



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 18, 2026 – 10:10 AM JST

PDB ID : 27EB / pdb_000027eb
Title : TCR-HLA-DQ2.5-glia-w2 complex
Authors : Loh, T.J.; Lim, J.J.; Rossjohn, J.
Deposited on : 2026-05-28
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 : 1.8.5 (274361), CSD as541be (2020)
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

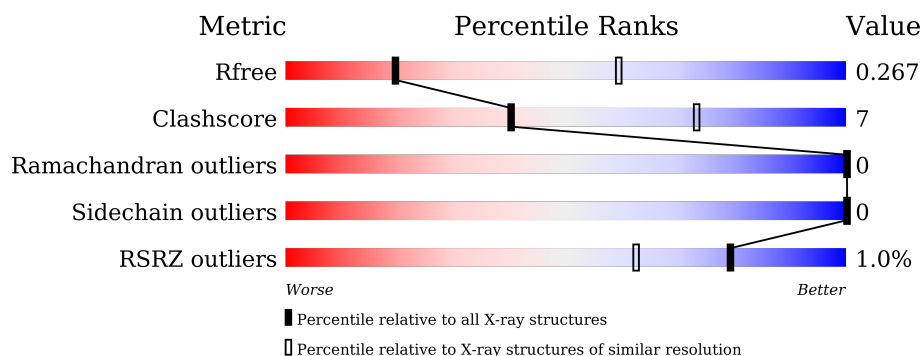
1 Overall quality at a glance

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.



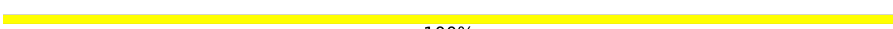
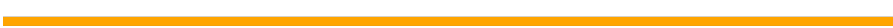
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	190	
1	D	190	
2	B	200	
2	E	200	
3	C	12	
3	F	12	

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Mol	Chain	Length	Quality of chain
4	G	207	 81% 18% .
4	I	207	%  74% 14% 11%
5	H	241	%  84% 16%
5	J	241	2%  82% 17% .
6	K	2	 100%
6	L	2	 100%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12810 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	183	Total	C	N	O	S	0	0	0
			1424	917	232	271	4			
1	D	182	Total	C	N	O	S	0	0	0
			1401	908	225	264	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	71	CYS	SER	conflict	UNP P01909
A	181	SER	-	expression tag	UNP P01909
A	182	GLY	-	expression tag	UNP P01909
A	183	ASP	-	expression tag	UNP P01909
A	184	ASP	-	expression tag	UNP P01909
A	185	ASP	-	expression tag	UNP P01909
A	186	ASP	-	expression tag	UNP P01909
A	187	LYS	-	expression tag	UNP P01909
D	71	CYS	SER	conflict	UNP P01909
D	181	SER	-	expression tag	UNP P01909
D	182	GLY	-	expression tag	UNP P01909
D	183	ASP	-	expression tag	UNP P01909
D	184	ASP	-	expression tag	UNP P01909
D	185	ASP	-	expression tag	UNP P01909
D	186	ASP	-	expression tag	UNP P01909
D	187	LYS	-	expression tag	UNP P01909

- Molecule 2 is a protein called cDNA FLJ59004, highly similar to HLA class II histocompatibility antigen, DQ(1)beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	181	Total	C	N	O	S	0	0	0
			1459	925	259	268	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	177	Total	C	N	O	S	0	0	0
			1417	903	245	262	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	229	THR	-	expression tag	UNP B4E328
B	230	GLY	-	expression tag	UNP B4E328
B	231	GLY	-	expression tag	UNP B4E328
B	232	ASP	-	expression tag	UNP B4E328
B	233	ASP	-	expression tag	UNP B4E328
B	234	ASP	-	expression tag	UNP B4E328
B	235	ASP	-	expression tag	UNP B4E328
B	236	LYS	-	expression tag	UNP B4E328
E	229	THR	-	expression tag	UNP B4E328
E	230	GLY	-	expression tag	UNP B4E328
E	231	GLY	-	expression tag	UNP B4E328
E	232	ASP	-	expression tag	UNP B4E328
E	233	ASP	-	expression tag	UNP B4E328
E	234	ASP	-	expression tag	UNP B4E328
E	235	ASP	-	expression tag	UNP B4E328
E	236	LYS	-	expression tag	UNP B4E328

- Molecule 3 is a protein called glia-omega 2 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	S	0	0	0
			100	66	16	17	1			
3	F	12	Total	C	N	O	S	0	0	0
			100	66	16	17	1			

- Molecule 4 is a protein called TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	204	Total	C	N	O	S	0	0	0
			1591	1002	256	322	11			
4	I	184	Total	C	N	O	S	0	0	0
			1399	883	225	280	11			

- Molecule 5 is a protein called TCR beta chain.

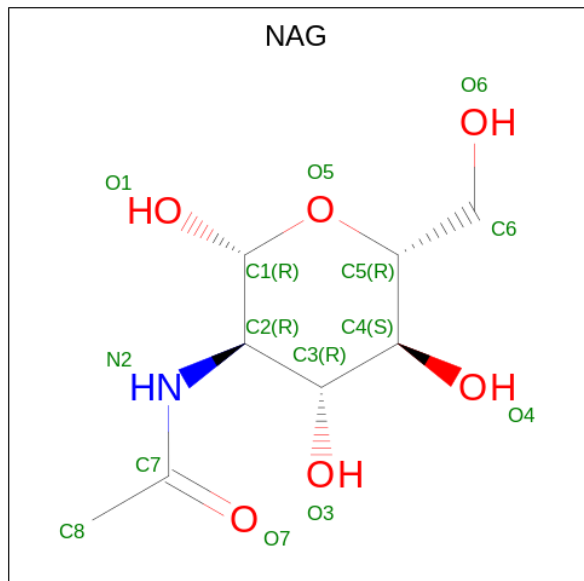
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	240	Total	C	N	O	S	0	0	0
			1902	1201	331	365	5			
5	J	237	Total	C	N	O	S	0	0	0
			1847	1170	315	357	5			

- 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			
6	L	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: $C_8H_{15}NO_6$).



