



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 11:56 PM BST

PDB ID : 4Z7W
Title : T316 complex
Authors : Petersen, J.; Rossjohn, J.; Reid, H.H.; Koning, F.
Deposited on : 2015-04-08
Resolution : 2.89 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 : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

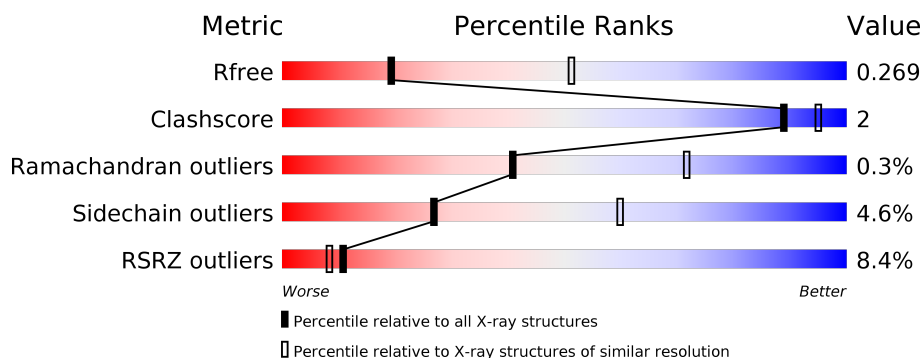
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	192	<div> <div></div> <div> <div></div> <div>88%</div> <div>6%</div> <div>6%</div> </div> </div>
1	C	192	<div> <div></div> <div> <div></div> <div>89%</div> <div>6%</div> <div>6%</div> </div> </div>
2	B	213	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>7%</div> <div>15%</div> </div> </div>
2	D	213	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>8%</div> <div>15%</div> </div> </div>
3	E	206	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>.</div> </div> </div>
3	G	206	<div> <div>25%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	F	241	<div><div></div><div>5%</div><div>93%</div><div>7%</div></div>
4	H	241	<div><div></div><div>21%</div><div>90%</div><div>8%</div><div>..</div></div>
5	I	18	<div><div></div><div>67%</div><div>17%</div><div>17%</div></div>
5	J	18	<div><div></div><div>67%</div><div>17%</div><div>17%</div></div>
6	K	6	<div><div></div><div>33%</div><div>50%</div><div>17%</div></div>
6	L	6	<div><div></div><div>17%</div><div>67%</div><div>17%</div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12983 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	181	Total	C	N	O	S	0	0	0
			1444	929	238	275	2			
1	C	181	Total	C	N	O	S	0	0	0
			1444	929	238	275	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	THR	-	expression tag	UNP Q30069
A	183	SER	-	expression tag	UNP Q30069
A	184	GLY	-	expression tag	UNP Q30069
A	185	ASP	-	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	LYS	-	expression tag	UNP Q30069
C	182	THR	-	expression tag	UNP Q30069
C	183	SER	-	expression tag	UNP Q30069
C	184	GLY	-	expression tag	UNP Q30069
C	185	ASP	-	expression tag	UNP Q30069
C	186	ASP	-	expression tag	UNP Q30069
C	187	ASP	-	expression tag	UNP Q30069
C	188	ASP	-	expression tag	UNP Q30069
C	189	LYS	-	expression tag	UNP Q30069

- Molecule 2 is a protein called MHC class II HLA-DQ-beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	180	Total	C	N	O	S	0	0	0
			1449	921	254	267	7			
2	D	180	Total	C	N	O	S	0	0	0
			1459	927	255	270	7			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	GLY	-	expression tag	UNP O19707
B	-11	GLY	-	expression tag	UNP O19707
B	-10	SER	-	expression tag	UNP O19707
B	-9	ILE	-	expression tag	UNP O19707
B	-8	GLU	-	expression tag	UNP O19707
B	-7	GLY	-	expression tag	UNP O19707
B	-6	ARG	-	expression tag	UNP O19707
B	-5	GLY	-	expression tag	UNP O19707
B	-4	GLY	-	expression tag	UNP O19707
B	-3	SER	-	expression tag	UNP O19707
B	-2	GLY	-	expression tag	UNP O19707
B	-1	ALA	-	expression tag	UNP O19707
B	0	SER	-	expression tag	UNP O19707
B	193	THR	-	expression tag	UNP O19707
B	194	GLY	-	expression tag	UNP O19707
B	195	GLY	-	expression tag	UNP O19707
B	196	ASP	-	expression tag	UNP O19707
B	197	ASP	-	expression tag	UNP O19707
B	198	ASP	-	expression tag	UNP O19707
B	199	ASP	-	expression tag	UNP O19707
B	200	LYS	-	expression tag	UNP O19707
D	-12	GLY	-	expression tag	UNP O19707
D	-11	GLY	-	expression tag	UNP O19707
D	-10	SER	-	expression tag	UNP O19707
D	-9	ILE	-	expression tag	UNP O19707
D	-8	GLU	-	expression tag	UNP O19707
D	-7	GLY	-	expression tag	UNP O19707
D	-6	ARG	-	expression tag	UNP O19707
D	-5	GLY	-	expression tag	UNP O19707
D	-4	GLY	-	expression tag	UNP O19707
D	-3	SER	-	expression tag	UNP O19707
D	-2	GLY	-	expression tag	UNP O19707
D	-1	ALA	-	expression tag	UNP O19707
D	0	SER	-	expression tag	UNP O19707
D	193	THR	-	expression tag	UNP O19707
D	194	GLY	-	expression tag	UNP O19707
D	195	GLY	-	expression tag	UNP O19707
D	196	ASP	-	expression tag	UNP O19707
D	197	ASP	-	expression tag	UNP O19707
D	198	ASP	-	expression tag	UNP O19707
D	199	ASP	-	expression tag	UNP O19707
D	200	LYS	-	expression tag	UNP O19707

