



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 21, 2024 – 02:52 PM EDT

PDB ID : 8US0
Title : Human antibody S8V1-157 in complex with the A/American black duck/New Brunswick/00464/2010(H4N6) HA head domain
Authors : McCarthy, K.R.
Deposited on : 2023-10-27
Resolution : 3.70 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

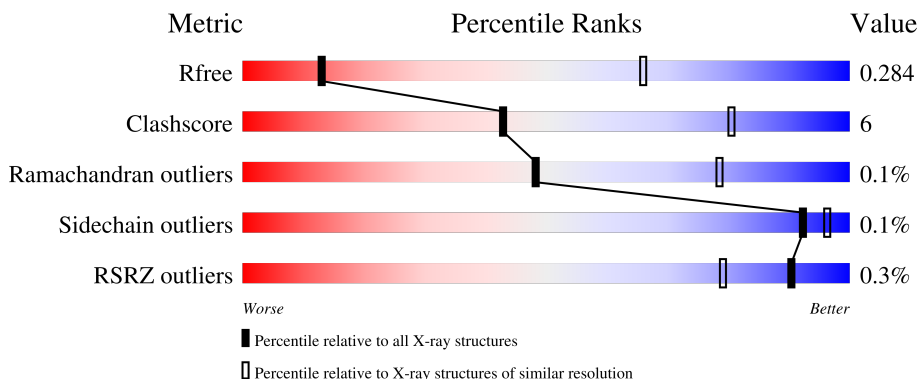
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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.











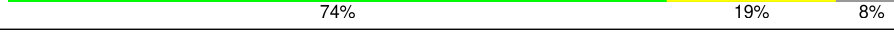
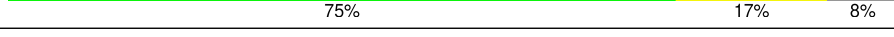
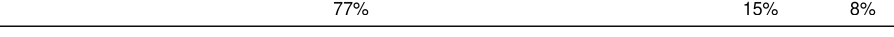

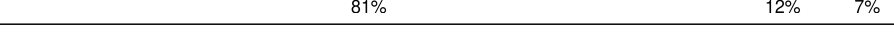
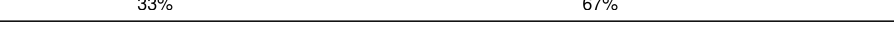
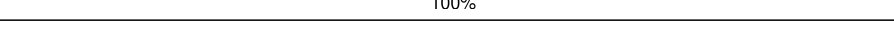


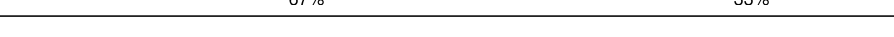
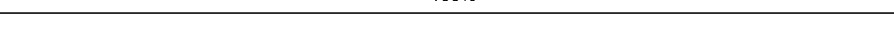

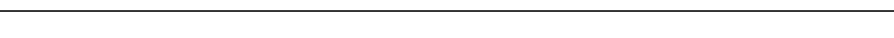

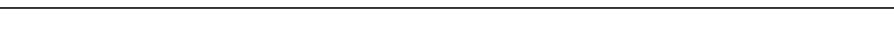
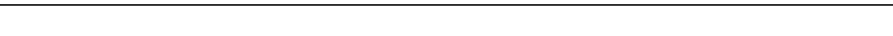
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1017 (3.80-3.60)
Clashscore	180529	1074 (3.80-3.60)
Ramachandran outliers	177936	1055 (3.80-3.60)
Sidechain outliers	177891	1052 (3.80-3.60)
RSRZ outliers	164620	1017 (3.80-3.60)

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	292	 84% 11% 5%
1	D	292	 83% 12% 5%
1	G	292	 79% 16% 5%
1	J	292	 79% 16% 5%
1	M	292	 81% 14% 5%

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Mol	Chain	Length	Quality of chain
1	P	292	 80% 14% 5%
2	C	221	 81% 16%
2	F	221	 82% 16%
2	I	221	 83% 14%
2	L	221	 84% 14%
2	O	221	 83% 14%
2	R	221	 88% 10%
3	B	231	 % 77% 16% 6%
3	E	231	 74% 19% 8%
3	H	231	 75% 17% 8%
3	K	231	 77% 15% 8%
3	N	231	 80% 12% 8%
3	Q	231	 81% 12% 7%
4	S	3	 33% 67%
4	T	3	 100%
4	U	3	 67% 33%
4	V	3	 67% 33%
4	W	3	 67% 33%
4	X	3	 100%
4	a	3	 100%
4	c	3	 100%
5	Y	2	 100%
5	Z	2	 50% 50%
5	b	2	 100%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 33101 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
			Total	C	N	O	S			
1	A	278	2174	1368	385	413	8	0	0	0
1	D	277	2166	1362	384	412	8	0	0	0
1	G	278	2175	1367	386	414	8	0	0	0
1	J	277	2166	1362	384	412	8	0	0	0
1	M	277	2166	1362	384	412	8	0	0	0
1	P	277	2166	1362	384	412	8	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	GLY	-	expression tag	UNP M1USN0
A	321	LEU	-	expression tag	UNP M1USN0
A	322	GLU	-	expression tag	UNP M1USN0
A	323	VAL	-	expression tag	UNP M1USN0
A	324	LEU	-	expression tag	UNP M1USN0
A	325	PHE	-	expression tag	UNP M1USN0
A	326	GLN	-	expression tag	UNP M1USN0
D	320	GLY	-	expression tag	UNP M1USN0
D	321	LEU	-	expression tag	UNP M1USN0
D	322	GLU	-	expression tag	UNP M1USN0
D	323	VAL	-	expression tag	UNP M1USN0
D	324	LEU	-	expression tag	UNP M1USN0
D	325	PHE	-	expression tag	UNP M1USN0
D	326	GLN	-	expression tag	UNP M1USN0
G	320	GLY	-	expression tag	UNP M1USN0
G	321	LEU	-	expression tag	UNP M1USN0
G	322	GLU	-	expression tag	UNP M1USN0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	323	VAL	-	expression tag	UNP M1USN0
G	324	LEU	-	expression tag	UNP M1USN0
G	325	PHE	-	expression tag	UNP M1USN0
G	326	GLN	-	expression tag	UNP M1USN0
J	320	GLY	-	expression tag	UNP M1USN0
J	321	LEU	-	expression tag	UNP M1USN0
J	322	GLU	-	expression tag	UNP M1USN0
J	323	VAL	-	expression tag	UNP M1USN0
J	324	LEU	-	expression tag	UNP M1USN0
J	325	PHE	-	expression tag	UNP M1USN0
J	326	GLN	-	expression tag	UNP M1USN0
M	320	GLY	-	expression tag	UNP M1USN0
M	321	LEU	-	expression tag	UNP M1USN0
M	322	GLU	-	expression tag	UNP M1USN0
M	323	VAL	-	expression tag	UNP M1USN0
M	324	LEU	-	expression tag	UNP M1USN0
M	325	PHE	-	expression tag	UNP M1USN0
M	326	GLN	-	expression tag	UNP M1USN0
P	320	GLY	-	expression tag	UNP M1USN0
P	321	LEU	-	expression tag	UNP M1USN0
P	322	GLU	-	expression tag	UNP M1USN0
P	323	VAL	-	expression tag	UNP M1USN0
P	324	LEU	-	expression tag	UNP M1USN0
P	325	PHE	-	expression tag	UNP M1USN0
P	326	GLN	-	expression tag	UNP M1USN0

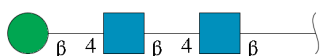
- Molecule 2 is a protein called human antibody S8V1-157 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	216	Total	C	N	O	S	0	0	0
			1665	1044	280	336	5			
2	I	216	Total	C	N	O	S	0	0	0
			1665	1044	280	336	5			
2	C	216	Total	C	N	O	S	0	0	0
			1665	1044	280	336	5			
2	R	216	Total	C	N	O	S	0	0	0
			1665	1044	280	336	5			
2	F	216	Total	C	N	O	S	0	0	0
			1665	1044	280	336	5			
2	L	216	Total	C	N	O	S	0	0	0
			1665	1044	280	336	5			

- Molecule 3 is a protein called human antibody S8V1-157 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	218	Total 1630	C 1027	N 268	O 327	S 8	0	0	0
3	H	213	Total 1596	C 1008	N 262	O 318	S 8	0	0	0
3	K	213	Total 1596	C 1008	N 262	O 318	S 8	0	0	0
3	N	213	Total 1596	C 1008	N 262	O 318	S 8	0	0	0
3	Q	214	Total 1602	C 1011	N 263	O 320	S 8	0	0	0
3	E	213	Total 1596	C 1008	N 262	O 318	S 8	0	0	0

- 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.