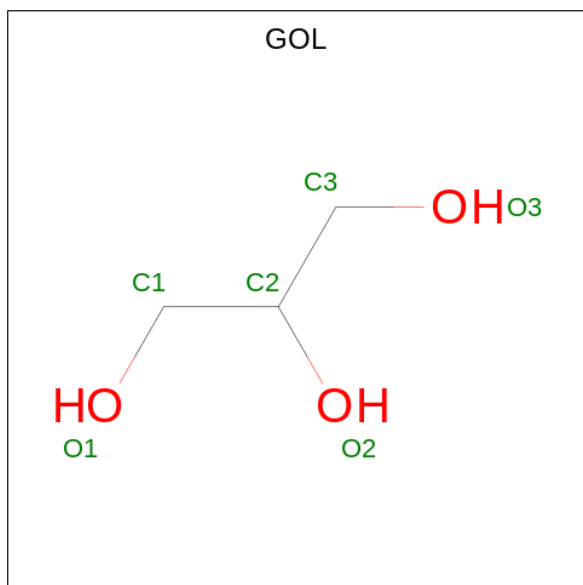
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		

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

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



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	7	Total	O	0	0
			7	7		
9	B	5	Total	O	0	0
			5	5		
9	D	4	Total	O	0	0
			4	4		
9	E	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	G	7	Total 7	O 7	0	0
9	H	5	Total 5	O 5	0	0
9	I	3	Total 3	O 3	0	0

3 Residue-property plots

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

Chain A: 



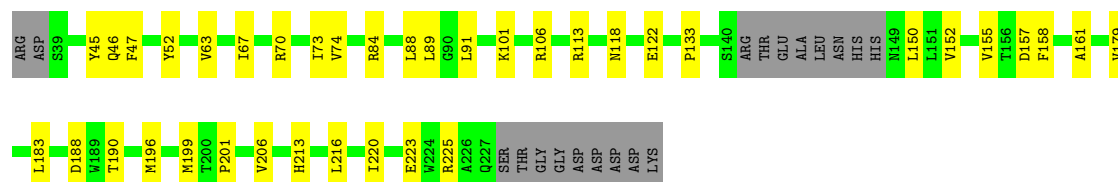
- Molecule 1: HLA class II histocompatibility antigen, DQ alpha 1 chain

Chain D: 



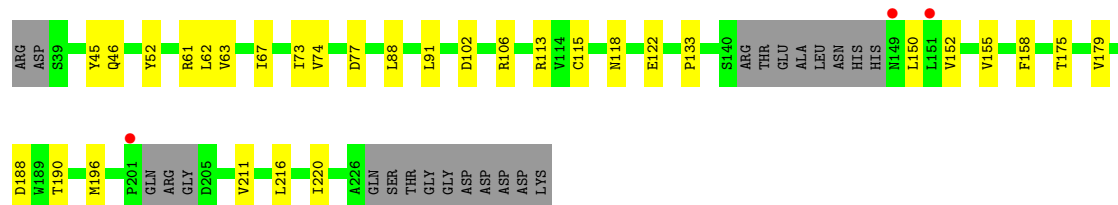
- Molecule 2: cDNA FLJ59004, highly similar to HLA class II histocompatibility antigen, DQ(1)beta chain

Chain B: 



- Molecule 2: cDNA FLJ59004, highly similar to HLA class II histocompatibility antigen, DQ(1)beta chain

Chain E: 



