



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 10:08 AM JST

PDB ID : 8K4Q
Title : Crystal structure of nanobody HuNb103 bound to human interleukin-4 receptor subunit alpha
Authors : Ding, Y.; Zhong, P.Y.
Deposited on : 2023-07-20
Resolution : 2.59 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 2.37.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

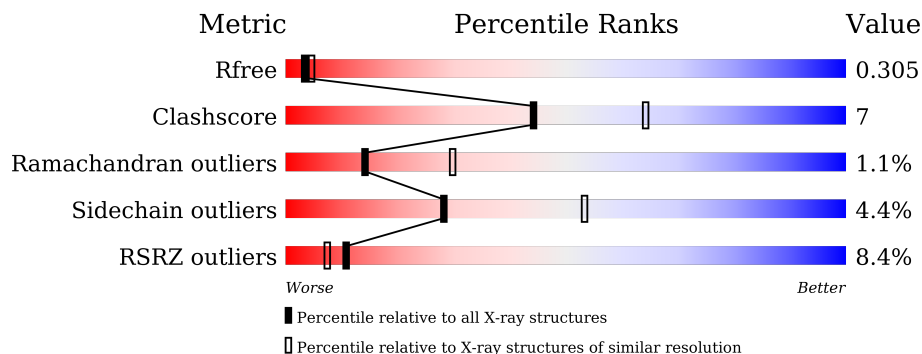
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	214	
1	C	214	
2	B	121	
2	D	121	
3	E	2	
3	G	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
4	F	3	 67%	 33%
4	H	3	 67%	 33%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5304 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 Interleukin-4 receptor subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	198	Total	C	N	O	S	0	0	0
			1588	1011	266	301	10			
1	C	199	Total	C	N	O	S	0	0	0
			1597	1017	268	302	10			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	208	GLU	-	expression tag	UNP Q53EP8
A	209	ASN	-	expression tag	UNP Q53EP8
A	210	LEU	-	expression tag	UNP Q53EP8
A	211	TYR	-	expression tag	UNP Q53EP8
A	212	PHE	-	expression tag	UNP Q53EP8
A	213	GLN	-	expression tag	UNP Q53EP8
A	214	GLY	-	expression tag	UNP Q53EP8
C	208	GLU	-	expression tag	UNP Q53EP8
C	209	ASN	-	expression tag	UNP Q53EP8
C	210	LEU	-	expression tag	UNP Q53EP8
C	211	TYR	-	expression tag	UNP Q53EP8
C	212	PHE	-	expression tag	UNP Q53EP8
C	213	GLN	-	expression tag	UNP Q53EP8
C	214	GLY	-	expression tag	UNP Q53EP8

- Molecule 2 is a protein called IL-4R nanobody HuNb103.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	118	Total	C	N	O	S	0	0	0
			896	550	162	177	7			
2	D	118	Total	C	N	O	S	0	0	0
			896	550	162	177	7			

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

cetamido-2-deoxy-beta-D-glucopyranose.



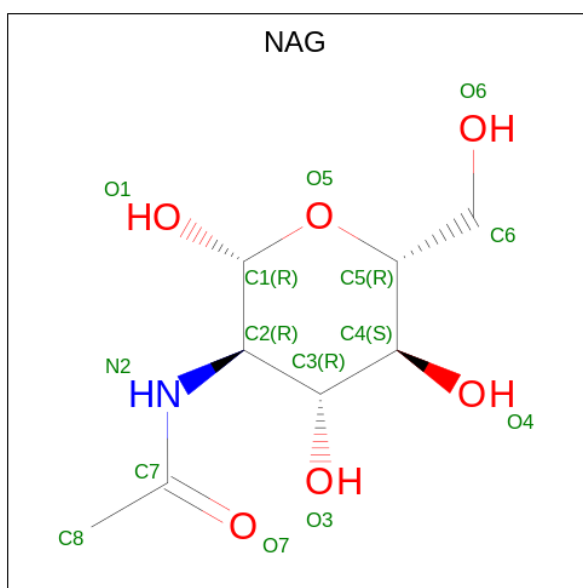
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	2	28	16	2	10	0	0	0
3	G	2	28	16	2	10	0	0	0

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



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

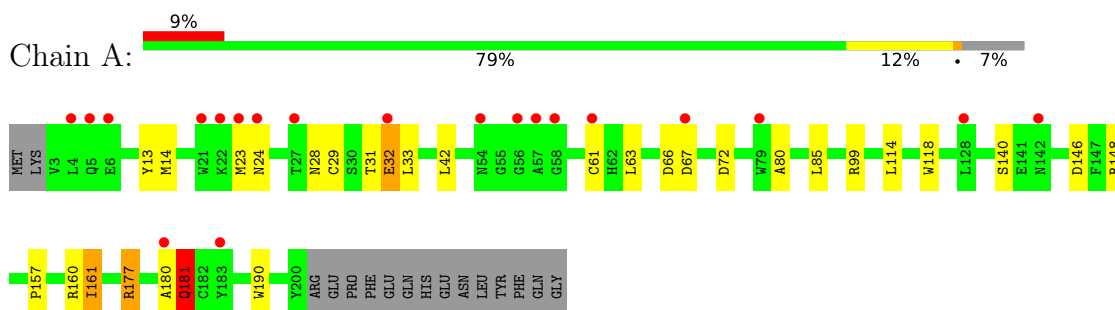
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	37	Total	O	0	0
			37	37		
6	B	30	Total	O	0	0
			30	30		
6	C	52	Total	O	0	0
			52	52		
6	D	18	Total	O	0	0
			18	18		

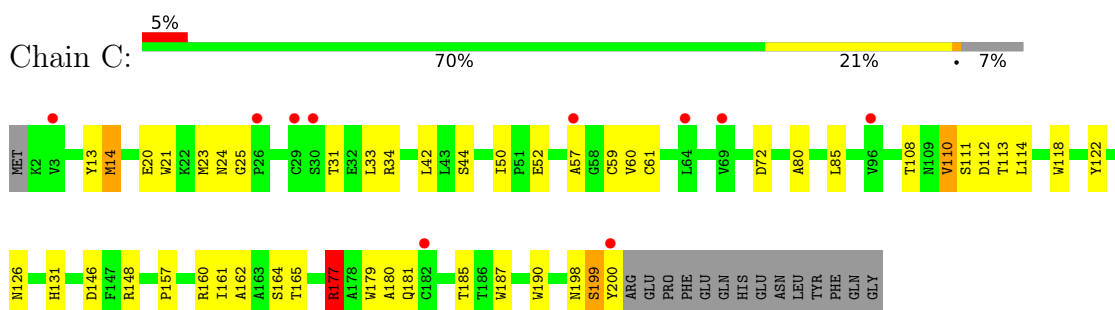
3 Residue-property plots [i](#)

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.

