



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2022 – 02:30 PM EDT

PDB ID : 7UBR
Title : Integrin α IIb β 3 complex with GR144053
Authors : Lin, F.-Y.; Zhu, J.; Zhu, J.; Springer, T.A.
Deposited on : 2022-03-15
Resolution : 2.05 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.29
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

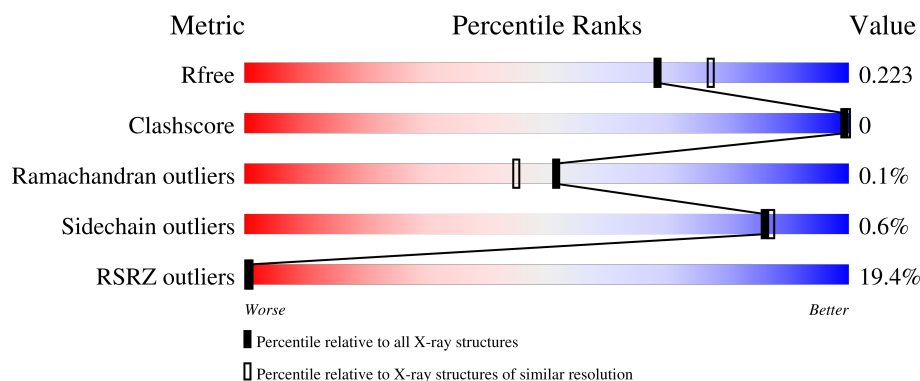
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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.



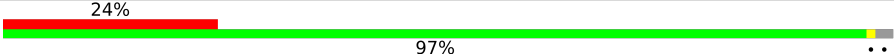
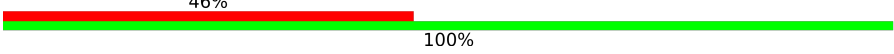
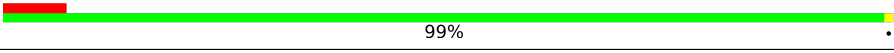

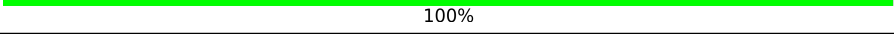
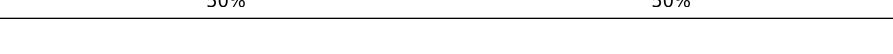
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	454	<div> <div>10%</div> <div>98%</div> </div>
1	C	454	<div> <div>9%</div> <div>98%</div> </div>
2	B	472	<div> <div>18%</div> <div>98%</div> </div>
2	D	472	<div> <div>15%</div> <div>99%</div> </div>
3	E	221	<div> <div>50%</div> <div>97%</div> </div>

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Mol	Chain	Length	Quality of chain
3	H	221	
4	F	214	
4	L	214	
5	G	5	
6	I	2	
6	K	2	
7	J	4	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 22310 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 Integrin alpha-IIb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	4	0
			3499	2226	601	664	8			
1	C	453	Total	C	N	O	S	0	4	0
			3502	2224	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	N	O	S	0	5	0
			3625	2257	618	716	34			
2	D	471	Total	C	N	O	S	0	1	0
			3633	2261	622	716	34			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	214	Total	C	N	O	S	0	0	0
			1631	1035	264	326	6			
3	H	216	Total	C	N	O	S	0	0	0
			1642	1041	266	329	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	214	Total	C	N	O	S	0	0	0
			1637	1019	268	341	9			
4	L	214	Total	C	N	O	S	0	0	0
			1637	1019	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	N	O	0	0	0
			61	34	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	N	O	0	0	0
			28	16	2	10			
6	K	2	Total	C	N	O	0	0	0
			28	16	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	N	O	0	0	0
			50	28	2	20			

- Molecule 8 is SULFATE ION (three-letter code: 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	A	1	Total	O	S	0	0
			5	4	1		
8	B	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	D	1	Total	O	S	0	0
			5	4	1		
8	L	1	Total	O	S	0	0
			5	4	1		

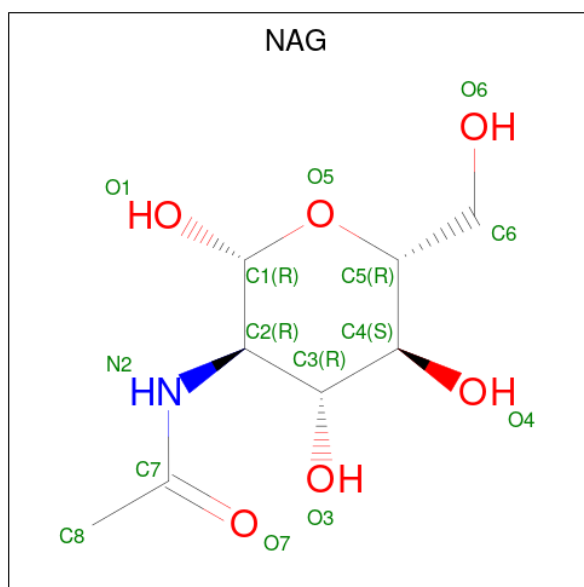
- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	4	Total	Ca	0	0
			4	4		
9	C	4	Total	Ca	0	0
			4	4		

- Molecule 10 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

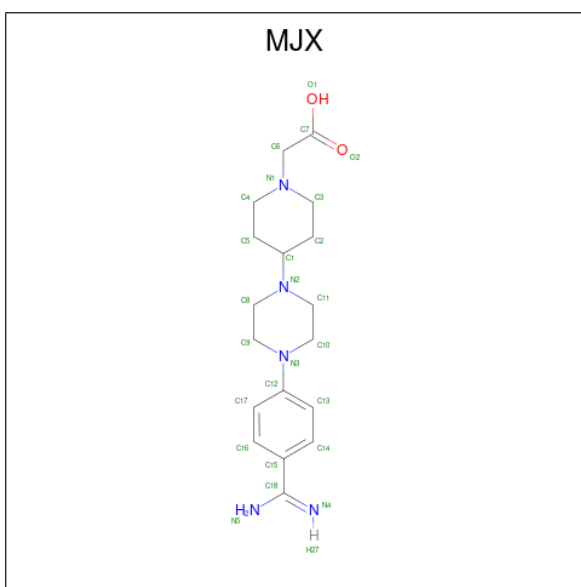
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	3	Total	Mn	0	0
			3	3		
10	D	3	Total	Mn	0	0
			3	3		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 12 is {4-[4-(4-carbamimidoylphenyl)piperazin-1-yl]piperidin-1-yl}acetic acid (three-letter code: MJX) (formula: C₁₈H₂₇N₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	N	O	0	0
			25	18	5	2		
12	D	1	Total	C	N	O	0	0
			25	18	5	2		

- Molecule 13 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	C	1	Total	Cl	0	0
			1	1		
13	D	1	Total	Cl	0	0
			1	1		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	428	Total	O	0	0
			428	428		
14	B	257	Total	O	0	0
			257	257		
14	C	214	Total	O	0	0
			214	214		
14	D	176	Total	O	0	0
			176	176		
14	E	16	Total	O	0	0
			16	16		

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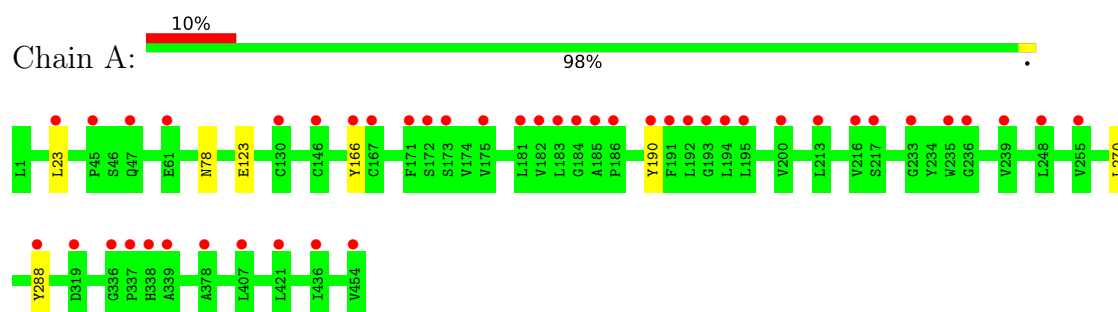
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	F	12	Total 12	O 12	0	0
14	H	34	Total 34	O 34	0	0
14	L	46	Total 46	O 46	0	0

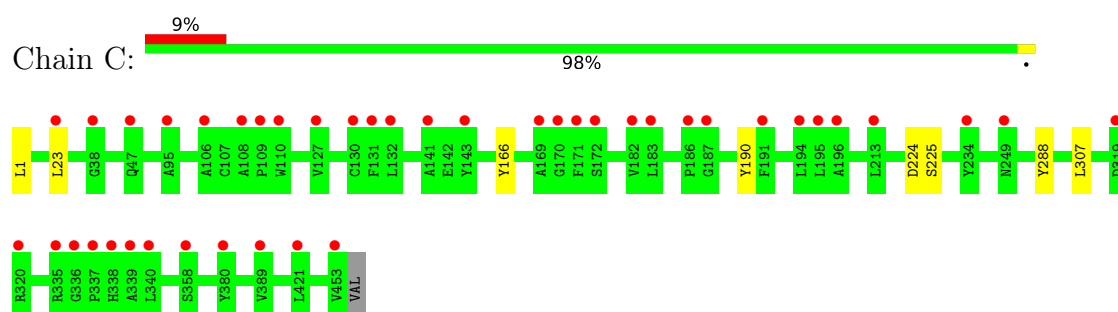
3 Residue-property plots [i](#)

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.

