wwPDB X-ray Structure Validation Summary Report (i)

Oct 14, 2023 – 06:13 PM EDT

PDB ID	:	7L8P
Title	:	Integrin alphaIIbbeta3 in complex with sibrafiban
Authors	:	Lin, F.-Y.; Springer, T.A.
Deposited on	:	2020-12-31
Resolution	:	2.35 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

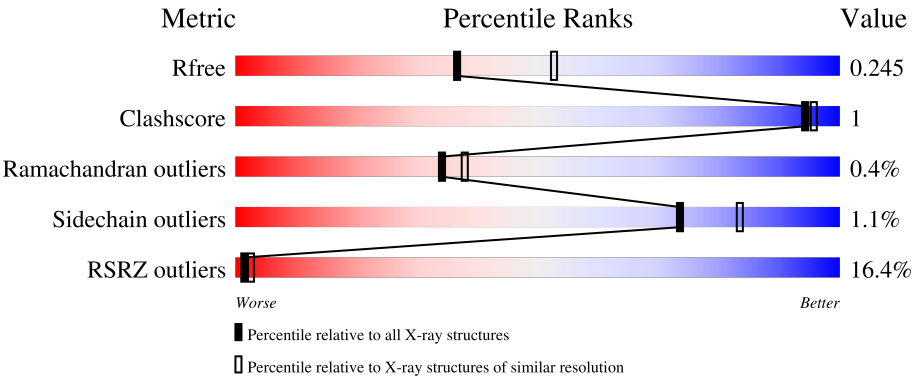
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (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 <=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	7% 96%
1	C	457	9% 95%
2	B	472	15% 93% 6%
2	D	472	14% 96%
3	E	221	48% 94%

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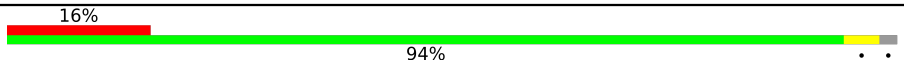
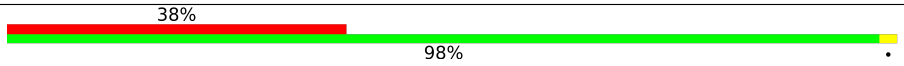
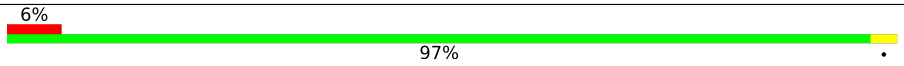
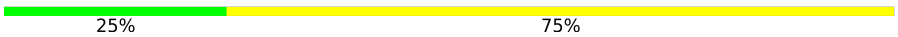
Mol	Chain	Length	Quality of chain
3	H	221	
4	F	214	
4	L	214	
5	G	5	
6	I	2	
6	K	2	
7	J	4	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CL	C	504	-	-	-	X

2 Entry composition (i)

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			

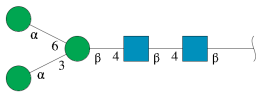
- Molecule 3 is a protein called Monoclonal antibody 10E5 heavy chain.

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			

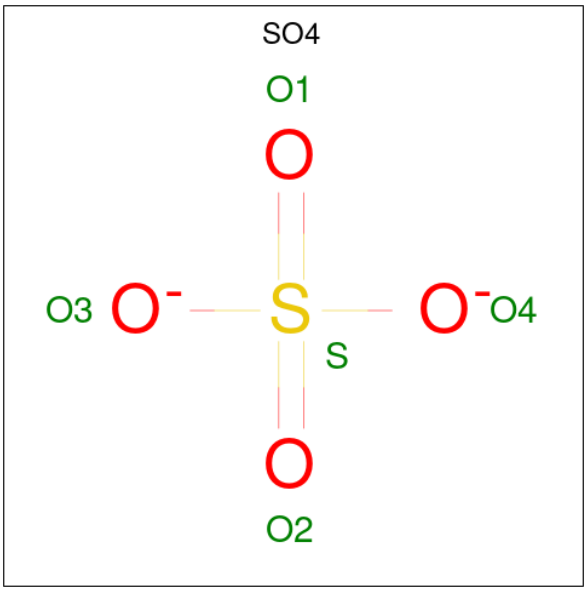
- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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.

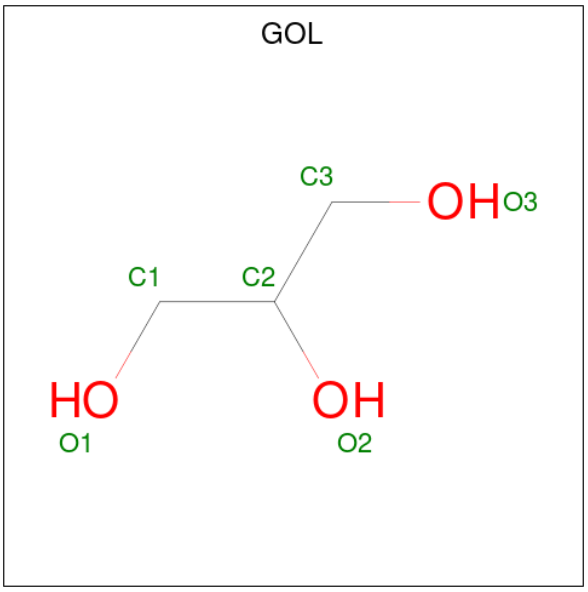
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	J	4	Total	C	H	N	O	0	0	0
			97	28	47	2	20			

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

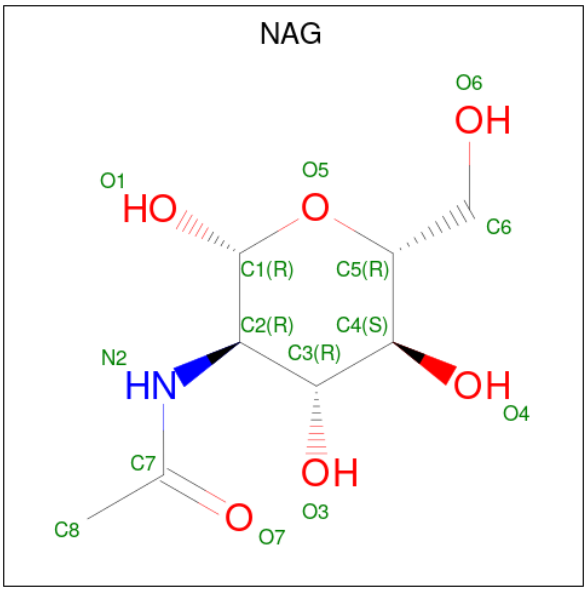
- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

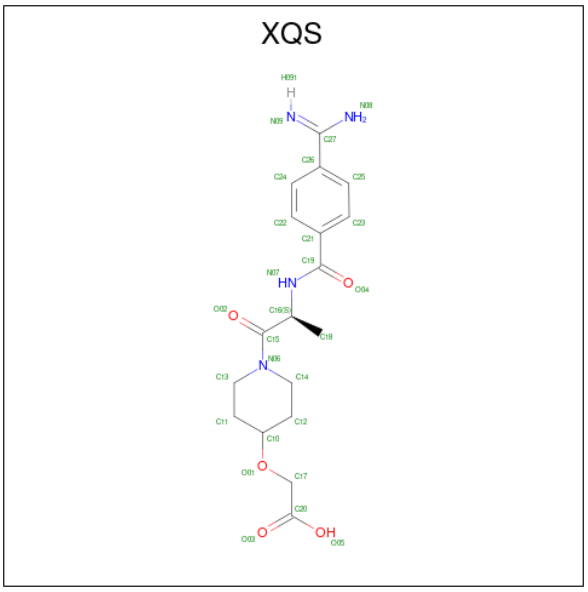
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total Mg 1 1	0	0
11	D	1	Total Mg 1 1	0	0

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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 sibrafiban (active form) (three-letter code: 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 (three-letter code: CL) (formula: Cl).

