wwPDB X-ray Structure Validation Summary Report (i)

Oct 26, 2023 – 10:31 PM EDT

PDB ID	:	3HUJ
Title	:	Crystal structure of human CD1d-alpha-Galactosylceramide in complex with semi-invariant NKT cell receptor
Authors	:	Pang, S.S.
Deposited on	:	2009-06-14
Resolution	:	2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

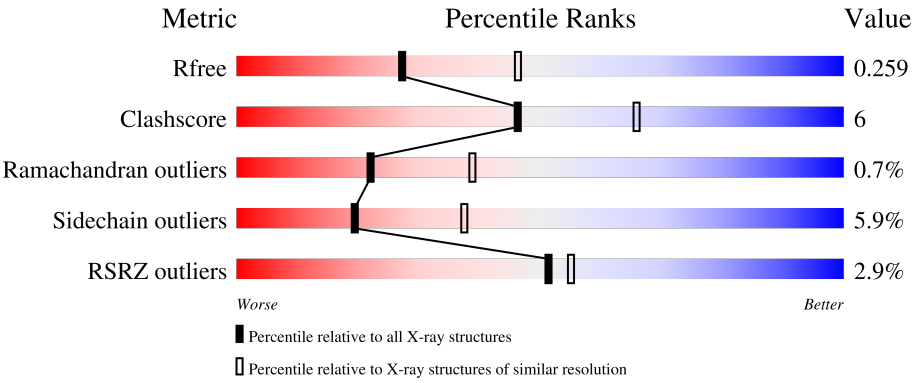
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	284	2% 77% 19%
1	C	284	7% 79% 16%
2	B	99	80% 17%
2	D	99	% 82% 16%
3	E	209	3% 81% 11% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	209	6% 79% 13%
4	F	246	82% 15%
4	H	246	% 84% 14%
5	I	2	50% 50%
6	J	3	33% 67%

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
5	NAG	I	1	X	-	-	-
7	NAG	C	2000	X	-	-	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 13690 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 T-cell surface glycoprotein CD1d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2181	1398	384	392	7			
1	C	274	Total	C	N	O	S	0	0	0
			2147	1378	374	388	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P15813
A	1	PRO	-	expression tag	UNP P15813
A	2	GLY	-	expression tag	UNP P15813
A	278	HIS	-	expression tag	UNP P15813
A	279	HIS	-	expression tag	UNP P15813
A	280	HIS	-	expression tag	UNP P15813
A	281	HIS	-	expression tag	UNP P15813
A	282	HIS	-	expression tag	UNP P15813
A	283	HIS	-	expression tag	UNP P15813
C	0	SER	-	expression tag	UNP P15813
C	1	PRO	-	expression tag	UNP P15813
C	2	GLY	-	expression tag	UNP P15813
C	278	HIS	-	expression tag	UNP P15813
C	279	HIS	-	expression tag	UNP P15813
C	280	HIS	-	expression tag	UNP P15813
C	281	HIS	-	expression tag	UNP P15813
C	282	HIS	-	expression tag	UNP P15813
C	283	HIS	-	expression tag	UNP P15813

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	97	Total	C	N	O	S	0	0	0
			805	514	138	151	2			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	99	Total	C	N	O	S	0	1	0
			830	527	140	160	3			

- Molecule 3 is a protein called NKT15 T cell receptor alpha-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	199	Total	C	N	O	S	0	1	0
			1562	967	265	321	9			
3	G	202	Total	C	N	O	S	0	1	0
			1566	973	261	323	9			

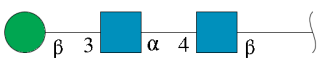
- Molecule 4 is a protein called NKT15 T cell receptor beta-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	242	Total	C	N	O	S	0	1	0
			1940	1222	336	374	8			
4	H	245	Total	C	N	O	S	0	1	0
			1964	1236	339	380	9			

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

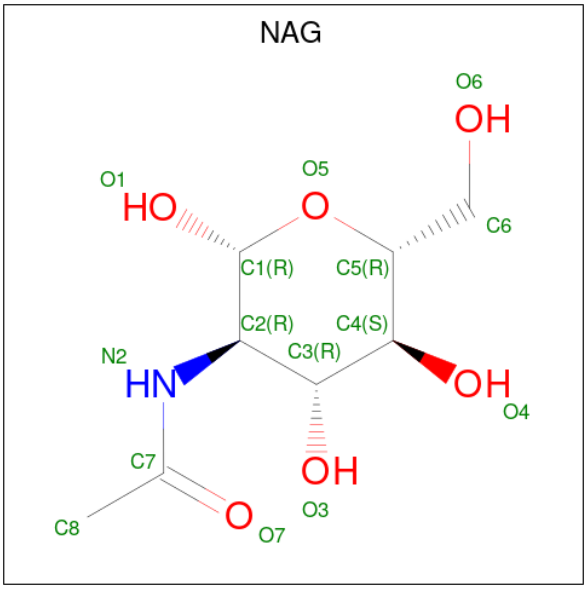
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	2	Total	C	N	O	0	0	0
			25	14	1	10			

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



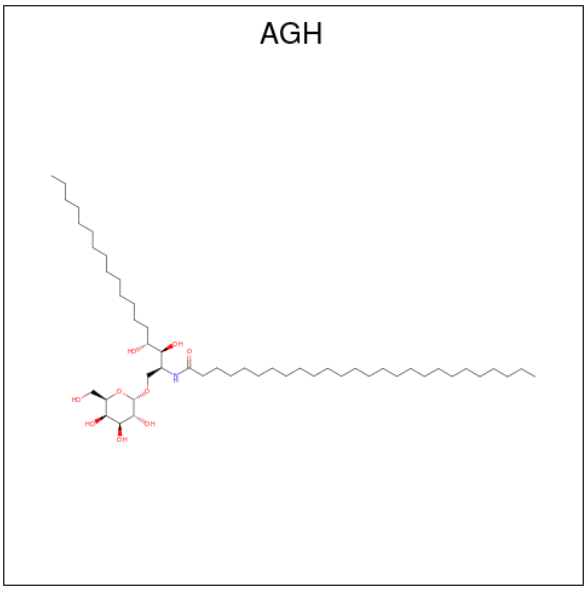
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is N-{(1S,2R,3S)-1-[(ALPHA-D-GALACTOPYRANOSYLOXY)METHYL]-2,3-DIHYDROXYHEPTADECYL}HEXACOSANAMIDE (three-letter code: AGH) (formula: $C_{50}H_{99}NO_9$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 60 50 1 9	0	0
8	C	1	Total C N O 60 50 1 9	0	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	H	1	Total Mg 1 1	0	0

