



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:51 PM UTC

PDB ID : 8DFW / pdb_00008dfw
Title : Crystal Structure of Human BTN2A1 in Complex With Vgamma9-Vdelta2 T Cell Receptor
Authors : Fulford, T.S.; Soliman, C.; Castle, R.G.; Rigau, M.; Ruan, Z.; Dolezal, O.; Seneviratna, R.; Brown, H.G.; Hanssen, E.; Hammet, A.; Li, S.; Redmond, S.J.; Chung, A.; Gorman, M.A.; Parker, M.W.; Patel, O.; Peat, T.S.; Newman, J.; Behren, A.; Gherardin, N.A.; Godfrey, D.I.; Uldrich, A.P.
Deposited on : 2022-06-22
Resolution : 2.10 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:

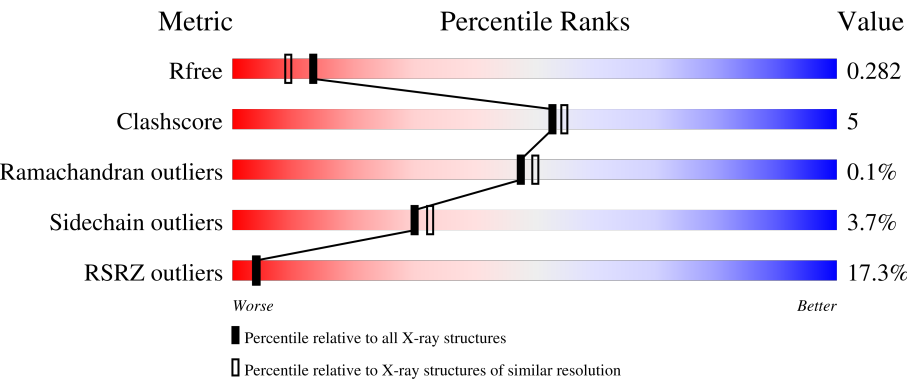
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



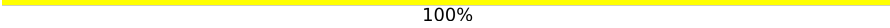
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	226	18% 83% 12% 6%
1	B	226	9% 78% 18% ..
2	D	239	7% 74% 11% 14%
3	G	252	29% 74% 15% 9%

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Mol	Chain	Length	Quality of chain
4	C	4	 50% 50%
5	E	3	 67% 33%
6	F	2	 100%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7186 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 Butyrophilin subfamily 2 member A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	51	1	0
			1680	1058	295	316	11			
1	B	220	Total	C	N	O	S	25	2	0
			1730	1090	301	326	13			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLU	-	expression tag	UNP Q7KYR7
A	-1	THR	-	expression tag	UNP Q7KYR7
A	0	GLY	-	expression tag	UNP Q7KYR7
A	218	HIS	-	expression tag	UNP Q7KYR7
A	219	HIS	-	expression tag	UNP Q7KYR7
A	220	HIS	-	expression tag	UNP Q7KYR7
A	221	HIS	-	expression tag	UNP Q7KYR7
A	222	HIS	-	expression tag	UNP Q7KYR7
A	223	HIS	-	expression tag	UNP Q7KYR7
B	-2	GLU	-	expression tag	UNP Q7KYR7
B	-1	THR	-	expression tag	UNP Q7KYR7
B	0	GLY	-	expression tag	UNP Q7KYR7
B	218	HIS	-	expression tag	UNP Q7KYR7
B	219	HIS	-	expression tag	UNP Q7KYR7
B	220	HIS	-	expression tag	UNP Q7KYR7
B	221	HIS	-	expression tag	UNP Q7KYR7
B	222	HIS	-	expression tag	UNP Q7KYR7
B	223	HIS	-	expression tag	UNP Q7KYR7

- Molecule 2 is a protein called T cell receptor delta variable chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	205	Total	C	N	O	S	37	0	0
			1606	1019	269	310	8			

- Molecule 3 is a protein called T cell receptor gamma variable chain.

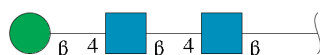
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	230	Total	C	N	O	S	74	0	0
			1832	1169	305	352	6			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 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.



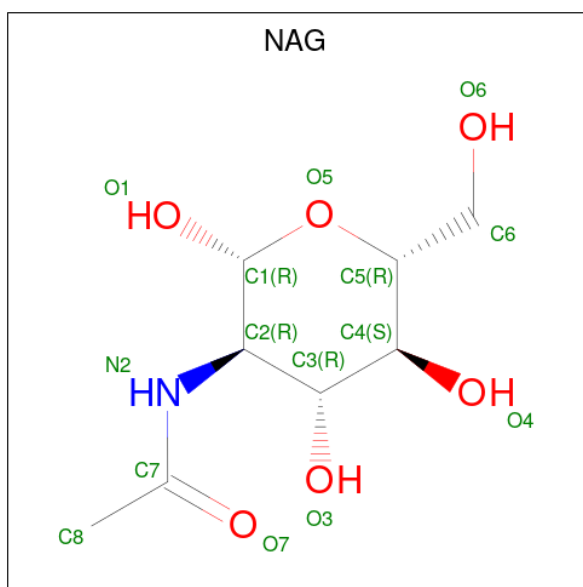
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 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
6	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

