Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 04:07 AM BST

PDB ID	:	4Z7N
Title	:	Integrin alphaIIbbeta3 in complex with AGDV peptide
Authors	:	Lin, F.-Y.; Zhu, J.; Springer, T.A.
Deposited on	:	2015-04-07
Resolution	:	2.60 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 following versions of software and data (see references ⓘ) were used in the production of this report:

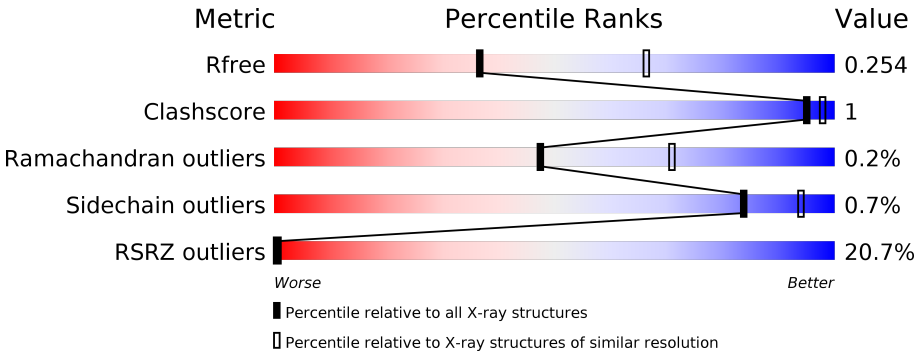
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on 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	455	10% 96%
1	C	455	11% 97%
2	B	469	21% 96%
2	D	469	22% 95%
3	E	219	45% 97%
3	H	219	22% 97%

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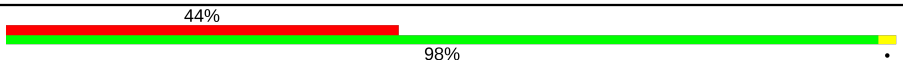
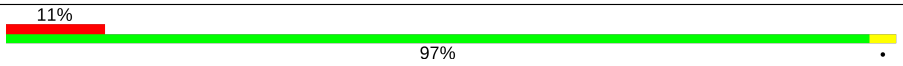
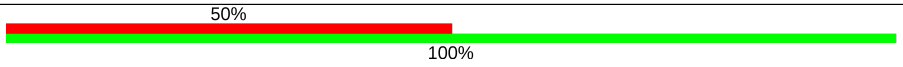
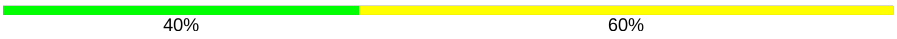
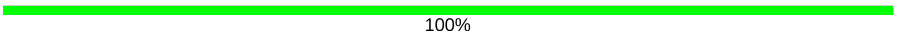
Mol	Chain	Length	Quality of chain
4	F	214	
4	L	214	
5	G	4	
5	J	4	
6	I	5	
7	K	2	
7	N	2	
8	M	4	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 41957 atoms, of which 20198 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	455	Total	C	H	N	O	S	1	2	0
			6839	2223	3341	602	665	8			
1	C	453	Total	C	H	N	O	S	0	0	0
			6782	2207	3308	598	661	8			

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	464	Total	C	H	N	O	S	4	0	0
			7075	2229	3496	611	706	33			
2	D	469	Total	C	H	N	O	S	10	0	0
			7140	2248	3528	617	713	34			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	216	Total	C	H	N	O	S	0	0	0
			3242	1041	1600	266	329	6			
3	H	216	Total	C	H	N	O	S	0	0	0
			3242	1041	1600	266	329	6			

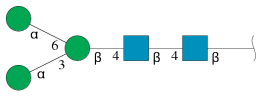
- Molecule 4 is a protein called Monoclonal antibody 10E5 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	214	Total	C	H	N	O	S	1	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 a protein called Tetrapeptide ALA-GLY-ASP-VAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	4	Total	C	H	N	O	0	0	0
			45	14	20	4	7			
5	J	4	Total	C	H	N	O	0	0	0
			45	14	20	4	7			

- Molecule 6 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.

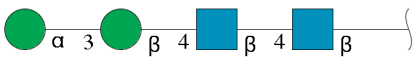


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	I	5	Total	C	H	N	O	0	0	0
			113	34	52	2	25			

- Molecule 7 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
7	K	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
7	N	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

- Molecule 8 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.

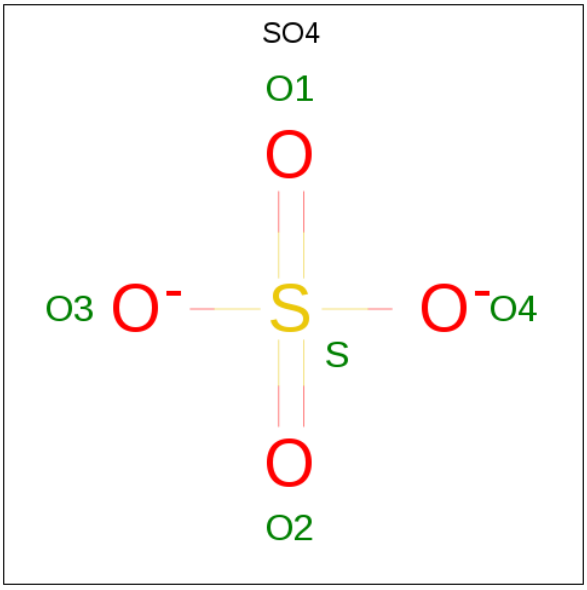


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	M	4	Total	C	H	N	O	0	0	0
			93	28	43	2	20			

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

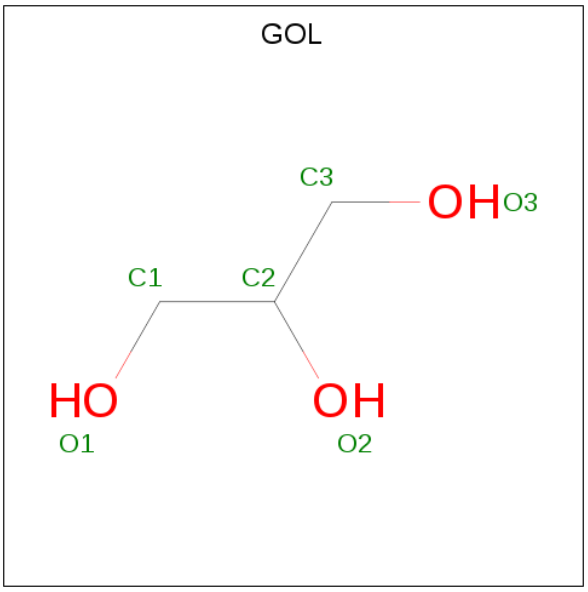
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	4	Total Ca 4 4	0	0
9	C	4	Total Ca 4 4	0	0

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 11 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

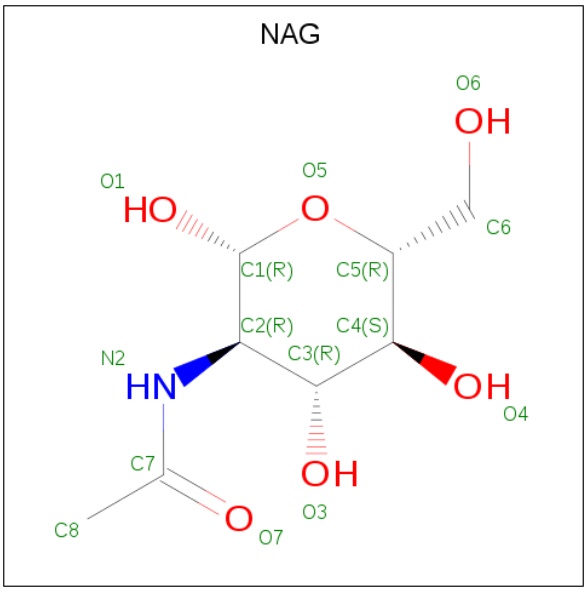


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C H O 14 3 8 3	0	0

- Molecule 12 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total C H N O 27 8 13 1 5	0	0
13	D	1	Total C H N O 27 8 13 1 5	0	0

- Molecule 14 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	1	Total Cl 1 1	0	0

- Molecule 15 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	319	Total O 319 319	0	0
15	B	144	Total O 144 144	0	0
15	C	123	Total O 123 123	0	0
15	D	75	Total O 75 75	0	0
15	E	9	Total O 9 9	0	0
15	F	9	Total O 9 9	0	0

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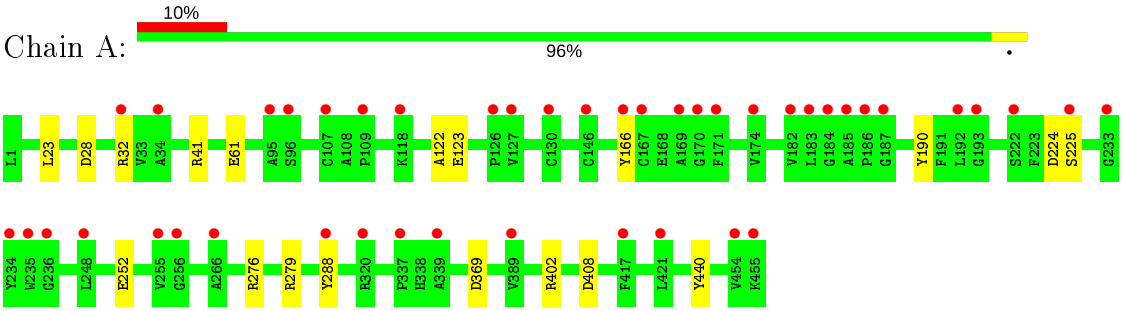
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	H	16	Total O 16 16	0	0
15	L	28	Total O 28 28	0	0
15	G	5	Total O 5 5	0	0
15	J	4	Total O 4 4	0	0

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.