- Molecule 3: glia-omega 2 peptide

Chain C:  83% 17%



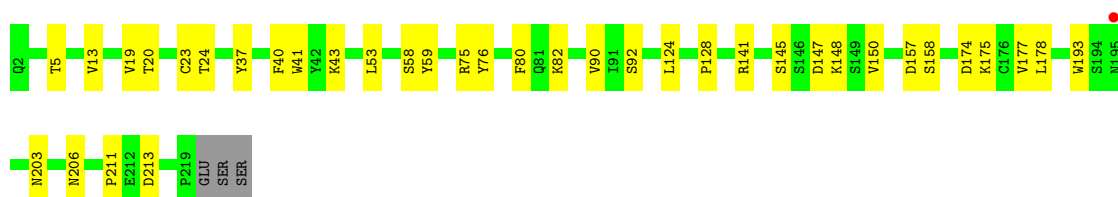
- Molecule 3: glia-omega 2 peptide

Chain F:  83% 17%



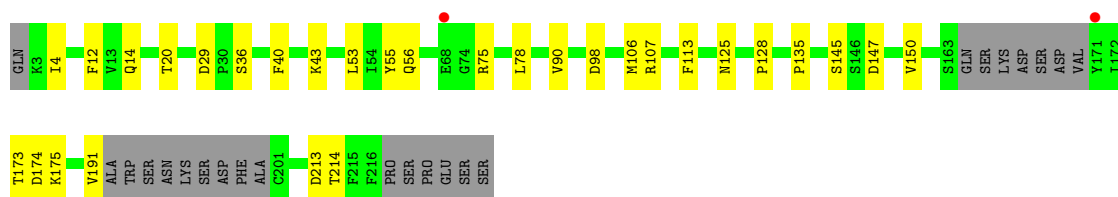
- Molecule 4: TCR alpha chain

Chain G:  81% 18%



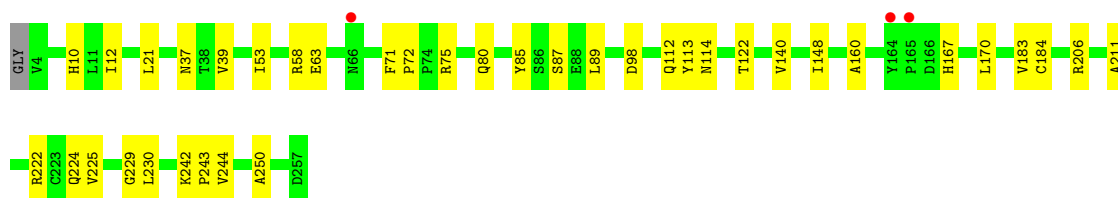
- Molecule 4: TCR alpha chain

Chain I:  74% 14% 11%



- Molecule 5: TCR beta chain

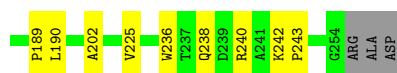
Chain H:  84% 16%



- Molecule 5: TCR beta chain

Chain J:  82% 17%





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

Chain K:  100%



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

Chain L:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.92Å 144.01Å 147.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.65 – 3.25 46.65 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.65-3.25) 99.8 (46.65-3.25)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.221 , 0.267 0.221 , 0.267	Depositor DCC
R_{free} test set	1842 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	83.9	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12810	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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	0.09	0/1466	0.25	0/2008
1	D	0.10	0/1443	0.28	0/1980
2	B	0.09	0/1492	0.29	0/2031
2	E	0.10	0/1449	0.27	0/1974
3	C	0.22	0/106	0.49	0/147
3	F	0.23	0/106	0.43	0/147
4	G	0.11	0/1628	0.36	0/2205
4	I	0.11	0/1429	0.33	0/1937
5	H	0.11	0/1956	0.34	0/2667
5	J	0.25	0/1901	0.45	0/2600
All	All	0.14	0/12976	0.33	0/17696

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
5	J	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	J	58	ARG	Sidechain

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	1424	0	1339	18	0
1	D	1401	0	1319	17	0
2	B	1459	0	1412	30	0
2	E	1417	0	1362	28	0
3	C	100	0	88	2	0
3	F	100	0	88	3	0
4	G	1591	0	1468	23	0
4	I	1399	0	1253	19	0
5	H	1902	0	1777	25	0
5	J	1847	0	1696	24	0
6	K	28	0	25	0	0
6	L	28	0	25	1	0
7	A	14	0	13	0	0
7	G	14	0	13	0	0
7	H	14	0	13	0	0
7	I	14	0	13	0	0
7	J	14	0	13	0	0
8	D	12	0	16	1	0
9	A	7	0	0	0	0
9	B	5	0	0	0	0
9	D	4	0	0	0	0
9	E	1	0	0	0	0
9	G	7	0	0	0	0
9	H	5	0	0	0	0
9	I	3	0	0	0	0
All	All	12810	0	11933	164	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 7.

