



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 16, 2022 – 12:24 PM EDT

PDB ID : 6BXA
Title : Crystal structure of N-terminal fragment of Zebrafish Toll-Like Receptor 5 (TLR5) with Lamprey Variable Lymphocyte Receptor 2 (VLR2) bound
Authors : Gunn, R.J.; Wilson, I.A.; Cooper, M.D.; Herrin, B.R.
Deposited on : 2017-12-18
Resolution : 2.30 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 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	:	2.27
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)	:	2.27

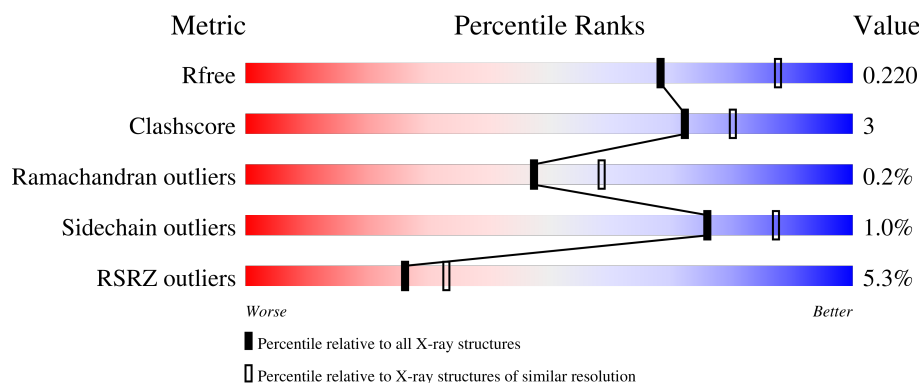
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	455	<div> <div style="width: 89%;"></div> <div style="width: 8%;"></div> <div style="width: 3%;"></div> <div style="width: 2%;"></div> </div>
1	B	455	<div> <div style="width: 8%;"></div> <div style="width: 91%;"></div> <div style="width: 6%;"></div> <div style="width: 5%;"></div> </div>
2	C	209	<div> <div style="width: 2%;"></div> <div style="width: 80%;"></div> <div style="width: 12%;"></div> <div style="width: 8%;"></div> </div>
2	D	209	<div> <div style="width: 11%;"></div> <div style="width: 81%;"></div> <div style="width: 10%;"></div> <div style="width: 8%;"></div> </div>
3	E	2	<div> <div style="width: 50%;"></div> <div style="width: 50%;"></div> </div>

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Mol	Chain	Length	Quality of chain
3	F	2	<div><div></div><div>50%</div><div></div><div>50%</div></div>
3	G	2	<div><div></div><div>100%</div><div></div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10281 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 Toll-like receptor 5b, Variable lymphocyte receptor B chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3487	2227	584	660	16			
1	B	441	Total	C	N	O	S	0	0	0
			3408	2184	562	646	16			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	ALA	-	expression tag	UNP F8W3J5
A	19	ASP	-	expression tag	UNP F8W3J5
A	20	PRO	-	expression tag	UNP F8W3J5
A	21	GLY	-	expression tag	UNP F8W3J5
A	466	SER	-	expression tag	UNP Q4G1L2
A	467	ALA	-	expression tag	UNP Q4G1L2
A	468	SER	-	expression tag	UNP Q4G1L2
A	469	LEU	-	expression tag	UNP Q4G1L2
A	470	VAL	-	expression tag	UNP Q4G1L2
A	471	PRO	-	expression tag	UNP Q4G1L2
A	472	ARG	-	expression tag	UNP Q4G1L2
B	18	ALA	-	expression tag	UNP F8W3J5
B	19	ASP	-	expression tag	UNP F8W3J5
B	20	PRO	-	expression tag	UNP F8W3J5
B	21	GLY	-	expression tag	UNP F8W3J5
B	466	SER	-	expression tag	UNP Q4G1L2
B	467	ALA	-	expression tag	UNP Q4G1L2
B	468	SER	-	expression tag	UNP Q4G1L2
B	469	LEU	-	expression tag	UNP Q4G1L2
B	470	VAL	-	expression tag	UNP Q4G1L2
B	471	PRO	-	expression tag	UNP Q4G1L2
B	472	ARG	-	expression tag	UNP Q4G1L2

- Molecule 2 is a protein called Variable Lymphocyte Receptor 2.

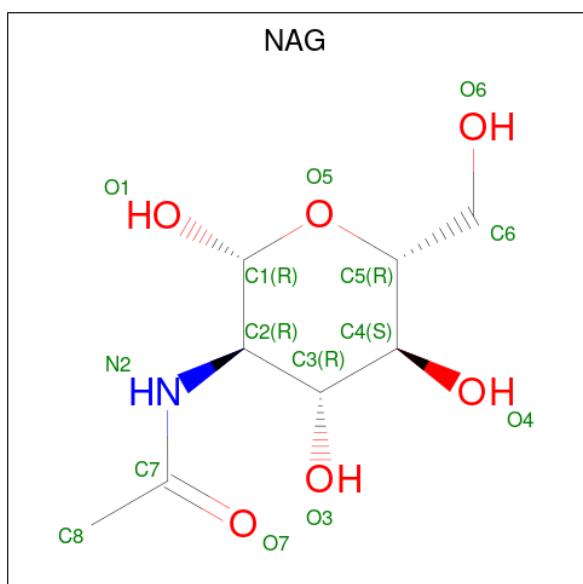
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	192	Total	C	N	O	S	0	0	0
			1440	904	240	288	8			
2	D	192	Total	C	N	O	S	0	0	0
			1441	905	240	288	8			

- 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	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	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: $C_8H_{15}NO_6$).