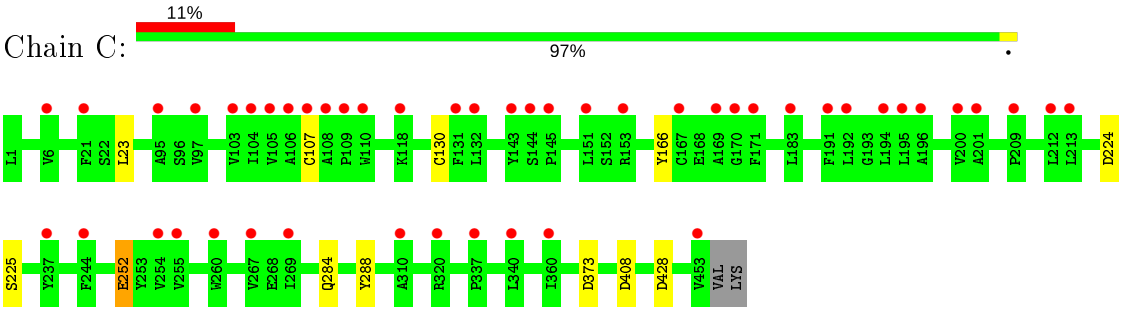
- Molecule 1: Integrin alpha-IIb

Chain A:



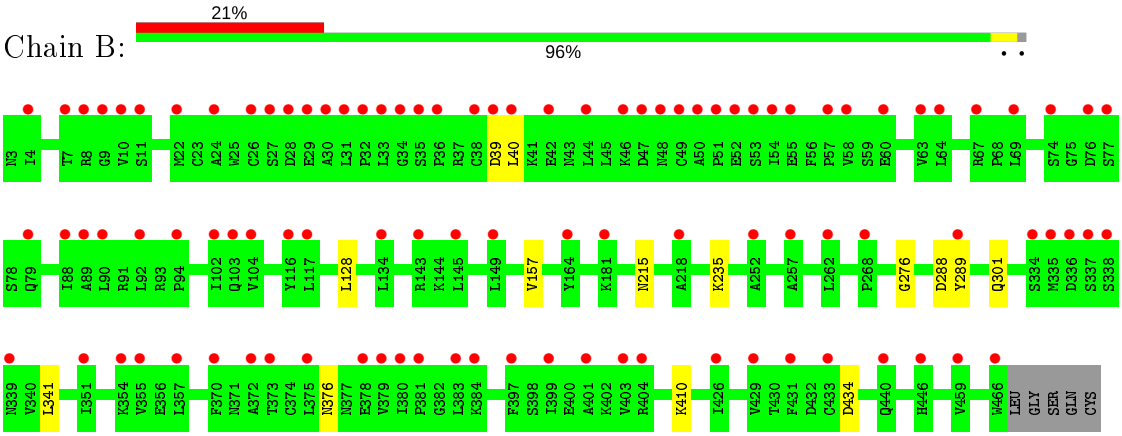
- Molecule 1: Integrin alpha-IIb

Chain C:



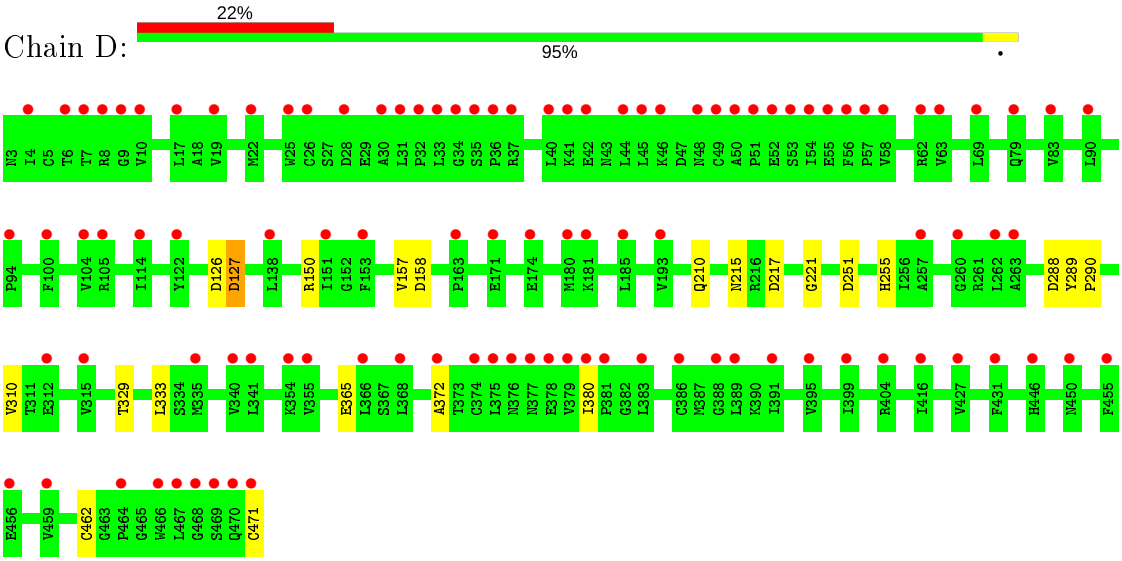
- Molecule 2: Integrin beta-3

Chain B:



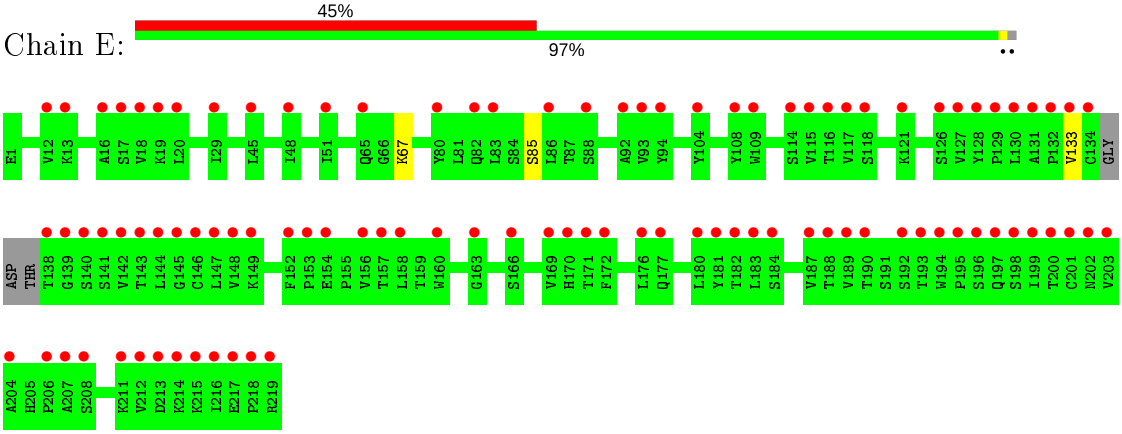
- Molecule 2: Integrin beta-3

Chain D:



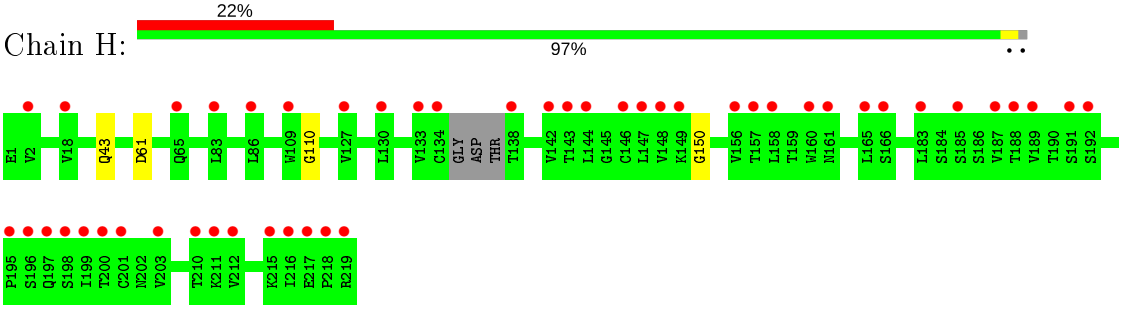
- Molecule 3: Monoclonal antibody 10E5 heavy chain

Chain E:



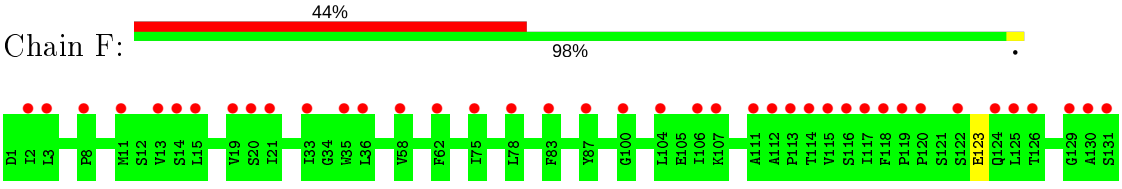
- Molecule 3: Monoclonal antibody 10E5 heavy chain