All (164) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:LEU:HD11	2:B:196:MET:HB3	1.72	0.71
1:D:117:ASN:HB2	1:D:165:GLU:HB2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:ARG:HD3	4:G:59:TYR:HD2	1.55	0.70
2:E:133:PRO:HD2	2:E:216:LEU:HD21	1.74	0.70
1:A:117:ASN:HB2	1:A:165:GLU:HB2	1.74	0.67
4:G:13:VAL:HG11	4:G:19:VAL:HB	1.76	0.66
5:H:39:VAL:HG11	5:H:87:SER:HB2	1.80	0.63
2:B:223:GLU:OE1	2:B:225:ARG:NH2	2.31	0.63
4:I:107:ARG:HH21	4:I:113:PHE:HB3	1.62	0.63
5:J:21:LEU:HD22	5:J:122:THR:HG21	1.80	0.62
4:I:40:PHE:HZ	5:J:113:TYR:O	1.82	0.62
4:I:43:LYS:HB2	4:I:53:LEU:HD11	1.80	0.62
2:B:73:ILE:HG13	2:B:74:VAL:HG23	1.81	0.60
1:A:121:LEU:HD11	1:A:163:LYS:HD2	1.84	0.60
2:B:88:LEU:HD11	2:E:196:MET:HE2	1.83	0.59
2:B:199:MET:HE3	2:B:201:PRO:HG3	1.84	0.59
1:D:119:THR:HB	1:D:163:LYS:HB3	1.84	0.59
4:I:75:ARG:NH1	4:I:98:ASP:OD2	2.36	0.59
1:D:69:LEU:HD13	2:E:45:TYR:HB2	1.85	0.58
2:B:152:VAL:HG22	2:B:196:MET:HG3	1.85	0.58
2:B:196:MET:HG2	2:E:88:LEU:HD21	1.86	0.58
2:B:216:LEU:HD13	2:B:220:ILE:HG13	1.85	0.58
2:E:46:GLN:HB2	2:E:67:ILE:HB	1.84	0.58
2:B:133:PRO:HB3	2:B:158:PHE:HB3	1.86	0.57
2:E:73:ILE:HG13	2:E:74:VAL:HG23	1.86	0.57
5:J:81:PHE:HB2	5:J:84:ASN:OD1	2.04	0.57
4:G:178:LEU:HB3	5:H:184:CYS:HB2	1.88	0.56
5:H:230:LEU:HD12	5:H:243:PRO:HD2	1.89	0.55
5:H:72:PRO:HB2	5:H:75:ARG:HG2	1.89	0.55
1:A:30:GLU:HB2	1:A:137:LEU:HD21	1.87	0.54
5:H:21:LEU:HD22	5:H:122:THR:HG21	1.89	0.54
1:D:121:LEU:HD12	1:D:174:LEU:HD11	1.89	0.54
2:B:46:GLN:HB2	2:B:67:ILE:HB	1.88	0.54
4:I:14:GLN:NE2	4:I:128:PRO:O	2.41	0.54
2:E:216:LEU:HD13	2:E:220:ILE:HG13	1.90	0.53
4:G:145:SER:O	4:G:148:LYS:HG2	2.09	0.53
4:G:23:CYS:HB2	4:G:41:TRP:CZ2	2.44	0.53
1:A:11:ASN:HB2	2:B:47:PHE:HB3	1.90	0.53
1:A:93:LYS:NZ	2:B:157:ASP:OD1	2.37	0.53
2:B:52:TYR:HE1	2:B:63:VAL:HG22	1.73	0.53
2:E:133:PRO:HB3	2:E:158:PHE:HB3	1.90	0.52
5:J:72:PRO:HB2	5:J:75:ARG:HG2	1.90	0.52
1:A:112:PHE:CG	2:B:70:ARG:HD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:12:PHE:HD1	4:I:125:ASN:HB2	1.75	0.51
1:D:109:ASP:OD2	8:D:202:GOL:O2	2.29	0.51
4:I:29:ASP:OD2	4:I:36:SER:OG	2.29	0.51
5:J:48:GLN:HG2	5:J:49:GLY:H	1.76	0.51
5:H:112:GLN:HE21	5:H:114:ASN:HD21	1.58	0.51
5:J:48:GLN:HG2	5:J:49:GLY:N	2.27	0.50
1:D:39:LYS:HG3	1:D:59:LEU:HD11	1.94	0.50
5:H:12:ILE:HD12	5:H:229:GLY:HA2	1.93	0.50
5:H:170:LEU:HG	5:H:225:VAL:HG22	1.94	0.50
4:G:203:ASN:OD1	4:G:206:ASN:ND2	2.45	0.49
1:A:62:ILE:O	1:A:66:LYS:HG3	2.13	0.49
4:G:157:ASP:OD1	4:G:158:SER:N	2.46	0.49
1:A:76:SER:HB3	2:B:89:LEU:HD21	1.95	0.49
5:J:134:PHE:HD1	5:J:135:PRO:HD2	1.77	0.49
5:J:12:ILE:HD11	5:J:165:PRO:HG3	1.94	0.49
1:D:96:VAL:HG21	1:D:177:TRP:HZ2	1.78	0.48
4:G:150:VAL:HG23	4:G:193:TRP:HB3	1.95	0.48
4:G:5:THR:HG1	4:G:24:THR:HG1	1.59	0.48
5:H:75:ARG:NH1	5:H:98:ASP:OD2	2.37	0.48
5:J:14:THR:HG22	5:J:130:LEU:HD13	1.95	0.48
2:B:161:ALA:HB1	2:B:183:LEU:HD21	1.96	0.48
2:B:179:VAL:HG13	2:E:91:LEU:HD13	1.95	0.48
5:J:166:ASP:OD1	5:J:189:PRO:HG3	2.14	0.48
1:D:119:THR:O	1:D:163:LYS:N	2.39	0.48
4:I:173:THR:HG22	4:I:191:VAL:H	1.78	0.48
2:E:150:LEU:HD22	2:E:196:MET:HB3	1.94	0.48
5:J:170:LEU:HG	5:J:225:VAL:HG22	1.95	0.48
2:B:91:LEU:HD13	2:E:179:VAL:HG13	1.95	0.47
2:E:118:ASN:O	2:E:122:GLU:HG2	2.15	0.47
5:H:63:GLU:HG3	5:H:80:GLN:O	2.14	0.47
1:A:67:HIS:HA	5:H:58:ARG:HH21	1.79	0.47
2:B:84:ARG:NH2	2:E:175:THR:HB	2.29	0.47
1:D:109:ASP:OD1	1:D:110:ASN:N	2.46	0.47
2:E:152:VAL:HG22	2:E:196:MET:HG3	1.94	0.47
4:I:4:ILE:HD11	4:I:106:MET:HB2	1.97	0.47
2:E:52:TYR:HE1	2:E:63:VAL:HG22	1.80	0.47
4:G:203:ASN:HA	4:G:206:ASN:HB3	1.96	0.46
2:E:102:ASP:OD2	4:I:55:TYR:OH	2.32	0.46
2:B:213:HIS:HB3	2:B:216:LEU:HG	1.97	0.46
1:D:46:PRO:HA	1:D:49:ARG:HE	1.80	0.46
1:A:119:THR:HB	1:A:163:LYS:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:14:THR:HA	5:J:127:LEU:O	2.16	0.46
1:D:30:GLU:HB2	1:D:137:LEU:HD21	1.96	0.46
1:D:169:LEU:HD13	1:D:173:LEU:HB2	1.98	0.46
1:A:150:LEU:O	1:A:150:LEU:HD23	2.16	0.46
2:B:188:ASP:OD1	2:B:190:THR:OG1	2.27	0.46
2:B:196:MET:SD	2:E:88:LEU:HD11	2.55	0.46
4:G:141:ARG:HD2	4:G:147:ASP:HB3	1.97	0.45
4:I:20:THR:HG23	4:I:90:VAL:HG22	1.98	0.45
5:J:190:LEU:HG	5:J:202:ALA:HB3	1.98	0.45
1:D:45:LEU:HD12	1:D:46:PRO:HD2	1.97	0.45
2:E:106:ARG:CD	3:F:7:PHE:HZ	2.29	0.45
4:I:174:ASP:OD1	4:I:175:LYS:N	2.44	0.45
