Full wwPDB X-ray Structure Validation Report

Aug 7, 2020 – 05:09 AM BST

PDB ID	:	3T3P
Title	:	A Novel High Affinity Integrin alphaIIbbeta3 Receptor Antagonist That Unexpectedly Displaces Mg2+ from the beta3 MIDAS
Authors	:	Zhu, J.; Zhu, J.; Springer, T.A.
Deposited on	:	2011-07-25
Resolution	:	2.20 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:

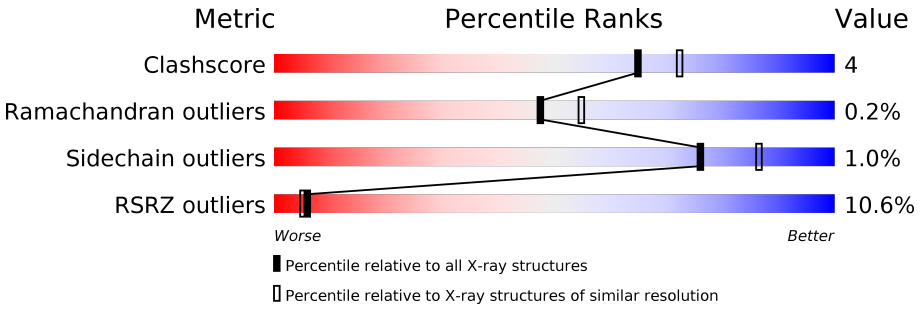
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.20 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))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	457	93% 6%
1	C	457	2% 91% 8%
2	B	472	8% 88% 10%
2	D	472	7% 91% 9%
3	E	221	33% 80% 17%
3	H	221	14% 85% 12%
4	F	214	40% 83% 17%

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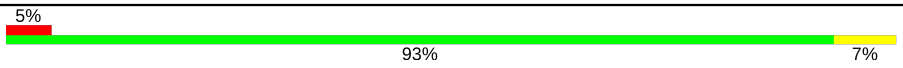
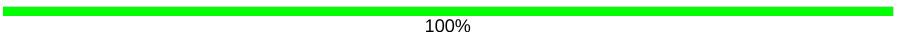
Mol	Chain	Length	Quality of chain
4	L	214	
5	G	5	
6	I	2	
6	K	2	
7	J	4	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 22411 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	8	0
			3532	2245	611	668	8			
1	C	453	Total	C	N	O	S	0	4	0
			3502	2224	604	666	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	466	Total	C	N	O	S	4	7	0
			3643	2269	622	718	34			
2	D	471	Total	C	N	O	S	3	2	0
			3642	2270	621	716	35			

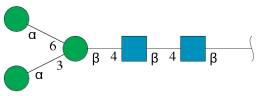
- Molecule 3 is a protein called Monoclonal antibody 10E5 heavy chain.

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 Monoclonal antibody 10E5 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			

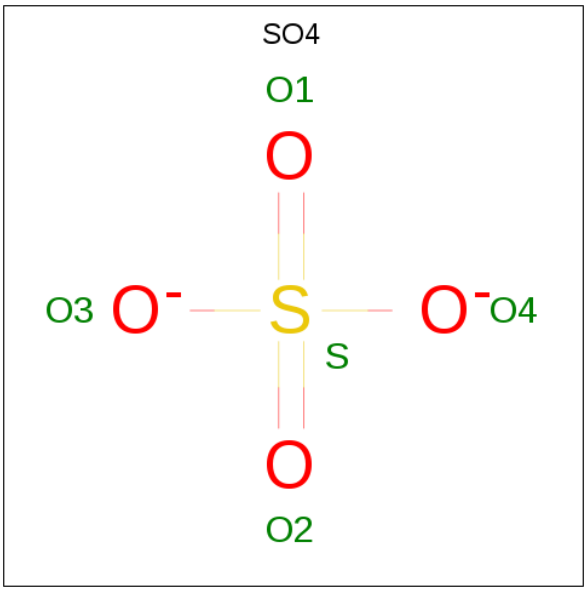
- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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.

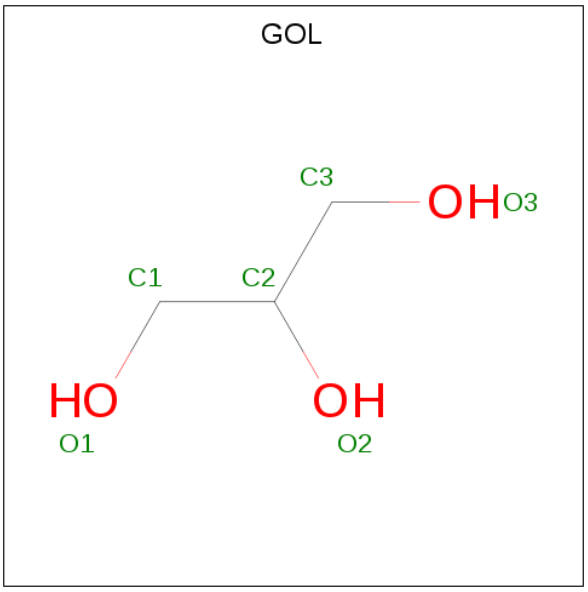
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	J	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: 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 O 6 3 3	0	0

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

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

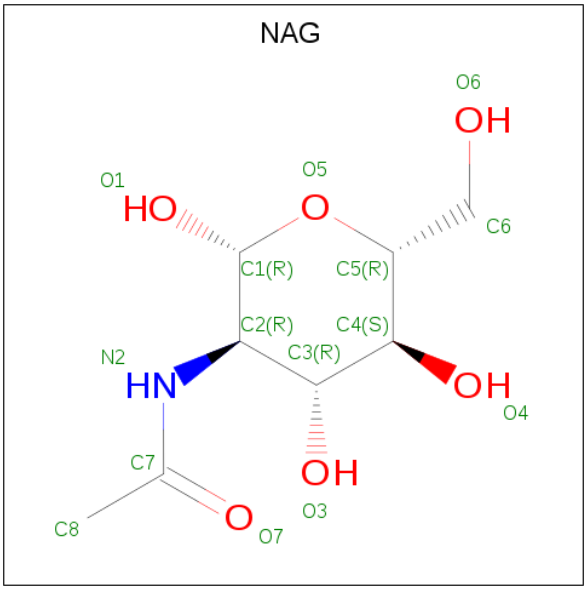
- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total Cl 1 1	0	0
11	D	1	Total Cl 1 1	0	0
11	C	2	Total Cl 2 2	0	0

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	463	Total O 463 463	0	0
14	B	249	Total O 249 249	0	0
14	C	274	Total O 274 274	0	0
14	D	200	Total O 200 200	0	0
14	E	17	Total O 17 17	0	0

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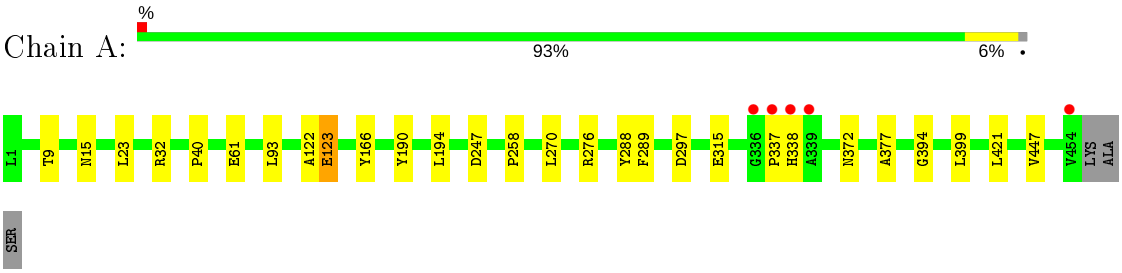
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	F	13	Total O 13 13	0	0
14	H	29	Total O 29 29	0	0
14	L	46	Total O 46 46	0	0

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.

