



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:56 PM UTC

PDB ID : 7L8P / pdb_00007l8p
Title : Integrin alphaIIb beta3 in complex with sibraxiban
Authors : Lin, F.-Y.; Springer, T.A.
Deposited on : 2020-12-31
Resolution : 2.35 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:

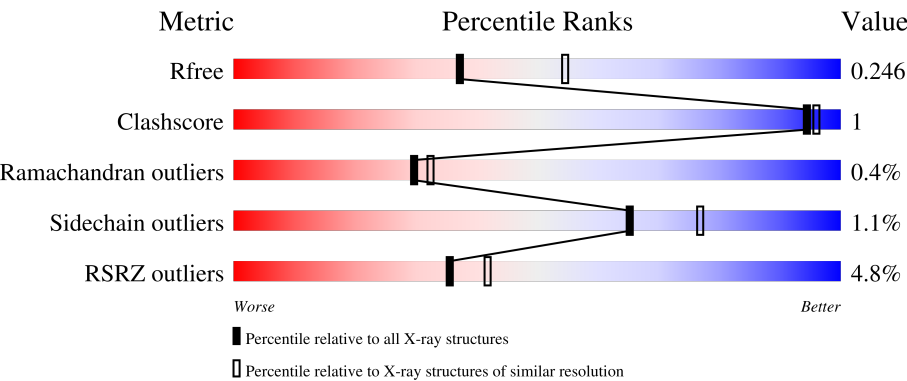
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	457	% 96% ..
1	C	457	% 96% ..
2	B	472	4% 93% 6% .
2	D	472	4% 96% .
3	E	221	18% 94% ..

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Mol	Chain	Length	Quality of chain
3	H	221	3% 94%
4	F	214	15% 98%
4	L	214	96%
5	G	5	60% 40%
6	I	2	100%
6	K	2	50% 50%
7	J	4	25% 75%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 42834 atoms, of which 20392 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 Isoform 3 of Integrin alpha-IIb.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	454	Total	C	H	N	O	S	0	10	0
			6919	2245	3387	611	668	8			
1	C	453	Total	C	H	N	O	S	0	6	0
			6840	2224	3338	604	666	8			

- Molecule 2 is a protein called Isoform Beta-3C of Integrin beta-3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	466	Total	C	H	N	O	S	6	10	0
			7202	2264	3568	621	715	34			
2	D	471	Total	C	H	N	O	S	10	3	0
			7206	2271	3561	622	717	35			

- Molecule 3 is a protein called Monoclonal antibody 10E5 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	214	Total	C	H	N	O	S	0	0	0
			3221	1035	1590	264	326	6			
3	H	216	Total	C	H	N	O	S	0	0	0
			3242	1041	1600	266	329	6			

- Molecule 4 is a protein called Monoclonal antibody 10E5 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	214	Total	C	H	N	O	S	0	0	0
			3190	1019	1553	268	341	9			
4	L	214	Total	C	H	N	O	S	0	0	0
			3190	1019	1553	268	341	9			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
5	G	5	Total	C	H	N	O	0	0	0
			118	34	57	2	25			

- 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	I	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
6	K	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
7	J	4	Total	C	H	N	O	0	0	0
			97	28	47	2	20			

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	0	0
			14	3	8	3		

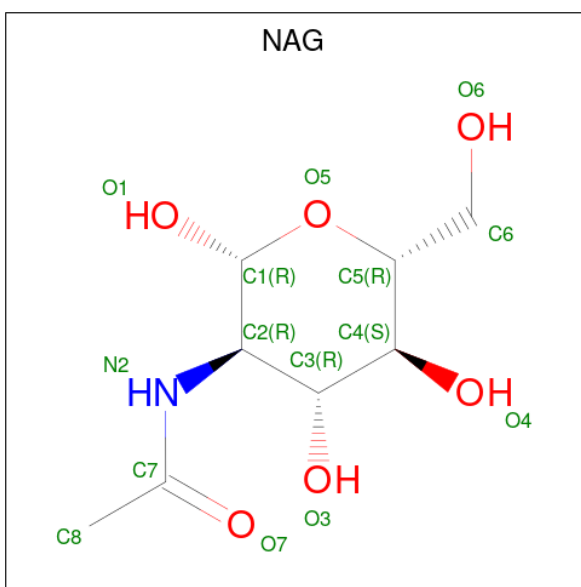
- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	4	Total	Ca	0	0
			4	4		
10	B	2	Total	Ca	0	0
			2	2		
10	C	4	Total	Ca	0	0
			4	4		
10	D	2	Total	Ca	0	0
			2	2		

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

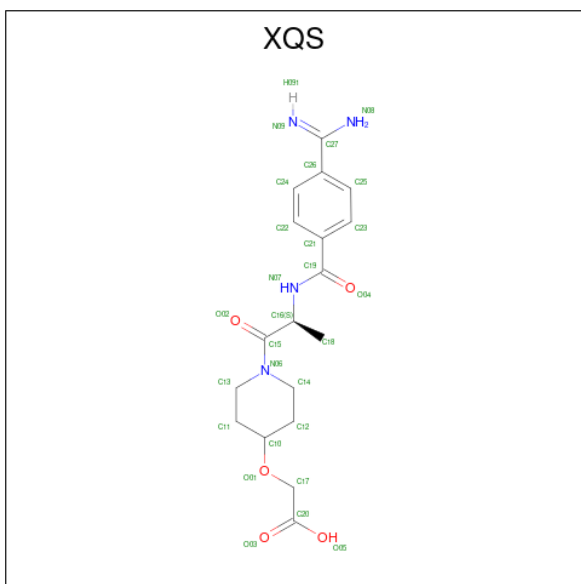
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	1	Total	Mg	0	0
			1	1		
11	D	1	Total	Mg	0	0
			1	1		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
12	D	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 13 is sibrafinan (active form) (CCD ID: XQS) (formula: $C_{18}H_{24}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	H	N	O	0	0
			51	18	24	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	H	N	O	0	0
			51	18	24	4	5		

- Molecule 14 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	2	Total	Cl	0	0
			2	2		

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	474	Total	O	0	0
			474	474		
15	B	245	Total	O	0	0
			245	245		
15	C	265	Total	O	0	0
			265	265		
15	D	193	Total	O	0	0
			193	193		
15	E	13	Total	O	0	0
			13	13		
15	F	11	Total	O	0	0
			11	11		
15	H	35	Total	O	0	0
			35	35		
15	L	40	Total	O	0	0
			40	40		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

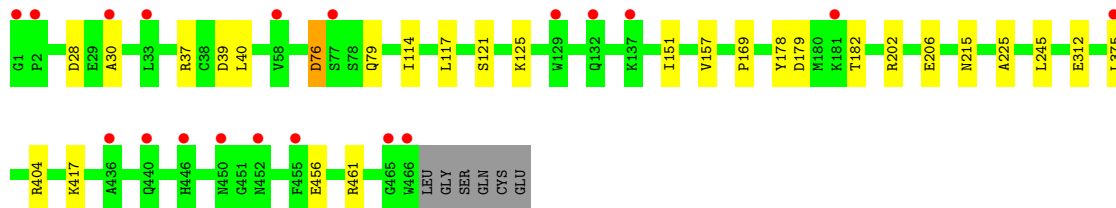
- Molecule 1: Isoform 3 of Integrin alpha-IIb



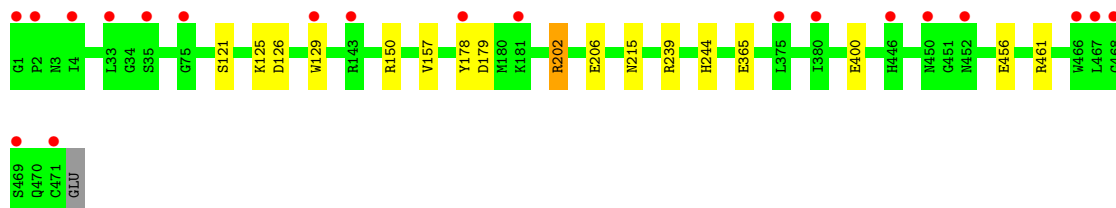
- Molecule 1: Isoform 3 of Integrin alpha-IIb