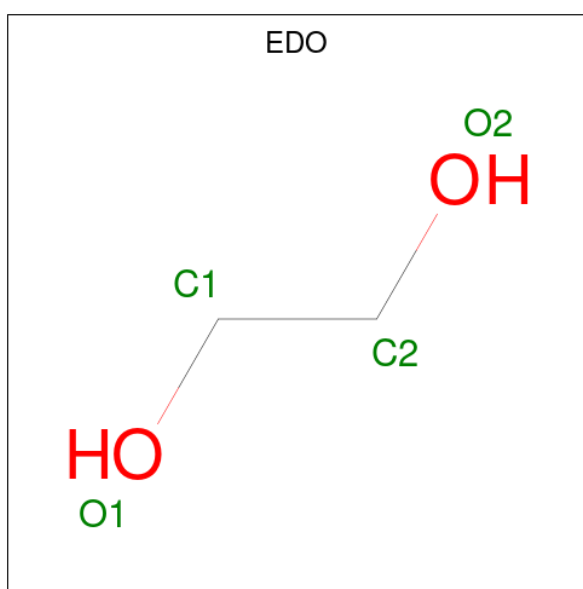
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	243	Total	O	0	0
			243	243		
6	B	63	Total	O	0	0
			63	63		

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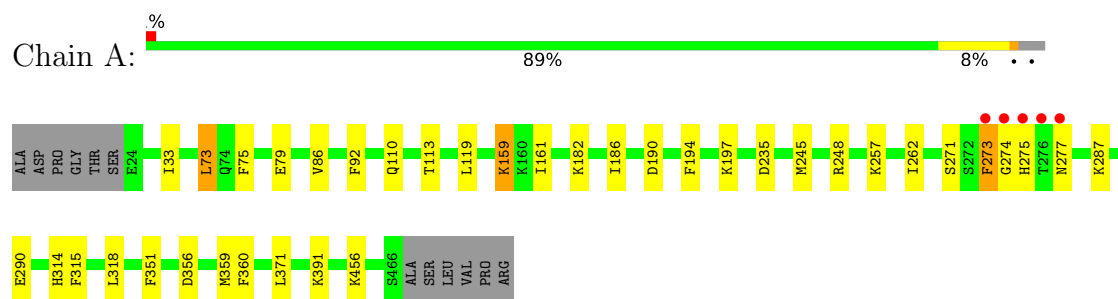
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	22	Total 22	O 22	0	0
6	D	11	Total 11	O 11	0	0

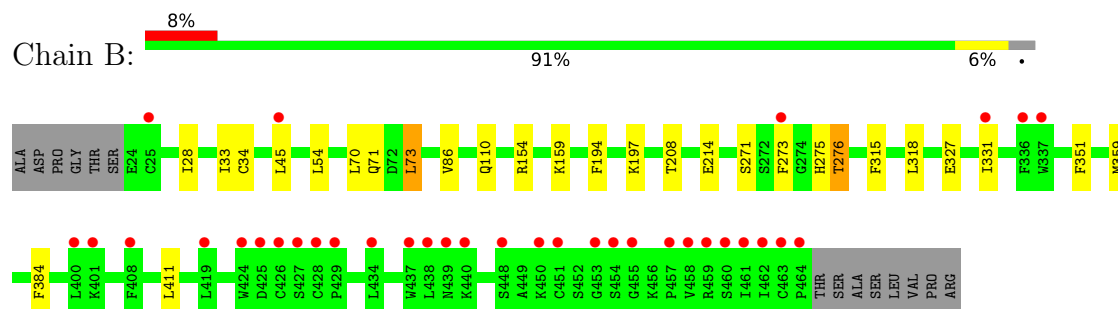
3 Residue-property plots [i](#)

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.

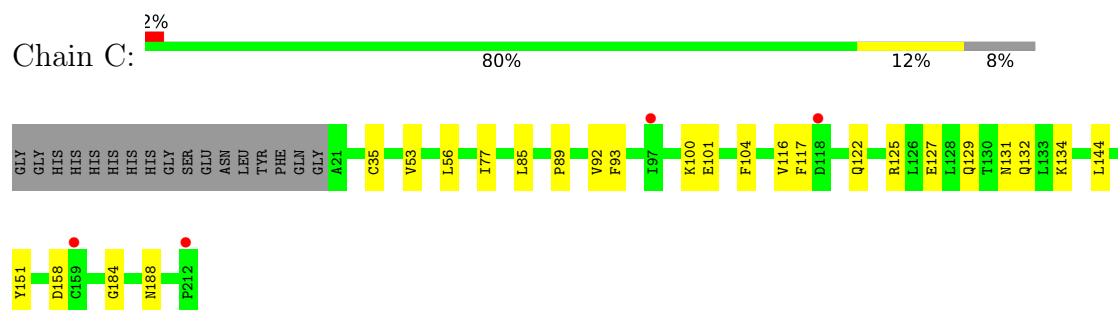
- Molecule 1: Toll-like receptor 5b, Variable lymphocyte receptor B chimera



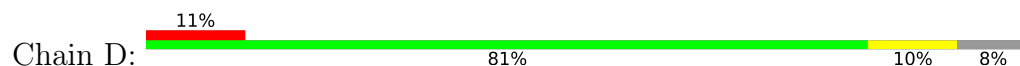
- Molecule 1: Toll-like receptor 5b, Variable lymphocyte receptor B chimera

