



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:02 PM UTC

PDB ID : 4KRM / pdb_00004krm
Title : Nanobody/VHH domain 7D12 in complex with domain III of the extracellular region of EGFR, pH 3.5
Authors : Ferguson, K.M.; Schmitz, K.R.
Deposited on : 2013-05-16
Resolution : 2.65 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

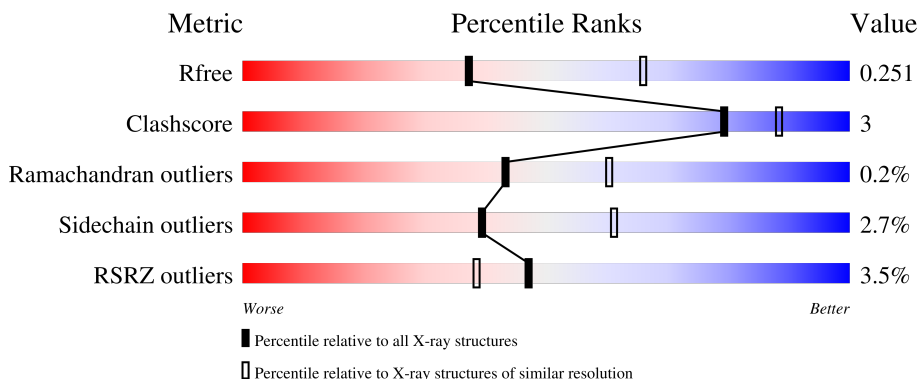
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	214	
1	C	214	
1	E	214	
1	G	214	
1	I	214	

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Mol	Chain	Length	Quality of chain
1	K	214	 5% 85% 6% 8%
2	B	133	 4% 86% 5% 7%
2	D	133	 4% 83% 8% 7%
2	F	133	 8% 79% 11% 8%
2	H	133	 4% 83% 8% 7%
2	J	133	 2% 86% 5% 7%
2	L	133	 3% 86% 6% 7%
3	M	4	 75% 25%
3	N	4	 75% 25%
3	P	4	 75% 25%
3	Q	4	 50% 50%
3	R	4	 75% 25%
3	S	4	 25% 75%
4	O	2	 50% 50%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 28686 atoms, of which 13827 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 Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	197	2885	924	1412	254	286	9	0	0	0
1	C	197	2906	927	1426	257	287	9	0	0	0
1	E	197	2885	923	1414	257	282	9	0	0	0
1	G	198	2912	930	1425	260	287	10	0	0	0
1	I	195	2851	912	1399	254	278	8	0	0	0
1	K	196	2847	913	1395	253	277	9	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	307	LEU	-	expression tag	UNP P00533
A	308	GLU	-	expression tag	UNP P00533
A	309	GLU	-	expression tag	UNP P00533
A	310	LYS	-	expression tag	UNP P00533
A	515	HIS	-	expression tag	UNP P00533
A	516	HIS	-	expression tag	UNP P00533
A	517	HIS	-	expression tag	UNP P00533
A	518	HIS	-	expression tag	UNP P00533
A	519	HIS	-	expression tag	UNP P00533
A	520	HIS	-	expression tag	UNP P00533
C	307	LEU	-	expression tag	UNP P00533
C	308	GLU	-	expression tag	UNP P00533
C	309	GLU	-	expression tag	UNP P00533
C	310	LYS	-	expression tag	UNP P00533
C	515	HIS	-	expression tag	UNP P00533
C	516	HIS	-	expression tag	UNP P00533
C	517	HIS	-	expression tag	UNP P00533

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Chain	Residue	Modelled	Actual	Comment	Reference
C	518	HIS	-	expression tag	UNP P00533
C	519	HIS	-	expression tag	UNP P00533
C	520	HIS	-	expression tag	UNP P00533
E	307	LEU	-	expression tag	UNP P00533
E	308	GLU	-	expression tag	UNP P00533
E	309	GLU	-	expression tag	UNP P00533
E	310	LYS	-	expression tag	UNP P00533
E	515	HIS	-	expression tag	UNP P00533
E	516	HIS	-	expression tag	UNP P00533
E	517	HIS	-	expression tag	UNP P00533
E	518	HIS	-	expression tag	UNP P00533
E	519	HIS	-	expression tag	UNP P00533
E	520	HIS	-	expression tag	UNP P00533
G	307	LEU	-	expression tag	UNP P00533
G	308	GLU	-	expression tag	UNP P00533
G	309	GLU	-	expression tag	UNP P00533
G	310	LYS	-	expression tag	UNP P00533
G	515	HIS	-	expression tag	UNP P00533
G	516	HIS	-	expression tag	UNP P00533
G	517	HIS	-	expression tag	UNP P00533
G	518	HIS	-	expression tag	UNP P00533
G	519	HIS	-	expression tag	UNP P00533
G	520	HIS	-	expression tag	UNP P00533
I	307	LEU	-	expression tag	UNP P00533
I	308	GLU	-	expression tag	UNP P00533
I	309	GLU	-	expression tag	UNP P00533
I	310	LYS	-	expression tag	UNP P00533
I	515	HIS	-	expression tag	UNP P00533
I	516	HIS	-	expression tag	UNP P00533
I	517	HIS	-	expression tag	UNP P00533
I	518	HIS	-	expression tag	UNP P00533
I	519	HIS	-	expression tag	UNP P00533
I	520	HIS	-	expression tag	UNP P00533
K	307	LEU	-	expression tag	UNP P00533
K	308	GLU	-	expression tag	UNP P00533
K	309	GLU	-	expression tag	UNP P00533
K	310	LYS	-	expression tag	UNP P00533
K	515	HIS	-	expression tag	UNP P00533
K	516	HIS	-	expression tag	UNP P00533
K	517	HIS	-	expression tag	UNP P00533
K	518	HIS	-	expression tag	UNP P00533
K	519	HIS	-	expression tag	UNP P00533

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Chain	Residue	Modelled	Actual	Comment	Reference
K	520	HIS	-	expression tag	UNP P00533

- Molecule 2 is a protein called Nanobody/VHH domain 7D12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
2	B	124	Total	C	H	N	O	S	0	0	0
			1753	568	835	159	187	4			
2	D	124	Total	C	H	N	O	S	0	0	0
			1717	562	810	155	186	4			
2	F	122	Total	C	H	N	O	S	0	0	0
			1666	549	782	151	180	4			
2	H	124	Total	C	H	N	O	S	0	0	0
			1770	571	846	162	187	4			
2	J	124	Total	C	H	N	O	S	0	0	0
			1771	572	845	160	190	4			
2	L	124	Total	C	H	N	O	S	0	0	0
			1732	565	821	156	186	4			

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



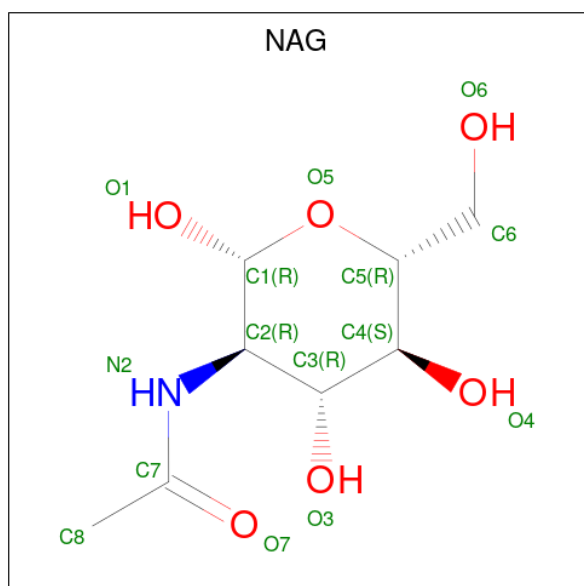
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	4	Total	C	H	N	O	0	0	0
			94	28	44	2	20			
3	N	4	Total	C	H	N	O	0	0	0
			94	28	44	2	20			
3	P	4	Total	C	H	N	O	0	0	0
			94	28	44	2	20			
3	Q	4	Total	C	H	N	O	0	0	0
			94	28	44	2	20			
3	R	4	Total	C	H	N	O	0	0	0
			94	28	44	2	20			
3	S	4	Total	C	H	N	O	0	0	0
			94	28	44	2	20			

- 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	O	2	28	16	2	10	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
5	A	1	28	8	14	1	5	0	0
5	A	1	28	8	14	1	5	0	0
5	C	1	27	8	13	1	5	0	0
5	E	1	28	8	14	1	5	0	0
5	E	1	28	8	14	1	5	0	0
5	G	1	28	8	14	1	5	0	0
5	G	1	28	8	14	1	5	0	0
5	I	1	28	8	14	1	5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	I	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	K	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	K	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

