



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 04:59 AM UTC

PDB ID : 2PO6 / pdb_00002po6
Title : Crystal structure of CD1d-lipid-antigen complexed with Beta-2-Microglobulin, NKT15 Alpha-Chain and NKT15 Beta-Chain
Authors : Borg, N.A.
Deposited on : 2007-04-25
Resolution : 3.20 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

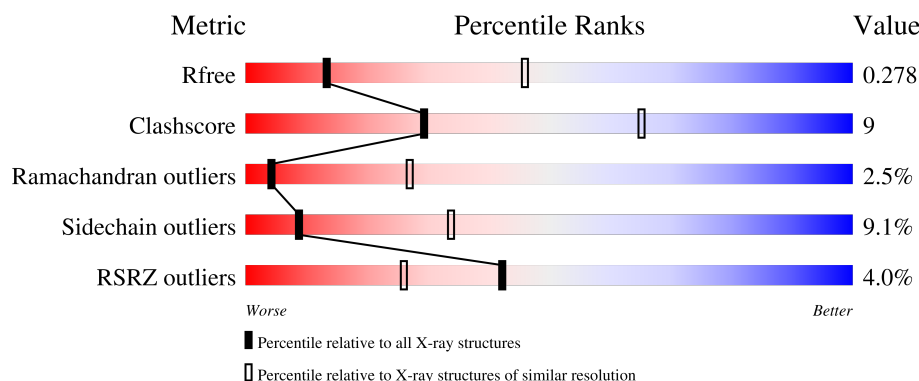
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	278	4% 69% 27% ..
1	E	278	5% 68% 24% ..
2	B	99	8% 75% 19% ..
2	F	99	2% 77% 19% ..
3	C	204	3% 79% 19% .

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Mol	Chain	Length	Quality of chain
3	G	204	4% 80% 17% .
4	D	244	2% 78% 18% .
4	H	244	3% 74% 22% ..
5	I	2	50% 50%
6	J	2	50% 50%

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	NAG	A	301	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13298 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
			2192	1400	383	402	7			
1	E	272	Total	C	N	O	S	0	0	0
			2171	1388	377	399	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
E	278	HIS	-	expression tag	UNP P15813
E	279	HIS	-	expression tag	UNP P15813
E	280	HIS	-	expression tag	UNP P15813
E	281	HIS	-	expression tag	UNP P15813
E	282	HIS	-	expression tag	UNP P15813
E	283	HIS	-	expression tag	UNP P15813

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			824	525	139	157	3			
2	F	98	Total	C	N	O	S	0	0	0
			813	517	138	156	2			

- Molecule 3 is a protein called NKT15 alpha-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	203	Total	C	N	O	S	0	0	0
			1581	979	267	326	9			
3	G	204	Total	C	N	O	S	0	0	0
			1588	984	268	327	9			

- Molecule 4 is a protein called NKT15 beta-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	244	Total	C	N	O	S	0	0	0
			1957	1230	340	379	8			
4	H	244	Total	C	N	O	S	0	0	0
			1957	1230	340	379	8			

- 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 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



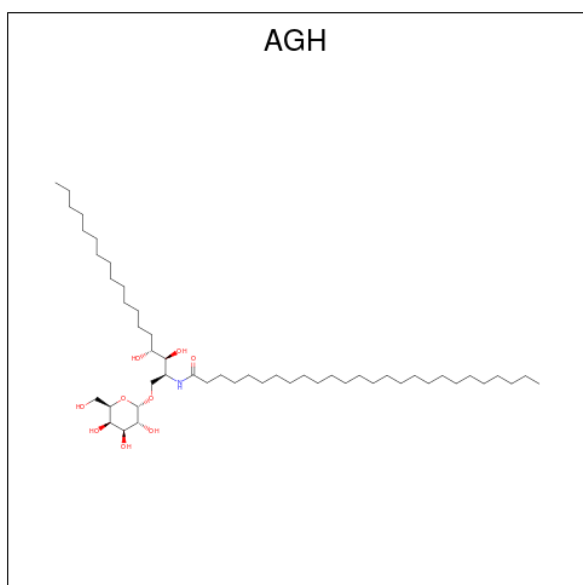
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



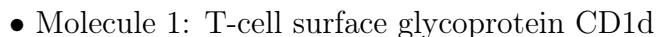
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		

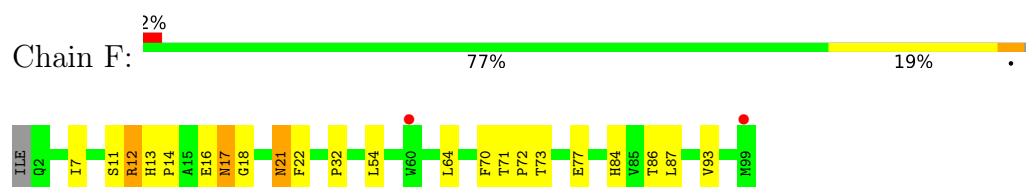
- Molecule 8 is N-{(1S,2R,3S)-1-[(ALPHA-D-GALACTOPYRANOSYLOXY)METHYL]-2,3-DIHYDROXYHEPTADECYL}HEXACOSANAMIDE (CCD ID: AGH) (formula: C₅₀H₉₉NO₉).



