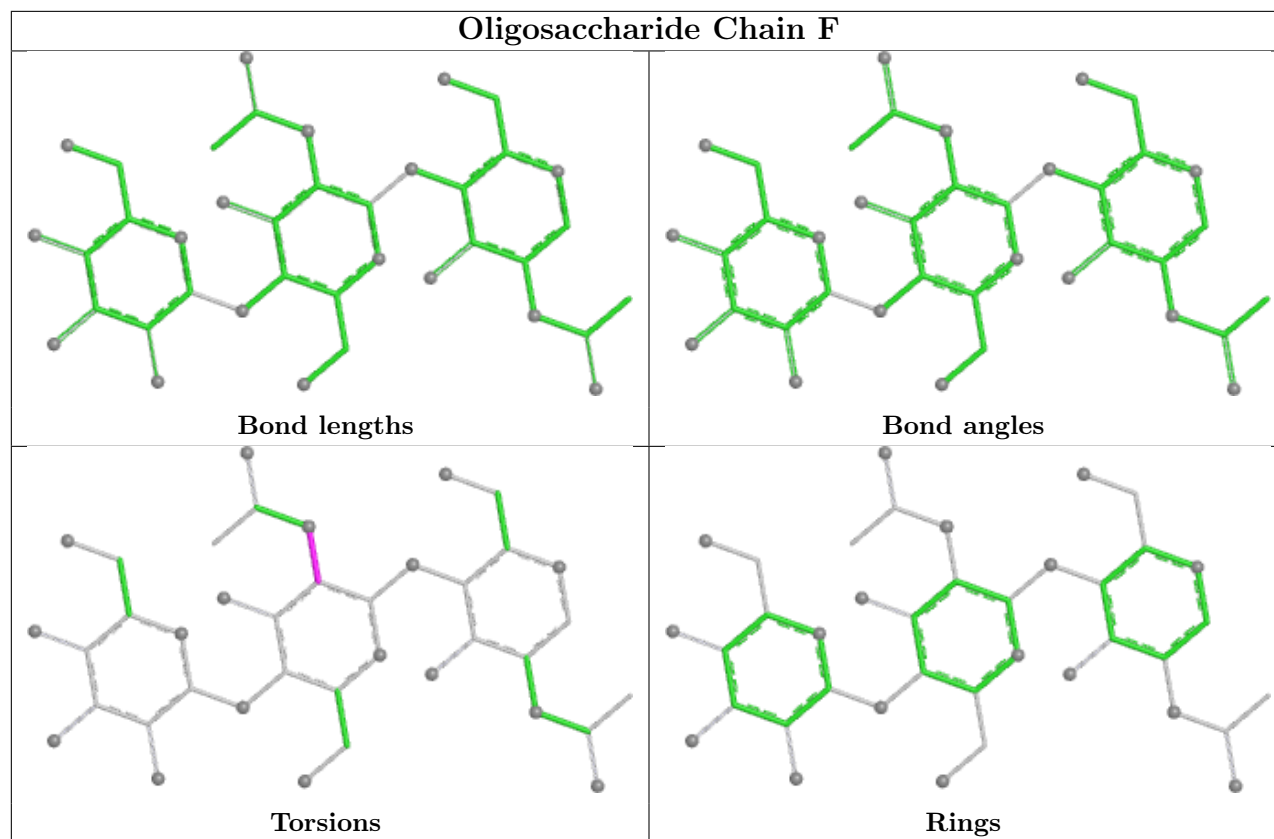
6 monomers are involved in 4 short contacts:

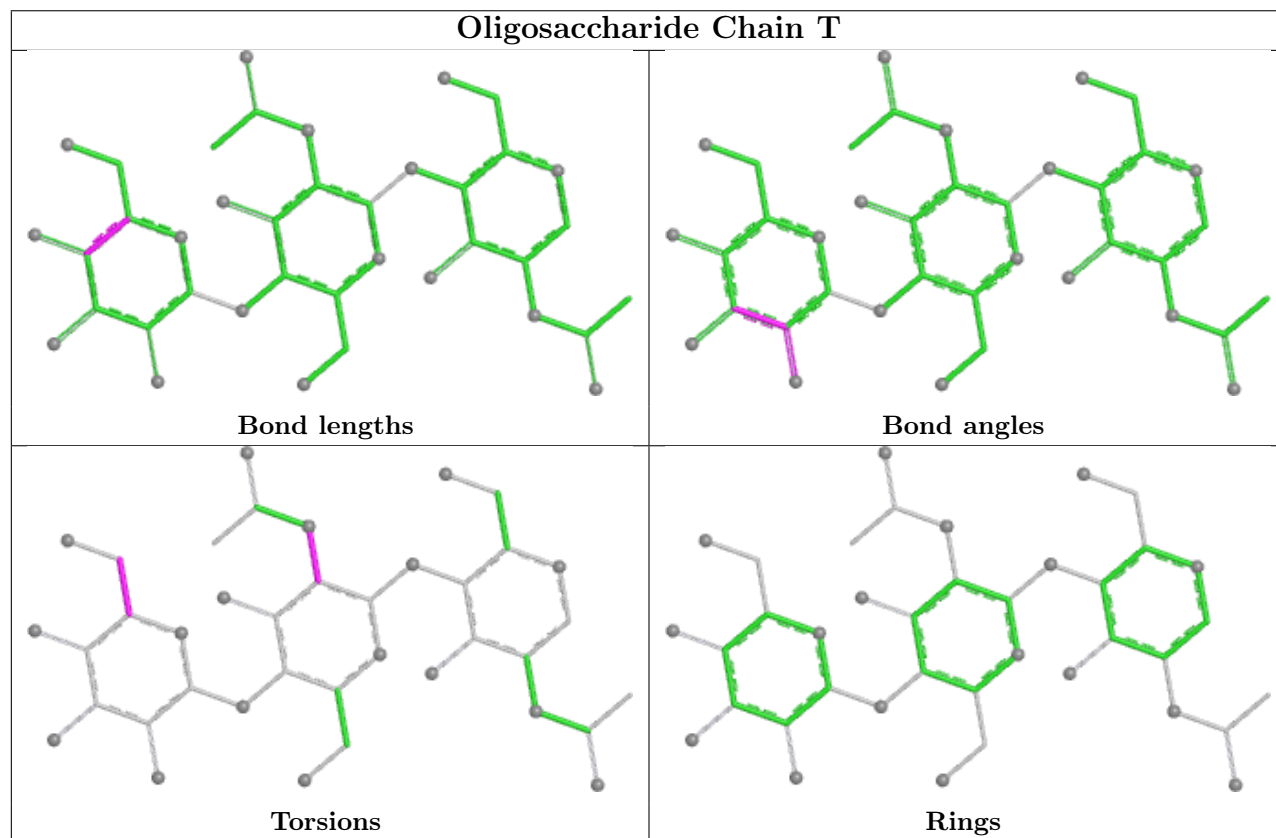
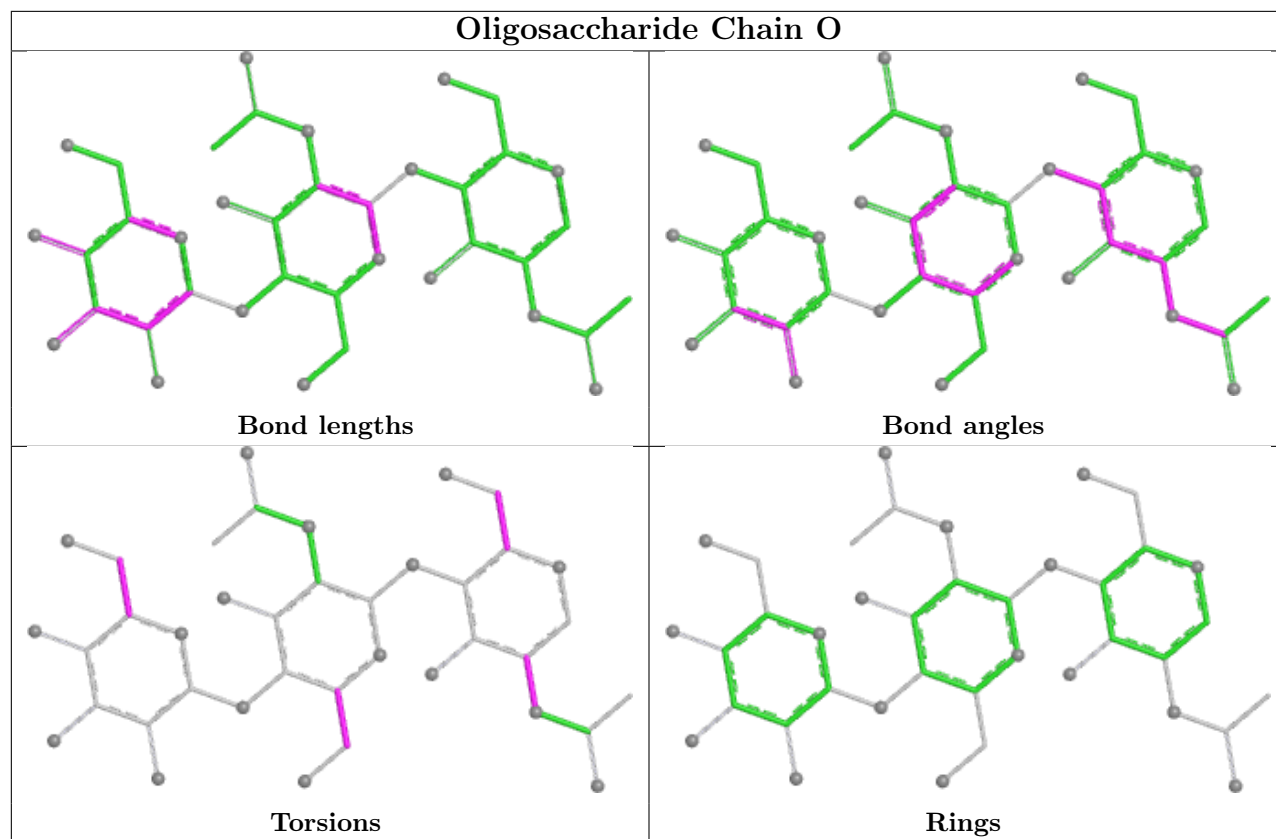
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	O	1	NAG	2	0
5	F	1	NAG	1	0
5	G	3	BMA	1	0
5	G	2	NAG	1	0
5	O	2	NAG	1	0
5	F	2	NAG	1	0

