Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2023 – 10:41 PM EDT

PDB ID	:	2HA2
Title	:	Crystal structure of mouse acetylcholinesterase complexed with succinylcholine
Authors	:	Bourne, Y.; Radic, Z.; Sulzenbacher, G.; Kim, E.; Taylor, P.; Marchot, P.
Deposited on	:	2006-06-12
Resolution	:	2.05 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 (i) 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 (i)) were used in the production of this report:

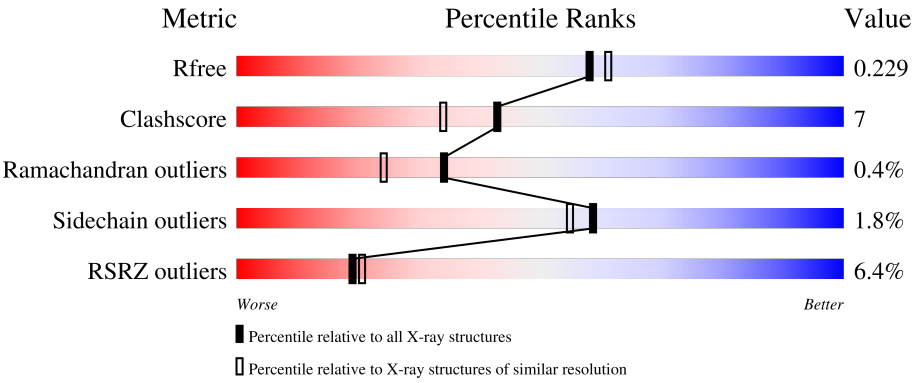
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 <=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	543	3% 85% 13%
1	B	543	9% 85% 12%
2	C	2	100%

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
2	NAG	C	2	-	-	-	X
3	FUC	A	2502	-	-	-	X
4	NAG	A	701	-	-	-	X
5	SCK	A	901[A]	-	-	X	X
5	SCK	B	951[A]	-	-	-	X
6	SCU	A	902[B]	-	-	X	X
6	SCU	B	952[B]	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 9313 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.

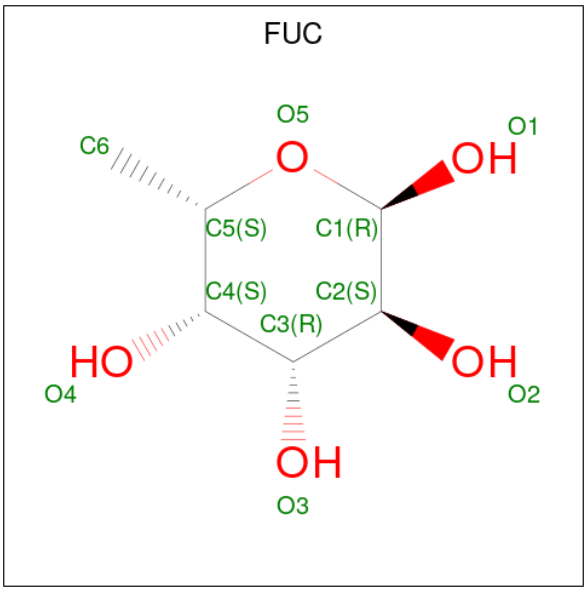
- Molecule 1 is a protein called Acetylcholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	2	0
			4202	2695	732	761	14			
1	B	534	Total	C	N	O	S	0	4	0
			4196	2694	727	760	15			

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

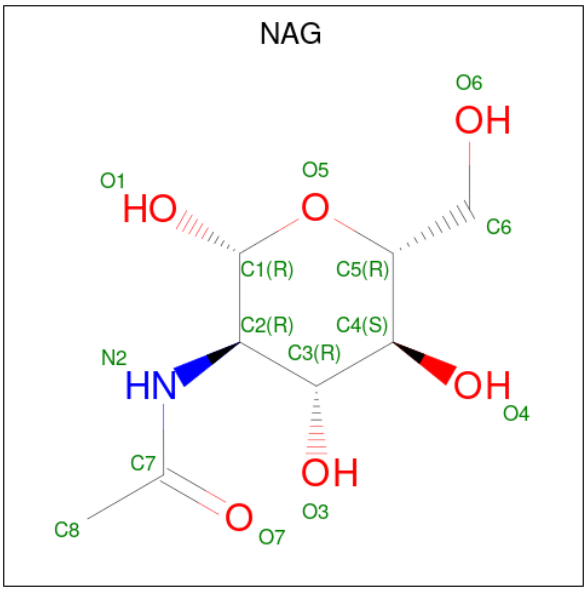
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is alpha-L-fucopyranose (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



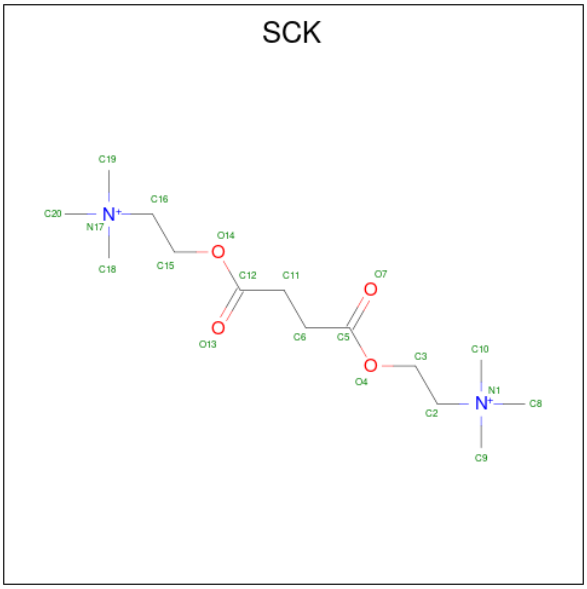
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 6 4	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



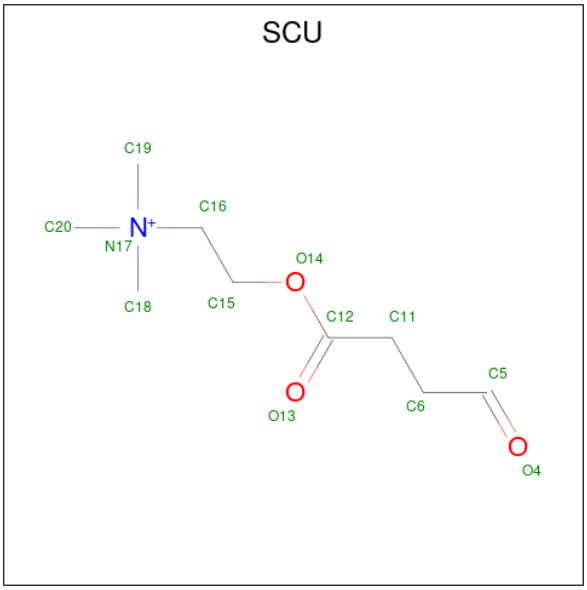
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is 2,2'-[(1,4-DIOXOBUTANE-1,4-DIYL)BIS(OXY)]BIS(N,N,N-TRIMETHYLE THANAMINIUM) (three-letter code: SCK) (formula: $C_{14}H_{30}N_2O_4$).



