Full wwPDB X-ray Structure Validation Report (i)

Mar 4, 2024 – 10:17 AM EST

PDB ID	:	3UBX
Title	:	Crystal structure of the mouse CD1d-C20:2-aGalCer-L363 mAb Fab complex
Authors	:	Yu, E.D.; Zajonc, D.M.
Deposited on	:	2011-10-25
Resolution	:	3.10 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

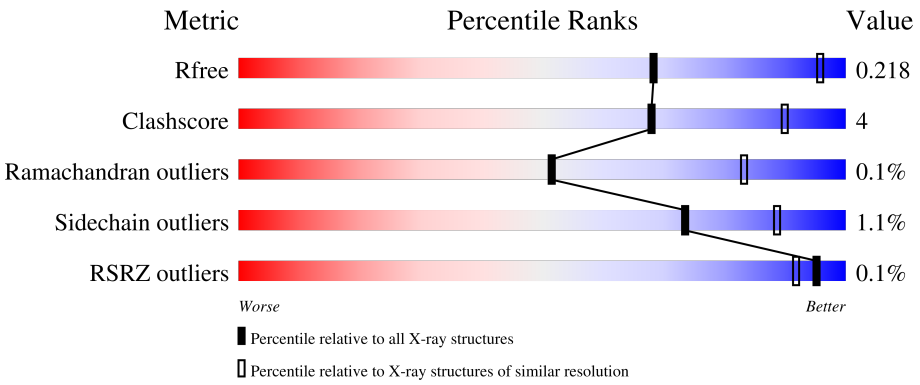
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	286	82% 14% •
1	D	286	81% 14% • •
2	B	99	87% 13%
2	E	99	87% 12% •
3	I	214	91% 9%

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Mol	Chain	Length	Quality of chain
3	L	214	90% 9%
4	G	222	90% 9%
4	H	222	91% 9%
5	C	2	50% 50%
5	F	2	50% 50%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12917 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 Antigen-presenting glycoprotein CD1d1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	275	2233	1420	395	406	12	0	1	0
1	D	276	2230	1419	393	406	12	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASP	SEE REMARK 999	UNP P11609
A	280	HIS	-	expression tag	UNP P11609
A	281	HIS	-	expression tag	UNP P11609
A	282	HIS	-	expression tag	UNP P11609
A	283	HIS	-	expression tag	UNP P11609
A	284	HIS	-	expression tag	UNP P11609
A	285	HIS	-	expression tag	UNP P11609
A	286	HIS	-	expression tag	UNP P11609
D	201	HIS	ASP	SEE REMARK 999	UNP P11609
D	280	HIS	-	expression tag	UNP P11609
D	281	HIS	-	expression tag	UNP P11609
D	282	HIS	-	expression tag	UNP P11609
D	283	HIS	-	expression tag	UNP P11609
D	284	HIS	-	expression tag	UNP P11609
D	285	HIS	-	expression tag	UNP P11609
D	286	HIS	-	expression tag	UNP P11609

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	99	832	531	142	152	7	0	2	0
2	E	98	805	514	136	148	7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ALA	ASP	SEE REMARK 999	UNP P01887
E	85	ALA	ASP	SEE REMARK 999	UNP P01887

- Molecule 3 is a protein called L363 light chain (IGKV13-84*01).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	214	1653	1027	278	341	7	0	0	0
3	I	214	1655	1028	279	341	7	0	0	0

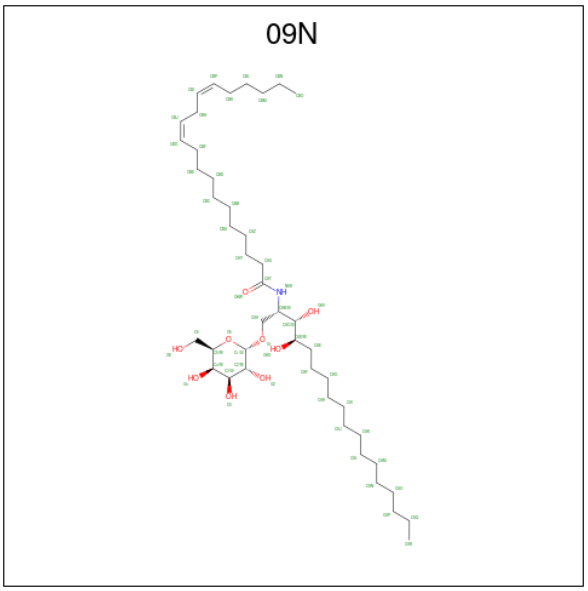
- Molecule 4 is a protein called L363 heavy chain (IGHV9-4*02).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	221	1660	1064	272	317	7	0	0	0
4	G	221	1657	1063	271	316	7	0	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

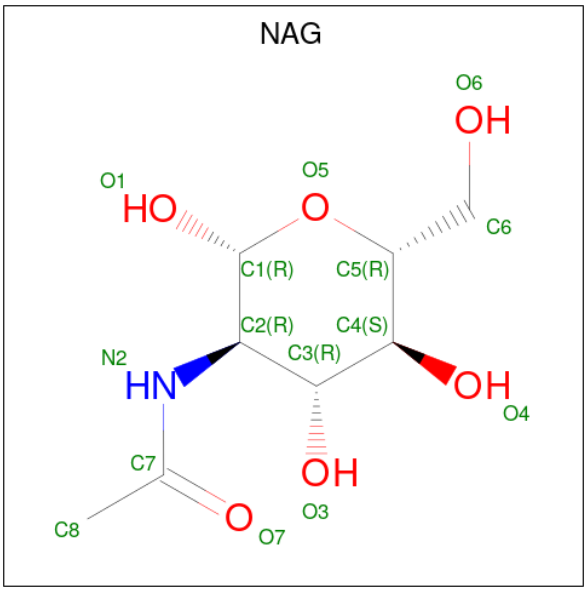
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	C	2	28	16	2	10	0	0	0
5	F	2	28	16	2	10	0	0	0

- Molecule 6 is (11Z,14Z)-N-[(2S,3S,4R)-1-(alpha-D-galactopyranosyloxy)-3,4-dihydroxyoctadecan-2-yl]icosa-11,14-dienamide (three-letter code: 09N) (formula: $C_{44}H_{83}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	54	44	1	9	0	0
			Total	C	N	O		
6	D	1	54	44	1	9	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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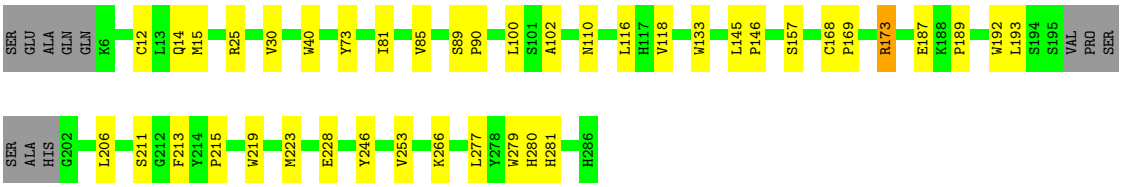
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	D	1	14	8	1	5	0	0

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.