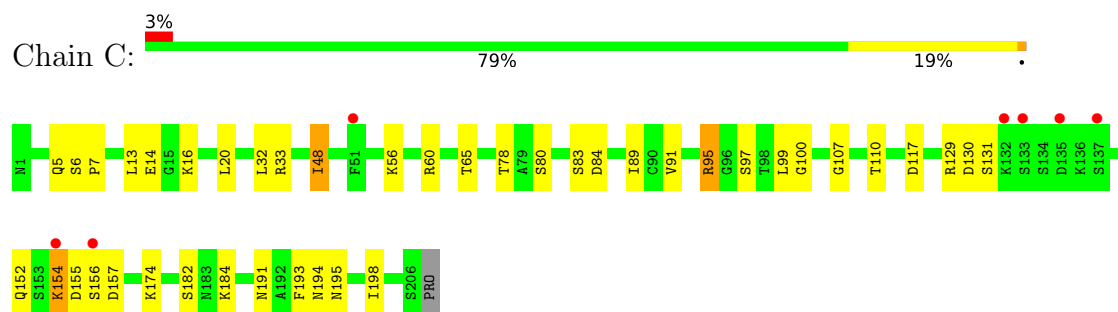
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			60	50	1	9		
8	E	1	Total	C	N	O	0	0
			60	50	1	9		

- Molecule 1: T-cell surface glycoprotein CD1d

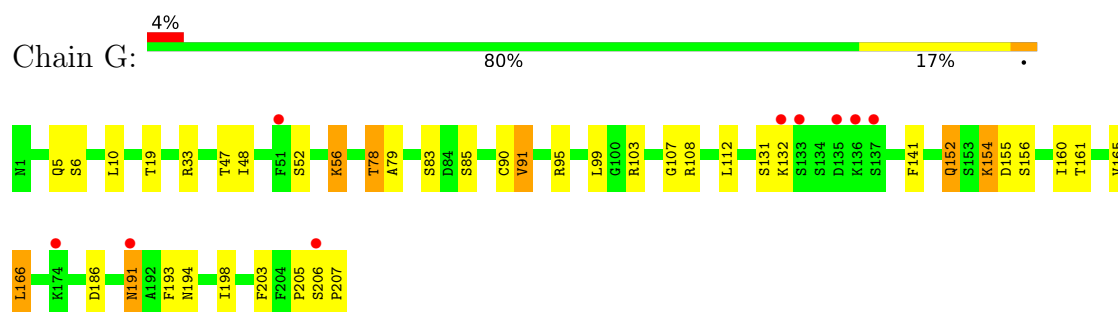




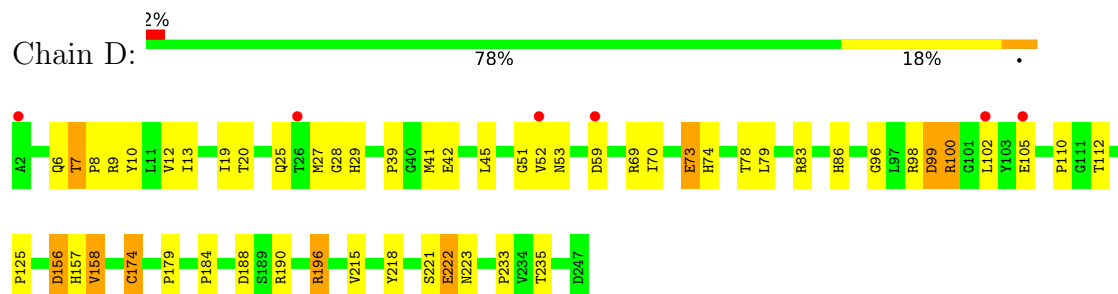
• Molecule 3: NKT15 alpha-chain



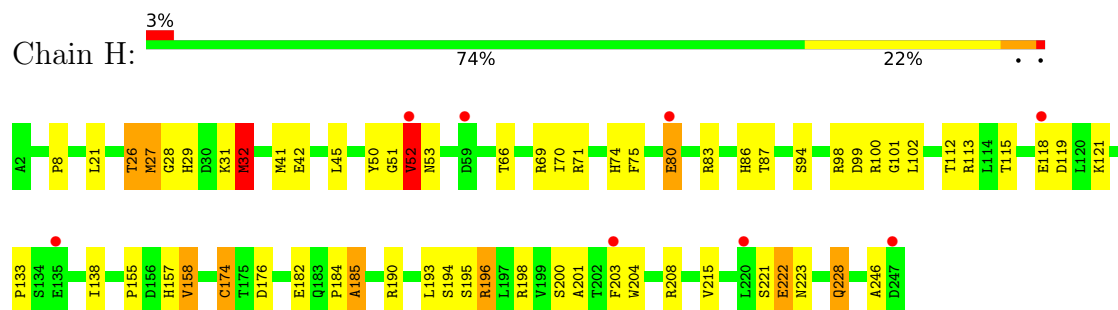
• Molecule 3: NKT15 alpha-chain



• Molecule 4: NKT15 beta-chain



• Molecule 4: NKT15 beta-chain



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

Chain I:  50% 50%

MAG1
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	204.01Å 155.64Å 85.98Å 90.00° 94.78° 90.00°	Depositor
Resolution (Å)	29.18 – 3.20 29.18 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.6 (29.18-3.20) 95.4 (29.18-3.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 3.18Å)	Xtriage
Refinement program	REFMAC refmac_5.2.0019	Depositor
R, R_{free}	0.226 , 0.293 0.217 , 0.278	Depositor DCC
R_{free} test set	2135 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	13298	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: AGH, BMA, 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	0.49	2/2257 (0.1%)	0.86	6/3076 (0.2%)
1	E	0.46	0/2236	0.89	8/3048 (0.3%)
2	B	0.45	0/847	0.85	2/1148 (0.2%)
2	F	0.45	0/836	0.79	0/1134
3	C	0.46	0/1612	0.77	0/2189
3	G	0.45	0/1620	0.77	0/2201
4	D	0.47	0/2011	0.78	0/2736
4	H	0.46	1/2011 (0.0%)	0.81	3/2736 (0.1%)
All	All	0.47	3/13430 (0.0%)	0.82	19/18268 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	GLU	CD-OE1	5.81	1.36	1.25
1	A	180	GLU	CD-OE2	5.56	1.35	1.25
4	H	52	VAL	CA-CB	5.12	1.61	1.54