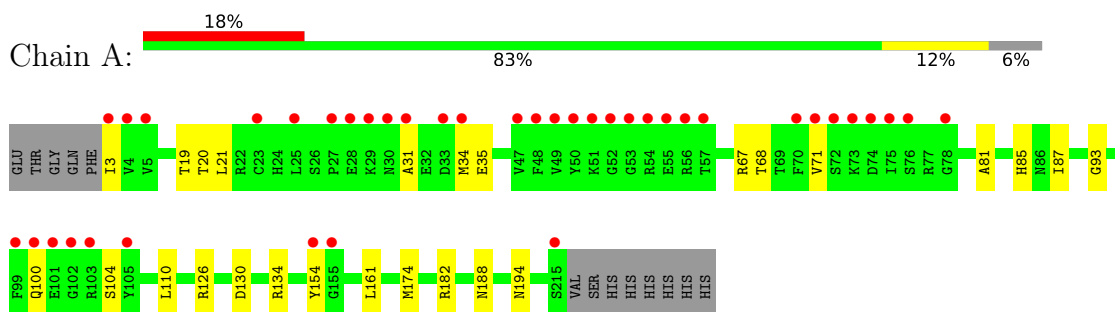
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	60	Total	O	0	0
			60	60		
8	B	41	Total	O	0	0
			41	41		
8	D	37	Total	O	0	0
			37	37		
8	G	27	Total	O	0	0
			27	27		

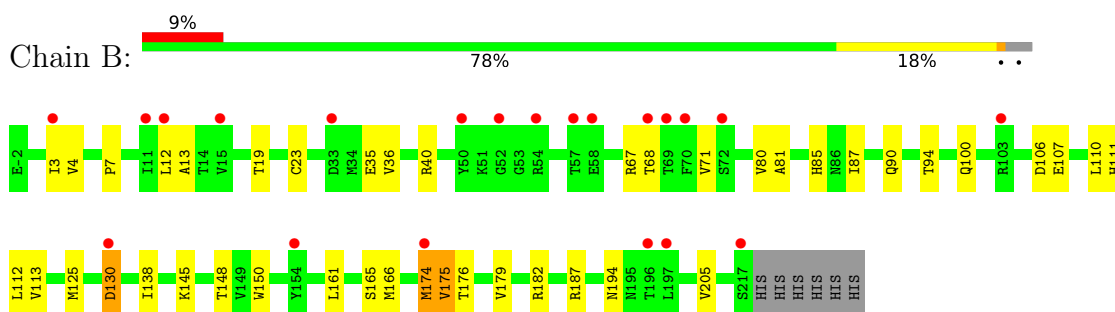
3 Residue-property plots [i](#)

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.

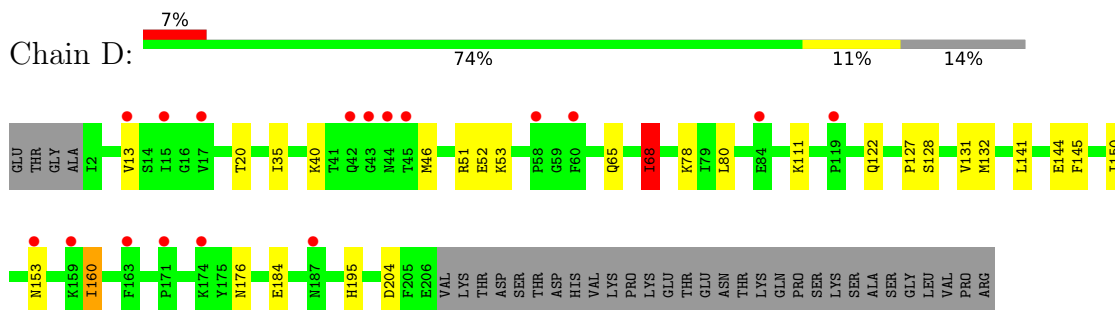
- Molecule 1: Butyrophilin subfamily 2 member A1



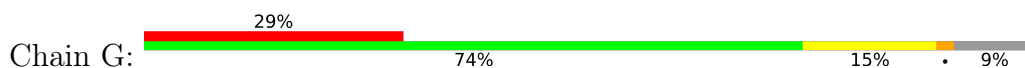
- Molecule 1: Butyrophilin subfamily 2 member A1