- Molecule 3 is a protein called T-CELL RECEPTOR, T316 ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	199	Total	C	N	O	S	0	0	0
			1529	967	248	307	7			
3	G	191	Total	C	N	O	S	0	0	0
			1419	896	235	282	6			

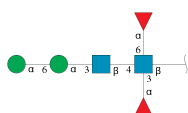
- Molecule 4 is a protein called T-CELL RECEPTOR, T316 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	241	Total	C	N	O	S	0	0	0
			1898	1193	333	363	9			
4	H	239	Total	C	N	O	S	0	0	0
			1847	1155	327	356	9			

- Molecule 5 is a protein called DQ8-glia-alpha1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	15	Total	C	N	O	0	0	0
			107	64	18	25			
5	J	15	Total	C	N	O	0	0	0
			111	66	19	26			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	K	6	Total	C	N	O	0	0	0
			70	40	2	28			
6	L	6	Total	C	N	O	0	0	0
			70	40	2	28			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	F	1	Total	O	S	0	0
			5	4	1		

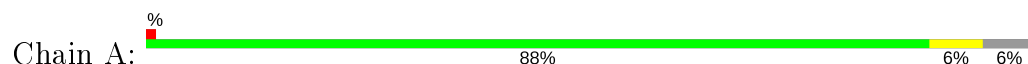
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	15	Total 15	O 15	0	0
9	B	18	Total 18	O 18	0	0
9	C	21	Total 21	O 21	0	0
9	D	8	Total 8	O 8	0	0
9	E	8	Total 8	O 8	0	0
9	F	15	Total 15	O 15	0	0
9	G	5	Total 5	O 5	0	0
9	H	12	Total 12	O 12	0	0
9	I	1	Total 1	O 1	0	0

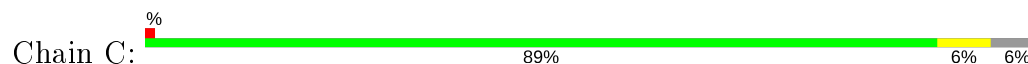
3 Residue-property plots [i](#)

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.

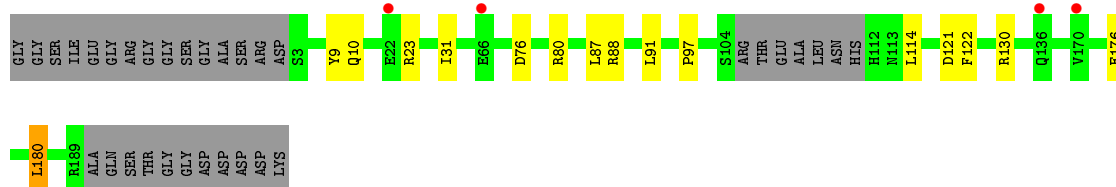
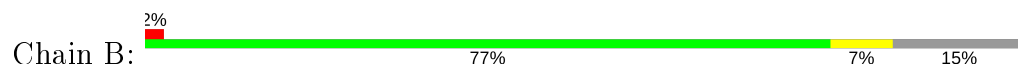
- Molecule 1: MHC class II HLA-DQ-alpha chain



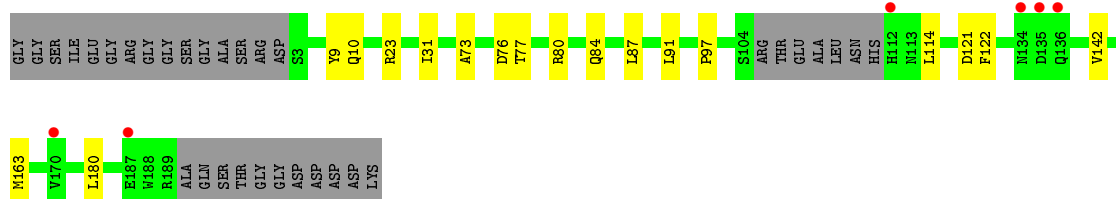
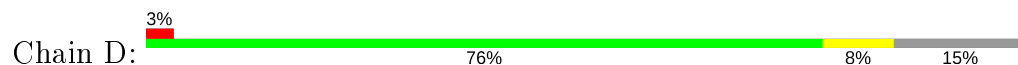
- Molecule 1: MHC class II HLA-DQ-alpha chain



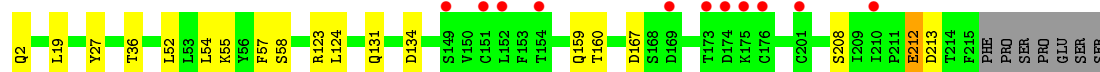
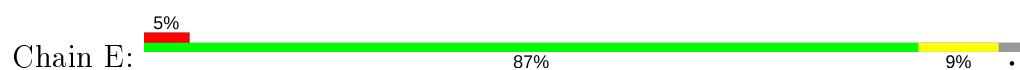
- Molecule 2: MHC class II HLA-DQ-beta-1



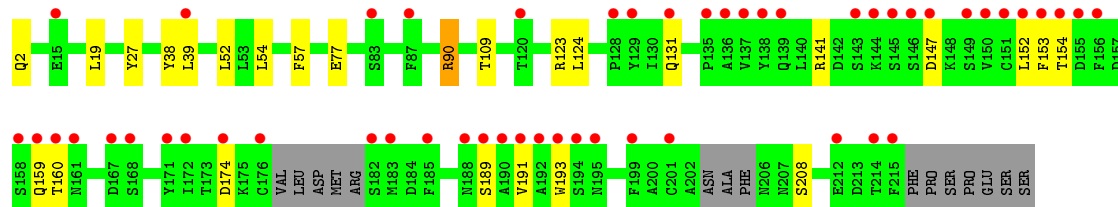
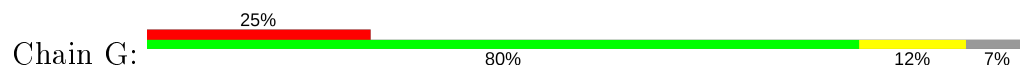
- Molecule 2: MHC class II HLA-DQ-beta-1



