



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 19, 2022 – 08:08 AM EST

PDB ID : 6XC9
Title : Immune receptor complex
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Tresoldi, M.C.E.; Cameron, J.F.; La-Gruta, L.N.; Purcell, W.A.; Mannering,
I.S.; Rossjohn, J.; Reid, H.H.
Deposited on : 2020-06-08
Resolution : 2.40 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 : 2.25
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) : 2.25

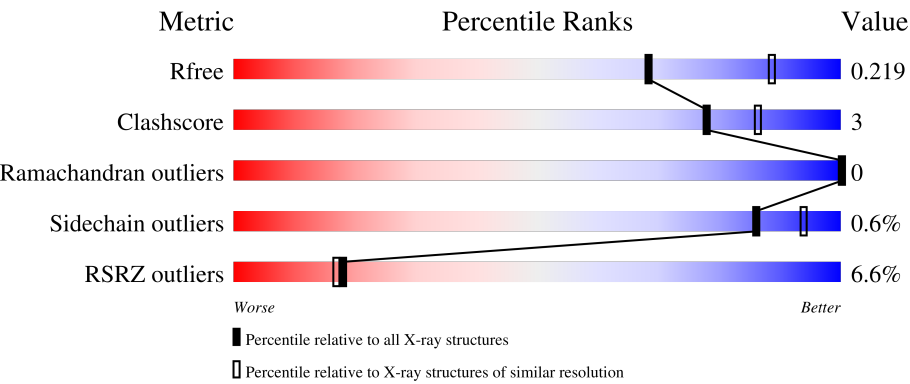
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	193	<div><div>3%</div><div></div><div>89%</div><div>7%</div><div>5%</div></div>
1	F	193	<div><div>2%</div><div></div><div>87%</div><div>7%</div><div>6%</div></div>
2	C	230	<div><div>14%</div><div></div><div>79%</div><div>7%</div><div>14%</div></div>
2	H	230	<div><div>3%</div><div></div><div>77%</div><div>8%</div><div>15%</div></div>
3	D	208	<div><div>13%</div><div></div><div>90%</div><div>8%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
3	I	208	
4	E	245	
4	J	245	
5	B	3	
6	G	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	B	2	-	-	-	X
5	MAN	B	3	-	-	-	X
6	NAG	G	1	-	-	-	X
6	NAG	G	2	-	-	-	X
7	NAG	A	204	-	-	-	X
7	NAG	C	302	-	-	-	X
7	NAG	F	204	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13543 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 MHC class II HLA-DQ-alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	0	0
			1479	950	243	283	3			
1	F	182	Total	C	N	O	S	0	0	0
			1463	941	241	278	3			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	CYS	ILE	engineered mutation	UNP Q30069
A	182	SER	-	expression tag	UNP Q30069
A	183	THR	-	expression tag	UNP Q30069
A	184	GLY	-	expression tag	UNP Q30069
A	185	GLY	-	expression tag	UNP Q30069
A	186	ASP	-	expression tag	UNP Q30069
A	187	ASP	-	expression tag	UNP Q30069
A	188	ASP	-	expression tag	UNP Q30069
A	189	ASP	-	expression tag	UNP Q30069
A	190	LYS	-	expression tag	UNP Q30069
F	72	CYS	ILE	engineered mutation	UNP Q30069
F	182	SER	-	expression tag	UNP Q30069
F	183	THR	-	expression tag	UNP Q30069
F	184	GLY	-	expression tag	UNP Q30069
F	185	GLY	-	expression tag	UNP Q30069
F	186	ASP	-	expression tag	UNP Q30069
F	187	ASP	-	expression tag	UNP Q30069
F	188	ASP	-	expression tag	UNP Q30069
F	189	ASP	-	expression tag	UNP Q30069
F	190	LYS	-	expression tag	UNP Q30069

- Molecule 2 is a protein called Hybrid Insulin Peptide, MHC class II HLA-DQ-beta chain fusion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	198	Total 1520	C 956	N 266	O 291	S 7	0	0	0
2	H	196	Total 1582	C 1000	N 276	O 298	S 8	0	1	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	14A	GLY	-	linker	PDB ?
C	14B	GLY	-	linker	PDB ?
C	14C	SER	-	linker	PDB ?
C	14D	ILE	-	linker	PDB ?
C	14E	GLU	-	linker	PDB ?
C	14F	GLY	-	linker	PDB ?
C	14G	ARG	-	linker	PDB ?
C	14H	GLY	-	linker	PDB ?
C	14I	GLY	-	linker	PDB ?
C	14J	SER	-	linker	PDB ?
C	14K	GLY	-	linker	PDB ?
C	14L	ALA	-	linker	PDB ?
C	14M	SER	-	linker	PDB ?
C	207	THR	-	expression tag	UNP A0A6B9KAL0
C	208	GLY	-	expression tag	UNP A0A6B9KAL0
C	209	GLY	-	expression tag	UNP A0A6B9KAL0
C	210	ASP	-	expression tag	UNP A0A6B9KAL0
C	211	ASP	-	expression tag	UNP A0A6B9KAL0
C	212	ASP	-	expression tag	UNP A0A6B9KAL0
C	213	ASP	-	expression tag	UNP A0A6B9KAL0
C	214	LYS	-	expression tag	UNP A0A6B9KAL0
H	14A	GLY	-	linker	PDB ?
H	14B	GLY	-	linker	PDB ?
H	14C	SER	-	linker	PDB ?
H	14D	ILE	-	linker	PDB ?
H	14E	GLU	-	linker	PDB ?
H	14F	GLY	-	linker	PDB ?
H	14G	ARG	-	linker	PDB ?
H	14H	GLY	-	linker	PDB ?
H	14I	GLY	-	linker	PDB ?
H	14J	SER	-	linker	PDB ?
H	14K	GLY	-	linker	PDB ?
H	14L	ALA	-	linker	PDB ?
H	14M	SER	-	linker	PDB ?
H	207	THR	-	expression tag	UNP A0A6B9KAL0