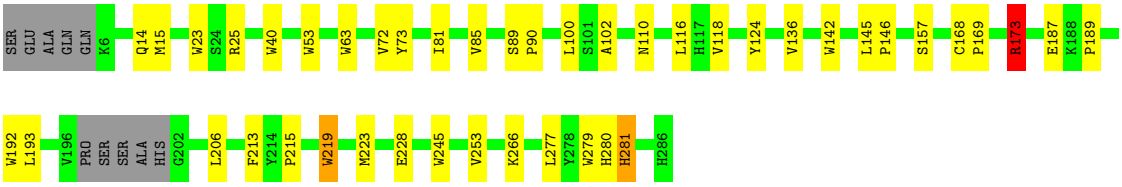
• Molecule 1: Antigen-presenting glycoprotein CD1d1

Chain A:



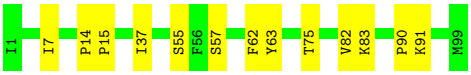
• Molecule 1: Antigen-presenting glycoprotein CD1d1

Chain D:



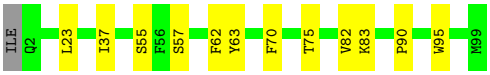
• Molecule 2: Beta-2-microglobulin

Chain B:



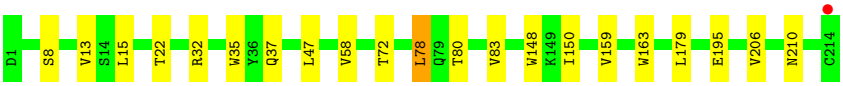
• Molecule 2: Beta-2-microglobulin

Chain E:



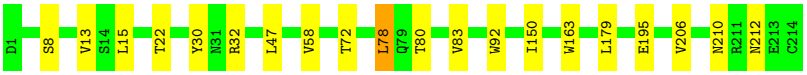
• Molecule 3: L363 light chain (IGKV13-84*01)

Chain L:



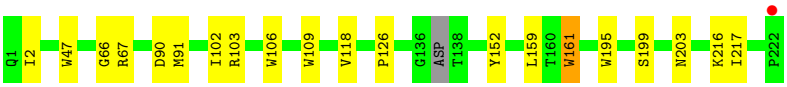
• Molecule 3: L363 light chain (IGKV13-84*01)

Chain I:



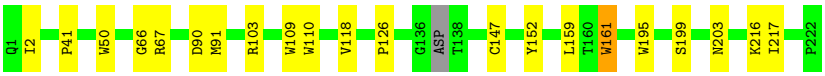
• Molecule 4: L363 heavy chain (IGHV9-4*02)

Chain H:



• Molecule 4: L363 heavy chain (IGHV9-4*02)

Chain G:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	234.95Å 234.95Å 99.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.89 – 3.10 37.89 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (37.89-3.10) 100.0 (37.89-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.63 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.202 , 0.230 0.192 , 0.218	Depositor DCC
R_{free} test set	2897 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	71.3	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 13.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12917	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 09N