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

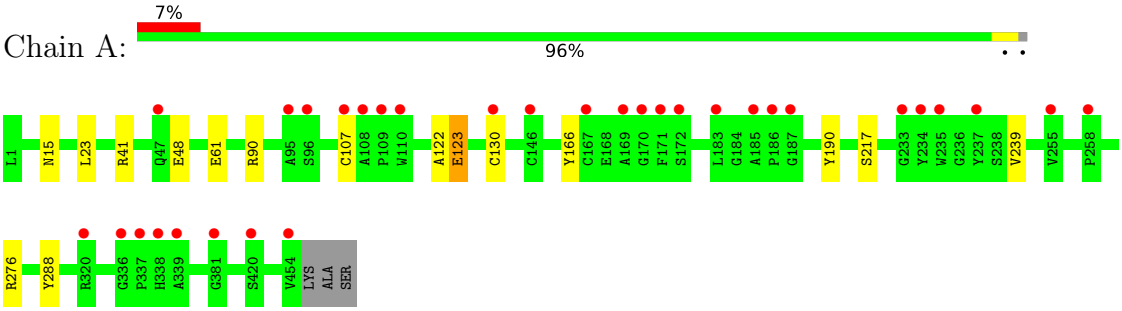
- Molecule 15 is water.

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		

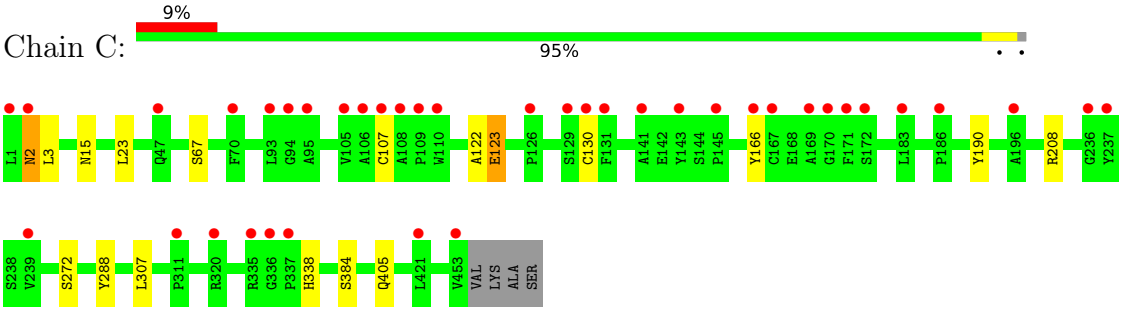
3 Residue-property plots (i)

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.

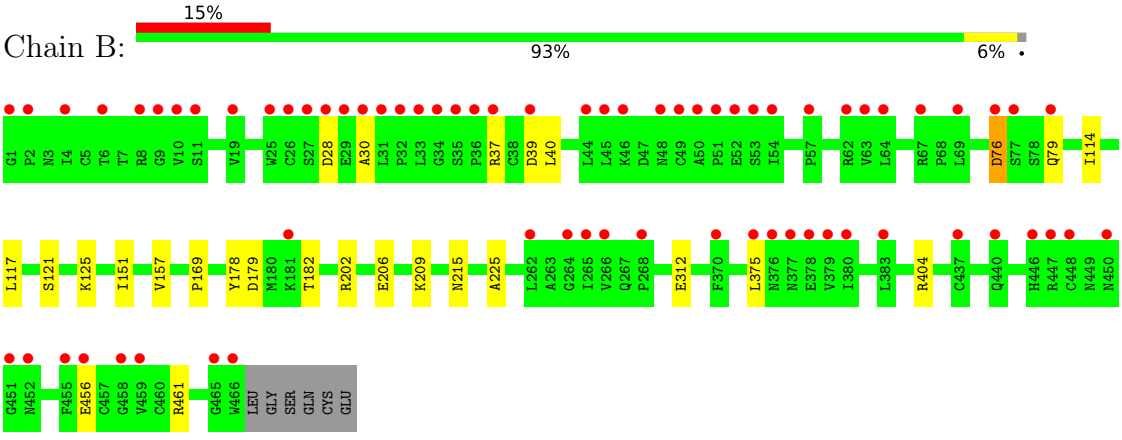
• Molecule 1: Isoform 3 of Integrin alpha-IIb



• Molecule 1: Isoform 3 of Integrin alpha-IIb

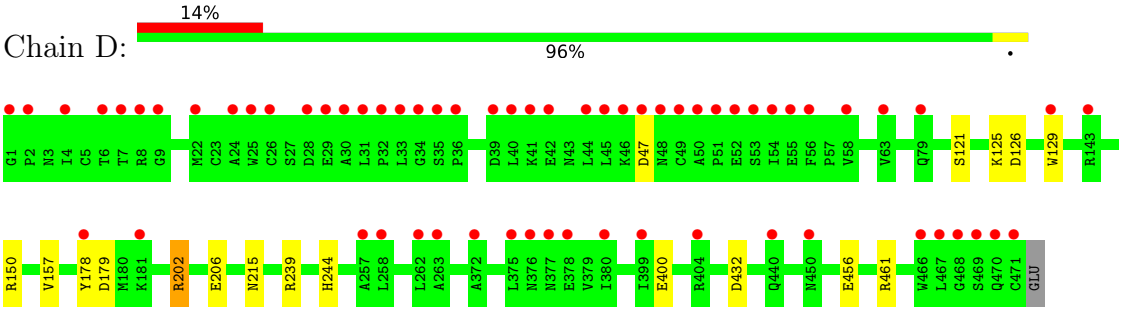


• Molecule 2: Isoform Beta-3C of Integrin beta-3



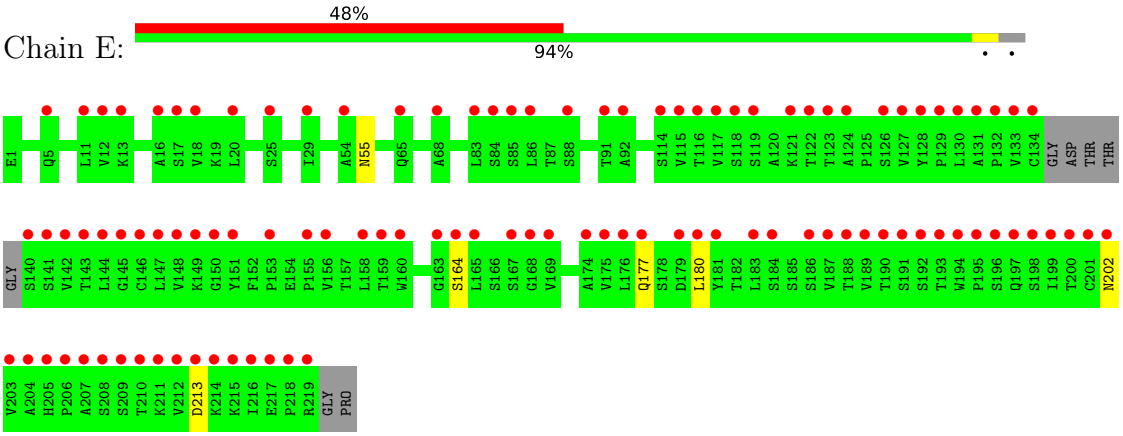
• Molecule 2: Isoform Beta-3C of Integrin beta-3

Chain D:



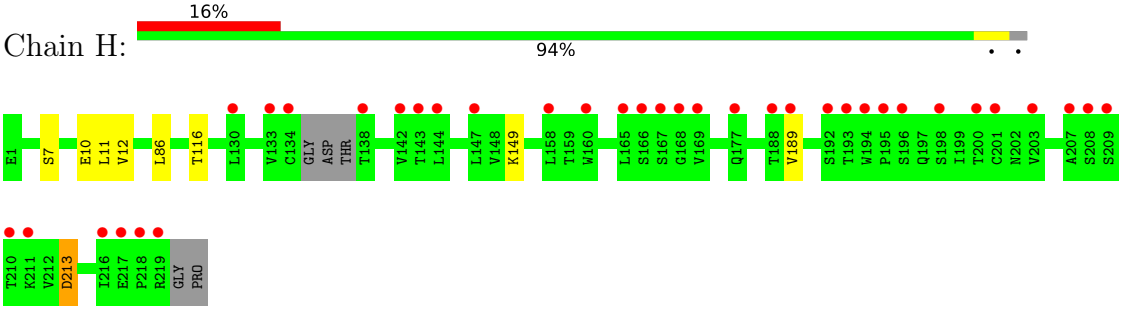
• Molecule 3: Monoclonal antibody 10E5 heavy chain

Chain E:



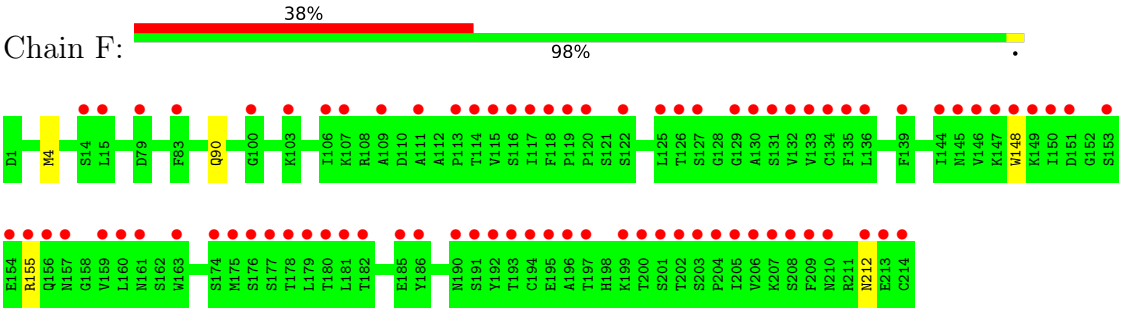
• Molecule 3: Monoclonal antibody 10E5 heavy chain

Chain H:



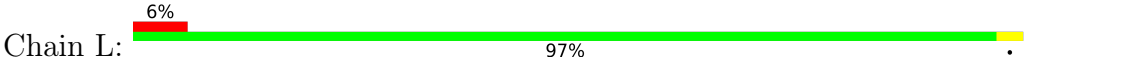
• Molecule 4: Monoclonal antibody 10E5 light chain

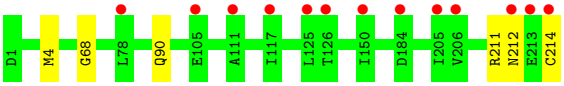
Chain F:



• Molecule 4: Monoclonal antibody 10E5 light chain

Chain L:



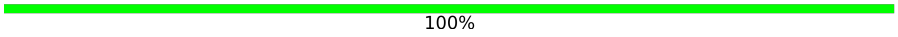


• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

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

Chain I:



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

Chain K:

• 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:

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 0.203 , 0.245	Depositor DCC
R_{free} test set	1992 reflections (1.24%)	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 , 49.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, GOL, CA, XQS, SO4, BMA, CL, MAN, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.30	0/3659	0.52	2/4986 (0.0%)
1	C	0.28	0/3618	0.48	0/4930
2	B	0.26	0/3743	0.46	0/5074
2	D	0.27	0/3726	0.46	0/5052
3	E	0.25	0/1673	0.44	0/2290
3	H	0.27	0/1684	0.46	0/2305
4	F	0.25	0/1673	0.43	0/2269
4	L	0.26	0/1673	0.46	0/2269
All	All	0.27	0/21449	0.47	2/29175 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	239[A]	VAL	CG1-CB-CG2	7.21	122.43	110.90
1	A	239[B]	VAL	CG1-CB-CG2	7.21	122.43	110.90

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	3532	3387	3371	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3502	3338	3320	6	0
2	B	3634	3568	3531	14	0
2	D	3645	3561	3549	13	0
3	E	1631	1590	1590	3	0
3	H	1642	1600	1600	5	0
4	F	1637	1553	1553	2	0
4	L	1637	1553	1553	3	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	3	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.

The worst 5 of 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
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

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	462/457 (101%)	445 (96%)	16 (4%)	1 (0%)	47	55
1	C	457/457 (100%)	443 (97%)	13 (3%)	1 (0%)	47	55
2	B	474/472 (100%)	453 (96%)	18 (4%)	3 (1%)	25	26
2	D	472/472 (100%)	447 (95%)	24 (5%)	1 (0%)	47	55
3	E	210/221 (95%)	190 (90%)	18 (9%)	2 (1%)	15	14
3	H	212/221 (96%)	199 (94%)	12 (6%)	1 (0%)	29	31
4	F	212/214 (99%)	194 (92%)	17 (8%)	1 (0%)	29	31
4	L	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	29	31
All	All	2711/2728 (99%)	2574 (95%)	126 (5%)	11 (0%)	34	38

5 of 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

5.3.2 Protein sidechains (i)

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%)	365 (98%)	6 (2%)	62 74
1	C	366/364 (100%)	356 (97%)	10 (3%)	44 55
2	B	422/417 (101%)	419 (99%)	3 (1%)	84 90
2	D	419/417 (100%)	415 (99%)	4 (1%)	76 85
3	E	186/190 (98%)	186 (100%)	0	100 100
3	H	187/190 (98%)	185 (99%)	2 (1%)	73 83
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%)	2302 (99%)	25 (1%)	73 83

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	190	TYR
1	C	307	LEU
3	H	213	ASP
1	C	288	TYR
1	C	338	HIS

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

13 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	G	1	2,5	14,14,15	0.39	0	17,19,21	0.48	0
5	NAG	G	2	5	14,14,15	0.43	0	17,19,21	0.59	0
5	BMA	G	3	5	11,11,12	0.88	0	15,15,17	0.79	0
5	MAN	G	4	5	11,11,12	0.61	0	15,15,17	1.19	2 (13%)
5	MAN	G	5	5	11,11,12	0.81	0	15,15,17	1.15	2 (13%)
6	NAG	I	1	2,6	14,14,15	0.51	0	17,19,21	0.47	0
6	NAG	I	2	6	14,14,15	0.14	0	17,19,21	0.59	0
7	NAG	J	1	2,7	14,14,15	0.17	0	17,19,21	0.57	0
7	NAG	J	2	7	14,14,15	0.65	1 (7%)	17,19,21	0.53	0
7	BMA	J	3	7	11,11,12	0.70	0	15,15,17	0.88	1 (6%)
7	MAN	J	4	7	11,11,12	0.71	0	15,15,17	0.97	1 (6%)
6	NAG	K	1	2,6	14,14,15	0.56	0	17,19,21	0.42	0
6	NAG	K	2	6	14,14,15	0.18	0	17,19,21	0.62	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	-	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	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	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	J	4	7	-	0/2/19/22	0/1/1/1
6	NAG	K	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	2	NAG	O5-C1	-2.29	1.40	1.43

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	4	MAN	C1-O5-C5	3.33	116.70	112.19
5	G	5	MAN	C1-O5-C5	2.69	115.83	112.19
7	J	4	MAN	C1-O5-C5	2.49	115.56	112.19
5	G	5	MAN	O2-C2-C3	-2.28	105.58	110.14
5	G	4	MAN	O2-C2-C3	-2.16	105.81	110.14

There are no chirality outliers.

5 of 6 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
5	G	5	MAN	O5-C5-C6-O6

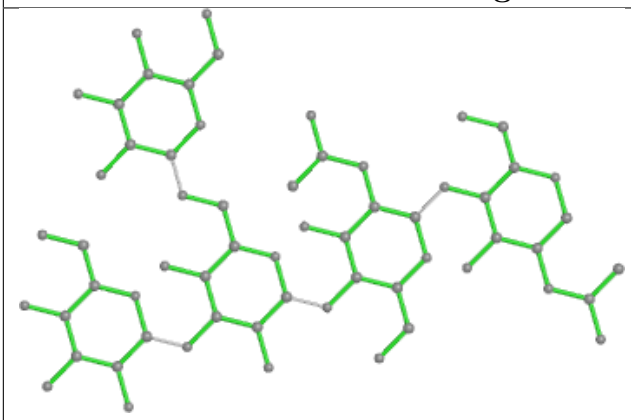
There are no ring outliers.

