



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 06:44 AM BST

PDB ID : 5XEZ
Title : Structure of the Full-length glucagon class B G protein-coupled receptor
Authors : Zhang, H.; Qiao, A.; Yang, D.; Yang, L.; Dai, A.; de Graaf, C.; Reedtz-Runge, S.; Dharmarajan, V.; Zhang, H.; Han, G.W.; Grant, T.; Sierra, R.; Weierstall, U.; Nelson, G.; Liu, W.; Wu, Y.; Ma, L.; Cai, X.; Lin, G.; Wu, X.; Geng, Z.; Dong, Y.; Song, G.; Griffin, P.; Lau, J.; Cherezov, V.; Yang, H.; Hanson, M.; Stevens, R.; Jiang, H.; Wang, M.; Zhao, Q.; Wu, B.
Deposited on : 2017-04-06
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

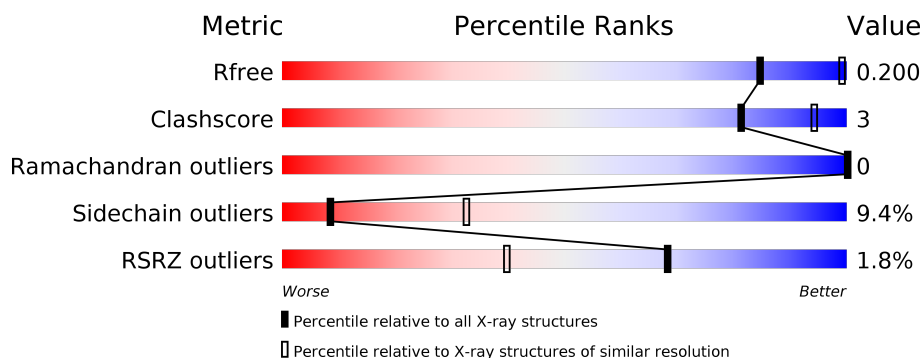
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	574	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>5%</div> </div> </div>
1	B	574	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>9%</div> <div>13%</div> </div> </div>
2	C	231	<div> <div></div> <div> <div></div> <div>87%</div> <div>13%</div> </div> </div>
2	H	231	<div> <div></div> <div> <div></div> <div>87%</div> <div>12%</div> </div> </div>
3	D	214	<div> <div></div> <div> <div></div> <div>84%</div> <div>14%</div> </div> </div>
3	L	214	<div> <div></div> <div> <div></div> <div>85%</div> <div>12%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	E	2	 50%50%
4	F	2	 100%
4	G	2	 100%
4	I	2	 100%
4	J	2	 100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 15068 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 Glucagon receptor,Endolysin,Glucagon receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	545	Total	C	N	O	S	0	0	0
			4234	2732	733	746	23			
1	B	499	Total	C	N	O	S	0	0	0
			3792	2447	654	669	22			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLY	-	expression tag	UNP P47871
A	25	ALA	-	expression tag	UNP P47871
A	26	PRO	-	expression tag	UNP P47871
A	1054	THR	CYS	engineered mutation	UNP D9IEF7
A	1097	ALA	CYS	engineered mutation	UNP D9IEF7
A	433	GLU	-	expression tag	UNP P47871
A	434	PHE	-	expression tag	UNP P47871
A	435	LEU	-	expression tag	UNP P47871
A	436	GLU	-	expression tag	UNP P47871
A	437	VAL	-	expression tag	UNP P47871
A	438	LEU	-	expression tag	UNP P47871
A	439	PHE	-	expression tag	UNP P47871
A	440	GLN	-	expression tag	UNP P47871
B	24	GLY	-	expression tag	UNP P47871
B	25	ALA	-	expression tag	UNP P47871
B	26	PRO	-	expression tag	UNP P47871
B	1054	THR	CYS	engineered mutation	UNP D9IEF7
B	1097	ALA	CYS	engineered mutation	UNP D9IEF7
B	433	GLU	-	expression tag	UNP P47871
B	434	PHE	-	expression tag	UNP P47871
B	435	LEU	-	expression tag	UNP P47871
B	436	GLU	-	expression tag	UNP P47871
B	437	VAL	-	expression tag	UNP P47871
B	438	LEU	-	expression tag	UNP P47871
B	439	PHE	-	expression tag	UNP P47871

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Chain	Residue	Modelled	Actual	Comment	Reference
B	440	GLN	-	expression tag	UNP P47871

- Molecule 2 is a protein called Antibody, mAb1, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	231	Total	C	N	O	S	0	0	0
			1756	1107	297	344	8			
2	H	231	Total	C	N	O	S	0	0	0
			1756	1107	297	344	8			

- Molecule 3 is a protein called Antibody, mAb1, light chain.

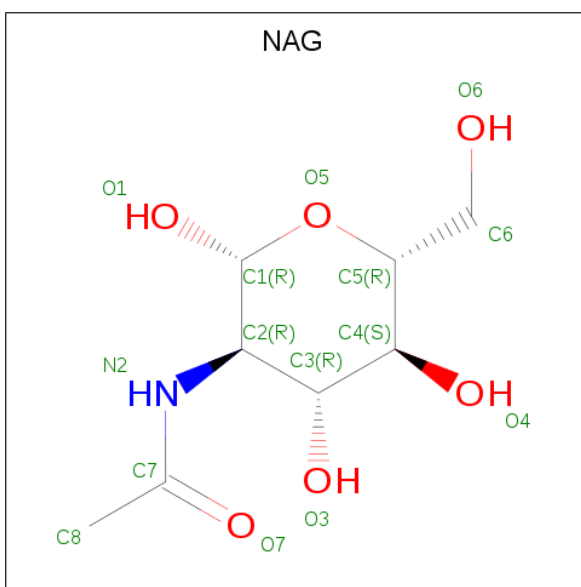
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	214	Total	C	N	O	S	0	0	0
			1633	1015	280	332	6			
3	L	214	Total	C	N	O	S	0	0	0
			1633	1015	280	332	6			

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



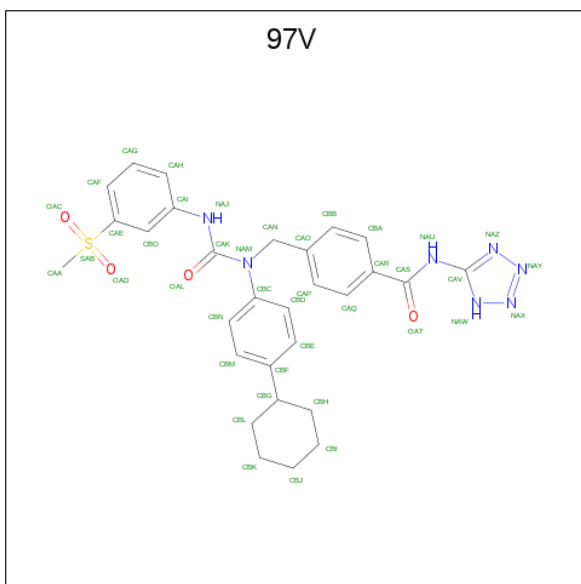
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is 4-[[[(4-cyclohexylphenyl){[3-(methylsulfonyl)phenyl]carbamoyl}amino]methyl]-N-(1H-tetrazol-5-yl)benzamide (three-letter code: 97V) (formula: C₂₉H₃₁N₇O₄S).

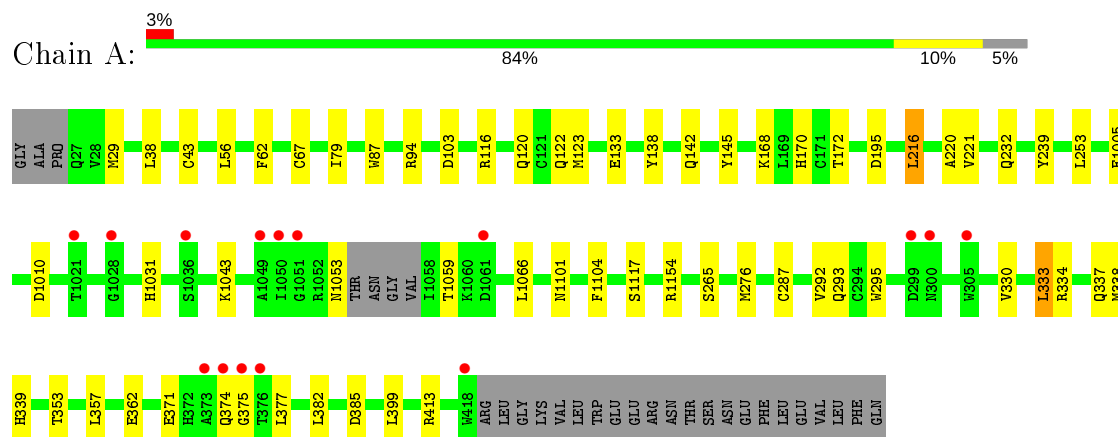


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			41	29	7	4	1		
6	B	1	Total	C	N	O	S	0	0
			41	29	7	4	1		

