



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:06 PM UTC

PDB ID : 1NQL / pdb_00001nql
Title : Structure of the extracellular domain of human epidermal growth factor (EGF) receptor in an inactive (low pH) complex with EGF.
Authors : Ferguson, K.M.; Lemmon, M.A.
Deposited on : 2003-01-21
Resolution : 2.80 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

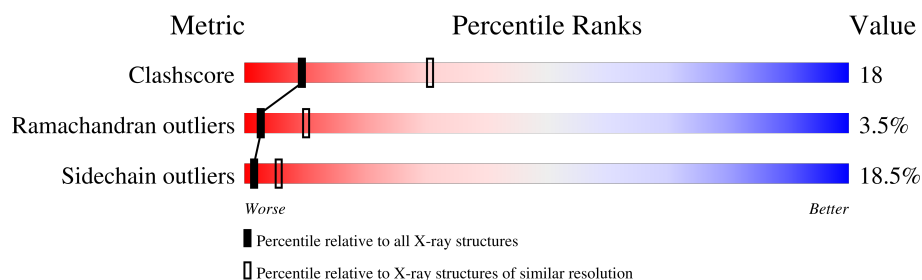
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	624	57% 33% 7% . .
2	B	53	55% 28% 8% 9%
3	C	3	100%
3	D	3	33% 67%
4	E	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	702	X	-	-	-
5	NAG	A	705	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5150 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.

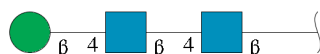
- Molecule 1 is a protein called epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	612	Total	C	N	O	S	10	0	0
			4597	2836	817	885	59			

- Molecule 2 is a protein called epidermal growth factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	48	Total	C	N	O	S	0	0	0
			377	235	62	73	7			

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



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

- Molecule 4 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
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



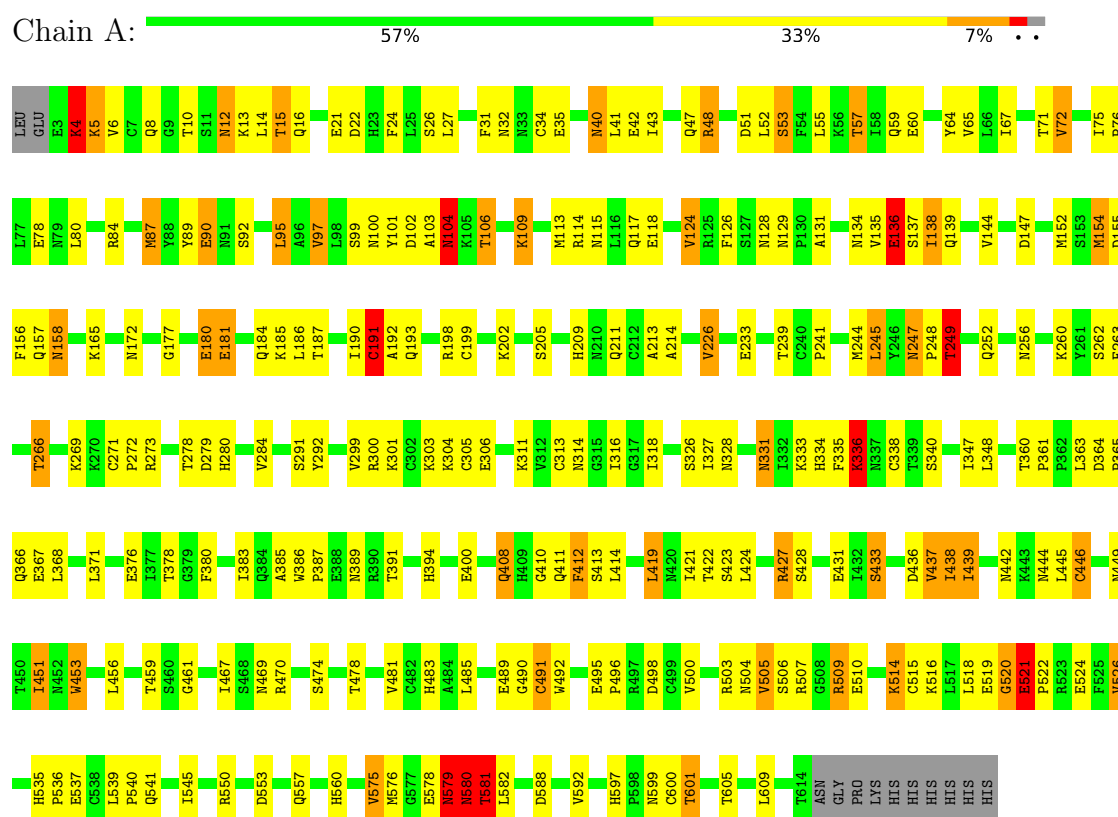
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots

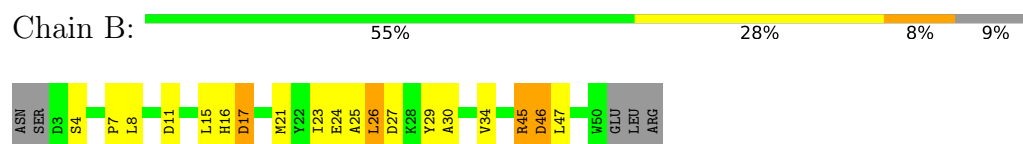
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



