



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:16 PM UTC

PDB ID : 3I2T / pdb_00003i2t
Title : Crystal structure of the unliganded Drosophila Epidermal Growth Factor Receptor ectodomain
Authors : Alvarado, D.; Klein, D.E.; Lemmon, M.A.
Deposited on : 2009-06-29
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

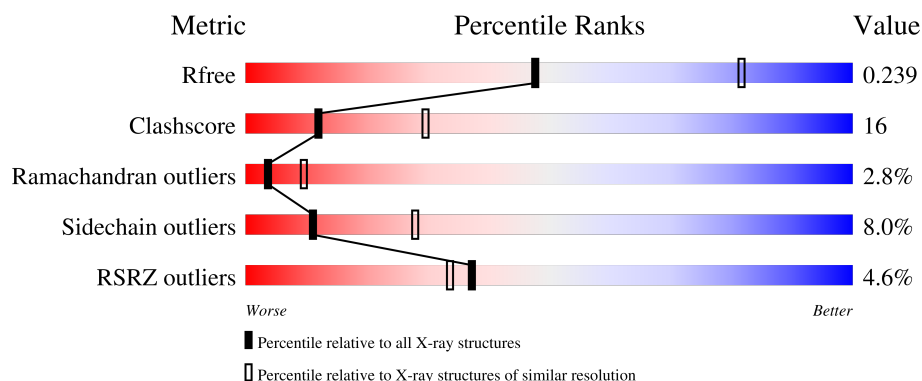
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.



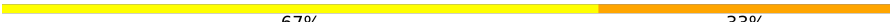
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	551	5% 67% 27% ...
2	B	2	50% 50%
3	C	2	100%
4	D	3	33% 67%
4	E	3	33% 67%

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Mol	Chain	Length	Quality of chain
5	F	3	 67% 33%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4381 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, isoform A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	542	Total	C	N	O	S	0	0	0
			4203	2617	737	798	51			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q8MLW0
A	-4	HIS	-	expression tag	UNP Q8MLW0
A	-3	HIS	-	expression tag	UNP Q8MLW0
A	-2	HIS	-	expression tag	UNP Q8MLW0
A	-1	HIS	-	expression tag	UNP Q8MLW0
A	0	HIS	-	expression tag	UNP Q8MLW0
A	2	ILE	VAL	SEE REMARK 999	UNP Q8MLW0
A	493	ASN	THR	SEE REMARK 999	UNP Q8MLW0

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



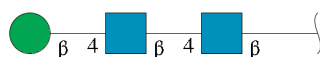
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



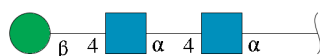
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 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
4	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



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

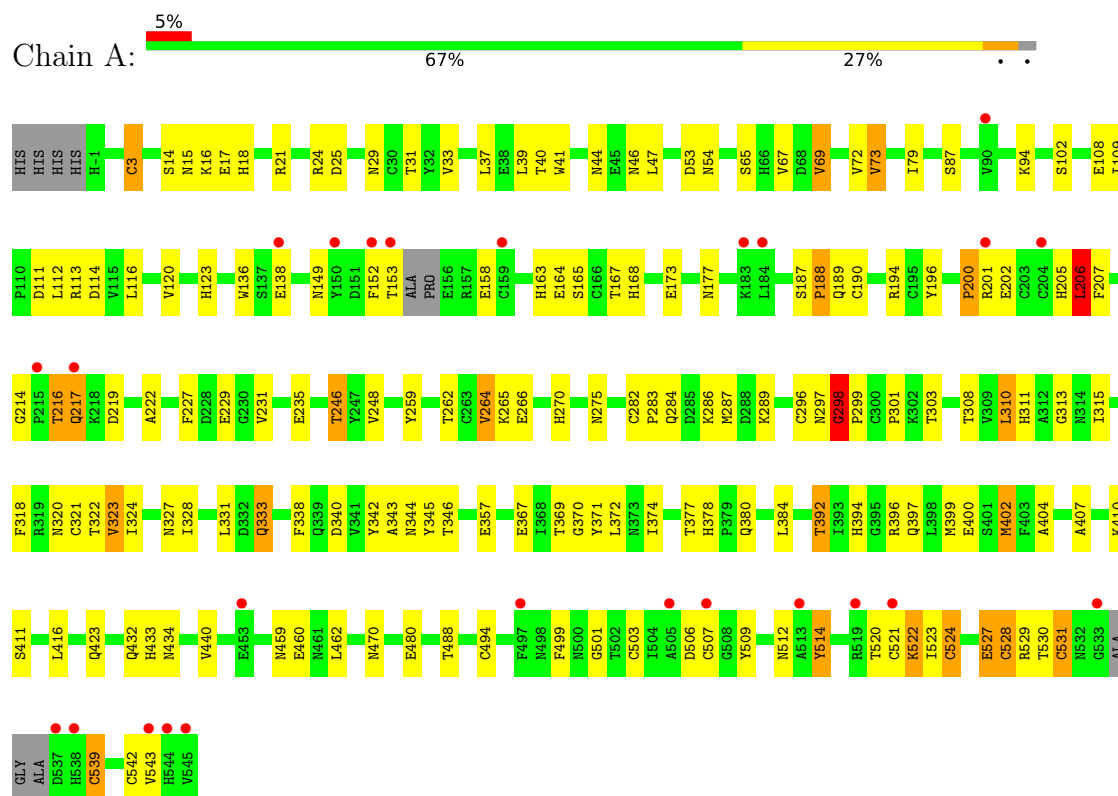
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total	O	0	0
			5	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 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: Epidermal growth factor receptor, isoform A



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



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



MAG1
MAG2

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

Chain E:  33% 67%

MAG1
MAG2
BMA3

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

Chain F:  67% 33%

NDG1
NDG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	74.38Å 174.80Å 161.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.68 – 2.70 36.68 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (36.68-2.70) 99.2 (36.68-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.68Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.224 , 0.264 0.235 , 0.239	Depositor DCC
R_{free} test set	1484 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	68.6	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 31.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4381	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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: NDG, BMA, 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	0.75	1/4298 (0.0%)	0.98	14/5826 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	VAL	CA-CB	5.27	1.60	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	CYS	CB-CA-C	-7.57	95.76	109.38
1	A	298	GLY	CA-C-N	-7.12	112.64	119.90
1	A	298	GLY	C-N-CA	-7.12	112.64	119.90
1	A	206	LEU	N-CA-C	-7.03	105.32	114.04
1	A	503	CYS	N-CA-C	6.87	119.66	108.26
1	A	53	ASP	N-CA-C	6.59	120.91	112.34
1	A	275	ASN	CB-CA-C	-5.94	109.15	117.23
1	A	494	CYS	CA-CB-SG	-5.62	101.47	114.40
1	A	494	CYS	N-CA-C	5.61	118.39	109.24
1	A	216	THR	N-CA-C	5.30	116.58	108.52
1	A	214	GLY	CA-C-N	5.25	126.41	119.84
1	A	214	GLY	C-N-CA	5.25	126.41	119.84
1	A	177	ASN	N-CA-C	5.20	119.60	113.16
1	A	531	CYS	N-CA-C	5.01	114.66	108.19

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4203	0	3924	133	0
2	B	28	0	24	5	0
3	C	28	0	25	3	0
4	D	39	0	34	0	0
4	E	39	0	34	0	0
5	F	39	0	32	5	0
6	A	5	0	0	0	0
All	All	4381	0	4073	133	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 16.