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Chain	Residue	Modelled	Actual	Comment	Reference
H	208	GLY	-	expression tag	UNP A0A6B9KAL0
H	209	GLY	-	expression tag	UNP A0A6B9KAL0
H	210	ASP	-	expression tag	UNP A0A6B9KAL0
H	211	ASP	-	expression tag	UNP A0A6B9KAL0
H	212	ASP	-	expression tag	UNP A0A6B9KAL0
H	213	ASP	-	expression tag	UNP A0A6B9KAL0
H	214	LYS	-	expression tag	UNP A0A6B9KAL0

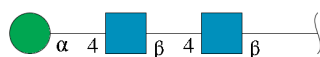
- Molecule 3 is a protein called T-CELL-RECEPTOR, A3.10-alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	203	Total	C	N	O	S	0	0	0
			1537	968	251	309	9			
3	I	204	Total	C	N	O	S	0	0	0
			1591	1001	260	320	10			

- Molecule 4 is a protein called T-CELL-RECEPTOR, A3.10-beta chain.

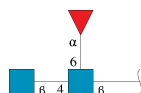
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	244	Total	C	N	O	S	0	1	0
			1903	1198	339	360	6			
4	J	244	Total	C	N	O	S	0	1	0
			1902	1196	338	362	6			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



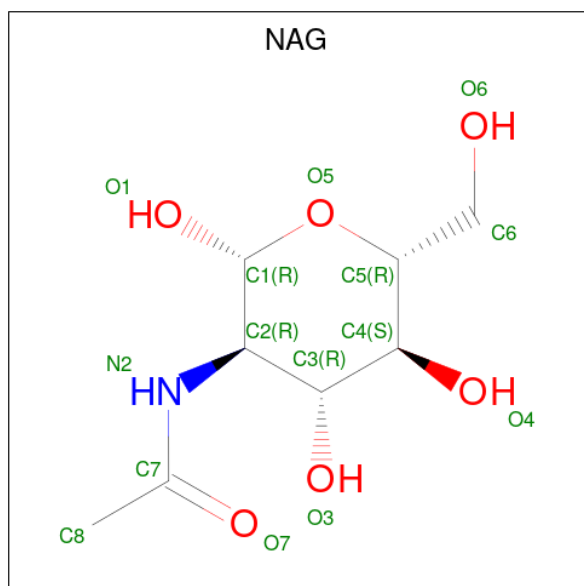
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	3	Total	C	N	O		0	0	0
			39	22	2	15				

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	G	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		
8	F	1	Total	C	O	0	0
			6	3	3		
8	F	1	Total	C	O	0	0
			6	3	3		
8	H	1	Total	C	O	0	0
			6	3	3		
8	I	1	Total	C	O	0	0
			6	3	3		
8	I	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	48	Total	O	0	0
			48	48		
9	C	40	Total	O	0	0
			40	40		
9	D	40	Total	O	0	0
			40	40		
9	E	58	Total	O	0	0
			58	58		
9	F	54	Total	O	0	0
			54	54		

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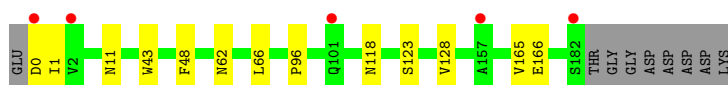
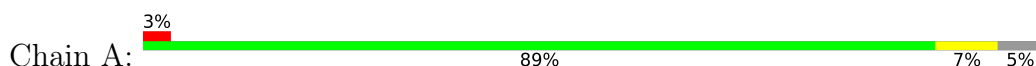
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	51	Total 51	O 51	0	0
9	I	44	Total 44	O 44	0	0
9	J	56	Total 56	O 56	0	0

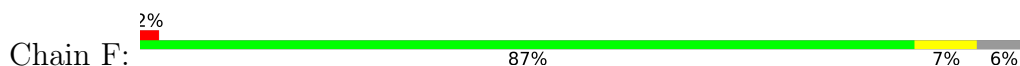
3 Residue-property plots [i](#)

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.

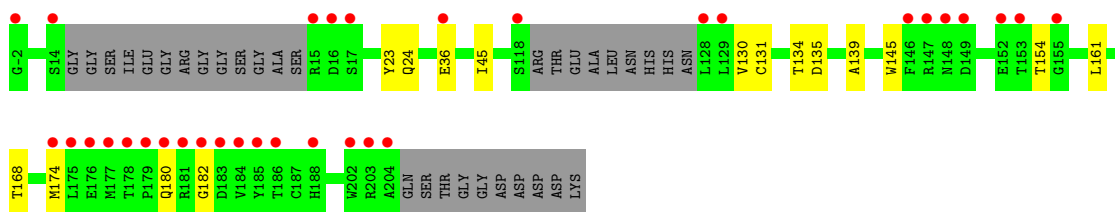
- Molecule 1: MHC class II HLA-DQ-alpha chain



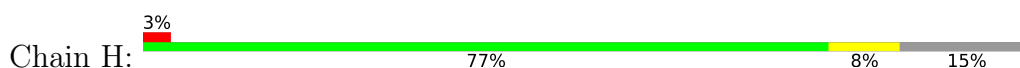
- Molecule 1: MHC class II HLA-DQ-alpha chain



