



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:36 AM UTC

PDB ID : 8VDU / pdb_00008vdu
Title : Crystal structure of hybrid insulin peptide (InsC8-15-IAPP74-80) bound to HLA-DQ8
Authors : Tran, T.M.; Lim, J.J.; Loh, T.Y.; Mannering, I.S.; Rossjohn, J.; Reid, H.H.
Deposited on : 2023-12-17
Resolution : 3.50 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)
Validation Pipeline (wwPDB-VP) : 2.49

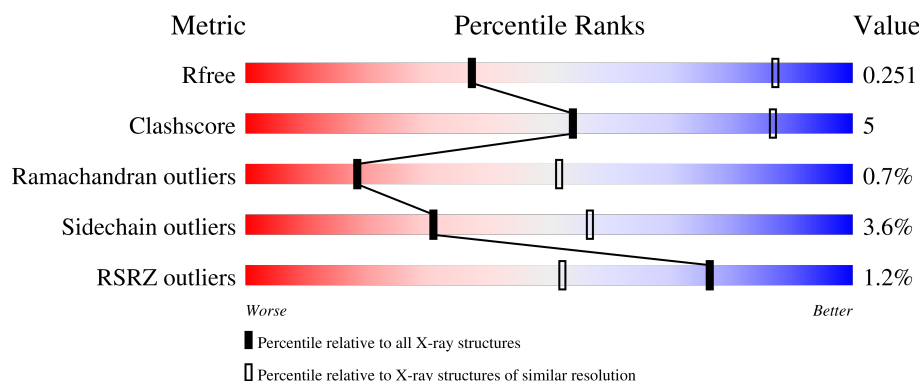
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	185	
1	D	185	
1	G	185	
1	J	185	
2	B	192	

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Mol	Chain	Length	Quality of chain
2	E	192	% 79%17% ••
2	H	192	% 85%12% ••
2	K	192	% 79%17% •
3	C	15	20% 60%27%7%7%
3	F	15	53%33%7%7%
3	I	15	67%27%7%
3	L	15	20% 60%27%13%
4	M	3	100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12192 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	183	Total	C	N	O	S	0	0	0
			1442	931	228	280	3			
1	D	183	Total	C	N	O	S	0	0	0
			1463	942	241	277	3			
1	G	182	Total	C	N	O	S	0	0	0
			1451	937	234	277	3			
1	J	183	Total	C	N	O	S	0	0	0
			1457	941	239	274	3			

There are 8 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
D	72	CYS	ILE	engineered mutation	UNP Q30069
D	182	SER	-	expression tag	UNP Q30069
G	72	CYS	ILE	engineered mutation	UNP Q30069
G	182	SER	-	expression tag	UNP Q30069
J	72	CYS	ILE	engineered mutation	UNP Q30069
J	182	SER	-	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	179	Total	C	N	O	S	0	0	0
			1436	915	244	271	6			
2	E	187	Total	C	N	O	S	0	0	0
			1498	950	256	285	7			
2	H	188	Total	C	N	O	S	0	0	0
			1532	970	268	287	7			
2	K	185	Total	C	N	O	S	0	0	0
			1458	929	250	272	7			

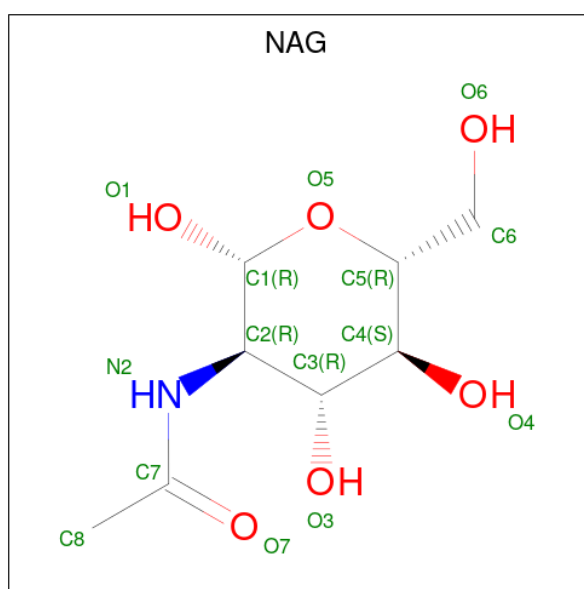
- Molecule 3 is a protein called Hybrid insulin peptide (HIP; InsC8-15-IAPP74-80).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	14	Total	C	N	O	S	0	0	0
			92	56	16	19	1			
3	F	14	Total	C	N	O	S	0	0	0
			92	55	16	20	1			
3	I	15	Total	C	N	O	S	0	0	0
			96	57	17	21	1			
3	L	13	Total	C	N	O	S	0	0	0
			79	48	14	16	1			