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	154	THR	N-CA-C	10.64	122.57	110.97
1	E	92	TYR	CA-C-N	-8.16	110.18	120.79
1	E	92	TYR	C-N-CA	-8.16	110.18	120.79
1	E	154	THR	CA-C-N	7.38	134.99	121.70
1	E	154	THR	C-N-CA	7.38	134.99	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	91	SER	Peptide
1	E	91	SER	Peptide

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	2192	0	2102	44	0
1	E	2171	0	2086	58	0
2	B	824	0	783	22	0
2	F	813	0	762	11	0
3	C	1581	0	1508	23	0
3	G	1588	0	1515	24	0
4	D	1957	0	1855	28	0
4	H	1957	0	1855	37	0
5	I	25	0	22	0	0
6	J	28	0	25	0	0
7	A	28	0	26	0	0
7	E	14	0	13	0	0
8	C	60	0	99	6	0
8	E	60	0	99	2	0
All	All	13298	0	12750	224	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 9.

The worst 5 of 224 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)
2:B:27:VAL:CA	2:B:28:SER:HB2	1.83	1.06
1:E:7:LEU:HB3	1:E:8:PHE:HA	1.36	1.06
2:B:27:VAL:HA	2:B:28:SER:CB	1.94	0.98
2:B:27:VAL:HA	2:B:28:SER:HB2	0.99	0.98
1:E:154:THR:HG22	1:E:155:ARG:HB2	1.51	0.91

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	273/278 (98%)	244 (89%)	24 (9%)	5 (2%)	6	34
1	E	270/278 (97%)	241 (89%)	16 (6%)	13 (5%)	2	14
2	B	97/99 (98%)	85 (88%)	10 (10%)	2 (2%)	5	31
2	F	96/99 (97%)	87 (91%)	8 (8%)	1 (1%)	12	45
3	C	201/204 (98%)	187 (93%)	12 (6%)	2 (1%)	12	45
3	G	202/204 (99%)	184 (91%)	16 (8%)	2 (1%)	12	45
4	D	242/244 (99%)	218 (90%)	18 (7%)	6 (2%)	4	27
4	H	242/244 (99%)	217 (90%)	16 (7%)	9 (4%)	2	18
All	All	1623/1650 (98%)	1463 (90%)	120 (7%)	40 (2%)	4	27

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	7	ILE
2	B	28	SER
3	C	156	SER
3	C	194	ASN
4	D	52	VAL

5.3.2 Protein sidechains ⓘ

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	236/244 (97%)	210 (89%)	26 (11%)	6	26
1	E	235/244 (96%)	218 (93%)	17 (7%)	13	44
2	B	93/94 (99%)	83 (89%)	10 (11%)	6	27
2	F	91/94 (97%)	81 (89%)	10 (11%)	6	26
3	C	185/186 (100%)	168 (91%)	17 (9%)	8	33
3	G	186/186 (100%)	170 (91%)	16 (9%)	10	36
4	D	215/215 (100%)	195 (91%)	20 (9%)	8	33
4	H	215/215 (100%)	198 (92%)	17 (8%)	11	40
All	All	1456/1478 (98%)	1323 (91%)	133 (9%)	9	34

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	198	ILE
4	H	66	THR
4	H	208	ARG
3	C	152	GLN
3	C	131	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	150	GLN
3	G	191	ASN
1	E	163	ASN
3	G	5	GLN
4	H	25	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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	I	1	5	14,14,15	0.73	0	17,19,21	1.19	1 (5%)
5	BMA	I	2	5	11,11,12	0.61	0	15,15,17	0.84	0
6	NAG	J	1	1,6	14,14,15	0.51	0	17,19,21	0.81	0
6	NAG	J	2	6	14,14,15	0.61	0	17,19,21	1.14	2 (11%)

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	-	3/6/23/26	0/1/1/1
5	BMA	I	2	5	-	0/2/19/22	0/1/1/1
6	NAG	J	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	2	6	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1	NAG	C4-C3-C2	3.89	116.73	111.02
6	J	2	NAG	C4-C3-C2	2.90	115.26	111.02
6	J	2	NAG	C3-C4-C5	2.43	114.64	110.23

There are no chirality outliers.