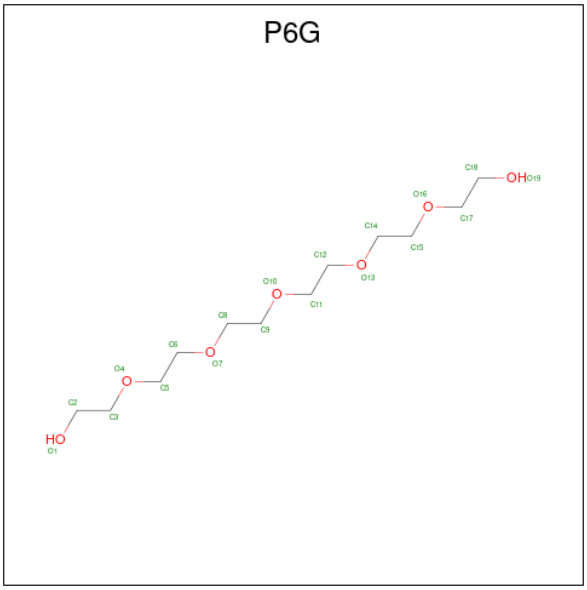
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	1
			20	14	2	4		
5	B	1	Total	C	N	O	0	1
			20	14	2	4		

- Molecule 6 is N,N,N-TRIMETHYL-2-[(4-OXOBUTANOYL)OXY]ETHANAMINIUM (three-letter code: SCU) (formula: $C_9H_{18}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 13 9 1 3	0	1
6	B	1	Total C N O 13 9 1 3	0	1

- Molecule 7 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



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

- Molecule 8 is water.

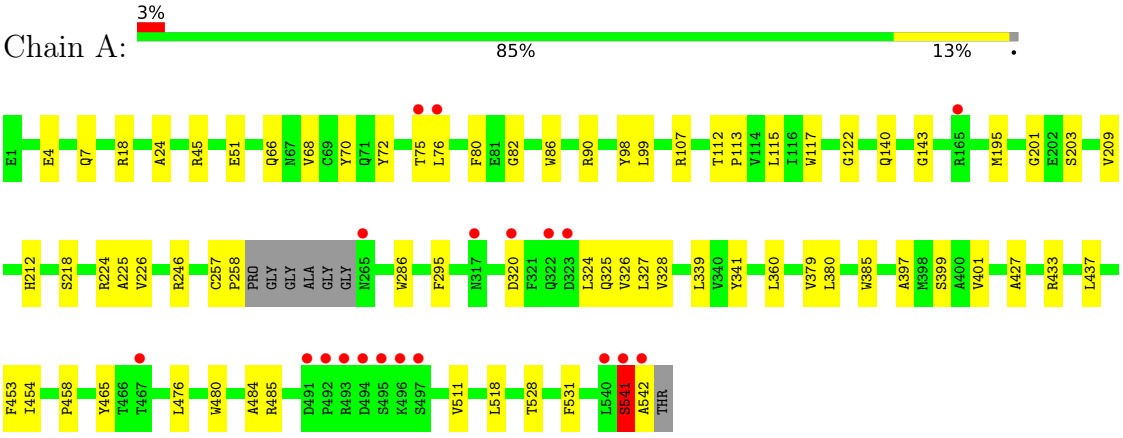
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	430	Total O 430 430	0	0
8	B	334	Total O 334 334	0	0

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.

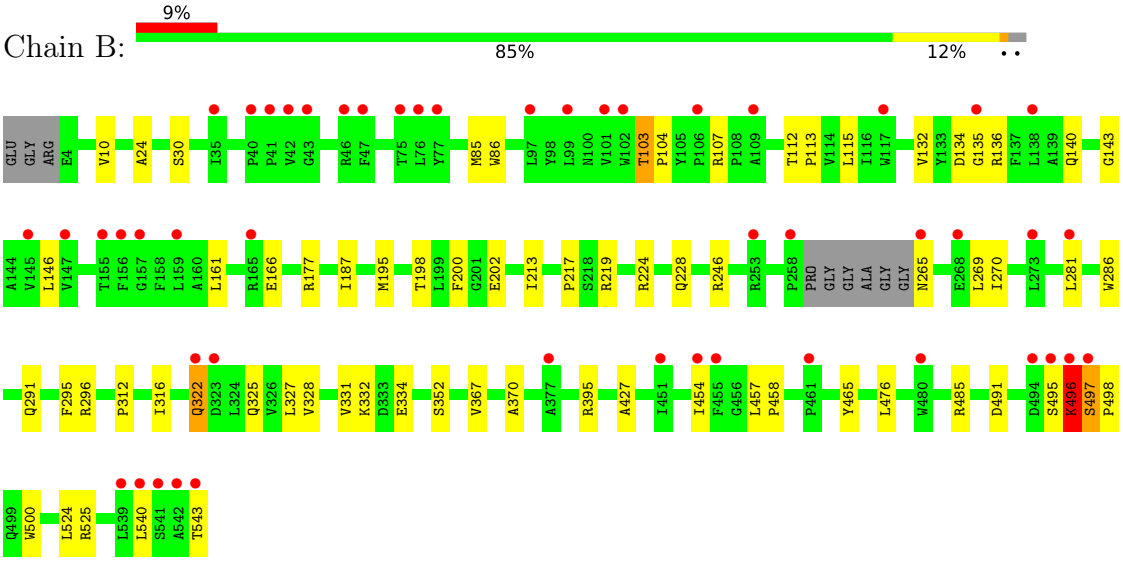
• Molecule 1: Acetylcholinesterase

Chain A:



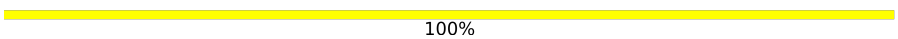
• Molecule 1: Acetylcholinesterase

Chain B:



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

Chain C:




NAG1
NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.94Å 110.49Å 227.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.05 29.09 – 2.05	Depositor EDS
% Data completeness (in resolution range)	89.9 (30.00-2.05) 77.8 (29.09-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.192 , 0.222 0.205 , 0.229	Depositor DCC
R_{free} test set	2255 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.804	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 56.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9313	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SCK, NAG, SCU, P6G, FUC

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	0.62	0/4330	0.73	1/5916 (0.0%)
1	B	0.50	0/4329	0.67	2/5914 (0.0%)
All	All	0.56	0/8659	0.70	3/11830 (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	B	1	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	433	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	B	322	GLN	N-CA-C	5.62	126.16	111.00
1	B	524	LEU	CA-CB-CG	5.35	127.61	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	322	GLN	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	496	LYS	Peptide
1	B	497	SER	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4202	0	4089	58	0
1	B	4196	0	4094	42	0
2	C	28	0	25	0	0
3	A	10	0	10	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
5	A	20	0	30	10	0
5	B	20	0	30	5	0
6	A	13	0	18	13	0
6	B	13	0	17	5	0
7	A	19	0	26	1	0
8	A	430	0	0	9	0
8	B	334	0	0	5	0
All	All	9313	0	8365	114	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 7.

