



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 02:50 PM BST

PDB ID : 1J07
Title : Crystal structure of the mouse acetylcholinesterase-decidium complex
Authors : Bourne, Y.; Taylor, P.; Radic, Z.; Marchot, P.
Deposited on : 2002-11-07
Resolution : 2.35 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

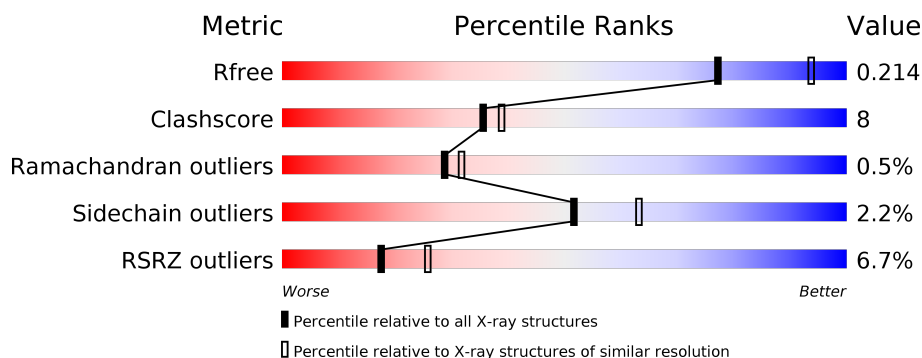
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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>83%</div> <div>15%</div> <div>..</div> </div>
1	B	543	<div> <div>7%</div> <div>80%</div> <div>17%</div> <div>..</div> </div>
2	C	2	<div> <div>50%</div> <div>50%</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	NAG	C	1	-	-	-	X
2	FUC	C	2	-	-	-	X
3	NAG	B	601	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 8904 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	0	0
			4184	2684	726	760	14			
1	B	534	Total	C	N	O	S	0	0	0
			4171	2678	722	757	14			

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



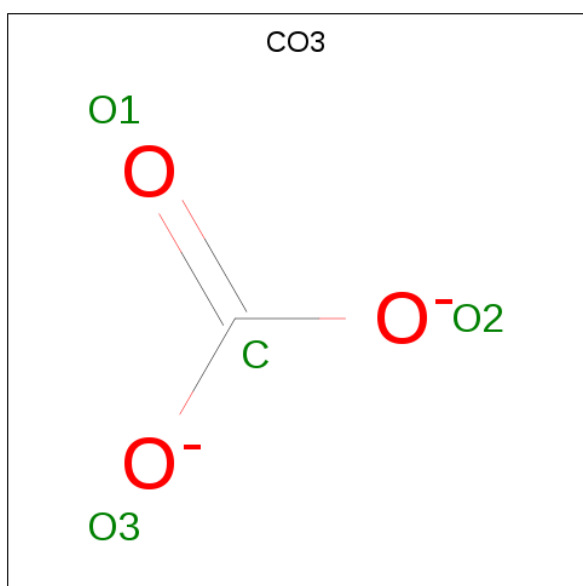
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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 CARBONATE ION (three-letter code: CO3) (formula: CO₃).

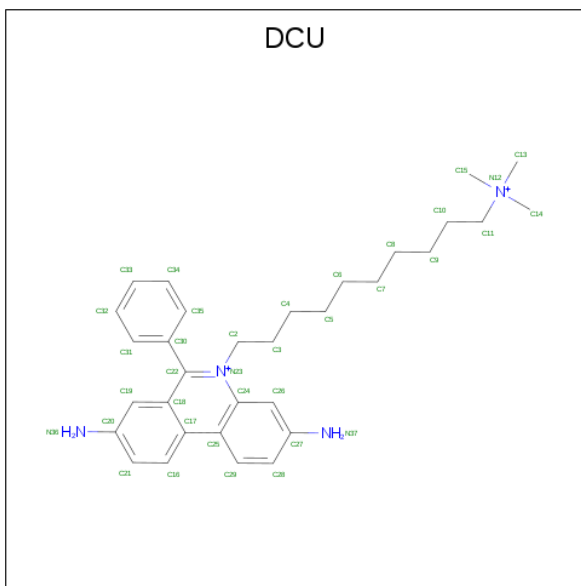


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	1	3		
4	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