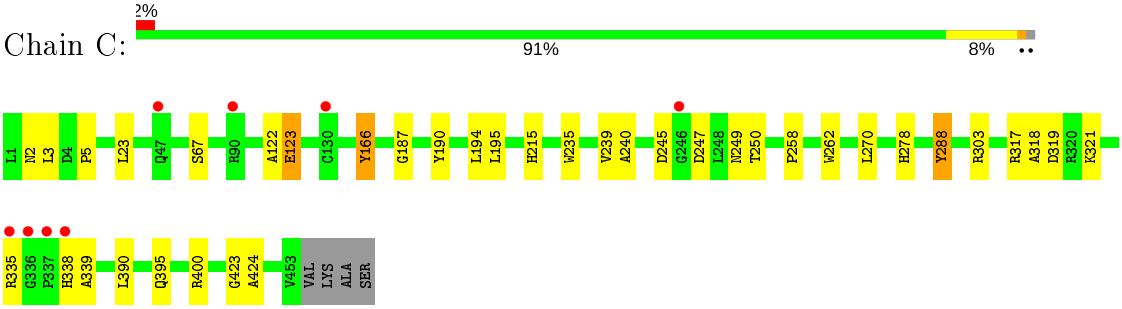
- Molecule 1: Integrin alpha-IIb

Chain A:



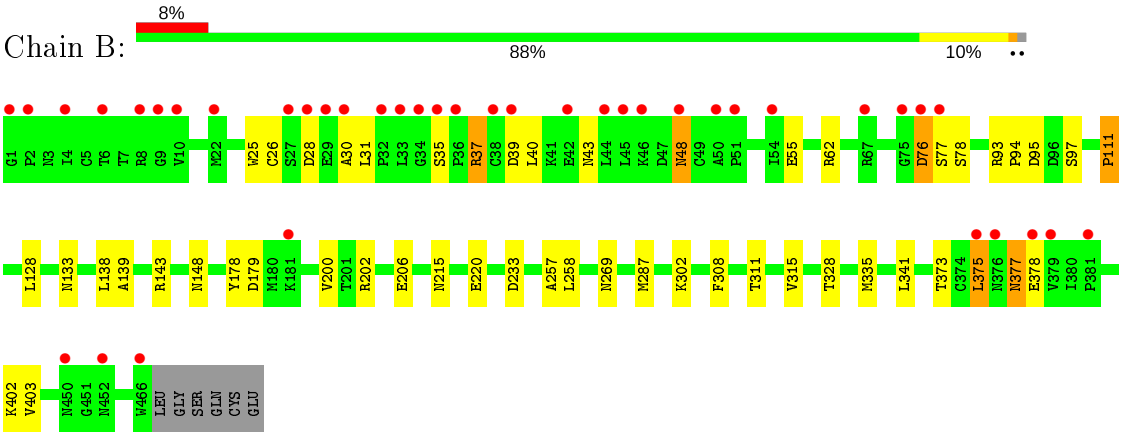
- Molecule 1: Integrin alpha-IIb

Chain C:



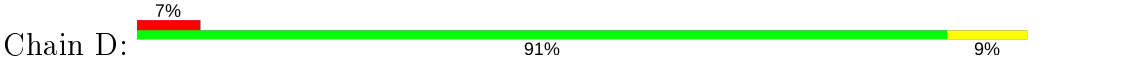
- Molecule 2: Integrin beta-3

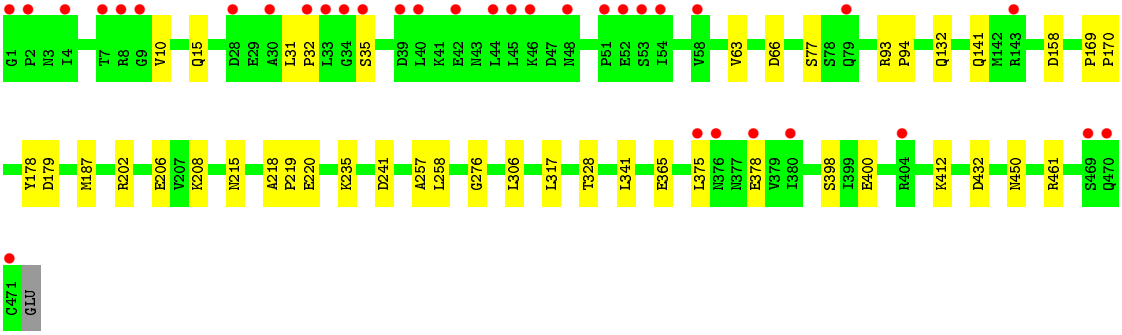
Chain B:



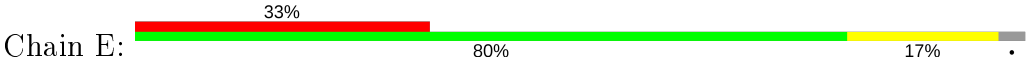
- Molecule 2: Integrin beta-3

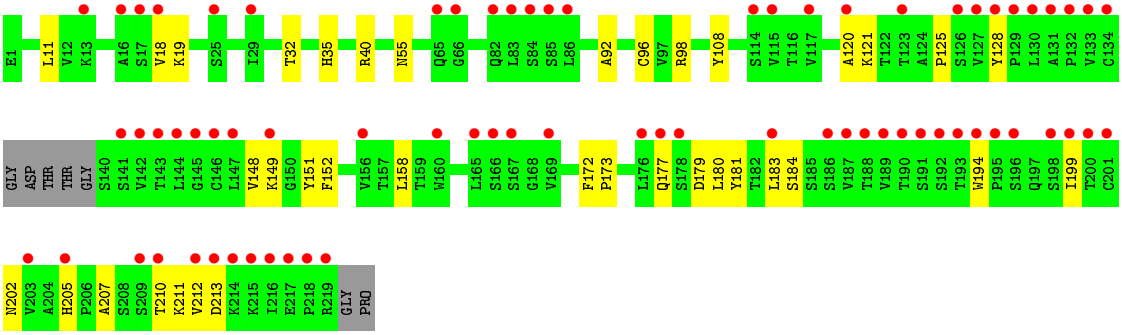
Chain D:



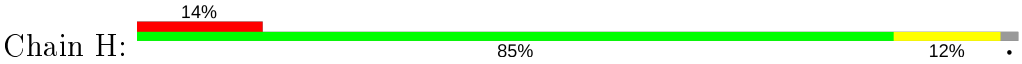


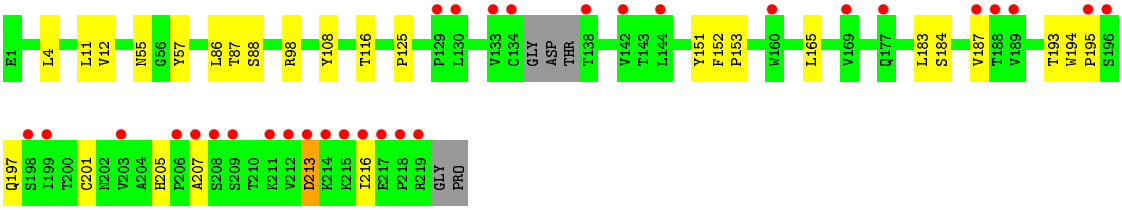
• Molecule 3: Monoclonal antibody 10E5 heavy chain



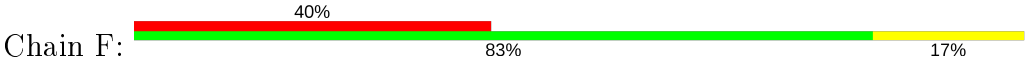


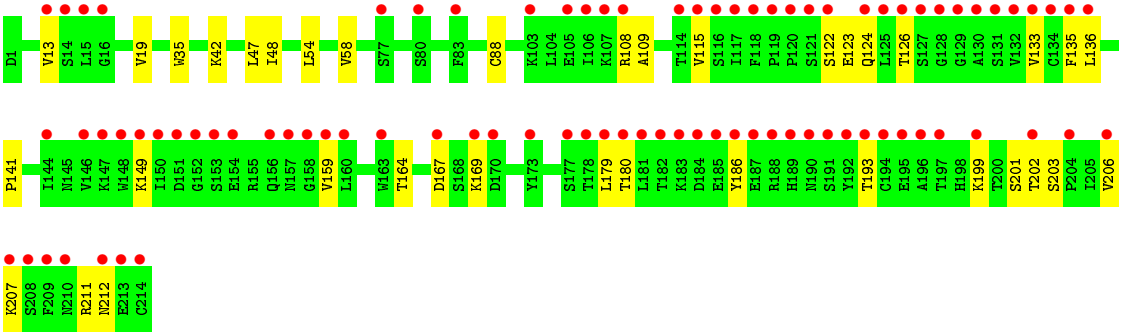
• Molecule 3: Monoclonal antibody 10E5 heavy chain





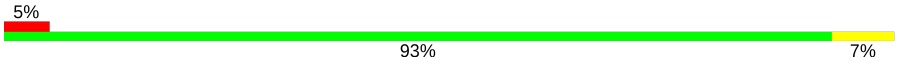
• Molecule 4: Monoclonal antibody 10E5 light chain

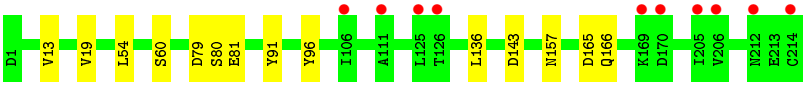




• Molecule 4: Monoclonal antibody 10E5 light chain

Chain L:



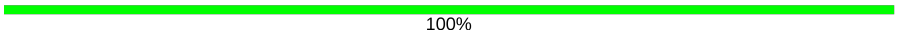


• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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	259.53Å 145.26Å 104.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.39 – 2.20 48.39 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.39-2.20) 99.3 (48.39-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.189 , 0.220 0.181 , (Not available)	Depositor DCC
R_{free} test set	991 reflections (0.50%)	wwPDB-VP
Wilson B-factor (Å^2)	33.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.0	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	22411	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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, MG, BMA, NAG, CL, CA, 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	0.36	0/3647	0.53	0/4969
1	C	0.31	0/3605	0.47	0/4912
2	B	0.32	0/3716	0.49	0/5037
2	D	0.29	0/3714	0.45	0/5036
3	E	0.22	0/1673	0.40	0/2290
3	H	0.26	0/1684	0.44	0/2305
4	F	0.24	0/1673	0.40	0/2269
4	L	0.27	0/1673	0.44	0/2269
All	All	0.30	0/21385	0.46	0/29087

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

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	0	3383	14	0
1	C	3502	0	3334	20	0
2	B	3643	0	3566	31	0
2	D	3642	0	3558	31	0
3	E	1631	0	1590	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1642	0	1600	18	0
4	F	1637	0	1553	25	0
4	L	1637	0	1553	8	0
5	G	61	0	52	0	0
6	I	28	0	25	0	0
6	K	28	0	25	2	0
7	J	50	0	43	0	0
8	A	15	0	0	1	0
8	C	15	0	0	0	0
8	L	5	0	0	0	0
9	A	6	0	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	C	2	0	0	0	0
11	D	1	0	0	0	0
12	B	1	0	0	0	0
12	D	1	0	0	0	0
13	B	14	0	13	0	0
13	D	14	0	13	0	0
14	A	463	0	0	4	0
14	B	249	0	0	6	0
14	C	274	0	0	0	0
14	D	200	0	0	2	0
14	E	17	0	0	0	0
14	F	13	0	0	0	0
14	H	29	0	0	0	0
14	L	46	0	0	1	0
All	All	22411	0	20316	171	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 4.

