wwPDB X-ray Structure Validation Summary Report (i)

Aug 26, 2024 – 02:23 PM JST

PDB ID	:	8ZES
Title	:	Crystal structure of the Wuhan SARS-CoV-2 RBD (333-541) complexed 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	:	3.70 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 (i) 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 (1)) were used in the production of this report:

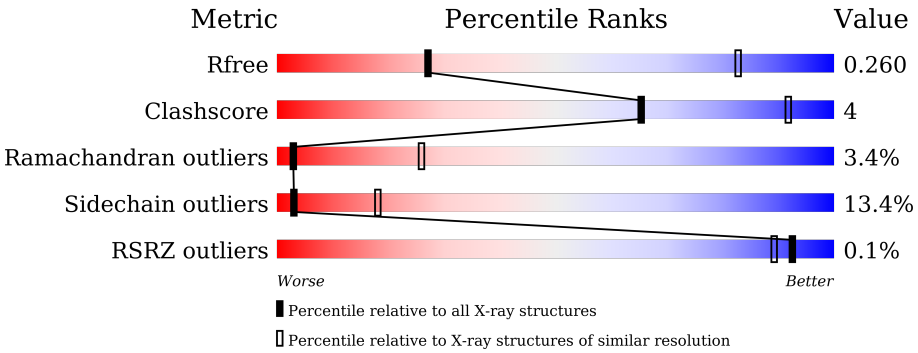
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance (i)

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 <=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	221	63% 16% 8% • 12%
1	C	221	56% 22% 8% • 12%
1	D	221	59% 23% 5% • 12%
1	G	221	57% 23% 5% • 13%
1	I	221	47% 29% 9% • 12%
2	B	146	59% 15% 8% • 17%

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Mol	Chain	Length	Quality of chain
2	E	146	54% 18% 9% 17%
2	F	146	59% 14% 7% 17%
2	H	146	55% 18% 8% 18%
2	J	146	49% 21% 9% 18%
3	K	2	100%
3	L	2	100%
3	M	2	100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12398 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
1	C	194	Total	C	N	O	S	0	0	0
			1530	983	254	285	8			
1	A	194	Total	C	N	O	S	0	0	0
			1528	981	253	286	8			
1	G	193	Total	C	N	O	S	0	0	0
			1520	977	251	284	8			
1	I	194	Total	C	N	O	S	0	0	0
			1531	982	254	287	8			
1	D	195	Total	C	N	O	S	0	0	0
			1540	988	256	288	8			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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
A	542	GLY	-	expression tag	UNP P0DTC2
A	543	SER	-	expression tag	UNP P0DTC2
A	544	HIS	-	expression tag	UNP P0DTC2
A	545	HIS	-	expression tag	UNP P0DTC2
A	546	HIS	-	expression tag	UNP P0DTC2
A	547	HIS	-	expression tag	UNP P0DTC2
A	548	HIS	-	expression tag	UNP P0DTC2

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

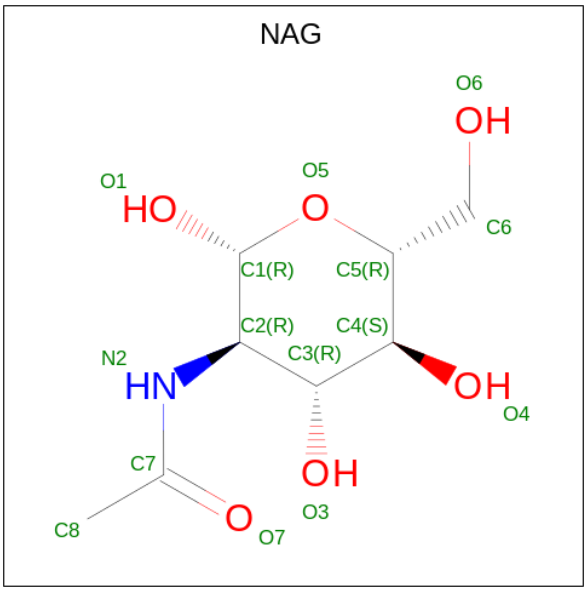
- Molecule 2 is a protein called Nanobody P2C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	121	Total	C	N	O	S	0	0	0
			931	576	158	190	7			
2	B	121	Total	C	N	O	S	0	0	0
			931	576	158	190	7			
2	F	121	Total	C	N	O	S	0	0	0
			931	576	158	190	7			
2	H	120	Total	C	N	O	S	0	0	0
			925	573	157	188	7			
2	J	119	Total	C	N	O	S	0	0	0
			919	570	156	186	7			

- Molecule 3 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
3	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



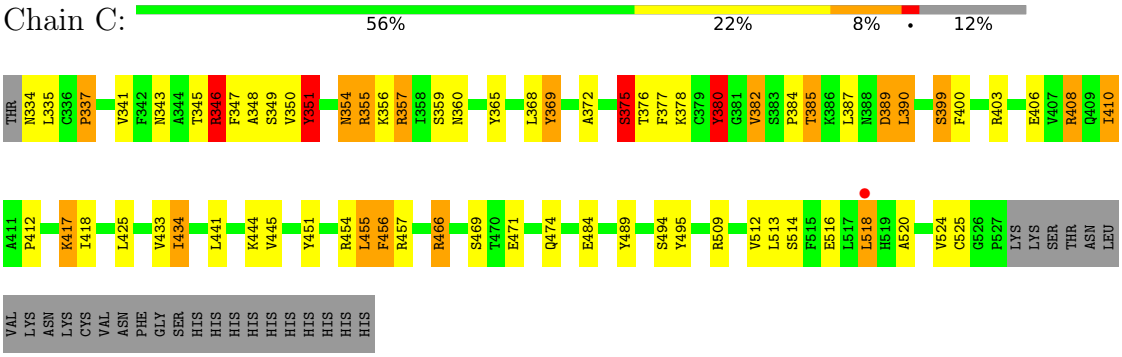
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0

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.