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

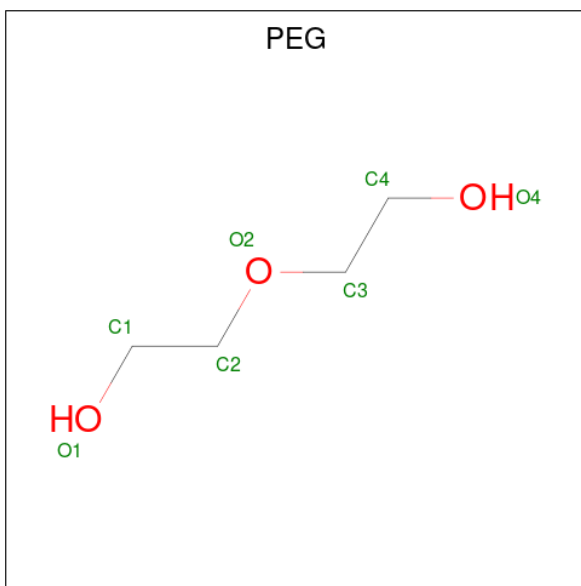
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	K	1	Total	C	O	0	0
			7	4	3		

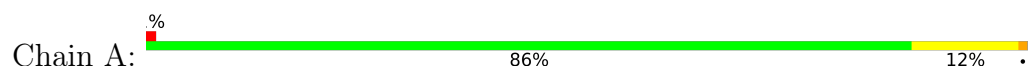
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	1	Total	O	0	0
			1	1		

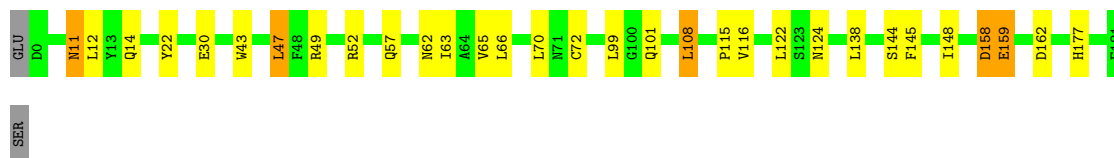
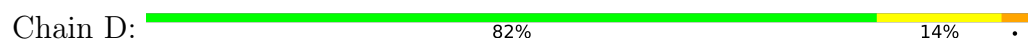
3 Residue-property plots [i](#)

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.

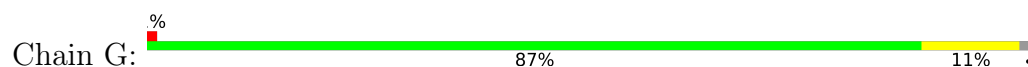
- Molecule 1: MHC class II HLA-DQ-alpha chain



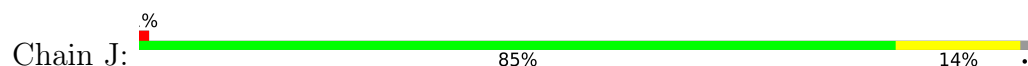
- Molecule 1: MHC class II HLA-DQ-alpha chain



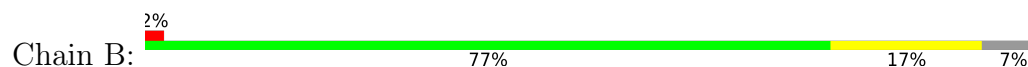
- Molecule 1: MHC class II HLA-DQ-alpha chain

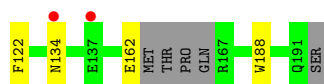


- Molecule 1: MHC class II HLA-DQ-alpha chain

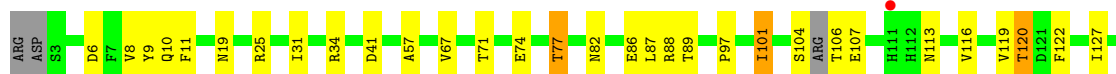
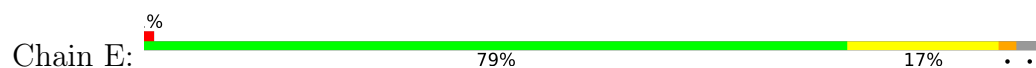


- Molecule 2: MHC class II HLA-DQ-beta-1

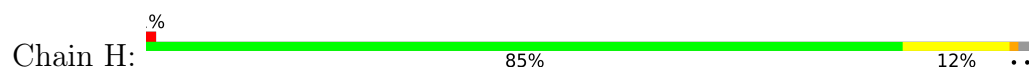




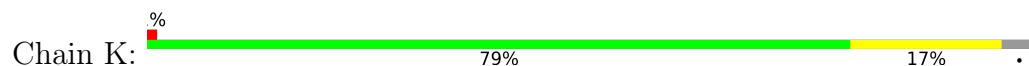
- Molecule 2: MHC class II HLA-DQ-beta-1