- Molecule 2: epidermal growth factor



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2
BMA3

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  33% 67%

MAG1
MAG2
BMA3

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

Chain E:  100%

MAG1
MAG2

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	119.17Å 103.66Å 101.49Å 90.00° 119.27° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	100.0 (20.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.241 , 0.310	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5150	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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: NAG, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.21	7/4688 (0.1%)	1.20	23/6365 (0.4%)
2	B	0.70	0/386	1.12	2/523 (0.4%)
All	All	1.17	7/5074 (0.1%)	1.19	25/6888 (0.4%)

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
1	A	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	LYS	C-N	-58.00	0.52	1.33
1	A	87	MET	SD-CE	8.57	2.00	1.79
1	A	4	LYS	CB-CG	-8.46	1.27	1.52
1	A	244	MET	CG-SD	8.12	2.01	1.80
1	A	419	LEU	C-O	5.64	1.31	1.23
1	A	97	VAL	CA-CB	5.55	1.59	1.53
1	A	124	VAL	CA-CB	5.33	1.61	1.54

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	LYS	O-C-N	21.23	150.83	122.59
1	A	4	LYS	CB-CG-CD	-12.09	83.50	111.30
1	A	4	LYS	CA-CB-CG	10.73	135.56	114.10
1	A	4	LYS	CA-C-N	-9.97	102.50	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	LYS	C-N-CA	-9.97	102.50	121.54
2	B	26	LEU	N-CA-C	-8.10	100.15	110.19
1	A	579	ASN	N-CA-C	7.63	127.05	110.80
1	A	520	GLY	N-CA-C	7.57	124.09	112.51
1	A	490	GLY	N-CA-C	7.21	121.22	110.97
1	A	280	HIS	N-CA-C	-7.03	104.73	113.38
1	A	249	THR	N-CA-C	-6.08	106.40	113.88
1	A	27	LEU	N-CA-C	-6.00	103.91	111.11
1	A	97	VAL	CB-CA-C	5.85	117.14	111.23
1	A	580	ASN	N-CA-C	5.80	123.15	110.80
1	A	581	THR	N-CA-C	5.61	116.79	108.60
1	A	109	LYS	N-CA-C	-5.50	106.25	113.12
1	A	433	SER	N-CA-C	5.47	117.10	111.03
2	B	4	SER	N-CA-C	5.44	117.39	108.52
1	A	412	PHE	N-CA-C	5.30	117.06	108.41
1	A	491	CYS	CB-CA-C	-5.26	99.26	109.68
1	A	305	CYS	N-CA-C	-5.21	102.14	109.96
1	A	187	THR	N-CA-C	5.14	117.46	110.88
1	A	157	GLN	N-CA-C	5.13	118.63	111.30
1	A	199	CYS	N-CA-C	5.12	116.97	109.24
1	A	244	MET	N-CA-C	-5.08	101.42	109.76

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	521	GLU	Peptide
1	A	578	GLU	Peptide