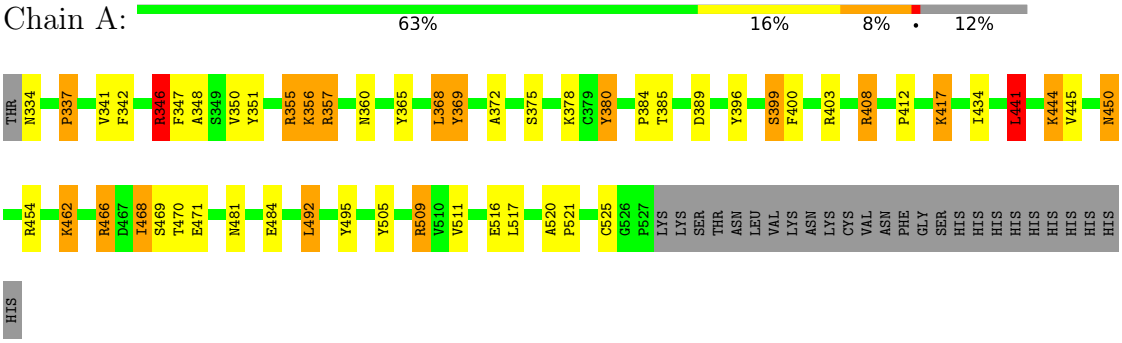
• Molecule 1: Spike protein S1

Chain C:



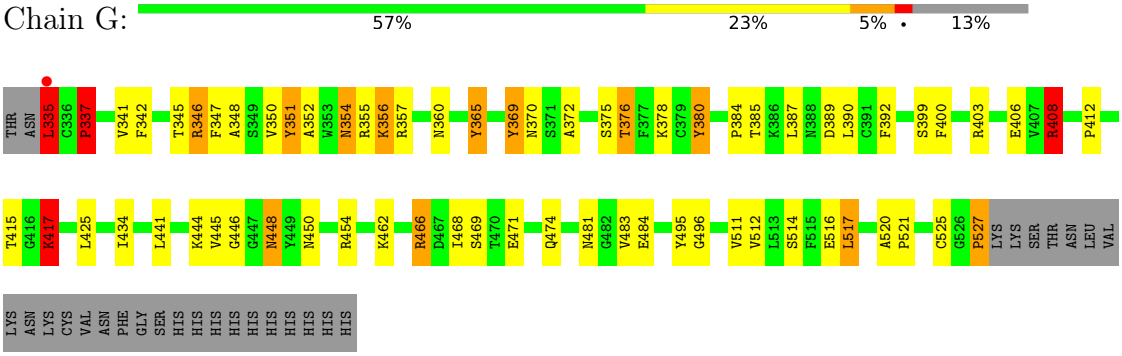
• Molecule 1: Spike protein S1

Chain A:



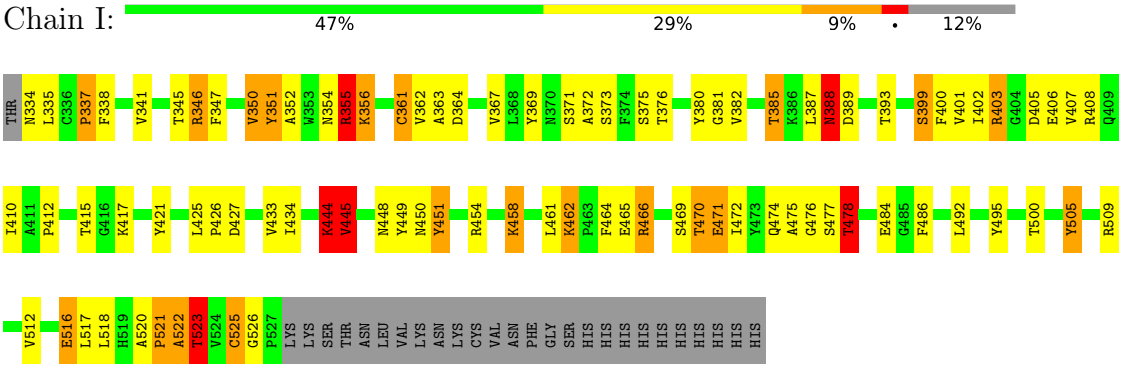
• Molecule 1: Spike protein S1

Chain G:



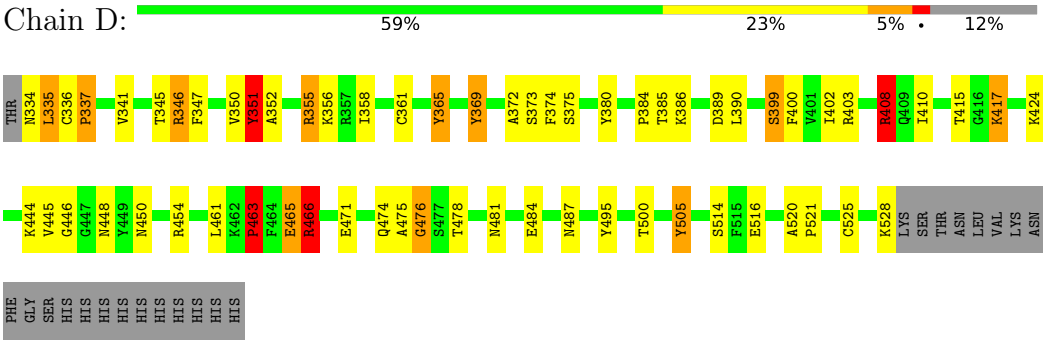
• Molecule 1: Spike protein S1

Chain I:



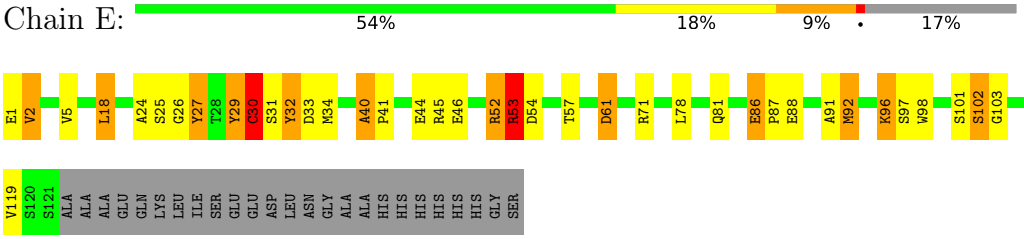
• Molecule 1: Spike protein S1

Chain D:



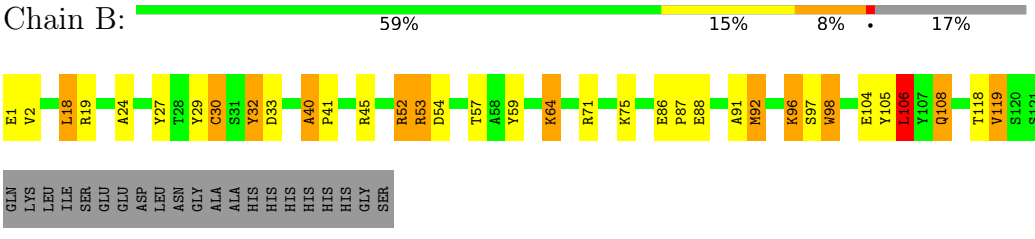
• Molecule 2: Nanobody P2C5

Chain E:



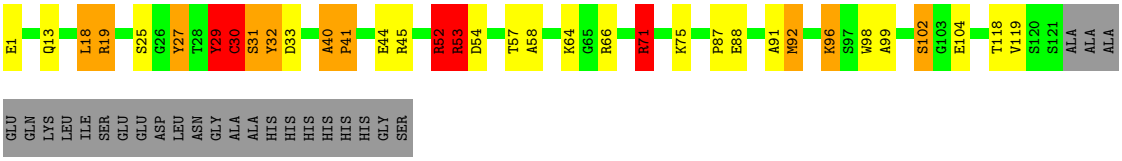
• Molecule 2: Nanobody P2C5

Chain B:



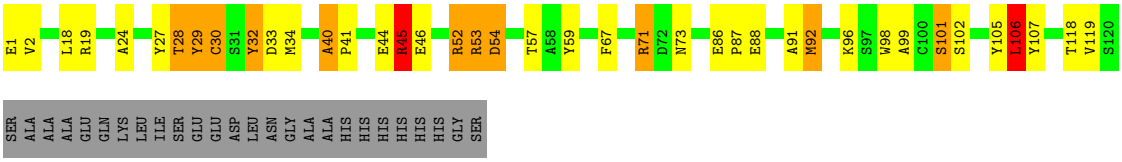
• Molecule 2: Nanobody P2C5

Chain F:



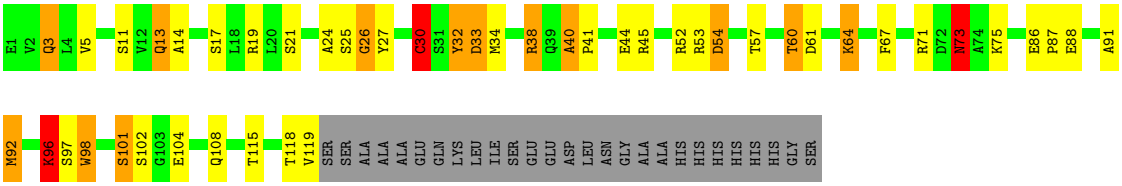
• Molecule 2: Nanobody P2C5

Chain H:



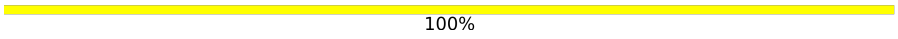
• Molecule 2: Nanobody P2C5

Chain J:



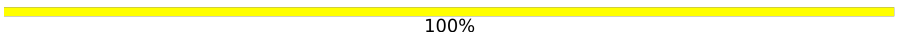
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



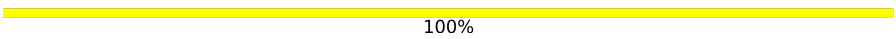
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



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

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	126.64Å 194.24Å 264.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.10 – 3.70 74.10 – 3.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (74.10-3.70) 98.9 (74.10-3.70)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.207 , 0.269 0.209 , 0.260	Depositor DCC
R_{free} test set	1810 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å^2)	150.3	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 173.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12398	wwPDB-VP
Average B, all atoms (Å^2)	195.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.93	1/1571 (0.1%)	1.71	38/2139 (1.8%)
1	C	0.92	1/1574 (0.1%)	1.75	48/2143 (2.2%)
1	D	0.86	1/1583 (0.1%)	1.62	26/2154 (1.2%)
1	G	0.94	2/1563 (0.1%)	1.77	49/2128 (2.3%)
1	I	1.01	3/1574 (0.2%)	1.80	47/2143 (2.2%)
2	B	0.89	0/950	1.75	27/1285 (2.1%)
2	E	0.88	0/950	1.72	24/1285 (1.9%)
2	F	0.90	1/950 (0.1%)	1.78	26/1285 (2.0%)
2	H	0.96	1/944 (0.1%)	1.75	27/1277 (2.1%)
2	J	0.88	0/938	1.79	29/1269 (2.3%)
All	All	0.92	10/12597 (0.1%)	1.74	341/17108 (2.0%)

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	A	0	8
1	C	0	18
1	D	0	9
1	G	0	11
1	I	0	19
2	B	0	7
2	E	0	16
2	F	0	11
2	H	0	17
2	J	0	16
All	All	0	132

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	514	SER	CA-CB	8.64	1.66	1.52
1	A	399	SER	CA-CB	7.53	1.64	1.52
1	G	406	GLU	CD-OE1	6.96	1.33	1.25
1	C	399	SER	CA-CB	6.53	1.62	1.52
1	I	373	SER	CA-CB	6.44	1.62	1.52

The worst 5 of 341 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	346	ARG	NE-CZ-NH1	14.08	127.34	120.30
1	G	346	ARG	NE-CZ-NH2	-13.18	113.71	120.30
2	H	45	ARG	CG-CD-NE	13.03	139.16	111.80
2	E	52	ARG	NE-CZ-NH2	12.78	126.69	120.30
2	F	32	TYR	N-CA-CB	12.60	133.28	110.60

There are no chirality outliers.