All (171) 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)
8:A:460:SO4:O4	14:A:691:HOH:O	2.14	0.65
1:A:122:ALA:O	1:A:123:GLU:HB2	1.99	0.62
2:B:202:ARG:NH2	2:B:206:GLU:OE2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:202:ASN:HA	3:E:213:ASP:HB3	1.83	0.60
2:D:178:TYR:CG	2:D:179:ASP:N	2.70	0.59
2:D:375:LEU:O	2:D:378:GLU:HG2	2.03	0.59
3:H:12:VAL:HG21	3:H:86:LEU:HD13	1.84	0.59
3:H:87:THR:HG22	3:H:88:SER:N	2.19	0.57
1:C:122:ALA:O	1:C:123:GLU:HB2	2.04	0.57
2:D:400:GLU:HB2	6:K:1:NAG:H83	1.86	0.56
1:A:337:PRO:O	1:A:338:HIS:CG	2.59	0.56
3:E:173:PRO:HD3	4:F:164:THR:HG22	1.88	0.56
4:F:193:THR:HG23	4:F:206:VAL:HG13	1.89	0.55
2:D:257:ALA:O	2:D:258:LEU:HB2	2.08	0.54
2:D:235:LYS:HE3	2:D:276:GLY:O	2.08	0.54
3:H:4:LEU:N	3:H:4:LEU:HD12	2.24	0.53
3:E:177:GLN:N	3:E:180:LEU:O	2.37	0.53
2:B:62:ARG:HD3	14:B:1066:HOH:O	2.09	0.53
2:D:202:ARG:NH2	2:D:206:GLU:OE2	2.39	0.53
2:B:26:CYS:O	2:B:37:ARG:NH1	2.42	0.53
3:H:194:TRP:CG	3:H:195:PRO:HA	2.44	0.52
3:E:125:PRO:HB2	3:E:148:VAL:HG13	1.92	0.52
3:E:98:ARG:HG3	3:E:108:TYR:HB2	1.91	0.52
4:F:159:VAL:HG22	4:F:179:LEU:HD13	1.91	0.52
4:F:141:PRO:HD3	4:F:199:LYS:HD3	1.93	0.51
3:H:193:THR:O	3:H:197:GLN:N	2.35	0.51
1:C:2:ASN:OD1	1:C:2:ASN:N	2.42	0.51
4:L:136:LEU:N	4:L:136:LEU:HD12	2.26	0.51
4:F:201:SER:OG	4:F:203:SER:O	2.19	0.51
1:C:245:ASP:OD1	1:C:250:THR:OG1	2.29	0.51
2:B:335:MET:HE2	14:B:518:HOH:O	2.10	0.51
3:E:40:ARG:CG	3:E:92:ALA:HB2	2.41	0.51
4:F:47:LEU:HA	4:F:58:VAL:HG21	1.93	0.50
3:E:205:HIS:CE1	3:E:207:ALA:HB3	2.46	0.50
1:C:303:ARG:NH1	1:C:335:ARG:HD3	2.27	0.50
4:F:136:LEU:N	4:F:136:LEU:HD12	2.26	0.50
4:F:149:LYS:HB2	4:F:193:THR:HB	1.93	0.50
2:D:202:ARG:HD3	14:D:754:HOH:O	2.12	0.50
3:E:149:LYS:NZ	4:F:180:THR:HG21	2.26	0.50
4:F:108:ARG:NE	4:F:109:ALA:O	2.43	0.50
2:B:93:ARG:HB2	2:B:94:PRO:HD2	1.94	0.49
1:A:194:LEU:C	1:A:194:LEU:HD12	2.32	0.49
3:E:120:ALA:HB2	3:E:179:ASP:HB3	1.93	0.49
4:F:167:ASP:OD1	4:F:169:LYS:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:125:PRO:HB3	3:H:151:TYR:HB3	1.94	0.48
2:D:178:TYR:CZ	2:D:179:ASP:HB3	2.48	0.48
2:D:93:ARG:HB2	2:D:94:PRO:HD2	1.95	0.48
1:A:270:LEU:HD23	1:A:276:ARG:HA	1.96	0.48
2:B:95:ASP:HA	2:B:403:VAL:O	2.14	0.47
2:D:306:LEU:HB3	2:D:328:THR:HG22	1.95	0.47
3:H:87:THR:CG2	3:H:88:SER:N	2.76	0.47
3:H:11:LEU:HD12	3:H:116:THR:HB	1.97	0.47
4:L:157:ASN:ND2	14:L:1197:HOH:O	2.47	0.47
1:A:15[B]:ASN:ND2	14:A:1000:HOH:O	2.34	0.47
2:D:218:ALA:HB3	2:D:219:PRO:HD3	1.95	0.47
4:F:141:PRO:CD	4:F:199:LYS:HD3	2.45	0.47
2:B:178:TYR:CG	2:B:179:ASP:N	2.83	0.47
1:A:32[A]:ARG:HD2	14:A:980:HOH:O	2.15	0.47
1:C:215:HIS:CE1	3:E:32:THR:HG22	2.50	0.47
4:F:206:VAL:HG12	4:F:207:LYS:N	2.29	0.46
2:B:76:ASP:OD2	2:B:76:ASP:N	2.47	0.46
1:A:247:ASP:OD2	1:A:247:ASP:C	2.54	0.46
2:B:133[A]:ASN:OD1	14:B:1138:HOH:O	2.21	0.46
3:E:128:TYR:CZ	4:F:124:GLN:HA	2.51	0.46
1:C:194:LEU:HD12	1:C:194:LEU:C	2.36	0.46
2:D:141:GLN:HG3	2:D:341:LEU:HD21	1.97	0.46
2:B:375:LEU:HB2	14:B:932:HOH:O	2.15	0.46
1:C:122:ALA:O	1:C:123:GLU:CB	2.63	0.46
4:L:79:ASP:OD1	4:L:80:SER:N	2.48	0.46
1:A:315:GLU:OE2	14:A:532:HOH:O	2.21	0.46
3:E:158:LEU:C	3:E:158:LEU:HD23	2.36	0.46
4:F:35:TRP:CZ3	4:F:88:CYS:HB3	2.51	0.46
2:D:398:SER:OG	6:K:1:NAG:O7	2.26	0.46
2:B:138:LEU:HA	2:B:341:LEU:CD1	2.45	0.46
2:D:63:VAL:HG11	2:D:66:ASP:HB2	1.98	0.46
4:F:115:VAL:HG12	4:F:207:LYS:HG3	1.97	0.46
3:H:201:CYS:O	3:H:213:ASP:HA	2.15	0.46
1:A:258:PRO:HA	1:A:289:PHE:O	2.15	0.45
2:B:97:SER:HB3	2:B:402:LYS:HG2	1.98	0.45
1:C:318:ALA:O	1:C:319:ASP:HB2	2.17	0.45
1:C:390:LEU:HD12	1:C:390:LEU:N	2.31	0.45
2:D:365:GLU:OE2	2:D:412:LYS:NZ	2.48	0.45
2:B:378:GLU:HB3	14:B:932:HOH:O	2.15	0.45
2:D:158:ASP:H	2:D:187[B]:MET:HE3	1.82	0.45
3:E:125:PRO:HB2	3:E:148:VAL:CG1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:ARG:HB2	2:B:94:PRO:CD	2.47	0.45
2:D:341:LEU:HD23	2:D:341:LEU:C	2.37	0.45
3:E:194:TRP:CD1	3:E:199:ILE:HD12	2.52	0.45
1:A:9:THR:HB	1:A:447:VAL:HB	1.98	0.45
3:E:183:LEU:HD23	3:E:183:LEU:C	2.37	0.45
3:E:205:HIS:HB3	3:E:210:THR:CG2	2.47	0.45
2:B:233:ASP:OD1	2:B:302:LYS:HD2	2.17	0.45
3:E:205:HIS:HB3	3:E:210:THR:HG22	1.99	0.45
3:E:212:VAL:HG12	3:E:213:ASP:N	2.31	0.44
2:B:31:LEU:CD2	2:B:35:SER:HB2	2.47	0.44
2:D:10:VAL:HA	2:D:15:GLN:NE2	2.32	0.44
1:A:394:GLY:HA2	1:A:399:LEU:HD23	1.99	0.44
4:F:122:SER:O	4:F:126:THR:HG23	2.17	0.44
1:C:278[A]:HIS:CE1	1:C:339:ALA:HB1	2.52	0.44
3:E:213:ASP:OD1	3:E:213:ASP:N	2.51	0.44
2:B:39:ASP:OD2	2:B:43:ASN:ND2	2.51	0.44
2:D:158:ASP:N	2:D:187[B]:MET:HE3	2.33	0.44
3:E:172:PHE:CD1	4:F:164:THR:HG23	2.53	0.44
4:F:186:TYR:CE2	4:F:211:ARG:HG3	2.53	0.44
4:L:54:LEU:HD21	4:L:60:SER:HA	1.99	0.44
1:C:317:ARG:HB2	1:C:321:LYS:HB2	1.99	0.44
2:B:39:ASP:OD2	2:B:40:LEU:N	2.51	0.44
2:D:77:SER:HB2	2:D:241:ASP:CG	2.38	0.44
4:F:133:VAL:HG11	4:F:135:PHE:CZ	2.52	0.44
2:B:373:THR:CG2	2:B:377:ASN:HA	2.49	0.43
4:F:123:GLU:O	4:F:126:THR:OG1	2.35	0.43
2:B:220:GLU:HA	2:B:220:GLU:OE1	2.17	0.43
1:C:166:TYR:O	1:C:187:GLY:HA3	2.18	0.43
2:D:132:GLN:OE1	2:D:208:LYS:HG2	2.18	0.43
3:E:210:THR:C	3:E:211:LYS:HG3	2.38	0.43
3:H:183:LEU:HD23	3:H:183:LEU:C	2.38	0.43
3:H:165:LEU:HD21	3:H:187:VAL:HG21	2.00	0.43
2:B:308:PHE:CE2	2:B:328:THR:HG21	2.54	0.43
3:H:55:ASN:CG	3:H:57:TYR:HD2	2.22	0.43
2:D:450:ASN:ND2	2:D:450:ASN:O	2.51	0.43
3:H:98:ARG:HG3	3:H:108:TYR:HB2	2.00	0.43
1:C:3:LEU:O	1:C:5:PRO:HD3	2.19	0.43
3:H:194:TRP:CZ2	3:H:216:ILE:HG22	2.54	0.43
3:H:205:HIS:CE1	3:H:207:ALA:HB3	2.54	0.43
1:C:258:PRO:HB2	1:C:288:TYR:CD1	2.54	0.42
3:E:11:LEU:N	3:E:11:LEU:HD12	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:121:LYS:HD2	3:E:121:LYS:N	2.34	0.42
1:A:297:ASP:O	1:A:372:ASN:HB2	2.19	0.42
3:E:40:ARG:HG3	3:E:92:ALA:HB2	2.01	0.42
1:A:40:PRO:HA	1:A:93:LEU:O	2.20	0.42
1:C:247:ASP:OD2	1:C:249:ASN:HB2	2.19	0.42
3:E:18:VAL:HG22	3:E:19:LYS:N	2.34	0.42
4:F:48:ILE:CD1	4:F:54:LEU:HD23	2.50	0.42
2:D:31:LEU:HD12	2:D:32:PRO:HD2	2.02	0.42
4:F:13:VAL:HG11	4:F:19:VAL:HG11	2.01	0.42
2:B:28:ASP:OD2	2:B:30:ALA:N	2.53	0.42
3:H:183:LEU:HD23	3:H:184:SER:N	2.35	0.42
2:D:461:ARG:NE	14:D:880:HOH:O	2.47	0.41
3:H:12:VAL:HG21	3:H:86:LEU:CD1	2.50	0.41
4:L:13:VAL:HG11	4:L:19:VAL:HG11	2.02	0.41
1:C:262:TRP:HB3	2:D:317:LEU:HD13	2.02	0.41
1:C:423:GLY:O	1:C:424:ALA:HB3	2.20	0.41
2:D:220:GLU:HA	2:D:220:GLU:OE1	2.20	0.41
4:F:202:THR:HG22	4:F:202:THR:O	2.20	0.41
4:L:81:GLU:N	4:L:81:GLU:OE1	2.54	0.41
2:B:139:ALA:HB2	2:B:200:VAL:HG11	2.02	0.41
1:C:395:GLN:OE1	1:C:400:ARG:HD3	2.21	0.41
3:H:152:PHE:CD1	3:H:153:PRO:HA	2.55	0.41
1:A:377:ALA:HB2	1:A:421:LEU:HD11	2.03	0.41
2:B:77:SER:O	2:B:78:SER:OG	2.29	0.41
2:D:93:ARG:HB2	2:D:94:PRO:CD	2.51	0.41
4:F:42:LYS:N	4:F:42:LYS:HD2	2.35	0.41
1:C:239:VAL:HG22	1:C:240:ALA:N	2.36	0.41
2:D:169:PRO:CB	2:D:170:PRO:CD	2.99	0.41
2:B:111:PRO:HB3	2:B:148:ASN:HB3	2.03	0.40
2:B:311:THR:O	2:B:315[B]:VAL:HG23	2.20	0.40
2:D:32:PRO:O	2:D:35:SER:HB3	2.21	0.40
3:E:183:LEU:HD23	3:E:184:SER:N	2.37	0.40
4:L:91:TYR:HB2	4:L:96:TYR:CZ	2.55	0.40
2:B:143:ARG:NH1	14:B:797:HOH:O	2.30	0.40
2:B:25:TRP:HB3	2:B:55:GLU:HB2	2.02	0.40
3:E:151:TYR:CZ	3:E:181:TYR:HB2	2.56	0.40
2:B:269:ASN:HA	2:B:287:MET:CG	2.51	0.40
2:D:341:LEU:HD23	2:D:341:LEU:O	2.21	0.40
3:E:152:PHE:CD2	3:E:152:PHE:C	2.94	0.40
3:E:35:HIS:O	3:E:96:CYS:HA	2.21	0.40
4:L:165:ASP:O	4:L:166:GLN:C	2.58	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:ASN:N	2:B:48:ASN:OD1	2.54	0.40
1:C:235:TRP:CZ2	1:C:270:LEU:HD11	2.56	0.40
2:B:257:ALA:O	2:B:258:LEU:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	460/457 (101%)	441 (96%)	18 (4%)	1 (0%)	47 55
1	C	455/457 (100%)	441 (97%)	13 (3%)	1 (0%)	47 55
2	B	471/472 (100%)	452 (96%)	17 (4%)	2 (0%)	34 37
2	D	471/472 (100%)	454 (96%)	17 (4%)	0	100 100
3	E	210/221 (95%)	193 (92%)	16 (8%)	1 (0%)	29 31
3	H	212/221 (96%)	197 (93%)	15 (7%)	0	100 100
4	F	212/214 (99%)	195 (92%)	16 (8%)	1 (0%)	29 31
4	L	212/214 (99%)	204 (96%)	8 (4%)	0	100 100
All	All	2703/2728 (99%)	2577 (95%)	120 (4%)	6 (0%)	47 55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
1	C	123	GLU
2	B	375	LEU
4	F	212	ASN
2	B	377	ASN
3	E	55	ASN