All (133) 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:320:ASN:ND2	3:C:1:NAG:C1	1.71	1.47
1:A:470:ASN:HD21	5:F:1:NDG:C1	1.28	1.44
1:A:29:ASN:ND2	2:B:1:NDG:C1	1.88	1.36
1:A:470:ASN:ND2	5:F:1:NDG:C1	1.90	1.32
1:A:399:MET:HE1	1:A:407:ALA:HB3	1.20	1.19
1:A:470:ASN:HD21	5:F:1:NDG:C2	1.65	1.09
1:A:114:ASP:OD2	1:A:116:LEU:HD23	1.59	1.02
1:A:399:MET:HE1	1:A:407:ALA:CB	1.90	1.01
1:A:205:HIS:ND1	1:A:216:THR:HG23	1.76	0.99
1:A:311:HIS:HD2	1:A:313:GLY:H	1.10	0.96
1:A:29:ASN:HD21	2:B:1:NDG:C1	1.60	0.92
1:A:378:HIS:HD2	1:A:380:GLN:H	1.21	0.87
1:A:15:ASN:HD22	1:A:18:HIS:H	1.22	0.86
1:A:531:CYS:CB	1:A:539:CYS:HB3	2.06	0.85
1:A:530:THR:O	1:A:539:CYS:HB2	1.75	0.85
1:A:205:HIS:CD2	1:A:206:LEU:H	1.97	0.83
1:A:303:THR:HG22	1:A:323:VAL:HG13	1.60	0.81
1:A:188:PRO:C	1:A:190:CYS:H	1.86	0.80
1:A:327:ASN:HD22	1:A:371:TYR:H	1.27	0.78
1:A:200:PRO:O	1:A:202:GLU:N	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:THR:HG22	1:A:248:VAL:HG23	1.67	0.75
1:A:378:HIS:CD2	1:A:380:GLN:H	2.04	0.75
1:A:114:ASP:OD2	1:A:116:LEU:CD2	2.33	0.74
1:A:459:ASN:HD22	1:A:460:GLU:HG3	1.52	0.73
1:A:531:CYS:HB2	1:A:539:CYS:HB3	1.69	0.73
1:A:111:ASP:OD1	1:A:113:ARG:NH1	2.21	0.72
1:A:163:HIS:HD2	1:A:165:SER:OG	1.73	0.72
1:A:512:ASN:HD22	1:A:524:CYS:HB2	1.55	0.71
1:A:320:ASN:ND2	3:C:1:NAG:O5	2.25	0.69
1:A:400:GLU:CD	1:A:400:GLU:H	2.00	0.69
1:A:29:ASN:CG	2:B:1:NDG:C1	2.66	0.67
1:A:402:MET:HA	1:A:402:MET:HE2	1.74	0.67
1:A:378:HIS:HD2	1:A:380:GLN:N	1.92	0.66
1:A:311:HIS:HD2	1:A:313:GLY:N	1.88	0.66
1:A:287:MET:HE3	1:A:296:CYS:HA	1.78	0.66
1:A:301:PRO:O	1:A:303:THR:HG23	1.97	0.64
1:A:531:CYS:HB3	1:A:539:CYS:HB3	1.79	0.64
1:A:324:ILE:HD13	1:A:328:ILE:HD11	1.80	0.63
1:A:311:HIS:CD2	1:A:313:GLY:H	2.02	0.63
1:A:470:ASN:ND2	5:F:1:NDG:C2	2.48	0.62
1:A:528:CYS:C	1:A:530:THR:H	2.08	0.62
1:A:512:ASN:HB3	1:A:524:CYS:H	1.65	0.61
1:A:246:THR:HG22	1:A:248:VAL:CG2	2.29	0.61
1:A:512:ASN:ND2	1:A:524:CYS:HB2	2.15	0.61
1:A:246:THR:CG2	1:A:248:VAL:HG23	2.30	0.60
1:A:196:TYR:CZ	1:A:202:GLU:HB2	2.36	0.60
1:A:297:ASN:O	1:A:298:GLY:O	2.20	0.60
1:A:367:GLU:OE1	1:A:394:HIS:HE1	1.85	0.60
1:A:399:MET:CE	1:A:407:ALA:CB	2.75	0.59
1:A:44:ASN:HB3	1:A:47:LEU:HG	1.85	0.59
1:A:259:TYR:O	1:A:262:THR:HB	2.02	0.58
1:A:411:SER:H	1:A:434:ASN:HD22	1.52	0.58
1:A:205:HIS:HD2	1:A:207:PHE:H	1.50	0.58
1:A:411:SER:H	1:A:434:ASN:ND2	2.00	0.58
1:A:24:ARG:NH1	1:A:25:ASP:OD2	2.37	0.57
1:A:338:PHE:HE2	1:A:340:ASP:OD1	1.88	0.56
1:A:343:ALA:C	1:A:345:TYR:H	2.12	0.56
1:A:521:CYS:O	1:A:522:LYS:CB	2.53	0.56
1:A:109:ILE:HG22	1:A:112:LEU:HB2	1.86	0.56
1:A:512:ASN:HB3	1:A:524:CYS:HB2	1.86	0.55
1:A:399:MET:HE3	1:A:404:ALA:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:HIS:HD2	1:A:206:LEU:H	1.53	0.54
1:A:246:THR:CG2	1:A:248:VAL:CG2	2.86	0.54
1:A:327:ASN:HD22	1:A:371:TYR:N	2.02	0.54
1:A:320:ASN:CG	3:C:1:NAG:C1	2.71	0.53
1:A:318:PHE:HA	1:A:321:CYS:SG	2.49	0.52
1:A:187:SER:O	1:A:190:CYS:HB2	2.10	0.52
1:A:310:LEU:HD11	1:A:315:ILE:HD12	1.92	0.52
1:A:138:GLU:O	1:A:194:ARG:NH2	2.42	0.52
1:A:531:CYS:HB3	1:A:539:CYS:CB	2.40	0.51
1:A:73:VAL:HB	1:A:108:GLU:HB2	1.92	0.51
1:A:21:ARG:HG3	1:A:24:ARG:HH22	1.75	0.51
1:A:123:HIS:HD2	1:A:149:ASN:HB3	1.76	0.51
1:A:327:ASN:ND2	1:A:370:GLY:HA3	2.26	0.50
1:A:205:HIS:HB2	1:A:217:GLN:H	1.76	0.50
1:A:527:GLU:O	1:A:528:CYS:SG	2.70	0.50
1:A:297:ASN:C	1:A:298:GLY:O	2.53	0.50
1:A:514:TYR:CD1	1:A:514:TYR:C	2.89	0.50
1:A:499:PHE:C	1:A:501:GLY:H	2.20	0.49
1:A:29:ASN:HD21	2:B:1:NDG:C2	2.21	0.49
1:A:287:MET:HE3	1:A:296:CYS:CA	2.40	0.49
1:A:205:HIS:ND1	1:A:216:THR:CG2	2.64	0.49
1:A:109:ILE:CG2	1:A:112:LEU:HB2	2.43	0.49
1:A:205:HIS:CG	1:A:206:LEU:H	2.29	0.49
1:A:528:CYS:O	1:A:530:THR:N	2.44	0.48
1:A:188:PRO:O	1:A:189:GLN:HB2	2.13	0.48
1:A:512:ASN:HB3	1:A:524:CYS:N	2.29	0.48
1:A:188:PRO:C	1:A:190:CYS:N	2.57	0.47
1:A:287:MET:HE2	1:A:301:PRO:HD3	1.96	0.47
1:A:163:HIS:CD2	1:A:165:SER:OG	2.61	0.47
1:A:470:ASN:CG	5:F:1:NDG:C1	2.80	0.47
1:A:15:ASN:ND2	1:A:18:HIS:H	2.01	0.47
1:A:289:LYS:HA	1:A:289:LYS:HD2	1.58	0.47
1:A:303:THR:HA	1:A:323:VAL:O	2.16	0.46
1:A:67:VAL:O	1:A:102:SER:HB3	2.15	0.46
1:A:333:GLN:H	1:A:333:GLN:CD	2.24	0.45
1:A:270:HIS:HA	1:A:396:ARG:HG2	1.98	0.45
1:A:369:THR:HA	1:A:394:HIS:HB2	1.98	0.45
1:A:287:MET:HE3	1:A:296:CYS:CB	2.47	0.45
1:A:392:THR:HB	1:A:423:GLN:HB3	1.99	0.45
1:A:531:CYS:CB	1:A:539:CYS:CB	2.86	0.45
1:A:283:PRO:HG2	1:A:286:LYS:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:HIS:CD2	1:A:207:PHE:H	2.34	0.44
1:A:416:LEU:HD11	1:A:440:VAL:HG12	1.99	0.44
1:A:87:SER:OG	1:A:94:LYS:HD3	2.18	0.44
1:A:120:VAL:HG11	1:A:136:TRP:CZ3	2.53	0.44
1:A:512:ASN:HD22	1:A:524:CYS:CB	2.27	0.43
1:A:433:HIS:HA	1:A:460:GLU:O	2.18	0.43
1:A:15:ASN:HD22	1:A:18:HIS:N	2.04	0.43
1:A:512:ASN:CB	1:A:524:CYS:HB2	2.48	0.43
1:A:372:LEU:HD11	1:A:374:ILE:HD11	1.99	0.43
1:A:506:ASP:O	1:A:507:CYS:CB	2.67	0.43
1:A:29:ASN:ND2	2:B:1:NDG:N2	2.67	0.43
1:A:298:GLY:O	1:A:299:PRO:C	2.61	0.42
1:A:227:PHE:CD2	1:A:227:PHE:C	2.97	0.42
1:A:342:TYR:O	1:A:343:ALA:C	2.63	0.42
1:A:152:PHE:O	1:A:153:THR:CB	2.67	0.42
1:A:167:THR:OG1	1:A:168:HIS:CD2	2.73	0.42
1:A:79:ILE:HD13	1:A:222:ALA:HB3	2.02	0.42
1:A:322:THR:HG22	1:A:323:VAL:HG12	2.01	0.42
1:A:327:ASN:HD22	1:A:370:GLY:HA3	1.84	0.41
1:A:410:LYS:HA	1:A:433:HIS:O	2.19	0.41
1:A:15:ASN:HD21	1:A:17:GLU:HB2	1.85	0.41
1:A:287:MET:HG2	1:A:296:CYS:SG	2.61	0.41
1:A:432:GLN:HA	1:A:459:ASN:O	2.20	0.41
1:A:528:CYS:C	1:A:530:THR:N	2.76	0.41
1:A:3:CYS:HB2	1:A:33:VAL:HA	2.03	0.41
1:A:114:ASP:OD1	1:A:194:ARG:NH1	2.54	0.41
1:A:264:VAL:HG13	1:A:266:GLU:O	2.21	0.41
1:A:31:THR:HA	1:A:54:ASN:O	2.20	0.41
1:A:40:THR:HA	1:A:65:SER:O	2.21	0.40
1:A:16:LYS:HE3	1:A:41:TRP:CE3	2.57	0.40
1:A:282:CYS:HB3	1:A:286:LYS:HB2	2.03	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	536/551 (97%)	463 (86%)	58 (11%)	15 (3%)	4 9

