



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 01:03 PM BST

PDB ID : 2PO6  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

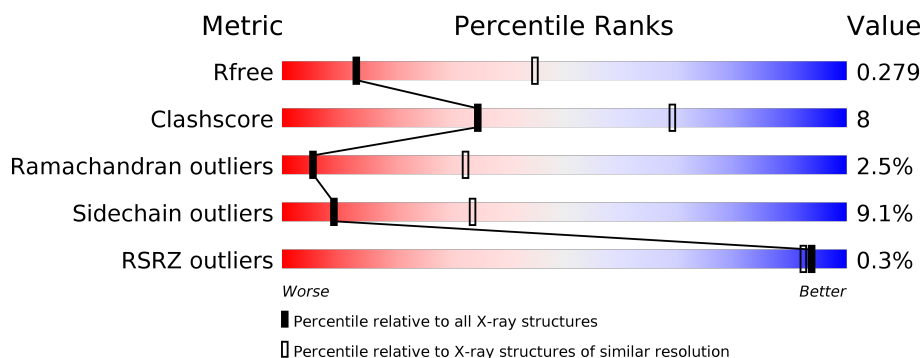
# 1 Overall quality at a glance

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.





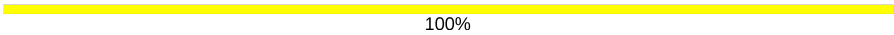

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
1	E	278	
2	B	99	
2	F	99	
3	C	204	
3	G	204	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
4	D	244	
4	H	244	
5	I	2	
6	J	2	

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	1000	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			

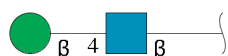
- Molecule 3 is a protein called NKT15 alpha-chain.

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.

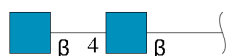
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	244	Total	C	N	O	S	0	0	0
			1957	1230	340	379	8			
4	H	244	Total	C	N	O	S	0	0	0
			1957	1230	340	379	8			

- 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.



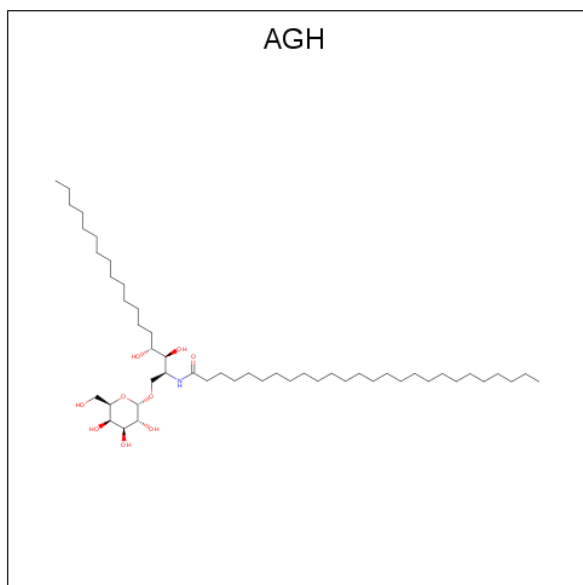
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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 (three-letter code: AGH) (formula: C<sub>50</sub>H<sub>99</sub>NO<sub>9</sub>).

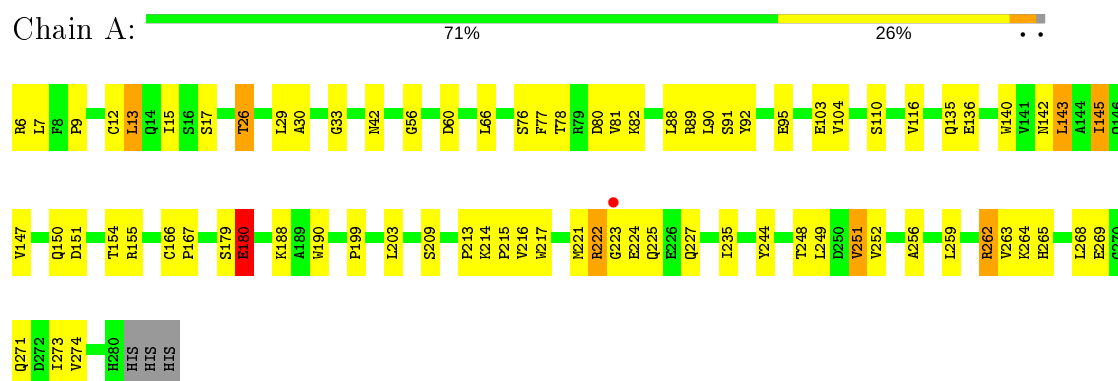


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			60	50	1	9		
8	E	1	Total	C	N	O	0	0
			60	50	1	9		

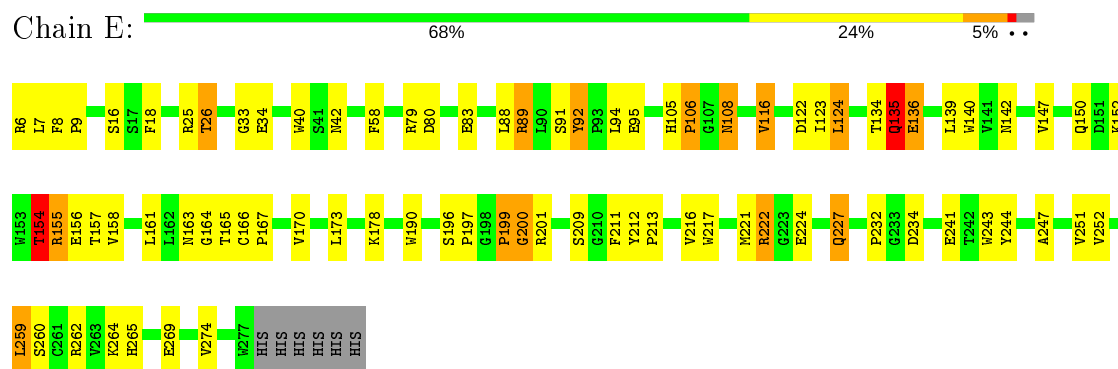
### 3 Residue-property plots

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.