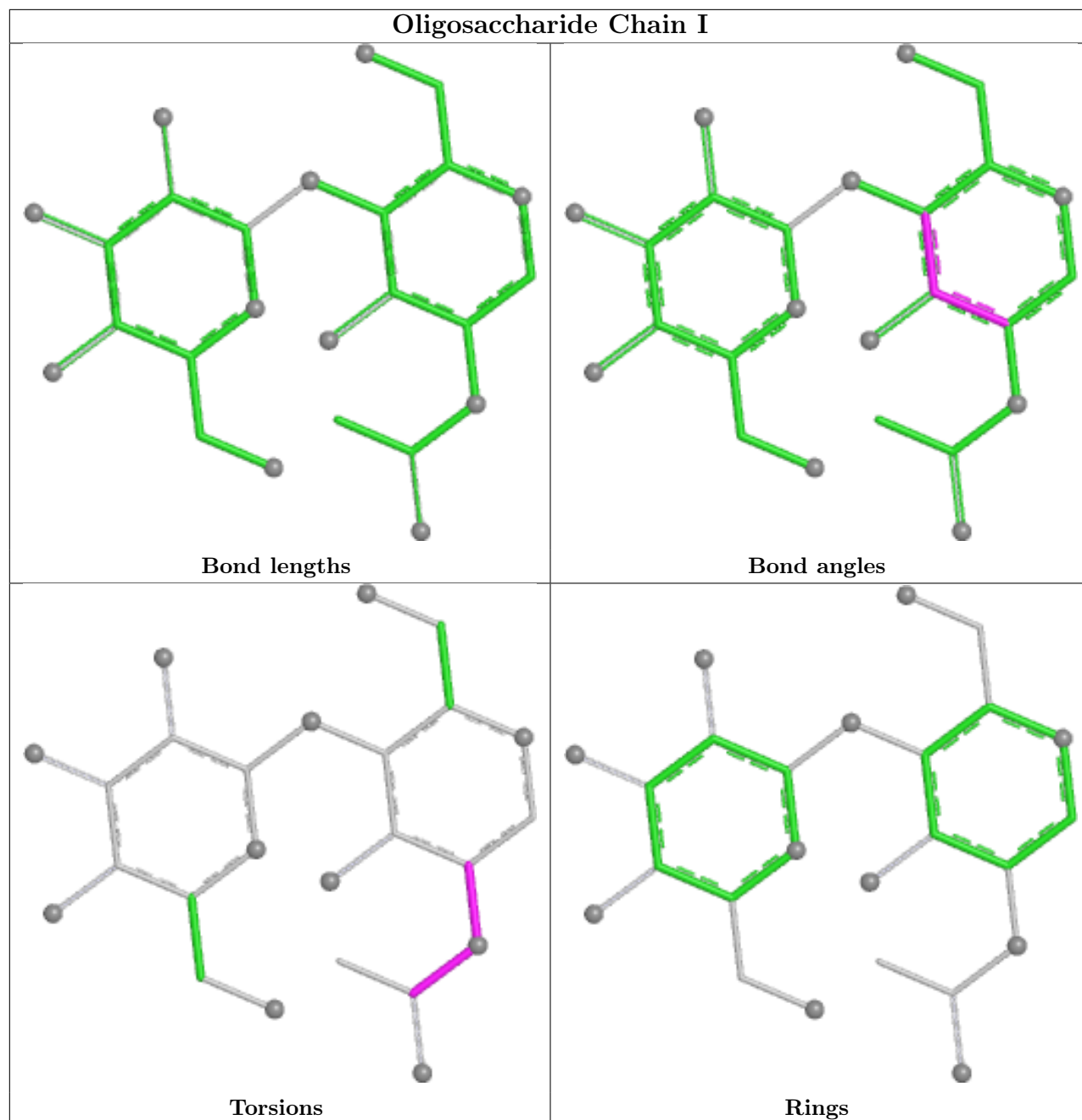
All (4) torsion outliers are listed below:

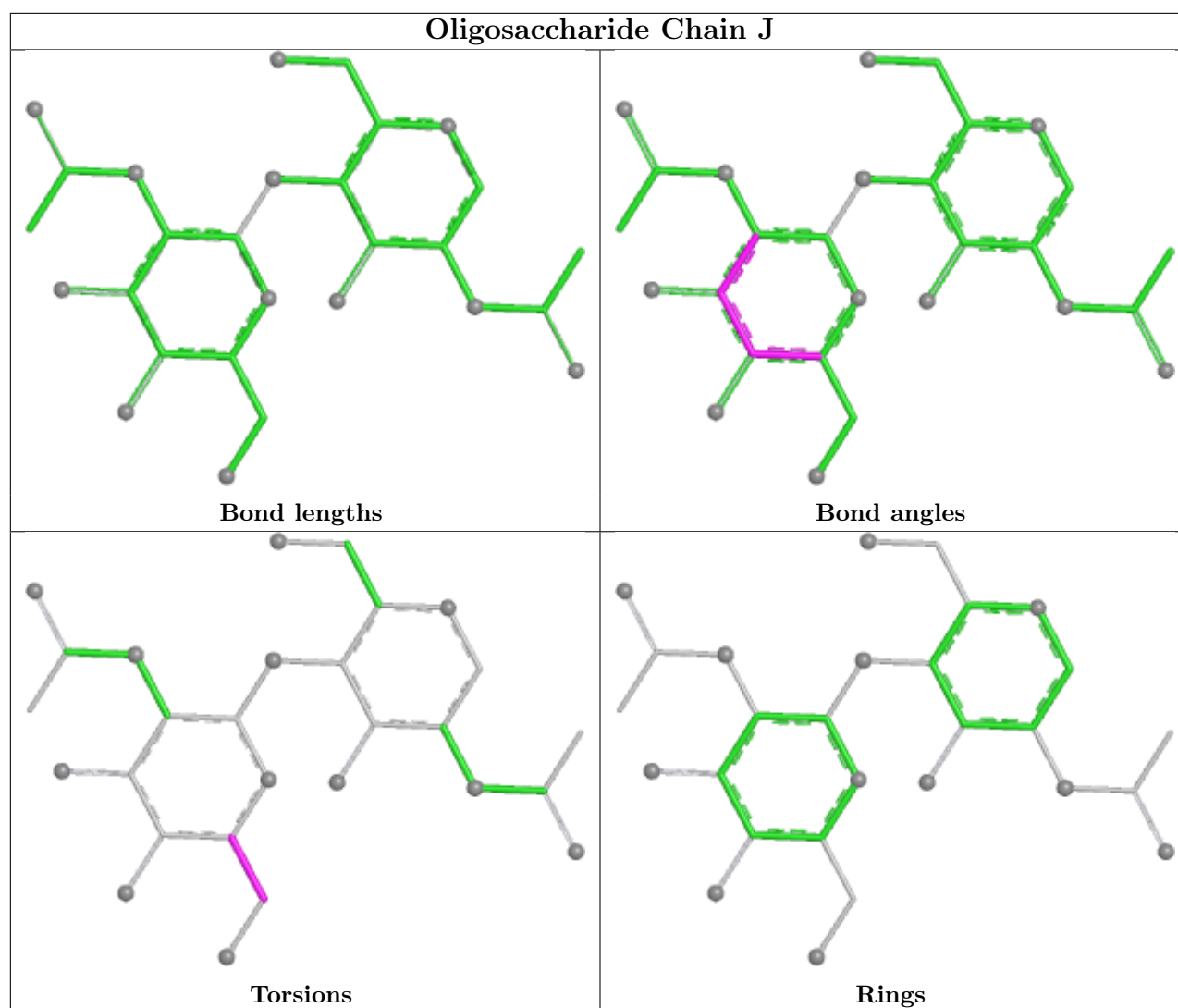
Mol	Chain	Res	Type	Atoms
5	I	1	NAG	O7-C7-N2-C2
5	I	1	NAG	C8-C7-N2-C2
6	J	2	NAG	O5-C5-C6-O6
5	I	1	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
7	NAG	E	301	-	14,14,15	0.45	0	17,19,21	1.33	1 (5%)
8	AGH	E	302	-	60,60,60	0.53	1 (1%)	66,69,69	0.90	3 (4%)
7	NAG	A	301	1	14,14,15	0.54	0	17,19,21	1.22	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	A	302	1	14,14,15	0.47	0	17,19,21	1.33	1 (5%)
8	AGH	C	301	-	60,60,60	0.41	0	66,69,69	0.76	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
7	NAG	E	301	-	-	3/6/23/26	0/1/1/1
8	AGH	E	302	-	-	25/58/78/78	0/1/1/1
7	NAG	A	301	1	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	A	302	1	-	2/6/23/26	0/1/1/1
8	AGH	C	301	-	-	28/58/78/78	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	302	AGH	O1A-C1A	2.75	1.44	1.40