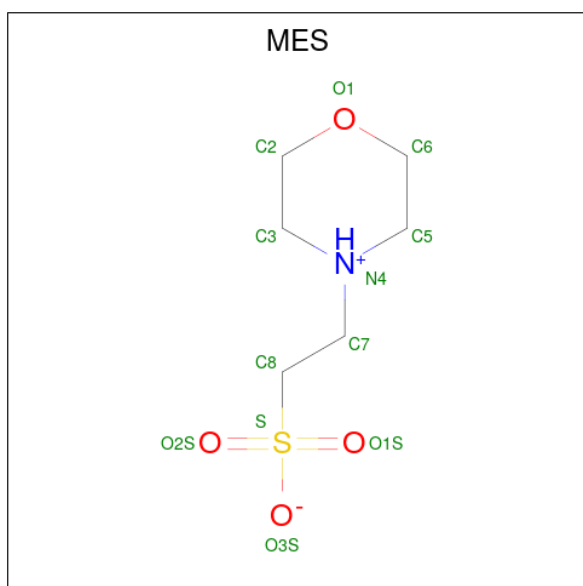
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	S	3	Total 39	C 22	N 2	O 15	0	0	0
4	T	3	Total 39	C 22	N 2	O 15	0	0	0
4	U	3	Total 39	C 22	N 2	O 15	0	0	0
4	V	3	Total 39	C 22	N 2	O 15	0	0	0
4	W	3	Total 39	C 22	N 2	O 15	0	0	0
4	X	3	Total 39	C 22	N 2	O 15	0	0	0
4	a	3	Total 39	C 22	N 2	O 15	0	0	0
4	c	3	Total 39	C 22	N 2	O 15	0	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



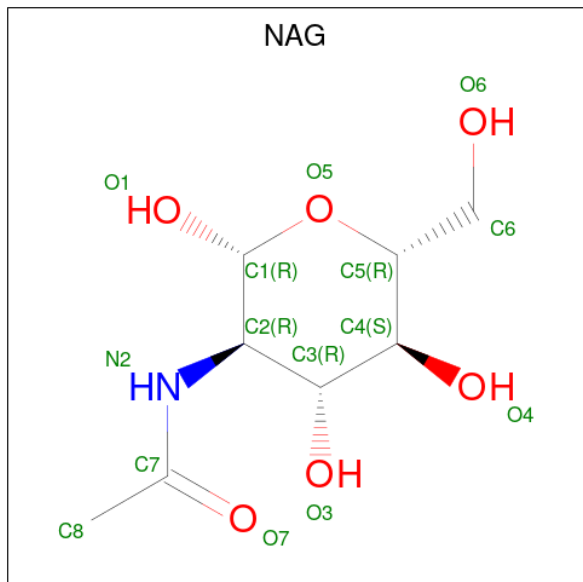
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	b	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	J	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	M	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	P	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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

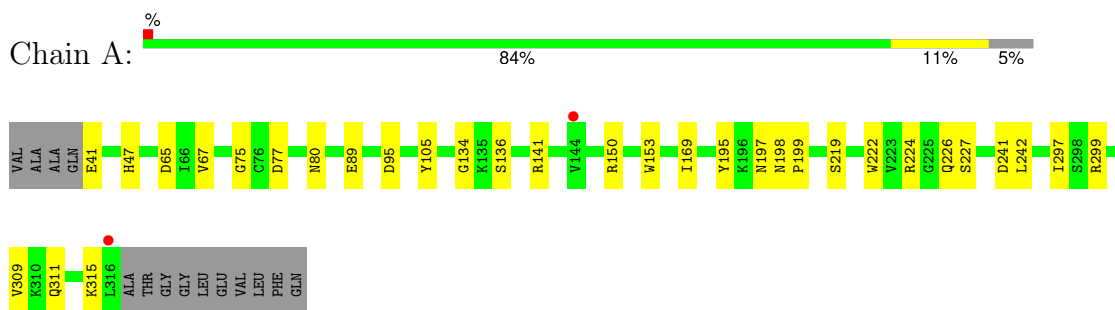


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	M	1	14	8	1	5	0	0

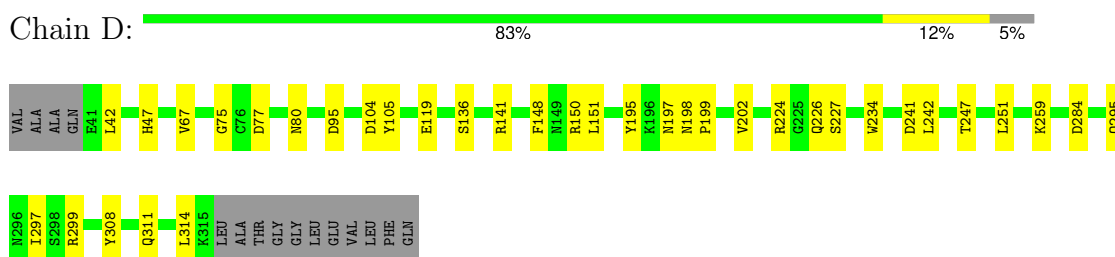
3 Residue-property plots [i](#)

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.

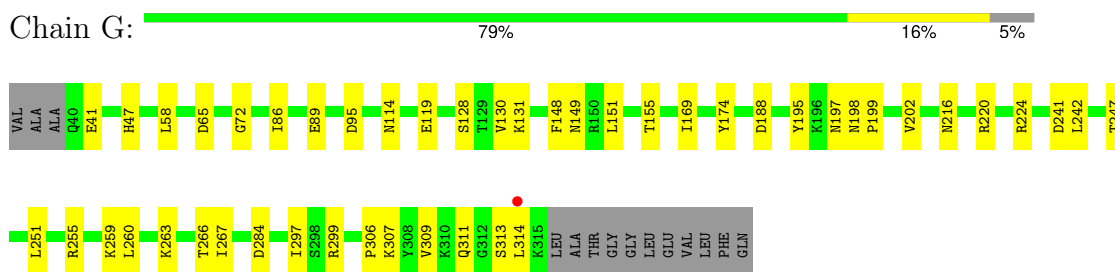
- Molecule 1: Hemagglutinin



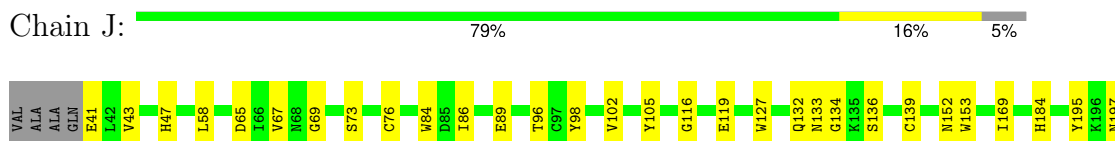
- Molecule 1: Hemagglutinin



- Molecule 1: Hemagglutinin

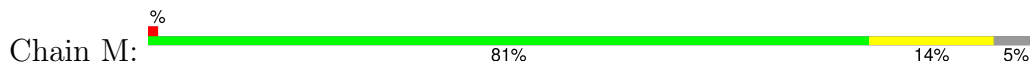


- Molecule 1: Hemagglutinin

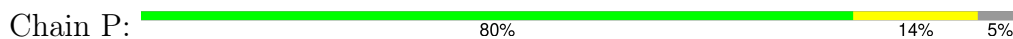




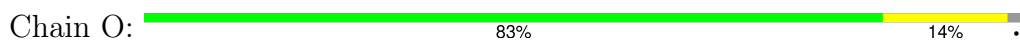
• Molecule 1: Hemagglutinin



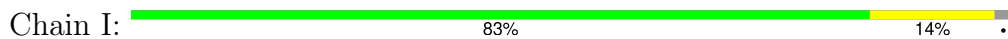
• Molecule 1: Hemagglutinin



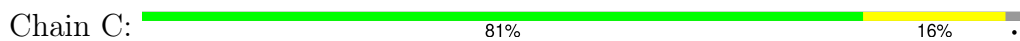
• Molecule 2: human antibody S8V1-157 light chain



• Molecule 2: human antibody S8V1-157 light chain

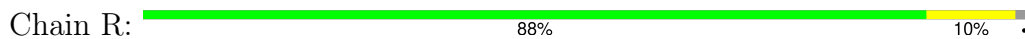


• Molecule 2: human antibody S8V1-157 light chain

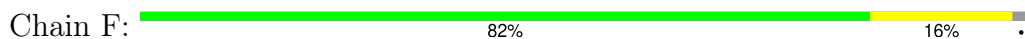




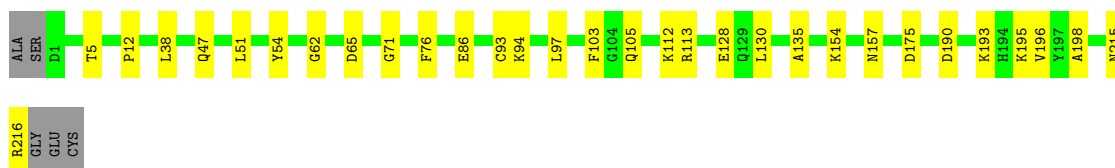
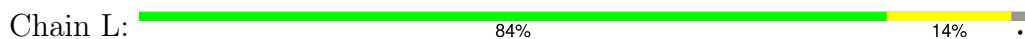
- Molecule 2: human antibody S8V1-157 light chain



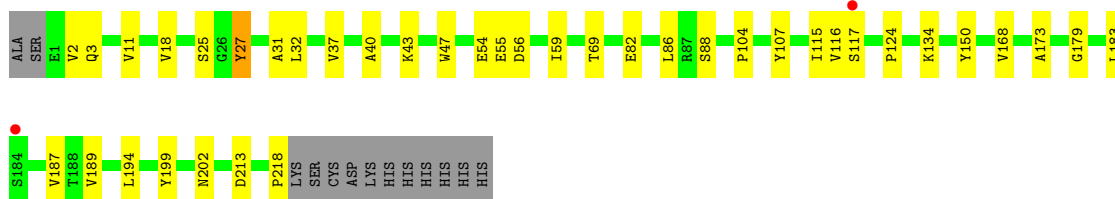
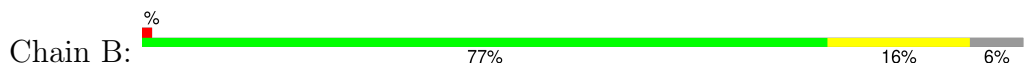
- Molecule 2: human antibody S8V1-157 light chain



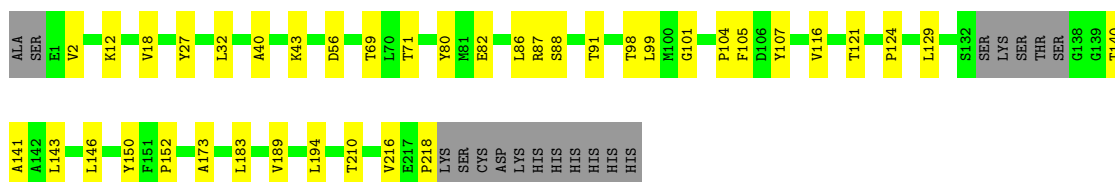
- Molecule 2: human antibody S8V1-157 light chain