All (114) 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:203:SER:OG	6:A:902[B]:SCU:H5	0.81	0.99
6:A:902[B]:SCU:H112	6:A:902[B]:SCU:H182	1.44	0.97
1:A:203:SER:CB	6:A:902[B]:SCU:H5	1.97	0.94
1:A:4:GLU:OE2	1:A:18:ARG:HD3	1.67	0.94
1:B:86:TRP:CE2	5:B:951[A]:SCK:H193	2.05	0.90
1:A:203:SER:HG	6:A:902[B]:SCU:H5	1.12	0.89
6:A:902[B]:SCU:H182	6:A:902[B]:SCU:C11	2.03	0.88
1:B:30:SER:HB2	1:B:103:THR:HG22	1.61	0.82
1:B:286:TRP:CE2	5:B:951[A]:SCK:H92	2.20	0.76
6:A:902[B]:SCU:H201	8:A:2768:HOH:O	1.92	0.69
1:B:112:THR:HG21	1:B:143:GLY:O	1.94	0.68
5:A:901[A]:SCK:H201	8:A:2768:HOH:O	1.94	0.67
1:A:117:TRP:CZ3	1:A:201:GLY:HA2	2.31	0.66
1:A:86:TRP:CD2	6:A:902[B]:SCU:H193	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:TRP:CZ2	5:A:901[A]:SCK:C8	2.83	0.62
1:A:541:SER:O	1:A:542:ALA:HB2	2.00	0.62
1:A:454:ILE:HD12	1:A:480:TRP:CE2	2.34	0.61
1:B:86:TRP:CD2	5:B:951[A]:SCK:H193	2.34	0.61
6:A:902[B]:SCU:H181	8:A:2768:HOH:O	2.02	0.60
1:A:99:LEU:C	1:A:99:LEU:HD12	2.23	0.60
1:A:212:HIS:HD2	1:A:218:SER:OG	1.86	0.59
5:B:951[A]:SCK:H183	8:B:1024:HOH:O	2.02	0.59
1:B:161:LEU:HD11	1:B:269:LEU:HD22	1.83	0.59
1:A:7:GLN:NE2	1:A:107:ARG:H	2.00	0.59
6:B:952[B]:SCU:H182	6:B:952[B]:SCU:H112	1.84	0.58
1:B:166:GLU:HG2	1:B:270:ILE:HD13	1.86	0.58
1:A:112:THR:HG21	1:A:143:GLY:O	2.03	0.57
1:A:66:GLN:HG3	1:A:98:TYR:CD2	2.40	0.57
1:A:113:PRO:HG2	1:A:485:ARG:HG2	1.89	0.55
1:B:10:VAL:HG22	1:B:107[A]:ARG:NH1	2.22	0.55
1:B:135:GLY:HA2	1:B:146:LEU:HD23	1.90	0.54
1:B:115:LEU:O	1:B:146:LEU:HD12	2.08	0.54
1:A:86:TRP:CE2	6:A:902[B]:SCU:H193	2.43	0.53
1:B:312:PRO:O	1:B:316:ILE:HG23	2.08	0.53
1:B:495:SER:O	1:B:496:LYS:HB2	2.08	0.52
1:B:86:TRP:CE3	6:B:952[B]:SCU:H202	2.45	0.52
1:A:286:TRP:CZ2	5:A:901[A]:SCK:H82	2.45	0.52
1:A:86:TRP:CE3	6:A:902[B]:SCU:H193	2.45	0.51
1:A:209:VAL:HG11	1:A:225:ALA:HB1	1.91	0.51
1:B:195:MET:HE3	8:B:1191:HOH:O	2.10	0.51
1:A:122:GLY:N	6:A:902[B]:SCU:O4	2.42	0.50
1:B:86:TRP:CE2	6:B:952[B]:SCU:H193	2.46	0.50
1:A:4:GLU:HB3	8:A:2798:HOH:O	2.11	0.50
1:A:224:ARG:HG2	1:A:325:GLN:HE21	1.77	0.50
1:A:209:VAL:CG1	1:A:225:ALA:HB1	2.41	0.49
1:B:24:ALA:HB3	1:B:140:GLN:HG3	1.94	0.49
1:B:367:VAL:HG12	1:B:370:ALA:HB2	1.93	0.49
1:A:66:GLN:HG3	1:A:98:TYR:CE2	2.48	0.48
1:B:454:ILE:HD13	1:B:476:LEU:HB3	1.94	0.48
1:B:332:LYS:NZ	8:B:1147:HOH:O	2.46	0.48
6:A:902[B]:SCU:H112	6:A:902[B]:SCU:C18	2.29	0.48
1:A:66:GLN:CG	1:A:98:TYR:CD2	2.97	0.48
1:B:30:SER:HB2	1:B:103:THR:CG2	2.39	0.48
1:B:115:LEU:HB2	1:B:146:LEU:HD13	1.95	0.48
5:A:901[A]:SCK:H83	5:A:901[A]:SCK:H32	1.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:VAL:HB	1:A:518:LEU:HD22	1.96	0.47
1:A:541:SER:O	1:A:542:ALA:CB	2.62	0.47
6:A:902[B]:SCU:H182	6:A:902[B]:SCU:C12	2.44	0.47
5:A:901[A]:SCK:H181	8:A:2768:HOH:O	2.14	0.47
1:B:115:LEU:HD23	1:B:198:THR:HB	1.97	0.47
1:A:320:ASP:C	1:A:320:ASP:OD1	2.53	0.46
1:A:286:TRP:CE2	5:A:901[A]:SCK:C8	2.99	0.46
1:A:454:ILE:HD12	1:A:480:TRP:CZ2	2.50	0.46
1:B:265:ASN:ND2	8:B:1154:HOH:O	2.48	0.46
1:A:195:MET:HE3	8:A:2632:HOH:O	2.14	0.46
1:A:397:ALA:O	1:A:401:VAL:HG23	2.16	0.46
1:B:85[A]:MET:HE3	1:B:132:VAL:HG11	1.98	0.45
1:A:360:LEU:CD2	1:A:379:VAL:HG11	2.46	0.45
1:A:380:LEU:HB3	7:A:1901:P6G:H152	1.98	0.45
1:B:286:TRP:CZ2	5:B:951[A]:SCK:H92	2.52	0.45
1:A:68:VAL:HG23	1:A:90:ARG:HB2	1.99	0.45
1:B:331:VAL:HG22	1:B:334:GLU:CD	2.37	0.45
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.52	0.45
1:B:103:THR:HG23	1:B:104:PRO:O	2.17	0.45
1:B:224:ARG:HG2	1:B:325:GLN:HB2	2.00	0.44
1:A:226:VAL:HG22	1:A:327:LEU:HB3	1.99	0.44
1:B:187:ILE:HD12	1:B:187:ILE:HA	1.91	0.44
1:A:286:TRP:CE2	5:A:901[A]:SCK:H82	2.53	0.44
1:A:453:PHE:HB3	1:A:476:LEU:HD12	1.98	0.44
1:A:115:LEU:HD21	1:A:484:ALA:HB2	1.99	0.44
1:B:135:GLY:CA	1:B:146:LEU:HD23	2.48	0.44
1:A:90:ARG:NE	8:A:2627:HOH:O	2.50	0.44
1:B:213:ILE:O	1:B:219:ARG:HD3	2.18	0.44
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.53	0.44
1:A:528:THR:O	1:A:531:PHE:HB3	2.18	0.44
1:A:7:GLN:HB2	8:A:2566:HOH:O	2.18	0.43
5:A:901[A]:SCK:H182	5:A:901[A]:SCK:H152	1.62	0.43
1:A:75:THR:HG22	8:A:2775:HOH:O	2.17	0.43
1:B:134:ASP:OD1	1:B:136:ARG:HD2	2.17	0.43
6:B:952[B]:SCU:H182	6:B:952[B]:SCU:C11	2.48	0.43
1:B:327:LEU:HD11	1:B:500:TRP:CH2	2.54	0.43
1:A:86:TRP:CE2	5:A:901[A]:SCK:H193	2.53	0.42
1:A:325:GLN:HE21	1:A:325:GLN:HB2	1.61	0.42
1:A:72:TYR:CE1	5:A:901[A]:SCK:H101	2.54	0.42
1:B:540:LEU:HB2	8:B:1125:HOH:O	2.20	0.42
1:A:324:LEU:HG	1:A:326:VAL:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:LEU:HD23	1:A:385:TRP:HZ2	1.85	0.42
1:B:177:ARG:CZ	1:B:217:PRO:HB2	2.50	0.42
1:B:457:LEU:N	1:B:458:PRO:CD	2.83	0.42
1:A:328:VAL:O	1:A:427:ALA:HA	2.19	0.42
1:A:45:ARG:CZ	1:A:51:GLU:OE1	2.68	0.42
1:A:80:PHE:CE2	1:A:82:GLY:HA3	2.55	0.42
1:A:24:ALA:HB3	1:A:140:GLN:HG3	2.01	0.42
1:A:380:LEU:CD2	1:A:385:TRP:HZ2	2.32	0.42
1:B:202:GLU:HA	1:B:228:GLN:O	2.19	0.42
1:A:257:CYS:HA	1:A:258:PRO:HD2	1.96	0.41
1:A:66:GLN:HG2	1:A:98:TYR:CG	2.55	0.41
1:B:113:PRO:HG2	1:B:485:ARG:HG2	2.01	0.41
1:B:328:VAL:O	1:B:427:ALA:HA	2.20	0.41
1:B:166:GLU:HG2	1:B:270:ILE:CD1	2.49	0.41
1:B:352:SER:O	1:B:395:ARG:HG3	2.20	0.41
6:B:952[B]:SCU:H183	6:B:952[B]:SCU:H151	1.85	0.41
1:A:76:LEU:HD22	1:A:341:TYR:CD2	2.56	0.41
1:A:339:LEU:HD11	1:A:399:SER:HA	2.04	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	534/543 (98%)	513 (96%)	20 (4%)	1 (0%)	47	39
1	B	534/543 (98%)	514 (96%)	17 (3%)	3 (1%)	25	15
All	All	1068/1086 (98%)	1027 (96%)	37 (4%)	4 (0%)	34	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	496	LYS
1	B	497	SER
1	B	498	PRO
1	A	541	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	442/443 (100%)	437 (99%)	5 (1%)	73	73
1	B	443/443 (100%)	432 (98%)	11 (2%)	47	40
All	All	885/886 (100%)	869 (98%)	16 (2%)	59	55