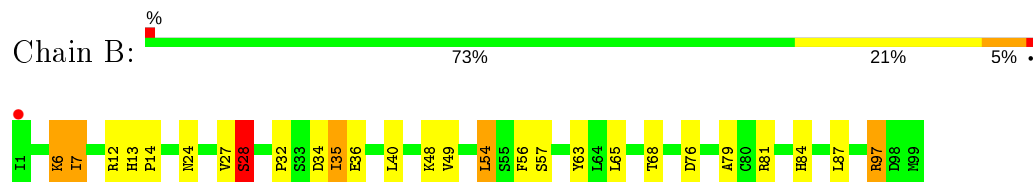
- Molecule 1: T-cell surface glycoprotein CD1d



- Molecule 1: T-cell surface glycoprotein CD1d



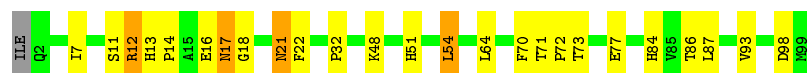
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin







- Molecule 3: NKT15 alpha-chain

Chain C: 81% 16% .



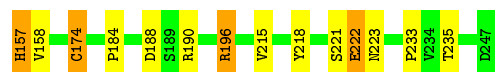
- Molecule 3: NKT15 alpha-chain

Chain G: 79% 17% .



- Molecule 4: NKT15 beta-chain

Chain D: 79% 18% .



- Molecule 4: NKT15 beta-chain

Chain H: 75% 20% .



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

Chain I: 100%

UAG1  
B/M2

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

Chain J:



UAG1  
UAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	204.01Å 155.64Å 85.98Å 90.00° 94.78° 90.00°	Depositor
Resolution (Å)	29.18 – 3.20 29.19 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.6 (29.18-3.20) 95.6 (29.19-3.20)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 3.18Å)	Xtriage
Refinement program	REFMAC refmac_5.2.0019	Depositor
R, $R_{free}$	0.226 , 0.293 0.217 , 0.279	Depositor DCC
$R_{free}$ test set	2135 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.6	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 41.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	13298	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: BMA, NAG, AGH

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	0.47	2/2257 (0.1%)	0.57	0/3076
1	E	0.37	0/2236	0.60	1/3048 (0.0%)
2	B	0.37	0/847	0.60	1/1148 (0.1%)
2	F	0.35	0/836	0.55	1/1134 (0.1%)
3	C	0.39	0/1612	0.56	1/2189 (0.0%)
3	G	0.38	0/1620	0.55	2/2201 (0.1%)
4	D	0.38	0/2011	0.54	0/2736
4	H	0.38	0/2011	0.58	0/2736
All	All	0.39	2/13430 (0.0%)	0.57	6/18268 (0.0%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	GLU	CD-OE1	9.77	1.36	1.25
1	A	180	GLU	CD-OE2	9.34	1.35	1.25

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	54	LEU	CA-CB-CG	6.29	129.77	115.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	54	LEU	CA-CB-CG	6.01	129.13	115.30
3	G	166	LEU	CA-CB-CG	5.51	127.98	115.30
1	E	154	THR	C-N-CA	5.32	134.99	121.70
3	G	32	LEU	CA-CB-CG	5.15	127.14	115.30

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 ⓘ

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	42	0
1	E	2171	0	2086	57	0
2	B	824	0	783	21	0
2	F	813	0	762	11	0
3	C	1581	0	1508	22	0
3	G	1588	0	1515	23	0
4	D	1957	0	1855	27	0
4	H	1957	0	1855	36	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	217	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 8.

The worst 5 of 217 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 [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	273/278 (98%)	244 (89%)	24 (9%)	5 (2%)	8	41
1	E	270/278 (97%)	241 (89%)	16 (6%)	13 (5%)	2	17
2	B	97/99 (98%)	85 (88%)	10 (10%)	2 (2%)	7	37
2	F	96/99 (97%)	87 (91%)	8 (8%)	1 (1%)	15	54
3	C	201/204 (98%)	187 (93%)	12 (6%)	2 (1%)	15	54
3	G	202/204 (99%)	184 (91%)	16 (8%)	2 (1%)	15	54
4	D	242/244 (99%)	218 (90%)	18 (7%)	6 (2%)	5	32
4	H	242/244 (99%)	217 (90%)	16 (7%)	9 (4%)	3	22
All	All	1623/1650 (98%)	1463 (90%)	120 (7%)	40 (2%)	5	32

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 [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	236/244 (97%)	211 (89%)	25 (11%)	6	27
1	E	235/244 (96%)	217 (92%)	18 (8%)	13	44
2	B	93/94 (99%)	81 (87%)	12 (13%)	4	19
2	F	91/94 (97%)	78 (86%)	13 (14%)	3	15
3	C	185/186 (100%)	169 (91%)	16 (9%)	10	38
3	G	186/186 (100%)	170 (91%)	16 (9%)	10	38
4	D	215/215 (100%)	198 (92%)	17 (8%)	12	43
4	H	215/215 (100%)	199 (93%)	16 (7%)	13	46
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
4	D	78	THR
1	E	92	TYR
4	H	98	ARG
4	D	98	ARG
4	D	190	ARG

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

Mol	Chain	Res	Type
4	D	86	HIS
1	E	55	GLN
4	H	183	GLN
4	D	106	GLN
4	D	236	GLN

### 5.3.3 RNA [i](#)

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	1.21	1 (5%)
5	BMA	I	2	5	11,11,12	0.63	0	15,15,17	1.00	2 (13%)
6	NAG	J	1	1,6	14,14,15	0.50	0	17,19,21	0.86	0
6	NAG	J	2	6	14,14,15	0.60	0	17,19,21	1.19	3 (17%)

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	-	4/6/23/26	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.

