



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 09:21 AM BST

PDB ID : 1N5M  
Title : Crystal structure of the mouse acetylcholinesterase-gallamine complex  
Authors : Bourne, Y.; Taylor, P.; Radic, Z.; Marchot, P.  
Deposited on : 2002-11-06  
Resolution : 2.20 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](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

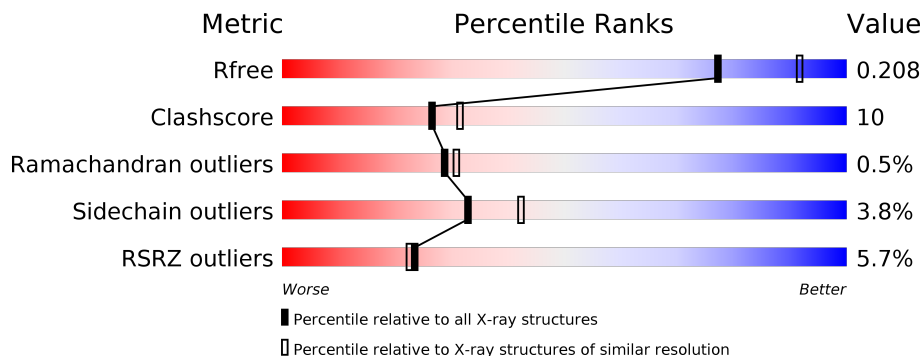
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*




The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	541	 6% 78% 19% ..
1	B	541	 6% 78% 18% ..
2	C	2	 50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IOD	A	990	-	-	X	-
5	GMN	A	951	-	X	-	-

## 2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 8970 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 acetylcholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	536	4184	2683	726	761	14	0	0	0
1	B	531	4143	2662	715	752	14	0	0	0

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

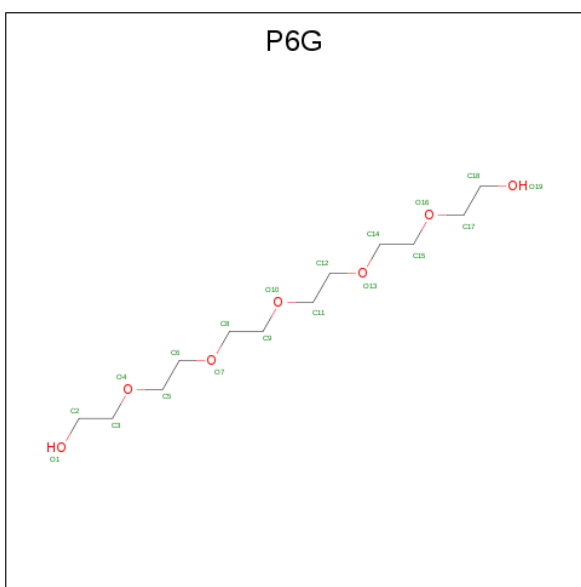


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	24	14	1	9	0	0	0

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

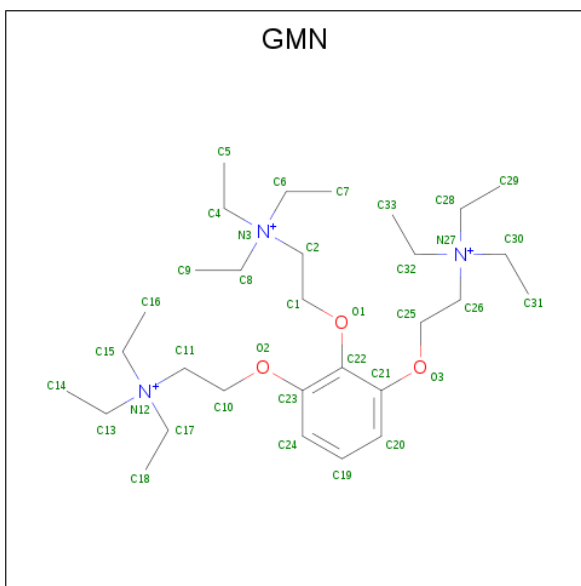
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	4	Total I 4 4	0	0
3	A	6	Total I 6 6	0	0

- Molecule 4 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C O	0	0
			19	12 7		

- Molecule 5 is 2,2',2''-[1,2,3-BENZENE-TRIYLTRIS(OXY)]TRIS[N,N,N-TRIETHYLETHANAMINIUM] (three-letter code: GMN) (formula:  $C_{30}H_{60}N_3O_3$ ).



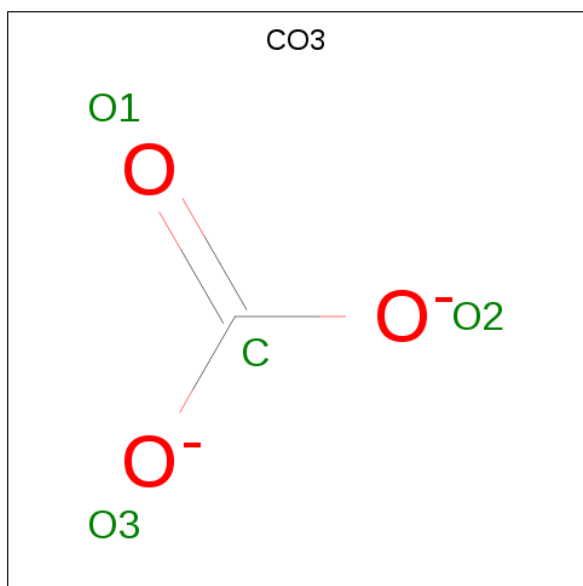
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C O	0	0
			9	6 3		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



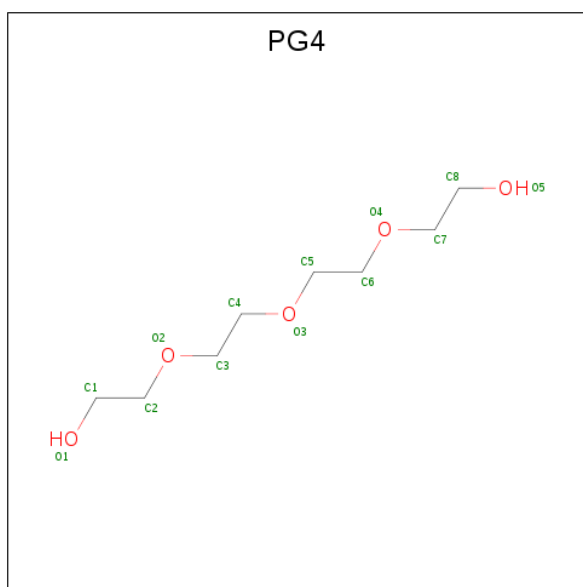
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
6	B	1	14	8	1	5	0	0