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	TYR
1	A	246	ARG
1	A	295	PHE
1	A	437	LEU
1	A	541	SER
1	B	103	THR
1	B	200	PHE
1	B	246	ARG
1	B	281	LEU
1	B	291	GLN
1	B	295	PHE
1	B	296	ARG
1	B	322	GLN
1	B	491	ASP
1	B	525	ARG
1	B	543	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	212	HIS
1	A	322	GLN
1	A	325	GLN
1	A	421	GLN
1	B	67	ASN
1	B	291	GLN
1	B	322	GLN

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	0.64	0	17,19,21	1.24	2 (11%)
2	NAG	C	2	2	14,14,15	0.53	0	17,19,21	0.97	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
2	NAG	C	1	1,2	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	NAG	O5-C1-C2	-2.64	107.11	111.29
2	C	2	NAG	O5-C5-C6	2.31	110.83	107.20
2	C	2	NAG	C4-C3-C2	2.17	114.20	111.02
2	C	1	NAG	C1-O5-C5	2.15	115.10	112.19

There are no chirality outliers.

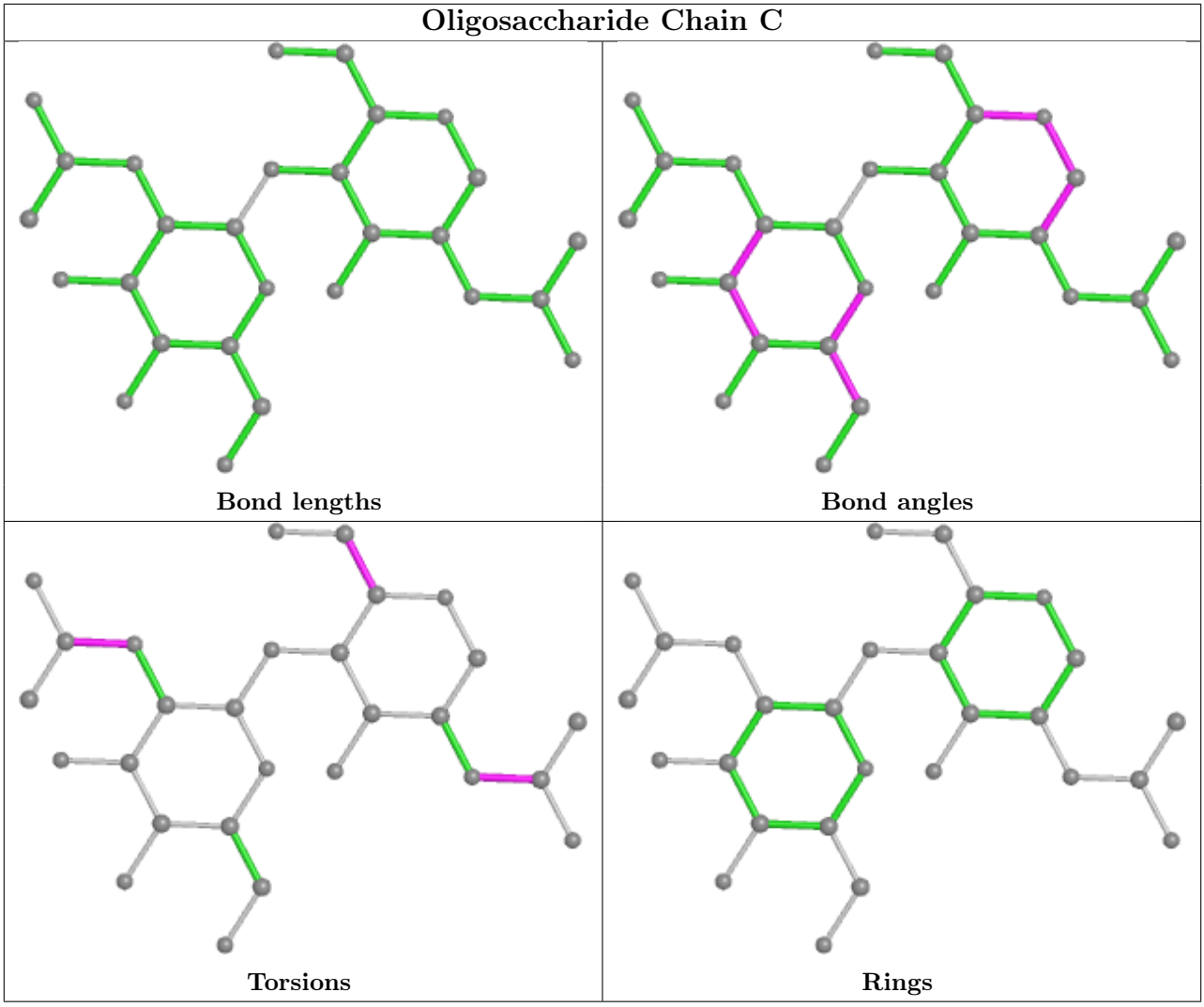
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6