5.2 Too-close contacts [i](#)

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	4597	0	4316	172	0
2	B	377	0	328	10	0
3	C	39	0	34	0	0
3	D	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	28	0	25	0	0
5	A	70	0	65	13	0
All	All	5150	0	4802	178	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 (178) 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:516:LYS:HB3	1:A:520:GLY:HA3	1.33	1.05
1:A:576:MET:SD	5:A:705:NAG:O3	2.15	1.05
1:A:576:MET:CG	5:A:705:NAG:H4	2.05	0.86
1:A:256:ASN:HD21	5:A:705:NAG:C6	1.89	0.85
1:A:541:GLN:HE22	1:A:557:GLN:HE21	1.24	0.84
1:A:209:HIS:HD2	1:A:211:GLN:H	1.26	0.83
1:A:576:MET:SD	5:A:705:NAG:H4	2.19	0.82
1:A:245:LEU:HB3	1:A:256:ASN:HB2	1.61	0.82
1:A:100:ASN:HD22	1:A:129:ASN:ND2	1.76	0.82
1:A:516:LYS:CB	1:A:520:GLY:HA3	2.10	0.82
2:B:17:ASP:HB3	2:B:34:VAL:HG21	1.63	0.80
1:A:256:ASN:HD21	5:A:705:NAG:H62	1.47	0.79
1:A:51:ASP:OD1	1:A:53:SER:HB2	1.82	0.79
1:A:483:HIS:HD2	1:A:485:LEU:H	1.37	0.72
1:A:213:ALA:HB3	1:A:226:VAL:HG12	1.71	0.71
1:A:99:SER:HA	1:A:128:ASN:O	1.91	0.70
1:A:247:ASN:HD22	1:A:247:ASN:C	1.99	0.70
1:A:514:LYS:NZ	1:A:518:LEU:H	1.90	0.70
1:A:521:GLU:HB2	1:A:522:PRO:CD	2.23	0.68
1:A:48:ARG:HH11	1:A:48:ARG:HG2	1.58	0.68
1:A:326:SER:HB3	1:A:348:LEU:HG	1.74	0.68
1:A:439:ILE:HG22	1:A:469:ASN:HD21	1.57	0.68
1:A:34:CYS:O	1:A:57:THR:HG22	1.94	0.67
1:A:101:TYR:HA	1:A:106:THR:O	1.95	0.67
1:A:136:GLU:HG2	1:A:137:SER:N	2.09	0.66
1:A:521:GLU:CB	1:A:522:PRO:CD	2.74	0.66
1:A:421:ILE:HD12	1:A:445:LEU:HD13	1.78	0.65
1:A:541:GLN:HE22	1:A:557:GLN:NE2	1.94	0.65
1:A:134:ASN:HD22	1:A:177:GLY:HA2	1.60	0.65
1:A:256:ASN:ND2	5:A:705:NAG:H62	2.13	0.64
1:A:600:CYS:O	1:A:601:THR:HB	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:GLU:OE1	1:A:560:HIS:HD2	1.80	0.63
1:A:180:GLU:HG2	1:A:181:GLU:N	2.14	0.63
1:A:100:ASN:HD22	1:A:129:ASN:HD21	1.46	0.63
1:A:333:LYS:O	1:A:336:LYS:HG2	1.99	0.62
1:A:576:MET:SD	5:A:705:NAG:C3	2.88	0.62
1:A:24:PHE:HE1	1:A:52:LEU:HD23	1.65	0.61
1:A:193:GLN:HA	1:A:193:GLN:OE1	2.00	0.61
1:A:241:PRO:HG2	1:A:260:LYS:HB2	1.81	0.61
1:A:535:HIS:HD2	1:A:537:GLU:H	1.48	0.61
1:A:576:MET:SD	5:A:705:NAG:C4	2.88	0.60
1:A:134:ASN:ND2	1:A:177:GLY:HA2	2.17	0.59
1:A:48:ARG:HG2	1:A:48:ARG:NH1	2.17	0.59
1:A:328:ASN:HB2	1:A:331:ASN:HB2	1.85	0.59
1:A:95:LEU:HD23	1:A:124:VAL:HG13	1.83	0.59
1:A:516:LYS:HB3	1:A:520:GLY:CA	2.20	0.59
1:A:247:ASN:HD21	1:A:249:THR:HB	1.67	0.58
1:A:576:MET:HG2	5:A:705:NAG:H4	1.82	0.58
1:A:328:ASN:H	1:A:331:ASN:CB	2.16	0.58
1:A:12:ASN:N	1:A:42:GLU:OE1	2.37	0.58
1:A:541:GLN:NE2	1:A:557:GLN:HE21	2.00	0.57
1:A:109:LYS:HA	1:A:131:ALA:O	2.05	0.57
1:A:453:TRP:HA	1:A:456:LEU:HD12	1.86	0.57
1:A:581:THR:HG22	1:A:582:LEU:H	1.70	0.57
1:A:247:ASN:HD22	1:A:249:THR:H	1.53	0.56
1:A:521:GLU:HB2	1:A:522:PRO:HD2	1.85	0.56
1:A:32:ASN:HD21	5:A:701:NAG:H2	1.71	0.56
1:A:256:ASN:ND2	5:A:705:NAG:C6	2.64	0.56
1:A:347:ILE:HD12	1:A:383:ILE:HG12	1.87	0.55
1:A:233:GLU:OE1	1:A:233:GLU:HA	2.05	0.55
1:A:451:ILE:HD12	1:A:491:CYS:O	2.05	0.55
1:A:16:GLN:HB3	2:B:21:MET:HE1	1.89	0.55
1:A:509:ARG:HG3	1:A:509:ARG:NH1	2.22	0.54
1:A:483:HIS:CD2	1:A:485:LEU:H	2.21	0.54
1:A:521:GLU:CB	1:A:522:PRO:HD3	2.38	0.54
1:A:588:ASP:OD1	1:A:592:VAL:N	2.41	0.53
1:A:80:LEU:HD23	1:A:113:MET:HE2	1.91	0.53
1:A:516:LYS:CG	1:A:520:GLY:HA3	2.38	0.53
1:A:414:LEU:HB3	1:A:437:VAL:HG22	1.90	0.53
1:A:158:ASN:HD22	1:A:158:ASN:H	1.56	0.53
1:A:496:PRO:HB2	1:A:510:GLU:HG2	1.92	0.52
1:A:192:ALA:O	1:A:193:GLN:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:LYS:HD3	1:A:521:GLU:H	1.73	0.52
1:A:504:ASN:OD1	5:A:704:NAG:O5	2.25	0.52
2:B:46:ASP:O	2:B:47:LEU:HB2	2.09	0.52
1:A:41:LEU:HD21	1:A:43:ILE:HD11	1.90	0.52
1:A:135:VAL:HA	1:A:138:ILE:CD1	2.39	0.51
1:A:539:LEU:HD12	1:A:540:PRO:HD2	1.92	0.51
1:A:247:ASN:ND2	1:A:249:THR:H	2.08	0.51
1:A:576:MET:CE	5:A:705:NAG:O3	2.59	0.51
1:A:495:GLU:HB2	1:A:498:ASP:OD2	2.11	0.51
1:A:385:ALA:O	1:A:386:TRP:HB2	2.11	0.50
1:A:35:GLU:HG2	1:A:59:GLN:HE21	1.77	0.50
1:A:209:HIS:CD2	1:A:211:GLN:H	2.18	0.50
1:A:535:HIS:HD2	1:A:537:GLU:N	2.09	0.50
1:A:311:LYS:HB3	1:A:338:CYS:HA	1.93	0.49
1:A:365:PRO:HB3	1:A:387:PRO:CG	2.43	0.49
