



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:25 AM UTC

PDB ID : 8TTZ / pdb_00008ttz
Title : Crystal structure of monkey TLR7 ectodomain with compound 20
Authors : Critton, D.A.
Deposited on : 2023-08-15
Resolution : 3.14 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

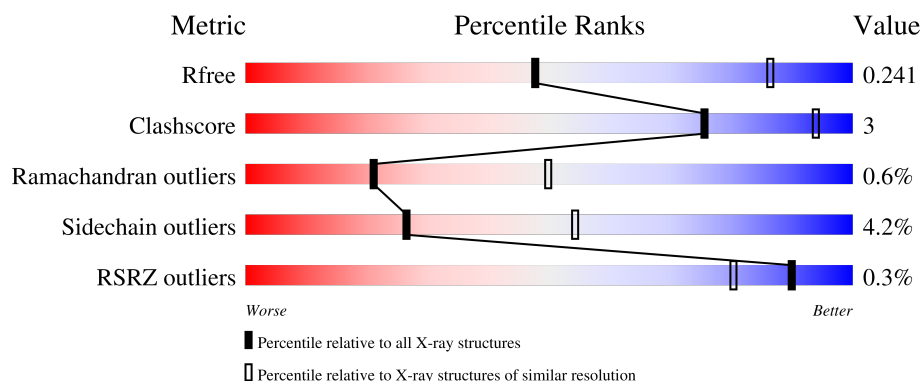
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

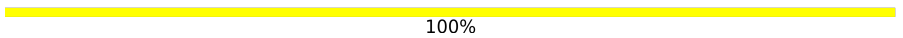
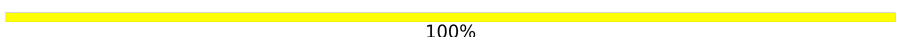
The reported resolution of this entry is 3.14 Å.

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	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)

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	817	
1	B	817	
2	C	2	
2	D	2	
2	E	2	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13077 atoms, of which 74 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 Toll-like receptor 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	772	Total	C	N	O	S	0	1	0
			6258	4010	1066	1152	30			
1	B	772	Total	C	N	O	S	0	3	0
			6272	4017	1068	1157	30			

There are 16 discrepancies between the modelled and reference sequences:

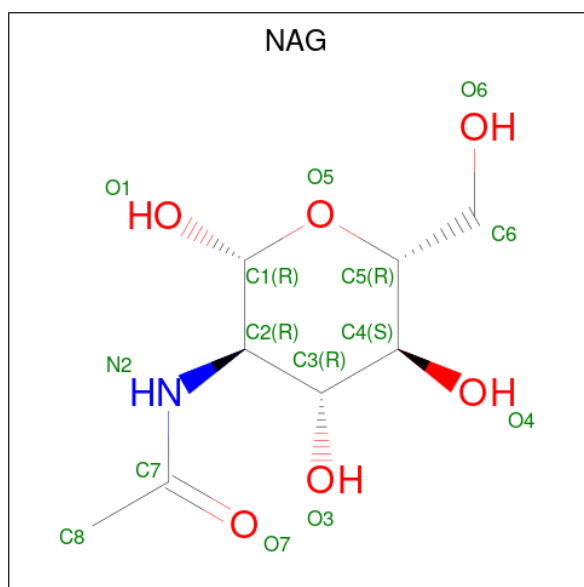
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	expression tag	UNP G8E2R2
A	24	SER	-	expression tag	UNP G8E2R2
A	25	PRO	-	expression tag	UNP G8E2R2
A	26	TRP	-	expression tag	UNP G8E2R2
A	167	GLN	ASN	conflict	UNP G8E2R2
A	389	GLN	ASN	conflict	UNP G8E2R2
A	488	GLN	ASN	conflict	UNP G8E2R2
A	799	GLN	ASN	conflict	UNP G8E2R2
B	23	ARG	-	expression tag	UNP G8E2R2
B	24	SER	-	expression tag	UNP G8E2R2
B	25	PRO	-	expression tag	UNP G8E2R2
B	26	TRP	-	expression tag	UNP G8E2R2
B	167	GLN	ASN	conflict	UNP G8E2R2
B	389	GLN	ASN	conflict	UNP G8E2R2
B	488	GLN	ASN	conflict	UNP G8E2R2
B	799	GLN	ASN	conflict	UNP G8E2R2

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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



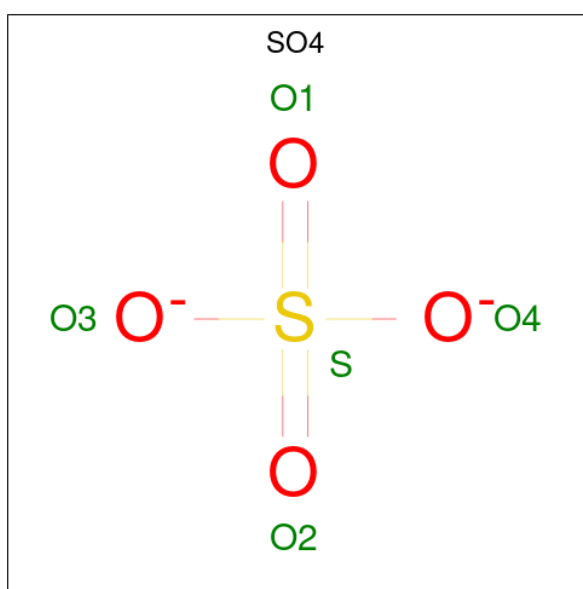
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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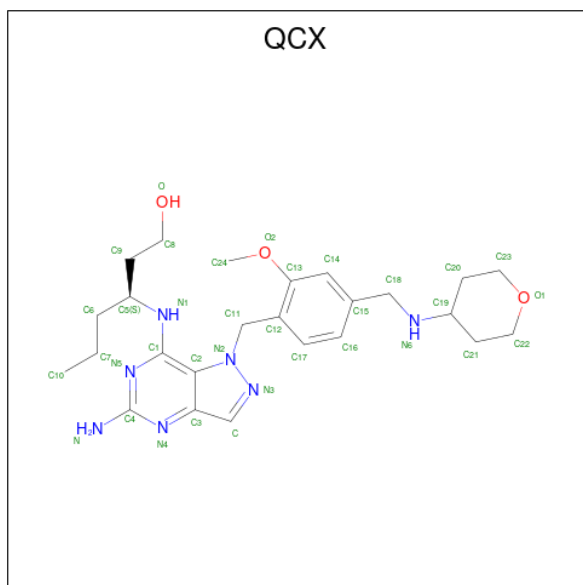
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total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

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

- Molecule 5 is (3S)-3-({5-amino-1-[(2-methoxy-4-[(oxan-4-yl)amino]methyl}phenyl)methyl]-1H-pyrazolo[4,3-d]pyrimidin-7-yl}amino)hexan-1-ol (CCD ID: QCX) (formula: C₂₅H₃₇N₇O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			72	25	37	7	3		
5	B	1	Total	C	H	N	O	0	0
			72	25	37	7	3		

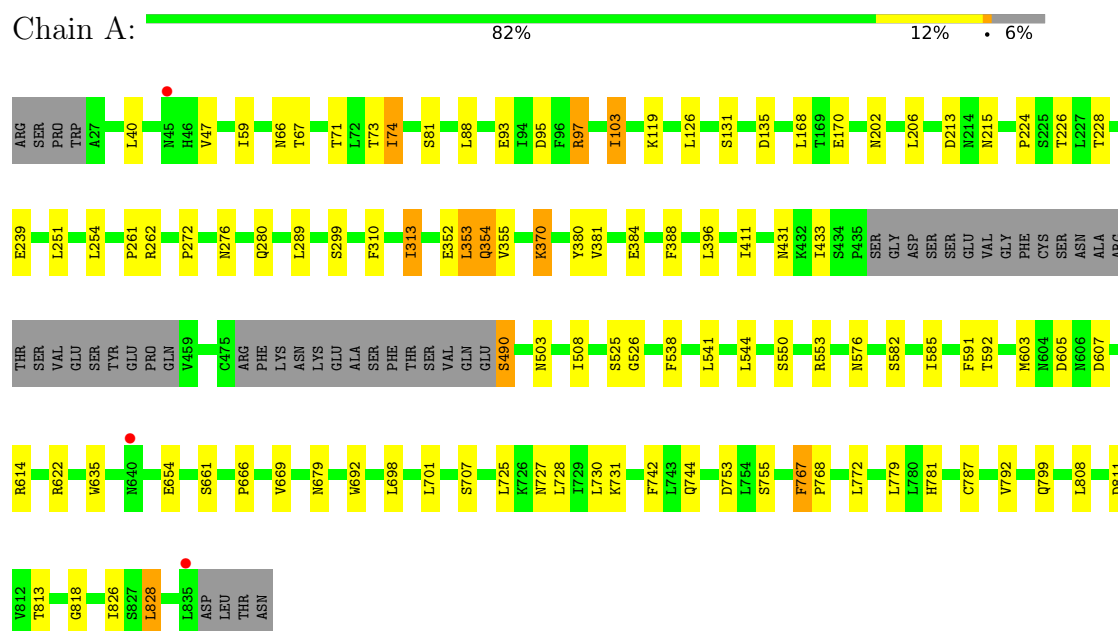
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total	O	0	0
			5	5		
6	B	1	Total	O	0	0
			1	1		