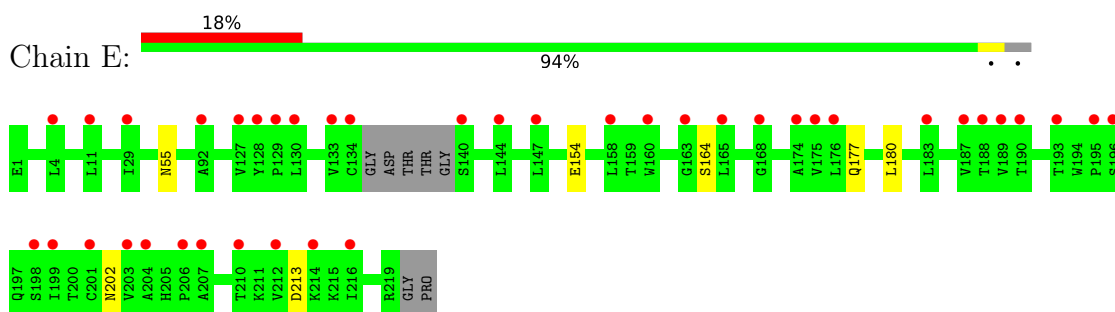
- Molecule 2: Isoform Beta-3C of Integrin beta-3



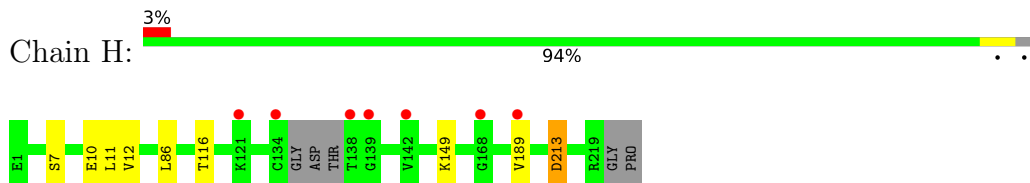
- Molecule 2: Isoform Beta-3C of Integrin beta-3



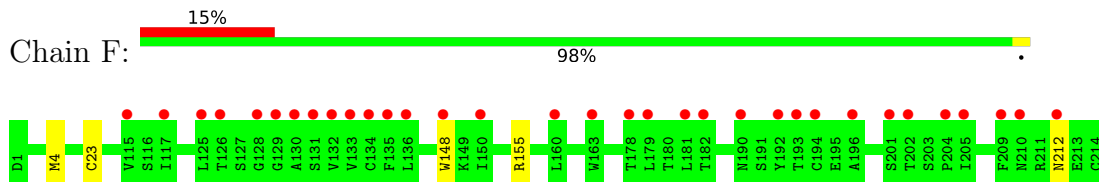
- Molecule 3: Monoclonal antibody 10E5 heavy chain



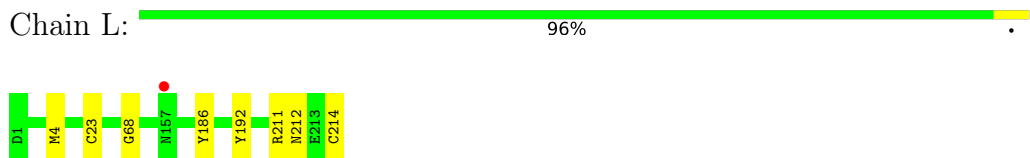
- Molecule 3: Monoclonal antibody 10E5 heavy chain



- Molecule 4: Monoclonal antibody 10E5 light chain



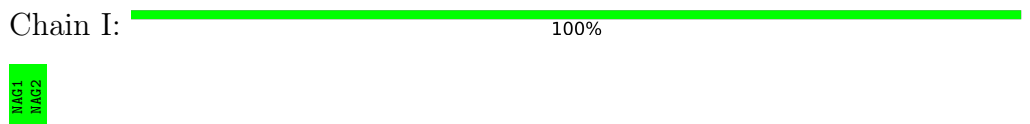
- Molecule 4: Monoclonal antibody 10E5 light chain



- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

Chain K:  50% 50%

MAG1
MAG2

- Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  25% 75%

MAG1
MAG2
EMA3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	257.50Å 144.68Å 104.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.22 – 2.35 49.22 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.22-2.35) 98.9 (49.22-2.35)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575, PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.204 , 0.245 0.205 , 0.246	Depositor DCC
R_{free} test set	2000 reflections (1.23%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	42834	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MG, CL, SO4, GOL, MAN, BMA, XQS, CA

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	0.15	0/3659	0.36	0/4986
1	C	0.14	0/3618	0.35	0/4930
2	B	0.15	0/3743	0.34	0/5074
2	D	0.15	0/3726	0.34	0/5052
3	E	0.13	0/1673	0.30	0/2290
3	H	0.13	0/1684	0.31	0/2305
4	F	0.12	0/1673	0.29	0/2269
4	L	0.12	0/1673	0.31	0/2269
All	All	0.14	0/21449	0.33	0/29175

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3532	3387	3371	9	0
1	C	3502	3338	3320	6	0
2	B	3634	3568	3531	13	0
2	D	3645	3561	3549	13	0
3	E	1631	1590	1590	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1642	1600	1600	5	0
4	F	1637	1553	1553	2	0
4	L	1637	1553	1553	4	0
5	G	61	57	52	0	0
6	I	28	27	25	0	0
6	K	28	27	25	1	0
7	J	50	47	43	0	0
8	A	15	0	0	0	0
8	C	15	0	0	0	0
8	L	5	0	0	0	0
9	A	6	8	8	0	0
10	A	4	0	0	0	0
10	B	2	0	0	0	0
10	C	4	0	0	0	0
10	D	2	0	0	0	0
11	B	1	0	0	0	0
11	D	1	0	0	0	0
12	B	14	14	13	0	0
12	D	14	14	13	0	0
13	B	27	24	0	1	0
13	C	27	24	0	1	0
14	C	2	0	0	0	0
15	A	474	0	0	5	0
15	B	245	0	0	2	0
15	C	265	0	0	2	0
15	D	193	0	0	3	0
15	E	13	0	0	0	0
15	F	11	0	0	0	0
15	H	35	0	0	3	0
15	L	40	0	0	0	0
All	All	22442	20392	20246	54	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 1.