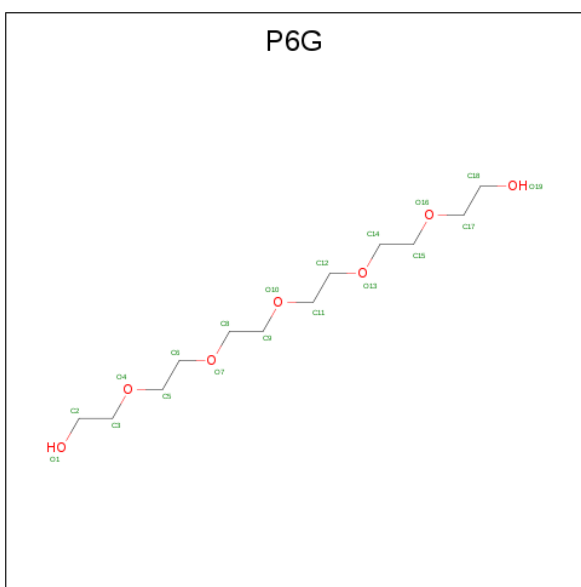
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Cl 2 2	0	0

- Molecule 6 is 3,8-DIAMINO-5,10'-(TRIMETHYLAMMONIUM)DECYL-6-PHENYL PHENANTHRIDINIUM (three-letter code: DCU) (formula: C₃₂H₄₄N₄).



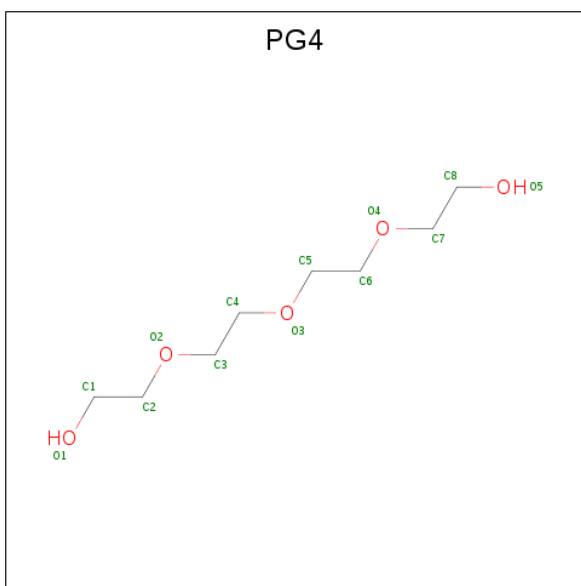
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N 36 32 4	0	0
6	B	1	Total C N 36 32 4	0	0

- Molecule 7 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



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

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			11	8	3		

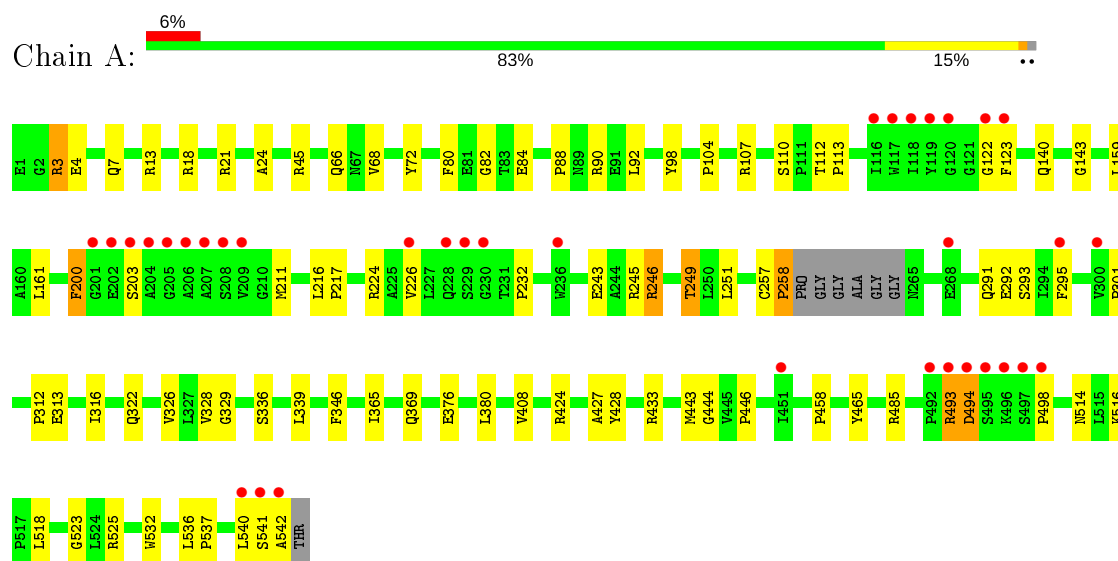
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	223	Total 223	O 223	0	0
9	B	162	Total 162	O 162	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 C:



Legend for Chain C:
H001 (yellow)
F002 (green)

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.53Å 112.31Å 226.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.91 – 2.35 39.42 – 2.35	Depositor EDS
% Data completeness (in resolution range)	92.8 (29.91-2.35) 92.9 (39.42-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.88 (at 2.34Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.199 , 0.227 0.191 , 0.214	Depositor DCC
R_{free} test set	1589 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.745	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.1	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	0.96	EDS
Total number of atoms	8904	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO3, NAG, CL, PG4, FUC, P6G, DCU

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	0.55	0/4308	0.79	4/5887 (0.1%)
1	B	0.52	0/4295	0.74	1/5869 (0.0%)
All	All	0.54	0/8603	0.77	5/11756 (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 (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	CYS	C-N-CD	-20.10	76.37	120.60
1	A	257	CYS	C-N-CA	13.68	179.44	122.00
1	B	494	ASP	N-CA-C	-6.96	92.21	111.00
1	A	258	PRO	CA-N-CD	-5.76	103.44	111.50
1	A	161	LEU	CA-CB-CG	-5.53	102.59	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	70	TYR	Sidechain

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	4184	0	4070	55	0
1	B	4171	0	4061	80	0
2	C	24	0	22	0	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	4	0	0	1	0
4	B	4	0	0	1	0
5	A	2	0	0	1	0
6	A	36	0	44	4	0
6	B	36	0	44	3	0
7	B	19	0	26	1	0
8	B	11	0	12	0	0
9	A	223	0	0	4	0
9	B	162	0	0	2	0
All	All	8904	0	8305	136	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 8.

