



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 13, 2026 – 12:13 PM EDT

PDB ID : 9YAF / pdb_00009yaf
Title : TCR-HLA-DQ2.5-glia-a1a complex
Authors : Lim, J.J.; Loh, T.J.; Rossjohn, J.
Deposited on : 2025-09-15
Resolution : 3.25 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

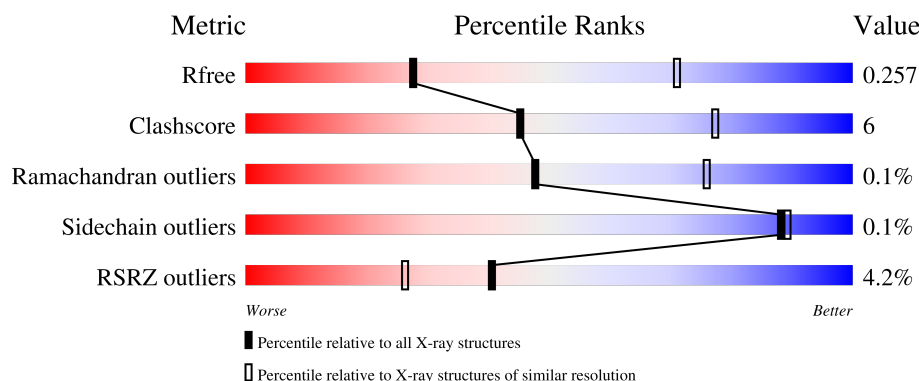
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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.



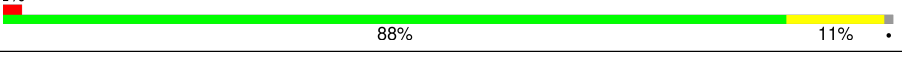
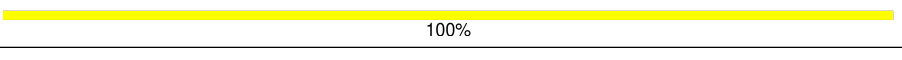
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	183	8% 87% 11% .
1	F	183	82% 16% .
2	B	192	3% 80% 14% 6%
2	G	192	2% 84% 9% 7%
3	C	13	8% 62% 31% 8%

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Mol	Chain	Length	Quality of chain
3	H	13	
4	D	206	
4	I	206	
5	E	244	
5	J	244	
6	K	2	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 12891 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 HLA class II histocompatibility antigen, DQ alpha 1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1390	901	224	263	2			
1	F	180	Total	C	N	O	S	0	0	0
			1399	905	228	264	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	SER	CYS	conflict	UNP P01909
F	46	SER	CYS	conflict	UNP P01909

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DQ 2.5 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	181	Total	C	N	O	S	0	0	0
			1456	923	258	268	7			
2	G	178	Total	C	N	O	S	0	0	0
			1436	912	255	262	7			

- Molecule 3 is a protein called GLIA-A1a peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	0	0	0
			102	69	15	18			
3	H	12	Total	C	N	O	0	0	0
			98	67	14	17			

- Molecule 4 is a protein called TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	202	Total	C	N	O	S	0	0	0
			1508	954	244	301	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	200	Total	C	N	O	S	0	0	0
			1486	938	242	297	9			

- Molecule 5 is a protein called TCR beta chain.

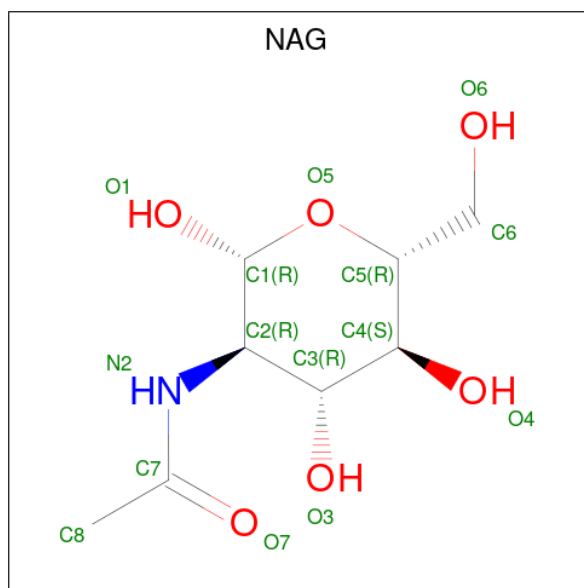
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	243	Total	C	N	O	S	0	0	0
			1919	1208	336	369	6			
5	J	241	Total	C	N	O	S	0	0	0
			1908	1204	337	361	6			

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



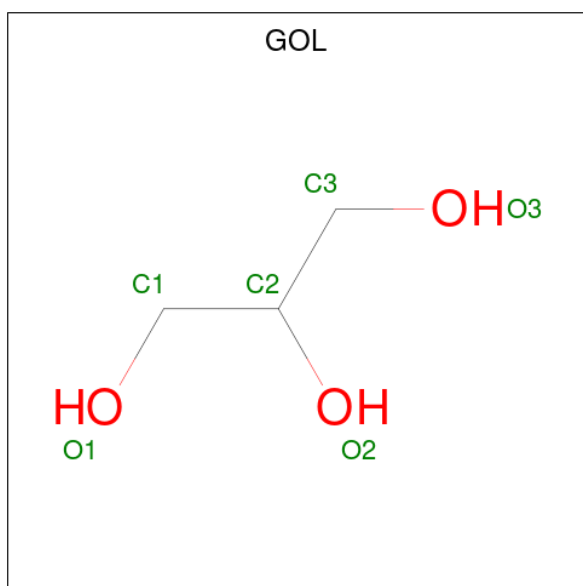
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	K	2	Total	C	N	O		0	0	0
			28	16	2	10				