1:A:514:LYS:HZ1	1:A:518:LEU:H	1.56	0.49
1:A:48:ARG:HH11	1:A:48:ARG:CG	2.25	0.49
1:A:507:ARG:NH2	1:A:516:LYS:HG3	2.28	0.49
1:A:24:PHE:HE1	1:A:52:LEU:CD2	2.25	0.48
2:B:24:GLU:O	2:B:26:LEU:O	2.30	0.48
1:A:41:LEU:HD23	1:A:65:VAL:HG13	1.94	0.48
1:A:135:VAL:O	1:A:136:GLU:C	2.56	0.48
1:A:263:PHE:O	1:A:266:THR:HB	2.12	0.48
1:A:78:GLU:OE1	1:A:114:ARG:NH2	2.46	0.48
1:A:421:ILE:CD1	1:A:445:LEU:HD13	2.43	0.48
1:A:333:LYS:C	1:A:335:PHE:H	2.21	0.48
1:A:364:ASP:HB3	1:A:367:GLU:HG3	1.95	0.48
1:A:408:GLN:C	1:A:410:GLY:H	2.20	0.48
1:A:291:SER:HB3	1:A:303:LYS:O	2.14	0.48
1:A:328:ASN:H	1:A:331:ASN:HB2	1.78	0.47
1:A:514:LYS:HD3	1:A:515:CYS:O	2.14	0.47
1:A:516:LYS:HD3	1:A:521:GLU:N	2.28	0.47
1:A:47:GLN:O	1:A:72:VAL:HG13	2.15	0.47
1:A:78:GLU:OE1	1:A:114:ARG:NH1	2.48	0.47
1:A:509:ARG:HG3	1:A:509:ARG:HH11	1.80	0.47
1:A:360:THR:HA	1:A:361:PRO:HD2	1.81	0.47
1:A:380:PHE:HB2	1:A:413:SER:O	2.15	0.47
1:A:446:CYS:SG	1:A:470:ARG:HD3	2.54	0.47
1:A:514:LYS:HZ3	1:A:518:LEU:H	1.63	0.47
1:A:14:LEU:CD1	2:B:23:ILE:HD13	2.45	0.47
1:A:509:ARG:HH11	1:A:509:ARG:CG	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:CYS:SG	1:A:526:VAL:HG13	2.55	0.46
1:A:575:VAL:O	1:A:582:LEU:HA	2.15	0.46
1:A:16:GLN:HB3	2:B:21:MET:CE	2.45	0.46
1:A:184:GLN:HG2	1:A:186:LEU:HD23	1.97	0.46
1:A:521:GLU:HB3	1:A:522:PRO:HD3	1.97	0.46
1:A:247:ASN:HA	1:A:248:PRO:HD3	1.78	0.46
1:A:60:GLU:OE2	1:A:84:ARG:NH2	2.49	0.46
1:A:67:ILE:HB	1:A:97:VAL:HG22	1.98	0.46
1:A:600:CYS:O	1:A:601:THR:CB	2.64	0.46
1:A:52:LEU:O	1:A:76:PRO:HG2	2.16	0.46
1:A:408:GLN:C	1:A:410:GLY:N	2.74	0.46
1:A:438:ILE:HG22	1:A:438:ILE:O	2.14	0.46
1:A:57:THR:HG22	1:A:57:THR:O	2.16	0.46
1:A:411:GLN:HG3	1:A:436:ASP:OD2	2.16	0.46
1:A:190:ILE:HD12	1:A:190:ILE:O	2.17	0.45
1:A:10:THR:OG1	1:A:12:ASN:ND2	2.50	0.45
1:A:100:ASN:HD22	1:A:129:ASN:HD22	1.60	0.45
1:A:597:HIS:CD2	1:A:599:ASN:H	2.34	0.45
1:A:57:THR:O	1:A:57:THR:CG2	2.64	0.45
1:A:516:LYS:N	1:A:524:GLU:OE1	2.40	0.45
1:A:505:VAL:HG11	1:A:515:CYS:SG	2.56	0.45
1:A:328:ASN:H	1:A:331:ASN:HB3	1.79	0.45
1:A:135:VAL:HA	1:A:138:ILE:HD13	1.99	0.45
2:B:25:ALA:C	2:B:26:LEU:O	2.57	0.44
1:A:597:HIS:CD2	1:A:599:ASN:HB2	2.52	0.44
1:A:117:GLN:HB2	1:A:214:ALA:HB1	1.98	0.44
1:A:444:ASN:HA	1:A:470:ARG:HD2	1.99	0.44
1:A:126:PHE:HD1	1:A:154:MET:HE1	1.81	0.44
1:A:247:ASN:C	1:A:247:ASN:ND2	2.70	0.44
1:A:412:PHE:CE2	1:A:438:ILE:HG13	2.53	0.44
1:A:419:LEU:HB2	1:A:442:ASN:OD1	2.18	0.44
1:A:126:PHE:HD1	1:A:154:MET:CE	2.31	0.43
1:A:515:CYS:SG	1:A:526:VAL:CG1	3.07	0.43
1:A:118:GLU:HG3	1:A:198:ARG:NH2	2.33	0.43
1:A:424:LEU:O	1:A:492:TRP:O	2.36	0.43
1:A:400:GLU:HA	1:A:428:SER:O	2.18	0.43
1:A:579:ASN:CG	1:A:580:ASN:H	2.26	0.43
1:A:365:PRO:HB3	1:A:387:PRO:HG3	2.00	0.43
1:A:31:PHE:CZ	1:A:41:LEU:HD12	2.54	0.43
1:A:144:VAL:HG21	1:A:152:MET:HE3	2.01	0.43
1:A:12:ASN:O	1:A:15:THR:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:HIS:CE1	2:B:45:ARG:HH21	2.36	0.43
1:A:75:ILE:HA	1:A:76:PRO:HD3	1.79	0.42
2:B:7:PRO:HG2	2:B:29:TYR:CG	2.53	0.42
1:A:427:ARG:H	1:A:427:ARG:HG2	1.69	0.42
1:A:271:CYS:HA	1:A:272:PRO:HD3	1.84	0.42
1:A:5:LYS:HD2	1:A:6:VAL:N	2.34	0.42
1:A:78:GLU:O	1:A:115:ASN:ND2	2.49	0.42
1:A:581:THR:HG22	1:A:582:LEU:N	2.34	0.42
1:A:516:LYS:HD3	1:A:520:GLY:HA3	2.02	0.42
1:A:333:LYS:O	1:A:335:PHE:N	2.53	0.42
1:A:89:TYR:CE2	1:A:90:GLU:HG3	2.56	0.41
1:A:40:ASN:HB3	1:A:64:TYR:O	2.20	0.41
1:A:71:THR:HG22	1:A:71:THR:O	2.21	0.41
1:A:102:ASP:O	1:A:104:ASN:N	2.53	0.41
1:A:78:GLU:OE1	1:A:114:ARG:CZ	2.69	0.41
1:A:138:ILE:CG2	1:A:139:GLN:N	2.83	0.41
1:A:21:GLU:O	1:A:22:ASP:C	2.64	0.41
1:A:35:GLU:CG	1:A:59:GLN:HE21	2.34	0.41
1:A:191:CYS:HB3	1:A:192:ALA:H	1.65	0.41
1:A:483:HIS:HD2	1:A:485:LEU:N	2.09	0.41
1:A:41:LEU:HD21	1:A:43:ILE:CD1	2.51	0.40
1:A:15:THR:HA	2:B:30:ALA:HB1	2.03	0.40
1:A:503:ARG:HG3	1:A:504:ASN:N	2.35	0.40
1:A:516:LYS:NZ	1:A:521:GLU:HG3	2.37	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	610/624 (98%)	514 (84%)	73 (12%)	23 (4%)	2 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	46/53 (87%)	37 (80%)	9 (20%)	0	100	100
All	All	656/677 (97%)	551 (84%)	82 (12%)	23 (4%)	3	10

