Full wwPDB X-ray Structure Validation Report (i)

Oct 22, 2023 – 03:04 AM EDT

PDB ID	:	3ARG
Title	:	Ternary crystal structure of the mouse NKT TCR-CD1d-alpha-glucosylceramide(C20:2)
Authors	:	Wun, K.S.; Rossjohn, J.
Deposited on	:	2010-11-27
Resolution	:	3.00 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:

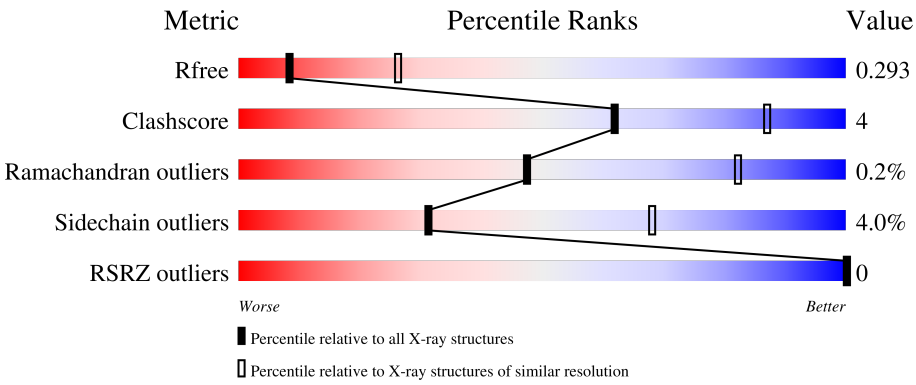
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	302	84% 12% ·
2	B	99	83% 14% · ·
3	C	207	88% 9% ·
4	D	244	87% 10% ·
5	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
5	F	2	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	DB6	A	650	X	-	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6177 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	290	2161	1381	386	382	12	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASP	conflict	UNP P11609
A	280	GLY	-	expression tag	UNP P11609
A	281	SER	-	expression tag	UNP P11609
A	282	LEU	-	expression tag	UNP P11609
A	283	HIS	-	expression tag	UNP P11609
A	284	HIS	-	expression tag	UNP P11609
A	285	ILE	-	expression tag	UNP P11609
A	286	LEU	-	expression tag	UNP P11609
A	287	ASP	-	expression tag	UNP P11609
A	288	ALA	-	expression tag	UNP P11609
A	289	GLN	-	expression tag	UNP P11609
A	290	LYS	-	expression tag	UNP P11609
A	291	MET	-	expression tag	UNP P11609
A	292	VAL	-	expression tag	UNP P11609
A	293	TRP	-	expression tag	UNP P11609
A	294	ASN	-	expression tag	UNP P11609
A	295	HIS	-	expression tag	UNP P11609
A	296	ARG	-	expression tag	UNP P11609
A	297	HIS	-	expression tag	UNP P11609
A	298	HIS	-	expression tag	UNP P11609
A	299	HIS	-	expression tag	UNP P11609
A	300	HIS	-	expression tag	UNP P11609
A	301	HIS	-	expression tag	UNP P11609
A	302	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	98	743	479	125	133	6	0	0	0

- Molecule 3 is a protein called NKT Valpha14-Jalpha18,NKT Valpha14-Jalpha18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	202	1432	896	244	285	7	0	0	0

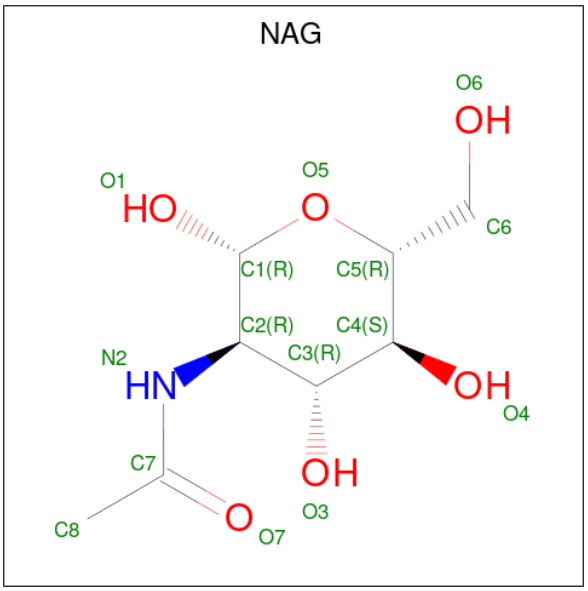
- Molecule 4 is a protein called Vbeta8.2,Vbeta8.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	236	1702	1090	294	312	6	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.