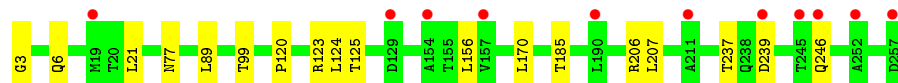
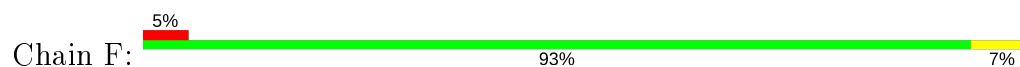
- Molecule 3: T-CELL RECEPTOR, T316 ALPHA CHAIN



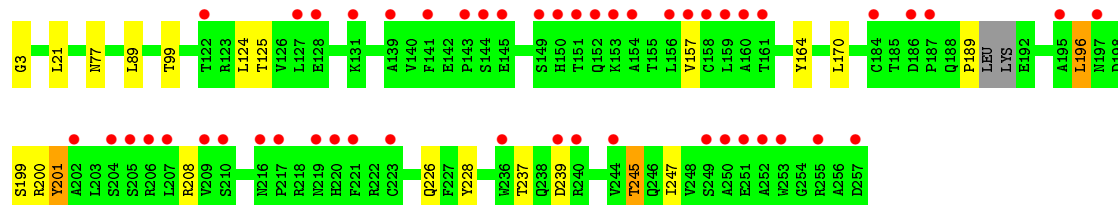
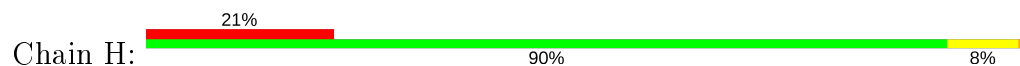
• Molecule 3: T-CELL RECEPTOR, T316 ALPHA CHAIN



• Molecule 4: T-CELL RECEPTOR, T316 BETA CHAIN



• Molecule 4: T-CELL RECEPTOR, T316 BETA CHAIN



• Molecule 5: DQ8-glia-alpha1

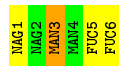


• Molecule 5: DQ8-glia-alpha1



- Molecule 6: α -D-mannopyranose-(1-6)- α -D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[α -L-fucopyranose-(1-3)][α -L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  33% 50% 17%



- Molecule 6: α -D-mannopyranose-(1-6)- α -D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[α -L-fucopyranose-(1-3)][α -L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  17% 67% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.62Å 200.52Å 87.18Å 90.00° 100.63° 90.00°	Depositor
Resolution (Å)	85.69 – 2.89 85.69 – 2.89	Depositor EDS
% Data completeness (in resolution range)	90.3 (85.69-2.89) 90.6 (85.69-2.89)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.228 , 0.247 0.250 , 0.269	Depositor DCC
R_{free} test set	2286 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	12983	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.12% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, NAG, SO4, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.36	0/1488	0.53	0/2035
1	C	0.36	0/1488	0.53	0/2035
2	B	0.36	0/1487	0.57	0/2034
2	D	0.36	0/1497	0.55	0/2047
3	E	0.36	0/1567	0.52	0/2135
3	G	0.37	0/1452	0.54	0/1982
4	F	0.35	0/1949	0.51	0/2653
4	H	0.35	0/1897	0.50	0/2585
5	I	0.31	0/110	0.42	0/148
5	J	0.28	0/114	0.38	0/153
All	All	0.36	0/13049	0.53	0/17807

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

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	1444	0	1354	7	0
1	C	1444	0	1354	6	0
2	B	1449	0	1358	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1459	0	1375	8	0
3	E	1529	0	1399	5	0
3	G	1419	0	1247	6	0
4	F	1898	0	1779	5	0
4	H	1847	0	1672	8	0
5	I	107	0	89	2	0
5	J	111	0	95	2	0
6	K	70	0	61	1	0
6	L	70	0	61	1	0
7	A	14	0	13	0	0
7	C	14	0	13	0	0
8	F	5	0	0	0	0
9	A	15	0	0	0	0
9	B	18	0	0	0	0
9	C	21	0	0	0	0
9	D	8	0	0	0	0
9	E	8	0	0	0	0
9	F	15	0	0	0	0
9	G	5	0	0	0	0
9	H	12	0	0	0	0
9	I	1	0	0	0	0
All	All	12983	0	11870	47	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 2.