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	5	LYS
1	A	104	ASN
1	A	191	CYS
1	A	521	GLU
1	A	579	ASN
1	A	172	ASN
1	A	273	ARG
1	A	314	ASN
1	A	453	TRP
1	A	580	ASN
1	A	13	LYS
1	A	55	LEU
1	A	136	GLU
1	A	334	HIS
1	A	92	SER
1	A	103	ALA
1	A	389	ASN
1	A	601	THR
1	A	336	LYS
1	A	292	TYR
1	A	461	GLY
1	A	536	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	507/545 (93%)	413 (82%)	94 (18%)	1 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	40/47 (85%)	33 (82%)	7 (18%)	2	7
All	All	547/592 (92%)	446 (82%)	101 (18%)	1	6

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	8	GLN
1	A	12	ASN
1	A	15	THR
1	A	26	SER
1	A	40	ASN
1	A	48	ARG
1	A	53	SER
1	A	57	THR
1	A	72	VAL
1	A	87	MET
1	A	90	GLU
1	A	95	LEU
1	A	104	ASN
1	A	106	THR
1	A	136	GLU
1	A	138	ILE
1	A	147	ASP
1	A	154	MET
1	A	155	ASP
1	A	156	PHE
1	A	158	ASN
1	A	165	LYS
1	A	180	GLU
1	A	181	GLU
1	A	185	LYS
1	A	191	CYS
1	A	202	LYS
1	A	205	SER
1	A	226	VAL
1	A	239	THR
1	A	245	LEU
1	A	247	ASN
1	A	249	THR
1	A	252	GLN
1	A	262	SER

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Mol	Chain	Res	Type
1	A	266	THR
1	A	269	LYS
1	A	278	THR
1	A	279	ASP
1	A	284	VAL
1	A	299	VAL
1	A	300	ARG
1	A	301	LYS
1	A	304	LYS
1	A	306	GLU
1	A	313	CYS
1	A	316	ILE
1	A	318	ILE
1	A	327	ILE
1	A	331	ASN
1	A	336	LYS
1	A	340	SER
1	A	363	LEU
1	A	366	GLN
1	A	368	LEU
1	A	371	LEU
1	A	376	GLU
1	A	378	THR
1	A	391	THR
1	A	394	HIS
1	A	408	GLN
1	A	422	THR
1	A	423	SER
1	A	427	ARG
1	A	431	GLU
1	A	433	SER
1	A	437	VAL
1	A	438	ILE
1	A	439	ILE
1	A	446	CYS
1	A	449	ASN
1	A	451	ILE
1	A	459	THR
1	A	467	ILE
1	A	474	SER
1	A	478	THR
1	A	481	VAL

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Mol	Chain	Res	Type
1	A	489	GLU
1	A	500	VAL
1	A	505	VAL
1	A	506	SER
1	A	509	ARG
1	A	514	LYS
1	A	519	GLU
1	A	526	VAL
1	A	545	ILE
1	A	550	ARG
1	A	553	ASP
1	A	575	VAL
1	A	579	ASN
1	A	581	THR
1	A	605	THR
1	A	609	LEU
2	B	8	LEU
2	B	11	ASP
2	B	15	LEU
2	B	17	ASP
2	B	27	ASP
2	B	45	ARG
2	B	46	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	12	ASN
1	A	59	GLN
1	A	79	ASN
1	A	81	GLN
1	A	104	ASN
1	A	128	ASN
1	A	129	ASN
1	A	134	ASN
1	A	139	GLN
1	A	158	ASN
1	A	209	HIS
1	A	210	ASN
1	A	247	ASN
1	A	256	ASN