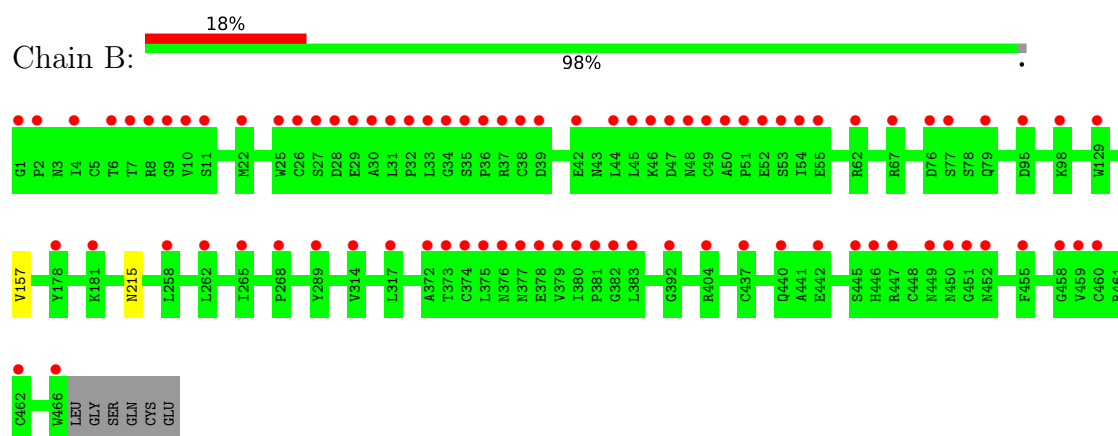
- Molecule 1: Integrin alpha-IIb



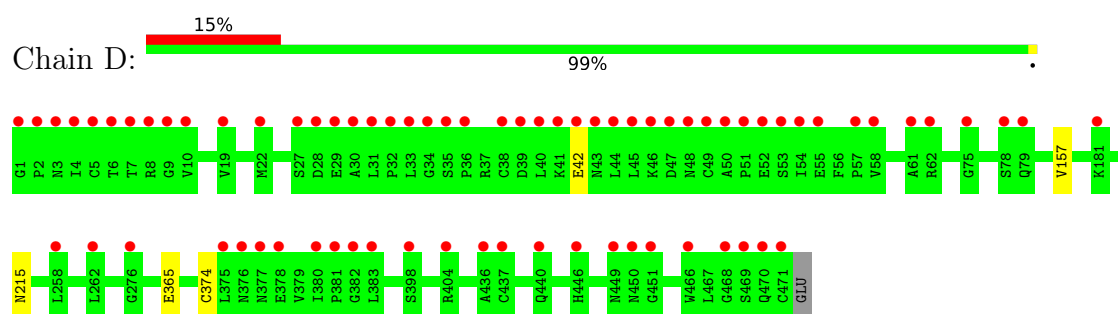
- Molecule 1: Integrin alpha-IIb



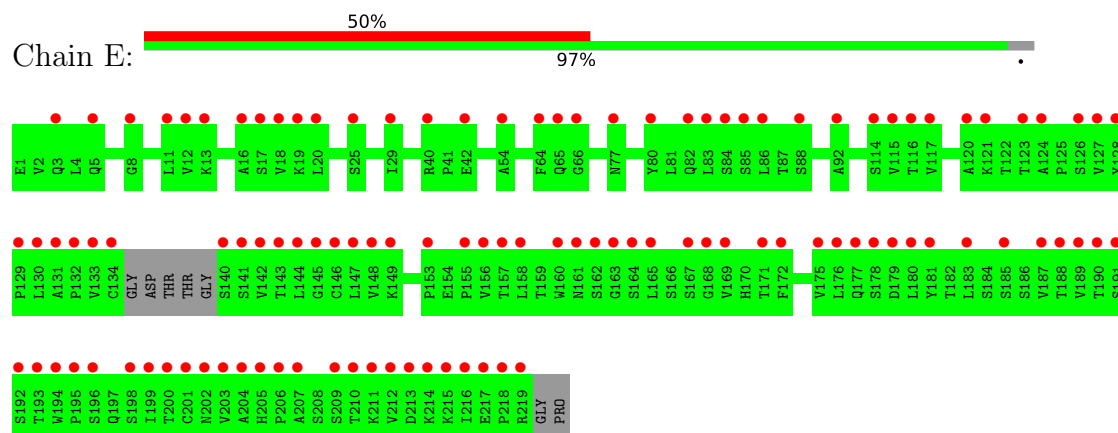
- Molecule 2: Isoform Beta-3C of Integrin beta-3



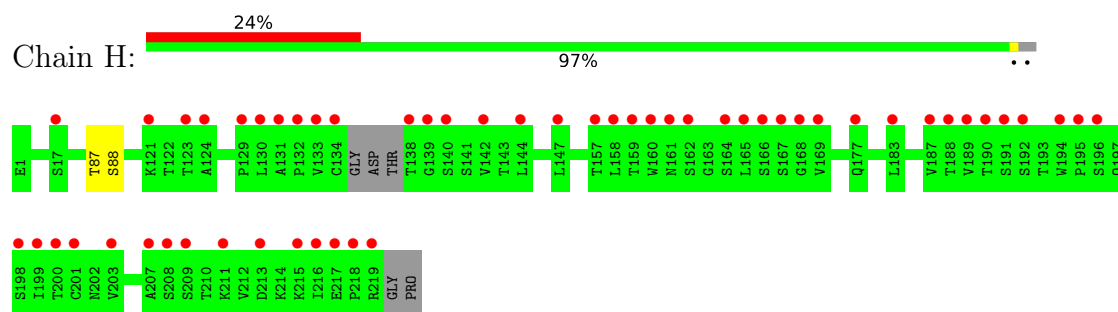
- Molecule 2: Isoform Beta-3C of Integrin beta-3



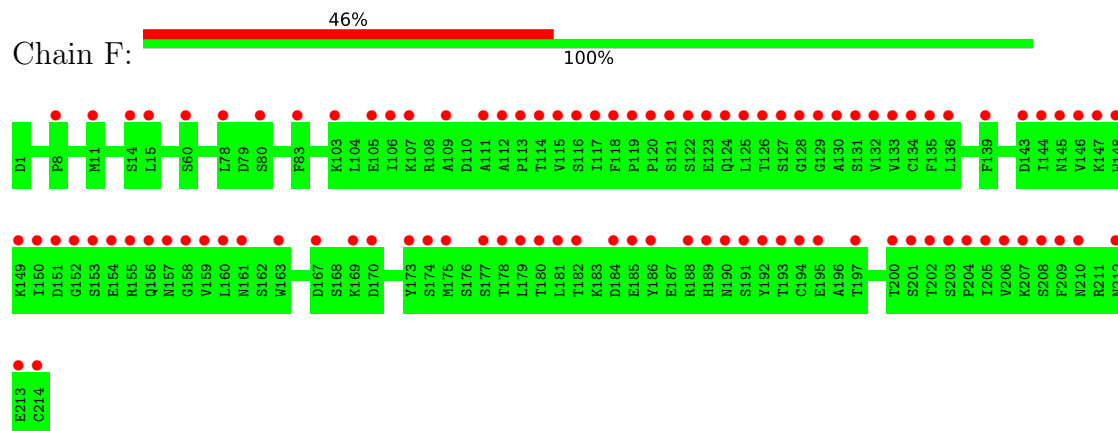
- Molecule 3: 10E5 Fab heavy chain



- Molecule 3: 10E5 Fab heavy chain

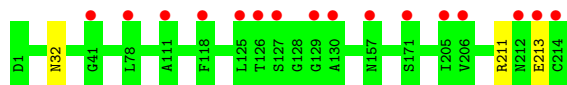


- Molecule 4: 10E5 Fab light chain



- Molecule 4: 10E5 Fab light chain

Chain L:  7% 99%



- 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

Chain G:  60% 40%



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

Chain I:  100%



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

Chain K:  100%



- 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:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	257.89Å 144.40Å 104.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.26 – 2.05 49.26 – 2.05	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.26-2.05) 97.0 (49.26-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.209 , 0.223 0.209 , 0.223	Depositor DCC
R_{free} test set	1944 reflections (0.82%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.5	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	0.96	EDS
Total number of atoms	22310	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: CL, SO4, BMA, MN, MAN, CA, NAG, MJX

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	0.22	0/3608	0.41	0/4918
1	C	0.21	0/3605	0.39	0/4912
2	B	0.22	0/3695	0.39	0/5010
2	D	0.21	0/3701	0.38	0/5018
3	E	0.21	0/1673	0.37	0/2290
3	H	0.21	0/1684	0.38	0/2305
4	F	0.21	0/1673	0.36	0/2269
4	L	0.22	0/1673	0.37	0/2269
All	All	0.21	0/21312	0.38	0/28991

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	3499	0	3345	1	0
1	C	3502	0	3334	3	0
2	B	3625	0	3541	0	0
2	D	3633	0	3546	1	0
3	E	1631	0	1590	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1642	0	1600	1	0
4	F	1637	0	1553	0	0
4	L	1637	0	1553	2	0
5	G	61	0	52	0	0
6	I	28	0	25	0	0
6	K	28	0	25	0	0
7	J	50	0	43	0	0
8	A	25	0	0	0	0
8	B	5	0	0	0	0
8	C	20	0	0	0	0
8	D	5	0	0	0	0
8	L	5	0	0	0	0
9	A	4	0	0	0	0
9	C	4	0	0	0	0
10	B	3	0	0	0	0
10	D	3	0	0	0	0
11	B	14	0	13	0	0
11	D	14	0	13	0	0
12	B	25	0	0	0	0
12	D	25	0	0	0	0
13	C	1	0	0	0	0
13	D	1	0	0	0	0
14	A	428	0	0	0	2
14	B	257	0	0	0	0
14	C	214	0	0	2	1
14	D	176	0	0	0	1
14	E	16	0	0	0	0
14	F	12	0	0	0	0
14	H	34	0	0	0	0
14	L	46	0	0	0	0
All	All	22310	0	20233	7	2

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 0.