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	0.66	2/2303 (0.1%)	0.60	2/3130 (0.1%)
1	D	0.66	8/2299 (0.3%)	0.59	2/3125 (0.1%)
2	B	0.57	0/859	0.53	0/1167
2	E	0.57	1/831 (0.1%)	0.54	0/1129
3	I	0.50	2/1691 (0.1%)	0.55	0/2297
3	L	0.51	2/1689 (0.1%)	0.55	0/2294
4	G	0.61	5/1706 (0.3%)	0.54	0/2336
4	H	0.61	5/1709 (0.3%)	0.54	0/2341
All	All	0.60	25/13087 (0.2%)	0.56	4/17819 (0.0%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	109	TRP	CD2-CE2	5.40	1.47	1.41
1	D	23	TRP	CD2-CE2	5.35	1.47	1.41
4	H	106	TRP	CD2-CE2	5.30	1.47	1.41
1	D	40	TRP	CD2-CE2	5.29	1.47	1.41
1	D	53	TRP	CD2-CE2	5.28	1.47	1.41
4	G	161	TRP	CD2-CE2	5.26	1.47	1.41
3	L	163	TRP	CD2-CE2	5.22	1.47	1.41
3	L	35	TRP	CD2-CE2	5.21	1.47	1.41
1	D	192	TRP	CD2-CE2	5.20	1.47	1.41
4	H	109	TRP	CD2-CE2	5.18	1.47	1.41
4	G	110	TRP	CD2-CE2	5.17	1.47	1.41
1	D	63	TRP	CD2-CE2	5.15	1.47	1.41
4	G	50	TRP	CD2-CE2	5.15	1.47	1.41
3	I	92	TRP	CD2-CE2	5.14	1.47	1.41
4	H	47	TRP	CD2-CE2	5.12	1.47	1.41
4	H	195	TRP	CD2-CE2	5.12	1.47	1.41
1	A	192	TRP	CD2-CE2	5.12	1.47	1.41
4	H	161	TRP	CD2-CE2	5.10	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	142	TRP	CD2-CE2	5.08	1.47	1.41
4	G	195	TRP	CD2-CE2	5.08	1.47	1.41
3	I	163	TRP	CD2-CE2	5.06	1.47	1.41
1	D	245	TRP	CD2-CE2	5.04	1.47	1.41
1	A	40	TRP	CD2-CE2	5.03	1.47	1.41
1	D	219	TRP	CD2-CE2	5.00	1.47	1.41
2	E	95	TRP	CD2-CE2	5.00	1.47	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	173	ARG	NE-CZ-NH1	9.43	125.01	120.30
1	A	173	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	D	173	ARG	NE-CZ-NH1	-7.81	116.39	120.30
1	D	173	ARG	NE-CZ-NH2	7.32	123.96	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2233	0	2106	28	0
1	D	2230	0	2109	24	0
2	B	832	0	799	7	0
2	E	805	0	772	5	0
3	I	1655	0	1581	9	0
3	L	1653	0	1580	10	0
4	G	1657	0	1595	10	0
4	H	1660	0	1605	11	0
5	C	28	0	25	1	0
5	F	28	0	25	1	0
6	A	54	0	83	5	0
6	D	54	0	83	1	0
7	A	14	0	13	0	0
7	D	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12917	0	12389	97	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 (97) 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)
4:H:91:MET:HG3	4:H:118:VAL:H	1.40	0.86
3:L:32:ARG:NH1	4:H:103:ARG:O	2.09	0.85
3:I:32:ARG:NH1	4:G:103:ARG:O	2.12	0.82
1:D:280:HIS:CD2	1:D:281:HIS:H	1.96	0.82
4:G:91:MET:HG3	4:G:118:VAL:H	1.44	0.80
1:A:15:MET:HG2	2:B:62:PHE:HE2	1.52	0.73
1:A:193:LEU:HD13	1:A:277:LEU:HD23	1.70	0.71
1:A:12:CYS:HB3	6:A:287:09N:H68	1.74	0.69
1:D:193:LEU:HD13	1:D:277:LEU:HD23	1.74	0.69
1:D:206:LEU:HG	1:D:253:VAL:HG21	1.74	0.68
3:L:22:THR:HG22	3:L:72:THR:HG22	1.76	0.67
1:A:206:LEU:HG	1:A:253:VAL:HG21	1.75	0.67
1:A:110:ASN:HA	1:A:173:ARG:NH2	2.09	0.67
1:D:15:MET:HG2	2:E:62:PHE:HE2	1.60	0.66
1:A:280:HIS:CD2	1:A:281:HIS:H	2.15	0.64
1:D:168:CYS:HB3	1:D:169:PRO:HD3	1.80	0.63
3:L:15:LEU:HD22	3:I:15:LEU:HD22	1.82	0.61
1:A:219:TRP:HB3	1:A:266:LYS:HB2	1.82	0.61
1:D:219:TRP:HB3	1:D:266:LYS:HB2	1.81	0.60
3:I:195:GLU:HG3	3:I:206:VAL:HG22	1.83	0.60
1:A:168:CYS:HB3	1:A:169:PRO:HD3	1.83	0.59
1:A:30:VAL:HG21	6:A:287:09N:H78	1.85	0.59
4:H:67:ARG:NH2	4:H:90:ASP:OD2	2.36	0.58
4:G:67:ARG:NH2	4:G:90:ASP:OD2	2.37	0.58
1:D:110:ASN:HA	1:D:173:ARG:HH22	1.69	0.58
1:D:145:LEU:HB3	1:D:146:PRO:HD3	1.85	0.58
3:L:195:GLU:HG3	3:L:206:VAL:HG22	1.87	0.57
3:I:22:THR:HG22	3:I:72:THR:HG22	1.86	0.57
1:A:25:ARG:HB3	5:C:1:NAG:H82	1.86	0.57
1:A:223:MET:HG2	1:A:228:GLU:HA	1.87	0.56
4:H:199:SER:HB2	4:H:216:LYS:HE3	1.89	0.55
4:G:199:SER:HB2	4:G:216:LYS:HE3	1.89	0.55
1:A:145:LEU:HB3	1:A:146:PRO:HD3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:MET:HG2	1:D:228:GLU:HA	1.90	0.54
4:H:66:GLY:O	4:H:67:ARG:HB2	2.08	0.53
3:I:80:THR:O	3:I:83:VAL:HG22	2.08	0.53
1:D:25:ARG:HB3	5:F:1:NAG:H82	1.91	0.53
1:A:280:HIS:CG	1:A:281:HIS:H	2.27	0.52
1:A:189:PRO:HB3	1:A:213:PHE:HB3	1.92	0.51
1:D:189:PRO:HB3	1:D:213:PHE:HB3	1.92	0.51
1:D:73:TYR:CE1	6:D:287:09N:H58	2.46	0.51
3:I:150:ILE:HD11	3:I:179:LEU:HD21	1.93	0.51
1:A:15:MET:HG2	2:B:62:PHE:CE2	2.41	0.51
1:D:280:HIS:CG	1:D:281:HIS:H	2.29	0.51
4:G:66:GLY:O	4:G:67:ARG:HB2	2.11	0.50
1:D:279:TRP:CE3	1:D:280:HIS:HA	2.48	0.49
1:A:100:LEU:HG	1:A:118:VAL:HG22	1.94	0.49
1:A:279:TRP:CE3	1:A:280:HIS:HA	2.47	0.49
1:D:14:GLN:HE22	1:D:73:TYR:HE2	1.59	0.49
3:L:80:THR:O	3:L:83:VAL:HG22	2.13	0.48
1:A:14:GLN:HE22	1:A:73:TYR:HE2	1.60	0.48
1:D:100:LEU:HG	1:D:118:VAL:HG22	1.95	0.48
3:L:150:ILE:HD11	3:L:179:LEU:HD21	1.96	0.47
4:H:91:MET:HG3	4:H:118:VAL:N	2.20	0.47
1:A:133:TRP:CH2	6:A:287:09N:H21	2.50	0.46
1:D:14:GLN:NE2	1:D:73:TYR:HE2	2.14	0.46
2:B:55:SER:HB3	2:B:63:TYR:CZ	2.51	0.46
1:A:110:ASN:HA	1:A:173:ARG:HH21	1.82	0.45
1:D:187:GLU:O	1:D:213:PHE:HA	2.17	0.45
1:A:14:GLN:NE2	1:A:73:TYR:HE2	2.15	0.45
3:I:13:VAL:HG23	3:I:78:LEU:HD22	1.98	0.45
2:E:83:LYS:HG3	2:E:90:PRO:HG3	1.97	0.45
1:D:89:SER:HA	1:D:90:PRO:C	2.36	0.44
1:D:72:VAL:HG13	3:I:30:TYR:HB3	2.00	0.44
2:E:37:ILE:HG12	2:E:82:VAL:HG22	1.99	0.43
1:D:102:ALA:HB2	1:D:116:LEU:HG	2.00	0.43
4:H:161:TRP:HZ3	4:H:217:ILE:HD11	1.81	0.43
4:G:147:CYS:HB2	4:G:161:TRP:CH2	2.54	0.43
1:A:73:TYR:CE1	6:A:287:09N:H58	2.54	0.43
2:B:83:LYS:HG3	2:B:90:PRO:HG3	1.99	0.43
1:A:81:ILE:O	1:A:85:VAL:HG23	2.18	0.43
2:B:7:ILE:HD12	2:B:91:LYS:HD2	2.01	0.43
1:A:102:ALA:HB2	1:A:116:LEU:HG	2.01	0.43
3:L:13:VAL:HG23	3:L:78:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:126:PRO:HB3	4:H:152:TYR:HB3	2.00	0.42
1:A:12:CYS:HB3	6:A:287:09N:CBJ	2.46	0.42
1:A:89:SER:HA	1:A:90:PRO:C	2.40	0.42
2:B:37:ILE:HG12	2:B:82:VAL:HG22	2.02	0.42
3:L:47:LEU:HA	3:L:58:VAL:HG21	2.02	0.42
4:G:2:ILE:H	4:G:2:ILE:HD12	1.83	0.42
2:B:14:PRO:HA	2:B:15:PRO:HD3	1.94	0.42
4:G:159:LEU:HA	4:G:203:ASN:O	2.20	0.42
4:G:126:PRO:HB3	4:G:152:TYR:HB3	2.01	0.42
1:A:187:GLU:O	1:A:213:PHE:HA	2.20	0.41
4:H:2:ILE:H	4:H:2:ILE:HD12	1.85	0.41
1:D:81:ILE:O	1:D:85:VAL:HG23	2.20	0.41
2:E:55:SER:HB3	2:E:63:TYR:CZ	2.55	0.41
4:H:159:LEU:HA	4:H:203:ASN:O	2.20	0.41
1:A:211:SER:HB2	1:A:246:TYR:HD1	1.85	0.41
3:L:37:GLN:HB2	3:L:47:LEU:HD11	2.02	0.41
4:H:102:ILE:HD12	4:H:102:ILE:C	2.41	0.41
4:G:161:TRP:HZ3	4:G:217:ILE:HD11	1.84	0.41
3:I:47:LEU:HA	3:I:58:VAL:HG21	2.03	0.41
2:E:23:LEU:HB2	2:E:70:PHE:CE2	2.56	0.40
1:D:280:HIS:HD2	1:D:281:HIS:H	1.58	0.40
3:L:148:TRP:CD1	3:L:159:VAL:HG11	2.57	0.40
1:D:124:TYR:CZ	1:D:136:VAL:HG11	2.56	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	272/286 (95%)	260 (96%)	12 (4%)	0	100 100
1	D	272/286 (95%)	258 (95%)	13 (5%)	1 (0%)	34 69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	99/99 (100%)	97 (98%)	2 (2%)	0	100	100
2	E	96/99 (97%)	94 (98%)	2 (2%)	0	100	100
3	I	212/214 (99%)	200 (94%)	12 (6%)	0	100	100
3	L	212/214 (99%)	201 (95%)	11 (5%)	0	100	100
4	G	217/222 (98%)	205 (94%)	11 (5%)	1 (0%)	29	64
4	H	217/222 (98%)	206 (95%)	11 (5%)	0	100	100
All	All	1597/1642 (97%)	1521 (95%)	74 (5%)	2 (0%)	51	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	281	HIS
4	G	41	PRO

