



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 02:16 AM BST

PDB ID : 2H9Y
Title : Crystal structure of mouse acetylcholinesterase complexed with m-(N,N,N-trimethylammonio)trifluoroacetophenone
Authors : Bourne, Y.; Radic, Z.; Sulzenbacher, G.; Kim, E.; Taylor, P.; Marchot, P.
Deposited on : 2006-06-12
Resolution : 2.40 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

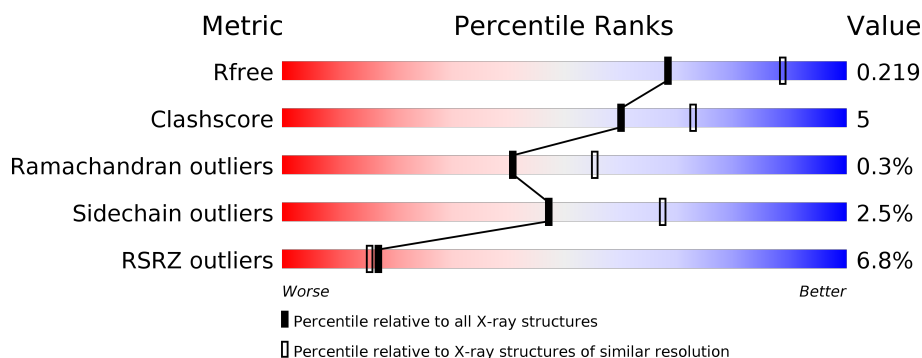
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	543	<div> <div>6%</div> <div>89%</div> <div>9%</div> <div>..</div> </div>
1	B	543	<div> <div>8%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
2	C	2	<div> <div>100%</div> </div>

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	FUC	C	2	X	-	-	-
3	NAG	A	701	-	-	-	X
3	NAG	B	601	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8911 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	1	0
			4190	2687	729	760	14			
1	B	534	Total	C	N	O	S	0	3	0
			4183	2685	723	761	14			

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



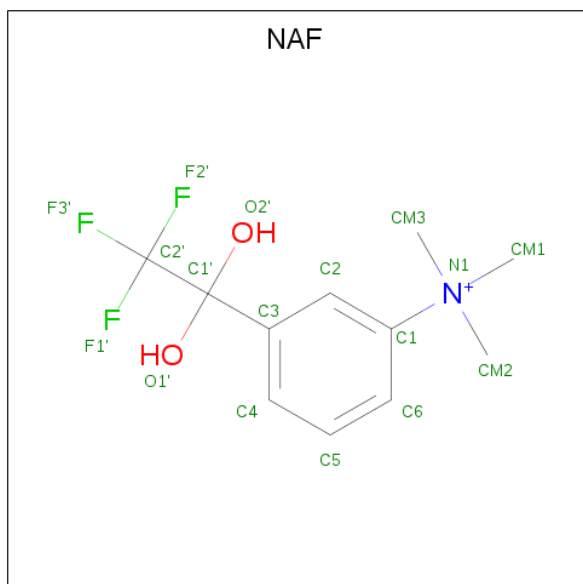
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is M-(N,N,N-TRIMETHYLAMMONIO)-2,2,2-TRIFLUORO-1,1-DIHYDROXY ETHYLBENZENE (three-letter code: NAF) (formula: $C_{11}H_{15}F_3NO_2$).



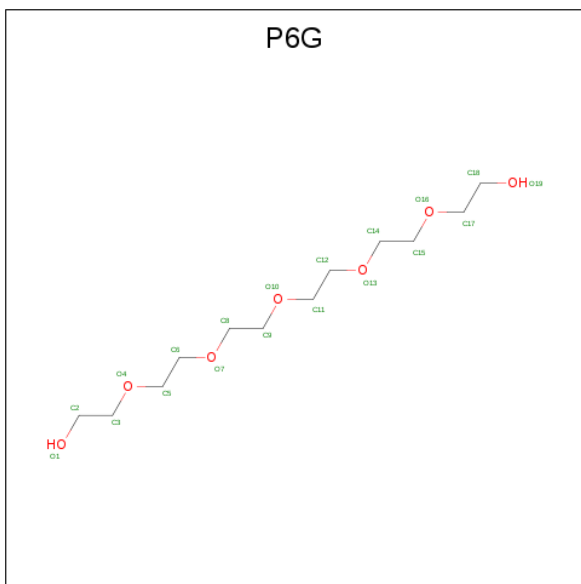
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			16	11	3	1	1		

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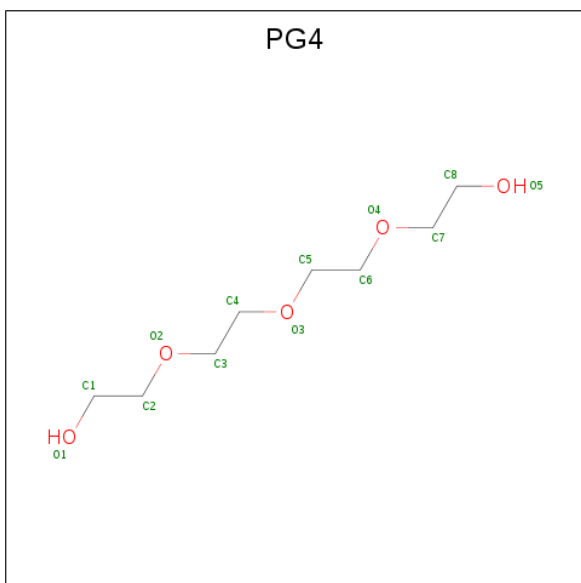
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	F	N	O	0	0
			16	11	3	1	1		