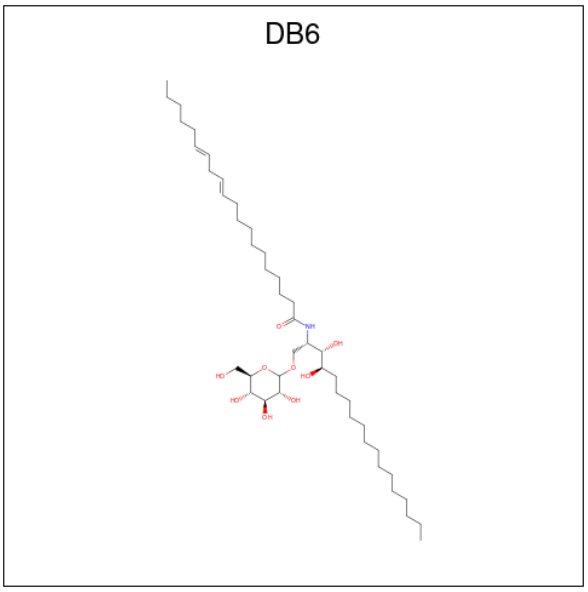
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	E	2	25	14	2	9	0	0	0
5	F	2	24	14	2	8	0	0	0

- Molecule 6 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		
6	A	1	14	8	1	5	0	0

- Molecule 7 is (11E,14E)-N-[(2S,3S,4R)-1-(alpha-D-glucopyranosyloxy)-3,4-dihydroxyoctadecan-2-yl]icosa-11,14-dienamide (three-letter code: DB6) (formula: $C_{44}H_{83}NO_9$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	10	10	10	0	0
			Total	O		
8	B	3	3	3	0	0
			Total	O		
8	C	4	4	4	0	0
			Total	O		
8	D	5	5	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 2: Beta-2-microglobulin

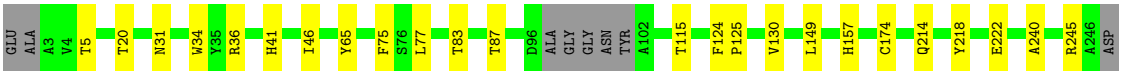
Chain B:

• Molecule 3: NKT Valpha14-Jalpha18,NKT Valpha14-Jalpha18

Chain C:

• Molecule 4: Vbeta8.2,Vbeta8.2

Chain D:



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

Chain E:

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

Chain F: 100%

NAG1
NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.16Å 85.77Å 237.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.56 – 3.00 42.21 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.3 (47.56-3.00) 93.4 (42.21-3.00)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.232 , 0.300 0.228 , 0.293	Depositor DCC
R_{free} test set	1197 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	65.5	Xtriage
Anisotropy	0.693	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 40.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6177	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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: DB6, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.33	0/2229	0.48	0/3050
2	B	0.34	0/769	0.52	0/1058
3	C	0.34	0/1459	0.49	0/1996
4	D	0.33	0/1752	0.47	0/2403
All	All	0.33	0/6209	0.49	0/8507