The worst 5 of 6 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	2.47	114.64	110.24
5	I	2	BMA	C1-C2-C3	2.33	112.53	109.67
5	I	2	BMA	O5-C5-C6	2.26	110.75	107.20



There are no chirality outliers.

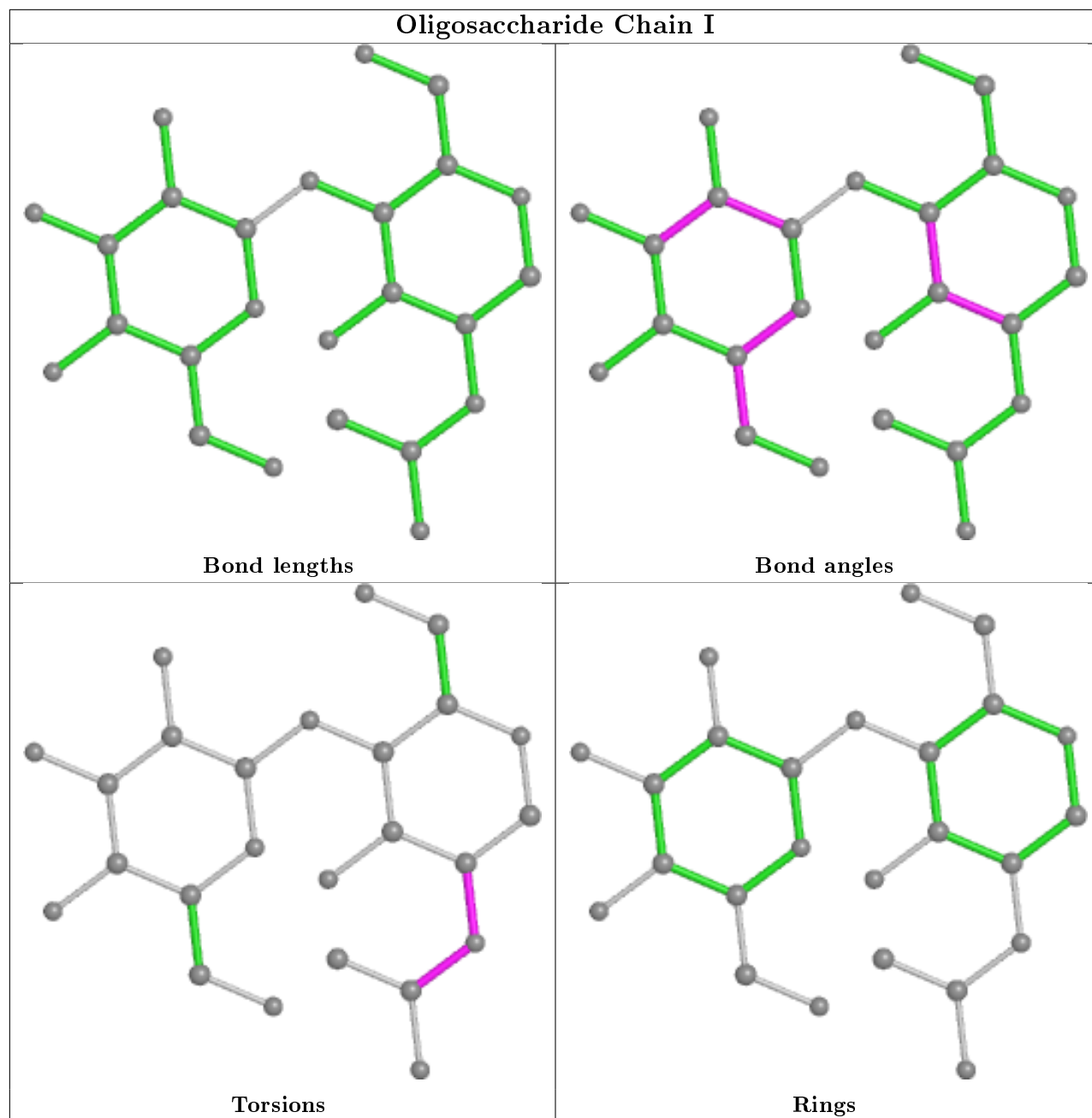
All (5) torsion outliers are listed below:

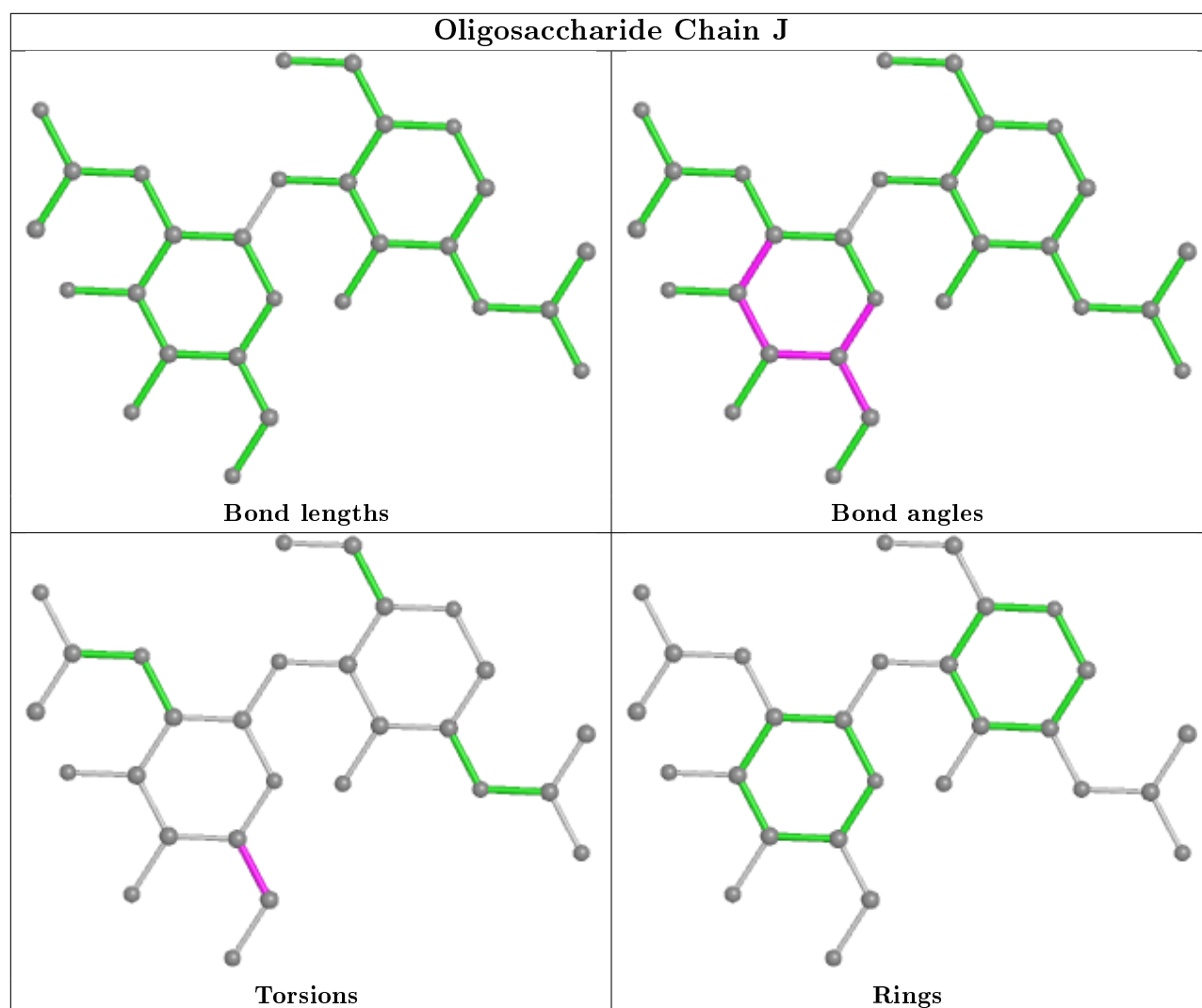
Mol	Chain	Res	Type	Atoms
5	I	1	NAG	O7-C7-N2-C2
5	I	1	NAG	C8-C7-N2-C2
5	I	1	NAG	C1-C2-N2-C7
6	J	2	NAG	O5-C5-C6-O6
5	I	1	NAG	C3-C2-N2-C7

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	$\# Z  > 2$
8	AGH	C	208	-	60,60,60	0.40	0	65,69,69	0.75	0
7	NAG	A	1000	1	14,14,15	0.54	0	17,19,21	1.19	1 (5%)
7	NAG	A	2000	1	14,14,15	0.46	0	17,19,21	1.35	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	AGH	E	2	-	60,60,60	0.52	1 (1%)	65,69,69	0.87	2 (3%)
7	NAG	E	4000	1	14,14,15	0.45	0	17,19,21	1.31	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
8	AGH	C	208	-	-	28/58/78/78	0/1/1/1
7	NAG	A	1000	1	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	A	2000	1	-	2/6/23/26	0/1/1/1
8	AGH	E	2	-	-	25/58/78/78	0/1/1/1
7	NAG	E	4000	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	2	AGH	O1A-C1A	2.69	1.44	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2000	NAG	C1-O5-C5	4.74	118.61	112.19
7	E	4000	NAG	C1-O5-C5	4.34	118.08	112.19
7	A	1000	NAG	C1-O5-C5	3.00	116.26	112.19
8	E	2	AGH	C1-C2-N2	-2.74	105.58	109.61
8	E	2	AGH	C1A-O6A-C5M	2.02	117.65	113.69

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	1000	NAG	C1

5 of 62 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	208	AGH	N2-C2-C3-O3
8	C	208	AGH	O3-C3-C4-C5
8	C	208	AGH	O4-C4-C5-C6