All (136) 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:197:VAL:H	1:B:223:HIS:HD2	1.06	0.95
1:B:424:ARG:HH11	1:B:424:ARG:HG3	1.37	0.89
1:A:245:ARG:O	1:A:249:THR:HG23	1.79	0.83
1:B:197:VAL:H	1:B:223:HIS:CD2	1.98	0.76
1:B:497:SER:HB2	1:B:498:PRO:C	2.07	0.75
1:B:351:GLU:OE2	1:B:351:GLU:HA	1.87	0.74
1:B:161:LEU:HD11	1:B:269:LEU:HD22	1.68	0.74
1:A:292:GLU:HA	6:A:951:DCU:H62	1.71	0.72
1:B:493:ARG:HB3	1:B:493:ARG:HH11	1.54	0.70
1:B:353:LEU:HB3	1:B:391:PRO:HB2	1.75	0.68
1:A:113:PRO:HG2	1:A:485:ARG:HG2	1.74	0.68
1:B:45:ARG:NH1	1:B:51:GLU:OE1	2.27	0.67
1:B:243:GLU:OE1	1:B:246:ARG:NH1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:ARG:HG3	1:B:424:ARG:NH1	2.00	0.66
1:B:493:ARG:CB	1:B:493:ARG:HH11	2.09	0.65
1:A:7:GLN:NE2	1:A:107:ARG:H	1.93	0.65
1:A:4:GLU:OE2	1:A:18:ARG:HD3	1.99	0.62
1:A:203:SER:OG	4:A:903:CO3:C	2.46	0.62
1:B:203:SER:OG	4:B:904:CO3:C	2.48	0.62
1:A:376:GLU:HG2	1:B:538:LYS:NZ	2.16	0.61
1:A:80:PHE:O	1:A:84:GLU:HG2	2.00	0.61
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.37	0.60
1:A:433:ARG:HD3	9:A:1971:HOH:O	2.02	0.60
1:B:166:GLU:HG2	1:B:270:ILE:HD12	1.82	0.60
1:A:7:GLN:HB2	9:A:2080:HOH:O	2.02	0.59
1:B:292:GLU:HA	6:B:952:DCU:H62	1.84	0.59
1:A:3:ARG:HH11	1:A:3:ARG:HG3	1.67	0.59
1:B:112:THR:HG21	1:B:143:GLY:O	2.05	0.57
1:A:243:GLU:OE1	1:A:246:ARG:NH1	2.38	0.57
1:B:408:VAL:HG11	1:B:525:ARG:HG3	1.87	0.56
1:A:541:SER:O	1:A:542:ALA:HB2	2.06	0.56
1:B:528:THR:O	1:B:531:PHE:HB3	2.06	0.56
1:B:197:VAL:N	1:B:223:HIS:HD2	1.90	0.56
1:B:161:LEU:HD12	1:B:270:ILE:HD11	1.88	0.55
1:B:161:LEU:HD12	1:B:270:ILE:CG1	2.35	0.55
1:A:369:GLN:HB2	9:A:1893:HOH:O	2.07	0.55
1:B:80:PHE:O	1:B:84:GLU:HG2	2.07	0.55
1:B:165:ARG:HB3	1:B:165:ARG:NH1	2.22	0.55
1:A:112:THR:HG21	1:A:143:GLY:O	2.07	0.55
1:B:356:ARG:HA	1:B:394:LEU:HD13	1.88	0.55
1:A:493:ARG:O	1:A:494:ASP:HB2	2.07	0.54
1:B:67:ASN:ND2	9:B:986:HOH:O	2.37	0.54
1:B:444:GLY:O	1:B:446:PRO:HD3	2.07	0.54
1:B:433:ARG:CZ	1:B:437:LEU:HD23	2.38	0.54
1:B:245:ARG:O	1:B:249:THR:HG23	2.08	0.53
1:B:541:SER:O	1:B:542:ALA:HB2	2.08	0.53
1:A:537:PRO:O	1:A:540:LEU:HB3	2.09	0.53
1:A:224:ARG:NH1	1:A:224:ARG:HG3	2.24	0.52
1:A:312:PRO:O	1:A:316:ILE:HG23	2.09	0.52
1:B:166:GLU:HG2	1:B:270:ILE:CD1	2.38	0.52
1:B:36:PRO:HB3	1:B:98:TYR:CE1	2.44	0.52
1:A:224:ARG:HH11	1:A:224:ARG:HG3	1.75	0.52
1:B:328:VAL:O	1:B:427:ALA:HA	2.09	0.52
1:B:493:ARG:CG	1:B:493:ARG:HH11	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:PRO:HG2	1:B:108:PRO:HG3	1.92	0.52
1:B:134:ASP:OD1	1:B:136:ARG:HD2	2.09	0.51
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.46	0.51
1:B:224:ARG:HG3	1:B:224:ARG:NH1	2.26	0.50
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.46	0.50
1:B:243:GLU:O	1:B:247:ARG:HG3	2.12	0.50
1:B:210:GLY:HA3	1:B:232:PRO:HD3	1.94	0.49
1:B:532:TRP:CE3	1:B:536:LEU:HD12	2.46	0.49
1:A:408:VAL:HG11	1:A:525:ARG:HG3	1.95	0.49
1:A:216:LEU:HB3	1:A:217:PRO:HD3	1.95	0.48
1:A:514:ASN:OD1	1:A:516:LYS:HB2	2.13	0.48
1:B:122:GLY:O	1:B:123:PHE:HB2	2.12	0.48
5:A:999:CL:CL	6:A:951:DCU:N37	2.84	0.48
1:A:326:VAL:HG12	1:A:328:VAL:HG13	1.95	0.48