All (54) 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)
15:H:324:HOH:O	4:L:214:CYS:SG	2.30	0.89
1:A:15[B]:ASN:ND2	15:A:601:HOH:O	2.21	0.69
1:C:208:ARG:O	15:C:602:HOH:O	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:SER:OG	15:C:601:HOH:O	2.12	0.65
3:H:149:LYS:NZ	15:H:302:HOH:O	2.33	0.61
2:D:129[A]:TRP:NE1	15:D:2104:HOH:O	2.34	0.60
3:H:10:GLU:O	15:H:301:HOH:O	2.16	0.60
1:A:48:GLU:OE2	1:A:90[B]:ARG:NH1	2.36	0.57
1:A:122:ALA:O	1:A:123:GLU:HB2	2.05	0.57
1:A:90[A]:ARG:NH2	15:A:616:HOH:O	2.38	0.56
2:D:125:LYS:NZ	15:D:2105:HOH:O	2.37	0.56
2:B:39:ASP:OD1	2:B:40:LEU:N	2.38	0.56
3:E:177:GLN:N	3:E:180:LEU:O	2.38	0.54
1:C:122:ALA:O	1:C:123:GLU:HB2	2.11	0.50
1:A:15[A]:ASN:ND2	15:A:622:HOH:O	2.44	0.49
2:B:125:LYS:NZ	15:B:2108:HOH:O	2.44	0.49
2:B:28:ASP:OD1	2:B:30:ALA:N	2.45	0.49
2:D:456:GLU:OE2	2:D:461:ARG:NH1	2.46	0.49
2:D:400:GLU:HB2	6:K:1:NAG:H83	1.95	0.49
1:C:2:ASN:N	1:C:2:ASN:OD1	2.47	0.48
2:B:404:ARG:NH1	15:B:2110:HOH:O	2.45	0.48
1:A:41:ARG:NH1	15:A:612:HOH:O	2.37	0.48
1:C:3:LEU:O	1:C:405:GLN:NE2	2.42	0.48
3:E:202:ASN:HA	3:E:213:ASP:HB3	1.96	0.47
4:L:4:MET:HE3	4:L:23:CYS:SG	2.55	0.47
2:D:126:ASP:OD1	2:D:126:ASP:N	2.48	0.47
2:D:239:ARG:O	2:D:244:HIS:NE2	2.44	0.46
2:D:178:TYR:CG	2:D:179:ASP:N	2.83	0.46
1:A:276:ARG:NH1	15:A:630:HOH:O	2.49	0.46
2:B:312:GLU:CD	2:D:125:LYS:HE2	2.41	0.46
1:C:107:CYS:HA	1:C:130:CYS:HA	1.99	0.45
3:E:213:ASP:OD1	3:E:213:ASP:N	2.50	0.45
3:H:12:VAL:HG21	3:H:86:LEU:HD13	1.99	0.45
2:B:456:GLU:OE2	2:B:461:ARG:NH1	2.50	0.45
2:D:150:ARG:NH1	15:D:2113:HOH:O	2.50	0.44
4:F:4:MET:HE3	4:F:23:CYS:SG	2.58	0.43
13:C:510:XQS:O03	2:D:121:SER:HB2	2.17	0.43
1:A:122:ALA:O	1:A:123:GLU:CB	2.67	0.43
2:B:121:SER:HB2	13:B:2005:XQS:O03	2.18	0.43
2:B:76:ASP:HB3	2:B:79:GLN:H	1.84	0.42
2:B:178:TYR:CG	2:B:179:ASP:N	2.87	0.42
2:B:202:ARG:NH2	2:B:206:GLU:OE2	2.52	0.42
2:D:150:ARG:HE	2:D:239:ARG:HD3	1.84	0.42
3:H:213:ASP:OD1	3:H:213:ASP:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:211:ARG:O	4:L:212:ASN:HB2	2.20	0.41
2:D:126:ASP:HA	2:D:129[A]:TRP:CE3	2.56	0.41
2:B:117:LEU:HD11	2:B:225:ALA:HB1	2.03	0.41
4:F:148:TRP:O	4:F:155:ARG:N	2.53	0.41
4:L:186:TYR:O	4:L:192:TYR:OH	2.34	0.41
2:B:114:ILE:O	2:B:151:ILE:HA	2.21	0.41
2:B:169:PRO:HD3	2:B:178:TYR:OH	2.20	0.41
2:D:202:ARG:NH2	2:D:206:GLU:OE2	2.50	0.41
1:A:107:CYS:HA	1:A:130:CYS:HA	2.02	0.40
3:H:11:LEU:HD12	3:H:116:THR:HB	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	462/457 (101%)	445 (96%)	16 (4%)	1 (0%)	43	50
1	C	457/457 (100%)	443 (97%)	13 (3%)	1 (0%)	43	50
2	B	474/472 (100%)	453 (96%)	18 (4%)	3 (1%)	21	22
2	D	472/472 (100%)	447 (95%)	24 (5%)	1 (0%)	43	50
3	E	210/221 (95%)	190 (90%)	18 (9%)	2 (1%)	12	11
3	H	212/221 (96%)	199 (94%)	12 (6%)	1 (0%)	24	26
4	F	212/214 (99%)	194 (92%)	17 (8%)	1 (0%)	24	26
4	L	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	24	26
All	All	2711/2728 (99%)	2574 (95%)	126 (5%)	11 (0%)	30	32

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
3	E	55	ASN
1	C	123	GLU
3	E	164	SER
2	B	76	ASP
2	B	375	LEU
4	F	212	ASN
4	L	68	GLY
3	H	189	VAL
2	B	157	VAL
2	D	157	VAL

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	371/364 (102%)	364 (98%)	7 (2%)	50	63
1	C	366/364 (100%)	358 (98%)	8 (2%)	45	58
2	B	422/417 (101%)	417 (99%)	5 (1%)	63	75
2	D	419/417 (100%)	416 (99%)	3 (1%)	76	84
3	E	186/190 (98%)	185 (100%)	1 (0%)	81	88
3	H	187/190 (98%)	185 (99%)	2 (1%)	65	77
4	F	188/188 (100%)	188 (100%)	0	100	100
4	L	188/188 (100%)	188 (100%)	0	100	100
All	All	2327/2318 (100%)	2301 (99%)	26 (1%)	65	77

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	61	GLU
1	A	166	TYR
1	A	195	LEU
1	A	217	SER

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Mol	Chain	Res	Type
1	A	270	LEU
1	A	288	TYR
2	B	37	ARG
2	B	182	THR
2	B	215	ASN
2	B	245	LEU
2	B	417	LYS
1	C	2	ASN
1	C	15	ASN
1	C	23	LEU
1	C	67	SER
1	C	166	TYR
1	C	195	LEU
1	C	272	SER
1	C	288	TYR
2	D	202	ARG
2	D	215	ASN
2	D	365	GLU
3	E	154	GLU
3	H	7	SER
3	H	213	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
2	B	141	GLN
2	B	272	GLN
2	B	301	GLN
2	B	305	ASN
1	C	158	ASN
1	C	215	HIS
1	C	444	GLN
2	D	82	GLN
2	D	210	GLN
2	D	408	GLN
2	D	440	GLN
4	F	138	ASN
4	L	93	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 ⓘ

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	$\# Z > 2$
5	NAG	G	1	5,2	14,14,15	0.39	0	17,19,21	0.50	0
5	NAG	G	2	5	14,14,15	0.41	0	17,19,21	0.60	0
5	BMA	G	3	5	11,11,12	0.87	0	15,15,17	0.75	0
5	MAN	G	4	5	11,11,12	0.62	0	15,15,17	1.15	2 (13%)
5	MAN	G	5	5	11,11,12	0.79	0	15,15,17	1.10	2 (13%)
6	NAG	I	1	6,2	14,14,15	0.48	0	17,19,21	0.48	0
6	NAG	I	2	6	14,14,15	0.14	0	17,19,21	0.60	0
7	NAG	J	1	7,2	14,14,15	0.16	0	17,19,21	0.58	0
7	NAG	J	2	7	14,14,15	0.62	1 (7%)	17,19,21	0.54	0
7	BMA	J	3	7	11,11,12	0.70	0	15,15,17	0.78	1 (6%)
7	MAN	J	4	7	11,11,12	0.71	0	15,15,17	0.95	1 (6%)
6	NAG	K	1	6,2	14,14,15	0.53	0	17,19,21	0.44	0
6	NAG	K	2	6	14,14,15	0.17	0	17,19,21	0.64	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
5	NAG	G	1	5,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	0/1/1/1
5	MAN	G	5	5	-	1/2/19/22	0/1/1/1
6	NAG	I	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	3/6/23/26	0/1/1/1
7	NAG	J	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	0/6/23/26	0/1/1/1
7	BMA	J	3	7	-	0/2/19/22	0/1/1/1
7	MAN	J	4	7	-	0/2/19/22	0/1/1/1
6	NAG	K	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	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)
7	J	2	NAG	O5-C1	-2.17	1.40	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	4	MAN	C1-O5-C5	3.37	116.70	112.19
5	G	5	MAN	C1-O5-C5	2.72	115.83	112.19
7	J	4	MAN	C1-O5-C5	2.52	115.56	112.19
5	G	5	MAN	O2-C2-C3	-2.21	105.58	110.15
5	G	4	MAN	O2-C2-C3	-2.10	105.81	110.15
7	J	3	BMA	O2-C2-C3	-2.01	105.99	110.15

There are no chirality outliers.