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	240/250 (96%)	238 (99%)	2 (1%)	81	92
1	D	240/250 (96%)	237 (99%)	3 (1%)	69	87
2	B	94/93 (101%)	92 (98%)	2 (2%)	53	79
2	E	91/93 (98%)	89 (98%)	2 (2%)	52	78
3	I	189/190 (100%)	185 (98%)	4 (2%)	53	79
3	L	189/190 (100%)	186 (98%)	3 (2%)	62	84
4	G	177/184 (96%)	177 (100%)	0	100	100
4	H	179/184 (97%)	179 (100%)	0	100	100
All	All	1399/1434 (98%)	1383 (99%)	16 (1%)	73	89

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	SER
1	A	215	PRO
2	B	57	SER
2	B	75	THR
1	D	157	SER
1	D	173	ARG
1	D	215	PRO
2	E	57	SER
2	E	75	THR
3	L	8	SER
3	L	78	LEU
3	L	210	ASN
3	I	8	SER
3	I	78	LEU
3	I	210	ASN
3	I	212	ASN

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

Mol	Chain	Res	Type
1	A	280	HIS
2	B	29	GLN
1	D	280	HIS
1	D	282	HIS
1	D	286	HIS
2	E	29	GLN
3	I	31	ASN

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)

4 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	C	1	1,5	14,14,15	0.55	0	17,19,21	1.03	1 (5%)
5	NAG	C	2	5	14,14,15	0.48	0	17,19,21	1.60	2 (11%)
5	NAG	F	1	1,5	14,14,15	0.53	0	17,19,21	1.30	1 (5%)
5	NAG	F	2	5	14,14,15	0.54	0	17,19,21	1.28	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
5	NAG	C	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	2	NAG	C1-O5-C5	4.90	118.83	112.19
5	F	1	NAG	C1-O5-C5	4.21	117.90	112.19
5	C	1	NAG	C1-O5-C5	3.30	116.66	112.19
5	F	2	NAG	O5-C5-C6	3.19	112.20	107.20
5	C	2	NAG	O3-C3-C2	-2.24	104.83	109.47

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	2	NAG	O5-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	C	1	NAG	C4-C5-C6-O6
5	C	1	NAG	O5-C5-C6-O6

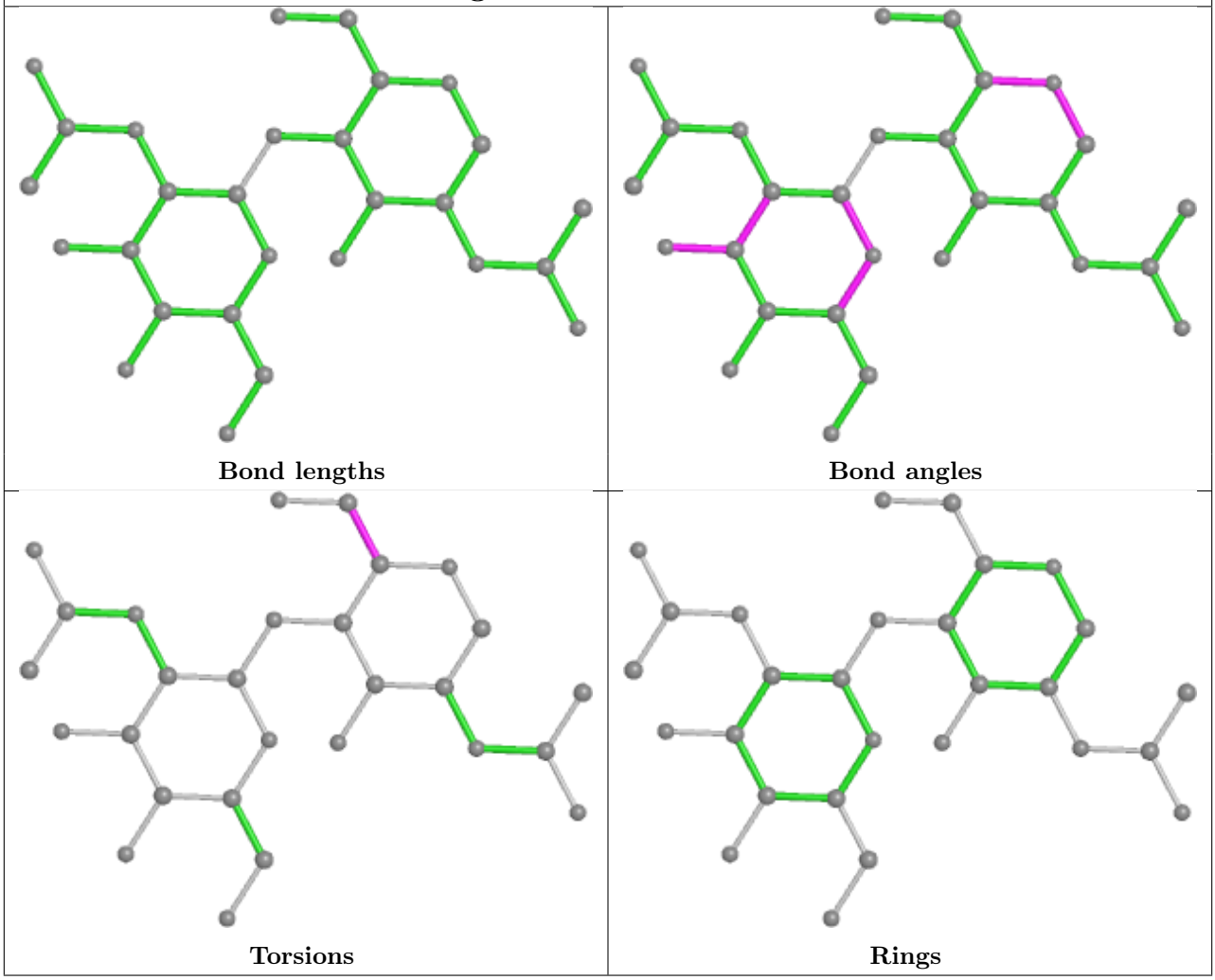
There are no ring outliers.