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Mol	Chain	Res	Type
1	A	442	ASN
1	A	449	ASN
1	A	469	ASN
1	A	480	GLN
1	A	483	HIS
1	A	535	HIS
1	A	557	GLN
1	A	560	HIS
1	A	594	HIS
1	A	597	HIS
1	A	599	ASN
2	B	16	HIS

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 ⓘ

8 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	1,3	14,14,15	0.72	1 (7%)	17,19,21	1.56	3 (17%)
3	NAG	C	2	3	14,14,15	0.64	0	17,19,21	1.58	4 (23%)
3	BMA	C	3	3	11,11,12	0.65	0	15,15,17	1.15	1 (6%)
3	NAG	D	1	1,3	14,14,15	0.69	0	17,19,21	1.35	3 (17%)
3	NAG	D	2	3	14,14,15	0.56	0	17,19,21	1.23	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	D	3	3	11,11,12	0.69	0	15,15,17	0.63	0
4	NAG	E	1	1,4	14,14,15	0.69	0	17,19,21	2.68	8 (47%)
4	NAG	E	2	4	14,14,15	0.59	0	17,19,21	1.39	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
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	1/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	4/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	NAG	C1-C2	2.10	1.55	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1	NAG	C1-O5-C5	8.31	123.32	112.19
4	E	2	NAG	C1-O5-C5	4.55	118.28	112.19
3	D	1	NAG	C4-C3-C2	3.96	116.83	111.02
3	C	2	NAG	C2-N2-C7	-3.67	117.98	122.90
3	C	1	NAG	C1-O5-C5	3.38	116.72	112.19
4	E	1	NAG	O3-C3-C2	-3.12	102.92	109.40
4	E	1	NAG	C2-N2-C7	-2.88	119.05	122.90
3	C	3	BMA	C1-C2-C3	2.85	113.79	109.64
3	D	2	NAG	C1-C2-N2	2.70	114.68	110.43
3	C	2	NAG	C4-C3-C2	2.67	114.93	111.02
3	C	2	NAG	O5-C1-C2	-2.66	107.17	111.29
4	E	1	NAG	C1-C2-N2	2.61	114.55	110.43
3	C	1	NAG	O6-C6-C5	-2.57	102.59	111.33
4	E	1	NAG	C6-C5-C4	-2.52	106.84	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	O7-C7-C8	-2.36	117.86	122.05
4	E	1	NAG	O3-C3-C4	-2.31	104.92	110.38
4	E	1	NAG	C3-C4-C5	2.27	114.35	110.23
3	D	2	NAG	C4-C3-C2	-2.27	107.70	111.02
3	C	2	NAG	O4-C4-C3	-2.22	105.14	110.38
3	D	1	NAG	O3-C3-C2	-2.17	104.90	109.40
3	D	1	NAG	C3-C4-C5	2.12	114.07	110.23
4	E	1	NAG	O4-C4-C5	2.05	114.37	109.32

There are no chirality outliers.