- Molecule 7 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	B	1	4	1	3	0	0

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			12	8	4		

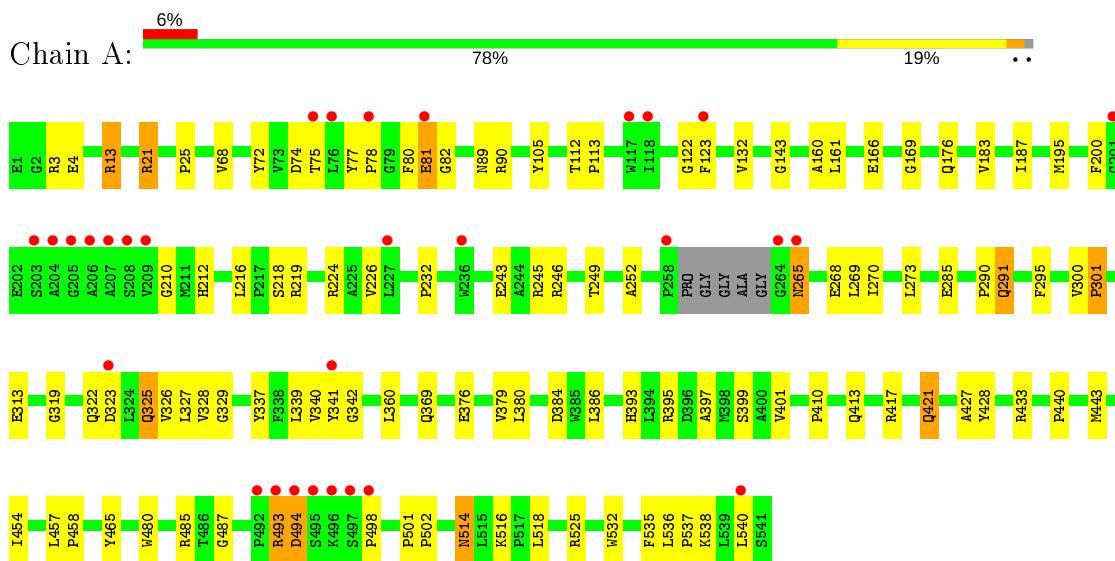
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	302	Total	O	0	0
			302	302		
9	B	249	Total	O	0	0
			249	249		

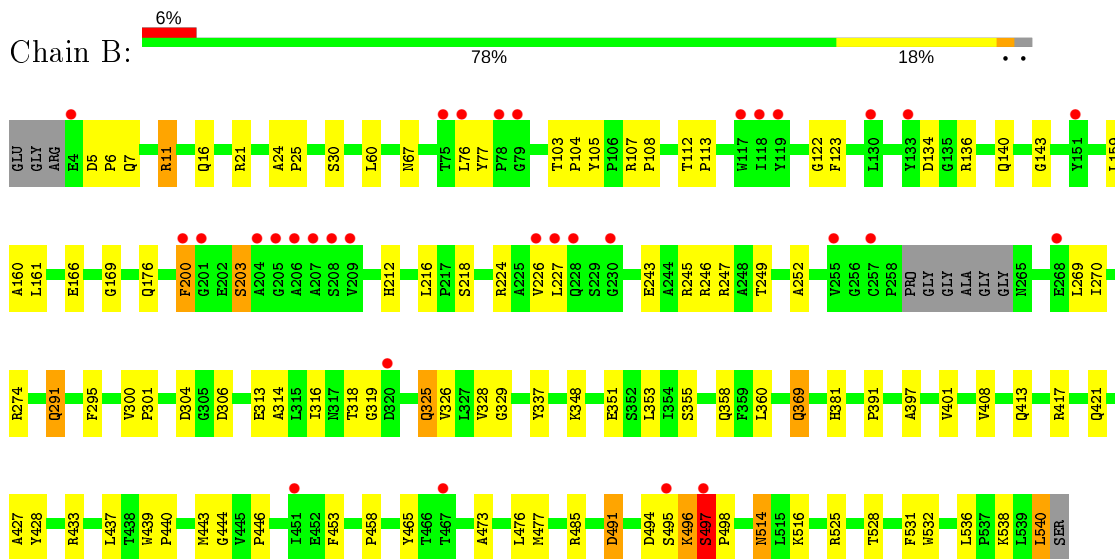
### 3 Residue-property plots [i](#)

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: acetylcholinesterase



- Molecule 1: acetylcholinesterase



- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.07Å 110.36Å 227.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.04 – 2.20 39.57 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.04-2.20) 99.0 (39.57-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.74 (at 2.20Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.198 , 0.213 0.190 , 0.208	Depositor DCC
$R_{free}$ test set	2010 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.4	Xtrriage
Anisotropy	0.833	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8970	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CO3, GMN, PG4, FUC, P6G, IOD, 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	0.66	0/4308	0.79	2/5885 (0.0%)
1	B	0.62	0/4267	0.77	0/5834
All	All	0.64	0/8575	0.78	2/11719 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	A	395	ARG	NE-CZ-NH2	-5.34	117.63	120.30

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	4184	0	4069	83	0
1	B	4143	0	4025	87	0
2	C	24	0	22	0	0
3	A	6	0	0	4	0
3	B	4	0	0	1	0
4	A	19	0	26	2	0
5	A	9	0	3	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	14	0	13	0	0
7	B	4	0	0	1	0
8	B	12	0	15	0	0
9	A	302	0	0	11	0
9	B	249	0	0	3	0
All	All	8970	0	8173	170	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 10.