- Molecule 3: human antibody S8V1-157 heavy chain

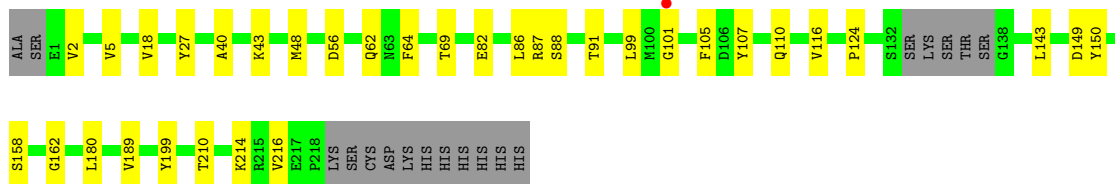


- Molecule 3: human antibody S8V1-157 heavy chain




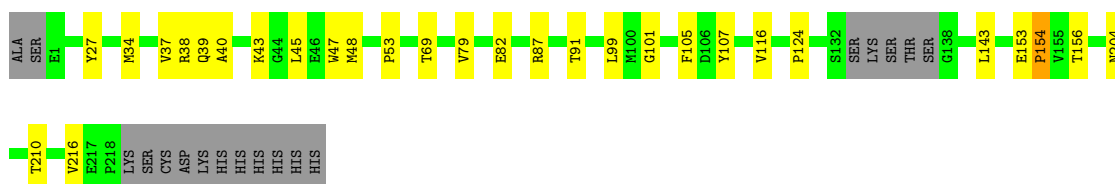
- Molecule 3: human antibody S8V1-157 heavy chain

Chain K:  77% 15% 8%




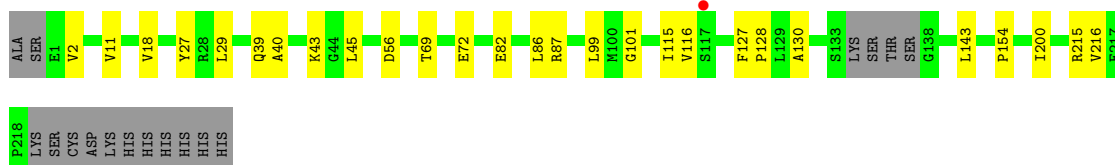
- Molecule 3: human antibody S8V1-157 heavy chain

Chain N:  80% 12% 8%



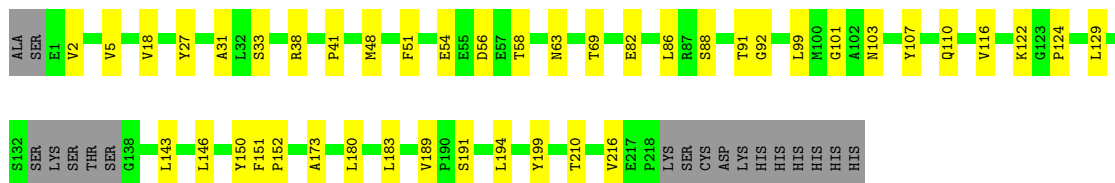
- Molecule 3: human antibody S8V1-157 heavy chain

Chain Q:  81% 12% 7%



- Molecule 3: human antibody S8V1-157 heavy chain

Chain E:  74% 19% 8%



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

Chain S:  33% 67%



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

Chain T:  100%



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

Chain U:  67% 33%



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

Chain V:  67% 33%



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

Chain W:  67% 33%



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

Chain X:  100%



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

Chain a:  100%



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

Chain c:  100%

MAG1
MAG2
BMA3

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

Chain Y:  100%

MAG1
MAG2

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

Chain Z:  50% 50%

MAG1
MAG2

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

Chain b:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	127.92Å 241.54Å 144.13Å 90.00° 101.62° 90.00°	Depositor
Resolution (Å)	49.33 – 3.70 49.33 – 3.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.33-3.70) 98.9 (49.33-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.67Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.246 , 0.293 0.242 , 0.284	Depositor DCC
R_{free} test set	4516 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	124.5	Xtrriage
Anisotropy	0.436	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 104.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	33101	wwPDB-VP
Average B, all atoms (Å ²)	144.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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

5.1 Standard geometry

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

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	0.24	0/2227	0.49	0/3030
1	D	0.24	0/2219	0.49	0/3019
1	G	0.24	0/2228	0.48	0/3031
1	J	0.24	0/2219	0.48	0/3019
1	M	0.24	0/2219	0.48	0/3019
1	P	0.24	0/2219	0.49	0/3019
2	C	0.24	0/1701	0.47	0/2310
2	F	0.24	0/1701	0.46	0/2310
2	I	0.24	0/1701	0.48	0/2310
2	L	0.25	0/1701	0.46	0/2310
2	O	0.24	0/1701	0.47	0/2310
2	R	0.24	0/1701	0.47	0/2310
3	B	0.24	0/1668	0.47	0/2274
3	E	0.25	0/1633	0.48	0/2226
3	H	0.24	0/1633	0.47	0/2226
3	K	0.25	0/1633	0.48	0/2226
3	N	0.25	0/1633	0.47	0/2226
3	Q	0.25	0/1639	0.47	0/2234
All	All	0.24	0/33376	0.48	0/45409

There are no bond length outliers.

There are no bond angle outliers.

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	2174	0	2117	22	0
1	D	2166	0	2108	25	0
1	G	2175	0	2116	36	0
1	J	2166	0	2108	31	0
1	M	2166	0	2108	25	0
1	P	2166	0	2108	30	0
2	C	1665	0	1626	23	0
2	F	1665	0	1626	27	0
2	I	1665	0	1626	23	0
2	L	1665	0	1626	24	0
2	O	1665	0	1626	22	0
2	R	1665	0	1626	18	0
3	B	1630	0	1593	25	0
3	E	1596	0	1557	26	0
3	H	1596	0	1557	29	0
3	K	1596	0	1557	27	0
3	N	1596	0	1557	16	0
3	Q	1602	0	1562	20	0
4	S	39	0	34	1	0
4	T	39	0	34	0	0
4	U	39	0	34	1	0
4	V	39	0	34	1	0
4	W	39	0	34	1	0
4	X	39	0	34	0	0
4	a	39	0	34	0	0
4	c	39	0	34	0	0
5	Y	28	0	25	0	0
5	Z	28	0	25	0	0
5	b	28	0	25	0	0
6	A	12	0	12	0	0
6	D	12	0	12	1	0
6	G	12	0	12	0	0
6	J	12	0	12	0	0
6	M	12	0	12	0	0
6	P	12	0	12	2	0
7	M	14	0	13	1	0
All	All	33101	0	32236	399	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 6.

The worst 5 of 399 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:I:29:LEU:HA	2:I:97:LEU:HD12	1.46	0.97
2:I:4:MET:SD	2:I:95:GLN:NE2	2.48	0.86
1:M:247:THR:HG21	1:M:251:LEU:HB2	1.69	0.75
1:J:216:ASN:O	1:J:220:ARG:NH2	2.21	0.74
2:O:4:MET:SD	2:O:95:GLN:NE2	2.54	0.73

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	276/292 (94%)	263 (95%)	13 (5%)	0	100	100
1	D	275/292 (94%)	263 (96%)	12 (4%)	0	100	100
1	G	276/292 (94%)	261 (95%)	15 (5%)	0	100	100
1	J	275/292 (94%)	259 (94%)	16 (6%)	0	100	100
1	M	275/292 (94%)	260 (94%)	14 (5%)	1 (0%)	30	62
1	P	275/292 (94%)	259 (94%)	16 (6%)	0	100	100
2	C	214/221 (97%)	206 (96%)	8 (4%)	0	100	100
2	F	214/221 (97%)	204 (95%)	10 (5%)	0	100	100
2	I	214/221 (97%)	201 (94%)	12 (6%)	1 (0%)	25	57
2	L	214/221 (97%)	205 (96%)	7 (3%)	2 (1%)	14	47
2	O	214/221 (97%)	203 (95%)	11 (5%)	0	100	100
2	R	214/221 (97%)	204 (95%)	10 (5%)	0	100	100
3	B	216/231 (94%)	205 (95%)	11 (5%)	0	100	100
3	E	209/231 (90%)	196 (94%)	13 (6%)	0	100	100
3	H	209/231 (90%)	200 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	K	209/231 (90%)	195 (93%)	14 (7%)	0	100	100
3	N	209/231 (90%)	200 (96%)	8 (4%)	1 (0%)	25	57
3	Q	210/231 (91%)	197 (94%)	12 (6%)	1 (0%)	25	57
All	All	4198/4464 (94%)	3981 (95%)	211 (5%)	6 (0%)	48	78

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	N	154	PRO
3	Q	154	PRO
2	L	97	LEU
2	L	157	ASN
1	M	196	LYS

5.3.2 Protein sidechains [i](#)

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	245/254 (96%)	245 (100%)	0	100	100
1	D	244/254 (96%)	244 (100%)	0	100	100
1	G	245/254 (96%)	245 (100%)	0	100	100
1	J	244/254 (96%)	244 (100%)	0	100	100
1	M	244/254 (96%)	244 (100%)	0	100	100
1	P	244/254 (96%)	244 (100%)	0	100	100
2	C	191/194 (98%)	190 (100%)	1 (0%)	86	92
2	F	191/194 (98%)	191 (100%)	0	100	100
2	I	191/194 (98%)	191 (100%)	0	100	100
2	L	191/194 (98%)	191 (100%)	0	100	100
2	O	191/194 (98%)	191 (100%)	0	100	100
2	R	191/194 (98%)	191 (100%)	0	100	100
3	B	184/196 (94%)	183 (100%)	1 (0%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	179/196 (91%)	179 (100%)	0	100	100
3	H	179/196 (91%)	179 (100%)	0	100	100
3	K	179/196 (91%)	179 (100%)	0	100	100
3	N	179/196 (91%)	178 (99%)	1 (1%)	84	90
3	Q	180/196 (92%)	180 (100%)	0	100	100
All	All	3692/3864 (96%)	3689 (100%)	3 (0%)	92	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	95	GLN
3	B	27	TYR
3	N	27	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