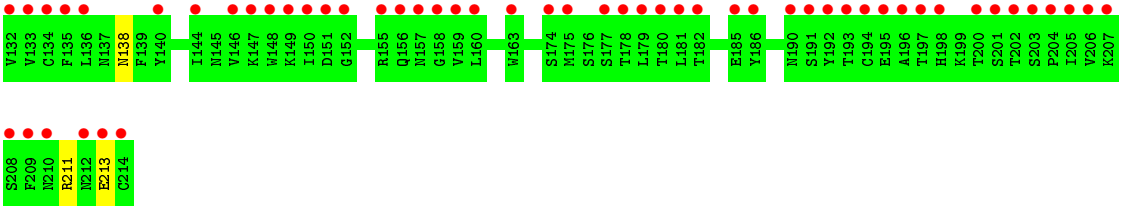
Chain H:



- Molecule 4: Monoclonal antibody 10E5 light chain

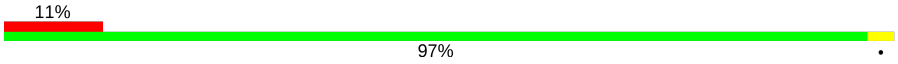
Chain F:

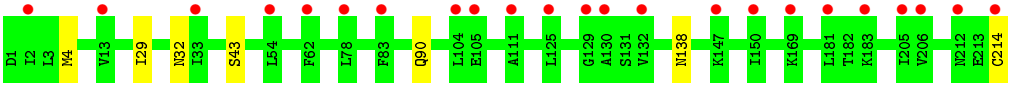




• Molecule 4: Monoclonal antibody 10E5 light chain

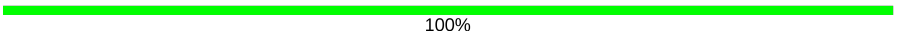
Chain L:





• Molecule 5: Tetrapeptide ALA-GLY-ASP-VAL

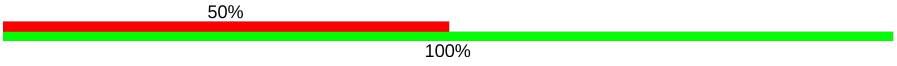
Chain G:



There are no outlier residues recorded for this chain.

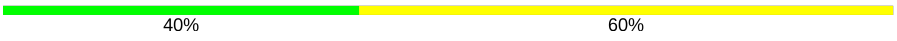
• Molecule 5: Tetrapeptide ALA-GLY-ASP-VAL

Chain J:



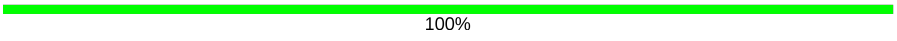
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



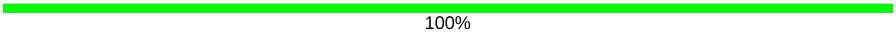
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



• Molecule 8: 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 M:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	256.88Å 144.37Å 104.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.19 – 2.60 49.19 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.9 (49.19-2.60) 84.0 (49.19-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.55 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.10pre_2104: ???)	Depositor
R, R_{free}	0.230 , 0.253 0.231 , 0.254	Depositor DCC
R_{free} test set	2000 reflections (1.71%)	wwPDB-VP
Wilson B-factor (Å^2)	50.6	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	41957	wwPDB-VP
Average B, all atoms (Å^2)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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: GOL, BMA, NAG, CL, CA, MN, SO4, MAN

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	0/3600	0.44	0/4905
1	C	0.27	0/3570	0.43	0/4865
2	B	0.25	0/3645	0.43	0/4942
2	D	0.25	0/3678	0.41	0/4986
3	E	0.25	0/1684	0.44	0/2305
3	H	0.25	0/1684	0.43	0/2305
4	F	0.24	0/1673	0.41	0/2269
4	L	0.24	0/1673	0.42	0/2269
5	G	0.19	0/24	0.45	0/30
5	J	0.21	0/24	0.37	0/30
All	All	0.26	0/21255	0.43	0/28906

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	341	LEU	Peptide

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	3498	3341	3341	13	0
1	C	3474	3308	3308	7	0
2	B	3579	3496	3496	5	0
2	D	3612	3528	3527	12	0
3	E	1642	1600	1600	1	0
3	H	1642	1600	1600	3	0
4	F	1637	1553	1553	2	0
4	L	1637	1553	1553	3	0
5	G	25	20	20	0	0
5	J	25	20	20	0	0
6	I	61	52	52	0	0
7	K	28	25	25	0	0
7	N	28	25	25	0	0
8	M	50	43	43	0	0
9	A	4	0	0	0	0
9	C	4	0	0	0	0
10	A	20	0	0	0	0
10	C	15	0	0	0	0
10	L	5	0	0	0	0
11	A	6	8	8	0	0
12	B	3	0	0	0	0
12	D	3	0	0	0	0
13	B	14	13	13	4	0
13	D	14	13	13	0	0
14	C	1	0	0	0	0
15	A	319	0	0	9	1
15	B	144	0	0	1	0
15	C	123	0	0	4	1
15	D	75	0	0	6	0
15	E	9	0	0	0	0
15	F	9	0	0	0	0
15	G	5	0	0	0	0
15	H	16	0	0	1	0
15	J	4	0	0	0	0
15	L	28	0	0	0	0
All	All	21759	20198	20197	49	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (49) 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:276:ARG:NH1	15:A:604:HOH:O	2.17	0.78
1:A:369:ASP:OD2	15:A:601:HOH:O	2.02	0.77
2:B:235:LYS:NZ	2:B:276:GLY:O	2.24	0.71
1:C:408:ASP:OD2	15:C:601:HOH:O	2.10	0.69
13:B:2004:NAG:H3	13:B:2004:NAG:H83	1.73	0.69
1:A:276:ARG:NH1	15:A:612:HOH:O	2.26	0.69
1:C:428:ASP:OD2	15:C:602:HOH:O	2.14	0.64
2:D:462:CYS:SG	2:D:471:CYS:N	2.71	0.64
1:C:373:ASP:O	15:C:603:HOH:O	2.14	0.63
1:A:402:ARG:O	15:A:602:HOH:O	2.15	0.63
1:A:369:ASP:CG	15:A:601:HOH:O	2.37	0.61
1:C:284:GLN:OE1	15:C:604:HOH:O	2.17	0.57
1:A:190:TYR:O	15:A:606:HOH:O	2.18	0.56
1:A:408:ASP:OD2	15:A:605:HOH:O	2.17	0.56
13:B:2004:NAG:C8	13:B:2004:NAG:H3	2.37	0.55
1:C:252:GLU:N	1:C:252:GLU:OE2	2.39	0.55
2:D:288:ASP:OD1	2:D:289:TYR:N	2.40	0.55
1:A:440:TYR:OH	15:A:603:HOH:O	2.16	0.55
2:D:210:GLN:OE1	15:D:2101:HOH:O	2.18	0.54
4:F:211:ARG:O	4:F:213:GLU:N	2.41	0.53
13:B:2004:NAG:C3	13:B:2004:NAG:H83	2.41	0.51
1:C:224:ASP:OD1	1:C:225:SER:N	2.41	0.51
2:B:288:ASP:OD1	2:B:289:TYR:N	2.40	0.50
2:B:410:LYS:NZ	2:B:434:ASP:OD2	2.44	0.49
2:D:221:GLY:O	15:D:2102:HOH:O	2.19	0.49
3:H:61:ASP:OD1	15:H:301:HOH:O	2.19	0.49
2:D:217:ASP:OD2	2:D:255:HIS:NE2	2.43	0.49
4:F:123:GLU:OE1	4:F:123:GLU:N	2.43	0.48
2:D:290:PRO:O	15:D:2103:HOH:O	2.20	0.48
2:D:372:ALA:O	2:D:380:ILE:N	2.47	0.47
3:H:43:GLN:N	3:H:43:GLN:OE1	2.46	0.46
2:D:310:VAL:O	2:D:333:LEU:N	2.44	0.46
1:C:107:CYS:HA	1:C:130:CYS:HA	1.98	0.46
3:E:67:LYS:NZ	3:E:85:SER:O	2.50	0.44
1:A:122:ALA:O	1:A:123:GLU:HB2	2.18	0.44
4:L:4:MET:HE1	4:L:90:GLN:HB3	2.01	0.43
2:D:251:ASP:OD2	15:D:2104:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ARG:NH2	15:A:634:HOH:O	2.44	0.42
1:A:224:ASP:OD1	1:A:225:SER:N	2.43	0.42
2:D:126:ASP:OD1	2:D:127:ASP:N	2.52	0.42
1:A:28:ASP:OD1	1:A:32:ARG:N	2.49	0.42
13:B:2004:NAG:C8	13:B:2004:NAG:C3	2.95	0.42
1:A:276:ARG:HD2	1:A:279:ARG:HB2	2.02	0.41
4:L:29:ILE:O	4:L:32:ASN:ND2	2.48	0.41
2:D:150:ARG:NH1	15:D:2111:HOH:O	2.45	0.41
2:B:301:GLN:NE2	15:B:2109:HOH:O	2.35	0.41
2:B:39:ASP:OD1	2:B:40:LEU:N	2.46	0.41
3:H:110:GLY:O	4:L:43:SER:OG	2.29	0.40
2:D:329:THR:N	15:D:2108:HOH:O	2.49	0.40

All (1) 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)
15:A:605:HOH:O	15:C:632:HOH:O[1_554]	2.13	0.07

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	455/455 (100%)	434 (95%)	21 (5%)	0	100	100
1	C	451/455 (99%)	432 (96%)	19 (4%)	0	100	100
2	B	462/469 (98%)	438 (95%)	23 (5%)	1 (0%)	47	71
2	D	467/469 (100%)	445 (95%)	21 (4%)	1 (0%)	47	71
3	E	212/219 (97%)	197 (93%)	14 (7%)	1 (0%)	29	52
3	H	212/219 (97%)	202 (95%)	9 (4%)	1 (0%)	29	52
4	F	212/214 (99%)	202 (95%)	9 (4%)	1 (0%)	29	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	L	212/214 (99%)	205 (97%)	6 (3%)	1 (0%)	29 52
5	G	2/4 (50%)	2 (100%)	0	0	100 100
5	J	2/4 (50%)	2 (100%)	0	0	100 100
All	All	2687/2722 (99%)	2559 (95%)	122 (4%)	6 (0%)	47 71