All (170) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:ARG:HG3	9:A:1692:HOH:O	1.62	0.97
1:B:497:SER:HB2	1:B:498:PRO:C	1.90	0.92
1:B:30:SER:HB2	1:B:103:THR:HG22	1.54	0.88
1:A:313:GLU:HG2	9:A:1700:HOH:O	1.71	0.88
1:B:161:LEU:HD12	1:B:270:ILE:HD11	1.54	0.86
1:A:245:ARG:O	1:A:249:THR:HG23	1.78	0.82
1:B:245:ARG:O	1:B:249:THR:HG23	1.78	0.82
1:B:113:PRO:HG3	1:B:485:ARG:HG2	1.62	0.81
1:A:72:TYR:CE1	5:A:951:GMN:H19	2.15	0.81
1:B:369:GLN:HG2	9:B:1828:HOH:O	1.81	0.79
1:A:21:ARG:NH2	3:A:991:IOD:I	2.87	0.78
1:A:113:PRO:HG2	1:A:485:ARG:HG2	1.69	0.75
1:B:497:SER:HB2	1:B:498:PRO:O	1.87	0.75
1:A:72:TYR:HE1	5:A:951:GMN:H19	1.54	0.72
1:B:203:SER:OG	7:B:904:CO3:C	2.38	0.72
1:A:376:GLU:HG2	1:B:538:LYS:HE3	1.72	0.71
1:A:325:GLN:HE21	1:A:487:GLY:HA3	1.55	0.71
1:B:212:HIS:HD2	1:B:218:SER:OG	1.75	0.68
1:A:13:ARG:NH2	9:A:1625:HOH:O	2.28	0.67
1:B:224:ARG:HD3	1:B:325:GLN:HE21	1.60	0.66
1:A:75:THR:O	1:A:78:PRO:HD3	1.96	0.66
1:A:393:HIS:HB2	9:A:1540:HOH:O	1.97	0.65
1:B:491:ASP:HB3	1:B:494:ASP:HB3	1.80	0.64
1:B:514:ASN:ND2	1:B:516:LYS:H	1.94	0.63
1:A:537:PRO:O	1:A:540:LEU:HB3	1.98	0.63
1:A:243:GLU:OE1	1:A:246:ARG:NH1	2.32	0.62
1:A:161:LEU:HD12	1:A:270:ILE:HD11	1.81	0.62
1:B:408:VAL:HG11	1:B:525:ARG:HG3	1.81	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:LYS:C	1:A:540:LEU:H	2.03	0.61
1:B:514:ASN:HD22	1:B:516:LYS:H	1.48	0.61
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.36	0.61
1:A:433:ARG:HD3	9:A:1542:HOH:O	2.01	0.61
1:B:7:GLN:O	1:B:107:ARG:NH1	2.34	0.60
1:B:224:ARG:HG2	1:B:325:GLN:NE2	2.16	0.60
1:B:161:LEU:HD12	1:B:270:ILE:CD1	2.28	0.60
1:A:393:HIS:HD2	9:A:1617:HOH:O	1.86	0.59
1:A:166:GLU:HB2	1:A:270:ILE:HD13	1.84	0.59
1:B:514:ASN:HD22	1:B:514:ASN:C	2.07	0.58
1:B:353:LEU:HB3	1:B:391:PRO:HB2	1.86	0.58
1:A:413:GLN:O	1:A:417:ARG:HG2	2.03	0.58
1:B:497:SER:HB2	1:B:498:PRO:CA	2.33	0.58
1:B:319:GLY:O	1:B:421:GLN:HG3	2.03	0.58
1:B:495:SER:O	1:B:496:LYS:O	2.23	0.57
1:B:166:GLU:HG2	1:B:270:ILE:HD13	1.86	0.57
1:A:265:ASN:OD1	1:A:268:GLU:HG3	2.05	0.57
1:B:30:SER:HB2	1:B:103:THR:CG2	2.29	0.57
1:A:291:GLN:NE2	3:A:990:IOD:I	3.08	0.55
1:B:355:SER:OG	1:B:358:GLN:HG3	2.07	0.55
1:B:224:ARG:HD3	1:B:325:GLN:NE2	2.22	0.55
1:A:212:HIS:HD2	1:A:218:SER:OG	1.92	0.53
1:A:224:ARG:HD3	1:A:325:GLN:NE2	2.24	0.53
1:A:360:LEU:HD22	1:A:379:VAL:HG21	1.90	0.53
1:A:243:GLU:CD	1:A:246:ARG:NH1	2.62	0.53
1:A:77:TYR:OH	1:A:340:VAL:HG11	2.07	0.53
1:A:75:THR:HG22	1:A:75:THR:O	2.09	0.52
1:B:514:ASN:HD22	1:B:516:LYS:N	2.08	0.52
1:A:195:MET:HE3	9:A:1679:HOH:O	2.09	0.52
1:B:24:ALA:HB3	1:B:140:GLN:HG3	1.90	0.52
1:B:313:GLU:OE2	1:B:316:ILE:HD11	2.09	0.52
1:A:326:VAL:HG12	1:A:328:VAL:HG13	1.91	0.51
1:B:538:LYS:C	1:B:540:LEU:H	2.14	0.51
1:B:413:GLN:O	1:B:417:ARG:HG2	2.10	0.51
1:A:514:ASN:HD22	1:A:516:LYS:H	1.58	0.51
1:A:300:VAL:HB	1:A:301:PRO:HD2	1.93	0.51
1:A:339:LEU:HD11	1:A:399:SER:HA	1.93	0.51
1:B:104:PRO:HG2	1:B:108:PRO:HG3	1.93	0.51
1:A:112:THR:HG21	1:A:143:GLY:O	2.11	0.50
1:B:328:VAL:O	1:B:427:ALA:HA	2.11	0.50
1:B:497:SER:CB	1:B:498:PRO:CA	2.89	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:THR:HG21	1:B:143:GLY:O	2.11	0.50
1:A:243:GLU:OE2	1:A:246:ARG:NH1	2.44	0.50
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.47	0.50
1:B:314:ALA:O	1:B:318:THR:HG23	2.12	0.50
1:B:319:GLY:O	1:B:421:GLN:CG	2.60	0.50
1:A:25:PRO:HD3	9:A:1598:HOH:O	2.12	0.50
1:B:532:TRP:CE3	1:B:536:LEU:HD12	2.47	0.50
1:B:122:GLY:O	1:B:123:PHE:HB2	2.12	0.49
1:B:444:GLY:O	1:B:446:PRO:HD3	2.13	0.49
1:A:291:GLN:HE22	1:A:369:GLN:NE2	2.11	0.49
1:A:74:ASP:HB2	9:A:1587:HOH:O	2.13	0.49
1:B:166:GLU:HG2	1:B:270:ILE:CD1	2.43	0.48
1:A:176:GLN:OE1	1:A:212:HIS:HE1	1.96	0.48
1:B:433:ARG:CZ	1:B:437:LEU:HD23	2.43	0.48
1:A:340:VAL:O	1:A:340:VAL:HG12	2.12	0.47
1:A:161:LEU:HD11	1:A:269:LEU:HD22	1.97	0.47
1:B:243:GLU:O	1:B:247:ARG:HG3	2.15	0.47