30 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	S	1	4,1	14,14,15	0.32	0	17,19,21	0.43	0
4	NAG	S	2	4	14,14,15	0.41	0	17,19,21	0.78	1 (5%)
4	BMA	S	3	4	11,11,12	0.82	1 (9%)	15,15,17	0.74	0
4	NAG	T	1	4,1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	T	2	4	14,14,15	0.29	0	17,19,21	0.44	0
4	BMA	T	3	4	11,11,12	0.55	0	15,15,17	0.69	0
4	NAG	U	1	4,1	14,14,15	0.45	0	17,19,21	0.54	0
4	NAG	U	2	4	14,14,15	0.43	0	17,19,21	0.56	0
4	BMA	U	3	4	11,11,12	0.78	0	15,15,17	0.81	0
4	NAG	V	1	4,1	14,14,15	0.27	0	17,19,21	0.41	0
4	NAG	V	2	4	14,14,15	0.45	0	17,19,21	1.33	2 (11%)
4	BMA	V	3	4	11,11,12	0.57	0	15,15,17	0.68	0
4	NAG	W	1	4,1	14,14,15	0.34	0	17,19,21	0.58	0
4	NAG	W	2	4	14,14,15	0.38	0	17,19,21	0.59	0
4	BMA	W	3	4	11,11,12	0.57	0	15,15,17	0.78	0
4	NAG	X	1	4,1	14,14,15	0.23	0	17,19,21	0.36	0
4	NAG	X	2	4	14,14,15	0.21	0	17,19,21	0.45	0
4	BMA	X	3	4	11,11,12	0.57	0	15,15,17	0.65	0
5	NAG	Y	1	5,1	14,14,15	0.27	0	17,19,21	0.46	0
5	NAG	Y	2	5	14,14,15	0.40	0	17,19,21	0.57	0
5	NAG	Z	1	5,1	14,14,15	0.22	0	17,19,21	0.44	0
5	NAG	Z	2	5	14,14,15	0.64	1 (7%)	17,19,21	0.63	0
4	NAG	a	1	4,1	14,14,15	0.20	0	17,19,21	0.49	0
4	NAG	a	2	4	14,14,15	0.36	0	17,19,21	0.45	0
4	BMA	a	3	4	11,11,12	0.58	0	15,15,17	0.72	0
5	NAG	b	1	5,1	14,14,15	0.25	0	17,19,21	0.42	0
5	NAG	b	2	5	14,14,15	0.29	0	17,19,21	0.65	0
4	NAG	c	1	4,1	14,14,15	0.35	0	17,19,21	0.52	0
4	NAG	c	2	4	14,14,15	0.22	0	17,19,21	0.40	0
4	BMA	c	3	4	11,11,12	0.53	0	15,15,17	0.76	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
4	NAG	S	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
4	BMA	S	3	4	-	1/2/19/22	0/1/1/1
4	NAG	T	1	4,1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
4	BMA	T	3	4	-	0/2/19/22	0/1/1/1
4	NAG	U	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1
4	BMA	U	3	4	-	2/2/19/22	0/1/1/1
4	NAG	V	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	V	2	4	-	4/6/23/26	0/1/1/1
4	BMA	V	3	4	-	1/2/19/22	0/1/1/1
4	NAG	W	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	W	2	4	-	4/6/23/26	0/1/1/1
4	BMA	W	3	4	-	1/2/19/22	0/1/1/1
4	NAG	X	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	X	2	4	-	2/6/23/26	0/1/1/1
4	BMA	X	3	4	-	0/2/19/22	0/1/1/1
5	NAG	Y	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	2/6/23/26	0/1/1/1
5	NAG	Z	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	1/6/23/26	0/1/1/1
4	NAG	a	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	a	2	4	-	0/6/23/26	0/1/1/1
4	BMA	a	3	4	-	0/2/19/22	0/1/1/1
5	NAG	b	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	b	2	5	-	2/6/23/26	0/1/1/1
4	NAG	c	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	c	2	4	-	3/6/23/26	0/1/1/1
4	BMA	c	3	4	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	3	BMA	C1-C2	2.23	1.57	1.52
5	Z	2	NAG	C1-C2	2.22	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	2	NAG	C2-N2-C7	4.57	129.03	122.90
4	S	2	NAG	C1-O5-C5	2.40	115.40	112.19
4	V	2	NAG	C1-C2-N2	2.16	113.84	110.43

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

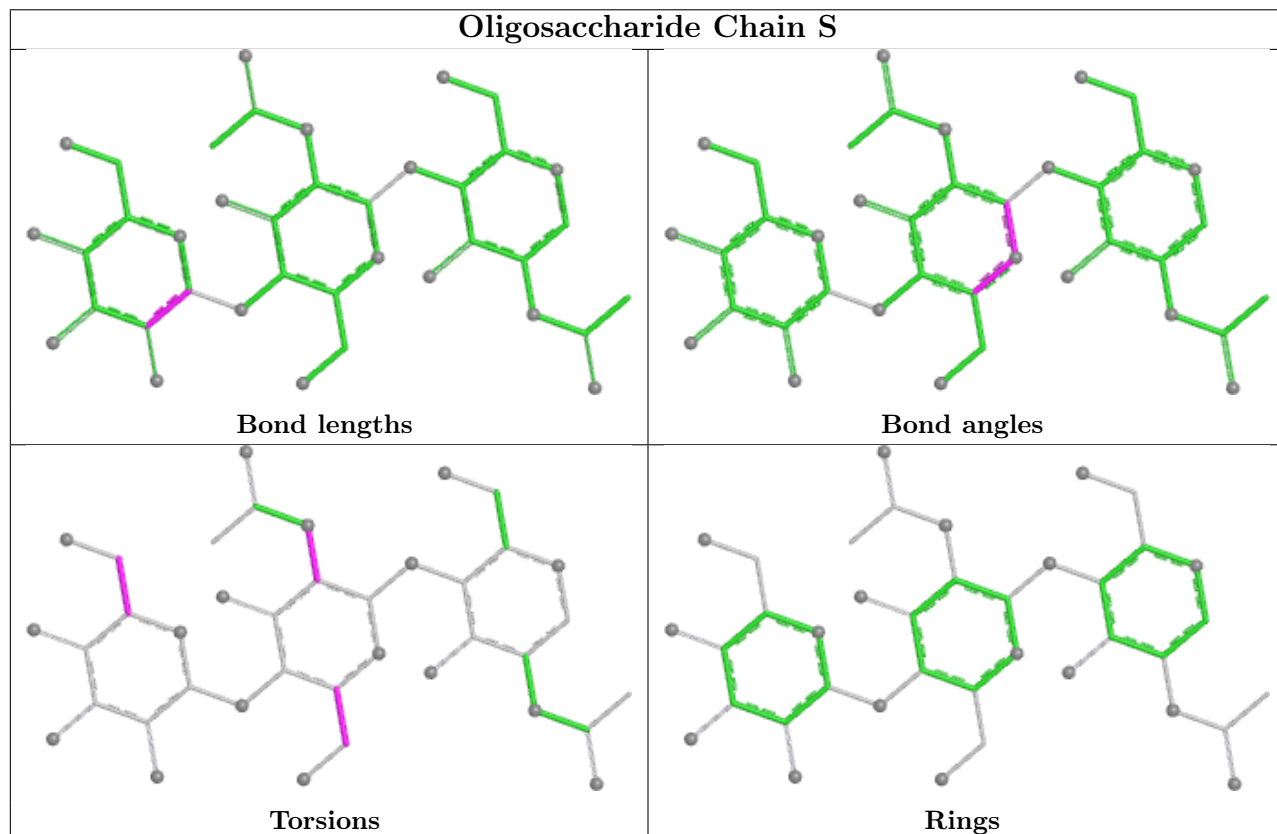
Mol	Chain	Res	Type	Atoms
4	a	1	NAG	O5-C5-C6-O6
4	U	3	BMA	O5-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	V	2	NAG	C8-C7-N2-C2
4	V	2	NAG	O7-C7-N2-C2