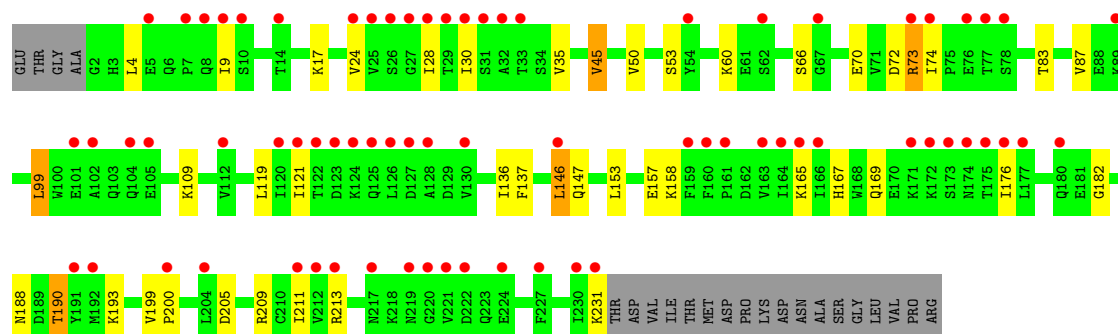


- Molecule 2: T cell receptor delta variable chain



- Molecule 3: T cell receptor gamma variable chain





- Molecule 4: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 50% 50%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 67% 33%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	112.03Å 218.46Å 107.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.72 – 2.10 49.72 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.72-2.10) 100.0 (49.72-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.10Å)	Xtrriage
Refinement program	BUSTER 2.10.4 (11-DEC-2020)	Depositor
R, R_{free}	0.261 , 0.287 0.252 , 0.282	Depositor DCC
R_{free} test set	3723 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtrriage
Anisotropy	0.071	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.2	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	0.93	EDS
Total number of atoms	7186	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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: MAN, NAG, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.76	0/1716	0.93	2/2322 (0.1%)
1	B	0.76	2/1773 (0.1%)	0.95	0/2399
2	D	0.73	1/1641 (0.1%)	1.00	4/2221 (0.2%)
3	G	0.80	1/1871 (0.1%)	1.05	4/2534 (0.2%)
All	All	0.77	4/7001 (0.1%)	0.99	10/9476 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	174	MET	SD-CE	-5.55	1.65	1.79
3	G	188	ASN	CA-C	5.37	1.57	1.52
1	B	125	MET	SD-CE	5.25	1.92	1.79
2	D	68	ILE	CG1-CD1	-5.19	1.31	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	ASN	CA-CB-CG	6.90	119.50	112.60
2	D	153	ASN	CA-CB-CG	6.12	118.72	112.60
3	G	72	ASP	CA-CB-CG	5.94	118.54	112.60
2	D	160	ILE	N-CA-C	-5.29	106.64	111.67
2	D	122	GLN	N-CA-CB	-5.22	105.91	111.29
1	A	93	GLY	N-CA-C	5.19	116.80	111.56
2	D	204	ASP	CA-CB-CG	5.12	117.72	112.60
3	G	190	THR	N-CA-CB	-5.02	103.48	111.62
3	G	30	ILE	CA-C-N	5.00	128.20	121.05
3	G	30	ILE	C-N-CA	5.00	128.20	121.05

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	1680	0	1659	10	0
1	B	1730	0	1710	22	0
2	D	1606	0	1588	13	0
3	G	1832	0	1848	24	0
4	C	50	0	43	0	0
5	E	39	0	34	0	0
6	F	28	0	25	1	0
7	A	28	0	26	0	0
7	B	28	0	26	1	0
8	A	60	0	0	1	0
8	B	41	0	0	1	0
8	D	37	0	0	0	0
8	G	27	0	0	0	0
All	All	7186	0	6959	67	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 5.

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:B:148:THR:HG21	1:B:175:VAL:HG21	1.58	0.86
2:D:132:MET:HE1	2:D:141:LEU:HB2	1.69	0.73
2:D:40:LYS:HE3	2:D:46:MET:HE1	1.72	0.71
3:G:158:LYS:HA	3:G:190:THR:CG2	2.24	0.67
2:D:35:ILE:HG13	2:D:68:ILE:HD11	1.75	0.66
3:G:158:LYS:HA	3:G:190:THR:HG21	1.78	0.65
1:B:138:ILE:HG22	1:B:176:THR:HG22	1.79	0.62
3:G:53:SER:O	3:G:73:ARG:NH1	2.34	0.60
1:A:31:ALA:HA	1:A:34:MET:HG3	1.83	0.60
2:D:35:ILE:CG1	2:D:68:ILE:HD11	2.33	0.58
3:G:167:HIS:NE2	3:G:169:GLN:NE2	2.51	0.58
3:G:165:LYS:HB3	3:G:213:ARG:HB3	1.85	0.58
3:G:87:VAL:HG11	3:G:119:LEU:HD21	1.86	0.57
3:G:146:LEU:HD12	3:G:147:GLN:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:127:PRO:HB3	2:D:145:PHE:HB3	1.85	0.56
2:D:65:GLN:HG3	2:D:80:LEU:HD11	1.87	0.55
3:G:167:HIS:CD2	3:G:169:GLN:HE21	2.25	0.55
2:D:160:ILE:HD11	2:D:184:GLU:HG2	1.88	0.54
3:G:137:PHE:HB2	3:G:153:LEU:HB3	1.89	0.54
1:B:19:THR:HG22	1:B:87:ILE:HD11	1.89	0.53
1:B:67:ARG:HG2	1:B:85:HIS:O	2.10	0.52
2:D:20:THR:HG22	2:D:78:LYS:HG3	1.91	0.52
3:G:70:GLU:HB3	3:G:83:THR:HB	1.92	0.51
1:B:194:ASN:HB2	8:B:437:HOH:O	2.10	0.51
1:A:194:ASN:HB3	8:A:445:HOH:O	2.10	0.51
1:A:67:ARG:HG2	1:A:85:HIS:O	2.09	0.51
1:B:4:VAL:HG23	1:B:106:ASP:HB3	1.93	0.51
1:B:12:LEU:HA	1:B:113:VAL:HG13	1.92	0.51
3:G:87:VAL:HG11	3:G:121:ILE:HD11	1.94	0.50
1:B:130:ASP:HB2	1:B:182:ARG:HH21	1.78	0.49
3:G:53:SER:C	3:G:73:ARG:HH12	2.21	0.49
1:A:19:THR:HG22	1:A:87:ILE:HD11	1.93	0.49
2:D:150:ILE:HG13	2:D:195:HIS:HB2	1.94	0.49
2:D:111:LYS:HG2	3:G:45:VAL:HG23	1.95	0.48
1:B:166:MET:HG2	1:B:174:MET:HE3	1.96	0.48
1:B:23[A]:CYS:SG	1:B:110:LEU:HD11	2.54	0.48
3:G:4:LEU:HD11	3:G:99:LEU:HG	1.97	0.47
3:G:209:ARG:HG3	3:G:211:ILE:HD11	1.96	0.47
1:B:35:GLU:HB3	1:B:100:GLN:HB3	1.95	0.47
1:B:205:VAL:HG11	7:B:302:NAG:H82	1.96	0.47
1:B:7:PRO:HD2	1:B:110:LEU:HG	1.96	0.46
1:A:35:GLU:HB3	1:A:100:GLN:HB3	1.97	0.45
1:A:126:ARG:HB2	1:A:134:ARG:HG2	1.97	0.45
1:A:130:ASP:HB3	1:A:182:ARG:HH21	1.82	0.45
1:B:150:TRP:NE1	1:B:179:VAL:HG13	2.32	0.45
1:B:13:ALA:HB2	1:B:112:LEU:HD11	1.99	0.45
1:B:166:MET:HE2	1:B:174:MET:HE2	1.97	0.45
3:G:136:ILE:HG12	6:F:1:NAG:O6	2.17	0.45
3:G:182:GLY:O	3:G:193:LYS:HE2	2.16	0.44
3:G:4:LEU:HD21	3:G:99:LEU:HD21	2.00	0.44
2:D:132:MET:HE1	2:D:141:LEU:CB	2.44	0.44
1:B:187:ARG:HA	1:B:187:ARG:NE	2.33	0.43
1:A:174:MET:HE2	1:A:174:MET:HB2	1.94	0.43
1:B:71:VAL:HB	1:B:81:ALA:HB3	2.00	0.43
2:D:52:GLU:HA	2:D:53:LYS:HA	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:LYS:HE2	1:B:165:SER:HB3	2.01	0.43
3:G:17:LYS:O	3:G:87:VAL:HG23	2.19	0.42
1:A:71:VAL:HB	1:A:81:ALA:HB3	2.01	0.42
1:B:40:ARG:NH2	1:B:90:GLN:O	2.52	0.42
3:G:205:ASP:HA	3:G:231:LYS:HB2	2.00	0.42
2:D:51:ARG:HD3	3:G:109:LYS:O	2.20	0.42
1:B:94:THR:HG22	1:B:111:HIS:CE1	2.54	0.42
3:G:199:VAL:HA	3:G:200:PRO:HD3	1.96	0.41
1:A:21:LEU:HB3	1:A:110:LEU:HD22	2.03	0.40
3:G:35:VAL:HG23	3:G:73:ARG:HH21	1.85	0.40
1:B:36:VAL:HG11	1:B:80:VAL:HG21	2.04	0.40
3:G:50:VAL:HG12	3:G:60:LYS:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	212/226 (94%)	205 (97%)	7 (3%)	0	100	100
1	B	220/226 (97%)	215 (98%)	5 (2%)	0	100	100
2	D	203/239 (85%)	198 (98%)	4 (2%)	1 (0%)	24	22
3	G	228/252 (90%)	214 (94%)	14 (6%)	0	100	100
All	All	863/943 (92%)	832 (96%)	30 (4%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	144	GLU