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)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	P6G	A	1901	-	18,18,18	2.19	6 (33%)	17,17,17	1.27	1 (5%)
4	NAG	A	701	1	14,14,15	0.65	0	17,19,21	1.43	2 (11%)
3	FUC	A	2502	-	10,10,11	0.64	0	14,14,16	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	SCK	A	901[A]	-	19,19,19	1.57	2 (10%)	26,26,26	1.20	3 (11%)
4	NAG	B	601	1	14,14,15	0.75	1 (7%)	17,19,21	1.91	3 (17%)
6	SCU	A	902[B]	1	12,12,12	1.50	1 (8%)	15,15,15	1.44	4 (26%)
5	SCK	B	951[A]	-	19,19,19	1.62	2 (10%)	26,26,26	1.14	3 (11%)
6	SCU	B	952[B]	1	12,12,12	1.32	1 (8%)	15,15,15	1.34	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	P6G	A	1901	-	-	5/16/16/16	-
4	NAG	A	701	1	-	2/6/23/26	0/1/1/1
3	FUC	A	2502	-	-	-	0/1/1/1
5	SCK	A	901[A]	-	-	4/19/19/19	-
4	NAG	B	601	1	-	2/6/23/26	0/1/1/1
6	SCU	A	902[B]	1	-	6/10/11/11	-
5	SCK	B	951[A]	-	-	3/19/19/19	-
6	SCU	B	952[B]	1	-	6/10/11/11	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	902[B]	SCU	O14-C12	4.55	1.46	1.33
7	A	1901	P6G	O10-C9	4.51	1.61	1.42
5	B	951[A]	SCK	O14-C12	4.44	1.46	1.33
5	B	951[A]	SCK	O4-C5	4.43	1.46	1.33
5	A	901[A]	SCK	O14-C12	4.09	1.45	1.33
5	A	901[A]	SCK	O4-C5	4.08	1.45	1.33
6	B	952[B]	SCU	O14-C12	4.08	1.45	1.33
7	A	1901	P6G	O13-C12	3.62	1.57	1.42
7	A	1901	P6G	O19-C18	3.46	1.59	1.42
7	A	1901	P6G	O4-C3	3.44	1.57	1.42
7	A	1901	P6G	O16-C15	3.41	1.56	1.42
7	A	1901	P6G	O7-C6	2.87	1.54	1.42
4	B	601	NAG	C1-C2	2.07	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	601	NAG	C1-O5-C5	6.08	120.42	112.19
4	A	701	NAG	O5-C5-C6	3.57	112.79	107.20
7	A	1901	P6G	O1-C2-C3	3.30	130.96	111.81
5	B	951[A]	SCK	O14-C12-C11	3.09	121.60	111.91
5	B	951[A]	SCK	O14-C12-O13	-2.76	116.62	123.59
6	B	952[B]	SCU	C11-C6-C5	-2.69	103.06	111.89
5	A	901[A]	SCK	O4-C5-C6	2.65	120.23	111.91
5	A	901[A]	SCK	O14-C12-C11	2.64	120.19	111.91
6	A	902[B]	SCU	O14-C15-C16	2.60	118.22	109.14
6	B	952[B]	SCU	O14-C12-O13	-2.33	117.72	123.59
5	B	951[A]	SCK	O4-C5-C6	2.31	119.15	111.91
5	A	901[A]	SCK	C15-C16-N17	-2.29	108.12	115.78
6	A	902[B]	SCU	C11-C6-C5	-2.29	104.37	111.89
4	B	601	NAG	O5-C5-C6	2.20	110.65	107.20
6	A	902[B]	SCU	O14-C12-C11	2.20	118.81	111.91
4	A	701	NAG	C3-C4-C5	-2.19	106.33	110.24
4	B	601	NAG	C1-C2-N2	2.17	114.19	110.49
6	A	902[B]	SCU	O14-C12-O13	-2.01	118.53	123.59

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	951[A]	SCK	O14-C15-C16-N17
6	A	902[B]	SCU	C12-C11-C6-C5
6	B	952[B]	SCU	C11-C12-O14-C15
6	B	952[B]	SCU	O14-C15-C16-N17
6	B	952[B]	SCU	O13-C12-O14-C15
5	B	951[A]	SCK	C11-C12-O14-C15
5	A	901[A]	SCK	O13-C12-O14-C15
5	B	951[A]	SCK	O13-C12-O14-C15
5	A	901[A]	SCK	C11-C12-O14-C15
6	A	902[B]	SCU	O13-C12-O14-C15
6	A	902[B]	SCU	C11-C12-O14-C15
4	B	601	NAG	C8-C7-N2-C2
4	B	601	NAG	O7-C7-N2-C2
4	A	701	NAG	C8-C7-N2-C2
6	A	902[B]	SCU	C15-C16-N17-C19
5	A	901[A]	SCK	C6-C5-O4-C3
7	A	1901	P6G	O13-C14-C15-O16
7	A	1901	P6G	O4-C5-C6-O7
5	A	901[A]	SCK	O7-C5-O4-C3
6	B	952[B]	SCU	C15-C16-N17-C18

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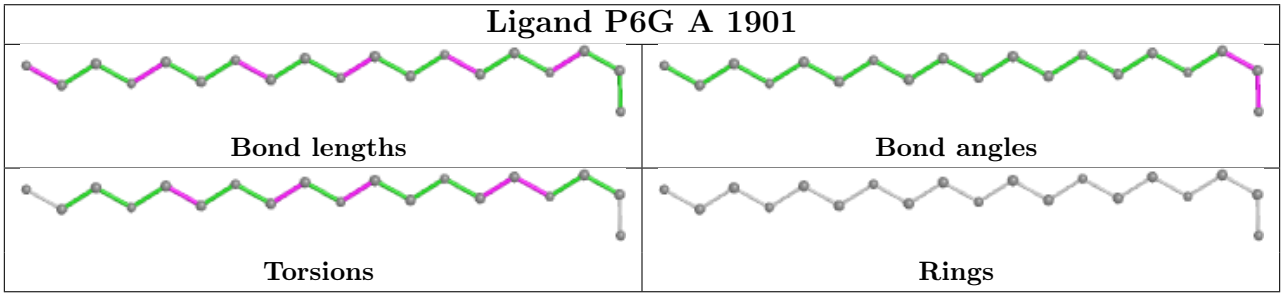
Mol	Chain	Res	Type	Atoms
6	B	952[B]	SCU	C15-C16-N17-C20
7	A	1901	P6G	C6-C5-O4-C3
4	A	701	NAG	O7-C7-N2-C2
6	A	902[B]	SCU	C15-C16-N17-C18
6	A	902[B]	SCU	C15-C16-N17-C20
7	A	1901	P6G	C8-C9-O10-C11
6	B	952[B]	SCU	C15-C16-N17-C19
7	A	1901	P6G	O10-C11-C12-O13

There are no ring outliers.