All (7) 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:C:1:LEU:N	14:C:607:HOH:O	2.44	0.50
4:L:211:ARG:O	4:L:213:GLU:N	2.46	0.45
1:A:78:ASN:O	4:L:32:ASN:ND2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:LEU:N	14:C:614:HOH:O	2.53	0.42
2:D:42:GLU:OE2	2:D:42:GLU:N	2.50	0.41
1:C:224:ASP:OD1	1:C:225:SER:N	2.49	0.40
3:H:87:THR:HG22	3:H:88:SER:N	2.35	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:894:HOH:O	14:D:2101:HOH:O[1_554]	2.08	0.12
14:A:935:HOH:O	14:C:784:HOH:O[1_554]	2.14	0.06

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	456/454 (100%)	439 (96%)	16 (4%)	1 (0%)	47	39
1	C	455/454 (100%)	435 (96%)	20 (4%)	0	100	100
2	B	469/472 (99%)	455 (97%)	13 (3%)	1 (0%)	47	39
2	D	470/472 (100%)	453 (96%)	15 (3%)	2 (0%)	34	24
3	E	210/221 (95%)	193 (92%)	17 (8%)	0	100	100
3	H	212/221 (96%)	197 (93%)	15 (7%)	0	100	100
4	F	212/214 (99%)	199 (94%)	13 (6%)	0	100	100
4	L	212/214 (99%)	201 (95%)	11 (5%)	0	100	100
All	All	2696/2722 (99%)	2572 (95%)	120 (4%)	4 (0%)	51	45

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	374	CYS
1	A	123	GLU
2	D	157	VAL
2	B	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	366/362 (101%)	361 (99%)	5 (1%)	67	65
1	C	365/362 (101%)	360 (99%)	5 (1%)	67	65
2	B	417/417 (100%)	416 (100%)	1 (0%)	93	94
2	D	417/417 (100%)	415 (100%)	2 (0%)	88	89
3	E	186/190 (98%)	186 (100%)	0	100	100
3	H	187/190 (98%)	187 (100%)	0	100	100
4	F	188/188 (100%)	188 (100%)	0	100	100
4	L	188/188 (100%)	188 (100%)	0	100	100
All	All	2314/2314 (100%)	2301 (99%)	13 (1%)	86	87

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	166	TYR
1	A	190	TYR
1	A	270	LEU
1	A	288	TYR
2	B	215	ASN
1	C	23	LEU
1	C	166	TYR
1	C	190	TYR
1	C	288	TYR
1	C	307	LEU
2	D	215	ASN

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Mol	Chain	Res	Type
2	D	365	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	2,5	14,14,15	0.24	0	17,19,21	0.37	0
5	NAG	G	2	5	14,14,15	0.24	0	17,19,21	0.40	0
5	BMA	G	3	5	11,11,12	0.76	0	15,15,17	0.70	0
5	MAN	G	4	5	11,11,12	0.76	0	15,15,17	1.07	2 (13%)
5	MAN	G	5	5	11,11,12	0.89	0	15,15,17	1.29	3 (20%)
6	NAG	I	1	2,6	14,14,15	0.19	0	17,19,21	0.36	0
6	NAG	I	2	6	14,14,15	0.23	0	17,19,21	0.47	0
7	NAG	J	1	2,7	14,14,15	0.18	0	17,19,21	0.46	0
7	NAG	J	2	7	14,14,15	0.15	0	17,19,21	0.47	0
7	BMA	J	3	7	11,11,12	1.25	2 (18%)	15,15,17	1.01	1 (6%)
7	MAN	J	4	7	11,11,12	0.91	0	15,15,17	1.12	1 (6%)
6	NAG	K	1	2,6	14,14,15	0.41	0	17,19,21	0.45	0
6	NAG	K	2	6	14,14,15	0.21	0	17,19,21	0.48	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	2,5	-	0/6/23/26	0/1/1/1
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	2,6	-	1/6/23/26	0/1/1/1
6	NAG	I	2	6	-	4/6/23/26	0/1/1/1
7	NAG	J	1	2,7	-	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	-	2/2/19/22	0/1/1/1
7	MAN	J	4	7	-	2/2/19/22	0/1/1/1
6	NAG	K	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	3	BMA	O5-C1	-3.03	1.38	1.43
7	J	3	BMA	C4-C5	2.18	1.57	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	4	MAN	C1-O5-C5	2.90	116.12	112.19
5	G	5	MAN	O5-C1-C2	2.61	114.79	110.77
5	G	4	MAN	C1-O5-C5	2.49	115.56	112.19
7	J	3	BMA	C3-C4-C5	2.27	114.30	110.24
5	G	5	MAN	O2-C2-C3	-2.08	105.98	110.14
5	G	5	MAN	C1-O5-C5	2.07	114.99	112.19
5	G	4	MAN	O2-C2-C3	-2.06	106.00	110.14

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	K	2	NAG	O5-C5-C6-O6

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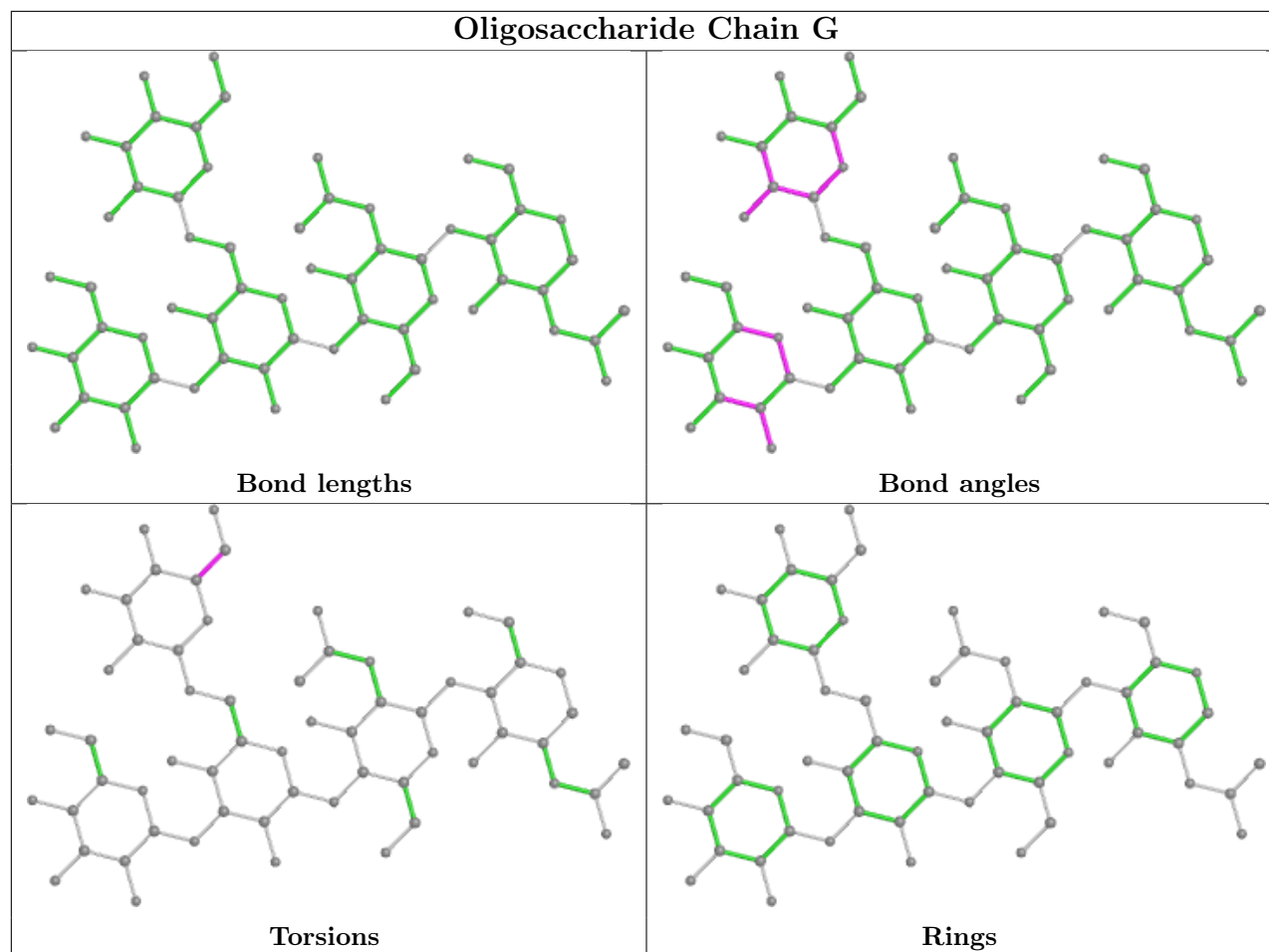
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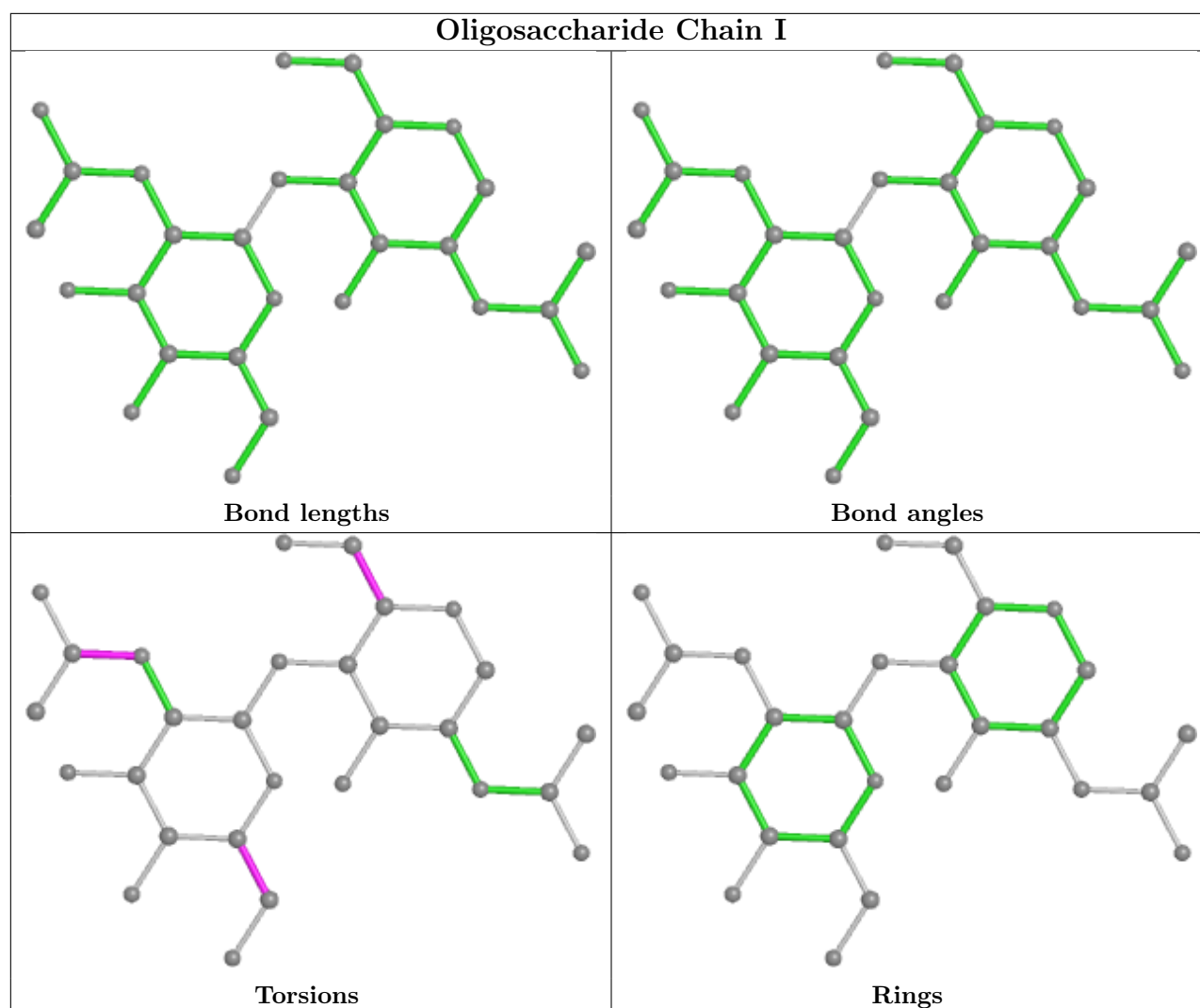
Mol	Chain	Res	Type	Atoms
6	I	2	NAG	O5-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
7	J	3	BMA	C4-C5-C6-O6
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
6	K	2	NAG	C8-C7-N2-C2
6	K	2	NAG	O7-C7-N2-C2
6	I	2	NAG	C4-C5-C6-O6
7	J	4	MAN	O5-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
7	J	3	BMA	O5-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6
5	G	5	MAN	O5-C5-C6-O6
7	J	4	MAN	C4-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6