5.3.2 Protein sidechains ⓘ

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	185/196 (94%)	179 (97%)	6 (3%)	34	38
1	B	192/196 (98%)	186 (97%)	6 (3%)	35	39
2	D	180/210 (86%)	175 (97%)	5 (3%)	38	43
3	G	209/227 (92%)	198 (95%)	11 (5%)	20	19
All	All	766/829 (92%)	738 (96%)	28 (4%)	30	33

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	20	THR
1	A	68	THR
1	A	104	SER
1	A	154	TYR
1	A	161	LEU
1	B	3	ILE
1	B	68	THR
1	B	107	GLU
1	B	130	ASP
1	B	161	LEU
1	B	175	VAL
2	D	13	VAL
2	D	68	ILE
2	D	128	SER
2	D	131	VAL
2	D	176	ASN
3	G	9	ILE
3	G	24	VAL
3	G	28	ILE
3	G	45	VAL
3	G	66	SER
3	G	73	ARG
3	G	74	ILE

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Mol	Chain	Res	Type
3	G	99	LEU
3	G	146	LEU
3	G	157	GLU
3	G	176	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	B	60	GLN
2	D	176	ASN
3	G	3	HIS
3	G	169	GLN
3	G	180	GLN
3	G	223	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

9 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	$\# Z > 2$
4	NAG	C	1	1,4	14,14,15	0.28	0	17,19,21	0.83	1 (5%)
4	NAG	C	2	4	14,14,15	0.31	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BMA	C	3	4	11,11,12	0.29	0	15,15,17	0.53	0
4	MAN	C	4	4	11,11,12	0.32	0	15,15,17	0.83	1 (6%)
5	NAG	E	1	1,5	14,14,15	0.35	0	17,19,21	0.95	2 (11%)
5	NAG	E	2	5	14,14,15	0.29	0	17,19,21	0.40	0
5	BMA	E	3	5	11,11,12	0.30	0	15,15,17	0.55	0
6	NAG	F	1	6,2	14,14,15	0.28	0	17,19,21	0.57	0
6	NAG	F	2	6	14,14,15	0.33	0	17,19,21	0.87	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1
4	BMA	C	3	4	-	1/2/19/22	0/1/1/1
4	MAN	C	4	4	-	0/2/19/22	0/1/1/1
5	NAG	E	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
6	NAG	F	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	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(°)
4	C	4	MAN	C1-O5-C5	2.80	115.94	112.19
6	F	2	NAG	C1-O5-C5	2.78	115.91	112.19
5	E	1	NAG	C1-C2-N2	-2.35	106.74	110.43
4	C	1	NAG	C1-O5-C5	2.17	115.10	112.19
5	E	1	NAG	C1-O5-C5	2.06	114.94	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