*Continued on next page...*

*Continued from previous page...*

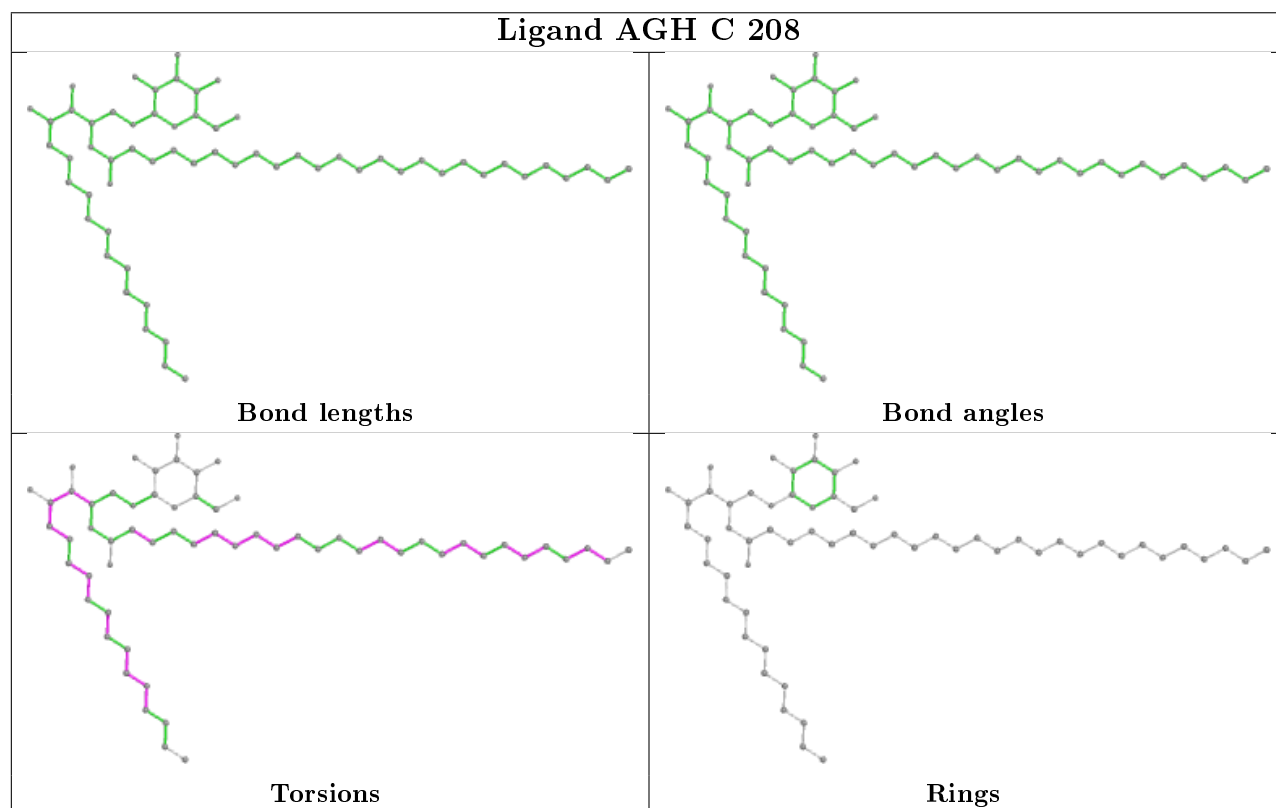
Mol	Chain	Res	Type	Atoms
7	A	1000	NAG	C8-C7-N2-C2
7	A	1000	NAG	O7-C7-N2-C2

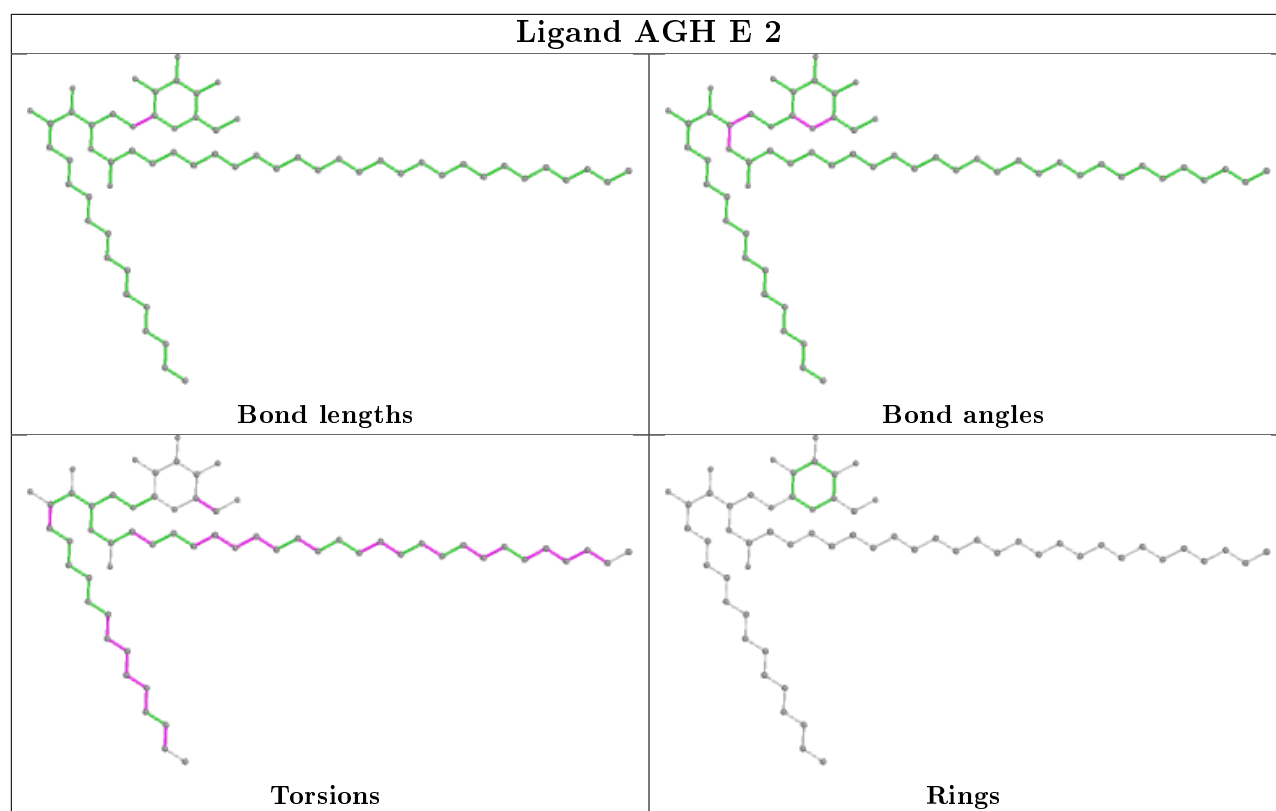
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	208	AGH	6	0
8	E	2	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	275/278 (98%)	-0.19	1 (0%) 92 89	52, 57, 61, 63	0
1	E	272/278 (97%)	-0.27	0 100 100	53, 58, 62, 65	0
2	B	99/99 (100%)	-0.13	1 (1%) 82 72	53, 58, 60, 64	0
2	F	98/99 (98%)	-0.23	0 100 100	54, 58, 61, 62	0
3	C	203/204 (99%)	-0.23	1 (0%) 91 86	52, 58, 61, 65	0
3	G	204/204 (100%)	-0.31	1 (0%) 91 86	51, 58, 62, 64	0
4	D	244/244 (100%)	-0.31	0 100 100	54, 57, 62, 64	0
4	H	244/244 (100%)	-0.30	1 (0%) 92 89	49, 57, 63, 66	0
All	All	1639/1650 (99%)	-0.25	5 (0%) 94 92	49, 58, 62, 66	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	ILE	3.0
3	C	154	LYS	2.7
3	G	135	ASP	2.7
1	A	223	GLY	2.4
4	H	222	GLU	2.4

