



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:21 PM UTC

PDB ID : 1TCR / pdb_00001tcr
Title : MURINE T-CELL ANTIGEN RECEPTOR 2C CLONE
Authors : Garcia, K.C.; Degano, M.; Stanfield, R.L.; Wilson, I.A.
Deposited on : 1996-09-12
Resolution : 2.50 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

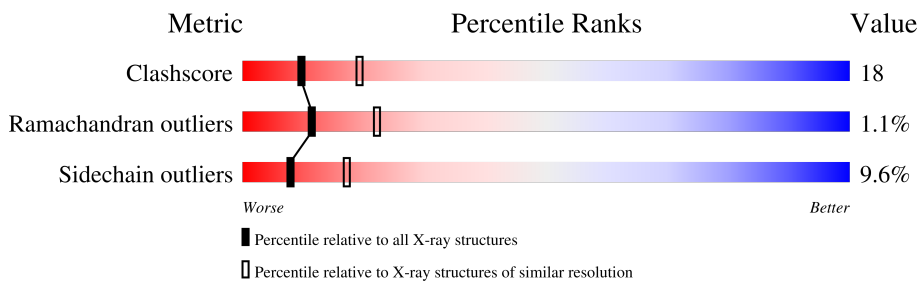
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	202	
2	B	237	
3	C	4	
4	D	3	
5	E	2	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3589 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 ALPHA, BETA T-CELL RECEPTOR (VB8.2DB2JB2.4CB2\;VA3JA58CA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	202	1570	999	253	310	8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	ALA	GLN	conflict	EMBL X01134
A	165	ALA	LYS	conflict	EMBL X01134

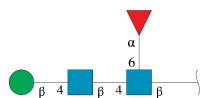
- Molecule 2 is a protein called ALPHA, BETA T-CELL RECEPTOR (VB8.2DB2JB2.4CB2\;VA3JA58CA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	237	1853	1160	331	355	7	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

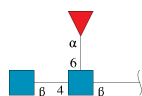
Chain	Residue	Modelled	Actual	Comment	Reference
B	97	GLY	GLN	conflict	GB 1791255
B	?	-	ARG	deletion	GB 1791255
B	?	-	ALA	deletion	GB 1791255
B	105	THR	GLU	conflict	GB 1791255
B	106	LEU	GLN	conflict	GB 1791255
B	107	TYR	PHE	conflict	GB 1791255
B	110	ALA	PRO	conflict	GB 1791255
B	115	SER	THR	conflict	GB 1791255

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



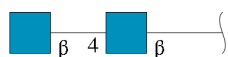
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



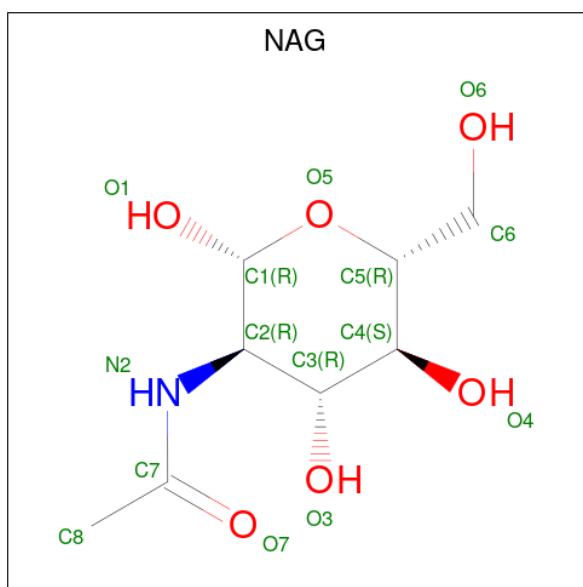
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



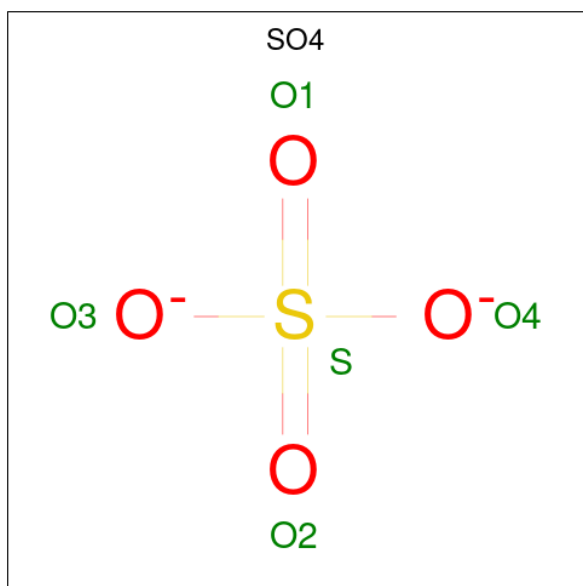
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	9	Total 9	O 9	0	0
8	B	13	Total 13	O 13	0	0