1 monomer is involved in 1 short contact:

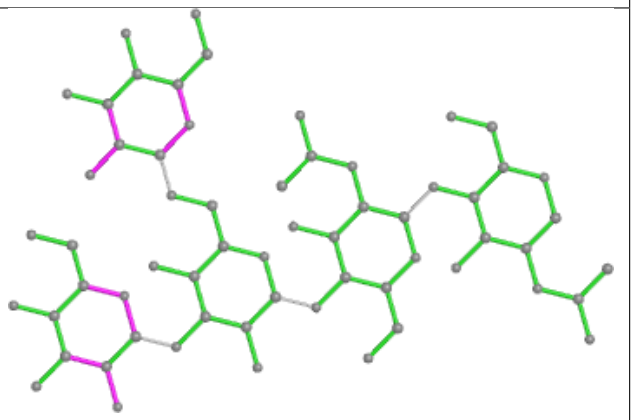
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	1	NAG	1	0

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

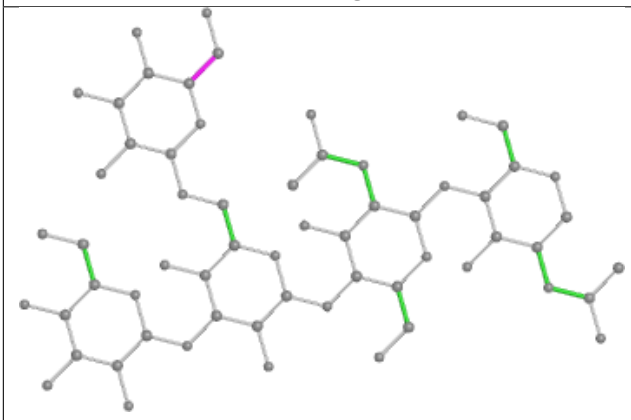
Oligosaccharide Chain G



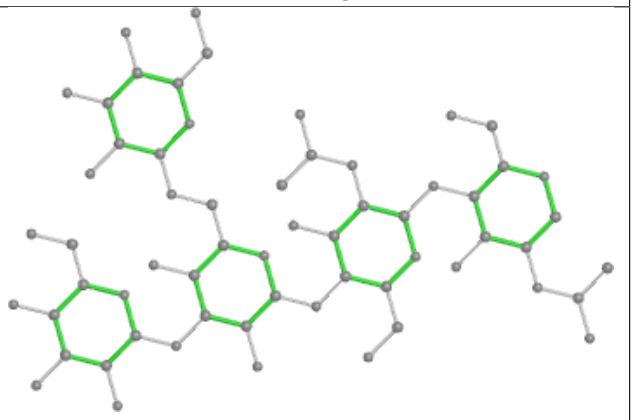
Bond lengths



Bond angles

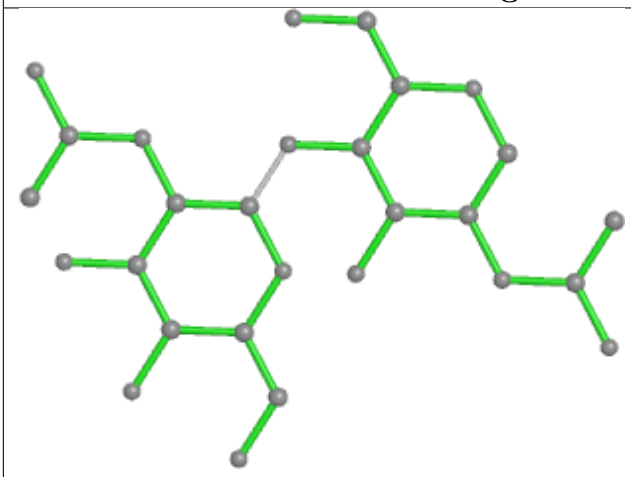


Torsions

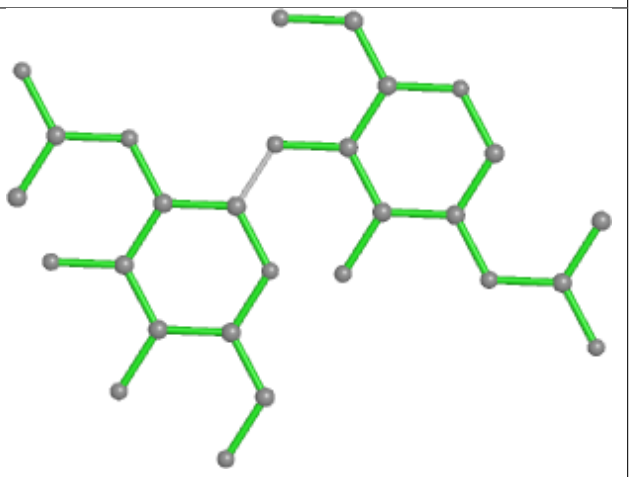


Rings

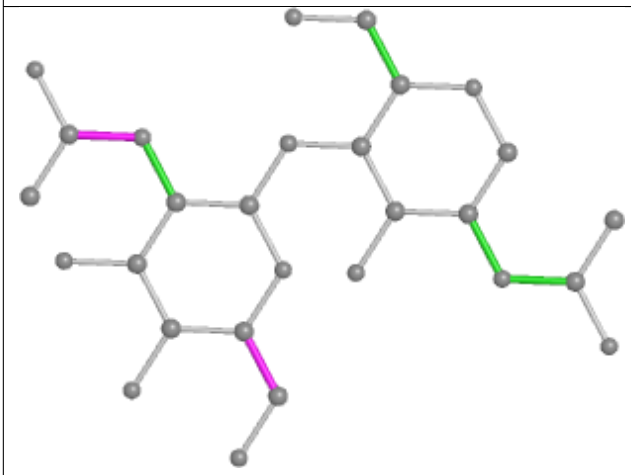
Oligosaccharide Chain I



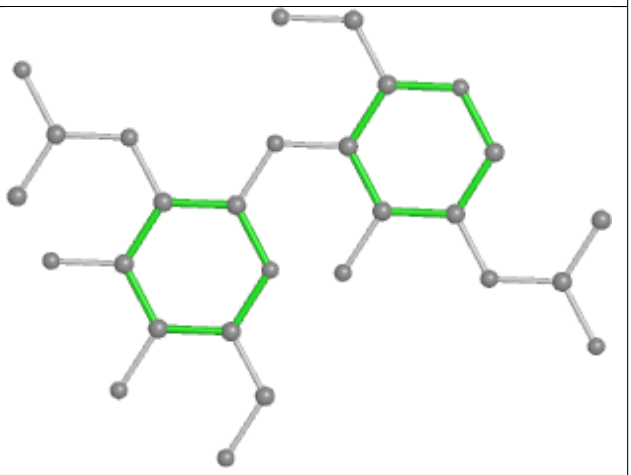
Bond lengths



Bond angles

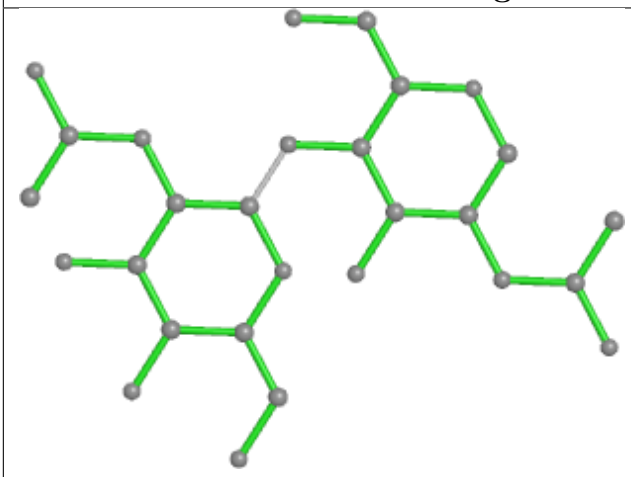


Torsions

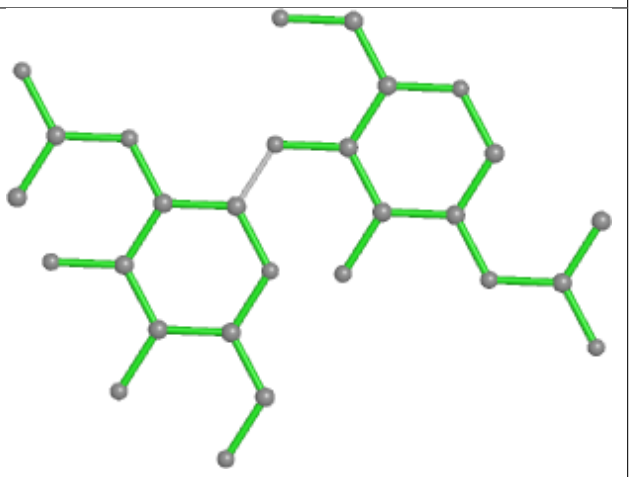


Rings

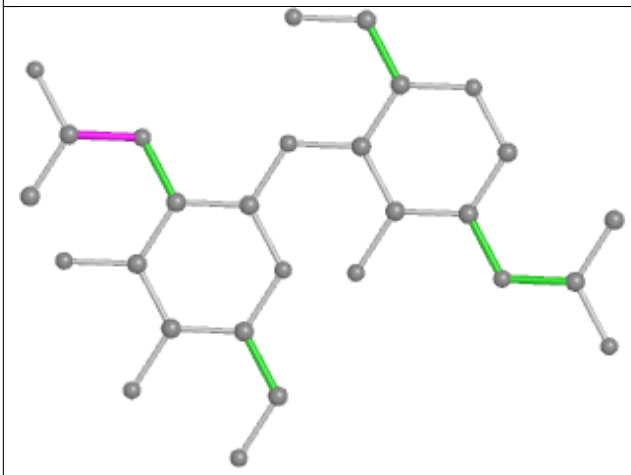
Oligosaccharide Chain K



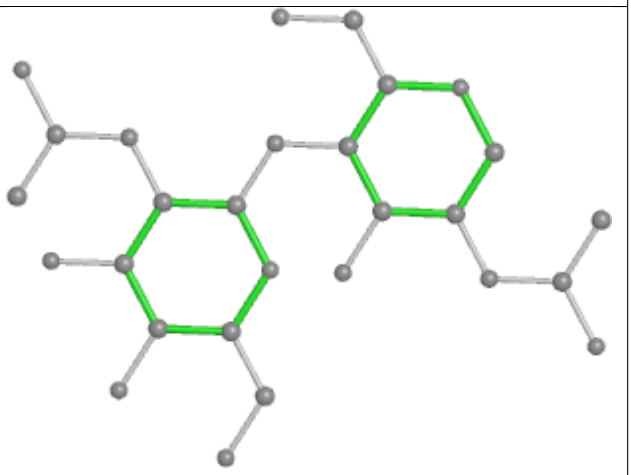
Bond lengths



Bond angles

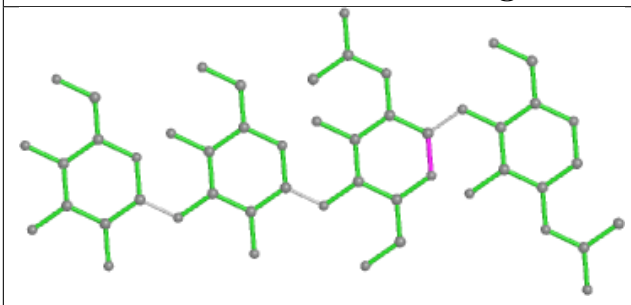


Torsions

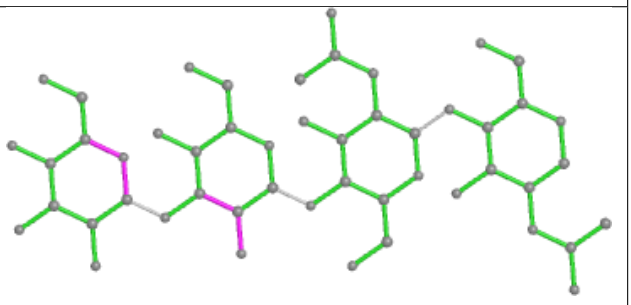


Rings

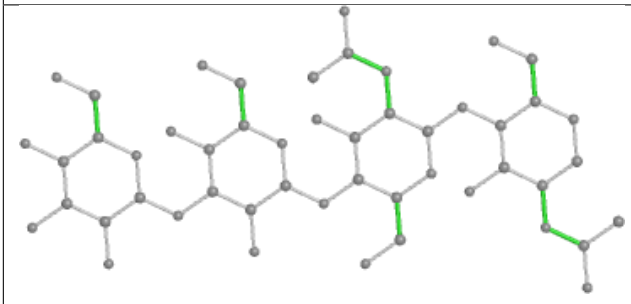
Oligosaccharide Chain J



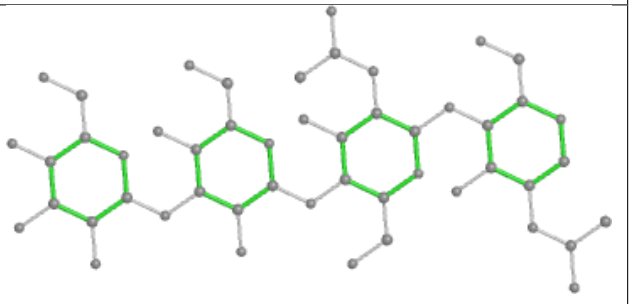
Bond lengths



Bond angles



Torsions



Rings

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	$\#\|Z\| > 2$
8	SO4	L	301	-	4,4,4	0.22	0	6,6,6	0.12	0
13	XQS	B	2005	11	28,28,28	0.79	0	33,38,38	2.06	8 (24%)
8	SO4	C	503	-	4,4,4	0.18	0	6,6,6	0.24	0
12	NAG	B	2004	2	14,14,15	0.45	0	17,19,21	0.57	0
8	SO4	A	502	-	4,4,4	0.22	0	6,6,6	0.27	0