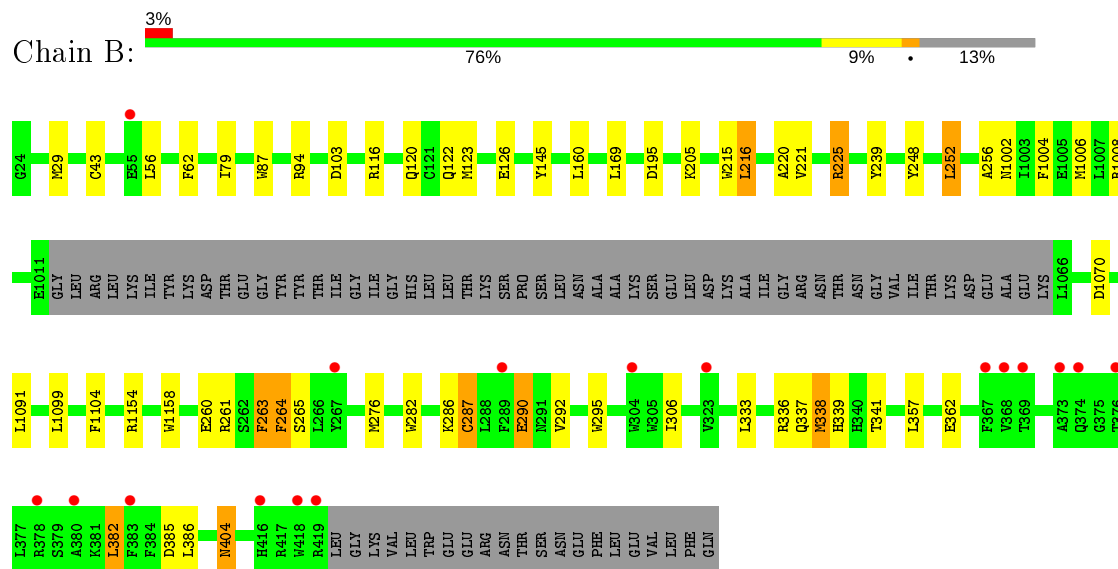
3 Residue-property plots [i](#)

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.

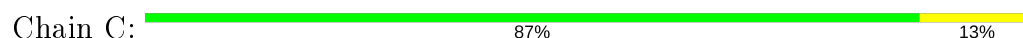
- Molecule 1: Glucagon receptor,Endolysin,Glucagon receptor

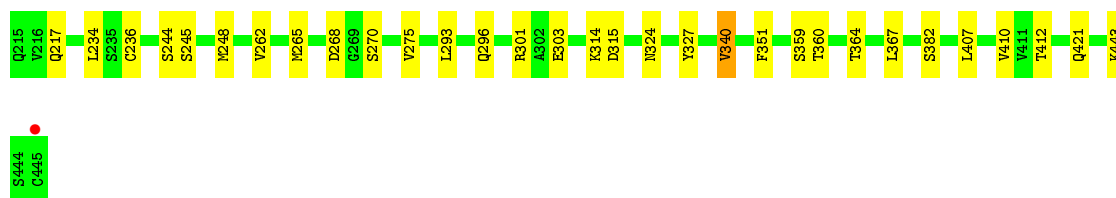


- Molecule 1: Glucagon receptor,Endolysin,Glucagon receptor

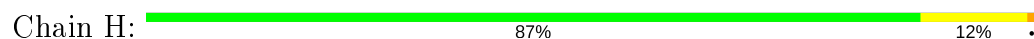


- Molecule 2: Antibody, mAb1, heavy chain

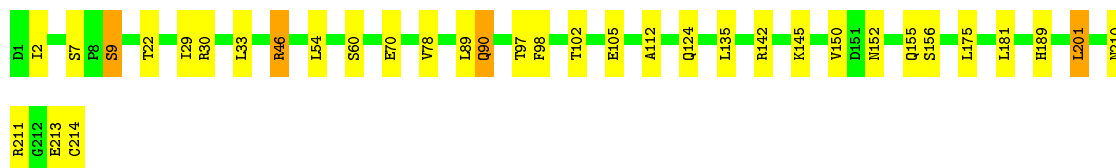
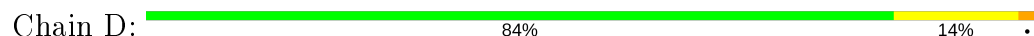




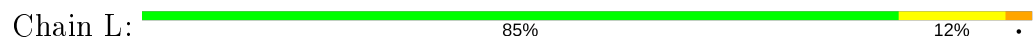
- Molecule 2: Antibody, mAb1, heavy chain



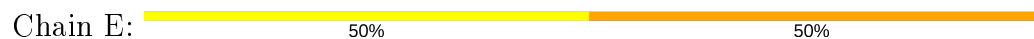
- Molecule 3: Antibody, mAb1, light chain



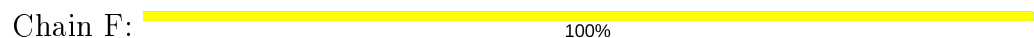
- Molecule 3: Antibody, mAb1, light chain



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



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



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



MAG1
MAG2

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

Chain I:  100%MAG1
MAG2

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

Chain J:  100%MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.61Å 245.33Å 96.15Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	31.78 – 3.00 31.78 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (31.78-3.00) 99.9 (31.78-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.210 , 0.243 0.173 , 0.200	Depositor DCC
R_{free} test set	3312 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 11.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.086 for h,-k,-l	Xtriage
Reported twinning fraction	0.501 for H, K, L 0.499 for h,-k,-l	Depositor
Outliers	0 of 66961 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15068	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: 97V, 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	0.45	0/4338	0.65	0/5901
1	B	0.45	0/3888	0.67	4/5306 (0.1%)
2	C	0.42	0/1799	0.70	0/2448
2	H	0.41	0/1799	0.71	0/2448
3	D	0.40	0/1666	0.70	0/2259
3	L	0.40	0/1666	0.71	1/2259 (0.0%)
All	All	0.43	0/15156	0.68	5/20621 (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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	B	145	TYR	CA-CB-CG	5.39	123.64	113.40
1	B	1154	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	B	1006	MET	CG-SD-CE	5.15	108.44	100.20
3	L	175	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	337	GLN	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	4234	0	4091	15	0
1	B	3792	0	3570	28	0
2	C	1756	0	1704	7	0
2	H	1756	0	1704	7	0
3	D	1633	0	1590	15	0
3	L	1633	0	1590	12	0
4	E	28	0	25	1	0
4	F	28	0	25	0	0
4	G	28	0	25	0	0
4	I	28	0	25	0	0
4	J	28	0	25	1	0
5	A	14	0	13	1	0
5	B	28	0	26	1	0
6	A	41	0	0	1	0
6	B	41	0	0	1	0
All	All	15068	0	14413	77	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 3.