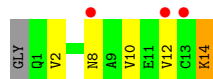
- Molecule 2: MHC class II HLA-DQ-beta-1



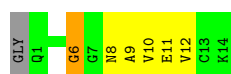
- Molecule 2: MHC class II HLA-DQ-beta-1



- Molecule 3: Hybrid insulin peptide (HIP; InsC8-15-IAPP74-80)



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- Molecule 3: Hybrid insulin peptide (HIP; InsC8-15-IAPP74-80)



- Molecule 4: beta-D-mannopyranose-(3-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-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	72.32Å 138.12Å 101.83Å 90.00° 102.50° 90.00°	Depositor
Resolution (Å)	49.04 – 3.50 49.04 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.04-3.50) 99.9 (49.04-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	50.00 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.207 , 0.246 0.209 , 0.251	Depositor DCC
R_{free} test set	1216 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	12192	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: PEG, 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	0.11	0/1486	0.33	0/2037
1	D	0.12	0/1507	0.35	0/2060
1	G	0.10	0/1494	0.29	0/2041
1	J	0.10	0/1501	0.31	0/2052
2	B	0.11	0/1473	0.34	0/2015
2	E	0.12	0/1536	0.33	0/2101
2	H	0.11	0/1571	0.33	0/2146
2	K	0.12	0/1496	0.36	1/2048 (0.0%)
3	C	0.15	0/91	0.50	0/121
3	F	0.10	0/91	0.49	0/122
3	I	0.13	0/95	0.59	0/127
3	L	0.16	0/78	0.40	0/105
All	All	0.11	0/12419	0.34	1/16975 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	167	ARG	CB-CA-C	-6.60	108.95	116.54