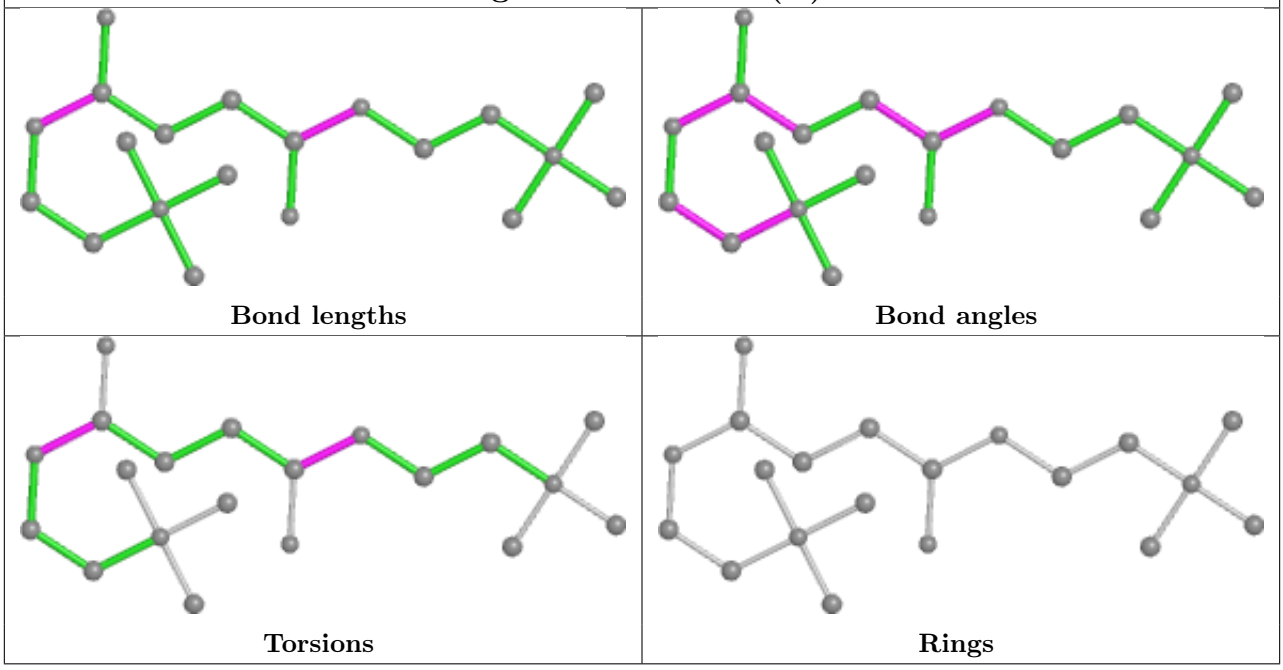
5 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1901	P6G	1	0
5	A	901[A]	SCK	10	0
6	A	902[B]	SCU	13	0
5	B	951[A]	SCK	5	0
6	B	952[B]	SCU	5	0

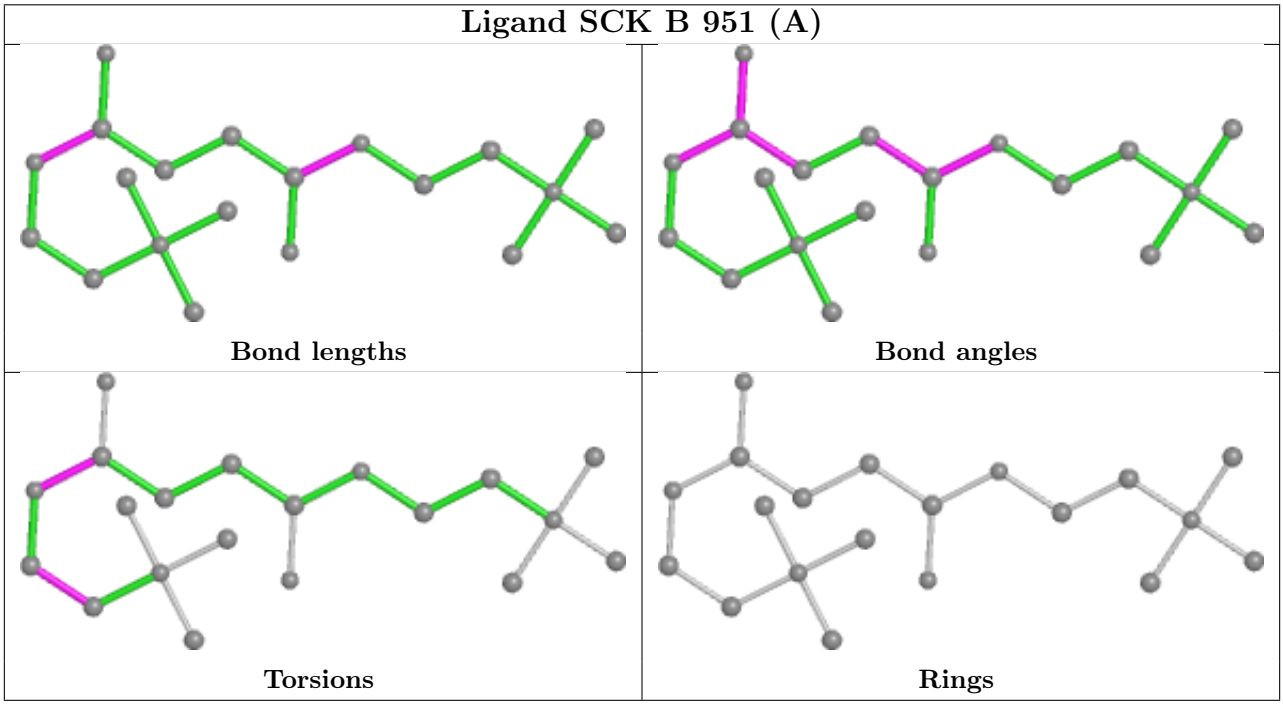
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.