All (77) 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:B:256:ALA:HB3	1:B:1002:ASN:HA	1.68	0.75
1:B:248:TYR:HA	1:B:264:PHE:HE2	1.57	0.67
1:B:248:TYR:HA	1:B:264:PHE:CE2	2.34	0.62
3:L:189:HIS:O	3:L:211:ARG:NH1	2.35	0.59
3:D:189:HIS:O	3:D:211:ARG:NH1	2.35	0.57
1:B:256:ALA:CB	1:B:1002:ASN:HA	2.34	0.55
1:B:382:LEU:HD23	1:B:386:LEU:HD12	1.88	0.55
1:B:286:LYS:O	1:B:290:GLU:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1091:LEU:HD12	1:B:1099:LEU:HD11	1.90	0.53
1:B:1004:PHE:O	1:B:1008:ARG:N	2.39	0.53
2:H:327:TYR:O	3:L:46:ARG:NH2	2.42	0.53
1:B:287:CYS:HB2	1:B:295:TRP:CH2	2.44	0.52
1:A:333:LEU:HD22	1:A:338:MET:O	2.10	0.52
2:C:327:TYR:O	3:D:46:ARG:NH2	2.43	0.51
3:L:150:VAL:HG12	3:L:155:GLN:CG	2.41	0.51
3:D:150:VAL:HG12	3:D:155:GLN:CG	2.41	0.51
1:B:87:TRP:HB3	1:B:215:TRP:CZ2	2.47	0.50
1:B:1158:TRP:O	1:B:260:GLU:HG3	2.11	0.50
1:B:126:GLU:HG3	3:D:152:ASN:HD22	1.76	0.50
1:B:239:TYR:OH	1:B:362:GLU:HG3	2.13	0.49
3:L:2:ILE:HD13	3:L:29:ILE:HG22	1.94	0.49
1:A:239:TYR:OH	1:A:362:GLU:HG3	2.12	0.48
2:C:443:LYS:NZ	3:D:213:GLU:OE1	2.38	0.48
3:D:2:ILE:HD13	3:D:29:ILE:HG22	1.94	0.48
5:B:1204:NAG:O4	3:D:7:SER:HB3	2.13	0.48
3:D:89:LEU:HD13	3:D:98:PHE:CZ	2.49	0.47
1:B:263:PHE:C	1:B:263:PHE:CD1	2.88	0.47
3:L:89:LEU:HD13	3:L:98:PHE:CZ	2.49	0.47
1:A:1031:HIS:CD2	1:A:1066:LEU:HD23	2.50	0.47
1:A:1010:ASP:OD2	1:A:1101:ASN:ND2	2.41	0.46
2:H:410:VAL:HG11	3:L:135:LEU:HD22	1.97	0.46
1:A:67:CYS:HB3	5:A:1201:NAG:H81	1.98	0.46
1:A:353:THR:HG21	6:A:1208:97V:CBE	2.45	0.46
1:A:374:GLN:CB	1:A:375:GLY:HA2	2.46	0.46
3:D:210:ASN:O	3:D:210:ASN:ND2	2.50	0.45
3:L:210:ASN:O	3:L:210:ASN:ND2	2.49	0.45
2:C:410:VAL:HG11	3:D:135:LEU:HD22	1.98	0.45
2:H:301:ARG:O	2:H:340:VAL:HG11	2.17	0.45
1:B:282:TRP:CB	1:B:306:ILE:CG2	2.95	0.45
2:C:301:ARG:O	2:C:340:VAL:HG11	2.17	0.45
1:A:94:ARG:HB3	1:A:120:GLN:HB3	1.98	0.45
1:B:94:ARG:HB3	1:B:120:GLN:HB3	1.98	0.44
1:B:252:LEU:HG	1:B:260:GLU:HG2	1.99	0.44
4:E:2:NAG:H82	4:E:2:NAG:O3	2.18	0.44
2:H:248:MET:HB3	2:H:293:LEU:HD22	1.99	0.44
1:B:337:GLN:O	1:B:338:MET:HG2	2.17	0.44
2:C:248:MET:HB3	2:C:293:LEU:HD22	1.99	0.44
2:H:410:VAL:HG11	3:L:135:LEU:CD2	2.47	0.44
1:A:292:VAL:O	1:A:295:TRP:NE1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:VAL:O	1:A:334:ARG:HG3	2.18	0.43
1:B:1091:LEU:CD1	1:B:1099:LEU:HD11	2.49	0.43
1:A:216:LEU:HD23	1:A:220:ALA:HB1	2.01	0.43
1:B:221:VAL:HG12	1:B:225:ARG:HD2	2.01	0.42
2:H:330:ASP:OD1	2:H:330:ASP:N	2.48	0.42
1:B:248:TYR:CE1	1:B:252:LEU:HD23	2.55	0.42
4:J:1:NAG:C6	4:J:2:NAG:O5	2.67	0.42
2:C:351:PHE:CE2	3:D:124:GLN:HG3	2.54	0.41
1:B:404:ASN:ND2	6:B:1207:97V:NAY	2.67	0.41
3:L:90:GLN:NE2	3:L:97:THR:OG1	2.54	0.41
1:A:87:TRP:CZ2	1:A:123:MET:HB3	2.56	0.41
2:C:410:VAL:HG11	3:D:135:LEU:CD2	2.51	0.41
1:B:292:VAL:O	1:B:295:TRP:NE1	2.50	0.41
1:B:382:LEU:HD23	1:B:386:LEU:CD1	2.51	0.41
3:D:90:GLN:NE2	3:D:97:THR:OG1	2.54	0.41
1:B:216:LEU:HD23	1:B:220:ALA:HB1	2.02	0.41
1:A:43:CYS:SG	1:A:62:PHE:HB2	2.61	0.41
1:B:248:TYR:CE1	1:B:252:LEU:CD2	3.04	0.41
2:H:361:SER:O	2:H:364:THR:HG23	2.21	0.41
1:A:142:GLN:HA	1:A:145:TYR:CE2	2.55	0.41
3:L:112:ALA:HB1	3:L:201:LEU:HD13	2.03	0.41
3:L:212:GLY:O	3:L:214:CYS:N	2.54	0.41
3:D:9:SER:O	3:D:102:THR:HA	2.21	0.41
1:B:87:TRP:CZ2	1:B:123:MET:HB3	2.57	0.40
3:L:9:SER:O	3:L:102:THR:HA	2.21	0.40
3:D:112:ALA:HB1	3:D:201:LEU:HD13	2.03	0.40
1:B:43:CYS:SG	1:B:62:PHE:HB2	2.62	0.40
1:A:221:VAL:HG13	1:A:293:GLN:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	541/574 (94%)	513 (95%)	28 (5%)	0	100	100
1	B	495/574 (86%)	467 (94%)	28 (6%)	0	100	100
2	C	229/231 (99%)	216 (94%)	13 (6%)	0	100	100
2	H	229/231 (99%)	216 (94%)	13 (6%)	0	100	100
3	D	212/214 (99%)	200 (94%)	12 (6%)	0	100	100
3	L	212/214 (99%)	201 (95%)	11 (5%)	0	100	100
All	All	1918/2038 (94%)	1813 (94%)	105 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	428/493 (87%)	393 (92%)	35 (8%)	11	39
1	B	371/493 (75%)	341 (92%)	30 (8%)	11	40
2	C	196/196 (100%)	172 (88%)	24 (12%)	5	21
2	H	196/196 (100%)	174 (89%)	22 (11%)	6	24
3	D	187/187 (100%)	169 (90%)	18 (10%)	8	32
3	L	187/187 (100%)	169 (90%)	18 (10%)	8	32
All	All	1565/1752 (89%)	1418 (91%)	147 (9%)	8	32

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	MET
1	A	38	LEU
1	A	56	LEU
1	A	79	ILE
1	A	103	ASP
1	A	116	ARG
1	A	122	GLN

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Mol	Chain	Res	Type
1	A	133	GLU
1	A	138	TYR
1	A	168	LYS
1	A	170	HIS
1	A	172	THR
1	A	195	ASP
1	A	216	LEU
1	A	232	GLN
1	A	253	LEU
1	A	1005	GLU
1	A	1043	LYS
1	A	1053	ASN
1	A	1059	THR
1	A	1104	PHE
1	A	1117	SER
1	A	1154	ARG
1	A	265	SER
1	A	276	MET
1	A	287	CYS
1	A	333	LEU
1	A	339	HIS
1	A	357	LEU
1	A	371	GLU
1	A	377	LEU
1	A	382	LEU
1	A	385	ASP
1	A	399	LEU
1	A	413	ARG
1	B	29	MET
1	B	56	LEU
1	B	79	ILE
1	B	103	ASP
1	B	116	ARG
1	B	122	GLN
1	B	160	LEU
1	B	169	LEU
1	B	195	ASP
1	B	205	LYS
1	B	216	LEU
1	B	252	LEU
1	B	1070	ASP
1	B	1104	PHE

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Mol	Chain	Res	Type
1	B	261	ARG
1	B	263	PHE
1	B	264	PHE
1	B	265	SER
1	B	276	MET
1	B	287	CYS
1	B	290	GLU
1	B	333	LEU
1	B	336	ARG
1	B	338	MET
1	B	339	HIS
1	B	341	THR
1	B	357	LEU
1	B	382	LEU
1	B	385	ASP
1	B	404	ASN
2	C	217	GLN
2	C	234	LEU
2	C	236	CYS
2	C	244	SER
2	C	245	SER
2	C	262	VAL
2	C	265	MET
2	C	268	ASP
2	C	270	SER
2	C	275	VAL
2	C	296	GLN
2	C	303	GLU
2	C	314	LYS
2	C	315	ASP
2	C	324	ASN
2	C	340	VAL
2	C	359	SER
2	C	360	THR
2	C	364	THR
2	C	367	LEU
2	C	382	SER
2	C	407	LEU
2	C	412	THR
2	C	421	GLN
3	D	9	SER
3	D	22	THR

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Mol	Chain	Res	Type
3	D	30	ARG
3	D	33	LEU
3	D	46	ARG
3	D	54	LEU
3	D	60	SER
3	D	70	GLU
3	D	78	VAL
3	D	90	GLN
3	D	105	GLU
3	D	142	ARG
3	D	145	LYS
3	D	156	SER
3	D	175	LEU
3	D	181	LEU
3	D	201	LEU
3	D	214	CYS
2	H	217	GLN
2	H	234	LEU
2	H	236	CYS
2	H	244	SER
2	H	245	SER
2	H	262	VAL
2	H	265	MET
2	H	268	ASP
2	H	275	VAL
2	H	296	GLN
2	H	303	GLU
2	H	314	LYS
2	H	315	ASP
2	H	324	ASN
2	H	340	VAL
2	H	359	SER
2	H	364	THR
2	H	367	LEU
2	H	382	SER
2	H	407	LEU
2	H	412	THR
2	H	421	GLN
3	L	9	SER
3	L	22	THR
3	L	30	ARG
3	L	33	LEU