All (47) 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:70:LEU:HD13	2:B:9:TYR:HB2	1.78	0.65
1:C:70:LEU:HD13	2:D:9:TYR:HB2	1.80	0.63
4:F:3:GLY:N	6:K:3:MAN:HO2	1.98	0.61
4:F:99:THR:HG23	4:F:125:THR:HA	1.84	0.59
1:C:118:ASN:HB2	1:C:166:GLU:HB2	1.85	0.58
4:H:99:THR:HG23	4:H:125:THR:HA	1.84	0.58
1:A:118:ASN:HB2	1:A:166:GLU:HB2	1.85	0.56
4:F:6:GLN:HG2	4:F:120:PRO:HD2	1.88	0.55
1:C:54:PHE:HD1	5:I:3:GLU:HB2	1.76	0.51
3:G:19:LEU:HD11	3:G:124:LEU:HD11	1.92	0.51
2:B:97:PRO:HD2	2:B:180:LEU:HD21	1.93	0.51
4:F:156:LEU:HD13	4:F:207:LEU:HD23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:19:LEU:HD11	3:E:124:LEU:HD11	1.93	0.49
4:H:21:LEU:HD13	4:H:89:LEU:HD23	1.95	0.48
2:B:76:ASP:HA	2:B:80:ARG:HB2	1.95	0.48
2:D:76:ASP:HA	2:D:80:ARG:HB2	1.95	0.48
4:F:21:LEU:HD13	4:F:89:LEU:HD23	1.96	0.48
3:G:191:VAL:HG21	4:H:157:VAL:HG21	1.95	0.48
2:D:77:THR:HA	3:E:36:THR:HG21	1.97	0.47
3:G:38:TYR:HE1	3:G:109:THR:HG22	1.79	0.47
1:A:54:PHE:HD1	5:J:3:GLU:HB2	1.78	0.46
4:H:196:LEU:HB3	4:H:199:SER:HB2	1.98	0.46
3:G:2:GLN:N	3:G:27:TYR:HH	2.15	0.44
4:H:189:PRO:HB2	4:H:201:TYR:HB2	1.99	0.44
1:A:43:TRP:CE3	1:A:48:PHE:HB3	2.51	0.44
2:B:97:PRO:HB3	2:B:122:PHE:HB3	2.00	0.44
1:C:43:TRP:CE3	1:C:48:PHE:HB3	2.52	0.44
2:D:97:PRO:HB3	2:D:122:PHE:HB3	1.98	0.44
1:A:69:ASN:O	1:A:73:VAL:HG23	2.18	0.44
1:C:65:VAL:HG13	5:I:10:GLN:HG2	2.00	0.44
2:D:73:ALA:HB1	3:E:58:SER:HB3	2.00	0.44
3:E:2:GLN:N	3:E:27:TYR:HH	2.15	0.44
1:C:69:ASN:O	1:C:73:VAL:HG23	2.18	0.44
1:A:65:VAL:HG13	5:J:10:GLN:HG2	2.01	0.43
2:B:87:LEU:HA	2:B:91:LEU:HB2	2.01	0.43
1:A:43:TRP:HB2	1:A:49:ARG:HG2	2.01	0.43
2:D:87:LEU:HA	2:D:91:LEU:HB2	2.01	0.42
4:H:228:TYR:HA	4:H:245:THR:HG22	2.00	0.42
3:G:154:THR:HG23	3:G:189:SER:HB3	2.01	0.42
4:H:3:GLY:N	6:L:3:MAN:HO2	2.18	0.42
2:B:10:GLN:HB2	2:B:31:ILE:HB	2.02	0.41
4:H:164:TYR:HB2	4:H:200:ARG:HG2	2.02	0.41
3:G:77:GLU:HG3	3:G:90:ARG:HG2	2.03	0.41
2:B:130:ARG:HH22	2:B:176:GLU:HG3	1.85	0.41
2:D:10:GLN:HB2	2:D:31:ILE:HB	2.02	0.41
3:E:212:GLU:H	3:E:212:GLU:HG3	1.60	0.41
2:D:84:GLN:HA	2:D:87:LEU:HD12	2.04	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	179/192 (93%)	176 (98%)	3 (2%)	0	100	100
1	C	179/192 (93%)	174 (97%)	5 (3%)	0	100	100
2	B	176/213 (83%)	163 (93%)	12 (7%)	1 (1%)	25	58
2	D	176/213 (83%)	162 (92%)	13 (7%)	1 (1%)	25	58
3	E	197/206 (96%)	188 (95%)	8 (4%)	1 (0%)	29	61
3	G	185/206 (90%)	175 (95%)	9 (5%)	1 (0%)	29	61
4	F	239/241 (99%)	233 (98%)	6 (2%)	0	100	100
4	H	235/241 (98%)	227 (97%)	8 (3%)	0	100	100
5	I	13/18 (72%)	13 (100%)	0	0	100	100
5	J	13/18 (72%)	13 (100%)	0	0	100	100
All	All	1592/1740 (92%)	1524 (96%)	64 (4%)	4 (0%)	41	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	121	ASP
2	D	121	ASP
3	E	208	SER
3	G	208	SER

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	160/176 (91%)	158 (99%)	2 (1%)	69	90
1	C	160/176 (91%)	158 (99%)	2 (1%)	69	90
2	B	154/189 (82%)	150 (97%)	4 (3%)	46	77
2	D	157/189 (83%)	152 (97%)	5 (3%)	39	73
3	E	166/182 (91%)	154 (93%)	12 (7%)	14	39
3	G	142/182 (78%)	127 (89%)	15 (11%)	6	20
4	F	202/210 (96%)	193 (96%)	9 (4%)	27	61
4	H	189/210 (90%)	178 (94%)	11 (6%)	20	50
5	I	12/14 (86%)	11 (92%)	1 (8%)	11	32
5	J	13/14 (93%)	12 (92%)	1 (8%)	13	35
All	All	1355/1542 (88%)	1293 (95%)	62 (5%)	27	60

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	101	GLN
2	B	23	ARG
2	B	88	ARG
2	B	114	LEU
2	B	180	LEU
1	C	62	ASN
1	C	101	GLN
2	D	23	ARG
2	D	114	LEU
2	D	142	VAL
2	D	163	MET
2	D	180	LEU
3	E	52	LEU
3	E	54	LEU
3	E	55	LYS
3	E	57	PHE
3	E	123	ARG
3	E	131	GLN
3	E	134	ASP
3	E	159	GLN
3	E	160	THR
3	E	167	ASP
3	E	212	GLU

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Mol	Chain	Res	Type
3	E	213	ASP
4	F	77	ASN
4	F	123	ARG
4	F	124	LEU
4	F	170	LEU
4	F	185	THR
4	F	206	ARG
4	F	237	THR
4	F	239	ASP
4	F	246	GLN
3	G	39	LEU
3	G	52	LEU
3	G	54	LEU
3	G	57	PHE
3	G	90	ARG
3	G	123	ARG
3	G	131	GLN
3	G	141	ARG
3	G	147	ASP
3	G	152	LEU
3	G	153	PHE
3	G	159	GLN
3	G	160	THR
3	G	174	ASP
3	G	193	TRP
4	H	77	ASN
4	H	124	LEU
4	H	170	LEU
4	H	196	LEU
4	H	201	TYR
4	H	208	ARG
4	H	226	GLN
4	H	237	THR
4	H	239	ASP
4	H	245	THR
4	H	247	ILE
5	I	11	GLU
5	J	11	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	64	GLN
4	F	28	ASN