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	1442	0	1335	15	0
1	D	1463	0	1387	22	0
1	G	1451	0	1373	12	0
1	J	1457	0	1381	15	0
2	B	1436	0	1341	15	0
2	E	1498	0	1401	22	0
2	H	1532	0	1465	14	0
2	K	1458	0	1354	17	0
3	C	92	0	91	3	0
3	F	92	0	86	4	0
3	I	96	0	89	2	0
3	L	79	0	74	3	0
4	M	39	0	34	0	0
5	A	14	0	13	0	0
5	H	14	0	13	1	0
5	J	14	0	13	0	0
6	A	7	0	10	1	0
6	K	7	0	10	1	0
7	E	1	0	0	0	0
All	All	12192	0	11470	117	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 (117) 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:J:62:ASN:ND2	3:L:6:GLY:O	2.16	0.78
1:D:14:GLN:NE2	2:E:6:ASP:OD2	2.20	0.75
1:A:39:LYS:HG3	1:A:60:LEU:HD11	1.67	0.75
1:D:30:GLU:HB2	1:D:138:LEU:HD21	1.68	0.74
1:G:11:ASN:HB3	1:G:66:LEU:HD11	1.72	0.71
2:K:78:VAL:O	2:K:82:ASN:ND2	2.23	0.71
1:D:43:TRP:HB2	1:D:49:ARG:HG2	1.75	0.69
2:E:97:PRO:HB3	2:E:122:PHE:HB3	1.73	0.69
2:E:10:GLN:HB2	2:E:31:ILE:HB	1.77	0.66
1:G:30:GLU:HB2	1:G:138:LEU:HD21	1.76	0.66
2:E:106:THR:O	2:E:113:ASN:ND2	2.31	0.64
1:J:11:ASN:HB3	1:J:66:LEU:HD11	1.78	0.64
1:J:70:LEU:HD13	2:K:9:TYR:HB2	1.80	0.64
1:A:11:ASN:HB3	1:A:66:LEU:HD11	1.81	0.62
1:G:70:LEU:HD13	2:H:9:TYR:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LYS:NZ	1:A:166:GLU:OE2	2.33	0.62
1:D:108:LEU:HD23	1:D:148:ILE:HG12	1.82	0.61
5:H:201:NAG:H83	5:H:201:NAG:H3	1.86	0.58
1:J:30:GLU:HB2	1:J:138:LEU:HD11	1.86	0.56
1:J:76:ARG:NH2	3:L:11:GLU:OE2	2.38	0.56
2:E:25:ARG:NH2	2:E:41:ASP:OD2	2.37	0.56
2:H:76:ASP:OD1	2:H:80:ARG:NH1	2.39	0.56
1:D:70:LEU:HD13	2:E:9:TYR:HB2	1.88	0.55
2:E:120:THR:HA	2:E:156:GLN:HG3	1.89	0.55
1:J:70:LEU:O	1:J:74:ILE:HG13	2.06	0.55
2:E:74:GLU:HA	2:E:77:THR:HG23	1.89	0.55
2:B:14:MET:SD	2:B:29:ARG:NH1	2.80	0.55
1:A:11:ASN:ND2	1:A:62:ASN:OD1	2.40	0.54
2:B:25:ARG:NH2	2:B:43:ASP:OD2	2.41	0.54
1:A:96:PRO:HD3	2:B:120:THR:HG21	1.90	0.53
1:D:122:LEU:HB2	1:D:162:ASP:HB2	1.91	0.52
2:H:116:VAL:HG22	2:H:160:MET:HG2	1.90	0.52
2:E:119:VAL:HG11	2:E:127:ILE:HD11	1.92	0.52
1:D:14:GLN:HG3	2:E:8:VAL:HG22	1.90	0.52
6:A:602:PEG:H21	2:K:178:PRO:O	2.10	0.51
2:E:104:SER:O	2:E:106:THR:OG1	2.28	0.51
2:B:10:GLN:HB2	2:B:31:ILE:HB	1.92	0.51
2:K:116:VAL:HG22	2:K:160:MET:HG2	1.92	0.51
2:B:61:TRP:NE1	3:C:10:VAL:O	2.37	0.51
1:J:122:LEU:HB2	1:J:162:ASP:HB2	1.94	0.50
1:G:62:ASN:ND2	3:I:6:GLY:O	2.41	0.49
2:B:8:VAL:HB	2:B:33:ASN:HA	1.93	0.49
1:A:159:GLU:HG2	1:A:161:TYR:CZ	2.48	0.49
2:E:101:ILE:HG21	2:E:188:TRP:HB2	1.94	0.49
1:A:122:LEU:HB2	1:A:162:ASP:HB2	1.95	0.48
1:G:122:LEU:HB2	1:G:162:ASP:HB2	1.94	0.48
2:H:169:ASP:HB3	2:H:171:TYR:CE1	2.48	0.48
2:K:115:LEU:HG	2:K:163:MET:HE2	1.96	0.47
1:D:11:ASN:HB3	1:D:22:TYR:HD2	1.79	0.47
1:A:62:ASN:HD21	3:C:8:ASN:H	1.61	0.47
1:D:158:ASP:OD1	1:D:158:ASP:N	2.47	0.47
1:D:63:ILE:HA	1:D:66:LEU:HD13	1.97	0.46
1:A:122:LEU:HD23	1:A:127:SER:HA	1.98	0.46
1:A:158:ASP:HA	2:H:112:HIS:NE2	2.30	0.46
1:D:144:SER:HB2	2:E:34:ARG:NH1	2.30	0.46
1:A:70:LEU:HD13	2:B:9:TYR:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:ARG:O	2:B:74:GLU:HG3	2.15	0.46
2:K:18:THR:HB	2:K:23:ARG:HB2	1.98	0.46
1:A:158:ASP:HA	2:H:112:HIS:CD2	2.51	0.46
2:E:181:GLN:HE22	2:H:162:GLU:HB2	1.81	0.46