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 14 8 1 5	0	0
7	D	1	Total C N O 14 8 1 5	0	0
7	D	1	Total C N O 14 8 1 5	0	0
7	E	1	Total C N O 14 8 1 5	0	0
7	I	1	Total C N O 14 8 1 5	0	0
7	I	1	Total C N O 14 8 1 5	0	0
7	J	1	Total C N O 14 8 1 5	0	0

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	F	1	Total C O 6 3 3	0	0
8	F	1	Total C O 6 3 3	0	0
8	G	1	Total C O 6 3 3	0	0
8	G	1	Total C O 6 3 3	0	0

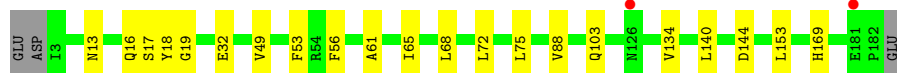
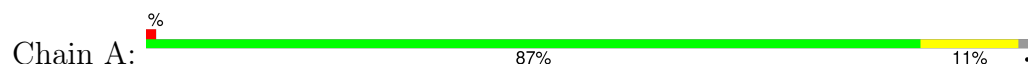
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total O 1 1	0	0
9	B	6	Total O 6 6	0	0
9	E	6	Total O 6 6	0	0
9	F	3	Total O 3 3	0	0
9	G	6	Total O 6 6	0	0
9	I	1	Total O 1 1	0	0
9	J	10	Total O 10 10	0	0

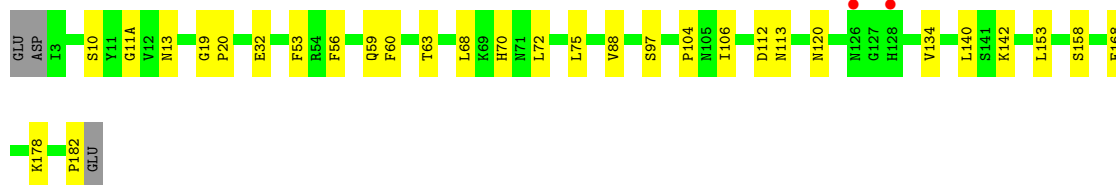
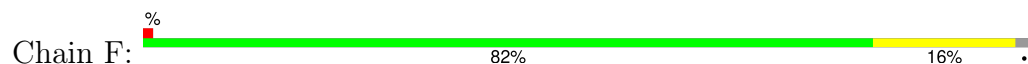
3 Residue-property plots [i](#)

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.

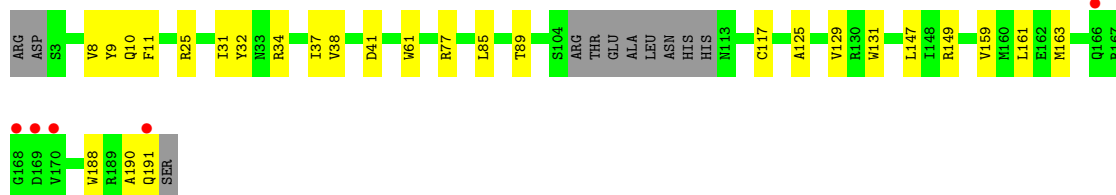
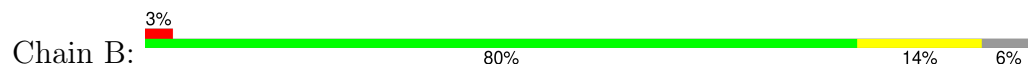
- Molecule 1: HLA class II histocompatibility antigen, DQ alpha 1 chain



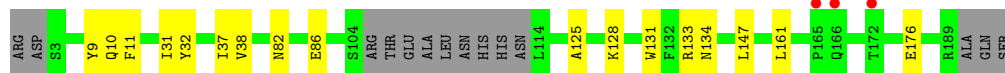
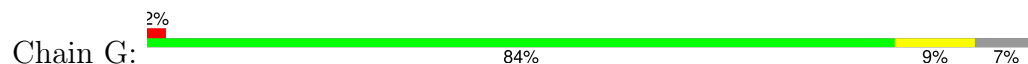
- Molecule 1: HLA class II histocompatibility antigen, DQ alpha 1 chain



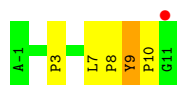
- Molecule 2: HLA class II histocompatibility antigen, DQ 2.5 beta chain



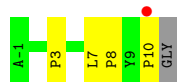
- Molecule 2: HLA class II histocompatibility antigen, DQ 2.5 beta chain



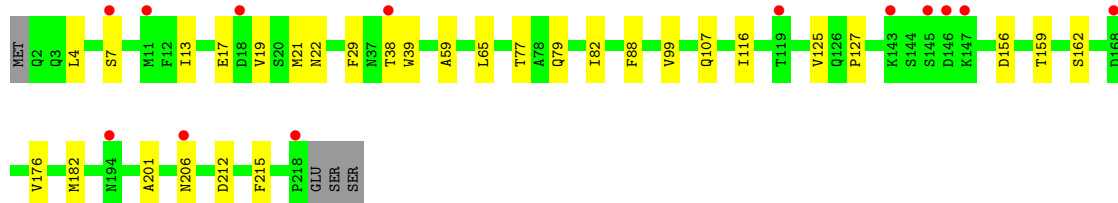
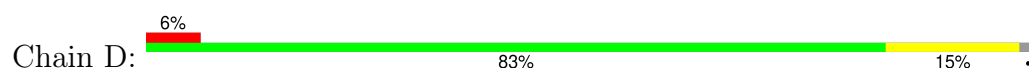
- Molecule 3: GLIA-A1a peptide