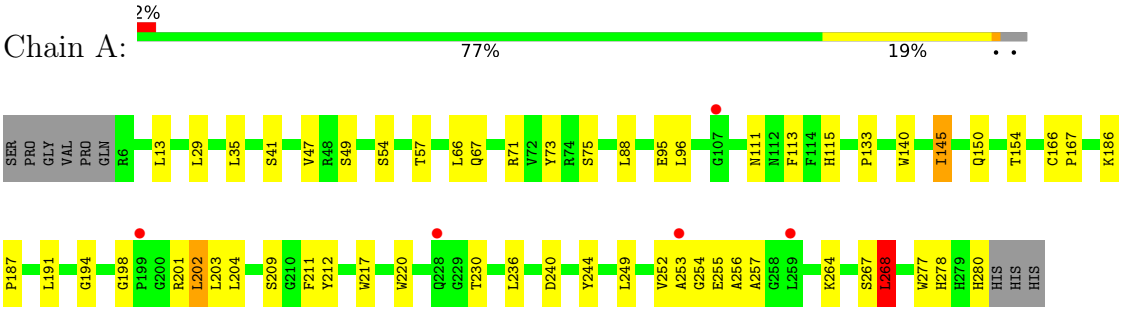
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	95	Total O 95 95	0	0
10	B	42	Total O 42 42	0	0
10	C	88	Total O 88 88	0	0
10	D	35	Total O 35 35	0	0
10	E	40	Total O 40 40	0	0
10	F	52	Total O 52 52	0	0
10	G	62	Total O 62 62	0	0
10	H	68	Total O 68 68	0	0

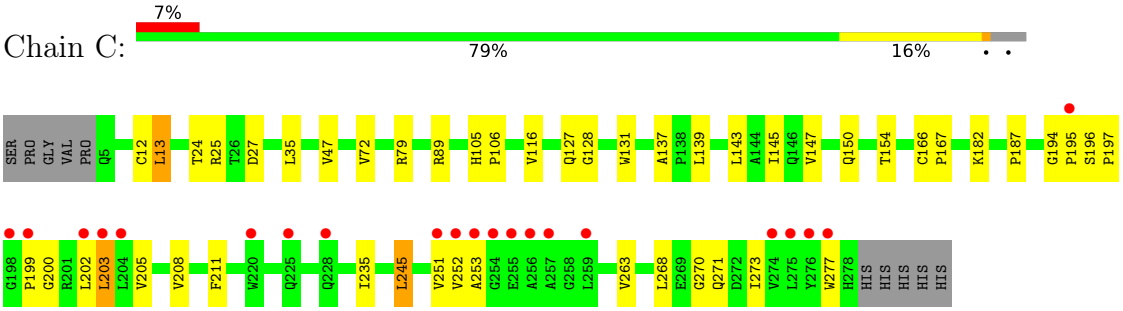
3 Residue-property plots (i)

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.

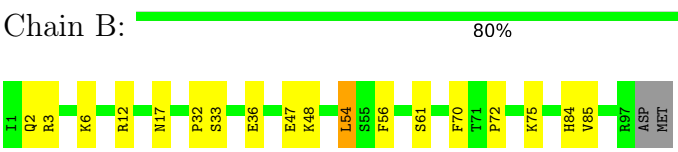
• Molecule 1: T-cell surface glycoprotein CD1d



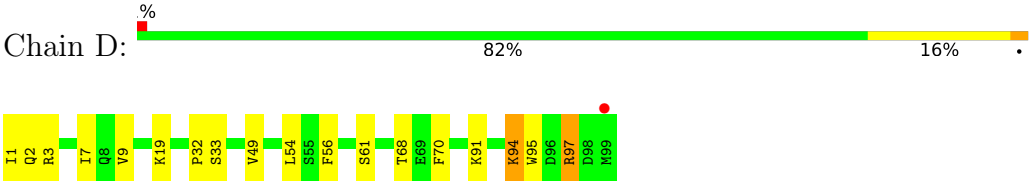
• Molecule 1: T-cell surface glycoprotein CD1d



• Molecule 2: Beta-2-microglobulin

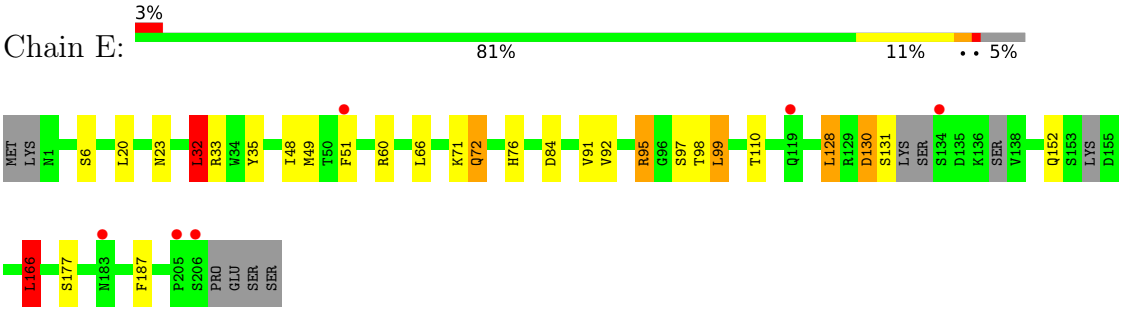


• Molecule 2: Beta-2-microglobulin



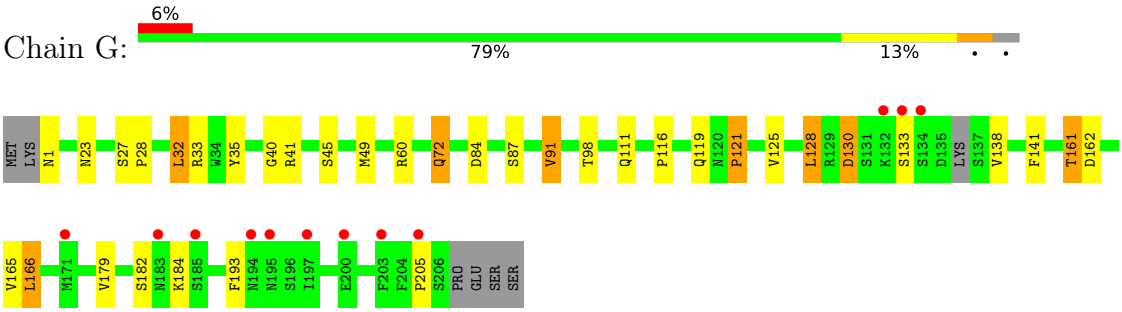
• Molecule 3: NKT15 T cell receptor alpha-chain