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

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

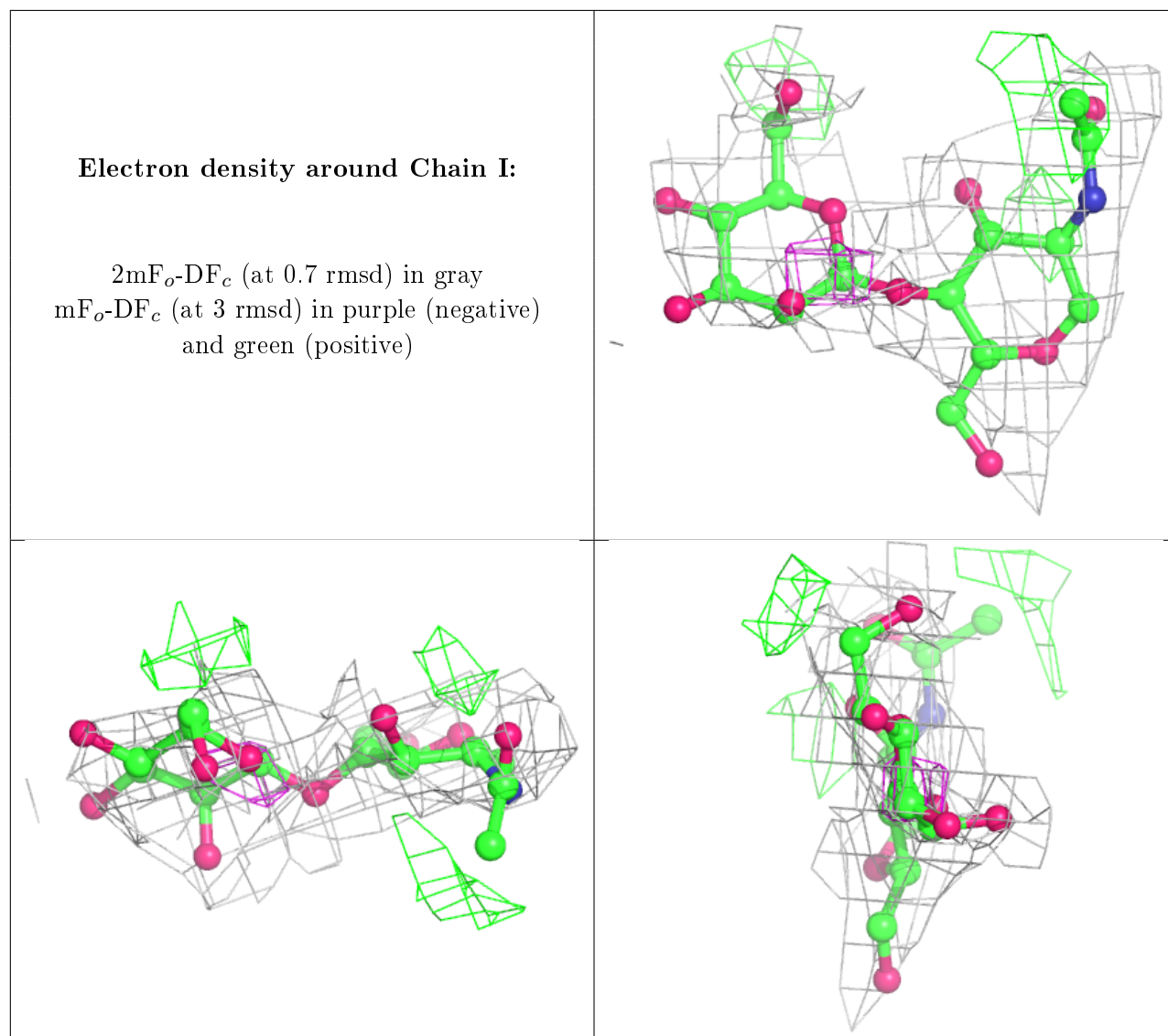
### 6.3 Carbohydrates [i](#)