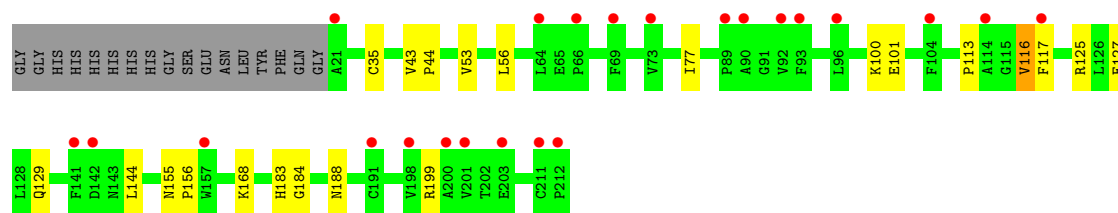


- Molecule 2: Variable Lymphocyte Receptor 2



- Molecule 2: Variable Lymphocyte Receptor 2





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

Chain E:  50%



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

Chain F:  50%



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

Chain G:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.69Å 112.10Å 148.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.45 – 2.30 49.45 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.45-2.30) 98.6 (49.45-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.185 , 0.218 0.188 , 0.220	Depositor DCC
R_{free} test set	3616 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10281	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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: EDO, 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	0.40	0/3556	0.52	0/4812
1	B	0.30	0/3476	0.46	0/4715
2	C	0.28	0/1467	0.46	0/2007
2	D	0.28	0/1468	0.45	0/2008
All	All	0.34	0/9967	0.48	0/13542

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	3487	0	3448	27	0
1	B	3408	0	3312	16	0
2	C	1440	0	1416	13	0
2	D	1441	0	1418	15	0
3	E	28	0	25	1	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
4	A	28	0	26	0	0
4	B	42	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	4	0	6	0	0
5	B	8	0	12	0	0
6	A	243	0	0	9	1
6	B	63	0	0	2	0
6	C	22	0	0	0	0
6	D	11	0	0	0	0
All	All	10281	0	9752	67	1

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.

All (67) 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:A:33:ILE:HG13	2:C:77:ILE:HD13	1.66	0.76
1:A:359:MET:HE2	6:A:1133:HOH:O	1.87	0.72
1:B:154:ARG:NH2	6:B:901:HOH:O	2.29	0.66
1:A:314:HIS:ND1	6:A:903:HOH:O	2.30	0.64
1:A:315:PHE:HB3	1:A:318:LEU:HB2	1.83	0.59
2:D:127:GLU:HG2	2:D:129:GLN:OE1	2.04	0.58
1:B:315:PHE:HB3	1:B:318:LEU:HB2	1.86	0.58
1:B:28:ILE:HD12	2:D:77:ILE:HD11	1.86	0.57
1:B:331:ILE:HD12	1:B:359:MET:HE3	1.86	0.56
1:A:159:LYS:HE2	1:A:182:LYS:O	2.06	0.56
2:C:134:LYS:HE3	2:C:158:ASP:HB2	1.88	0.55
1:A:359:MET:HB3	6:A:1133:HOH:O	2.06	0.55
2:D:35:CYS:HB2	2:D:56:LEU:HD23	1.90	0.54
2:C:184:GLY:HA3	2:C:188:ASN:HB2	1.89	0.54
2:C:93:PHE:HZ	2:C:104:PHE:HZ	1.57	0.52
1:B:86:VAL:HG22	1:B:110:GLN:HB2	1.92	0.52
2:C:127:GLU:HG2	2:C:129:GLN:OE1	2.10	0.52
1:B:271:SER:O	1:B:276:THR:OG1	2.27	0.52
2:D:168:LYS:HG3	2:D:199:ARG:HA	1.93	0.51
2:D:184:GLY:HA3	2:D:188:ASN:HB2	1.93	0.50
1:B:384:PHE:HB3	1:B:411:LEU:HD21	1.94	0.50
2:D:101:GLU:HG2	2:D:125:ARG:HB3	1.94	0.49
1:A:356:ASP:OD2	6:A:901:HOH:O	2.20	0.49
1:A:159:LYS:HD2	1:B:159:LYS:HE2	1.94	0.48
1:A:275:HIS:CE1	1:A:277:ASN:HD22	2.32	0.48
1:A:360:PHE:HZ	1:A:371:LEU:HD21	1.79	0.47
2:D:53:VAL:HG22	2:D:77:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:LYS:O	1:A:290:GLU:HB2	2.13	0.47
1:B:45:LEU:HB2	1:B:70:LEU:HD21	1.96	0.47
1:A:248:ARG:NH2	6:A:913:HOH:O	2.48	0.47
2:D:127:GLU:HG2	2:D:129:GLN:HE22	1.81	0.46
1:B:34:CYS:HB2	1:B:54:LEU:HD23	1.97	0.46
1:A:194:PHE:O	1:A:197:LYS:HB2	2.16	0.46
1:A:161:ILE:HD12	1:A:186:ILE:HD12	1.99	0.45
1:A:92:PHE:HB3	1:A:119:LEU:HD21	1.98	0.45
1:B:73:LEU:HD12	1:B:73:LEU:HA	1.85	0.45
2:C:100:LYS:HE3	2:C:122:GLN:HB3	1.98	0.45
1:A:113:THR:OG1	3:E:1:NAG:H5	2.16	0.45
2:C:89:PRO:HG2	2:C:92:VAL:HB	1.99	0.44
1:A:73:LEU:HD12	1:A:73:LEU:HA	1.83	0.44
1:B:33:ILE:HG13	2:D:77:ILE:HD13	2.00	0.44
2:D:183:HIS:O	2:D:188:ASN:ND2	2.38	0.44
2:D:117:PHE:HB3	2:D:144:LEU:HD21	1.99	0.44
1:B:327:GLU:HG2	1:B:351:PHE:HE2	1.83	0.43
1:B:208:THR:HG23	6:B:904:HOH:O	2.19	0.43
1:A:79:GLU:OE2	6:A:902:HOH:O	2.21	0.43
1:A:275:HIS:NE2	1:A:277:ASN:HB2	2.33	0.43
1:A:161:ILE:O	1:A:190:ASP:HB3	2.19	0.43
1:A:257:LYS:HE2	6:A:976:HOH:O	2.18	0.43
1:A:273:PHE:HE2	1:A:351:PHE:CE1	2.36	0.43
2:C:101:GLU:HG2	2:C:125:ARG:HB3	2.01	0.43
2:C:131:ASN:HB3	2:C:132:GLN:H	1.73	0.43
2:C:117:PHE:HB3	2:C:144:LEU:HD21	2.01	0.42
1:A:271:SER:O	1:A:275:HIS:HB3	2.19	0.42
2:D:155:ASN:HA	2:D:156:PRO:HD3	1.90	0.42
1:A:235:ASP:HA	1:A:262:ILE:HB	2.01	0.42
1:A:391:LYS:NZ	6:A:906:HOH:O	2.38	0.41
2:D:43:VAL:HA	2:D:44:PRO:HD3	1.94	0.41
1:B:194:PHE:O	1:B:197:LYS:HB2	2.20	0.41
2:C:35:CYS:HB2	2:C:56:LEU:HD23	2.02	0.41
2:C:53:VAL:HG22	2:C:77:ILE:HD12	2.03	0.41
2:D:113:PRO:HD2	2:D:116:VAL:HG11	2.03	0.41
2:C:127:GLU:HG3	2:C:151:TYR:CD1	2.55	0.41
1:A:245:MET:HE2	6:A:1024:HOH:O	2.20	0.41
2:D:100:LYS:HZ2	2:D:100:LYS:HG2	1.62	0.41
1:A:86:VAL:HG22	1:A:110:GLN:HB2	2.02	0.40
1:B:214:GLU:CD	1:B:214:GLU:H	2.25	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:901:HOH:O	6:A:1090:HOH:O[2_565]	1.96	0.24