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	370/364 (102%)	365 (99%)	5 (1%)	67 80
1	C	365/364 (100%)	358 (98%)	7 (2%)	57 71
2	B	419/417 (100%)	413 (99%)	6 (1%)	67 80
2	D	418/417 (100%)	416 (100%)	2 (0%)	88 94
3	E	186/190 (98%)	186 (100%)	0	100 100
3	H	187/190 (98%)	186 (100%)	1 (0%)	88 94
4	F	188/188 (100%)	188 (100%)	0	100 100
4	L	188/188 (100%)	187 (100%)	1 (0%)	88 94
All	All	2321/2318 (100%)	2299 (99%)	22 (1%)	76 88

All (22) 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	190	TYR
1	A	288	TYR
2	B	37	ARG
2	B	48	ASN
2	B	76	ASP
2	B	111	PRO
2	B	128	LEU
2	B	215	ASN
1	C	23	LEU
1	C	67	SER
1	C	166	TYR
1	C	190	TYR
1	C	195	LEU
1	C	288	TYR
1	C	338	HIS
2	D	215	ASN

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Mol	Chain	Res	Type
2	D	432	ASP
3	H	213	ASP
4	L	143	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	C	197	GLN
2	D	15	GLN
2	D	450	ASN
2	D	452	ASN
4	F	27	GLN
4	F	93	GLN