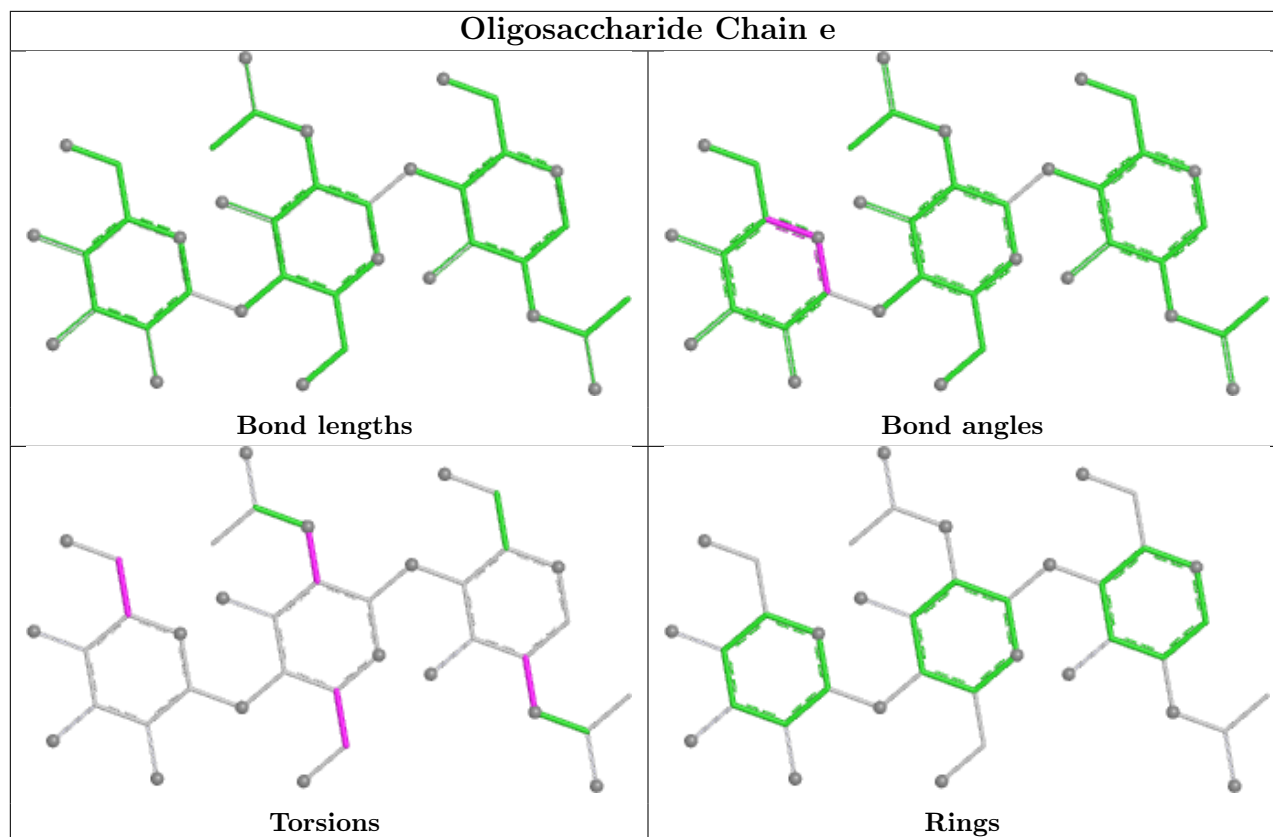
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