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.49	0.47
1:A:369:GLN:HB2	9:A:1754:HOH:O	2.14	0.47
1:A:493:ARG:HB2	1:A:494:ASP:H	1.51	0.47
1:A:540:LEU:HD12	1:A:540:LEU:C	2.35	0.47
1:B:491:ASP:CB	1:B:494:ASP:HB3	2.45	0.47
1:B:76:LEU:HG	1:B:77:TYR:CE2	2.50	0.47
1:A:89:ASN:O	1:A:90:ARG:NH1	2.42	0.47
1:B:351:GLU:OE2	1:B:351:GLU:HA	2.14	0.46
1:A:74:ASP:OD1	1:A:341:TYR:HE2	1.98	0.46
1:A:433:ARG:NH2	1:A:440:PRO:O	2.48	0.46
1:A:81:GLU:HB2	9:A:1548:HOH:O	2.15	0.46
3:A:1463:IOD:I	5:A:951:GMN:O3	3.03	0.46
1:A:328:VAL:O	1:A:427:ALA:HA	2.15	0.46
1:B:514:ASN:HD21	1:B:516:LYS:HB2	1.81	0.46
1:A:252:ALA:HA	1:A:273:LEU:HD21	1.97	0.45
1:A:21:ARG:HG3	1:A:105:TYR:CE1	2.52	0.45
1:A:337:TYR:HA	1:A:443:MET:HE1	1.98	0.45
1:B:224:ARG:HG3	1:B:224:ARG:NH1	2.31	0.45
1:B:77:TYR:CD1	1:B:348:LYS:HE3	2.51	0.45
1:B:453:PHE:HB3	1:B:476:LEU:HD12	1.98	0.45
1:A:122:GLY:O	1:A:123:PHE:HB2	2.15	0.45
1:A:300:VAL:HB	1:A:301:PRO:CD	2.46	0.45
1:A:319:GLY:O	1:A:421:GLN:CG	2.65	0.45
1:B:103:THR:HG23	1:B:104:PRO:O	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:SER:O	1:B:496:LYS:C	2.55	0.45
1:B:300:VAL:HB	1:B:301:PRO:HD2	1.99	0.45
1:A:514:ASN:ND2	1:A:516:LYS:H	2.14	0.45
1:A:68:VAL:HG23	1:A:90:ARG:HB2	1.98	0.45
1:A:80:PHE:CE2	1:A:82:GLY:HA3	2.52	0.45
1:B:67:ASN:ND2	9:B:1617:HOH:O	2.46	0.45
1:A:161:LEU:HA	1:A:161:LEU:HD23	1.85	0.44
1:A:384:ASP:OD1	1:A:384:ASP:C	2.55	0.44
1:A:322:GLN:O	1:A:323:ASP:HB2	2.17	0.44
1:A:329:GLY:HA3	1:A:428:TYR:CZ	2.52	0.44
1:A:210:GLY:HA3	1:A:232:PRO:HD3	1.98	0.44
1:A:200:PHE:CB	1:A:226:VAL:HB	2.48	0.44
1:B:134:ASP:OD1	1:B:136:ARG:HD2	2.16	0.44
1:B:200:PHE:CB	1:B:226:VAL:HB	2.47	0.44
1:A:376:GLU:O	1:A:380:LEU:HG	2.17	0.44
1:B:200:PHE:HB2	1:B:226:VAL:HB	2.00	0.44
1:B:337:TYR:HA	1:B:443:MET:CE	2.47	0.44
1:A:498:PRO:HG2	1:A:518:LEU:HB2	2.00	0.44
1:B:176:GLN:OE1	1:B:212:HIS:HE1	2.00	0.44
1:B:252:ALA:HB2	1:B:269:LEU:HD21	1.99	0.44
1:A:514:ASN:C	1:A:514:ASN:HD22	2.20	0.43
1:B:528:THR:O	1:B:531:PHE:HB3	2.18	0.43
1:A:200:PHE:HB2	1:A:226:VAL:HB	2.01	0.43
1:A:457:LEU:N	1:A:458:PRO:CD	2.82	0.42
1:B:224:ARG:HH11	1:B:325:GLN:HE22	1.65	0.42
1:A:219:ARG:HD2	1:A:219:ARG:HA	1.78	0.42
1:A:397:ALA:O	1:A:401:VAL:HG23	2.19	0.42
1:B:473:ALA:O	1:B:477:MET:HG3	2.19	0.42
1:B:5:ASP:HA	1:B:6:PRO:HD2	1.89	0.42
1:B:11:ARG:NH1	1:B:16:GLN:CG	2.83	0.42
1:B:397:ALA:O	1:B:401:VAL:HG23	2.20	0.42
1:A:160:ALA:HB2	1:A:169:GLY:HA2	2.02	0.42
1:A:428:TYR:CD1	1:A:428:TYR:C	2.93	0.42
1:A:454:ILE:HD12	1:A:480:TRP:CE2	2.55	0.42
1:B:304:ASP:OD2	1:B:306:ASP:HB3	2.19	0.42
4:A:901:P6G:H182	1:B:381:HIS:HE1	1.85	0.42
1:B:104:PRO:CG	1:B:108:PRO:HG3	2.49	0.42
1:B:291:GLN:NE2	3:B:1335:IOD:I	3.23	0.42
1:B:159:LEU:HD23	1:B:159:LEU:C	2.41	0.41
1:B:536:LEU:HD23	1:B:536:LEU:HA	1.76	0.41
1:A:532:TRP:CE3	1:A:536:LEU:HD12	2.55	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:PHE:CE2	4:A:901:P6G:H112	2.56	0.41
1:B:21:ARG:HG3	1:B:105:TYR:CE1	2.56	0.41
1:B:326:VAL:HG12	1:B:328:VAL:HG13	2.03	0.41
1:A:290:PRO:HD2	3:A:990:IOD:I	2.90	0.41
1:B:439:TRP:HB3	1:B:440:PRO:HD2	2.02	0.41
1:B:161:LEU:HD12	1:B:270:ILE:CG1	2.50	0.41
1:B:227:LEU:HB2	1:B:328:VAL:HG12	2.02	0.41
1:A:337:TYR:HA	1:A:443:MET:CE	2.51	0.41
1:B:274:ARG:HD3	9:B:1782:HOH:O	2.20	0.41
1:A:183:VAL:HG13	1:A:187:ILE:HB	2.03	0.40
1:A:77:TYR:OH	1:A:340:VAL:CG1	2.69	0.40
1:B:160:ALA:HB2	1:B:169:GLY:HA2	2.02	0.40
1:B:76:LEU:HG	1:B:77:TYR:CD2	2.57	0.40
1:A:386:LEU:HA	1:A:386:LEU:HD23	1.80	0.40
1:A:501:PRO:HA	1:A:502:PRO:HD3	1.94	0.40
1:B:107:ARG:HA	1:B:108:PRO:HD3	1.96	0.40
1:B:291:GLN:HE21	1:B:291:GLN:HB2	1.53	0.40
1:B:514:ASN:ND2	1:B:516:LYS:N	2.63	0.40
1:B:269:LEU:C	1:B:269:LEU:HD23	2.42	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	532/541 (98%)	514 (97%)	15 (3%)	3 (1%)	25 26
1	B	527/541 (97%)	509 (97%)	16 (3%)	2 (0%)	34 37
All	All	1059/1082 (98%)	1023 (97%)	31 (3%)	5 (0%)	29 31