5:J:29:HIS:ND1	5:J:106:SER:OG	2.42	0.45
2:E:188:ASP:OD1	2:E:190:THR:OG1	2.26	0.45
4:G:20:THR:HG23	4:G:90:VAL:HG22	1.99	0.44
4:I:145:SER:O	4:I:147:ASP:N	2.41	0.44
5:H:222:ARG:NH1	5:H:224:GLN:HB2	2.32	0.44
5:J:236:TRP:HB2	5:J:242:LYS:HD2	1.99	0.44
5:H:112:GLN:HE21	5:H:114:ASN:ND2	2.15	0.44
4:I:213:ASP:OD1	4:I:213:ASP:N	2.47	0.44
1:A:43:TRP:HH2	3:C:1:PRO:HG3	1.83	0.44
5:H:160:ALA:HB2	5:H:225:VAL:HG21	1.99	0.44
4:G:53:LEU:HD22	4:G:76:TYR:CE2	2.52	0.44
4:G:211:PRO:HB2	4:G:213:ASP:OD1	2.18	0.44
2:E:61:ARG:NH2	2:E:77:ASP:OD2	2.47	0.44
5:J:39:VAL:HG11	5:J:87:SER:HB2	2.00	0.44
6:L:1:NAG:H4	6:L:2:NAG:H2	1.79	0.44
4:G:128:PRO:HB3	4:G:177:VAL:HG21	2.00	0.44
5:J:53:ILE:HA	5:J:71:PHE:CD2	2.52	0.44
1:A:67:HIS:HA	5:H:58:ARG:NH2	2.32	0.43
2:E:106:ARG:HD3	3:F:7:PHE:HZ	1.82	0.43
4:G:75:ARG:HD2	4:G:92:SER:O	2.19	0.43
4:G:43:LYS:HB2	4:G:53:LEU:HD11	2.01	0.43
4:I:56:GLN:HB2	4:I:78:LEU:HD13	2.00	0.43
5:J:129:ASP:OD1	5:J:129:ASP:N	2.51	0.43
1:A:104:LEU:HD23	1:A:104:LEU:HA	1.85	0.43
5:J:46:LEU:H	5:J:46:LEU:HD22	1.83	0.43
2:E:102:ASP:O	2:E:106:ARG:HG2	2.18	0.43
2:E:155:VAL:HG21	2:E:211:VAL:HG11	2.00	0.43
1:A:96:VAL:HG21	1:A:177:TRP:HZ2	1.83	0.43
5:J:242:LYS:HA	5:J:243:PRO:HD3	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:LEU:HG	2:E:45:TYR:CD2	2.53	0.43
2:E:113:ARG:NH1	3:F:3:PRO:O	2.46	0.42
4:G:37:TYR:H	4:G:58:SER:CB	2.32	0.42
5:H:37:ASN:HA	5:H:85:TYR:CG	2.54	0.42
1:A:8:SER:HB2	1:A:25:GLU:HB2	2.00	0.42
2:B:113:ARG:NH1	3:C:3:PRO:O	2.49	0.42
4:G:19:VAL:HG21	4:G:124:LEU:HD13	2.00	0.42
4:I:150:VAL:HG13	4:I:191:VAL:HG13	2.01	0.42
5:J:63:GLU:HA	5:J:80:GLN:HB3	2.02	0.42
5:H:140:VAL:HG23	5:H:250:ALA:HB3	2.01	0.42
2:E:102:ASP:OD2	4:I:55:TYR:CE2	2.72	0.42
5:H:53:ILE:HA	5:H:71:PHE:CD2	2.55	0.42
5:J:238:GLN:CG	5:J:240:ARG:HG2	2.50	0.42
1:A:8:SER:HB3	1:A:10:VAL:HG23	2.02	0.42
4:G:40:PHE:HZ	5:H:113:TYR:O	2.03	0.42
5:J:12:ILE:HD13	5:J:125:THR:HB	2.02	0.41
4:I:12:PHE:CD1	4:I:125:ASN:HB2	2.53	0.41
2:B:118:ASN:O	2:B:122:GLU:HG2	2.20	0.41
5:H:21:LEU:HD12	5:H:89:LEU:HD22	2.02	0.41
5:H:58:ARG:NH1	5:H:85:TYR:OH	2.53	0.41
4:I:135:PRO:HG2	4:I:214:THR:HA	2.01	0.41
2:B:133:PRO:HD2	2:B:216:LEU:HD21	2.01	0.41
1:D:161:ASP:HB3	1:D:174:LEU:HD12	2.03	0.41
5:H:242:LYS:O	5:H:244:VAL:N	2.49	0.41
2:B:101:LYS:HA	2:B:101:LYS:HD3	1.83	0.41
1:A:69:LEU:HD13	2:B:45:TYR:HB2	2.03	0.41
1:D:76:SER:O	1:D:79:THR:HG23	2.20	0.41
1:D:104:LEU:HD23	1:D:104:LEU:HA	1.88	0.41
5:H:183:VAL:HA	5:H:206:ARG:O	2.21	0.41
2:B:133:PRO:HB2	2:B:155:VAL:CG2	2.51	0.41
2:E:150:LEU:HD23	2:E:150:LEU:HA	1.92	0.41
4:G:37:TYR:H	4:G:58:SER:HB3	1.85	0.41
4:G:174:ASP:OD1	4:G:175:LYS:N	2.46	0.41
5:H:148:ILE:HG23	5:H:211:ALA:HB1	2.02	0.40
2:B:206:VAL:HG22	2:B:225:ARG:HG2	2.04	0.40
2:E:62:LEU:HB2	2:E:115:CYS:SG	2.62	0.40
4:G:80:PHE:CZ	4:G:82:LYS:HG2	2.56	0.40
5:H:10:HIS:CD2	5:H:167:HIS:HB3	2.56	0.40
5:J:133:VAL:O	5:J:243:PRO:HG2	2.21	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	181/190 (95%)	175 (97%)	6 (3%)	0	100	100
1	D	180/190 (95%)	175 (97%)	5 (3%)	0	100	100
2	B	177/200 (88%)	168 (95%)	9 (5%)	0	100	100
2	E	171/200 (86%)	162 (95%)	9 (5%)	0	100	100
3	C	10/12 (83%)	10 (100%)	0	0	100	100
3	F	10/12 (83%)	10 (100%)	0	0	100	100
4	G	202/207 (98%)	191 (95%)	11 (5%)	0	100	100
4	I	178/207 (86%)	159 (89%)	19 (11%)	0	100	100
5	H	238/241 (99%)	229 (96%)	9 (4%)	0	100	100
5	J	235/241 (98%)	229 (97%)	6 (3%)	0	100	100
All	All	1582/1700 (93%)	1508 (95%)	74 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	158/173 (91%)	158 (100%)	0	100	100
1	D	154/173 (89%)	154 (100%)	0	100	100
2	B	159/182 (87%)	159 (100%)	0	100	100
2	E	154/182 (85%)	154 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	11/11 (100%)	11 (100%)	0	100	100
3	F	11/11 (100%)	11 (100%)	0	100	100
4	G	176/185 (95%)	176 (100%)	0	100	100
4	I	147/185 (80%)	147 (100%)	0	100	100
5	H	205/209 (98%)	205 (100%)	0	100	100
5	J	197/209 (94%)	197 (100%)	0	100	100
All	All	1372/1520 (90%)	1372 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
2	B	100	GLN
2	B	186	ASN
2	B	192	GLN
4	G	44	GLN
4	G	81	GLN
4	G	139	GLN
4	G	159	GLN
5	H	51	GLN
5	H	92	ASN
5	H	114	ASN
5	H	152	GLN
4	I	110	ASN
4	I	188	ASN
5	J	17	GLN
5	J	18	GLN
5	J	55	GLN
5	J	66	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 ⓘ

