



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2022 – 02:24 PM EDT

PDB ID : 7TD8
Title : Integrin α IIb β 3 complex with Tirofiban
Authors : Zhu, J.; Lin, F.-Y.; Zhu, J.; Springer, T.A.
Deposited on : 2021-12-30
Resolution : 2.60 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
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)	:	2.29

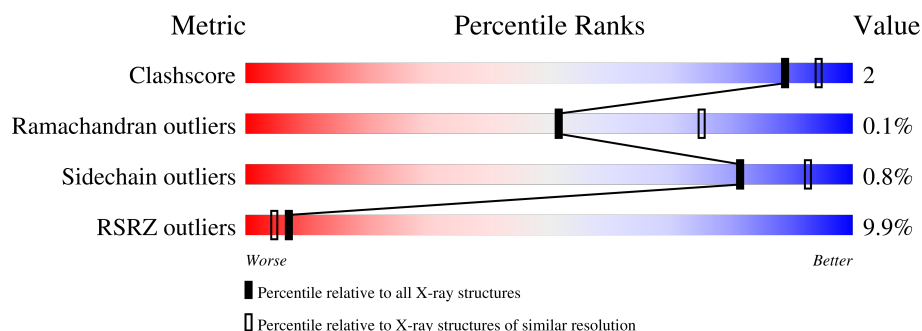
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	453	<div> <div></div> <div>94%6%</div> </div>
1	C	453	<div> <div></div> <div>93%7%</div> </div>
2	B	471	<div> <div>10%</div> <div>92%7%</div> </div>
2	D	471	<div> <div>8%</div> <div>94%5%</div> </div>
3	E	216	<div> <div>38%</div> <div>94%6%</div> </div>
3	H	216	<div> <div>7%</div> <div>98%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	214	
4	L	214	
5	G	5	
6	I	2	
6	K	2	
7	J	4	

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
10	SO4	A	506	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 21949 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 Integrin alpha-IIb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	6	0
			3511	2232	607	664	8			
1	C	453	Total	C	N	O	S	0	4	0
			3502	2224	604	666	8			

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	466	Total	C	N	O	S	4	7	0
			3638	2265	621	718	34			
2	D	471	Total	C	N	O	S	4	4	0
			3647	2272	623	717	35			

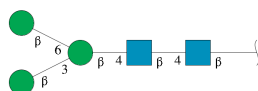
- Molecule 3 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	214	Total	C	N	O	S	0	0	0
			1631	1035	264	326	6			
3	H	216	Total	C	N	O	S	0	0	0
			1642	1041	266	329	6			

- Molecule 4 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	214	Total	C	N	O	S	0	0	0
			1637	1019	268	341	9			
4	L	214	Total	C	N	O	S	0	0	0
			1637	1019	268	341	9			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

- 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	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	J	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	4	Total	Ca	0	0
			4	4		
8	B	2	Total	Ca	0	0
			2	2		
8	C	4	Total	Ca	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Ca	0	0
			2	2		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	1	Total	Mg	0	0
			1	1		
11	D	1	Total	Mg	0	0
			1	1		

- Molecule 12 is TIROFIBAN (three-letter code: AGG) (formula: C₂₂H₃₆N₂O₅S) (labeled as "Ligand of Interest" by depositor).



- Molecule 13 is water.



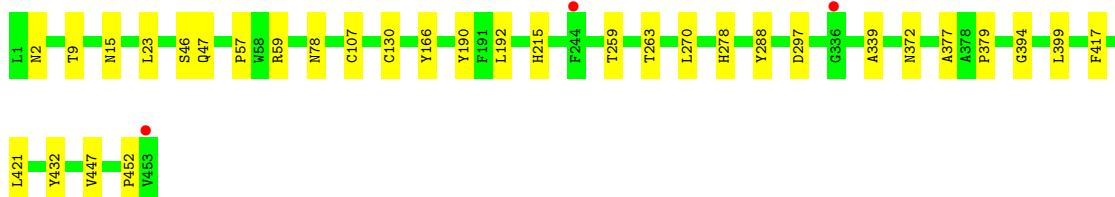
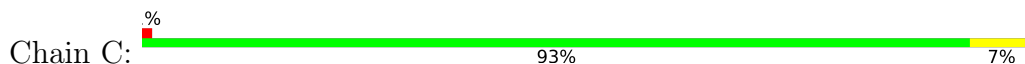
3 Residue-property plots [i](#)

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.

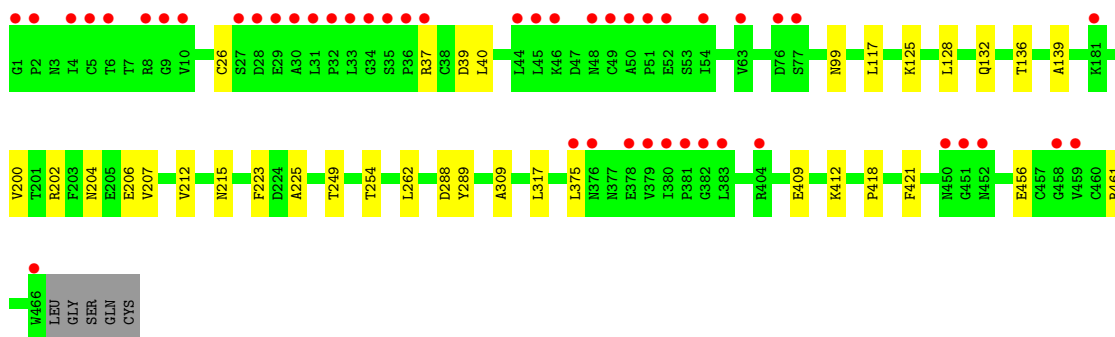
- Molecule 1: Integrin alpha-IIb



- Molecule 1: Integrin alpha-IIb

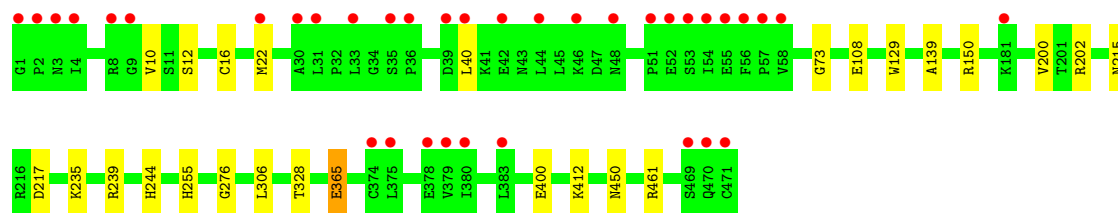


- Molecule 2: Integrin beta-3

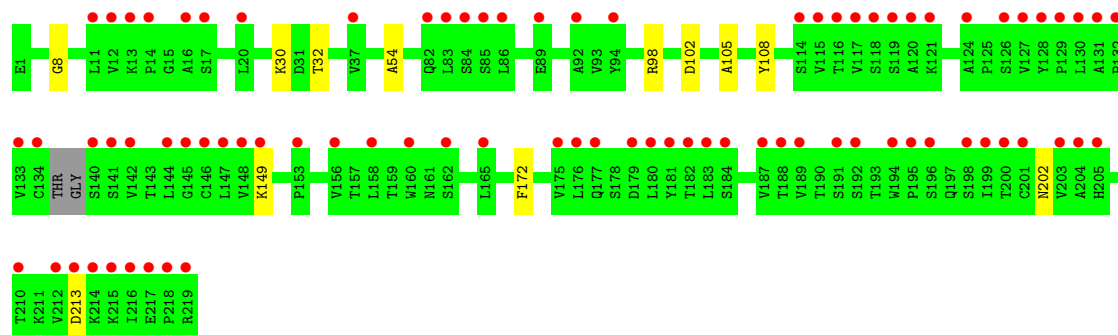
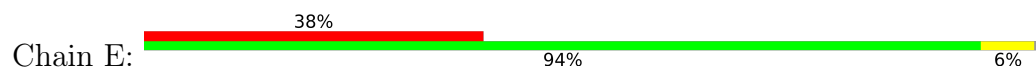