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2161	0	1858	24	0
2	B	743	0	647	10	0
3	C	1432	0	1245	12	0
4	D	1702	0	1466	8	0
5	E	25	0	21	0	0
5	F	24	0	18	1	0
6	A	14	0	13	0	0
7	A	54	0	82	2	0
8	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	3	0	0	0	0
8	C	4	0	0	0	0
8	D	5	0	0	0	0
All	All	6177	0	5350	51	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 (51) 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)
3:C:95:ARG:HH21	3:C:95:ARG:HG3	1.43	0.83
3:C:95:ARG:HG3	3:C:95:ARG:NH2	2.06	0.69
4:D:36:ARG:HB2	4:D:46:ILE:HD11	1.75	0.68
1:A:168:CYS:SG	1:A:169:PRO:HD3	2.38	0.64
1:A:156:THR:HG23	7:A:650:DB6:HABA	1.80	0.63
2:B:10:TYR:CD1	2:B:10:TYR:N	2.68	0.60
1:A:207:VAL:HG11	1:A:209:HIS:NE2	2.19	0.58
4:D:87:THR:HG23	4:D:115:THR:HA	1.86	0.57
3:C:138:VAL:HG12	3:C:181:TRP:HB3	1.88	0.55
2:B:28:THR:HG22	2:B:63:TYR:HB2	1.89	0.55
1:A:163:LEU:HA	1:A:167:THR:HB	1.89	0.55
4:D:65:TYR:HB3	4:D:77:LEU:HD11	1.89	0.54
1:A:280:GLY:H	1:A:284:HIS:HD2	1.55	0.53
2:B:79:ALA:HB2	2:B:94:TYR:CD2	2.43	0.52
3:C:123:PRO:HB2	3:C:202:THR:HA	1.91	0.52
1:A:73:TYR:HE1	7:A:650:DB6:H7	1.75	0.51
3:C:116:PRO:HG3	3:C:165:VAL:HG11	1.92	0.51
1:A:239:PRO:HG2	2:B:65:LEU:HD13	1.92	0.51
1:A:207:VAL:HG11	1:A:209:HIS:CE1	2.45	0.51
1:A:240:ASN:HD22	2:B:12:ARG:HG2	1.76	0.51
2:B:40:LEU:HD23	2:B:45:LYS:HA	1.93	0.51
1:A:212:GLY:HA3	2:B:12:ARG:NH2	2.26	0.51
1:A:281:SER:O	1:A:285:ILE:HG12	2.12	0.49
1:A:280:GLY:N	1:A:284:HIS:HD2	2.12	0.48
1:A:30:VAL:HB	1:A:38:HIS:HB2	1.94	0.48
1:A:280:GLY:H	1:A:284:HIS:CD2	2.31	0.48
1:A:209:HIS:HD2	1:A:246:TYR:OH	1.97	0.46
5:F:1:NAG:O3	5:F:2:NAG:N2	2.48	0.46
3:C:12:VAL:HG23	3:C:114:VAL:HG22	1.97	0.45
1:A:208:CYS:HB2	1:A:222:TRP:CZ2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:157:HIS:HB3	4:D:218:TYR:HB2	1.99	0.44
2:B:23:LEU:HB2	2:B:70:PHE:CD1	2.53	0.44
1:A:219:TRP:HB3	1:A:266:LYS:HB2	2.00	0.44
1:A:187:GLU:HB2	1:A:214:TYR:N	2.33	0.44
3:C:116:PRO:HG3	3:C:165:VAL:CG1	2.47	0.44
1:A:258:GLU:HB3	1:A:279:TRP:NE1	2.32	0.43
3:C:89:ILE:HG12	3:C:109:GLY:HA3	1.99	0.43
4:D:34:TRP:CD1	4:D:75:PHE:CE2	3.07	0.43
1:A:207:VAL:CG1	1:A:209:HIS:CE1	3.01	0.43
3:C:22:CYS:HB3	3:C:73:SER:HB3	2.01	0.43
2:B:17:ASN:HA	2:B:72:PRO:O	2.20	0.42
4:D:130:VAL:HG23	4:D:240:ALA:HB3	2.02	0.42
3:C:95:ARG:HH21	3:C:95:ARG:CG	2.21	0.42
2:B:26:TYR:CE2	2:B:28:THR:HG21	2.55	0.41
1:A:136:VAL:HG22	1:A:139:ALA:HB2	2.01	0.41
1:A:224:ARG:HG2	1:A:261:LEU:HD23	2.02	0.41
1:A:147:ILE:HD13	1:A:147:ILE:HA	1.92	0.41
3:C:206:SER:HA	3:C:207:PRO:HD3	1.88	0.41
3:C:98:ALA:HB1	4:D:31:ASN:HD21	1.86	0.41
4:D:124:PHE:HA	4:D:125:PRO:HD3	1.94	0.40
1:A:168:CYS:SG	1:A:169:PRO:CD	3.08	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	282/302 (93%)	268 (95%)	14 (5%)	0	100 100
2	B	96/99 (97%)	93 (97%)	2 (2%)	1 (1%)	15 53
3	C	196/207 (95%)	183 (93%)	13 (7%)	0	100 100
4	D	232/244 (95%)	219 (94%)	12 (5%)	1 (0%)	34 72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	806/852 (95%)	763 (95%)	41 (5%)	2 (0%)	47 82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	222	GLU
2	B	97	ARG

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	192/264 (73%)	186 (97%)	6 (3%)	40 75
2	B	71/93 (76%)	68 (96%)	3 (4%)	30 66
3	C	137/186 (74%)	132 (96%)	5 (4%)	35 70
4	D	145/206 (70%)	137 (94%)	8 (6%)	21 57
All	All	545/749 (73%)	523 (96%)	22 (4%)	31 68

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	CYS
1	A	157	SER
1	A	159	THR
1	A	168	CYS
1	A	182	ASP
1	A	296	ARG
2	B	10	TYR
2	B	12	ARG
2	B	39	MET
3	C	8	GLN
3	C	33	ARG
3	C	48	VAL
3	C	80	THR

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Mol	Chain	Res	Type
3	C	95	ARG
4	D	5	THR
4	D	20	THR
4	D	41	HIS
4	D	83	THR
4	D	149	LEU
4	D	174	CYS
4	D	214	GLN
4	D	245	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	203	HIS
1	A	209	HIS
1	A	248	GLN
1	A	284	HIS
2	B	42	ASN
3	C	30	ASN
3	C	194	ASN
3	C	195	ASN
4	D	6	GLN
4	D	27	ASN
4	D	214	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)