1:B:369:GLN:HB2	9:B:1037:HOH:O	2.13	0.48
6:B:952:DCU:H22	6:B:952:DCU:H26	1.76	0.48
1:B:187:ILE:HA	1:B:187:ILE:HD12	1.77	0.47
1:A:3:ARG:NH1	1:A:3:ARG:HG3	2.28	0.47
1:B:497:SER:CB	1:B:498:PRO:C	2.81	0.47
1:A:328:VAL:O	1:A:427:ALA:HA	2.14	0.47
1:A:336:SER:HB2	1:A:443:MET:HG2	1.95	0.47
1:A:104:PRO:HG3	1:A:143:GLY:HA2	1.97	0.47
1:A:200:PHE:HB2	1:A:226:VAL:HB	1.97	0.47
1:B:165:ARG:HB3	1:B:165:ARG:HH11	1.81	0.46
1:A:200:PHE:CB	1:A:226:VAL:HB	2.46	0.46
1:B:66:GLN:HG3	1:B:98:TYR:CG	2.50	0.46
1:A:376:GLU:O	1:A:380:LEU:HG	2.15	0.46
1:B:360:LEU:HD22	1:B:379:VAL:HG21	1.98	0.46
1:A:7:GLN:HE21	1:A:107:ARG:HG3	1.80	0.46
1:B:104:PRO:CG	1:B:108:PRO:HG3	2.46	0.46
1:A:211:MET:HG3	1:A:232:PRO:HB3	1.99	0.45
1:B:224:ARG:HG3	1:B:224:ARG:HH11	1.82	0.45
1:B:374:ALA:HB2	1:B:540:LEU:HD21	1.99	0.45
1:B:536:LEU:HA	1:B:536:LEU:HD23	1.70	0.45
1:B:339:LEU:HD11	1:B:399:SER:HA	1.98	0.45
1:B:10:VAL:HG23	1:B:32:PHE:CE2	2.52	0.45
1:B:134:ASP:CG	1:B:136:ARG:HD2	2.37	0.45
1:B:211:MET:HG2	1:B:308:LEU:HD21	1.98	0.45
1:B:326:VAL:HG12	1:B:328:VAL:HG13	2.00	0.44
1:B:491:ASP:HA	1:B:492:PRO:HD3	1.73	0.44
1:B:134:ASP:OD2	1:B:136:ARG:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ARG:HH12	1:B:16:GLN:NE2	2.15	0.44
1:B:428:TYR:CD1	1:B:428:TYR:C	2.90	0.44
1:B:66:GLN:HG3	1:B:98:TYR:CD1	2.52	0.44
1:B:200:PHE:CB	1:B:226:VAL:HB	2.47	0.44
1:A:122:GLY:O	1:A:123:PHE:HB2	2.17	0.44
1:B:439:TRP:HB3	1:B:440:PRO:HD2	1.99	0.44
1:B:200:PHE:HB2	1:B:226:VAL:HB	1.99	0.44
1:A:24:ALA:HB3	1:A:140:GLN:HG3	1.99	0.43
1:A:80:PHE:CE2	1:A:82:GLY:HA3	2.53	0.43
1:A:444:GLY:O	1:A:446:PRO:HD3	2.18	0.43
1:A:376:GLU:HG2	1:B:538:LYS:HZ3	1.82	0.43
1:A:329:GLY:HA3	1:A:428:TYR:CZ	2.54	0.43
1:A:339:LEU:HD13	1:A:346:PHE:CE2	2.52	0.43
1:B:136:ARG:HG2	1:B:137:PHE:N	2.34	0.43
1:B:11:ARG:NH1	1:B:16:GLN:HG2	2.33	0.43
1:A:293:SER:HA	1:A:365:ILE:HG23	2.01	0.43
1:A:66:GLN:HG3	1:A:98:TYR:CD1	2.54	0.43
1:A:13:ARG:NH2	9:A:1888:HOH:O	2.52	0.43
1:A:159:LEU:C	1:A:159:LEU:HD23	2.39	0.42
1:A:428:TYR:C	1:A:428:TYR:CD1	2.93	0.42
1:B:433:ARG:NH1	1:B:437:LEU:HD23	2.34	0.42
1:A:88:PRO:HG2	1:A:92:LEU:HD21	2.01	0.42
1:B:46:ARG:HD3	1:B:47:PHE:CZ	2.54	0.42
1:A:537:PRO:O	1:A:540:LEU:N	2.53	0.42
1:A:68:VAL:HG23	1:A:90:ARG:HB2	2.02	0.42
1:B:72:TYR:CZ	6:B:952:DCU:H29	2.55	0.42
1:A:251:LEU:O	1:A:251:LEU:HG	2.20	0.42
1:B:395:ARG:CZ	1:B:442:TRP:HB2	2.50	0.42
1:B:161:LEU:HD12	1:B:270:ILE:CD1	2.48	0.42
1:B:541:SER:O	1:B:542:ALA:CB	2.68	0.41
1:A:498:PRO:HG2	1:A:518:LEU:HB2	2.03	0.41
1:A:541:SER:O	1:A:542:ALA:CB	2.68	0.41
1:A:532:TRP:CE3	1:A:536:LEU:HD12	2.55	0.41
1:A:72:TYR:CZ	6:A:951:DCU:H29	2.56	0.41
1:B:497:SER:OG	1:B:499:GLN:NE2	2.52	0.41
6:A:951:DCU:H22	6:A:951:DCU:H26	1.71	0.41
1:B:293:SER:HB3	1:B:368:PRO:HB3	2.03	0.41
1:B:4:GLU:HG3	1:B:5:ASP:H	1.86	0.41
1:B:493:ARG:CG	1:B:493:ARG:NH1	2.82	0.40
1:A:537:PRO:O	1:A:540:LEU:CB	2.69	0.40
1:B:380:LEU:HB2	7:B:901:P6G:H81	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	532/543 (98%)	506 (95%)	24 (4%)	2 (0%)	34	38
1	B	530/543 (98%)	509 (96%)	18 (3%)	3 (1%)	25	27
All	All	1062/1086 (98%)	1015 (96%)	42 (4%)	5 (0%)	29	32