1 ligand is 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	NAG	V	601	-	14,14,15	0.27	0	17,19,21	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	V	601	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

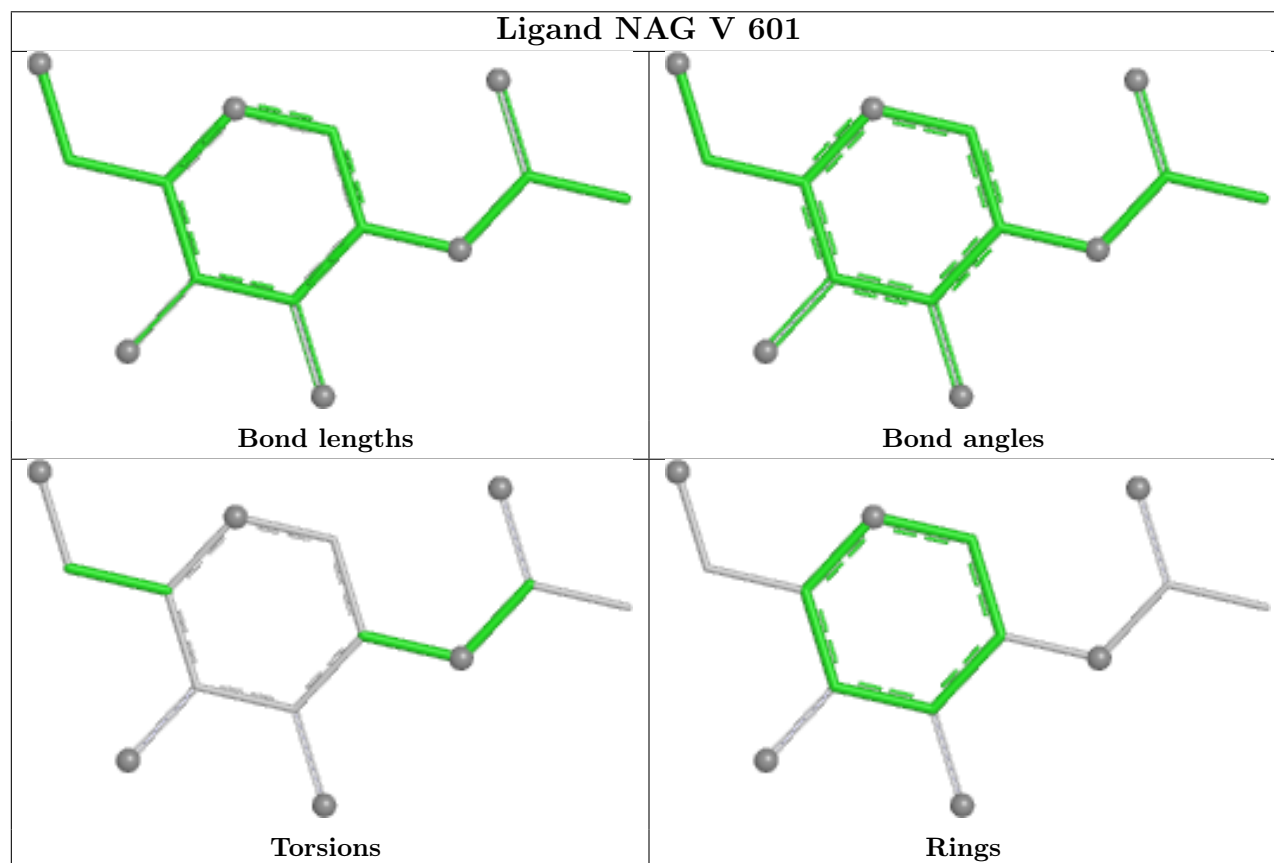
There are no chirality outliers.