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

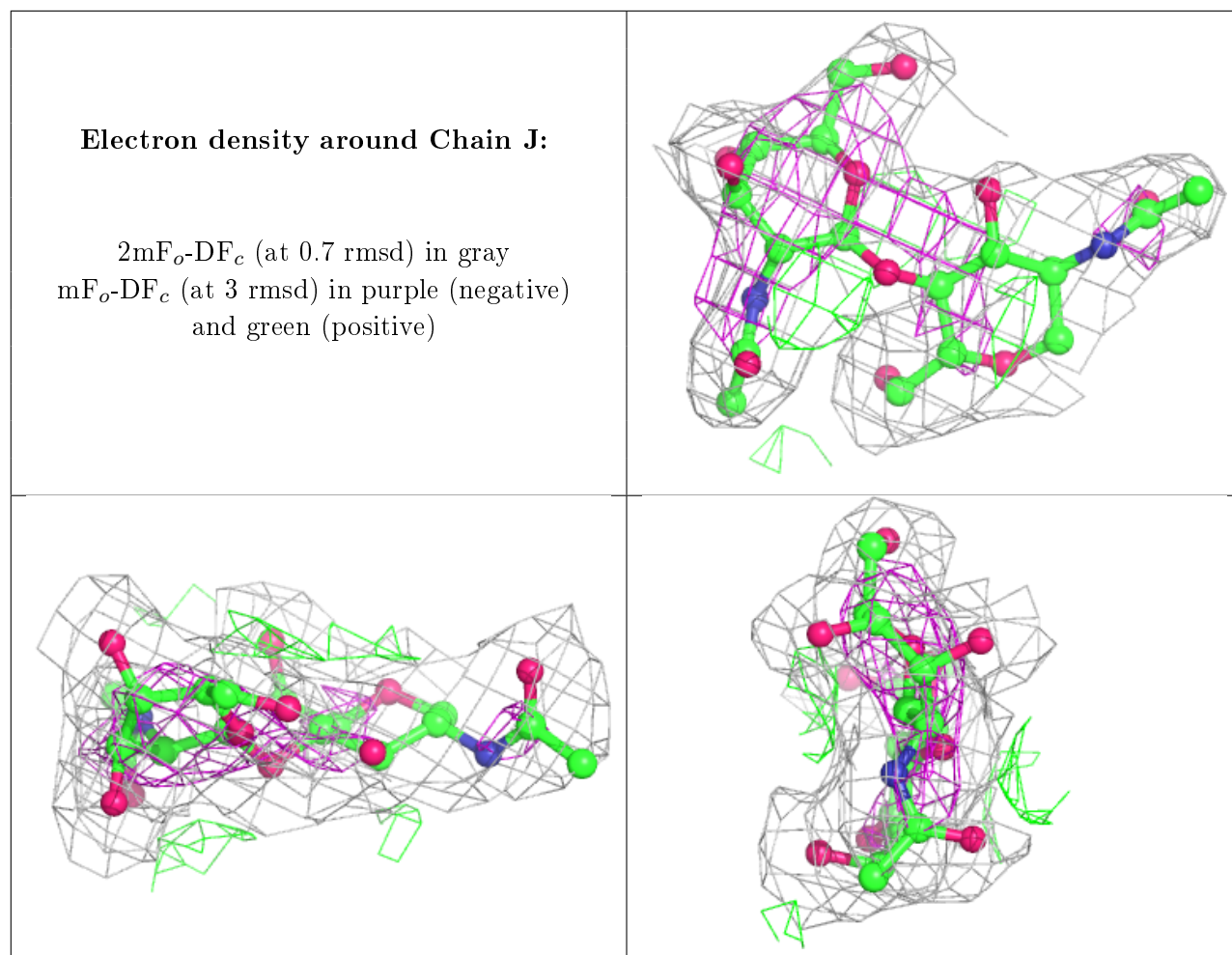
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	BMA	I	2	11/12	0.52	0.37	156,156,156,156	0
5	NAG	I	1	14/15	0.56	0.33	154,155,156,156	0
6	NAG	J	2	14/15	0.86	0.26	82,83,83,83	0
6	NAG	J	1	14/15	0.95	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](#)