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	E	1	1,5	14,14,15	0.62	0	17,19,21	1.00	1 (5%)
5	NAG	E	2	5	11,11,15	0.62	0	12,15,21	0.61	0
5	NAG	F	1	1,5	14,14,15	0.54	0	17,19,21	1.32	2 (11%)
5	NAG	F	2	5	10,10,15	0.82	1 (10%)	11,14,21	0.82	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	E	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	1/2/19/26	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	2	NAG	C1-C2	2.07	1.54	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	1	NAG	C4-C3-C2	3.37	115.96	111.02
5	F	1	NAG	O5-C1-C2	-3.02	106.53	111.29
5	E	1	NAG	C1-O5-C5	2.69	115.84	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1	NAG	C4-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6

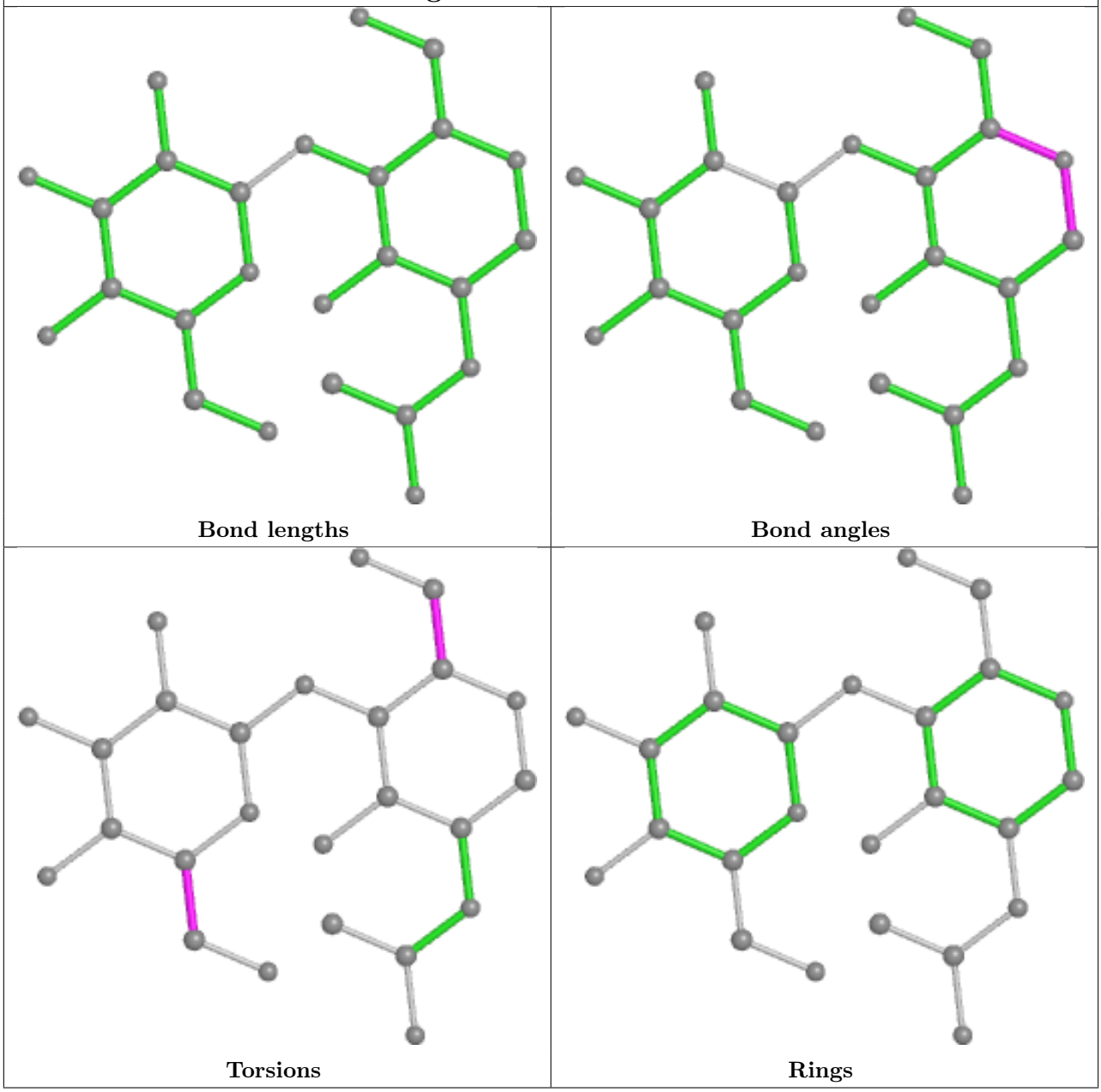
There are no ring outliers.