- Molecule 2: Integrin beta-3

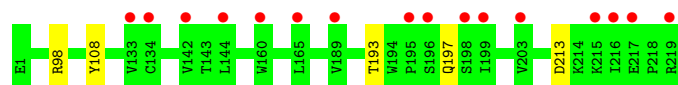




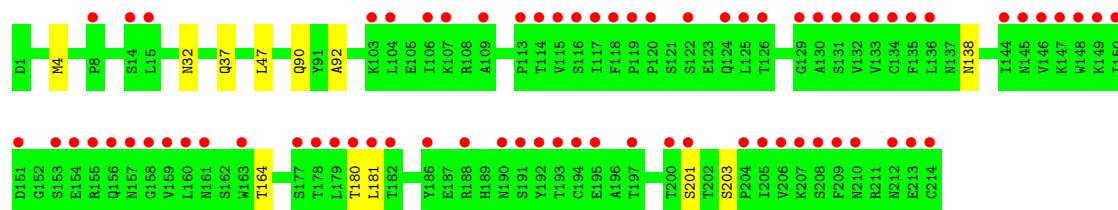
• Molecule 3: Fab heavy chain



• Molecule 3: Fab heavy chain



• Molecule 4: Fab light chain



• Molecule 4: Fab light chain



• Molecule 5: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  40% 20% 40%

BAG1
BAG2
BMA3
BMA4
BMA5

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

Chain I:  100%

BAG1
BAG2

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

Chain K:  50% 50%

BAG1
BAG2

- Molecule 7: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%

BAG1
BAG2
BMA3
BMA4

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	256.56Å 144.37Å 104.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.31 – 2.60 48.35 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.31-2.60) 99.9 (48.35-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.181 , 0.210 0.181 , (Not available)	Depositor DCC
R_{free} test set	1000 reflections (0.84%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.1	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	0.96	EDS
Total number of atoms	21949	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, SO4, CA, AGG, MG, 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	0.26	0/3623	0.53	0/4936
1	C	0.26	0/3605	0.52	0/4912
2	B	0.25	0/3714	0.48	0/5036
2	D	0.24	0/3723	0.48	0/5046
3	E	0.24	0/1673	0.46	0/2290
3	H	0.24	0/1684	0.46	0/2305
4	F	0.24	0/1673	0.46	0/2269
4	L	0.24	0/1673	0.47	0/2269
All	All	0.25	0/21368	0.49	0/29063

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	3511	0	3360	11	0
1	C	3502	0	3334	16	0
2	B	3638	0	3556	18	0
2	D	3647	0	3577	14	0
3	E	1631	0	1590	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1642	0	1600	2	0
4	F	1637	0	1553	7	0
4	L	1637	0	1553	3	0
5	G	61	0	52	1	0
6	I	28	0	25	0	0
6	K	28	0	25	1	0
7	J	50	0	43	0	0
8	A	4	0	0	0	0
8	B	2	0	0	0	0
8	C	4	0	0	0	0
8	D	2	0	0	0	0
9	A	14	0	13	0	0
9	B	14	0	13	1	0
9	D	14	0	13	0	0
10	A	25	0	0	3	0
10	C	15	0	0	0	0
11	B	1	0	0	0	0
11	D	1	0	0	0	0
12	B	30	0	35	0	0
12	D	30	0	35	1	0
13	A	314	0	0	4	0
13	B	132	0	0	1	0
13	C	167	0	0	2	0
13	D	105	0	0	2	0
13	E	7	0	0	1	0
13	F	10	0	0	0	0
13	H	17	0	0	0	0
13	L	29	0	0	0	0
All	All	21949	0	20377	79	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 2.

The worst 5 of 79 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:E:8:GLY:O	13:E:301:HOH:O	2.13	0.67
1:A:90[A]:ARG:NH2	13:A:604:HOH:O	2.28	0.65
10:A:506:SO4:O2	13:A:601:HOH:O	2.14	0.64
2:D:365:GLU:OE2	2:D:412:LYS:NZ	2.30	0.64
2:D:129:TRP:NE1	13:D:2103:HOH:O	2.32	0.60

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	457/453 (101%)	444 (97%)	12 (3%)	1 (0%)	47	71
1	C	455/453 (100%)	439 (96%)	16 (4%)	0	100	100
2	B	471/471 (100%)	449 (95%)	21 (4%)	1 (0%)	47	71
2	D	473/471 (100%)	455 (96%)	18 (4%)	0	100	100
3	E	210/216 (97%)	196 (93%)	14 (7%)	0	100	100
3	H	212/216 (98%)	205 (97%)	7 (3%)	0	100	100
4	F	212/214 (99%)	200 (94%)	11 (5%)	1 (0%)	29	52
4	L	212/214 (99%)	205 (97%)	6 (3%)	1 (0%)	29	52
All	All	2702/2708 (100%)	2593 (96%)	105 (4%)	4 (0%)	51	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	B	375	LEU
4	F	138	ASN
4	L	77	SER

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	367/361 (102%)	361 (98%)	6 (2%)	62	82
1	C	365/361 (101%)	359 (98%)	6 (2%)	62	82
2	B	419/416 (101%)	417 (100%)	2 (0%)	88	96
2	D	420/416 (101%)	417 (99%)	3 (1%)	84	94
3	E	186/187 (100%)	186 (100%)	0	100	100
3	H	187/187 (100%)	186 (100%)	1 (0%)	88	96
4	F	188/188 (100%)	187 (100%)	1 (0%)	88	96
4	L	188/188 (100%)	188 (100%)	0	100	100
All	All	2320/2304 (101%)	2301 (99%)	19 (1%)	81	92

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	202	ARG
4	F	181	LEU
3	H	213	ASP
2	D	365	GLU
1	C	15	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	333	GLN
2	D	450	ASN