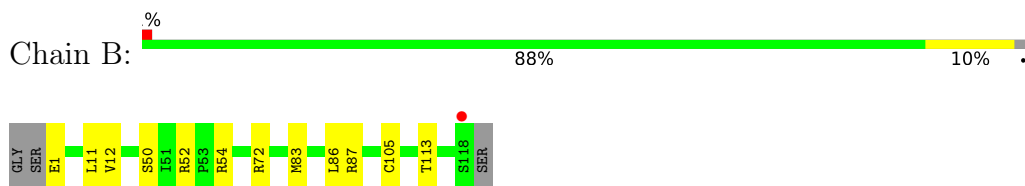
- Molecule 1: Interleukin-4 receptor subunit alpha



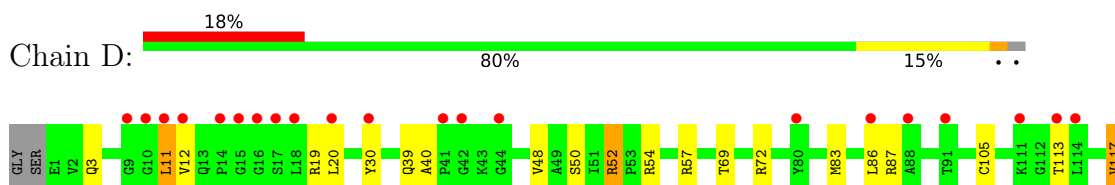
- Molecule 1: Interleukin-4 receptor subunit alpha



- Molecule 2: IL-4R nanobody HuNb103



- Molecule 2: IL-4R nanobody HuNb103





SER
SER


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

Chain E:  100%



MAG1
MAG2

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

Chain G:  50% 50%



MAG1
MAG2

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

Chain F:  67% 33%



MAG1
MAG2
BMA3

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

Chain H:  67% 33%



MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.87Å 109.60Å 64.17Å 90.00° 98.48° 90.00°	Depositor
Resolution (Å)	57.30 – 2.59 57.24 – 2.59	Depositor EDS
% Data completeness (in resolution range)	100.0 (57.30-2.59) 100.0 (57.24-2.59)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.58Å)	Xtrriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.222 , 0.280 0.260 , 0.305	Depositor DCC
R_{free} test set	1186 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtrriage
Anisotropy	0.567	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.1	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	0.90	EDS
Total number of atoms	5304	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.33	0/1638	0.60	0/2248
1	C	0.34	0/1647	0.58	0/2259
2	B	0.34	0/912	0.62	0/1230
2	D	0.33	0/912	0.61	0/1230
All	All	0.34	0/5109	0.60	0/6967

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	2
1	C	0	1
2	B	0	1
2	D	0	3
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	ARG	Sidechain
1	A	181	GLN	Peptide
2	B	54	ARG	Sidechain
1	C	177	ARG	Sidechain
2	D	52	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	D	54	ARG	Sidechain
2	D	57	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	A	1588	0	1498	14	0
1	C	1597	0	1511	29	0
2	B	896	0	857	11	0
2	D	896	0	857	11	0
3	E	28	0	25	0	0
3	G	28	0	25	1	0
4	F	39	0	34	2	0
4	H	39	0	34	1	0
5	A	14	0	13	0	0
5	C	42	0	39	1	0
6	A	37	0	0	0	0
6	B	30	0	0	1	0
6	C	52	0	0	2	0
6	D	18	0	0	2	0
All	All	5304	0	4893	66	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 7.