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	441/455 (97%)	421 (96%)	19 (4%)	1 (0%)	47	58
1	B	439/455 (96%)	420 (96%)	17 (4%)	2 (0%)	29	35
2	C	190/209 (91%)	185 (97%)	5 (3%)	0	100	100
2	D	190/209 (91%)	184 (97%)	6 (3%)	0	100	100
All	All	1260/1328 (95%)	1210 (96%)	47 (4%)	3 (0%)	47	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	275	HIS
1	B	276	THR
1	A	274	GLY

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	393/409 (96%)	388 (99%)	5 (1%)	69	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	374/409 (91%)	371 (99%)	3 (1%)	81	91
2	C	169/185 (91%)	167 (99%)	2 (1%)	71	84
2	D	169/185 (91%)	168 (99%)	1 (1%)	86	94
All	All	1105/1188 (93%)	1094 (99%)	11 (1%)	76	87

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	LEU
1	A	75	PHE
1	A	159	LYS
1	A	273	PHE
1	A	456	LYS
1	B	71	GLN
1	B	73	LEU
1	B	273	PHE
2	C	85	LEU
2	C	116	VAL
2	D	116	VAL

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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	E	1	1,3	14,14,15	0.58	0	17,19,21	0.63	0
3	NAG	E	2	3	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	F	1	1,3	14,14,15	0.58	0	17,19,21	0.60	0
3	NAG	F	2	3	14,14,15	0.37	0	17,19,21	0.71	1 (5%)
3	NAG	G	1	1,3	14,14,15	0.35	0	17,19,21	0.50	0
3	NAG	G	2	3	14,14,15	0.22	0	17,19,21	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	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	NAG	C1-O5-C5	2.55	115.64	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6

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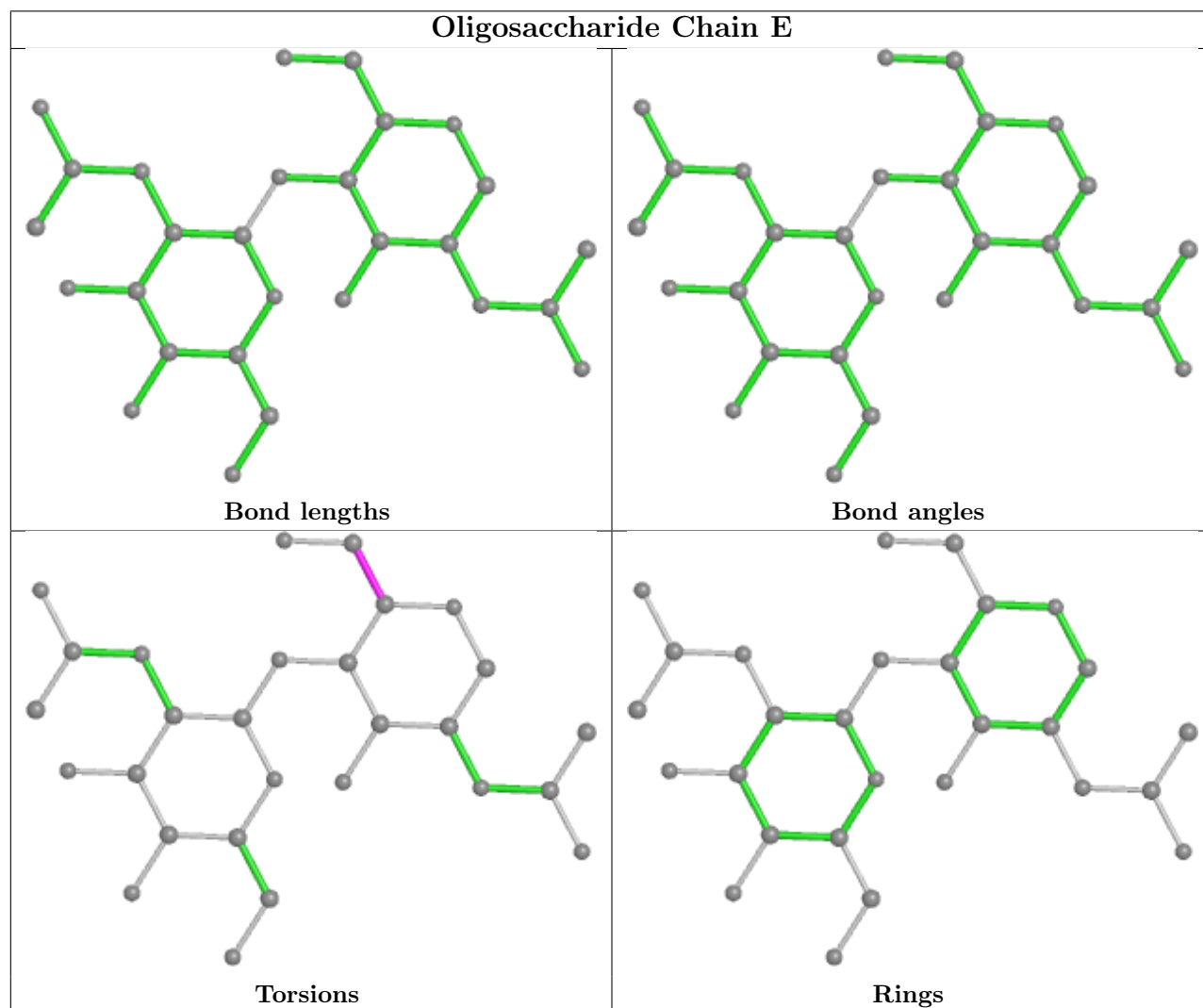
Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6