3 Residue-property plots

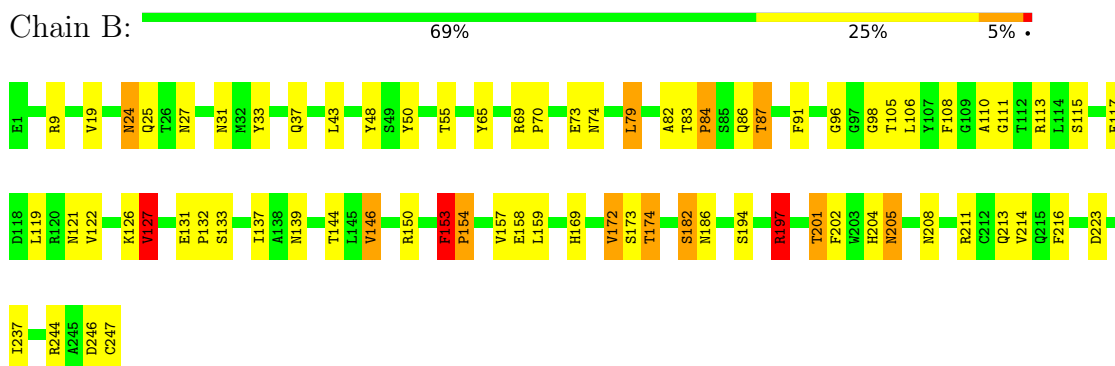
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

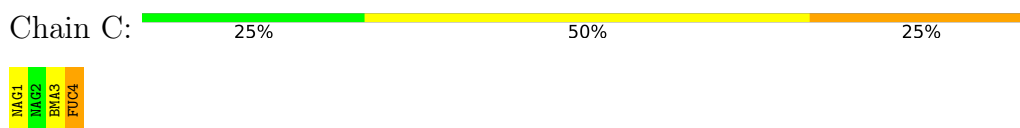
- Molecule 1: ALPHA, BETA T-CELL RECEPTOR (VB8.2DB2JB2.4CB2\;VA3JA58CA)



- Molecule 2: ALPHA, BETA T-CELL RECEPTOR (VB8.2DB2JB2.4CB2\;VA3JA58CA)



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



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





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

Chain E:  100%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.00Å 72.90Å 57.30Å 90.00° 101.20° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	93.4 ((Not available)-2.50)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.208 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3589	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.00	7/1611 (0.4%)	1.27	18/2193 (0.8%)
2	B	0.76	0/1904	1.21	16/2586 (0.6%)
All	All	0.88	7/3515 (0.2%)	1.24	34/4779 (0.7%)

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
2	B	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	THR	N-CA	-12.88	1.32	1.46
1	A	28	ALA	C-N	-10.93	1.17	1.33
1	A	29	THR	CA-C	-8.68	1.41	1.52
1	A	28	ALA	CA-C	-8.20	1.41	1.52
1	A	29	THR	C-N	-7.60	1.23	1.33
1	A	27	SER	C-N	-6.69	1.24	1.33
1	A	29	THR	CA-CB	-6.46	1.45	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	153	PHE	O-C-N	-16.15	102.75	121.32
1	A	29	THR	CB-CA-C	12.81	123.40	110.33
1	A	52	GLY	N-CA-C	9.27	120.20	111.67
1	A	5	GLN	CA-C-N	8.85	129.02	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	GLN	C-N-CA	8.85	129.02	119.28
1	A	29	THR	O-C-N	8.39	129.72	120.83
1	A	68	LYS	N-CA-C	-8.10	102.53	111.36
1	A	209	SER	N-CA-C	-8.01	96.50	109.96
1	A	206	TYR	CA-C-N	7.23	126.99	119.76
1	A	206	TYR	C-N-CA	7.23	126.99	119.76
2	B	205	ASN	CA-C-N	6.88	126.58	119.56
2	B	205	ASN	C-N-CA	6.88	126.58	119.56
2	B	153	PHE	CA-CB-CG	-5.99	107.81	113.80
1	A	40	ARG	NE-CZ-NH2	5.99	124.59	119.20
2	B	108	PHE	N-CA-C	5.93	119.24	110.46
1	A	211	VAL	CA-C-N	5.83	125.52	119.05
1	A	211	VAL	C-N-CA	5.83	125.52	119.05
2	B	131	GLU	CA-C-N	5.70	125.63	119.76
2	B	131	GLU	C-N-CA	5.70	125.63	119.76
1	A	158	SER	N-CA-C	-5.64	101.35	110.32
2	B	126	LYS	N-CA-C	-5.61	99.27	108.41
1	A	39	PRO	O-C-N	5.43	128.90	122.98
2	B	117	GLU	N-CA-C	-5.34	105.50	112.23
2	B	127	VAL	N-CA-C	5.30	115.49	107.80
1	A	28	ALA	CA-C-N	-5.23	112.93	122.35
1	A	28	ALA	C-N-CA	-5.23	112.93	122.35
2	B	197	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	A	120	ASN	CA-C-N	5.17	125.97	120.13
1	A	120	ASN	C-N-CA	5.17	125.97	120.13
2	B	153	PHE	N-CA-CB	5.15	119.54	110.37
2	B	223	ASP	N-CA-C	5.12	117.90	110.42
2	B	153	PHE	CA-C-N	-5.08	113.49	119.84
2	B	153	PHE	C-N-CA	-5.08	113.49	119.84
2	B	139	ASN	N-CA-C	5.08	116.89	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	153	PHE	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	1570	0	1502	73	0
2	B	1853	0	1762	61	0
3	C	49	0	43	2	0
4	D	38	0	34	2	0
5	E	28	0	25	0	0
6	A	14	0	13	0	0
7	B	15	0	0	1	0
8	A	9	0	0	0	0
8	B	13	0	0	0	0
All	All	3589	0	3379	122	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 18.