2:K:78:VAL:HG22	3:L:5:GLY:HA2	1.97	0.46
1:D:115:PRO:HG3	1:D:145:PHE:CD2	2.52	0.45
2:K:94:ARG:HG3	6:K:201:PEG:H42	1.98	0.45
1:J:77:SER:HB3	2:K:53:LEU:HD21	1.98	0.45
2:K:10:GLN:HB2	2:K:31:ILE:HB	1.99	0.45
2:B:113:ASN:O	2:B:162:GLU:HA	2.17	0.45
2:K:117:CYS:HB2	2:K:131:TRP:CZ2	2.52	0.44
1:A:107:CYS:HB2	1:A:121:TRP:CH2	2.53	0.44
2:K:148:ILE:HB	2:K:156:GLN:HG3	1.99	0.44
1:G:76:ARG:NH2	3:I:11:GLU:OE2	2.49	0.44
2:B:97:PRO:HB3	2:B:122:PHE:HB3	2.00	0.44
1:D:62:ASN:ND2	3:F:6:GLY:O	2.50	0.44
1:J:105:LEU:HG	1:J:153:PHE:CE1	2.53	0.44
2:E:107:GLU:N	2:E:107:GLU:OE1	2.50	0.44
2:E:82:ASN:O	2:E:86:GLU:HG2	2.18	0.43
1:J:0:ASP:HB3	1:J:1:ILE:HD12	2.00	0.43
1:J:61:THR:O	1:J:65:VAL:HG23	2.18	0.43
1:J:94:LYS:NZ	2:K:154:THR:OG1	2.51	0.43
1:D:11:ASN:OD1	2:E:11:PHE:HB3	2.18	0.43
1:J:11:ASN:HB2	2:K:11:PHE:HB3	2.00	0.43
1:A:105:LEU:HD23	1:A:121:TRP:CZ3	2.54	0.43
1:D:47:LEU:HD11	2:E:89:THR:HB	2.01	0.43
2:K:44:VAL:HG11	2:K:48:ARG:HE	1.83	0.43
2:E:116:VAL:HG22	2:E:160:MET:HG2	2.00	0.43
3:F:8:ASN:OD1	3:F:9:ALA:N	2.51	0.43
2:H:119:VAL:HG11	2:H:127:ILE:HD11	2.00	0.43
1:D:52:ARG:HH22	2:E:86:GLU:CD	2.26	0.43
1:D:162:ASP:OD1	1:D:177:HIS:ND1	2.51	0.43
1:J:119:ILE:HD12	1:J:147:LYS:HD2	2.01	0.43
2:B:115:LEU:HD23	2:B:115:LEU:HA	1.91	0.43
1:G:122:LEU:HD23	1:G:127:SER:HA	2.01	0.43
1:D:11:ASN:HB3	1:D:22:TYR:CD2	2.54	0.42
1:G:105:LEU:HD23	1:G:105:LEU:HA	1.88	0.42
2:H:97:PRO:HB3	2:H:122:PHE:HB3	2.01	0.42
1:G:105:LEU:HG	1:G:153:PHE:CE1	2.55	0.42
1:D:12:LEU:HD21	1:D:115:PRO:HG2	2.00	0.42
1:D:65:VAL:HG13	3:F:10:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:148:ILE:HB	2:H:156:GLN:HG3	2.01	0.42
2:H:82:ASN:O	2:H:86:GLU:HG2	2.20	0.42
2:B:55:PRO:N	2:B:56:PRO:HD2	2.35	0.42
1:G:69:ASN:O	1:G:73:VAL:HG23	2.20	0.42
2:K:97:PRO:HB3	2:K:122:PHE:HB3	2.00	0.42
1:D:14:GLN:HE22	1:D:116:VAL:HG23	1.85	0.42
2:B:64:GLN:HB2	2:B:67:VAL:HG12	2.02	0.41
1:J:140:LYS:HD3	1:J:144:SER:OG	2.21	0.41
2:E:57:ALA:HB2	3:F:11:GLU:OE2	2.20	0.41
1:G:61:THR:O	1:G:65:VAL:HG23	2.21	0.41
2:H:55:PRO:N	2:H:56:PRO:HD2	2.36	0.41
1:A:43:TRP:CE3	1:A:48:PHE:HB3	2.55	0.41
3:C:14:LYS:HE3	3:C:14:LYS:HB2	1.89	0.41
1:G:76:ARG:HD2	2:H:53:LEU:HD12	2.03	0.41
2:K:25:ARG:NH2	2:K:41:ASP:OD2	2.46	0.40
2:B:54:GLY:H	2:B:55:PRO:CD	2.35	0.40
2:B:101:ILE:HD13	2:B:188:TRP:HB3	2.04	0.40
2:E:88:ARG:HG3	2:E:89:THR:HG23	2.03	0.40
1:D:124:ASN:OD1	1:D:159:GLU:HA	2.21	0.40
2:H:31:ILE:HA	2:H:36:GLU:HA	2.03	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	181/185 (98%)	171 (94%)	9 (5%)	1 (1%)	21 54
1	D	181/185 (98%)	169 (93%)	10 (6%)	2 (1%)	11 43
1	G	178/185 (96%)	170 (96%)	7 (4%)	1 (1%)	21 54
1	J	181/185 (98%)	171 (94%)	10 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	173/192 (90%)	165 (95%)	6 (4%)	2 (1%)	10	41
2	E	183/192 (95%)	175 (96%)	8 (4%)	0	100	100
2	H	186/192 (97%)	175 (94%)	10 (5%)	1 (0%)	24	57
2	K	181/192 (94%)	170 (94%)	10 (6%)	1 (1%)	21	54
3	C	12/15 (80%)	11 (92%)	1 (8%)	0	100	100
3	F	12/15 (80%)	11 (92%)	0	1 (8%)	0	7
3	I	13/15 (87%)	12 (92%)	0	1 (8%)	1	8
3	L	11/15 (73%)	10 (91%)	1 (9%)	0	100	100
All	All	1492/1568 (95%)	1410 (94%)	72 (5%)	10 (1%)	18	51