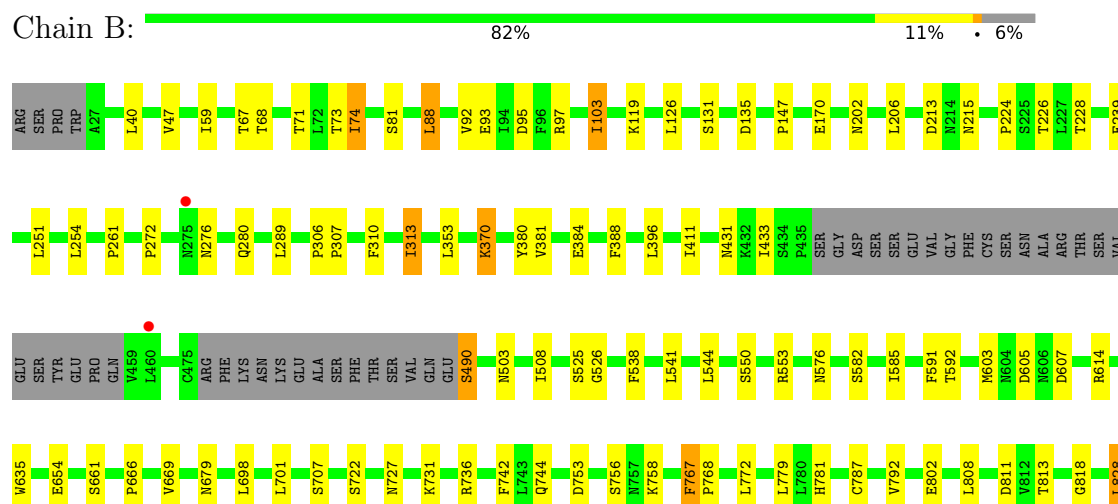
3 Residue-property plots

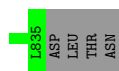
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Toll-like receptor 7



• Molecule 1: Toll-like receptor 7





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

Chain C:  100%



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

Chain D:  50% 50%



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

Chain E:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.81Å 138.69Å 148.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.80 – 3.14 41.80 – 3.14	Depositor EDS
% Data completeness (in resolution range)	92.9 (41.80-3.14) 93.1 (41.80-3.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.194 , 0.241 (Not available) , 0.241	Depositor DCC
R_{free} test set	1633 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	68.2	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13077	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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: QCX, NAG, SO4

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	0.76	0/6389	1.21	20/8657 (0.2%)
1	B	0.76	0/6403	1.21	20/8676 (0.2%)
All	All	0.76	0/12792	1.21	40/17333 (0.2%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	TYR	N-CA-C	-7.21	103.46	112.90
1	B	380	TYR	N-CA-C	-6.83	103.28	111.69
1	B	576	ASN	CA-C-N	6.57	129.74	120.28
1	B	576	ASN	C-N-CA	6.57	129.74	120.28
1	A	490	SER	CA-C-N	6.54	131.06	120.60
1	A	490	SER	C-N-CA	6.54	131.06	120.60
1	B	490	SER	CA-C-N	6.51	131.02	120.60
1	B	490	SER	C-N-CA	6.51	131.02	120.60
1	A	576	ASN	CA-C-N	6.35	129.42	120.28
1	A	576	ASN	C-N-CA	6.35	129.42	120.28
1	A	126	LEU	CA-C-N	6.14	128.80	120.38
1	A	126	LEU	C-N-CA	6.14	128.80	120.38
1	B	126	LEU	CA-C-N	6.14	128.79	120.38
1	B	126	LEU	C-N-CA	6.14	128.79	120.38
1	A	767	PHE	CA-CB-CG	5.84	119.64	113.80
1	B	591	PHE	CA-C-N	5.56	128.29	120.28
1	B	591	PHE	C-N-CA	5.56	128.29	120.28
1	A	591	PHE	CA-C-N	5.56	128.29	120.28
1	A	591	PHE	C-N-CA	5.56	128.29	120.28
1	A	396	LEU	CA-C-N	5.43	127.82	120.38
1	A	396	LEU	C-N-CA	5.43	127.82	120.38
1	B	396	LEU	CA-C-N	5.42	127.81	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	396	LEU	C-N-CA	5.42	127.81	120.38
1	A	215	ASN	CA-CB-CG	5.26	117.86	112.60
1	A	592	THR	CA-C-N	5.23	127.28	120.28
1	A	592	THR	C-N-CA	5.23	127.28	120.28
1	A	276	ASN	CA-C-N	5.22	128.08	120.51
1	A	276	ASN	C-N-CA	5.22	128.08	120.51
1	B	592	THR	CA-C-N	5.18	127.22	120.28
1	B	592	THR	C-N-CA	5.18	127.22	120.28
1	B	276	ASN	CA-C-N	5.17	128.00	120.51
1	B	276	ASN	C-N-CA	5.17	128.00	120.51
1	A	742	PHE	CA-CB-CG	5.09	118.89	113.80
1	B	802	GLU	CA-C-N	5.08	128.10	120.69
1	B	802	GLU	C-N-CA	5.08	128.10	120.69
1	B	767	PHE	CA-CB-CG	5.04	118.84	113.80
1	B	147	PRO	N-CA-C	5.02	115.29	110.47
1	B	215	ASN	CA-CB-CG	5.02	117.62	112.60
1	A	97	ARG	CA-C-N	5.02	129.54	122.46
1	A	97	ARG	C-N-CA	5.02	129.54	122.46

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	6258	0	6301	41	0
1	B	6272	0	6309	38	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
3	A	98	0	91	0	0
3	B	70	0	65	0	0
4	A	95	0	0	0	0
4	B	50	0	0	0	0
5	A	35	37	0	1	0
5	B	35	37	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	5	0	0	0	0
6	B	1	0	0	0	0
All	All	13003	74	12841	77	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 3.