4 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	6,1	14,14,15	0.79	0	17,19,21	1.31	2 (11%)
6	NAG	K	2	6	14,14,15	0.70	0	17,19,21	1.21	1 (5%)
6	NAG	L	1	6,1	14,14,15	0.74	0	17,19,21	2.37	4 (23%)
6	NAG	L	2	6	14,14,15	0.79	0	17,19,21	0.96	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
6	NAG	K	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	K	2	6	-	1/6/23/26	0/1/1/1
6	NAG	L	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1	NAG	C2-N2-C7	7.98	134.27	122.90
6	K	2	NAG	C2-N2-C7	3.15	127.39	122.90
6	L	1	NAG	O4-C4-C3	-2.77	103.94	110.35
6	K	1	NAG	C1-O5-C5	2.59	115.70	112.19
6	L	1	NAG	O5-C1-C2	-2.52	107.31	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1	NAG	C8-C7-N2	2.39	120.15	116.10
6	L	2	NAG	O5-C1-C2	-2.24	107.75	111.29
6	K	1	NAG	O4-C4-C3	-2.22	105.23	110.35

There are no chirality outliers.

All (6) torsion outliers are listed below:

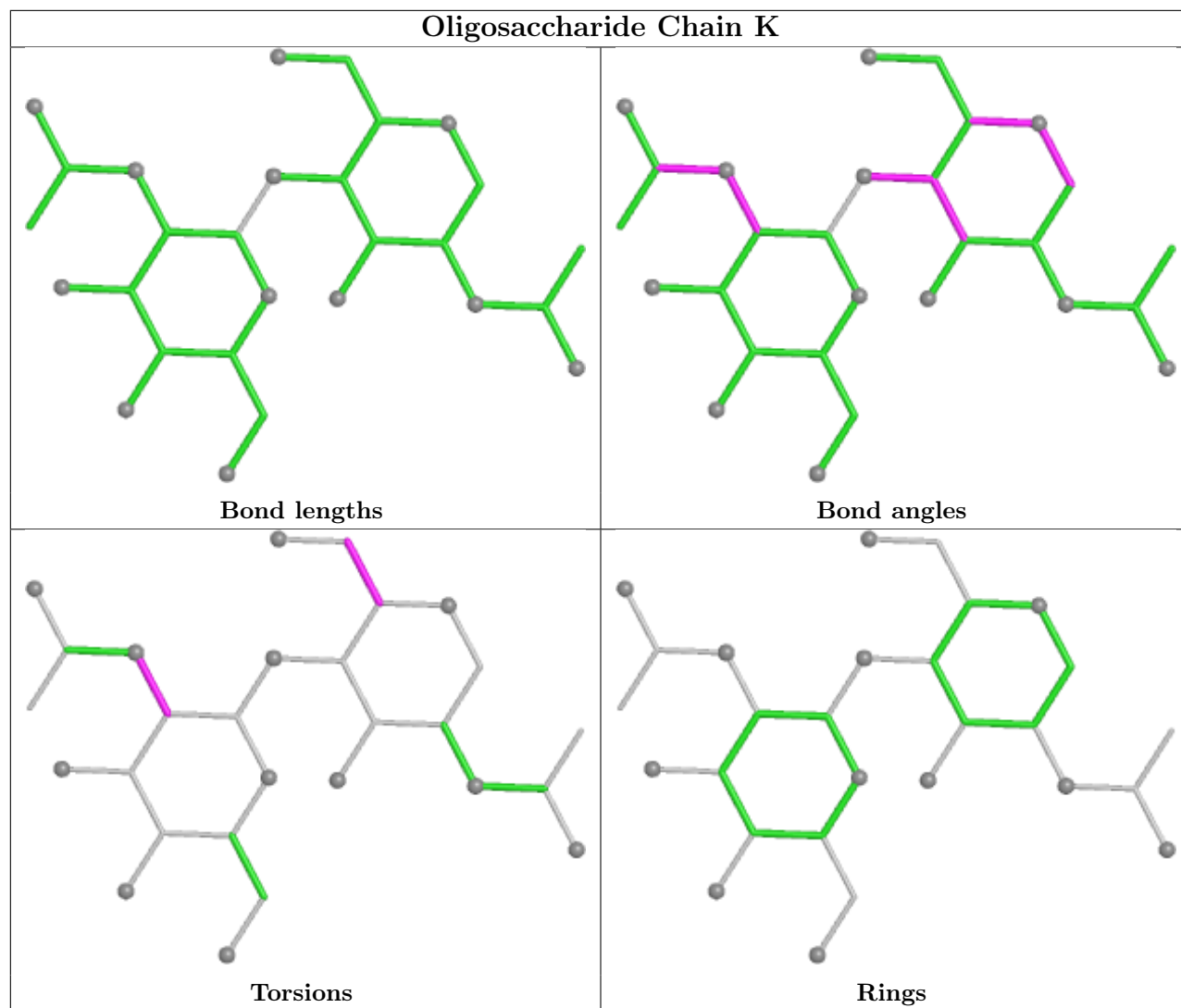
Mol	Chain	Res	Type	Atoms
6	L	1	NAG	C8-C7-N2-C2
6	L	1	NAG	O7-C7-N2-C2
6	K	2	NAG	C3-C2-N2-C7
6	L	1	NAG	O5-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
6	L	1	NAG	C3-C2-N2-C7