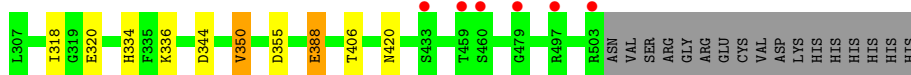
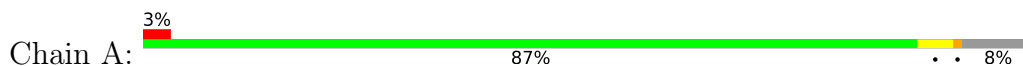
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total	O	0	0
			9	9		
6	B	8	Total	O	0	0
			8	8		
6	C	12	Total	O	0	0
			12	12		
6	D	3	Total	O	0	0
			3	3		
6	E	14	Total	O	0	0
			14	14		
6	F	3	Total	O	0	0
			3	3		
6	G	10	Total	O	0	0
			10	10		
6	H	5	Total	O	0	0
			5	5		
6	I	7	Total	O	0	0
			7	7		
6	J	10	Total	O	0	0
			10	10		
6	K	5	Total	O	0	0
			5	5		
6	L	6	Total	O	0	0
			6	6		

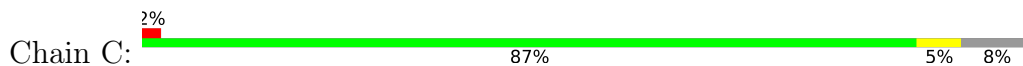
3 Residue-property plots [i](#)

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.

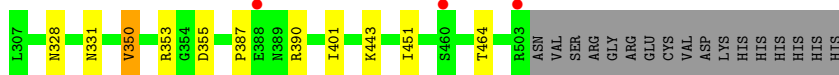
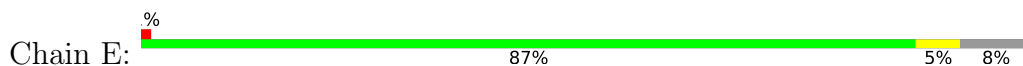
- Molecule 1: Epidermal growth factor receptor



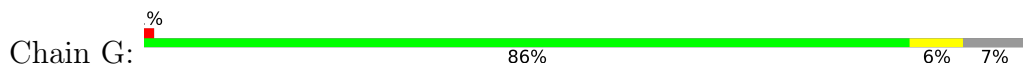
- Molecule 1: Epidermal growth factor receptor



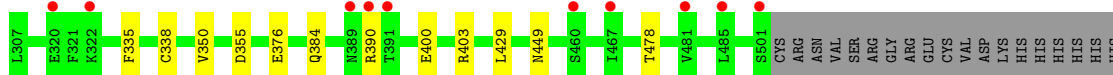
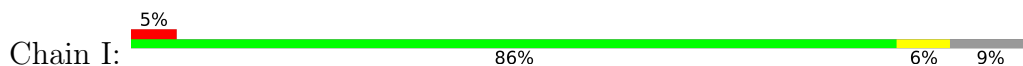
- Molecule 1: Epidermal growth factor receptor



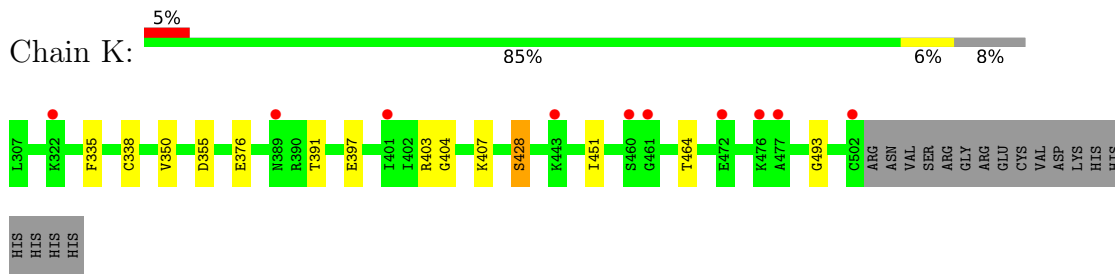
- Molecule 1: Epidermal growth factor receptor



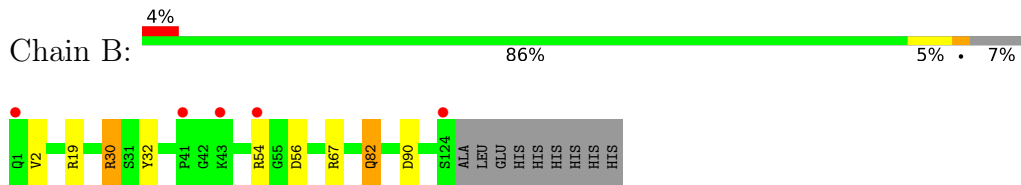
- Molecule 1: Epidermal growth factor receptor



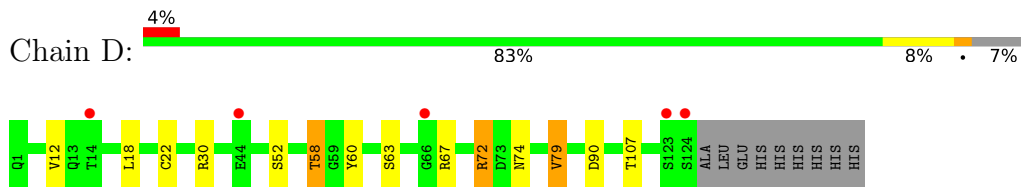
- Molecule 1: Epidermal growth factor receptor



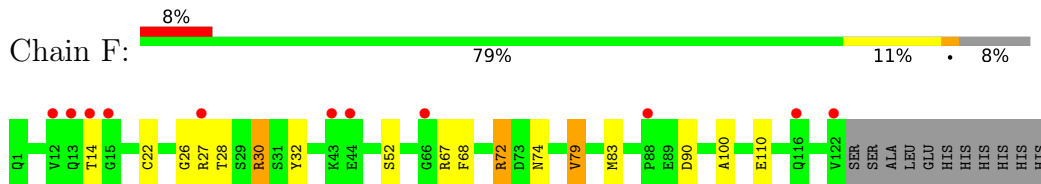
• Molecule 2: Nanobody/VHH domain 7D12



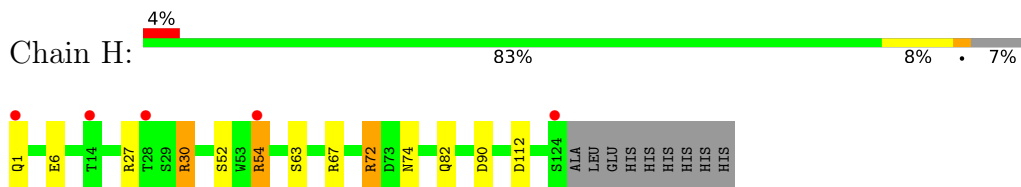
• Molecule 2: Nanobody/VHH domain 7D12



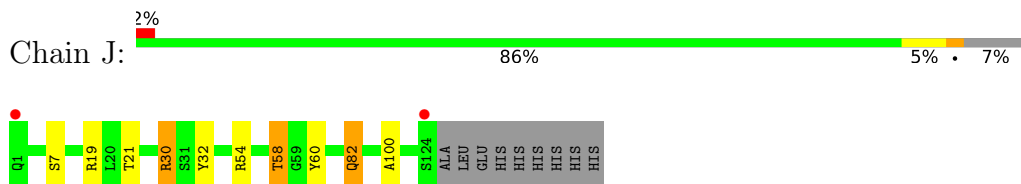
• Molecule 2: Nanobody/VHH domain 7D12



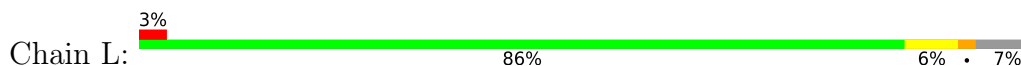
• Molecule 2: Nanobody/VHH domain 7D12



• Molecule 2: Nanobody/VHH domain 7D12



• Molecule 2: Nanobody/VHH domain 7D12





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

Chain M: 75% 25%



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

Chain N: 75% 25%



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

Chain P: 75% 25%



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

Chain Q: 50% 50%



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

Chain R: 75% 25%



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

Chain S: 25% 75%



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

Chain O:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.70Å 147.25Å 254.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.51 – 2.65 49.51 – 2.65	Depositor EDS
% Data completeness (in resolution range)	96.1 (49.51-2.65) 96.1 (49.51-2.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.65Å)	Xtrriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.208 , 0.244 0.215 , 0.251	Depositor DCC
R_{free} test set	4233 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	47.6	Xtrriage
Anisotropy	0.267	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	28686	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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, BMA, MAN