All (77) 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:781:HIS:HB2	1:A:811:ASP:HB3	1.65	0.78
1:B:781:HIS:HB2	1:B:811:ASP:HB3	1.66	0.76
1:A:767:PHE:HB3	1:A:772:LEU:HD11	1.73	0.70
1:B:767:PHE:HB3	1:B:772:LEU:HD11	1.75	0.68
1:B:73:THR:HG22	1:B:74:ILE:HG13	1.82	0.62
1:A:73:THR:HG22	1:A:74:ILE:HG13	1.82	0.62
1:B:261:PRO:HD2	1:B:272:PRO:HA	1.84	0.60
1:A:384:GLU:HG3	1:A:411:ILE:HB	1.84	0.60
1:B:384:GLU:HG3	1:B:411:ILE:HB	1.85	0.59
1:B:433:ILE:H	1:B:503:ASN:HD22	1.51	0.57
1:A:261:PRO:HD2	1:A:272:PRO:HA	1.85	0.57
1:B:753:ASP:HA	1:B:779:LEU:HB2	1.86	0.57
1:A:433:ILE:H	1:A:503:ASN:HD22	1.52	0.56
1:A:753:ASP:HA	1:A:779:LEU:HB2	1.86	0.56
1:B:736:ARG:HG2	1:B:758:LYS:HB2	1.87	0.56
1:B:97:ARG:HG2	1:B:135:ASP:HB2	1.87	0.56
1:A:352:GLU:HG3	1:A:355:VAL:HB	1.88	0.56
1:A:239:GLU:HG2	1:A:280:GLN:HB2	1.89	0.55
1:B:698:LEU:HD23	1:B:701:LEU:HD13	1.90	0.54
1:A:97:ARG:HG2	1:A:135:ASP:HB2	1.89	0.54
1:B:93:GLU:HG3	1:B:131:SER:HB2	1.89	0.54
1:B:635:TRP:HB3	1:B:666:PRO:HG2	1.90	0.53
1:B:239:GLU:HG2	1:B:280:GLN:HB2	1.90	0.53
1:A:635:TRP:HB3	1:A:666:PRO:HG2	1.90	0.52
1:A:431:ASN:HB2	1:A:503:ASN:HD21	1.74	0.52
1:A:310:PHE:HA	1:A:313:ILE:HD12	1.92	0.52
1:A:654:GLU:HG3	1:A:679[A]:ASN:HB3	1.92	0.52
1:B:654:GLU:HG3	1:B:679[A]:ASN:HB3	1.92	0.52
1:B:431:ASN:HB2	1:B:503:ASN:HD21	1.75	0.51
1:A:744:GLN:HA	1:A:768:PRO:HG3	1.93	0.51
1:A:206:LEU:O	1:A:226:THR:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:ILE:HG23	5:A:926:QCX:N	2.26	0.50
1:B:310:PHE:HA	1:B:313:ILE:HD12	1.92	0.50
1:A:47:VAL:HB	1:A:67:THR:HA	1.94	0.49
1:A:725:LEU:HD21	1:A:728:LEU:HB2	1.95	0.49
1:B:206:LEU:O	1:B:226:THR:HG23	2.13	0.49
1:B:538:PHE:HB3	1:B:541:LEU:HD12	1.95	0.48
1:A:698:LEU:HD23	1:A:701:LEU:HD13	1.94	0.48
1:B:47:VAL:HB	1:B:67:THR:HA	1.95	0.48
1:A:538:PHE:HB3	1:A:541:LEU:HD12	1.96	0.47
1:A:353:LEU:O	1:A:354:GLN:HB2	2.15	0.47
1:A:224:PRO:HB2	1:A:226:THR:HG22	1.97	0.47
1:B:525:SER:HA	1:B:550:SER:O	2.14	0.47
1:A:354:GLN:HB2	1:A:354:GLN:HE21	1.64	0.46
1:A:787:CYS:HB3	1:A:828:LEU:HD21	1.97	0.46
1:B:787:CYS:HB3	1:B:828:LEU:HD21	1.96	0.46
1:A:779:LEU:HD23	1:A:781:HIS:HE1	1.80	0.46
1:A:582:SER:HB2	1:A:585:ILE:HD12	1.98	0.45
1:B:71:THR:HA	1:B:95:ASP:HB3	1.99	0.45
1:B:224:PRO:HB2	1:B:226:THR:HG22	1.98	0.45
1:B:779:LEU:HD23	1:B:781:HIS:HE1	1.81	0.45
1:A:81:SER:HA	1:A:119:LYS:HB2	1.99	0.44
1:A:228:THR:HA	1:A:251:LEU:HA	2.00	0.44
1:B:81:SER:HA	1:B:119:LYS:HB2	1.99	0.44
1:B:228:THR:HA	1:B:251:LEU:HA	2.00	0.43
1:A:654:GLU:HG3	1:A:679[B]:ASN:HB2	2.00	0.43
1:B:68:THR:HB	1:B:92:VAL:HG22	2.00	0.43
1:A:71:THR:HA	1:A:95:ASP:HB3	1.99	0.43
1:A:553:ARG:HH22	1:B:526:GLY:C	2.26	0.43
1:B:582:SER:HB2	1:B:585:ILE:HD12	2.00	0.43
1:B:654:GLU:HG3	1:B:679[B]:ASN:HB2	2.01	0.43
1:A:251:LEU:HD21	1:A:254:LEU:HB2	2.01	0.42
1:B:251:LEU:HD21	1:B:254:LEU:HB2	2.00	0.42
1:A:666:PRO:HD2	1:A:669:VAL:HG21	2.01	0.42
1:B:744:GLN:HA	1:B:768:PRO:HG3	2.00	0.42
1:B:88:LEU:H	1:B:88:LEU:HG	1.60	0.42
1:B:767:PHE:CD1	1:B:772:LEU:HD21	2.55	0.42
1:B:666:PRO:HD2	1:B:669:VAL:HG21	2.02	0.41
1:A:526:GLY:C	1:B:553:ARG:HH22	2.28	0.41
1:A:707:SER:HA	1:A:731:LYS:O	2.20	0.41
1:A:692:TRP:HH2	1:A:730:LEU:HD21	1.85	0.41
1:B:306:PRO:HA	1:B:307:PRO:HD3	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:SER:HA	1:A:550:SER:O	2.21	0.41
1:B:707:SER:HA	1:B:731:LYS:O	2.21	0.41
1:A:799:GLN:HA	1:A:826:ILE:HD12	2.03	0.41
1:A:93:GLU:HG3	1:A:131:SER:HB2	2.03	0.41
1:A:353:LEU:H	1:A:353:LEU:HG	1.47	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	767/817 (94%)	700 (91%)	63 (8%)	4 (0%)	24	54
1	B	769/817 (94%)	693 (90%)	71 (9%)	5 (1%)	18	47
All	All	1536/1634 (94%)	1393 (91%)	134 (9%)	9 (1%)	21	50

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	818	GLY
1	B	818	GLY
1	A	370	LYS
1	B	370	LYS
1	B	742	PHE
1	A	103	ILE
1	A	381	VAL
1	B	103	ILE
1	B	381	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	726/768 (94%)	693 (96%)	33 (4%)	24	52
1	B	728/768 (95%)	700 (96%)	28 (4%)	29	56
All	All	1454/1536 (95%)	1393 (96%)	61 (4%)	26	54

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	59	ILE
1	A	66	ASN
1	A	74	ILE
1	A	88	LEU
1	A	103	ILE
1	A	168	LEU
1	A	170	GLU
1	A	202	ASN
1	A	213	ASP
1	A	262	ARG
1	A	289	LEU
1	A	299	SER
1	A	313	ILE
1	A	353	LEU
1	A	354	GLN
1	A	370	LYS
1	A	388	PHE
1	A	490	SER
1	A	508	ILE
1	A	544	LEU
1	A	603	MET
1	A	605	ASP
1	A	607	ASP
1	A	614	ARG
1	A	622	ARG
1	A	661	SER

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Mol	Chain	Res	Type
1	A	727	ASN
1	A	755	SER
1	A	792	VAL
1	A	808	LEU
1	A	813	THR
1	A	828	LEU
1	B	40	LEU
1	B	59	ILE
1	B	74	ILE
1	B	88	LEU
1	B	103	ILE
1	B	170	GLU
1	B	202	ASN
1	B	213	ASP
1	B	289	LEU
1	B	313	ILE
1	B	353	LEU
1	B	370	LYS
1	B	388	PHE
1	B	490	SER
1	B	508	ILE
1	B	544	LEU
1	B	603	MET
1	B	605	ASP
1	B	607	ASP
1	B	614	ARG
1	B	661	SER
1	B	722	SER
1	B	727	ASN
1	B	756	SER
1	B	792	VAL
1	B	808	LEU
1	B	813	THR
1	B	828	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	76	HIS
1	A	159	ASN
1	A	167	GLN

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Mol	Chain	Res	Type
1	A	323	GLN
1	A	337	HIS
1	A	354	GLN
1	A	389	GLN
1	A	398	ASN
1	A	503	ASN
1	A	587	HIS
1	A	594	ASN
1	A	599	GLN
1	A	734	GLN
1	A	760	GLN
1	A	781	HIS
1	B	45	ASN
1	B	76	HIS
1	B	159	ASN
1	B	167	GLN
1	B	181	GLN
1	B	300	ASN
1	B	323	GLN
1	B	337	HIS
1	B	398	ASN
1	B	503	ASN
1	B	594	ASN
1	B	640	ASN
1	B	734	GLN
1	B	760	GLN
1	B	781	HIS

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](#)

6 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	NAG	C	1	1,2	14,14,15	0.29	0	17,19,21	0.76	1 (5%)
2	NAG	C	2	2	14,14,15	0.32	0	17,19,21	0.91	2 (11%)
2	NAG	D	1	1,2	14,14,15	0.30	0	17,19,21	0.49	0
2	NAG	D	2	2	14,14,15	0.31	0	17,19,21	0.75	1 (5%)
2	NAG	E	1	1,2	14,14,15	0.35	0	17,19,21	0.74	1 (5%)
2	NAG	E	2	2	14,14,15	0.33	0	17,19,21	0.85	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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C1-O5-C5	2.63	115.71	112.19
2	E	2	NAG	C1-O5-C5	2.62	115.69	112.19
2	C	2	NAG	O5-C1-C2	-2.57	107.31	111.29
2	C	1	NAG	O5-C1-C2	-2.16	107.94	111.29
2	C	2	NAG	C1-O5-C5	2.14	115.06	112.19
2	E	1	NAG	O5-C1-C2	-2.05	108.12	111.29

There are no chirality outliers.