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Mol	Chain	Res	Type
3	L	46	ARG
3	L	54	LEU
3	L	60	SER
3	L	70	GLU
3	L	78	VAL
3	L	90	GLN
3	L	105	GLU
3	L	142	ARG
3	L	145	LYS
3	L	156	SER
3	L	175	LEU
3	L	181	LEU
3	L	201	LEU
3	L	214	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1132	ASN
1	A	404	ASN
3	D	152	ASN
3	D	155	GLN
3	D	158	ASN
3	L	155	GLN
3	L	158	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 ⓘ

10 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
4	NAG	E	1	1,4	14,14,15	0.55	0	17,19,21	1.62	2 (11%)
4	NAG	E	2	4	14,14,15	0.60	0	17,19,21	1.94	3 (17%)
4	NAG	F	1	1,4	14,14,15	0.26	0	17,19,21	1.12	2 (11%)
4	NAG	F	2	4	14,14,15	0.35	0	17,19,21	1.18	2 (11%)
4	NAG	G	1	1,4	14,14,15	0.68	0	17,19,21	1.90	3 (17%)
4	NAG	G	2	4	14,14,15	0.44	0	17,19,21	1.57	3 (17%)
4	NAG	I	1	1,4	14,14,15	0.67	0	17,19,21	1.68	4 (23%)
4	NAG	I	2	4	14,14,15	0.23	0	17,19,21	1.13	2 (11%)
4	NAG	J	1	1,4	14,14,15	0.72	0	17,19,21	2.22	7 (41%)
4	NAG	J	2	4	14,14,15	0.60	0	17,19,21	1.60	6 (35%)

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
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	5/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	4/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2	NAG	C2-N2-C7	5.17	130.27	122.90
4	G	1	NAG	O5-C1-C2	-5.11	103.22	111.29
4	E	1	NAG	C1-O5-C5	5.01	118.99	112.19
4	J	1	NAG	O5-C1-C2	-4.58	104.05	111.29
4	E	2	NAG	C8-C7-N2	3.66	122.29	116.10
4	I	1	NAG	O5-C1-C2	-3.46	105.82	111.29
4	J	1	NAG	O4-C4-C5	3.46	117.89	109.30
4	G	1	NAG	C1-C2-N2	3.40	116.29	110.49
4	J	1	NAG	C1-C2-N2	3.33	116.17	110.49
4	J	1	NAG	C3-C4-C5	-3.25	104.44	110.24
4	G	2	NAG	C8-C7-N2	3.17	121.46	116.10
4	G	2	NAG	C2-N2-C7	3.03	127.22	122.90
4	J	2	NAG	C2-N2-C7	3.00	127.18	122.90
4	I	2	NAG	C2-N2-C7	2.99	127.15	122.90
4	I	1	NAG	O5-C5-C6	-2.93	102.60	107.20
4	G	2	NAG	O5-C5-C6	2.90	111.74	107.20
4	F	1	NAG	C1-C2-N2	2.84	115.34	110.49
4	J	2	NAG	C8-C7-N2	2.74	120.75	116.10
4	I	1	NAG	O4-C4-C3	-2.70	104.10	110.35
4	J	1	NAG	O5-C5-C6	-2.57	103.17	107.20
4	E	1	NAG	C4-C3-C2	-2.53	107.31	111.02
4	G	1	NAG	O5-C5-C4	-2.48	104.79	110.83
4	F	2	NAG	C8-C7-N2	2.48	120.29	116.10
4	J	1	NAG	O4-C4-C3	-2.47	104.64	110.35
4	F	2	NAG	C2-N2-C7	2.46	126.41	122.90
4	J	2	NAG	O5-C5-C6	2.36	110.91	107.20
4	J	1	NAG	C6-C5-C4	2.30	118.38	113.00
4	I	1	NAG	C6-C5-C4	2.25	118.26	113.00
4	J	2	NAG	O5-C1-C2	-2.23	107.77	111.29
4	J	2	NAG	O5-C5-C4	-2.19	105.50	110.83
4	I	2	NAG	C8-C7-N2	2.17	119.78	116.10
4	F	1	NAG	C4-C3-C2	-2.09	107.96	111.02
4	E	2	NAG	C4-C3-C2	2.08	114.07	111.02
4	J	2	NAG	C1-O5-C5	2.08	115.01	112.19

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	2	NAG	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	E	2	NAG	C8-C7-N2-C2

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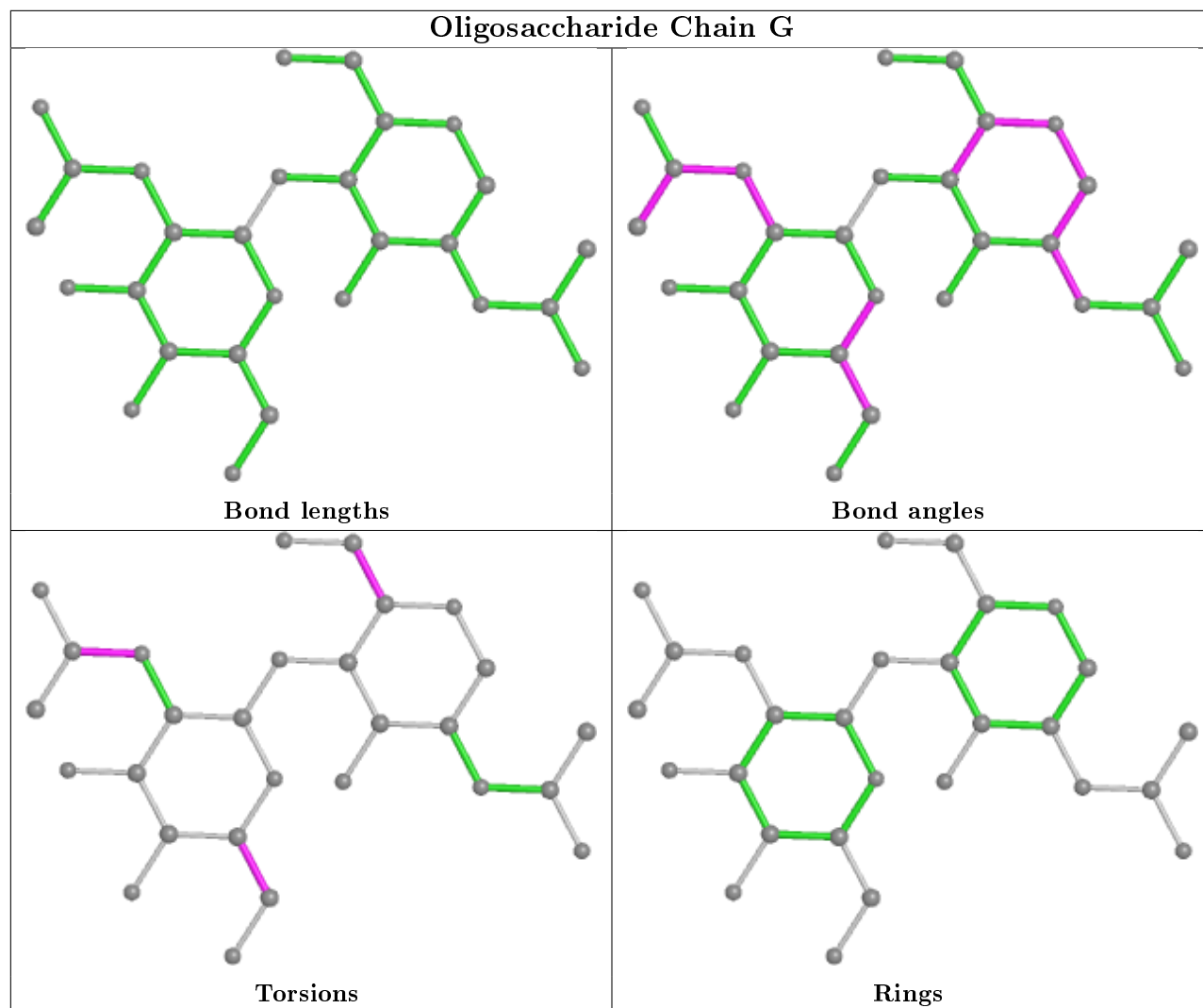
Mol	Chain	Res	Type	Atoms
4	E	2	NAG	O7-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
4	I	2	NAG	C8-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
4	G	2	NAG	O5-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	I	1	NAG	C3-C2-N2-C7
4	J	1	NAG	C3-C2-N2-C7
4	G	1	NAG	O5-C5-C6-O6
4	E	2	NAG	C1-C2-N2-C7
4	I	1	NAG	C1-C2-N2-C7
4	G	1	NAG	C4-C5-C6-O6
4	J	1	NAG	C1-C2-N2-C7