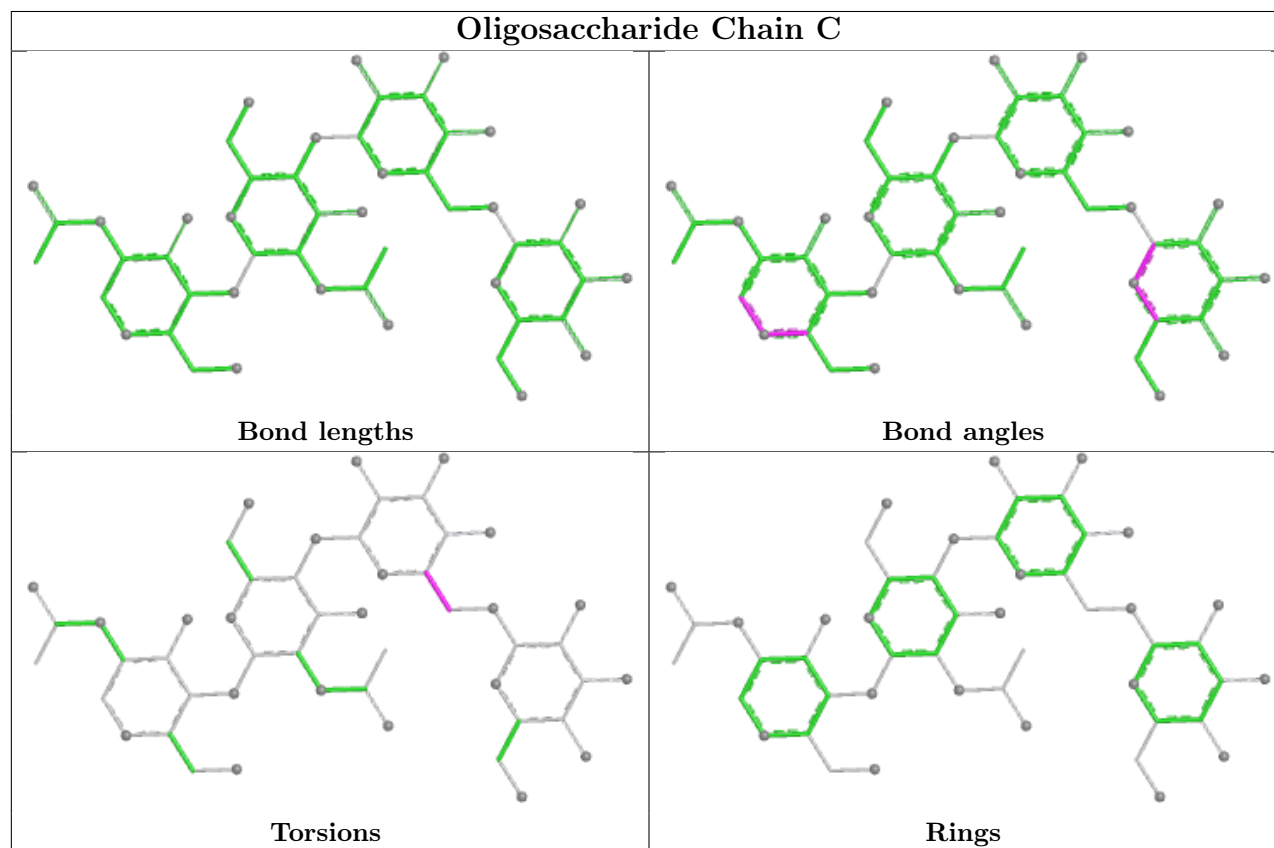
Mol	Chain	Res	Type	Atoms
4	C	3	BMA	O5-C5-C6-O6

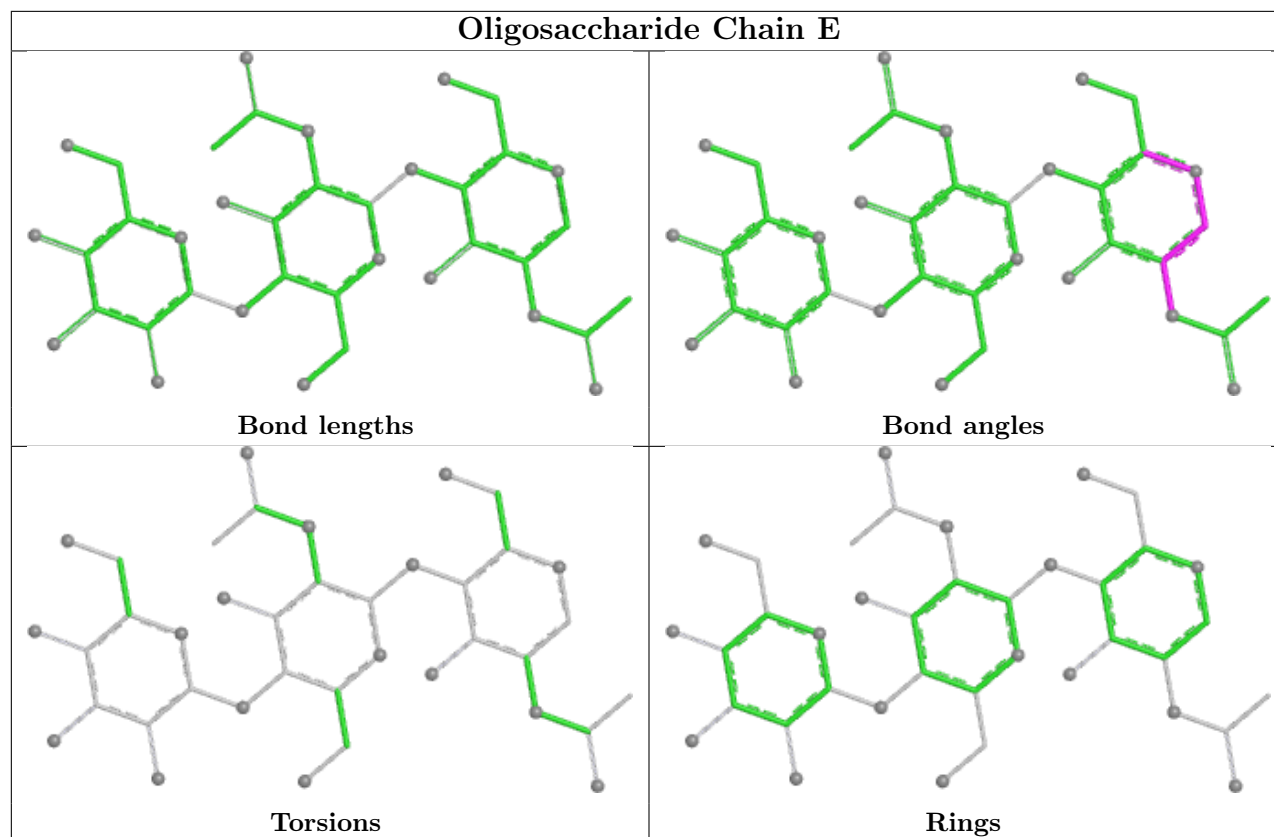
There are no ring outliers.