5 of 132 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	343	ASN	Mainchain
1	C	346	ARG	Sidechain
1	C	348	ALA	Peptide
1	C	351	TYR	Sidechain
1	C	354	ASN	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	A	1528	0	1443	12	0
1	C	1530	0	1444	11	0
1	D	1540	0	1460	11	0
1	G	1520	0	1437	16	0
1	I	1531	0	1446	25	0
2	B	931	0	864	4	0
2	E	931	0	864	3	0
2	F	931	0	864	3	0
2	H	925	0	859	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	919	0	854	6	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
4	A	14	0	13	0	0
4	D	14	0	13	0	0
All	All	12398	0	11636	90	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 4.

The worst 5 of 90 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:361:CYS:SG	1:I:362:VAL:N	2.45	0.90
1:I:382:VAL:HG11	1:I:387:LEU:HD23	1.61	0.81
1:C:380:TYR:CE2	1:C:412:PRO:HD2	2.25	0.71
1:A:380:TYR:CE2	1:A:412:PRO:HD2	2.24	0.71
1:I:401:VAL:HG11	1:I:451:TYR:CD2	2.27	0.70

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	192/221 (87%)	160 (83%)	29 (15%)	3 (2%)	8 37
1	C	192/221 (87%)	163 (85%)	24 (12%)	5 (3%)	4 29
1	D	193/221 (87%)	162 (84%)	25 (13%)	6 (3%)	3 27
1	G	191/221 (86%)	161 (84%)	25 (13%)	5 (3%)	4 29
1	I	192/221 (87%)	153 (80%)	29 (15%)	10 (5%)	1 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	119/146 (82%)	107 (90%)	8 (7%)	4 (3%)	3 26
2	E	119/146 (82%)	105 (88%)	9 (8%)	5 (4%)	2 21
2	F	119/146 (82%)	102 (86%)	11 (9%)	6 (5%)	1 18
2	H	118/146 (81%)	105 (89%)	9 (8%)	4 (3%)	3 26
2	J	117/146 (80%)	104 (89%)	8 (7%)	5 (4%)	2 20
All	All	1552/1835 (85%)	1322 (85%)	177 (11%)	53 (3%)	3 26

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	445	VAL
1	C	456	PHE
2	E	40	ALA
1	A	445	VAL
2	B	40	ALA

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	165/193 (86%)	147 (89%)	18 (11%)	5 24
1	C	165/193 (86%)	145 (88%)	20 (12%)	4 20
1	D	167/193 (86%)	141 (84%)	26 (16%)	2 14
1	G	164/193 (85%)	145 (88%)	19 (12%)	4 22
1	I	166/193 (86%)	142 (86%)	24 (14%)	2 16
2	B	98/117 (84%)	85 (87%)	13 (13%)	3 18
2	E	98/117 (84%)	83 (85%)	15 (15%)	2 14
2	F	98/117 (84%)	84 (86%)	14 (14%)	2 16
2	H	97/117 (83%)	85 (88%)	12 (12%)	4 20
2	J	96/117 (82%)	81 (84%)	15 (16%)	2 14
All	All	1314/1550 (85%)	1138 (87%)	176 (13%)	3 18

5 of 176 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	350	VAL
2	J	60	THR
1	I	367	VAL
1	I	472	ILE
1	D	334	ASN

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

Mol	Chain	Res	Type
1	D	501	ASN
2	J	108	GLN
1	I	501	ASN
1	G	501	ASN
2	J	13	GLN

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)

6 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	14,14,15	2.54	4 (28%)	17,19,21	4.25	6 (35%)
3	NAG	K	2	3	14,14,15	2.16	3 (21%)	17,19,21	4.30	10 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	L	1	3,1	14,14,15	1.89	1 (7%)	17,19,21	3.64	8 (47%)
3	NAG	L	2	3	14,14,15	1.24	2 (14%)	17,19,21	1.99	5 (29%)
3	NAG	M	1	3,1	14,14,15	0.77	0	17,19,21	2.70	10 (58%)
3	NAG	M	2	3	14,14,15	0.79	0	17,19,21	1.95	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	K	1	3	-	3/6/23/26	0/1/1/1
3	NAG	K	2	3	-	6/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	L	2	3	-	6/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	6/6/23/26	0/1/1/1
3	NAG	M	2	3	-	1/6/23/26	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	1	NAG	O4-C4	7.70	1.61	1.43
3	K	2	NAG	C1-C2	6.90	1.62	1.52
3	L	1	NAG	O4-C4	5.14	1.55	1.43
3	L	2	NAG	C1-C2	3.63	1.57	1.52
3	K	1	NAG	O5-C5	2.39	1.48	1.43

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	1	NAG	C1-O5-C5	12.48	129.10	112.19
3	K	2	NAG	C1-C2-N2	11.53	130.19	110.49
3	L	1	NAG	C2-N2-C7	8.95	135.65	122.90
3	L	1	NAG	C1-O5-C5	8.43	123.61	112.19
3	K	1	NAG	C2-N2-C7	8.01	134.31	122.90

There are no chirality outliers.