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	133	VAL
2	B	157	VAL
4	L	138	ASN
2	D	157	VAL
4	F	138	ASN
3	H	150	GLY

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	365/363 (101%)	360 (99%)	5 (1%)	67 85
1	C	361/363 (99%)	357 (99%)	4 (1%)	73 88
2	B	411/415 (99%)	408 (99%)	3 (1%)	84 94
2	D	415/415 (100%)	411 (99%)	4 (1%)	76 90
3	E	187/189 (99%)	187 (100%)	0	100 100
3	H	187/189 (99%)	187 (100%)	0	100 100
4	F	188/188 (100%)	188 (100%)	0	100 100
4	L	188/188 (100%)	187 (100%)	1 (0%)	88 96
5	G	2/2 (100%)	2 (100%)	0	100 100
5	J	2/2 (100%)	2 (100%)	0	100 100
All	All	2306/2314 (100%)	2289 (99%)	17 (1%)	84 94

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	61	GLU
1	A	166	TYR
1	A	252	GLU
1	A	288	TYR
2	B	128	LEU
2	B	215	ASN
2	B	376	ASN
1	C	23	LEU
1	C	166	TYR
1	C	252	GLU
1	C	288	TYR
2	D	127	ASP
2	D	158	ASP
2	D	215	ASN
2	D	365	GLU
4	L	214	CYS

Some 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	$\#\|Z\|>2$
6	NAG	I	1	2,6	14,14,15	0.30	0	17,19,21	0.43	0
6	NAG	I	2	6	14,14,15	0.22	0	17,19,21	0.42	0
6	BMA	I	3	6	11,11,12	0.80	1 (9%)	15,15,17	0.72	0
6	MAN	I	4	6	11,11,12	0.70	0	15,15,17	1.08	2 (13%)
6	MAN	I	5	6	11,11,12	0.70	0	15,15,17	1.06	2 (13%)
7	NAG	K	1	2,7	14,14,15	0.32	0	17,19,21	0.34	0
7	NAG	K	2	7	14,14,15	0.24	0	17,19,21	0.40	0
8	NAG	M	1	8,2	14,14,15	0.26	0	17,19,21	0.41	0
8	NAG	M	2	8	14,14,15	0.24	0	17,19,21	0.41	0
8	BMA	M	3	8	11,11,12	0.61	0	15,15,17	0.73	0
8	MAN	M	4	8	11,11,12	0.74	0	15,15,17	1.02	2 (13%)
7	NAG	N	1	2,7	14,14,15	0.41	0	17,19,21	0.34	0
7	NAG	N	2	7	14,14,15	0.24	0	17,19,21	0.42	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
6	NAG	I	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	2/6/23/26	0/1/1/1
6	BMA	I	3	6	-	0/2/19/22	0/1/1/1
6	MAN	I	4	6	-	2/2/19/22	0/1/1/1
6	MAN	I	5	6	-	1/2/19/22	0/1/1/1
7	NAG	K	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	K	2	7	-	1/6/23/26	0/1/1/1
8	NAG	M	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	M	2	8	-	0/6/23/26	0/1/1/1
8	BMA	M	3	8	-	2/2/19/22	0/1/1/1
8	MAN	M	4	8	-	0/2/19/22	0/1/1/1
7	NAG	N	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	N	2	7	-	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)
6	I	3	BMA	O5-C1	-2.10	1.40	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	4	MAN	O2-C2-C3	-2.40	105.33	110.14
8	M	4	MAN	O2-C2-C3	-2.31	105.52	110.14
6	I	5	MAN	C1-O5-C5	2.29	115.30	112.19
6	I	5	MAN	O2-C2-C3	-2.24	105.65	110.14
8	M	4	MAN	C1-O5-C5	2.11	115.05	112.19
6	I	4	MAN	C1-O5-C5	2.07	115.00	112.19

There are no chirality outliers.

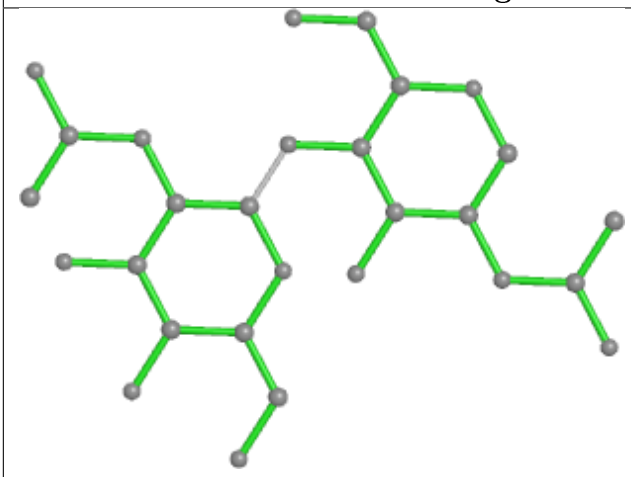
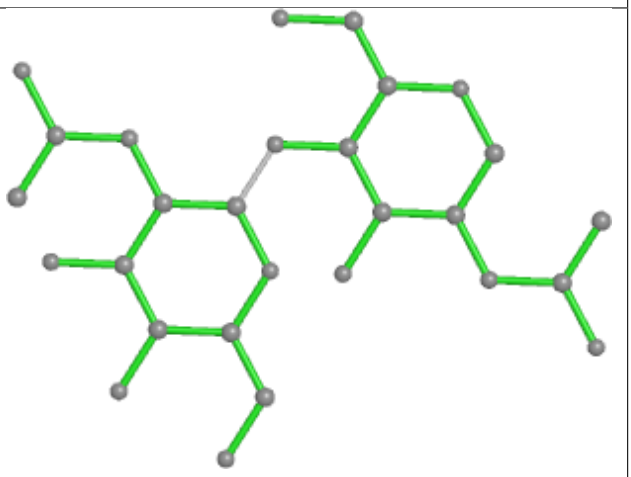
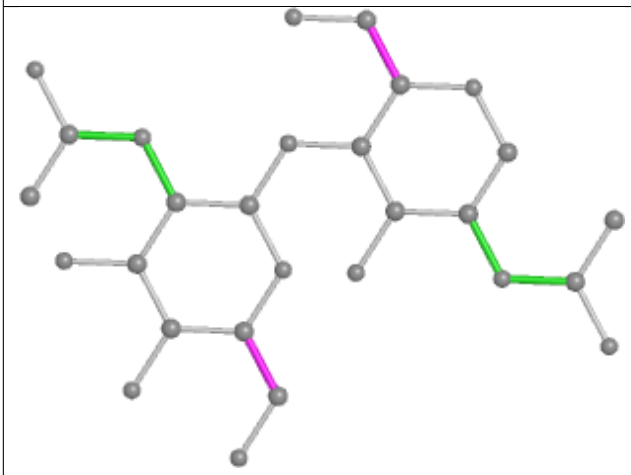
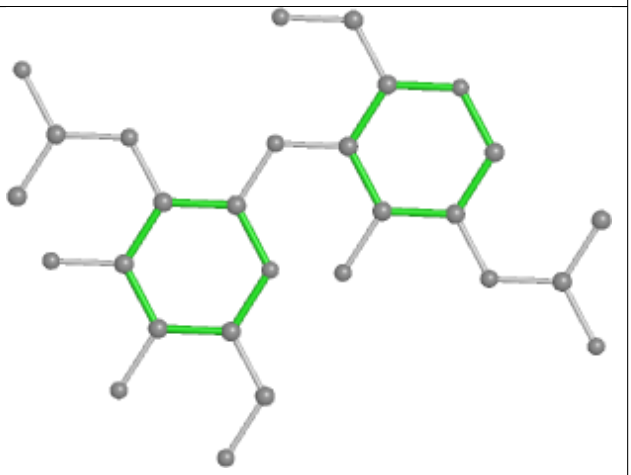
All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	N	2	NAG	O5-C5-C6-O6
7	N	1	NAG	O5-C5-C6-O6
6	I	4	MAN	C4-C5-C6-O6
6	I	4	MAN	O5-C5-C6-O6
8	M	3	BMA	O5-C5-C6-O6
7	N	1	NAG	C4-C5-C6-O6
8	M	3	BMA	C4-C5-C6-O6
7	N	2	NAG	C4-C5-C6-O6
7	K	1	NAG	O5-C5-C6-O6
6	I	5	MAN	O5-C5-C6-O6
7	K	1	NAG	C4-C5-C6-O6
7	K	2	NAG	O5-C5-C6-O6
6	I	2	NAG	C4-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6

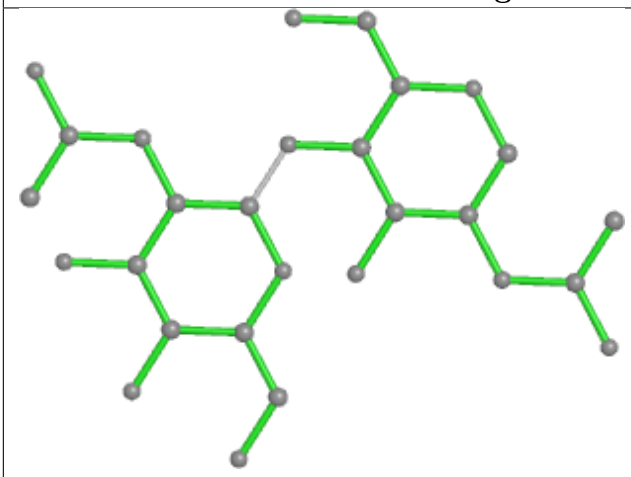
There are no ring outliers.