Ligand SCK A 901 (A)



Ligand SCK B 951 (A)



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^{th} 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	536/543 (98%)	0.21	19 (3%) 44 48	34, 54, 74, 106	0
1	B	534/543 (98%)	0.53	49 (9%) 9 9	44, 61, 83, 105	0
All	All	1070/1086 (98%)	0.37	68 (6%) 19 21	34, 57, 80, 106	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	495	SER	6.8
1	B	543	THR	6.4
1	A	493	ARG	6.1
1	B	42	VAL	4.9
1	B	495	SER	4.4
1	B	156	PHE	4.2
1	B	542	ALA	4.0
1	A	494	ASP	4.0
1	A	75	THR	4.0
1	B	540	LEU	3.9
1	B	461	PRO	3.9
1	B	497	SER	3.8
1	B	109	ALA	3.7
1	A	497	SER	3.7
1	B	494	ASP	3.7
1	A	542	ALA	3.6
1	B	138	LEU	3.6
1	B	41	PRO	3.5
1	B	323	ASP	3.5
1	A	492	PRO	3.4
1	A	265	ASN	3.3
1	B	541	SER	3.3
1	A	541	SER	3.3
1	B	75	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	159	LEU	3.3
1	A	540	LEU	3.3
1	A	496	LYS	3.2
1	B	165	ARG	3.2
1	A	323	ASP	3.1
1	B	47	PHE	3.1
1	B	147	VAL	3.1
1	B	273	LEU	3.0
1	B	97	LEU	3.0
1	B	265	ASN	2.9
1	B	99	LEU	2.8
1	B	322	GLN	2.8
1	B	157	GLY	2.8
1	B	451	ILE	2.8
1	B	101	VAL	2.8
1	A	165	ARG	2.8
1	B	77	TYR	2.7
1	B	455	PHE	2.7
1	B	496	LYS	2.6
1	B	155	THR	2.6
1	B	454	ILE	2.6
1	A	317	ASN	2.5
1	A	467	THR	2.5
1	B	46	ARG	2.5
1	B	281	LEU	2.5
1	B	35	ILE	2.5
1	B	539	LEU	2.4
1	B	76	LEU	2.4
1	A	320	ASP	2.4
1	B	40	PRO	2.4
1	B	135	GLY	2.3
1	B	106	PRO	2.3
1	B	43	GLY	2.3
1	B	117	TRP	2.3
1	B	480	TRP	2.3
1	B	258	PRO	2.3
1	B	268	GLU	2.2
1	A	76	LEU	2.2
1	A	322	GLN	2.2
1	B	145	VAL	2.1
1	B	102	TRP	2.1
1	B	253	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	491	ASP	2.0
1	B	377	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)

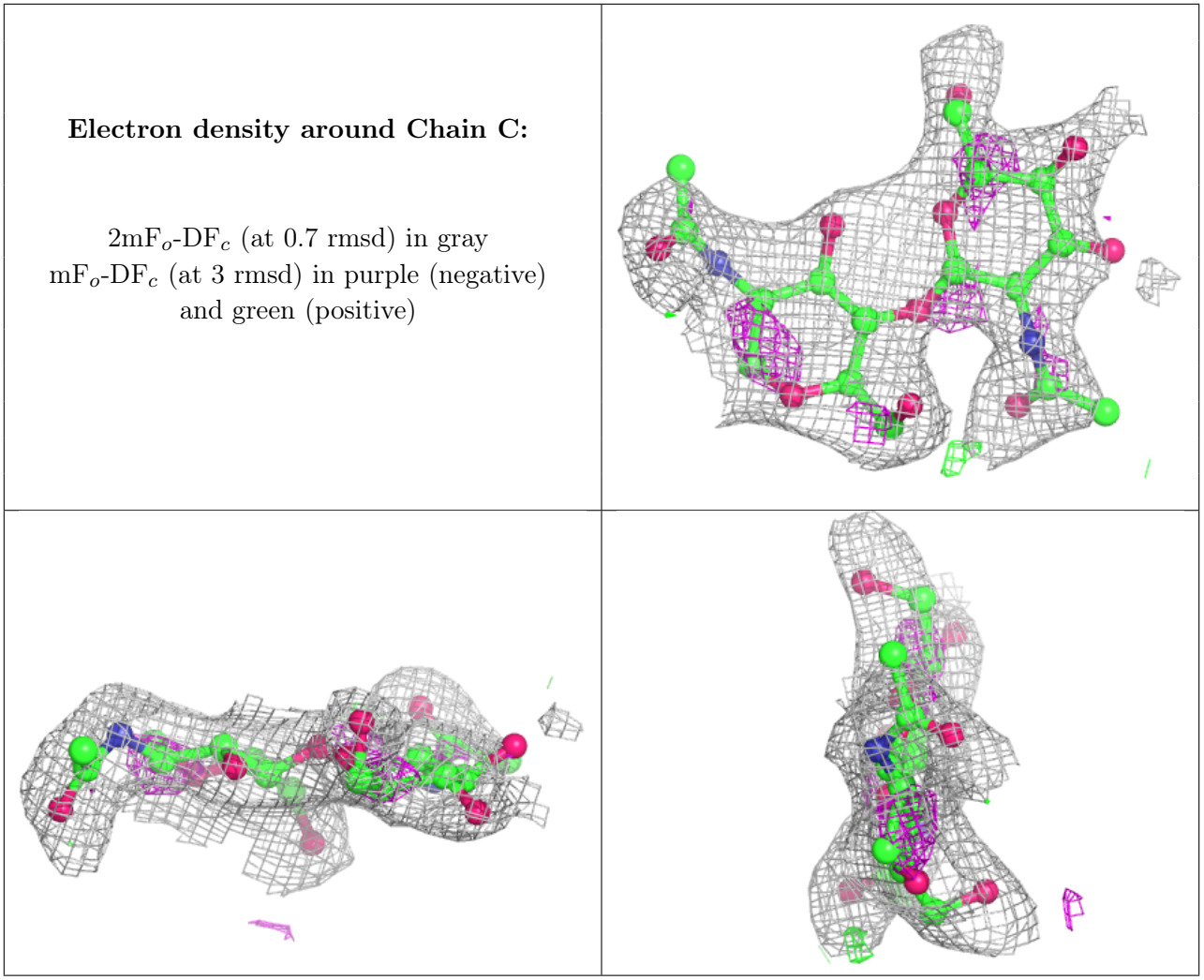
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	NAG	C	2	14/15	0.73	0.42	99,100,101,101	0
2	NAG	C	1	14/15	0.83	0.34	82,89,90,96	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 C:

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



6.4 Ligands

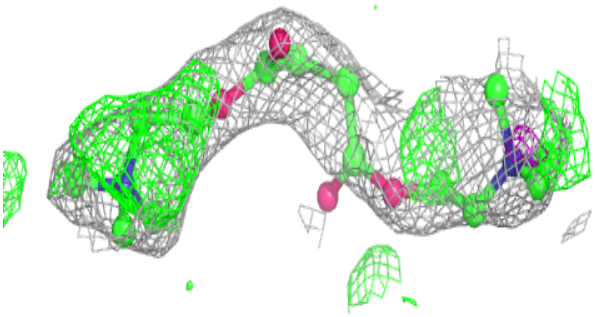
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