Chain E:



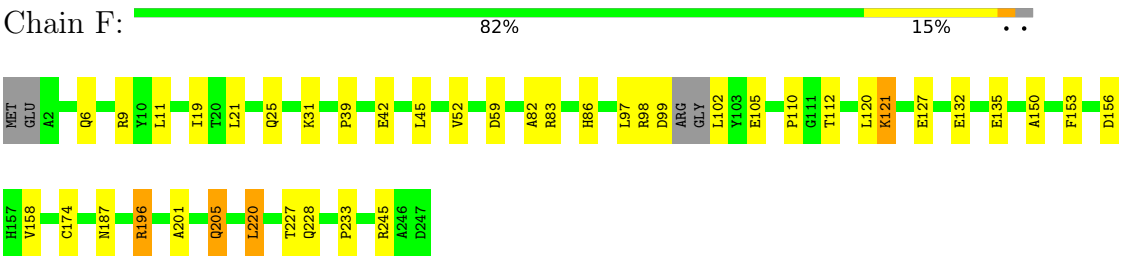
• Molecule 3: NKT15 T cell receptor alpha-chain

Chain G:



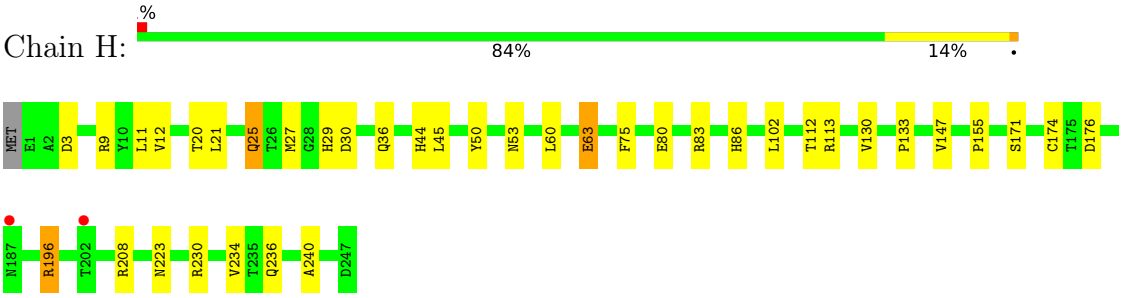
• Molecule 4: NKT15 T cell receptor beta-chain

Chain F:



• Molecule 4: NKT15 T cell receptor beta-chain

Chain H:



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

Chain I:

• Molecule 6: beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-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 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	112.11Å 82.36Å 117.18Å 90.00° 101.26° 90.00°	Depositor
Resolution (Å)	47.28 – 2.50 47.28 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.5 (47.28-2.50) 90.5 (47.28-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.216 , 0.279 0.233 , 0.259	Depositor DCC
R_{free} test set	3288 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	41.9	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 18.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.057 for l,-k,h	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	13690	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BMA, AGH, NAG, NDG

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	0.41	0/2249	0.57	0/3066
1	C	0.39	0/2213	0.53	0/3022
2	B	0.42	0/828	0.54	0/1122
2	D	0.43	0/853	0.57	0/1156
3	E	0.40	0/1590	0.59	3/2156 (0.1%)
3	G	0.41	0/1598	0.59	2/2176 (0.1%)
4	F	0.38	0/1993	0.53	0/2712
4	H	0.41	0/2018	0.54	0/2747
All	All	0.40	0/13342	0.56	5/18157 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	32	LEU	CA-CB-CG	7.54	132.64	115.30
3	G	32	LEU	CA-CB-CG	7.18	131.82	115.30
3	G	166	LEU	CA-CB-CG	6.26	129.70	115.30
3	E	166	LEU	CA-CB-CG	5.42	127.76	115.30
3	E	128	LEU	CA-CB-CG	5.31	127.51	115.30

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	2181	0	2091	42	0
1	C	2147	0	2040	25	0
2	B	805	0	768	8	0
2	D	830	0	779	10	0
3	E	1562	0	1481	20	0
3	G	1566	0	1465	24	0
4	F	1940	0	1833	26	0
4	H	1964	0	1859	21	0
5	I	25	0	22	0	0
6	J	39	0	33	1	0
7	A	14	0	13	0	0
7	C	14	0	13	0	0
8	A	60	0	99	2	0
8	C	60	0	99	4	0
9	H	1	0	0	0	0
10	A	95	0	0	2	0
10	B	42	0	0	0	0
10	C	88	0	0	2	0
10	D	35	0	0	1	0
10	E	40	0	0	2	0
10	F	52	0	0	1	0
10	G	62	0	0	1	0
10	H	68	0	0	8	0
All	All	13690	0	12595	162	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 6.

The worst 5 of 162 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:SER:HB2	1:A:268:LEU:HB2	1.29	1.15
1:A:253:ALA:HB1	1:A:254:GLY:HA3	1.11	1.05
1:A:253:ALA:CB	1:A:254:GLY:HA3	1.90	1.01
4:F:98:ARG:HB3	4:F:99:ASP:HB2	1.45	0.97
2:D:94:LYS:H	2:D:94:LYS:HE2	1.35	0.91

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	273/284 (96%)	263 (96%)	9 (3%)	1 (0%)	34 54
1	C	272/284 (96%)	244 (90%)	21 (8%)	7 (3%)	5 8
2	B	95/99 (96%)	94 (99%)	1 (1%)	0	100 100
2	D	98/99 (99%)	93 (95%)	4 (4%)	1 (1%)	15 28
3	E	192/209 (92%)	184 (96%)	7 (4%)	1 (0%)	29 48
3	G	199/209 (95%)	190 (96%)	9 (4%)	0	100 100
4	F	239/246 (97%)	230 (96%)	8 (3%)	1 (0%)	34 54
4	H	244/246 (99%)	234 (96%)	10 (4%)	0	100 100
All	All	1612/1676 (96%)	1532 (95%)	69 (4%)	11 (1%)	22 39