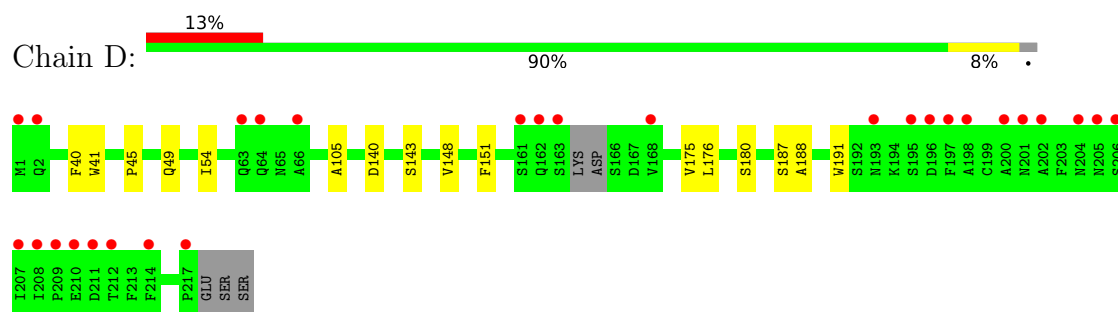
- Molecule 2: Hybrid Insulin Peptide, MHC class II HLA-DQ-beta chain fusion



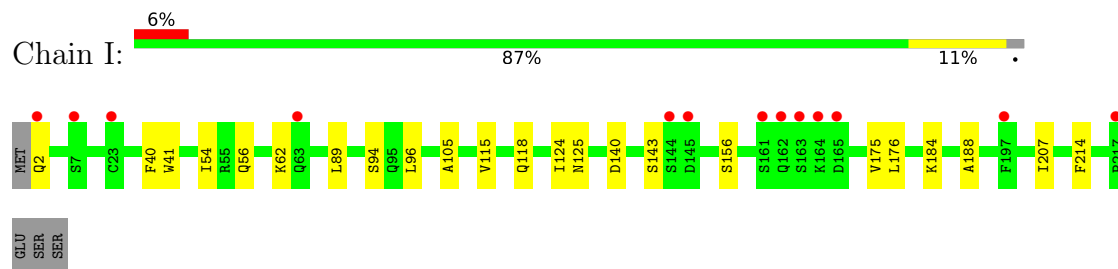
- Molecule 2: Hybrid Insulin Peptide, MHC class II HLA-DQ-beta chain fusion



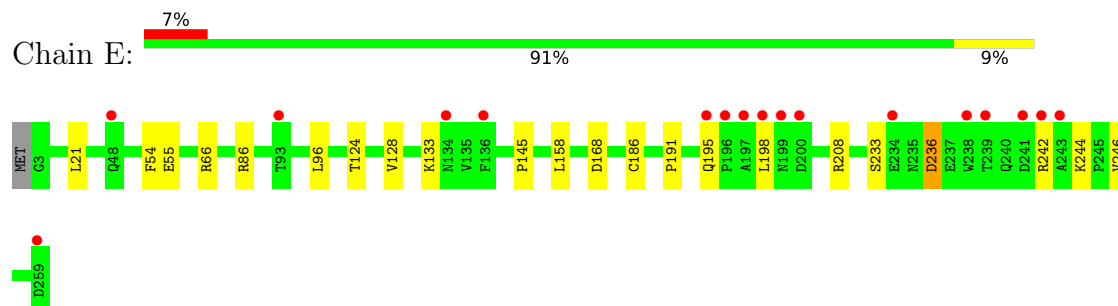
- Molecule 3: T-CELL-RECEPTOR, A3.10-alpha chain



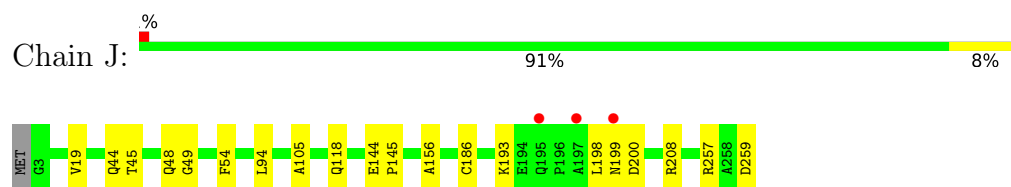
- Molecule 3: T-CELL-RECEPTOR, A3.10-alpha chain



- Molecule 4: T-CELL-RECEPTOR, A3.10-beta chain



- Molecule 4: T-CELL-RECEPTOR, A3.10-beta chain



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



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.99Å 114.79Å 153.93Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	46.01 – 2.40 46.01 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.01-2.40) 100.0 (46.01-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.184 , 0.219 0.184 , 0.219	Depositor DCC
R_{free} test set	4465 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13543	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: FUC, NAG, GOL, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.29	0/1523	0.47	0/2079
1	F	0.29	0/1507	0.48	0/2058
2	C	0.27	0/1552	0.48	0/2117
2	H	0.27	0/1621	0.48	0/2208
3	D	0.29	0/1570	0.48	0/2136
3	I	0.29	0/1626	0.49	0/2207
4	E	0.29	0/1954	0.47	0/2660
4	J	0.30	0/1953	0.48	0/2659
All	All	0.29	0/13306	0.48	0/18124