All (66) 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:C:162:ALA:O	1:C:165:THR:HG22	1.78	0.83
1:C:180:ALA:O	1:C:185:THR:HG21	1.84	0.78
1:C:177:ARG:HD3	1:C:187:TRP:CE3	2.19	0.77
2:B:87:ARG:HH11	2:B:87:ARG:HG2	1.50	0.75
1:C:164:SER:HA	1:C:200:TYR:OH	1.87	0.74
1:A:28:ASN:O	1:A:31:THR:O	2.07	0.72
1:C:177:ARG:HG2	1:C:190:TRP:CZ3	2.27	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ARG:HG2	1:A:190:TRP:CZ3	2.32	0.64
1:A:14:MET:SD	1:A:99:ARG:NH1	2.73	0.62
1:C:20:GLU:HG2	1:C:60:VAL:HG12	1.81	0.61
2:D:12:VAL:HG11	2:D:86:LEU:HD13	1.83	0.60
1:C:110:VAL:HG13	1:C:113:THR:O	2.01	0.60
1:C:161:ILE:HD11	1:C:165:THR:HG21	1.84	0.59
1:C:161:ILE:HD12	6:C:438:HOH:O	2.04	0.58
1:A:180:ALA:O	1:A:181:GLN:HB2	2.05	0.56
4:F:1:NAG:H5	4:F:2:NAG:H82	1.87	0.56
2:D:19:ARG:HH11	2:D:19:ARG:HG3	1.72	0.55
1:C:114:LEU:HB2	1:C:161:ILE:HG23	1.87	0.55
1:A:29:CYS:SG	1:A:33:LEU:HD12	2.47	0.55
2:D:83:MET:HB3	2:D:86:LEU:HD21	1.88	0.55
2:B:83:MET:HB3	2:B:86:LEU:HD21	1.90	0.54
1:C:34:ARG:NH1	1:C:50:ILE:HG23	2.22	0.54
1:C:14:MET:HG2	1:C:126:ASN:ND2	2.25	0.52
2:B:12:VAL:HG11	2:B:86:LEU:HD12	1.92	0.51
1:C:21:TRP:CE2	1:C:59:CYS:HB2	2.45	0.51
2:B:11:LEU:HD12	2:B:12:VAL:H	1.76	0.50
1:A:118:TRP:O	1:A:157:PRO:HB2	2.13	0.48
2:B:11:LEU:HD12	2:B:12:VAL:N	2.29	0.48
3:G:1:NAG:H62	3:G:2:NAG:H82	1.96	0.48
2:D:30:TYR:O	2:D:30:TYR:CG	2.66	0.48
1:C:52:GLU:HG2	1:C:60:VAL:HG23	1.96	0.48
1:C:131:HIS:O	1:C:181:GLN:HG2	2.14	0.47
1:C:118:TRP:O	1:C:157:PRO:HB2	2.15	0.47
4:F:1:NAG:N2	4:F:1:NAG:O4	2.48	0.47
1:C:198:ASN:O	1:C:199:SER:HB2	2.16	0.46
1:A:80:ALA:HB2	1:A:85:LEU:HD11	1.96	0.46
2:D:39:GLN:HG2	6:D:216:HOH:O	2.13	0.46
1:C:25:GLY:O	1:C:57:ALA:HB2	2.16	0.46
1:C:42:LEU:HD23	2:D:50:SER:HB3	1.97	0.46
5:C:303:NAG:H4	6:C:410:HOH:O	2.15	0.46
2:D:11:LEU:HD13	2:D:12:VAL:N	2.31	0.46
1:C:108:THR:HG22	1:C:108:THR:O	2.16	0.46
1:C:111:SER:O	1:C:112:ASP:HB2	2.15	0.46
2:B:87:ARG:HH11	2:B:87:ARG:CG	2.22	0.45
1:C:80:ALA:HB2	1:C:85:LEU:HD11	1.99	0.45
1:A:114:LEU:HB2	1:A:161:ILE:HG12	1.99	0.45
1:A:72:ASP:OD1	2:B:52:ARG:NH1	2.48	0.44
1:C:23:MET:CE	1:C:33:LEU:HD11	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:LEU:O	1:C:160:ARG:HA	2.17	0.44
2:D:87:ARG:O	2:D:117:VAL:HG11	2.17	0.43
1:A:31:THR:O	1:A:32:GLU:HB2	2.19	0.43
1:C:72:ASP:OD1	2:D:52:ARG:NH2	2.51	0.43
1:C:146:ASP:OD1	1:C:148:ARG:NH1	2.51	0.43
1:A:114:LEU:O	1:A:160:ARG:HA	2.19	0.43
2:B:87:ARG:CG	2:B:87:ARG:NH1	2.82	0.43
2:D:20:LEU:HD12	2:D:20:LEU:N	2.34	0.43
1:A:146:ASP:OD1	1:A:148:ARG:NH1	2.52	0.42
4:H:1:NAG:H83	4:H:1:NAG:H3	2.01	0.42
2:D:3:GLN:HB3	6:D:212:HOH:O	2.19	0.42
1:C:160:ARG:HG2	1:C:160:ARG:HH11	1.85	0.41
1:C:14:MET:HG3	1:C:122:TYR:CE1	2.55	0.41
1:C:179:TRP:HB2	1:C:187:TRP:CZ3	2.56	0.41
2:B:1:GLU:HG3	2:B:1:GLU:O	2.20	0.41
1:A:42:LEU:HD23	2:B:50:SER:HB3	2.03	0.41
2:B:1:GLU:HB3	6:B:225:HOH:O	2.20	0.41
1:A:63:LEU:HD12	1:A:63:LEU:N	2.36	0.40

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	196/214 (92%)	178 (91%)	13 (7%)	5 (3%)	5 9
1	C	197/214 (92%)	181 (92%)	15 (8%)	1 (0%)	29 52
2	B	116/121 (96%)	116 (100%)	0	0	100 100
2	D	116/121 (96%)	113 (97%)	2 (2%)	1 (1%)	17 35
All	All	625/670 (93%)	588 (94%)	30 (5%)	7 (1%)	14 30

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	ASP
1	A	67	ASP
1	A	32	GLU
1	A	181	GLN
1	C	199	SER
1	A	23	MET
2	D	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	178/193 (92%)	172 (97%)	6 (3%)	37	63
1	C	179/193 (93%)	171 (96%)	8 (4%)	27	52
2	B	93/95 (98%)	90 (97%)	3 (3%)	39	65
2	D	93/95 (98%)	86 (92%)	7 (8%)	13	27
All	All	543/576 (94%)	519 (96%)	24 (4%)	28	53

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	TYR
1	A	24	ASN
1	A	61	CYS
1	A	140	SER
1	A	161	ILE
1	A	181	GLN
2	B	72	ARG
2	B	105	CYS
2	B	113	THR
1	C	13	TYR
1	C	14	MET
1	C	24	ASN
1	C	31	THR
1	C	44	SER
1	C	61	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	110	VAL
1	C	177	ARG
2	D	11	LEU
2	D	48	VAL
2	D	69	THR
2	D	72	ARG
2	D	105	CYS
2	D	113	THR
2	D	117	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	GLN
2	B	77	ASN
2	D	77	ASN
2	D	101	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](#)

10 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	E	1	1,3	14,14,15	0.36	0	17,19,21	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	2	3	14,14,15	0.32	0	17,19,21	0.63	0
4	NAG	F	1	1,4	14,14,15	0.28	0	17,19,21	0.84	0
4	NAG	F	2	4	14,14,15	0.32	0	17,19,21	1.16	1 (5%)
4	BMA	F	3	4	11,11,12	0.58	0	15,15,17	0.89	1 (6%)
3	NAG	G	1	1,3	14,14,15	0.30	0	17,19,21	0.85	1 (5%)
3	NAG	G	2	3	14,14,15	0.28	0	17,19,21	0.52	0
4	NAG	H	1	1,4	14,14,15	0.34	0	17,19,21	1.76	2 (11%)
4	NAG	H	2	4	14,14,15	0.33	0	17,19,21	0.65	0
4	BMA	H	3	4	11,11,12	0.39	0	15,15,17	0.55	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
3	NAG	E	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	F	2	4	-	4/6/23/26	0/1/1/1
4	BMA	F	3	4	-	1/2/19/22	1/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	5/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	BMA	H	3	4	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	NAG	C2-N2-C7	4.99	130.01	122.90
4	H	1	NAG	C1-C2-N2	3.85	117.07	110.49
4	F	2	NAG	C1-C2-N2	2.71	115.11	110.49
4	F	3	BMA	C1-O5-C5	2.56	115.66	112.19
3	G	1	NAG	C1-C2-N2	2.08	114.03	110.49