No monomer is involved in short contacts.

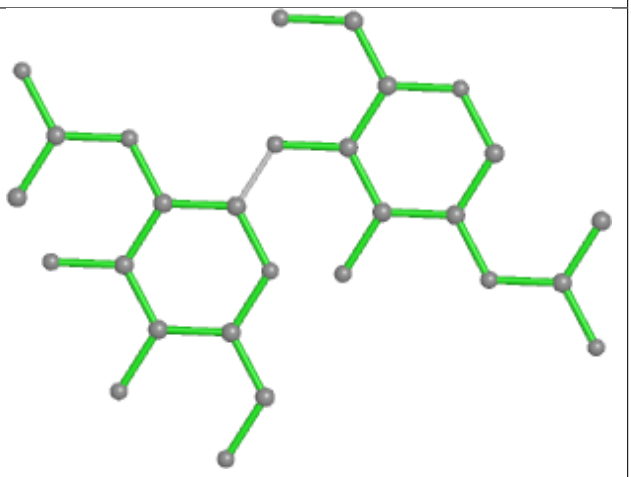
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain K	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

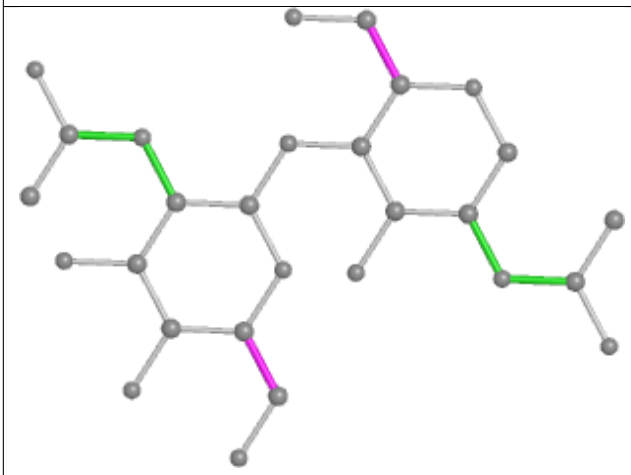
Oligosaccharide Chain N



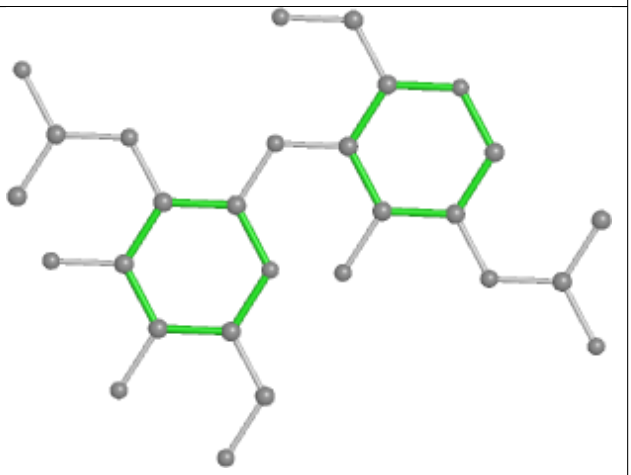
Bond lengths



Bond angles

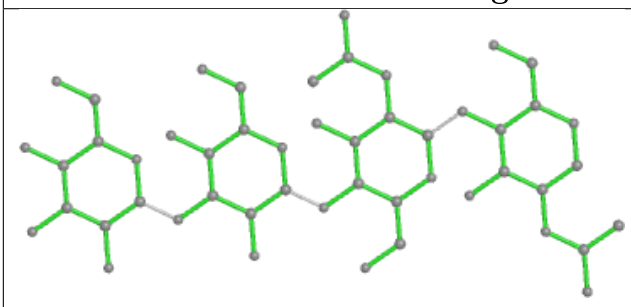


Torsions

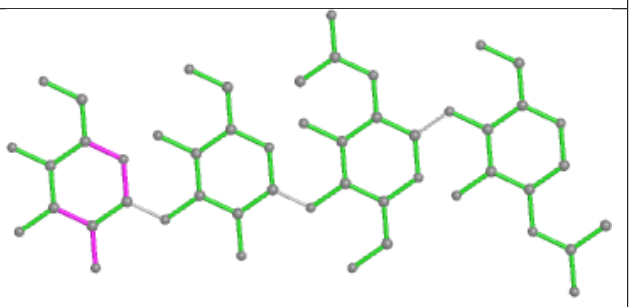


Rings

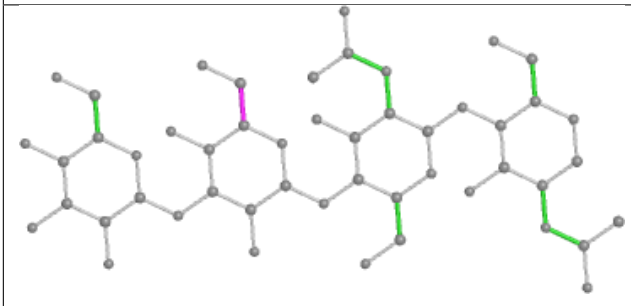
Oligosaccharide Chain M



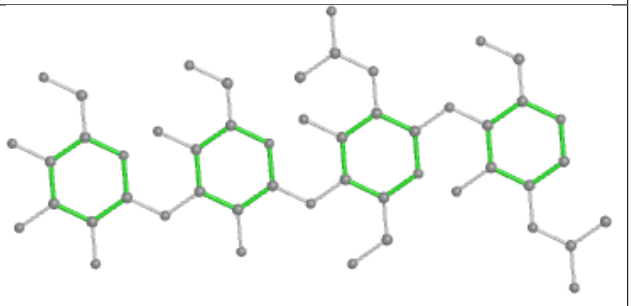
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 15 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
10	SO4	A	506	-	4,4,4	0.14	0	6,6,6	0.05	0
10	SO4	A	505	-	4,4,4	0.15	0	6,6,6	0.04	0
13	NAG	D	2004	2	14,14,15	0.25	0	17,19,21	0.38	0
13	NAG	B	2004	2	14,14,15	0.45	0	17,19,21	1.41	2 (11%)
10	SO4	C	507	-	4,4,4	0.14	0	6,6,6	0.05	0
10	SO4	A	507	-	4,4,4	0.14	0	6,6,6	0.05	0
10	SO4	L	301	-	4,4,4	0.14	0	6,6,6	0.05	0
10	SO4	C	508	-	4,4,4	0.15	0	6,6,6	0.06	0
11	GOL	A	509	-	5,5,5	0.41	0	5,5,5	0.25	0
10	SO4	A	508	-	4,4,4	0.15	0	6,6,6	0.06	0
10	SO4	C	501	-	4,4,4	0.13	0	6,6,6	0.05	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	NAG	B	2004	2	-	5/6/23/26	0/1/1/1
13	NAG	D	2004	2	-	0/6/23/26	0/1/1/1
11	GOL	A	509	-	-	0/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	2004	NAG	C2-N2-C7	4.00	128.60	122.90
13	B	2004	NAG	C1-O5-C5	2.66	115.79	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	B	2004	NAG	O5-C5-C6-O6
13	B	2004	NAG	C8-C7-N2-C2
13	B	2004	NAG	O7-C7-N2-C2
13	B	2004	NAG	C4-C5-C6-O6
13	B	2004	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	2004	NAG	4	0

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	455/455 (100%)	1.00	44 (9%) 7 5	43, 58, 83, 169	1 (0%)
1	C	453/455 (99%)	0.98	48 (10%) 6 4	52, 76, 104, 137	0
2	B	464/469 (98%)	1.35	100 (21%) 0 0	47, 89, 159, 185	1 (0%)
2	D	469/469 (100%)	1.25	104 (22%) 0 0	58, 98, 147, 177	1 (0%)
3	E	216/219 (98%)	2.61	99 (45%) 0 0	86, 135, 218, 243	0
3	H	216/219 (98%)	1.26	48 (22%) 0 0	69, 113, 158, 181	0
4	F	214/214 (100%)	2.70	94 (43%) 0 0	93, 135, 219, 252	1 (0%)
4	L	214/214 (100%)	0.86	23 (10%) 6 3	70, 101, 124, 160	0
5	G	4/4 (100%)	1.04	0 100 100	54, 64, 67, 68	0
5	J	4/4 (100%)	2.20	2 (50%) 0 0	80, 81, 81, 86	0
All	All	2709/2722 (99%)	1.37	562 (20%) 1 0	43, 92, 170, 252	4 (0%)

All (562) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	179	LEU	14.9
3	E	198	SER	14.8
3	E	144	LEU	13.7
3	E	131	ALA	12.9
4	F	193	THR	12.6
4	F	130	ALA	12.2
4	F	194	CYS	12.0
3	E	142	VAL	11.5
3	E	132	PRO	11.3
4	F	195	GLU	11.0
3	E	133	VAL	10.9
4	F	148	TRP	10.5
4	F	206	VAL	10.4