All (5) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	494	ASP
1	B	497	SER
1	B	496	LYS
1	A	493	ARG
1	A	342	GLY

### 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	440/442 (100%)	423 (96%)	17 (4%)	32	41
1	B	436/442 (99%)	420 (96%)	16 (4%)	34	43
All	All	876/884 (99%)	843 (96%)	33 (4%)	33	42

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	4	GLU
1	A	21	ARG
1	A	81	GLU
1	A	132	VAL
1	A	216	LEU
1	A	265	ASN
1	A	285	GLU
1	A	291	GLN
1	A	295	PHE
1	A	301	PRO
1	A	325	GLN
1	A	327	LEU
1	A	410	PRO
1	A	421	GLN
1	A	514	ASN
1	A	525	ARG
1	B	11	ARG
1	B	25	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	60	LEU
1	B	200	PHE
1	B	203	SER
1	B	216	LEU
1	B	246	ARG
1	B	291	GLN
1	B	295	PHE
1	B	325	GLN
1	B	360	LEU
1	B	369	GLN
1	B	491	ASP
1	B	497	SER
1	B	514	ASN
1	B	540	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	HIS
1	A	284	HIS
1	A	291	GLN
1	A	325	GLN
1	A	508	GLN
1	A	514	ASN
1	B	212	HIS
1	B	291	GLN
1	B	325	GLN
1	B	514	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

2 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
2	NAG	C	1	1,2	14,14,15	0.83	0	17,19,21	0.97	1 (5%)
2	FUC	C	2	2	10,10,11	0.67	0	14,14,16	0.47	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
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	FUC	C	2	2	-	-	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	C	1	NAG	C2-N2-C7	-2.10	119.91	122.90

There are no chirality outliers.

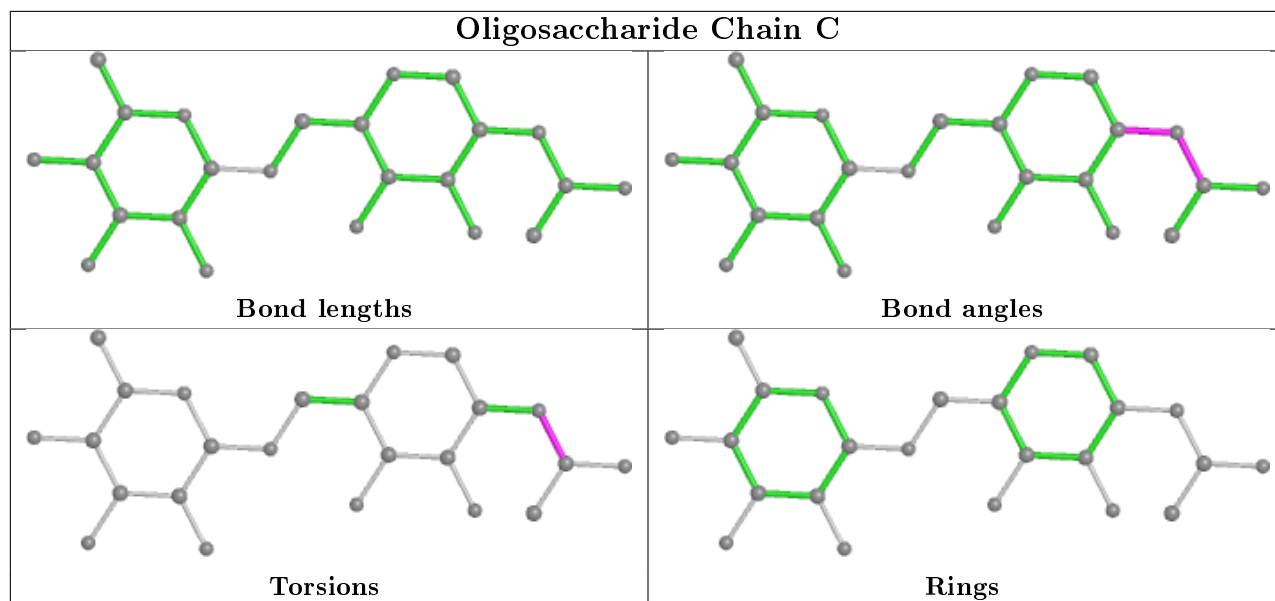
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2

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](#)

Of 15 ligands modelled in this entry, 10 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
7	CO3	B	904	-	0,3,3	0.00	-	0,3,3	0.00	-
6	NAG	B	601	1	14,14,15	0.99	1 (7%)	17,19,21	1.15	2 (11%)
4	P6G	A	901	-	18,18,18	2.17	6 (33%)	17,17,17	0.96	0
5	GMN	A	951	-	9,9,36	5.89	7 (77%)	12,12,48	2.18	3 (25%)
8	PG4	B	902	-	11,11,12	2.15	3 (27%)	10,10,11	1.08	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
6	NAG	B	601	1	-	3/6/23/26	0/1/1/1
4	P6G	A	901	-	-	5/16/16/16	-

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GMN	A	951	-	-	-	0/1/1/1
8	PG4	B	902	-	-	4/9/9/10	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	951	GMN	C21-C22	12.46	1.55	1.40
5	A	951	GMN	C23-C22	6.98	1.48	1.40
5	A	951	GMN	C20-C21	6.70	1.51	1.39
5	A	951	GMN	C19-C24	5.34	1.50	1.38
8	B	902	PG4	O4-C6	4.69	1.62	1.42
4	A	901	P6G	O10-C9	4.17	1.60	1.42
5	A	951	GMN	O3-C21	3.85	1.44	1.36
4	A	901	P6G	O13-C12	3.76	1.58	1.42
8	B	902	PG4	O2-C2	3.62	1.57	1.42
4	A	901	P6G	O4-C3	3.42	1.56	1.42
4	A	901	P6G	O16-C15	3.41	1.56	1.42
4	A	901	P6G	O19-C18	3.23	1.58	1.42
5	A	951	GMN	C24-C23	3.05	1.44	1.39
8	B	902	PG4	O3-C4	2.68	1.53	1.42
4	A	901	P6G	O7-C6	2.51	1.52	1.42
6	B	601	NAG	C1-C2	2.22	1.55	1.52
5	A	951	GMN	O2-C23	2.16	1.40	1.36

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	951	GMN	C24-C23-C22	-4.21	115.75	120.06
5	A	951	GMN	C23-C22-C21	4.03	122.08	119.51
5	A	951	GMN	C19-C24-C23	2.98	123.81	120.05
6	B	601	NAG	C1-C2-N2	2.72	115.14	110.49
6	B	601	NAG	C1-O5-C5	2.04	114.96	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	601	NAG	C8-C7-N2-C2
6	B	601	NAG	O7-C7-N2-C2
8	B	902	PG4	O3-C5-C6-O4
8	B	902	PG4	C5-C6-O4-C7

Continued on next page...

Continued from previous page...