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
4	H	2	NAG	O5-C5-C6-O6
4	F	2	NAG	C8-C7-N2-C2
3	G	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
3	E	2	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O7-C7-N2-C2
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
3	E	2	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
4	F	3	BMA	O5-C5-C6-O6
4	H	1	NAG	C3-C2-N2-C7
3	E	1	NAG	O7-C7-N2-C2
4	F	1	NAG	C8-C7-N2-C2
4	H	3	BMA	O5-C5-C6-O6
4	F	1	NAG	O7-C7-N2-C2
4	H	1	NAG	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	F	1	NAG	C1-C2-N2-C7
4	H	1	NAG	O5-C5-C6-O6

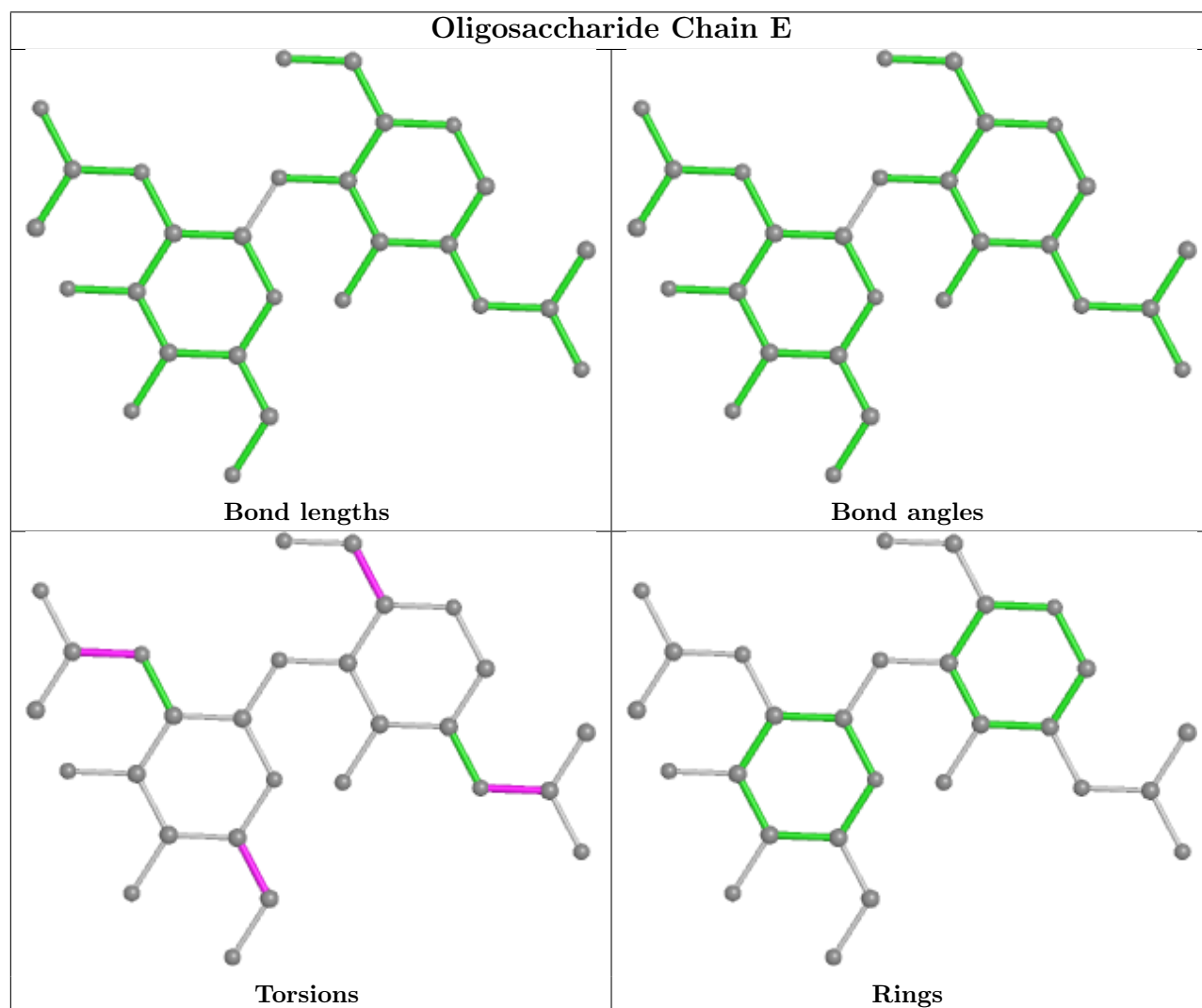
All (1) ring outliers are listed below:

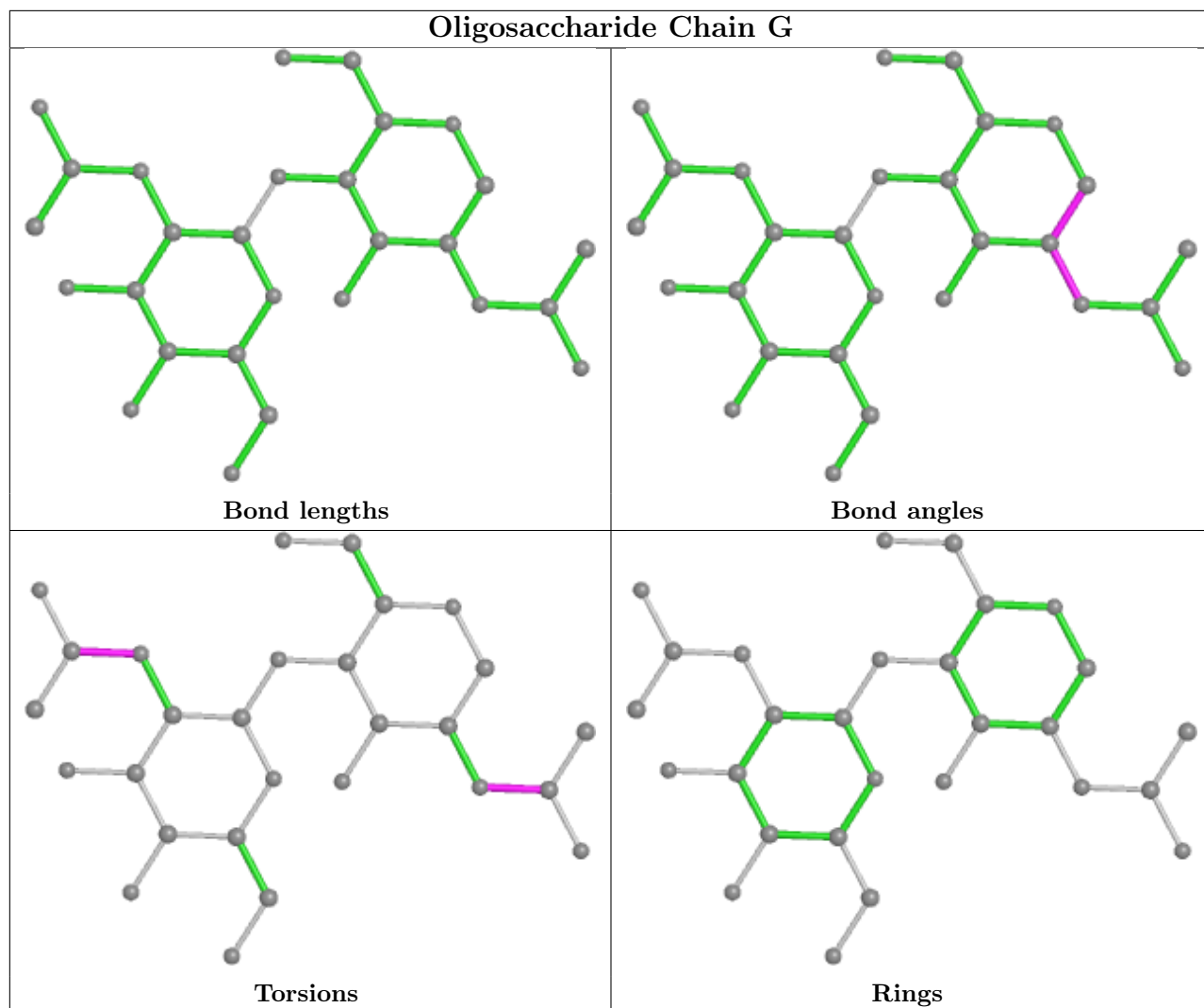
Mol	Chain	Res	Type	Atoms
4	F	3	BMA	C1-C2-C3-C4-C5-O5