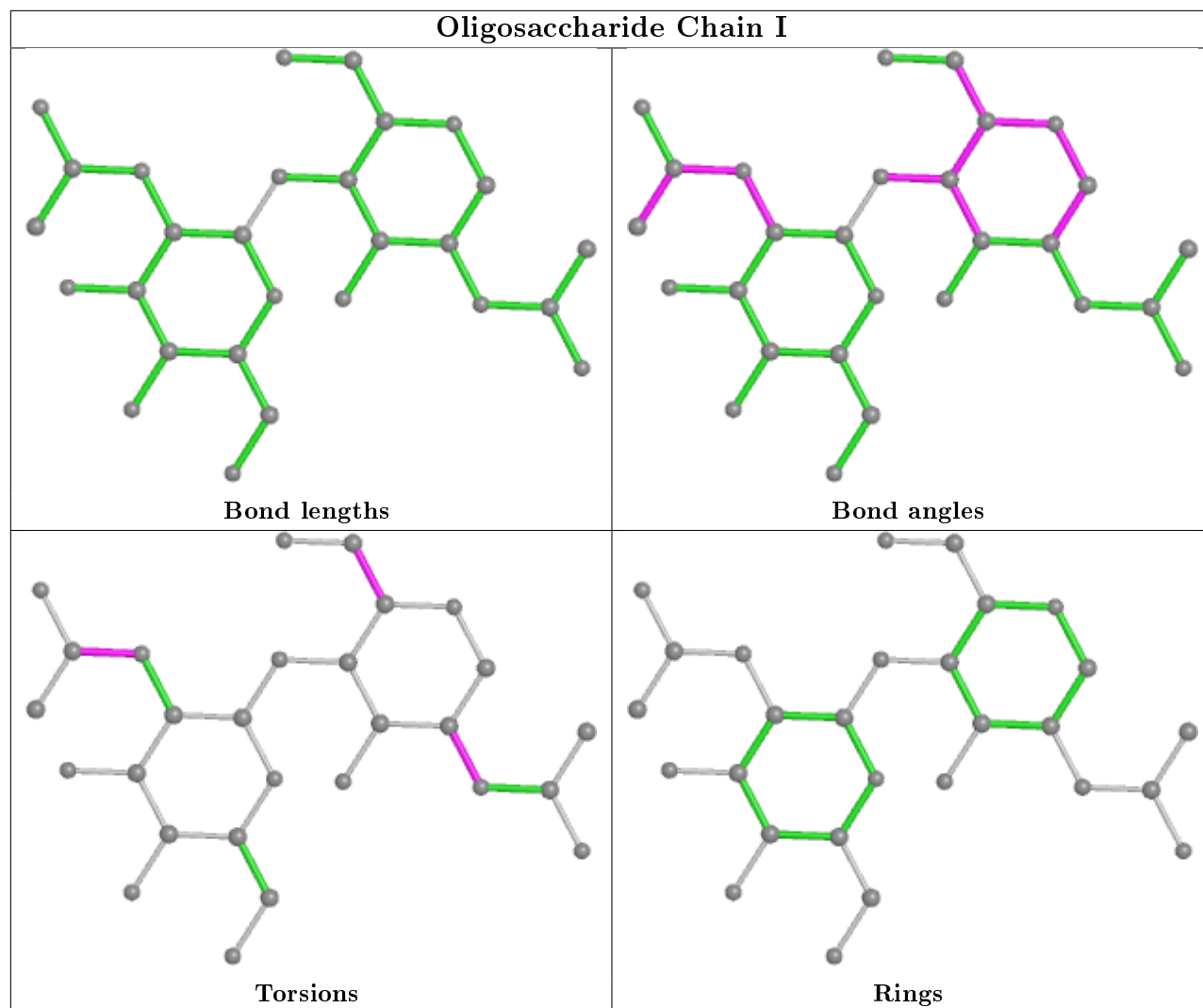
There are no ring outliers.

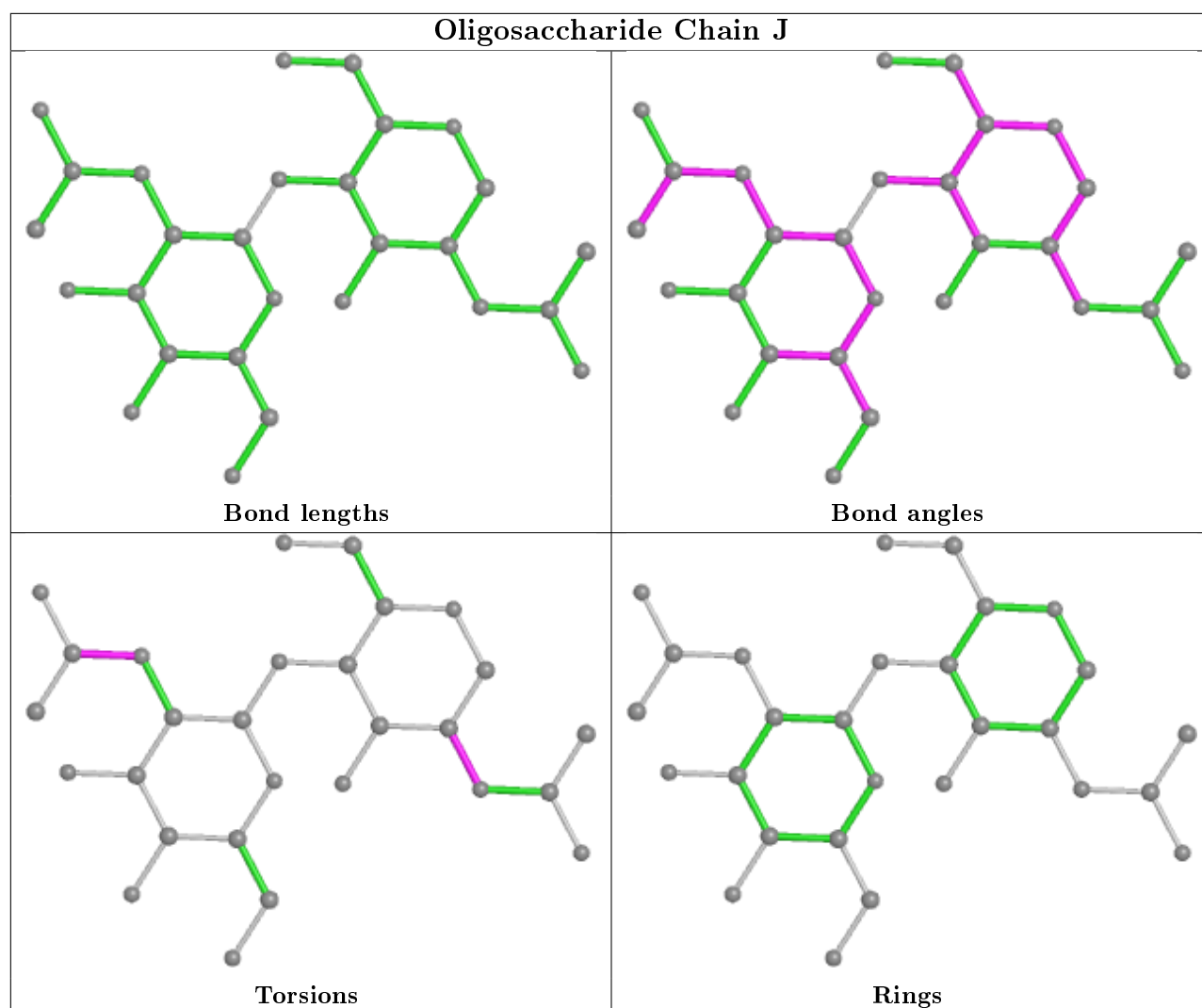
3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	NAG	1	0
4	J	1	NAG	1	0
4	J	2	NAG	1	0

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







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
6	97V	A	1208	-	43,45,45	1.91	8 (18%)	55,63,63	1.65	12 (21%)
5	NAG	B	1204	1	14,14,15	0.91	1 (7%)	17,19,21	2.09	7 (41%)
5	NAG	B	1203	1	14,14,15	0.47	0	17,19,21	1.55	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	97V	B	1207	-	43,45,45	1.91	8 (18%)	55,63,63	1.51	9 (16%)
5	NAG	A	1201	1	14,14,15	0.40	0	17,19,21	1.39	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
6	97V	A	1208	-	-	12/32/42/42	0/5/5/5
5	NAG	B	1204	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1203	1	-	1/6/23/26	0/1/1/1
6	97V	B	1207	-	-	12/32/42/42	0/5/5/5
5	NAG	A	1201	1	-	2/6/23/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1207	97V	CAN-CAO	-5.53	1.41	1.51
6	A	1208	97V	CAN-CAO	-5.42	1.41	1.51
6	A	1208	97V	CAR-CAS	-4.94	1.39	1.50
6	B	1207	97V	CBF-CBG	-4.93	1.42	1.52
6	B	1207	97V	CAR-CAS	-4.92	1.39	1.50
6	A	1208	97V	CBF-CBG	-4.41	1.43	1.52
6	B	1207	97V	CBC-NAM	-3.97	1.35	1.43
6	A	1208	97V	CBC-NAM	-3.74	1.35	1.43
6	A	1208	97V	CAV-NAU	-3.66	1.34	1.38
6	A	1208	97V	CAI-NAJ	-3.45	1.34	1.41
6	B	1207	97V	CAV-NAU	-3.45	1.34	1.38
6	B	1207	97V	OAD-SAB	3.42	1.53	1.44
6	A	1208	97V	OAC-SAB	3.41	1.53	1.44
6	A	1208	97V	OAD-SAB	3.40	1.53	1.44
6	B	1207	97V	OAC-SAB	3.34	1.53	1.44
5	B	1204	NAG	C1-C2	2.82	1.56	1.52
6	B	1207	97V	CAI-NAJ	-2.31	1.37	1.41