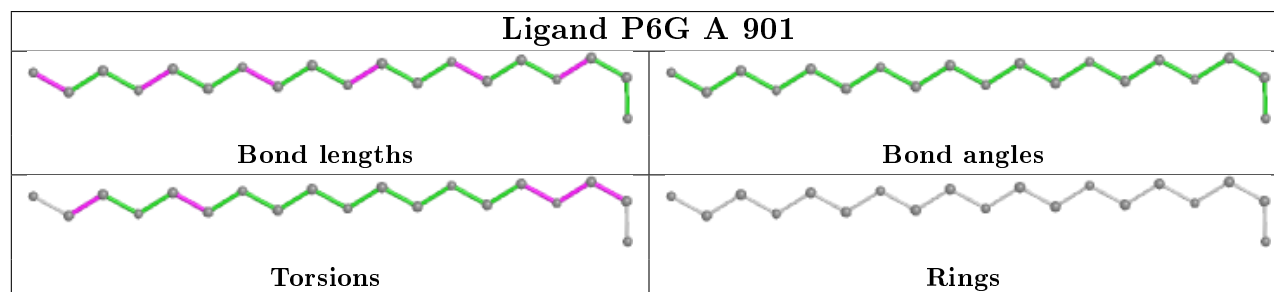
Mol	Chain	Res	Type	Atoms
8	B	902	PG4	O1-C1-C2-O2
4	A	901	P6G	O13-C14-C15-O16
6	B	601	NAG	C1-C2-N2-C7
4	A	901	P6G	O16-C17-C18-O19
4	A	901	P6G	O1-C2-C3-O4
4	A	901	P6G	C6-C5-O4-C3
8	B	902	PG4	C4-C3-O2-C2
4	A	901	P6G	C2-C3-O4-C5

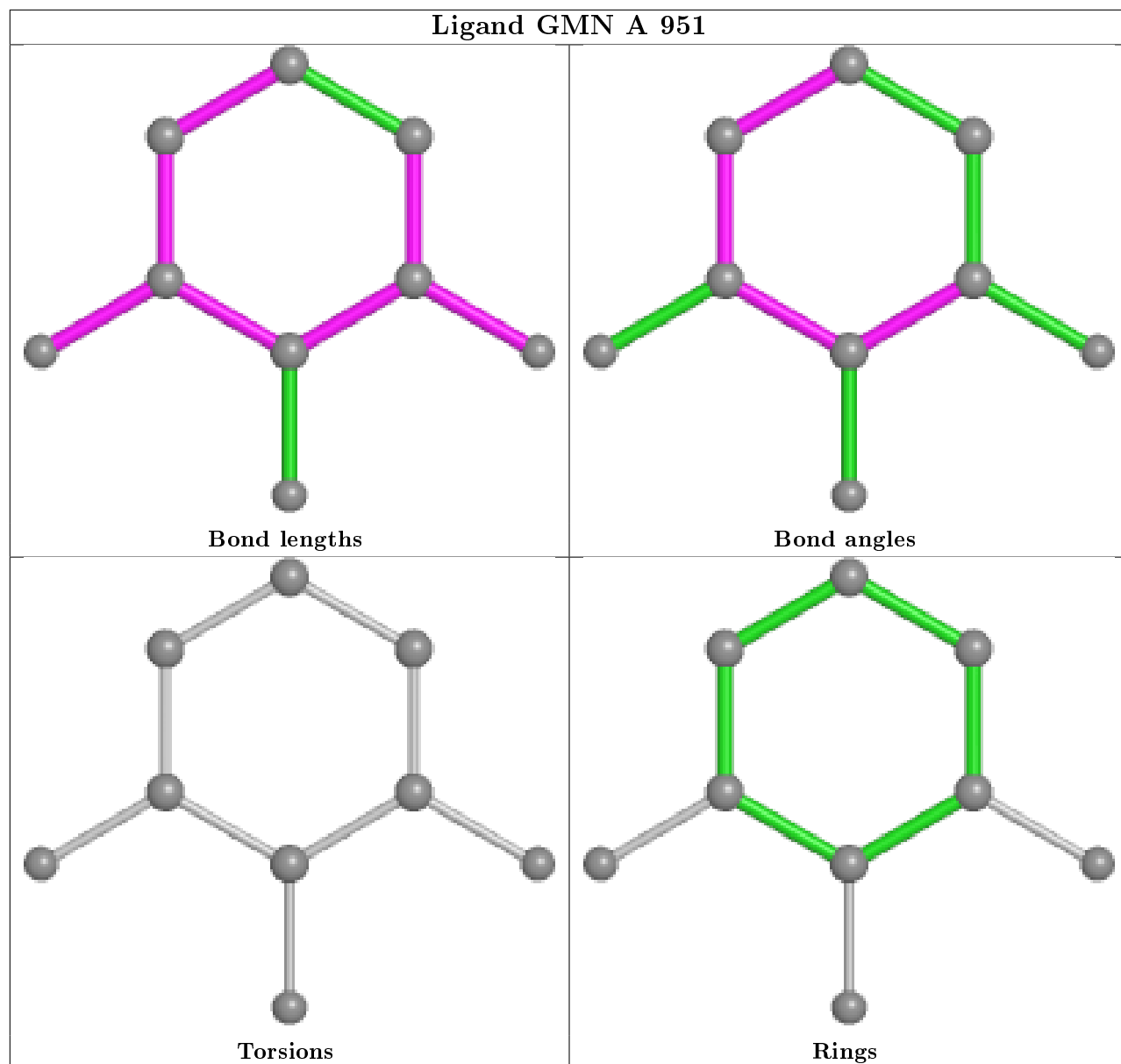
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	904	CO3	1	0
4	A	901	P6G	2	0
5	A	951	GMN	3	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, 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	536/541 (99%)	-0.07	30 (5%) 24 23	29, 42, 70, 97	0
1	B	531/541 (98%)	0.04	31 (5%) 23 22	29, 44, 70, 86	0
All	All	1067/1082 (98%)	-0.02	61 (5%) 23 22	29, 43, 70, 97	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	495	SER	6.6
1	A	496	LYS	6.2
1	B	118	ILE	4.8
1	A	497	SER	4.4
1	A	76	LEU	4.4
1	B	117	TRP	4.3
1	A	493	ARG	4.1
1	A	264	GLY	3.8
1	A	494	ASP	3.8
1	A	492	PRO	3.8
1	B	204	ALA	3.6
1	A	341	TYR	3.6
1	A	118	ILE	3.2
1	B	200	PHE	3.2
1	A	207	ALA	3.2
1	B	257	CYS	3.1
1	A	204	ALA	3.1
1	B	201	GLY	3.1
1	A	209	VAL	3.0
1	A	75	THR	3.0
1	B	75	THR	3.0
1	B	227	LEU	2.9
1	A	206	ALA	2.9
1	B	207	ALA	2.9

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	323	ASP	2.8
1	A	123	PHE	2.8
1	B	133	TYR	2.8
1	B	119	TYR	2.6
1	B	467	THR	2.6
1	A	81	GLU	2.5
1	B	4	GLU	2.5
1	A	78	PRO	2.4
1	A	117	TRP	2.4
1	A	540	LEU	2.4
1	B	497	SER	2.4
1	B	79	GLY	2.3
1	A	236	TRP	2.3
1	A	258	PRO	2.3
1	A	227	LEU	2.3
1	B	209	VAL	2.3
1	A	265	ASN	2.2
1	B	151	TYR	2.2
1	A	201	GLY	2.2
1	B	226	VAL	2.2
1	A	498	PRO	2.2
1	B	206	ALA	2.1
1	B	78	PRO	2.1
1	B	208	SER	2.1
1	B	205	GLY	2.1
1	B	255	VAL	2.1
1	B	130	LEU	2.1
1	B	230	GLY	2.1
1	B	451	ILE	2.1
1	A	205	GLY	2.1
1	B	76	LEU	2.1
1	A	203	SER	2.1
1	B	228	GLN	2.0
1	A	208	SER	2.0
1	B	320	ASP	2.0
1	B	268	GLU	2.0
1	B	495	SER	2.0