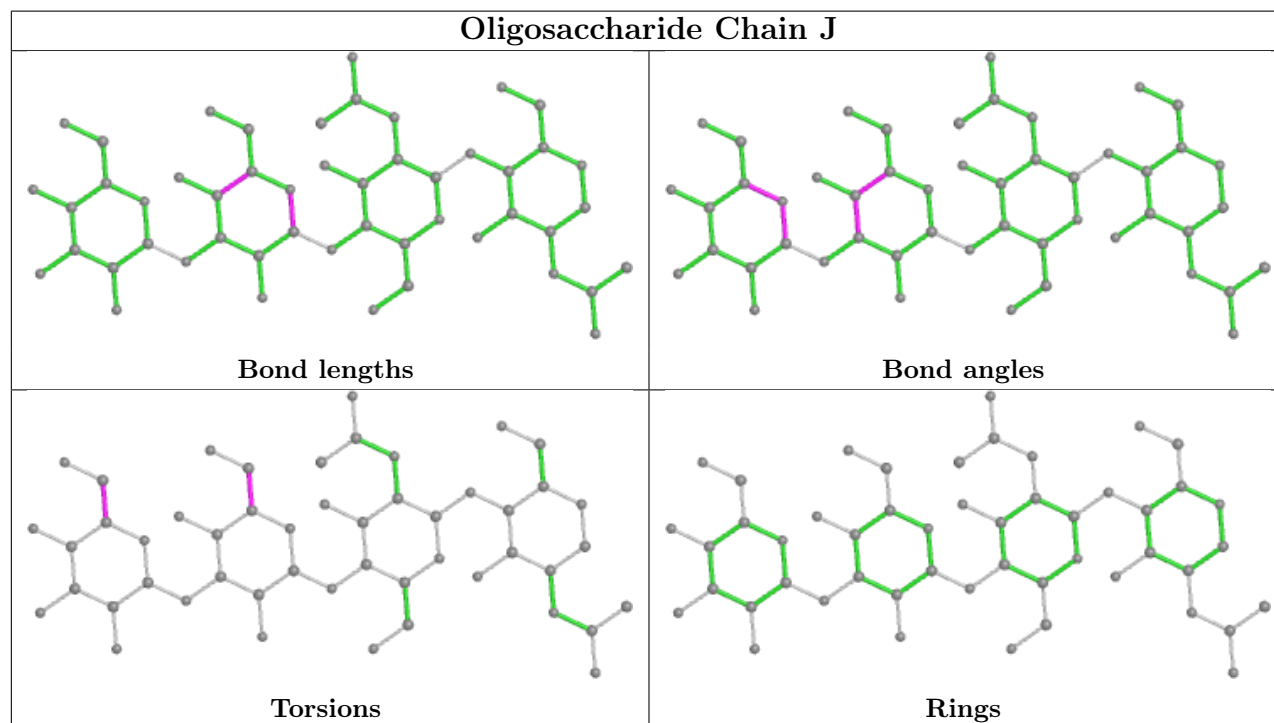
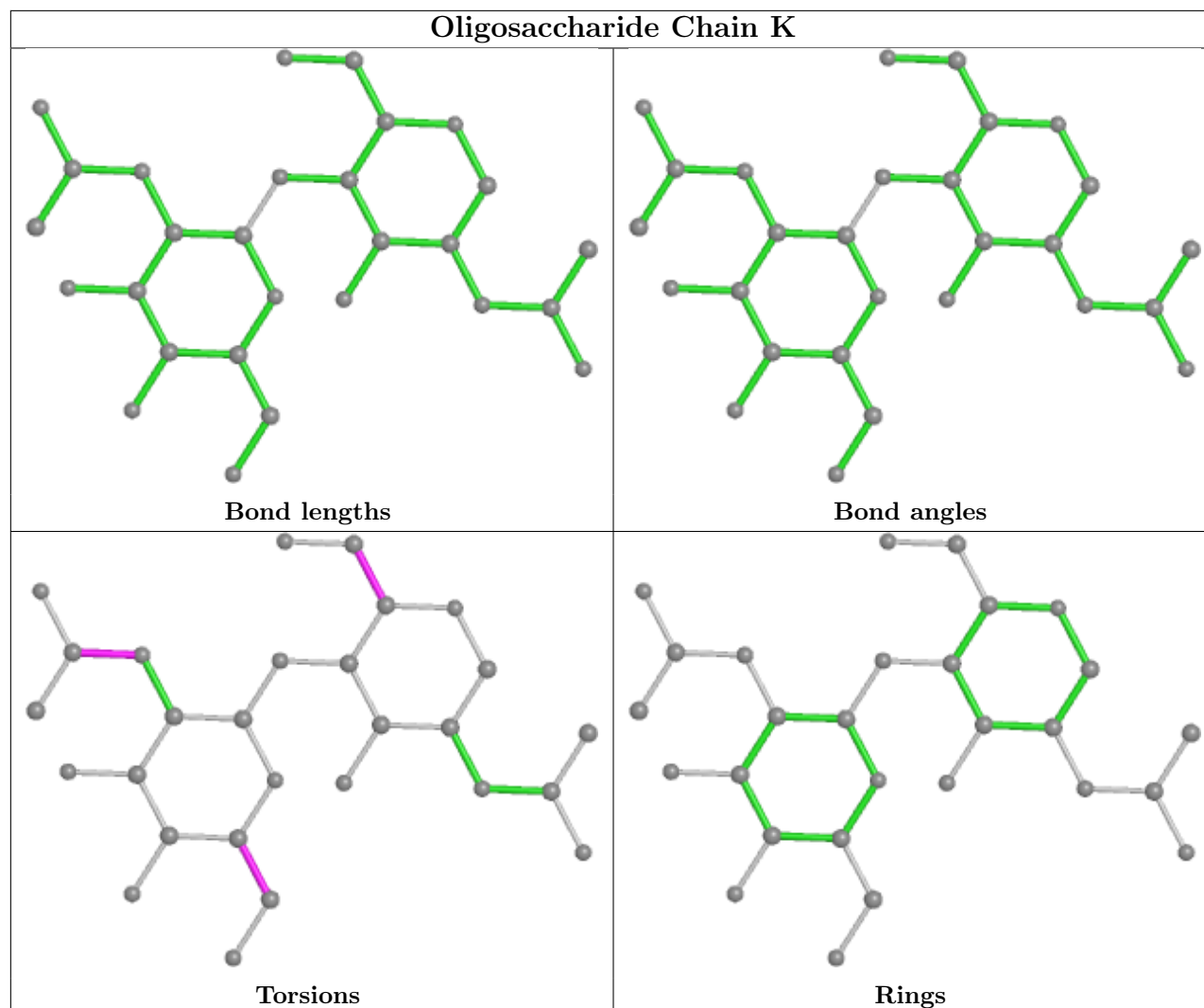
There are no ring outliers.