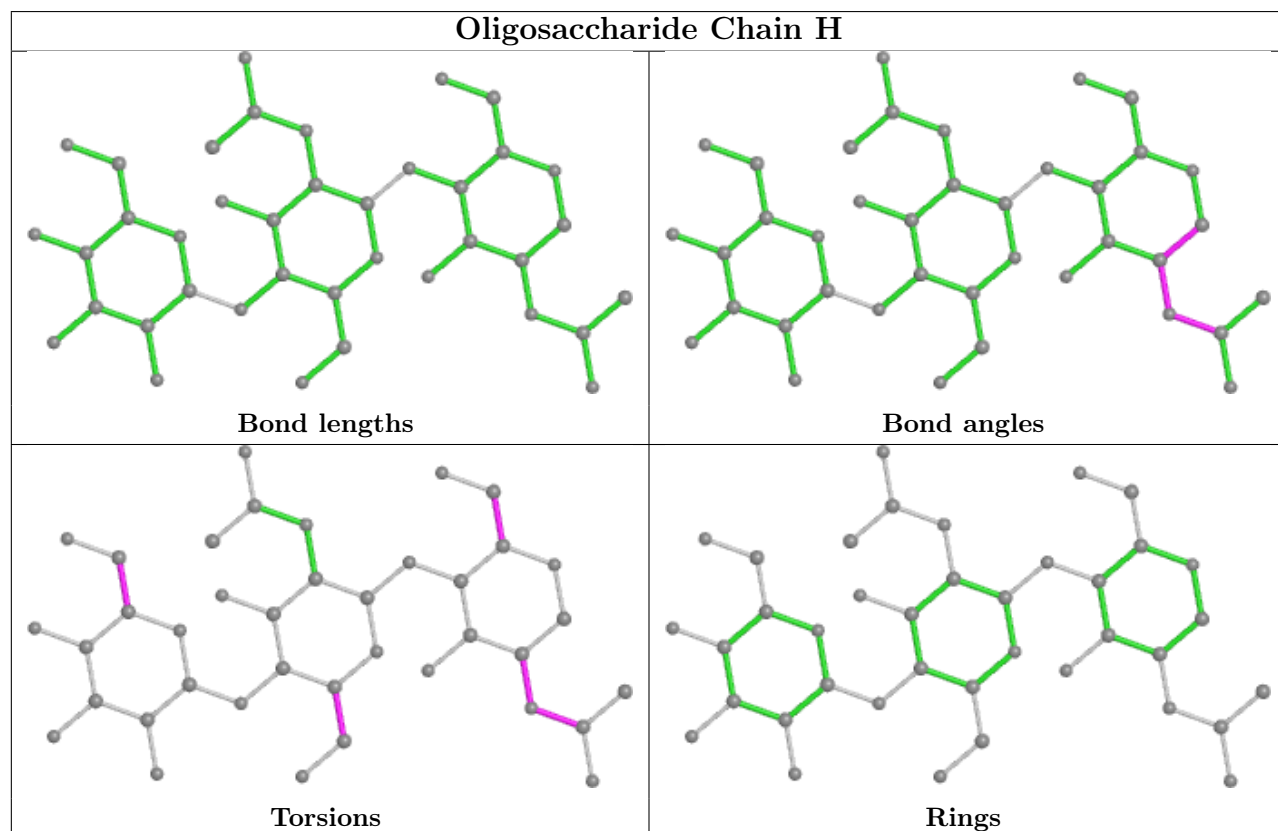
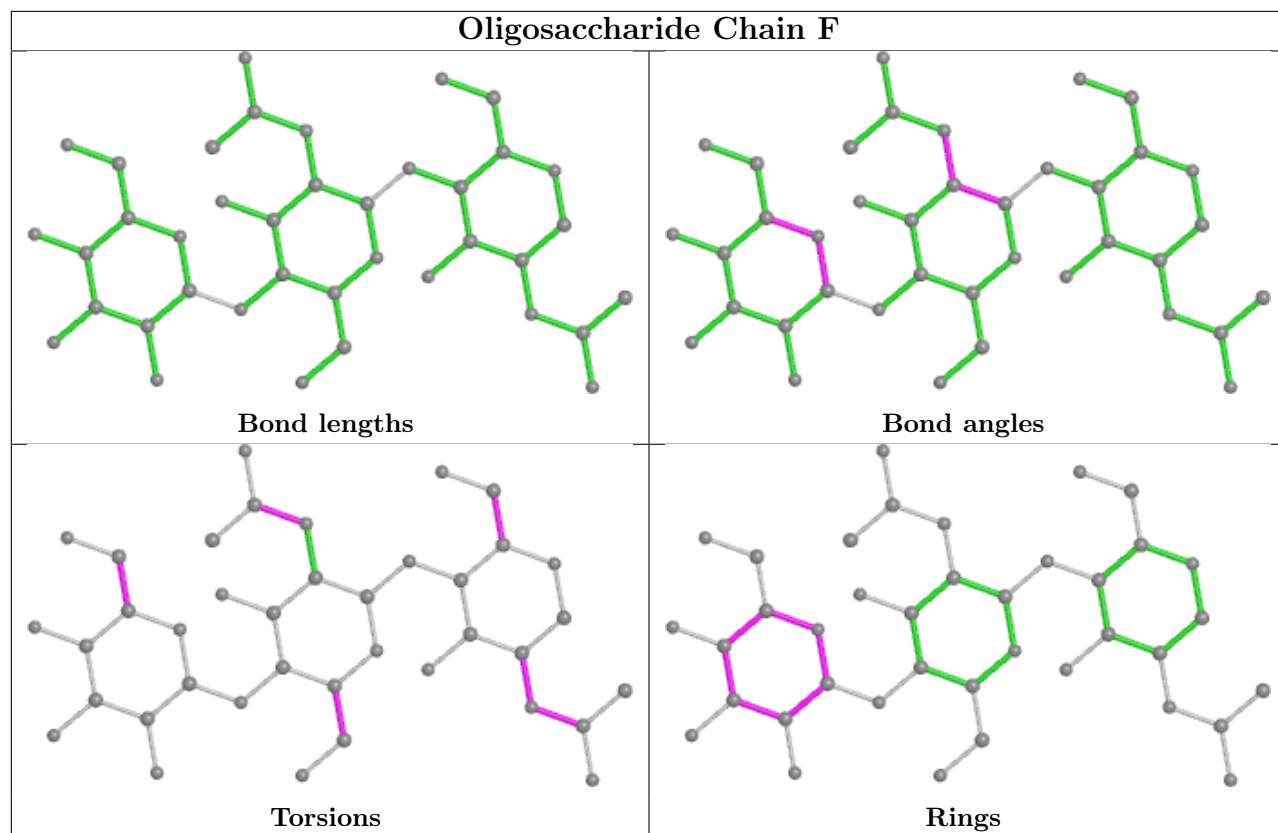
5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2	NAG	1	0
3	G	2	NAG	1	0
4	H	1	NAG	1	0
4	F	1	NAG	2	0
3	G	1	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

4 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	A	301	1	14,14,15	0.34	0	17,19,21	0.71	1 (5%)
5	NAG	C	302	1	14,14,15	0.36	0	17,19,21	1.27	1 (5%)
5	NAG	C	301	1	14,14,15	0.33	0	17,19,21	0.65	0
5	NAG	C	303	1	14,14,15	0.36	0	17,19,21	1.10	3 (17%)

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	A	301	1	-	2/6/23/26	0/1/1/1
5	NAG	C	302	1	-	4/6/23/26	0/1/1/1
5	NAG	C	301	1	-	4/6/23/26	0/1/1/1
5	NAG	C	303	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	302	NAG	C1-C2-N2	4.66	118.45	110.49
5	C	303	NAG	C4-C3-C2	2.71	114.99	111.02
5	C	303	NAG	C2-N2-C7	2.30	126.18	122.90
5	A	301	NAG	C4-C3-C2	2.11	114.11	111.02
5	C	303	NAG	O5-C5-C4	-2.08	105.77	110.83