All (122) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:TYR:CE2	1:A:28:ALA:HB3	1.75	1.20
2:B:153:PHE:O	2:B:154:PRO:O	1.72	1.08
1:A:27:SER:O	1:A:28:ALA:HB2	1.55	1.04
1:A:123:PRO:O	1:A:204:ALA:HB3	1.65	0.97
2:B:153:PHE:O	2:B:154:PRO:C	1.98	0.93
1:A:27:SER:O	1:A:28:ALA:CB	2.10	0.93
1:A:170:MET:HB2	1:A:175:SER:HB3	1.55	0.88
1:A:40:ARG:O	1:A:40:ARG:HD3	1.73	0.87
2:B:84:PRO:O	2:B:87:THR:HG23	1.79	0.82
1:A:28:ALA:O	1:A:30:PRO:HD3	1.79	0.81
1:A:91:ALA:HB1	1:A:104:LEU:HD22	1.60	0.81
2:B:174:THR:HB	2:B:194:SER:HB2	1.62	0.80
1:A:192:GLN:HG3	1:A:205:THR:HG21	1.69	0.75
1:A:26:TYR:CE2	1:A:28:ALA:CB	2.64	0.74
2:B:87:THR:HB	2:B:115:SER:HA	1.70	0.71
1:A:26:TYR:CD2	1:A:28:ALA:HB3	2.26	0.70
1:A:143:PHE:CZ	1:A:198:THR:HG21	2.26	0.70
1:A:67:SER:HB3	4:D:1:NAG:H82	1.73	0.70
2:B:205:ASN:HB3	2:B:208:ASN:ND2	2.06	0.69
1:A:128:LEU:HD12	2:B:146:VAL:HG13	1.75	0.68
2:B:133:SER:O	2:B:137:ILE:HG13	1.94	0.66
1:A:49:TYR:HB2	1:A:56:VAL:HG21	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:CYS:H	1:A:74:HIS:HD2	1.43	0.66
1:A:170:MET:HB2	1:A:175:SER:CB	2.26	0.66
2:B:127:VAL:HG13	2:B:237:ILE:HG22	1.77	0.65
2:B:174:THR:HB	2:B:194:SER:CB	2.26	0.65
2:B:246:ASP:O	2:B:247:CYS:HB2	1.97	0.65
2:B:37:GLN:HB2	2:B:43:LEU:CD2	2.26	0.65
1:A:48:LYS:O	1:A:56:VAL:HG11	1.96	0.65
1:A:172:ALA:HB3	1:A:175:SER:OG	1.98	0.64
1:A:132:ASP:HB3	1:A:138:SER:HB3	1.79	0.64
2:B:65:TYR:HD1	2:B:79:LEU:HD22	1.63	0.62
2:B:24:ASN:HA	2:B:73:GLU:O	2.00	0.62
1:A:22:CYS:H	1:A:74:HIS:CD2	2.19	0.60
2:B:169:HIS:O	2:B:172:VAL:HG13	2.02	0.60
1:A:42:GLY:HA2	2:B:91:PHE:CE2	2.36	0.60
2:B:83:THR:H	2:B:86:GLN:HE21	1.49	0.59
2:B:82:ALA:HA	2:B:86:GLN:NE2	2.17	0.59
2:B:204:HIS:HA	2:B:244:ARG:O	2.02	0.59
1:A:182:ALA:HB1	1:A:194:ILE:CD1	2.32	0.59
1:A:2:SER:HB3	1:A:25:SER:HB3	1.85	0.58
1:A:26:TYR:HE2	1:A:28:ALA:HB3	1.57	0.57
2:B:65:TYR:CD1	2:B:79:LEU:HD22	2.37	0.57
2:B:9:ARG:NH1	2:B:110:ALA:HB3	2.20	0.57
1:A:18:LEU:HD11	1:A:20:LEU:HD21	1.86	0.57
1:A:168:LEU:C	1:A:168:LEU:HD12	2.30	0.56
1:A:168:LEU:HB3	2:B:173:SER:CB	2.36	0.56
1:A:129:LYS:HG2	1:A:139:THR:HG22	1.89	0.56
2:B:69:ARG:HD2	2:B:74:ASN:O	2.05	0.55
1:A:82:TRP:HA	1:A:114:VAL:HG22	1.89	0.55
1:A:40:ARG:O	1:A:40:ARG:CD	2.49	0.54
1:A:67:SER:CB	4:D:1:NAG:H82	2.35	0.54
1:A:128:LEU:HD12	2:B:146:VAL:CG1	2.38	0.54
1:A:182:ALA:HB1	1:A:194:ILE:HD11	1.90	0.53
1:A:12:VAL:O	1:A:114:VAL:HA	2.08	0.53
1:A:111:LYS:HD3	1:A:113:ILE:HD11	1.89	0.53
1:A:115:LEU:HB3	1:A:148:SER:HB3	1.89	0.52
2:B:82:ALA:HA	2:B:86:GLN:HE22	1.73	0.52
1:A:147:ASP:O	1:A:150:ILE:HG22	2.09	0.52
2:B:48:TYR:HE2	2:B:50:TYR:CE2	2.27	0.52
1:A:28:ALA:O	1:A:30:PRO:CD	2.54	0.52
2:B:119:LEU:O	2:B:122:VAL:HG23	2.10	0.51
1:A:42:GLY:HA2	2:B:91:PHE:HE2	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:PRO:HB2	2:B:137:ILE:HD11	1.91	0.51