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	0.36	0/1501	0.69	1/2040 (0.0%)
1	C	0.34	0/1508	0.73	2/2048 (0.1%)
1	E	0.36	0/1499	0.73	1/2037 (0.0%)
1	G	0.34	0/1514	0.71	0/2055
1	I	0.34	0/1479	0.69	0/2009
1	K	0.33	0/1480	0.70	2/2013 (0.1%)
2	B	0.33	0/938	0.60	0/1273
2	D	0.33	0/927	0.59	0/1261
2	F	0.34	0/904	0.60	0/1232
2	H	0.34	0/944	0.61	0/1280
2	J	0.34	0/946	0.62	0/1283
2	L	0.34	0/931	0.61	0/1265
All	All	0.34	0/14571	0.67	6/19796 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	350	VAL	CB-CA-C	-6.07	103.94	112.14
1	E	350	VAL	CB-CA-C	-5.63	103.83	112.05
1	C	493	GLY	CA-C-N	5.20	124.89	119.64
1	C	493	GLY	C-N-CA	5.20	124.89	119.64
1	K	493	GLY	CA-C-N	5.04	124.73	119.64

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	1473	1412	1408	7	0
1	C	1480	1426	1422	6	0
1	E	1471	1414	1410	8	0
1	G	1487	1425	1421	6	0
1	I	1452	1399	1397	8	0
1	K	1452	1395	1390	6	0
2	B	918	835	835	6	0
2	D	907	810	810	8	0
2	F	884	782	782	11	0
2	H	924	846	846	10	0
2	J	926	845	845	7	0
2	L	911	821	821	6	0
3	M	50	44	43	0	0
3	N	50	44	43	0	0
3	P	50	44	43	0	0
3	Q	50	44	43	0	0
3	R	50	44	43	0	0
3	S	50	44	43	0	0
4	O	28	0	25	1	0
5	A	28	28	26	2	0
5	C	14	13	13	0	0
5	E	28	28	26	0	0
5	G	28	28	26	0	0
5	I	28	28	26	0	0
5	K	28	28	26	0	0
6	A	9	0	0	0	0
6	B	8	0	0	0	0
6	C	12	0	0	1	0
6	D	3	0	0	0	0
6	E	14	0	0	0	0
6	F	3	0	0	0	0
6	G	10	0	0	2	0
6	H	5	0	0	0	0
6	I	7	0	0	2	0
6	J	10	0	0	0	0
6	K	5	0	0	0	0
6	L	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14859	13827	13813	76	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 76 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:384:GLN:NE2	6:I:705:HOH:O	2.14	0.80
1:E:328:ASN:OD1	1:E:331:ASN:ND2	2.19	0.76
1:A:336:LYS:HG2	5:A:605:NAG:O7	1.87	0.75
2:F:67:ARG:NH2	2:F:90:ASP:OD1	2.19	0.74
1:E:328:ASN:OD1	1:E:331:ASN:CG	2.32	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	195/214 (91%)	186 (95%)	9 (5%)	0	100	100
1	C	195/214 (91%)	190 (97%)	5 (3%)	0	100	100
1	E	195/214 (91%)	183 (94%)	12 (6%)	0	100	100
1	G	195/214 (91%)	187 (96%)	8 (4%)	0	100	100
1	I	193/214 (90%)	186 (96%)	7 (4%)	0	100	100
1	K	194/214 (91%)	183 (94%)	11 (6%)	0	100	100
2	B	122/133 (92%)	118 (97%)	4 (3%)	0	100	100
2	D	122/133 (92%)	119 (98%)	3 (2%)	0	100	100
2	F	120/133 (90%)	116 (97%)	2 (2%)	2 (2%)	7	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	122/133 (92%)	121 (99%)	1 (1%)	0	100	100
2	J	122/133 (92%)	119 (98%)	3 (2%)	0	100	100
2	L	122/133 (92%)	120 (98%)	1 (1%)	1 (1%)	16	27
All	All	1897/2082 (91%)	1828 (96%)	66 (4%)	3 (0%)	43	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	14	THR
2	F	27	ARG
2	L	27	ARG

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	161/188 (86%)	158 (98%)	3 (2%)	50	71
1	C	163/188 (87%)	163 (100%)	0	100	100
1	E	160/188 (85%)	156 (98%)	4 (2%)	42	64
1	G	163/188 (87%)	156 (96%)	7 (4%)	26	44
1	I	157/188 (84%)	155 (99%)	2 (1%)	61	77
1	K	157/188 (84%)	153 (98%)	4 (2%)	42	64
2	B	90/104 (86%)	87 (97%)	3 (3%)	33	55
2	D	87/104 (84%)	83 (95%)	4 (5%)	24	41
2	F	83/104 (80%)	80 (96%)	3 (4%)	31	51
2	H	91/104 (88%)	87 (96%)	4 (4%)	25	43
2	J	92/104 (88%)	88 (96%)	4 (4%)	26	44
2	L	88/104 (85%)	86 (98%)	2 (2%)	44	66
All	All	1492/1752 (85%)	1452 (97%)	40 (3%)	39	61

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	390	ARG
1	K	428	SER
1	I	478	THR
2	J	58	THR
1	K	464	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	384	GLN
1	K	442	ASN
1	K	483	HIS
1	C	480	GLN
1	C	359	HIS

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](#)

26 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	M	1	3,1	14,14,15	0.36	0	17,19,21	0.38	0
3	NAG	M	2	3	14,14,15	0.47	0	17,19,21	0.47	0
3	BMA	M	3	3	11,11,12	0.43	0	15,15,17	1.02	0
3	MAN	M	4	3	11,11,12	1.00	1 (9%)	15,15,17	1.83	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	N	1	3,1	14,14,15	0.27	0	17,19,21	0.41	0
3	NAG	N	2	3	14,14,15	0.52	0	17,19,21	0.39	0
3	BMA	N	3	3	11,11,12	0.32	0	15,15,17	0.92	0
3	MAN	N	4	3	11,11,12	1.04	1 (9%)	15,15,17	1.69	4 (26%)
4	NAG	O	1	4,1	14,14,15	0.33	0	17,19,21	0.42	0
4	NAG	O	2	4	14,14,15	0.27	0	17,19,21	0.49	0
3	NAG	P	1	3,1	14,14,15	0.28	0	17,19,21	0.46	0
3	NAG	P	2	3	14,14,15	0.47	0	17,19,21	0.43	0
3	BMA	P	3	3	11,11,12	0.46	0	15,15,17	0.91	0
3	MAN	P	4	3	11,11,12	1.00	1 (9%)	15,15,17	1.74	4 (26%)
3	NAG	Q	1	3,1	14,14,15	0.39	0	17,19,21	0.41	0
3	NAG	Q	2	3	14,14,15	0.44	0	17,19,21	0.44	0
3	BMA	Q	3	3	11,11,12	0.36	0	15,15,17	1.12	1 (6%)
3	MAN	Q	4	3	11,11,12	0.86	1 (9%)	15,15,17	1.54	4 (26%)
3	NAG	R	1	3,1	14,14,15	0.26	0	17,19,21	0.45	0
3	NAG	R	2	3	14,14,15	0.38	0	17,19,21	0.39	0
3	BMA	R	3	3	11,11,12	0.31	0	15,15,17	0.72	0
3	MAN	R	4	3	11,11,12	1.01	1 (9%)	15,15,17	1.62	5 (33%)
3	NAG	S	1	3,1	14,14,15	0.30	0	17,19,21	0.51	0
3	NAG	S	2	3	14,14,15	0.59	1 (7%)	17,19,21	0.38	0
3	BMA	S	3	3	11,11,12	0.42	0	15,15,17	0.99	1 (6%)
3	MAN	S	4	3	11,11,12	0.81	1 (9%)	15,15,17	1.57	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	M	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	BMA	M	3	3	-	0/2/19/22	0/1/1/1
3	MAN	M	4	3	-	2/2/19/22	0/1/1/1
3	NAG	N	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	1/6/23/26	0/1/1/1
3	BMA	N	3	3	-	0/2/19/22	0/1/1/1
3	MAN	N	4	3	-	2/2/19/22	0/1/1/1
4	NAG	O	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
3	NAG	P	1	3,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	BMA	P	3	3	-	0/2/19/22	0/1/1/1
3	MAN	P	4	3	-	2/2/19/22	0/1/1/1
3	NAG	Q	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	0/2/19/22	0/1/1/1
3	MAN	Q	4	3	-	2/2/19/22	0/1/1/1
3	NAG	R	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
3	BMA	R	3	3	-	0/2/19/22	0/1/1/1
3	MAN	R	4	3	-	2/2/19/22	0/1/1/1
3	NAG	S	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	BMA	S	3	3	-	0/2/19/22	0/1/1/1
3	MAN	S	4	3	-	0/2/19/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	4	MAN	C1-C2	2.74	1.58	1.52
3	N	4	MAN	C1-C2	2.70	1.58	1.52
3	R	4	MAN	C1-C2	2.31	1.57	1.52
3	M	4	MAN	C1-C2	2.26	1.57	1.52
3	Q	4	MAN	C1-C2	2.22	1.57	1.52