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	LEU
1	D	99	LEU
2	H	169	ASP
3	I	6	GLY
2	K	134	ASN
2	B	112	HIS
2	B	134	ASN
1	D	159	GLU
1	G	16	TYR
3	F	6	GLY

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	160/170 (94%)	155 (97%)	5 (3%)	35	59
1	D	164/170 (96%)	157 (96%)	7 (4%)	26	51
1	G	163/170 (96%)	159 (98%)	4 (2%)	42	63
1	J	162/170 (95%)	159 (98%)	3 (2%)	50	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	155/177 (88%)	150 (97%)	5 (3%)	34	59
2	E	161/177 (91%)	154 (96%)	7 (4%)	26	51
2	H	168/177 (95%)	165 (98%)	3 (2%)	51	69
2	K	153/177 (86%)	148 (97%)	5 (3%)	33	58
3	C	9/10 (90%)	6 (67%)	3 (33%)	0	2
3	F	9/10 (90%)	8 (89%)	1 (11%)	6	25
3	I	9/10 (90%)	6 (67%)	3 (33%)	0	2
3	L	7/10 (70%)	6 (86%)	1 (14%)	3	18
All	All	1320/1428 (92%)	1273 (96%)	47 (4%)	31	57

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	52	ARG
1	A	62	ASN
1	A	129	THR
1	A	159	GLU
2	B	19	ASN
2	B	23	ARG
2	B	75	LEU
2	B	98	THR
2	B	111	HIS
3	C	2	VAL
3	C	12	VAL
3	C	14	LYS
1	D	11	ASN
1	D	47	LEU
1	D	57	GLN
1	D	72	CYS
1	D	101	GLN
1	D	108	LEU
1	D	158	ASP
2	E	19	ASN
2	E	67	VAL
2	E	71	THR
2	E	77	THR
2	E	87	LEU
2	E	101	ILE

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Mol	Chain	Res	Type
2	E	120	THR
3	F	12	VAL
1	G	86	VAL
1	G	98	THR
1	G	103	ASN
1	G	159	GLU
2	H	10	GLN
2	H	34	ARG
2	H	135	ASP
3	I	2	VAL
3	I	12	VAL
3	I	13	CYS
1	J	72	CYS
1	J	124	ASN
1	J	126	HIS
2	K	21	THR
2	K	67	VAL
2	K	70	ARG
2	K	120	THR
2	K	169	ASP
3	L	2	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	62	ASN
1	D	14	GLN
1	D	101	GLN
1	D	126	HIS
2	E	136	GLN
2	E	150	ASN
2	E	166	GLN
1	G	71	ASN
1	G	84	ASN
1	G	118	ASN
1	J	71	ASN
2	K	81	HIS
2	K	182	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 ⓘ

3 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	M	1	4,1	14,14,15	0.31	0	17,19,21	0.56	0
4	NAG	M	2	4	14,14,15	0.35	0	17,19,21	0.39	0
4	BMA	M	3	4	11,11,12	0.54	0	14,15,17	0.81	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
4	NAG	M	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	BMA	M	3	4	-	2/2/18/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