All (7) torsion outliers are listed below:

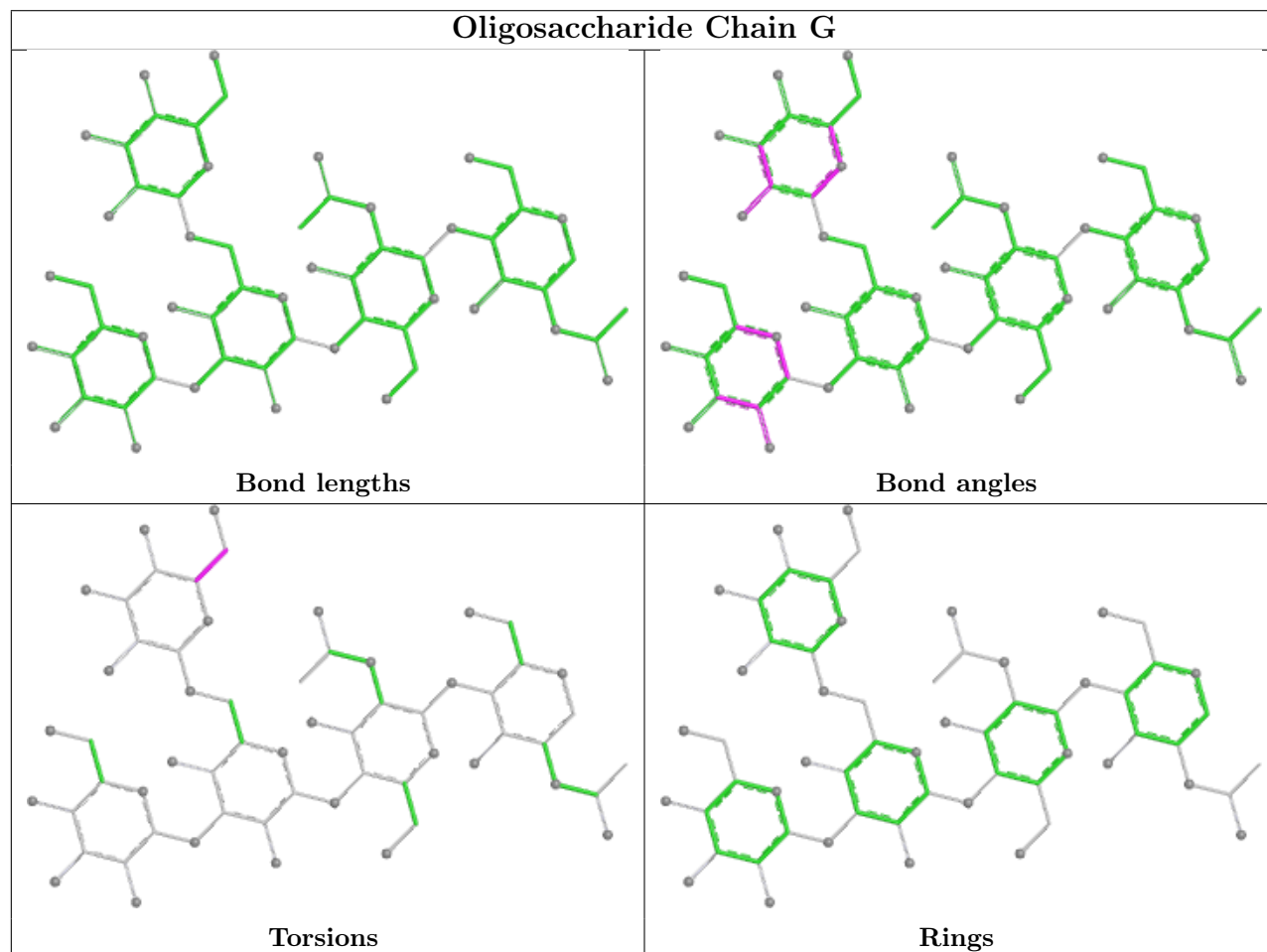
Mol	Chain	Res	Type	Atoms
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
6	K	2	NAG	C8-C7-N2-C2
6	K	2	NAG	O7-C7-N2-C2
6	I	2	NAG	O5-C5-C6-O6
5	G	5	MAN	O5-C5-C6-O6
6	K	2	NAG	C1-C2-N2-C7

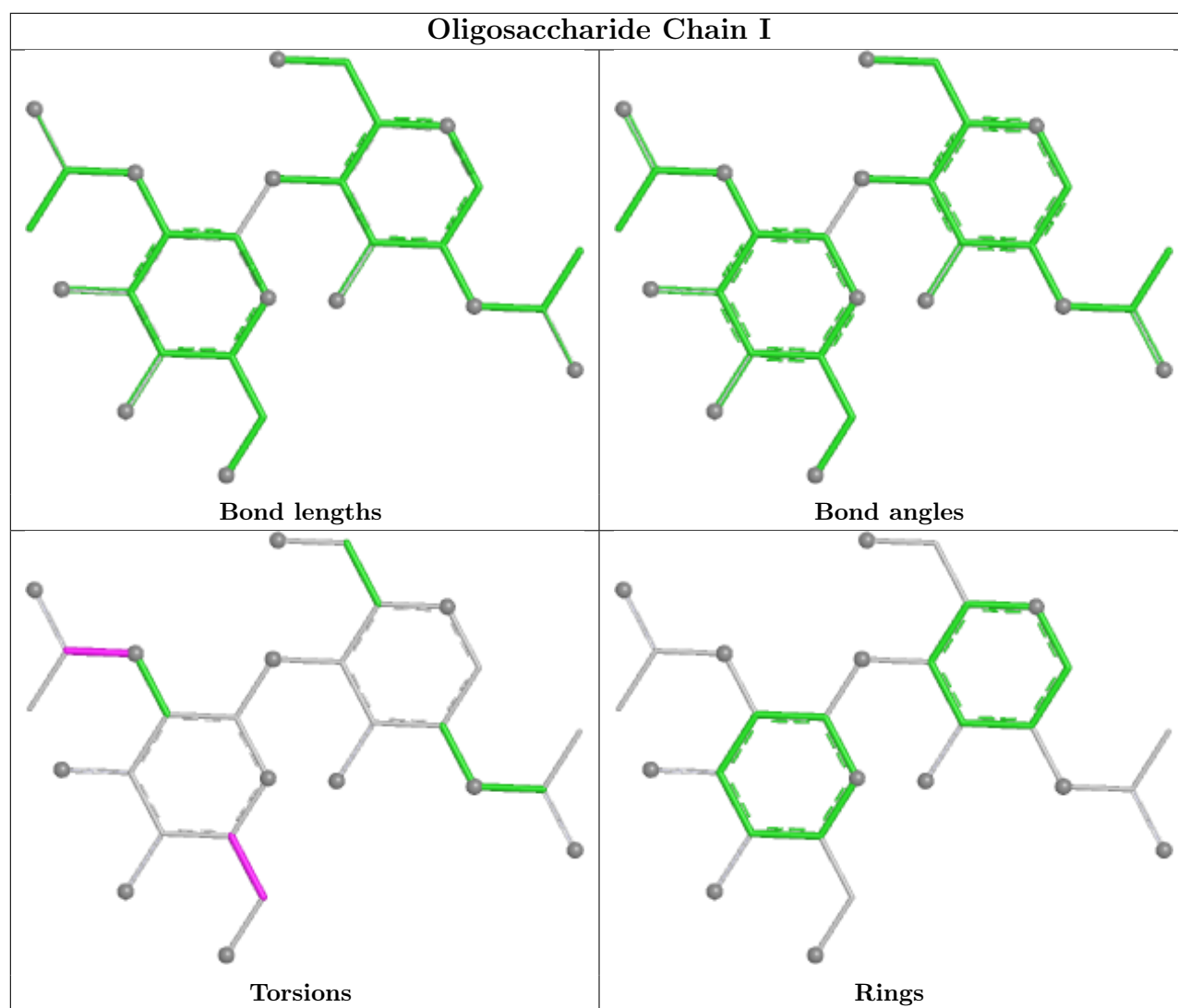
There are no ring outliers.