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	0.47	0	17,19,21	0.83	1 (5%)
5	NAG	G	2	5	14,14,15	0.62	0	17,19,21	0.91	0
5	BMA	G	3	5	11,11,12	0.64	0	15,15,17	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	MAN	G	4	5	11,11,12	0.59	0	15,15,17	0.81	0
5	MAN	G	5	5	11,11,12	0.64	0	15,15,17	0.72	0
6	NAG	I	1	2,6	14,14,15	0.60	0	17,19,21	0.82	0
6	NAG	I	2	6	14,14,15	0.53	0	17,19,21	0.70	0
7	NAG	J	1	2,7	14,14,15	0.61	0	17,19,21	0.80	0
7	NAG	J	2	7	14,14,15	0.68	0	17,19,21	1.13	1 (5%)
7	BMA	J	3	7	11,11,12	0.68	0	15,15,17	0.88	1 (6%)
7	MAN	J	4	7	11,11,12	0.61	0	15,15,17	0.86	0
6	NAG	K	1	2,6	14,14,15	0.65	0	17,19,21	0.67	0
6	NAG	K	2	6	14,14,15	0.54	0	17,19,21	0.72	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	-	2/6/23/26	0/1/1/1
7	NAG	J	2	7	-	0/6/23/26	0/1/1/1
7	BMA	J	3	7	-	0/2/19/22	0/1/1/1
7	MAN	J	4	7	-	0/2/19/22	0/1/1/1
6	NAG	K	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	J	2	NAG	C4-C3-C2	2.93	115.31	111.02
5	G	1	NAG	O5-C5-C6	2.27	110.76	107.20
7	J	3	BMA	C1-C2-C3	2.04	112.18	109.67

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

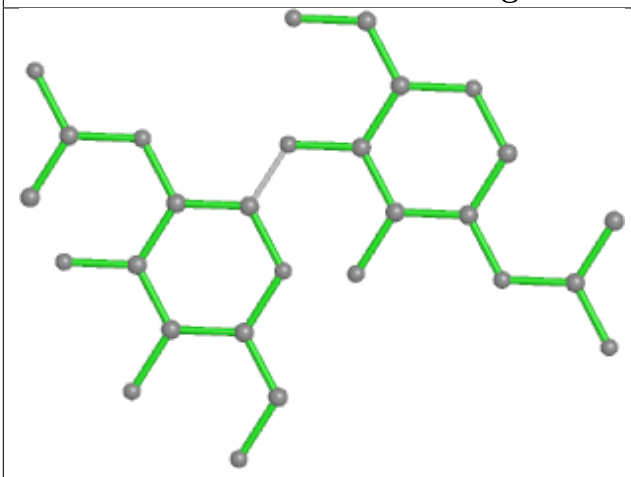
There are no ring outliers.

1 monomer is involved in 2 short contacts:

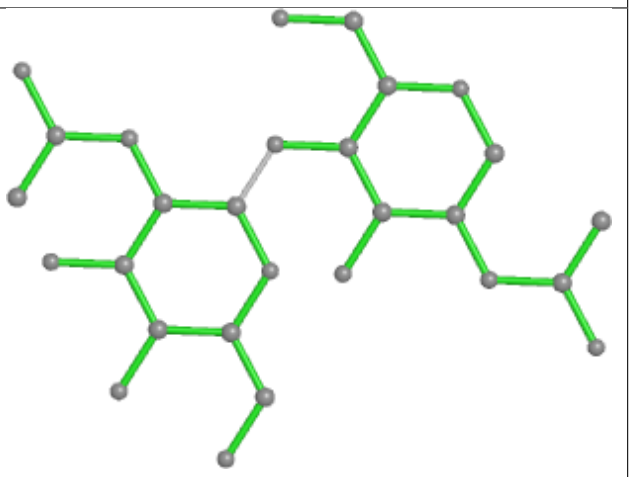
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	1	NAG	2	0