2 monomers are involved in 2 short contacts:

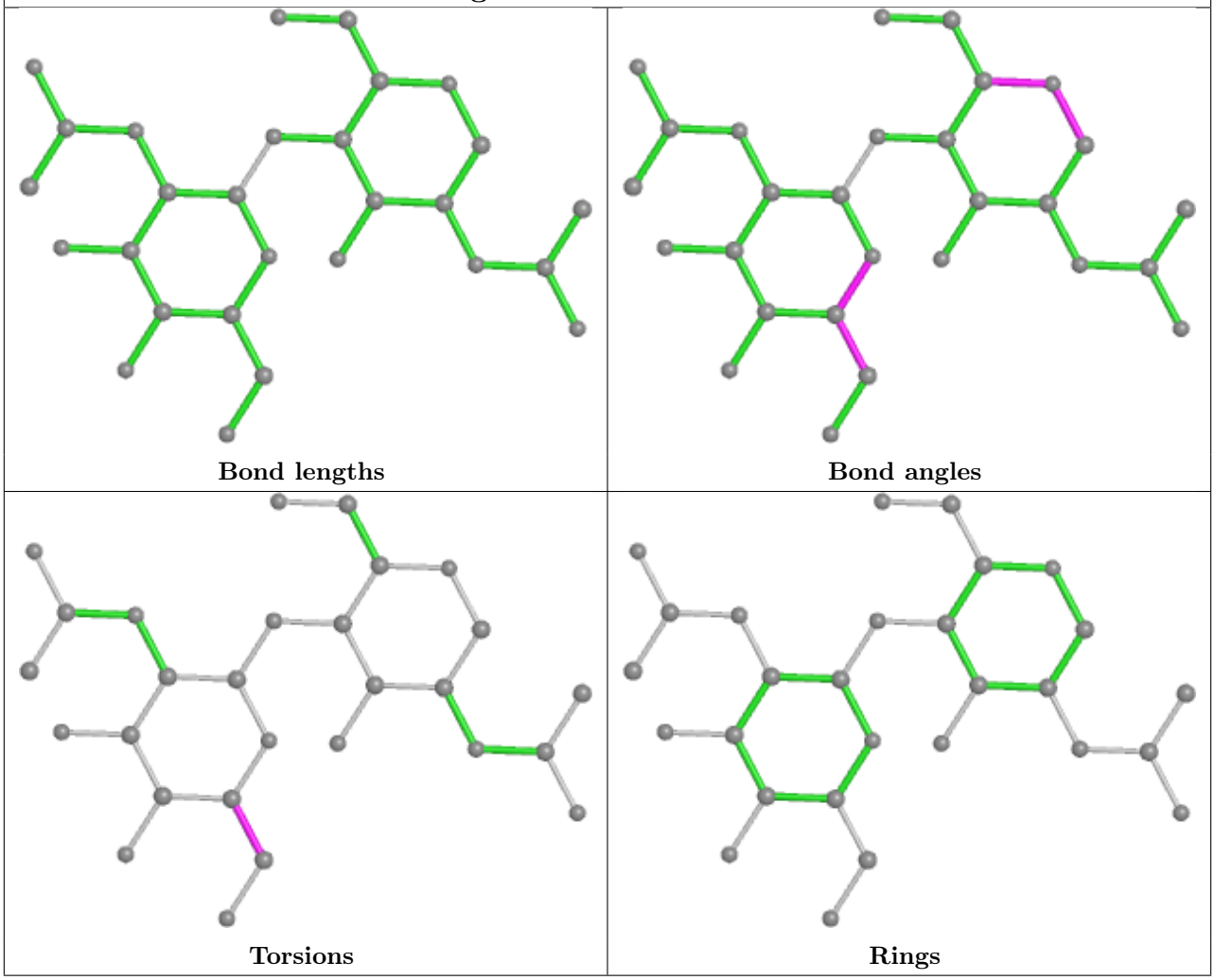
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1	NAG	1	0
5	C	1	NAG	1	0

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

Oligosaccharide Chain C



Oligosaccharide Chain F



5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	09N	D	287	-	54,54,54	0.81	0	59,63,63	0.62	0
7	NAG	D	512	1	14,14,15	0.42	0	17,19,21	1.34	1 (5%)
7	NAG	A	512	1	14,14,15	0.44	0	17,19,21	1.16	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	09N	A	287	-	54,54,54	0.87	2 (3%)	59,63,63	0.66	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	09N	D	287	-	-	23/52/72/72	0/1/1/1
7	NAG	D	512	1	-	0/6/23/26	0/1/1/1
7	NAG	A	512	1	-	0/6/23/26	0/1/1/1
6	09N	A	287	-	-	22/52/72/72	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	287	09N	O1-C1	2.77	1.44	1.40
6	A	287	09N	O5-C1	2.43	1.48	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	512	NAG	C1-O5-C5	4.55	118.35	112.19
7	A	512	NAG	C1-O5-C5	3.90	117.47	112.19