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	4	MAN	C1-O5-C5	5.20	119.15	112.19
3	P	4	MAN	C1-O5-C5	4.45	118.15	112.19
3	S	4	MAN	C1-O5-C5	4.11	117.69	112.19
3	N	4	MAN	C1-O5-C5	4.05	117.62	112.19
3	Q	4	MAN	C1-O5-C5	3.56	116.95	112.19

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	N	4	MAN	O5-C5-C6-O6
3	R	4	MAN	O5-C5-C6-O6

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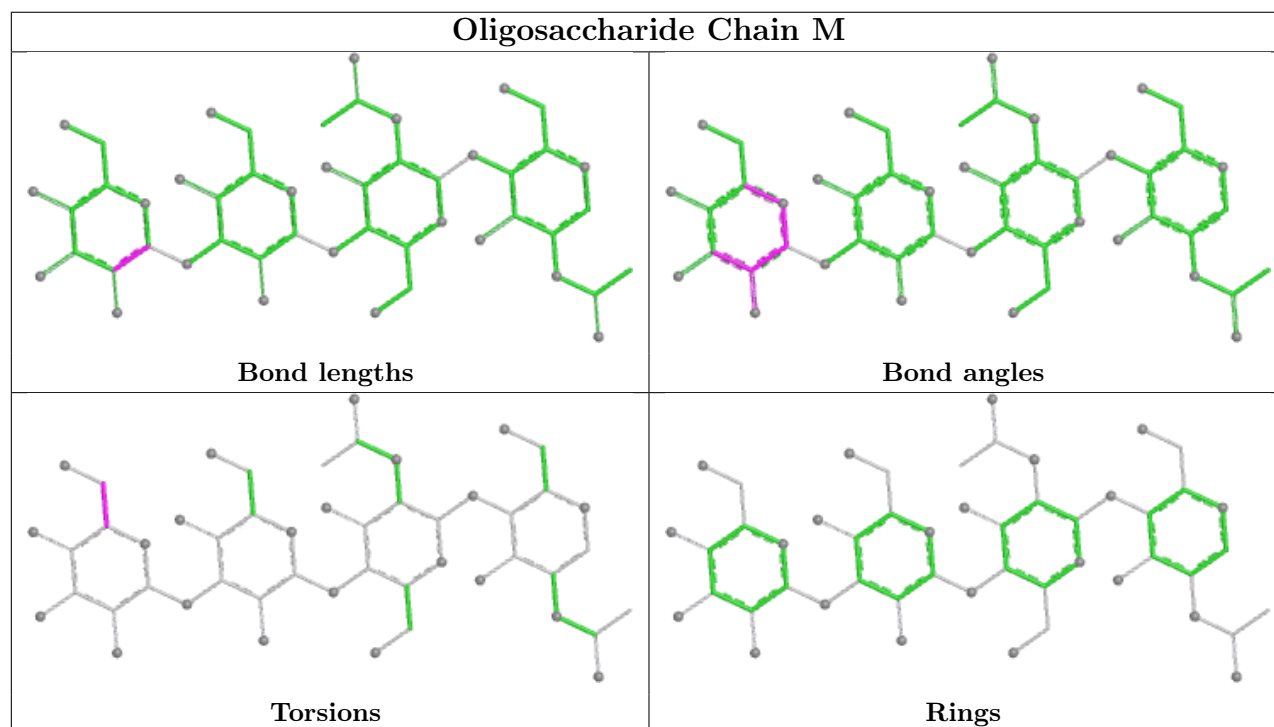
Mol	Chain	Res	Type	Atoms
3	N	4	MAN	C4-C5-C6-O6
4	O	2	NAG	C8-C7-N2-C2
4	O	2	NAG	O7-C7-N2-C2

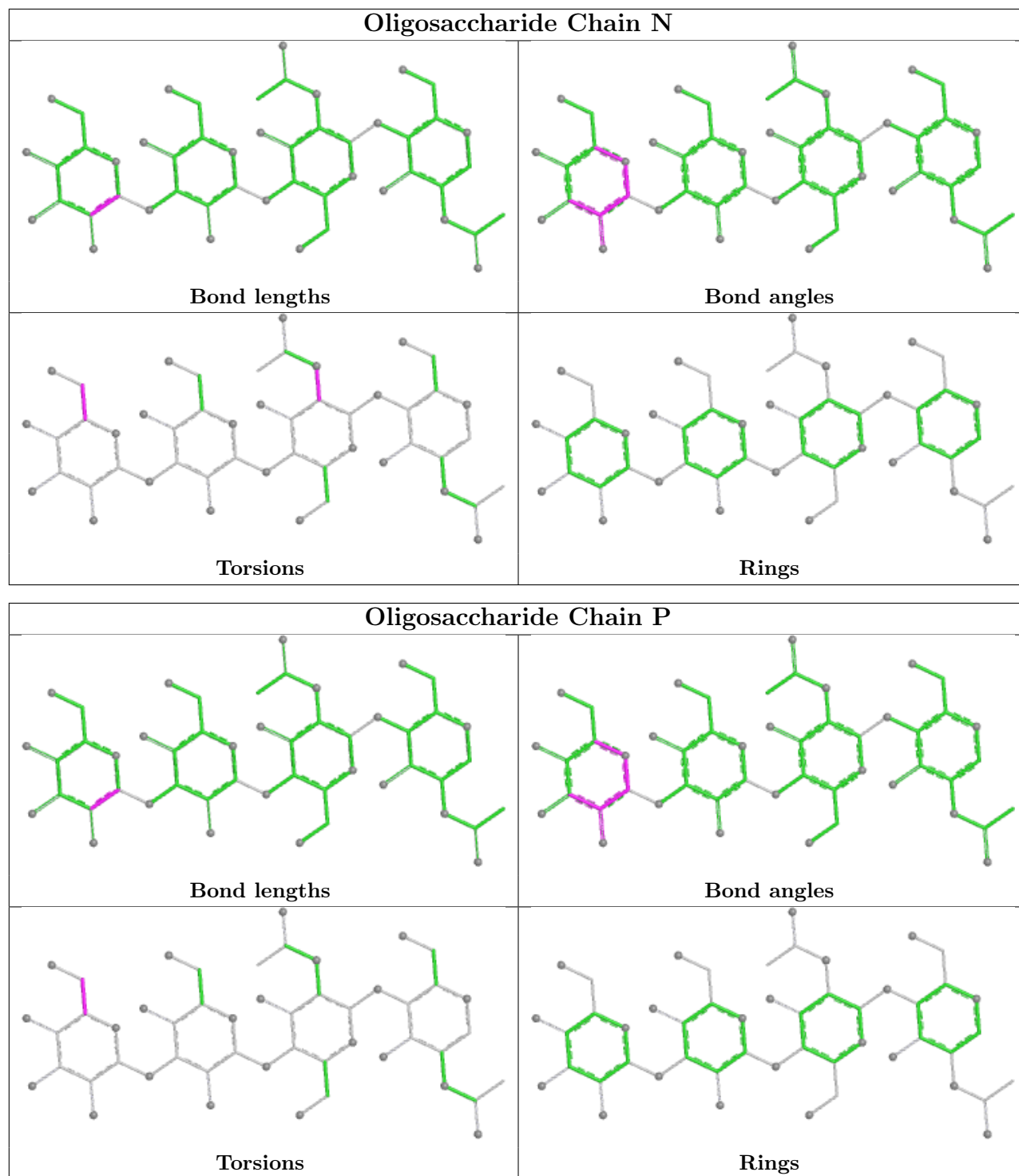
There are no ring outliers.