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 ⓘ

13 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	G	1	2,5	14,14,15	0.39	0	17,19,21	0.67	0
5	NAG	G	2	5	14,14,15	0.40	0	17,19,21	0.58	0
5	BMA	G	3	5	11,11,12	1.73	3 (27%)	15,15,17	2.57	5 (33%)
5	BMA	G	4	5	11,11,12	1.12	1 (9%)	15,15,17	1.19	2 (13%)
5	BMA	G	5	5	11,11,12	1.52	2 (18%)	15,15,17	1.74	3 (20%)
6	NAG	I	1	2,6	14,14,15	0.68	0	17,19,21	0.57	0
6	NAG	I	2	6	14,14,15	0.17	0	17,19,21	0.38	0
7	NAG	J	1	2,7	14,14,15	0.38	0	17,19,21	0.50	0
7	NAG	J	2	7	14,14,15	0.45	0	17,19,21	0.47	0
7	BMA	J	3	7	11,11,12	0.96	1 (9%)	15,15,17	2.11	3 (20%)
7	BMA	J	4	7	11,11,12	1.29	2 (18%)	15,15,17	1.53	3 (20%)
6	NAG	K	1	2,6	14,14,15	0.49	0	17,19,21	0.55	0
6	NAG	K	2	6	14,14,15	0.30	0	17,19,21	0.43	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	G	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	2/2/19/22	0/1/1/1
5	BMA	G	4	5	-	0/2/19/22	0/1/1/1
5	BMA	G	5	5	-	2/2/19/22	0/1/1/1
6	NAG	I	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	4/6/23/26	0/1/1/1
7	NAG	J	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	0/6/23/26	0/1/1/1
7	BMA	J	3	7	-	2/2/19/22	0/1/1/1
7	BMA	J	4	7	-	0/2/19/22	0/1/1/1
6	NAG	K	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	5	BMA	C1-C2	3.51	1.60	1.52
5	G	3	BMA	C2-C3	2.92	1.56	1.52
5	G	3	BMA	O5-C1	2.91	1.48	1.43
5	G	4	BMA	O5-C5	-2.62	1.38	1.43
5	G	3	BMA	O5-C5	2.49	1.48	1.43

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	3	BMA	O5-C5-C6	5.71	116.16	107.20
7	J	3	BMA	C1-C2-C3	-5.66	102.71	109.67
5	G	3	BMA	O3-C3-C2	5.51	120.55	109.99
7	J	3	BMA	O3-C3-C2	5.20	119.95	109.99
5	G	3	BMA	C1-C2-C3	-4.27	104.42	109.67

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

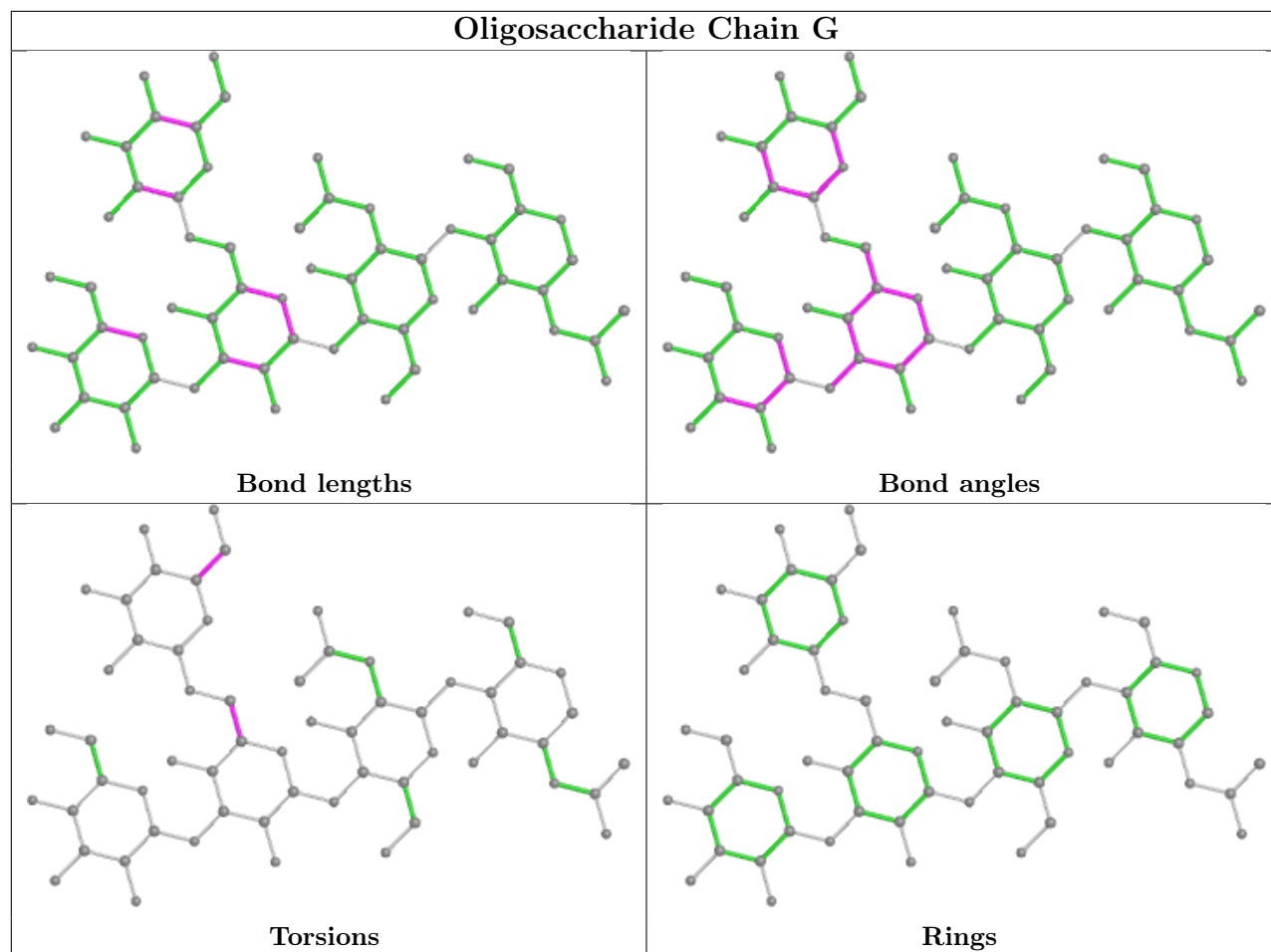
Mol	Chain	Res	Type	Atoms
5	G	3	BMA	O5-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
5	G	3	BMA	C4-C5-C6-O6
5	G	5	BMA	O5-C5-C6-O6