2 monomers are involved in 1 short contact:

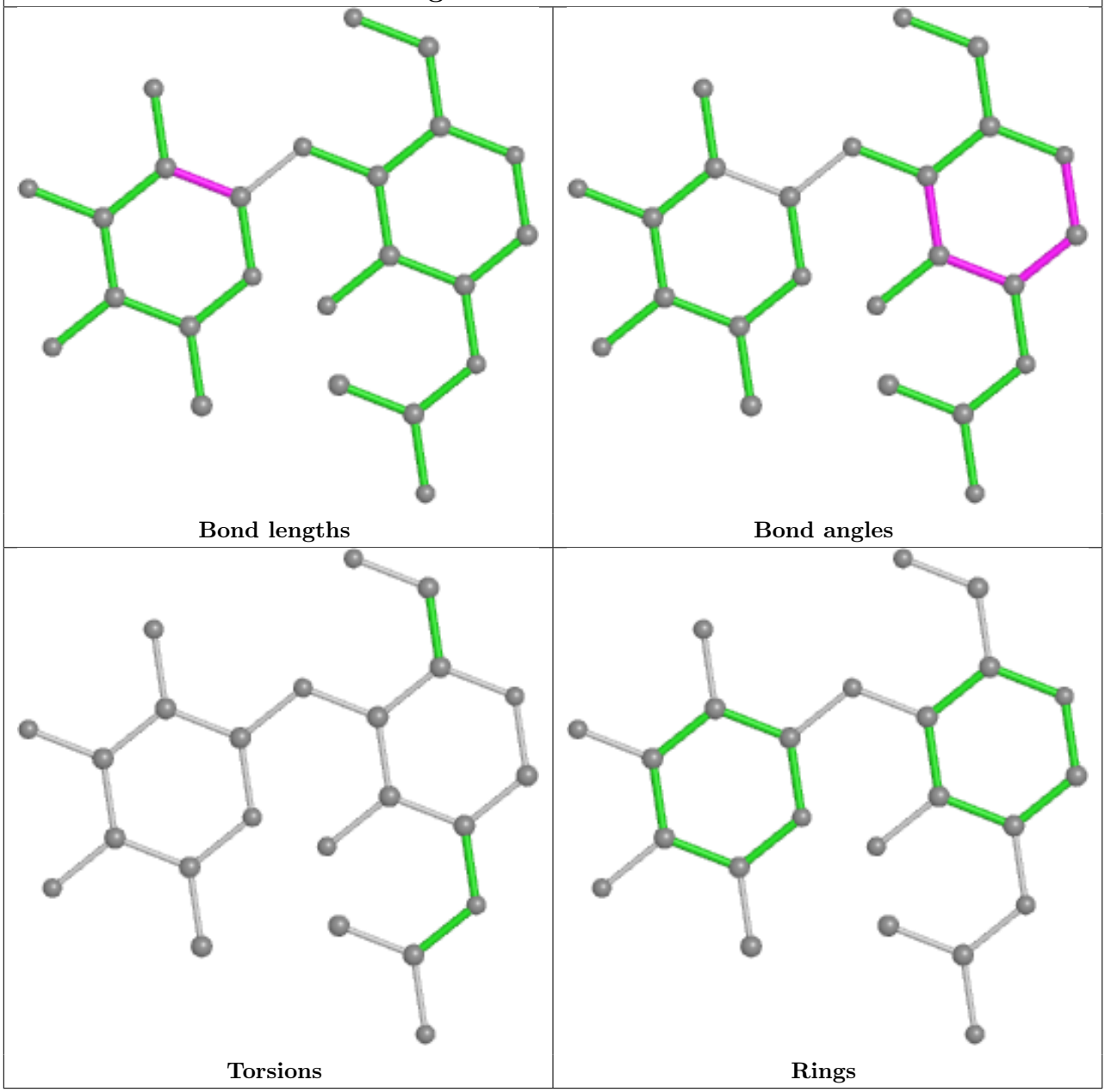
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	2	NAG	1	0
5	F	1	NAG	1	0

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 E



Oligosaccharide Chain F



5.6 Ligand geometry (i)

2 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	NAG	A	314	1	14,14,15	0.50	0	17,19,21	1.34	1 (5%)
7	DB6	A	650	-	54,54,54	0.60	1 (1%)	59,63,63	1.80	8 (13%)