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

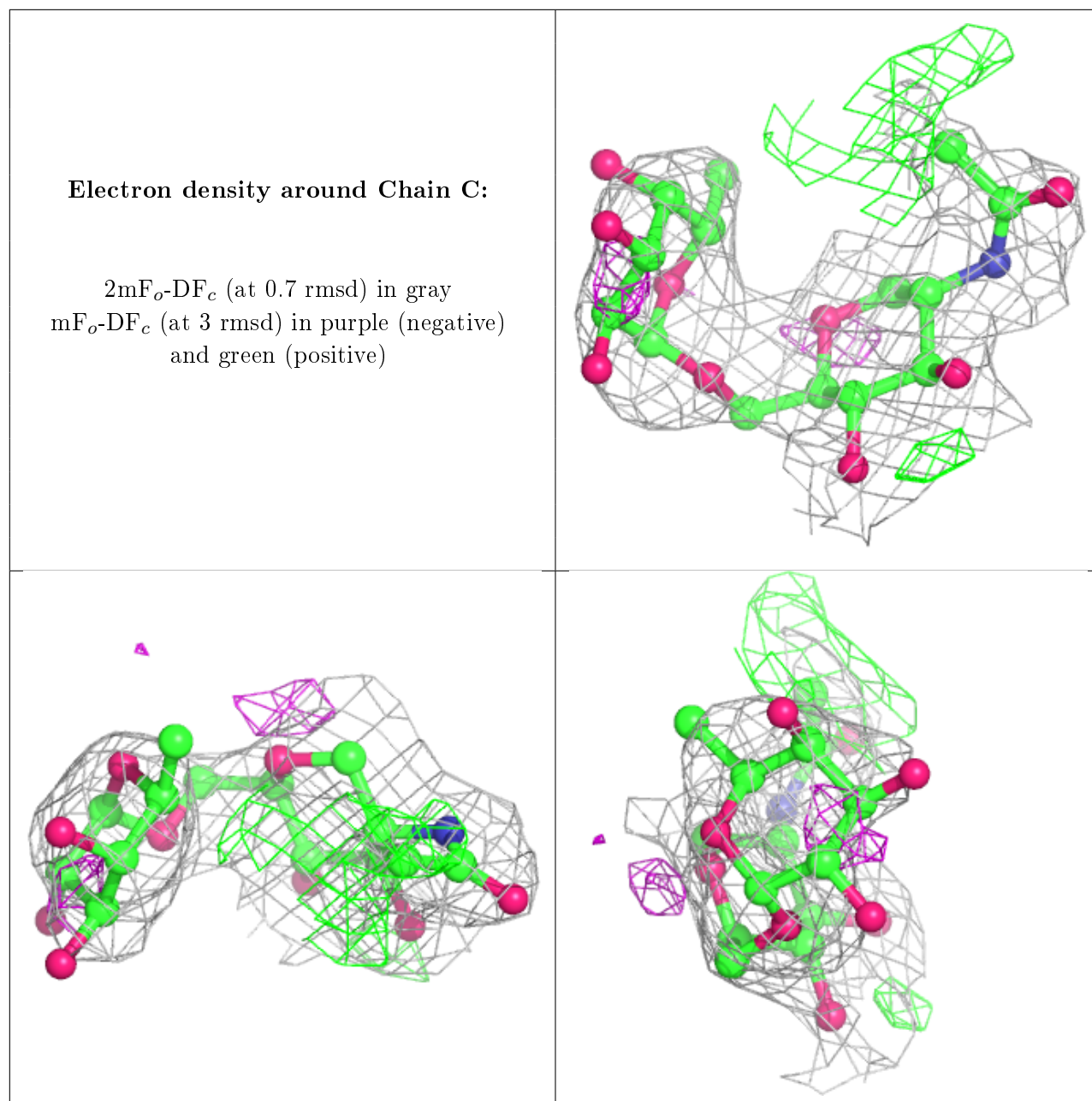
There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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(Å <sup>2</sup> )	Q<0.9
2	NAG	C	1	14/15	0.78	0.35	78,83,88,93	0
2	FUC	C	2	10/11	0.89	0.53	95,97,99,99	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.

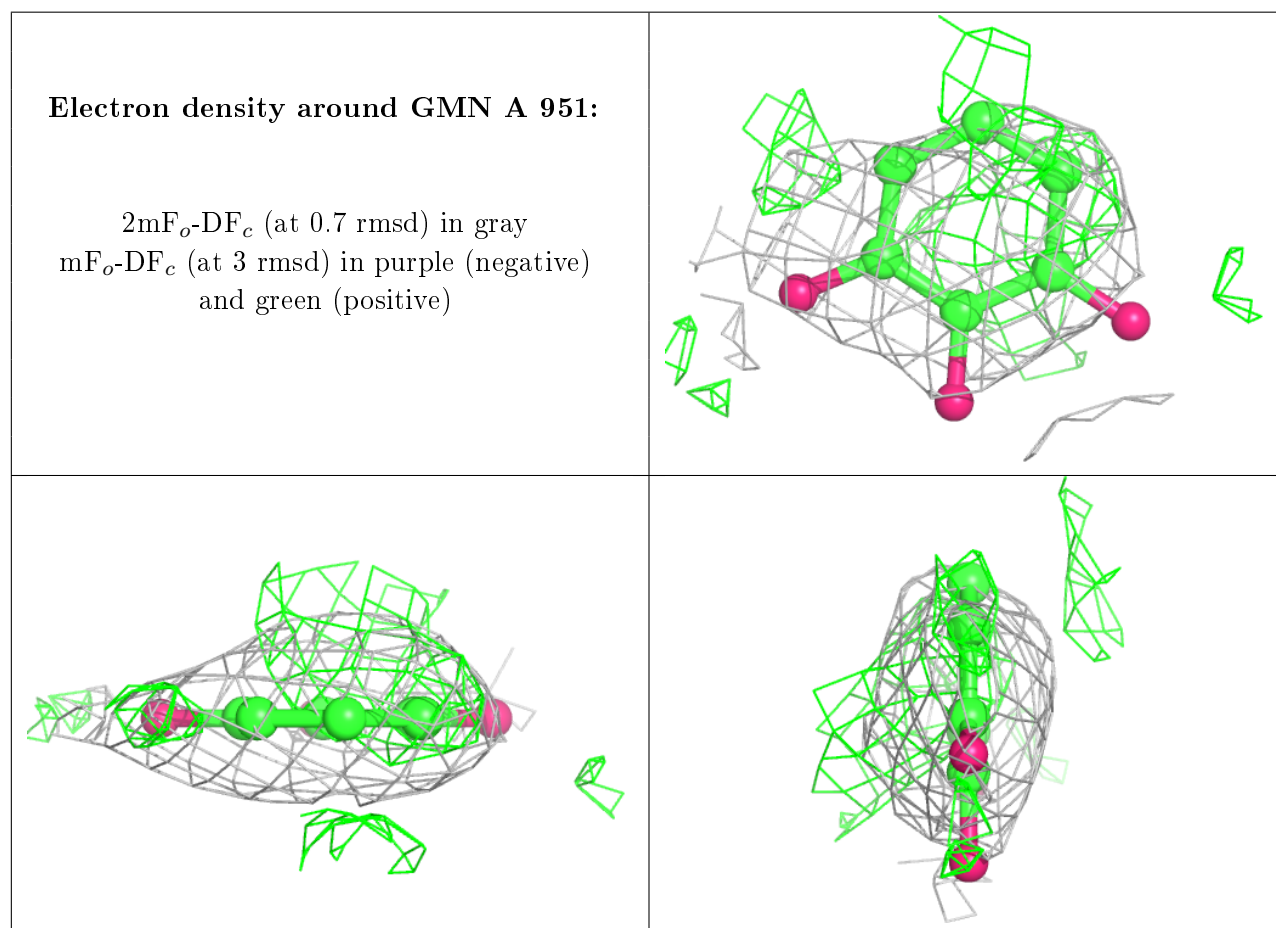
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	NAG	B	601	14/15	0.53	0.36	86,89,90,90	0
8	PG4	B	902	12/13	0.66	0.21	87,89,91,91	0
5	GMN	A	951	9/36	0.80	0.42	78,79,79,80	9