8	SO4	A	501	-	4,4,4	0.27	0	6,6,6	0.23	0
8	SO4	A	503	-	4,4,4	0.16	0	6,6,6	0.18	0
12	NAG	D	2004	2	14,14,15	0.40	0	17,19,21	0.57	0
9	GOL	A	504	-	5,5,5	0.31	0	5,5,5	0.24	0
13	XQS	C	510	11	28,28,28	0.82	0	33,38,38	1.97	8 (24%)
8	SO4	C	502	-	4,4,4	0.24	0	6,6,6	0.18	0
8	SO4	C	501	-	4,4,4	0.22	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
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
12	NAG	D	2004	2	-	0/6/23/26	0/1/1/1
9	GOL	A	504	-	-	2/4/4/4	-
13	XQS	C	510	11	-	4/25/35/35	0/2/2/2

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	2005	XQS	C13-C11-C10	-7.17	102.43	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	510	XQS	C13-C11-C10	-7.08	102.53	110.32
13	B	2005	XQS	C11-C13-N06	-4.55	103.91	110.82
13	C	510	XQS	C11-C13-N06	-4.31	104.27	110.82
13	B	2005	XQS	C14-C12-C10	-4.09	105.82	110.32

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

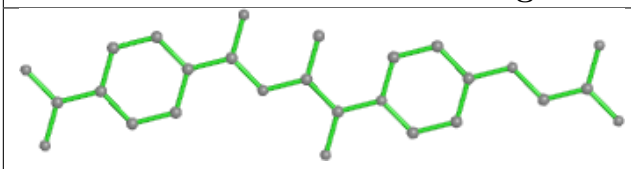
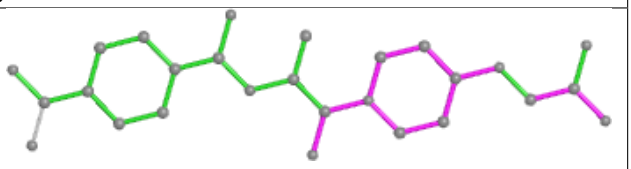
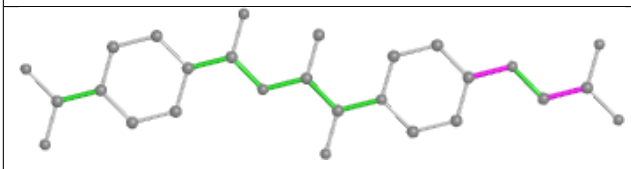
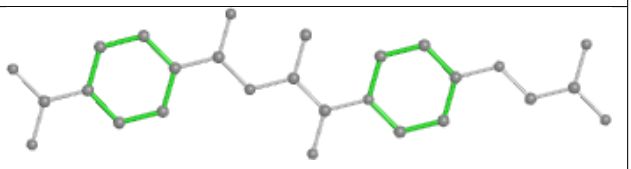
Mol	Chain	Res	Type	Atoms
9	A	504	GOL	O1-C1-C2-C3
13	C	510	XQS	O01-C17-C20-O05
9	A	504	GOL	O1-C1-C2-O2
13	C	510	XQS	O01-C17-C20-O03
13	B	2005	XQS	C12-C10-O01-C17

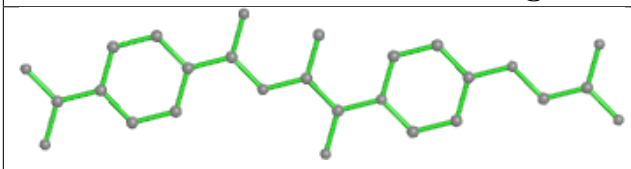
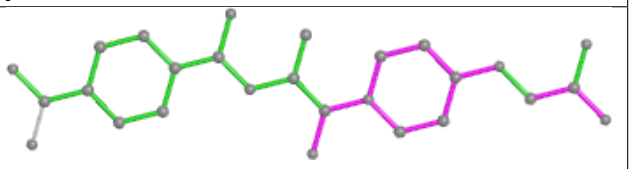
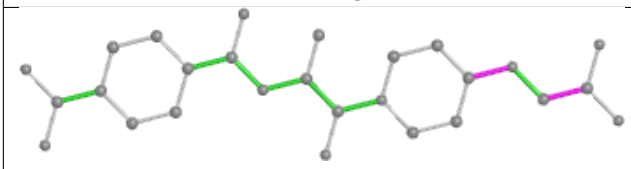
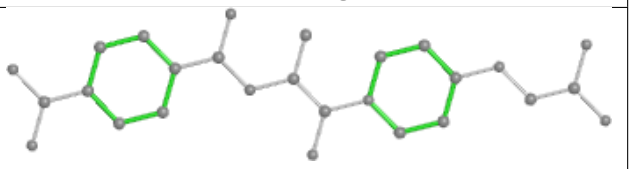
There are no ring outliers.