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

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 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
8	SO4	A	507	-	4,4,4	0.15	0	6,6,6	0.06	0
8	SO4	C	501	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	L	301	-	4,4,4	0.14	0	6,6,6	0.05	0
11	NAG	B	2004	2	14,14,15	0.28	0	17,19,21	0.60	0
8	SO4	A	508	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	C	503	-	4,4,4	0.14	0	6,6,6	0.04	0
8	SO4	C	509	-	4,4,4	0.14	0	6,6,6	0.05	0
12	MJX	D	2006	10	27,27,27	0.94	0	33,37,37	1.05	2 (6%)
8	SO4	C	502	-	4,4,4	0.14	0	6,6,6	0.05	0
11	NAG	D	2004	2	14,14,15	0.22	0	17,19,21	0.37	0
8	SO4	A	501	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	A	502	-	4,4,4	0.14	0	6,6,6	0.05	0
12	MJX	B	2005	10	27,27,27	0.91	0	33,37,37	1.02	0
8	SO4	B	2006	-	4,4,4	0.15	0	6,6,6	0.09	0
8	SO4	A	509	-	4,4,4	0.15	0	6,6,6	0.04	0
8	SO4	D	2007	-	4,4,4	0.14	0	6,6,6	0.06	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
11	NAG	D	2004	2	-	2/6/23/26	0/1/1/1
12	MJX	D	2006	10	-	4/16/36/36	0/3/3/3
11	NAG	B	2004	2	-	0/6/23/26	0/1/1/1
12	MJX	B	2005	10	-	3/16/36/36	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	2006	MJX	C6-N1-C3	2.25	114.58	111.09
12	D	2006	MJX	C2-C1-C5	-2.06	106.45	111.19

There are no chirality outliers.

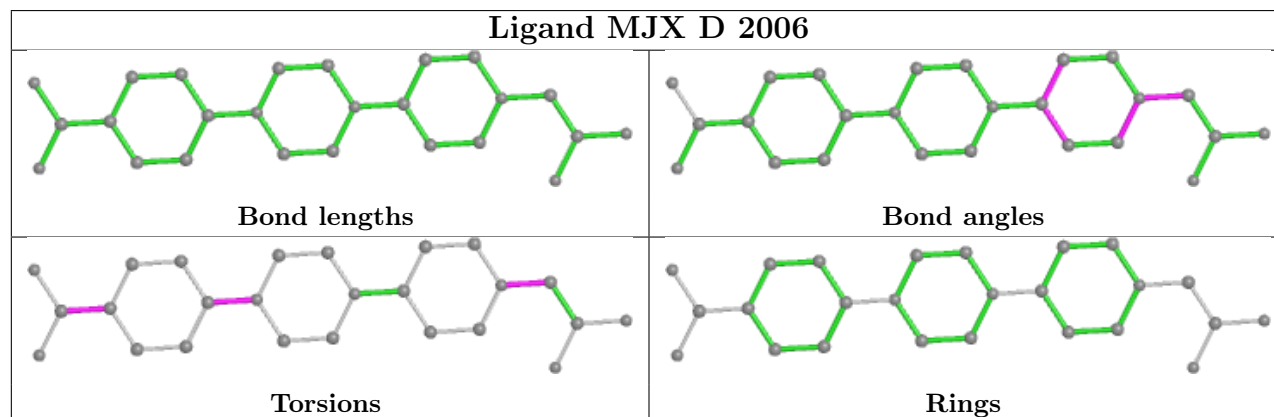
All (9) torsion outliers are listed below:

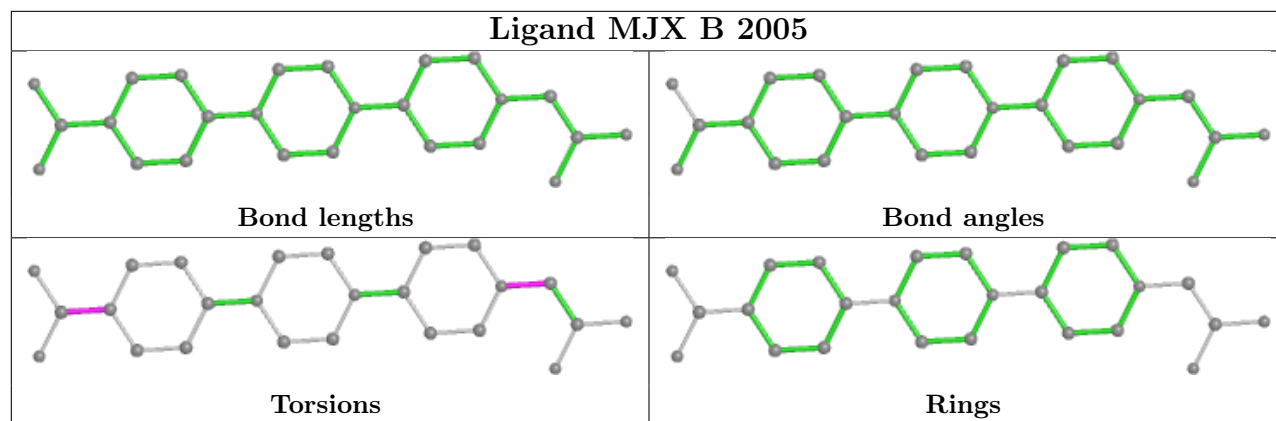
Mol	Chain	Res	Type	Atoms
12	B	2005	MJX	C14-C15-C18-N5
12	B	2005	MJX	C16-C15-C18-N5
11	D	2004	NAG	O5-C5-C6-O6
11	D	2004	NAG	C4-C5-C6-O6
12	D	2006	MJX	C14-C15-C18-N4
12	D	2006	MJX	C16-C15-C18-N5
12	B	2005	MJX	C7-C6-N1-C4
12	D	2006	MJX	C7-C6-N1-C4
12	D	2006	MJX	C13-C12-N3-C9

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 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	454/454 (100%)	1.00	45 (9%) 7 8	29, 41, 64, 104	0
1	C	453/454 (99%)	0.88	42 (9%) 8 9	36, 55, 80, 109	0
2	B	466/472 (98%)	1.33	85 (18%) 1 1	29, 63, 136, 158	0
2	D	471/472 (99%)	1.06	73 (15%) 2 1	38, 71, 123, 143	0
3	E	214/221 (96%)	2.70	111 (51%) 0 0	66, 115, 163, 188	0
3	H	216/221 (97%)	1.32	54 (25%) 0 0	47, 92, 138, 159	0
4	F	214/214 (100%)	2.42	98 (45%) 0 0	68, 114, 163, 186	0
4	L	214/214 (100%)	0.71	16 (7%) 14 15	53, 80, 104, 140	0
All	All	2702/2722 (99%)	1.29	524 (19%) 1 0	29, 68, 142, 188	0

All (524) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	165	LEU	12.8
3	E	212	VAL	12.7
4	L	214	CYS	12.3
2	B	33	LEU	11.9
3	E	216	ILE	11.3
4	F	125	LEU	11.3
2	B	77	SER	11.3
3	E	201	CYS	11.2
4	F	214	CYS	11.1
4	F	181	LEU	10.9
3	E	134	CYS	10.4
4	F	148	TRP	9.9
2	D	375	LEU	9.5
3	E	194	TRP	9.5
3	E	142	VAL	9.3
3	E	160	TRP	9.2

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Mol	Chain	Res	Type	RSRZ
3	E	133	VAL	9.0
4	F	206	VAL	9.0
4	F	126	THR	8.9
2	B	44	LEU	8.9
4	F	130	ALA	8.8
2	B	375	LEU	8.7
4	F	160	LEU	8.5
3	E	127	VAL	8.3
2	B	10	VAL	8.2
2	D	469	SER	8.1
2	D	33	LEU	8.1
3	E	144	LEU	8.1
3	H	165	LEU	8.1
2	B	34	GLY	8.0
3	H	216	ILE	7.9
3	E	219	ARG	7.7
2	B	49	CYS	7.4
4	F	119	PRO	7.4
2	B	1	GLY	7.3
3	E	129	PRO	7.3
2	B	51	PRO	7.2
4	L	212	ASN	7.2
4	F	122	SER	7.1
2	B	54	ILE	7.0
4	F	209	PHE	7.0
2	D	2	PRO	6.9
3	E	147	LEU	6.8
3	E	196	SER	6.8
2	B	2	PRO	6.8
3	H	134	CYS	6.8
4	F	135	PHE	6.7
3	E	169	VAL	6.6
3	E	128	TYR	6.6
4	F	201	SER	6.6
4	F	179	LEU	6.5
2	D	470	GLN	6.5
2	D	471	CYS	6.5
2	D	35	SER	6.5
4	F	194	CYS	6.4
3	E	132	PRO	6.4
4	F	180	THR	6.4
2	B	36	PRO	6.4