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	1479	0	1402	9	0
1	F	1463	0	1389	8	0
2	C	1520	0	1394	8	0
2	H	1582	0	1520	11	0
3	D	1537	0	1397	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	1591	0	1485	13	0
4	E	1903	0	1793	14	0
4	J	1902	0	1787	12	0
5	B	39	0	34	1	0
6	G	38	0	34	1	0
7	A	14	0	13	0	0
7	C	14	0	13	0	0
7	F	28	0	26	0	0
8	C	6	0	8	0	0
8	D	6	0	8	1	0
8	F	12	0	16	0	0
8	H	6	0	8	0	0
8	I	12	0	16	0	0
9	A	48	0	0	0	0
9	C	40	0	0	0	0
9	D	40	0	0	0	0
9	E	58	0	0	0	0
9	F	54	0	0	0	0
9	H	51	0	0	0	0
9	I	44	0	0	0	0
9	J	56	0	0	0	0
All	All	13543	0	12343	73	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (73) 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)
2:C:130:VAL:HG22	2:C:174:MET:HG2	1.71	0.72
3:D:41:TRP:HB2	3:D:54:ILE:HG22	1.75	0.68
3:I:41:TRP:HB2	3:I:54:ILE:HG22	1.77	0.66
3:I:125:ASN:HB3	3:I:156:SER:HB3	1.78	0.66
2:H:130:VAL:HG22	2:H:174:MET:HG2	1.76	0.66
3:I:176:LEU:HB3	4:J:186:CYS:HB2	1.77	0.66
3:D:40:PHE:HB2	3:D:105:ALA:HB3	1.79	0.64
2:C:24:GLN:HB2	2:C:45:ILE:HB	1.80	0.64
2:H:24:GLN:HB2	2:H:45:ILE:HB	1.81	0.63
1:A:118:ASN:HB2	1:A:166:GLU:HB2	1.81	0.62
4:E:233:SER:HB3	4:E:236:ASP:OD1	1.99	0.62
1:F:89:VAL:O	1:F:176:LYS:NZ	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:94:SER:HB3	3:I:124:ILE:HD12	1.86	0.58
1:F:43:TRP:CE3	1:F:48:PHE:HB3	2.40	0.56
3:I:40:PHE:HB2	3:I:105:ALA:HB3	1.87	0.55
1:F:11:ASN:HB3	1:F:66:LEU:HD11	1.89	0.55
2:H:33:ASN:ND2	6:G:1:NAG:H61	2.21	0.55
3:I:2:GLN:OE1	3:I:118:GLN:NE2	2.39	0.55
1:A:43:TRP:CE3	1:A:48:PHE:HB3	2.43	0.54
4:E:133:LYS:O	4:E:242:ARG:NH2	2.38	0.54
3:D:176:LEU:HB3	4:E:186:CYS:HB2	1.89	0.53
1:A:96:PRO:HD3	2:C:134:THR:HG21	1.91	0.52
1:F:96:PRO:HD3	2:H:134:THR:HG21	1.92	0.52
1:A:166:GLU:HB3	5:B:1:NAG:H83	1.92	0.51
1:F:118:ASN:HB2	1:F:166:GLU:HB2	1.92	0.50
4:E:145:PRO:HD3	4:E:158:LEU:HG	1.94	0.49
1:A:66:LEU:HD22	2:C:23:TYR:CD1	2.47	0.49
1:A:11:ASN:HB3	1:A:66:LEU:HD11	1.95	0.48
2:C:139:ALA:HB1	2:C:161:LEU:HD21	1.95	0.48
3:D:45:PRO:HD2	3:D:49:GLN:O	2.14	0.48
3:D:188:ALA:HA	4:E:208:ARG:HH11	1.79	0.48
2:H:180:GLN:HG2	2:H:183:ASP:OD2	2.13	0.47
3:I:96:LEU:HD11	3:I:184:LYS:HD3	1.95	0.47
2:H:142:LYS:HB2	2:H:190:GLU:HB2	1.96	0.47
3:D:140:ASP:HB3	3:D:143:SER:O	2.16	0.46
3:D:180:SER:H	8:D:301:GOL:H32	1.81	0.46
3:I:140:ASP:HB3	3:I:143:SER:O	2.16	0.46
4:J:145:PRO:HG3	4:J:156:ALA:HB1	1.97	0.45
1:F:0:ASP:OD1	1:F:1:ILE:N	2.47	0.45
4:E:86:ARG:HE	4:J:259:ASP:C	2.20	0.45
3:I:41:TRP:CE2	3:I:89:LEU:HB2	2.51	0.45
3:I:175:VAL:N	4:J:186:CYS:SG	2.90	0.45
4:J:193:LYS:NZ	4:J:199:ASN:HA	2.32	0.45
3:D:188:ALA:HA	4:E:208:ARG:NH1	2.33	0.44
4:E:21:LEU:HD22	4:E:124:THR:HG21	2.00	0.44
3:I:188:ALA:HA	4:J:208:ARG:HH11	1.83	0.44
4:E:195:GLN:HB3	4:E:198:LEU:HD13	2.00	0.44
4:J:19:VAL:HG13	4:J:94:LEU:HD11	1.99	0.43
4:E:55:GLU:OE2	4:E:66:ARG:HB2	2.18	0.43
2:H:101:LEU:O	2:H:106:GLN:HG2	2.19	0.43
2:H:147:ARG:NH2	2:H:183:ASP:OD2	2.51	0.43
4:E:168:ASP:HB2	4:E:191:PRO:HG2	2.00	0.43
4:E:96:LEU:HD23	4:E:128:VAL:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ASN:O	1:A:165:VAL:HA	2.20	0.42
3:I:56:GLN:NE2	3:I:62:LYS:O	2.52	0.42
1:F:9(A):GLY:O	2:H:26:LYS:HA	2.20	0.42
1:F:26:PHE:CD2	2:H:104:THR:HG21	2.55	0.42
2:H:135:ASP:HA	2:H:168:THR:HB	2.02	0.41
4:J:144:GLU:OE1	4:J:257:ARG:NE	2.53	0.41
3:I:207:ILE:HG21	3:I:214:PHE:HZ	1.86	0.41
4:J:105:ALA:HB1	4:J:118:GLN:HB3	2.01	0.41
4:J:44:GLN:HA	4:J:49:GLY:O	2.21	0.41
1:A:0:ASP:OD1	1:A:1:ILE:N	2.52	0.41
1:A:123:SER:HB3	1:A:128:VAL:HG21	2.03	0.41
2:C:135:ASP:HA	2:C:168:THR:HB	2.03	0.41
4:J:45:THR:OG1	4:J:48:GLN:HB2	2.21	0.40
4:J:198:LEU:C	4:J:200:ASP:H	2.23	0.40
2:C:180:GLN:HG3	2:C:182:GLY:H	1.86	0.40
4:E:244:LYS:HG2	4:E:246:VAL:HG13	2.03	0.40
3:D:175:VAL:N	4:E:186:CYS:SG	2.95	0.40
2:C:131:CYS:HB2	2:C:145:TRP:CZ2	2.57	0.40
3:D:148:VAL:HG12	3:D:191:TRP:HB3	2.04	0.40
3:D:151:PHE:O	3:D:187:SER:HA	2.21	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	182/193 (94%)	178 (98%)	4 (2%)	0	100	100
1	F	180/193 (93%)	177 (98%)	3 (2%)	0	100	100
2	C	192/230 (84%)	187 (97%)	5 (3%)	0	100	100
2	H	191/230 (83%)	186 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	199/208 (96%)	194 (98%)	5 (2%)	0	100	100
3	I	202/208 (97%)	197 (98%)	5 (2%)	0	100	100
4	E	243/245 (99%)	238 (98%)	5 (2%)	0	100	100
4	J	243/245 (99%)	238 (98%)	5 (2%)	0	100	100
All	All	1632/1752 (93%)	1595 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	167/176 (95%)	166 (99%)	1 (1%)	86	94
1	F	165/176 (94%)	164 (99%)	1 (1%)	86	94
2	C	155/200 (78%)	153 (99%)	2 (1%)	69	84
2	H	173/200 (86%)	172 (99%)	1 (1%)	86	94
3	D	163/189 (86%)	163 (100%)	0	100	100
3	I	177/189 (94%)	176 (99%)	1 (1%)	86	94
4	E	203/212 (96%)	201 (99%)	2 (1%)	76	88
4	J	203/212 (96%)	202 (100%)	1 (0%)	88	95
All	All	1406/1554 (90%)	1397 (99%)	9 (1%)	86	94