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	A	314	1	-	4/6/23/26	0/1/1/1
7	DB6	A	650	-	1/1/9/14	21/52/72/72	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	650	DB6	O1A-C1A	3.41	1.46	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	650	DB6	O1A-C1A-C2A	8.92	122.24	108.30
7	A	650	DB6	O6A-C1A-O1A	4.81	121.36	109.97
7	A	650	DB6	C3A-C4A-C5M	4.66	118.56	110.24
6	A	314	NAG	C1-O5-C5	4.31	118.03	112.19
7	A	650	DB6	C1-O1A-C1A	3.25	120.08	113.74
7	A	650	DB6	C4A-C3A-C2A	3.13	116.28	110.82
7	A	650	DB6	C1-C2-N2	-2.94	105.29	109.61
7	A	650	DB6	O6A-C1A-C2A	2.85	116.39	110.35
7	A	650	DB6	O6A-C5M-C4A	2.33	113.92	109.69

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	650	DB6	C1A

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	650	DB6	O1A-C1-C2-N2
7	A	650	DB6	O1A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
7	A	650	DB6	O6A-C1A-O1A-C1
7	A	650	DB6	O6A-C5M-C6A-O5A
6	A	314	NAG	C8-C7-N2-C2
6	A	314	NAG	O7-C7-N2-C2
7	A	650	DB6	C4A-C5M-C6A-O5A
6	A	314	NAG	O5-C5-C6-O6
6	A	314	NAG	C4-C5-C6-O6
7	A	650	DB6	C11-C10-C9-C8
7	A	650	DB6	C6-C7-C8-C9
7	A	650	DB6	C12-C13-C14-C15
7	A	650	DB6	C10-C11-C12-C13
7	A	650	DB6	C13-C14-C15-C16
7	A	650	DB6	CAD-CAE-CAF-CAG
7	A	650	DB6	CAP-CAQ-CAR-CAS
7	A	650	DB6	CAG-CAH-CAI-CAJ
7	A	650	DB6	C15-C16-C17-C18
7	A	650	DB6	O4-C4-C5-C6
7	A	650	DB6	C14-C15-C16-C17
7	A	650	DB6	CAN-CAO-CAP-CAQ
7	A	650	DB6	C4-C5-C6-C7
7	A	650	DB6	CAC-CAD-CAE-CAF
7	A	650	DB6	C2-C1-O1A-C1A
7	A	650	DB6	CAE-CAF-CAG-CAH

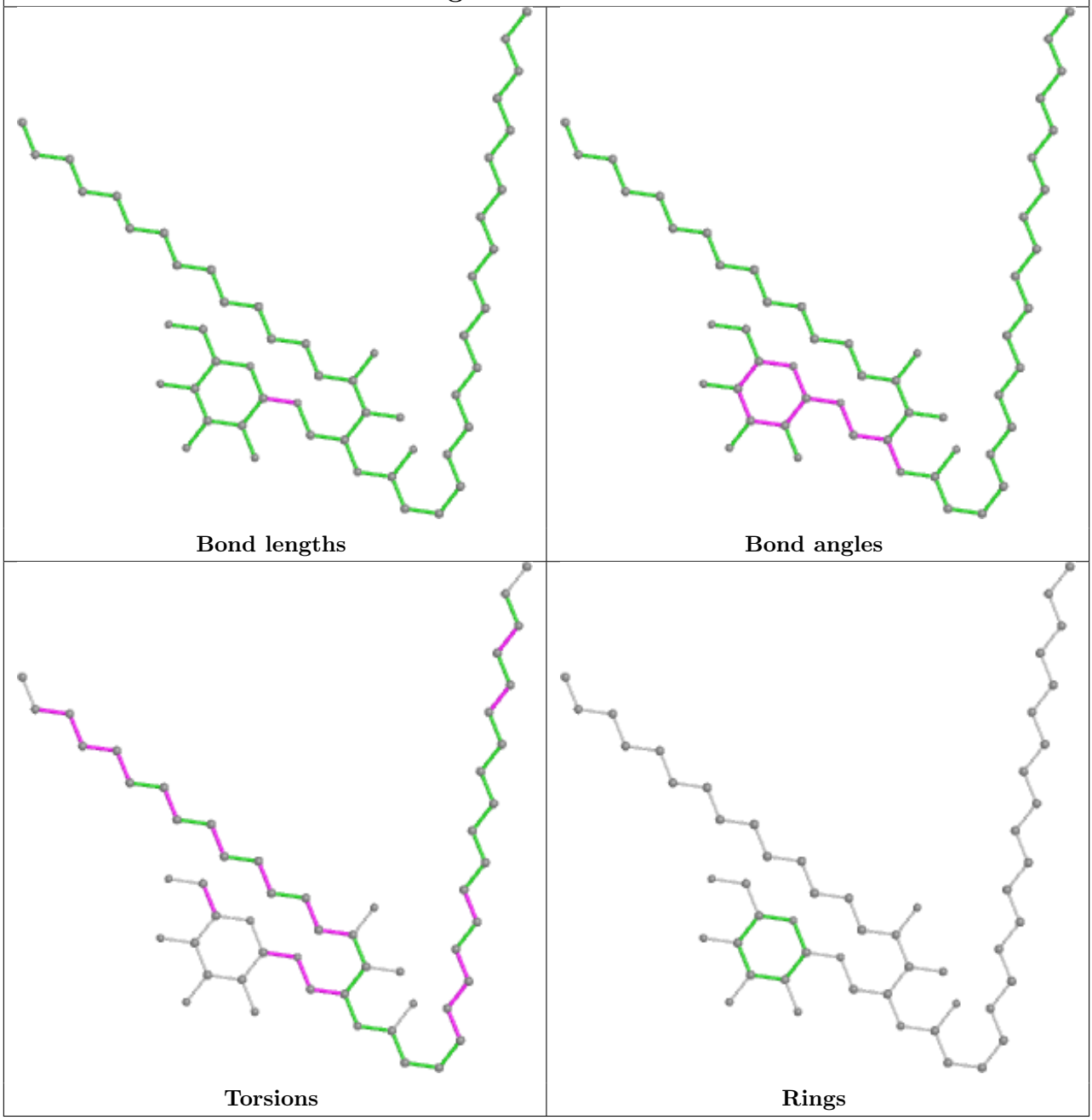
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	650	DB6	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 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 DB6 A 650