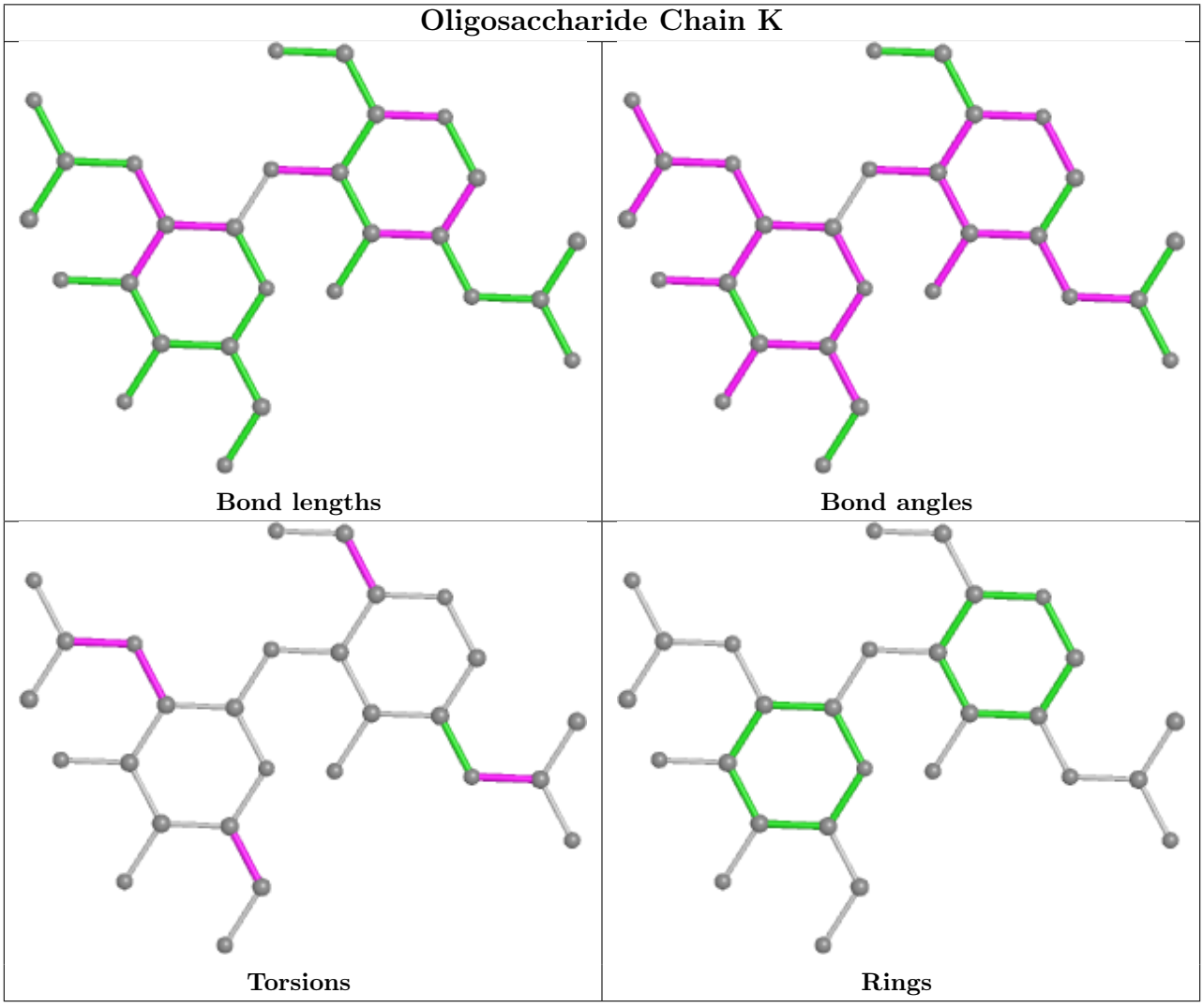
5 of 25 torsion outliers are listed below:

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

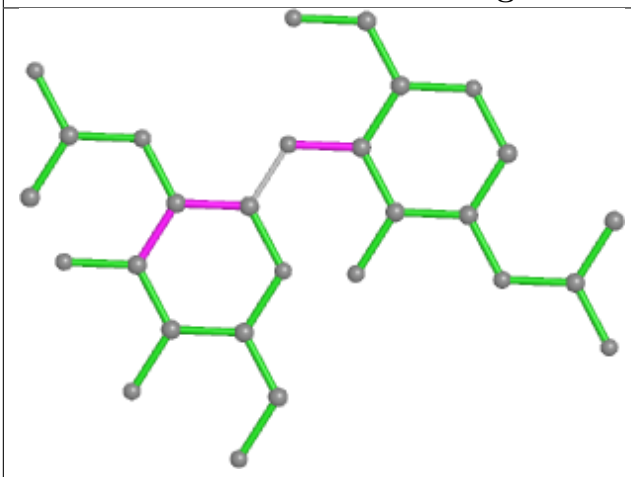
There are no ring outliers.

No monomer is involved in short contacts.

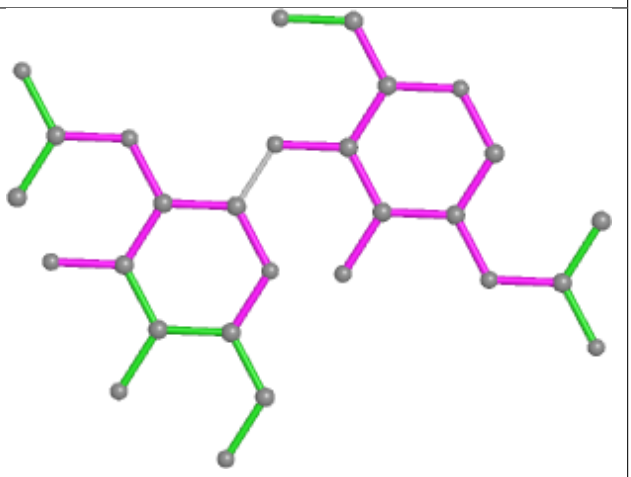
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