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
2	C	36	GLU
2	C	154	THR
4	E	54	PHE
4	E	236	ASP
1	F	62	ASN

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Mol	Chain	Res	Type
2	H	36	GLU
3	I	115	VAL
4	J	54	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	180	GLN

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	$\# Z > 2$
5	NAG	B	1	1,5	14,14,15	0.49	0	17,19,21	0.56	0
5	NAG	B	2	5	14,14,15	0.26	0	17,19,21	0.52	0
5	MAN	B	3	5	11,11,12	0.78	0	15,15,17	1.08	2 (13%)
6	NAG	G	1	6,2	14,14,15	0.76	1 (7%)	17,19,21	1.69	3 (17%)
6	NAG	G	2	6	14,14,15	0.55	0	17,19,21	0.59	0
6	FUC	G	3	6	10,10,11	1.15	1 (10%)	14,14,16	1.35	3 (21%)

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	B	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	B	2	5	-	4/6/23/26	0/1/1/1
5	MAN	B	3	5	-	0/2/19/22	1/1/1/1
6	NAG	G	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	G	2	6	-	2/6/23/26	0/1/1/1
6	FUC	G	3	6	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	1	NAG	O5-C1	-2.55	1.39	1.43
6	G	3	FUC	C2-C3	2.28	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	1	NAG	C3-C4-C5	4.60	118.44	110.24
6	G	1	NAG	C4-C3-C2	3.97	116.83	111.02
5	B	3	MAN	C1-O5-C5	2.78	115.96	112.19
6	G	1	NAG	C1-O5-C5	2.75	115.92	112.19
6	G	3	FUC	O5-C5-C4	2.48	113.96	109.52
6	G	3	FUC	C1-C2-C3	2.37	112.58	109.67
6	G	3	FUC	C1-O5-C5	2.22	117.80	112.78
5	B	3	MAN	O2-C2-C3	-2.20	105.72	110.14

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	1	NAG	C4-C5-C6-O6
5	B	1	NAG	C8-C7-N2-C2
5	B	1	NAG	O7-C7-N2-C2
5	B	2	NAG	C8-C7-N2-C2
5	B	2	NAG	O7-C7-N2-C2
6	G	2	NAG	C8-C7-N2-C2
6	G	2	NAG	O7-C7-N2-C2
5	B	2	NAG	O5-C5-C6-O6
6	G	1	NAG	O5-C5-C6-O6
5	B	2	NAG	C4-C5-C6-O6