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	302	NAG	C1-O5-C5	4.80	118.61	112.19
7	E	301	NAG	C1-O5-C5	4.39	118.08	112.19
7	A	301	NAG	C1-O5-C5	3.04	116.26	112.19
8	E	302	AGH	C1-C2-N2	-2.86	105.58	109.66
8	E	302	AGH	C5-C4-C3	2.13	117.34	113.97

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	301	NAG	C1

5 of 62 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	301	NAG	C8-C7-N2-C2
7	A	301	NAG	O7-C7-N2-C2
7	E	301	NAG	C8-C7-N2-C2

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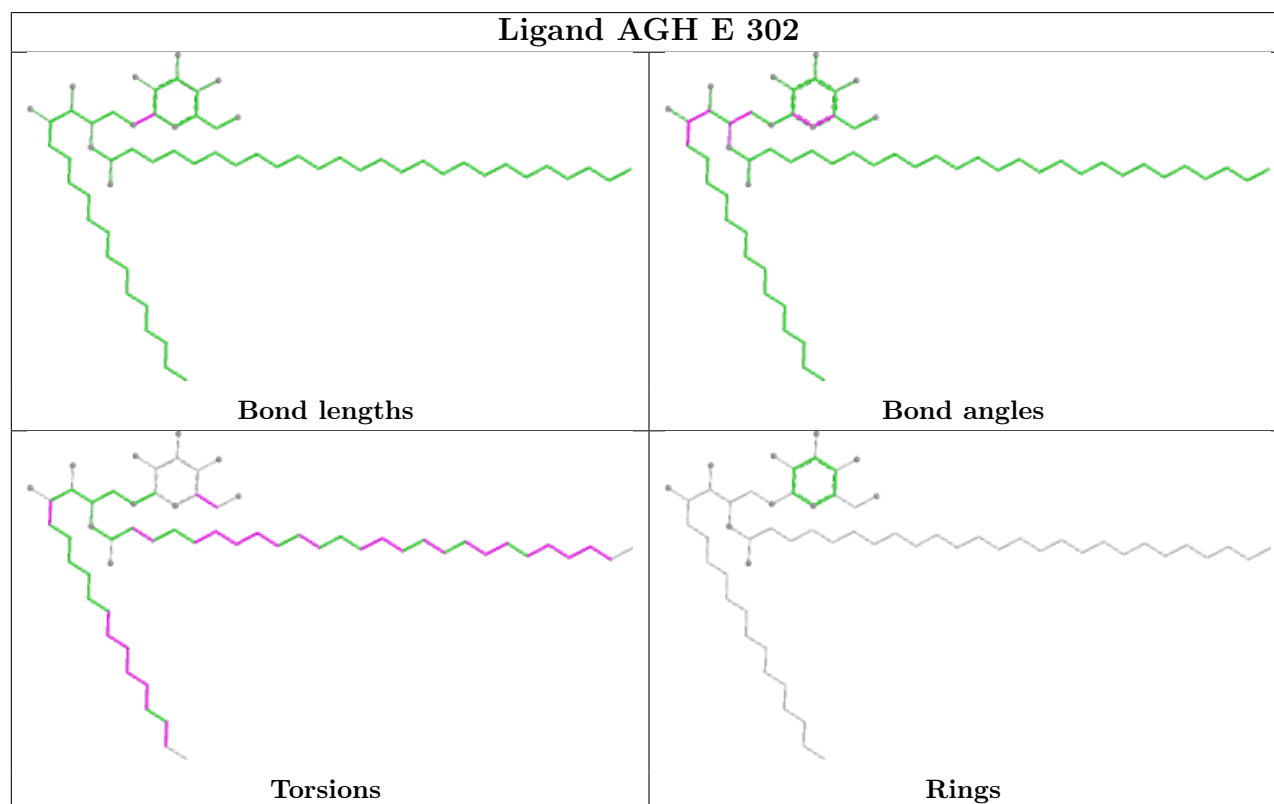
Mol	Chain	Res	Type	Atoms
7	E	301	NAG	O7-C7-N2-C2
8	C	301	AGH	N2-C2-C3-O3