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	302	NAG	C8-C7-N2-C2
5	C	302	NAG	O7-C7-N2-C2
5	C	301	NAG	O5-C5-C6-O6
5	C	302	NAG	O5-C5-C6-O6
5	C	302	NAG	C4-C5-C6-O6
5	C	301	NAG	C4-C5-C6-O6
5	C	303	NAG	O5-C5-C6-O6
5	C	303	NAG	C4-C5-C6-O6
5	C	301	NAG	C1-C2-N2-C7
5	A	301	NAG	C8-C7-N2-C2
5	A	301	NAG	O7-C7-N2-C2
5	C	301	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	303	NAG	1	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	198/214 (92%)	0.77	20 (10%) 7 4	10, 30, 62, 89	0
1	C	199/214 (92%)	0.73	10 (5%) 28 23	12, 32, 49, 69	0
2	B	118/121 (97%)	0.52	1 (0%) 86 84	20, 27, 39, 52	0
2	D	118/121 (97%)	1.10	22 (18%) 1 0	20, 30, 41, 49	0
All	All	633/670 (94%)	0.77	53 (8%) 11 7	10, 30, 54, 89	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	TYR	5.3
1	A	5	GLN	5.0
1	A	32	GLU	4.7
2	D	30	TYR	4.7
1	C	57	ALA	4.7
2	D	18	LEU	4.5
1	A	22	LYS	4.1
1	A	23	MET	4.1
1	C	200	TYR	4.1
2	D	9	GLY	3.7
2	B	118	SER	3.6
2	D	17	SER	3.6
1	A	27	THR	3.5
2	D	88	ALA	3.5
2	D	91	THR	3.5
1	A	79	TRP	3.5
1	A	4	LEU	3.4
2	D	42	GLY	3.3
1	A	61	CYS	3.3
1	A	128	LEU	3.1
2	D	15	GLY	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	64	LEU	3.0
1	A	6	GLU	3.0
1	A	56	GLY	3.0
2	D	44	GLY	2.9
2	D	86	LEU	2.9
1	A	67	ASP	2.8
1	A	57	ALA	2.8
2	D	41	PRO	2.7
2	D	10	GLY	2.7
2	D	111	LYS	2.6
2	D	11	LEU	2.6
2	D	114	LEU	2.6
1	C	3	VAL	2.5
1	A	54	ASN	2.5
1	A	142	ASN	2.5
2	D	16	GLY	2.5
1	C	26	PRO	2.4
2	D	80	TYR	2.4
2	D	113	THR	2.4
2	D	118	SER	2.4
1	A	21	TRP	2.4
1	C	96	VAL	2.4
1	A	180	ALA	2.3
1	C	30	SER	2.3
2	D	20	LEU	2.2
1	C	182	CYS	2.2
1	A	58	GLY	2.2
1	C	29	CYS	2.2
2	D	12	VAL	2.1
1	C	69	VAL	2.1
2	D	14	PRO	2.0
1	A	24	ASN	2.0

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

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

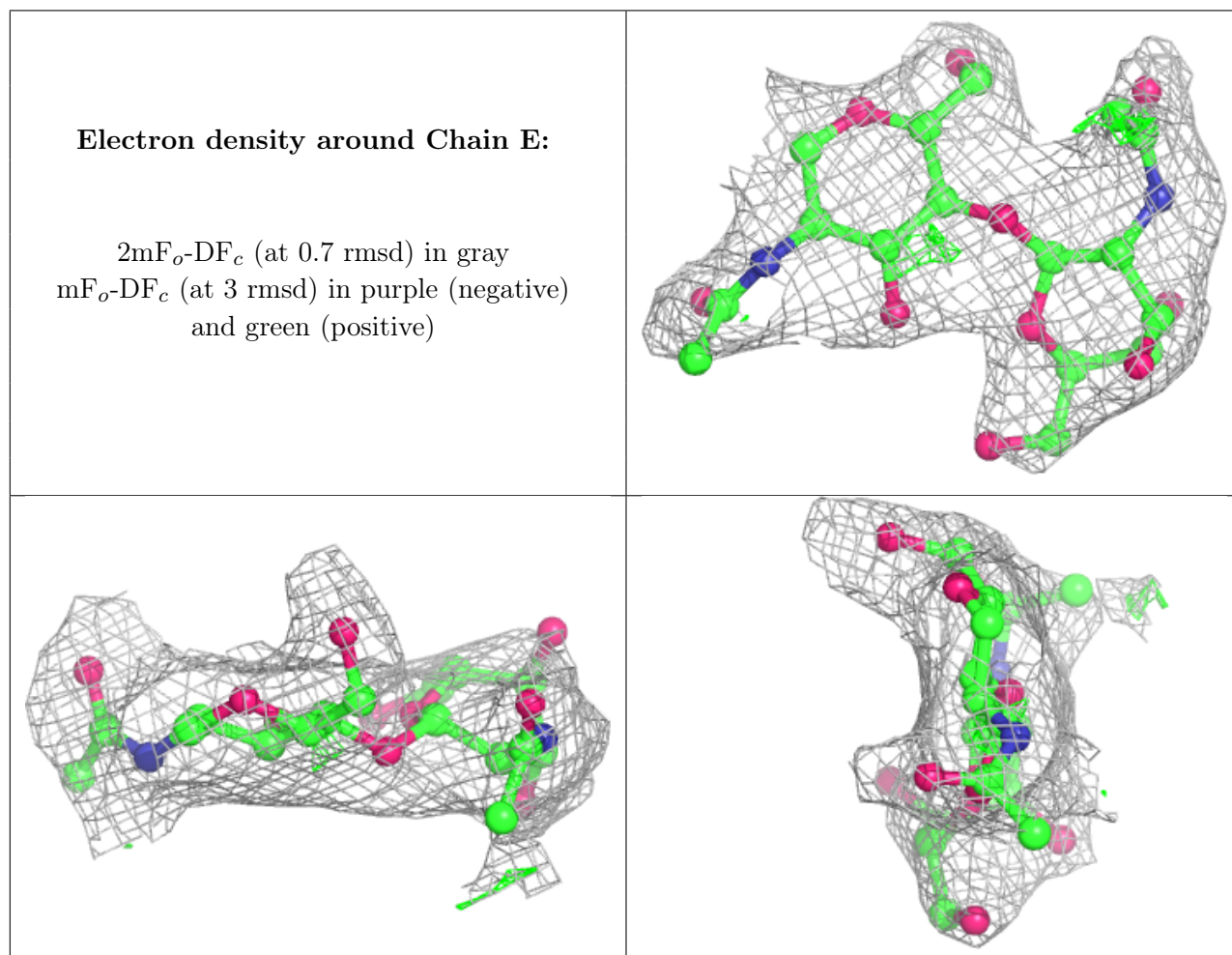
6.3 Carbohydrates [i](#)

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.