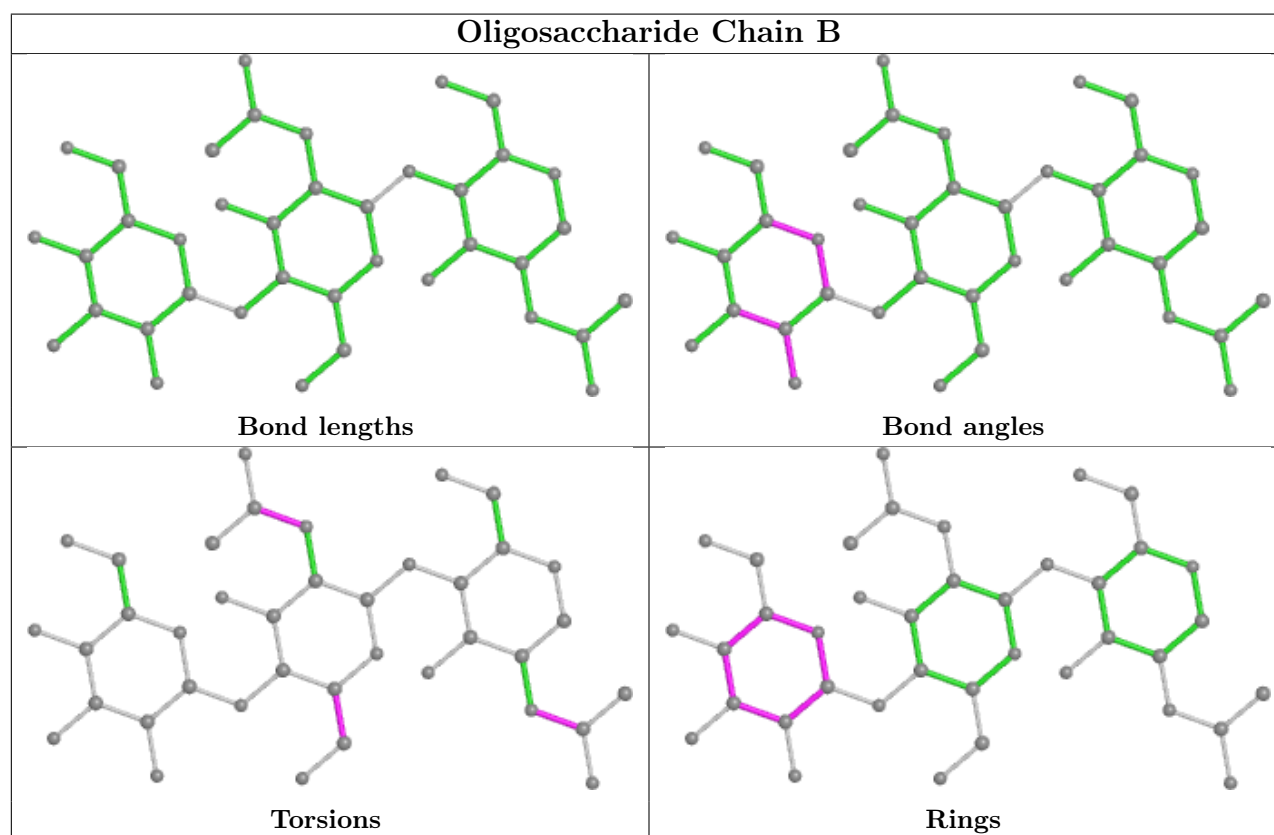
All (1) ring outliers are listed below:

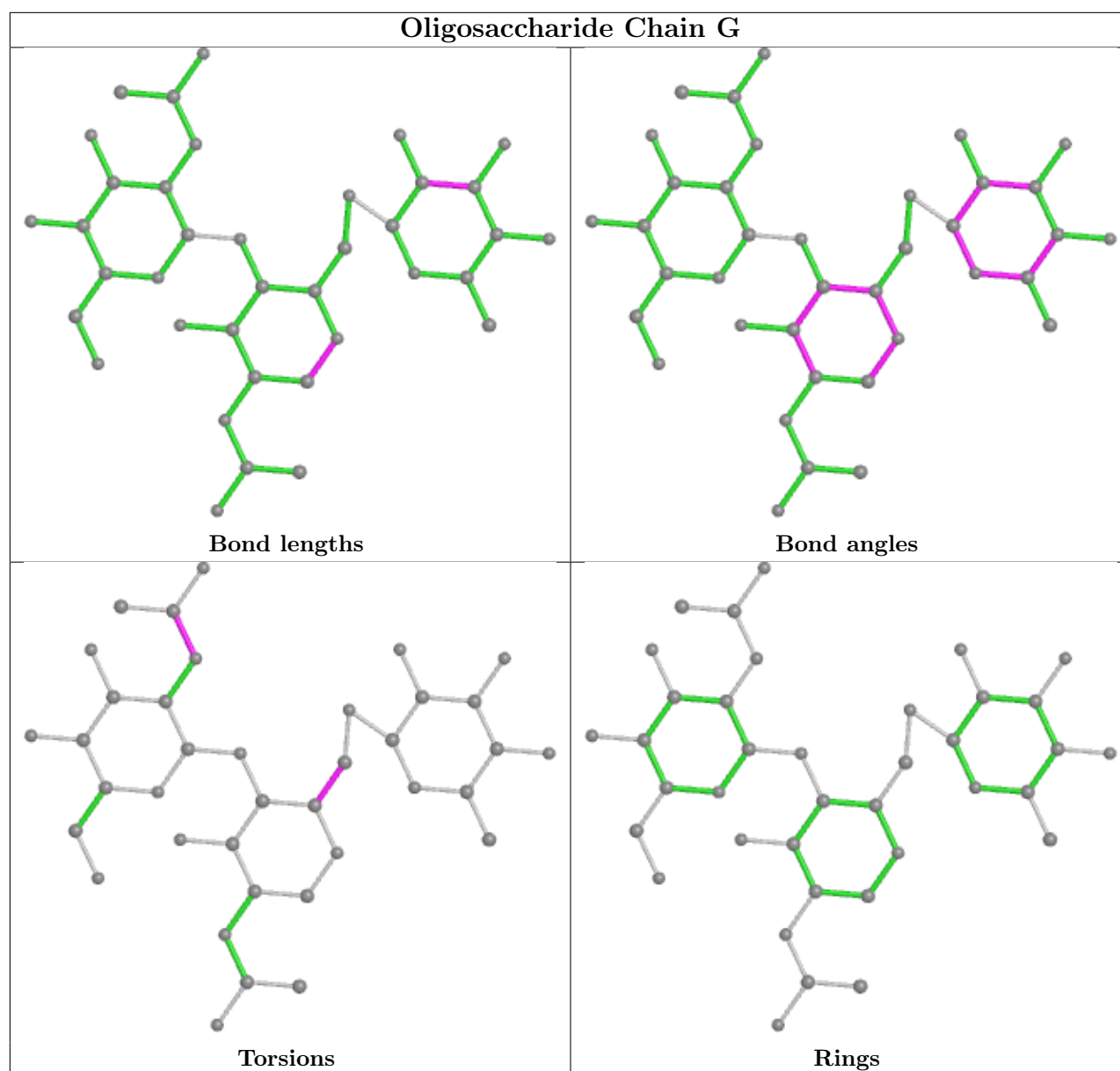
Mol	Chain	Res	Type	Atoms
5	B	3	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	1	NAG	1	0
5	B	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](#)