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Mol	Chain	Res	Type	RSRZ
4	F	120	PRO	6.4
3	E	205	HIS	6.4
4	F	115	VAL	6.3
3	E	192	SER	6.3
2	B	466	TRP	6.2
1	C	453	VAL	6.2
2	B	8	ARG	6.2
4	F	182	THR	6.2
2	D	181	LYS	6.2
4	F	150	ILE	6.1
1	A	337	PRO	6.0
2	B	45	LEU	6.0
3	E	168	GLY	6.0
4	F	213	GLU	6.0
3	H	189	VAL	6.0
2	B	4	ILE	6.0
2	B	46	LYS	6.0
4	F	136	LEU	6.0
2	D	34	GLY	5.9
3	H	133	VAL	5.9
2	B	32	PRO	5.9
3	E	140	SER	5.9
3	E	200	THR	5.9
2	B	376	ASN	5.9
3	E	203	VAL	5.8
3	E	218	PRO	5.8
2	D	8	ARG	5.8
3	E	131	ALA	5.7
2	D	48	ASN	5.7
2	B	181	LYS	5.7
4	F	117	ILE	5.7
2	D	1	GLY	5.6
3	H	201	CYS	5.6
2	D	7	THR	5.6
2	B	28	ASP	5.6
2	B	30	ALA	5.6
4	F	128	GLY	5.6
3	E	199	ILE	5.6
2	B	31	LEU	5.5
2	B	26	CYS	5.5
4	F	134	CYS	5.5
2	D	51	PRO	5.5

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Mol	Chain	Res	Type	RSRZ
2	D	468	GLY	5.4
3	H	203	VAL	5.3
2	D	4	ILE	5.3
3	E	183	LEU	5.3
3	E	210	THR	5.3
4	F	159	VAL	5.3
4	F	191	SER	5.3
3	E	146	CYS	5.3
2	D	46	LYS	5.2
2	D	54	ILE	5.2
4	F	132	VAL	5.2
3	E	177	GLN	5.1
4	F	193	THR	5.1
2	B	450	ASN	5.1
4	F	129	GLY	5.1
3	E	195	PRO	5.1
2	D	30	ALA	5.1
2	D	50	ALA	5.1
4	F	195	GLU	5.1
3	E	176	LEU	5.1
3	E	11	LEU	5.0
3	E	191	SER	5.0
3	H	160	TRP	5.0
4	F	210	ASN	5.0
4	F	157	ASN	5.0
2	B	76	ASP	4.9
4	F	205	ILE	4.9
3	H	158	LEU	4.9
2	D	9	GLY	4.9
2	B	9	GLY	4.9
4	F	197	THR	4.9
2	D	44	LEU	4.8
2	D	31	LEU	4.8
3	E	198	SER	4.8
3	E	167	SER	4.7
4	F	156	GLN	4.7
3	E	143	THR	4.6
1	C	320	ARG	4.6
3	E	217	GLU	4.6
4	F	204	PRO	4.6
3	E	141	SER	4.6
4	F	178	THR	4.6

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Mol	Chain	Res	Type	RSRZ
2	D	36	PRO	4.6
2	D	32	PRO	4.5
2	D	52	GLU	4.5
1	C	337	PRO	4.5
4	F	190	ASN	4.5
4	F	118	PHE	4.5
2	B	42	GLU	4.5
2	B	48	ASN	4.4
2	B	53	SER	4.4
3	H	192	SER	4.4
1	A	454	VAL	4.4
3	E	12	VAL	4.4
4	L	213	GLU	4.4
3	H	218	PRO	4.3
3	H	144	LEU	4.3
4	F	146	VAL	4.3
4	F	152	GLY	4.2
3	E	115	VAL	4.2
2	D	376	ASN	4.2
2	D	42	GLU	4.2
4	F	154	GLU	4.2
3	E	175	VAL	4.2
3	H	198	SER	4.2
4	F	144	ILE	4.2
4	F	145	ASN	4.2
4	F	200	THR	4.2
3	H	196	SER	4.2
2	D	40	LEU	4.2
3	E	215	LYS	4.2
4	F	163	TRP	4.1
2	B	455	PHE	4.1
3	E	148	VAL	4.1
2	D	380	ILE	4.1
3	H	166	SER	4.1
2	B	452	ASN	4.1
4	F	151	ASP	4.0
4	F	174	SER	4.0
4	F	113	PRO	4.0
2	D	378	GLU	4.0
3	E	130	LEU	4.0
4	F	186	TYR	4.0
1	A	339	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
3	H	219	ARG	4.0
3	H	217	GLU	4.0
4	F	15	LEU	3.9
4	F	147	LYS	3.9
3	E	162	SER	3.9
3	H	167	SER	3.9
3	H	199	ILE	3.9
2	B	451	GLY	3.9
2	D	53	SER	3.9
3	H	162	SER	3.9
2	B	35	SER	3.8
2	B	440	GLN	3.8
3	E	8	GLY	3.8
4	F	133	VAL	3.8
2	B	50	ALA	3.8
3	H	195	PRO	3.8
4	F	192	TYR	3.8
3	H	159	THR	3.8
2	B	380	ILE	3.7
2	D	3	ASN	3.7
2	B	29	GLU	3.7
4	F	212	ASN	3.7
2	D	79	GLN	3.7
3	E	204	ALA	3.7
2	B	55	GLU	3.7
3	H	211	LYS	3.7
4	L	111	ALA	3.7
3	E	156	VAL	3.7
3	H	138	THR	3.7
4	F	158	GLY	3.6
3	H	130	LEU	3.6
4	F	202	THR	3.6
3	E	16	ALA	3.6
3	E	193	THR	3.6
1	C	338	HIS	3.6
3	H	194	TRP	3.6
2	B	7	THR	3.6
3	E	123	THR	3.6
3	E	145	GLY	3.6
3	E	164	SER	3.6
3	E	83	LEU	3.5
2	B	379	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	378	GLU	3.5
3	E	25	SER	3.5
2	B	129	TRP	3.5
3	E	187	VAL	3.5
3	E	124	ALA	3.5
1	C	171	PHE	3.5
3	E	178	SER	3.5
2	D	10	VAL	3.5
1	A	217	SER	3.5
4	F	127	SER	3.5
4	F	103	LYS	3.5
4	F	107	LYS	3.5
2	B	47	ASP	3.4
3	H	157	THR	3.4
4	F	153	SER	3.4
4	F	149	LYS	3.4
3	H	131	ALA	3.4
2	B	6	THR	3.4
1	A	183	LEU	3.4
1	C	339	ALA	3.3
2	D	383	LEU	3.3
2	D	466	TRP	3.3
3	E	65	GLN	3.3
2	B	404	ARG	3.3
3	E	29	ILE	3.3
3	E	188	THR	3.3
3	H	208	SER	3.3
3	E	82	GLN	3.3
4	L	206	VAL	3.3
4	F	14	SER	3.3
1	C	131	PHE	3.3
4	F	83	PHE	3.3
2	D	45	LEU	3.3
3	H	187	VAL	3.3
2	B	437	CYS	3.3
4	F	106	ILE	3.3
3	E	189	VAL	3.2
3	E	121	LYS	3.2
2	B	39	ASP	3.2
1	A	171	PHE	3.2
2	B	27	SER	3.2
2	B	67	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	47	GLN	3.1
4	F	207	LYS	3.1
4	F	123	GLU	3.1
2	B	381	PRO	3.1
2	D	382	GLY	3.1
3	E	64	PHE	3.1
4	F	114	THR	3.1
3	E	120	ALA	3.1
1	A	45	PRO	3.1
2	B	178	TYR	3.1
3	E	17	SER	3.1
3	E	85	SER	3.1
3	H	142	VAL	3.1
2	B	79	GLN	3.1
3	E	213	ASP	3.1
2	B	442	GLU	3.1
1	A	336	GLY	3.0
2	B	377	ASN	3.0
3	E	206	PRO	3.0
2	D	29	GLU	3.0
3	H	200	THR	3.0
4	F	189	HIS	3.0
2	D	58	VAL	3.0
3	H	17	SER	3.0
3	H	209	SER	3.0
1	C	183	LEU	3.0
4	F	184	ASP	3.0
4	F	169	LYS	3.0
1	A	186	PRO	3.0
3	H	169	VAL	3.0
3	E	13	LYS	3.0
4	F	208	SER	2.9
4	L	78	LEU	2.9
1	C	319	ASP	2.9
2	B	265	ILE	2.9
3	E	54	ALA	2.9
1	A	194	LEU	2.9
2	D	39	ASP	2.9
3	E	179	ASP	2.9
1	A	235	TRP	2.9
1	A	338	HIS	2.9
3	E	66	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
3	H	124	ALA	2.9
2	B	382	GLY	2.8
2	B	458	GLY	2.8
4	L	127	SER	2.8
2	D	258	LEU	2.8
4	L	125	LEU	2.8
2	B	374	CYS	2.8
2	B	460	CYS	2.8
1	A	185	ALA	2.8
4	F	167	ASP	2.8
3	H	164	SER	2.8
2	B	22	MET	2.8
4	F	188	ARG	2.8
1	C	213	LEU	2.8
2	D	450	ASN	2.8
4	F	111	ALA	2.8
4	L	118	PHE	2.8
3	E	126	SER	2.8
2	D	22	MET	2.8
4	F	170	ASP	2.8
1	A	288	TYR	2.7
1	C	143	TYR	2.7
4	F	60	SER	2.7
2	D	377	ASN	2.7
3	E	92	ALA	2.7
3	E	42	GLU	2.7
2	B	462	CYS	2.7
2	D	38	CYS	2.7
3	E	153	PRO	2.7
1	C	191	PHE	2.7
3	E	202	ASN	2.7
2	D	62	ARG	2.7
1	C	195	LEU	2.7
2	D	5	CYS	2.7
3	E	80	TYR	2.7
4	F	203	SER	2.7
2	B	446	HIS	2.7
1	A	195	LEU	2.7
1	A	190	TYR	2.7
2	B	38	CYS	2.7
2	D	449	ASN	2.7
3	H	121	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	335	ARG	2.7
3	H	161	ASN	2.7
2	D	78	SER	2.6
4	L	129	GLY	2.6
3	E	3	GLN	2.6
1	A	248	LEU	2.6
1	A	130	CYS	2.6
2	B	449	ASN	2.6
3	E	77	ASN	2.6
3	E	171	THR	2.6
4	F	121	SER	2.6
3	E	163	GLY	2.6
3	E	149	LYS	2.6
1	C	130	CYS	2.6
2	B	373	THR	2.6
1	C	194	LEU	2.6
1	A	175	VAL	2.6
2	D	43	ASN	2.6
3	E	117	VAL	2.6
1	A	436	ILE	2.6
4	L	126	THR	2.6
1	A	181	LEU	2.6
1	A	47	GLN	2.6
4	F	143	ASP	2.6
2	D	451	GLY	2.6
2	D	436	ALA	2.5
3	E	114	SER	2.5
4	F	105	GLU	2.5
3	H	213	ASP	2.5
2	D	49	CYS	2.5
2	D	398	SER	2.5
2	D	440	GLN	2.5
1	C	109	PRO	2.5
1	C	340	LEU	2.5
2	B	52	GLU	2.5
4	F	116	SER	2.5
4	F	177	SER	2.5
3	E	158	LEU	2.5
3	E	190	THR	2.5
2	D	446[A]	HIS	2.5
3	E	180	LEU	2.5
4	F	78	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	196	ALA	2.5
4	F	173	TYR	2.5
4	F	155	ARG	2.5
2	B	25	TRP	2.5
3	E	155	PRO	2.5
1	A	167	CYS	2.5
2	D	75	GLY	2.5
4	F	112	ALA	2.5
4	F	139	PHE	2.5
1	A	421	LEU	2.4
3	H	129	PRO	2.4
3	E	172	PHE	2.4
4	F	8	PRO	2.4
3	E	86	LEU	2.4
2	D	47	ASP	2.4
3	H	215	LYS	2.4
4	L	171	SER	2.4
3	H	177	GLN	2.4
2	D	55	GLU	2.4
3	E	185	SER	2.4
1	A	216	VAL	2.4
4	F	124	GLN	2.4
2	D	6	THR	2.4
2	D	437	CYS	2.4
3	E	116	THR	2.4
2	B	62	ARG	2.4
1	C	336	GLY	2.4
2	B	262	LEU	2.4
1	C	141	ALA	2.4
2	D	404	ARG	2.4
3	E	211	LYS	2.4
3	H	188	THR	2.4
1	A	146	CYS	2.3
1	A	239[A]	VAL	2.3
2	D	27	SER	2.3
2	D	61	ALA	2.3
3	H	168	GLY	2.3
1	C	421	LEU	2.3
3	H	139	GLY	2.3
3	H	191	SER	2.3
2	D	19	VAL	2.3
1	C	95	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
4	F	161	ASN	2.3
1	C	172	SER	2.3
2	D	262	LEU	2.3
3	E	19	LYS	2.3
3	E	209	SER	2.3
2	B	37	ARG	2.3
3	H	207	ALA	2.3
4	F	11	MET	2.3
2	B	95	ASP	2.3
3	E	214	LYS	2.3
3	H	183	LEU	2.3
2	B	372	ALA	2.3
2	B	459	VAL	2.3
1	C	110	TRP	2.3
1	C	132	LEU	2.2
2	B	317	LEU	2.2
3	E	5	GLN	2.2
3	E	18	VAL	2.2
2	B	98	LYS	2.2
2	B	445	SER	2.2
2	D	381	PRO	2.2
4	F	109	ALA	2.2
3	E	161	ASN	2.2
4	L	157	ASN	2.2
1	A	166	TYR	2.2
1	C	380	TYR	2.2
1	A	182	VAL	2.2
1	A	193	GLY	2.2
1	C	182	VAL	2.2
2	B	11	SER	2.2
2	D	276	GLY	2.2
3	E	84	SER	2.2
3	H	132	PRO	2.2
2	B	258	LEU	2.2
3	E	20	LEU	2.2
2	D	28	ASP	2.2
4	F	185	GLU	2.2
1	C	108	ALA	2.2
3	E	207	ALA	2.2
4	L	130	ALA	2.2
1	A	172	SER	2.2
1	A	407	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	H	147	LEU	2.2
1	A	200	VAL	2.2
1	C	389	VAL	2.2
1	C	249	ASN	2.2
1	A	233	GLY	2.2
2	B	383	LEU	2.1
1	C	169	ALA	2.1
2	B	447	ARG	2.1
3	H	140	SER	2.1
1	C	186	PRO	2.1
1	A	192	LEU	2.1
1	C	23	LEU	2.1
1	A	236	GLY	2.1
1	C	38	GLY	2.1
1	C	234	TYR	2.1
4	L	41	GLY	2.1
3	E	88	SER	2.1
1	C	170	GLY	2.1
1	A	173	SER	2.1
1	A	378	ALA	2.1
1	C	106	ALA	2.1
2	B	289	TYR	2.1
3	E	181	TYR	2.1
3	H	123	THR	2.1
1	C	358[A]	SER	2.1
2	B	392	GLY	2.1
2	D	41	LYS	2.1
4	F	80	SER	2.1
4	L	205	ILE	2.1
2	B	268	PRO	2.1
2	D	57	PRO	2.1
3	H	190	THR	2.1
1	A	191	PHE	2.1
4	F	175	MET	2.0
1	C	127	VAL	2.0
2	B	314	VAL	2.0
1	A	61	GLU	2.0
1	A	255	VAL	2.0
1	A	319	ASP	2.0
4	F	131	SER	2.0
1	A	23	LEU	2.0
1	A	213	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
3	E	157	THR	2.0
3	E	40	ARG	2.0
1	A	184	GLY	2.0
1	C	187	GLY	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](#)