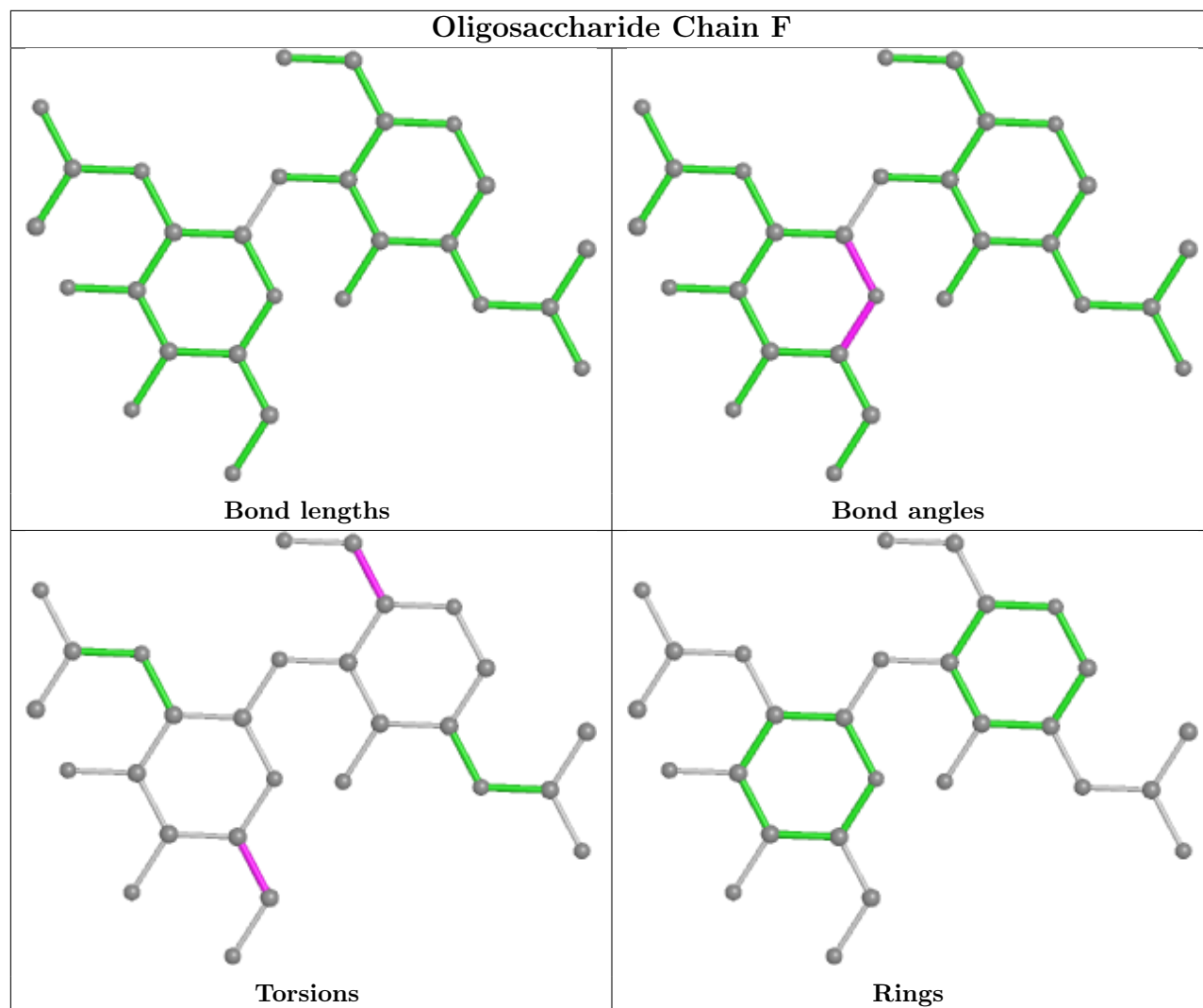
There are no ring outliers.