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	290/302 (96%)	-0.65	0	100	100	44, 73, 101, 128	9 (3%)
2	B	98/99 (98%)	-0.65	0	100	100	42, 64, 81, 98	2 (2%)
3	C	202/207 (97%)	-0.63	0	100	100	40, 73, 102, 120	6 (2%)
4	D	236/244 (96%)	-0.58	0	100	100	49, 74, 112, 137	4 (1%)
All	All	826/852 (96%)	-0.63	0	100	100	40, 72, 107, 137	21 (2%)

There are no RSRZ outliers to report.

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)

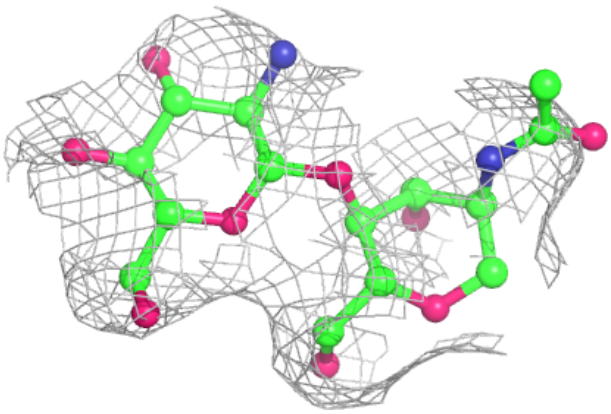
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

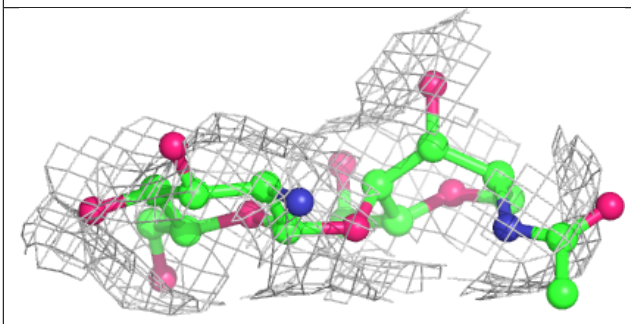
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	F	2	10/15	0.82	0.19	115,121,131,133	0
5	NAG	E	2	11/15	0.84	0.24	106,121,134,137	0
5	NAG	E	1	14/15	0.89	0.27	103,118,125,128	0
5	NAG	F	1	14/15	0.92	0.17	105,109,113,116	0

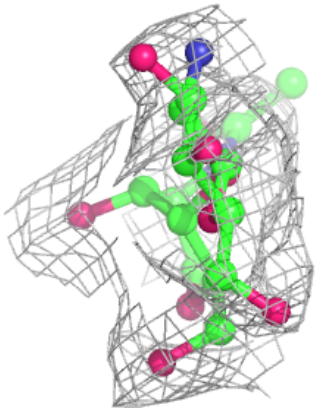
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