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GOL	C	301	-	5,5,5	0.96	0	5,5,5	1.04	0
7	NAG	C	302	2	14,14,15	0.28	0	17,19,21	0.50	0
8	GOL	I	302	-	5,5,5	1.02	0	5,5,5	0.90	0
8	GOL	H	304	-	5,5,5	0.82	0	5,5,5	1.08	0
8	GOL	I	301	-	5,5,5	0.96	0	5,5,5	0.98	0
8	GOL	D	301	-	5,5,5	0.82	0	5,5,5	1.04	0
7	NAG	F	204	1	14,14,15	0.33	0	17,19,21	0.58	0
8	GOL	F	201	-	5,5,5	0.94	0	5,5,5	0.99	0
7	NAG	F	203	1	14,14,15	0.34	0	17,19,21	0.47	0
8	GOL	F	202	-	5,5,5	0.94	0	5,5,5	0.98	0
7	NAG	A	204	1	14,14,15	0.39	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
8	GOL	C	301	-	-	0/4/4/4	-
7	NAG	C	302	2	-	0/6/23/26	0/1/1/1
8	GOL	I	302	-	-	0/4/4/4	-
8	GOL	H	304	-	-	0/4/4/4	-
8	GOL	I	301	-	-	0/4/4/4	-
8	GOL	D	301	-	-	4/4/4/4	-
7	NAG	F	204	1	-	1/6/23/26	0/1/1/1
8	GOL	F	201	-	-	1/4/4/4	-
7	NAG	F	203	1	-	1/6/23/26	0/1/1/1
8	GOL	F	202	-	-	0/4/4/4	-
7	NAG	A	204	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	301	GOL	O1-C1-C2-C3
8	D	301	GOL	C1-C2-C3-O3
8	D	301	GOL	O1-C1-C2-O2
8	D	301	GOL	O2-C2-C3-O3
7	F	203	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	F	204	NAG	C3-C2-N2-C7
8	F	201	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	301	GOL	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	184/193 (95%)	0.32	5 (2%) 54 52	27, 41, 74, 110	0
1	F	182/193 (94%)	0.18	4 (2%) 62 60	26, 40, 75, 99	0
2	C	198/230 (86%)	0.81	33 (16%) 1 1	28, 45, 103, 138	0
2	H	196/230 (85%)	0.12	7 (3%) 42 42	29, 40, 78, 121	0
3	D	203/208 (97%)	0.62	28 (13%) 2 2	30, 52, 93, 108	0
3	I	204/208 (98%)	0.35	13 (6%) 19 18	30, 49, 91, 124	0
4	E	244/245 (99%)	0.39	17 (6%) 16 15	29, 49, 86, 113	0
4	J	244/245 (99%)	0.25	3 (1%) 79 77	30, 44, 81, 124	0
All	All	1655/1752 (94%)	0.38	110 (6%) 18 17	26, 45, 88, 138	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	16	ASP	7.3
2	C	181	ARG	6.4
2	C	179	PRO	6.3
3	D	200	ALA	6.2
4	E	241	ASP	6.2
2	C	177	MET	6.2
3	I	161	SER	5.9
2	C	15	ARG	5.6
2	H	17	SER	5.4
2	C	182	GLY	5.4
2	C	185	TYR	5.3
3	D	1	MET	5.2
2	C	204	ALA	5.1
4	E	259	ASP	5.0
3	D	217	PRO	4.8
2	C	17	SER	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	182	SER	4.7
2	C	202	TRP	4.7
2	C	180	GLN	4.6
3	D	168	VAL	4.4
4	J	197	ALA	4.2
2	H	180	GLN	4.2
3	D	197	PHE	4.2
3	D	208	ILE	4.2
3	D	205	ASN	4.1
3	I	63	GLN	4.1
1	A	2	VAL	4.1
3	I	217	PRO	3.9
3	D	212	THR	3.8
2	C	128	LEU	3.8
2	C	183	ASP	3.7
3	D	63	GLN	3.7
3	D	206	SER	3.7
3	D	201	ASN	3.6
3	D	162	GLN	3.6
3	I	2	GLN	3.6
1	F	51	PHE	3.6
3	D	207	ILE	3.6
4	J	199	ASN	3.6
2	C	147	ARG	3.6
2	H	179	PRO	3.6
2	C	146	PHE	3.5
4	E	197	ALA	3.5
2	C	129	LEU	3.5
4	E	134	ASN	3.5
3	D	214	PHE	3.3
3	D	2	GLN	3.3
4	E	199	ASN	3.3
3	D	195	SER	3.3
2	C	178	THR	3.2
3	D	64	GLN	3.2
3	I	145	ASP	3.2
4	E	243	ALA	3.2
2	H	182	GLY	3.2
2	C	14	SER	3.2
3	D	196	ASP	3.1
4	E	239	THR	3.1
2	C	184	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	180	PRO	3.1
1	A	157	ALA	3.0
2	C	155	GLY	3.0
3	I	164	LYS	3.0
2	C	175	LEU	2.9
2	C	153	THR	2.9
3	I	162	GLN	2.9
3	D	202	ALA	2.8
2	C	176	GLU	2.8
2	C	149	ASP	2.8
3	I	163	SER	2.8
3	D	209	PRO	2.8
4	E	198	LEU	2.8
3	D	193	ASN	2.7
3	D	161	SER	2.6
3	D	204	ASN	2.6
3	D	198	ALA	2.6
2	C	186	THR	2.6
3	I	165	ASP	2.5
1	F	169	GLY	2.5
2	C	148	ASN	2.5
4	E	242	ARG	2.4
1	A	0	ASP	2.4
2	C	188	HIS	2.4
4	J	195	GLN	2.4
2	C	203	ARG	2.4
1	A	101	GLN	2.4
3	D	211	ASP	2.3
3	I	144	SER	2.3
3	I	197	PHE	2.3
4	E	238	TRP	2.3
2	H	203	ARG	2.2
3	D	163	SER	2.2
2	H	181	ARG	2.2
4	E	196	PRO	2.2
1	F	47	LEU	2.2
2	C	36	GLU	2.2
4	E	93	THR	2.2
2	C	174	MET	2.1
3	D	210	GLU	2.1
2	H	178	THR	2.1
4	E	195	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	152	GLU	2.1
2	C	-2	GLY	2.1
4	E	48	GLN	2.1
3	I	7	SER	2.0
4	E	200	ASP	2.0
3	D	66	ALA	2.0
4	E	234	GLU	2.0
3	I	23	CYS	2.0
2	C	118	SER	2.0
4	E	136	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](#)