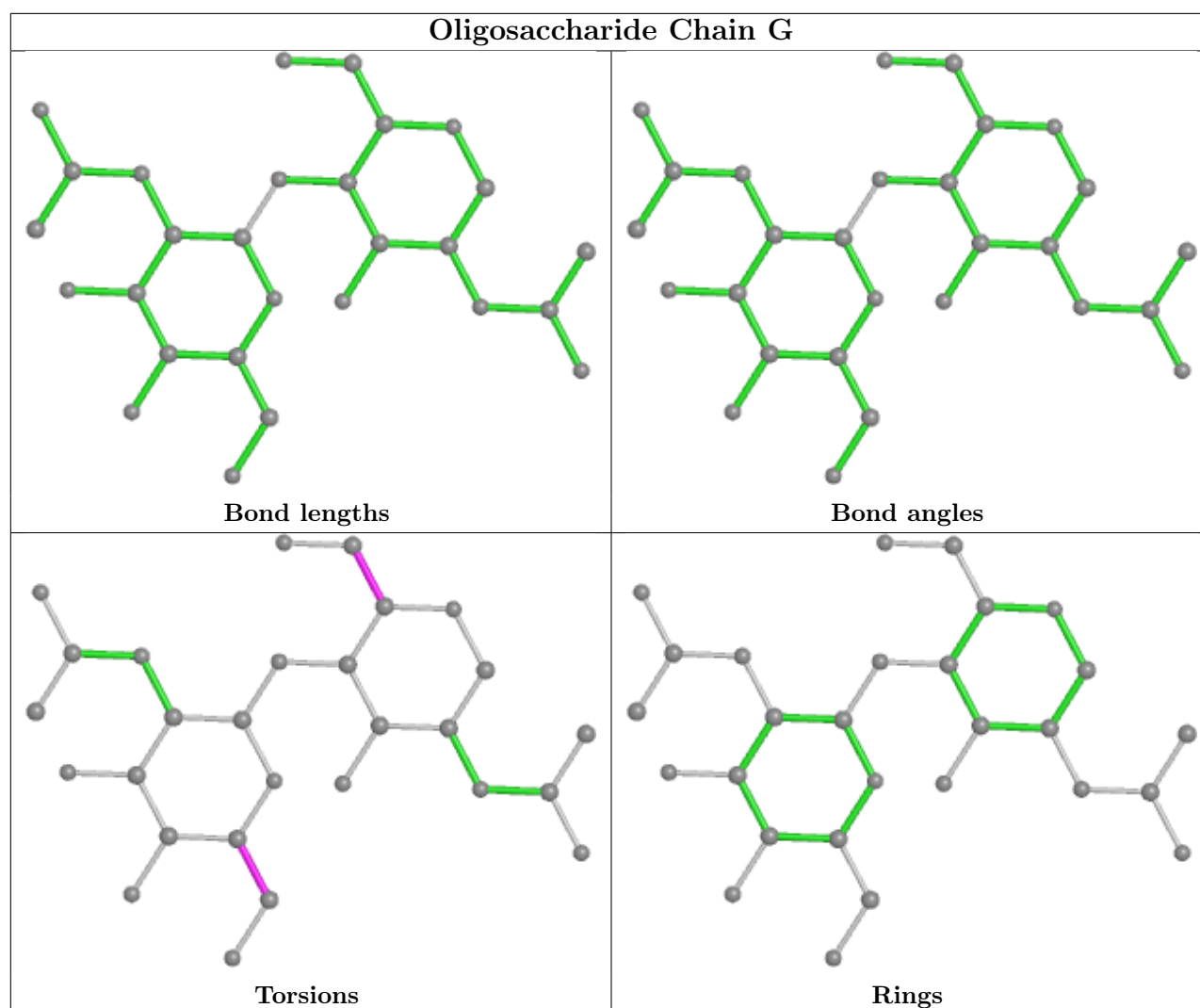
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	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 [i](#)