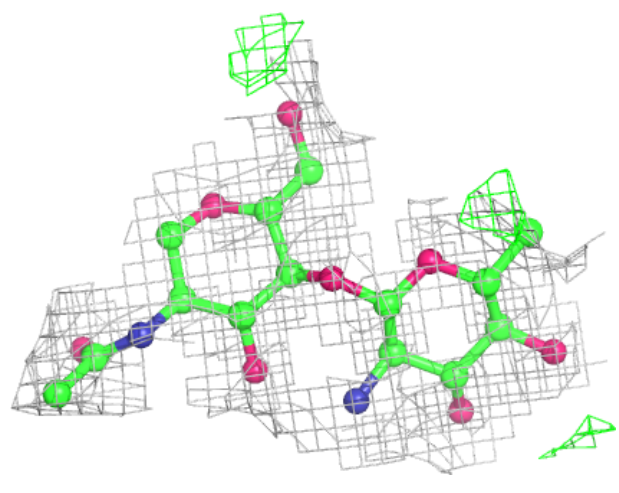


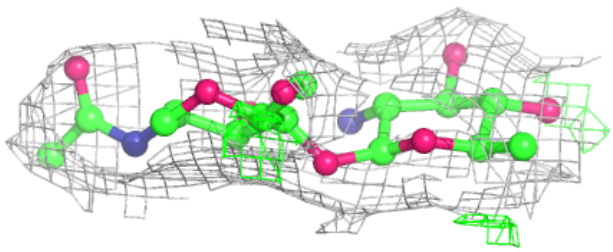


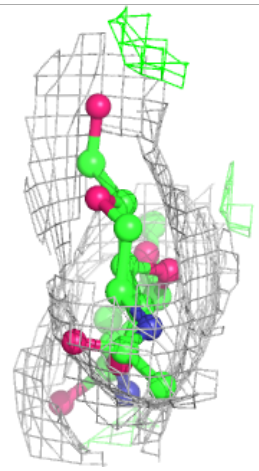


Electron density around Chain F:

$2mF_o$-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)

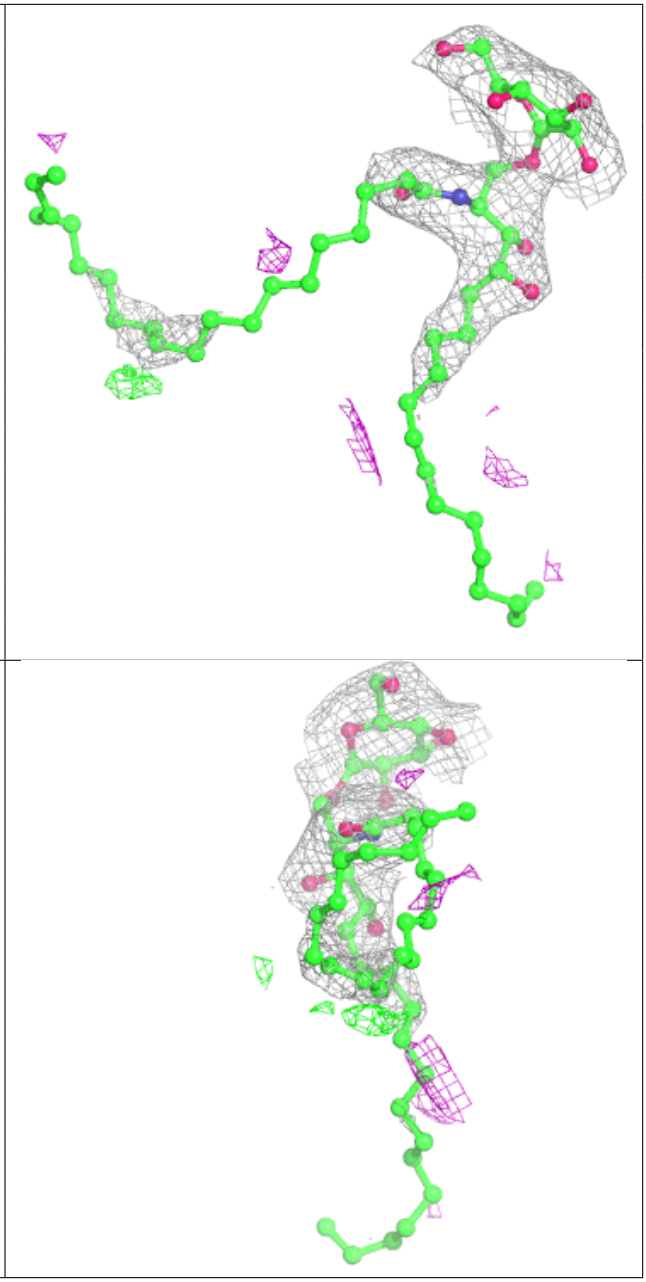
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	A	314	14/15	0.86	0.17	84,89,97,98	0
7	DB6	A	650	54/54	0.89	0.35	60,73,93,96	23

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 DB6 A 650:

$2mF_o$-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.