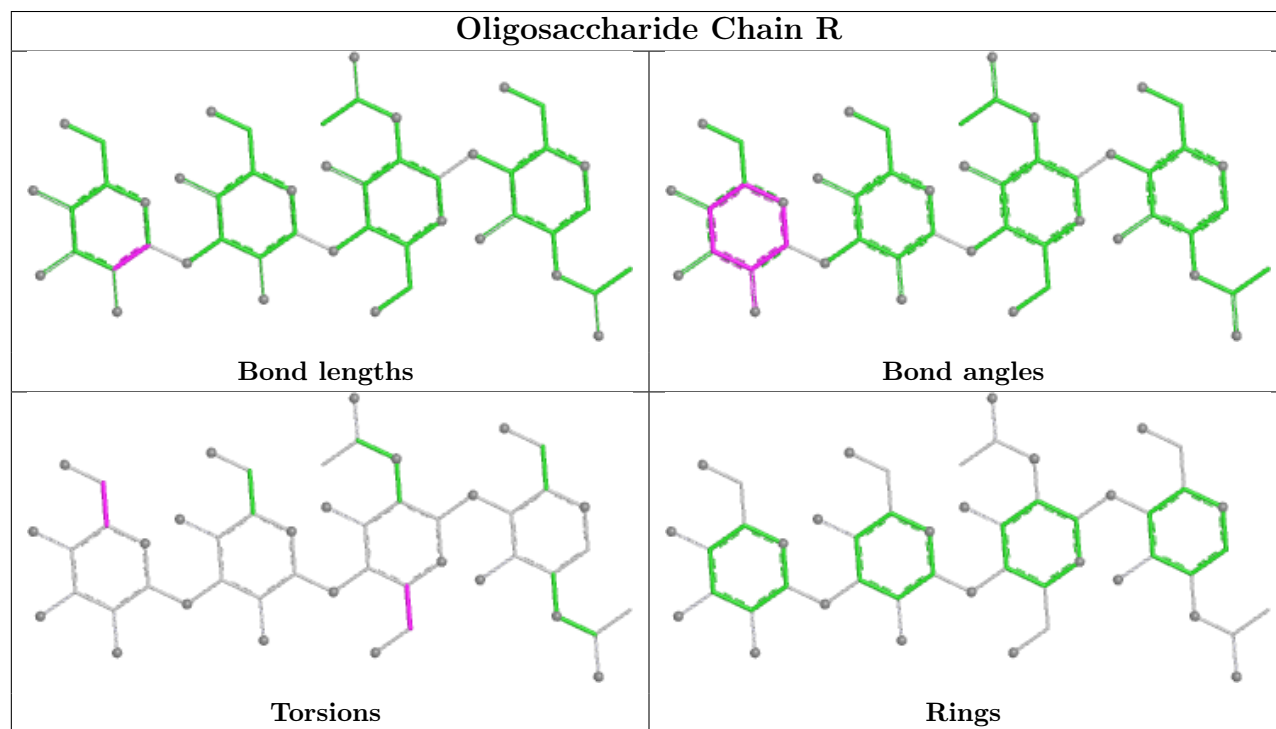
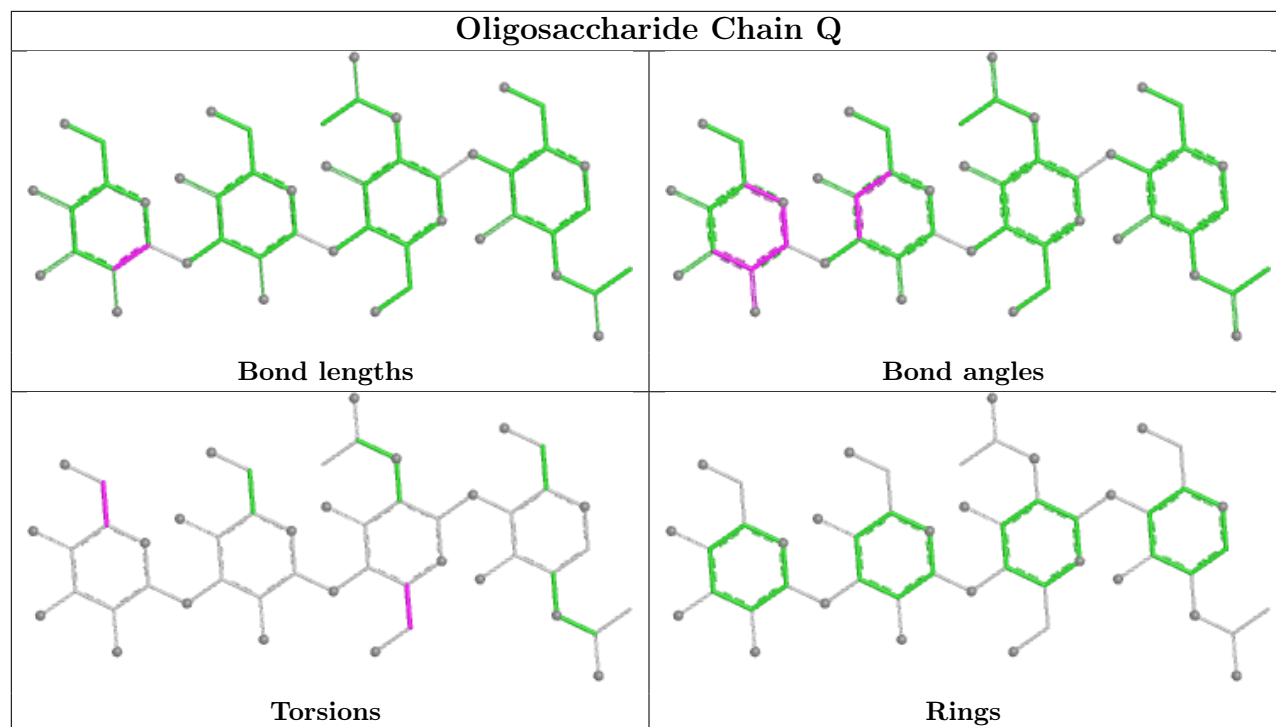
1 monomer is involved in 1 short contact:

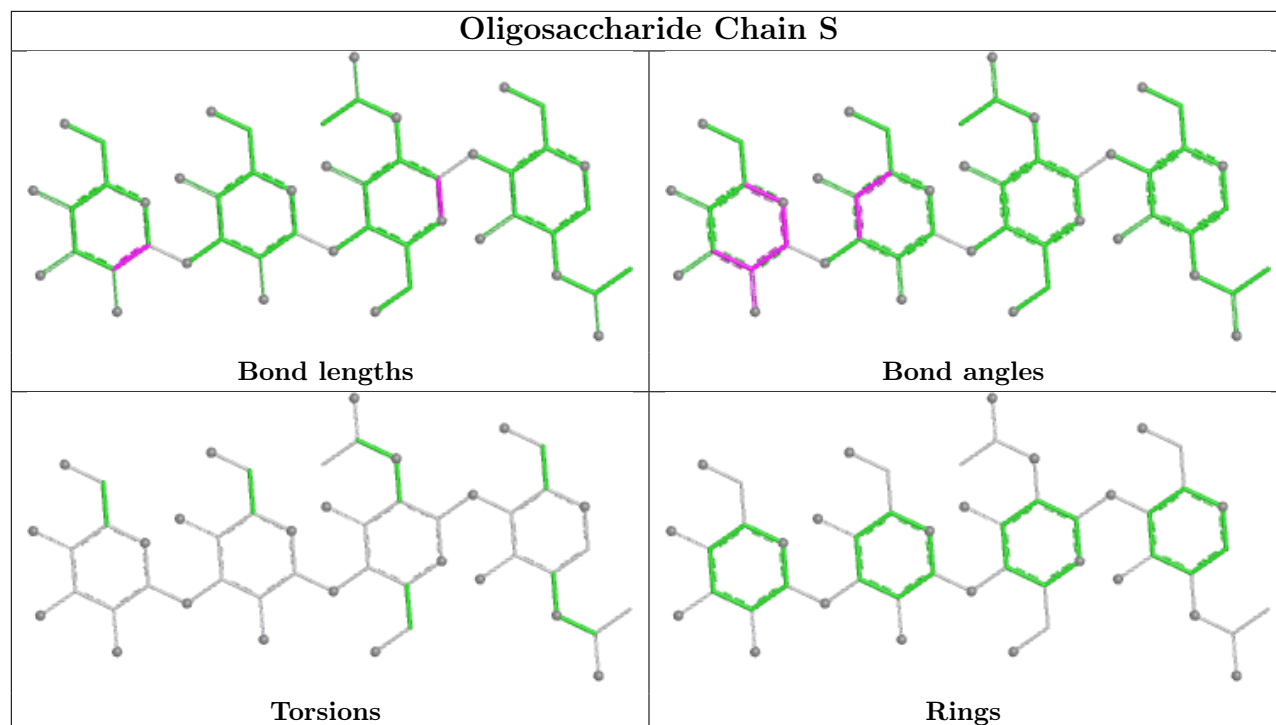
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	O	2	NAG	1	0