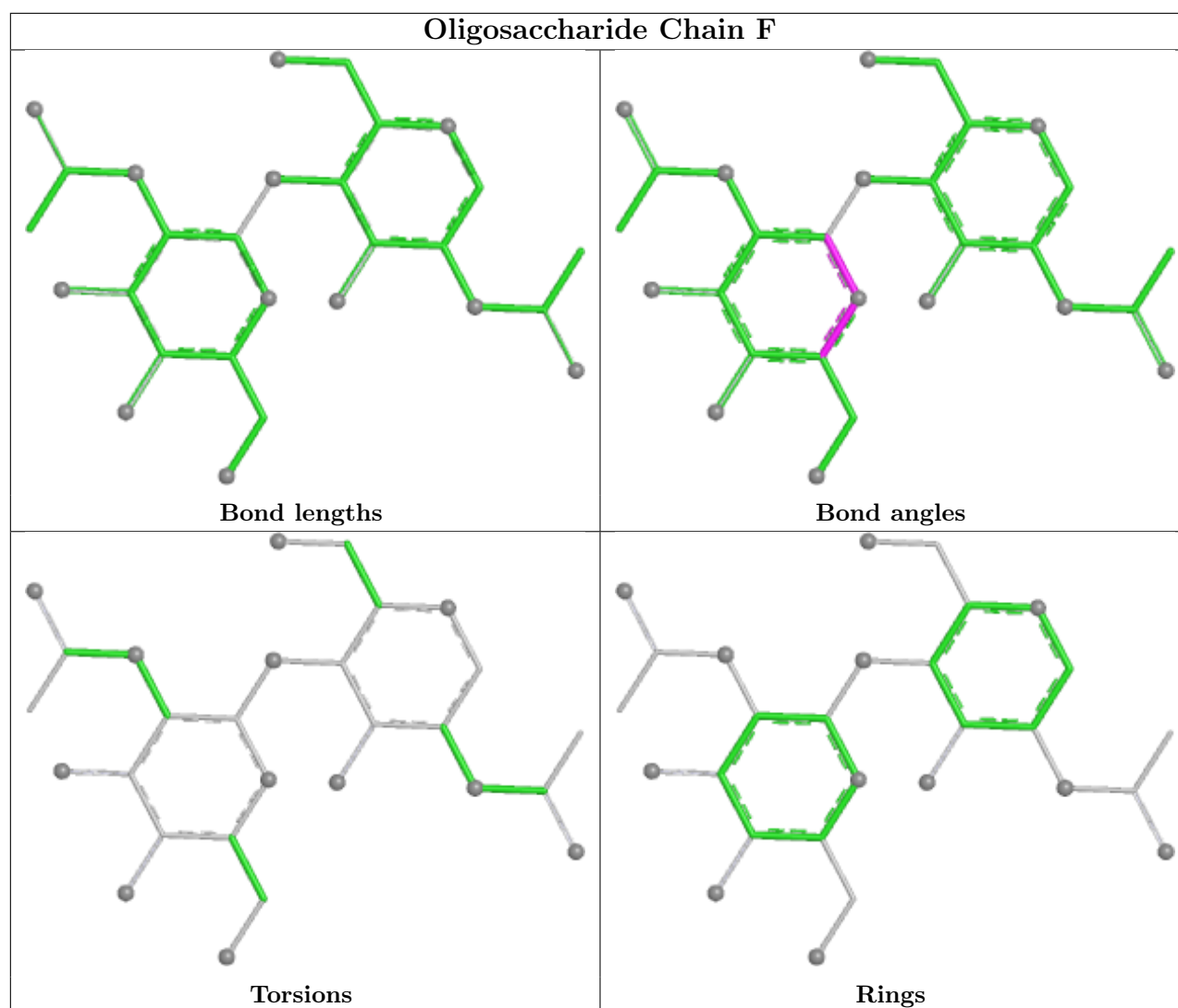
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	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](#)

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	$\# Z > 2$
7	NAG	A	301	1	14,14,15	0.31	0	17,19,21	0.88	1 (5%)
7	NAG	A	302	1	14,14,15	0.39	0	17,19,21	1.08	2 (11%)
7	NAG	B	301	1	14,14,15	0.27	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	B	302	1	14,14,15	0.38	0	17,19,21	0.50	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
7	NAG	A	301	1	-	0/6/23/26	0/1/1/1
7	NAG	A	302	1	-	0/6/23/26	0/1/1/1
7	NAG	B	301	1	-	1/6/23/26	0/1/1/1
7	NAG	B	302	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	302	NAG	C1-C2-N2	3.41	115.81	110.43
7	A	302	NAG	C1-O5-C5	2.61	115.69	112.19
7	A	301	NAG	C1-C2-N2	-2.57	106.38	110.43

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	301	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	302	NAG	1	0

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	213/226 (94%)	0.81	40 (18%) 3 3	22, 41, 99, 118	12 (5%)
1	B	220/226 (97%)	0.82	21 (9%) 14 14	22, 49, 73, 89	10 (4%)
2	D	205/239 (85%)	0.74	17 (8%) 17 18	23, 48, 66, 76	11 (5%)
3	G	230/252 (91%)	1.60	72 (31%) 1 1	27, 57, 83, 106	22 (9%)
All	All	868/943 (92%)	1.01	150 (17%) 4 4	22, 50, 82, 118	55 (6%)