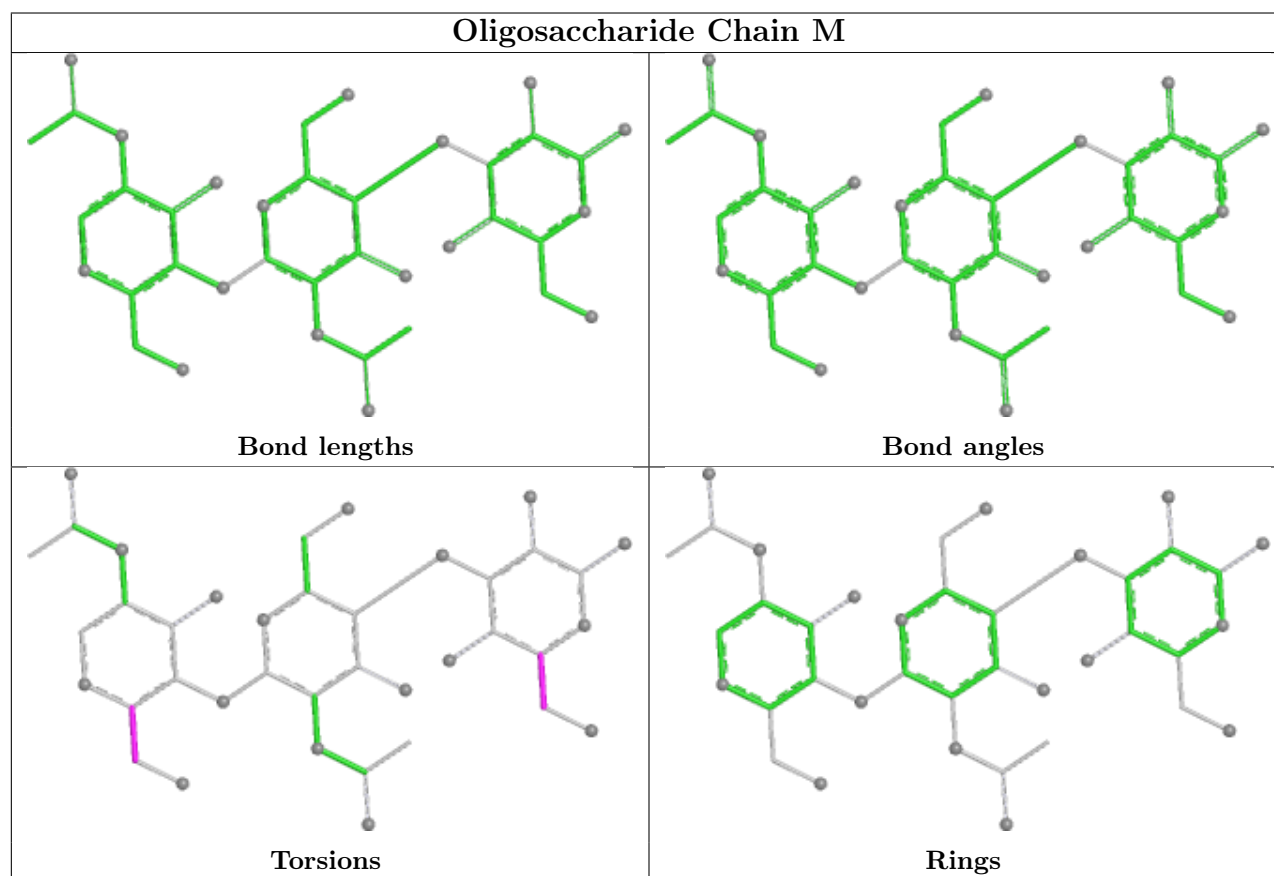
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	1	NAG	O5-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
4	M	3	BMA	O5-C5-C6-O6
4	M	3	BMA	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	601	1	14,14,15	0.44	0	17,19,21	0.36	0
6	PEG	A	602	-	6,6,6	0.09	0	5,5,5	0.12	0
5	NAG	J	201	1	14,14,15	0.32	0	17,19,21	0.51	0
5	NAG	H	201	2	14,14,15	0.55	0	17,19,21	1.35	2 (11%)
6	PEG	K	201	-	6,6,6	0.08	0	5,5,5	0.16	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	601	1	-	0/6/23/26	0/1/1/1
6	PEG	A	602	-	-	2/4/4/4	-
5	NAG	J	201	1	-	2/6/23/26	0/1/1/1
5	NAG	H	201	2	-	6/6/23/26	0/1/1/1
6	PEG	K	201	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	201	NAG	C2-N2-C7	4.61	129.07	122.90
5	H	201	NAG	C1-C2-N2	2.35	114.14	110.43

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	201	NAG	O5-C5-C6-O6
5	H	201	NAG	C4-C5-C6-O6
5	H	201	NAG	C8-C7-N2-C2
5	H	201	NAG	O7-C7-N2-C2
6	K	201	PEG	O1-C1-C2-O2
5	J	201	NAG	O5-C5-C6-O6
6	A	602	PEG	O1-C1-C2-O2
6	A	602	PEG	C4-C3-O2-C2
6	K	201	PEG	C1-C2-O2-C3
5	J	201	NAG	C4-C5-C6-O6
5	H	201	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
5	H	201	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	602	PEG	1	0
5	H	201	NAG	1	0
6	K	201	PEG	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	183/185 (98%)	0.06	1 (0%) 87 68	20, 33, 58, 96	0
1	D	183/185 (98%)	0.10	0 100 100	22, 36, 62, 93	0
1	G	182/185 (98%)	0.05	2 (1%) 78 54	22, 39, 68, 100	0
1	J	183/185 (98%)	0.21	1 (0%) 87 68	27, 45, 72, 91	0
2	B	179/192 (93%)	0.22	3 (1%) 69 43	19, 39, 73, 95	0
2	E	187/192 (97%)	0.10	1 (0%) 87 68	22, 38, 64, 84	0
2	H	188/192 (97%)	0.11	2 (1%) 78 54	21, 34, 66, 93	0
2	K	185/192 (96%)	0.22	2 (1%) 78 54	26, 47, 79, 108	0
3	C	14/15 (93%)	1.15	3 (21%) 2 3	35, 53, 72, 85	0
3	F	14/15 (93%)	0.84	0 100 100	41, 48, 76, 94	0
3	I	15/15 (100%)	0.83	0 100 100	38, 50, 64, 71	0
3	L	13/15 (86%)	1.19	3 (23%) 2 2	42, 61, 79, 85	0
All	All	1526/1568 (97%)	0.17	18 (1%) 76 52	19, 39, 72, 108	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	13	CYS	3.5
1	A	181	GLU	3.3
1	G	18	PRO	3.1
3	L	1	GLN	2.5
2	K	88	ARG	2.4
2	B	134	ASN	2.4
3	C	12	VAL	2.4
2	E	111	HIS	2.3
3	C	8	ASN	2.3
2	B	103	PRO	2.3
2	H	168	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
3	L	13	CYS	2.2
1	G	171	ASP	2.2
2	H	135	ASP	2.2
1	J	58	PHE	2.1
2	B	137	GLU	2.1
3	L	2	VAL	2.1
2	K	169	ASP	2.0

