



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 26, 2024 – 02:26 PM JST

PDB ID : 8ZER
Title : Crystal structure of the complex of Wuhan SARS-CoV-2 RBD (319-541) with P2C5 nanobody
Authors : Sluchanko, N.N.; Varfolomeeva, L.A.; Shcheblyakov, D.V.; Logunov, D.Y.; Gintsburg, A.L.; Popov, V.O.; Boyko, K.M.
Deposited on : 2024-05-06
Resolution : 3.10 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.002 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.2

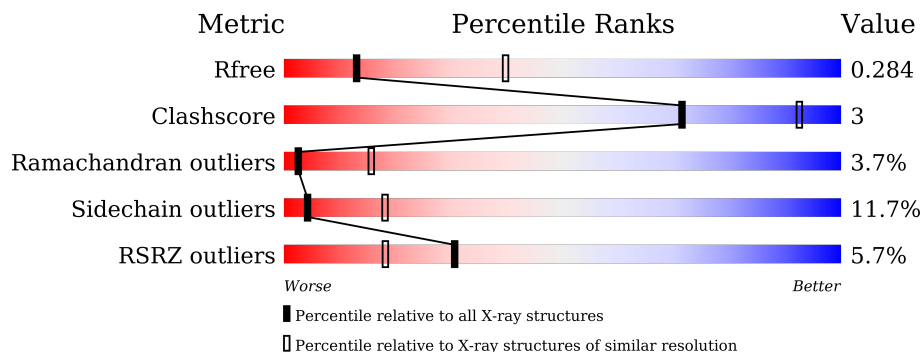
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	235	<p>3% 57% 21% 17%</p>
1	C	235	<p>5% 55% 20% 18%</p>
1	E	235	<p>4% 53% 23% 17%</p>
1	G	235	<p>9% 53% 18% 18%</p>
1	I	235	<p>6% 60% 17% 18%</p>
2	A	146	<p>% 63% 15% 18%</p>

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Mol	Chain	Length	Quality of chain
2	D	146	<p>7% 65% 14% 18%</p>
2	F	146	<p>2% 67% 12% 18%</p>
2	H	146	<p>2% 65% 15% 16%</p>
2	J	146	<p>6% 70% 9% 18%</p>
3	K	3	<p>100%</p>
3	N	3	<p>100%</p>
4	L	2	<p>100%</p>
4	M	2	<p>100%</p>
5	O	7	<p>100%</p>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12475 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	195	1542	988	259	287	8	0	1	0
1	C	192	1514	972	252	282	8	0	0	0
1	E	194	1525	977	254	286	8	0	0	0
1	G	192	1520	976	253	283	8	0	0	0
1	I	193	1521	975	253	285	8	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	542	GLY	-	expression tag	UNP P0DTC2
B	543	SER	-	expression tag	UNP P0DTC2
B	544	HIS	-	expression tag	UNP P0DTC2
B	545	HIS	-	expression tag	UNP P0DTC2
B	546	HIS	-	expression tag	UNP P0DTC2
B	547	HIS	-	expression tag	UNP P0DTC2
B	548	HIS	-	expression tag	UNP P0DTC2
B	549	HIS	-	expression tag	UNP P0DTC2
B	550	HIS	-	expression tag	UNP P0DTC2
B	551	HIS	-	expression tag	UNP P0DTC2
B	552	HIS	-	expression tag	UNP P0DTC2
B	553	HIS	-	expression tag	UNP P0DTC2
C	542	GLY	-	expression tag	UNP P0DTC2
C	543	SER	-	expression tag	UNP P0DTC2
C	544	HIS	-	expression tag	UNP P0DTC2
C	545	HIS	-	expression tag	UNP P0DTC2
C	546	HIS	-	expression tag	UNP P0DTC2
C	547	HIS	-	expression tag	UNP P0DTC2
C	548	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	549	HIS	-	expression tag	UNP P0DTC2
C	550	HIS	-	expression tag	UNP P0DTC2
C	551	HIS	-	expression tag	UNP P0DTC2
C	552	HIS	-	expression tag	UNP P0DTC2
C	553	HIS	-	expression tag	UNP P0DTC2
E	542	GLY	-	expression tag	UNP P0DTC2
E	543	SER	-	expression tag	UNP P0DTC2
E	544	HIS	-	expression tag	UNP P0DTC2
E	545	HIS	-	expression tag	UNP P0DTC2
E	546	HIS	-	expression tag	UNP P0DTC2
E	547	HIS	-	expression tag	UNP P0DTC2
E	548	HIS	-	expression tag	UNP P0DTC2
E	549	HIS	-	expression tag	UNP P0DTC2
E	550	HIS	-	expression tag	UNP P0DTC2
E	551	HIS	-	expression tag	UNP P0DTC2
E	552	HIS	-	expression tag	UNP P0DTC2
E	553	HIS	-	expression tag	UNP P0DTC2
G	542	GLY	-	expression tag	UNP P0DTC2
G	543	SER	-	expression tag	UNP P0DTC2
G	544	HIS	-	expression tag	UNP P0DTC2
G	545	HIS	-	expression tag	UNP P0DTC2
G	546	HIS	-	expression tag	UNP P0DTC2
G	547	HIS	-	expression tag	UNP P0DTC2
G	548	HIS	-	expression tag	UNP P0DTC2
G	549	HIS	-	expression tag	UNP P0DTC2
G	550	HIS	-	expression tag	UNP P0DTC2
G	551	HIS	-	expression tag	UNP P0DTC2
G	552	HIS	-	expression tag	UNP P0DTC2
G	553	HIS	-	expression tag	UNP P0DTC2
I	542	GLY	-	expression tag	UNP P0DTC2
I	543	SER	-	expression tag	UNP P0DTC2
I	544	HIS	-	expression tag	UNP P0DTC2
I	545	HIS	-	expression tag	UNP P0DTC2
I	546	HIS	-	expression tag	UNP P0DTC2
I	547	HIS	-	expression tag	UNP P0DTC2
I	548	HIS	-	expression tag	UNP P0DTC2
I	549	HIS	-	expression tag	UNP P0DTC2
I	550	HIS	-	expression tag	UNP P0DTC2
I	551	HIS	-	expression tag	UNP P0DTC2
I	552	HIS	-	expression tag	UNP P0DTC2
I	553	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Nanobody P2C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	120	Total 922	C 572	N 157	O 186	S 7	0	0	0
2	D	120	Total 929	C 575	N 160	O 187	S 7	0	1	0
2	F	120	Total 914	C 567	N 155	O 185	S 7	0	0	0
2	H	123	Total 945	C 585	N 161	O 192	S 7	0	0	0
2	J	120	Total 923	C 572	N 157	O 187	S 7	0	1	0