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	287	09N	CBI-CBH-CBJ-CBG
6	A	287	09N	O5-C5-C6-O6
6	D	287	09N	O5-C5-C6-O6
6	D	287	09N	C4-C5-C6-O6
6	A	287	09N	C4-C5-C6-O6
6	D	287	09N	CAM-CAN-CAO-CAP
6	A	287	09N	CBA-CBB-CBC-CBD
6	A	287	09N	CBD-CBE-CBF-CBG
6	A	287	09N	CAL-CAM-CAN-CAO
6	A	287	09N	CAI-CAJ-CAK-CAL
6	A	287	09N	CAM-CAN-CAO-CAP

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Mol	Chain	Res	Type	Atoms
6	D	287	09N	CAL-CAM-CAN-CAO
6	D	287	09N	CBB-CBC-CBD-CBE
6	D	287	09N	CBD-CBE-CBF-CBG
6	D	287	09N	CAJ-CAK-CAL-CAM
6	D	287	09N	CBK-CBL-CBM-CBN
6	A	287	09N	CBB-CBC-CBD-CBE
6	D	287	09N	CBL-CBM-CBN-CBO
6	A	287	09N	CBK-CBL-CBM-CBN
6	D	287	09N	CAN-CAO-CAP-CAQ
6	D	287	09N	CBA-CBB-CBC-CBD
6	A	287	09N	CAO-CAP-CAQ-CAR
6	D	287	09N	CAO-CAP-CAQ-CAR
6	A	287	09N	CAN-CAO-CAP-CAQ
6	D	287	09N	CAT-CAU-CAY-CAZ
6	A	287	09N	CBI-CBH-CBJ-CBG
6	A	287	09N	CBL-CBM-CBN-CBO
6	D	287	09N	CBC-CBD-CBE-CBF
6	A	287	09N	CBP-CBK-CBL-CBM
6	A	287	09N	CAK-CAL-CAM-CAN
6	D	287	09N	CAK-CAL-CAM-CAN
6	D	287	09N	CAI-CAJ-CAK-CAL
6	A	287	09N	CAG-CAH-CAI-CAJ
6	D	287	09N	CBP-CBK-CBL-CBM
6	D	287	09N	OAX-CAD-CAE-CAF
6	A	287	09N	CAT-CAU-CAY-CAZ
6	A	287	09N	CBL-CBK-CBP-CBI
6	A	287	09N	CAJ-CAK-CAL-CAM
6	D	287	09N	CAZ-CBA-CBB-CBC
6	A	287	09N	CAE-CAF-CAG-CAH
6	D	287	09N	CBL-CBK-CBP-CBI
6	A	287	09N	CAC-CAB-NAS-CAT
6	D	287	09N	CAY-CAZ-CBA-CBB
6	A	287	09N	CAF-CAG-CAH-CAI
6	D	287	09N	CAF-CAG-CAH-CAI

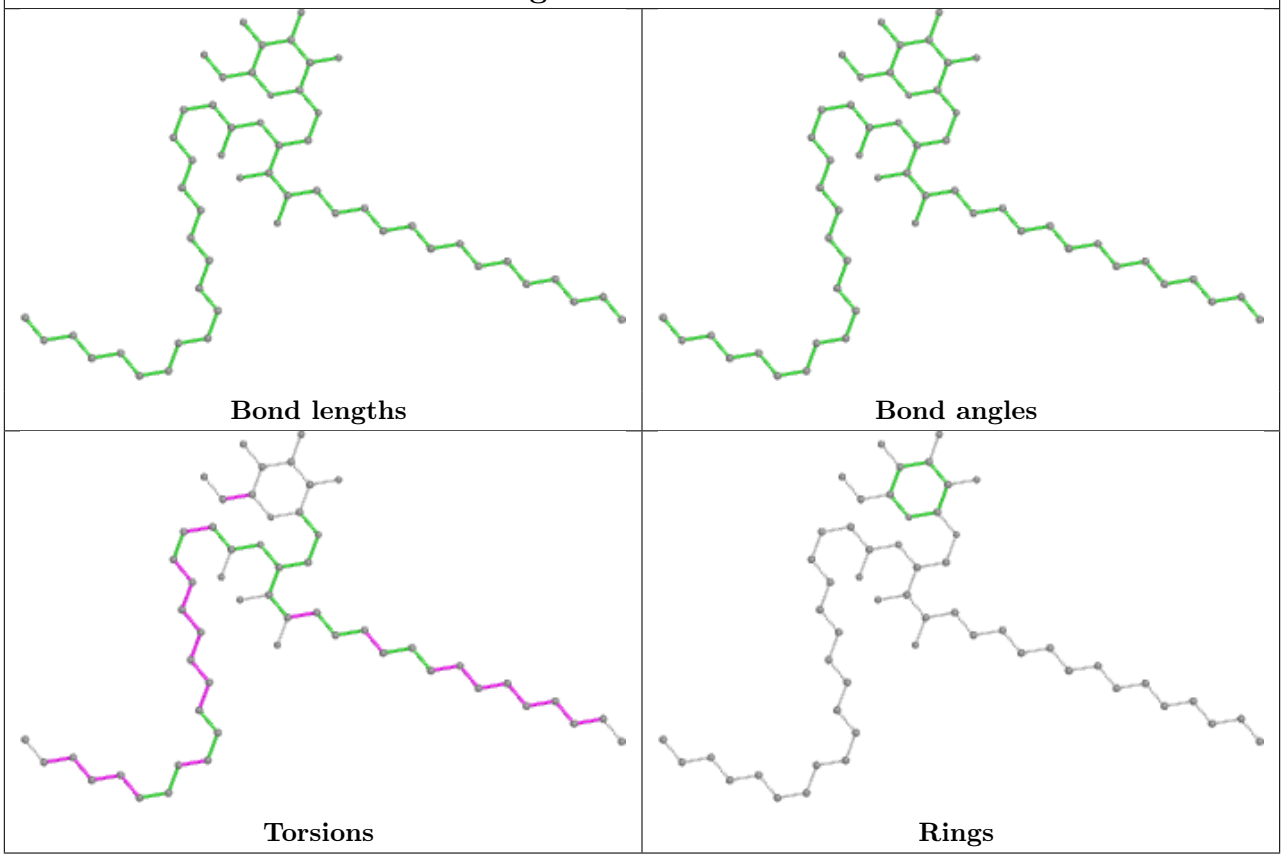
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	287	09N	1	0
6	A	287	09N	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 09N D 287