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	LEU
1	C	271	GLN
3	E	187	PHE
1	C	137	ALA
1	C	195	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	233/249 (94%)	220 (94%)	13 (6%)	21 40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	226/249 (91%)	212 (94%)	14 (6%)	18 35
2	B	90/94 (96%)	83 (92%)	7 (8%)	12 24
2	D	93/94 (99%)	89 (96%)	4 (4%)	29 53
3	E	182/191 (95%)	173 (95%)	9 (5%)	25 47
3	G	180/191 (94%)	170 (94%)	10 (6%)	21 40
4	F	212/217 (98%)	199 (94%)	13 (6%)	18 36
4	H	215/217 (99%)	201 (94%)	14 (6%)	17 33
All	All	1431/1502 (95%)	1347 (94%)	84 (6%)	19 37

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	205	GLN
4	H	11	LEU
4	F	227	THR
3	G	121	PRO
4	H	45	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	21	GLN
4	H	140	HIS
3	G	23	ASN
3	G	149	ASN
2	D	8	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)

5 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	I	1	5,1	14,14,15	0.55	0	17,19,21	1.20	2 (11%)
5	BMA	I	2	5	11,11,12	0.55	0	15,15,17	0.74	0
6	NAG	J	1	6,1	14,14,15	0.50	0	17,19,21	1.37	4 (23%)
6	NDG	J	2	6	14,14,15	0.77	0	17,19,21	1.25	3 (17%)
6	BMA	J	3	6	11,11,12	0.69	0	15,15,17	0.96	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	I	1	5,1	1/1/5/7	2/6/23/26	0/1/1/1
5	BMA	I	2	5	-	2/2/19/22	0/1/1/1
6	NAG	J	1	6,1	-	2/6/23/26	0/1/1/1
6	NDG	J	2	6	-	2/6/23/26	0/1/1/1
6	BMA	J	3	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	2	NDG	C4-C3-C2	3.44	116.07	111.02
6	J	1	NAG	C1-O5-C5	3.01	116.28	112.19
5	I	1	NAG	C1-O5-C5	2.80	115.99	112.19
6	J	1	NAG	O4-C4-C3	-2.64	104.23	110.35
6	J	2	NDG	O5-C5-C6	2.37	110.92	107.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	I	1	NAG	C1

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	2	BMA	O5-C5-C6-O6
5	I	1	NAG	C8-C7-N2-C2
5	I	2	BMA	C4-C5-C6-O6
5	I	1	NAG	O7-C7-N2-C2
6	J	2	NDG	O5-C5-C6-O6

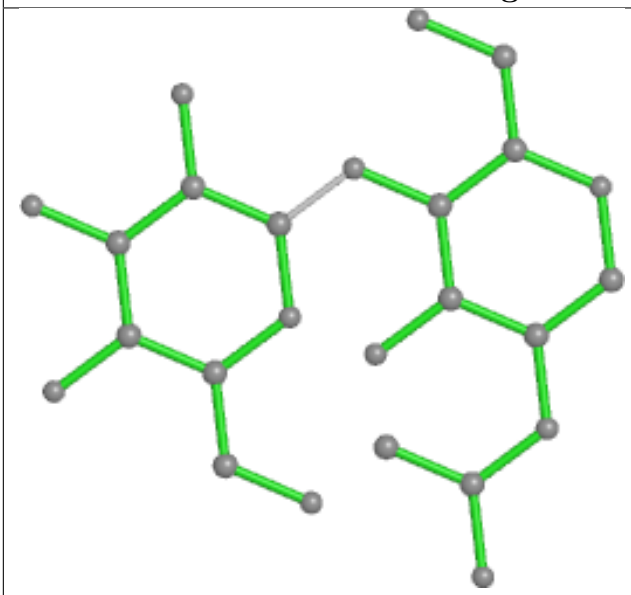
There are no ring outliers.

2 monomers are involved in 1 short contact:

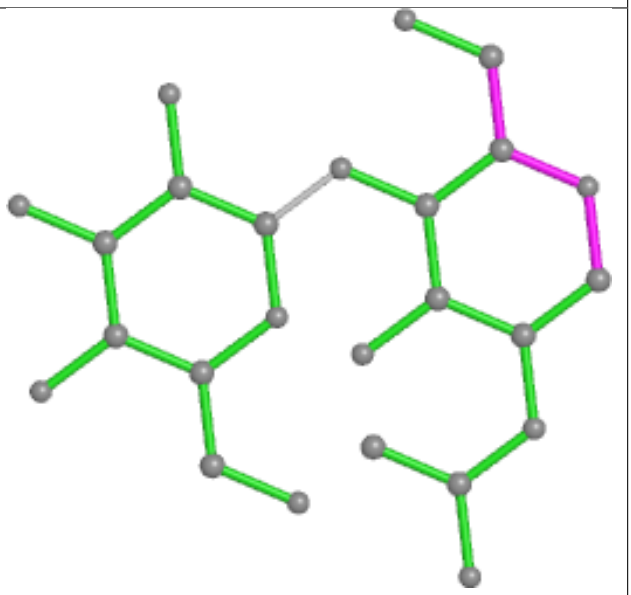
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	1	NAG	1	0
6	J	2	NDG	1	0