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 ⓘ

12 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$
6	NAG	K	1	1,6	14,14,15	0.33	0	17,19,21	0.95	1 (5%)
6	NAG	K	2	6	14,14,15	0.33	0	17,19,21	0.69	0
6	MAN	K	3	6	11,11,12	0.37	0	15,15,17	1.08	1 (6%)
6	MAN	K	4	6	11,11,12	0.46	0	15,15,17	0.75	0
6	FUC	K	5	6	10,10,11	0.39	0	14,14,16	0.90	1 (7%)
6	FUC	K	6	6	10,10,11	0.67	0	14,14,16	2.24	3 (21%)
6	NAG	L	1	1,6	14,14,15	0.31	0	17,19,21	0.66	0
6	NAG	L	2	6	14,14,15	0.32	0	17,19,21	0.69	1 (5%)
6	MAN	L	3	6	11,11,12	0.42	0	15,15,17	1.06	1 (6%)
6	MAN	L	4	6	11,11,12	0.33	0	15,15,17	1.13	1 (6%)
6	FUC	L	5	6	10,10,11	0.41	0	14,14,16	1.16	2 (14%)
6	FUC	L	6	6	10,10,11	0.32	0	14,14,16	0.90	1 (7%)

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

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	6	FUC	C1-O5-C5	6.69	127.94	112.78
6	K	6	FUC	C1-C2-C3	4.14	114.75	109.67
6	L	4	MAN	C1-O5-C5	3.99	117.60	112.19
6	K	3	MAN	C1-O5-C5	3.74	117.26	112.19
6	L	3	MAN	C1-O5-C5	3.68	117.17	112.19
6	L	5	FUC	C1-O5-C5	3.18	119.99	112.78
6	L	6	FUC	C1-O5-C5	3.08	119.76	112.78
6	K	5	FUC	C1-O5-C5	2.92	119.39	112.78
6	K	1	NAG	C1-O5-C5	2.34	115.37	112.19
6	L	2	NAG	C1-O5-C5	2.18	115.15	112.19
6	L	5	FUC	C1-C2-C3	2.11	112.26	109.67
6	K	6	FUC	O5-C1-C2	2.01	113.87	110.77

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	K	1	NAG	O5-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6
6	K	4	MAN	O5-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
6	L	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	L	2	NAG	O5-C5-C6-O6
6	L	3	MAN	O5-C5-C6-O6
6	K	4	MAN	C4-C5-C6-O6

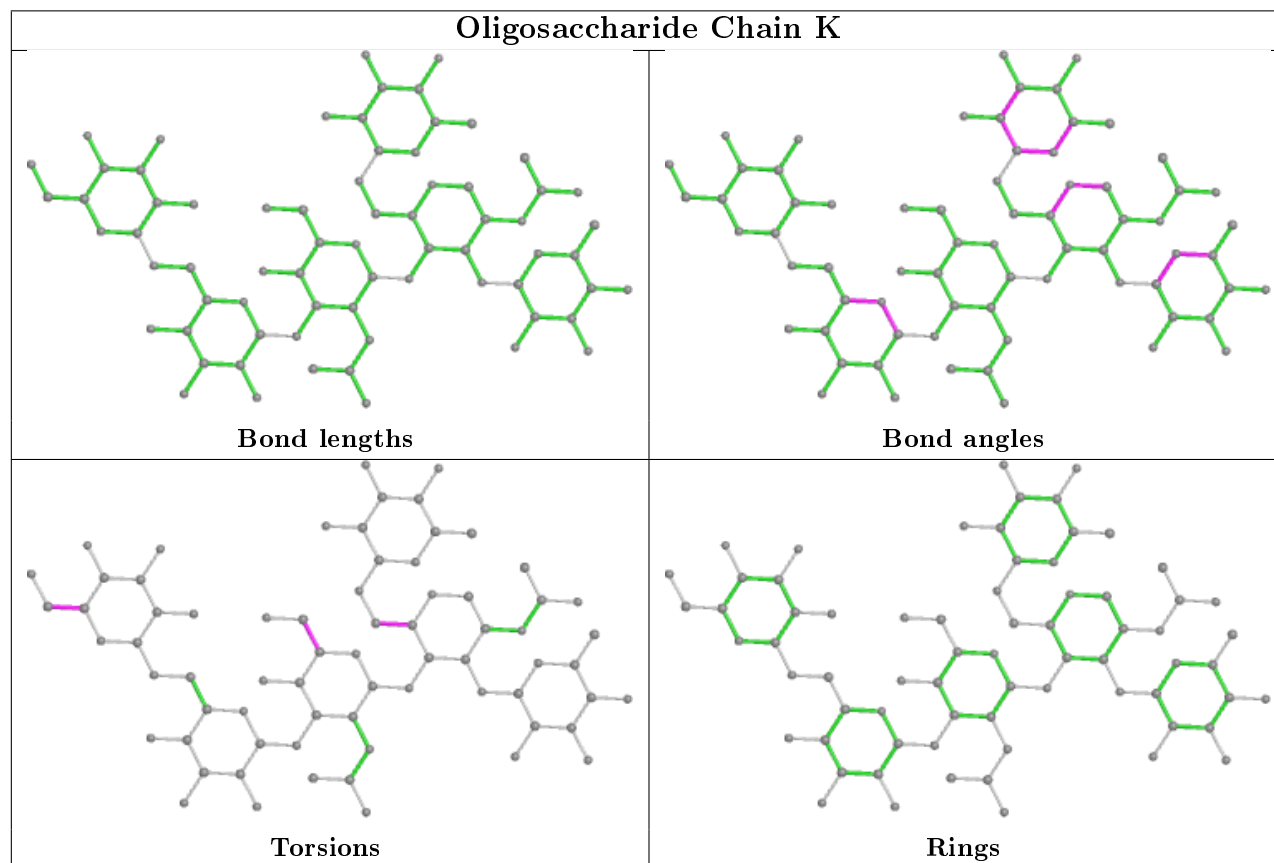
All (1) ring outliers are listed below:

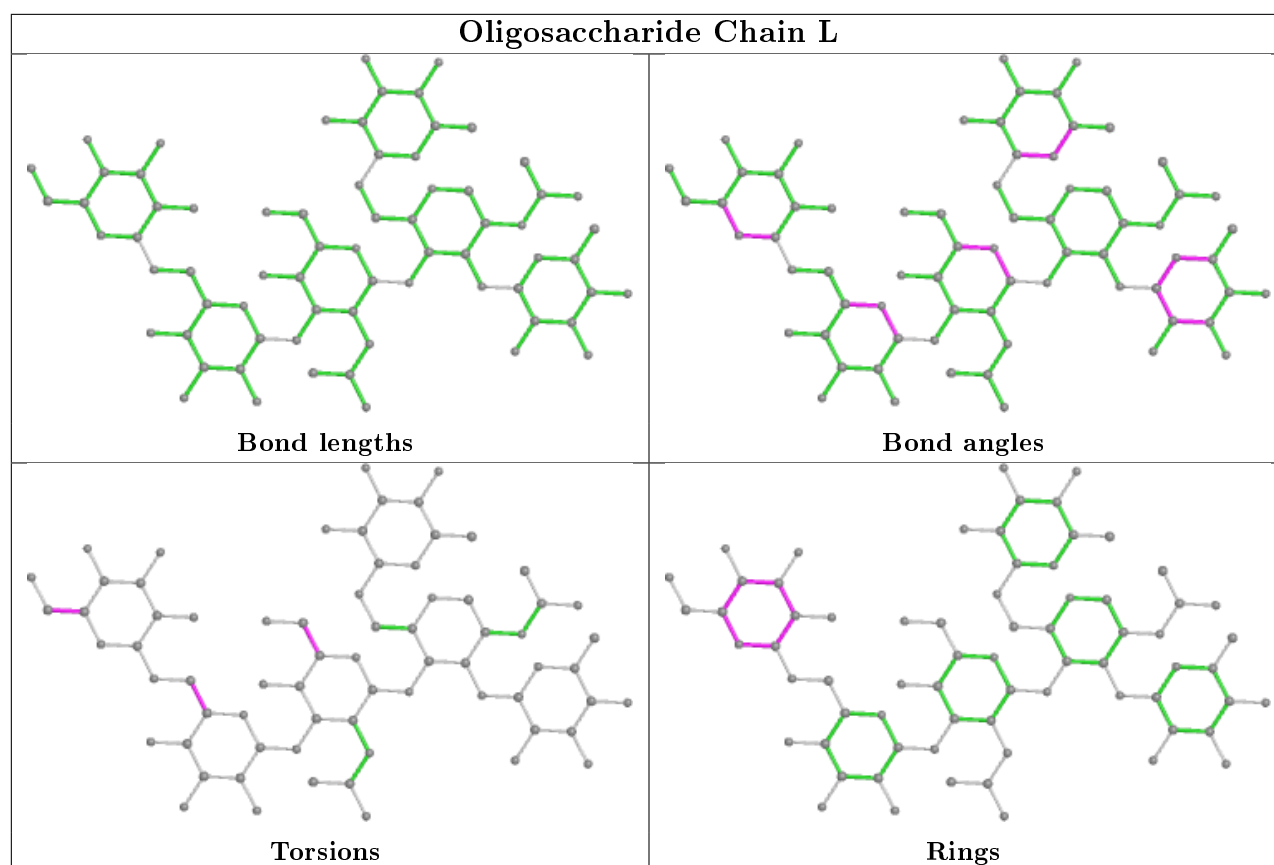
Mol	Chain	Res	Type	Atoms
6	L	4	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	3	MAN	1	0
6	L	3	MAN	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](#)

3 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	SO4	F	301	-	4,4,4	0.13	0	6,6,6	0.05	0
7	NAG	C	207	1	14,14,15	0.27	0	17,19,21	0.56	0
7	NAG	A	207	1	14,14,15	0.27	0	17,19,21	0.57	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
7	NAG	C	207	1	-	1/6/23/26	0/1/1/1
7	NAG	A	207	1	-	0/6/23/26	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($^{\circ}$)	Ideal($^{\circ}$)
7	A	207	NAG	C1-O5-C5	2.02	114.92	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	207	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	181/192 (94%)	0.30	1 (0%) 89 89	24, 45, 74, 87	0
1	C	181/192 (94%)	0.17	2 (1%) 80 80	20, 37, 62, 77	0
2	B	180/213 (84%)	0.35	4 (2%) 62 59	21, 47, 91, 106	0
2	D	180/213 (84%)	0.29	6 (3%) 46 41	19, 40, 79, 98	0
3	E	199/206 (96%)	0.57	11 (5%) 25 21	26, 59, 90, 115	0
3	G	191/206 (92%)	1.44	52 (27%) 0 0	40, 81, 150, 171	0
4	F	241/241 (100%)	0.57	11 (4%) 32 29	20, 57, 92, 118	0
4	H	239/241 (99%)	1.16	50 (20%) 1 0	28, 84, 128, 145	0
5	I	15/18 (83%)	0.06	0 100 100	21, 34, 46, 50	0
5	J	15/18 (83%)	0.42	0 100 100	26, 40, 55, 84	0
All	All	1622/1740 (93%)	0.62	137 (8%) 11 8	19, 55, 121, 171	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	159	GLN	8.3
3	G	158	SER	8.1
3	G	151	CYS	6.9
3	G	215	PHE	6.3
3	G	152	LEU	6.1
4	H	157	VAL	5.8
4	H	160	ALA	5.7
3	G	135	PRO	5.5
3	G	190	ALA	5.4
3	G	149	SER	5.4
4	H	257	ASP	5.3
3	G	212	GLU	5.2
4	H	219	ASN	4.9