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	ARG
1	A	217	GLN
1	A	229	GLU
1	A	522	LYS
1	A	529	ARG
1	A	200	PRO
1	A	298	GLY
1	A	344	ASN
1	A	528	CYS
1	A	539	CYS
1	A	520	THR
1	A	543	VAL
1	A	14	SER
1	A	509	TYR
1	A	188	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	463/489 (95%)	426 (92%)	37 (8%)	11 28

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	39	LEU
1	A	46	ASN
1	A	69	VAL

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Mol	Chain	Res	Type
1	A	72	VAL
1	A	73	VAL
1	A	158	GLU
1	A	164	GLU
1	A	173	GLU
1	A	206	LEU
1	A	219	ASP
1	A	231	VAL
1	A	235	GLU
1	A	246	THR
1	A	264	VAL
1	A	265	LYS
1	A	284	GLN
1	A	308	THR
1	A	310	LEU
1	A	323	VAL
1	A	331	LEU
1	A	333	GLN
1	A	346	THR
1	A	357	GLU
1	A	377	THR
1	A	384	LEU
1	A	392	THR
1	A	397	GLN
1	A	402	MET
1	A	462	LEU
1	A	480	GLU
1	A	488	THR
1	A	514	TYR
1	A	523	ILE
1	A	524	CYS
1	A	527	GLU
1	A	542	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	29	ASN
1	A	66	HIS
1	A	119	GLN
1	A	123	HIS

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Mol	Chain	Res	Type
1	A	163	HIS
1	A	168	HIS
1	A	205	HIS
1	A	270	HIS
1	A	284	GLN
1	A	311	HIS
1	A	327	ASN
1	A	333	GLN
1	A	378	HIS
1	A	394	HIS
1	A	423	GLN
1	A	434	ASN
1	A	459	ASN
1	A	470	ASN
1	A	512	ASN
1	A	518	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