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

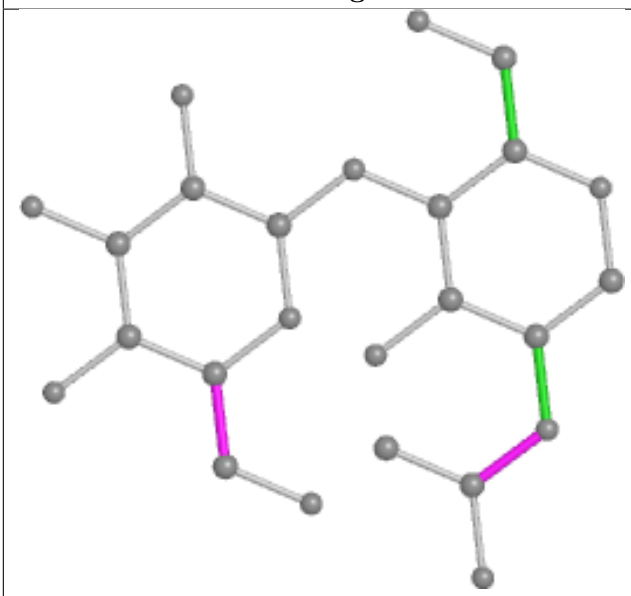
Oligosaccharide Chain I



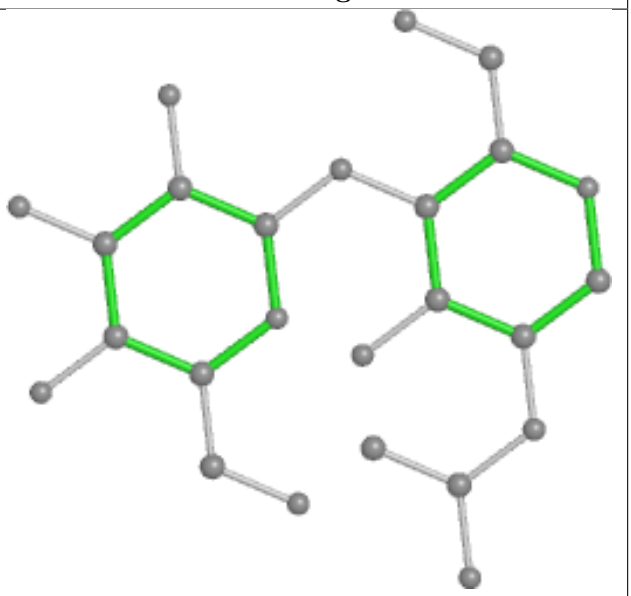
Bond lengths



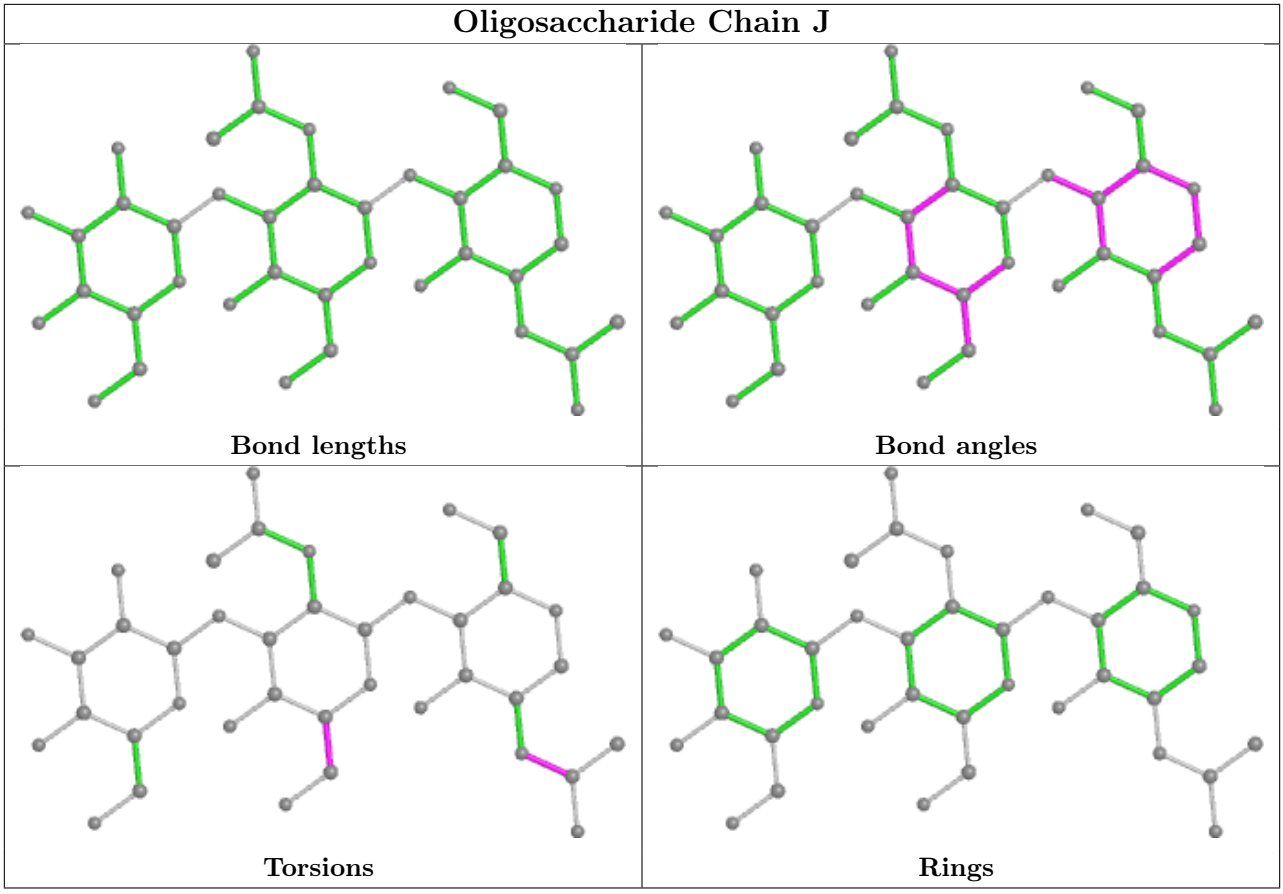
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\#\|Z\| > 2$
7	NAG	A	2000	1	14,14,15	0.52	0	17,19,21	2.70	6 (35%)
8	AGH	C	3000	-	60,60,60	0.41	0	65,69,69	0.76	1 (1%)
7	NAG	C	2000	1	14,14,15	0.48	0	17,19,21	1.40	3 (17%)
8	AGH	A	3000	-	60,60,60	0.48	1 (1%)	65,69,69	0.75	1 (1%)

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
7	NAG	A	2000	1	-	4/6/23/26	0/1/1/1
8	AGH	C	3000	-	-	23/58/78/78	0/1/1/1
7	NAG	C	2000	1	1/1/5/7	5/6/23/26	0/1/1/1
8	AGH	A	3000	-	-	19/58/78/78	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	3000	AGH	O1A-C1A	2.64	1.44	1.40

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	2000	NAG	C1-O5-C5	8.12	123.20	112.19
7	A	2000	NAG	C4-C3-C2	-3.76	105.51	111.02
7	A	2000	NAG	C2-N2-C7	3.74	128.23	122.90
7	C	2000	NAG	C1-O5-C5	3.65	117.14	112.19
8	C	3000	AGH	C1-C2-N2	-3.02	105.16	109.61

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	C	2000	NAG	C1

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2000	NAG	C8-C7-N2-C2
7	A	2000	NAG	O7-C7-N2-C2
7	C	2000	NAG	C8-C7-N2-C2
7	C	2000	NAG	O7-C7-N2-C2
8	C	3000	AGH	C14-C15-C16-C17

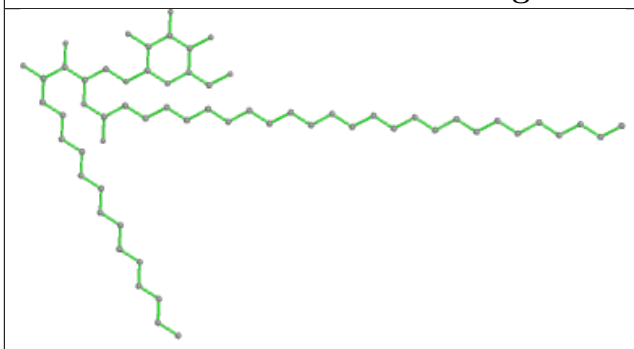
There are no ring outliers.