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Mol	Chain	Res	Type	RSRZ
4	F	181	LEU	10.3
4	F	214	CYS	10.2
3	H	216	ILE	10.1
3	E	183	LEU	10.1
3	E	194	TRP	9.4
3	E	219	ARG	9.2
3	E	130	LEU	8.9
4	F	205	ILE	8.8
3	E	216	ILE	8.7
3	E	148	VAL	8.7
4	F	208	SER	8.7
4	F	180	THR	8.3
4	F	209	PHE	8.3
3	E	200	THR	8.2
2	D	375	LEU	8.2
3	E	189	VAL	8.1
2	B	33	LEU	8.0
4	F	126	THR	8.0
4	F	135	PHE	7.9
4	F	132	VAL	7.9
3	E	199	ILE	7.8
4	F	160	LEU	7.6
4	L	214	CYS	7.5
4	F	117	ILE	7.3
1	A	455	LYS	7.3
4	F	125	LEU	7.2
4	F	178	THR	7.2
4	F	118	PHE	7.2
2	B	36	PRO	7.1
2	D	471	CYS	7.1
4	F	192	TYR	7.0
4	F	115	VAL	6.9
2	B	338	SER	6.9
3	E	147	LEU	6.9
2	B	51	PRO	6.9
3	H	158	LEU	6.9
4	F	159	VAL	6.9
4	F	116	SER	6.8
3	E	146	CYS	6.7
3	E	195	PRO	6.7
4	F	119	PRO	6.6
3	H	144	LEU	6.6

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Mol	Chain	Res	Type	RSRZ
2	B	337	SER	6.6
2	D	44	LEU	6.6
3	E	207	ALA	6.5
4	F	134	CYS	6.5
3	E	218	PRO	6.4
4	F	120	PRO	6.4
1	A	454	VAL	6.4
3	E	160	TRP	6.4
2	B	339	ASN	6.3
4	F	204	PRO	6.3
3	E	127	VAL	6.2
2	D	54	ILE	6.2
4	F	104	LEU	6.2
2	B	10	VAL	6.1
3	E	134	CYS	6.1
3	E	176	LEU	6.1
2	B	46	LYS	6.1
4	F	207	LYS	5.9
4	F	133	VAL	5.9
3	E	129	PRO	5.9
2	D	380	ILE	5.9
3	E	187	VAL	5.9
2	B	54	ILE	5.8
2	B	336	ASP	5.8
4	F	157	ASN	5.8
4	F	155	ARG	5.7
2	D	33	LEU	5.7
3	E	190	THR	5.7
4	F	147	LYS	5.7
4	F	136	LEU	5.6
4	F	196	ALA	5.6
2	D	9	GLY	5.5
2	B	440	GLN	5.5
3	E	201	CYS	5.5
3	E	145	GLY	5.5
3	E	138	THR	5.5
2	B	380	ILE	5.4
2	D	468	GLY	5.4
2	B	30	ALA	5.4
5	J	411	VAL	5.4
2	B	44	LEU	5.3
2	B	53	SER	5.3

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Mol	Chain	Res	Type	RSRZ
3	E	217	GLU	5.2
3	H	138	THR	5.2
3	E	139	GLY	5.2
3	E	128	TYR	5.2
4	F	78	LEU	5.1
3	E	12	VAL	5.1
3	E	83	LEU	5.1
4	F	144	ILE	5.1
3	E	188	THR	5.0
2	D	36	PRO	5.0
3	H	133	VAL	5.0
4	F	150	ILE	5.0
3	H	160	TRP	5.0
3	H	198	SER	4.9
2	B	181	LYS	4.9
2	B	92	LEU	4.8
3	E	215	LYS	4.8
4	F	151	ASP	4.8
3	E	86	LEU	4.7
4	F	212	ASN	4.7
2	D	379	VAL	4.7
3	H	134	CYS	4.7
3	H	142	VAL	4.7
2	B	28	ASP	4.7
3	E	212	VAL	4.7
3	E	115	VAL	4.6
3	E	143	THR	4.6
3	H	201	CYS	4.6
3	E	156	VAL	4.6
3	E	181	TYR	4.6
3	H	203	VAL	4.6
4	F	129	GLY	4.6
2	B	8	ARG	4.5
3	E	211	LYS	4.5
3	H	189	VAL	4.5
2	B	76	ASP	4.5
3	E	157	THR	4.5
2	B	34	GLY	4.5
4	F	146	VAL	4.5
4	L	212	ASN	4.5
1	C	453	VAL	4.5
2	D	35	SER	4.4

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Mol	Chain	Res	Type	RSRZ
4	F	131	SER	4.4
4	L	104	LEU	4.4
2	B	375	LEU	4.4
4	F	87	TYR	4.4
4	F	149	LYS	4.4
2	B	48	ASN	4.4
4	F	202	THR	4.4
2	D	51	PRO	4.4
2	B	49	CYS	4.4
2	B	9	GLY	4.2
3	E	204	ALA	4.2
2	D	48	ASN	4.2
2	D	450	ASN	4.2
2	B	4	ILE	4.2
3	E	197	GLN	4.2
4	L	129	GLY	4.1
4	F	113	PRO	4.1
4	F	83	PHE	4.1
3	H	215	LYS	4.1
3	H	197	GLN	4.1
2	D	34	GLY	4.1
2	D	381	PRO	4.0
3	H	219	ARG	4.0
4	F	21	ILE	4.0
1	C	320	ARG	4.0
2	D	58	VAL	4.0
4	F	191	SER	3.9
4	F	124	GLN	3.9
4	F	158	GLY	3.9
2	D	376	ASN	3.9
2	B	466	TRP	3.9
4	F	15	LEU	3.9
2	D	404	ARG	3.9
2	B	69	LEU	3.8
1	A	337	PRO	3.8
3	E	140	SER	3.8
2	D	8	ARG	3.8
4	F	11	MET	3.8
3	E	18	VAL	3.8
2	D	181	LYS	3.8
2	D	378	GLU	3.7
2	B	381	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
3	E	184	SER	3.7
3	E	149	LYS	3.7
3	H	212	VAL	3.7
3	E	19	LYS	3.7
2	D	63	VAL	3.7
3	E	182	THR	3.7
4	L	206	VAL	3.7
4	F	33	ILE	3.6
2	D	17	LEU	3.6
2	B	459	VAL	3.6
4	F	106	ILE	3.6
2	B	88	ILE	3.6
2	D	31	LEU	3.6
1	C	337	PRO	3.6
3	E	126	SER	3.6
4	L	183	LYS	3.5
3	H	188	THR	3.5
3	E	196	SER	3.5
3	E	16	ALA	3.5
4	F	182	THR	3.5
3	E	48	ILE	3.5
3	E	203	VAL	3.5
2	D	466	TRP	3.4
4	F	107	LYS	3.4
2	D	90	LEU	3.4
4	F	186	TYR	3.4
2	B	90	LEU	3.4
2	D	40	LEU	3.4
2	D	377	ASN	3.4
3	H	210	THR	3.4
4	L	111	ALA	3.4
2	B	370	PHE	3.3
1	A	417	PHE	3.3
2	D	30	ALA	3.3
2	B	50	ALA	3.3
2	B	373	THR	3.3
3	E	193	THR	3.3
2	D	22	MET	3.3
2	B	383	LEU	3.3
3	E	172	PHE	3.3
4	F	175	MET	3.3
2	D	83	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
4	F	122	SER	3.2
4	F	8	PRO	3.2
4	L	83	PHE	3.2
2	B	26	CYS	3.2
2	D	171	GLU	3.2
3	H	217	GLU	3.2
2	B	117	LEU	3.2
2	D	56	PHE	3.2
2	D	354	LYS	3.2
3	H	127	VAL	3.2
3	H	200	THR	3.1
3	E	65	GLN	3.1
3	E	177	GLN	3.1
3	E	180	LEU	3.1
3	H	166	SER	3.1
3	E	141	SER	3.1
2	D	10	VAL	3.1
2	D	45	LEU	3.1
3	H	165	LEU	3.1
2	D	62	ARG	3.1
4	F	20	SER	3.1
2	B	289	TYR	3.1
2	B	29	GLU	3.1
4	F	201	SER	3.1
2	B	32	PRO	3.0
4	F	156	GLN	3.0
2	D	46	LYS	3.0
2	B	145	LEU	3.0
4	L	181	LEU	3.0
2	D	470	GLN	3.0
3	E	169	VAL	3.0
2	D	26	CYS	3.0
4	F	197	THR	3.0
2	D	7	THR	3.0
2	D	459	VAL	3.0
4	F	13	VAL	3.0
1	C	131	PHE	3.0
3	E	29	ILE	3.0
1	C	143	TYR	3.0
2	D	37	ARG	3.0
2	B	42	GLU	3.0
3	E	214	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	52	GLU	3.0
2	D	469	SER	3.0
3	H	147	LEU	3.0
1	A	339	ALA	2.9
2	D	57	PRO	2.9
4	F	198	HIS	2.9
1	A	320	ARG	2.9
3	H	192	SER	2.9
2	B	35	SER	2.9
3	E	45	LEU	2.9
3	H	130	LEU	2.9
4	F	200	THR	2.9
2	D	456	GLU	2.9
3	E	202	ASN	2.9
3	H	199	ILE	2.9
1	A	183	LEU	2.9
5	J	408	ALA	2.9
1	C	269	ILE	2.9
2	D	391	ILE	2.9
2	B	7	THR	2.9
3	E	116	THR	2.9
1	C	255	VAL	2.8
2	B	429	VAL	2.8
2	B	384	LYS	2.8
2	D	185	LEU	2.8
2	B	399	ILE	2.8
4	F	35	TRP	2.8
2	B	77	SER	2.8
3	E	88	SER	2.8
2	D	42	GLU	2.8
4	L	205	ILE	2.8
1	C	106	ALA	2.8
2	B	52	GLU	2.8
4	L	33	ILE	2.8
4	L	62	PHE	2.8
2	B	74	SER	2.8
2	B	39	ASP	2.8
2	B	149	LEU	2.8
3	H	196	SER	2.8
1	C	200	VAL	2.8
2	D	455	PHE	2.8
2	B	334	SER	2.8