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



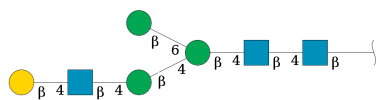
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	K	3	Total 39	C 22	N 2	O 15	0	0	0
3	N	3	Total 39	C 22	N 2	O 15	0	0	0

- 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
			Total	C	N	O			
4	L	2	Total 28	C 16	N 2	O 10	0	0	0
4	M	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 5 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-mannopyranose-(1-4)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

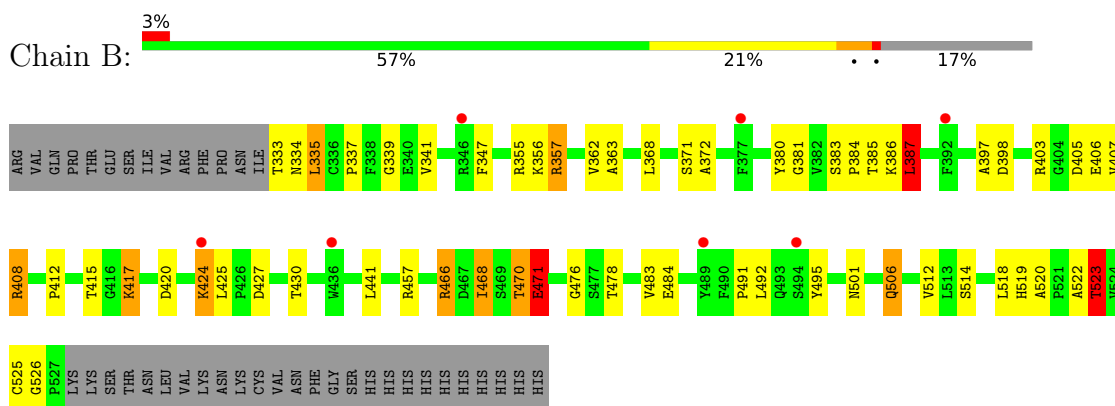


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
5	O	7	86	48	3	35	0	0	0

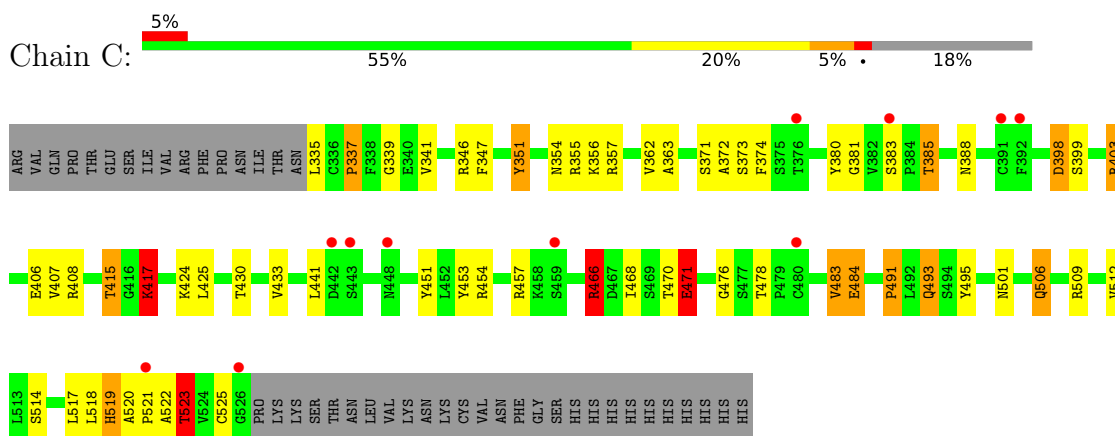
3 Residue-property plots [i](#)

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.

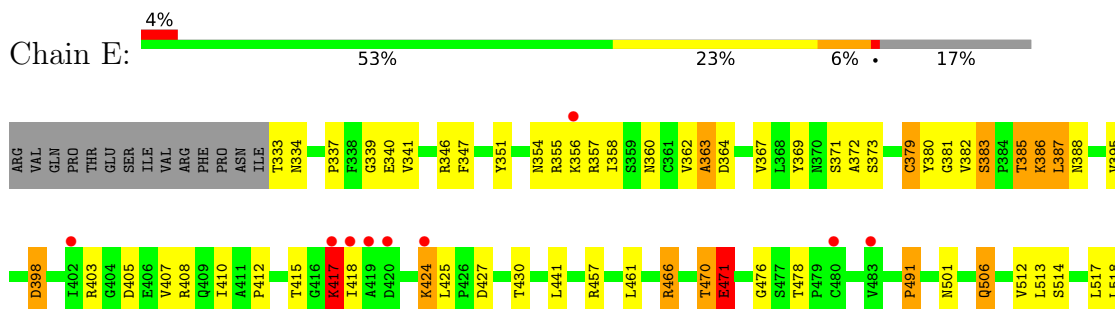
- Molecule 1: Spike protein S1



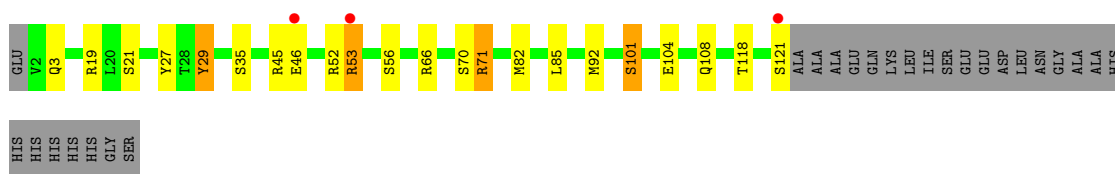
- Molecule 1: Spike protein S1



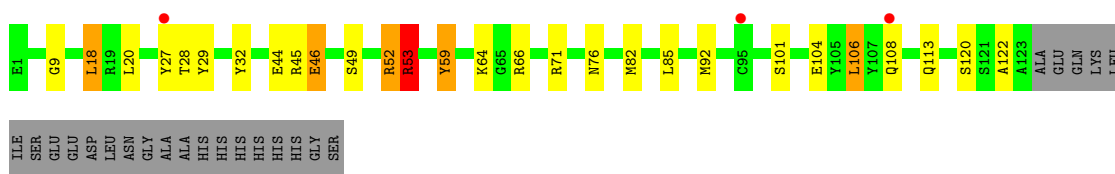
- Molecule 1: Spike protein S1



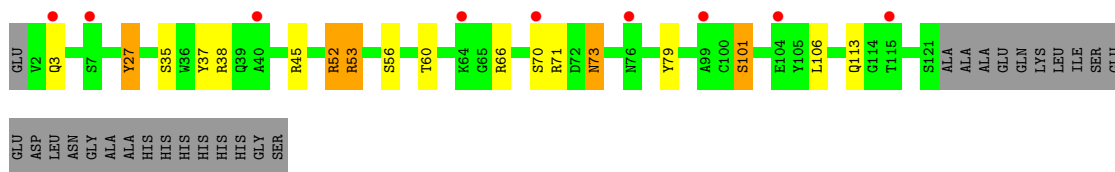
- Molecule 2: Nanobody P2C5



- Molecule 2: Nanobody P2C5



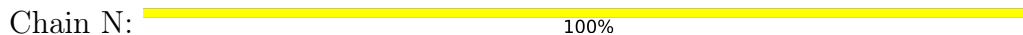
- Molecule 2: Nanobody P2C5



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



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



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



MAG1
MAG2

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

Chain M:

100%

MAG1
MAG2

- Molecule 5: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-mannopyranose-(1-4)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

100%

MAG1
MAG2
BMA3
BMA4
MAG5
GAL6
BMA7

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.48Å 177.46Å 209.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.17 – 3.10 45.17 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (45.17-3.10) 98.7 (45.17-3.10)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 3.12Å)	Xtrriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.222 , 0.283 0.224 , 0.284	Depositor DCC
R_{free} test set	2386 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	76.1	Xtrriage
Anisotropy	0.683	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12475	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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: NAG, GAL, BMA

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	0.83	1/1591 (0.1%)	1.56	22/2167 (1.0%)
1	C	0.87	1/1557 (0.1%)	1.59	25/2120 (1.2%)
1	E	0.88	2/1568 (0.1%)	1.62	31/2137 (1.5%)
1	G	0.86	4/1563 (0.3%)	1.66	37/2128 (1.7%)
1	I	0.80	0/1564	1.53	21/2132 (1.0%)
2	A	0.76	1/941 (0.1%)	1.53	14/1272 (1.1%)
2	D	0.81	2/952 (0.2%)	1.73	27/1287 (2.1%)
2	F	0.79	1/933 (0.1%)	1.62	17/1263 (1.3%)
2	H	0.77	0/964	1.57	15/1303 (1.2%)
2	J	0.82	1/946 (0.1%)	1.53	8/1280 (0.6%)
All	All	0.83	13/12579 (0.1%)	1.60	217/17089 (1.3%)

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	B	0	8
1	C	0	6
1	E	0	7
1	G	0	10
1	I	0	6
2	A	0	5
2	D	0	5
2	F	0	3
2	H	0	4
2	J	0	4
All	All	0	58

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	417	LYS	CB-CG	7.90	1.73	1.52
2	J	35	SER	CA-CB	-6.74	1.42	1.52
1	G	346	ARG	NE-CZ	6.30	1.41	1.33
1	B	468	ILE	CB-CG1	-5.94	1.37	1.54
2	D	46	GLU	CG-CD	5.79	1.60	1.51

The worst 5 of 217 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	346	ARG	NE-CZ-NH1	15.11	127.85	120.30
1	B	466	ARG	NE-CZ-NH1	12.49	126.54	120.30
1	B	466	ARG	NE-CZ-NH2	-11.75	114.42	120.30
2	F	92	MET	CG-SD-CE	11.70	118.92	100.20
1	E	417	LYS	CB-CG-CD	11.11	140.49	111.60

There are no chirality outliers.

5 of 58 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	333	THR	Peptide
1	B	357	ARG	Sidechain
1	B	371	SER	Peptide
1	B	381	GLY	Peptide
1	B	408	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	1542	0	1455	12	0
1	C	1514	0	1426	10	0
1	E	1525	0	1428	10	0
1	G	1520	0	1435	13	0
1	I	1521	0	1425	7	0
2	A	922	0	860	9	0
2	D	929	0	864	8	0
2	F	914	0	843	4	0
2	H	945	0	885	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	923	0	853	3	0
3	K	39	0	34	0	0
3	N	39	0	34	0	0
4	L	28	0	25	0	0
4	M	28	0	25	0	0
5	O	86	0	73	0	0
All	All	12475	0	11665	74	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 3.

The worst 5 of 74 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:466:ARG:HH21	2:J:106:LEU:HD22	1.59	0.68
2:A:53:ARG:HH11	2:A:53:ARG:HB3	1.59	0.67
1:I:425:LEU:HD21	1:I:512:VAL:HG11	1.85	0.58
2:D:19:ARG:HH11	2:D:19:ARG:HG3	1.68	0.58
1:B:406:GLU:OE2	1:B:495:TYR:OH	2.22	0.56

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	B	194/235 (83%)	161 (83%)	21 (11%)	12 (6%)	1 7
1	C	190/235 (81%)	157 (83%)	22 (12%)	11 (6%)	1 8
1	E	192/235 (82%)	158 (82%)	21 (11%)	13 (7%)	1 6
1	G	190/235 (81%)	158 (83%)	21 (11%)	11 (6%)	1 8
1	I	191/235 (81%)	162 (85%)	19 (10%)	10 (5%)	1 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	118/146 (81%)	111 (94%)	7 (6%)	0	100	100
2	D	119/146 (82%)	113 (95%)	6 (5%)	0	100	100
2	F	118/146 (81%)	110 (93%)	8 (7%)	0	100	100
2	H	121/146 (83%)	112 (93%)	8 (7%)	1 (1%)	16	48
2	J	119/146 (82%)	110 (92%)	9 (8%)	0	100	100
All	All	1552/1905 (82%)	1352 (87%)	142 (9%)	58 (4%)	2	16

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	363	ALA
1	B	372	ALA
1	C	363	ALA
1	C	372	ALA
1	C	417	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	B	167/207 (81%)	147 (88%)	20 (12%)	4	16
1	C	163/207 (79%)	136 (83%)	27 (17%)	2	8
1	E	164/207 (79%)	140 (85%)	24 (15%)	2	11
1	G	164/207 (79%)	144 (88%)	20 (12%)	4	16
1	I	164/207 (79%)	143 (87%)	21 (13%)	3	15
2	A	97/117 (83%)	87 (90%)	10 (10%)	6	22
2	D	98/117 (84%)	91 (93%)	7 (7%)	12	39
2	F	95/117 (81%)	86 (90%)	9 (10%)	7	26
2	H	99/117 (85%)	91 (92%)	8 (8%)	9	33
2	J	97/117 (83%)	88 (91%)	9 (9%)	7	27
All	All	1308/1620 (81%)	1153 (88%)	155 (12%)	4	17

5 of 155 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	514	SER
1	I	514	SER
2	H	46	GLU
1	I	387	LEU
2	J	56	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	73	ASN
1	G	474	GLN
1	G	354	ASN
1	E	409	GLN
1	G	450	ASN

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](#)