2:B:121:ASN:O	2:B:153:PHE:CB	2.58	0.51
1:A:31:TYR:O	1:A:32:LEU:HD23	2.11	0.51
2:B:37:GLN:CB	2:B:43:LEU:HD23	2.41	0.51
2:B:144:THR:OG1	2:B:197:ARG:HD3	2.12	0.50
1:A:192:GLN:CG	1:A:205:THR:HG21	2.41	0.50
1:A:141:CYS:HG	1:A:191:CYS:CB	2.18	0.50
1:A:203:ASN:OD1	1:A:203:ASN:N	2.44	0.50
1:A:43:LEU:HD11	2:B:43:LEU:HD12	1.94	0.49
1:A:43:LEU:HD11	2:B:43:LEU:CD1	2.41	0.49
1:A:70:ASN:N	1:A:70:ASN:OD1	2.45	0.49
2:B:37:GLN:HB2	2:B:43:LEU:HD23	1.93	0.49
2:B:84:PRO:O	2:B:87:THR:CG2	2.57	0.49
2:B:9:ARG:NH1	2:B:111:GLY:O	2.46	0.49
1:A:212:PRO:HB3	2:B:247:CYS:O	2.14	0.48
2:B:246:ASP:CG	2:B:247:CYS:N	2.71	0.48
2:B:121:ASN:O	2:B:153:PHE:HB3	2.14	0.47
1:A:168:LEU:CB	2:B:173:SER:HB2	2.45	0.47
1:A:168:LEU:HB3	2:B:173:SER:HB3	1.96	0.47
1:A:182:ALA:HB1	1:A:194:ILE:HD13	1.97	0.47
2:B:150:ARG:HH21	3:C:4:FUC:H5	1.79	0.47
1:A:85:SER:OG	1:A:114:VAL:HG13	2.15	0.47
1:A:155:THR:HG22	1:A:156:MET:N	2.31	0.46
1:A:197:GLU:O	1:A:198:THR:HG23	2.16	0.46
1:A:205:THR:O	1:A:207:PRO:HD3	2.15	0.46
1:A:188:SER:C	1:A:189:PHE:HD1	2.24	0.46
1:A:24:TYR:CD1	1:A:24:TYR:C	2.93	0.46
1:A:20:LEU:HD12	1:A:75:LEU:HD23	1.98	0.46
1:A:128:LEU:N	1:A:128:LEU:HD23	2.31	0.45
2:B:201:THR:HG22	2:B:202:PHE:N	2.31	0.45
1:A:136:GLN:HE21	1:A:137:ASP:H	1.64	0.45
1:A:5:GLN:HA	1:A:6:PRO:HD2	1.74	0.45
2:B:246:ASP:O	2:B:247:CYS:CB	2.65	0.45
2:B:25:GLN:OE1	2:B:27:ASN:HB2	2.17	0.44
2:B:96:GLY:C	2:B:98:GLY:H	2.25	0.44
1:A:37:GLN:HB2	1:A:43:LEU:HD22	1.99	0.44
1:A:48:LYS:HD2	1:A:50:TYR:CE2	2.53	0.43
1:A:168:LEU:HB3	2:B:173:SER:HB2	2.00	0.43
1:A:91:ALA:HA	1:A:105:THR:O	2.17	0.43
2:B:31:ASN:OD1	2:B:50:TYR:CD1	2.72	0.43
2:B:19:VAL:HB	2:B:79:LEU:HG	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:MET:CB	1:A:175:SER:HB3	2.39	0.42
2:B:182:SER:HB3	3:C:4:FUC:O3	2.19	0.42
1:A:75:LEU:C	1:A:76:ARG:HG3	2.44	0.42
2:B:113:ARG:NH2	2:B:158:GLU:OE2	2.53	0.41
2:B:157:VAL:HG12	2:B:216:PHE:HA	2.02	0.41
2:B:159:LEU:C	2:B:159:LEU:HD23	2.46	0.41
1:A:26:TYR:CD2	1:A:30:PRO:HB3	2.56	0.41
2:B:79:LEU:N	2:B:79:LEU:HD23	2.35	0.41
1:A:32:LEU:HD12	1:A:66:PHE:CD1	2.55	0.41
2:B:174:THR:HA	2:B:194:SER:HA	2.02	0.41
1:A:196:LYS:O	1:A:196:LYS:HG2	2.20	0.41
2:B:211:ARG:HD3	7:B:251:SO4:O3	2.20	0.41
2:B:205:ASN:HB3	2:B:208:ASN:HD22	1.81	0.41
1:A:104:LEU:HD12	2:B:106:LEU:HG	2.03	0.40
1:A:206:TYR:HA	1:A:207:PRO:HD2	1.90	0.40
2:B:70:PRO:HG2	2:B:74:ASN:HB2	2.02	0.40
2:B:213:GLN:HG2	2:B:214:VAL:N	2.35	0.40
1:A:141:CYS:SG	1:A:191:CYS:CB	3.09	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	200/202 (99%)	177 (88%)	20 (10%)	3 (2%)	8	16
2	B	235/237 (99%)	222 (94%)	11 (5%)	2 (1%)	14	27
All	All	435/439 (99%)	399 (92%)	31 (7%)	5 (1%)	11	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ALA
1	A	175	SER
2	B	153	PHE
1	A	135	SER
2	B	154	PRO