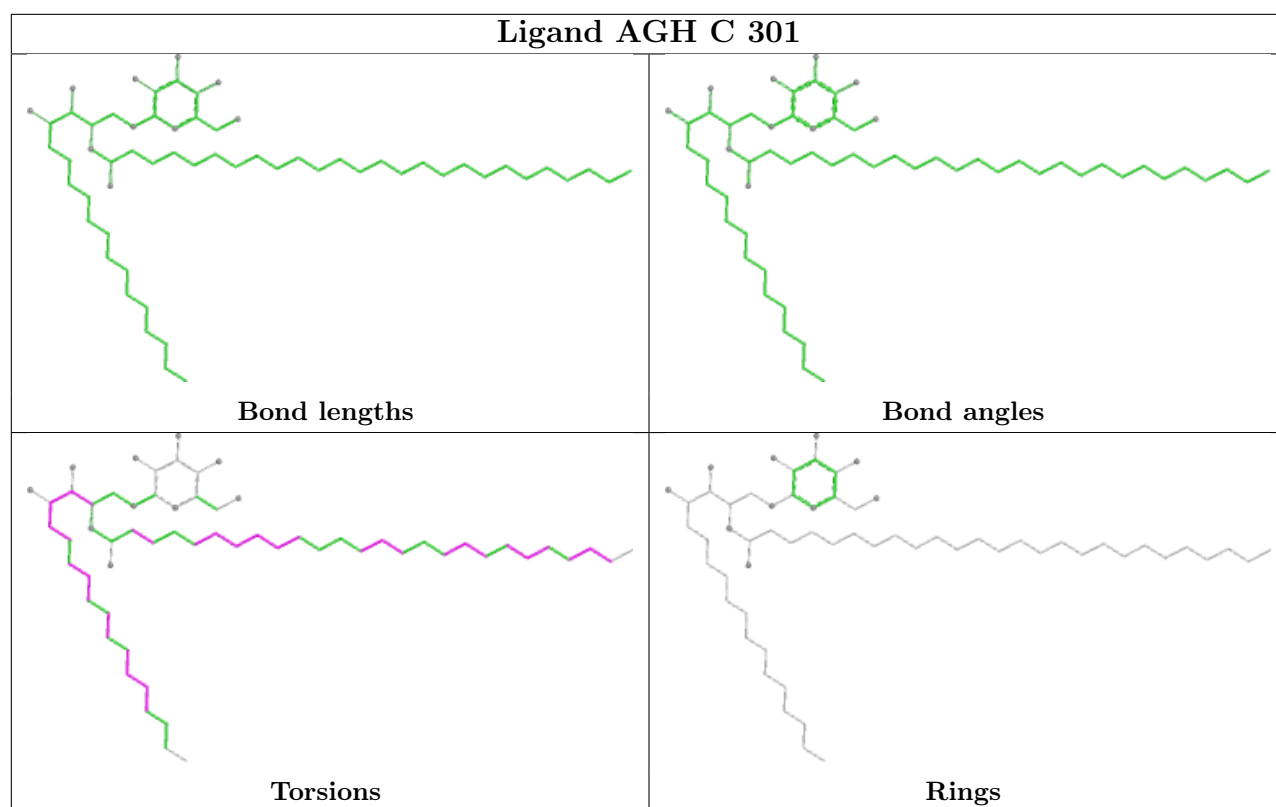
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	302	AGH	2	0
8	C	301	AGH	6	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 than 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.





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	275/278 (98%)	0.57	12 (4%) 39 24	52, 57, 61, 63	0
1	E	272/278 (97%)	0.74	14 (5%) 33 21	53, 58, 62, 65	0
2	B	99/99 (100%)	0.94	8 (8%) 18 11	53, 58, 60, 64	0
2	F	98/99 (98%)	0.63	2 (2%) 65 45	54, 58, 61, 62	0
3	C	203/204 (99%)	0.37	7 (3%) 48 30	52, 58, 61, 65	0
3	G	204/204 (100%)	0.43	9 (4%) 39 24	51, 58, 62, 64	0
4	D	244/244 (100%)	0.33	6 (2%) 58 39	54, 57, 62, 64	0
4	H	244/244 (100%)	0.28	8 (3%) 49 30	49, 57, 63, 66	0
All	All	1639/1650 (99%)	0.50	66 (4%) 42 26	49, 58, 62, 66	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	ILE	4.5
3	C	154	LYS	4.3
4	H	247	ASP	3.8
3	C	133	SER	3.4
1	A	226	GLU	3.3