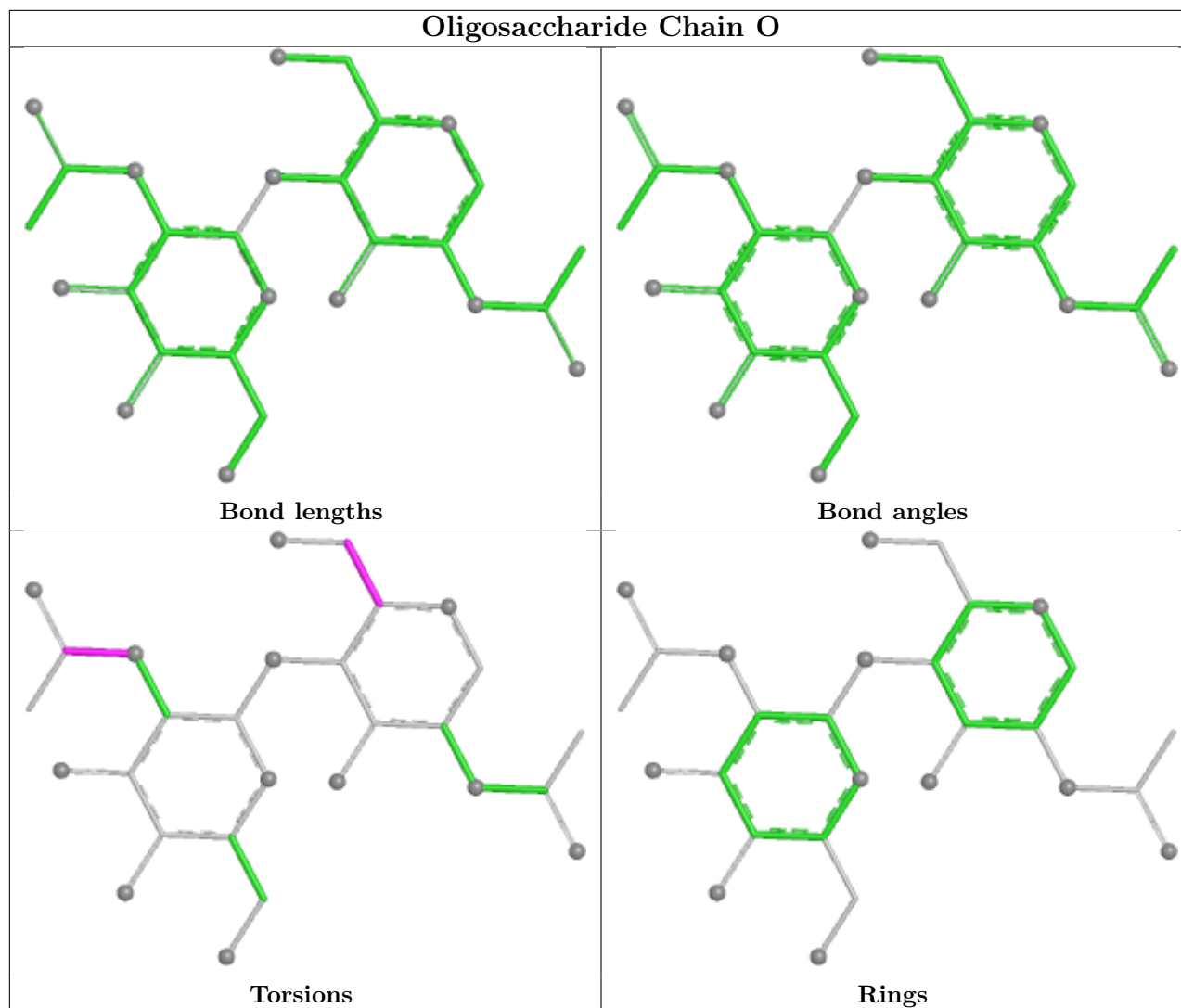
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

11 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	$\# Z > 2$
5	NAG	K	606	1	14,14,15	0.19	0	17,19,21	0.46	0
5	NAG	I	606	1	14,14,15	0.28	0	17,19,21	0.37	0
5	NAG	A	606	1	14,14,15	0.36	0	17,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	K	605	1	14,14,15	0.65	0	17,19,21	0.56	0
5	NAG	A	605	1	14,14,15	0.54	0	17,19,21	1.26	0
5	NAG	C	605	1	14,14,15	0.51	0	17,19,21	1.19	1 (5%)
5	NAG	E	606	1	14,14,15	0.58	1 (7%)	17,19,21	0.45	0
5	NAG	G	605	1	14,14,15	0.36	0	17,19,21	0.50	0
5	NAG	G	606	1	14,14,15	0.28	0	17,19,21	0.50	0
5	NAG	E	605	1	14,14,15	0.45	0	17,19,21	0.67	1 (5%)
5	NAG	I	605	1	14,14,15	0.25	0	17,19,21	0.53	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
5	NAG	K	606	1	-	0/6/23/26	0/1/1/1
5	NAG	I	606	1	-	0/6/23/26	0/1/1/1
5	NAG	A	606	1	-	3/6/23/26	0/1/1/1
5	NAG	K	605	1	-	2/6/23/26	0/1/1/1
5	NAG	A	605	1	-	2/6/23/26	0/1/1/1
5	NAG	C	605	1	-	3/6/23/26	0/1/1/1
5	NAG	E	606	1	-	0/6/23/26	0/1/1/1
5	NAG	G	605	1	-	0/6/23/26	0/1/1/1
5	NAG	G	606	1	-	2/6/23/26	0/1/1/1
5	NAG	E	605	1	-	2/6/23/26	0/1/1/1
5	NAG	I	605	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	606	NAG	C1-C2	2.00	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	605	NAG	C1-O5-C5	2.45	115.47	112.19
5	C	605	NAG	C4-C3-C2	-2.22	107.76	111.02

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	605	NAG	C1-C2-N2-C7
5	G	606	NAG	O5-C5-C6-O6
5	E	605	NAG	O5-C5-C6-O6
5	G	606	NAG	C4-C5-C6-O6
5	C	605	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	605	NAG	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	197/214 (92%)	0.11	6 (3%) 52 45	43, 56, 74, 82	0
1	C	197/214 (92%)	0.06	4 (2%) 65 59	42, 55, 73, 87	0
1	E	197/214 (92%)	0.11	3 (1%) 72 67	46, 57, 72, 82	0
1	G	198/214 (92%)	0.10	3 (1%) 72 67	47, 59, 78, 90	0
1	I	195/214 (91%)	0.47	10 (5%) 33 26	45, 64, 89, 101	0
1	K	196/214 (91%)	0.71	10 (5%) 33 26	54, 73, 93, 103	0
2	B	124/133 (93%)	0.00	5 (4%) 42 34	42, 56, 72, 83	0
2	D	124/133 (93%)	0.32	5 (4%) 42 34	45, 62, 78, 92	0
2	F	122/133 (91%)	0.62	11 (9%) 15 12	43, 70, 91, 96	0
2	H	124/133 (93%)	0.10	5 (4%) 42 34	46, 59, 75, 83	0
2	J	124/133 (93%)	0.09	2 (1%) 70 66	45, 56, 70, 88	0
2	L	124/133 (93%)	0.34	4 (3%) 50 42	49, 62, 75, 88	0
All	All	1922/2082 (92%)	0.25	68 (3%) 47 38	42, 60, 84, 103	0

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	124	SER	6.4
2	D	124	SER	4.8
1	I	460	SER	4.5
1	K	502	CYS	4.2
1	G	503	ARG	3.9

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](#)