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	176/176 (100%)	155 (88%)	21 (12%)	5	11
2	B	200/200 (100%)	185 (92%)	15 (8%)	12	26
All	All	376/376 (100%)	340 (90%)	36 (10%)	8	17

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	69	SER
1	A	70	ASN
1	A	102	SER
1	A	111	LYS
1	A	114	VAL
1	A	128	LEU
1	A	134	ARG
1	A	137	ASP
1	A	138	SER
1	A	140	LEU
1	A	168	LEU
1	A	174	ASP
1	A	181	ILE
1	A	198	THR
1	A	203	ASN
1	A	206	TYR
1	A	208	SER
1	A	209	SER

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Mol	Chain	Res	Type
1	A	210	ASP
1	A	211	VAL
2	B	24	ASN
2	B	33	TYR
2	B	55	THR
2	B	79	LEU
2	B	84	PRO
2	B	87	THR
2	B	105	THR
2	B	127	VAL
2	B	146	VAL
2	B	172	VAL
2	B	174	THR
2	B	182	SER
2	B	186	ASN
2	B	197	ARG
2	B	201	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	60	ASN
1	A	74	HIS
1	A	136	GLN
2	B	28	ASN
2	B	74	ASN
2	B	86	GLN
2	B	215	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 ⓘ

9 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$
3	NAG	C	1	3,1	14,14,15	0.88	1 (7%)	17,19,21	0.64	0
3	NAG	C	2	3	14,14,15	0.61	0	17,19,21	0.65	0
3	BMA	C	3	3	11,11,12	1.36	2 (18%)	15,15,17	0.76	0
3	FUC	C	4	3	10,10,11	1.03	1 (10%)	14,14,16	1.86	2 (14%)