- Molecule 5 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



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

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	8	5		

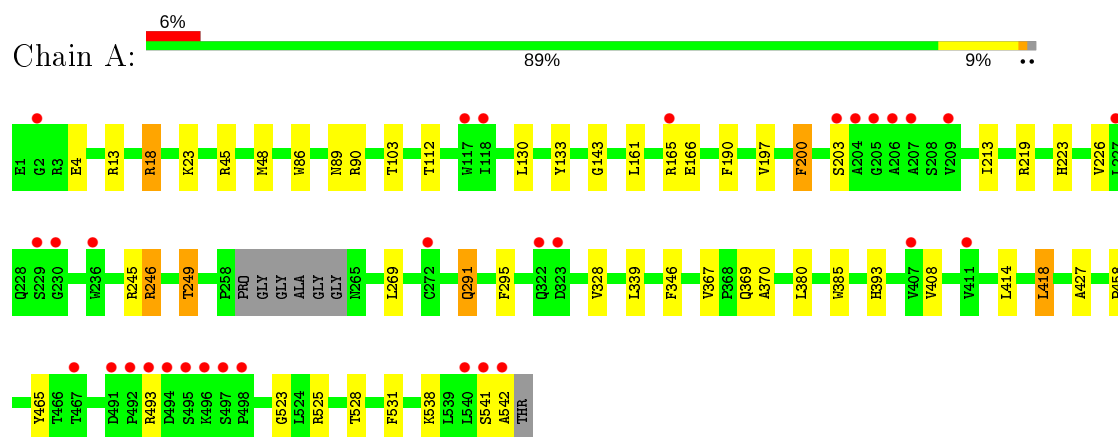
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	237	Total	O	0	0
			237	237		
7	B	185	Total	O	0	0
			185	185		

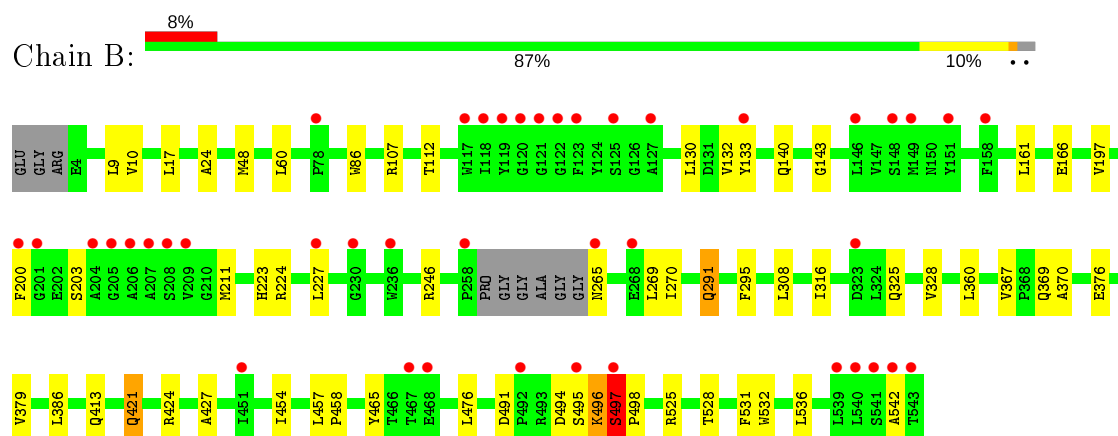
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

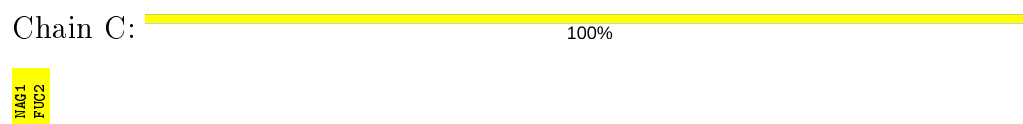
• Molecule 1: Acetylcholinesterase



• 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, α , β , γ	79.01Å 111.39Å 226.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 39.36 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.40) 91.0 (39.36-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.186 , 0.214 0.200 , 0.219	Depositor DCC
R_{free} test set	1564 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.793	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8911	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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: PG4, NAF, NAG, 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	0.54	0/4319	0.65	3/5901 (0.1%)
1	B	0.48	0/4319	0.62	0/5901
All	All	0.51	0/8638	0.64	3/11802 (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	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	246	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	246	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	18	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	496	LYS	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	4190	0	4079	39	0
1	B	4183	0	4068	38	0
2	C	24	0	22	0	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	16	0	14	4	0
4	B	16	0	14	4	0
5	A	19	0	26	0	0
6	A	13	0	18	0	0
7	A	237	0	0	2	0
7	B	185	0	0	1	0
All	All	8911	0	8267	75	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 5.