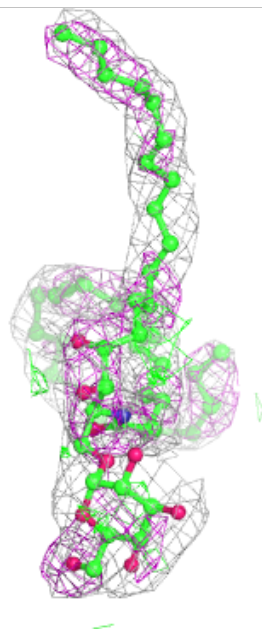
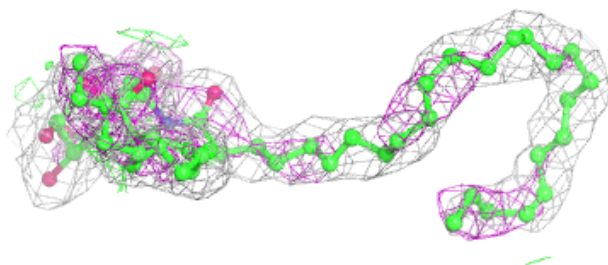
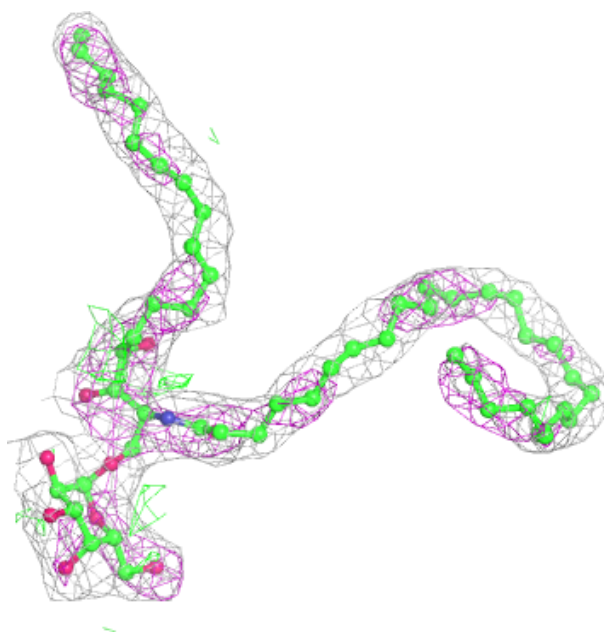
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

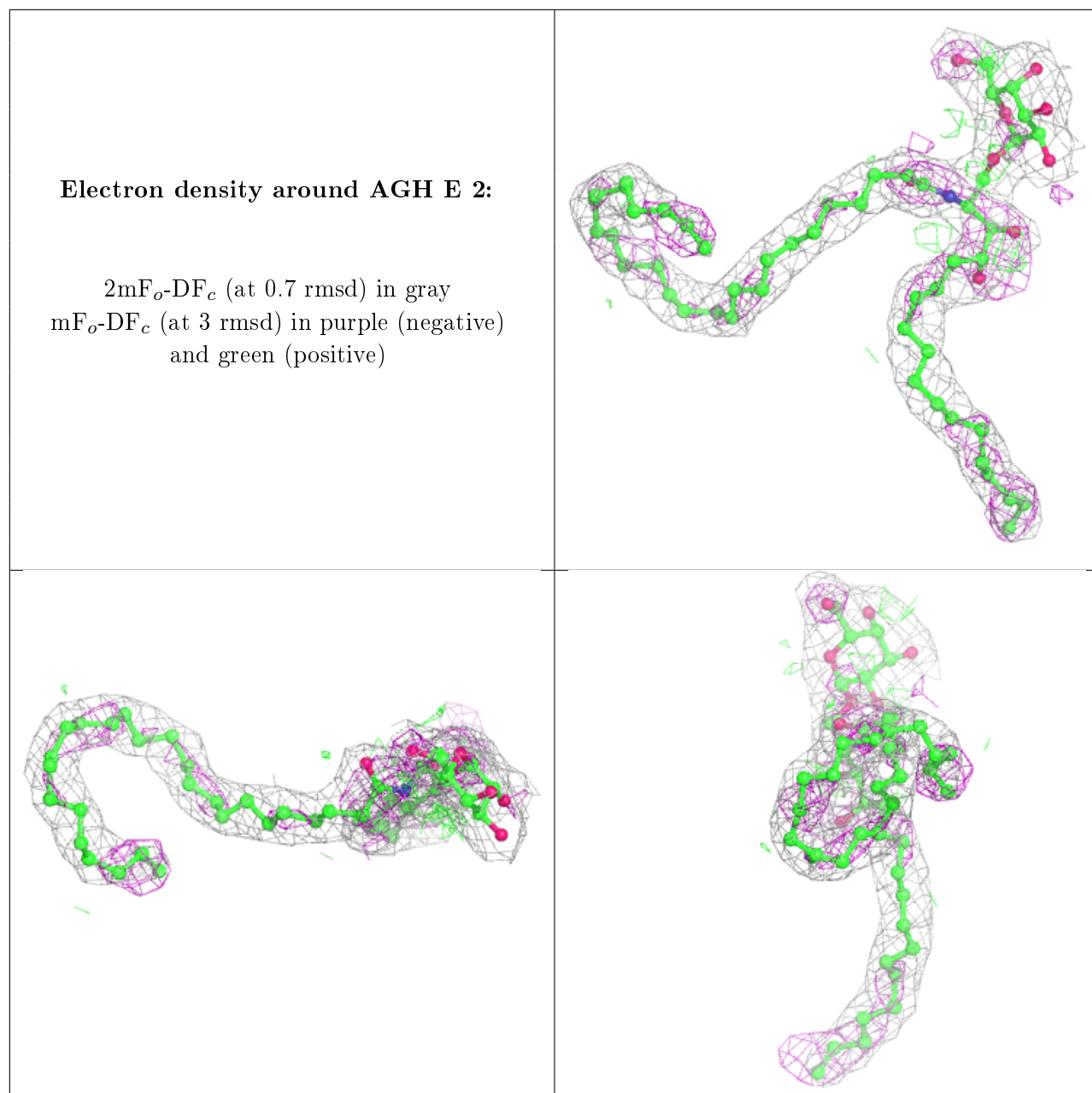
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NAG	A	2000	14/15	0.91	0.17	66,68,69,69	0
7	NAG	E	4000	14/15	0.92	0.19	65,65,67,67	0
7	NAG	A	1000	14/15	0.94	0.14	62,63,64,64	0
8	AGH	C	208	60/60	0.96	0.28	29,37,55,55	0
8	AGH	E	2	60/60	0.97	0.26	30,35,47,48	0

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 208:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.