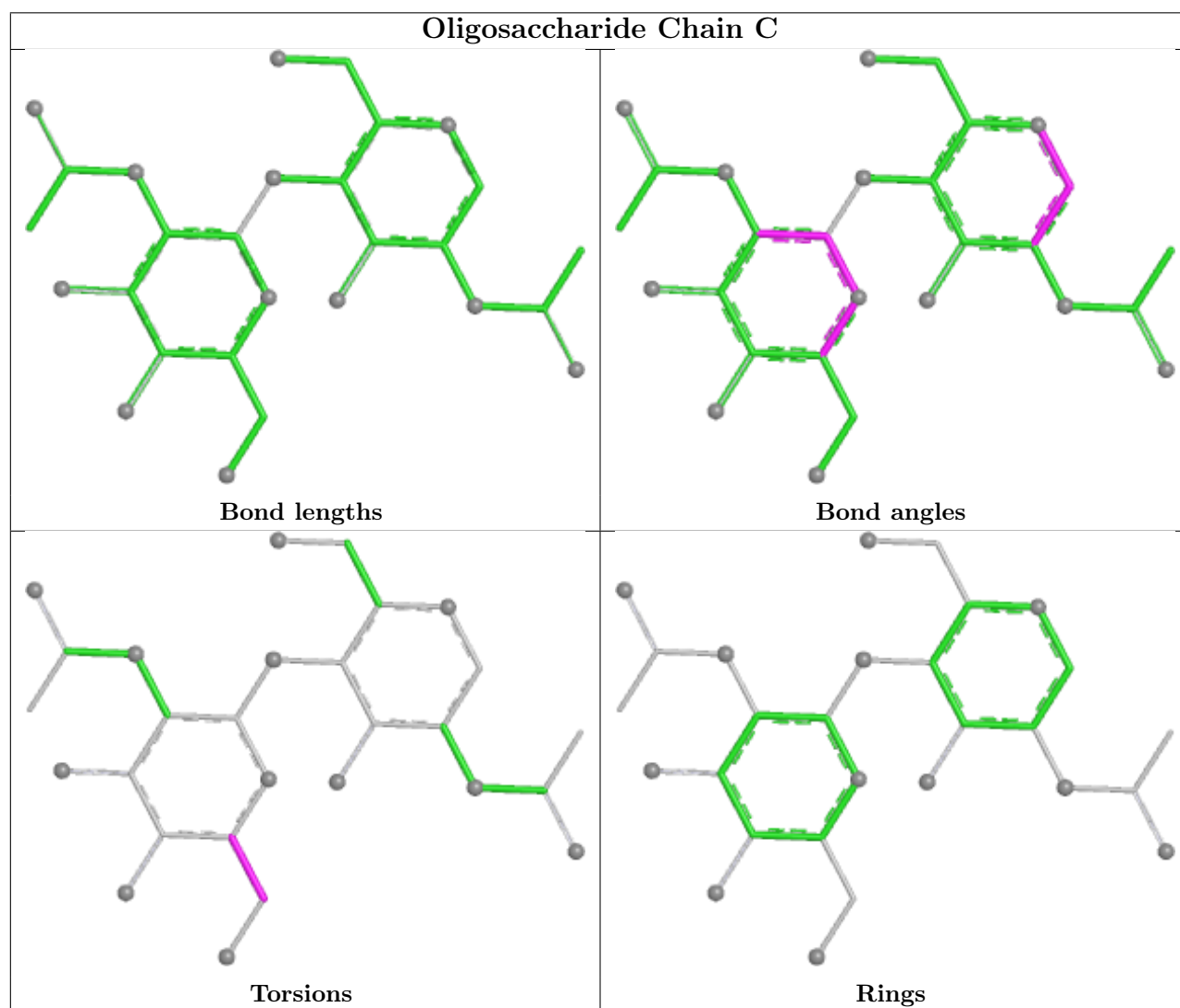
All (5) torsion outliers are listed below:

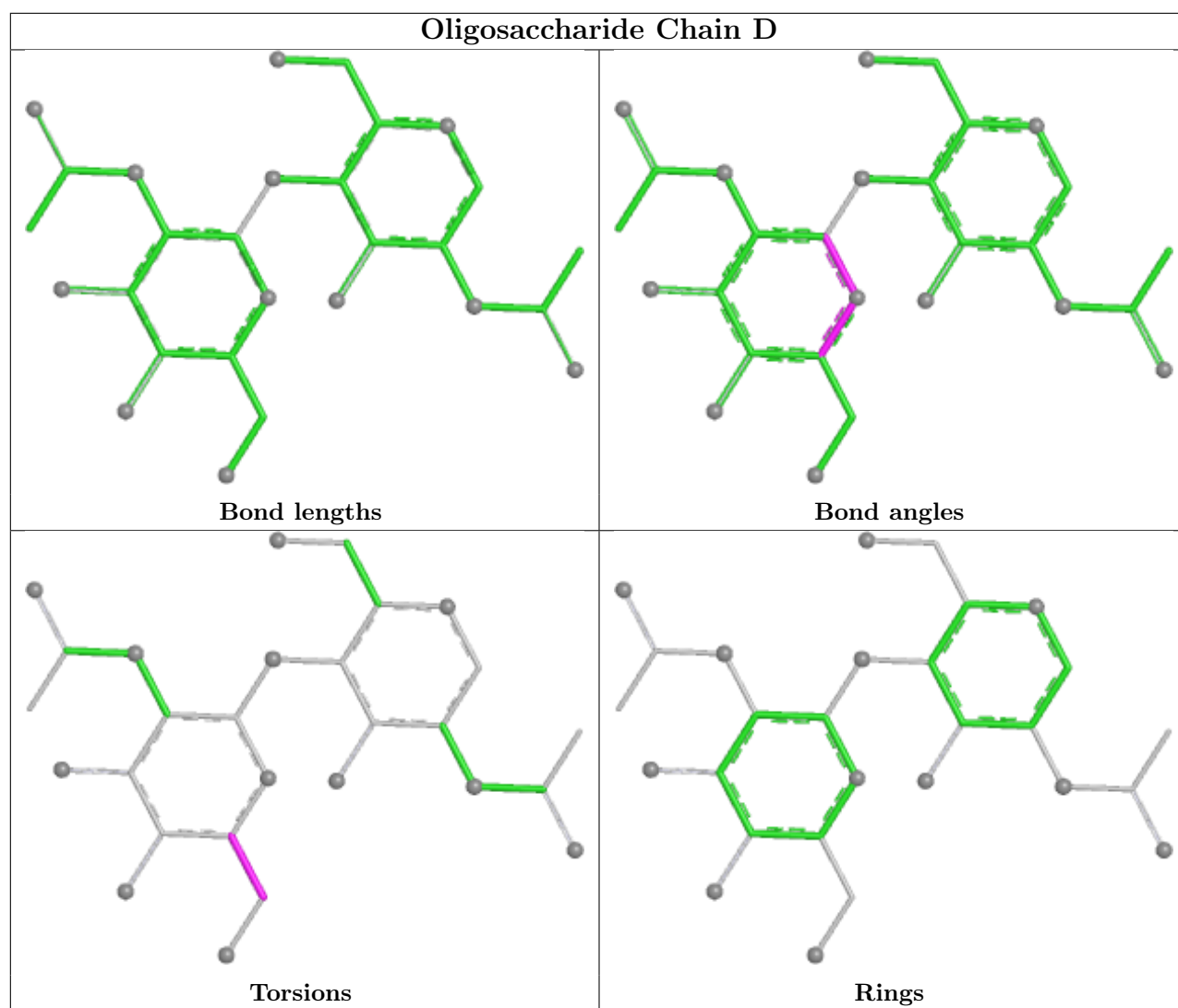
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6