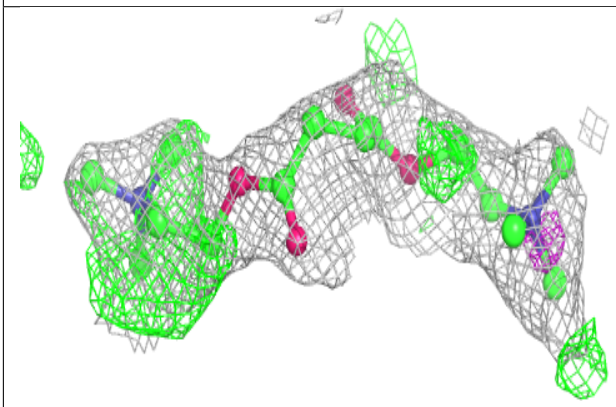
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SCU	A	902[B]	13/13	0.42	0.70	72,79,82,82	13
5	SCK	B	951[A]	20/20	0.53	0.68	83,86,90,92	20
5	SCK	A	901[A]	20/20	0.55	0.68	77,81,88,89	20
3	FUC	A	2502	10/11	0.62	0.64	138,138,139,139	0
4	NAG	A	701	14/15	0.63	0.43	86,92,94,94	0
6	SCU	B	952[B]	13/13	0.65	0.56	73,85,86,86	13
4	NAG	B	601	14/15	0.78	0.33	87,92,95,96	0
7	P6G	A	1901	19/19	0.86	0.16	67,69,81,81	0

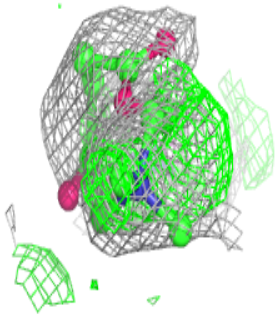
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SCK B 951 (A):

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

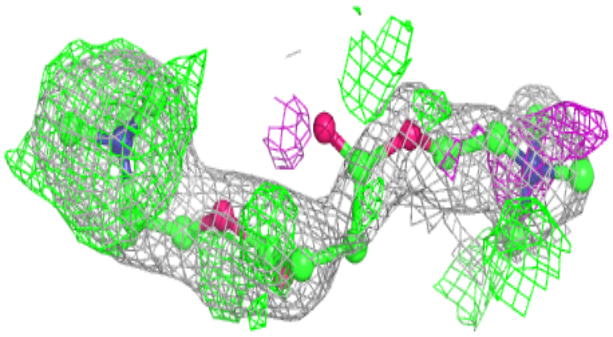


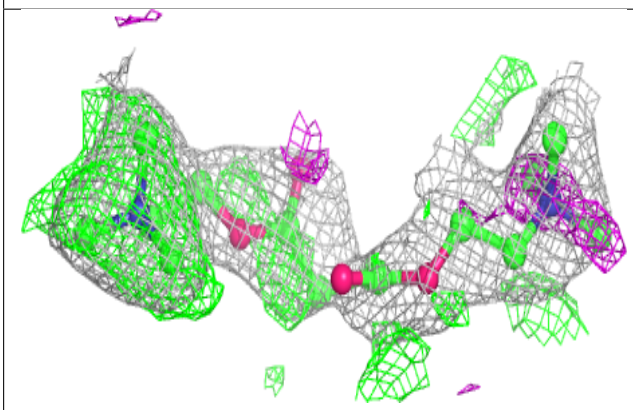


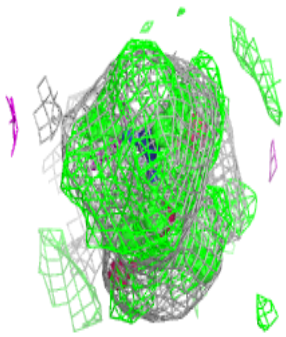


Electron density around SCK A 901 (A):

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

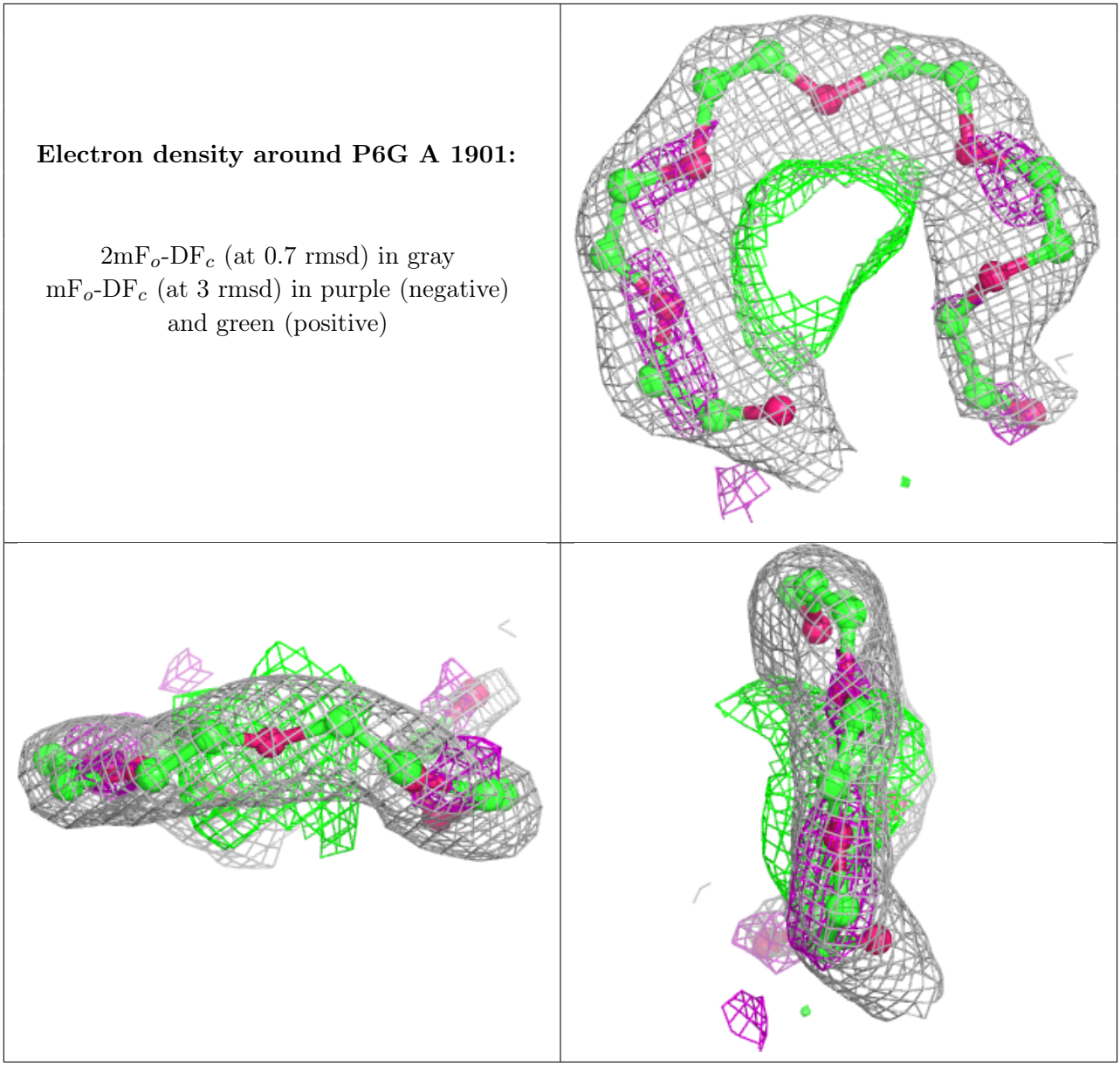






Electron density around P6G A 1901:

$2mF_o$-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.