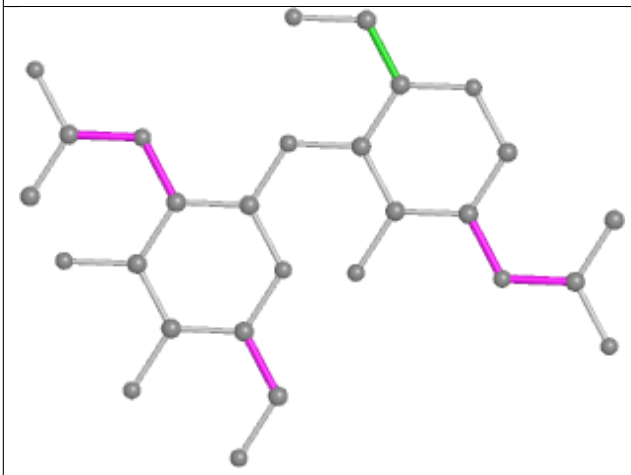
Oligosaccharide Chain L



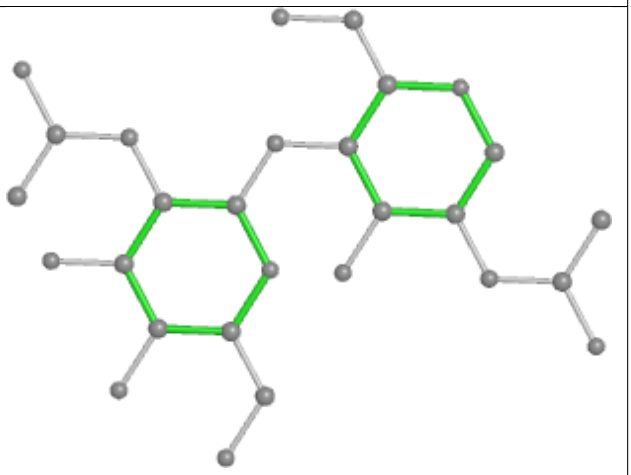
Bond lengths



Bond angles

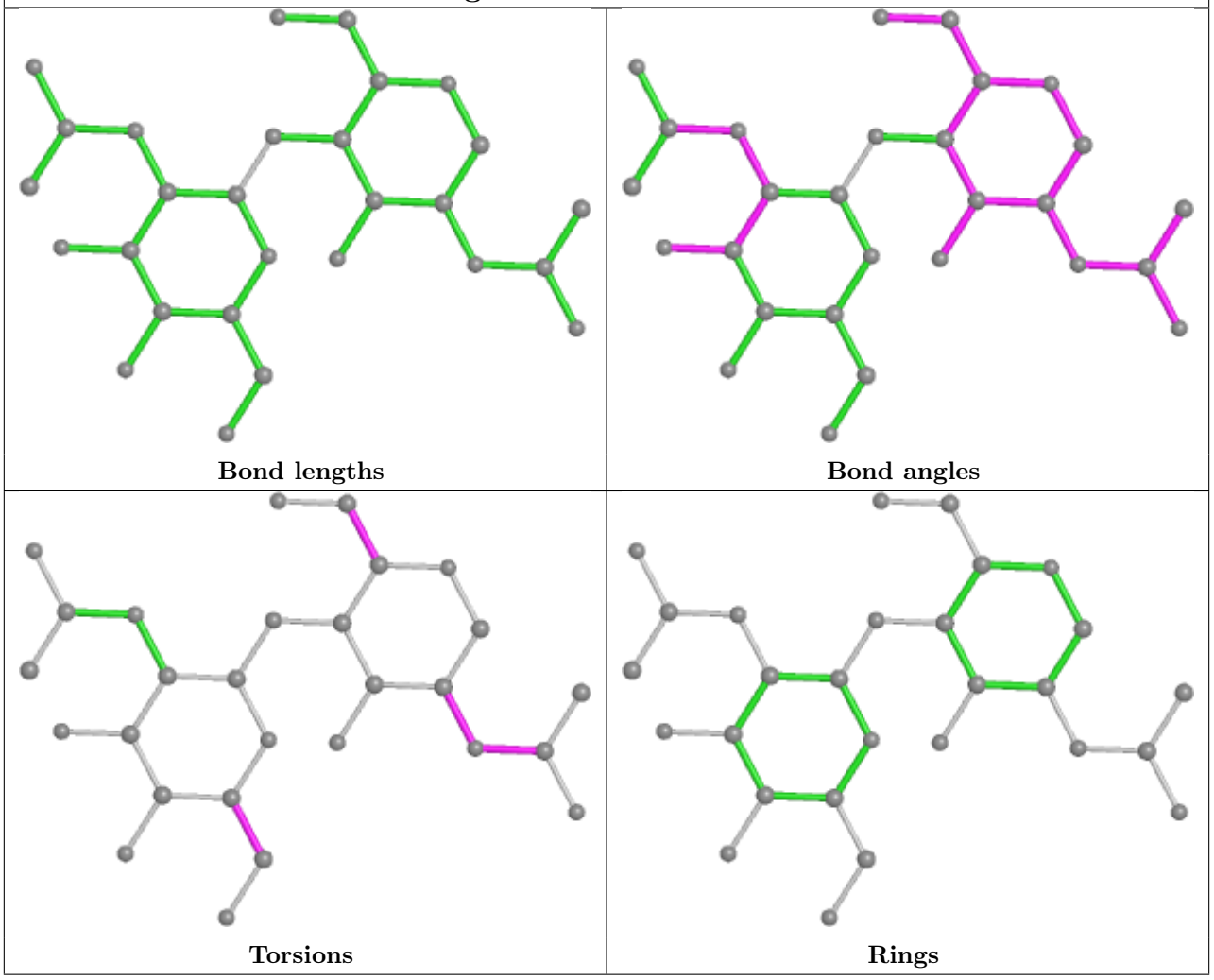


Torsions



Rings

Oligosaccharide Chain M



5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	601	-	14,14,15	1.75	3 (21%)	17,19,21	2.65	7 (41%)
4	NAG	D	601	1	14,14,15	1.26	1 (7%)	17,19,21	2.82	6 (35%)