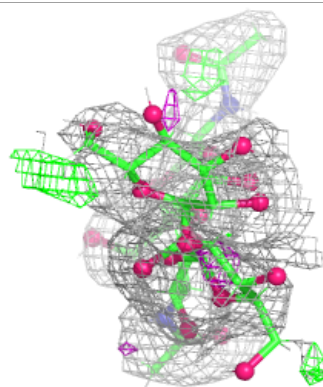
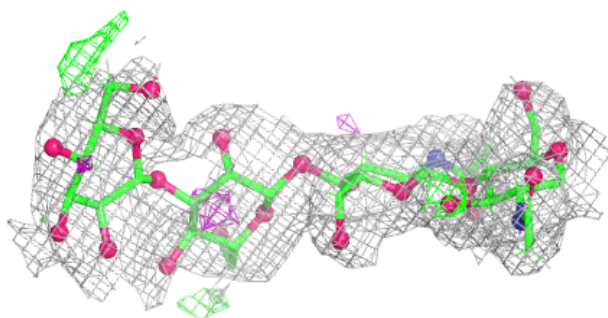
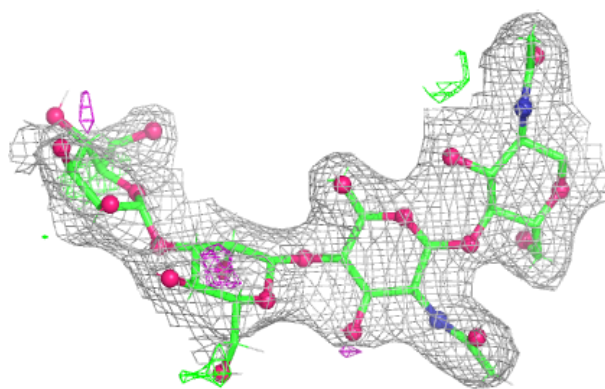
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MAN	S	4	11/12	0.32	0.22	102,113,135,136	0
3	MAN	P	4	11/12	0.38	0.20	94,111,130,133	0
3	MAN	N	4	11/12	0.43	0.19	96,105,127,128	0
3	BMA	P	3	11/12	0.49	0.18	89,107,128,131	0
3	MAN	R	4	11/12	0.52	0.20	90,109,128,132	0
3	MAN	M	4	11/12	0.52	0.19	86,103,118,124	0
3	MAN	Q	4	11/12	0.53	0.17	97,106,121,128	0
3	BMA	M	3	11/12	0.54	0.18	80,99,121,122	0
3	BMA	S	3	11/12	0.60	0.17	91,106,127,140	0
3	BMA	N	3	11/12	0.61	0.16	86,100,120,121	0
3	BMA	Q	3	11/12	0.62	0.18	88,100,120,125	0
4	NAG	O	2	14/15	0.65	0.23	68,85,93,97	0
3	BMA	R	3	11/12	0.72	0.16	76,95,118,121	0
4	NAG	O	1	14/15	0.86	0.14	64,77,78,82	0
3	NAG	P	2	14/15	0.88	0.12	62,77,90,98	0
3	NAG	M	2	14/15	0.90	0.10	55,67,84,90	0
3	NAG	N	2	14/15	0.91	0.11	49,68,81,89	0
3	NAG	S	2	14/15	0.91	0.12	63,77,91,92	0
3	NAG	P	1	14/15	0.91	0.12	50,61,73,81	0
3	NAG	R	2	14/15	0.92	0.10	56,67,80,81	0
3	NAG	Q	2	14/15	0.92	0.11	59,72,81,93	0
3	NAG	S	1	14/15	0.93	0.11	51,62,74,87	0
3	NAG	R	1	14/15	0.94	0.11	51,59,71,84	0
3	NAG	Q	1	14/15	0.94	0.09	48,58,69,76	0
3	NAG	M	1	14/15	0.95	0.09	41,53,67,77	0
3	NAG	N	1	14/15	0.96	0.08	46,55,65,76	0

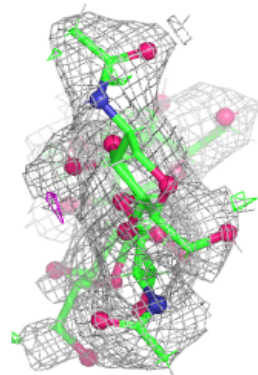
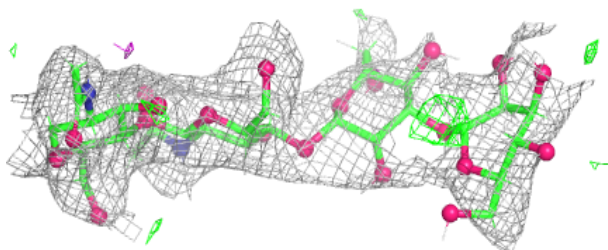
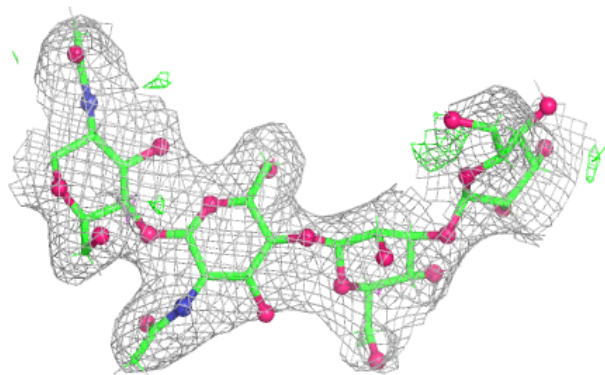
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain M:

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

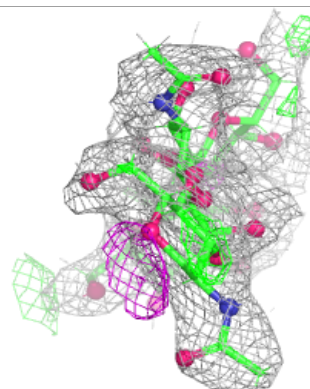
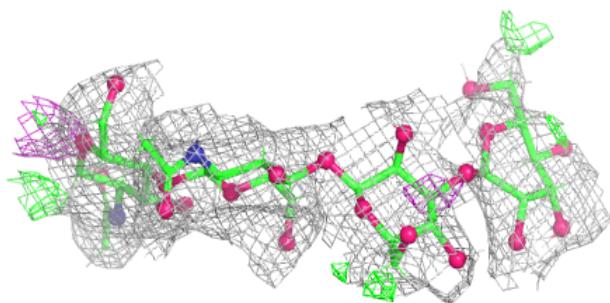
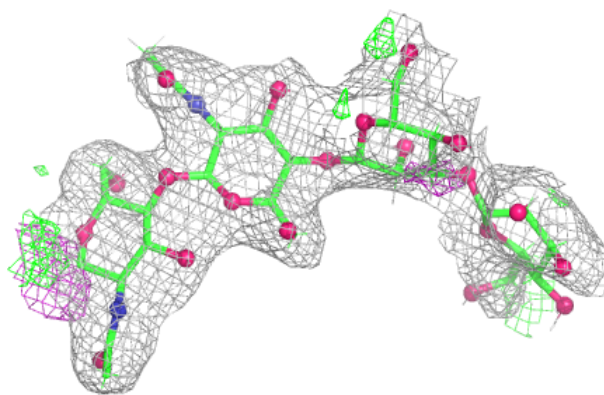
**Electron density around Chain N:**

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

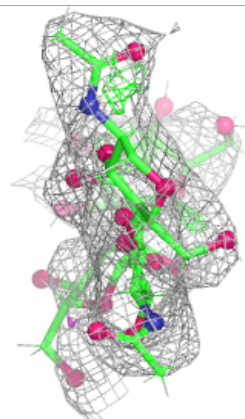
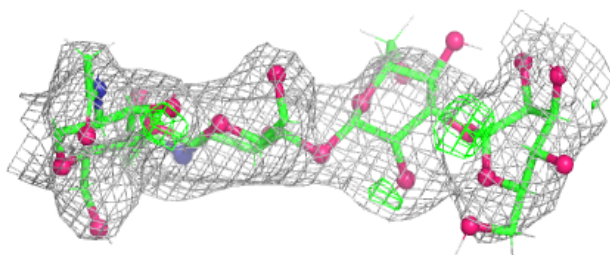
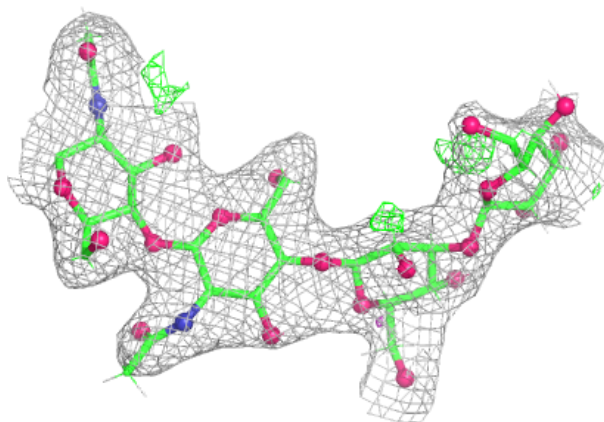