2 monomers are involved in 6 short contacts:

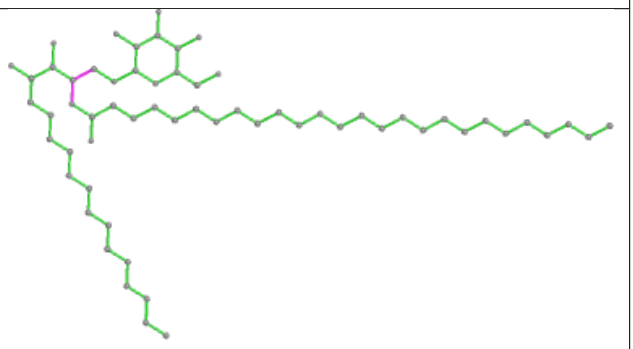
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	3000	AGH	4	0
8	A	3000	AGH	2	0

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.

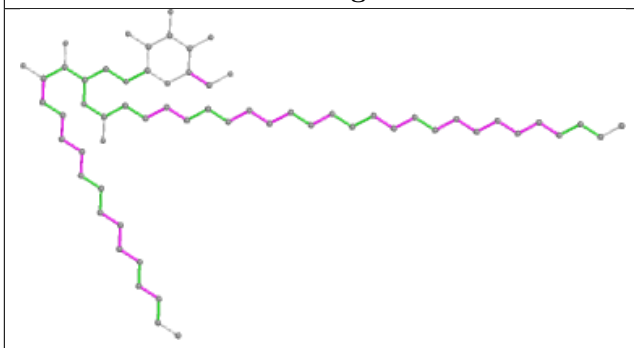
Ligand AGH C 3000



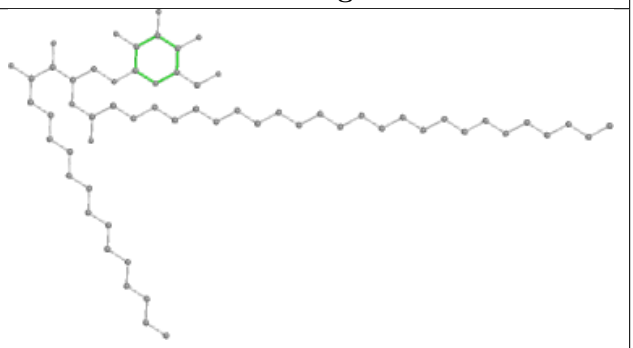
Bond lengths



Bond angles

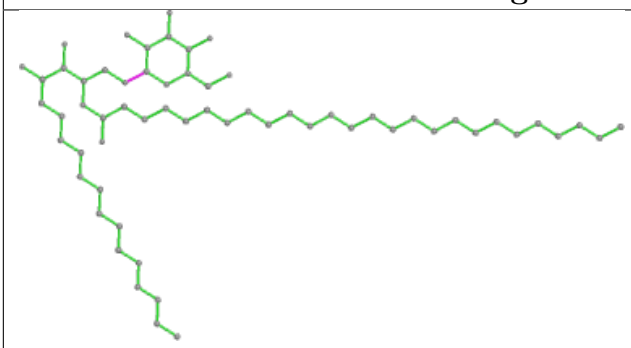


Torsions

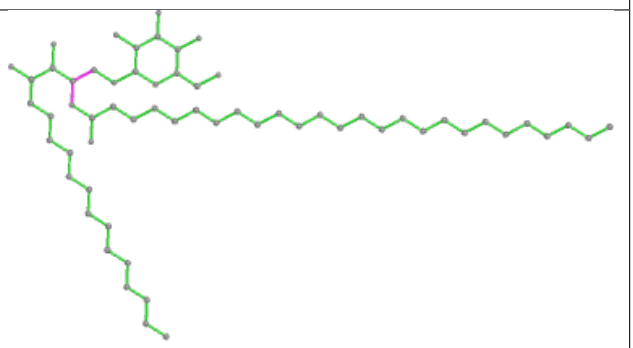


Rings

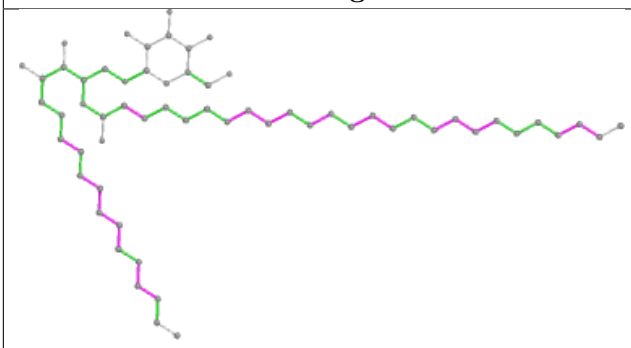
Ligand AGH A 3000



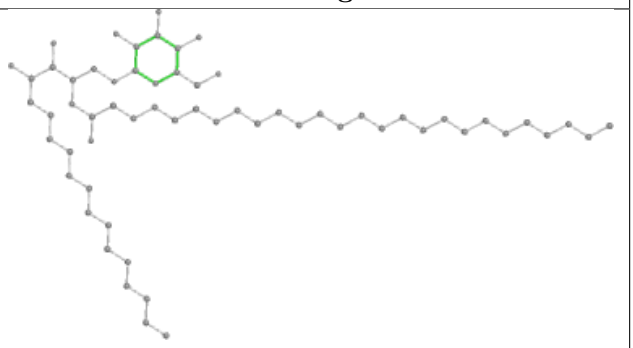
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	275/284 (96%)	0.17	5 (1%) 68 71	22, 39, 59, 68	0
1	C	274/284 (96%)	0.48	21 (7%) 13 13	29, 43, 69, 74	0
2	B	97/99 (97%)	-0.11	0 100 100	23, 31, 40, 43	0
2	D	99/99 (100%)	0.01	1 (1%) 82 84	30, 35, 44, 55	0
3	E	199/209 (95%)	0.22	6 (3%) 50 53	27, 37, 70, 70	0
3	G	202/209 (96%)	0.32	12 (5%) 22 23	24, 36, 70, 73	0
4	F	242/246 (98%)	0.23	0 100 100	31, 47, 56, 61	0
4	H	245/246 (99%)	0.08	2 (0%) 86 87	22, 43, 54, 55	1 (0%)
All	All	1633/1676 (97%)	0.22	47 (2%) 51 55	22, 41, 64, 74	1 (0%)