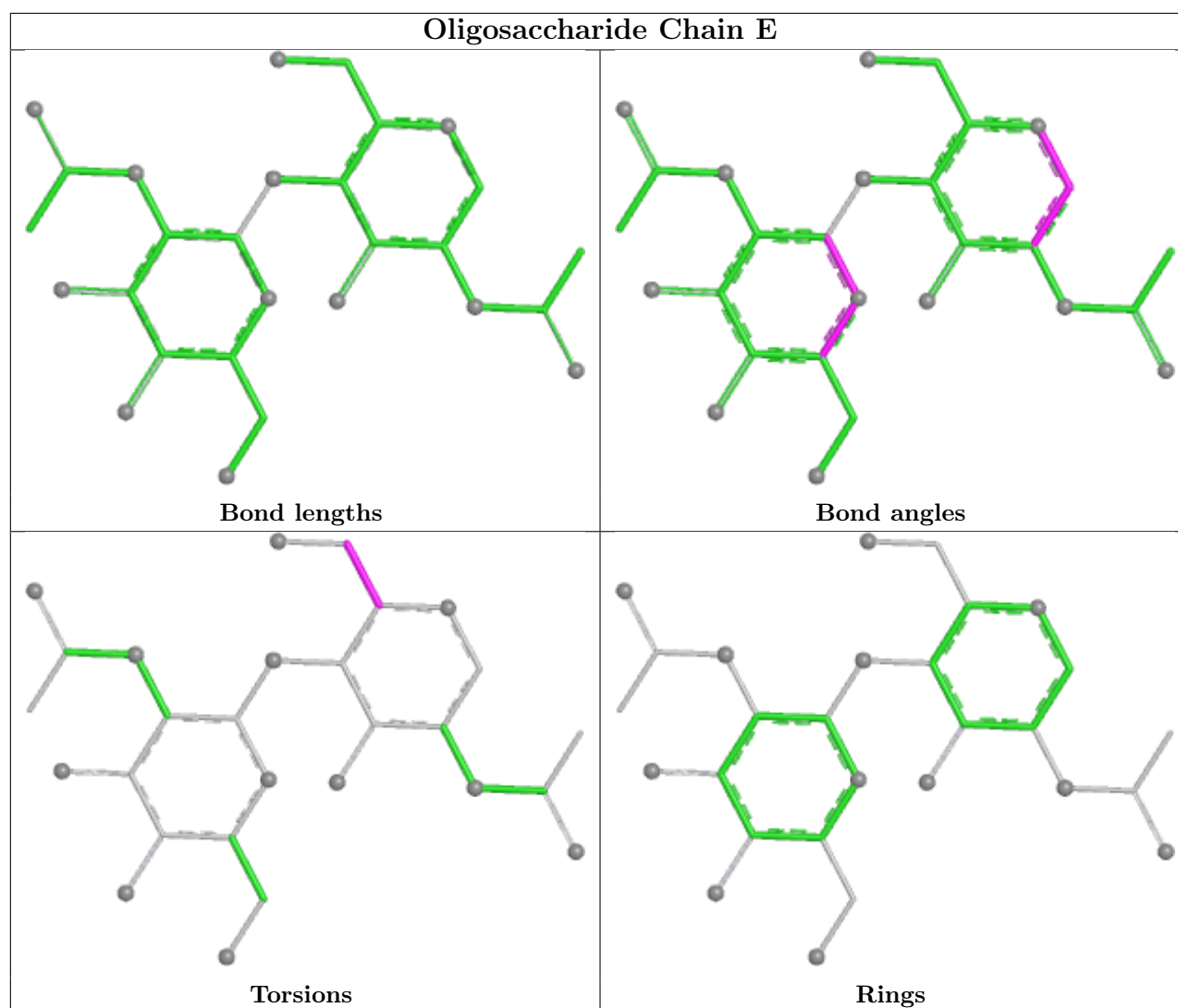
There are no ring outliers.

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](#)

43 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	$\# Z > 2$
4	SO4	A	913	-	4,4,4	0.26	0	6,6,6	0.14	0
4	SO4	B	910	-	4,4,4	0.20	0	6,6,6	0.18	0
4	SO4	A	915	-	4,4,4	0.26	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	904	1	14,14,15	0.31	0	17,19,21	0.70	1 (5%)
4	SO4	A	921	-	4,4,4	0.22	0	6,6,6	0.21	0
5	QCX	B	901	-	38,38,38	0.40	0	45,51,51	1.24	4 (8%)
4	SO4	A	920	-	4,4,4	0.29	0	6,6,6	0.06	0
3	NAG	B	906	1	14,14,15	0.32	0	17,19,21	0.69	1 (5%)
4	SO4	A	919	-	4,4,4	0.28	0	6,6,6	0.08	0
4	SO4	B	907	-	4,4,4	0.29	0	6,6,6	0.14	0
4	SO4	B	908	-	4,4,4	0.24	0	6,6,6	0.09	0
4	SO4	A	914	-	4,4,4	0.23	0	6,6,6	0.09	0
4	SO4	A	912	-	4,4,4	0.25	0	6,6,6	0.13	0
3	NAG	A	907	1	14,14,15	0.33	0	17,19,21	0.68	1 (5%)
4	SO4	B	915	-	4,4,4	0.24	0	6,6,6	0.12	0
4	SO4	A	922	-	4,4,4	0.26	0	6,6,6	0.10	0
3	NAG	B	905	1	14,14,15	0.33	0	17,19,21	0.42	0
3	NAG	A	906	1	14,14,15	0.32	0	17,19,21	0.69	0
4	SO4	A	918	-	4,4,4	0.25	0	6,6,6	0.08	0
4	SO4	B	909	-	4,4,4	0.20	0	6,6,6	0.09	0
4	SO4	B	916	-	4,4,4	0.26	0	6,6,6	0.08	0
3	NAG	B	904	1	14,14,15	0.33	0	17,19,21	0.48	0
5	QCX	A	926	-	38,38,38	0.44	0	45,51,51	1.24	4 (8%)
4	SO4	A	923	-	4,4,4	0.27	0	6,6,6	0.11	0
4	SO4	A	925	-	4,4,4	0.24	0	6,6,6	0.11	0
4	SO4	A	911	-	4,4,4	0.24	0	6,6,6	0.16	0
4	SO4	B	914	-	4,4,4	0.27	0	6,6,6	0.10	0
4	SO4	B	912	-	4,4,4	0.26	0	6,6,6	0.08	0
3	NAG	B	902	1	14,14,15	0.29	0	17,19,21	0.90	1 (5%)
4	SO4	A	927	-	4,4,4	0.28	0	6,6,6	0.06	0
4	SO4	B	913	-	4,4,4	0.26	0	6,6,6	0.06	0
4	SO4	A	916	-	4,4,4	0.28	0	6,6,6	0.22	0
3	NAG	A	901	1	14,14,15	0.30	0	17,19,21	0.96	1 (5%)
3	NAG	A	905	1	14,14,15	0.31	0	17,19,21	0.62	0
4	SO4	A	909	-	4,4,4	0.24	0	6,6,6	0.11	0
4	SO4	A	910	-	4,4,4	0.27	0	6,6,6	0.14	0
3	NAG	A	903	1	14,14,15	0.30	0	17,19,21	1.10	2 (11%)
3	NAG	A	902	1	14,14,15	0.34	0	17,19,21	0.84	1 (5%)
4	SO4	A	917	-	4,4,4	0.21	0	6,6,6	0.12	0
4	SO4	B	911	-	4,4,4	0.24	0	6,6,6	0.10	0
3	NAG	B	903	1	14,14,15	0.36	0	17,19,21	2.05	2 (11%)
4	SO4	A	908	-	4,4,4	0.25	0	6,6,6	0.19	0
4	SO4	A	924	-	4,4,4	0.24	0	6,6,6	0.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	901	1	-	0/6/23/26	0/1/1/1
5	QCX	A	926	-	-	2/21/29/29	0/4/4/4
3	NAG	A	905	1	-	0/6/23/26	0/1/1/1
3	NAG	A	907	1	-	1/6/23/26	0/1/1/1
3	NAG	B	902	1	-	0/6/23/26	0/1/1/1
3	NAG	A	903	1	-	2/6/23/26	0/1/1/1
3	NAG	A	904	1	-	2/6/23/26	0/1/1/1
3	NAG	A	902	1	-	0/6/23/26	0/1/1/1
3	NAG	B	905	1	-	0/6/23/26	0/1/1/1
3	NAG	A	906	1	-	0/6/23/26	0/1/1/1
5	QCX	B	901	-	-	1/21/29/29	0/4/4/4
3	NAG	B	906	1	-	1/6/23/26	0/1/1/1
3	NAG	B	903	1	-	0/6/23/26	0/1/1/1
3	NAG	B	904	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	903	NAG	C1-O5-C5	7.17	121.80	112.19
5	A	926	QCX	C3-C2-C1	-5.25	113.47	119.59
5	B	901	QCX	C3-C2-C1	-4.72	114.08	119.59
5	B	901	QCX	C6-C5-C9	-4.38	105.29	112.41
5	A	926	QCX	C6-C5-C9	-4.02	105.86	112.41
3	B	903	NAG	O5-C1-C2	3.45	116.63	111.29
5	B	901	QCX	C1-N1-C5	3.33	129.80	124.18
3	A	903	NAG	O5-C1-C2	-3.23	106.29	111.29
5	A	926	QCX	N1-C1-N5	-3.00	112.78	118.55
5	B	901	QCX	N1-C1-N5	-2.68	113.38	118.55
3	A	903	NAG	C1-O5-C5	2.62	115.69	112.19
3	A	902	NAG	C1-O5-C5	2.48	115.51	112.19
3	A	904	NAG	C1-O5-C5	2.40	115.41	112.19
3	A	907	NAG	C1-O5-C5	2.40	115.41	112.19
3	B	906	NAG	C1-O5-C5	2.38	115.37	112.19
5	A	926	QCX	C1-N1-C5	2.37	128.18	124.18
3	A	901	NAG	C1-C2-N2	-2.32	106.78	110.43
3	B	902	NAG	C1-C2-N2	-2.03	107.24	110.43

There are no chirality outliers.