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Mol	Chain	Res	Type	RSRZ
4	F	100	GLY	2.7
1	C	340	LEU	2.7
2	D	174	GLU	2.7
4	F	213	GLU	2.7
3	E	171	THR	2.7
4	F	2	ILE	2.7
2	B	357	LEU	2.7
3	H	83	LEU	2.7
4	F	14	SER	2.7
2	B	79	GLN	2.7
2	B	102	ILE	2.7
4	F	177	SER	2.7
2	B	378	GLU	2.7
3	H	18	VAL	2.7
1	A	185	ALA	2.7
3	E	92	ALA	2.7
2	B	38	CYS	2.7
2	B	397	PHE	2.7
4	L	105	GLU	2.6
3	E	117	VAL	2.6
3	H	218	PRO	2.6
2	B	27	SER	2.6
2	D	69	LEU	2.6
4	F	75	ILE	2.6
1	C	109	PRO	2.6
3	H	191	SER	2.6
3	E	93	VAL	2.6
2	D	467	LEU	2.6
3	E	163	GLY	2.6
2	B	104	VAL	2.6
3	E	13	LYS	2.6
2	D	427	VAL	2.6
3	E	158	LEU	2.6
2	D	431	PHE	2.6
2	D	79	GLN	2.6
1	A	32	ARG	2.6
1	C	105	VAL	2.5
1	C	167	CYS	2.5
1	C	196	ALA	2.5
1	C	171	PHE	2.5
2	D	28	ASP	2.5
1	A	248	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
3	H	86	LEU	2.5
2	B	143	ARG	2.5
1	C	244	PHE	2.5
4	F	62	PHE	2.5
2	D	340	VAL	2.5
3	H	146	CYS	2.5
1	A	187	GLY	2.5
1	C	183	LEU	2.5
2	B	403	VAL	2.5
3	E	20	LEU	2.5
1	A	96	SER	2.5
2	B	24	ALA	2.5
1	A	255	VAL	2.5
2	B	134	LEU	2.5
3	E	192	SER	2.5
2	B	354	LYS	2.5
1	C	95	ALA	2.5
1	A	192	LEU	2.4
2	B	67	ARG	2.4
2	D	341	LEU	2.4
1	C	267	VAL	2.4
2	B	58	VAL	2.4
2	B	31	LEU	2.4
4	F	3	LEU	2.4
1	C	103	VAL	2.4
2	B	55	GLU	2.4
1	A	118	LYS	2.4
1	A	256	GLY	2.4
2	D	104	VAL	2.4
3	E	17	SER	2.4
3	E	118	SER	2.4
1	C	144	SER	2.4
2	D	53	SER	2.4
4	L	125	LEU	2.4
1	A	182	VAL	2.4
3	E	121	LYS	2.4
1	C	237	TYR	2.4
2	D	464	PRO	2.4
1	A	235	TRP	2.4
1	A	266	ALA	2.4
1	C	192	LEU	2.4
3	H	148	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	236	GLY	2.4
2	D	260	GLY	2.4
1	C	107	CYS	2.4
2	D	372	ALA	2.4
1	C	153	ARG	2.4
1	A	109	PRO	2.4
2	B	11	SER	2.4
4	F	152	GLY	2.3
1	C	145	PRO	2.3
2	D	114	ILE	2.3
3	E	108	TYR	2.3
3	H	183	LEU	2.3
1	C	110	TRP	2.3
2	B	63	VAL	2.3
2	B	379	VAL	2.3
2	D	386	CYS	2.3
3	E	213	ASP	2.3
2	D	399	ILE	2.3
4	F	111	ALA	2.3
4	L	130	ALA	2.3
1	A	222	SER	2.3
3	E	114	SER	2.3
2	D	19	VAL	2.3
3	H	161	ASN	2.3
1	A	184	GLY	2.3
2	D	138	LEU	2.3
2	D	368	LEU	2.3
1	A	389	VAL	2.3
2	D	25	TRP	2.3
4	F	163	TRP	2.3
2	D	4	ILE	2.3
1	A	233	GLY	2.3
2	B	401	ALA	2.3
2	D	263	ALA	2.3
2	D	395	VAL	2.3
2	B	335	MET	2.3
2	B	404	ARG	2.3
3	H	157	THR	2.3
2	D	49	CYS	2.3
3	E	104	TYR	2.3
1	A	186	PRO	2.3
3	H	211	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	6	THR	2.3
2	D	374	CYS	2.3
2	D	41	LYS	2.2
2	D	180	MET	2.2
2	D	335	MET	2.2
2	D	50	ALA	2.2
2	D	416	ILE	2.2
2	B	64	LEU	2.2
4	L	54	LEU	2.2
2	D	122	TYR	2.2
2	B	57	PRO	2.2
1	C	108	ALA	2.2
4	F	112	ALA	2.2
4	L	150	ILE	2.2
3	E	152	PHE	2.2
1	C	260	TRP	2.2
2	B	60	GLU	2.2
1	A	127	VAL	2.2
1	A	174	VAL	2.2
2	B	433	CYS	2.2
1	A	34	ALA	2.2
1	C	201	ALA	2.2
3	H	143	THR	2.2
2	D	366	LEU	2.2
3	H	195	PRO	2.2
4	F	174	SER	2.2
1	A	130	CYS	2.2
2	B	426	ILE	2.2
1	C	195	LEU	2.2
2	D	389	LEU	2.2
3	E	206	PRO	2.2
2	B	22	MET	2.2
4	F	58	VAL	2.2
1	C	310	ALA	2.2
2	B	257	ALA	2.2
2	D	257	ALA	2.2
2	D	312	GLU	2.2
1	C	360	ILE	2.2
2	D	151	ILE	2.2
4	F	114	THR	2.2
1	A	193	GLY	2.2
1	C	213	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	446	HIS	2.2
1	A	169	ALA	2.2
1	C	151	LEU	2.2
3	E	80	TYR	2.1
3	E	94	TYR	2.1
2	D	315	VAL	2.1
3	E	109	TRP	2.1
2	B	372	ALA	2.1
2	D	163	PRO	2.1
4	F	185	GLU	2.1
2	B	40	LEU	2.1
4	L	78	LEU	2.1
1	C	118	LYS	2.1
3	E	208	SER	2.1
3	H	65	GLN	2.1
2	D	193	VAL	2.1
3	H	187	VAL	2.1
4	L	13	VAL	2.1
2	D	388	GLY	2.1
1	C	104	ILE	2.1
4	L	169	LYS	2.1
1	A	171	PHE	2.1
3	E	166	SER	2.1
1	A	146	CYS	2.1
1	A	166	TYR	2.1
1	A	288	TYR	2.1
2	B	355	VAL	2.1
3	H	156	VAL	2.1
3	E	153	PRO	2.1
4	F	36	LEU	2.1
2	B	218	ALA	2.1
4	F	140	TYR	2.1
4	L	132	VAL	2.1
1	A	167	CYS	2.1
2	B	351	ILE	2.1
2	D	262	LEU	2.1
3	E	170	HIS	2.1
3	E	82	GLN	2.1
1	C	254	VAL	2.1
2	D	55	GLU	2.1
2	D	94	PRO	2.1
4	F	19	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	47	ASP	2.1
1	C	212	LEU	2.1
2	B	446	HIS	2.1
2	D	383	LEU	2.1
4	F	210	ASN	2.1
1	C	170	GLY	2.1
1	A	95	ALA	2.1
3	H	2	VAL	2.1
3	E	51	ILE	2.1
1	C	21	PHE	2.1
1	C	191	PHE	2.1
2	B	262	LEU	2.1
2	D	100	PHE	2.1
1	A	107	CYS	2.1
2	B	103	GLN	2.1
2	B	252	ALA	2.0
2	D	32	PRO	2.0
1	C	97	VAL	2.0
2	D	355	VAL	2.0
1	A	234	TYR	2.0
1	C	132	LEU	2.0
1	C	194	LEU	2.0
4	F	190	ASN	2.0
4	L	147	LYS	2.0
2	D	105	ARG	2.0
3	H	109	TRP	2.0
1	C	169	ALA	2.0
2	B	268	PRO	2.0
3	E	154	GLU	2.0
1	A	225	SER	2.0
3	H	185	SER	2.0
1	A	170	GLY	2.0
2	B	164	TYR	2.0
4	L	2	ILE	2.0
2	D	153	PHE	2.0
1	A	126	PRO	2.0
2	B	89	ALA	2.0
3	H	149	LYS	2.0
1	C	6	VAL	2.0
4	F	203	SER	2.0
1	A	421	LEU	2.0
2	B	116	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	431	PHE	2.0
1	C	209	PRO	2.0
2	B	94	PRO	2.0

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

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

6.3 Carbohydrates (i)

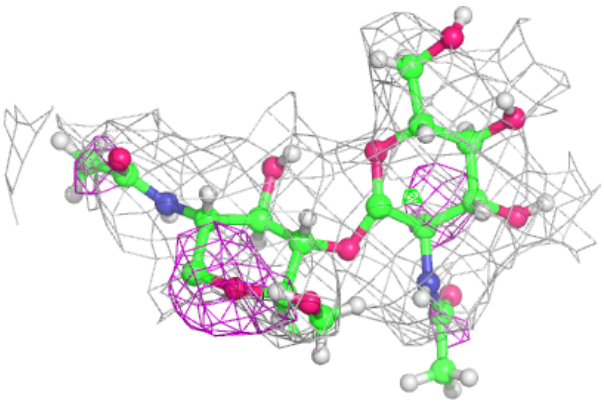
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