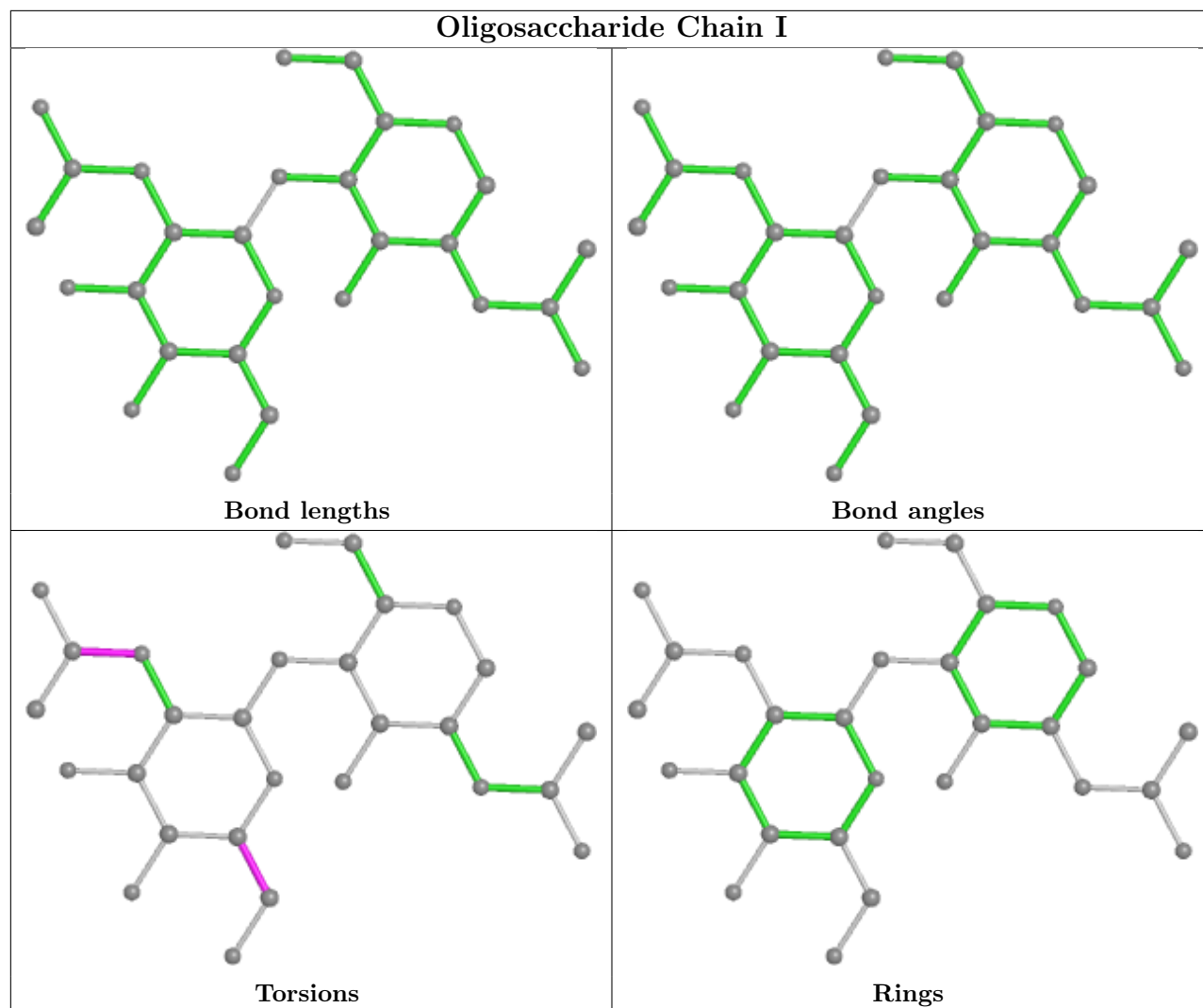
There are no ring outliers.

3 monomers are involved in 2 short contacts:

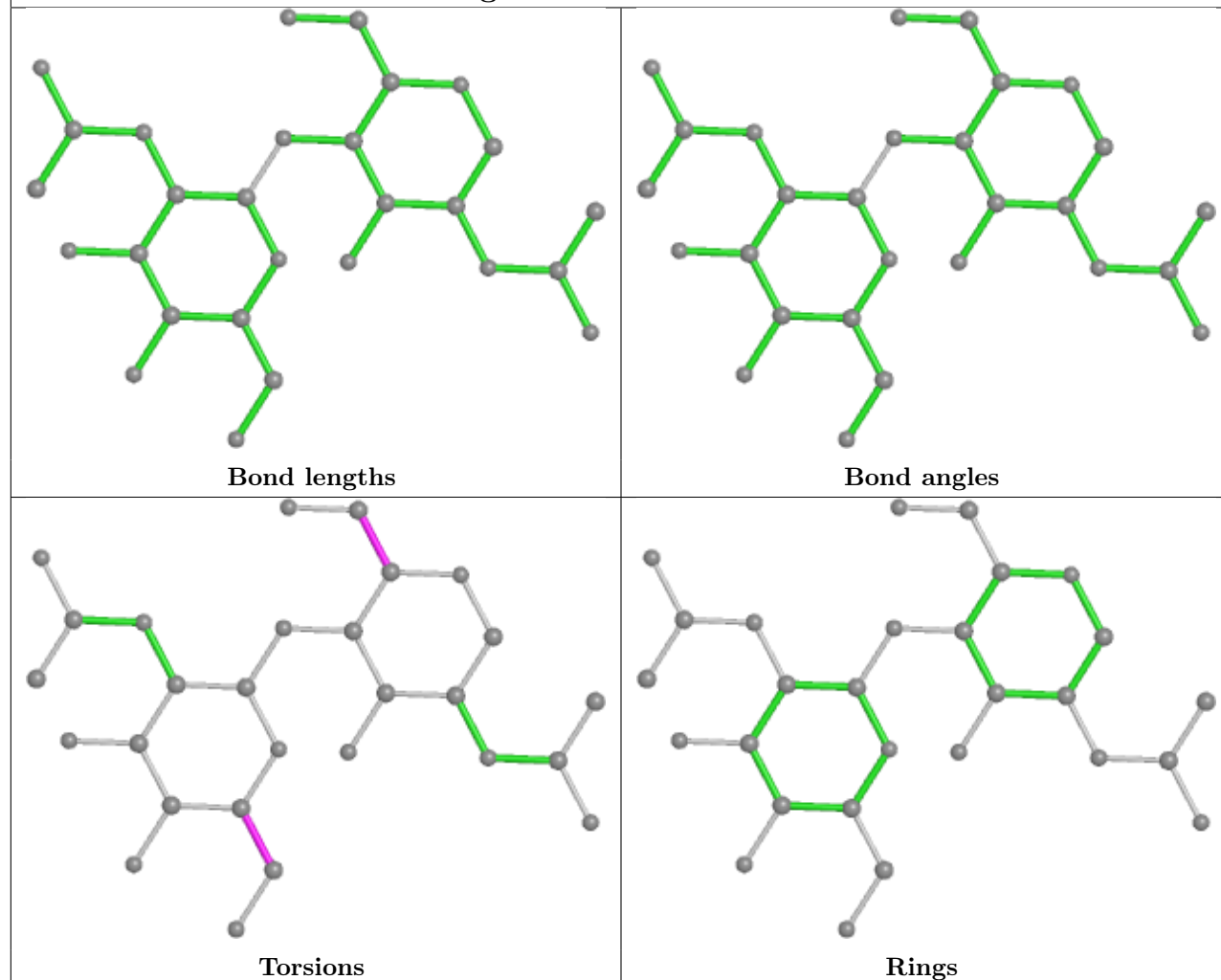
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	1	NAG	1	0
5	G	5	BMA	1	0
5	G	3	BMA	1	0