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	228	GLN	6.6
1	C	198	GLY	4.8
3	E	206	SER	4.8
1	C	256	ALA	4.5
1	C	257	ALA	4.2

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

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

6.3 Carbohydrates

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

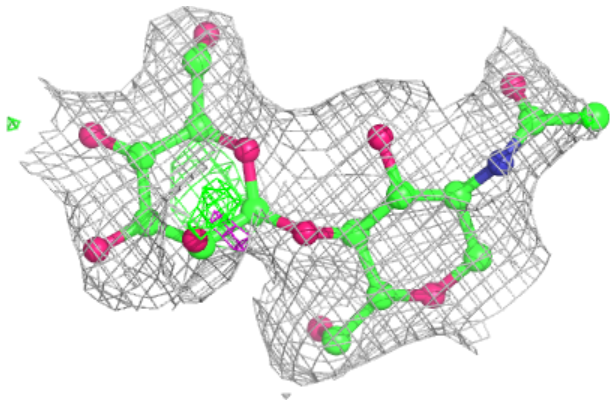
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

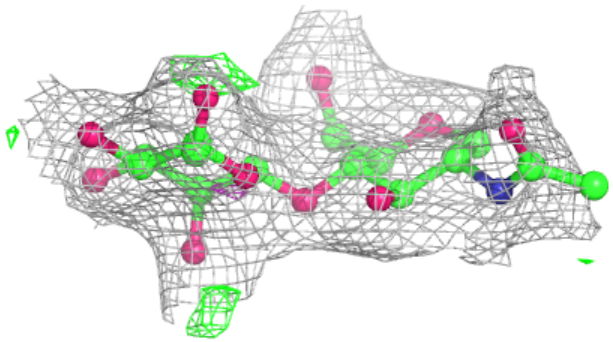
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BMA	I	2	11/12	0.77	0.17	55,56,56,57	0
6	BMA	J	3	11/12	0.84	0.15	65,65,65,65	0
5	NAG	I	1	14/15	0.87	0.17	45,50,52,53	0
6	NDG	J	2	14/15	0.93	0.15	60,63,63,64	0
6	NAG	J	1	14/15	0.95	0.13	46,49,53,57	0

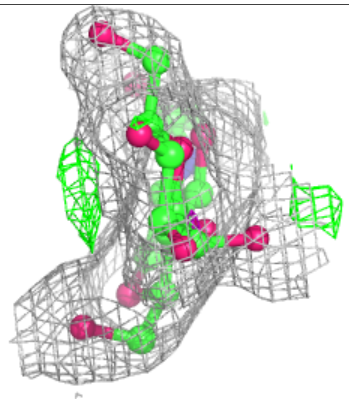
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

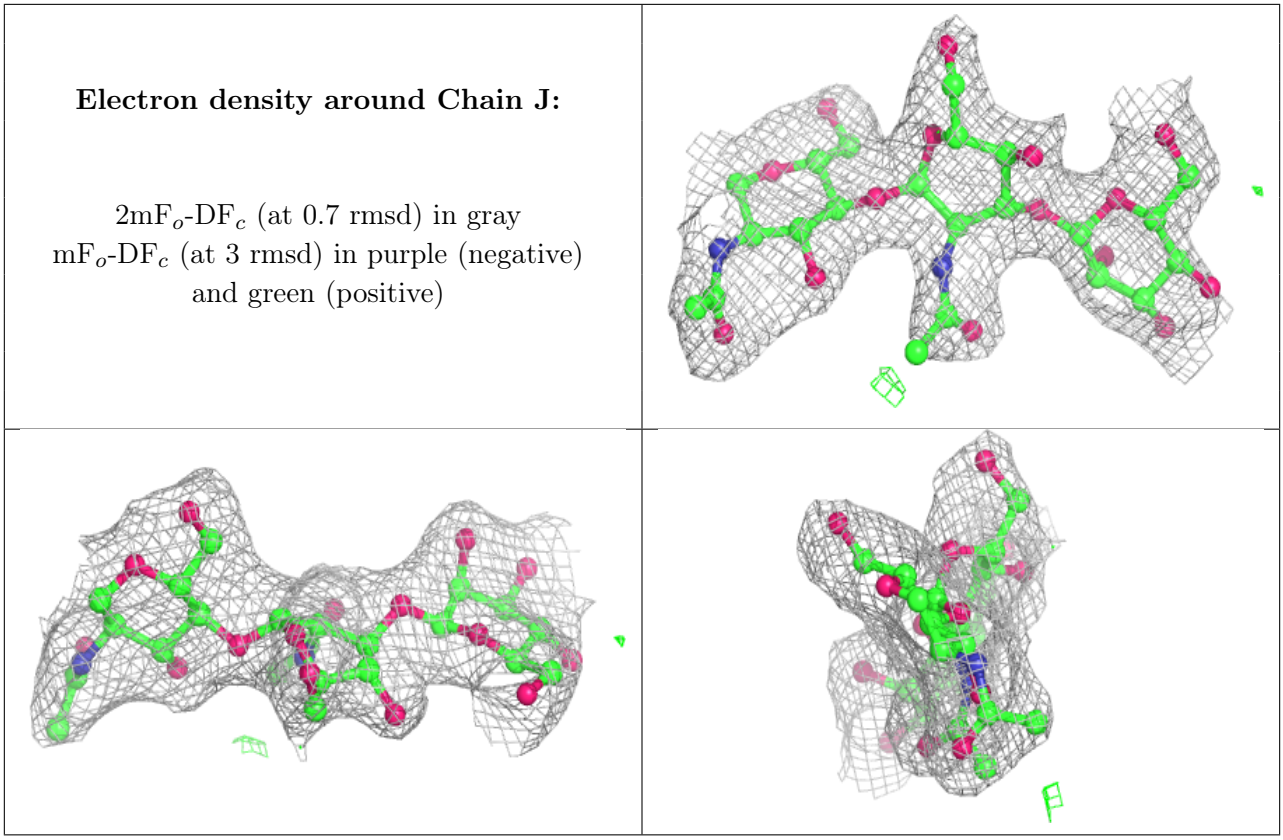






Electron density around Chain J:

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



6.4 Ligands

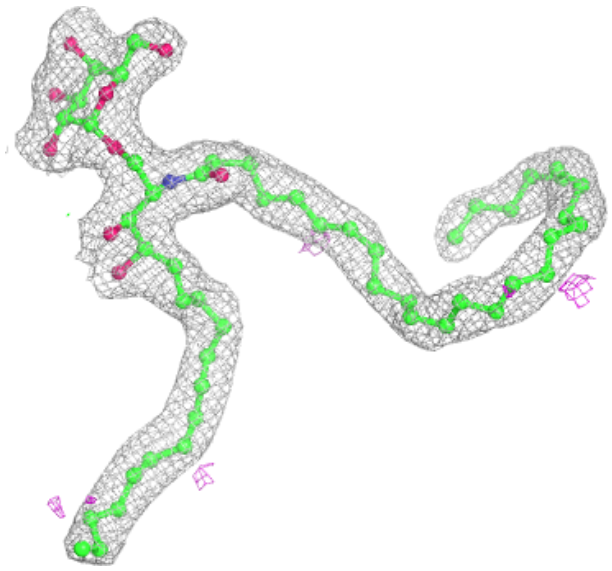
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

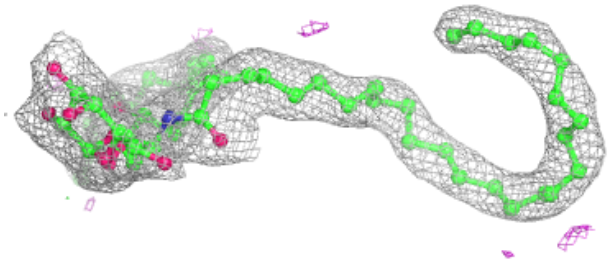
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	A	2000	14/15	0.90	0.13	38,40,41,41	0
7	NAG	C	2000	14/15	0.92	0.13	43,44,45,46	0
9	MG	H	1000	1/1	0.94	0.21	27,27,27,27	1
8	AGH	C	3000	60/60	0.96	0.18	26,31,34,35	0
8	AGH	A	3000	60/60	0.96	0.17	22,26,37,38	0

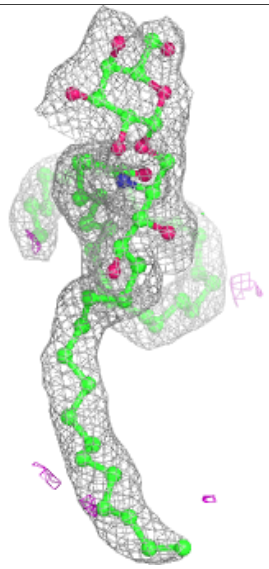
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AGH C 3000:

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

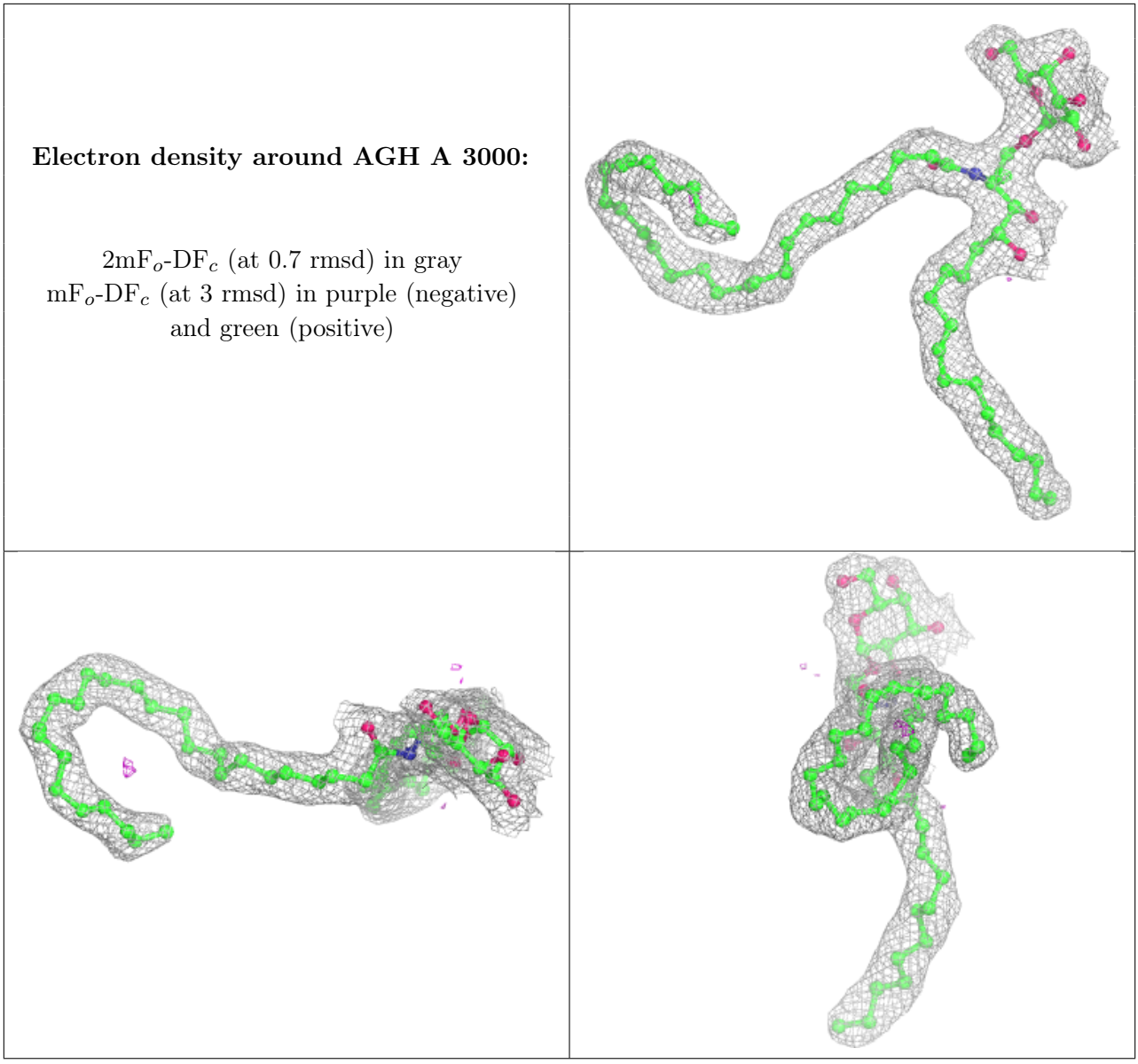






Electron density around AGH A 3000:

$2mF_o$-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.