All (9) torsion outliers are listed below:

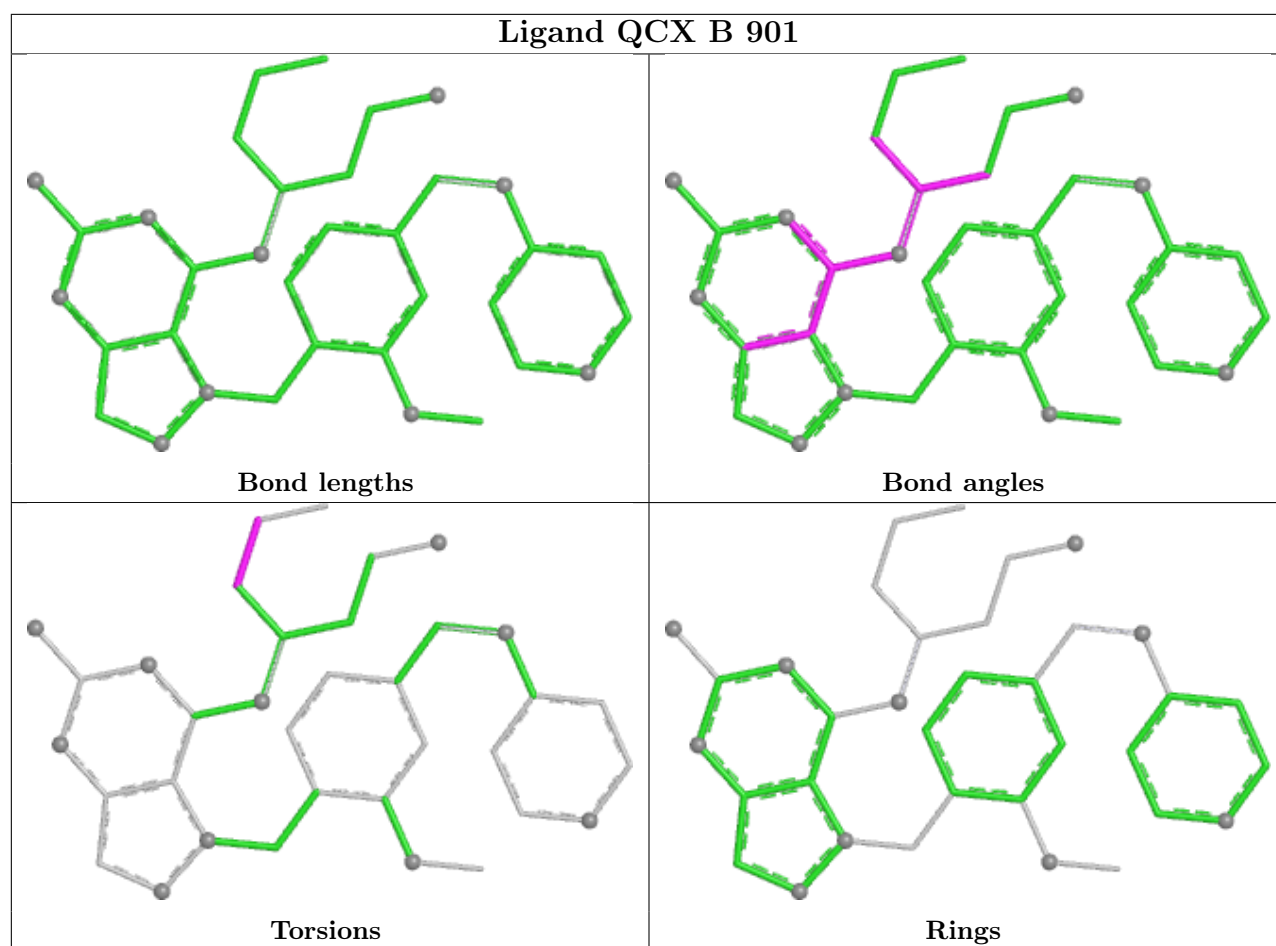
Mol	Chain	Res	Type	Atoms
5	A	926	QCX	C21-C19-N6-C18
3	A	903	NAG	O5-C5-C6-O6
3	A	904	NAG	C4-C5-C6-O6
3	A	904	NAG	O5-C5-C6-O6
5	B	901	QCX	C5-C6-C7-C10
5	A	926	QCX	C5-C6-C7-C10
3	A	903	NAG	C4-C5-C6-O6
3	A	907	NAG	C1-C2-N2-C7
3	B	906	NAG	C1-C2-N2-C7

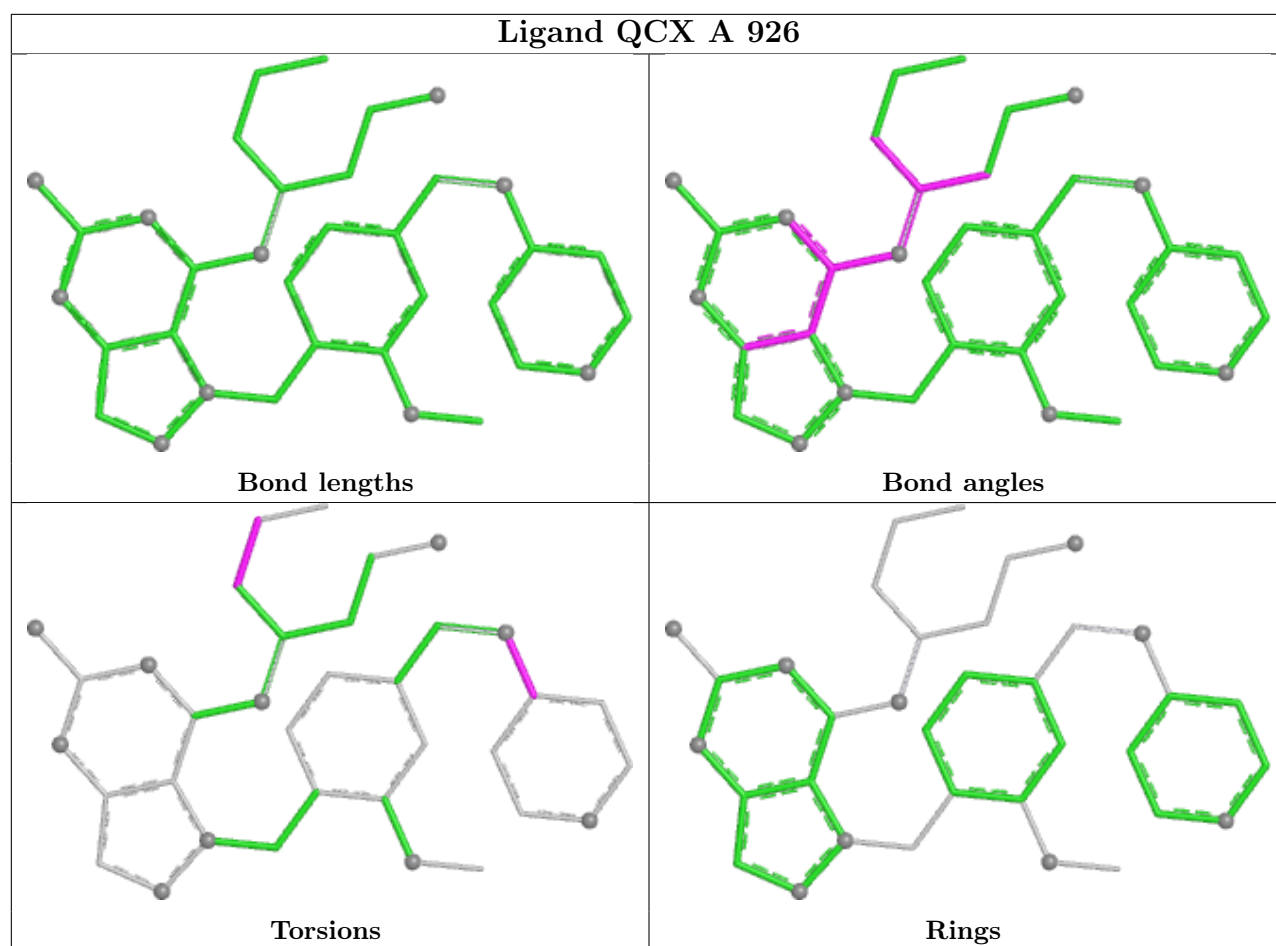
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	926	QCX	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	772/817 (94%)	-0.19	3 (0%) 88 76	22, 67, 95, 123	1 (0%)
1	B	772/817 (94%)	-0.09	2 (0%) 90 80	26, 77, 107, 124	3 (0%)
All	All	1544/1634 (94%)	-0.14	5 (0%) 90 80	22, 72, 105, 124	4 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	835	LEU	2.9
1	A	640	ASN	2.6
1	B	275	ASN	2.3
1	A	45	ASN	2.0
1	B	460	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