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

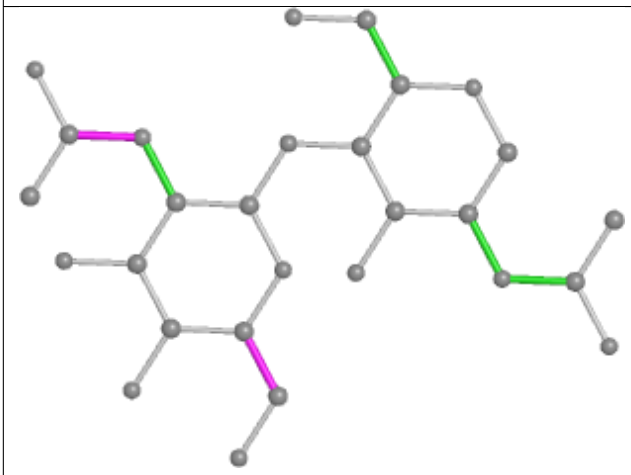
Oligosaccharide Chain I



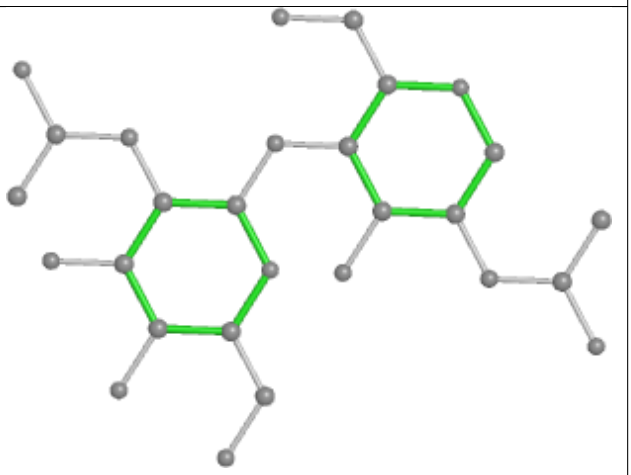
Bond lengths



Bond angles

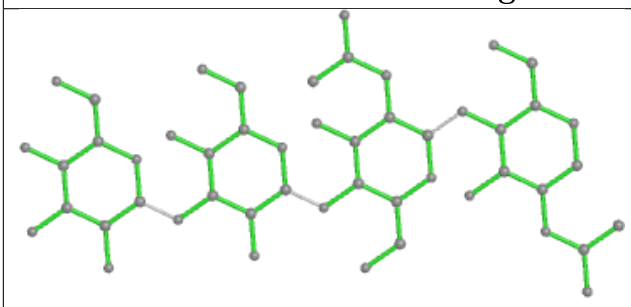


Torsions

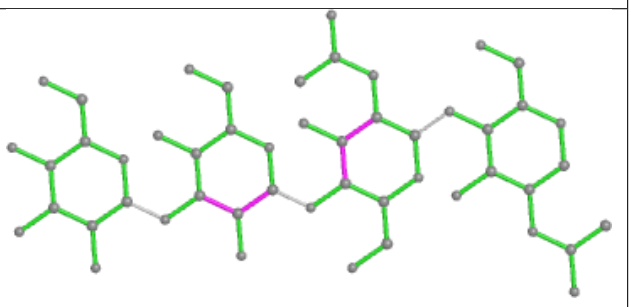


Rings

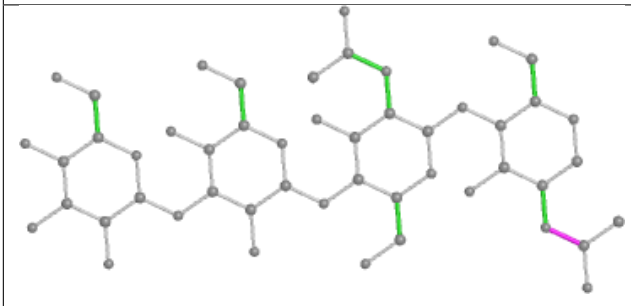
Oligosaccharide Chain J



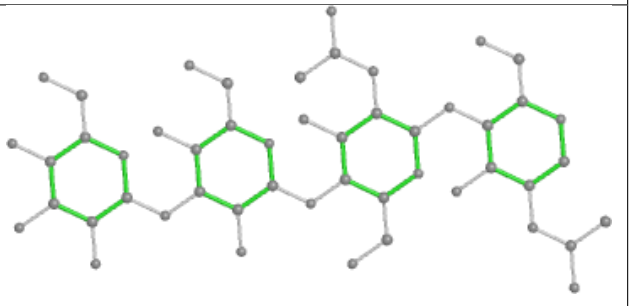
Bond lengths



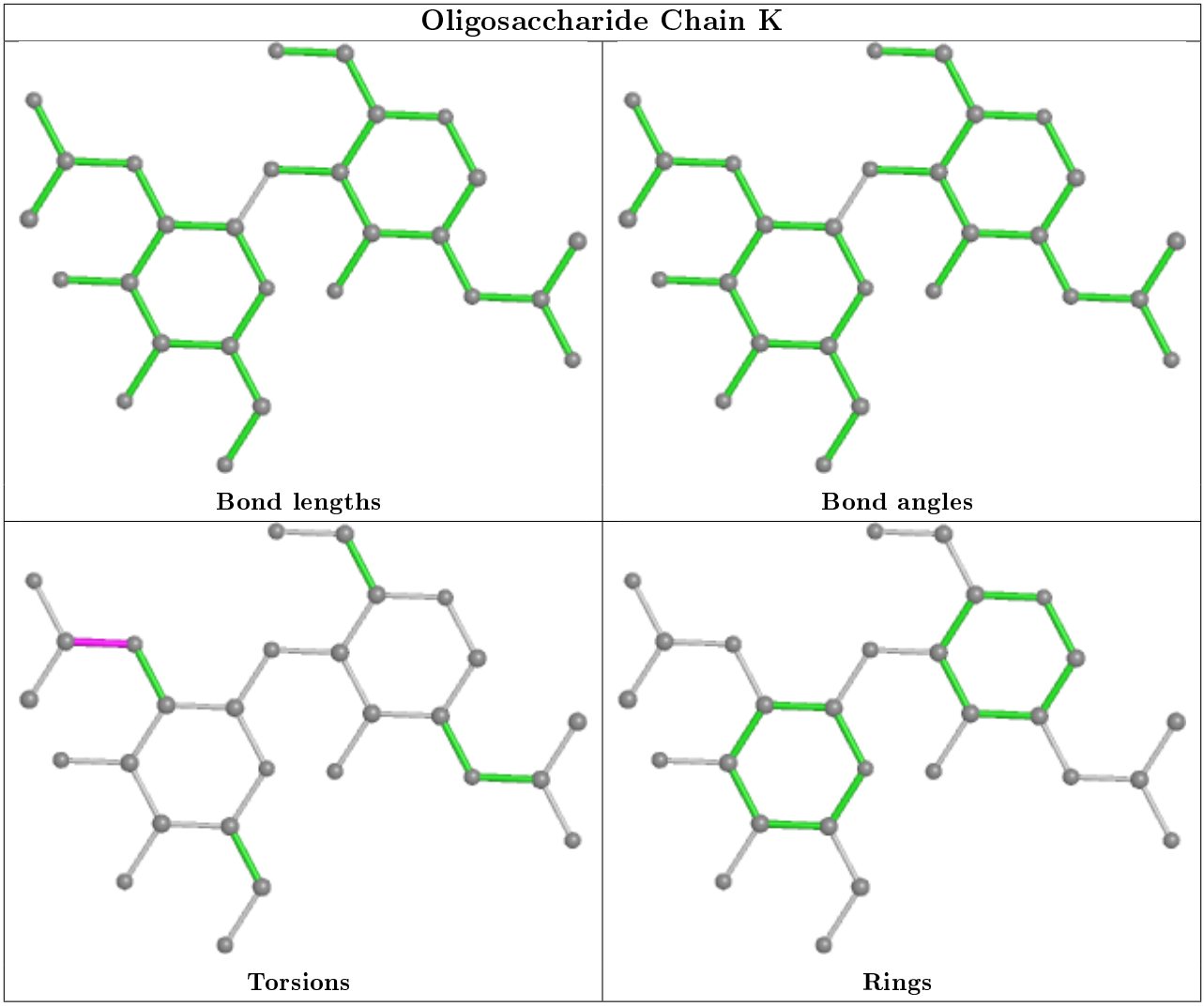
Bond angles



Torsions



Rings



5.6 Ligand geometry

Of 28 ligands modelled in this entry, 18 are monoatomic - leaving 10 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	459	-	4,4,4	0.16	0	6,6,6	0.14	0
13	NAG	D	3099	2	14,14,15	0.51	0	17,19,21	0.78	0
8	SO4	C	459	-	4,4,4	0.16	0	6,6,6	0.07	0
9	GOL	A	461	-	5,5,5	0.36	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	SO4	A	460	-	4,4,4	0.10	0	6,6,6	0.18	0
8	SO4	C	458	-	4,4,4	0.18	0	6,6,6	0.11	0
8	SO4	C	460	-	4,4,4	0.14	0	6,6,6	0.09	0
8	SO4	A	458	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	L	215	-	4,4,4	0.14	0	6,6,6	0.06	0
13	NAG	B	3099	2	14,14,15	0.56	0	17,19,21	0.86	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	D	3099	2	-	0/6/23/26	0/1/1/1
13	NAG	B	3099	2	-	0/6/23/26	0/1/1/1
9	GOL	A	461	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	3099	NAG	C1-O5-C5	2.46	115.52	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	461	GOL	O1-C1-C2-C3
9	A	461	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	460	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.01	5 (1%) 80 79	3, 11, 34, 73	0
1	C	453/457 (99%)	0.00	8 (1%) 68 66	9, 24, 50, 77	0
2	B	466/472 (98%)	0.37	40 (8%) 10 9	2, 32, 90, 112	1 (0%)
2	D	471/472 (99%)	0.10	34 (7%) 15 14	11, 33, 78, 142	1 (0%)
3	E	214/221 (96%)	1.74	72 (33%) 0 0	33, 85, 137, 155	0
3	H	216/221 (97%)	0.46	31 (14%) 2 2	16, 59, 103, 118	0
4	F	214/214 (100%)	1.81	86 (40%) 0 0	33, 81, 134, 157	1 (0%)
4	L	214/214 (100%)	0.08	10 (4%) 31 30	20, 44, 70, 95	1 (0%)
All	All	2702/2728 (99%)	0.41	286 (10%) 6 5	2, 34, 109, 157	4 (0%)

All (286) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	214	CYS	11.4
2	D	469	SER	10.3
3	E	133	VAL	10.2
3	E	144	LEU	9.1
2	B	33	LEU	8.8
3	E	165	LEU	8.6
3	E	134	CYS	8.5
3	E	216	ILE	8.2
3	E	142	VAL	8.2
3	E	196	SER	8.1
3	E	212	VAL	7.6
4	F	130	ALA	7.5
4	L	214	CYS	7.5
2	B	36	PRO	7.4
3	E	194	TRP	7.2
4	F	193	THR	7.2