All (75) 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:161:LEU:HD11	1:B:269:LEU:HD22	1.64	0.80
1:A:380:LEU:HD23	1:A:385:TRP:HZ2	1.53	0.73
1:A:291:GLN:HE22	1:A:369:GLN:NE2	1.90	0.68
1:A:245:ARG:O	1:A:249:THR:CG2	2.42	0.67
1:B:166:GLU:HG2	1:B:270:ILE:HD13	1.80	0.64
1:A:380:LEU:HD23	1:A:385:TRP:CZ2	2.34	0.63
1:B:86:TRP:CD2	4:B:952:NAF:HM11	2.34	0.62
1:B:227:LEU:HB2	1:B:328:VAL:HG12	1.81	0.62
1:B:203:SER:HG	4:B:952:NAF:C1'	2.10	0.62
1:A:291:GLN:NE2	1:A:369:GLN:NE2	2.48	0.61
1:B:112:THR:HG21	1:B:143:GLY:O	2.01	0.61
1:A:245:ARG:O	1:A:249:THR:HG22	2.01	0.60
1:A:86:TRP:CD2	4:A:951:NAF:HM11	2.36	0.60
1:A:291:GLN:NE2	1:A:369:GLN:HE21	1.98	0.60
1:A:291:GLN:HE22	1:A:369:GLN:HE21	1.48	0.60
1:B:316:ILE:O	1:B:421:GLN:NE2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:GLU:OE2	1:A:18:ARG:HD3	2.02	0.59
1:B:367:VAL:HG12	1:B:370:ALA:HB2	1.84	0.58
1:B:497:SER:HB2	1:B:498:PRO:O	2.06	0.56
1:A:203:SER:OG	4:A:951:NAF:C2'	2.53	0.56
1:A:414:LEU:HG	1:A:418:LEU:HD22	1.88	0.55
1:A:203:SER:HG	4:A:951:NAF:C1'	2.13	0.55
1:B:197:VAL:H	1:B:223:HIS:HD2	1.55	0.55
1:A:203:SER:CB	4:A:951:NAF:C1'	2.84	0.55
1:A:245:ARG:O	1:A:249:THR:HG23	2.06	0.55
1:B:291:GLN:HE22	1:B:369:GLN:NE2	2.05	0.54
1:B:24:ALA:HB3	1:B:140:GLN:HG3	1.90	0.54
1:B:203:SER:OG	4:B:952:NAF:C2'	2.55	0.53
1:B:17:LEU:HD23	1:B:60:LEU:HB3	1.91	0.53
1:A:197:VAL:H	1:A:223:HIS:HD2	1.56	0.53
1:A:112:THR:HG21	1:A:143:GLY:O	2.08	0.52
1:A:103:THR:HG21	1:A:190:PHE:HB3	1.91	0.52
1:A:328:VAL:O	1:A:427:ALA:HA	2.08	0.52
1:A:538:LYS:HD3	1:B:376[A]:GLU:HG2	1.91	0.52
1:B:161:LEU:HD11	1:B:269:LEU:CD2	2.39	0.51
1:B:265:ASN:ND2	7:B:1104:HOH:O	2.37	0.50
1:B:161:LEU:CD1	1:B:269:LEU:HD22	2.38	0.49
1:A:408:VAL:HG11	1:A:525:ARG:HG3	1.95	0.49
1:B:497:SER:HB2	1:B:498:PRO:C	2.33	0.49
1:B:211:MET:HG2	1:B:308:LEU:HD21	1.94	0.48
1:B:197:VAL:H	1:B:223:HIS:CD2	2.31	0.48
1:A:197:VAL:H	1:A:223:HIS:CD2	2.31	0.48
1:B:10:VAL:HG22	1:B:107:ARG:NH1	2.28	0.48
1:A:130:LEU:HD12	1:A:133:TYR:CE2	2.48	0.48
1:B:360:LEU:HD22	1:B:379:VAL:HG21	1.95	0.48
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.49	0.47
1:B:491:ASP:HB3	1:B:494:ASP:HB3	1.95	0.47
1:B:166:GLU:HG2	1:B:270:ILE:CD1	2.45	0.46
1:B:130:LEU:HD12	1:B:133:TYR:CE2	2.50	0.46
1:A:48:MET:HE1	1:A:166:GLU:HA	1.98	0.44
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.52	0.44
1:A:523:GLY:HA3	1:B:386:LEU:HD21	1.98	0.44
1:A:541:SER:O	1:A:542:ALA:HB3	2.18	0.44
1:B:203:SER:CB	4:B:952:NAF:C1'	2.89	0.44
1:A:291:GLN:HB2	1:A:291:GLN:HE21	1.66	0.43
1:B:457:LEU:N	1:B:458:PRO:CD	2.81	0.43
1:A:89:ASN:O	1:A:90:ARG:NH1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:PHE:CB	1:A:226:VAL:HB	2.49	0.43
1:A:339:LEU:HD13	1:A:346:PHE:CE2	2.54	0.43
1:B:328:VAL:O	1:B:427:ALA:HA	2.19	0.43
1:B:224:ARG:HG2	1:B:325:GLN:HB2	2.00	0.42
1:A:48:MET:HE1	1:A:165:ARG:O	2.19	0.42
1:A:393:HIS:CD2	7:A:995:HOH:O	2.73	0.42
1:A:45:ARG:HG3	7:A:1164:HOH:O	2.19	0.42
1:B:367:VAL:CG1	1:B:370:ALA:HB2	2.50	0.42
1:B:454:ILE:HD13	1:B:476:LEU:HB3	2.01	0.42
1:B:532:TRP:CE3	1:B:536:LEU:HD12	2.55	0.41
1:A:213:ILE:O	1:A:219:ARG:HD3	2.19	0.41
1:B:291:GLN:HE21	1:B:291:GLN:HB2	1.66	0.41
1:A:161:LEU:HD11	1:A:269:LEU:HD22	2.02	0.41
1:B:161:LEU:HD12	1:B:270:ILE:CG1	2.51	0.41
1:A:528:THR:O	1:A:531:PHE:HB3	2.21	0.41
1:A:367:VAL:HG12	1:A:370:ALA:HB2	2.03	0.41
1:A:269:LEU:C	1:A:269:LEU:HD23	2.42	0.40
1:B:528:THR:O	1:B:531:PHE:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	533/543 (98%)	511 (96%)	22 (4%)	0	100	100
1	B	533/543 (98%)	513 (96%)	17 (3%)	3 (1%)	25	36
All	All	1066/1086 (98%)	1024 (96%)	39 (4%)	3 (0%)	41	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	497	SER
1	B	542	ALA
1	B	495	SER

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	441/443 (100%)	432 (98%)	9 (2%)	55	74
1	B	442/443 (100%)	429 (97%)	13 (3%)	42	62
All	All	883/886 (100%)	861 (98%)	22 (2%)	47	67