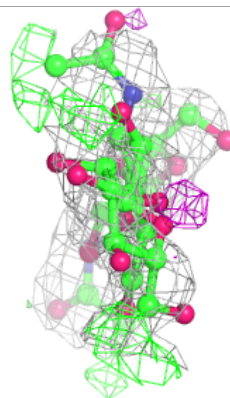
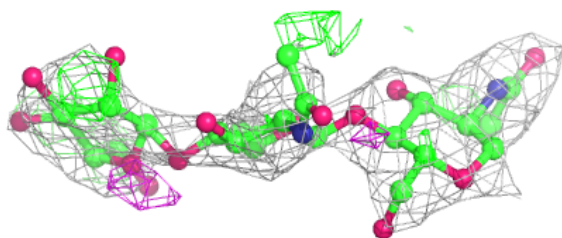
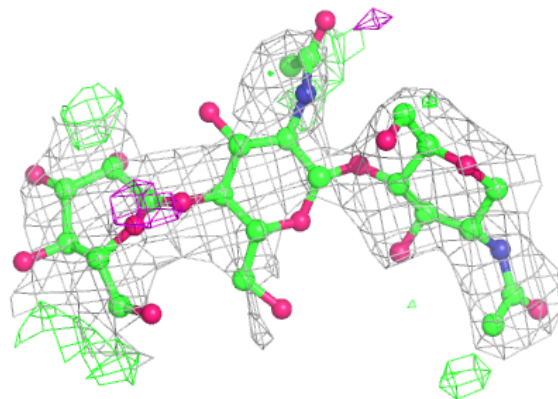
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	B	2	14/15	0.55	0.46	116,121,128,128	0
5	MAN	B	3	11/12	0.58	0.46	122,125,128,129	0
6	NAG	G	2	14/15	0.60	0.47	133,157,161,161	0
6	NAG	G	1	14/15	0.66	0.49	125,133,142,157	0
6	FUC	G	3	10/11	0.83	0.41	117,121,124,125	0
5	NAG	B	1	14/15	0.84	0.18	64,88,101,112	0

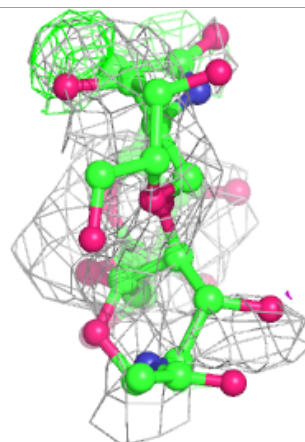
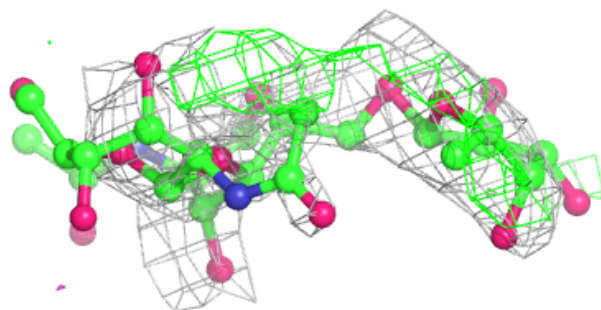
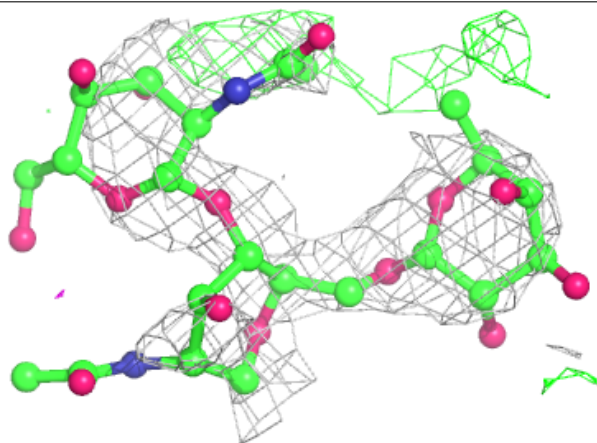
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

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

**Electron density around Chain G:**

$2mF_o-DF_c$ (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	A	204	14/15	0.57	0.61	85,102,108,111	0
7	NAG	C	302	14/15	0.70	0.47	102,111,115,116	0
8	GOL	C	301	6/6	0.73	0.33	65,73,76,76	0
7	NAG	F	204	14/15	0.74	0.47	100,115,120,123	0
8	GOL	I	302	6/6	0.82	0.27	61,73,74,78	0
8	GOL	F	202	6/6	0.85	0.23	65,67,69,70	0
8	GOL	D	301	6/6	0.86	0.17	69,71,72,80	0
7	NAG	F	203	14/15	0.87	0.31	46,73,84,89	0
8	GOL	F	201	6/6	0.90	0.28	60,66,70,72	0
8	GOL	H	304	6/6	0.91	0.26	48,51,57,60	0
8	GOL	I	301	6/6	0.93	0.28	61,69,72,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.