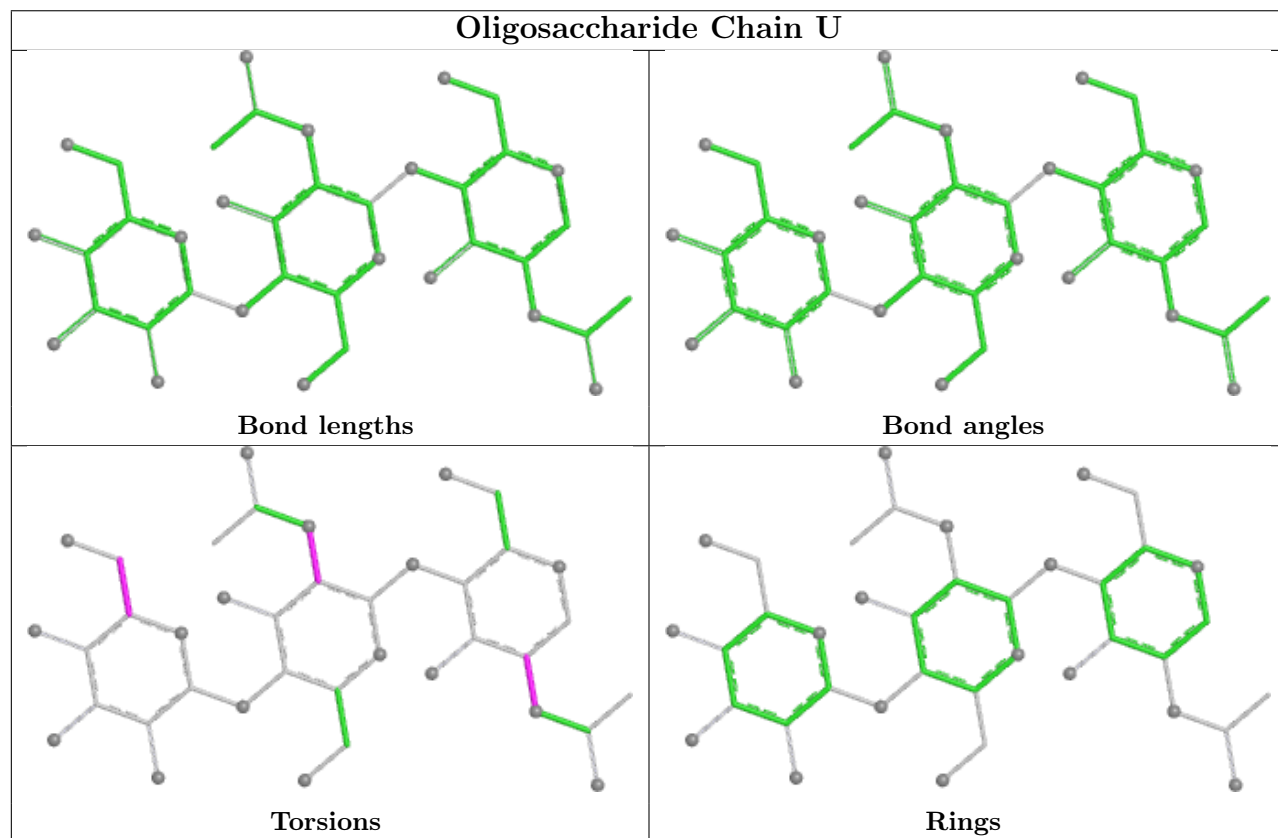
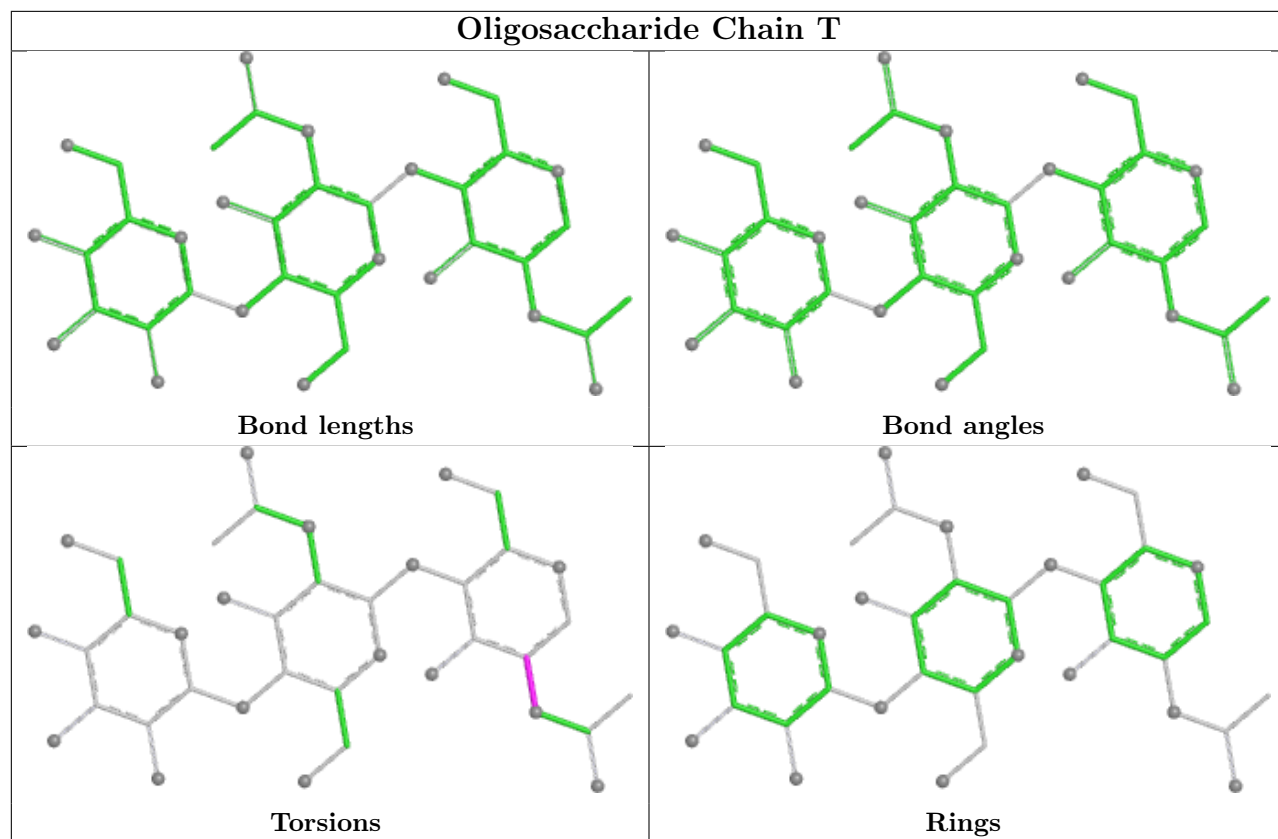
There are no ring outliers.

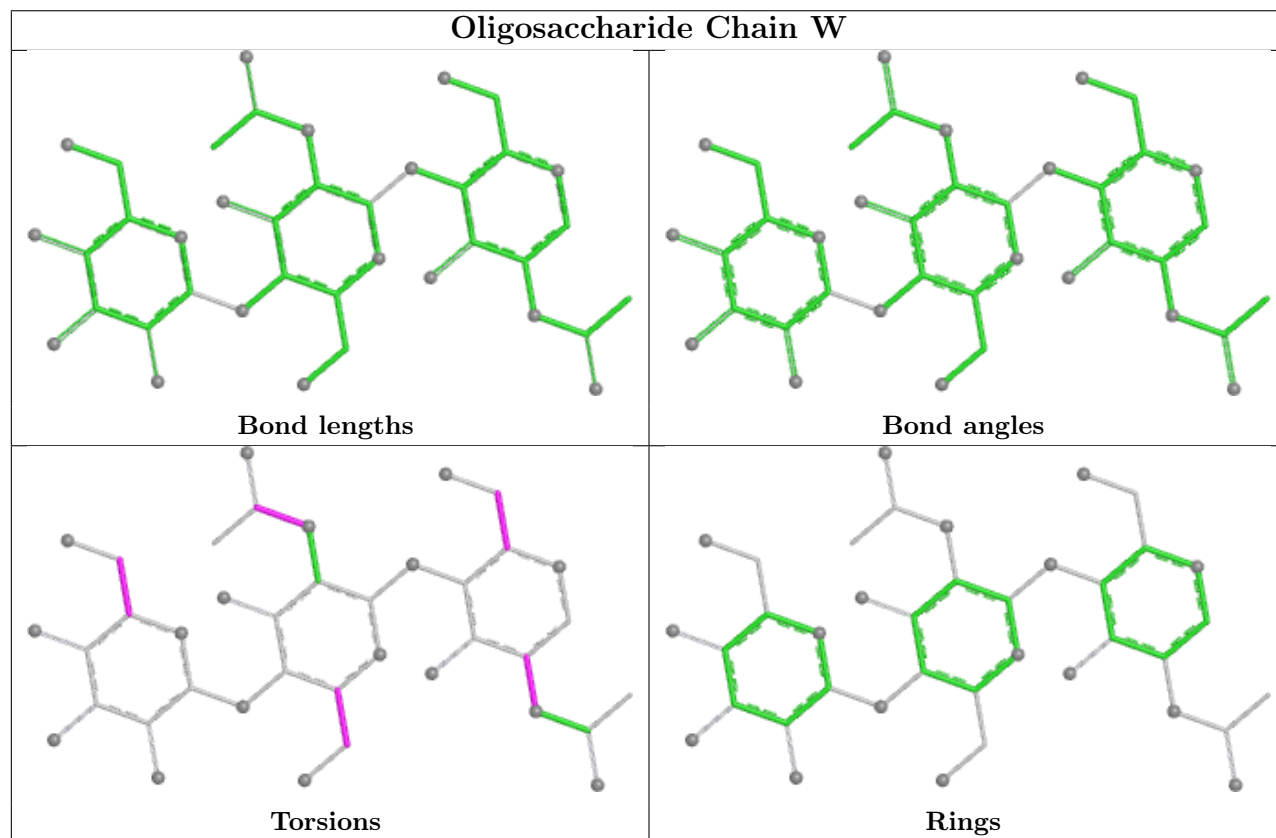
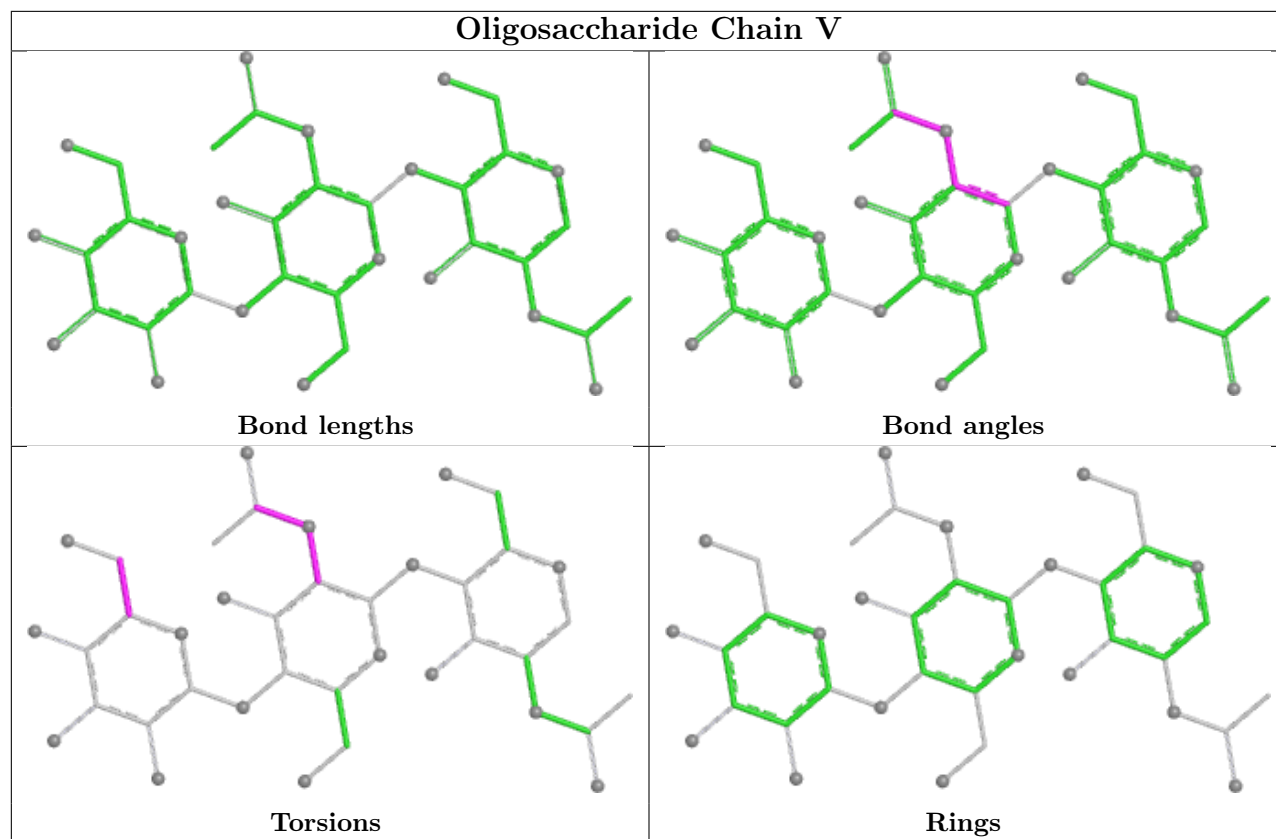
5 monomers are involved in 4 short contacts:

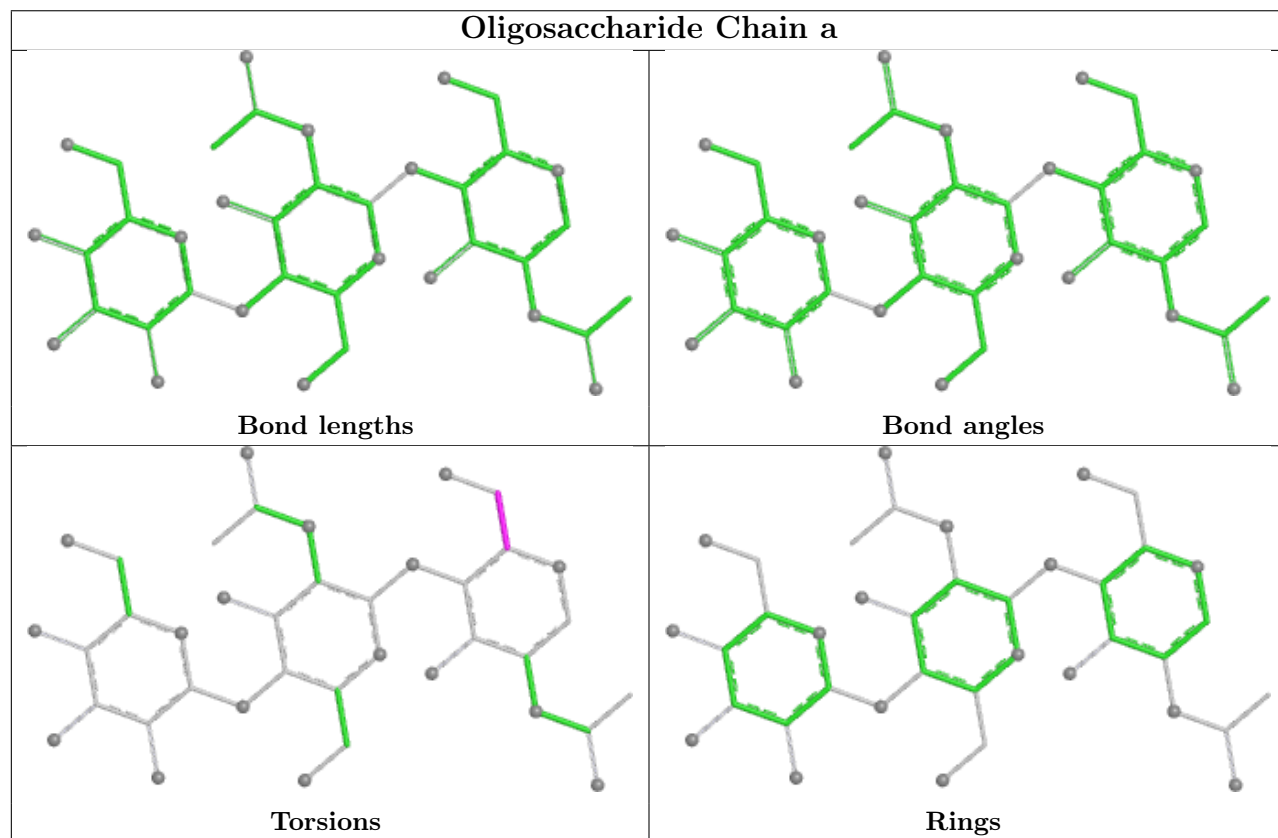
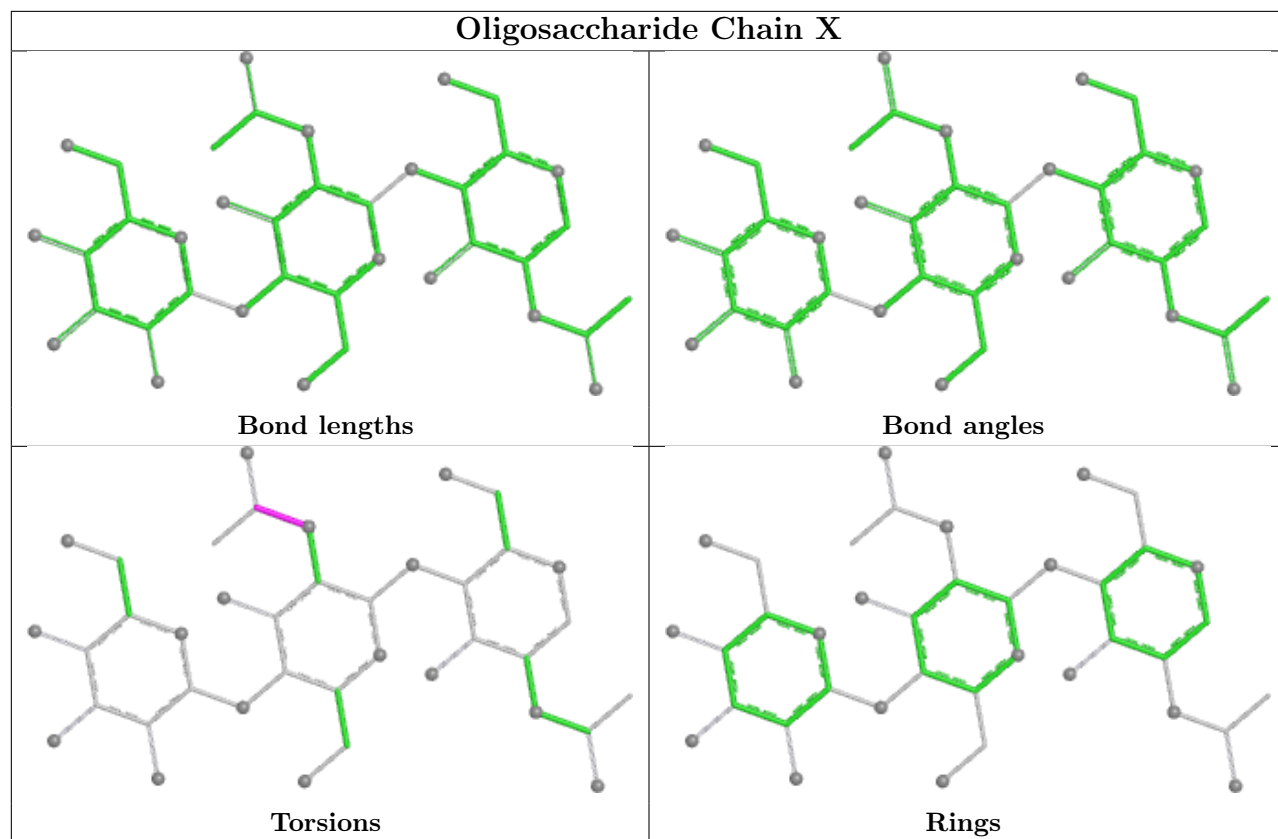
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	3	BMA	1	0
4	W	1	NAG	1	0
4	U	1	NAG	1	0
4	S	2	NAG	1	0
4	V	2	NAG	1	0