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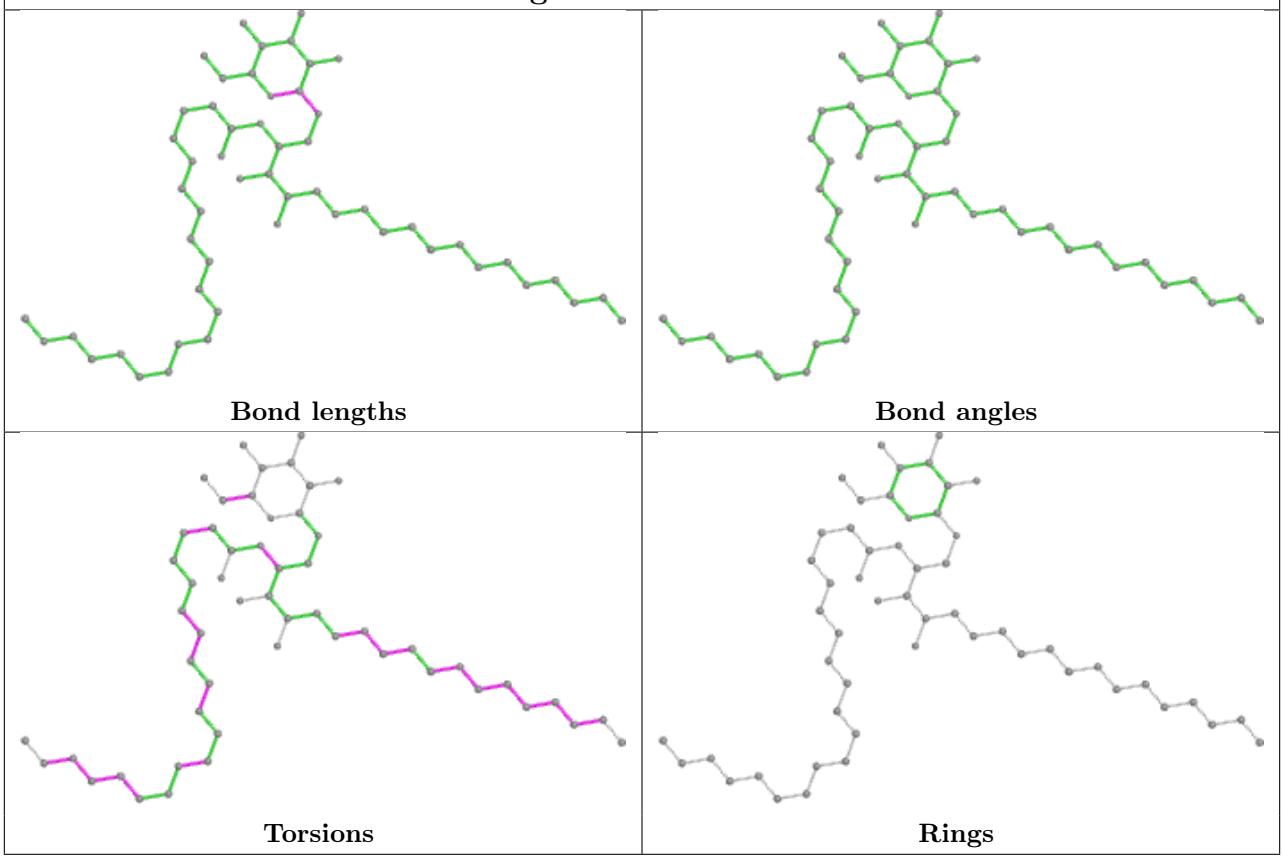


5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	275/286 (96%)	-0.45	0	100	100	46, 61, 86, 113	0
1	D	276/286 (96%)	-0.40	0	100	100	46, 66, 96, 125	0
2	B	99/99 (100%)	-0.35	0	100	100	46, 58, 82, 105	0
2	E	98/99 (98%)	-0.28	0	100	100	46, 64, 81, 96	0
3	I	214/214 (100%)	-0.47	0	100	100	47, 59, 84, 113	0
3	L	214/214 (100%)	-0.42	1 (0%)	91	81	39, 56, 87, 118	0
4	G	221/222 (99%)	-0.36	0	100	100	51, 71, 105, 133	0
4	H	221/222 (99%)	-0.33	1 (0%)	91	81	43, 72, 107, 139	0
All	All	1618/1642 (98%)	-0.39	2 (0%)	95	92	39, 64, 96, 139	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	222	PRO	2.3
3	L	214	CYS	2.2

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

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

6.3 Carbohydrates (i)

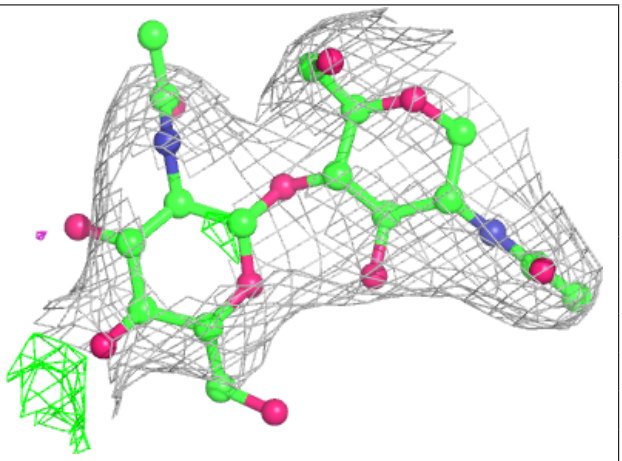
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

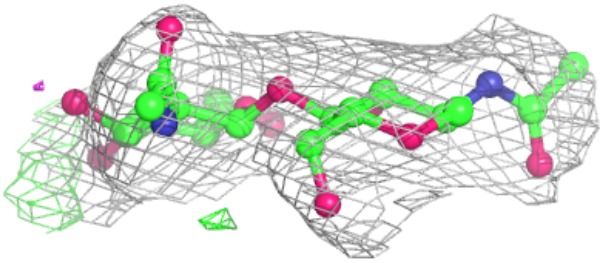
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	F	2	14/15	0.85	0.19	74,78,83,85	0
5	NAG	C	2	14/15	0.88	0.34	82,86,92,96	0
5	NAG	C	1	14/15	0.95	0.17	64,67,71,75	0
5	NAG	F	1	14/15	0.96	0.10	65,68,72,73	0

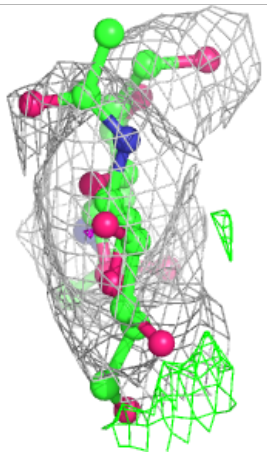
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