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	23	LYS
1	A	200	PHE
1	A	246	ARG
1	A	249	THR
1	A	291	GLN
1	A	295	PHE
1	A	418	LEU
1	A	493	ARG
1	B	9	LEU
1	B	48	MET
1	B	132	VAL
1	B	200	PHE
1	B	246	ARG
1	B	291	GLN
1	B	295	PHE
1	B	413	GLN
1	B	421	GLN
1	B	424	ARG
1	B	496	LYS
1	B	497	SER

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Mol	Chain	Res	Type
1	B	525	ARG

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	223	HIS
1	A	287	HIS
1	A	291	GLN
1	B	223	HIS
1	B	291	GLN
1	B	421	GLN
1	B	499	GLN

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 ⓘ

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	0.58	0	17,19,21	1.55	2 (11%)
2	FUC	C	2	2	10,10,11	0.64	0	14,14,16	1.25	2 (14%)

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	1/1/4/5	-	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(°)	Ideal(°)
2	C	1	NAG	C1-O5-C5	4.35	118.09	112.19
2	C	1	NAG	C2-N2-C7	-2.50	119.34	122.90
2	C	2	FUC	C6-C5-C4	-2.11	109.18	113.07
2	C	2	FUC	O5-C1-C2	2.05	113.94	110.77

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	2	FUC	C1

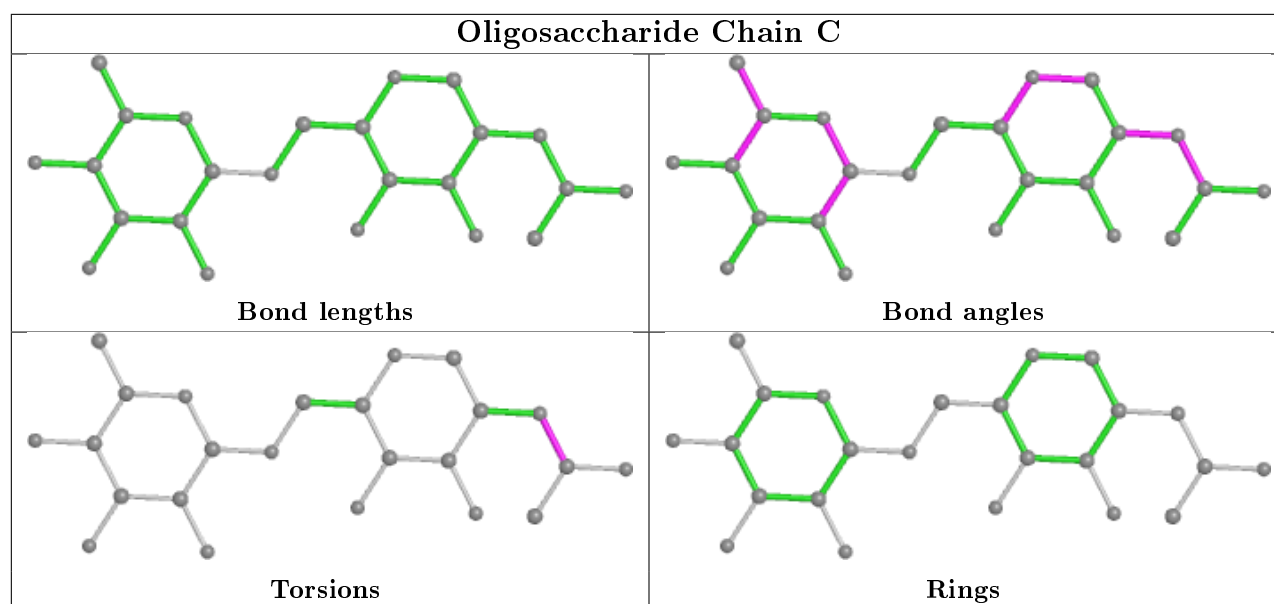
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-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](#)

6 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	$\# Z > 2$
3	NAG	B	601	1	14,14,15	0.64	0	17,19,21	1.67	3 (17%)
5	P6G	A	901	-	18,18,18	2.17	6 (33%)	17,17,17	1.23	1 (5%)
4	NAF	A	951	1	16,16,17	1.37	2 (12%)	24,25,28	1.29	3 (12%)
3	NAG	A	701	1	14,14,15	0.54	0	17,19,21	1.10	1 (5%)
4	NAF	B	952	1	16,16,17	1.46	2 (12%)	24,25,28	1.58	4 (16%)
6	PG4	A	902	-	12,12,12	0.68	0	11,11,11	0.75	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
3	NAG	B	601	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	P6G	A	901	-	-	6/16/16/16	-
4	NAF	A	951	1	-	4/16/16/21	0/1/1/1
3	NAG	A	701	1	-	2/6/23/26	0/1/1/1
4	NAF	B	952	1	-	4/16/16/21	0/1/1/1
6	PG4	A	902	-	-	5/10/10/10	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	901	P6G	O10-C9	4.43	1.61	1.42
5	A	901	P6G	O13-C12	3.77	1.58	1.42
4	B	952	NAF	C3-C1'	-3.50	1.48	1.51
5	A	901	P6G	O16-C15	3.49	1.57	1.42
5	A	901	P6G	O19-C18	3.41	1.59	1.42
4	B	952	NAF	C1-N1	-3.41	1.42	1.50
4	A	951	NAF	C1-N1	-3.39	1.42	1.50
5	A	901	P6G	O4-C3	3.35	1.56	1.42
4	A	951	NAF	C3-C1'	-3.12	1.48	1.51
5	A	901	P6G	O7-C6	2.80	1.54	1.42