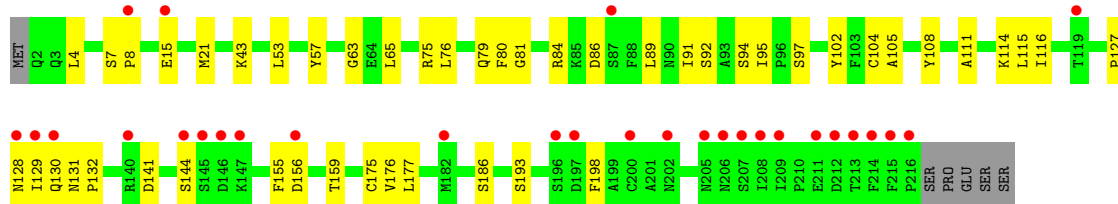
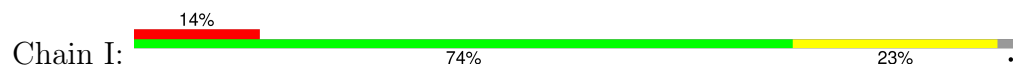
- Molecule 3: GLIA-A1a peptide



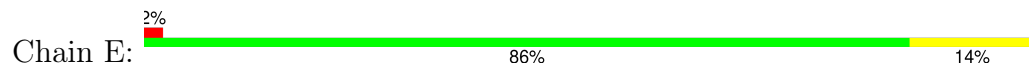
- Molecule 4: TCR alpha chain



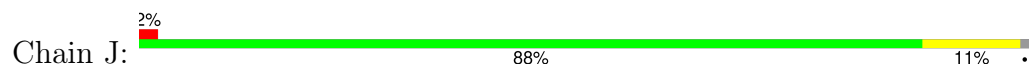
- Molecule 4: TCR alpha chain

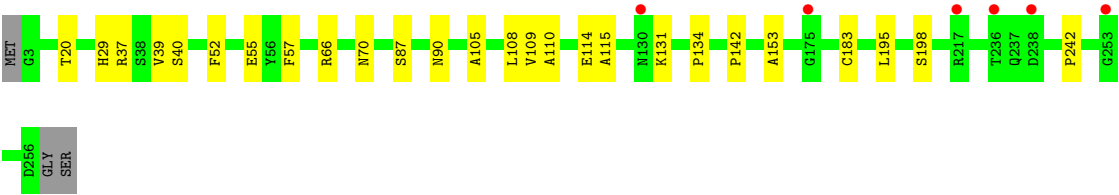


- Molecule 5: TCR beta chain



- Molecule 5: TCR beta chain





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

Chain K: 100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.62Å 122.67Å 252.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.59 – 3.25 49.59 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.59-3.25) 99.7 (49.59-3.25)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.222 , 0.257 0.223 , 0.257	Depositor DCC
R_{free} test set	2347 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	54.7	Xtriage
Anisotropy	1.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12891	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: GOL, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.21	1/1432 (0.1%)	0.35	0/1965
1	F	0.28	2/1441 (0.1%)	0.34	0/1976
2	B	0.13	0/1489	0.36	0/2027
2	G	0.14	0/1469	0.37	0/1999
3	C	0.31	0/108	0.64	0/150
3	H	0.24	0/104	0.48	0/145
4	D	0.27	0/1542	0.55	0/2102
4	I	0.24	0/1518	0.57	0/2070
5	E	0.14	0/1971	0.34	0/2683
5	J	0.15	0/1960	0.36	0/2667
All	All	0.20	3/13034 (0.0%)	0.42	0/17784

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
4	I	0	1
5	E	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	97	SER	N-CA	6.37	1.51	1.45
1	F	88	VAL	CA-C	-6.14	1.48	1.53
1	A	88	VAL	CA-C	5.81	1.57	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	9	TYR	Peptide
5	E	75	ARG	Sidechain
4	I	7	SER	Peptide

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	1390	0	1309	18	0
1	F	1399	0	1324	22	0
2	B	1456	0	1409	22	0
2	G	1436	0	1395	11	0
3	C	102	0	96	6	0
3	H	98	0	93	6	0
4	D	1508	0	1397	19	0
4	I	1486	0	1372	31	0
5	E	1919	0	1806	25	0
5	J	1908	0	1809	21	0
6	K	28	0	25	0	0
7	A	14	0	13	1	0
7	D	28	0	26	0	0
7	E	14	0	13	1	0
7	I	28	0	26	0	0
7	J	14	0	13	0	0
8	A	6	0	8	1	0
8	F	12	0	16	1	0
8	G	12	0	16	0	0
9	A	1	0	0	0	0
9	B	6	0	0	0	0
9	E	6	0	0	0	0
9	F	3	0	0	0	0
9	G	6	0	0	0	0
9	I	1	0	0	0	0
9	J	10	0	0	0	0
All	All	12891	0	12166	147	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 6.