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

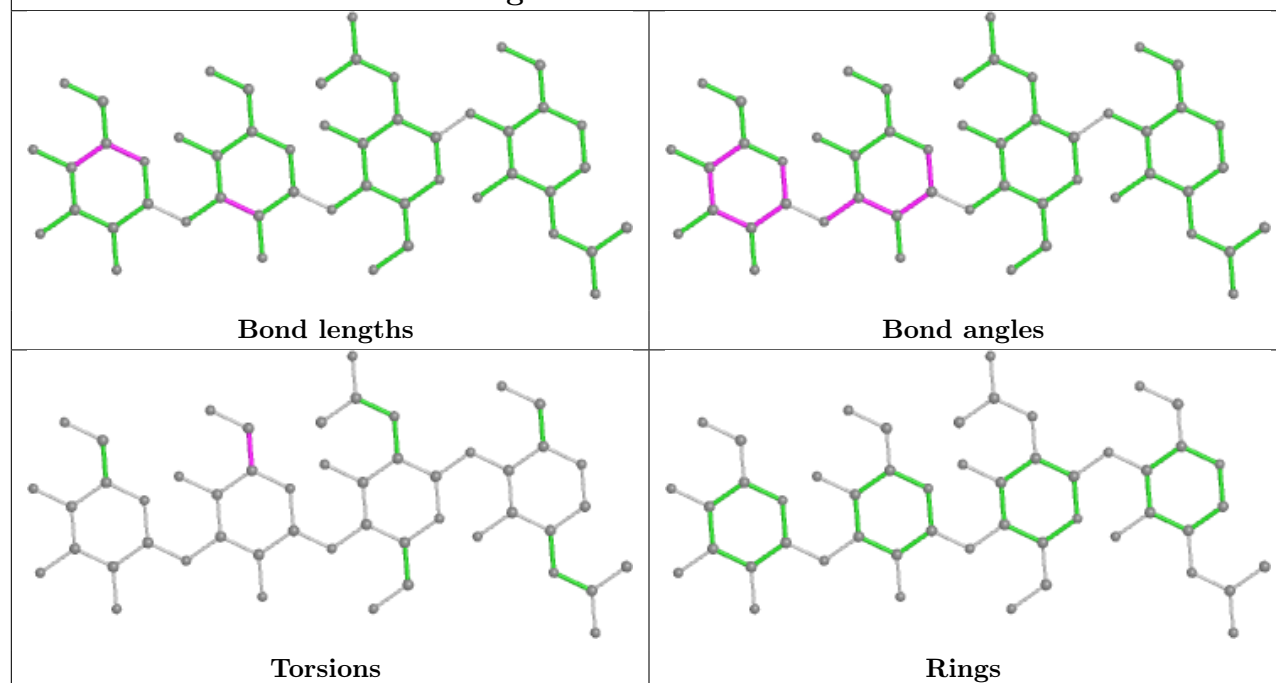




Oligosaccharide Chain K



Oligosaccharide Chain J



5.6 Ligand geometry

Of 27 ligands modelled in this entry, 14 are monoatomic - leaving 13 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
10	SO4	C	506	-	4,4,4	0.14	0	6,6,6	0.05	0
9	NAG	B	2004	2	14,14,15	0.36	0	17,19,21	0.37	0
9	NAG	D	2004	2	14,14,15	0.40	0	17,19,21	0.43	0
9	NAG	A	505	1	14,14,15	0.79	1 (7%)	17,19,21	1.32	2 (11%)
10	SO4	A	509	-	4,4,4	0.14	0	6,6,6	0.07	0
12	AGG	D	2005	11	31,31,31	0.72	2 (6%)	38,40,40	0.71	2 (5%)
10	SO4	C	507	-	4,4,4	0.14	0	6,6,6	0.05	0
12	AGG	B	2005	11	31,31,31	0.73	2 (6%)	38,40,40	0.73	2 (5%)
10	SO4	A	507	-	4,4,4	0.14	0	6,6,6	0.05	0
10	SO4	C	505	-	4,4,4	0.14	0	6,6,6	0.04	0
10	SO4	A	508	-	4,4,4	0.14	0	6,6,6	0.06	0
10	SO4	A	506	-	4,4,4	0.14	0	6,6,6	0.11	0
10	SO4	A	510	-	4,4,4	0.15	0	6,6,6	0.05	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
12	AGG	D	2005	11	-	6/26/34/34	0/2/2/2
9	NAG	B	2004	2	-	0/6/23/26	0/1/1/1
9	NAG	D	2004	2	-	2/6/23/26	0/1/1/1
9	NAG	A	505	1	-	3/6/23/26	0/1/1/1
12	AGG	B	2005	11	-	6/26/34/34	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2005	AGG	O-C	2.84	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	2005	AGG	O-C	2.84	1.30	1.22
12	B	2005	AGG	OXT-C	-2.73	1.21	1.30
12	D	2005	AGG	OXT-C	-2.72	1.21	1.30
9	A	505	NAG	C1-C2	2.39	1.55	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	505	NAG	C1-O5-C5	4.24	117.94	112.19
12	D	2005	AGG	O-C-CA	-2.75	113.24	122.26
12	B	2005	AGG	O-C-CA	-2.74	113.26	122.26
12	D	2005	AGG	OXT-C-CA	2.66	122.24	113.40
12	B	2005	AGG	OXT-C-CA	2.65	122.20	113.40

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	2005	AGG	C1-C2-C3-C4
12	D	2005	AGG	C13-C14-C15-C16
9	D	2004	NAG	O5-C5-C6-O6
12	D	2005	AGG	C1-C2-C3-C4
12	D	2005	AGG	CE2-CZ-OH-C11

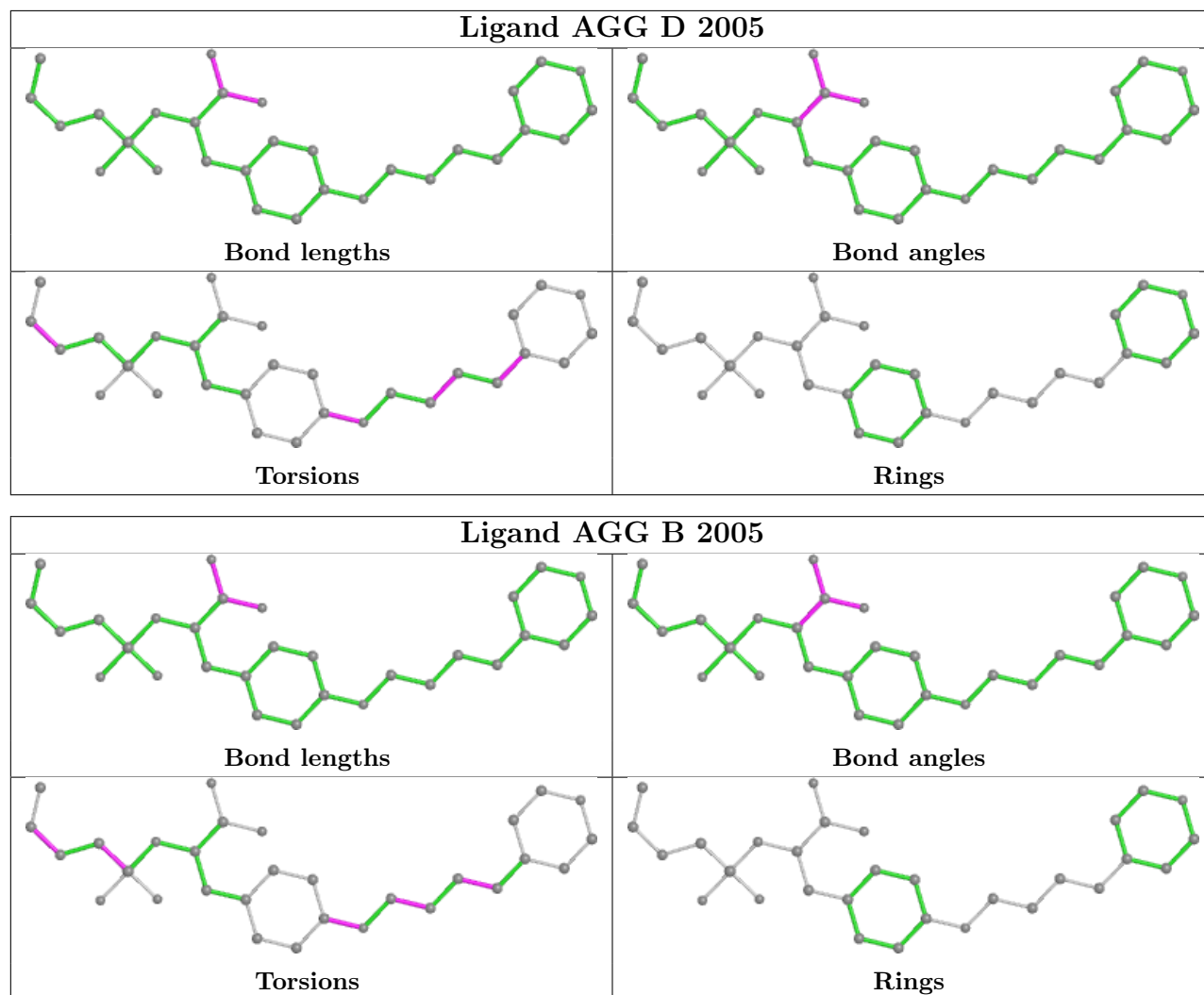
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	2004	NAG	1	0
12	D	2005	AGG	1	0
10	A	506	SO4	2	0
10	A	510	SO4	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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	134:CYS	C	138:THR	N	7.15