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 then 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.

Ligand XQS B 2005	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand XQS C 510	
 Bond lengths	 Bond angles
 Torsions	 Rings

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, 95^{th} 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%)	0.84	32 (7%) 16 24	27, 39, 62, 97	0
1	C	453/457 (99%)	0.74	39 (8%) 10 16	32, 52, 76, 104	0
2	B	466/472 (98%)	1.00	70 (15%) 2 3	27, 61, 124, 152	1 (0%)
2	D	471/472 (99%)	0.94	64 (13%) 3 4	35, 70, 120, 148	1 (0%)
3	E	214/221 (96%)	2.48	106 (49%) 0 0	57, 110, 168, 185	0
3	H	216/221 (97%)	0.99	36 (16%) 1 2	43, 87, 131, 149	0
4	F	214/214 (100%)	2.15	82 (38%) 0 0	60, 106, 160, 174	0
4	L	214/214 (100%)	0.62	13 (6%) 21 30	48, 78, 102, 133	0
All	All	2702/2728 (99%)	1.09	442 (16%) 1 2	27, 65, 137, 185	2 (0%)

The worst 5 of 442 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	201	CYS	14.2
3	E	212	VAL	11.8
3	E	134	CYS	10.6
2	B	33	LEU	10.5
3	E	210	THR	10.0

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

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

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

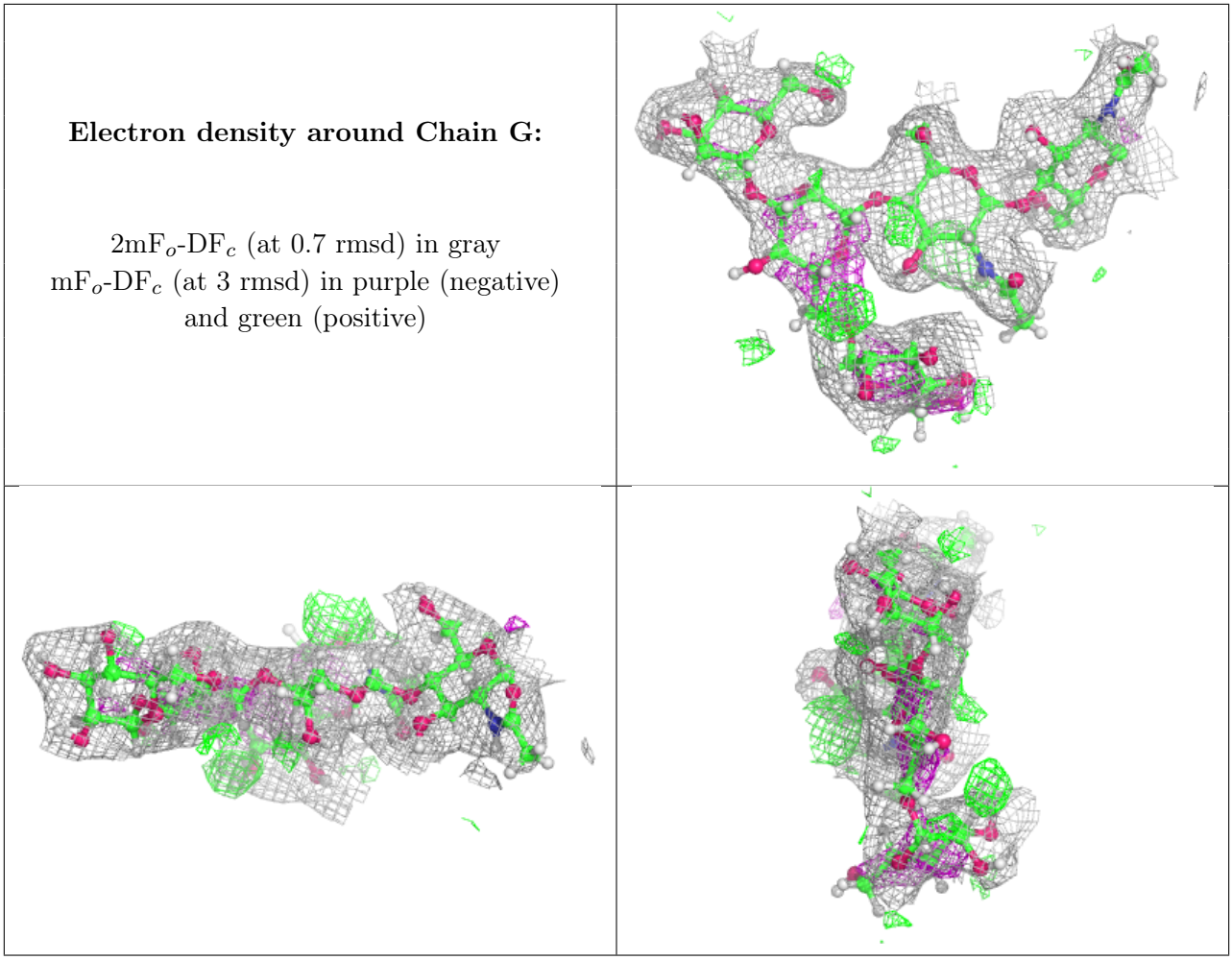
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MAN	G	5	11/12	0.69	0.32	71,88,113,113	0
7	BMA	J	3	11/12	0.81	0.32	73,94,102,117	0
5	BMA	G	3	11/12	0.83	0.25	57,85,105,106	0
5	MAN	G	4	11/12	0.84	0.19	51,77,94,106	0
7	MAN	J	4	11/12	0.84	0.35	58,92,110,111	0
7	NAG	J	2	14/15	0.86	0.27	53,74,114,117	0
6	NAG	K	1	14/15	0.88	0.29	67,82,95,105	0
6	NAG	I	1	14/15	0.88	0.25	62,79,93,95	0
6	NAG	K	2	14/15	0.89	0.35	70,92,110,121	0
6	NAG	I	2	14/15	0.91	0.31	70,94,106,128	0
5	NAG	G	2	14/15	0.94	0.10	56,74,101,103	0
5	NAG	G	1	14/15	0.95	0.13	40,57,71,85	0
7	NAG	J	1	14/15	0.96	0.13	46,58,82,83	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.