All (147) 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)
3:C:9:TYR:CD2	3:C:10:PRO:HD3	2.14	0.81
3:C:9:TYR:CG	3:C:10:PRO:HD3	2.24	0.70
3:H:8:PRO:HD2	5:J:108:LEU:HG	1.73	0.70
5:E:57:PHE:HB3	5:E:66:ARG:HE	1.56	0.69
5:J:40:SER:HB2	5:J:105:ALA:HB3	1.74	0.68
5:E:134:PRO:HD3	5:E:242:PRO:HB3	1.79	0.64
2:G:37:ILE:HG13	2:G:38:VAL:HG23	1.79	0.64
5:E:44:GLN:HG3	5:E:50:LEU:HG	1.80	0.63
5:E:50:LEU:HD21	5:E:103:LEU:HD12	1.79	0.63
2:B:37:ILE:HG13	2:B:38:VAL:HG23	1.80	0.63
1:A:13:ASN:HB2	2:B:11:PHE:HB3	1.81	0.61
1:A:75:LEU:HD13	2:B:32:TYR:HB2	1.81	0.61
5:E:40:SER:HB3	5:E:105:ALA:HB3	1.81	0.61
4:D:182:MET:HE1	5:E:152:LYS:HE3	1.81	0.60
1:F:72:LEU:HD13	2:G:9:TYR:HB2	1.83	0.60
1:F:59:GLN:HG2	5:J:66:ARG:CZ	2.32	0.60
5:J:134:PRO:HD3	5:J:242:PRO:HB3	1.83	0.59
4:I:177:LEU:HB3	5:J:183:CYS:HB2	1.84	0.59
4:I:76:LEU:HD22	4:I:89:LEU:HD11	1.83	0.58
4:I:15:GLU:HG3	4:I:128:ASN:ND2	2.19	0.58
5:E:29:HIS:HA	5:E:108:LEU:HD12	1.85	0.57
1:F:32:GLU:HB2	1:F:140:LEU:HD21	1.85	0.57
5:E:188:PRO:HB2	5:E:200:TYR:HB3	1.86	0.57
5:E:52:PHE:HZ	5:E:55:GLU:HB2	1.69	0.56
1:A:72:LEU:HD13	2:B:9:TYR:HB2	1.88	0.56
2:B:125:ALA:HB1	2:B:147:LEU:HD21	1.86	0.55
4:I:175:CYS:HG	5:J:183:CYS:HG	1.55	0.55
4:I:127:PRO:HD3	4:I:176:VAL:HG21	1.88	0.54
4:D:156:ASP:OD1	4:D:159:THR:OG1	2.22	0.54
1:F:59:GLN:HG3	1:F:63:THR:HG23	1.90	0.54
4:I:141:ASP:HB3	4:I:144:SER:O	2.09	0.53
4:I:80:PHE:HE1	4:I:84:ARG:HA	1.73	0.53
1:F:13:ASN:HB2	2:G:11:PHE:HB3	1.90	0.53
1:F:75:LEU:HD13	2:G:32:TYR:HB2	1.90	0.53
2:B:77:ARG:HH12	4:D:38:THR:HG22	1.74	0.52
4:D:13:ILE:HD13	4:D:19:VAL:CG1	2.40	0.52
2:B:25:ARG:NH2	2:B:41:ASP:OD2	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:57:PHE:HB3	5:E:66:ARG:NE	2.24	0.52
4:I:4:LEU:HG	4:I:116:ILE:HG12	1.91	0.51
4:I:177:LEU:HD23	4:I:186:SER:O	2.10	0.51
5:J:52:PHE:HZ	5:J:55:GLU:HB2	1.76	0.51
3:C:8:PRO:HD2	5:E:108:LEU:HG	1.93	0.51
1:A:103:GLN:NE2	5:J:131:LYS:NZ	2.60	0.50
5:E:109:VAL:CG2	5:E:111:TRP:O	2.59	0.50
5:J:105:ALA:HB1	5:J:115:ALA:HB1	1.92	0.50
5:E:214:GLN:HA	5:E:254:ARG:O	2.12	0.50
4:I:65:LEU:HD13	4:I:79:GLN:HB2	1.93	0.50
4:I:130:GLN:O	4:I:132:PRO:HD3	2.12	0.50
2:G:128:LYS:HB3	2:G:176:GLU:HB2	1.93	0.49
8:A:202:GOL:H31	2:B:149:ARG:HB3	1.94	0.49
4:I:21:MET:HE1	4:I:102:TYR:CD1	2.47	0.49
1:A:169:HIS:HA	7:A:201:NAG:H81	1.94	0.49
4:D:21:MET:O	4:D:88:PHE:HA	2.12	0.49
4:D:79:GLN:HB3	4:D:88:PHE:CE1	2.48	0.49
2:G:125:ALA:HB1	2:G:147:LEU:HD21	1.95	0.49
4:I:15:GLU:HG3	4:I:128:ASN:CG	2.39	0.48
2:B:190:ALA:N	2:B:191:GLN:HA	2.28	0.48
2:B:190:ALA:HB3	2:B:191:GLN:C	2.39	0.48
2:B:117:CYS:HB2	2:B:131:TRP:CZ2	2.49	0.48
4:D:7:SER:HB3	4:D:22:ASN:HB2	1.94	0.48
4:I:129:ILE:HG21	4:I:156:ASP:HA	1.94	0.48
4:I:111:ALA:HB3	5:J:66:ARG:HH21	1.77	0.48
1:A:68:LEU:HG	2:B:9:TYR:CD1	2.48	0.48
4:D:59:ALA:HB1	4:D:82:ILE:HA	1.95	0.48
2:G:131:TRP:HB3	2:G:161:LEU:HD22	1.96	0.47
4:I:57:TYR:OH	5:J:114:GLU:OE2	2.31	0.47
2:G:82:ASN:O	2:G:86:GLU:HG2	2.15	0.47
1:A:103:GLN:NE2	5:J:131:LYS:HZ1	2.13	0.47
5:J:29:HIS:HA	5:J:108:LEU:HD12	1.97	0.47
1:F:56:PHE:CE1	3:H:3:PRO:HG3	2.49	0.47
1:F:68:LEU:HG	2:G:9:TYR:CD1	2.49	0.47
4:D:127:PRO:HD3	4:D:176:VAL:HG21	1.96	0.47
5:E:39:VAL:HG21	5:E:87:SER:HB2	1.96	0.46
2:B:61:TRP:CE2	3:C:7:LEU:HB2	2.50	0.46
2:B:129:VAL:HB	2:B:159:VAL:HG21	1.97	0.46
5:J:142:PRO:HG2	5:J:153:ALA:HB1	1.97	0.46
5:E:128:ASP:HB2	1:F:104:PRO:HG3	1.97	0.46
5:J:39:VAL:HG21	5:J:87:SER:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:10:GLN:HB2	2:G:31:ILE:HB	1.98	0.45
4:D:13:ILE:HD13	4:D:19:VAL:HG12	1.98	0.45