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1204	NAG	C2-N2-C7	5.17	130.26	122.90
6	B	1207	97V	OAD-SAB-OAC	-4.93	109.43	117.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1208	97V	OAD-SAB-OAC	-4.81	109.64	117.92
6	B	1207	97V	CAI-CBO-CAE	4.28	122.12	118.89
6	B	1207	97V	CAA-SAB-CAE	3.98	109.29	104.58
6	A	1208	97V	CAI-CBO-CAE	3.68	121.66	118.89
6	A	1208	97V	CAF-CAE-SAB	3.64	122.96	119.58
6	A	1208	97V	CAA-SAB-CAE	3.47	108.67	104.58
6	A	1208	97V	CBD-CBC-NAM	3.36	125.09	120.18
5	A	1201	NAG	C1-C2-N2	3.32	116.17	110.49
5	B	1203	NAG	O5-C1-C2	-3.23	106.19	111.29
5	B	1204	NAG	C1-O5-C5	2.90	116.12	112.19
6	B	1207	97V	CBJ-CBI-CBH	-2.89	105.53	111.42
6	A	1208	97V	CAI-NAJ-CAK	-2.86	120.37	126.12
6	A	1208	97V	CBJ-CBI-CBH	-2.80	105.71	111.42
5	A	1201	NAG	C2-N2-C7	2.60	126.60	122.90
6	A	1208	97V	CAO-CAN-NAM	2.57	117.73	113.39
6	A	1208	97V	OAD-SAB-CAE	2.56	110.33	108.25
5	B	1203	NAG	C2-N2-C7	2.52	126.49	122.90
5	B	1204	NAG	O5-C1-C2	-2.51	107.32	111.29
6	B	1207	97V	NAW-NAX-NAY	-2.50	107.90	109.53
5	B	1203	NAG	C4-C3-C2	-2.45	107.43	111.02
5	B	1204	NAG	O7-C7-N2	2.39	126.36	121.95
6	B	1207	97V	CAH-CAI-CBO	-2.25	116.98	119.65
5	B	1204	NAG	C6-C5-C4	-2.24	107.76	113.00
6	B	1207	97V	OAD-SAB-CAE	2.20	110.04	108.25
6	B	1207	97V	CAH-CAI-NAJ	2.19	127.78	120.40
6	A	1208	97V	NAW-NAX-NAY	-2.13	108.14	109.53
5	B	1204	NAG	O3-C3-C4	-2.11	105.47	110.35
5	B	1204	NAG	O5-C5-C6	2.06	110.44	107.20
6	A	1208	97V	CBO-CAE-SAB	-2.06	117.43	119.06
6	A	1208	97V	NAZ-NAY-NAX	-2.04	108.20	109.53
6	B	1207	97V	CAF-CAE-SAB	2.02	121.45	119.58

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1208	97V	NAJ-CAK-NAM-CAN
6	A	1208	97V	OAL-CAK-NAM-CAN
5	B	1204	NAG	C3-C2-N2-C7
6	B	1207	97V	NAJ-CAK-NAM-CAN
6	B	1207	97V	OAL-CAK-NAM-CAN
6	A	1208	97V	CBA-CAR-CAS-OAT

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Mol	Chain	Res	Type	Atoms
6	A	1208	97V	CAQ-CAR-CAS-OAT
6	B	1207	97V	CBO-CAE-SAB-OAC
6	A	1208	97V	CBA-CAR-CAS-NAU
6	B	1207	97V	CAF-CAE-SAB-OAC
6	A	1208	97V	CAQ-CAR-CAS-NAU
6	B	1207	97V	CBA-CAR-CAS-OAT
6	B	1207	97V	CAQ-CAR-CAS-OAT
6	B	1207	97V	CBO-CAE-SAB-CAA
5	A	1201	NAG	C1-C2-N2-C7
5	B	1203	NAG	C3-C2-N2-C7
6	B	1207	97V	CBA-CAR-CAS-NAU
6	B	1207	97V	CAQ-CAR-CAS-NAU
6	B	1207	97V	CAF-CAE-SAB-CAA
6	A	1208	97V	CBO-CAI-NAJ-CAK
6	A	1208	97V	CAH-CAI-NAJ-CAK
5	A	1201	NAG	C4-C5-C6-O6
6	A	1208	97V	CBM-CBF-CBG-CBH
6	A	1208	97V	OAL-CAK-NAM-CBC
6	B	1207	97V	OAL-CAK-NAM-CBC
6	A	1208	97V	NAJ-CAK-NAM-CBC
6	B	1207	97V	NAJ-CAK-NAM-CBC
6	A	1208	97V	CBE-CBF-CBG-CBH

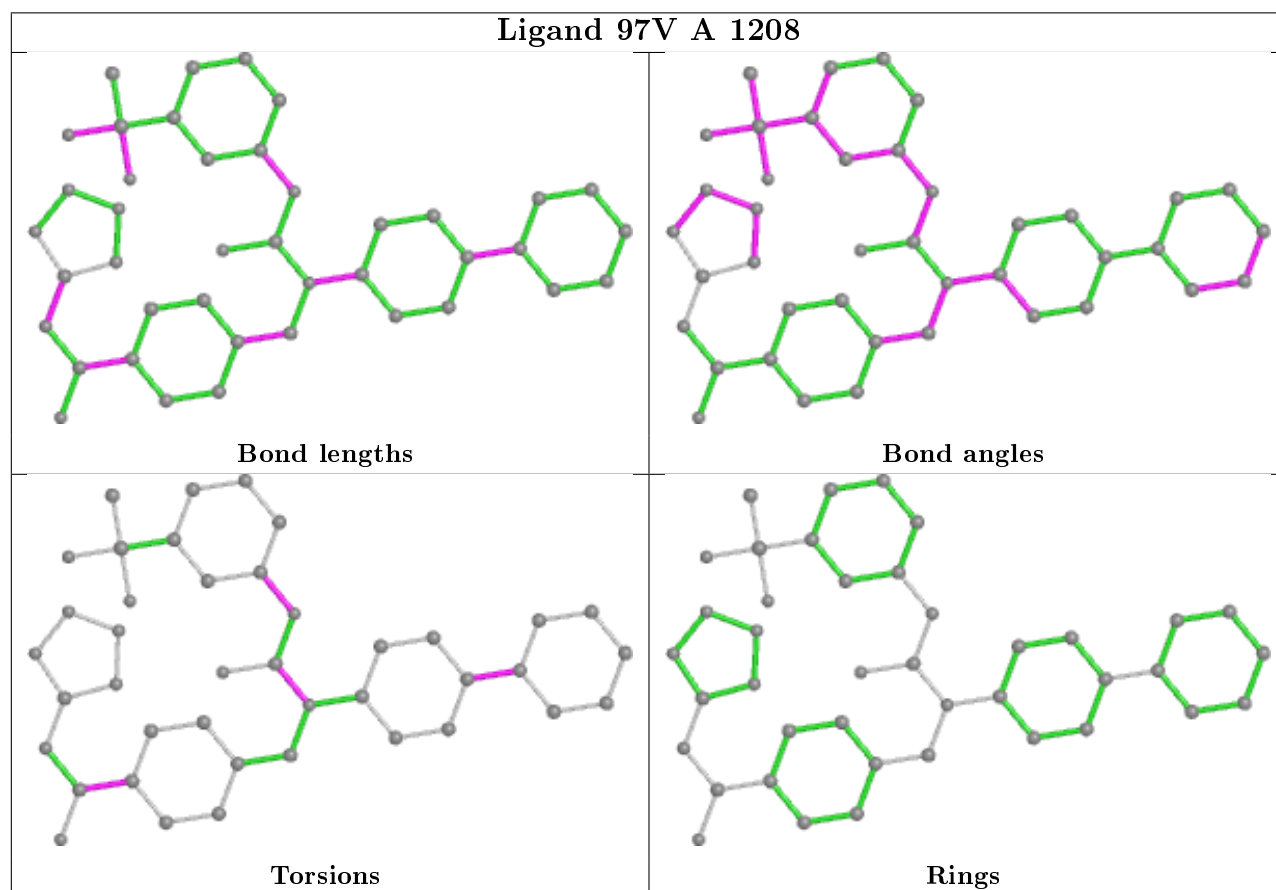
There are no ring outliers.