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Mol	Chain	Res	Type	RSRZ
4	H	252	ALA	4.9
4	H	159	LEU	4.7
3	G	145	SER	4.7
3	G	192	ALA	4.5
3	G	191	VAL	4.5
3	G	155	ASP	4.3
4	H	152	GLN	4.3
3	G	168	SER	4.3
4	H	255	ARG	4.2
4	H	143	PRO	4.0
4	H	220	HIS	4.0
4	F	257	ASP	4.0
3	G	146	SER	4.0
4	H	154	ALA	4.0
2	D	135	ASP	3.8
4	H	250	ALA	3.8
3	G	194	SER	3.7
3	E	149	SER	3.6
4	H	156	LEU	3.6
3	G	154	THR	3.5
3	G	171	TYR	3.5
3	G	147	ASP	3.4
4	H	131	LYS	3.4
4	F	154	ALA	3.4
3	G	167	ASP	3.3
4	H	158	CYS	3.3
3	G	185	PHE	3.3
3	G	131	GLN	3.3
3	G	201	CYS	3.2
2	D	136	GLN	3.2
3	E	151	CYS	3.2
3	G	137	VAL	3.1
3	G	120	THR	3.1
4	H	149	SER	3.1
3	G	214	THR	3.1
4	H	151	THR	3.1
4	H	221	PHE	3.0
4	H	127	LEU	3.0
3	G	138	TYR	3.0
3	G	176	CYS	3.0
4	H	209	VAL	3.0
3	G	139	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
3	G	160	THR	2.8
3	G	189	SER	2.8
4	H	249	SER	2.8
4	H	253	TRP	2.8
4	H	122	THR	2.8
4	H	161	THR	2.8
3	G	182	SER	2.7
4	H	204	SER	2.7
4	H	217	PRO	2.7
1	C	157	ALA	2.7
3	G	193	TRP	2.7
3	E	174	ASP	2.6
3	G	83	SER	2.6
4	H	128	GLU	2.6
4	H	184	CYS	2.6
3	E	173	THR	2.6
4	F	211	ALA	2.6
4	H	141	PHE	2.5
4	H	202	ALA	2.5
3	G	161	ASN	2.5
4	H	197	ASN	2.5
4	H	206	ARG	2.5
3	G	136	ALA	2.5
4	F	19	MET	2.5
4	H	244	VAL	2.5
4	H	210	SER	2.5
4	F	157	VAL	2.5
3	E	201	CYS	2.4
3	G	153	PHE	2.4
4	F	252	ALA	2.4
2	D	112	HIS	2.4
3	G	128	PRO	2.4
3	G	174	ASP	2.4
4	H	195	ALA	2.4
1	C	126	HIS	2.4
3	E	169	ASP	2.4
2	B	136	GLN	2.4
3	G	143	SER	2.4
3	G	15	GLU	2.3
4	F	245	THR	2.3
4	H	240	ARG	2.3
3	G	195	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
3	E	175	LYS	2.3
4	H	239	ASP	2.2
4	H	139	ALA	2.2
2	D	170	VAL	2.2
2	B	170	VAL	2.2
4	H	207	LEU	2.2
3	E	176	CYS	2.2
4	H	153	LYS	2.2
4	H	144	SER	2.2
3	E	152	LEU	2.2
2	D	134	ASN	2.2
4	H	216	ASN	2.2
3	G	129	TYR	2.2
4	H	186	ASP	2.1
3	G	188	ASN	2.1
3	G	144	LYS	2.1
4	H	150	HIS	2.1
4	H	223	CYS	2.1
3	G	39	LEU	2.1
4	F	239	ASP	2.1
1	A	123	SER	2.1
3	G	156	PHE	2.1
2	D	187	GLU	2.1
4	H	236	TRP	2.1
3	G	183	MET	2.1
4	F	190	LEU	2.1
3	G	150	VAL	2.1
4	F	129	ASP	2.1
3	E	210	ILE	2.1
3	G	87	PHE	2.1
4	H	145	GLU	2.1
4	F	246	GLN	2.1
3	G	172	ILE	2.1
2	B	66	GLU	2.1
4	H	251	GLU	2.1
4	H	205	SER	2.0
2	B	22	GLU	2.0
4	H	187	PRO	2.0
3	E	154	THR	2.0
3	G	199	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

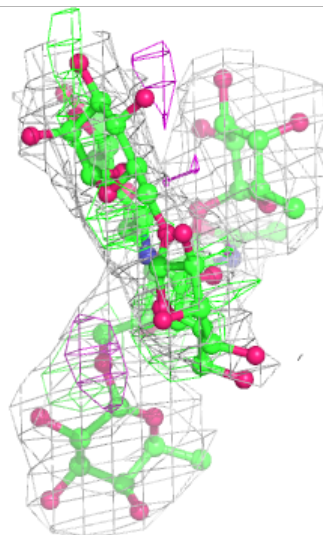
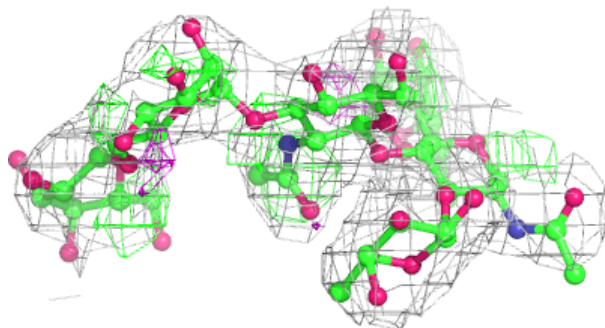
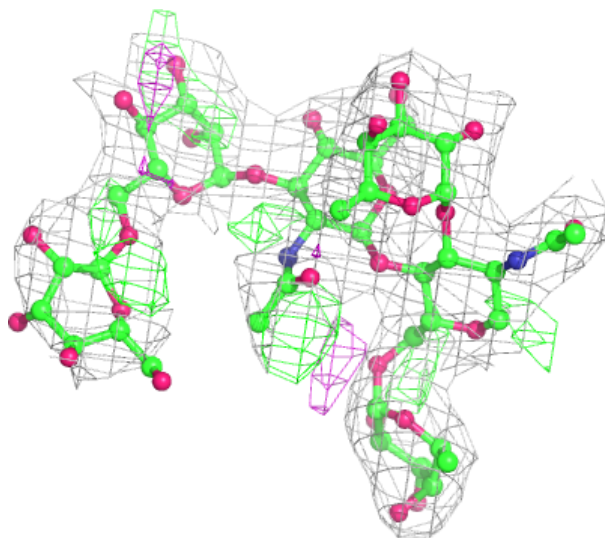
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