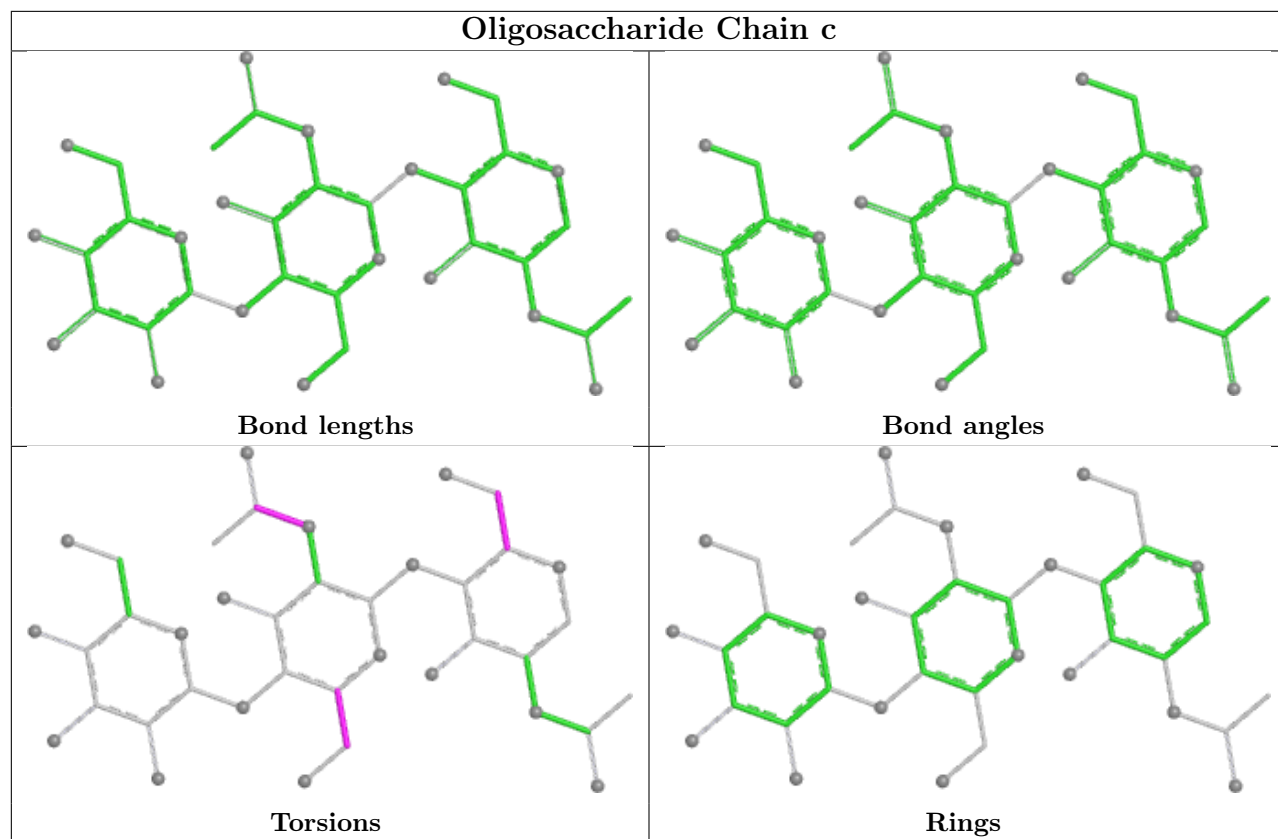
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