13 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	$\# Z > 2$
2	NDG	B	1	2	14,14,15	0.50	0	17,19,21	1.94	2 (11%)
2	NAG	B	2	2	14,14,15	0.53	0	17,19,21	0.90	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	1	3	14,14,15	0.67	0	17,19,21	0.98	0
3	NAG	C	2	3	14,14,15	0.83	1 (7%)	17,19,21	1.29	2 (11%)
4	NAG	D	1	4,1	14,14,15	0.67	0	17,19,21	2.42	6 (35%)
4	NAG	D	2	4	14,14,15	0.85	1 (7%)	17,19,21	1.43	1 (5%)
4	BMA	D	3	4	11,11,12	0.77	0	15,15,17	0.87	0
4	NAG	E	1	4,1	14,14,15	0.55	0	17,19,21	1.91	5 (29%)
4	NAG	E	2	4	14,14,15	0.55	0	17,19,21	0.98	0
4	BMA	E	3	4	11,11,12	0.84	0	15,15,17	1.47	3 (20%)
5	NDG	F	1	5	14,14,15	0.60	0	17,19,21	1.66	5 (29%)
5	NDG	F	2	5	14,14,15	0.64	0	17,19,21	1.64	2 (11%)
5	BMA	F	3	5	11,11,12	0.85	0	15,15,17	1.47	2 (13%)

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
2	NDG	B	1	2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
3	NAG	C	1	3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
4	NAG	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	1/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	0/1/1/1
5	NDG	F	1	5	-	3/6/23/26	0/1/1/1
5	NDG	F	2	5	-	1/6/23/26	0/1/1/1
5	BMA	F	3	5	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	C1-C2	2.32	1.55	1.52
4	D	2	NAG	C1-C2	2.30	1.55	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	NAG	C1-O5-C5	6.94	121.49	112.19
2	B	1	NDG	O5-C1-C2	5.85	120.34	111.29
4	E	1	NAG	C2-N2-C7	-5.15	116.00	122.90
4	D	2	NAG	C1-O5-C5	-4.66	105.94	112.19
5	F	2	NDG	C2-N2-C7	-4.35	117.08	122.90
2	B	1	NDG	C1-O5-C5	4.08	117.66	112.19
5	F	3	BMA	C1-O5-C5	3.98	117.52	112.19
5	F	2	NDG	C1-O5-C5	3.96	117.50	112.19
4	D	1	NAG	C2-N2-C7	3.56	127.67	122.90
4	D	1	NAG	O5-C1-C2	3.33	116.44	111.29
4	E	1	NAG	O5-C1-C2	-3.26	106.24	111.29
4	D	1	NAG	C1-C2-N2	-3.12	105.52	110.43
3	C	2	NAG	C1-O5-C5	3.11	116.36	112.19
4	E	3	BMA	O5-C5-C6	3.09	113.68	107.66
5	F	1	NDG	C1-O5-C5	2.96	116.15	112.19
5	F	1	NDG	C1-C2-N2	2.76	114.79	110.43
3	C	2	NAG	O5-C5-C6	2.69	112.89	107.66
5	F	1	NDG	C2-N2-C7	2.65	126.45	122.90
4	D	1	NAG	O7-C7-C8	-2.52	117.56	122.05
5	F	1	NDG	O5-C1-C2	-2.40	107.58	111.29
5	F	3	BMA	C1-C2-C3	2.39	113.12	109.64
4	D	1	NAG	O7-C7-N2	2.28	126.01	121.98
5	F	1	NDG	O4-C4-C5	-2.25	103.79	109.32
4	E	1	NAG	O3-C3-C4	-2.17	105.26	110.38
4	E	3	BMA	C3-C4-C5	-2.15	106.33	110.23
4	E	3	BMA	O3-C3-C4	2.14	115.42	110.38
4	E	1	NAG	C8-C7-N2	2.09	119.58	116.12
4	E	1	NAG	C1-C2-N2	2.08	113.71	110.43
2	B	2	NAG	C1-C2-N2	-2.04	107.22	110.43

There are no chirality outliers.

All (15) torsion outliers are listed below:

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

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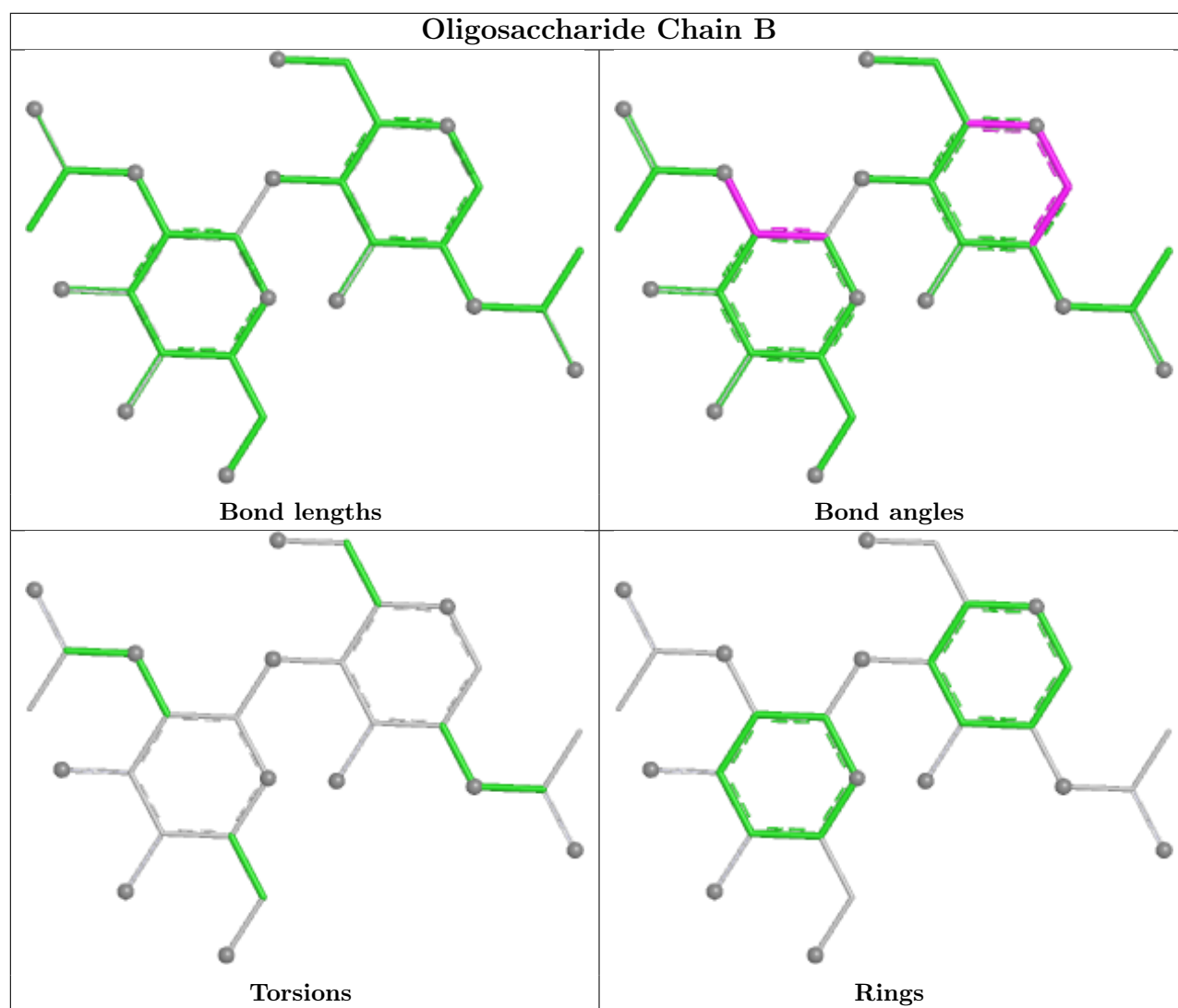
Mol	Chain	Res	Type	Atoms
4	D	3	BMA	C4-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
5	F	2	NDG	O5-C5-C6-O6
5	F	1	NDG	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
5	F	1	NDG	C3-C2-N2-C7