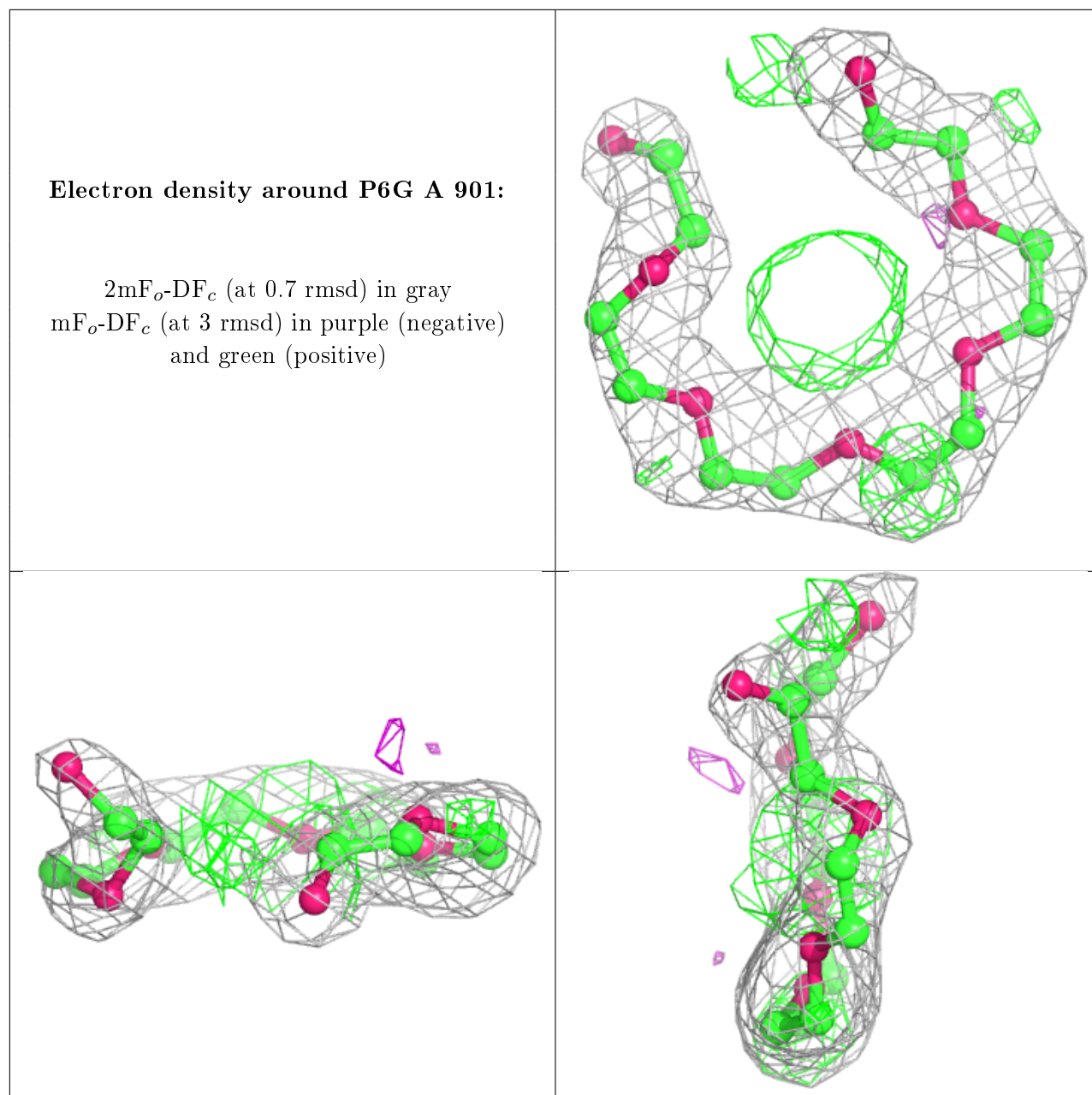
*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	IOD	A	991	1/1	0.83	0.05	80,80,80,80	1
7	CO3	B	904	4/4	0.84	0.28	60,61,61,62	0
3	IOD	B	1448	1/1	0.85	0.05	93,93,93,93	1
4	P6G	A	901	19/19	0.86	0.19	55,67,70,70	0
3	IOD	B	1485	1/1	0.95	0.08	60,60,60,60	1
3	IOD	A	1367	1/1	0.97	0.04	62,62,62,62	1
3	IOD	B	1335	1/1	0.97	0.09	51,51,51,51	1
3	IOD	A	990	1/1	0.99	0.04	51,51,51,51	1
3	IOD	A	802	1/1	0.99	0.11	40,40,40,40	1
3	IOD	B	1590	1/1	0.99	0.09	57,57,57,57	1
3	IOD	A	1463	1/1	0.99	0.11	45,45,45,45	1
3	IOD	A	1243	1/1	0.99	0.10	50,50,50,50	1

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 ⓘ

There are no such residues in this entry.