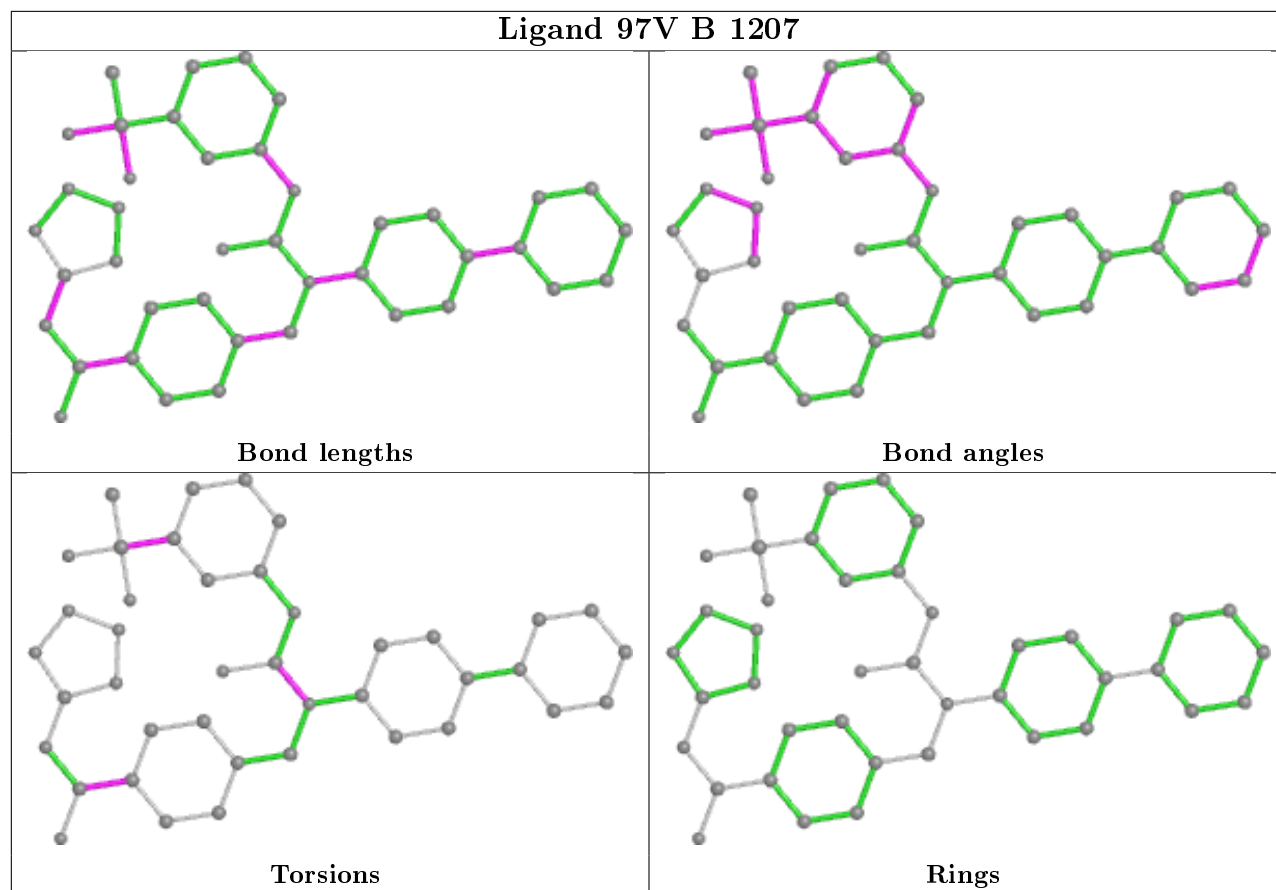
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1208	97V	1	0
5	B	1204	NAG	1	0
6	B	1207	97V	1	0
5	A	1201	NAG	1	0

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

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, 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	545/574 (94%)	-0.23	15 (2%) 53 25	40, 91, 150, 161	0
1	B	499/574 (86%)	-0.26	17 (3%) 45 19	38, 105, 152, 177	0
2	C	231/231 (100%)	-0.66	1 (0%) 92 79	36, 59, 90, 129	0
2	H	231/231 (100%)	-0.66	1 (0%) 92 79	35, 56, 83, 125	0
3	D	214/214 (100%)	-0.70	0 100 100	38, 54, 82, 132	0
3	L	214/214 (100%)	-0.77	0 100 100	29, 48, 76, 118	0
All	All	1934/2038 (94%)	-0.45	34 (1%) 68 40	29, 74, 144, 177	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1050	ILE	6.0
2	H	445	CYS	6.0
1	A	374	GLN	5.2
1	B	374	GLN	3.6
1	B	289	PHE	3.4
1	A	373	ALA	3.3
1	A	1051	GLY	3.3
1	A	1021	THR	3.1
1	A	1036	SER	3.0
1	A	1028	GLY	2.9
1	A	1061	ASP	2.9
1	A	376	THR	2.9
1	B	376	THR	2.6
1	A	418	TRP	2.6
1	B	418	TRP	2.6
1	B	323	VAL	2.5
1	B	367	PHE	2.5
1	B	378	ARG	2.4
1	B	267	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	373	ALA	2.3
1	B	368	VAL	2.3
1	A	375	GLY	2.2
1	A	300	ASN	2.2
1	B	383	PHE	2.2
1	B	369	THR	2.2
1	A	1049	ALA	2.2
1	B	416	HIS	2.2
1	B	419	ARG	2.2
1	A	299	ASP	2.1
2	C	445	CYS	2.1
1	B	304	TRP	2.1
1	A	305	TRP	2.0
1	B	55	GLU	2.0
1	B	380	ALA	2.0

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](#)

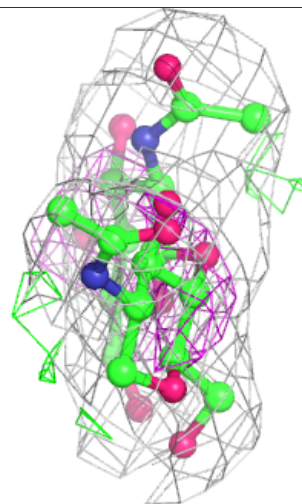
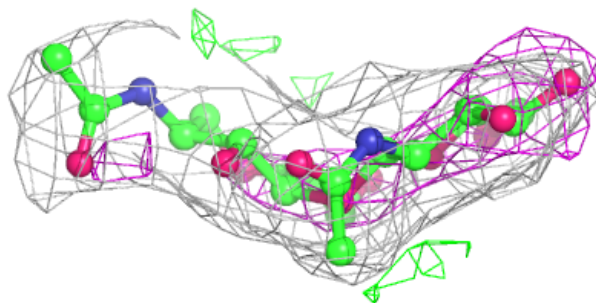
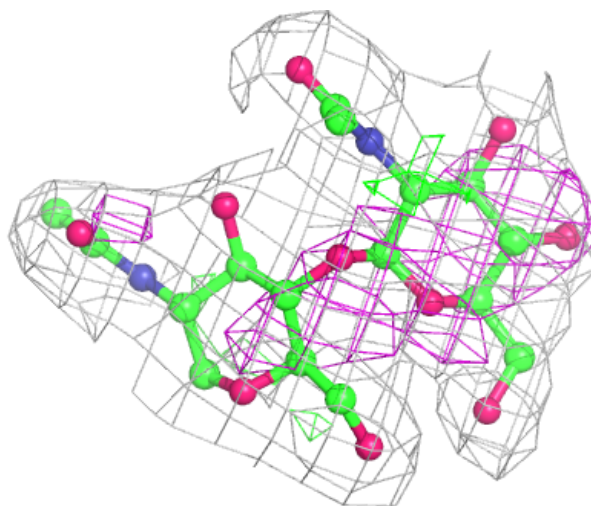
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	I	2	14/15	0.89	0.15	67,69,74,76	0
4	NAG	J	2	14/15	0.91	0.30	61,63,73,76	0
4	NAG	E	2	14/15	0.93	0.21	63,65,67,67	0
4	NAG	G	2	14/15	0.93	0.34	58,60,61,62	0
4	NAG	G	1	14/15	0.94	0.24	55,58,60,61	0
4	NAG	J	1	14/15	0.94	0.15	57,59,63,65	0
4	NAG	E	1	14/15	0.94	0.23	62,65,67,67	0
4	NAG	F	1	14/15	0.95	0.11	55,58,59,60	0
4	NAG	I	1	14/15	0.96	0.10	63,65,68,68	0
4	NAG	F	2	14/15	0.97	0.17	57,58,59,61	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.