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	NAG	C1-O5-C5	4.89	118.81	112.19
4	B	952	NAF	C4-C3-C1'	4.51	125.77	120.78
4	B	952	NAF	F2'-C2'-F1'	3.76	115.28	106.87
5	A	901	P6G	O1-C2-C3	3.42	131.66	111.81
4	A	951	NAF	C4-C3-C1'	3.04	124.15	120.78
4	A	951	NAF	F2'-C2'-F1'	2.82	113.17	106.87
4	A	951	NAF	F2'-C2'-C1'	-2.76	105.94	112.27
3	B	601	NAG	O5-C5-C6	2.74	111.50	107.20
3	B	601	NAG	O5-C1-C2	-2.55	107.26	111.29
3	A	701	NAG	O5-C5-C6	2.39	110.95	107.20
4	B	952	NAF	F1'-C2'-C1'	-2.38	106.80	112.27
4	B	952	NAF	C5-C4-C3	-2.35	117.73	120.65

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	951	NAF	C2'-C1'-C3-C2
4	B	952	NAF	C2'-C1'-C3-C2
4	B	952	NAF	C2'-C1'-C3-C4
6	A	902	PG4	C8-C7-O4-C6
3	B	601	NAG	O5-C5-C6-O6
3	B	601	NAG	C8-C7-N2-C2
3	B	601	NAG	O7-C7-N2-C2
3	B	601	NAG	C4-C5-C6-O6
4	A	951	NAF	O1'-C1'-C3-C2
4	A	951	NAF	O1'-C1'-C3-C4
4	B	952	NAF	O1'-C1'-C3-C2
4	B	952	NAF	O1'-C1'-C3-C4
5	A	901	P6G	C11-C12-O13-C14
3	A	701	NAG	C8-C7-N2-C2
5	A	901	P6G	C2-C3-O4-C5
6	A	902	PG4	C4-C3-O2-C2
5	A	901	P6G	O4-C5-C6-O7
4	A	951	NAF	C2'-C1'-C3-C4
5	A	901	P6G	O13-C14-C15-O16
6	A	902	PG4	O2-C3-C4-O3
5	A	901	P6G	C18-C17-O16-C15
3	A	701	NAG	O7-C7-N2-C2
5	A	901	P6G	O16-C17-C18-O19
6	A	902	PG4	O4-C7-C8-O5
6	A	902	PG4	O3-C5-C6-O4

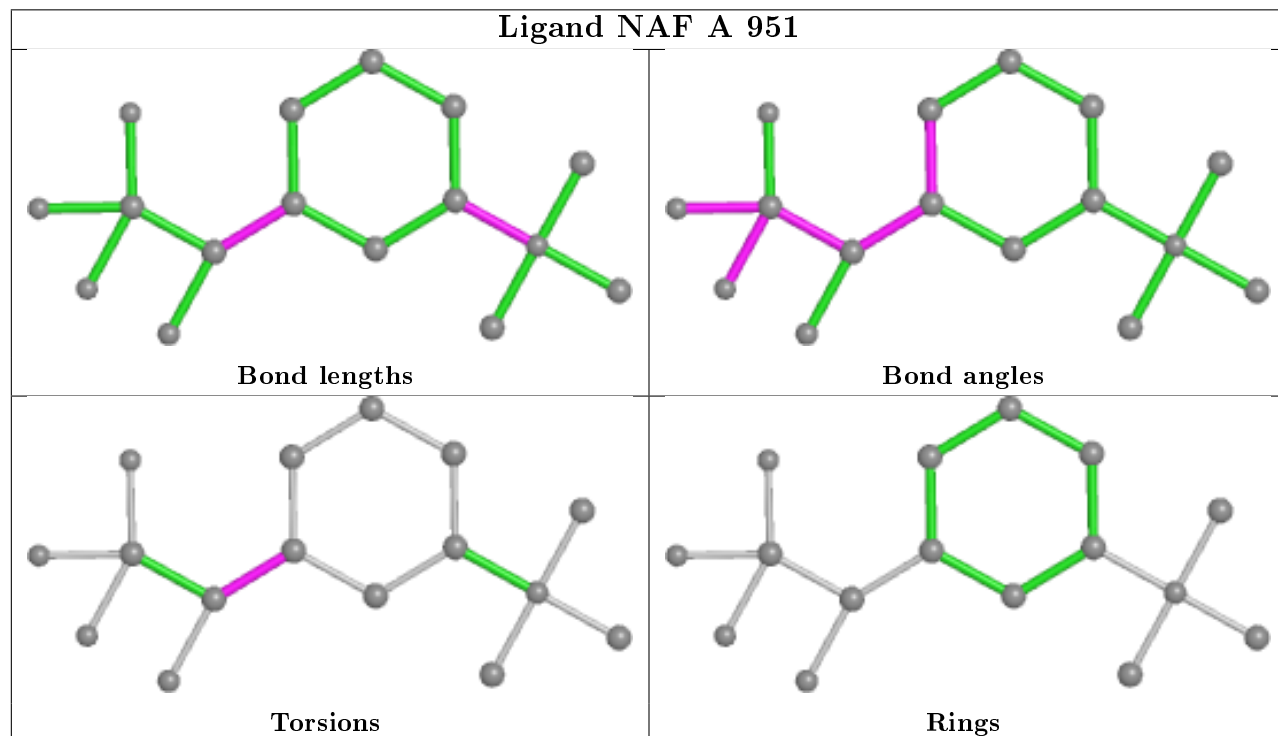
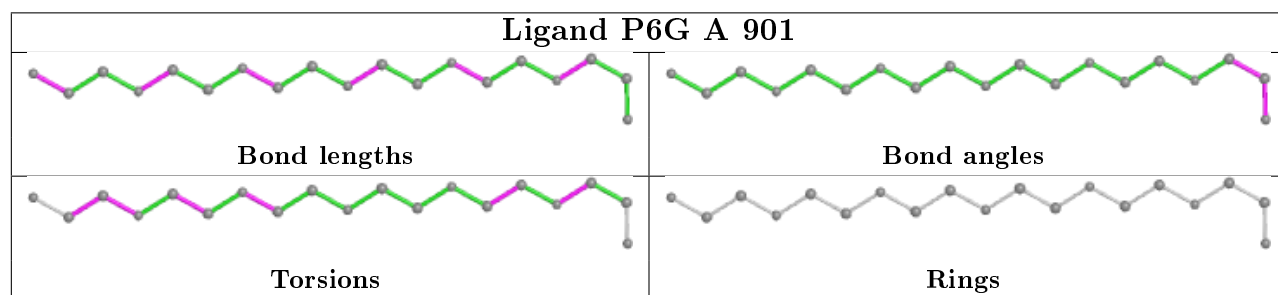
There are no ring outliers.