1:A:53:PHE:O	5:J:70:ASN:ND2	2.49	0.45
4:D:162:SER:HB2	4:D:206:ASN:O	2.16	0.45
5:E:57:PHE:CD2	5:E:110:ALA:HB2	2.50	0.45
1:F:60:PHE:CG	3:H:3:PRO:HG2	2.52	0.45
5:E:70:ASN:ND2	1:F:53:PHE:O	2.50	0.44
5:E:105:ALA:HB1	5:E:115:ALA:HB1	1.98	0.44
1:F:112:ASP:OD1	1:F:113:ASN:N	2.50	0.44
1:F:134:VAL:HG22	1:F:153:LEU:HD13	1.98	0.44
4:D:65:LEU:HD22	4:D:77:THR:HG22	1.99	0.44
5:E:65:GLN:HG2	5:E:66:ARG:N	2.31	0.44
4:D:38:THR:OG1	4:D:107:GLN:HB3	2.16	0.44
4:I:86:ASP:OD1	4:I:86:ASP:N	2.51	0.44
4:I:155:PHE:HD1	4:I:159:THR:HB	1.81	0.44
1:A:32:GLU:HB2	1:A:140:LEU:HD21	2.00	0.44
1:A:16:GLN:HB3	2:B:8:VAL:HG22	1.98	0.44
1:A:144:ASP:HB2	2:B:34:ARG:HH21	1.82	0.44
1:F:106:ILE:HD13	8:F:201:GOL:H12	2.00	0.44
4:I:155:PHE:CD1	4:I:159:THR:HB	2.53	0.43
4:D:13:ILE:HD12	4:D:17:GLU:HB2	1.99	0.43
1:F:178:LYS:HD3	1:F:178:LYS:HA	1.90	0.43
5:E:109:VAL:HG23	5:E:111:TRP:O	2.18	0.43
4:I:76:LEU:CD2	4:I:91:ILE:HG12	2.48	0.43
4:I:92:SER:C	4:I:94:SER:H	2.26	0.43
5:E:109:VAL:HG21	5:E:111:TRP:O	2.18	0.43
1:F:120:ASN:HB2	1:F:168:GLU:HB2	1.98	0.43
4:D:4:LEU:HG	4:D:116:ILE:HG12	2.00	0.43
1:F:142:LYS:HB3	1:F:142:LYS:HE3	1.88	0.43
4:I:43:LYS:HB2	4:I:53:LEU:HD11	2.00	0.43
1:A:61:ALA:O	1:A:65:ILE:HG12	2.19	0.43
4:D:99:VAL:HG22	4:D:125:VAL:H	1.83	0.42
3:C:3:PRO:HB2	5:E:111:TRP:CH2	2.54	0.42
4:I:80:PHE:HD1	4:I:81:GLY:N	2.17	0.42
5:J:195:LEU:HB2	5:J:198:SER:HB2	2.02	0.42
1:F:70:HIS:NE2	3:H:10:PRO:HB3	2.34	0.42
2:B:131:TRP:HB3	2:B:161:LEU:HD22	2.01	0.42
4:I:95:ILE:O	4:I:97:SER:N	2.52	0.42
4:I:75:ARG:NH1	4:I:92:SER:O	2.45	0.42
5:J:20:THR:HG23	5:J:90:ASN:OD1	2.20	0.42
4:I:80:PHE:CE1	4:I:84:ARG:HG2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:108:TYR:HD1	4:I:114:LYS:O	2.02	0.42
1:A:17:SER:O	1:A:19:GLY:HA2	2.20	0.42
4:I:63:GLY:HA2	4:I:79:GLN:HE21	1.85	0.42
5:J:57:PHE:CD2	5:J:110:ALA:HB2	2.55	0.42
2:B:163:MET:HE1	2:B:188:TRP:CH2	2.55	0.41
4:D:212:ASP:OD1	4:D:212:ASP:N	2.52	0.41
4:I:105:ALA:HB1	4:I:115:LEU:HD22	2.03	0.41
4:I:193:SER:HB3	4:I:198:PHE:CG	2.56	0.41
4:D:201:ALA:HA	4:D:215:PHE:CE2	2.55	0.41
5:E:24:SER:HA	5:E:25:PRO:HD3	1.92	0.41
1:F:10:SER:C	1:F:11(A):GLY:HA2	2.45	0.41
1:F:70:HIS:CE1	5:J:37:ARG:HH21	2.38	0.41
2:B:131:TRP:CD1	2:B:161:LEU:HB2	2.55	0.41
1:F:19:GLY:N	1:F:20:PRO:HA	2.36	0.41
1:F:158:SER:O	1:F:182:PRO:HG3	2.21	0.41
4:I:177:LEU:HD23	4:I:177:LEU:H	1.86	0.41
2:B:10:GLN:HB2	2:B:31:ILE:HB	2.02	0.41
1:A:56:PHE:CE1	3:C:3:PRO:HG3	2.56	0.40
5:E:190:LYS:HD2	5:E:198:SER:HB3	2.03	0.40
3:H:8:PRO:HD3	5:J:109:VAL:HG13	2.02	0.40
5:E:77:SER:OG	7:E:301:NAG:O7	2.32	0.40
1:A:134:VAL:HG22	1:A:153:LEU:HD13	2.04	0.40
4:D:29:PHE:O	4:D:39:TRP:NE1	2.54	0.40
1:A:49:VAL:HG22	2:B:89:THR:HG22	2.03	0.40
2:G:133:ARG:HA	2:G:134:ASN:HA	1.90	0.40
1:A:18:TYR:HA	1:A:19:GLY:HA2	1.70	0.40
1:A:53:PHE:CE1	2:B:85:LEU:HD22	2.57	0.40
3:H:7:LEU:HA	3:H:8:PRO:HD3	1.89	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	178/183 (97%)	173 (97%)	5 (3%)	0	100	100
1	F	178/183 (97%)	173 (97%)	5 (3%)	0	100	100
2	B	177/192 (92%)	172 (97%)	5 (3%)	0	100	100
2	G	174/192 (91%)	167 (96%)	7 (4%)	0	100	100
3	C	11/13 (85%)	10 (91%)	1 (9%)	0	100	100
3	H	10/13 (77%)	10 (100%)	0	0	100	100
4	D	200/206 (97%)	187 (94%)	13 (6%)	0	100	100
4	I	198/206 (96%)	181 (91%)	15 (8%)	2 (1%)	12	40
5	E	241/244 (99%)	228 (95%)	13 (5%)	0	100	100
5	J	239/244 (98%)	226 (95%)	13 (5%)	0	100	100
All	All	1606/1676 (96%)	1527 (95%)	77 (5%)	2 (0%)	48	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	I	8	PRO
4	I	131	ASN