4	NAG	D	1	4,1	14,14,15	1.12	1 (7%)	17,19,21	0.60	0
4	NAG	D	2	4	14,14,15	0.91	0	17,19,21	0.55	0
4	FUC	D	3	4	10,10,11	1.16	1 (10%)	14,14,16	1.26	2 (14%)
5	NAG	E	1	2,5	14,14,15	0.61	0	17,19,21	0.50	0
5	NAG	E	2	5	14,14,15	0.65	0	17,19,21	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
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	1/2/19/22	0/1/1/1
3	FUC	C	4	3	-	-	0/1/1/1
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	FUC	D	3	4	-	-	0/1/1/1
5	NAG	E	1	2,5	-	1/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	NAG	C1-C2	2.96	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3	FUC	C2-C3	2.69	1.56	1.52
3	C	3	BMA	C2-C3	2.58	1.56	1.52
3	C	3	BMA	C1-C2	2.33	1.57	1.52
3	C	4	FUC	C4-C3	2.13	1.57	1.52
3	C	1	NAG	C1-C2	2.13	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	FUC	C6-C5-C4	4.90	122.04	113.08
3	C	4	FUC	C3-C4-C5	3.96	115.83	109.81
4	D	3	FUC	C6-C5-C4	3.12	118.79	113.08
4	D	3	FUC	C1-C2-C3	2.87	113.82	109.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

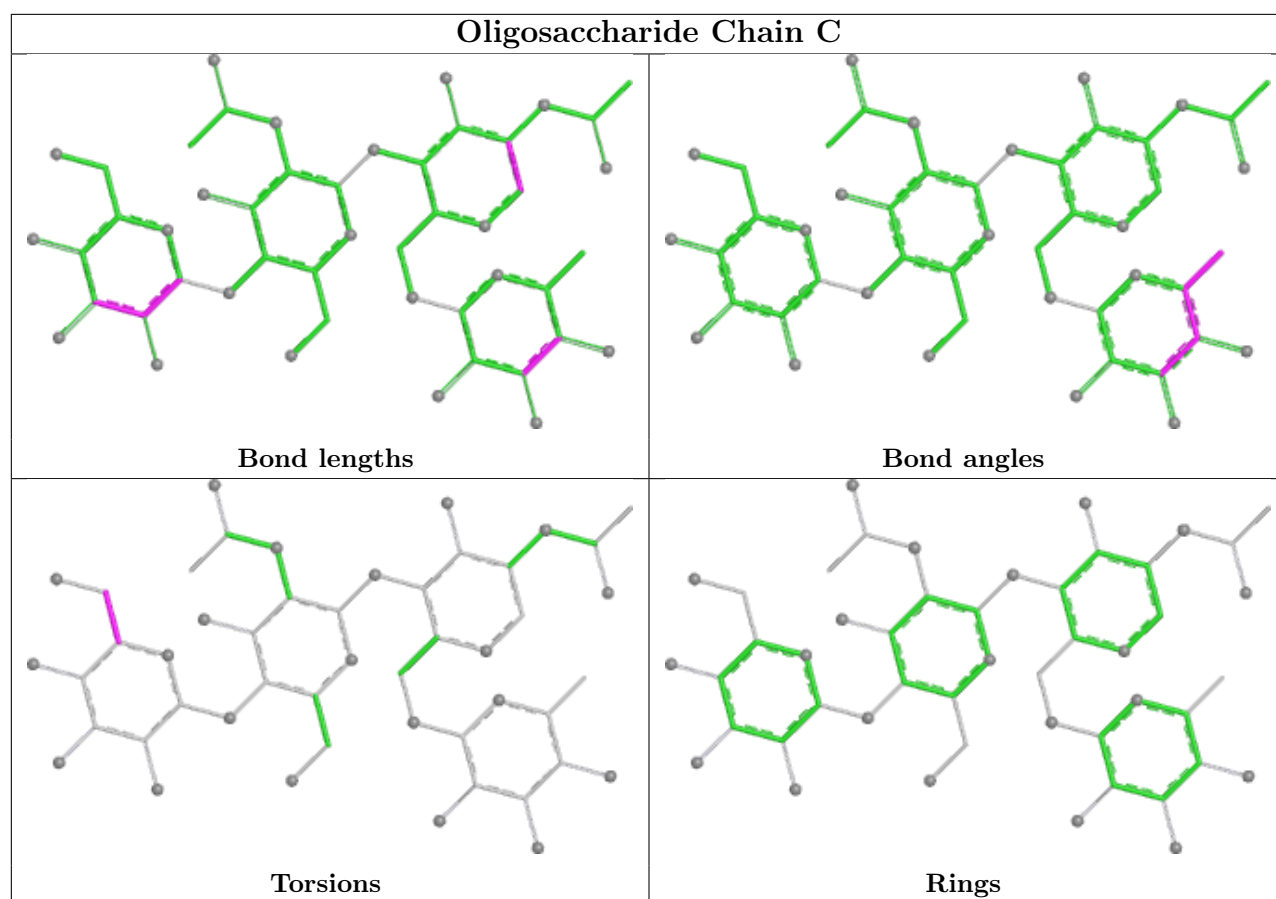
Mol	Chain	Res	Type	Atoms
5	E	2	NAG	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
5	E	1	NAG	C1-C2-N2-C7