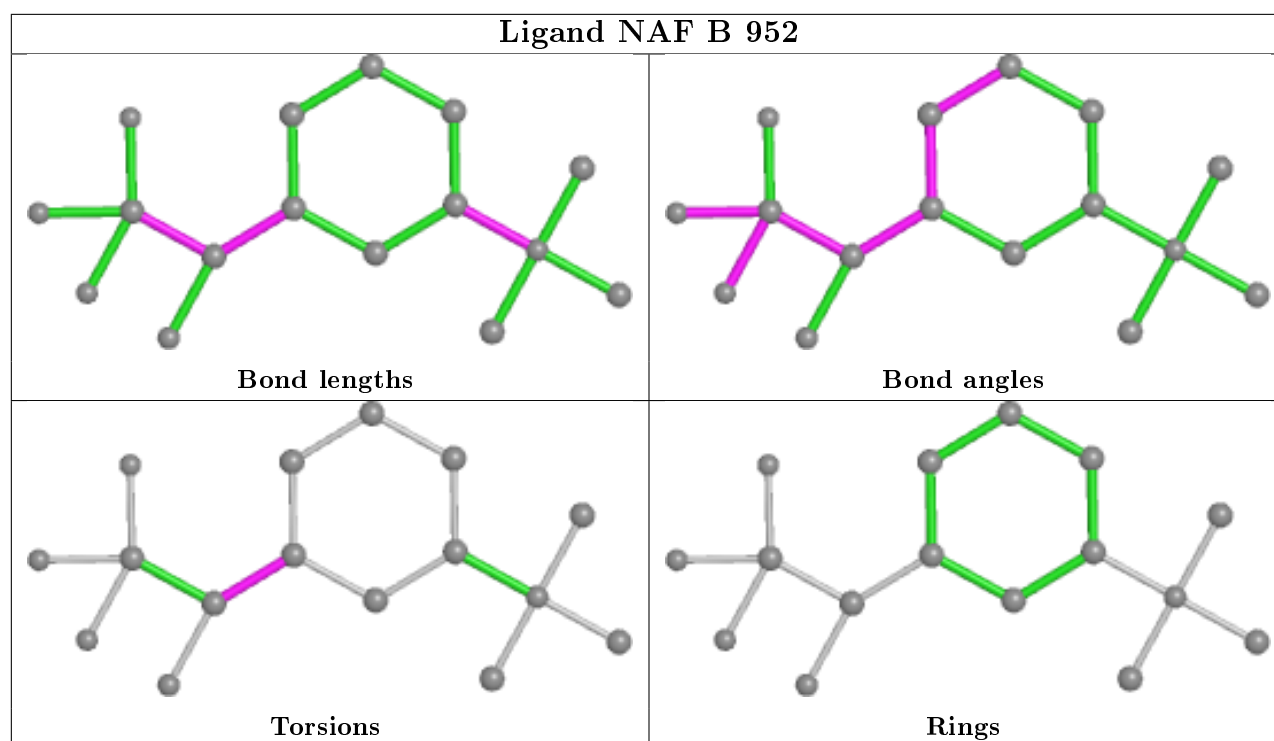
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	951	NAF	4	0
4	B	952	NAF	4	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	536/543 (98%)	0.22	31 (5%)	23 22	46, 61, 85, 110	0
1	B	534/543 (98%)	0.41	42 (7%)	12 11	50, 67, 89, 116	0
All	All	1070/1086 (98%)	0.31	73 (6%)	17 15	46, 64, 88, 116	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	495	SER	8.8
1	B	543	THR	6.7
1	B	542	ALA	5.8
1	A	497	SER	5.6
1	B	497	SER	5.5
1	B	540	LEU	5.2
1	B	118	ILE	5.0
1	B	541	SER	4.9
1	B	495	SER	4.8
1	A	494	ASP	4.5
1	B	204	ALA	4.2
1	A	496	LYS	4.1
1	B	117	TRP	4.0
1	A	542	ALA	3.8
1	A	493	ARG	3.8
1	B	268	GLU	3.7
1	B	451	ILE	3.6
1	A	498	PRO	3.5
1	A	272	CYS	3.2
1	A	204	ALA	3.1
1	B	539	LEU	3.1
1	A	492	PRO	3.0
1	B	123	PHE	2.9
1	B	121	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	206	ALA	2.8
1	A	117	TRP	2.8
1	B	205	GLY	2.8
1	A	209	VAL	2.8
1	A	491	ASP	2.8
1	B	209	VAL	2.8
1	A	118	ILE	2.8
1	B	265	ASN	2.8
1	A	323	ASP	2.8
1	A	236	TRP	2.7
1	B	206	ALA	2.7
1	A	205	GLY	2.7
1	A	322	GLN	2.6
1	A	467	THR	2.6
1	B	467	THR	2.6
1	A	2	GLY	2.6
1	A	227	LEU	2.6
1	B	133	TYR	2.6
1	A	165	ARG	2.6
1	B	208	SER	2.6
1	A	230	GLY	2.6
1	B	120	GLY	2.5
1	B	119	TYR	2.5
1	B	207	ALA	2.5
1	B	227	LEU	2.5
1	B	230	GLY	2.4
1	B	125	SER	2.4
1	A	540	LEU	2.4
1	B	258	PRO	2.3
1	B	323	ASP	2.3
1	A	203	SER	2.3
1	B	200	PHE	2.3
1	B	127	ALA	2.3
1	B	149	MET	2.2
1	A	411	VAL	2.2
1	A	541	SER	2.2
1	A	207	ALA	2.2
1	A	229	SER	2.2
1	B	151	TYR	2.1
1	A	407	VAL	2.1
1	B	78	PRO	2.1
1	B	468	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	492	PRO	2.1
1	B	201	GLY	2.1
1	B	148	SER	2.1
1	B	236	TRP	2.1
1	B	122	GLY	2.1
1	B	158	PHE	2.0
1	B	146	LEU	2.0