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	153/167 (92%)	153 (100%)	0	100	100
1	F	155/167 (93%)	155 (100%)	0	100	100
2	B	159/176 (90%)	159 (100%)	0	100	100
2	G	157/176 (89%)	157 (100%)	0	100	100
3	C	11/11 (100%)	11 (100%)	0	100	100
3	H	11/11 (100%)	11 (100%)	0	100	100
4	D	163/181 (90%)	163 (100%)	0	100	100
4	I	159/181 (88%)	158 (99%)	1 (1%)	78	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	209/212 (99%)	209 (100%)	0	100	100
5	J	207/212 (98%)	207 (100%)	0	100	100
All	All	1384/1494 (93%)	1383 (100%)	1 (0%)	88	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	I	104	CYS

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

Mol	Chain	Res	Type
1	A	16	GLN
1	A	103	GLN
2	B	191	GLN
5	E	192	GLN
5	E	225	GLN
2	G	84	GLN
2	G	156	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 ⓘ

2 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	0.83	0	17,19,21	0.97	1 (5%)
6	NAG	K	2	6	14,14,15	0.78	0	17,19,21	1.37	2 (11%)

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	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	2	NAG	C2-N2-C7	3.61	127.73	122.90
6	K	1	NAG	C1-O5-C5	2.21	115.14	112.19
6	K	2	NAG	O5-C1-C2	-2.13	108.00	111.29

There are no chirality outliers.

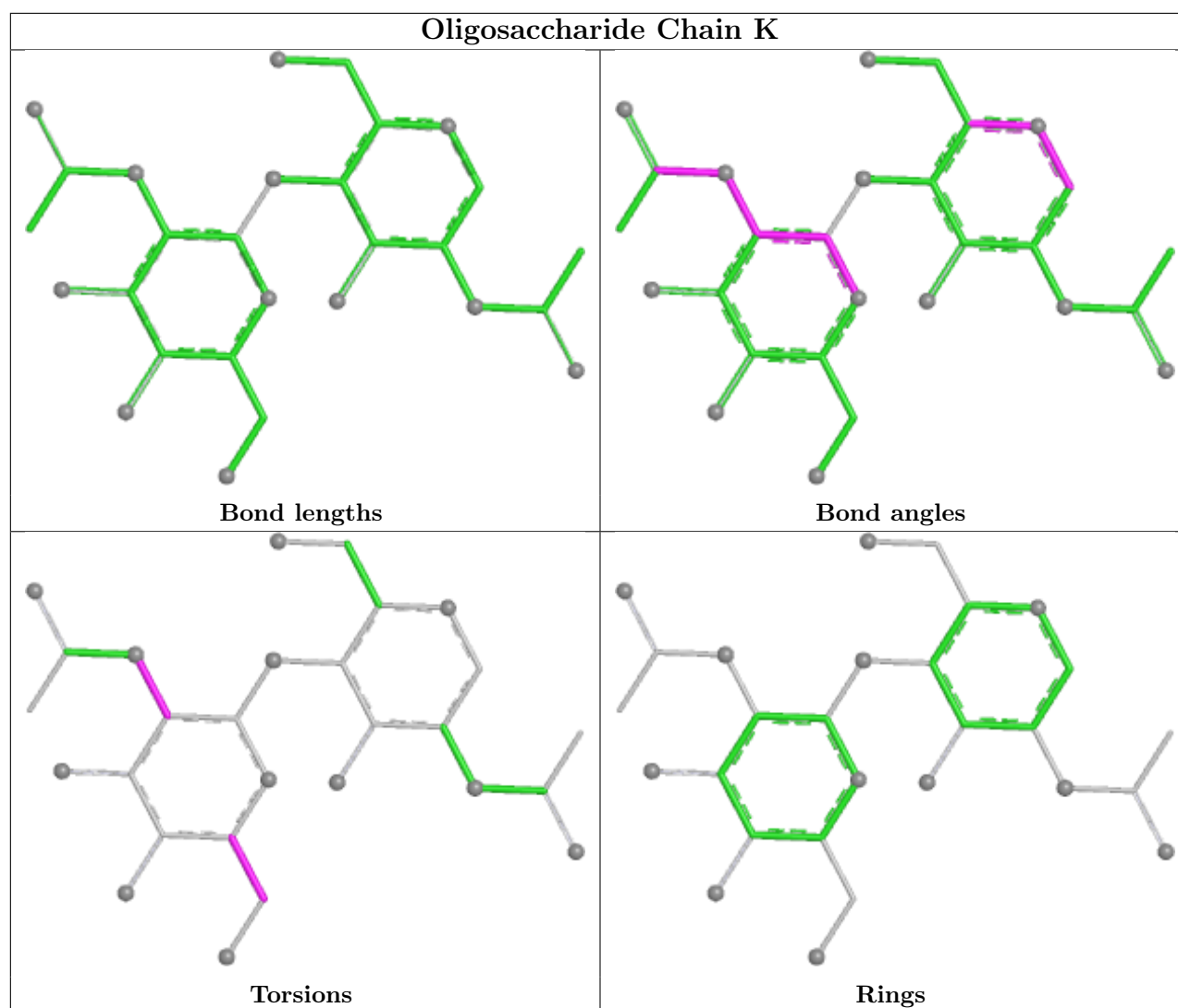
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	K	2	NAG	O5-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
6	K	2	NAG	C3-C2-N2-C7
6	K	2	NAG	C1-C2-N2-C7