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Mol	Chain	Res	Type	RSRZ
4	F	181	LEU	6.9
3	E	210	THR	6.9
3	E	131	ALA	6.9
3	E	219	ARG	6.8
4	F	134	CYS	6.6
4	F	212	ASN	6.6
4	F	179	LEU	6.5
3	E	201	CYS	6.4
2	B	77	SER	6.3
4	F	125	LEU	6.2
3	E	199	ILE	6.0
4	F	117	ILE	5.9
3	E	160	TRP	5.9
3	E	129	PRO	5.9
4	F	115	VAL	5.8
4	F	213	GLU	5.7
4	F	126	THR	5.6
4	F	182	THR	5.6
2	B	44	LEU	5.5
4	L	212	ASN	5.5
3	E	128	TYR	5.5
3	E	147	LEU	5.4
3	E	215	LYS	5.4
4	F	120	PRO	5.3
3	H	142	VAL	5.3
2	B	34	GLY	5.3
2	B	8	ARG	5.3
4	F	206	VAL	5.2
3	E	132	PRO	5.2
4	F	116	SER	5.1
3	H	133	VAL	5.0
4	F	135	PHE	5.0
4	F	195	GLU	5.0
4	F	119	PRO	4.9
4	F	148	TRP	4.9
2	D	471	CYS	4.8
3	H	189	VAL	4.8
1	A	337	PRO	4.8
4	F	151	ASP	4.7
3	E	130	LEU	4.7
2	B	375	LEU	4.6
2	B	10	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
4	F	180	THR	4.6
2	B	46	LYS	4.6
4	F	118	PHE	4.6
4	F	194	CYS	4.6
3	E	195	PRO	4.6
3	E	218	PRO	4.5
3	E	187	VAL	4.5
3	E	141	SER	4.5
4	F	150	ILE	4.5
3	E	127	VAL	4.4
4	F	129	GLY	4.4
4	F	169	LYS	4.4
2	B	2	PRO	4.4
4	F	122	SER	4.3
1	C	336	GLY	4.3
4	F	184	ASP	4.3
2	B	35	SER	4.3
3	E	200	THR	4.2
3	H	198	SER	4.2
2	B	4	ILE	4.2
4	F	191	SER	4.2
3	E	177	GLN	4.2
4	F	156	GLN	4.2
2	B	1	GLY	4.2
2	B	32	PRO	4.1
3	E	217	GLU	4.1
3	E	16	ALA	4.1
4	F	186	TYR	4.1
4	F	209	PHE	4.1
3	E	143	THR	4.0
4	F	152	GLY	4.0
4	F	127	SER	4.0
2	B	30	ALA	4.0
3	E	83	LEU	4.0
3	H	207	ALA	4.0
3	E	190	THR	3.9
3	E	198	SER	3.9
4	F	210	ASN	3.9
3	E	149	LYS	3.9
4	F	146	VAL	3.9
4	F	147	LYS	3.9
2	B	9	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
2	D	1	GLY	3.8
4	F	149	LYS	3.8
4	F	14	SER	3.8
2	D	8	ARG	3.8
3	E	183	LEU	3.8
4	F	133	VAL	3.8
4	F	136	LEU	3.8
2	B	466	TRP	3.8
2	B	51	PRO	3.7
3	H	160	TRP	3.7
4	F	190	ASN	3.7
3	H	215	LYS	3.7
3	H	134	CYS	3.7
1	A	339	ALA	3.7
4	F	128	GLY	3.7
4	F	158	GLY	3.6
4	L	169	LYS	3.6
2	B	22	MET	3.6
3	E	167	SER	3.6
2	D	2	PRO	3.6
3	E	29	ILE	3.6
2	D	470	GLN	3.6
2	D	48	ASN	3.5
3	E	65	GLN	3.5
4	F	107	LYS	3.5
4	F	183	LYS	3.5
4	F	197	THR	3.5
2	B	54	ILE	3.5
4	F	132	VAL	3.5
2	D	375	LEU	3.5
4	F	192	TYR	3.4
3	H	188	THR	3.4
4	F	131	SER	3.4
2	D	42	GLU	3.4
4	F	154	GLU	3.4
3	E	84	SER	3.4
4	F	188	ARG	3.3
4	F	124	GLN	3.3
2	B	45	LEU	3.3
2	D	33	LEU	3.3
4	F	208	SER	3.3
2	D	51	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
3	E	192	SER	3.2
3	E	169	VAL	3.2
3	H	138	THR	3.2
1	A	338	HIS	3.2
4	F	121	SER	3.2
2	D	46	LYS	3.2
3	H	203	VAL	3.2
2	B	181	LYS	3.2
3	E	13	LYS	3.2
3	E	188	THR	3.2
4	F	159	VAL	3.2
4	F	15	LEU	3.1
2	D	380	ILE	3.1
1	C	335	ARG	3.1
4	F	185	GLU	3.1
2	D	4	ILE	3.1
3	H	217	GLU	3.1
3	H	211	LYS	3.1
3	H	213	ASP	3.1
4	F	207	LYS	3.1
4	F	106	ILE	3.1
3	E	17	SER	3.0
2	B	381	PRO	3.0
3	H	208	SER	3.0
2	B	450	ASN	3.0
3	E	156	VAL	3.0
2	D	34	GLY	3.0
2	D	404	ARG	3.0
2	D	52	GLU	3.0
4	F	144	ILE	3.0
3	E	203	VAL	3.0
3	E	126	SER	2.9
3	E	166	SER	2.9
3	H	199	ILE	2.9
2	D	44	LEU	2.9
3	E	191	SER	2.9
3	H	216	ILE	2.9
3	H	144	LEU	2.9
2	D	54	ILE	2.9
2	B	75	GLY	2.9
3	E	214	LYS	2.9
2	B	28	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	79	GLN	2.8
2	B	76	ASP	2.8
2	D	32	PRO	2.8
4	F	178	THR	2.8
3	E	85	SER	2.8
1	A	336	GLY	2.7
3	H	187	VAL	2.7
4	F	170	ASP	2.7
2	B	452	ASN	2.7
3	E	189	VAL	2.7
3	H	209	SER	2.7
2	D	376	ASN	2.7
3	E	117	VAL	2.7
4	L	126	THR	2.7
2	D	40	LEU	2.6
3	E	115	VAL	2.6
2	B	42	GLU	2.6
3	E	178	SER	2.6
4	F	153	SER	2.6
4	F	105	GLU	2.6
2	D	39	ASP	2.6
3	E	205	HIS	2.6
2	B	39	ASP	2.6
2	B	379	VAL	2.6
4	F	83	PHE	2.6
4	F	177	SER	2.6
2	D	143	ARG	2.6
3	H	177	GLN	2.6
2	D	53	SER	2.6
2	D	45	LEU	2.6
4	F	160	LEU	2.5
1	C	47	GLN	2.5
3	H	219	ARG	2.5
2	D	35	SER	2.5
3	E	120	ALA	2.5
1	C	338	HIS	2.5
3	E	213	ASP	2.5
3	H	218	PRO	2.5
2	B	376	ASN	2.5
2	D	9	GLY	2.5
3	E	145	GLY	2.5
3	E	86	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	90	ARG	2.4
2	D	58	VAL	2.4
3	E	82	GLN	2.4
2	B	378	GLU	2.4
4	F	80	SER	2.4
3	H	195	PRO	2.4
1	C	246	GLY	2.4
3	H	196	SER	2.4
1	A	454	VAL	2.4
2	B	67	ARG	2.4
2	B	50	ALA	2.4
3	E	146	CYS	2.4
4	F	157	ASN	2.4
3	E	209	SER	2.3
1	C	337	PRO	2.3
3	E	25	SER	2.3
4	F	103	LYS	2.3
4	F	13	VAL	2.3
3	H	214	LYS	2.3
2	B	27	SER	2.3
3	E	186	SER	2.3
3	H	169	VAL	2.2
4	F	163	TRP	2.2
4	F	187	GLU	2.2
2	B	48	ASN	2.2
4	L	170	ASP	2.2
2	B	38	CYS	2.2
3	H	206	PRO	2.2
2	D	30	ALA	2.2
4	L	106	ILE	2.2
4	L	205	ILE	2.2
3	H	130	LEU	2.2
2	D	28	ASP	2.2
2	D	378	GLU	2.2
4	L	125	LEU	2.2
4	F	199	LYS	2.2
4	F	173	TYR	2.2
4	F	189	HIS	2.2
3	E	66	GLY	2.2
3	E	123	THR	2.2
2	B	29	GLU	2.2
4	F	114	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	7	THR	2.1
4	F	108	ARG	2.1
4	L	111	ALA	2.1
3	E	114	SER	2.1
4	F	16	GLY	2.1
4	F	204	PRO	2.1
3	H	212	VAL	2.1
4	L	206	VAL	2.1
1	C	130	CYS	2.1
3	E	193	THR	2.1
4	F	167	ASP	2.1
4	F	202	THR	2.1
3	E	18	VAL	2.1
3	H	129	PRO	2.1
2	B	6	THR	2.0
3	E	176	LEU	2.0
4	F	77	SER	2.0
4	F	196	ALA	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
7	MAN	J	4	11/12	0.64	0.21	99,105,107,108	0
7	BMA	J	3	11/12	0.77	0.23	100,108,112,113	0
6	NAG	K	2	14/15	0.78	0.39	93,108,114,117	0
5	BMA	G	3	11/12	0.79	0.25	62,94,110,118	0
5	MAN	G	5	11/12	0.80	0.27	114,116,117,117	0
5	MAN	G	4	11/12	0.81	0.23	45,79,95,96	0
6	NAG	I	1	14/15	0.83	0.23	51,69,76,85	0
6	NAG	K	1	14/15	0.90	0.25	49,69,80,94	0
6	NAG	I	2	14/15	0.90	0.27	78,86,91,94	0
7	NAG	J	2	14/15	0.90	0.19	38,59,76,89	0

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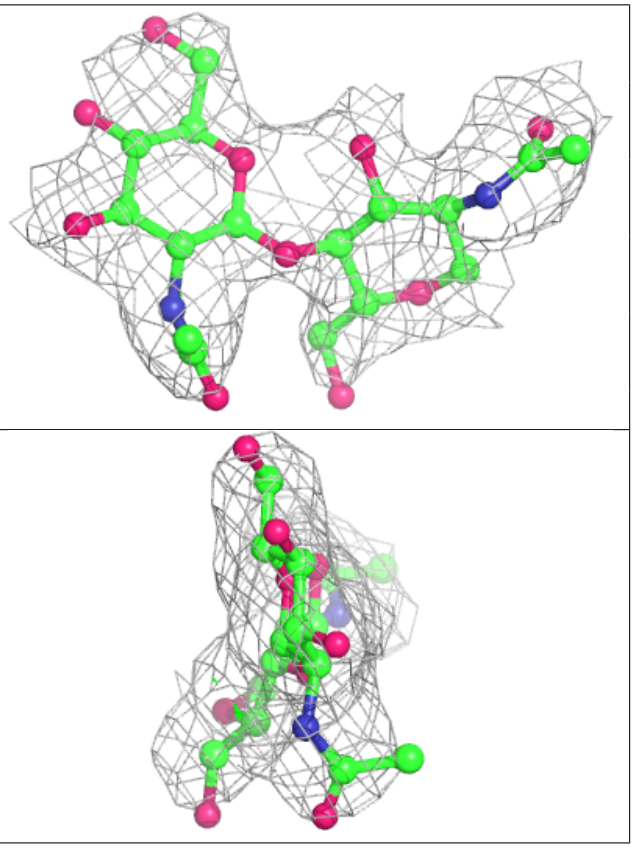
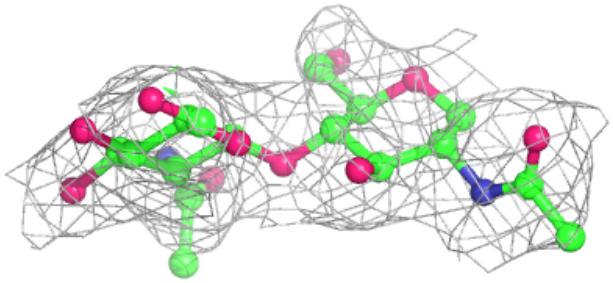
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	G	2	14/15	0.92	0.11	29,49,58,65	0
5	NAG	G	1	14/15	0.97	0.07	5,18,26,28	0
7	NAG	J	1	14/15	0.97	0.08	15,30,43,45	0

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

Electron density around Chain I:

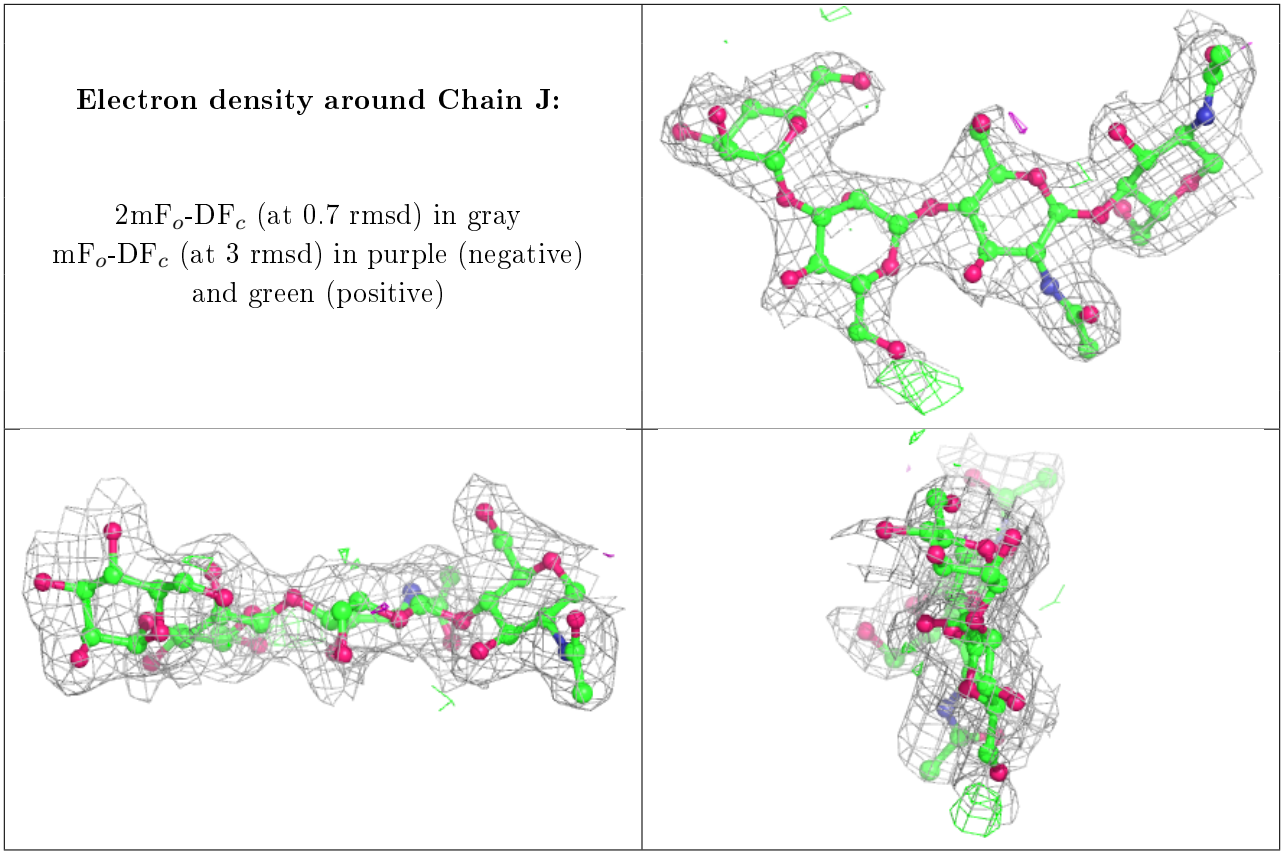
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





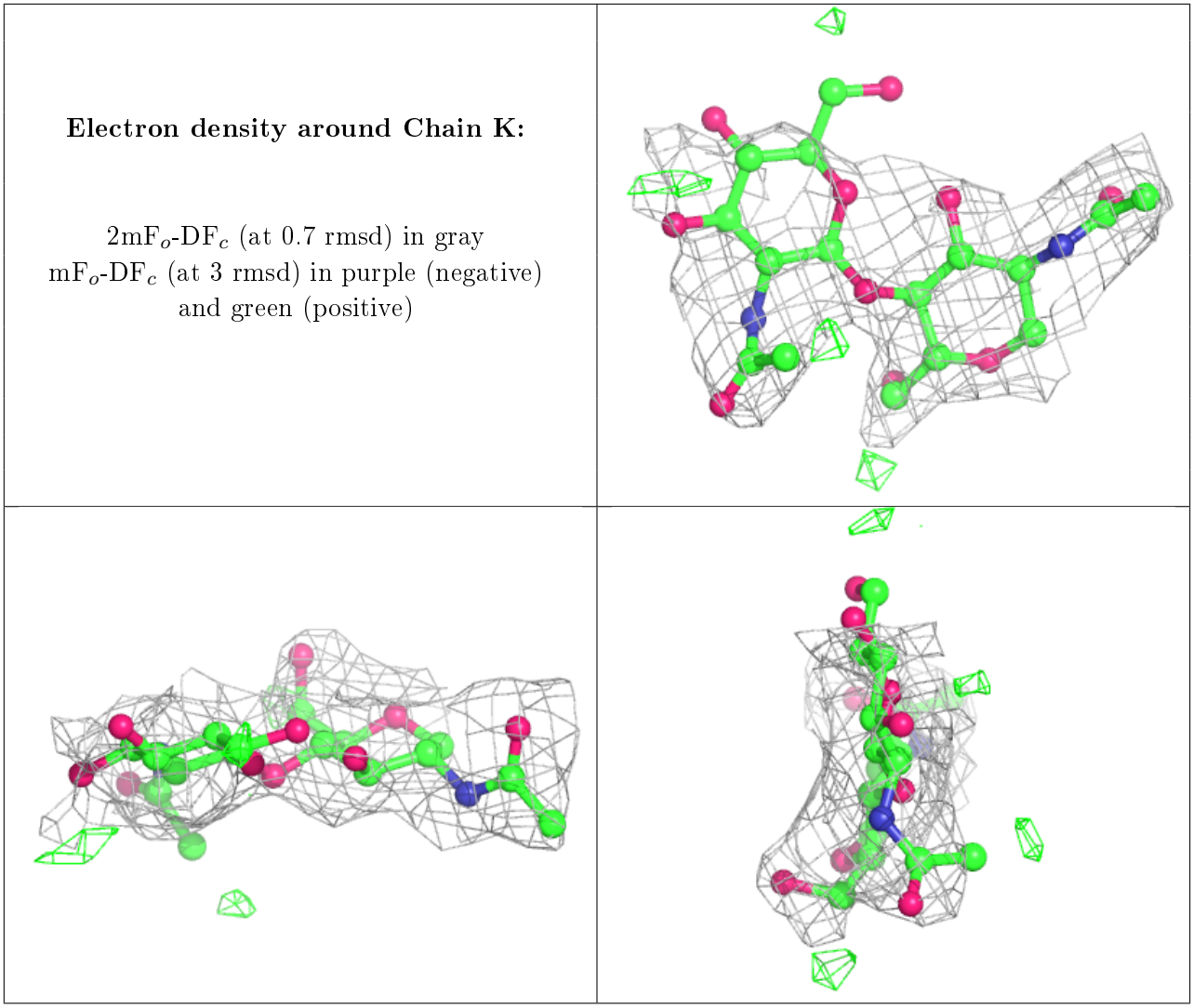
Electron density around Chain J:

$2mF_o$-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)



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
13	NAG	B	3099	14/15	0.86	0.40	75,90,97,102	0
9	GOL	A	461	6/6	0.87	0.18	38,52,57,64	0
13	NAG	D	3099	14/15	0.88	0.30	61,76,81,81	0
8	SO4	C	458	5/5	0.88	0.18	63,79,88,91	0
8	SO4	C	460	5/5	0.88	0.23	42,44,45,63	5
8	SO4	A	458	5/5	0.89	0.14	86,97,100,104	0
11	CL	C	462	1/1	0.90	0.25	57,57,57,57	0
8	SO4	C	459	5/5	0.91	0.17	85,97,101,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	CL	C	461	1/1	0.93	0.06	42,42,42,42	0
8	SO4	A	459	5/5	0.93	0.16	34,51,66,77	0
12	MG	D	2001	1/1	0.94	0.06	7,7,7,7	1
8	SO4	L	215	5/5	0.94	0.17	79,80,86,89	0
10	CA	C	2005	1/1	0.95	0.04	29,29,29,29	0
10	CA	C	2004	1/1	0.96	0.03	34,34,34,34	0
10	CA	A	2004	1/1	0.98	0.03	11,11,11,11	0
10	CA	C	2007	1/1	0.98	0.08	25,25,25,25	0
8	SO4	A	460	5/5	0.98	0.12	40,46,55,60	0
10	CA	A	2005	1/1	0.98	0.05	3,3,3,3	0
11	CL	D	473	1/1	0.98	0.07	22,22,22,22	0
11	CL	B	473	1/1	0.99	0.06	13,13,13,13	0
10	CA	D	2003	1/1	0.99	0.13	13,13,13,13	0
12	MG	B	2001	1/1	0.99	0.09	0,0,0,0	1
10	CA	C	2006	1/1	0.99	0.08	24,24,24,24	0
10	CA	B	2002	1/1	0.99	0.04	14,14,14,14	0
10	CA	D	2002	1/1	0.99	0.07	17,17,17,17	0
10	CA	A	2006	1/1	0.99	0.08	0,0,0,0	0
10	CA	A	2007	1/1	1.00	0.05	1,1,1,1	0
10	CA	B	2003	1/1	1.00	0.11	0,0,0,0	0

6.5 Other polymers (i)

There are no such residues in this entry.