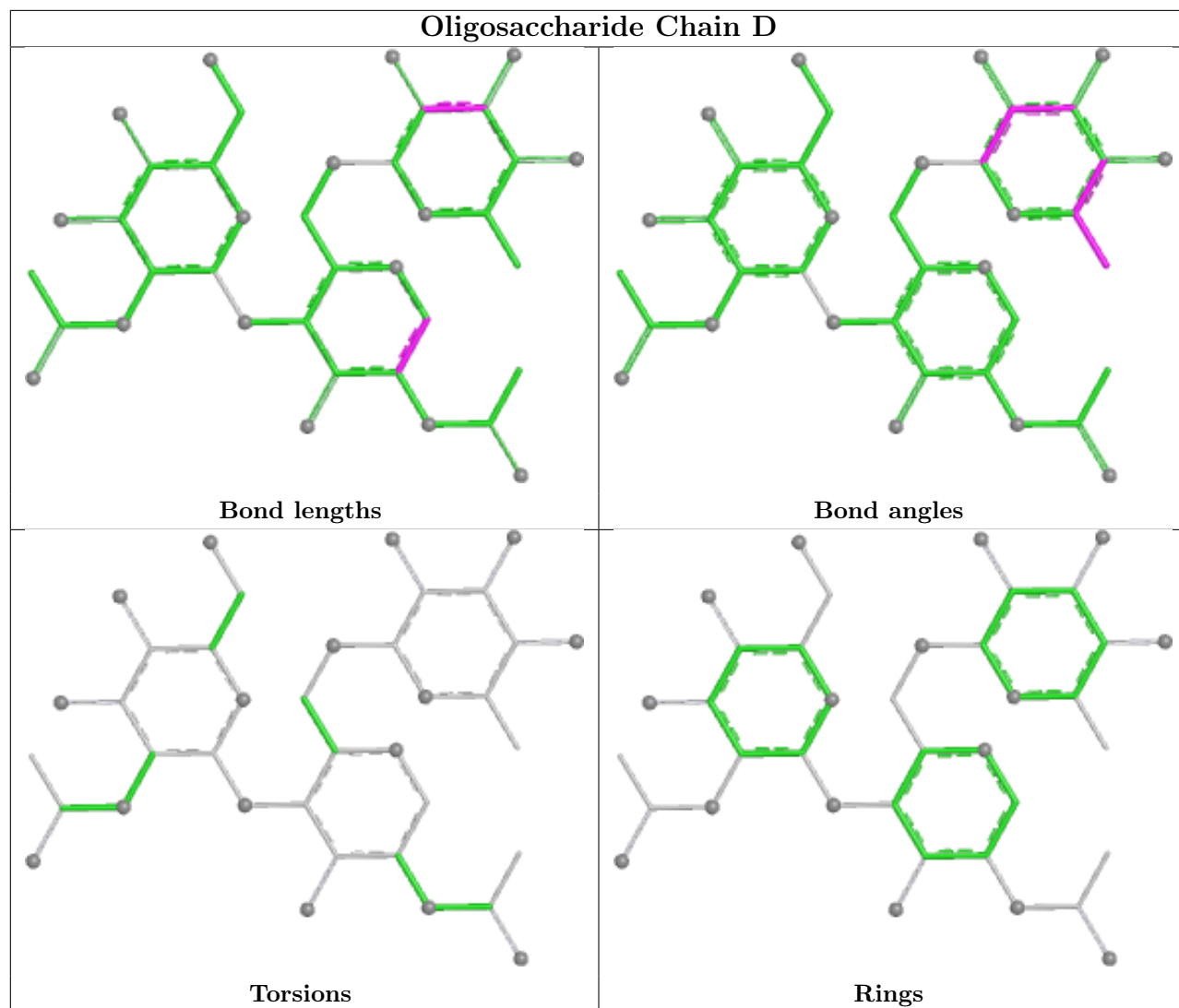
There are no ring outliers.