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	453/453 (100%)	0.16	3 (0%) 87 86	32, 43, 71, 131	0
1	C	453/453 (100%)	0.05	3 (0%) 87 86	35, 58, 94, 143	0
2	B	466/471 (98%)	0.47	47 (10%) 7 4	32, 69, 152, 218	2 (0%)
2	D	471/471 (100%)	0.34	36 (7%) 13 10	41, 77, 142, 205	3 (0%)
3	E	214/216 (99%)	1.76	82 (38%) 0 0	70, 135, 209, 268	0
3	H	216/216 (100%)	0.30	16 (7%) 14 10	46, 98, 153, 169	0
4	F	214/214 (100%)	1.71	73 (34%) 0 0	73, 128, 210, 229	0
4	L	214/214 (100%)	0.14	7 (3%) 46 39	50, 82, 116, 207	0
All	All	2701/2708 (99%)	0.49	267 (9%) 7 5	32, 74, 169, 268	5 (0%)

The worst 5 of 267 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	179	LEU	9.1
4	F	181	LEU	9.1
4	F	115	VAL	8.5
4	F	193	THR	8.4
4	F	148	TRP	8.2

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

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

6.3 Carbohydrates [i](#)

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

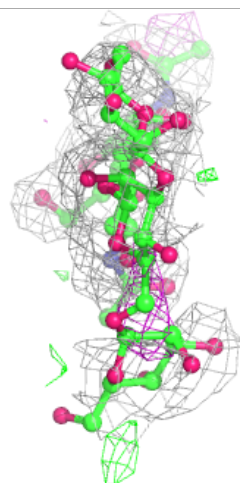
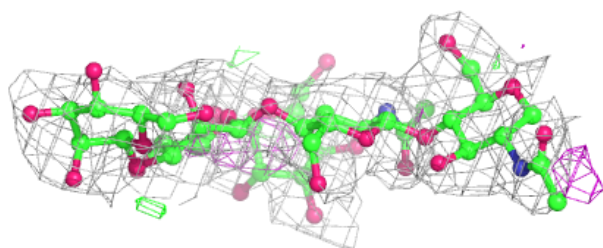
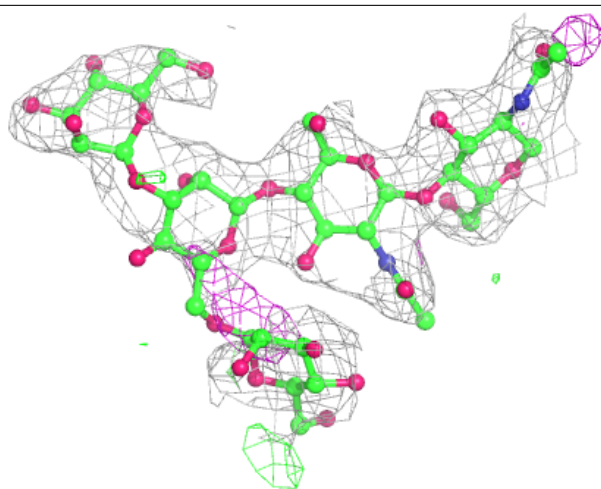
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BMA	G	5	11/12	0.55	0.39	131,137,145,147	0
5	BMA	G	3	11/12	0.78	0.20	102,128,148,148	0
7	BMA	J	4	11/12	0.84	0.32	136,139,148,149	0
7	BMA	J	3	11/12	0.85	0.33	125,133,142,142	0
5	BMA	G	4	11/12	0.86	0.23	115,124,128,128	0
6	NAG	I	1	14/15	0.86	0.26	89,101,107,114	0
6	NAG	K	2	14/15	0.87	0.36	123,128,132,134	0
7	NAG	J	2	14/15	0.87	0.29	92,110,122,123	0
6	NAG	K	1	14/15	0.88	0.29	86,101,109,117	0
5	NAG	G	2	14/15	0.91	0.18	84,92,103,110	0
6	NAG	I	2	14/15	0.92	0.29	119,121,123,124	0
7	NAG	J	1	14/15	0.93	0.16	59,75,81,94	0
5	NAG	G	1	14/15	0.95	0.15	48,57,64,75	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.

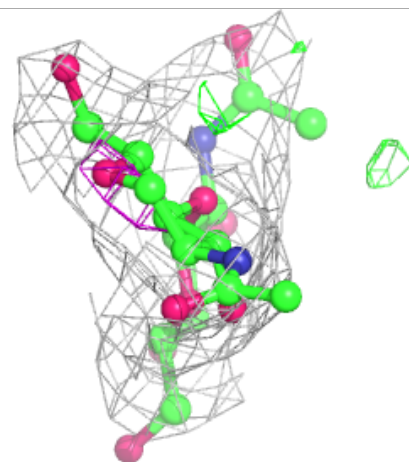
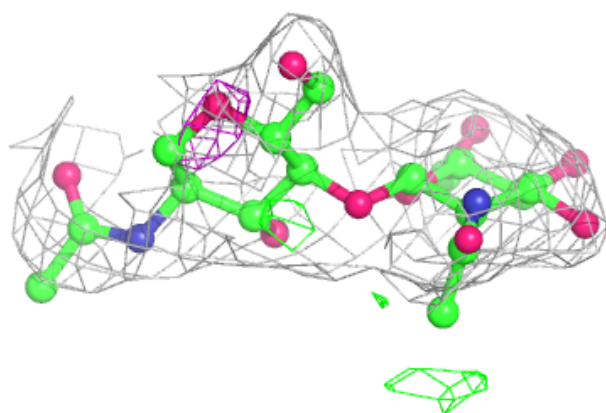
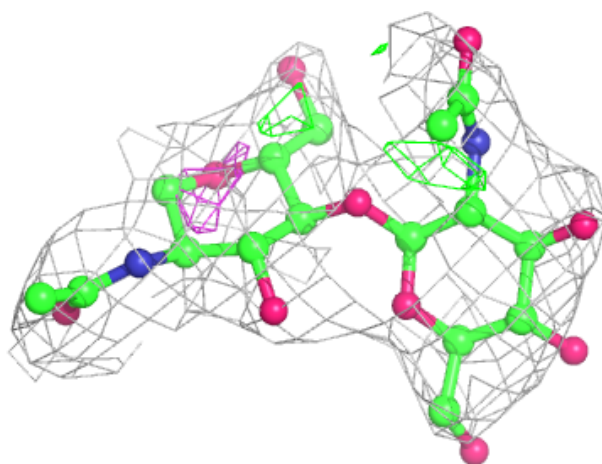
Electron density around Chain G:

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



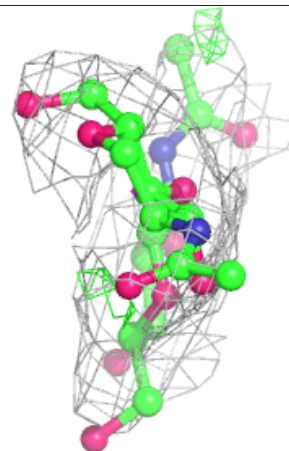
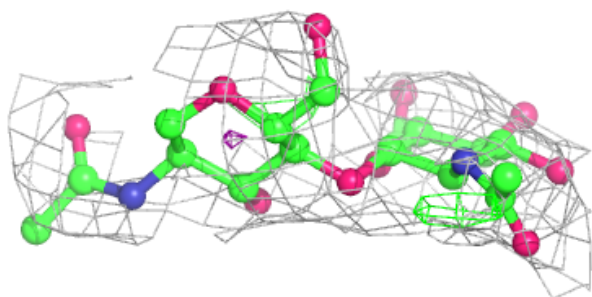
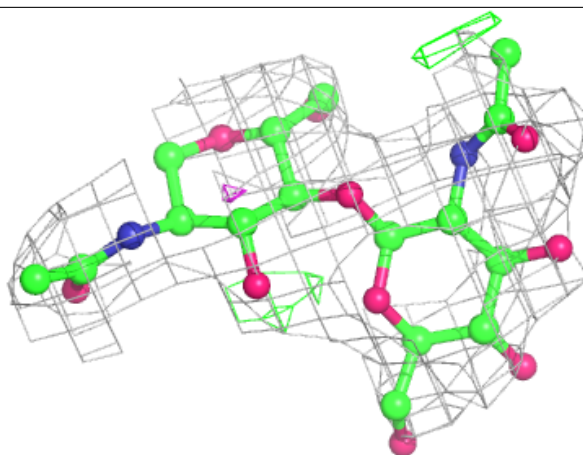
Electron density around Chain I:

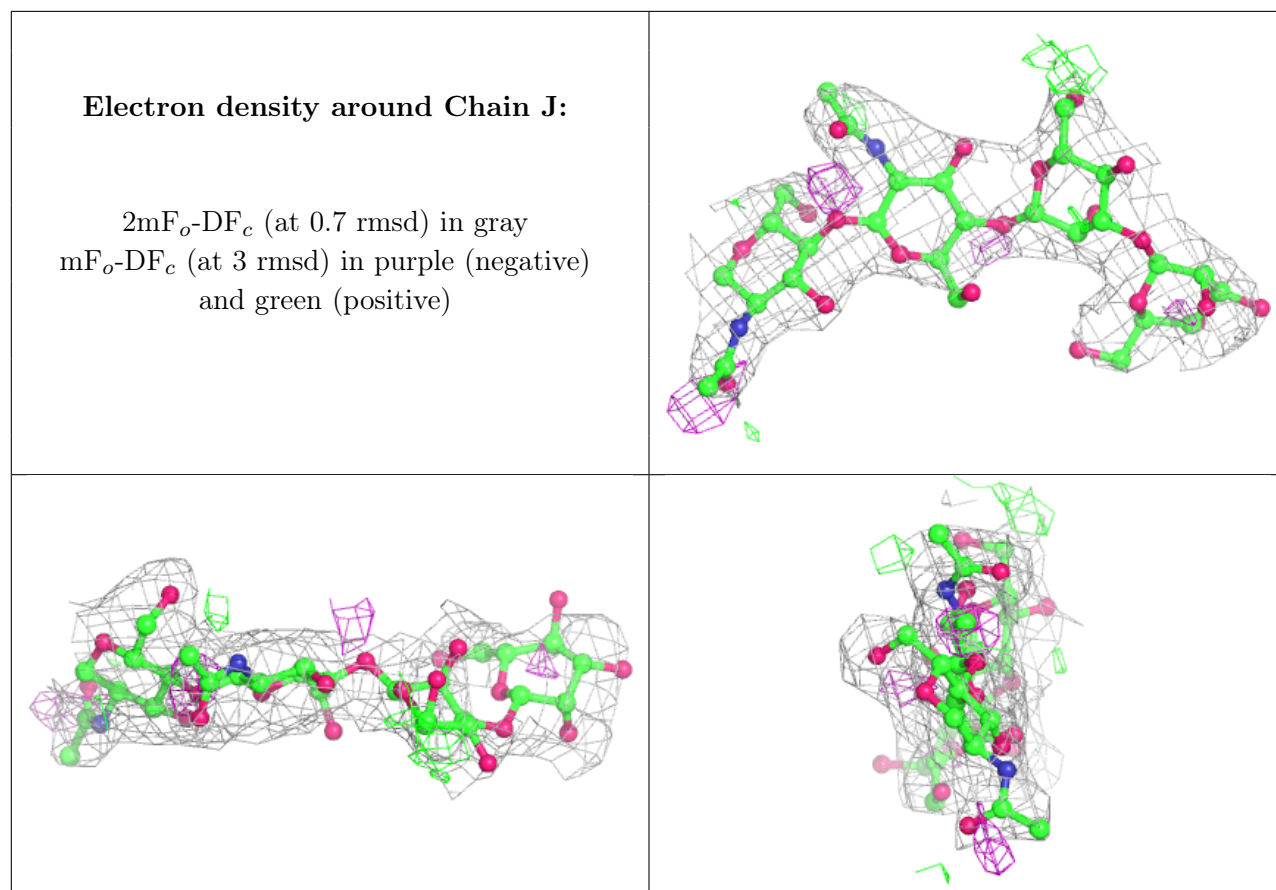
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain K:

$2mF_o-DF_c$ (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, 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.