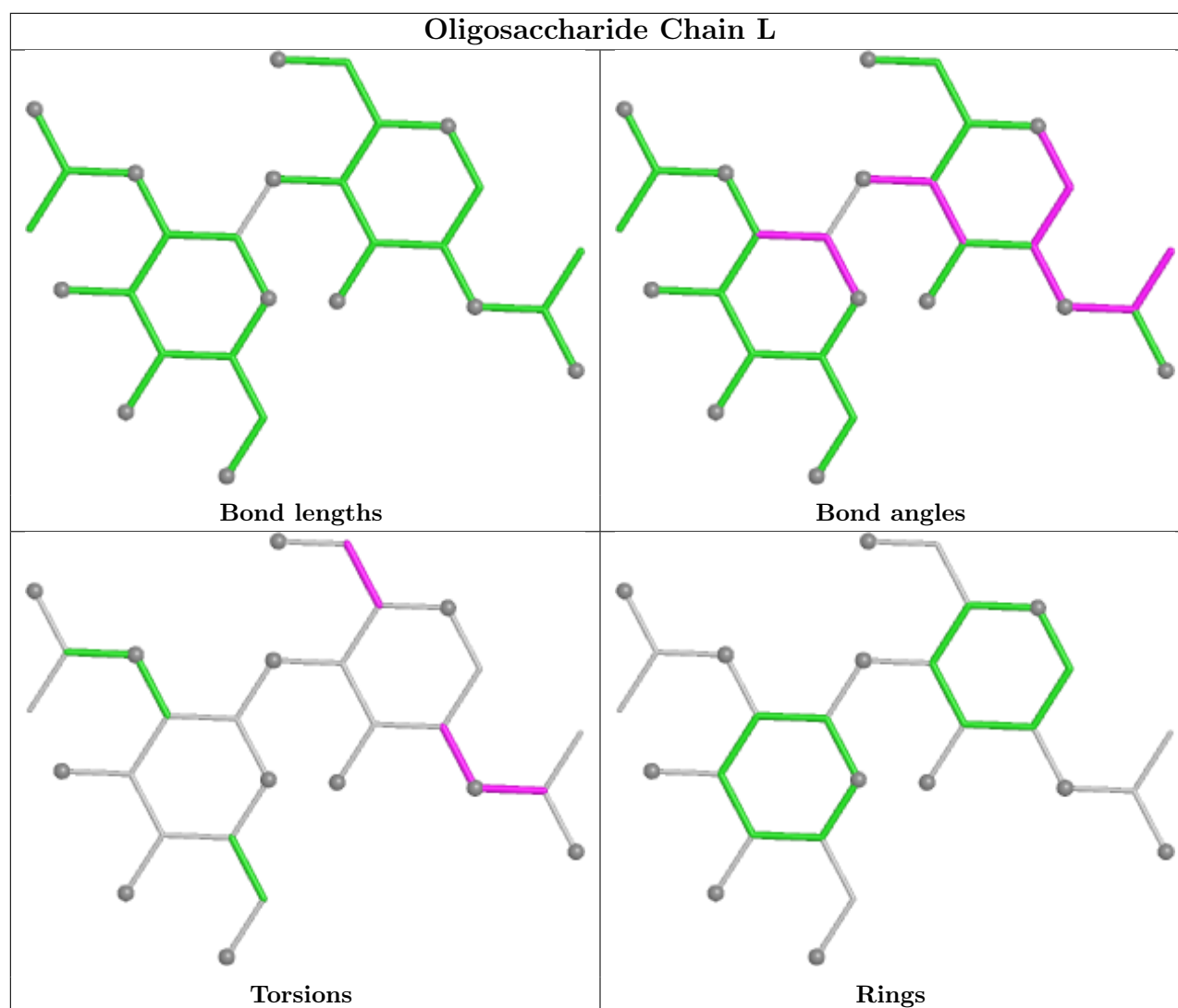
There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	1	NAG	1	0
6	L	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

7 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	0.76	0	17,19,21	2.07	2 (11%)
8	GOL	D	201	-	5,5,5	0.34	0	5,5,5	0.36	0
7	NAG	A	201	1	14,14,15	0.73	0	17,19,21	1.20	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	H	301	5	14,14,15	0.78	0	17,19,21	0.80	0
7	NAG	G	301	4	14,14,15	0.67	0	17,19,21	1.25	1 (5%)
8	GOL	D	202	-	5,5,5	0.34	0	5,5,5	0.36	0
7	NAG	J	301	5	14,14,15	0.58	0	17,19,21	1.27	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
7	NAG	I	301	4	-	1/6/23/26	0/1/1/1
8	GOL	D	201	-	-	0/4/4/4	-
7	NAG	A	201	1	-	2/6/23/26	0/1/1/1
7	NAG	H	301	5	-	2/6/23/26	0/1/1/1
7	NAG	G	301	4	-	1/6/23/26	0/1/1/1
8	GOL	D	202	-	-	0/4/4/4	-
7	NAG	J	301	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	301	NAG	C2-N2-C7	7.22	133.18	122.90
7	J	301	NAG	O5-C1-C2	-3.44	105.86	111.29
7	G	301	NAG	C2-N2-C7	3.32	127.63	122.90
7	A	201	NAG	C2-N2-C7	3.27	127.56	122.90
7	I	301	NAG	O7-C7-N2	2.58	126.70	121.95
7	J	301	NAG	C2-N2-C7	2.35	126.25	122.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	301	NAG	C3-C2-N2-C7
7	H	301	NAG	O5-C5-C6-O6
7	H	301	NAG	C4-C5-C6-O6
7	J	301	NAG	C8-C7-N2-C2
7	J	301	NAG	O7-C7-N2-C2
7	A	201	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	A	201	NAG	C3-C2-N2-C7
7	G	301	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	202	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	183/190 (96%)	-0.26	0 100 100	44, 67, 91, 122	0
1	D	182/190 (95%)	0.13	3 (1%) 70 52	58, 86, 119, 141	0
2	B	181/200 (90%)	-0.17	0 100 100	49, 68, 91, 117	0
2	E	177/200 (88%)	0.06	3 (1%) 69 50	51, 74, 115, 141	0
3	C	12/12 (100%)	0.59	0 100 100	58, 67, 88, 96	0
3	F	12/12 (100%)	0.30	0 100 100	56, 67, 96, 106	0
4	G	204/207 (98%)	-0.01	1 (0%) 87 76	46, 77, 121, 150	0
4	I	184/207 (88%)	0.20	2 (1%) 78 60	46, 79, 151, 168	0
5	H	240/241 (99%)	-0.04	3 (1%) 75 56	55, 83, 124, 147	0
5	J	237/241 (98%)	0.34	4 (1%) 69 50	61, 97, 132, 147	0
All	All	1612/1700 (94%)	0.05	16 (0%) 79 62	44, 79, 129, 168	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	149	ASN	4.0
4	G	195	ASN	2.9
5	H	165	PRO	2.8
4	I	171	TYR	2.4
1	D	65	LEU	2.3
4	I	68	GLU	2.2
5	J	37	ASN	2.2
1	D	114	PRO	2.2
5	H	164	TYR	2.2
1	D	180	GLU	2.2
2	E	201	PRO	2.1
2	E	151	LEU	2.1
5	H	66	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
5	J	158	CYS	2.1
5	J	133	VAL	2.0
5	J	11	LEU	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](#)