17 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	K	1	3,1	14,14,15	1.41	3 (21%)	17,19,21	2.81	8 (47%)
3	NAG	K	2	3	14,14,15	0.84	1 (7%)	17,19,21	1.45	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	K	3	3	11,11,12	0.74	0	15,15,17	2.68	3 (20%)
4	NAG	L	1	1,4	14,14,15	0.66	0	17,19,21	2.78	9 (52%)
4	NAG	L	2	4	14,14,15	1.27	2 (14%)	17,19,21	3.46	10 (58%)
4	NAG	M	1	1,4	14,14,15	1.04	1 (7%)	17,19,21	2.62	5 (29%)
4	NAG	M	2	4	14,14,15	0.71	0	17,19,21	2.53	7 (41%)
3	NAG	N	1	3,1	14,14,15	0.56	0	17,19,21	2.09	6 (35%)
3	NAG	N	2	3	14,14,15	0.81	1 (7%)	17,19,21	1.92	4 (23%)
3	BMA	N	3	3	11,11,12	1.92	3 (27%)	15,15,17	2.72	6 (40%)
5	NAG	O	1	1,5	14,14,15	0.86	0	17,19,21	3.58	4 (23%)
5	NAG	O	2	5	14,14,15	0.76	0	17,19,21	3.26	7 (41%)
5	BMA	O	3	5	11,11,12	1.87	2 (18%)	15,15,17	2.47	7 (46%)
5	BMA	O	4	5	11,11,12	1.95	2 (18%)	15,15,17	2.64	5 (33%)
5	NAG	O	5	5	14,14,15	0.94	1 (7%)	17,19,21	1.54	3 (17%)
5	GAL	O	6	5	11,11,12	0.94	0	15,15,17	1.51	1 (6%)
5	BMA	O	7	5	11,11,12	1.19	2 (18%)	15,15,17	1.52	3 (20%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	O	5	5	-	2/6/23/26	0/1/1/1
5	GAL	O	6	5	-	2/2/19/22	0/1/1/1
5	BMA	O	7	5	-	2/2/19/22	0/1/1/1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	3	BMA	C2-C3	4.89	1.59	1.52
5	O	4	BMA	C2-C3	4.40	1.59	1.52
5	O	3	BMA	O5-C5	3.97	1.51	1.43
5	O	4	BMA	O5-C5	3.44	1.50	1.43
5	O	3	BMA	C2-C3	3.44	1.57	1.52

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	1	NAG	C1-O5-C5	10.48	126.39	112.19
4	L	2	NAG	C2-N2-C7	9.67	136.67	122.90
5	O	2	NAG	C2-N2-C7	9.06	135.80	122.90
5	O	1	NAG	C1-C2-N2	7.45	123.22	110.49
3	K	3	BMA	C1-O5-C5	7.30	122.08	112.19

There are no chirality outliers.

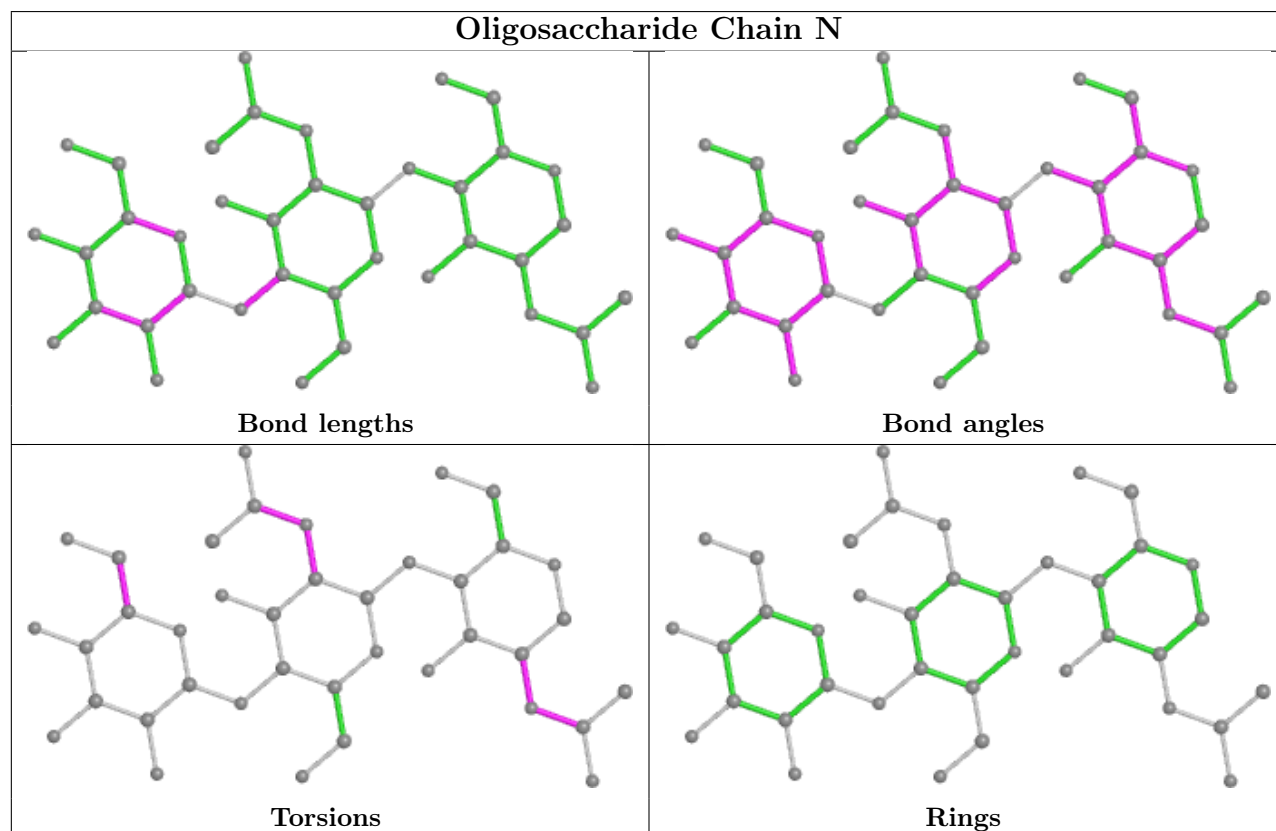
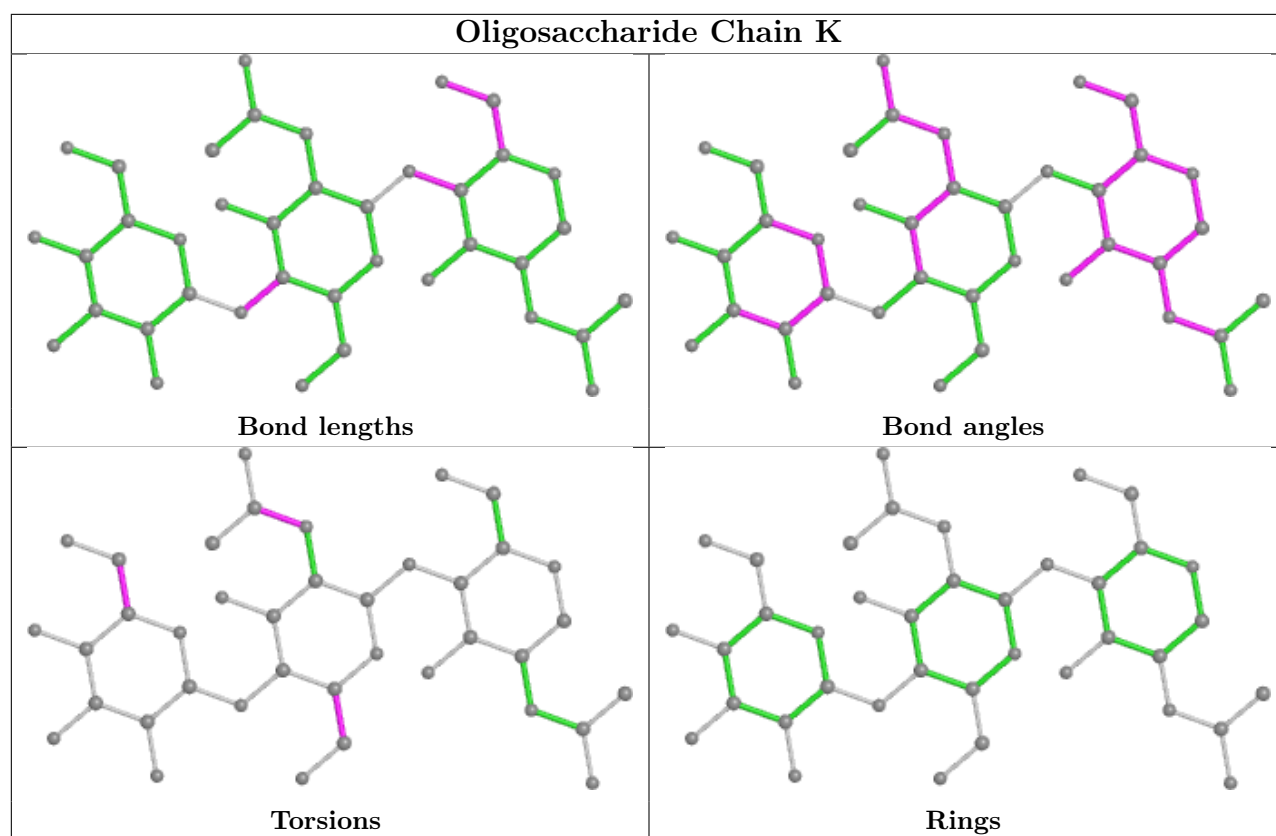
5 of 41 torsion outliers are listed below:

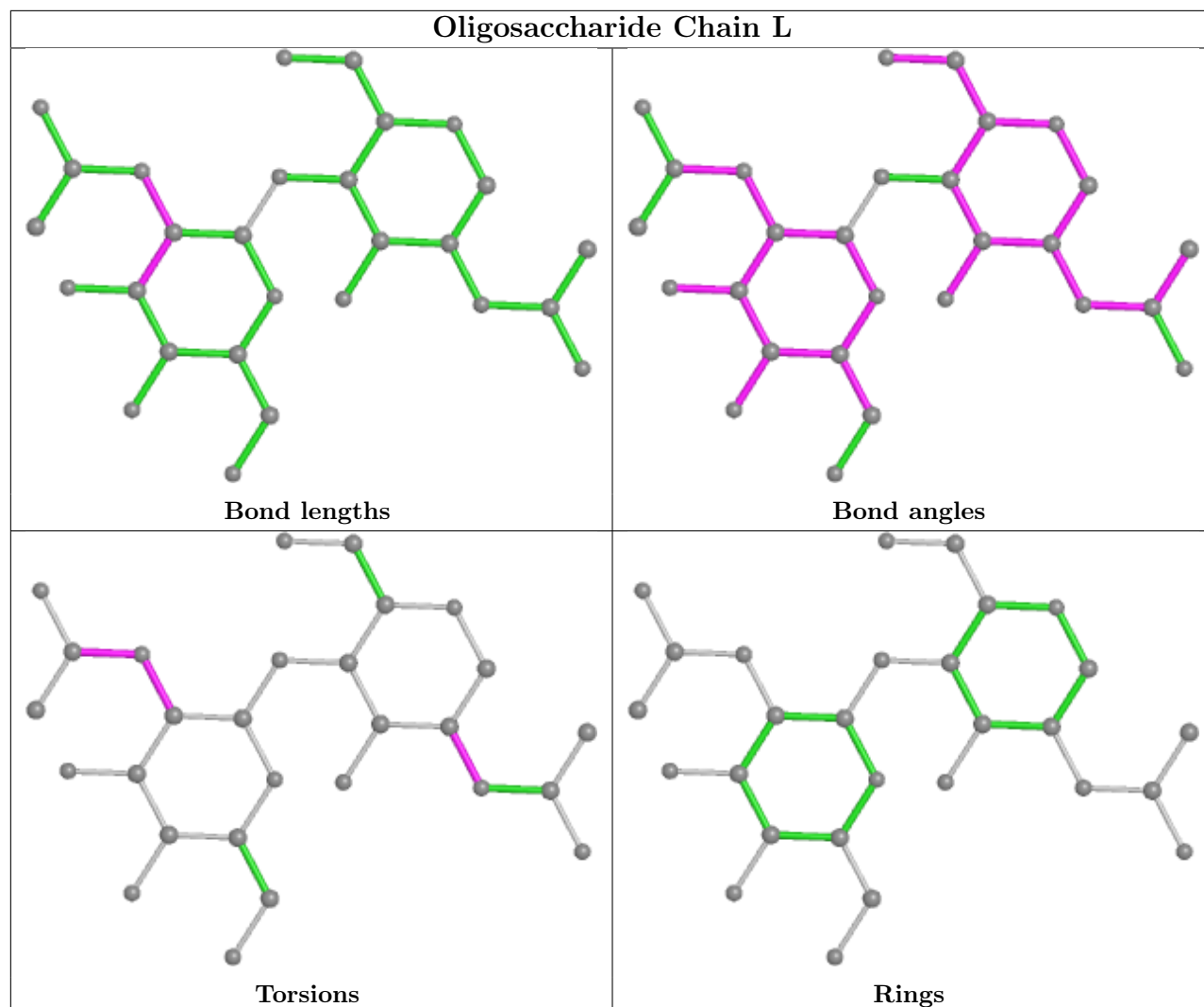
Mol	Chain	Res	Type	Atoms
3	K	2	NAG	C8-C7-N2-C2
3	K	2	NAG	O7-C7-N2-C2
3	N	1	NAG	C8-C7-N2-C2
3	N	1	NAG	O7-C7-N2-C2
3	N	2	NAG	C8-C7-N2-C2