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](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	I	301	4	14,14,15	0.72	0	17,19,21	0.68	0
8	GOL	F	202	-	5,5,5	0.25	0	5,5,5	0.30	0
8	GOL	G	202	-	5,5,5	0.25	0	5,5,5	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	D	301	4	14,14,15	0.84	0	17,19,21	0.88	0
7	NAG	J	301	5	14,14,15	0.77	0	17,19,21	0.80	1 (5%)
7	NAG	D	302	4	14,14,15	0.83	1 (7%)	17,19,21	1.59	2 (11%)
7	NAG	A	201	1	14,14,15	0.77	0	17,19,21	1.11	0
8	GOL	G	201	-	5,5,5	0.24	0	5,5,5	0.37	0
7	NAG	I	302	4	14,14,15	0.85	0	17,19,21	1.52	2 (11%)
7	NAG	E	301	5	14,14,15	0.77	0	17,19,21	0.87	0
8	GOL	A	202	-	5,5,5	0.24	0	5,5,5	0.39	0
8	GOL	F	201	-	5,5,5	0.25	0	5,5,5	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	I	301	4	-	3/6/23/26	0/1/1/1
8	GOL	F	202	-	-	0/4/4/4	-
8	GOL	G	202	-	-	0/4/4/4	-
7	NAG	D	301	4	-	2/6/23/26	0/1/1/1
7	NAG	J	301	5	-	1/6/23/26	0/1/1/1
7	NAG	D	302	4	-	0/6/23/26	0/1/1/1
7	NAG	A	201	1	-	0/6/23/26	0/1/1/1
8	GOL	G	201	-	-	0/4/4/4	-
7	NAG	I	302	4	-	0/6/23/26	0/1/1/1
7	NAG	E	301	5	-	1/6/23/26	0/1/1/1
8	GOL	A	202	-	-	2/4/4/4	-
8	GOL	F	201	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	302	NAG	O5-C1	-2.04	1.40	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	302	NAG	C2-N2-C7	4.93	129.51	122.90
7	I	302	NAG	C2-N2-C7	-4.12	117.38	122.90
7	I	302	NAG	C1-C2-N2	3.07	115.26	110.43
7	D	302	NAG	O5-C1-C2	-2.72	107.08	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	301	NAG	C1-O5-C5	2.11	115.02	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	202	GOL	C1-C2-C3-O3
8	A	202	GOL	O2-C2-C3-O3
7	D	301	NAG	C4-C5-C6-O6
7	E	301	NAG	O5-C5-C6-O6
7	J	301	NAG	O5-C5-C6-O6
7	D	301	NAG	O5-C5-C6-O6
7	I	301	NAG	C4-C5-C6-O6
7	I	301	NAG	O5-C5-C6-O6
7	I	301	NAG	C1-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	201	NAG	1	0
7	E	301	NAG	1	0
8	A	202	GOL	1	0
8	F	201	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	180/183 (98%)	0.28	2 (1%) 78 60	34, 58, 83, 124	0
1	F	180/183 (98%)	0.28	2 (1%) 78 60	34, 54, 80, 117	0
2	B	181/192 (94%)	0.32	5 (2%) 55 36	38, 55, 89, 112	0
2	G	178/192 (92%)	0.26	3 (1%) 69 50	34, 52, 78, 105	0
3	C	13/13 (100%)	0.72	1 (7%) 19 14	42, 49, 92, 97	0
3	H	12/13 (92%)	0.64	1 (8%) 17 13	37, 48, 83, 92	0
4	D	202/206 (98%)	0.70	13 (6%) 25 17	32, 67, 103, 133	0
4	I	200/206 (97%)	0.99	29 (14%) 6 5	33, 76, 126, 155	0
5	E	243/244 (99%)	0.24	6 (2%) 58 39	35, 54, 79, 94	0
5	J	241/244 (98%)	0.38	6 (2%) 58 39	37, 57, 94, 120	0
All	All	1630/1676 (97%)	0.44	68 (4%) 40 26	32, 58, 100, 155	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	130	GLN	4.6
3	H	10	PRO	3.9
5	E	66	ARG	3.9
4	D	147	LYS	3.9
5	E	67	ASN	3.9
4	I	145	SER	3.8
4	I	212	ASP	3.7
4	D	206	ASN	3.5
4	I	206	ASN	3.5
4	I	200	CYS	3.3
3	C	11	GLY	3.3
4	I	209	ILE	3.3
1	F	128	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
4	I	15	GLU	3.3
4	I	208	ILE	3.3
4	I	213	THR	3.2
4	D	168	ASP	3.2
5	E	112	ASP	3.1
4	I	197	ASP	3.1
4	I	129	ILE	3.0
5	J	238	ASP	2.9
4	I	140	ARG	2.8
4	I	144	SER	2.8
4	D	146	ASP	2.8
4	I	146	ASP	2.7
4	I	87	SER	2.7
4	I	147	LYS	2.7
4	D	11	MET	2.6
4	I	215	PHE	2.6
5	E	40	SER	2.6
4	D	145	SER	2.6
5	E	27	SER	2.6
2	B	191	GLN	2.5
4	D	143	LYS	2.5
2	B	166	GLN	2.4
2	B	170	VAL	2.4
4	D	38	THR	2.3
5	J	253	GLY	2.3
4	I	128	ASN	2.3
5	J	217	ARG	2.3
2	G	165	PRO	2.3
5	J	175	GLY	2.3
4	I	205	ASN	2.3
4	I	182	MET	2.3
4	I	214	PHE	2.3
5	J	130	ASN	2.3
4	I	211	GLU	2.2
1	F	126	ASN	2.2
4	D	194	ASN	2.2
4	I	202	ASN	2.2
4	I	216	PRO	2.2
1	A	126	ASN	2.2
4	D	218	PRO	2.2
4	I	119	THR	2.2
2	G	172	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	G	166	GLN	2.1
4	D	18	ASP	2.1
1	A	181	GLU	2.1
5	J	236	THR	2.1
2	B	169	ASP	2.1
4	D	7	SER	2.0
4	I	196	SER	2.0
4	I	207	SER	2.0
4	D	119	THR	2.0
4	I	156	ASP	2.0
2	B	168	GLY	2.0
4	I	8	PRO	2.0
5	E	111	TRP	2.0