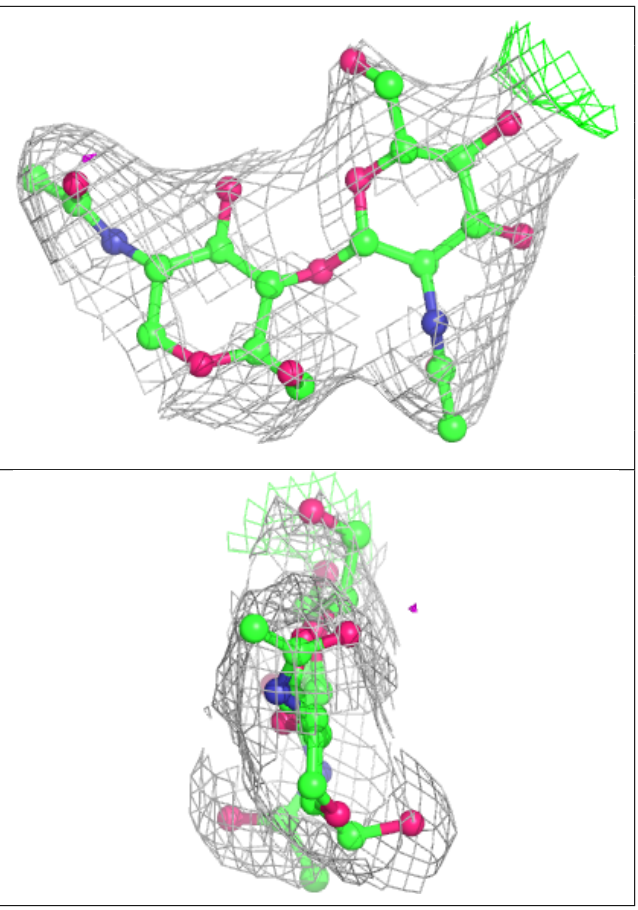






Electron density around Chain F:

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



6.4 Ligands (i)

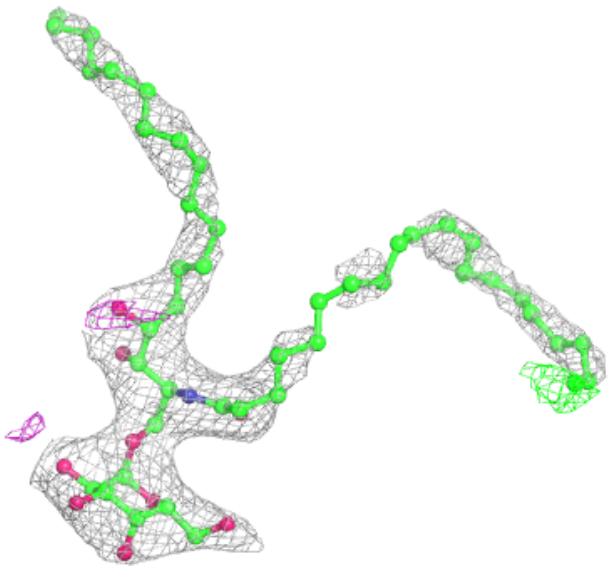
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

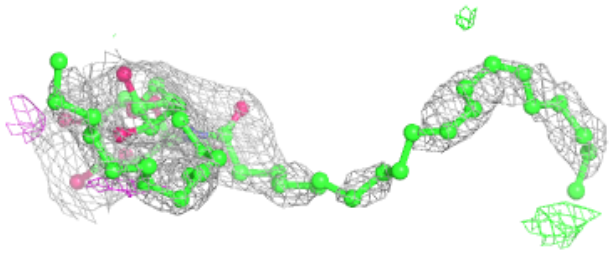
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	A	512	14/15	0.91	0.16	74,78,81,83	0
7	NAG	D	512	14/15	0.91	0.18	84,87,90,91	0
6	09N	D	287	54/54	0.96	0.26	52,59,71,72	0
6	09N	A	287	54/54	0.97	0.23	44,49,62,67	0

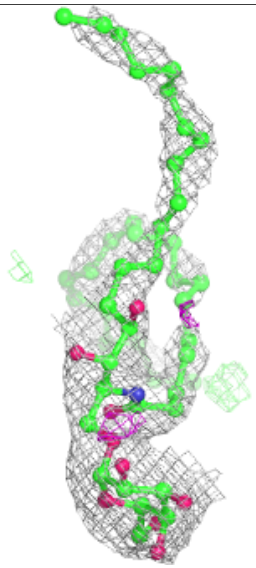
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 09N D 287:

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

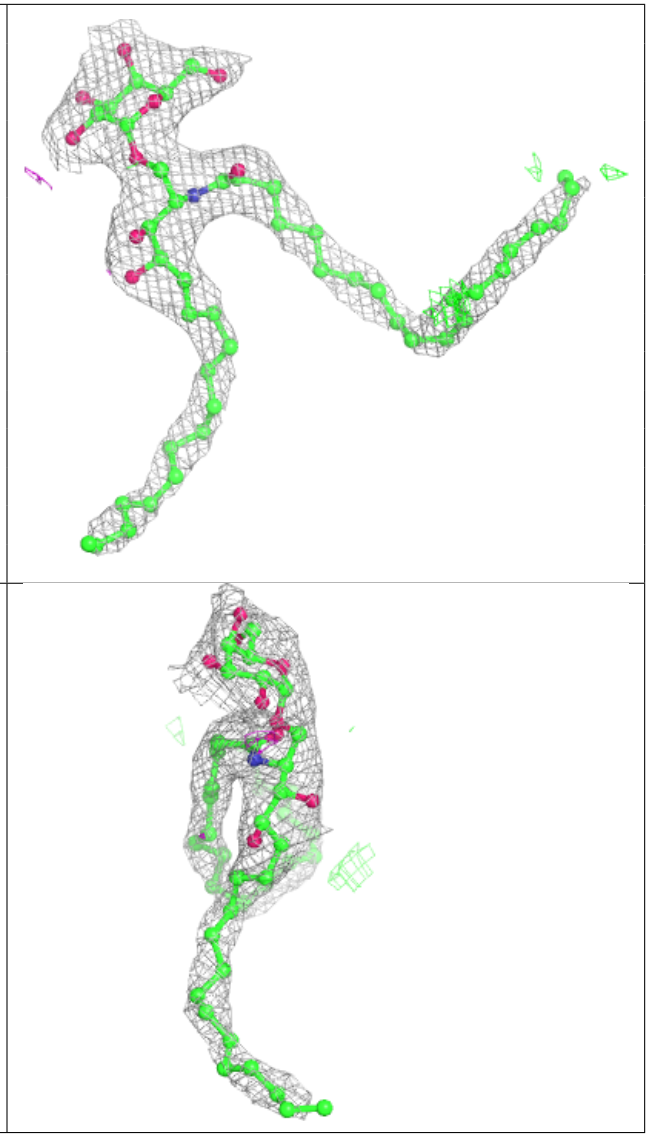






Electron density around 09N A 287:

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



6.5 Other polymers (i)

There are no such residues in this entry.