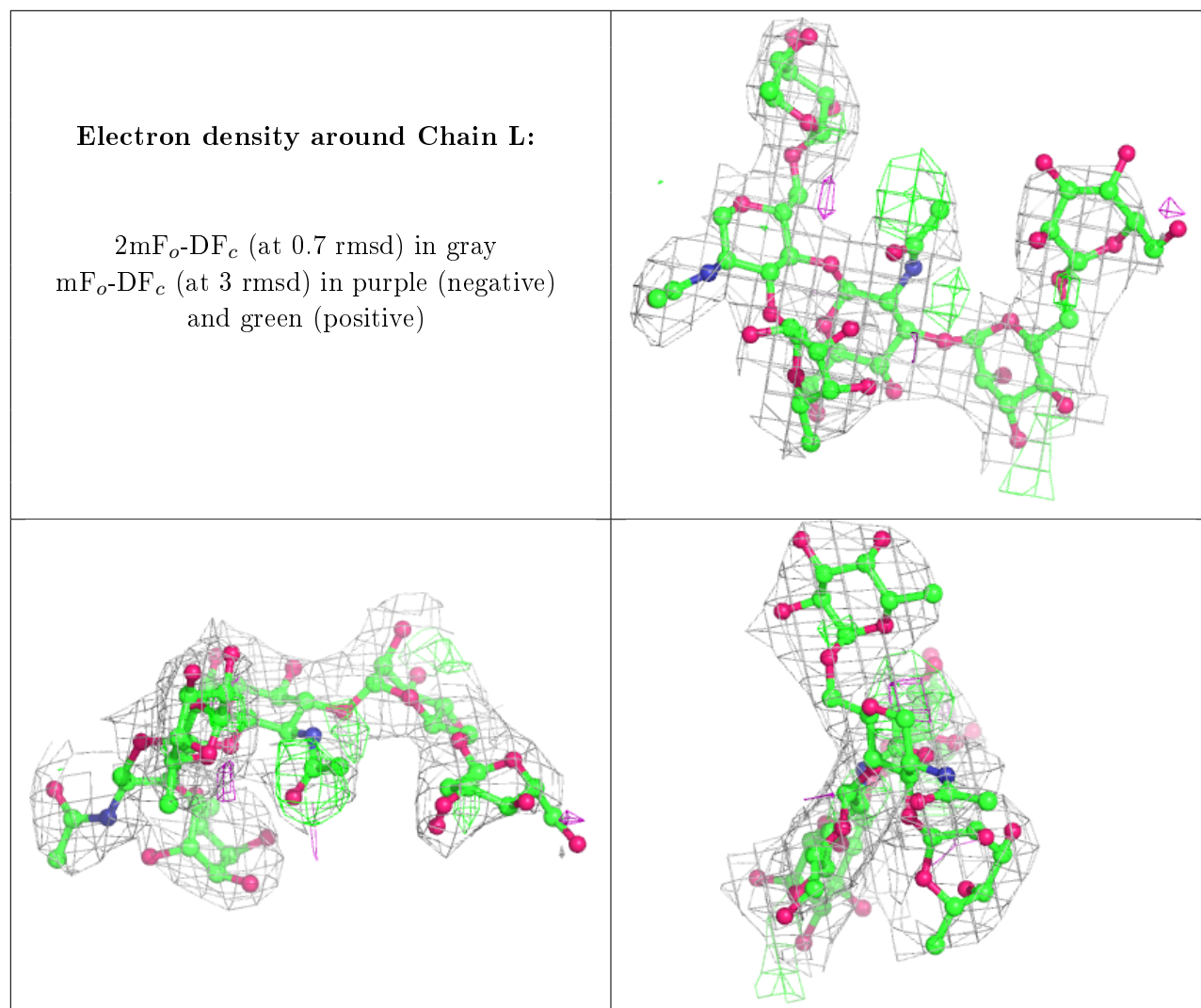
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MAN	K	4	11/12	0.78	0.37	73,75,79,79	0
6	MAN	K	3	11/12	0.78	0.28	68,71,74,75	0
6	NAG	L	2	14/15	0.81	0.22	69,72,77,77	0
6	MAN	L	3	11/12	0.81	0.21	79,82,86,88	0
6	NAG	K	2	14/15	0.83	0.25	59,62,65,66	0
6	MAN	L	4	11/12	0.84	0.35	78,83,88,89	0
6	NAG	K	1	14/15	0.88	0.23	49,51,52,56	0
6	NAG	L	1	14/15	0.92	0.18	57,59,63,66	0
6	FUC	K	6	10/11	0.93	0.22	47,48,49,49	0
6	FUC	K	5	10/11	0.93	0.14	52,54,56,56	0
6	FUC	L	5	10/11	0.94	0.21	64,68,71,71	0
6	FUC	L	6	10/11	0.95	0.25	56,56,58,58	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 K:

$2mF_o-DF_c$ (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(\AA^2)	Q<0.9
7	NAG	A	207	14/15	0.76	0.23	77,80,84,84	0
7	NAG	C	207	14/15	0.82	0.23	58,62,66,67	0
8	SO4	F	301	5/5	0.98	0.12	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.