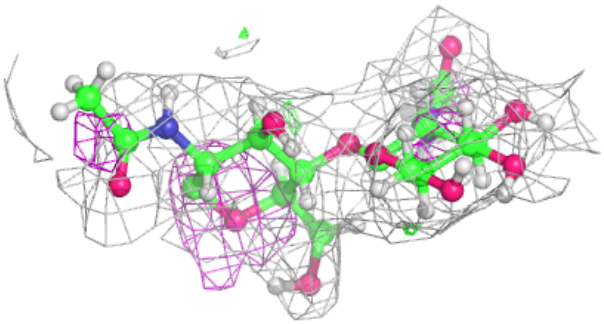
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MAN	I	5	11/12	0.66	0.37	85,99,119,121	0
7	NAG	K	1	14/15	0.75	0.33	72,89,105,105	0
8	BMA	M	3	11/12	0.79	0.28	85,91,109,109	0
6	BMA	I	3	11/12	0.79	0.19	76,89,110,110	0
7	NAG	N	2	14/15	0.83	0.30	83,100,117,125	0
7	NAG	K	2	14/15	0.83	0.30	88,101,122,122	0
8	NAG	M	2	14/15	0.83	0.28	79,94,113,113	0
7	NAG	N	1	14/15	0.85	0.28	70,88,104,105	0
6	NAG	I	2	14/15	0.86	0.17	75,87,101,106	0
8	MAN	M	4	11/12	0.87	0.31	82,92,110,111	0
6	MAN	I	4	11/12	0.87	0.21	79,87,104,106	0
6	NAG	I	1	14/15	0.93	0.17	51,69,94,100	0
8	NAG	M	1	14/15	0.94	0.13	59,78,93,94	0

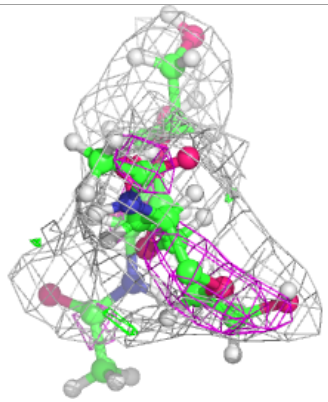
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain K:

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

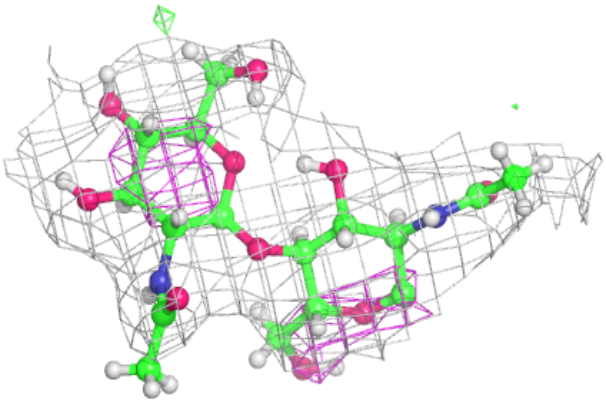


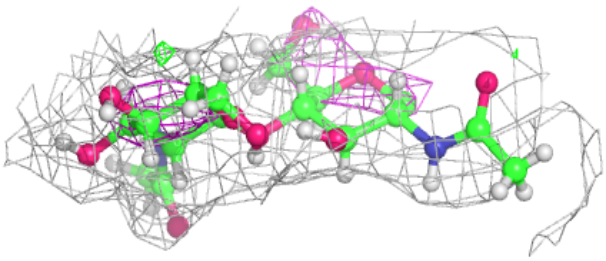


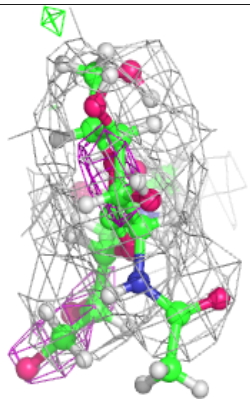


Electron density around Chain N:

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

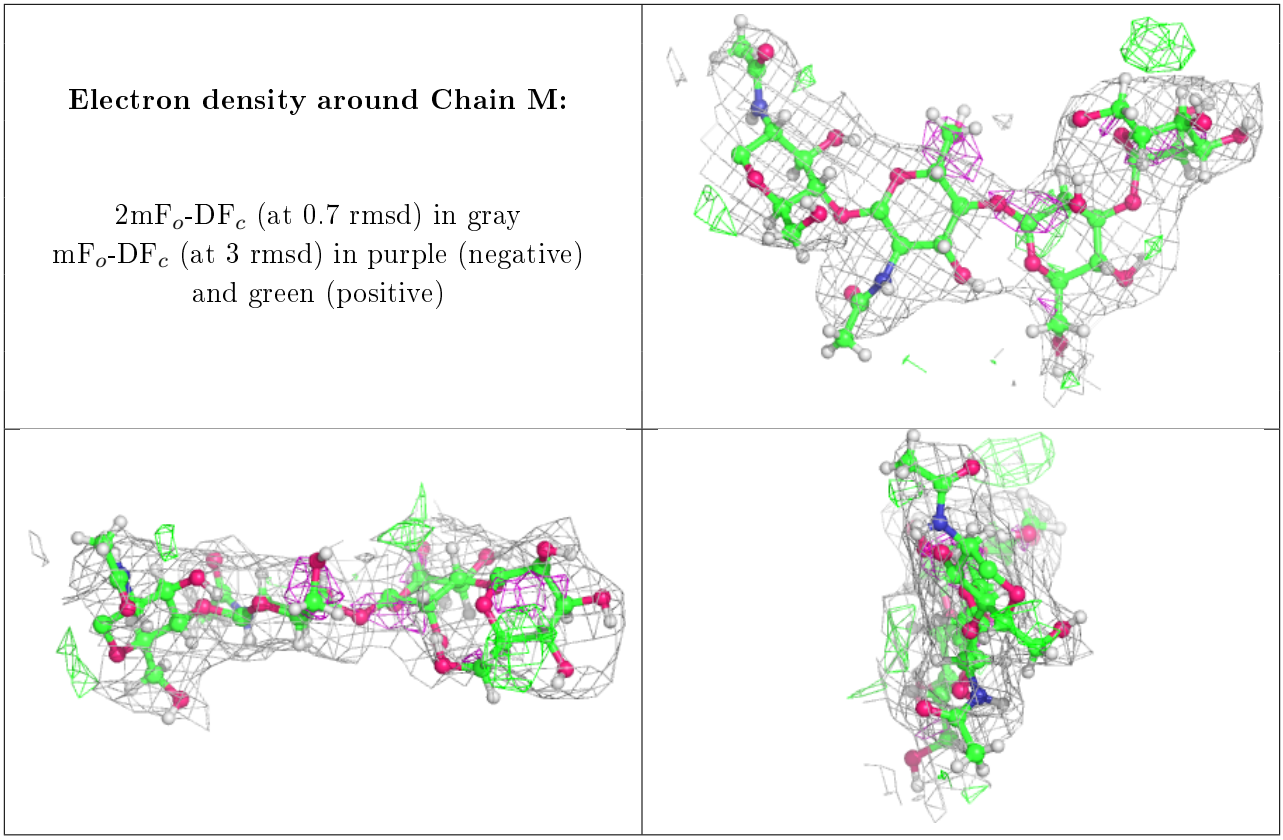






Electron density around Chain M:

$2mF_o$-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
12	MN	B	2002	1/1	0.59	0.32	145,145,145,145	0
12	MN	D	2002	1/1	0.69	0.33	247,247,247,247	0
9	CA	C	504	1/1	0.72	0.14	123,123,123,123	0
9	CA	C	503	1/1	0.73	0.19	141,141,141,141	0
13	NAG	D	2004	14/15	0.78	0.25	70,91,107,107	0
10	SO4	A	505	5/5	0.78	0.37	125,126,127,132	0
12	MN	D	2003	1/1	0.80	0.31	143,143,143,143	0
10	SO4	C	508	5/5	0.84	0.21	108,116,120,122	0
10	SO4	L	301	5/5	0.85	0.14	123,123,124,125	0
11	GOL	A	509	6/6	0.85	0.28	70,84,91,94	0
10	SO4	C	507	5/5	0.86	0.19	124,125,126,131	0
10	SO4	C	501	5/5	0.86	0.24	134,134,135,137	0
12	MN	B	2003	1/1	0.88	0.17	65,65,65,65	0
9	CA	A	501	1/1	0.88	0.17	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	NAG	B	2004	14/15	0.88	0.33	72,92,108,110	0
10	SO4	A	508	5/5	0.90	0.30	99,103,110,111	0
9	CA	C	506	1/1	0.91	0.20	75,75,75,75	0
12	MN	D	2001	1/1	0.91	0.29	109,109,109,109	0
14	CL	C	502	1/1	0.94	0.40	95,95,95,95	0
9	CA	C	505	1/1	0.94	0.16	73,73,73,73	0
9	CA	A	503	1/1	0.94	0.23	53,53,53,53	0
10	SO4	A	507	5/5	0.94	0.16	102,102,102,108	0
9	CA	A	502	1/1	0.95	0.16	46,46,46,46	0
10	SO4	A	506	5/5	0.95	0.21	110,113,114,115	0
12	MN	B	2001	1/1	0.96	0.23	46,46,46,46	0
9	CA	A	504	1/1	0.98	0.15	53,53,53,53	0

6.5 Other polymers (i)

There are no such residues in this entry.