Electron density around Chain P:

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

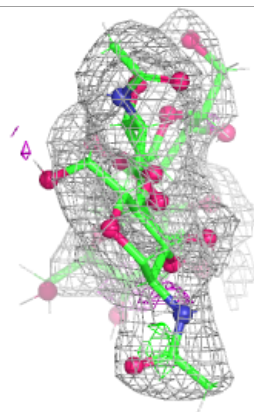
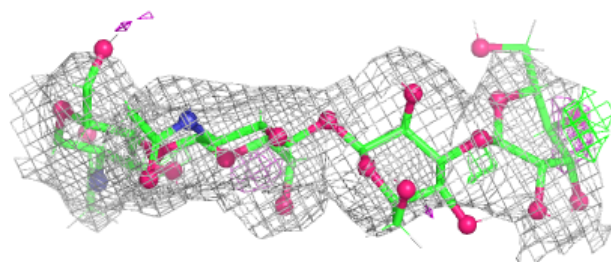
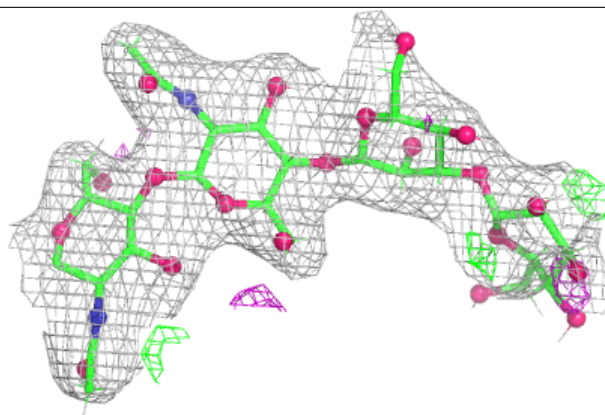
**Electron density around Chain Q:**

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

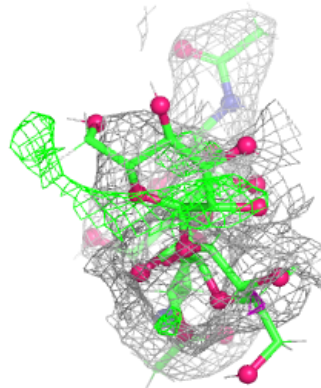
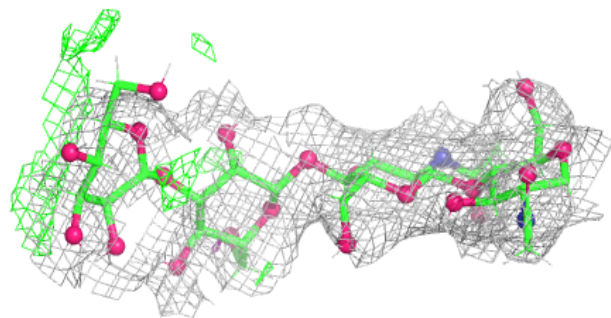
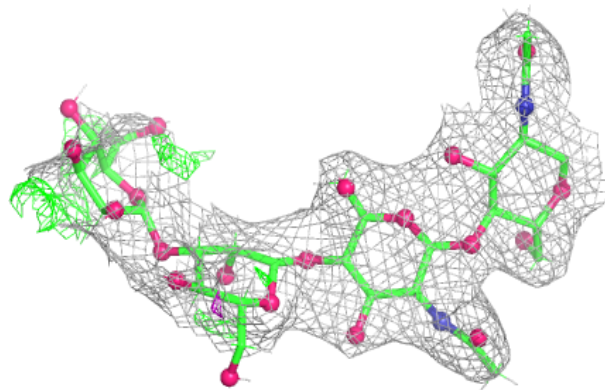


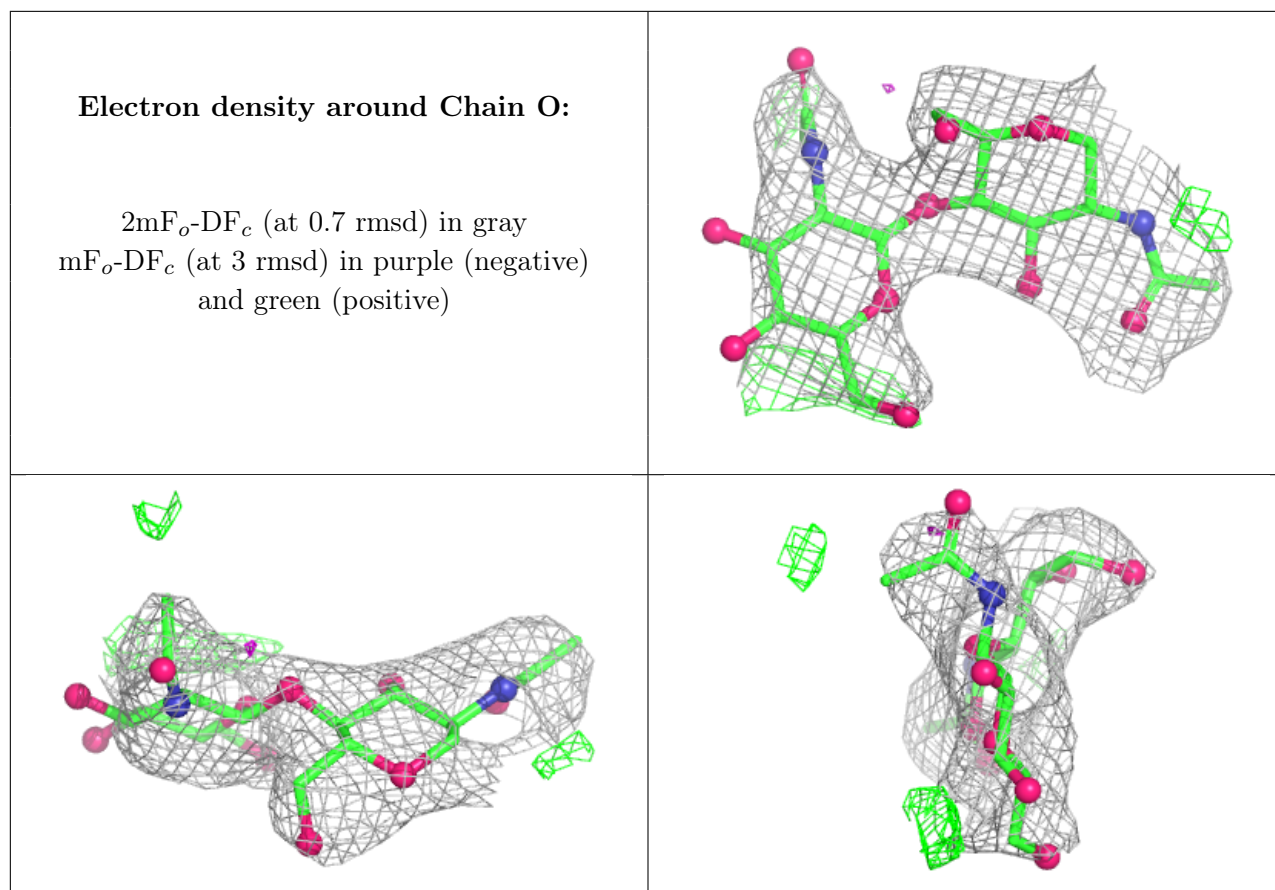
Electron density around Chain R:

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

**Electron density around Chain S:**

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	A	605	14/15	0.48	0.20	77,93,112,113	0
5	NAG	K	605	14/15	0.55	0.18	89,103,119,122	0
5	NAG	I	605	14/15	0.61	0.19	85,101,118,121	0
5	NAG	C	605	14/15	0.63	0.18	79,95,107,116	0
5	NAG	K	606	14/15	0.69	0.17	80,96,112,116	0
5	NAG	E	605	14/15	0.71	0.16	80,96,113,119	0
5	NAG	E	606	14/15	0.72	0.20	81,94,107,111	0
5	NAG	A	606	14/15	0.72	0.17	69,88,98,106	0
5	NAG	G	606	14/15	0.74	0.17	75,89,99,102	0
5	NAG	G	605	14/15	0.74	0.13	69,87,106,119	0
5	NAG	I	606	14/15	0.83	0.15	54,75,88,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.