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	601	-	-	4/6/23/26	0/1/1/1
4	NAG	D	601	1	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	NAG	C1-C2	4.02	1.58	1.52
4	A	601	NAG	O5-C5	2.79	1.49	1.43
4	A	601	NAG	C3-C2	2.69	1.58	1.52
4	D	601	NAG	C3-C2	2.29	1.57	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	601	NAG	C1-O5-C5	6.95	121.60	112.19
4	A	601	NAG	O3-C3-C2	6.55	123.02	109.47
4	A	601	NAG	C1-O5-C5	6.49	120.99	112.19
4	D	601	NAG	C2-N2-C7	5.66	130.97	122.90
4	D	601	NAG	C4-C3-C2	3.96	116.83	111.02

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	NAG	C8-C7-N2-C2
4	A	601	NAG	O7-C7-N2-C2
4	A	601	NAG	O5-C5-C6-O6
4	A	601	NAG	C4-C5-C6-O6
4	D	601	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	194/221 (87%)	-0.99	0 100 100	108, 191, 268, 314	0
1	C	194/221 (87%)	-0.85	1 (0%) 87 72	126, 200, 265, 299	0
1	D	195/221 (88%)	-0.99	0 100 100	120, 190, 253, 284	0
1	G	193/221 (87%)	-1.01	1 (0%) 87 72	130, 195, 266, 329	0
1	I	194/221 (87%)	-0.94	0 100 100	108, 191, 245, 285	0
2	B	121/146 (82%)	-0.96	0 100 100	147, 196, 244, 302	0
2	E	121/146 (82%)	-1.08	0 100 100	150, 208, 252, 293	0
2	F	121/146 (82%)	-1.12	0 100 100	133, 181, 228, 255	0
2	H	120/146 (82%)	-0.96	0 100 100	133, 190, 235, 255	0
2	J	119/146 (81%)	-1.03	0 100 100	140, 199, 248, 277	0
All	All	1572/1835 (85%)	-0.98	2 (0%) 92 89	108, 195, 254, 329	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	335	LEU	3.1
1	C	518	LEU	2.2

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

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

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

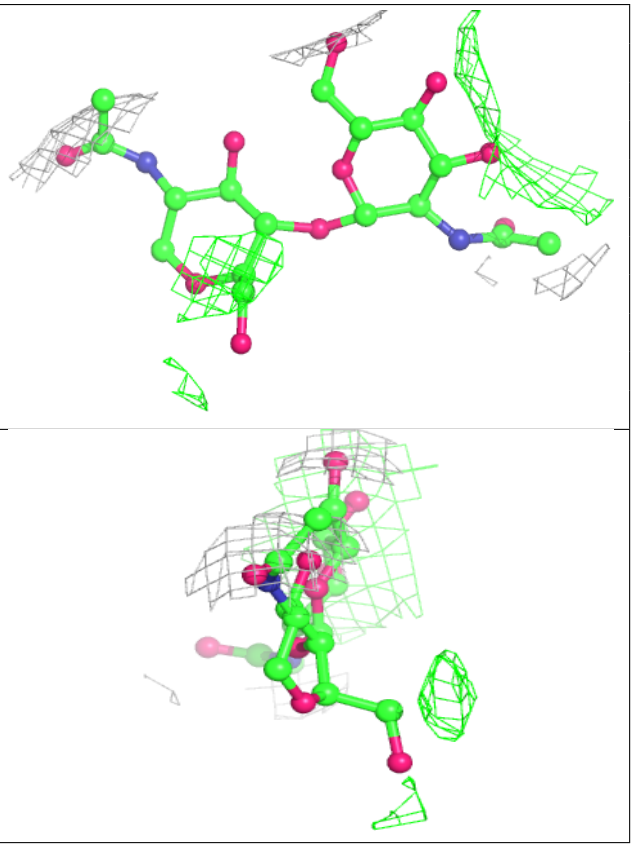
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

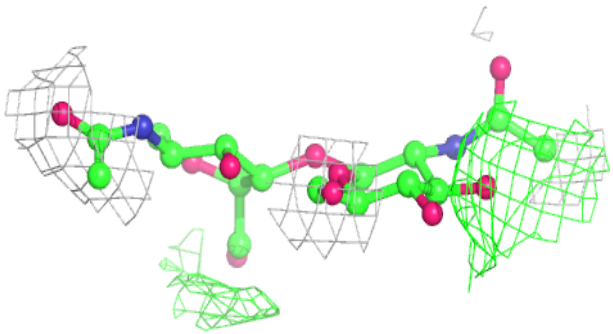
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	M	2	14/15	0.59	0.08	161,292,339,373	0
3	NAG	K	2	14/15	0.71	0.08	151,267,342,348	0
3	NAG	L	2	14/15	0.79	0.08	135,256,330,342	0
3	NAG	L	1	14/15	0.93	0.05	118,180,228,241	0
3	NAG	M	1	14/15	0.94	0.04	118,210,251,254	0
3	NAG	K	1	14/15	0.96	0.04	137,213,244,256	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:

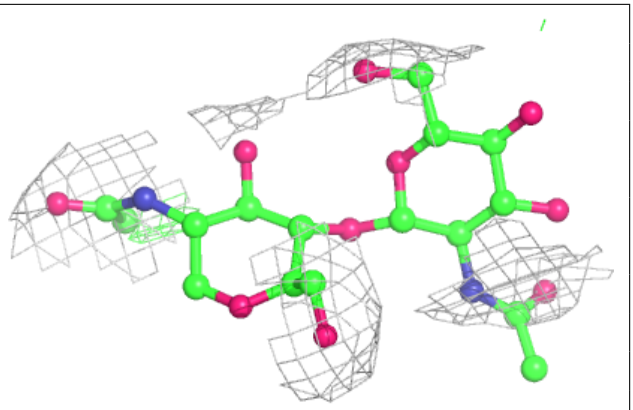
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

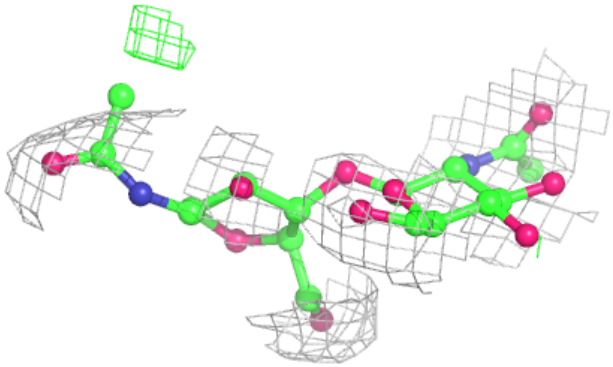


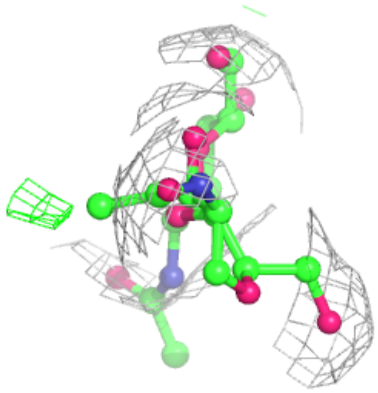


Electron density around Chain L:

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

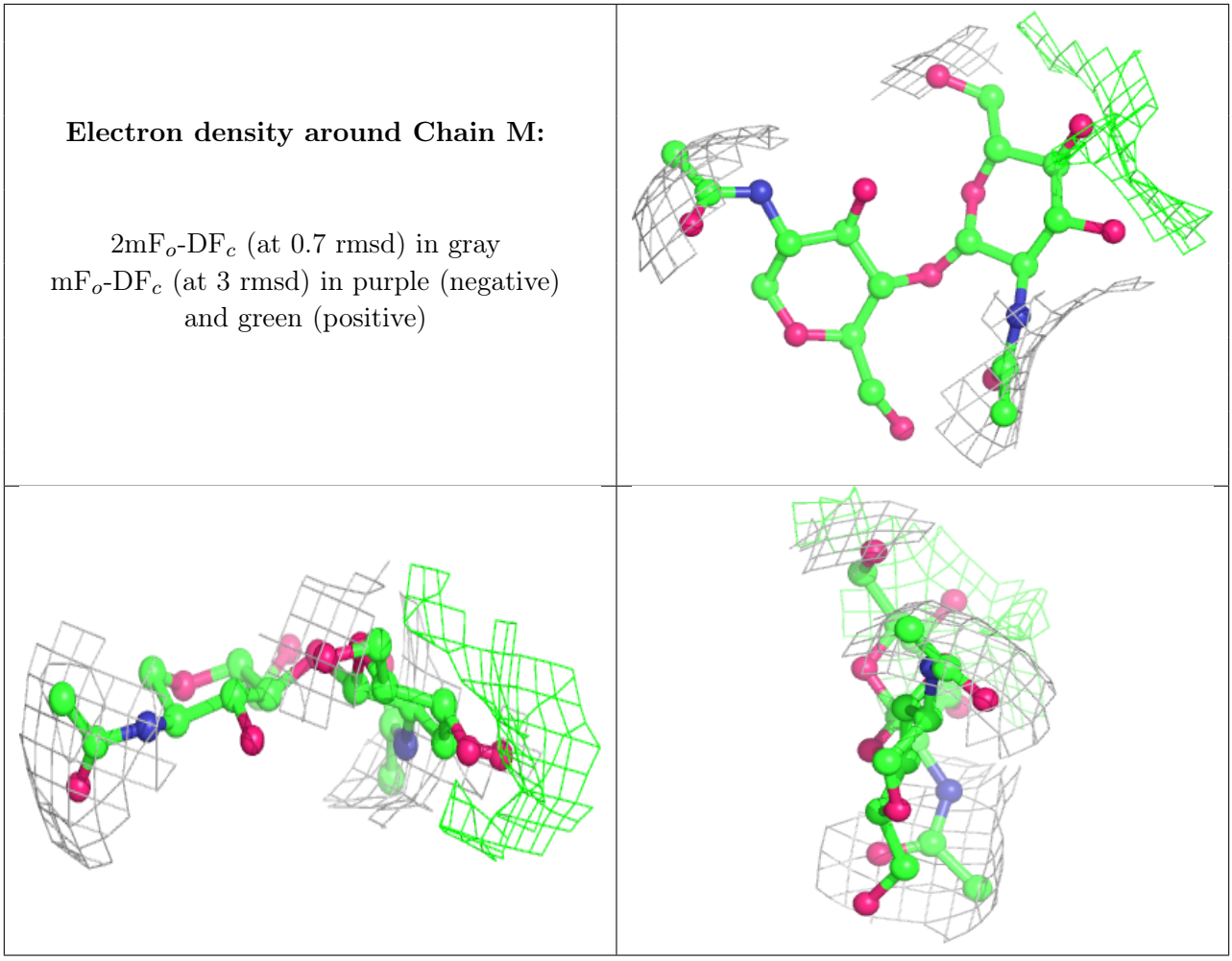






Electron density around Chain M:

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	A	601	14/15	0.91	0.07	145,224,264,268	0
4	NAG	D	601	14/15	0.92	0.07	116,180,245,254	0

6.5 Other polymers

There are no such residues in this entry.