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

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

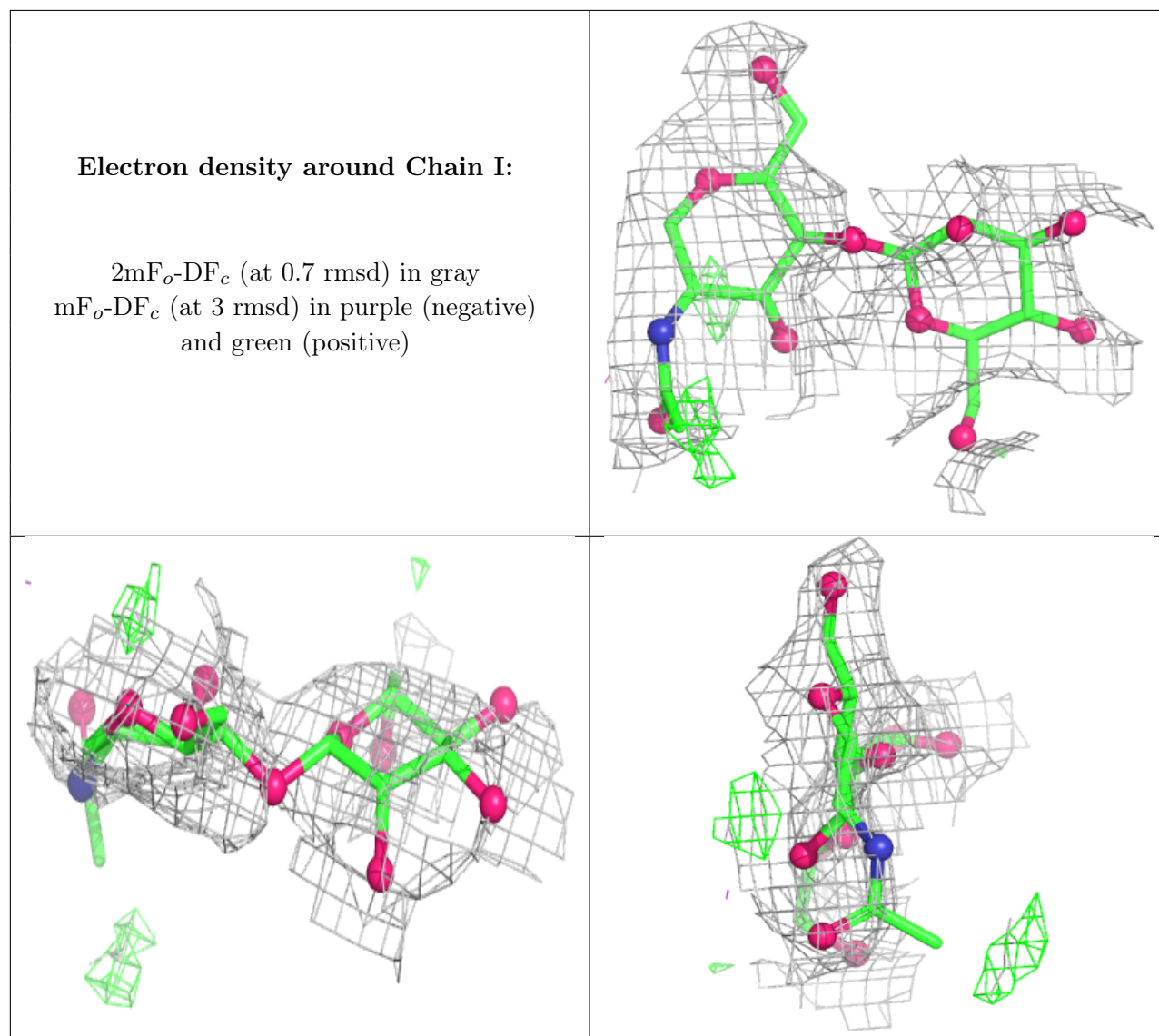
6.3 Carbohydrates [i](#)

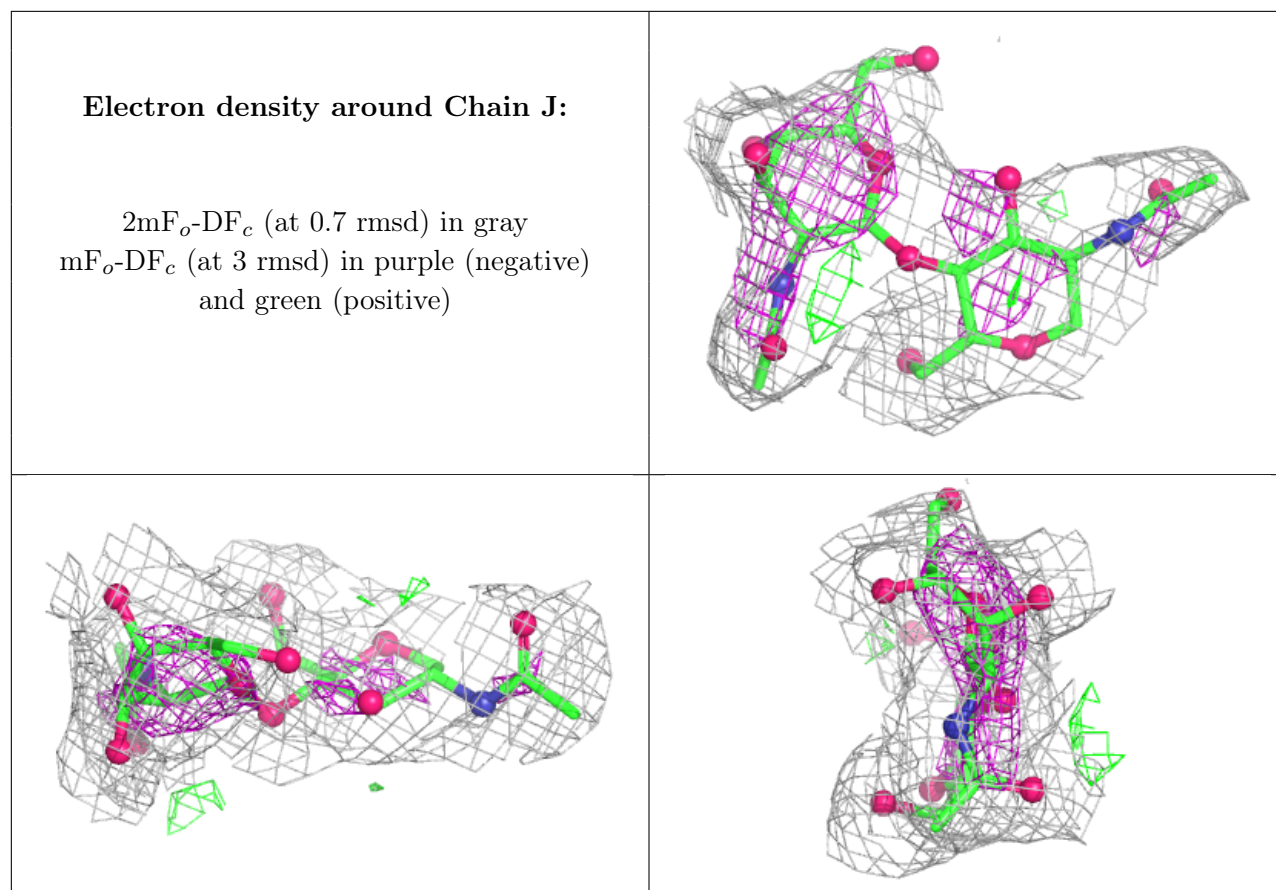
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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	BMA	I	2	11/12	0.35	0.16	156,156,156,156	0
5	NAG	I	1	14/15	0.38	0.21	154,155,156,156	0
6	NAG	J	2	14/15	0.50	0.16	82,83,83,83	0
6	NAG	J	1	14/15	0.63	0.14	73,76,78,80	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.