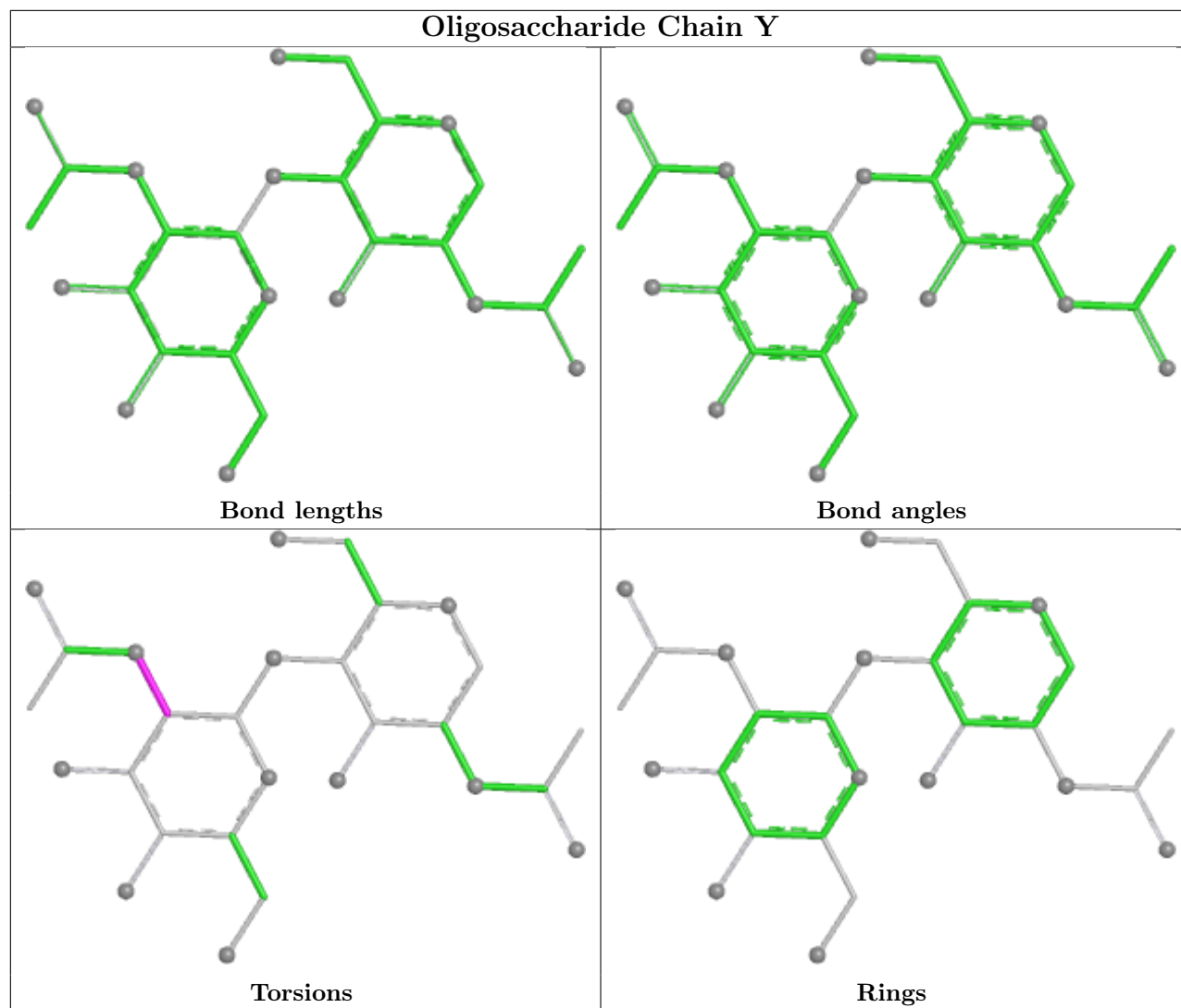


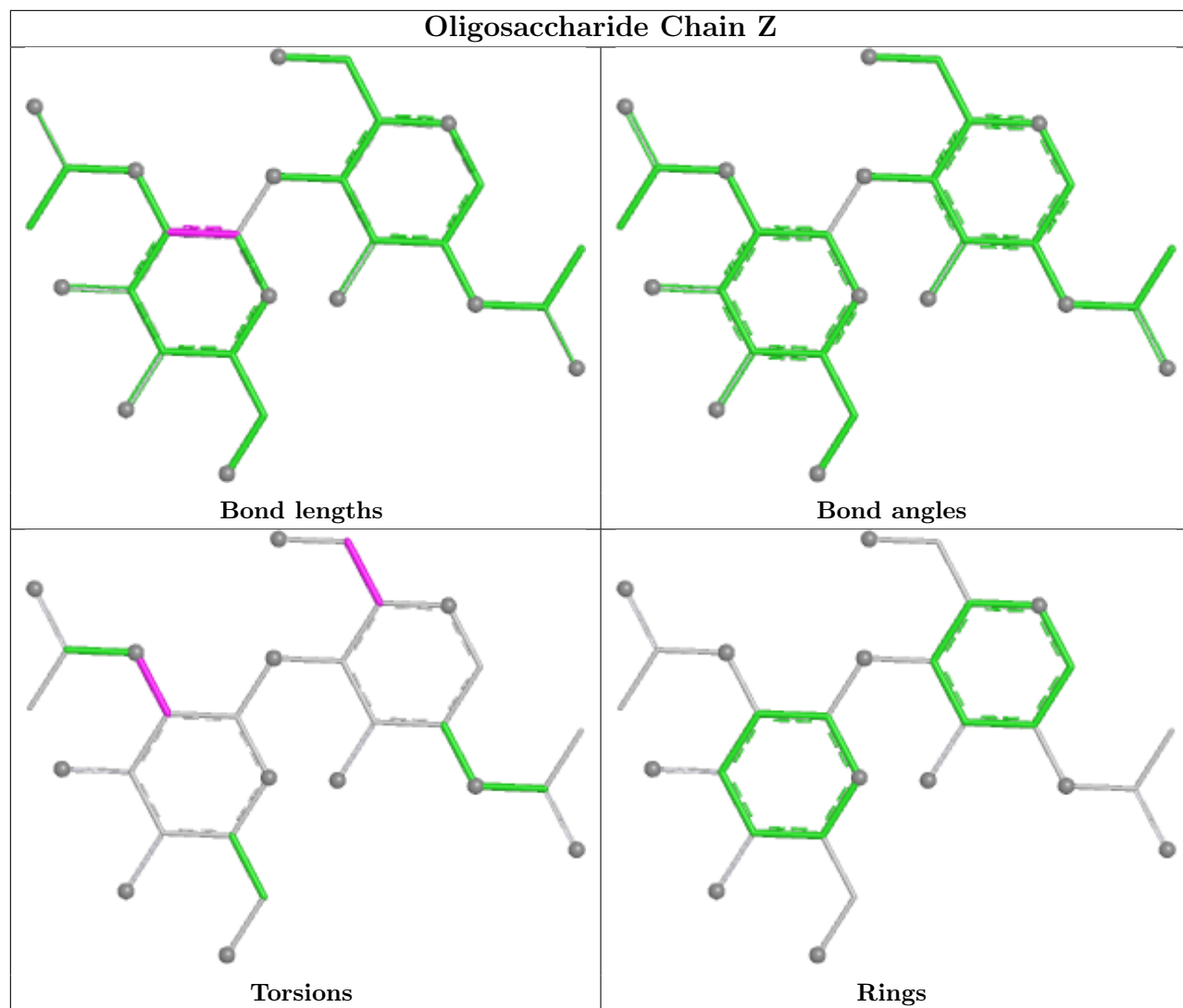


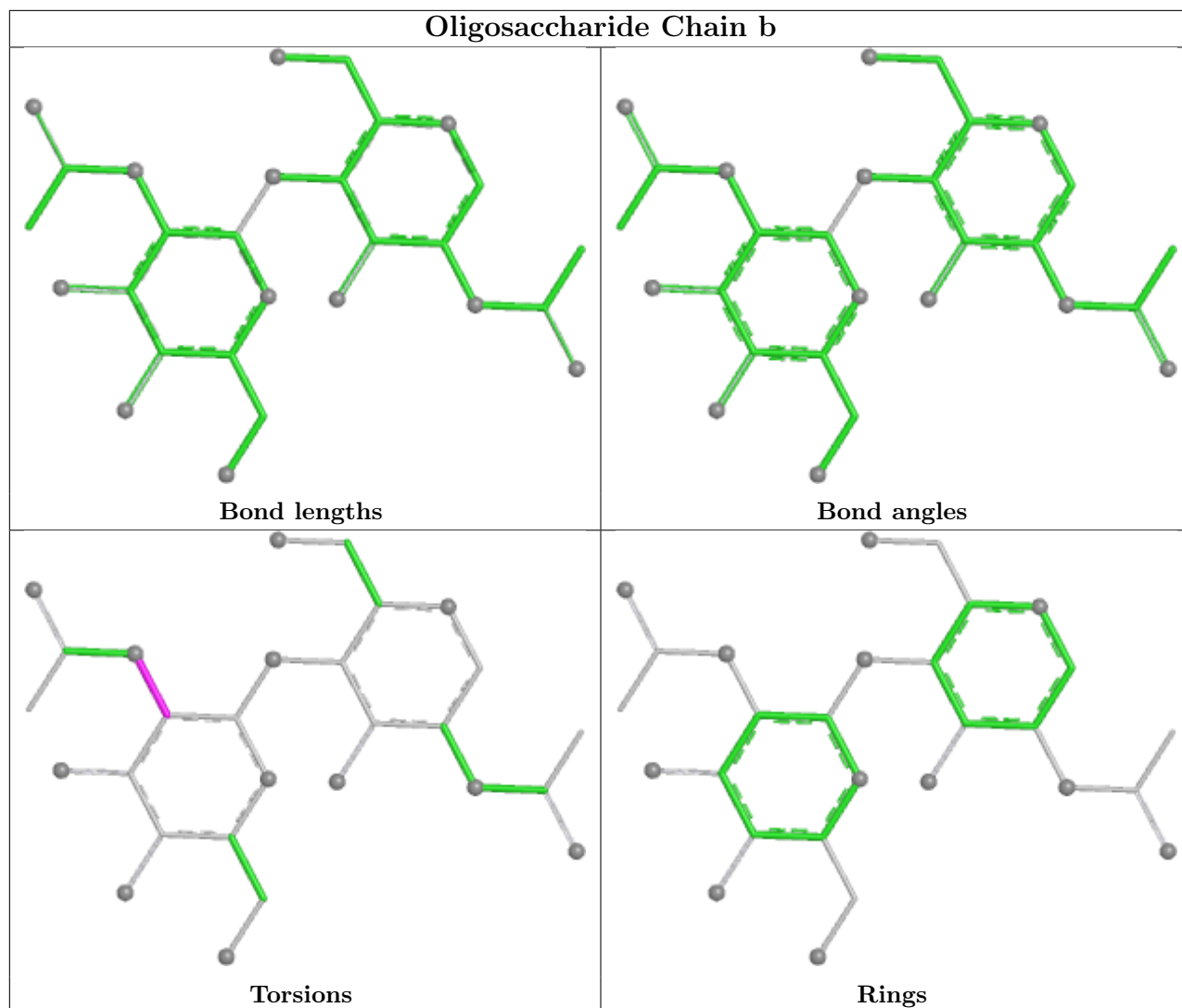












5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	MES	D	401	-	12,12,12	2.33	1 (8%)	15,16,16	2.19	7 (46%)
6	MES	A	401	-	12,12,12	2.37	1 (8%)	15,16,16	2.36	7 (46%)
6	MES	J	401	-	12,12,12	2.32	1 (8%)	15,16,16	1.89	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MES	G	401	-	12,12,12	2.34	1 (8%)	15,16,16	2.16	6 (40%)
7	NAG	M	401	1	14,14,15	0.32	0	17,19,21	0.44	0
6	MES	P	401	-	12,12,12	2.29	1 (8%)	15,16,16	1.82	4 (26%)
6	MES	M	402	-	12,12,12	2.35	1 (8%)	15,16,16	1.86	4 (26%)

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	MES	D	401	-	-	5/6/14/14	0/1/1/1
6	MES	A	401	-	-	1/6/14/14	0/1/1/1
6	MES	J	401	-	-	4/6/14/14	0/1/1/1
6	MES	G	401	-	-	6/6/14/14	0/1/1/1
7	NAG	M	401	1	-	2/6/23/26	0/1/1/1
6	MES	P	401	-	-	1/6/14/14	0/1/1/1
6	MES	M	402	-	-	1/6/14/14	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	401	MES	C8-S	-7.93	1.66	1.77
6	M	402	MES	C8-S	-7.87	1.66	1.77
6	G	401	MES	C8-S	-7.82	1.66	1.77
6	D	401	MES	C8-S	-7.79	1.66	1.77
6	J	401	MES	C8-S	-7.74	1.66	1.77

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	401	MES	C5-N4-C3	5.23	120.11	108.84
6	D	401	MES	C5-N4-C3	5.01	119.62	108.84
6	G	401	MES	C5-N4-C3	5.00	119.62	108.84
6	J	401	MES	C5-N4-C3	4.72	119.00	108.84
6	M	402	MES	C5-N4-C3	4.57	118.69	108.84

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	M	401	NAG	O5-C5-C6-O6
6	D	401	MES	C7-C8-S-O3S
6	G	401	MES	C7-C8-S-O3S
6	J	401	MES	C7-C8-S-O3S
7	M	401	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	401	MES	1	0
7	M	401	NAG	1	0
6	P	401	MES	2	0

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	278/292 (95%)	-0.38	2 (0%) 84 68	84, 118, 162, 228	0
1	D	277/292 (94%)	-0.45	0 100 100	84, 127, 174, 200	0
1	G	278/292 (95%)	-0.41	1 (0%) 89 76	86, 128, 177, 219	0
1	J	277/292 (94%)	-0.37	0 100 100	82, 134, 175, 224	0
1	M	277/292 (94%)	-0.40	2 (0%) 84 68	87, 141, 178, 232	0
1	P	277/292 (94%)	-0.41	1 (0%) 89 76	90, 133, 183, 218	0
2	C	216/221 (97%)	-0.33	1 (0%) 87 72	95, 148, 202, 238	0
2	F	216/221 (97%)	-0.30	0 100 100	92, 177, 237, 273	0
2	I	216/221 (97%)	-0.39	0 100 100	93, 140, 195, 231	0
2	L	216/221 (97%)	-0.42	0 100 100	88, 135, 189, 233	0
2	O	216/221 (97%)	-0.44	0 100 100	92, 141, 202, 226	0
2	R	216/221 (97%)	-0.44	0 100 100	95, 142, 194, 239	0
3	B	218/231 (94%)	-0.37	2 (0%) 81 64	106, 157, 212, 250	0
3	E	213/231 (92%)	-0.48	0 100 100	107, 158, 203, 256	0
3	H	213/231 (92%)	-0.36	0 100 100	105, 150, 200, 267	0
3	K	213/231 (92%)	-0.46	1 (0%) 87 72	95, 139, 209, 290	0
3	N	213/231 (92%)	-0.40	0 100 100	99, 147, 196, 227	0
3	Q	214/231 (92%)	-0.44	1 (0%) 87 72	108, 153, 193, 246	0
All	All	4244/4464 (95%)	-0.40	11 (0%) 90 79	82, 140, 201, 290	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	184	SER	3.4
1	P	314	LEU	2.9
1	M	312	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	181	SER	2.5
1	M	314	LEU	2.3

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	MES	D	401	12/12	0.31	0.15	154,186,199,203	0
6	MES	G	401	12/12	0.54	0.14	163,185,207,229	0
6	MES	A	401	12/12	0.60	0.16	174,207,218,220	0
6	MES	J	401	12/12	0.64	0.15	149,175,198,205	0
7	NAG	M	401	14/15	0.72	0.13	89,128,166,192	0
6	MES	M	402	12/12	0.75	0.13	152,177,181,184	0
6	MES	P	401	12/12	0.79	0.13	145,176,200,204	0

6.5 Other polymers [i](#)

There are no such residues in this entry.