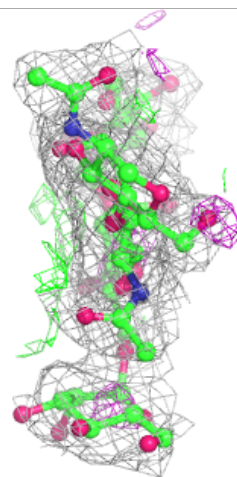
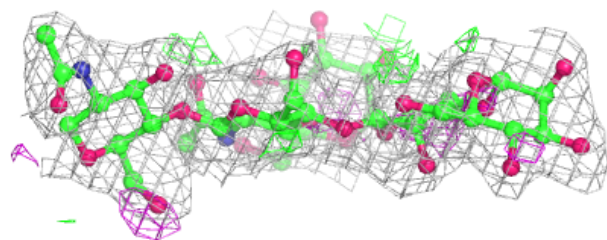
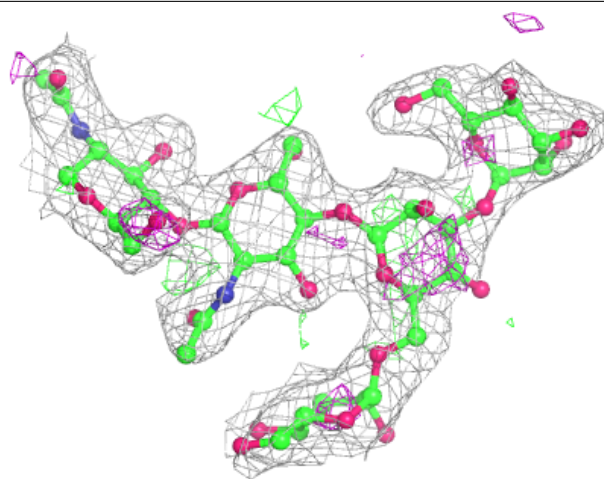
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	MAN	J	4	11/12	0.69	0.34	96,96,96,96	0
7	BMA	J	3	11/12	0.70	0.40	96,96,96,96	0
5	BMA	G	3	11/12	0.72	0.24	88,88,88,88	0
5	MAN	G	4	11/12	0.81	0.20	84,84,84,84	0
6	NAG	K	2	14/15	0.81	0.26	102,102,102,102	0
5	MAN	G	5	11/12	0.83	0.29	98,98,98,98	0
7	NAG	J	2	14/15	0.84	0.31	82,82,82,82	0
5	NAG	G	2	14/15	0.88	0.12	69,69,69,69	0
6	NAG	K	1	14/15	0.88	0.20	97,97,97,97	0
7	NAG	J	1	14/15	0.89	0.15	65,65,65,65	0
6	NAG	I	1	14/15	0.91	0.26	93,93,93,93	0
6	NAG	I	2	14/15	0.92	0.23	98,98,98,98	0
5	NAG	G	1	14/15	0.93	0.13	51,51,51,51	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.

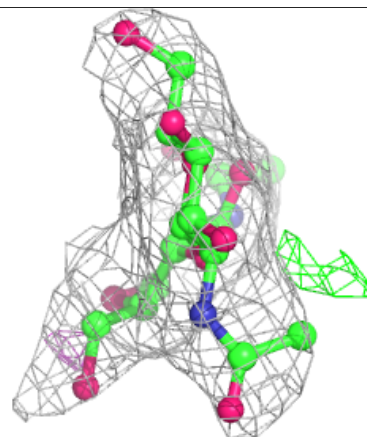
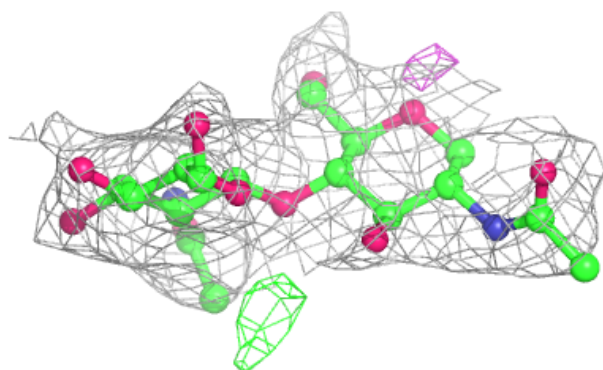
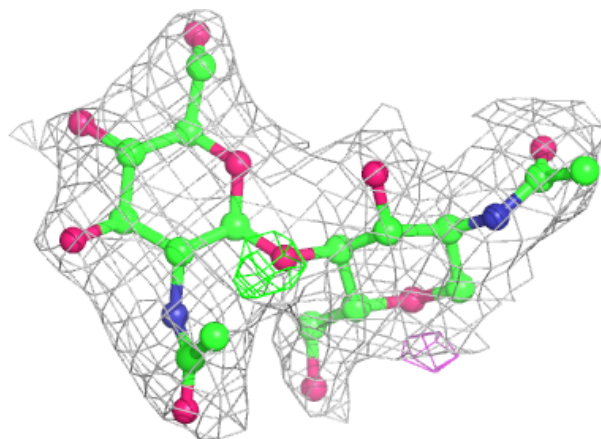
Electron density around Chain G:

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



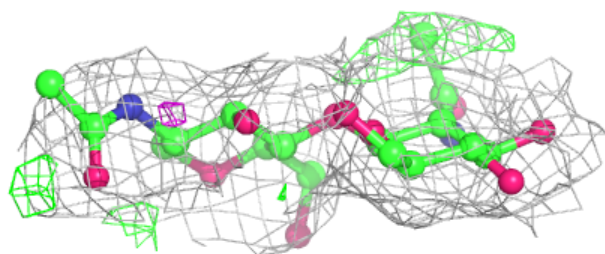
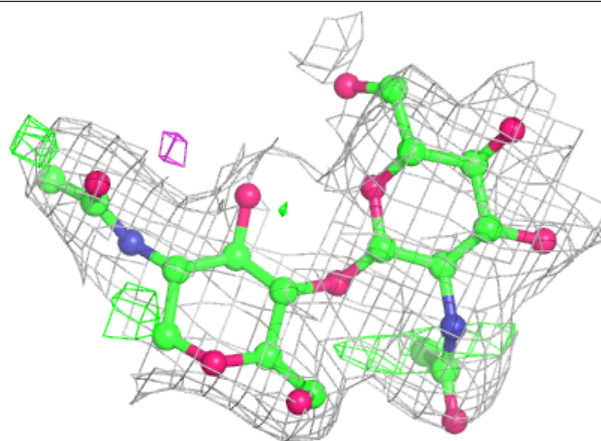
Electron density around Chain I:

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

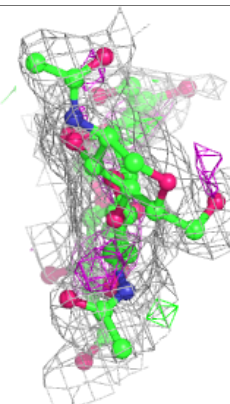
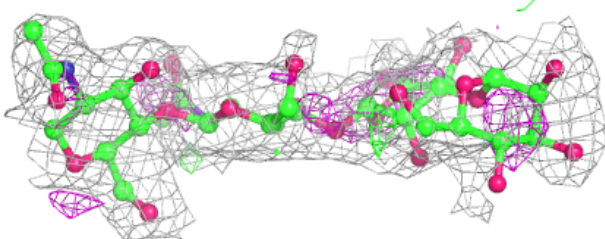
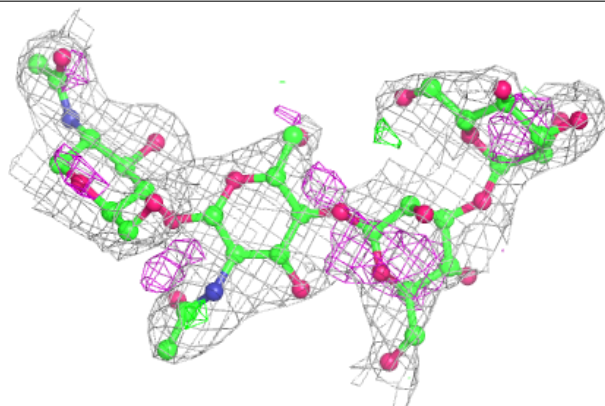


Electron density around Chain K:

$2mF_o-DF_c$ (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 ⓘ

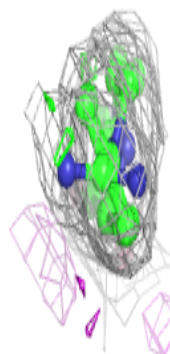
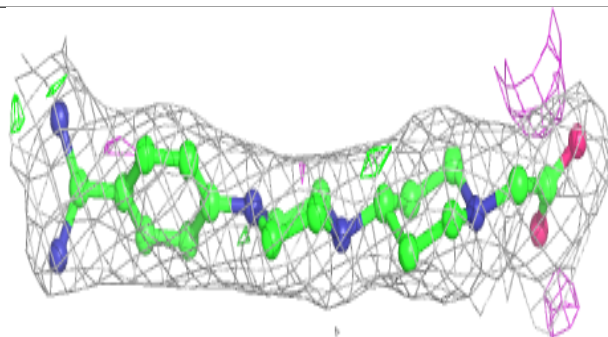
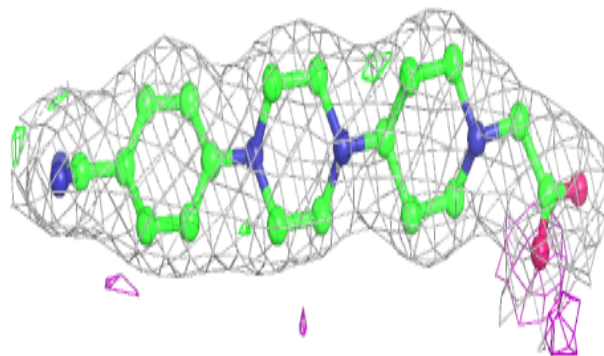
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	NAG	D	2004	14/15	0.78	0.27	96,96,96,96	0
8	SO4	C	502	5/5	0.82	0.28	89,89,89,89	0
8	SO4	A	508	5/5	0.82	0.22	91,91,91,91	0
8	SO4	A	507	5/5	0.85	0.20	80,80,80,80	0
8	SO4	A	509	5/5	0.86	0.25	73,73,73,73	0
9	CA	C	505	1/1	0.87	0.06	71,71,71,71	0
11	NAG	B	2004	14/15	0.89	0.29	101,101,101,101	0
8	SO4	C	501	5/5	0.89	0.19	83,83,83,83	0
8	SO4	A	501	5/5	0.91	0.18	70,70,70,70	0
10	MN	B	2002	1/1	0.92	0.13	73,73,73,73	0
13	CL	C	504	1/1	0.93	0.32	80,80,80,80	0
8	SO4	C	503	5/5	0.94	0.20	98,98,98,98	0
9	CA	C	508	1/1	0.94	0.11	53,53,53,53	0
8	SO4	C	509	5/5	0.94	0.24	90,90,90,90	0
13	CL	D	2005	1/1	0.94	0.22	84,84,84,84	0
8	SO4	B	2006	5/5	0.95	0.21	45,45,45,45	5
12	MJX	D	2006	25/25	0.95	0.16	51,51,51,51	0
8	SO4	D	2007	5/5	0.96	0.17	55,55,55,55	5
9	CA	C	507	1/1	0.96	0.15	53,53,53,53	0
8	SO4	L	301	5/5	0.96	0.25	85,85,85,85	0
12	MJX	B	2005	25/25	0.97	0.19	39,39,39,39	0
10	MN	D	2002	1/1	0.97	0.09	59,59,59,59	0
9	CA	C	506	1/1	0.97	0.07	60,60,60,60	0
9	CA	A	503	1/1	0.97	0.07	44,44,44,44	0
8	SO4	A	502	5/5	0.98	0.11	60,60,60,60	0
9	CA	A	505	1/1	0.98	0.17	34,34,34,34	0
10	MN	B	2003	1/1	0.99	0.14	34,34,34,34	0
10	MN	D	2001	1/1	0.99	0.14	43,43,43,43	0
9	CA	A	506	1/1	0.99	0.16	36,36,36,36	0
10	MN	D	2003	1/1	0.99	0.12	44,44,44,44	0
9	CA	A	504	1/1	0.99	0.12	36,36,36,36	0
10	MN	B	2001	1/1	1.00	0.22	34,34,34,34	0

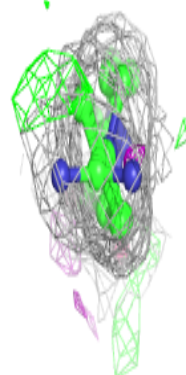
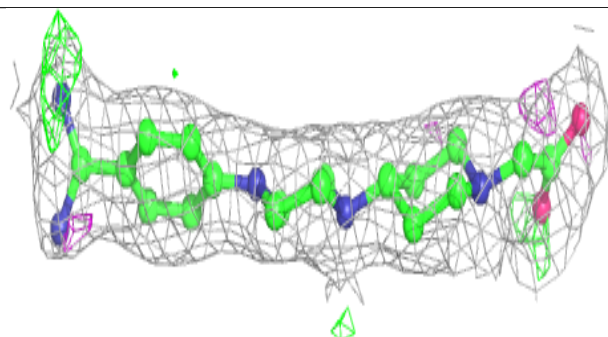
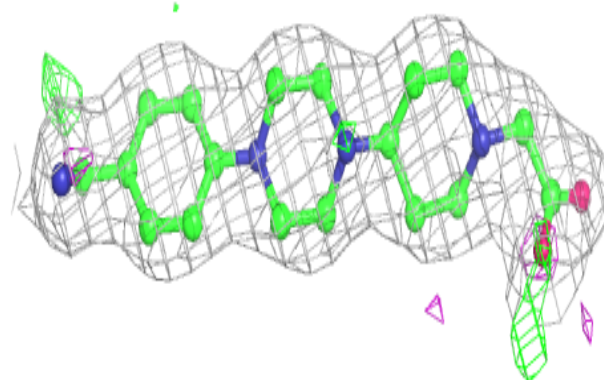
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MJX D 2006:

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

**Electron density around MJX 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.