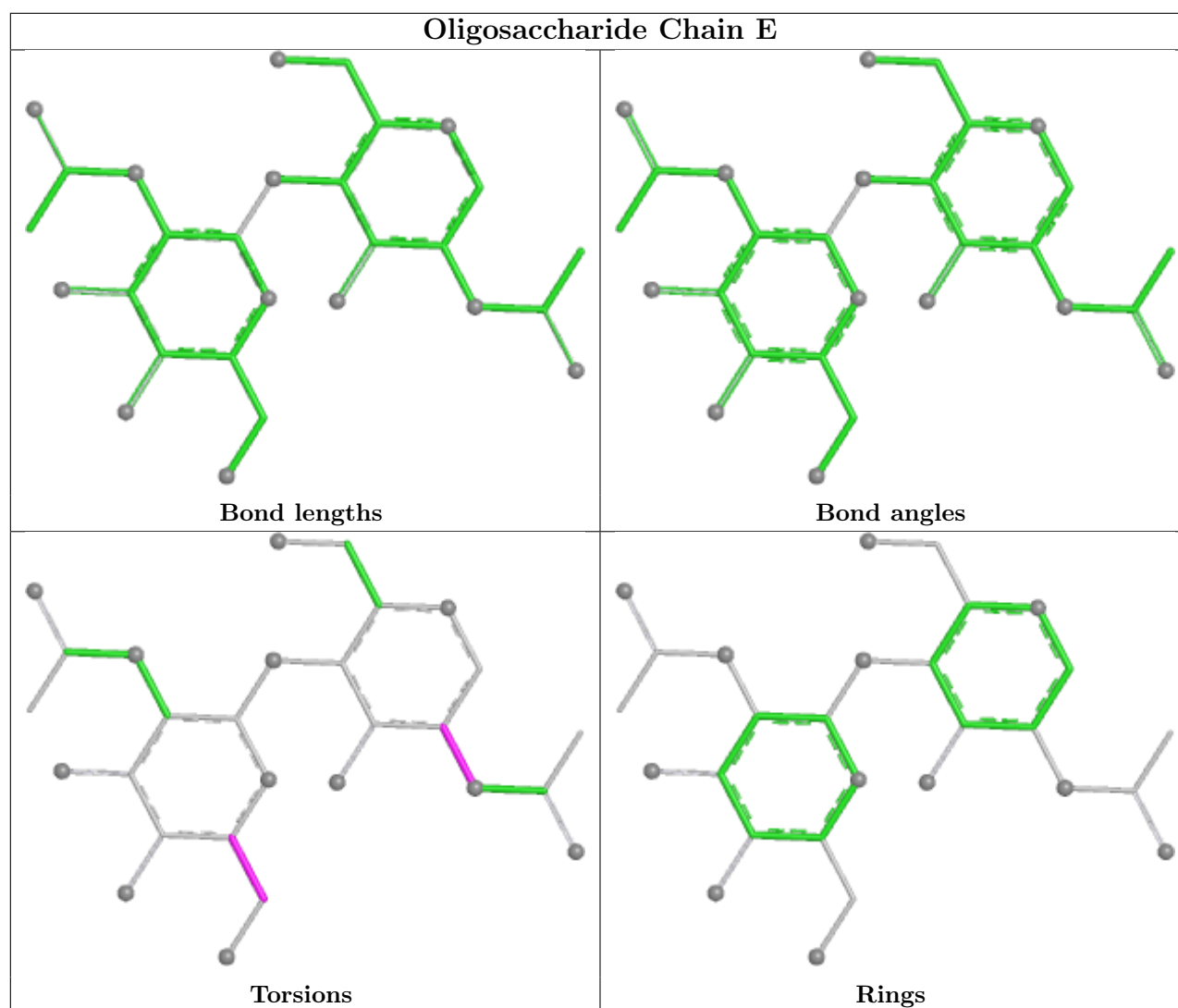
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	2	0
3	C	4	FUC	2	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](#)

4 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	SO4	B	252	-	4,4,4	0.32	0	6,6,6	0.77	0
7	SO4	B	250	-	4,4,4	0.53	0	6,6,6	0.70	0
6	NAG	A	200	1	14,14,15	1.25	2 (14%)	17,19,21	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SO4	B	251	-	4,4,4	0.35	0	6,6,6	0.40	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
6	NAG	A	200	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	200	NAG	C1-C2	3.49	1.57	1.52
6	A	200	NAG	C3-C2	2.61	1.58	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	200	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
7	B	251	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	28:ALA	C	29:THR	N	1.17

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.