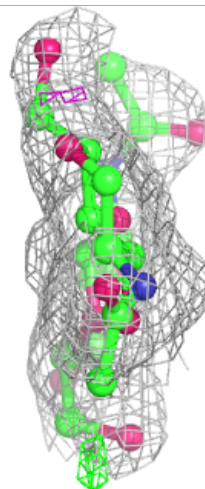
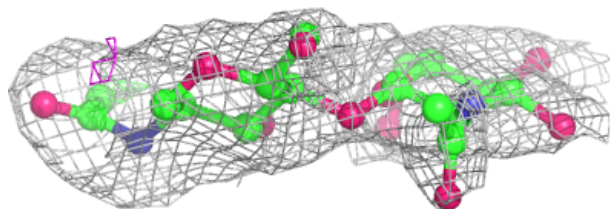
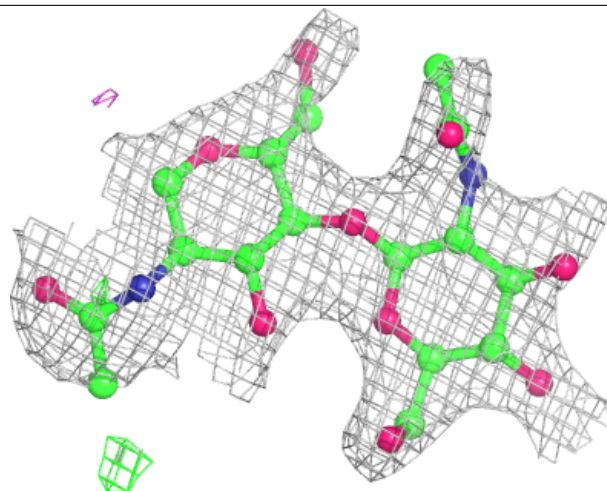
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	H	3	11/12	0.68	0.21	79,88,92,93	0
4	BMA	F	3	11/12	0.70	0.22	84,95,107,122	0
3	NAG	G	1	14/15	0.77	0.22	68,72,81,87	0
4	NAG	F	2	14/15	0.78	0.28	59,73,84,89	0
4	NAG	F	1	14/15	0.83	0.29	40,54,72,80	0
4	NAG	H	2	14/15	0.86	0.24	58,72,82,92	0
3	NAG	E	2	14/15	0.86	0.20	81,90,92,96	0
3	NAG	E	1	14/15	0.87	0.21	60,70,76,79	0
3	NAG	G	2	14/15	0.88	0.22	70,83,87,92	0
4	NAG	H	1	14/15	0.92	0.19	41,50,59,60	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.



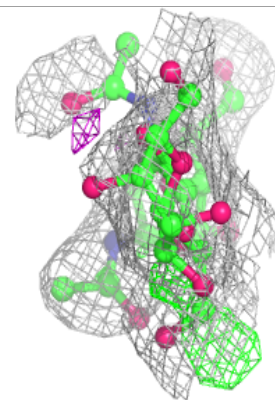
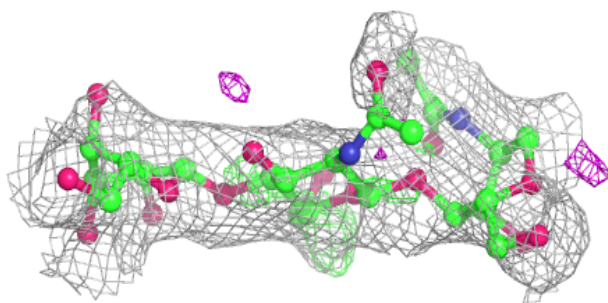
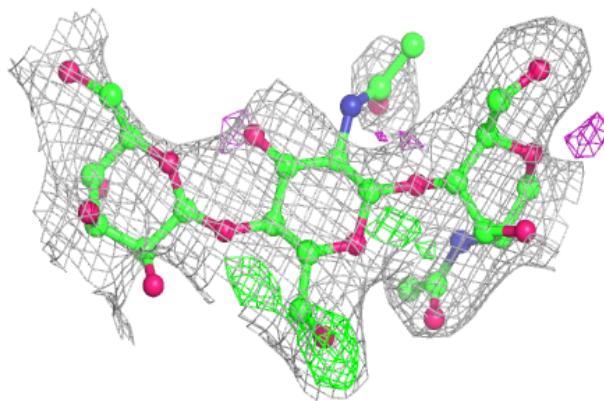
Electron density around Chain G:

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

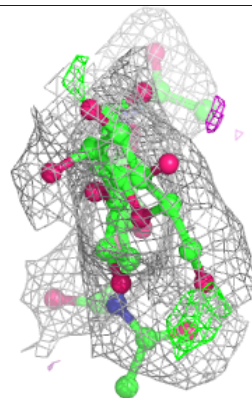
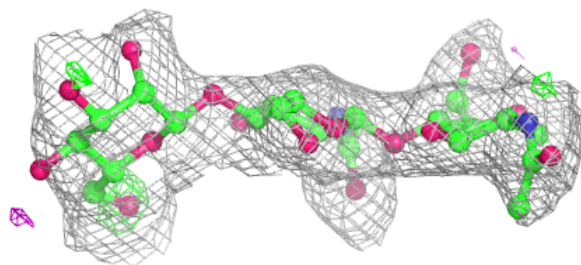
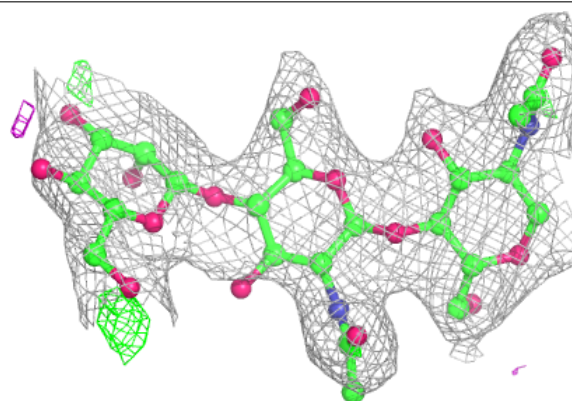


Electron density around Chain F:

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

**Electron density around Chain H:**

$2mF_o-DF_c$ (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	301	14/15	0.66	0.26	93,109,113,118	0
5	NAG	C	303	14/15	0.78	0.17	73,89,95,96	0
5	NAG	C	301	14/15	0.81	0.26	79,92,103,105	0
5	NAG	C	302	14/15	0.87	0.21	75,88,97,102	0

6.5 Other polymers [i](#)

There are no such residues in this entry.