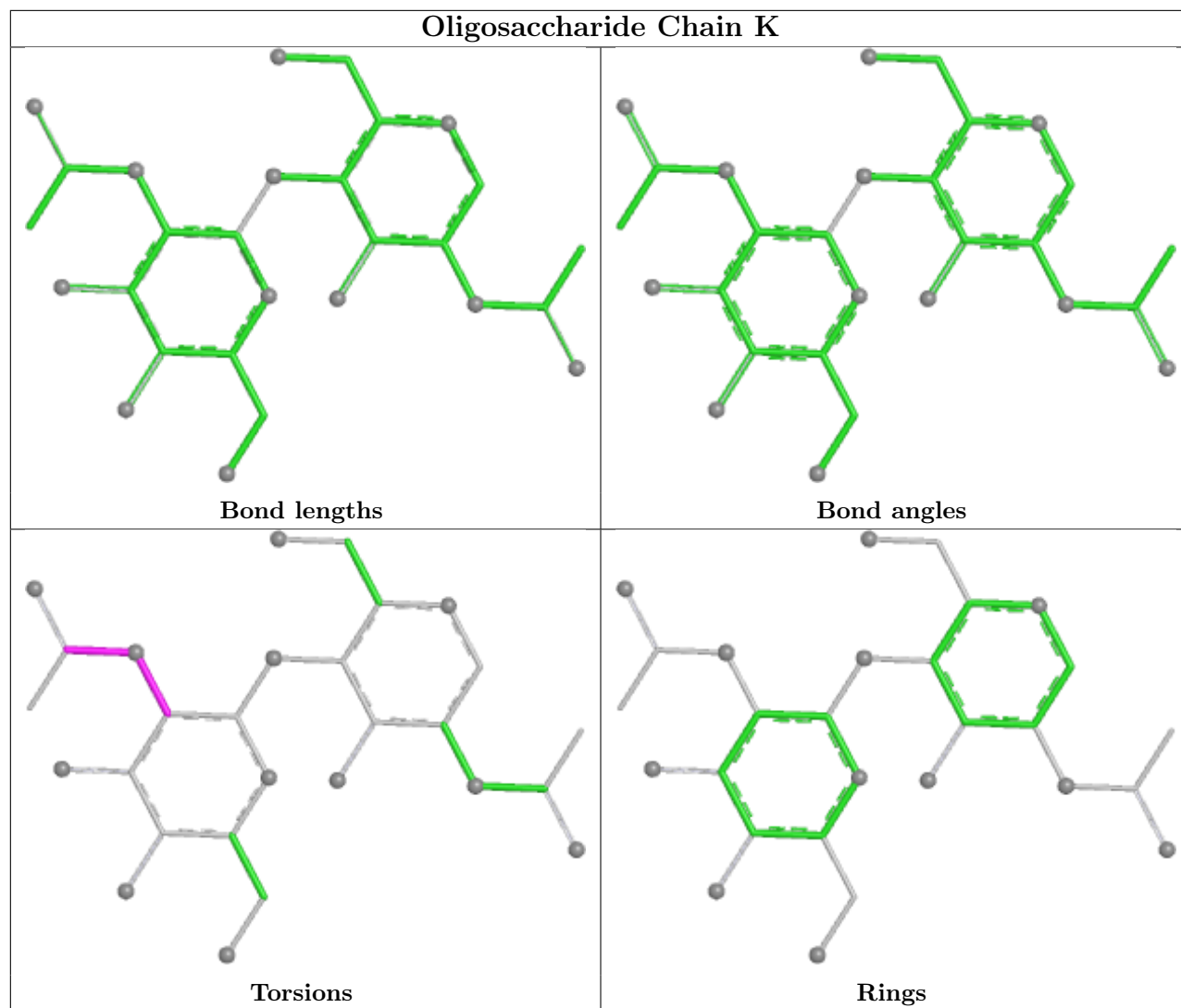
1 monomer is involved in 1 short contact:

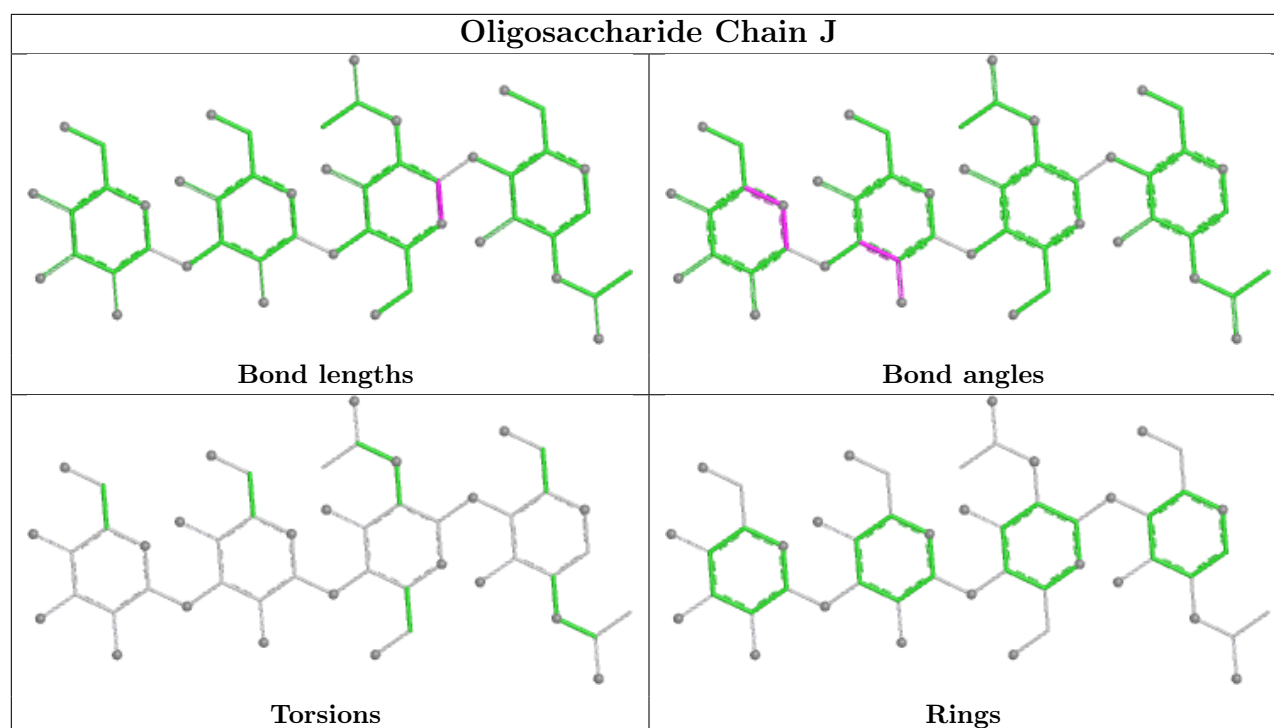
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	1	NAG	1	0

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](#)

Of 28 ligands modelled in this entry, 16 are monoatomic - leaving 12 for Mogul analysis.

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	$\# Z > 2$
9	GOL	A	504	-	5,5,5	0.32	0	5,5,5	0.27	0
8	SO4	C	501	-	4,4,4	0.34	0	6,6,6	0.21	0
8	SO4	L	301	-	4,4,4	0.33	0	6,6,6	0.12	0
12	NAG	D	2004	2	14,14,15	0.42	0	17,19,21	0.58	0
13	XQS	B	2005	11	28,28,28	0.80	0	33,38,38	1.97	6 (18%)
8	SO4	A	502	-	4,4,4	0.34	0	6,6,6	0.32	0
8	SO4	A	503	-	4,4,4	0.28	0	6,6,6	0.17	0
8	SO4	C	503	-	4,4,4	0.30	0	6,6,6	0.24	0
12	NAG	B	2004	2	14,14,15	0.45	0	17,19,21	0.58	0
8	SO4	A	501	-	4,4,4	0.38	0	6,6,6	0.26	0
13	XQS	C	510	11	28,28,28	0.82	0	33,38,38	1.90	7 (21%)
8	SO4	C	502	-	4,4,4	0.35	0	6,6,6	0.21	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
9	GOL	A	504	-	-	2/4/4/4	-
12	NAG	D	2004	2	-	0/6/23/26	0/1/1/1
13	XQS	B	2005	11	-	4/25/35/35	0/2/2/2
12	NAG	B	2004	2	-	0/6/23/26	0/1/1/1
13	XQS	C	510	11	-	4/25/35/35	0/2/2/2

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	2005	XQS	C13-C11-C10	-7.29	102.43	110.32
13	C	510	XQS	C13-C11-C10	-7.20	102.53	110.32
13	B	2005	XQS	C14-C12-C10	-4.16	105.82	110.32
13	B	2005	XQS	C11-C13-N06	-3.45	103.91	110.66
13	C	510	XQS	C11-C13-N06	-3.26	104.27	110.66
13	C	510	XQS	C14-N06-C13	3.10	119.02	112.68
13	C	510	XQS	C14-C12-C10	-2.75	107.34	110.32
13	B	2005	XQS	O01-C10-C12	2.64	118.08	109.22
13	B	2005	XQS	C14-N06-C13	2.56	117.91	112.68
13	C	510	XQS	O01-C10-C12	2.41	117.31	109.22
13	C	510	XQS	O02-C15-N06	2.30	124.35	121.61
13	B	2005	XQS	O02-C15-N06	2.07	124.08	121.61
13	C	510	XQS	C21-C19-N07	-2.02	113.29	117.04