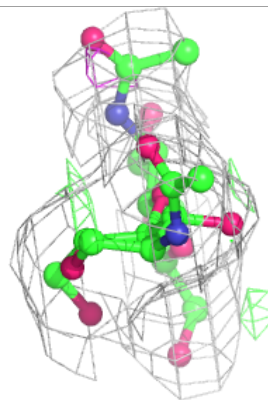
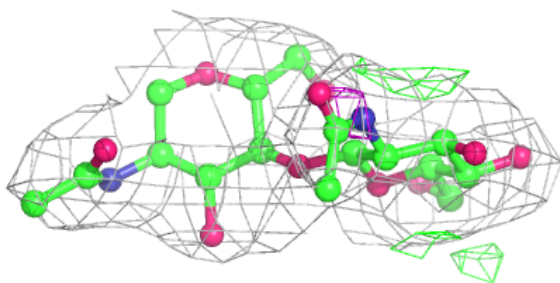
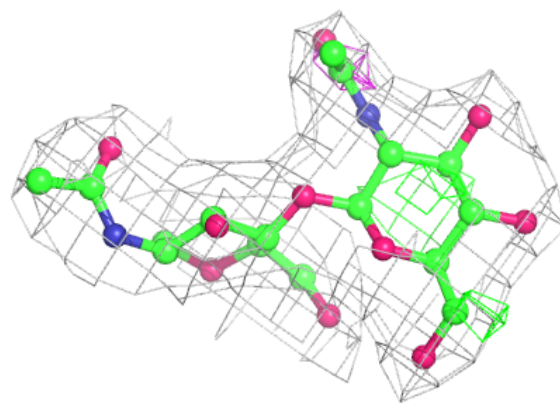
Electron density around Chain G:

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

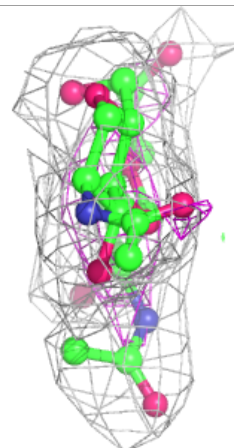
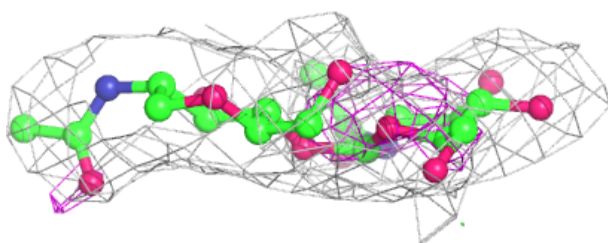
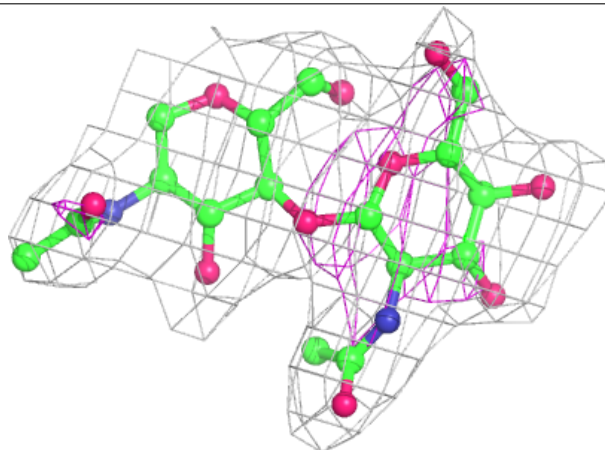


Electron density around Chain I:

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

**Electron density around Chain J:**

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

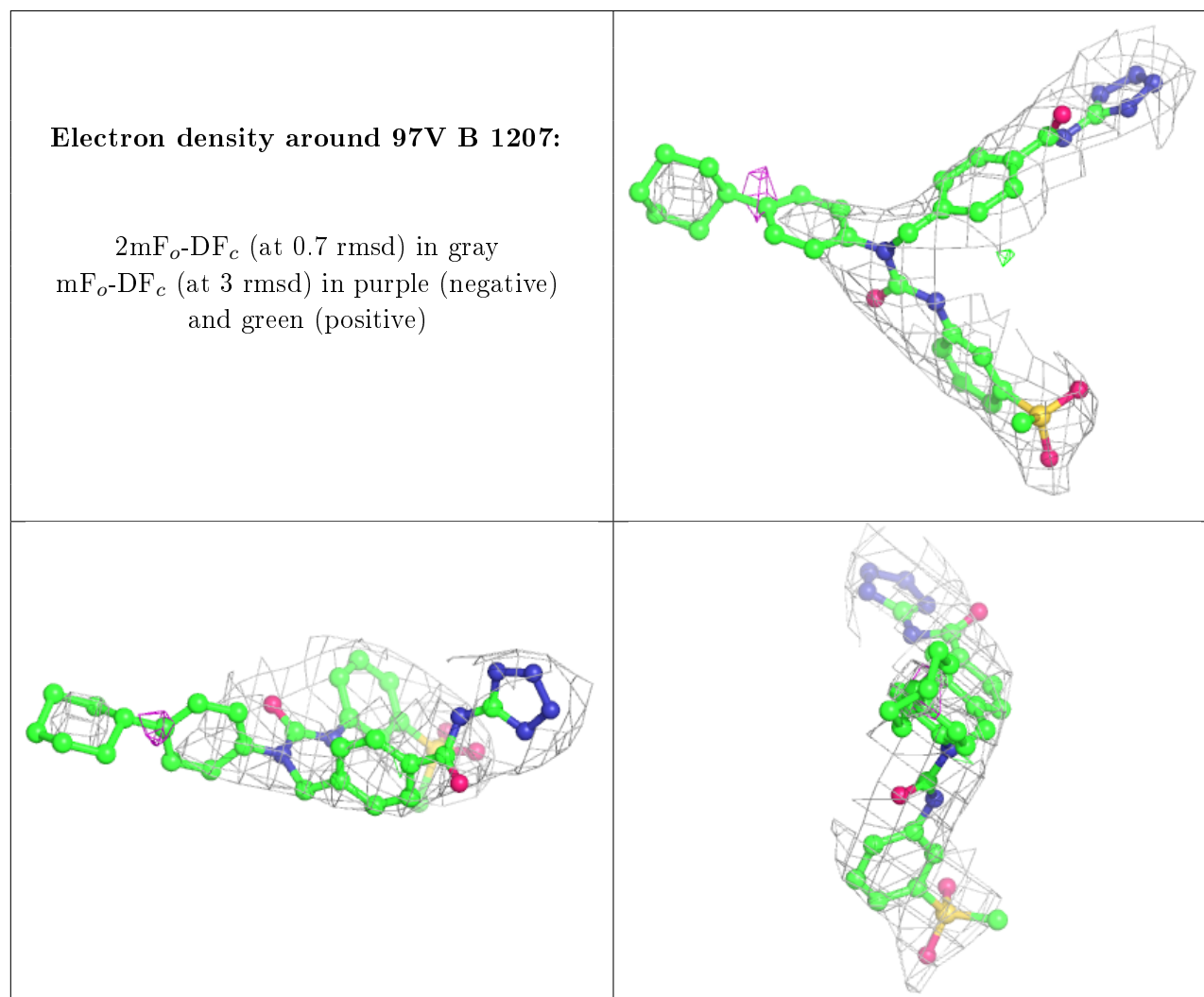


6.4 Ligands ⓘ

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, 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.

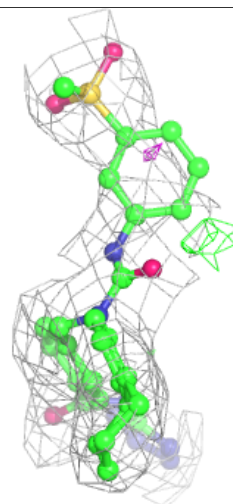
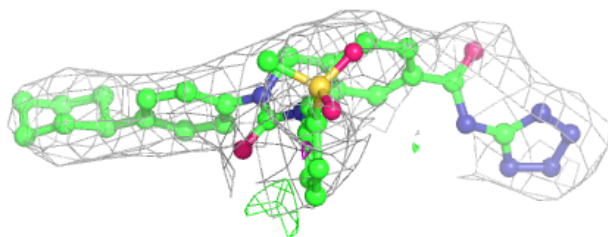
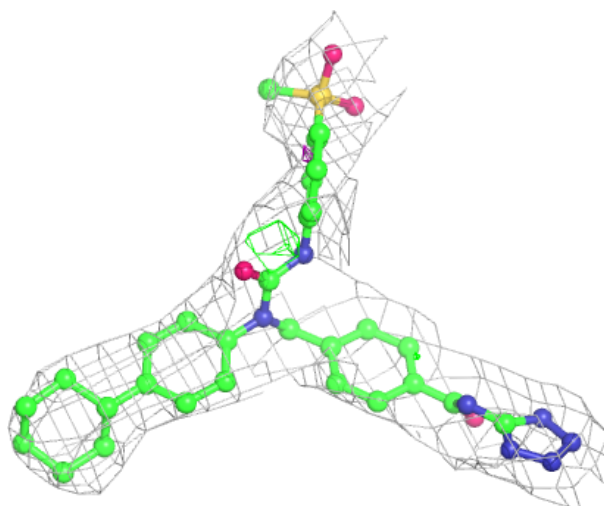
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	97V	B	1207	41/41	0.86	0.30	133,146,153,154	0
6	97V	A	1208	41/41	0.87	0.23	83,107,140,141	0
5	NAG	B	1203	14/15	0.92	0.20	62,64,68,70	0
5	NAG	B	1204	14/15	0.94	0.28	67,70,72,72	0
5	NAG	A	1201	14/15	0.95	0.16	61,64,65,65	0

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 97V A 1208:

$2mF_o-DF_c$ (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.