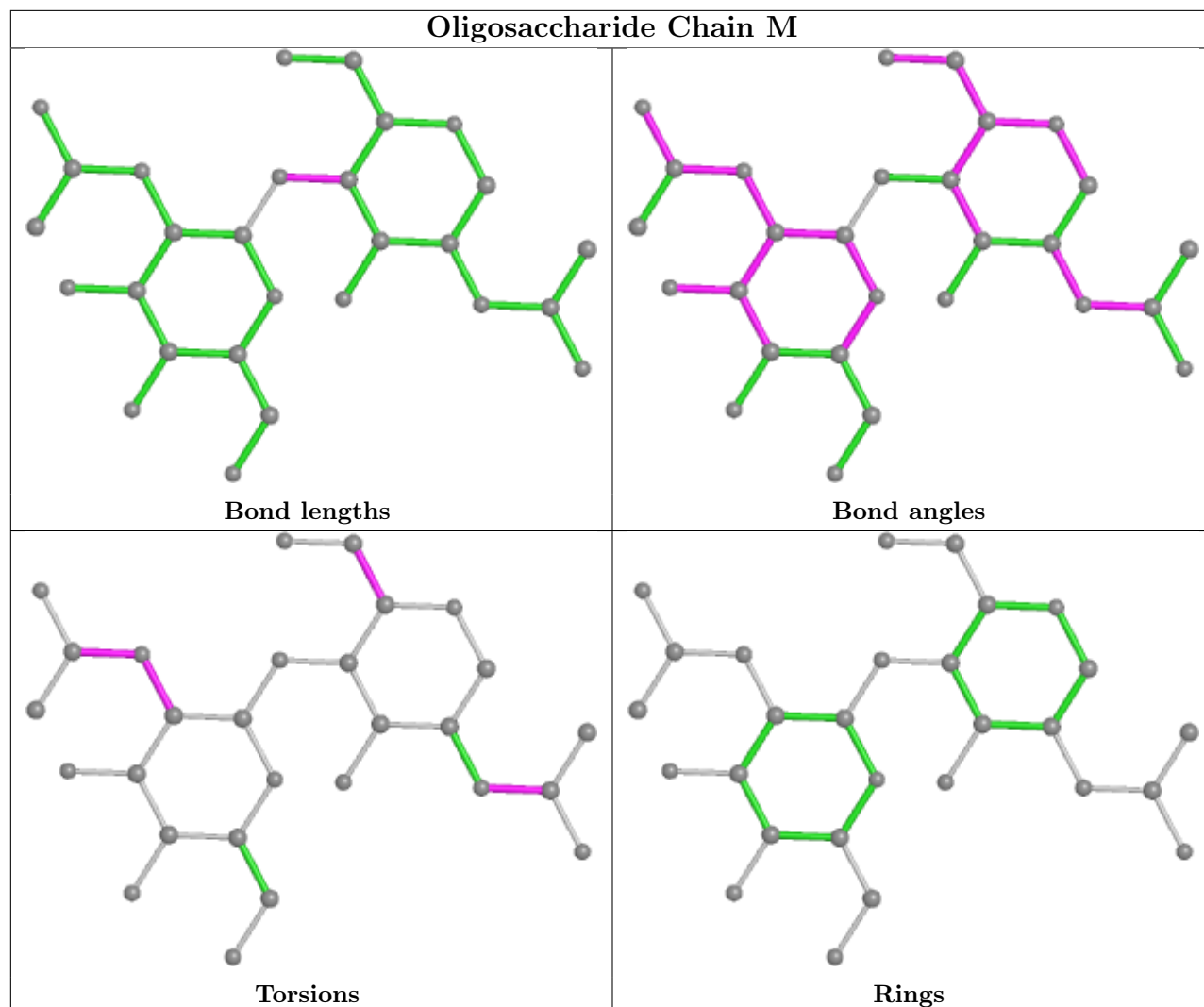
There are no ring outliers.

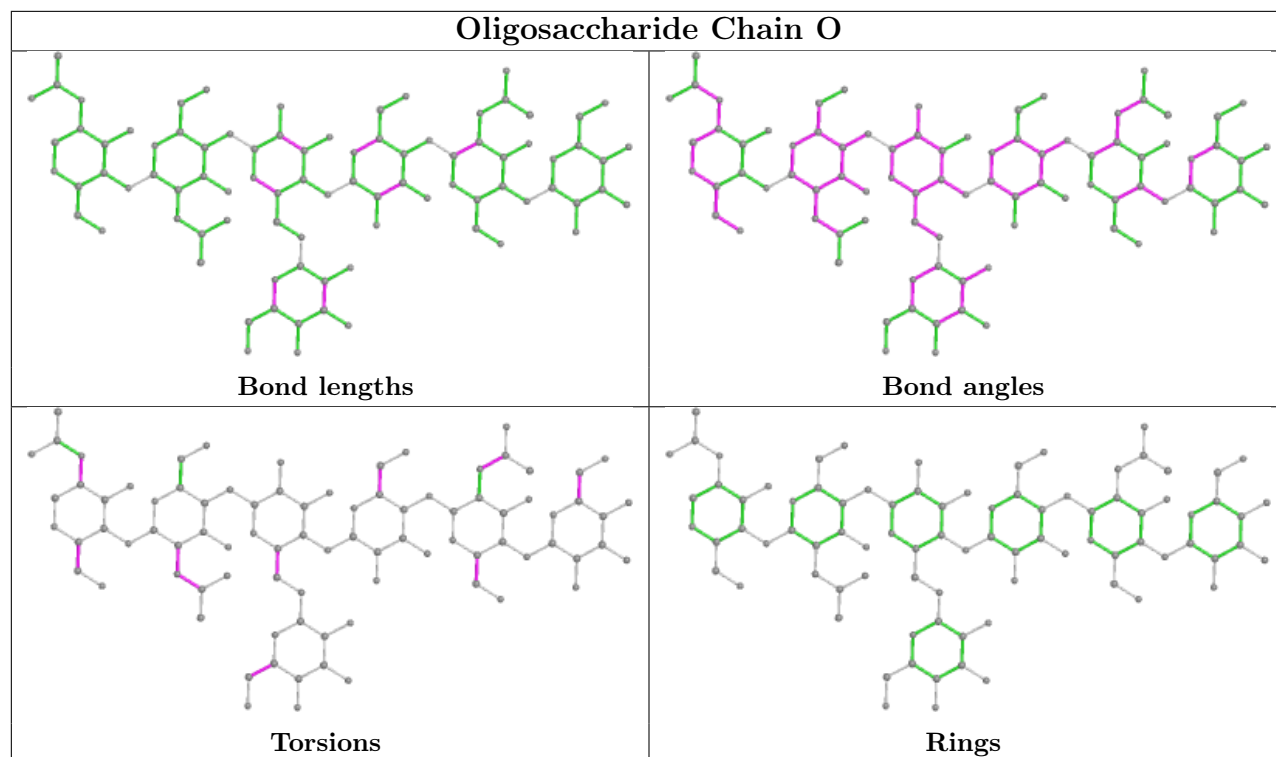
No monomer is involved in short contacts.