There are no torsion outliers.

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 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	168/504 (33%)	0.04	1 (0%) 85 74	143, 193, 240, 248	0
1	C	323/504 (64%)	0.26	15 (4%) 38 31	159, 225, 243, 254	0
1	H	168/504 (33%)	0.15	6 (3%) 46 35	133, 170, 239, 251	0
1	I	168/504 (33%)	0.29	5 (2%) 52 39	147, 180, 248, 258	0
1	L	323/504 (64%)	0.15	6 (1%) 66 50	87, 193, 207, 218	0
1	P	168/504 (33%)	0.25	7 (4%) 41 32	161, 184, 266, 273	0
1	Q	323/504 (64%)	0.21	10 (3%) 51 39	171, 239, 258, 266	0
1	U	168/504 (33%)	0.16	4 (2%) 59 45	174, 224, 269, 277	0
1	V	323/504 (64%)	0.26	14 (4%) 40 32	175, 266, 280, 295	0
1	Y	323/504 (64%)	0.23	14 (4%) 40 32	146, 212, 228, 240	0
1	a	168/504 (33%)	0.22	7 (4%) 41 32	135, 180, 255, 267	0
1	b	323/504 (64%)	0.14	8 (2%) 58 44	30, 228, 247, 258	0
2	D	212/214 (99%)	0.21	9 (4%) 41 32	202, 249, 297, 303	0
2	J	212/214 (99%)	-0.05	1 (0%) 87 76	142, 171, 208, 222	0
2	M	212/214 (99%)	0.23	10 (4%) 37 31	118, 152, 179, 190	0
2	R	212/214 (99%)	0.01	5 (2%) 59 45	153, 191, 222, 226	0
2	W	211/214 (98%)	0.43	11 (5%) 34 27	263, 324, 370, 376	0
2	c	212/214 (99%)	0.13	7 (3%) 49 38	124, 153, 184, 204	0
3	E	221/224 (98%)	0.26	2 (0%) 81 67	126, 257, 310, 317	0
3	K	221/224 (98%)	0.02	1 (0%) 87 76	77, 165, 177, 188	0
3	N	221/224 (98%)	0.12	4 (1%) 67 52	82, 149, 197, 224	0
3	S	221/224 (98%)	0.08	4 (1%) 67 52	87, 183, 212, 223	0
3	X	221/224 (98%)	0.38	4 (1%) 67 52	152, 325, 375, 379	0
3	d	221/224 (98%)	0.06	9 (4%) 42 33	83, 148, 186, 210	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	5543/8676 (63%)	0.18	164 (2%) 52 39	30, 199, 308, 379	0

The worst 5 of 164 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Y	185	VAL	6.4
1	V	71	ILE	6.2
1	Y	13	LEU	4.9
3	N	146	LEU	4.6
1	V	115	PHE	4.5

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](#)

SUGAR-RSR INFOmissingINFO

6.4 Ligands [i](#)

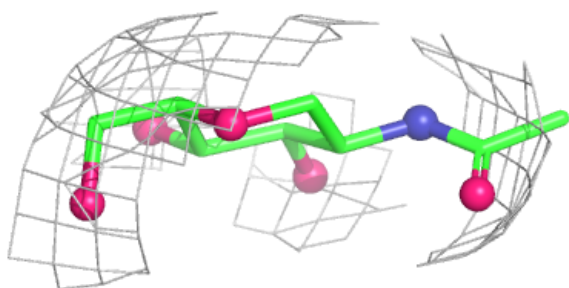
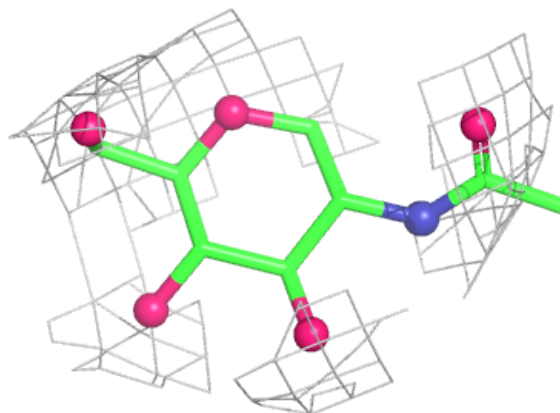
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	V	601	14/15	0.89	0.10	160,160,160,160	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 V 601:

$2mF_o-DF_c$ (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.