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

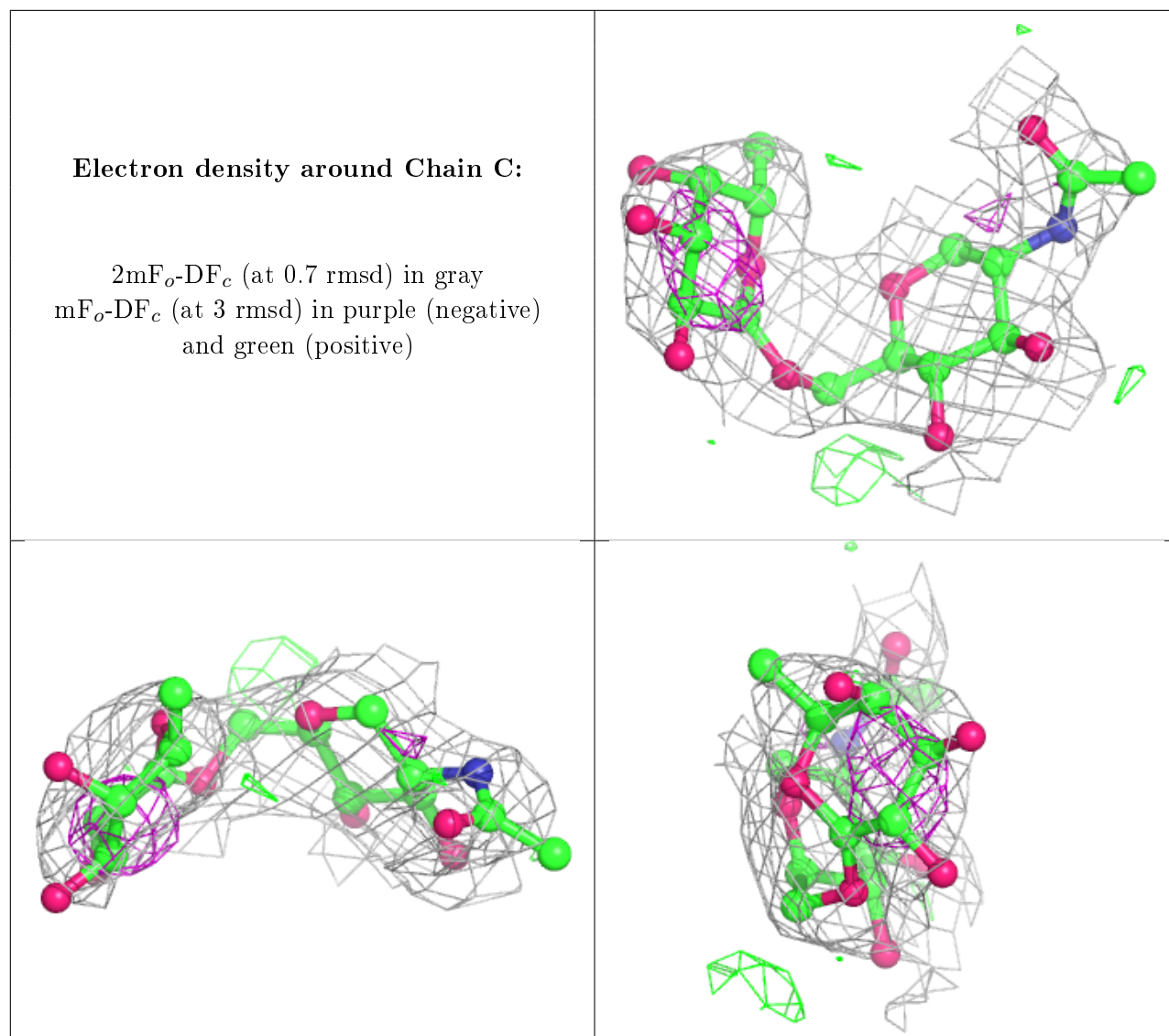
There are no non-standard protein/DNA/RNA residues in this entry.

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
2	FUC	C	2	10/11	0.85	0.60	108,109,111,111	0
2	NAG	C	1	14/15	0.86	0.41	95,99,101,105	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 ⓘ