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









5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	B	195/235 (82%)	0.45	7 (3%) 46 27	47, 83, 143, 190	1 (0%)
1	C	192/235 (81%)	0.54	11 (5%) 30 18	46, 76, 136, 203	0
1	E	194/235 (82%)	0.39	10 (5%) 34 20	50, 80, 128, 189	0
1	G	192/235 (81%)	0.67	20 (10%) 13 8	50, 85, 134, 161	0
1	I	193/235 (82%)	0.79	15 (7%) 20 11	54, 91, 144, 172	0
2	A	120/146 (82%)	0.19	2 (1%) 69 50	45, 74, 113, 145	0
2	D	120/146 (82%)	0.52	10 (8%) 19 10	43, 86, 112, 127	1 (0%)
2	F	120/146 (82%)	0.27	3 (2%) 58 39	52, 86, 117, 130	0
2	H	123/146 (84%)	0.39	3 (2%) 59 41	56, 78, 104, 133	0
2	J	120/146 (82%)	0.60	9 (7%) 22 12	53, 86, 111, 122	1 (0%)
All	All	1569/1905 (82%)	0.50	90 (5%) 30 18	43, 83, 132, 203	3 (0%)

The worst 5 of 90 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	432	CYS	6.0
2	D	24	ALA	5.7
1	I	363	ALA	5.5
1	G	382	VAL	4.2
1	I	442	ASP	4.2

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](#)

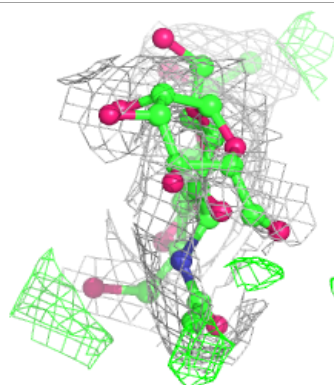
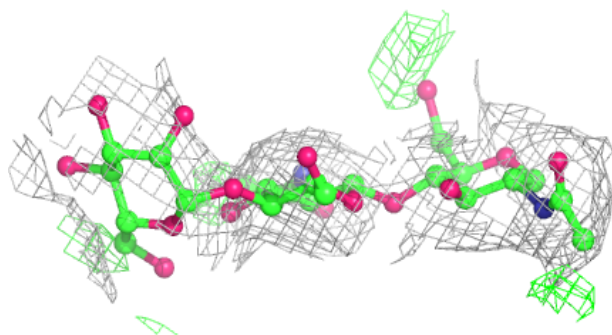
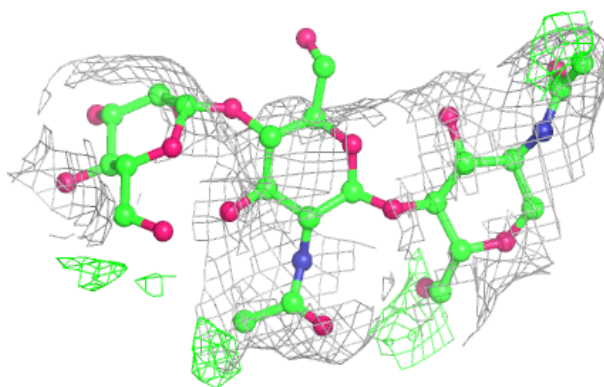
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	K	2	14/15	0.31	0.17	131,161,185,186	0
3	BMA	K	3	11/12	0.33	0.13	143,161,167,179	0
5	BMA	O	7	11/12	0.47	0.11	138,152,190,227	0
4	NAG	L	2	14/15	0.54	0.14	102,128,155,155	0
5	GAL	O	6	11/12	0.61	0.10	163,175,189,199	0
5	NAG	O	2	14/15	0.64	0.13	115,158,190,205	0
5	NAG	O	5	14/15	0.64	0.11	156,203,221,233	0
4	NAG	M	2	14/15	0.65	0.14	97,146,175,191	0
3	BMA	N	3	11/12	0.67	0.11	104,137,168,173	0
5	BMA	O	3	11/12	0.68	0.10	177,189,208,248	0
5	BMA	O	4	11/12	0.69	0.11	144,206,244,258	0
3	NAG	K	1	14/15	0.78	0.12	77,91,110,126	0
3	NAG	N	2	14/15	0.79	0.09	82,130,160,164	0
4	NAG	L	1	14/15	0.86	0.10	77,100,111,125	0
5	NAG	O	1	14/15	0.87	0.11	82,111,127,146	0
4	NAG	M	1	14/15	0.88	0.10	96,106,112,131	0
3	NAG	N	1	14/15	0.90	0.13	90,116,137,140	0

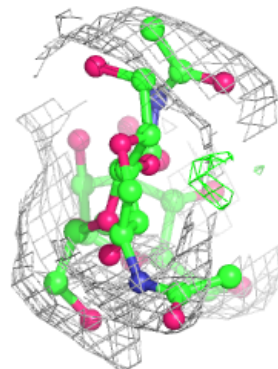
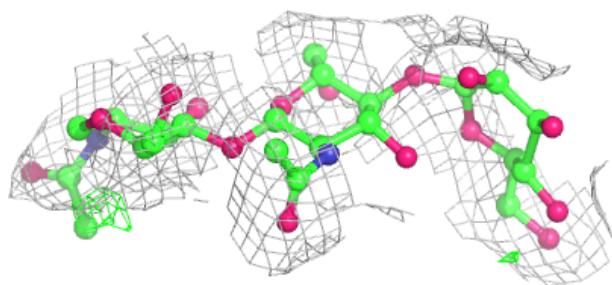
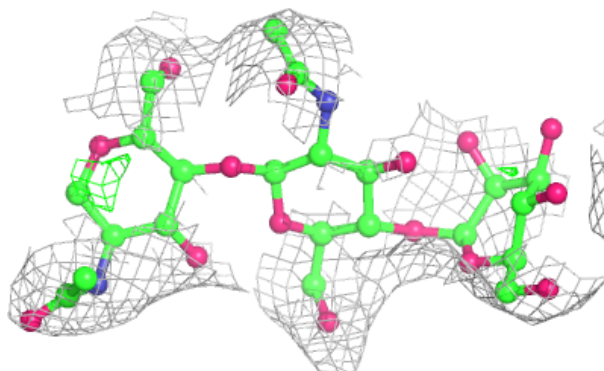
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain K:

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

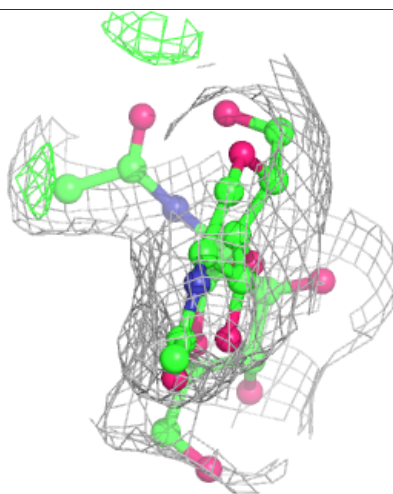
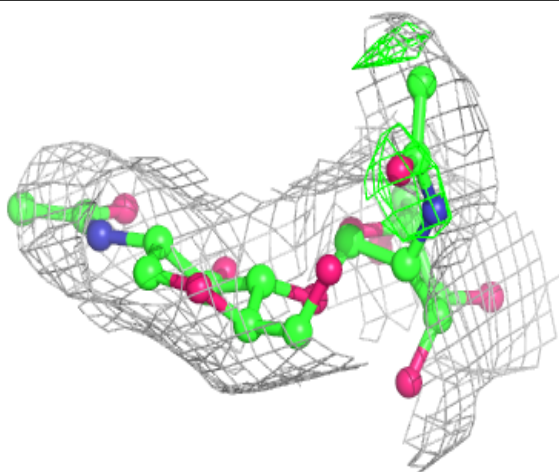
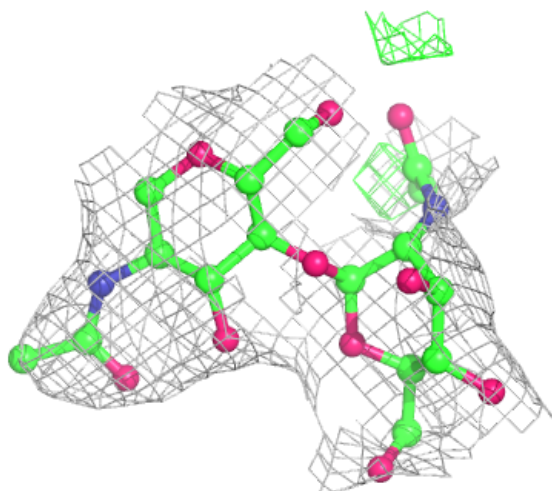
**Electron density around Chain N:**

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



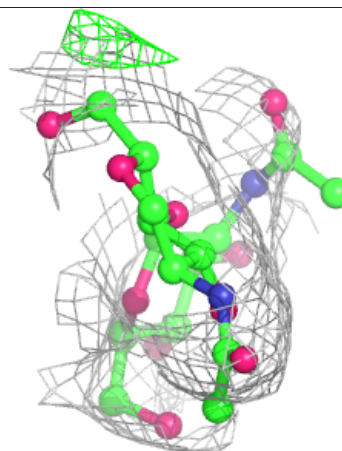
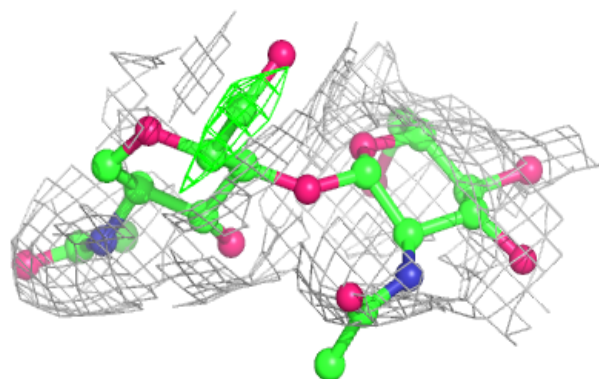
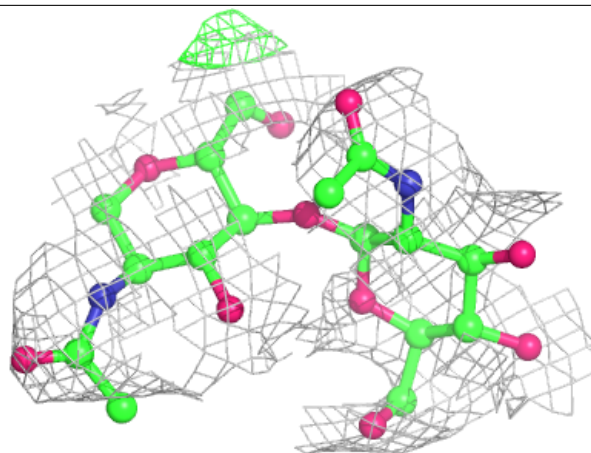
Electron density around Chain L:

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

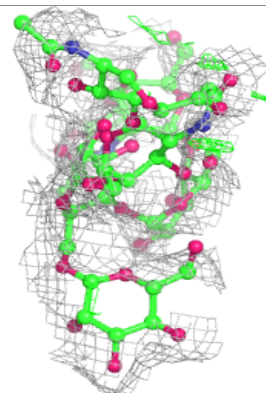
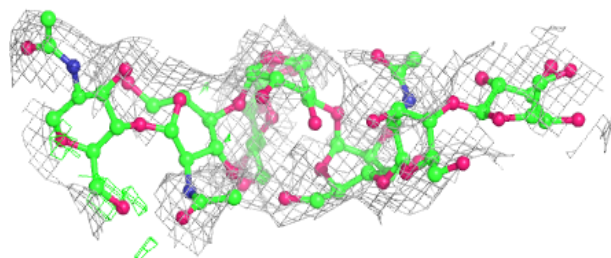
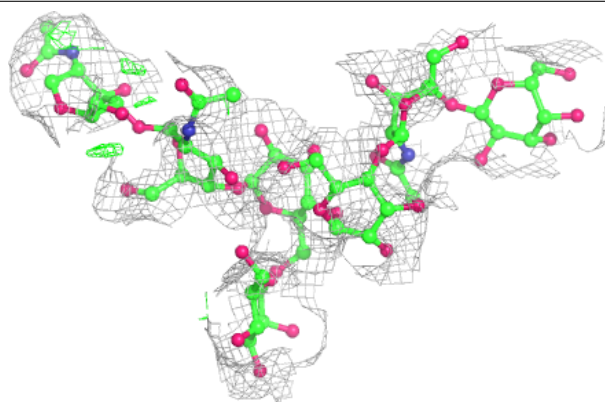


Electron density around Chain M:

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

**Electron density around Chain O:**

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.