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

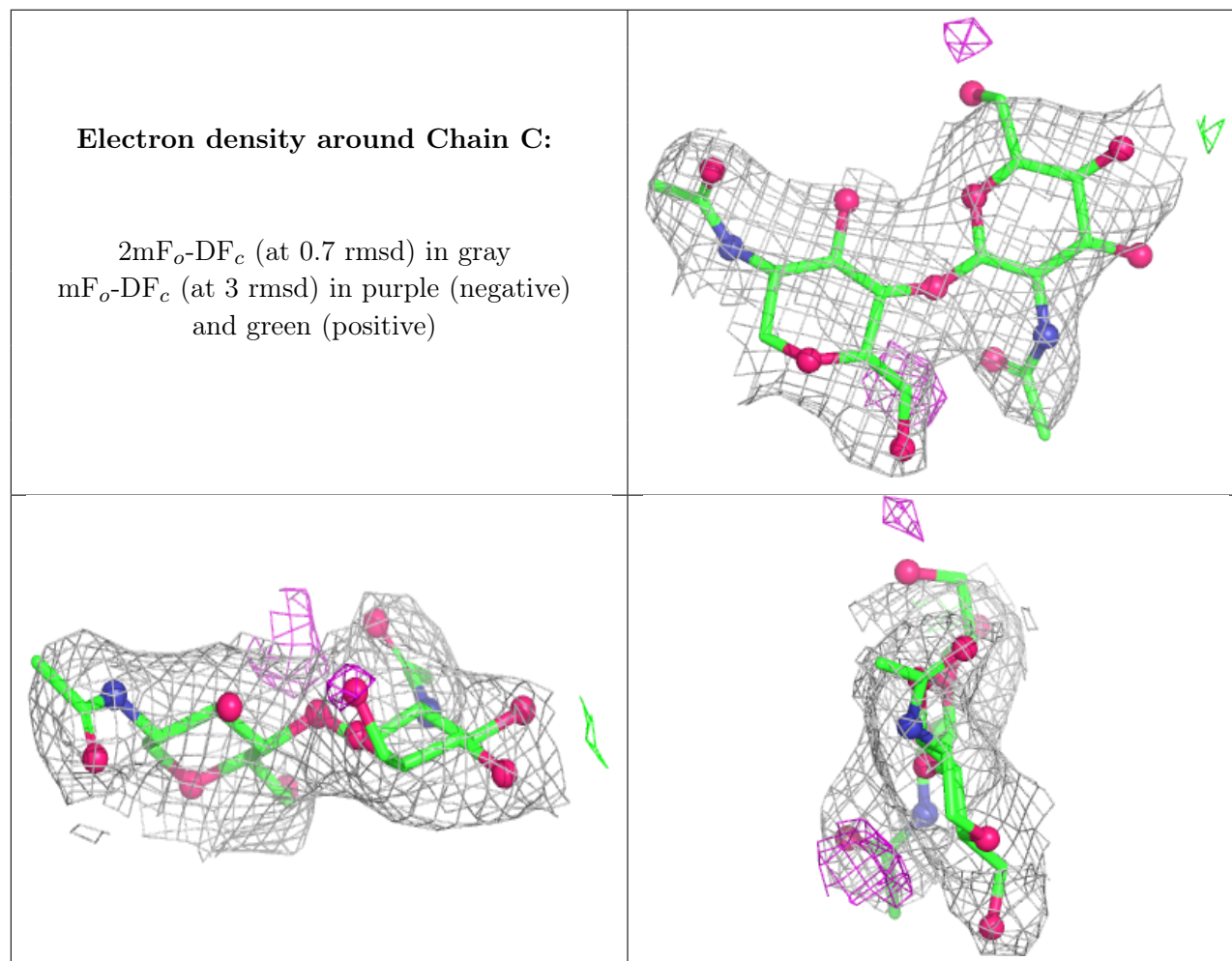
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	E	2	14/15	0.69	0.14	106,108,111,112	0
2	NAG	C	2	14/15	0.78	0.12	68,73,77,79	0
2	NAG	D	2	14/15	0.80	0.09	79,82,83,84	0
2	NAG	D	1	14/15	0.91	0.08	69,72,77,79	0

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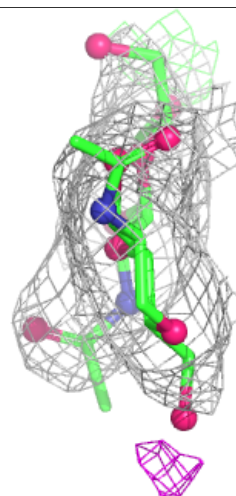
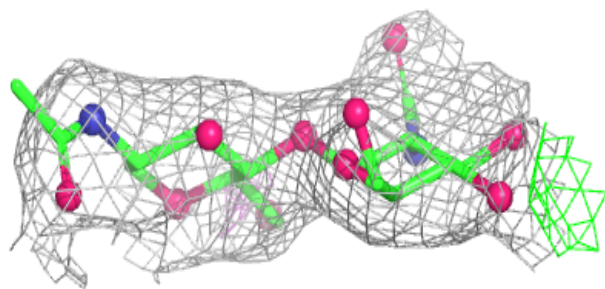
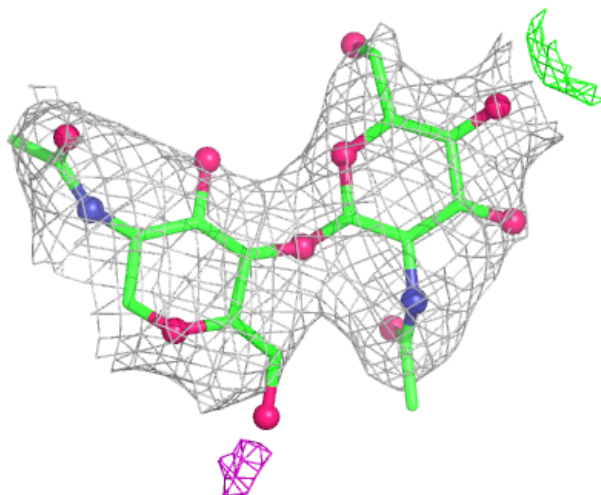
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	E	1	14/15	0.92	0.08	94,97,99,103	0
2	NAG	C	1	14/15	0.94	0.07	54,56,58,62	0