8 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	EDO	B	806	-	3,3,3	0.48	0	2,2,2	0.33	0
5	EDO	A	807	-	3,3,3	0.51	0	2,2,2	0.14	0
5	EDO	B	807	-	3,3,3	0.30	0	2,2,2	0.74	0
4	NAG	B	802	1	14,14,15	0.59	0	17,19,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	804	1	14,14,15	0.85	1 (7%)	17,19,21	0.62	0
4	NAG	B	803	1	14,14,15	0.71	0	17,19,21	0.54	0
4	NAG	A	801	1	14,14,15	0.32	0	17,19,21	0.42	0
4	NAG	B	801	1	14,14,15	0.32	0	17,19,21	0.34	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	EDO	B	806	-	-	0/1/1/1	-
5	EDO	A	807	-	-	0/1/1/1	-
5	EDO	B	807	-	-	0/1/1/1	-
4	NAG	B	802	1	-	2/6/23/26	0/1/1/1
4	NAG	A	804	1	-	0/6/23/26	0/1/1/1
4	NAG	B	803	1	-	0/6/23/26	0/1/1/1
4	NAG	A	801	1	-	2/6/23/26	0/1/1/1
4	NAG	B	801	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)
4	A	804	NAG	O5-C1	2.53	1.47	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	802	NAG	O5-C5-C6-O6
4	B	801	NAG	O5-C5-C6-O6
4	B	802	NAG	C4-C5-C6-O6
4	B	801	NAG	C4-C5-C6-O6
4	A	801	NAG	O5-C5-C6-O6
4	A	801	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	443/455 (97%)	-0.05	5 (1%) 80 85	26, 39, 70, 162	0
1	B	441/455 (96%)	0.21	35 (7%) 12 17	34, 67, 121, 147	0
2	C	192/209 (91%)	0.03	4 (2%) 63 70	44, 72, 98, 127	0
2	D	192/209 (91%)	0.73	23 (11%) 4 6	54, 88, 111, 150	0
All	All	1268/1328 (95%)	0.17	67 (5%) 26 33	26, 63, 109, 162	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	212	PRO	10.4
1	B	463	CYS	6.0
2	D	200	ALA	5.8
1	B	426	CYS	5.4
1	A	273	PHE	4.4
1	B	427	SER	4.4
2	D	21	ALA	4.3
1	B	451	CYS	4.2
1	B	428	CYS	4.2
1	A	276	THR	4.1
1	B	424	TRP	4.0
1	B	458	VAL	4.0
1	B	437	TRP	4.0
2	C	212	PRO	3.8
1	B	429	PRO	3.5
1	B	462	ILE	3.4
1	B	434	LEU	3.4
2	D	89	PRO	3.4
1	B	464	PRO	3.3
2	D	69	PHE	3.3
1	A	274	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	419	LEU	3.2
1	B	460	SER	3.1
1	B	439	ASN	3.1
1	B	425	ASP	3.0
1	B	400	LEU	3.0
1	B	25	CYS	3.0
1	B	337	TRP	2.9
2	D	114	ALA	2.8
2	D	201	VAL	2.8
1	B	457	PRO	2.8
1	A	277	ASN	2.8
2	D	191	CYS	2.8
1	B	408	PHE	2.7
2	C	97	ILE	2.7
1	B	45	LEU	2.7
2	D	64	LEU	2.7
1	B	401	LYS	2.6
2	D	104	PHE	2.6
1	B	455	GLY	2.6
2	D	211	CYS	2.5
1	B	448	SER	2.5
2	C	159	CYS	2.5
2	D	66	PRO	2.4
2	D	203	GLU	2.4
2	D	73	VAL	2.4
1	B	438	LEU	2.4
1	B	331	ILE	2.4
2	D	96	LEU	2.4
1	B	273	PHE	2.3
1	B	461	ILE	2.3
1	B	459	ARG	2.3
2	D	157	TRP	2.3
1	B	450	LYS	2.3
2	D	142	ASP	2.2
2	D	198	VAL	2.2
1	B	453	GLY	2.2
2	D	92	VAL	2.2
1	A	275	HIS	2.2
2	D	117	PHE	2.1
2	D	90	ALA	2.1
2	C	118	ASP	2.1
1	B	454	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	440	LYS	2.1
2	D	93	PHE	2.1
1	B	336	PHE	2.0
2	D	141	PHE	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](#)

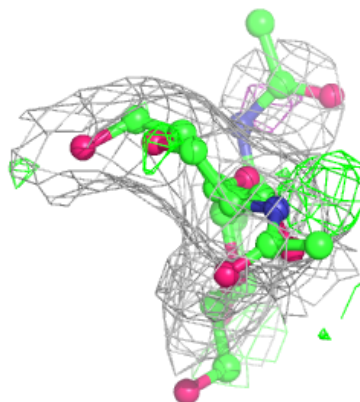
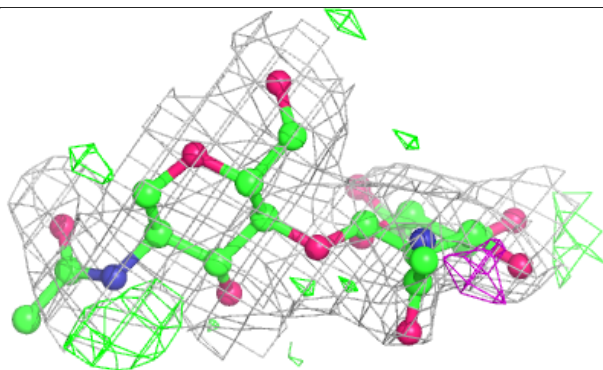
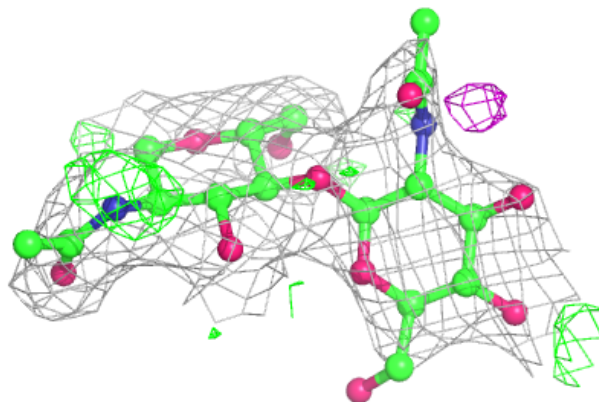
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	E	2	14/15	0.79	0.20	86,91,94,95	0
3	NAG	E	1	14/15	0.87	0.17	50,67,74,77	0
3	NAG	G	2	14/15	0.89	0.18	84,93,99,101	0
3	NAG	F	2	14/15	0.92	0.12	52,65,76,79	0
3	NAG	G	1	14/15	0.95	0.09	57,66,70,79	0
3	NAG	F	1	14/15	0.98	0.12	28,34,41,43	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.