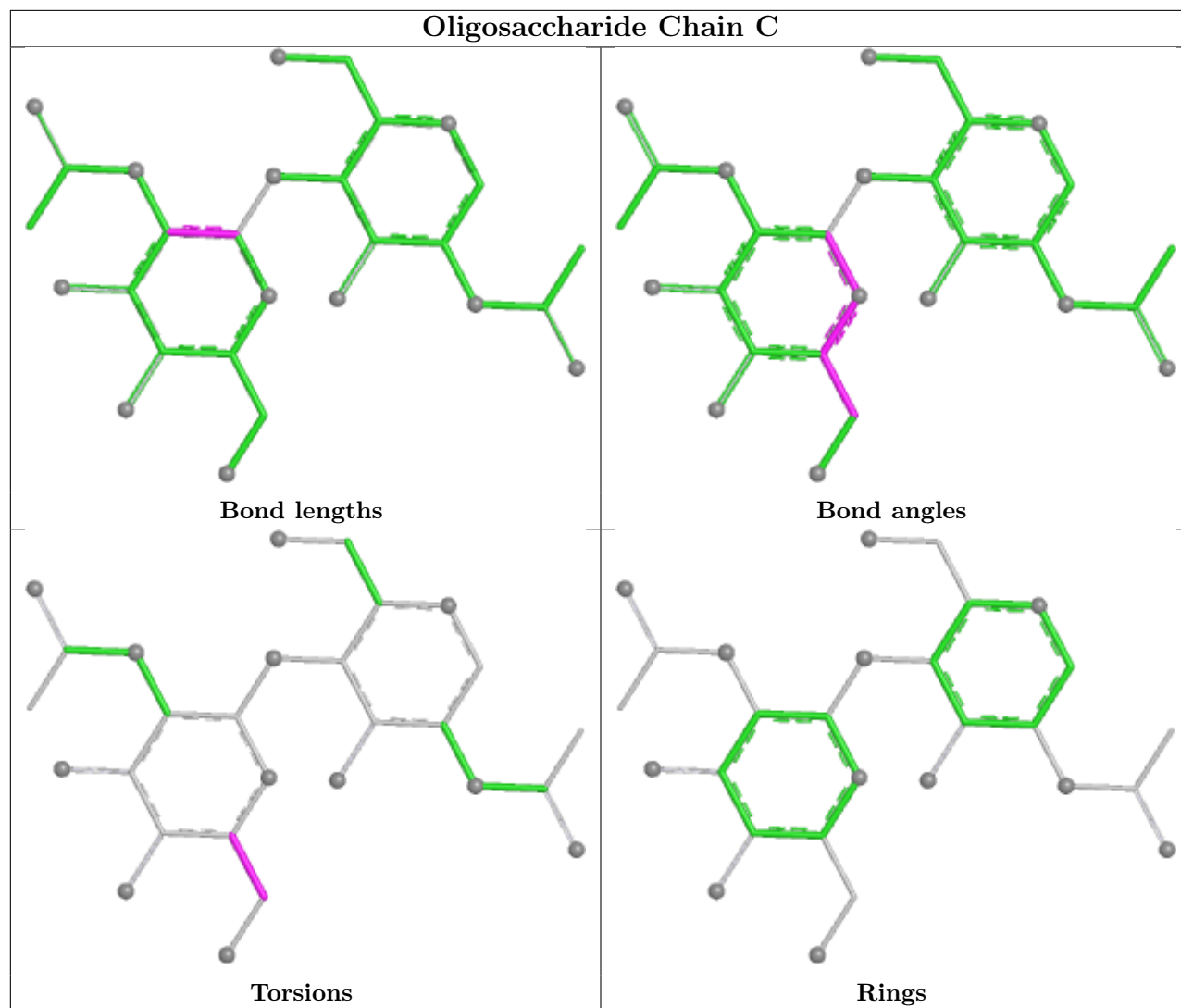
There are no ring outliers.