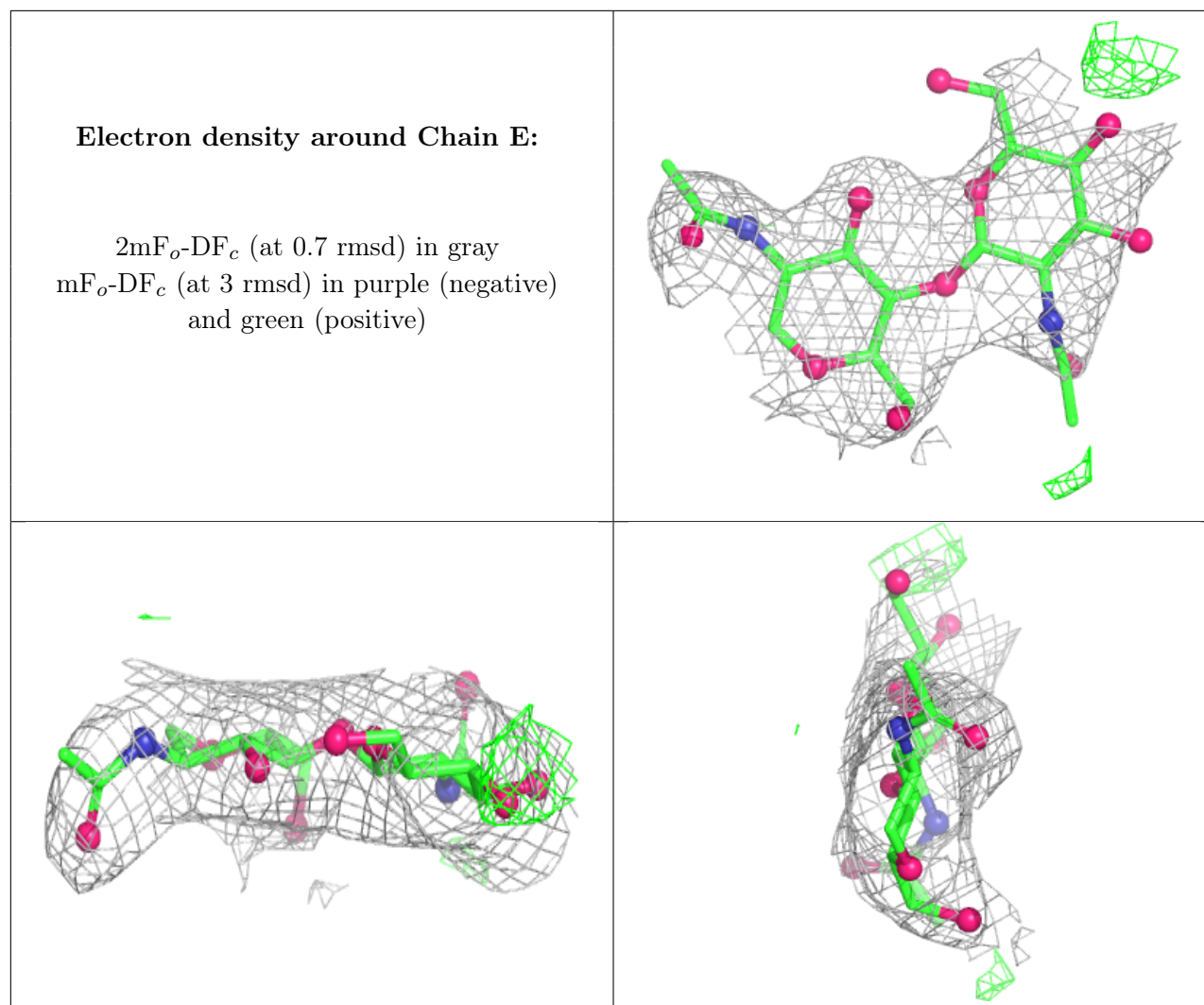
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain D:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	915	5/5	0.41	0.11	228,228,229,229	0
3	NAG	A	907	14/15	0.45	0.16	106,110,111,112	0
4	SO4	A	919	5/5	0.50	0.11	164,164,164,164	0
4	SO4	B	912	5/5	0.51	0.12	186,186,186,187	0
4	SO4	A	922	5/5	0.52	0.11	163,163,163,163	0
4	SO4	B	913	5/5	0.53	0.12	182,182,182,182	0
4	SO4	A	927	5/5	0.56	0.15	162,162,162,163	0
4	SO4	A	912	5/5	0.66	0.13	165,165,165,165	0

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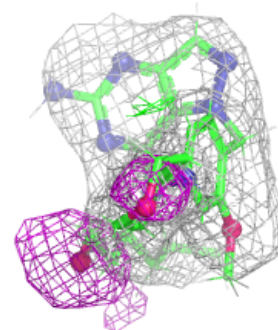
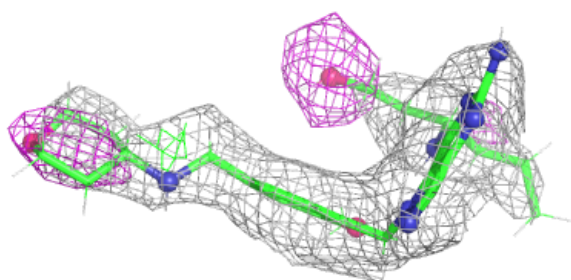
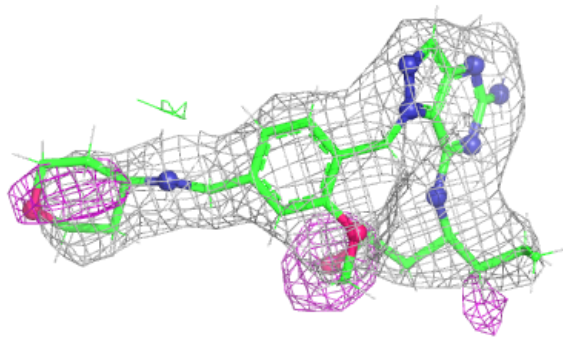
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	914	5/5	0.66	0.14	151,151,151,152	0
3	NAG	A	906	14/15	0.67	0.13	116,117,118,118	0
3	NAG	B	904	14/15	0.67	0.11	114,116,117,117	0
4	SO4	A	923	5/5	0.69	0.11	149,149,149,150	0
4	SO4	A	909	5/5	0.70	0.10	167,167,167,167	0
4	SO4	B	908	5/5	0.72	0.07	187,187,187,187	0
4	SO4	A	920	5/5	0.72	0.12	147,147,147,147	0
3	NAG	B	906	14/15	0.72	0.11	116,118,122,123	0
4	SO4	A	925	5/5	0.73	0.10	139,139,139,140	0
4	SO4	B	915	5/5	0.74	0.11	159,159,159,159	0
3	NAG	B	905	14/15	0.76	0.11	130,131,135,135	0
4	SO4	B	907	5/5	0.76	0.11	128,128,128,129	0
4	SO4	B	914	5/5	0.77	0.14	207,207,207,208	0
4	SO4	B	916	5/5	0.77	0.18	141,141,142,142	0
3	NAG	A	904	14/15	0.79	0.10	77,81,84,85	0
4	SO4	A	913	5/5	0.80	0.11	147,147,147,147	0
4	SO4	A	911	5/5	0.80	0.15	124,126,126,126	0
4	SO4	B	911	5/5	0.81	0.07	169,170,170,170	0
4	SO4	A	910	5/5	0.82	0.11	121,122,122,123	0
3	NAG	A	905	14/15	0.84	0.11	118,119,122,123	0
4	SO4	A	924	5/5	0.84	0.10	164,164,165,165	0
4	SO4	A	916	5/5	0.86	0.22	112,113,113,114	0
5	QCX	B	901	35/35	0.86	0.10	46,54,64,67	0
4	SO4	A	918	5/5	0.87	0.19	143,143,144,144	0
4	SO4	A	921	5/5	0.87	0.12	156,156,156,156	0
3	NAG	A	901	14/15	0.88	0.11	59,62,65,69	0
4	SO4	A	908	5/5	0.88	0.14	147,148,148,148	0
3	NAG	A	902	14/15	0.89	0.09	80,84,86,86	0
4	SO4	B	910	5/5	0.89	0.18	124,124,124,124	0
3	NAG	A	903	14/15	0.89	0.09	84,85,93,93	0
5	QCX	A	926	35/35	0.90	0.09	48,57,70,73	0
3	NAG	B	903	14/15	0.90	0.08	72,76,79,81	0
4	SO4	B	909	5/5	0.91	0.10	116,117,117,117	0
4	SO4	A	917	5/5	0.92	0.17	142,142,143,143	0
3	NAG	B	902	14/15	0.94	0.07	66,66,68,69	0

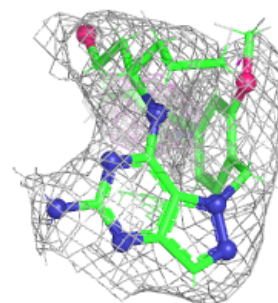
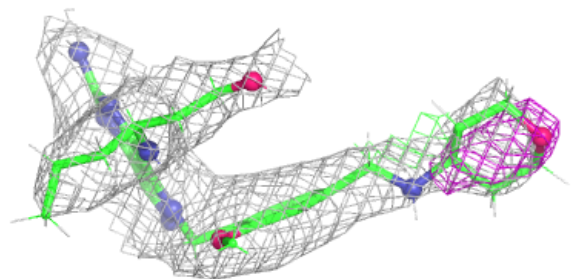
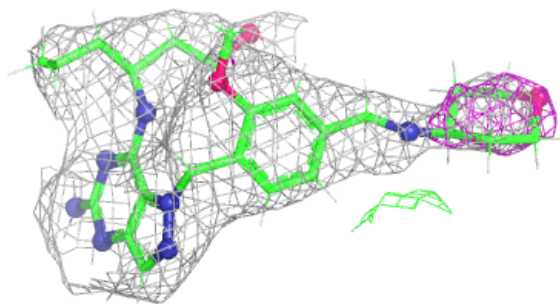
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around QCX B 901:

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

**Electron density around QCX A 926:**

$2mF_o-DF_c$ (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.