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

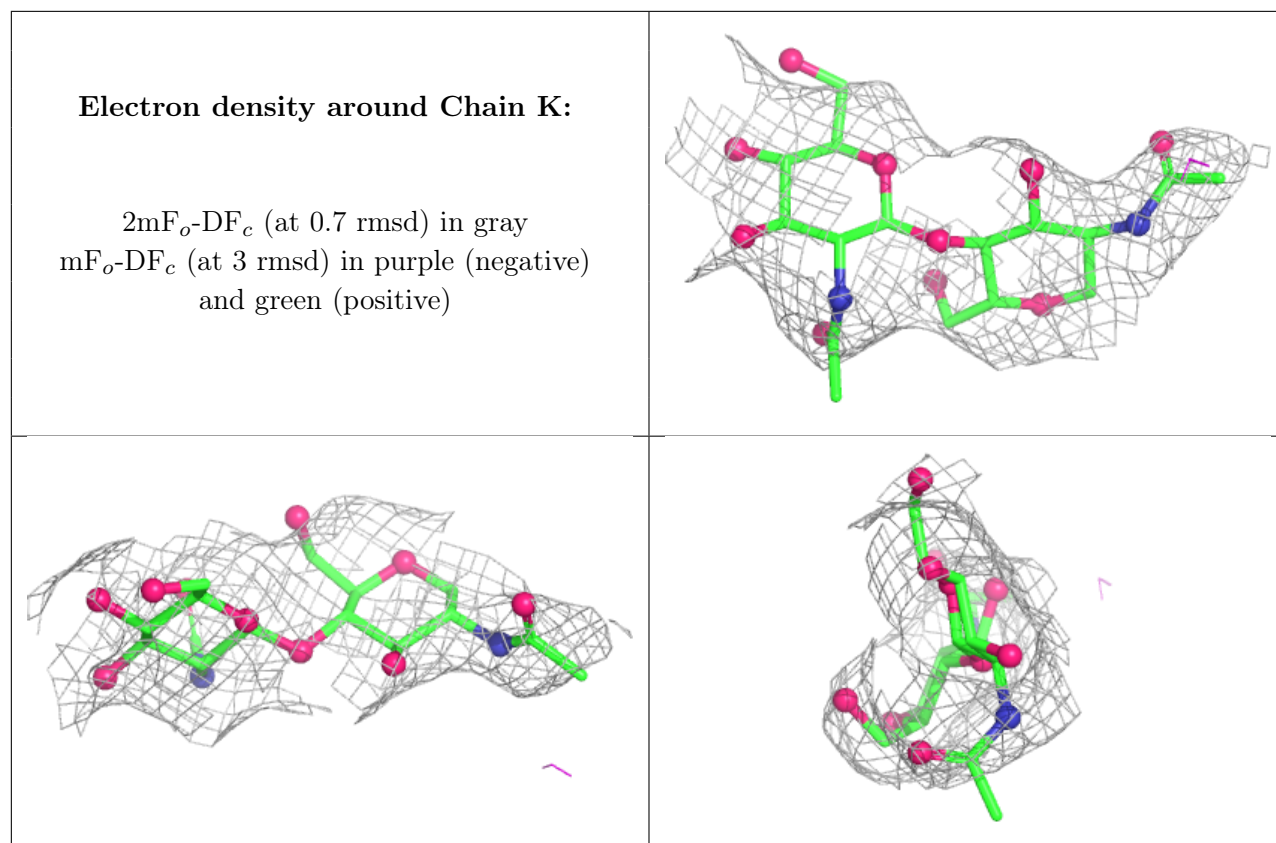
There are no non-standard protein/DNA/RNA residues in this entry.

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
6	NAG	K	2	14/15	0.66	0.16	122,122,122,122	0
6	NAG	K	1	14/15	0.81	0.15	81,96,117,120	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
7	NAG	D	302	14/15	0.51	0.22	111,111,111,111	0
7	NAG	I	302	14/15	0.70	0.18	103,103,103,103	0
7	NAG	A	201	14/15	0.79	0.17	79,93,113,115	0
8	GOL	G	201	6/6	0.80	0.24	73,73,73,73	0
7	NAG	D	301	14/15	0.81	0.14	66,76,92,106	0
8	GOL	F	201	6/6	0.83	0.19	61,61,61,61	0
8	GOL	A	202	6/6	0.83	0.15	41,47,62,64	0
7	NAG	E	301	14/15	0.85	0.14	54,73,84,91	0
7	NAG	I	301	14/15	0.85	0.12	71,84,105,106	0
7	NAG	J	301	14/15	0.88	0.12	52,64,79,89	0
8	GOL	F	202	6/6	0.91	0.11	65,65,65,65	0
8	GOL	G	202	6/6	0.94	0.10	43,75,84,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.