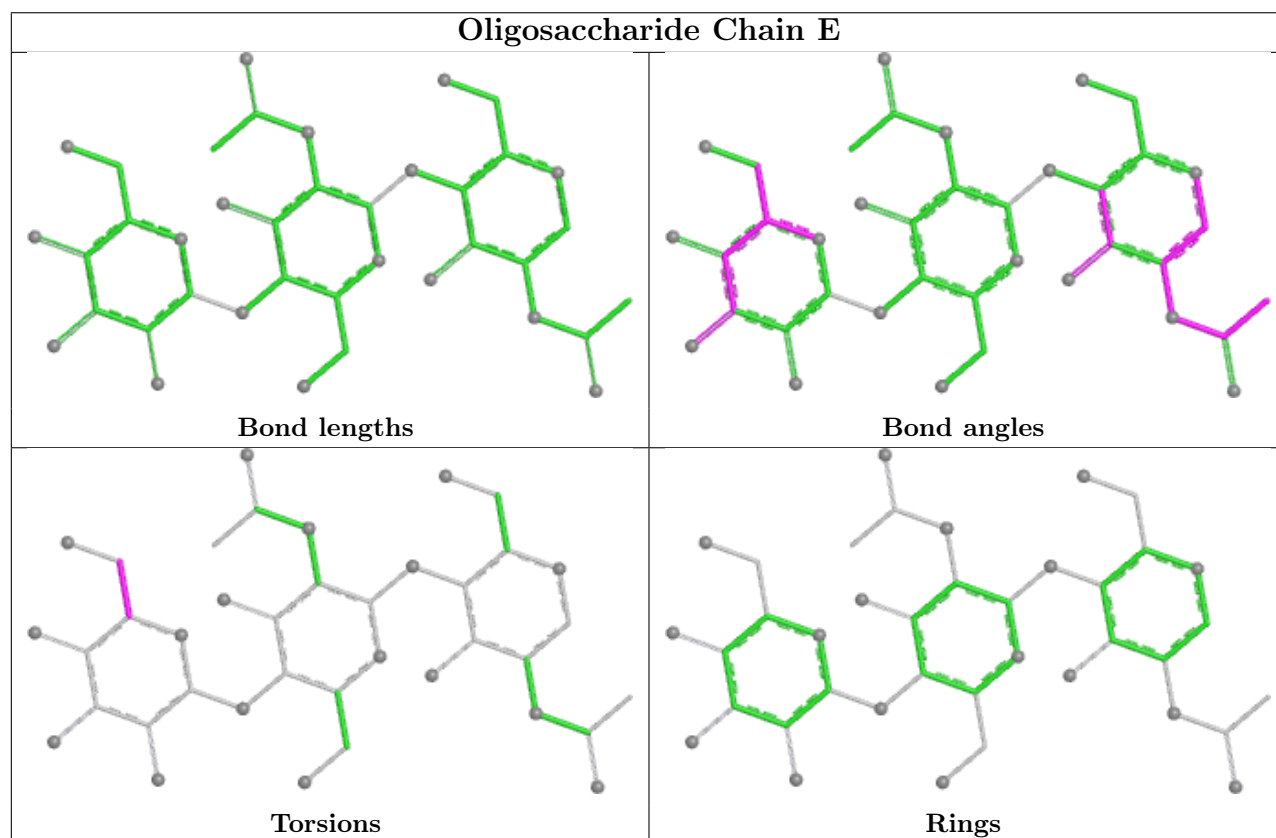
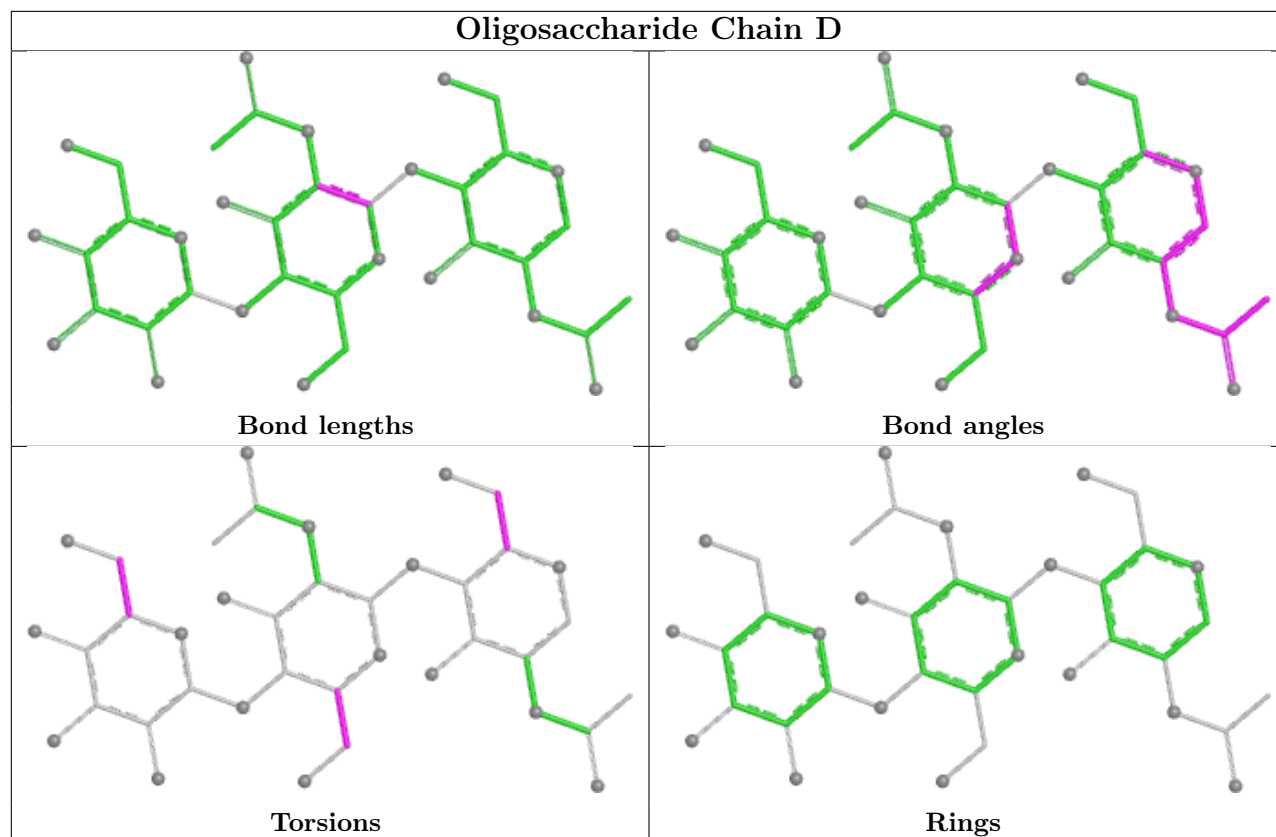
3 monomers are involved in 13 short contacts:

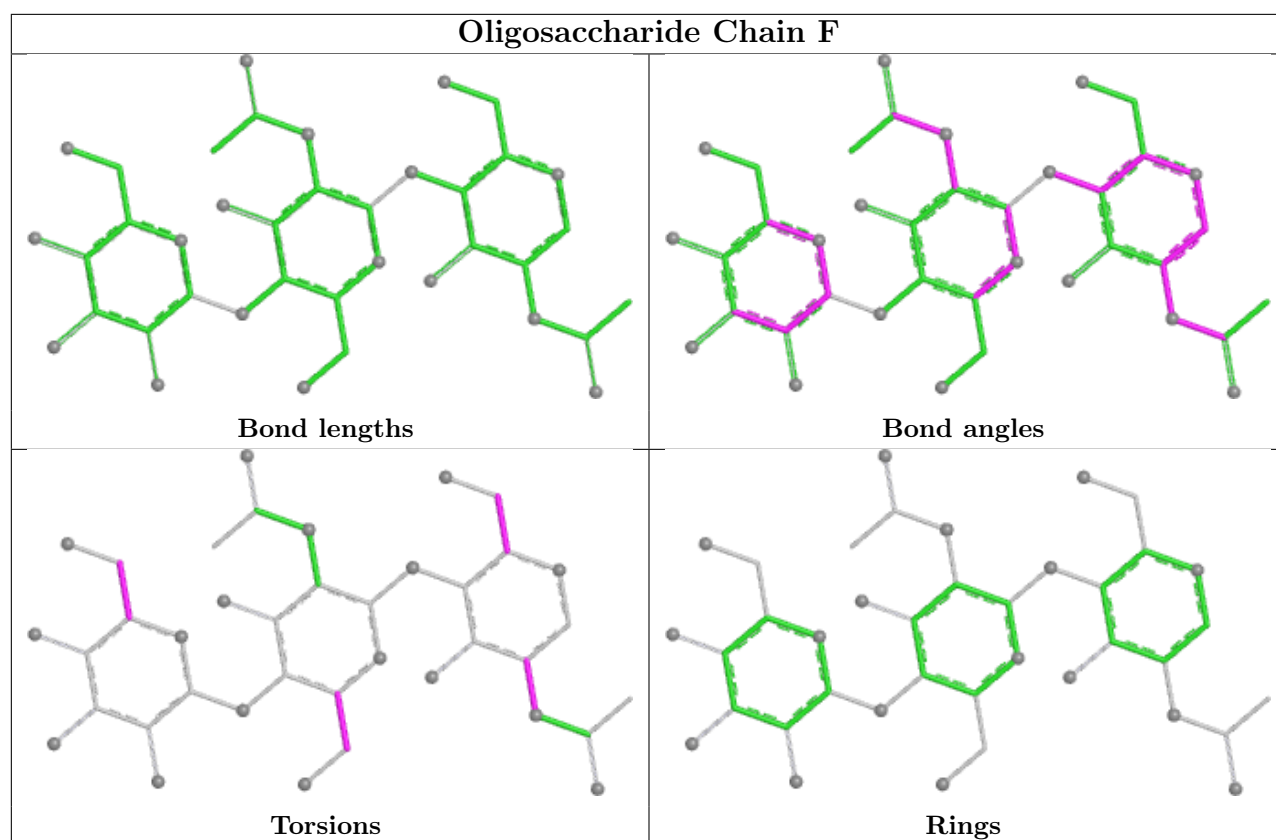
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NDG	5	0
3	C	1	NAG	3	0
5	F	1	NDG	5	0

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](#)

There are no ligands in this entry.

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	542/551 (98%)	0.35	25 (4%) 37 34	31, 45, 69, 78	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	537	ASP	7.2
1	A	533	GLY	6.4
1	A	545	VAL	6.0
1	A	217	GLN	4.6
1	A	215	PRO	4.3
1	A	153	THR	3.8
1	A	150	TYR	3.7
1	A	497	PHE	3.5
1	A	538	HIS	3.3
1	A	159	CYS	3.1
1	A	505	ALA	3.1
1	A	204	CYS	2.9
1	A	152	PHE	2.9
1	A	544	HIS	2.7
1	A	90	VAL	2.6
1	A	519	ARG	2.6
1	A	453	GLU	2.6
1	A	138	GLU	2.5
1	A	521	CYS	2.5
1	A	507	CYS	2.5
1	A	183	LYS	2.5
1	A	184	LEU	2.4
1	A	543	VAL	2.3
1	A	201	ARG	2.1
1	A	513	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

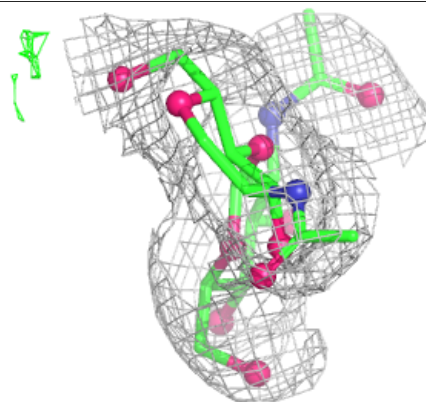
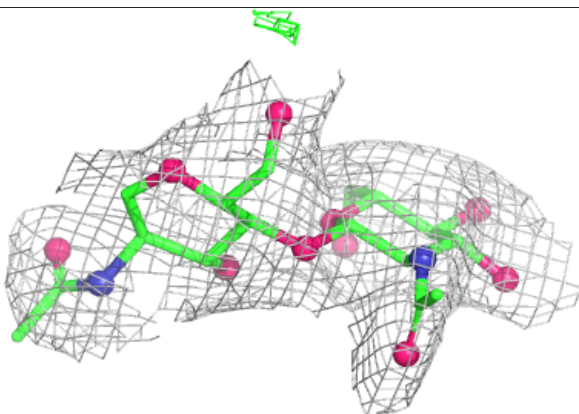
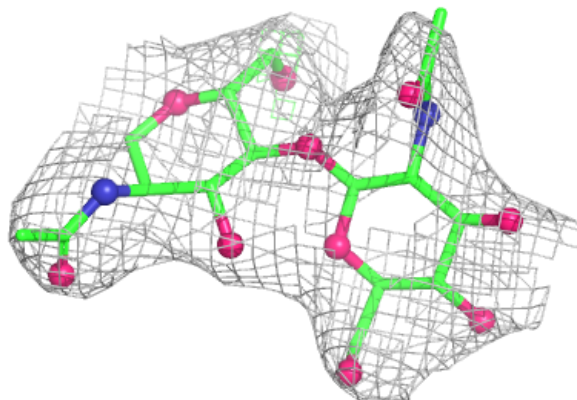
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	2	14/15	0.38	0.17	99,102,103,103	0
4	BMA	E	3	11/12	0.39	0.19	96,98,100,101	0
4	BMA	D	3	11/12	0.42	0.16	94,98,99,100	0
2	NAG	B	2	14/15	0.70	0.13	98,100,102,102	0
4	NAG	D	2	14/15	0.75	0.19	80,85,87,91	0
3	NAG	C	1	14/15	0.78	0.15	89,94,97,100	0
5	BMA	F	3	11/12	0.79	0.13	73,75,77,78	0
2	NDG	B	1	14/15	0.80	0.13	85,88,90,95	0
4	NAG	E	2	14/15	0.84	0.14	89,91,96,96	0
4	NAG	D	1	14/15	0.85	0.13	56,64,68,73	0
4	NAG	E	1	14/15	0.86	0.12	76,82,86,86	0
5	NDG	F	1	14/15	0.91	0.12	69,72,77,79	0
5	NDG	F	2	14/15	0.92	0.11	66,69,71,72	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.