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	504	GOL	O1-C1-C2-C3
13	C	510	XQS	O01-C17-C20-O05
9	A	504	GOL	O1-C1-C2-O2
13	C	510	XQS	O01-C17-C20-O03
13	B	2005	XQS	C12-C10-O01-C17
13	C	510	XQS	C11-C10-O01-C17
13	C	510	XQS	C12-C10-O01-C17
13	B	2005	XQS	O01-C17-C20-O03
13	B	2005	XQS	O01-C17-C20-O05

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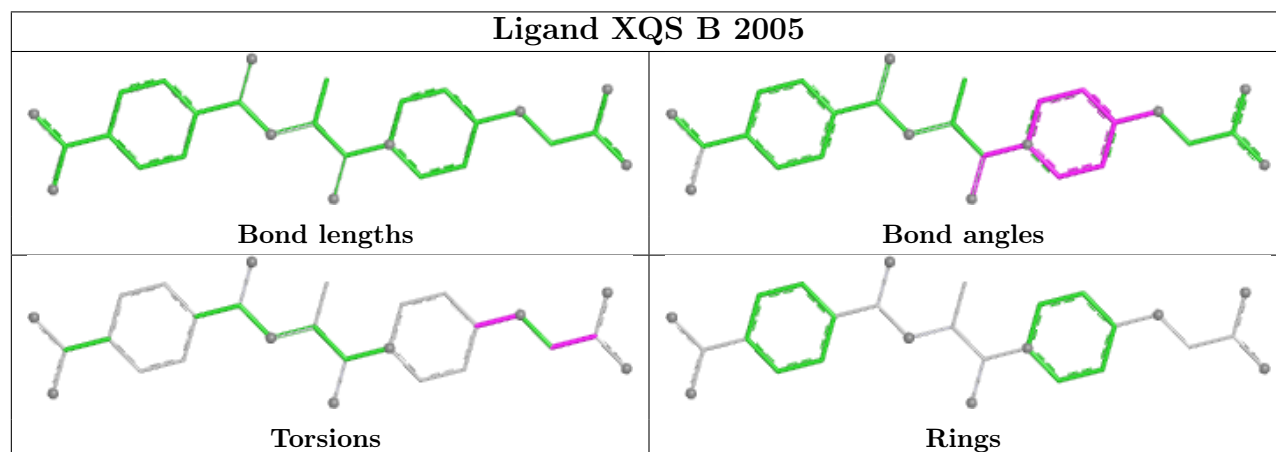
Mol	Chain	Res	Type	Atoms
13	B	2005	XQS	C11-C10-O01-C17

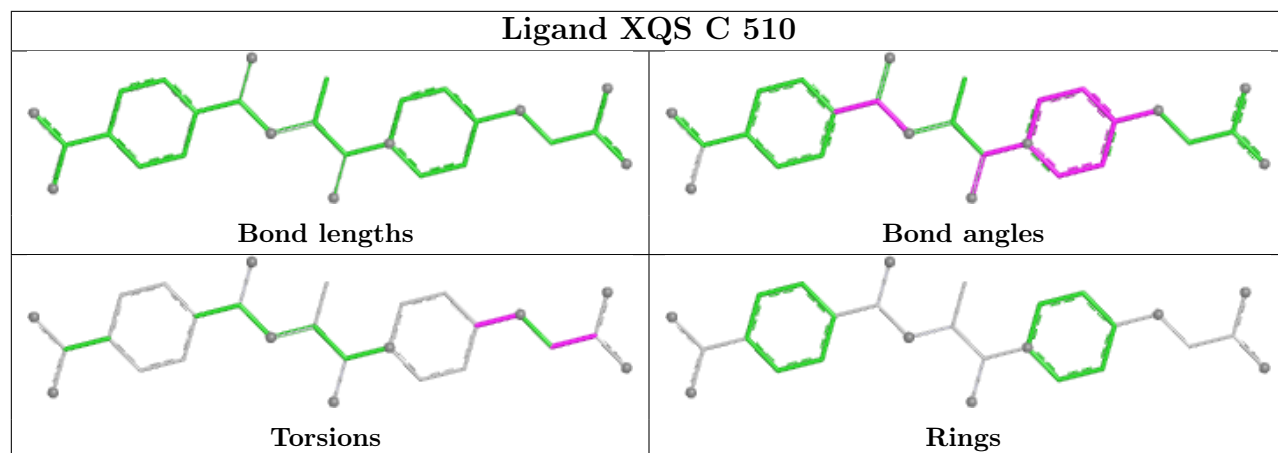
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	2005	XQS	1	0
13	C	510	XQS	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	454/457 (99%)	-0.43	4 (0%) 81 84	23, 43, 68, 111	8 (1%)
1	C	453/457 (99%)	-0.18	6 (1%) 75 79	22, 57, 85, 113	4 (0%)
2	B	466/472 (98%)	0.15	19 (4%) 41 47	19, 69, 136, 173	7 (1%)
2	D	471/472 (99%)	0.29	20 (4%) 40 46	28, 77, 133, 159	3 (0%)
3	E	214/221 (96%)	1.23	40 (18%) 3 3	61, 122, 186, 203	0
3	H	216/221 (97%)	0.70	7 (3%) 50 57	45, 97, 144, 163	0
4	F	214/214 (100%)	0.98	33 (15%) 5 5	67, 116, 174, 188	0
4	L	214/214 (100%)	0.32	1 (0%) 87 89	54, 86, 112, 143	0
All	All	2702/2728 (99%)	0.23	130 (4%) 35 42	19, 72, 151, 203	22 (0%)

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	LEU	5.8
1	A	454	VAL	5.7
3	E	165	LEU	5.3
3	E	212	VAL	5.1
1	C	453	VAL	4.4
3	E	133	VAL	4.3
3	E	147	LEU	4.0
3	E	189	VAL	4.0
2	D	471	CYS	4.0
2	B	33	LEU	3.9
2	B	446	HIS	3.9
2	D	466	TRP	3.9
2	D	467	LEU	3.9
2	B	375	LEU	3.8
4	F	178	THR	3.7
2	D	4	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	375	LEU	3.6
2	B	466	TRP	3.6
4	F	115	VAL	3.6
2	B	137[A]	LYS	3.5
2	B	132[A]	GLN	3.5
3	E	201	CYS	3.4
3	E	11	LEU	3.4
2	D	446	HIS	3.3
4	F	204	PRO	3.3
4	F	179	LEU	3.3
1	C	2	ASN	3.3
2	D	33	LEU	3.3
4	F	160	LEU	3.3
3	E	160	TRP	3.2
4	F	181	LEU	3.2
3	E	199	ILE	3.2
3	E	214	LYS	3.1
4	F	209	PHE	3.1
1	A	217	SER	3.1
4	F	125	LEU	3.1
4	F	202	THR	3.1
3	E	203	VAL	3.1
3	E	204	ALA	3.1
2	D	2	PRO	3.0
3	E	216	ILE	3.0
4	F	192	TYR	3.0
3	E	163	GLY	2.9
2	B	129	TRP	2.9
2	B	436	ALA	2.9
4	F	128	GLY	2.9
4	F	205	ILE	2.9
2	B	450	ASN	2.8
3	E	206	PRO	2.8
2	D	380	ILE	2.8
2	B	465	GLY	2.7
3	H	168	GLY	2.7
4	F	130	ALA	2.7
4	F	117	ILE	2.7
2	B	77	SER	2.7
3	E	127	VAL	2.6
3	E	210	THR	2.6
4	F	182	THR	2.6