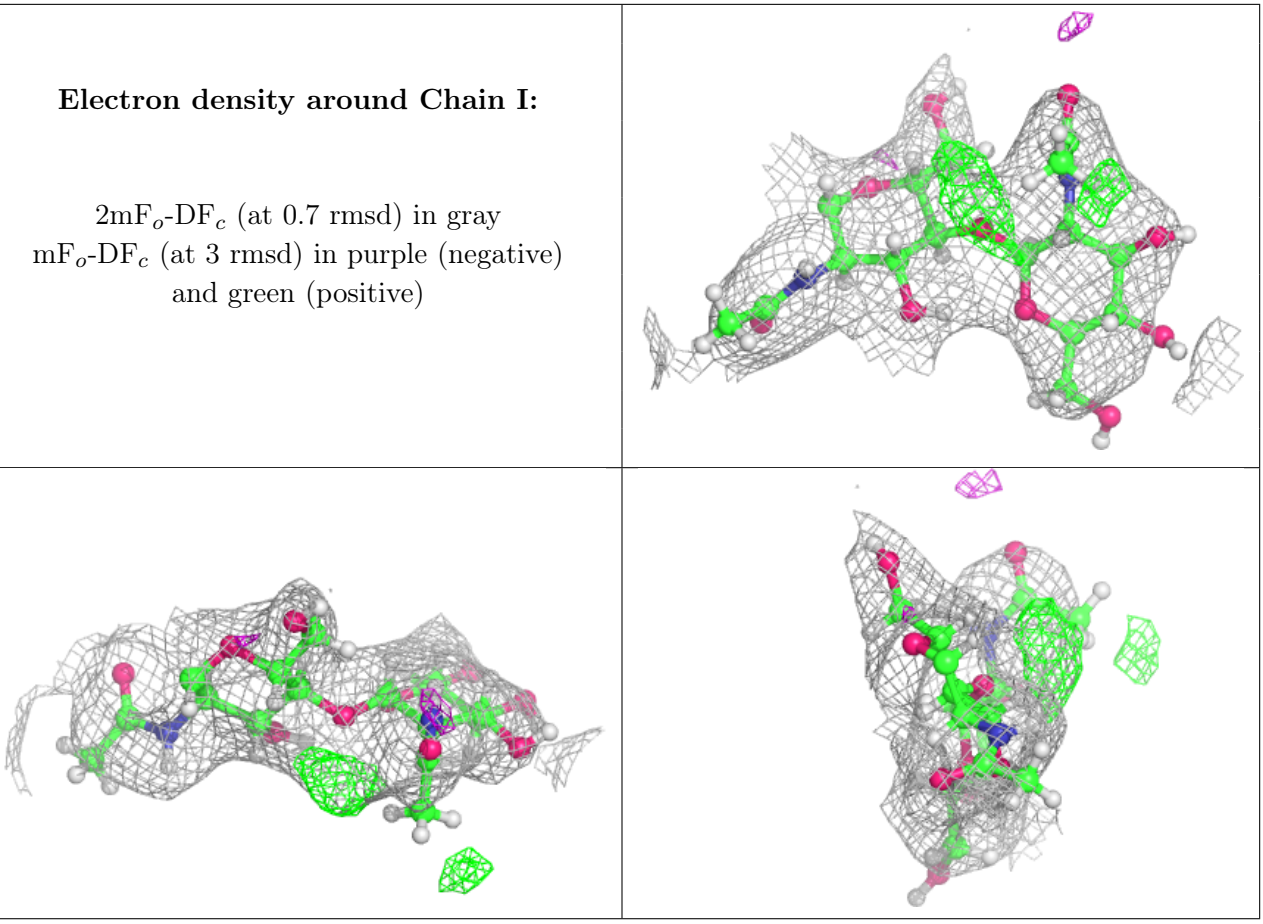
Electron density around Chain G:

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



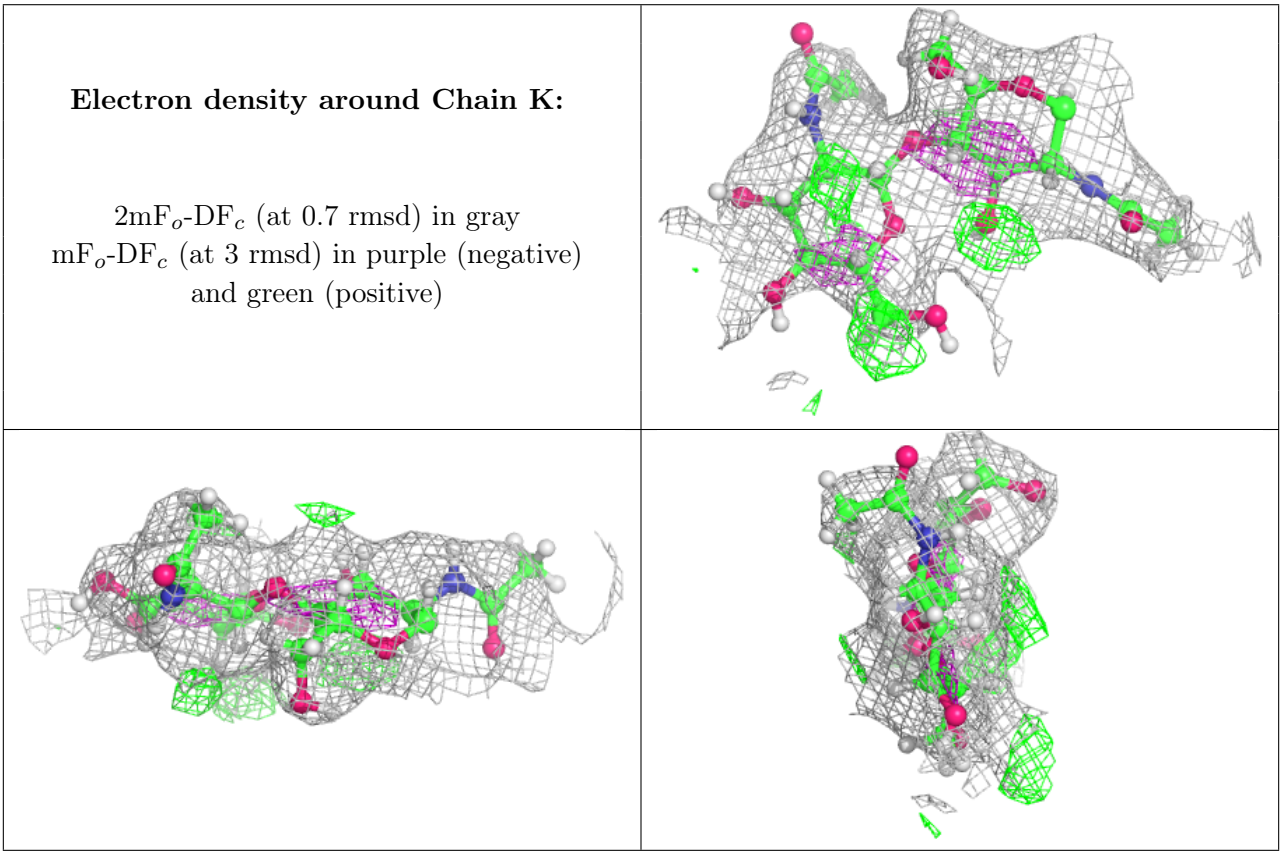
Electron density around Chain I:

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



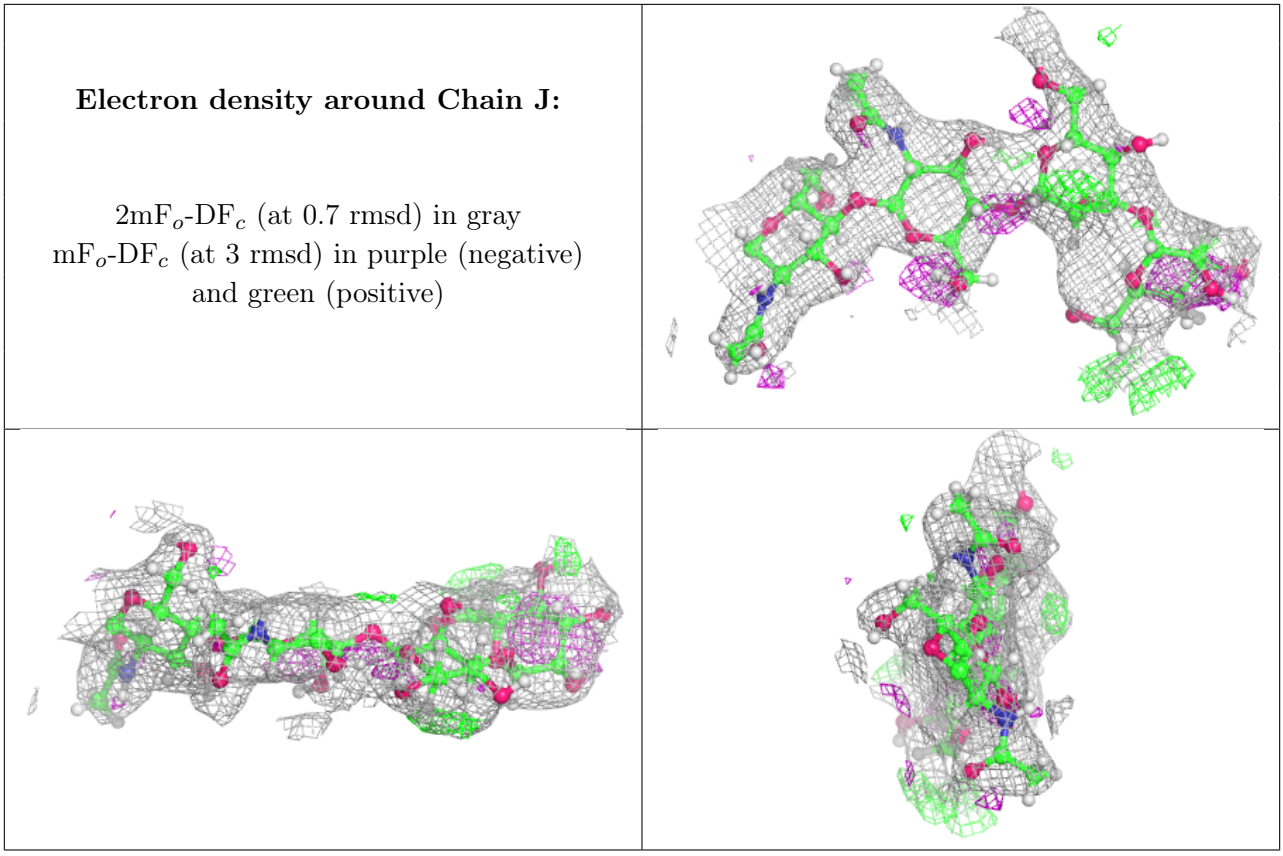
Electron density around Chain K:

$2mF_o$-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, 95^{th} 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
14	CL	C	505	1/1	0.35	0.36	136,136,136,136	0
14	CL	C	504	1/1	0.48	0.67	101,101,101,101	0
10	CA	C	506	1/1	0.74	0.15	108,108,108,108	0
12	NAG	B	2004	14/15	0.84	0.34	75,90,111,118	0
8	SO4	C	502	5/5	0.87	0.20	70,78,102,172	0
12	NAG	D	2004	14/15	0.88	0.29	64,80,103,121	0
8	SO4	A	502	5/5	0.89	0.23	51,54,88,128	0
8	SO4	C	501	5/5	0.89	0.17	57,74,88,168	0
8	SO4	A	501	5/5	0.89	0.29	58,84,105,171	0
8	SO4	L	301	5/5	0.89	0.14	66,70,77,146	0
9	GOL	A	504	6/6	0.89	0.27	31,71,87,92	0
11	MG	D	2001	1/1	0.91	0.20	30,30,30,30	0
11	MG	B	2001	1/1	0.92	0.30	30,30,30,30	0
8	SO4	C	503	5/5	0.92	0.15	60,74,79,139	0

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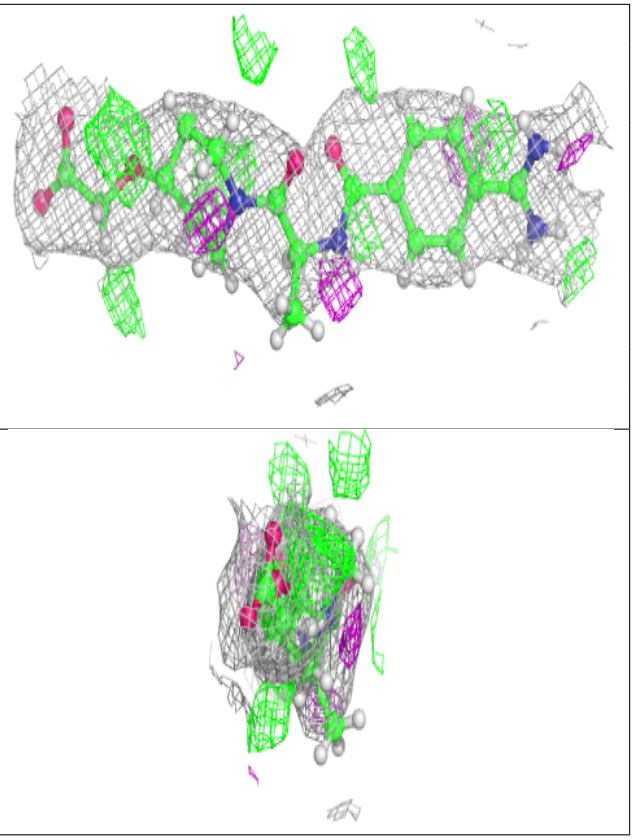
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	XQS	C	510	27/27	0.93	0.18	30,47,76,79	0
13	XQS	B	2005	27/27	0.94	0.22	30,39,69,77	0
10	CA	D	2002	1/1	0.94	0.13	48,48,48,48	0
10	CA	A	506	1/1	0.95	0.11	30,30,30,30	0
10	CA	A	505	1/1	0.96	0.13	57,57,57,57	0
10	CA	C	509	1/1	0.97	0.15	47,47,47,47	0
10	CA	B	2002	1/1	0.97	0.15	67,67,67,67	0
10	CA	A	508	1/1	0.98	0.17	30,30,30,30	0
10	CA	C	508	1/1	0.98	0.14	47,47,47,47	0
10	CA	A	507	1/1	0.98	0.19	30,30,30,30	0
10	CA	B	2003	1/1	0.98	0.20	30,30,30,30	0
10	CA	D	2003	1/1	0.99	0.21	43,43,43,43	0
10	CA	C	507	1/1	0.99	0.09	54,54,54,54	0
8	SO4	A	503	5/5	0.99	0.15	51,58,64,66	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.

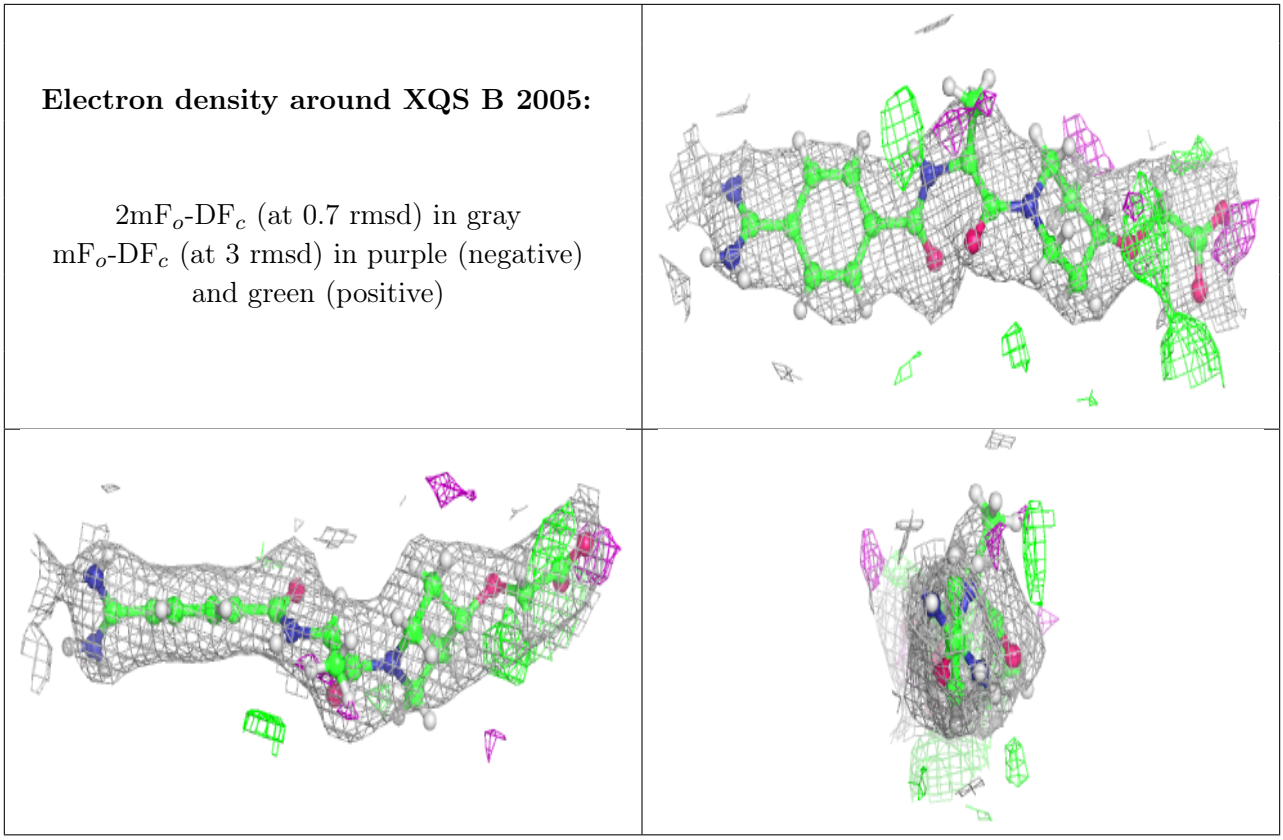
Electron density around XQS C 510:

$2mF_o$-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.