6.4 Ligands [i](#)

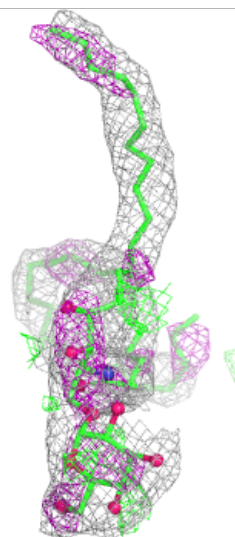
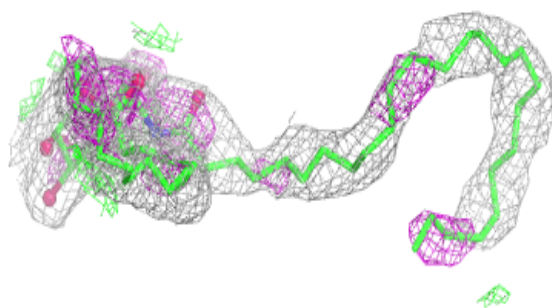
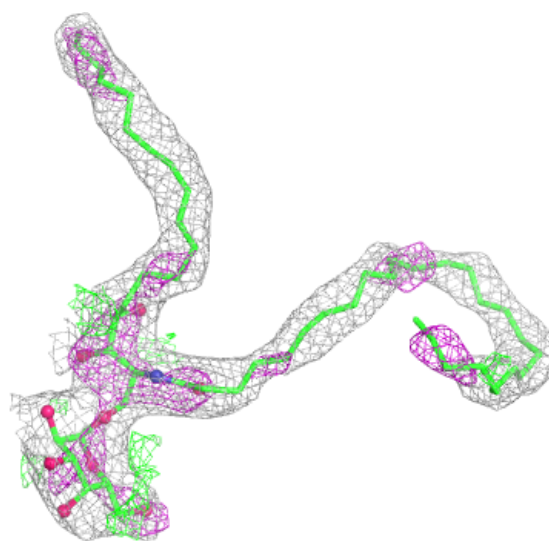
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	302	14/15	0.62	0.15	66,68,69,69	0
7	NAG	E	301	14/15	0.69	0.14	65,65,67,67	0
7	NAG	A	301	14/15	0.81	0.15	62,63,64,64	0
8	AGH	C	301	60/60	0.91	0.15	29,37,55,55	0
8	AGH	E	302	60/60	0.91	0.13	30,35,47,48	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.

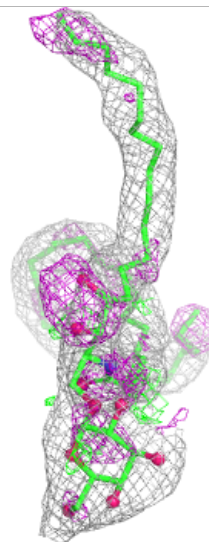
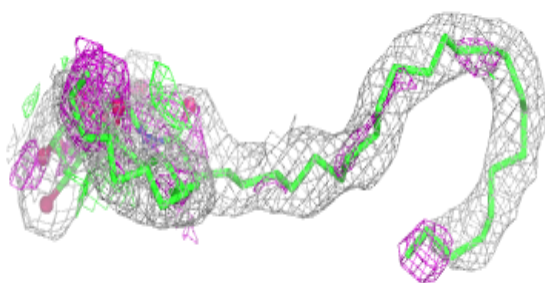
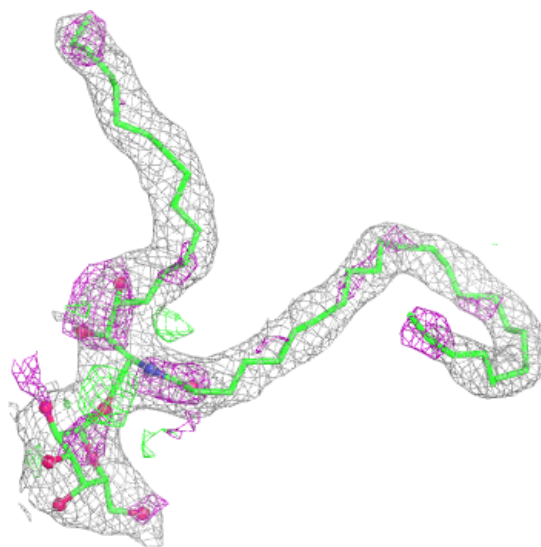
Electron density around AGH C 301:

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



Electron density around AGH E 302:

$2mF_o-DF_c$ (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.