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Mol	Chain	Res	Type	RSRZ
3	E	128	TYR	2.6
4	F	210	ASN	2.6
4	F	133	VAL	2.6
3	E	140	SER	2.6
2	D	181	LYS	2.6
1	C	339	ALA	2.6
1	A	45	PRO	2.6
4	F	150	ILE	2.6
3	E	158	LEU	2.5
1	A	339	ALA	2.5
3	E	196	SER	2.5
4	F	132	VAL	2.5
3	E	92	ALA	2.5
3	H	121	LYS	2.5
4	F	134	CYS	2.5
2	B	440	GLN	2.5
4	F	148	TRP	2.5
2	D	75	GLY	2.5
3	E	176	LEU	2.4
2	B	30	ALA	2.4
3	E	207	ALA	2.4
3	H	139	GLY	2.4
3	H	138	THR	2.4
3	H	134	CYS	2.4
2	B	58	VAL	2.4
2	D	452	ASN	2.4
4	F	212	ASN	2.4
2	D	468	GLY	2.4
2	D	129[A]	TRP	2.4
3	E	195	PRO	2.4
3	E	168	GLY	2.4
4	F	193	THR	2.4
4	F	129	GLY	2.3
3	E	188	THR	2.3
2	D	469	SER	2.3
3	E	144	LEU	2.3
2	B	2	PRO	2.3
4	F	196	ALA	2.3
2	B	452	ASN	2.3
4	F	201	SER	2.3
4	F	126	THR	2.3
3	E	183	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	E	187	VAL	2.3
1	C	46	SER	2.2
1	C	217	SER	2.2
4	F	131	SER	2.2
3	E	4	LEU	2.2
2	B	455	PHE	2.2
4	F	135	PHE	2.2
3	E	134	CYS	2.2
2	D	1	GLY	2.2
3	E	130	LEU	2.2
4	F	136	LEU	2.2
2	D	450	ASN	2.2
4	L	157	ASN	2.2
3	E	190	THR	2.2
4	F	163	TRP	2.2
2	D	143	ARG	2.2
3	E	175	VAL	2.2
4	F	194	CYS	2.2
3	E	198	SER	2.1
2	D	178	TYR	2.1
3	H	189	VAL	2.1
2	B	1	GLY	2.1
2	B	181	LYS	2.1
4	F	190	ASN	2.1
3	H	142	VAL	2.1
3	E	193	THR	2.0
3	E	174	ALA	2.0
2	D	35	SER	2.0
3	E	29	ILE	2.0
3	E	129	PRO	2.0

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

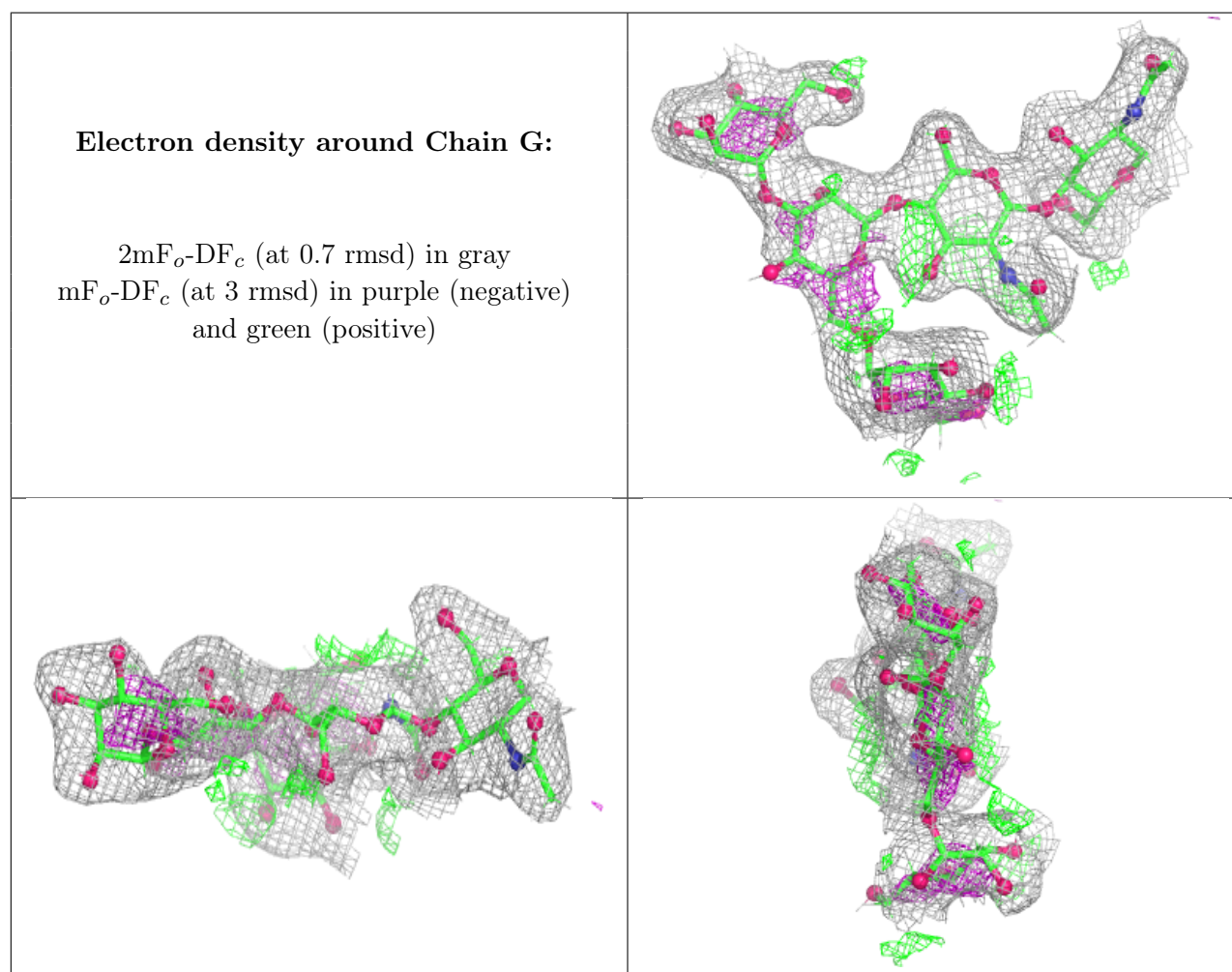
There are no non-standard protein/DNA/RNA residues in this entry.

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.

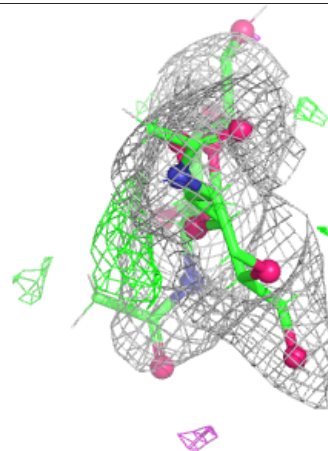
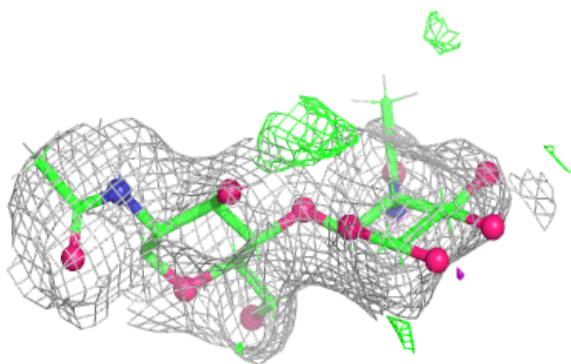
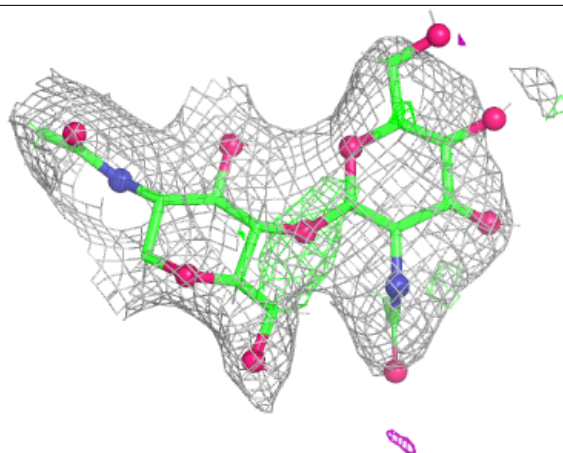
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	G	1	14/15	-	-	40,57,71,85	0
5	NAG	G	2	14/15	-	-	56,74,101,103	0
5	BMA	G	3	11/12	-	-	57,85,105,106	0
5	MAN	G	4	11/12	-	-	51,77,94,106	0
5	MAN	G	5	11/12	-	-	71,88,113,113	0
7	NAG	J	2	14/15	0.66	0.14	53,74,114,117	0
6	NAG	K	2	14/15	0.81	0.12	70,92,110,121	0
7	NAG	J	1	14/15	0.82	0.10	46,58,82,83	0
6	NAG	I	2	14/15	0.85	0.12	70,94,106,128	0
6	NAG	K	1	14/15	0.93	0.08	67,82,95,105	0
6	NAG	I	1	14/15	0.94	0.07	62,79,93,95	0
7	BMA	J	3	11/12	-	-	73,94,102,117	0
7	MAN	J	4	11/12	-	-	58,92,110,111	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.