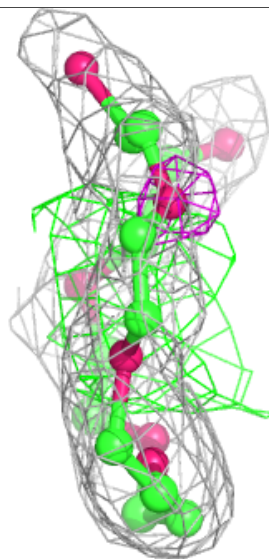
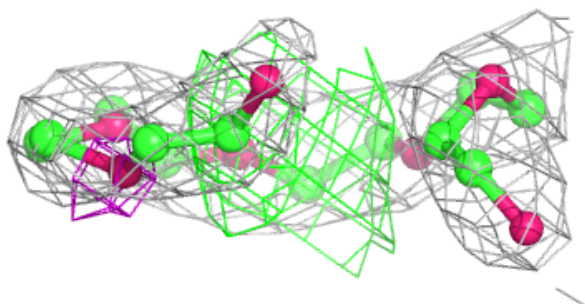
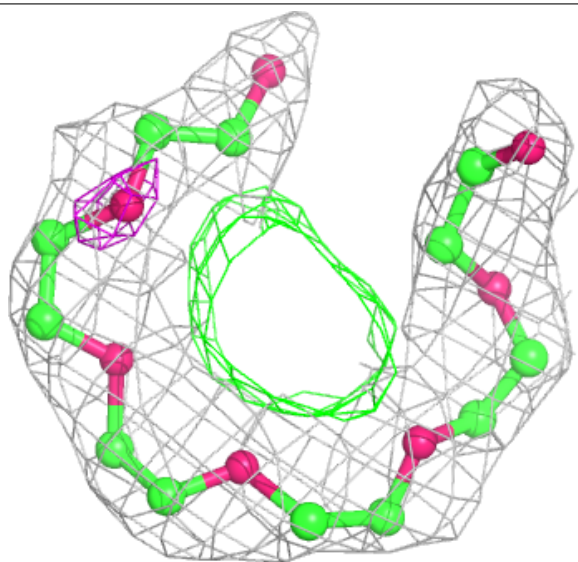
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	B	601	14/15	0.58	0.45	96,99,102,102	0
6	PG4	A	902	13/13	0.71	0.25	87,93,99,99	0
3	NAG	A	701	14/15	0.76	0.41	98,101,103,104	0
5	P6G	A	901	19/19	0.89	0.20	76,82,86,87	0
4	NAF	B	952	16/17	0.96	0.17	57,60,61,64	0
4	NAF	A	951	16/17	0.96	0.20	51,55,56,56	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.

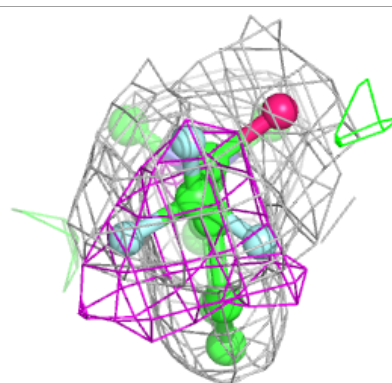
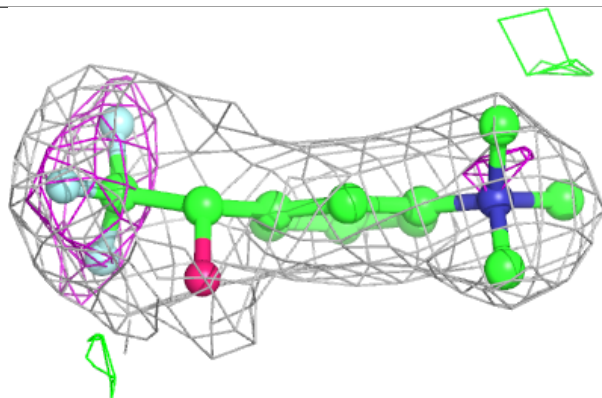
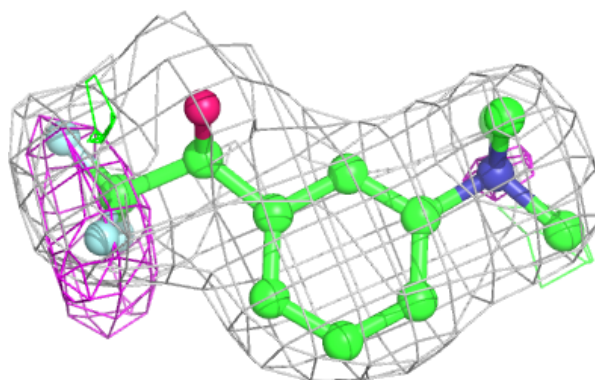
Electron density around P6G A 901:

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

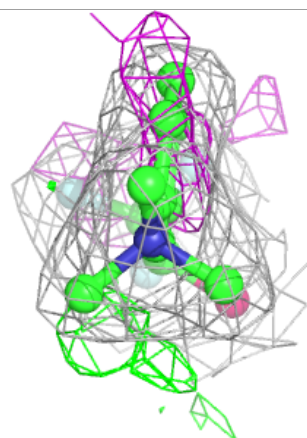
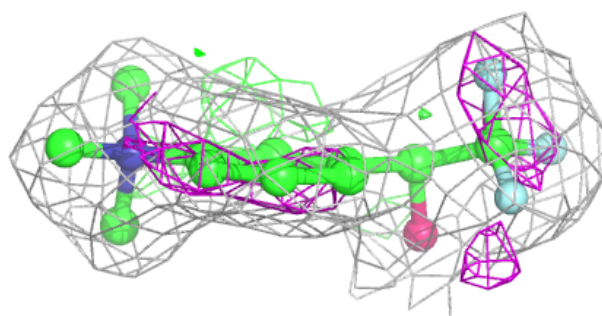
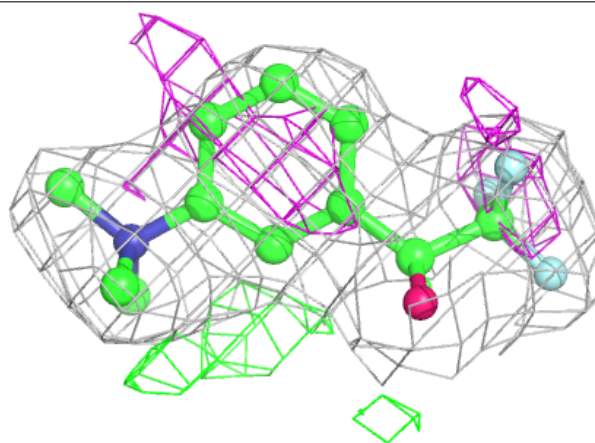


Electron density around NAF B 952:

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

**Electron density around NAF A 951:**

$2mF_o-DF_c$ (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.