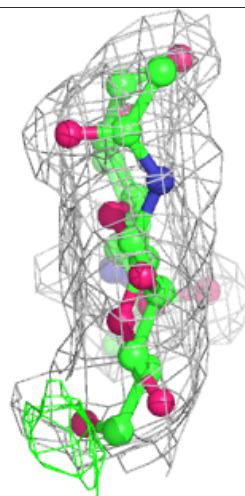
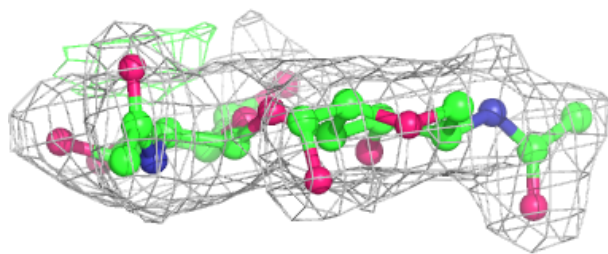
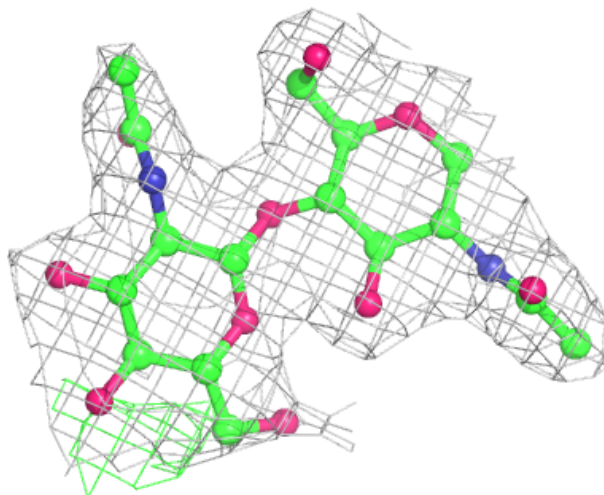
Electron density around Chain E:

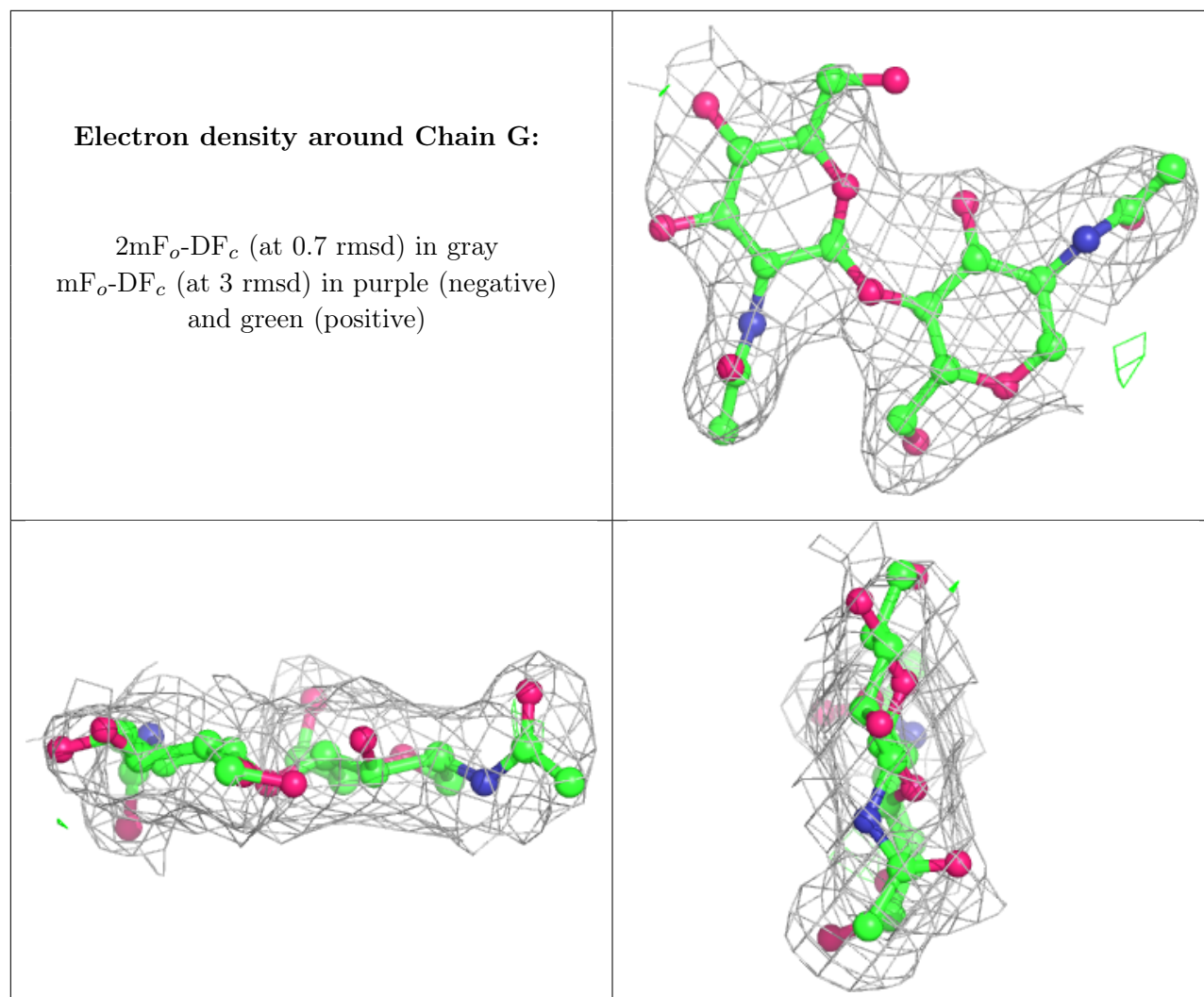
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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, 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	NAG	B	803	14/15	0.66	0.24	77,84,90,95	0
4	NAG	A	804	14/15	0.71	0.25	61,68,77,78	0
4	NAG	A	801	14/15	0.83	0.17	70,85,87,89	0
4	NAG	B	801	14/15	0.84	0.17	72,85,89,91	0
4	NAG	B	802	14/15	0.91	0.10	54,64,70,73	0
5	EDO	B	807	4/4	0.92	0.23	53,54,54,57	0
5	EDO	B	806	4/4	0.96	0.18	43,46,46,48	0
5	EDO	A	807	4/4	0.96	0.15	41,46,51,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.