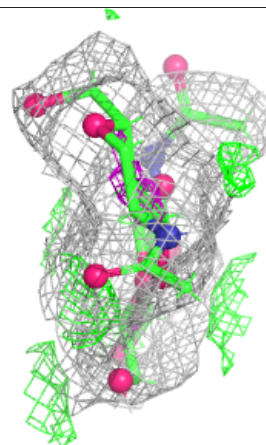
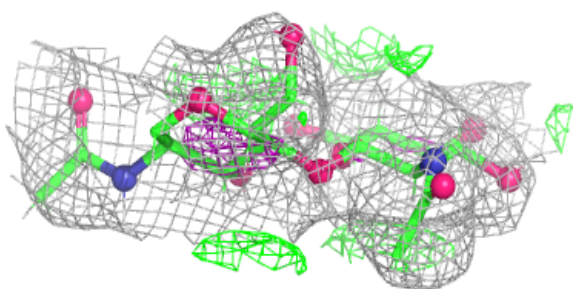
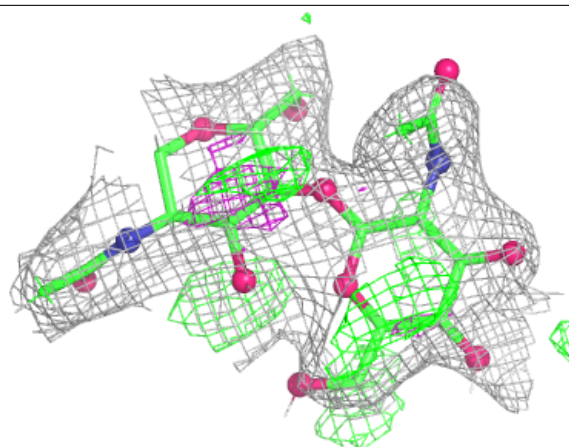
Electron density around Chain I:

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

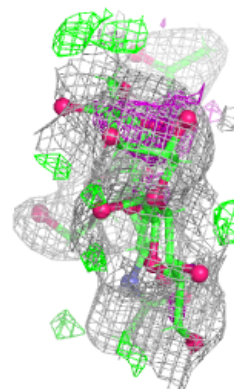
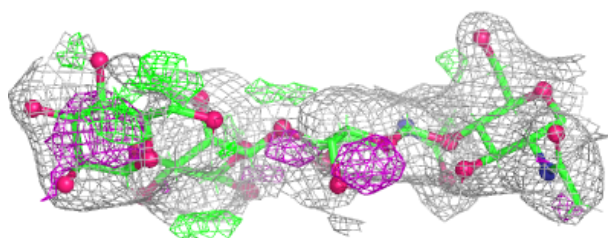
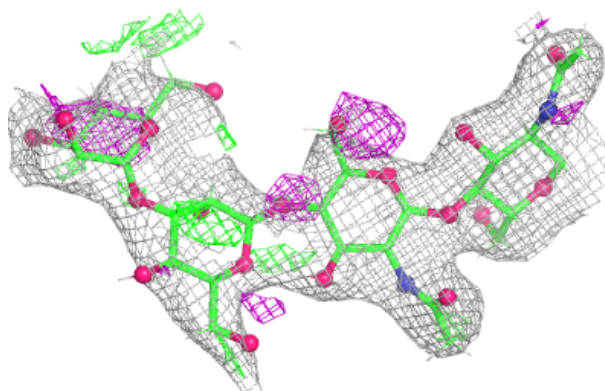


Electron density around Chain K:

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

**Electron density around Chain J:**

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



6.4 Ligands ⓘ

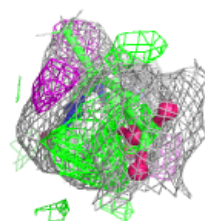
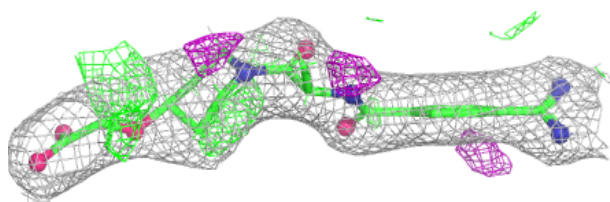
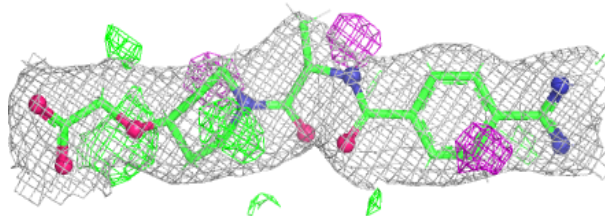
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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
12	NAG	B	2004	14/15	0.60	0.16	75,90,111,118	0
12	NAG	D	2004	14/15	0.67	0.14	64,80,103,121	0
14	CL	C	505	1/1	0.79	0.27	136,136,136,136	0
8	SO4	C	502	5/5	0.85	0.12	70,78,102,172	0
9	GOL	A	504	6/6	0.86	0.15	31,71,87,92	0
8	SO4	L	301	5/5	0.87	0.09	66,70,77,146	0
13	XQS	C	510	27/27	0.91	0.10	30,47,76,79	0
8	SO4	C	501	5/5	0.91	0.11	57,74,88,168	0
8	SO4	A	502	5/5	0.92	0.13	51,54,88,128	0
8	SO4	A	501	5/5	0.93	0.13	58,84,105,171	0
8	SO4	C	503	5/5	0.93	0.08	60,74,79,139	0
13	XQS	B	2005	27/27	0.94	0.09	30,39,69,77	0
14	CL	C	504	1/1	0.95	0.31	101,101,101,101	0
8	SO4	A	503	5/5	0.97	0.05	51,58,64,66	0
10	CA	C	506	1/1	0.98	0.09	108,108,108,108	0
10	CA	D	2002	1/1	0.98	0.05	48,48,48,48	0
10	CA	A	507	1/1	0.98	0.03	30,30,30,30	0
10	CA	A	508	1/1	0.98	0.03	30,30,30,30	0
10	CA	A	506	1/1	0.99	0.03	30,30,30,30	0
10	CA	D	2003	1/1	0.99	0.04	43,43,43,43	0
11	MG	B	2001	1/1	0.99	0.13	30,30,30,30	0
11	MG	D	2001	1/1	0.99	0.04	30,30,30,30	0
10	CA	B	2002	1/1	0.99	0.04	67,67,67,67	0
10	CA	B	2003	1/1	0.99	0.02	30,30,30,30	0
10	CA	A	505	1/1	0.99	0.04	57,57,57,57	0
10	CA	C	507	1/1	0.99	0.02	54,54,54,54	0
10	CA	C	508	1/1	0.99	0.03	47,47,47,47	0
10	CA	C	509	1/1	0.99	0.02	47,47,47,47	0

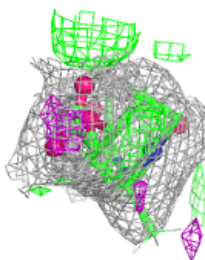
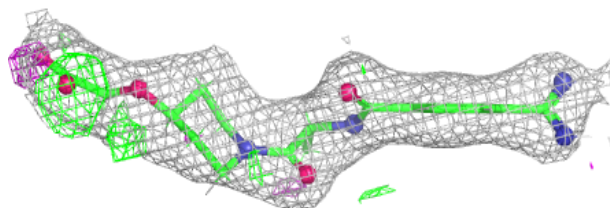
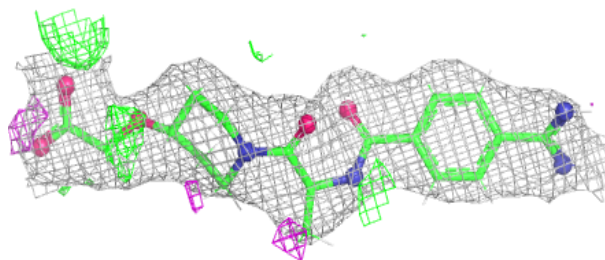
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around XQS C 510:

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

**Electron density around XQS B 2005:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.