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	28	ILE	7.1
3	G	160	PHE	5.3
3	G	176	ILE	5.3
3	G	30	ILE	5.3
1	A	78	GLY	5.0
1	A	25	LEU	4.9
3	G	33	THR	4.9
1	A	3	ILE	4.7
3	G	76	GLU	4.7
3	G	27	GLY	4.6
1	A	53	GLY	4.5
1	A	75	ILE	4.5
3	G	54	TYR	4.3
3	G	123	ASP	4.2
3	G	221	VAL	4.2
3	G	161	PRO	4.1
1	A	27	PRO	4.0
3	G	9	ILE	4.0
1	A	57	THR	3.9
1	B	196	THR	3.9
3	G	32	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
3	G	26	SER	3.9
3	G	77	THR	3.9
2	D	43	GLY	3.8
1	A	99	PHE	3.8
3	G	159	PHE	3.8
3	G	173	SER	3.7
2	D	44	ASN	3.7
3	G	102	ALA	3.7
2	D	42	GLN	3.7
3	G	31	SER	3.6
1	A	28	GLU	3.6
3	G	231	LYS	3.6
3	G	25	VAL	3.5
1	A	73	LYS	3.5
1	A	101	GLU	3.5
1	B	68	THR	3.4
3	G	121	ILE	3.4
1	B	50	TYR	3.4
3	G	122	THR	3.4
3	G	230	ILE	3.4
1	A	30	ASN	3.4
1	A	102	GLY	3.4
2	D	45	THR	3.3
1	A	31	ALA	3.3
3	G	74	ILE	3.3
3	G	213	ARG	3.3
1	B	174	MET	3.3
1	B	217	SER	3.3
3	G	163	VAL	3.3
3	G	78	SER	3.2
1	B	12	LEU	3.2
1	A	52	GLY	3.2
1	A	154	TYR	3.2
3	G	164	ILE	3.2
1	A	33	ASP	3.2
3	G	24	VAL	3.2
3	G	29	THR	3.2
3	G	222	ASP	3.1
3	G	191	TYR	3.1
2	D	171	PRO	3.1
3	G	174	ASN	3.1
3	G	204	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	15	VAL	3.0
3	G	175	THR	2.9
3	G	146	LEU	2.9
2	D	15	ILE	2.9
3	G	14	THR	2.8
1	A	29	LYS	2.8
3	G	172	LYS	2.8
1	B	103	ARG	2.8
1	A	5	VAL	2.8
3	G	112	VAL	2.8
1	A	76	SER	2.7
3	G	220	GLY	2.7
3	G	192	MET	2.7
1	A	105	TYR	2.7
1	A	54	ARG	2.7
3	G	8	GLN	2.7
1	A	23	CYS	2.7
2	D	119	PRO	2.6
3	G	124	LYS	2.6
1	A	70	PHE	2.6
1	A	56	ARG	2.6
2	D	17	VAL	2.6
3	G	7	PRO	2.6
3	G	126	LEU	2.6
1	A	100	GLN	2.6
1	B	3	ILE	2.6
3	G	165	LYS	2.6
2	D	163	PHE	2.5
1	B	154	TYR	2.5
3	G	89	LYS	2.5
3	G	171	LYS	2.5
3	G	130	VAL	2.5
1	B	130	ASP	2.5
1	B	197	LEU	2.5
1	B	11	ILE	2.5
3	G	120	ILE	2.5
3	G	219	ASN	2.5
3	G	105	GLU	2.4
3	G	180	GLN	2.4
3	G	224	GLU	2.4
3	G	128	ALA	2.4
2	D	153	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	33	ASP	2.4
3	G	73	ARG	2.4
3	G	177	LEU	2.4
2	D	60	PHE	2.4
1	A	4	VAL	2.4
1	A	71	VAL	2.4
1	B	54	ARG	2.4
2	D	13	VAL	2.4
1	A	215	SER	2.4
3	G	5	GLU	2.3
3	G	101	GLU	2.3
2	D	187	ASN	2.3
2	D	159	LYS	2.3
1	B	72	SER	2.3
1	A	49	VAL	2.3
1	A	74	ASP	2.3
3	G	217	ASN	2.3
1	A	72	SER	2.2
3	G	10	SER	2.2
1	B	57	THR	2.2
2	D	84	GLU	2.2
3	G	127	ASP	2.2
1	B	52	GLY	2.2
3	G	67	GLY	2.2
1	A	103	ARG	2.2
1	A	50	TYR	2.2
2	D	174	LYS	2.2
3	G	211	ILE	2.1
3	G	227	PHE	2.1
1	A	47	VAL	2.1
1	A	51	LYS	2.1
1	A	55	GLU	2.1
3	G	200	PRO	2.1
1	B	70	PHE	2.1
3	G	166	ILE	2.1
3	G	212	VAL	2.1
1	A	34	MET	2.1
1	B	58	GLU	2.1
2	D	58	PRO	2.1
1	A	155	GLY	2.1
3	G	104	GLN	2.1
3	G	125	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	69	THR	2.1
1	A	48	PHE	2.0
3	G	62	SER	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](#)