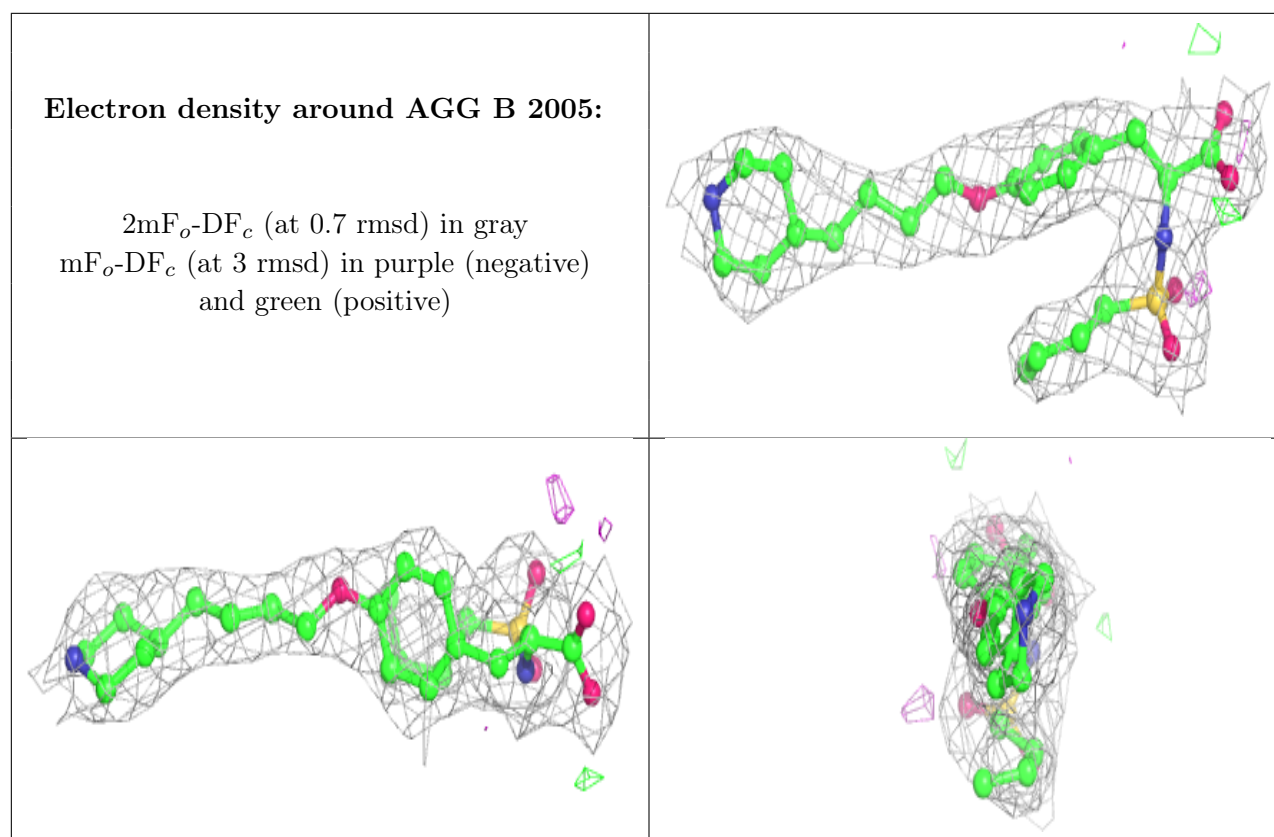
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	NAG	A	505	14/15	0.69	0.26	95,116,120,121	0
8	CA	D	2002	1/1	0.78	0.09	112,112,112,112	0
8	CA	B	2002	1/1	0.81	0.29	206,206,206,206	0
10	SO4	A	508	5/5	0.84	0.32	136,136,139,139	0
10	SO4	A	507	5/5	0.85	0.21	136,137,138,138	0
10	SO4	C	507	5/5	0.85	0.18	141,141,142,143	0
10	SO4	C	505	5/5	0.86	0.23	130,132,133,134	0
10	SO4	C	506	5/5	0.86	0.24	141,142,144,144	0
9	NAG	B	2004	14/15	0.86	0.31	92,110,112,113	0
9	NAG	D	2004	14/15	0.88	0.34	86,99,108,109	0
10	SO4	A	509	5/5	0.92	0.22	105,106,108,111	0
10	SO4	A	506	5/5	0.95	0.21	89,93,95,96	0
8	CA	A	501	1/1	0.97	0.07	54,54,54,54	0

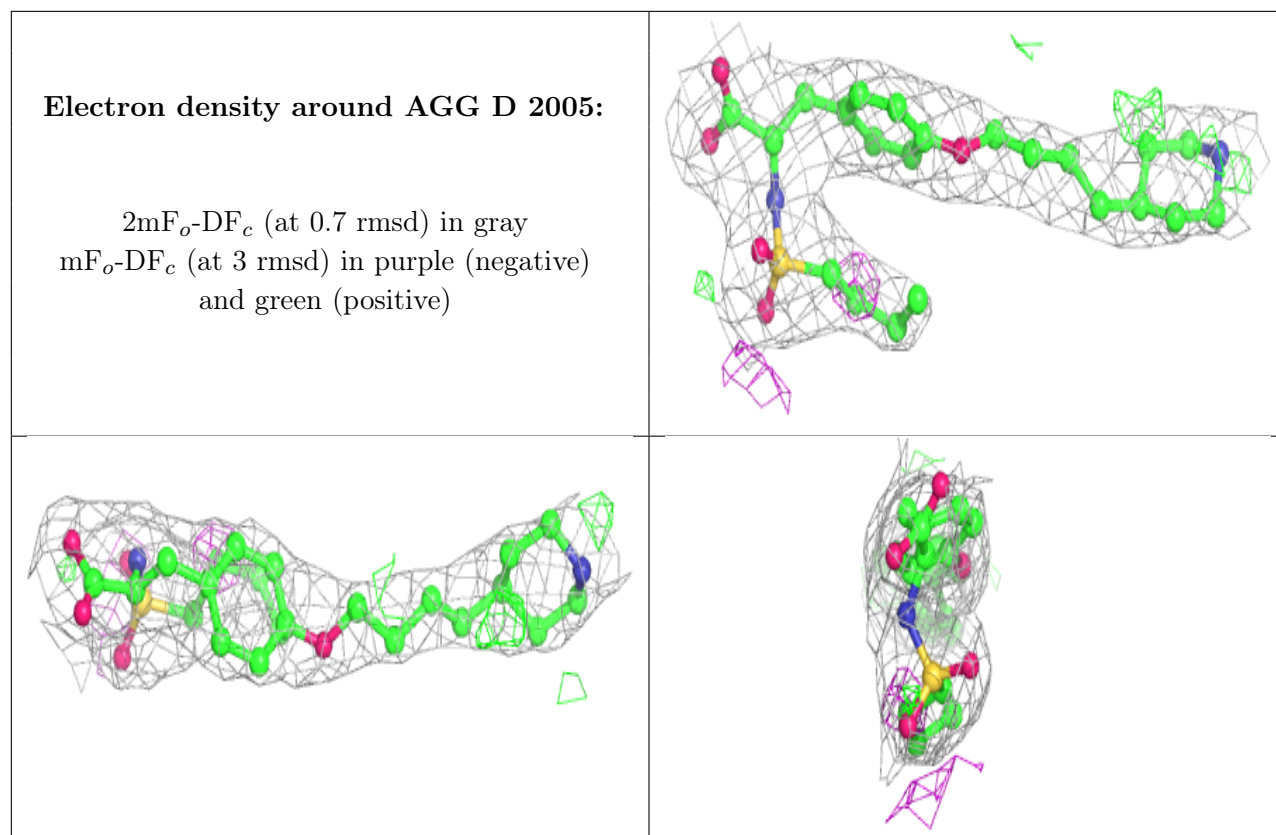
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	CA	C	504	1/1	0.97	0.14	54,54,54,54	0
10	SO4	A	510	5/5	0.97	0.13	88,90,91,92	0
11	MG	B	2001	1/1	0.97	0.24	33,33,33,33	0
11	MG	D	2001	1/1	0.97	0.16	48,48,48,48	0
12	AGG	B	2005	30/30	0.97	0.20	32,47,56,57	0
12	AGG	D	2005	30/30	0.97	0.20	37,57,80,80	0
8	CA	C	501	1/1	0.98	0.04	95,95,95,95	0
8	CA	C	502	1/1	0.98	0.04	69,69,69,69	0
8	CA	D	2003	1/1	0.98	0.17	44,44,44,44	0
8	CA	A	504	1/1	0.99	0.18	37,37,37,37	0
8	CA	C	503	1/1	0.99	0.15	59,59,59,59	0
8	CA	A	502	1/1	0.99	0.12	42,42,42,42	0
8	CA	A	503	1/1	0.99	0.20	39,39,39,39	0
8	CA	B	2003	1/1	1.00	0.18	31,31,31,31	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.