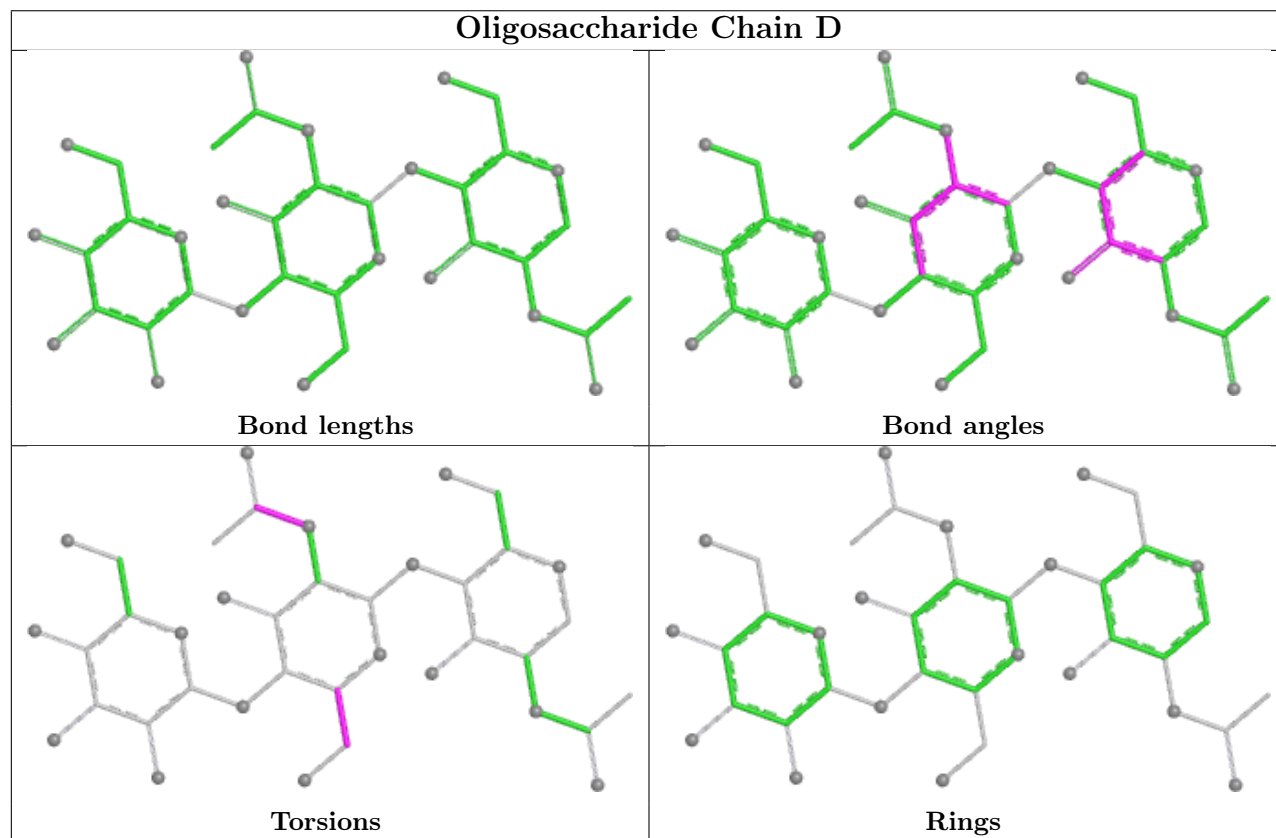
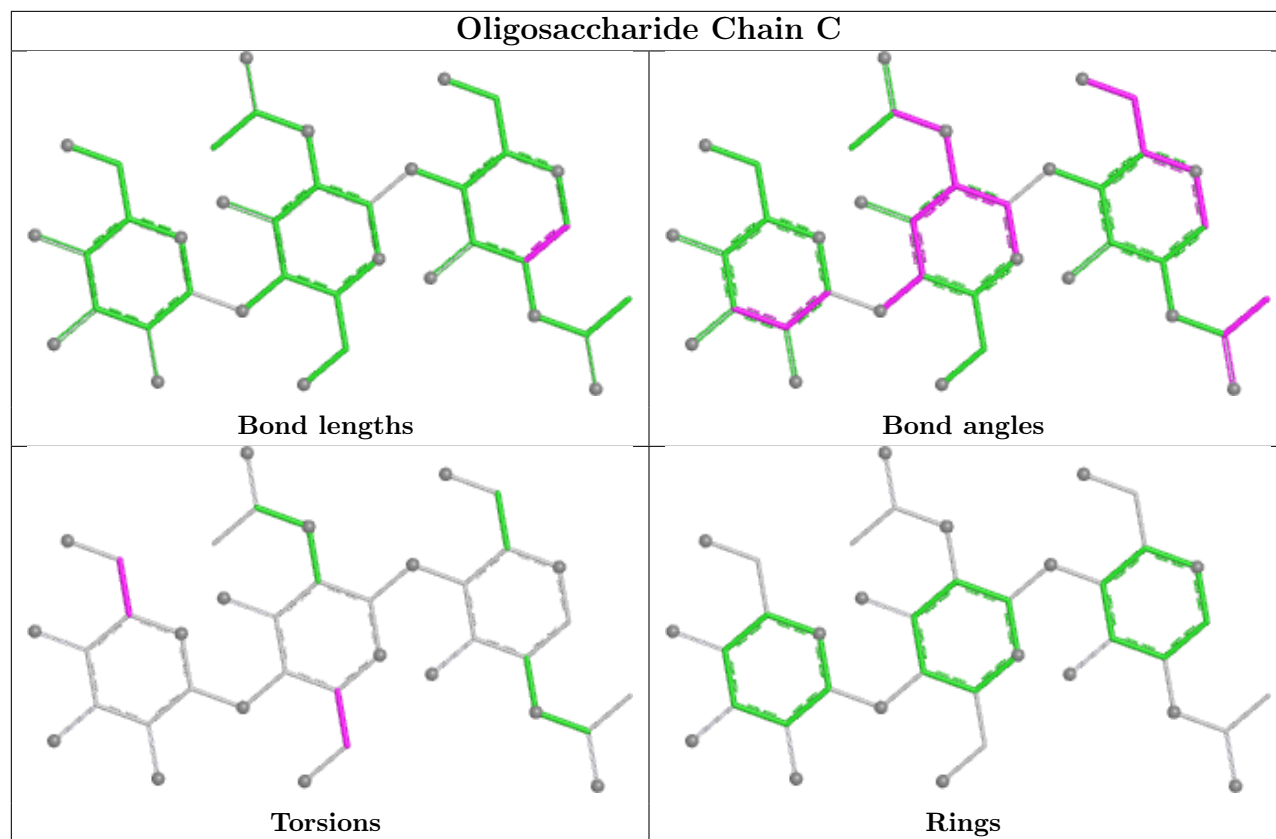
All (11) torsion outliers are listed below:

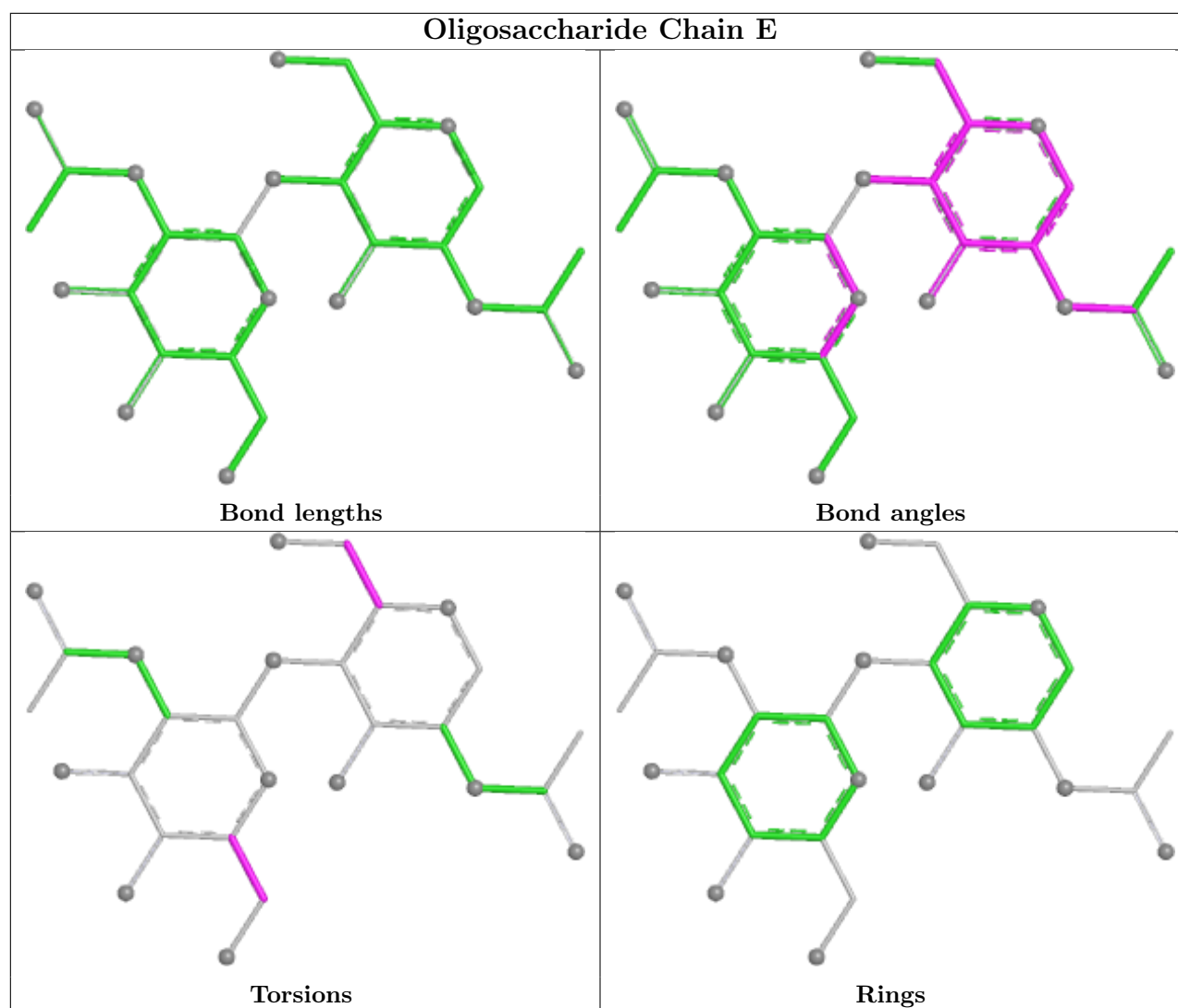
Mol	Chain	Res	Type	Atoms
4	E	2	NAG	O5-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	C	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	703	-	14,14,15	0.58	0	17,19,21	1.75	4 (23%)
5	NAG	A	705	1	14,14,15	0.89	1 (7%)	17,19,21	1.75	2 (11%)
5	NAG	A	702	1	14,14,15	0.68	0	17,19,21	1.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	704	1	14,14,15	0.58	0	17,19,21	2.34	2 (11%)
5	NAG	A	701	-	14,14,15	0.64	0	17,19,21	0.93	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
5	NAG	A	703	-	-	2/6/23/26	0/1/1/1
5	NAG	A	705	1	-	5/6/23/26	0/1/1/1
5	NAG	A	702	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	A	704	1	-	4/6/23/26	0/1/1/1
5	NAG	A	701	-	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	705	NAG	O5-C5	-2.12	1.39	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	704	NAG	C1-O5-C5	8.39	123.43	112.19
5	A	705	NAG	C1-O5-C5	-6.12	103.99	112.19
5	A	703	NAG	C3-C4-C5	4.03	117.53	110.23
5	A	703	NAG	O5-C1-C2	-3.21	106.33	111.29
5	A	703	NAG	C4-C3-C2	2.60	114.83	111.02
5	A	703	NAG	C1-O5-C5	2.55	115.60	112.19
5	A	701	NAG	O5-C1-C2	-2.37	107.62	111.29
5	A	704	NAG	C6-C5-C4	-2.35	107.25	113.02
5	A	705	NAG	O6-C6-C5	-2.05	104.37	111.33

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	702	NAG	C1

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	704	NAG	C8-C7-N2-C2
5	A	704	NAG	O7-C7-N2-C2
5	A	705	NAG	C8-C7-N2-C2
5	A	705	NAG	O7-C7-N2-C2
5	A	701	NAG	C8-C7-N2-C2
5	A	705	NAG	O5-C5-C6-O6
5	A	703	NAG	C8-C7-N2-C2
5	A	701	NAG	O7-C7-N2-C2
5	A	704	NAG	C3-C2-N2-C7
5	A	703	NAG	O7-C7-N2-C2
5	A	705	NAG	C4-C5-C6-O6
5	A	704	NAG	C4-C5-C6-O6
5	A	705	NAG	C3-C2-N2-C7
5	A	701	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	705	NAG	11	0
5	A	704	NAG	1	0
5	A	701	NAG	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	4:LYS	C	5:LYS	N	0.52

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.