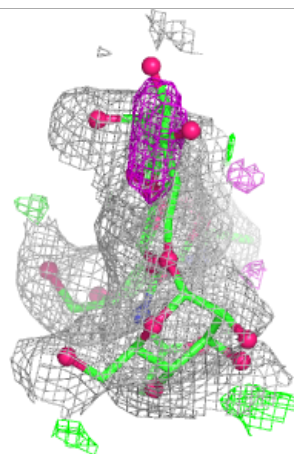
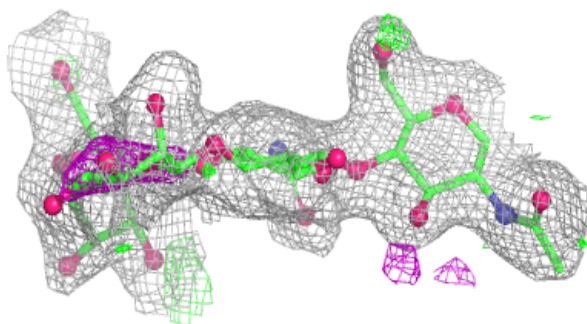
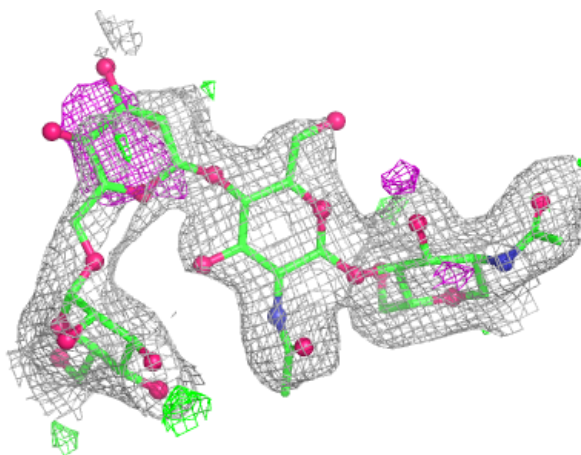
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NAG	C	1	14/15	-	-	43,46,50,55	0
4	NAG	C	2	14/15	-	-	59,62,66,70	0
4	BMA	C	3	11/12	-	-	73,76,78,79	0
4	MAN	C	4	11/12	-	-	80,80,81,81	0
5	BMA	E	3	11/12	0.45	0.21	75,77,78,78	0
5	NAG	E	2	14/15	0.81	0.15	65,67,70,73	0
6	NAG	F	2	14/15	0.82	0.14	70,74,75,76	0
6	NAG	F	1	14/15	0.91	0.12	56,59,62,66	0
5	NAG	E	1	14/15	0.92	0.10	54,55,58,62	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.

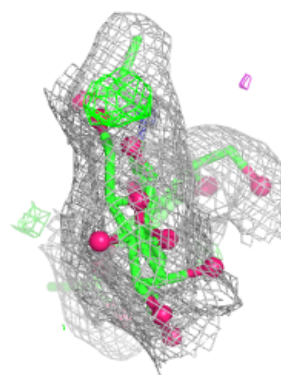
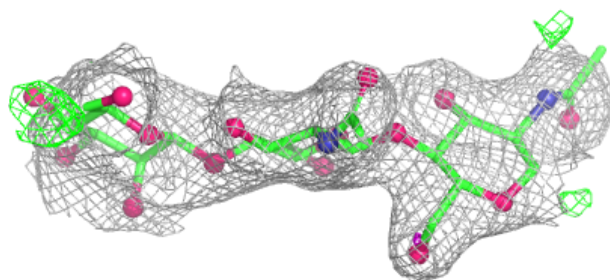
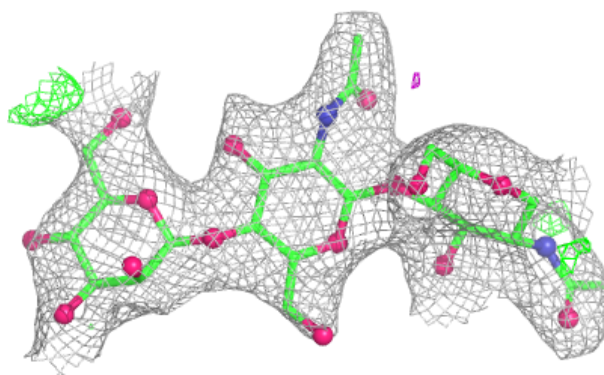
Electron density around Chain C:

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

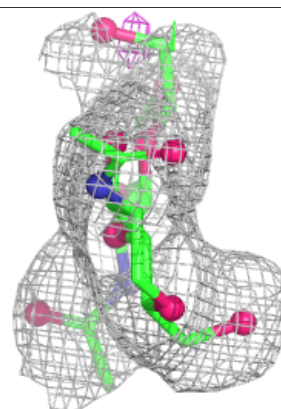
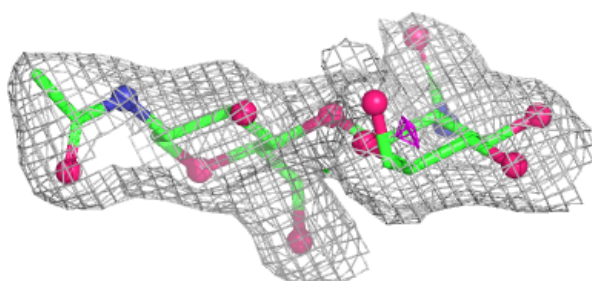
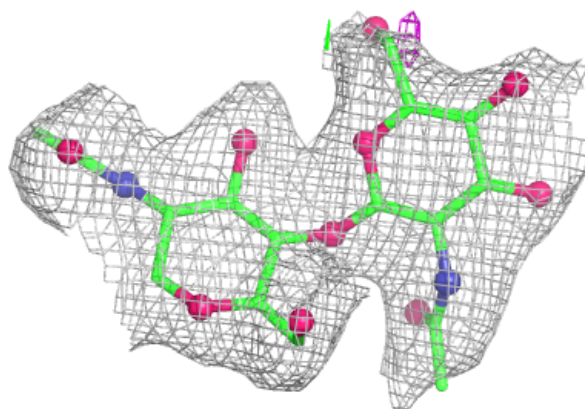


Electron density around Chain E:

$2mF_o - DF_c$ (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 [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
7	NAG	B	301	14/15	0.55	0.18	76,78,79,79	0
7	NAG	A	301	14/15	0.64	0.14	78,81,81,81	0
7	NAG	A	302	14/15	0.69	0.16	89,92,93,93	0
7	NAG	B	302	14/15	0.78	0.14	61,63,65,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.