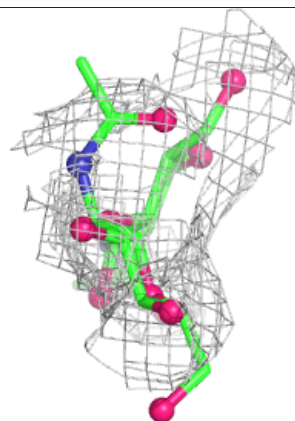
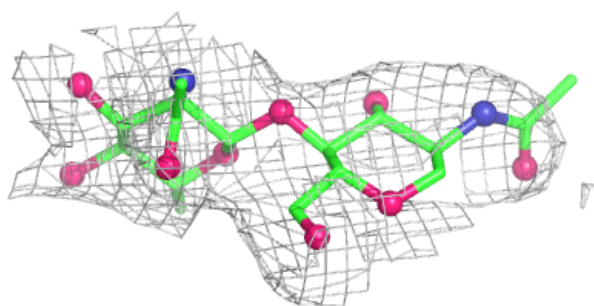
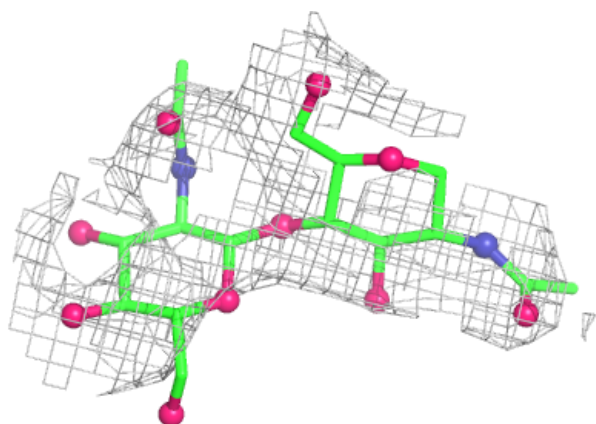
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	K	2	14/15	0.31	0.13	125,152,172,177	0
6	NAG	L	2	14/15	0.63	0.13	117,150,167,169	0
6	NAG	L	1	14/15	0.71	0.12	86,134,147,163	0
6	NAG	K	1	14/15	0.87	0.09	85,104,125,141	0

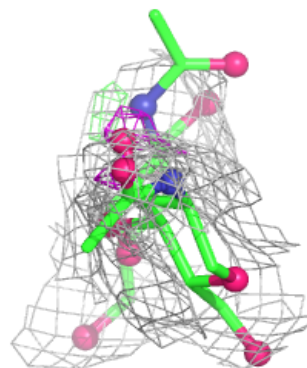
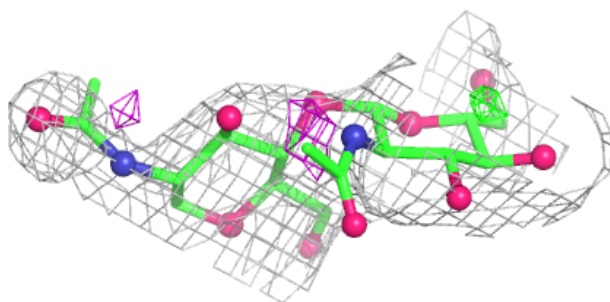
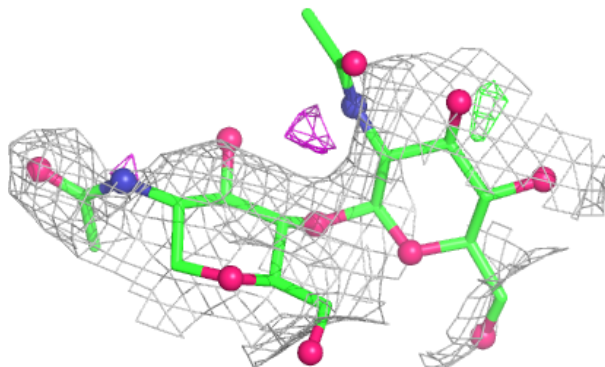
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

**Electron density around Chain L:**

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



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	A	201	14/15	0.55	0.10	109,127,138,141	0
7	NAG	J	301	14/15	0.55	0.13	127,127,127,127	0
8	GOL	D	201	6/6	0.55	0.13	79,88,101,104	0
7	NAG	G	301	14/15	0.69	0.12	93,128,145,148	0
8	GOL	D	202	6/6	0.79	0.14	74,82,92,97	0
7	NAG	H	301	14/15	0.81	0.14	92,101,124,127	0
7	NAG	I	301	14/15	0.85	0.15	54,69,108,119	0

6.5 Other polymers [i](#)

There are no such residues in this entry.