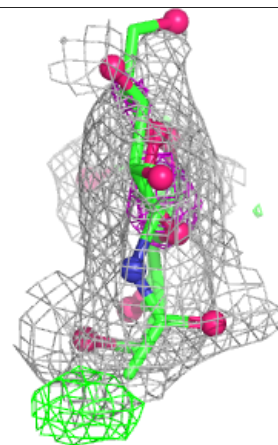
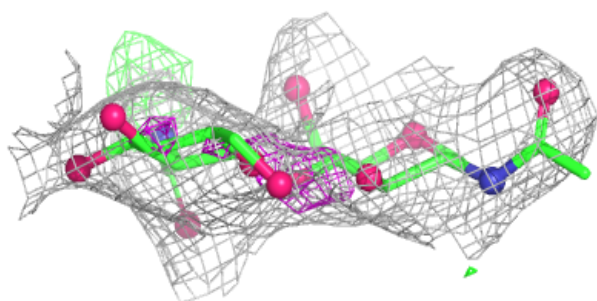
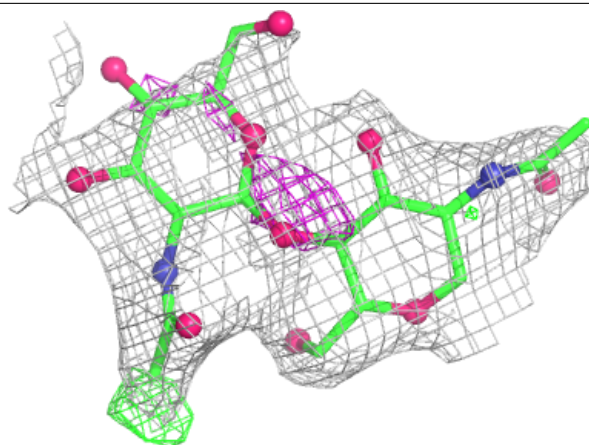
Electron density around Chain B:

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

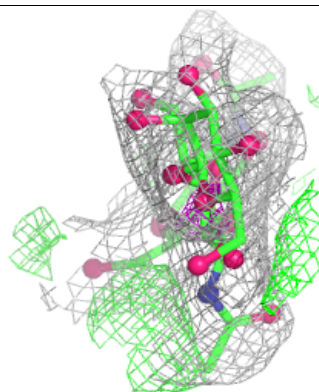
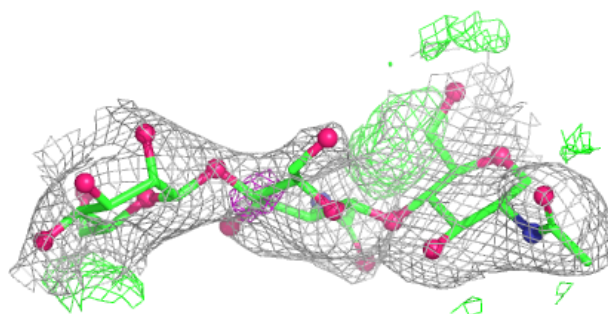
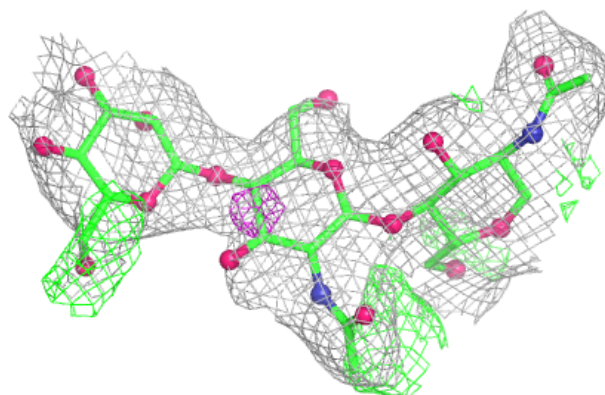


Electron density around Chain C:

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

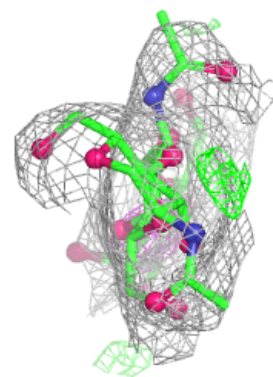
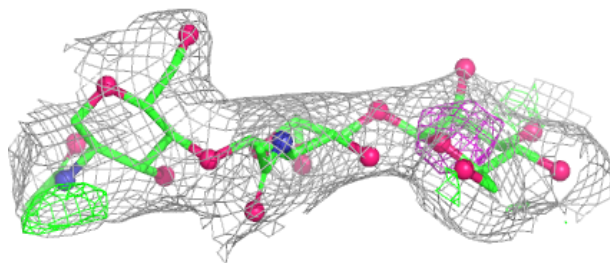
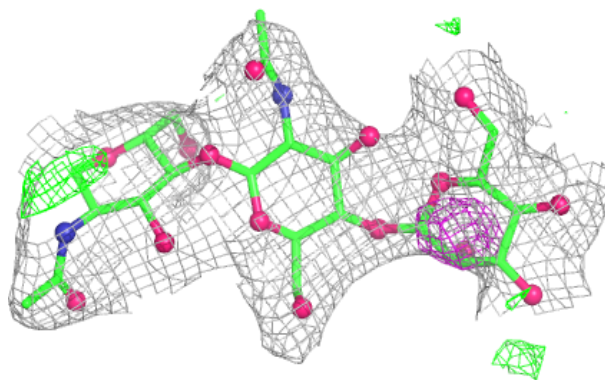
**Electron density around Chain D:**

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

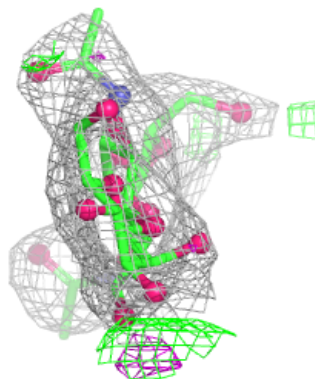
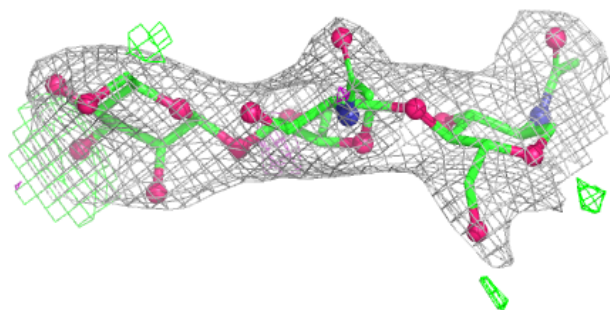
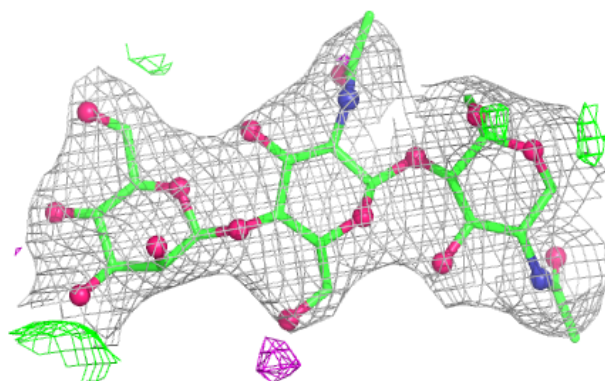


Electron density around Chain E:

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

**Electron density around Chain F:**

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



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.