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

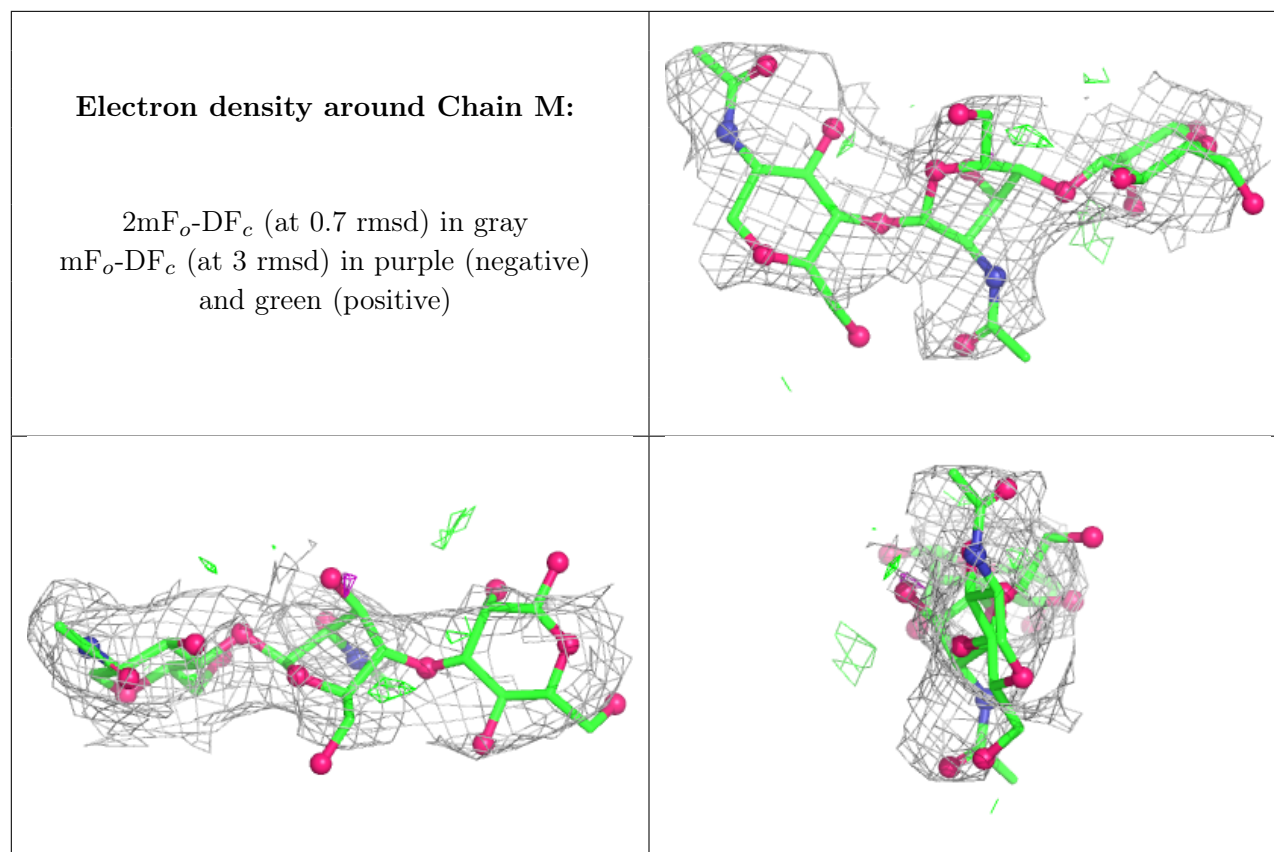
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	M	3	11/12	0.56	0.18	87,96,107,108	0
4	NAG	M	2	14/15	0.76	0.20	71,84,105,116	0
4	NAG	M	1	14/15	0.77	0.15	55,66,83,96	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.



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($\text{\AA}^2$)	Q<0.9
5	NAG	H	201	14/15	0.61	0.15	82,85,92,94	0
5	NAG	A	601	14/15	0.72	0.17	42,62,80,87	0
6	PEG	A	602	7/7	0.78	0.18	38,44,47,50	0
5	NAG	J	201	14/15	0.80	0.11	63,80,99,103	0
6	PEG	K	201	7/7	0.91	0.14	22,26,34,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.