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	494	ASP
1	B	542	ALA
1	A	494	ASP
1	B	497	SER
1	A	523	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	440/443 (99%)	425 (97%)	15 (3%)	37	46
1	B	439/443 (99%)	435 (99%)	4 (1%)	78	87
All	All	879/886 (99%)	860 (98%)	19 (2%)	52	63

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	21	ARG
1	A	45	ARG
1	A	110	SER
1	A	200	PHE
1	A	246	ARG
1	A	249	THR
1	A	258	PRO
1	A	291	GLN
1	A	295	PHE
1	A	301	PRO
1	A	313	GLU
1	A	322	GLN
1	A	424	ARG
1	A	493	ARG
1	B	23	LYS
1	B	295	PHE
1	B	493	ARG
1	B	543	THR

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	7	GLN
1	A	291	GLN
1	A	509	GLN
1	B	16	GLN
1	B	223	HIS
1	B	322	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	0.85	1 (7%)	17,19,21	0.74	0
2	FUC	C	2	2	10,10,11	0.78	0	14,14,16	0.64	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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	C1-C2	2.22	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

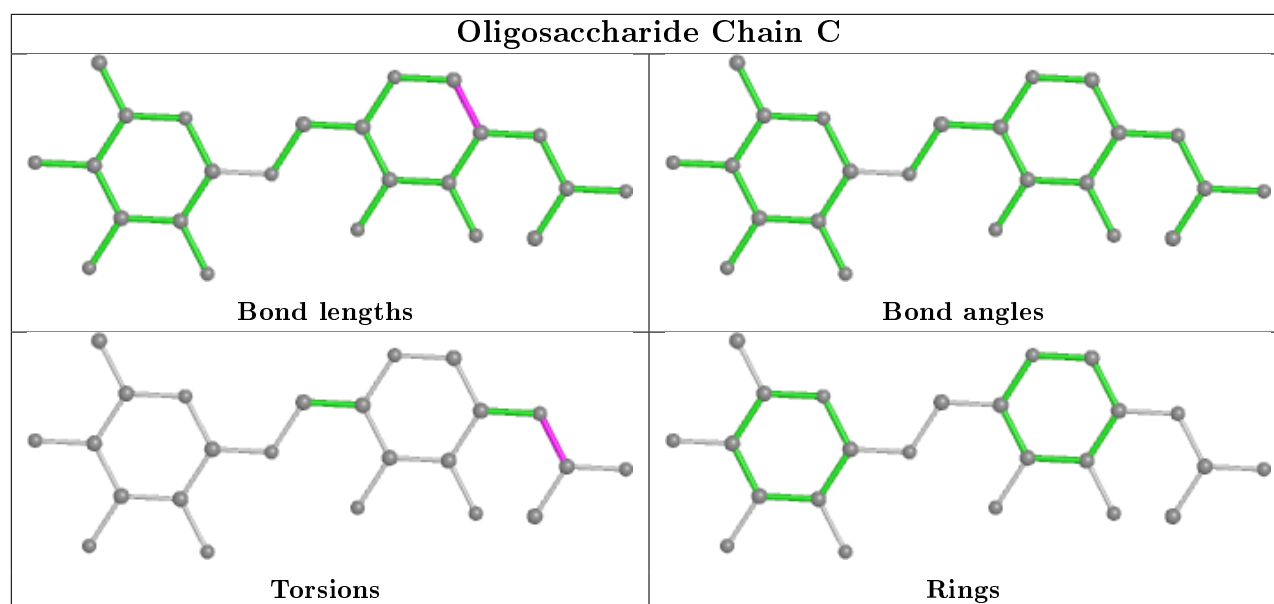
All (2) torsion outliers are listed below:

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 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\# Z > 2$
6	DCU	B	952	-	37,39,39	1.77	9 (24%)	47,54,54	1.41	6 (12%)
3	NAG	B	601	1	14,14,15	0.86	0	17,19,21	0.69	0
3	NAG	A	701	1	14,14,15	0.71	0	17,19,21	0.74	1 (5%)
6	DCU	A	951	-	37,39,39	1.73	8 (21%)	47,54,54	1.34	5 (10%)
8	PG4	B	902	-	10,10,12	1.91	2 (20%)	9,9,11	0.81	0
4	CO3	B	904	-	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	A	903	-	0,3,3	0.00	-	0,3,3	0.00	-
7	P6G	B	901	-	18,18,18	2.17	6 (33%)	17,17,17	1.19	1 (5%)

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	DCU	B	952	-	-	9/18/18/18	0/4/4/4
3	NAG	B	601	1	-	4/6/23/26	0/1/1/1
3	NAG	A	701	1	-	2/6/23/26	0/1/1/1
6	DCU	A	951	-	-	8/18/18/18	0/4/4/4
8	PG4	B	902	-	-	4/8/8/10	-
7	P6G	B	901	-	-	8/16/16/16	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	902	PG4	O2-C3	4.70	1.62	1.42
6	B	952	DCU	C18-C17	4.62	1.49	1.42
6	A	951	DCU	C18-C17	4.59	1.49	1.42
7	B	901	P6G	O10-C9	4.47	1.61	1.42
6	B	952	DCU	C25-C24	4.08	1.49	1.41
7	B	901	P6G	O13-C12	3.70	1.58	1.42
6	A	951	DCU	C25-C24	3.51	1.48	1.41
7	B	901	P6G	O4-C3	3.46	1.57	1.42
7	B	901	P6G	O16-C15	3.41	1.56	1.42
7	B	901	P6G	O19-C18	3.36	1.59	1.42
6	A	951	DCU	C16-C21	3.17	1.43	1.36
6	B	952	DCU	C16-C21	3.13	1.43	1.36
6	B	952	DCU	C24-N23	3.05	1.44	1.40
6	B	952	DCU	C29-C28	2.95	1.42	1.36
8	B	902	PG4	O3-C5	2.79	1.54	1.42
7	B	901	P6G	O7-C6	2.78	1.54	1.42
6	A	951	DCU	C24-N23	2.75	1.43	1.40
6	A	951	DCU	C29-C28	2.74	1.42	1.36
6	B	952	DCU	C26-C24	2.46	1.45	1.40
6	A	951	DCU	C26-C24	2.31	1.45	1.40
6	A	951	DCU	C31-C30	2.24	1.44	1.39
6	B	952	DCU	C31-C30	2.24	1.44	1.39
6	B	952	DCU	C26-C27	2.23	1.43	1.39
6	B	952	DCU	C34-C35	2.16	1.43	1.38
6	A	951	DCU	C34-C35	2.15	1.43	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	952	DCU	C26-C24-C25	-4.50	114.90	120.61
6	A	951	DCU	C26-C24-C25	-4.48	114.93	120.61
6	B	952	DCU	C20-C19-C18	4.11	124.47	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	952	DCU	C2-N23-C24	-3.92	115.41	118.90
6	A	951	DCU	C20-C19-C18	3.68	124.09	120.90
6	A	951	DCU	C2-N23-C24	-3.66	115.64	118.90
7	B	901	P6G	O1-C2-C3	3.37	131.38	111.81
6	B	952	DCU	C18-C22-N23	2.69	122.54	119.12
6	A	951	DCU	C28-C29-C25	2.55	125.31	121.63
6	B	952	DCU	C28-C29-C25	2.41	125.11	121.63
3	A	701	NAG	C2-N2-C7	-2.24	119.71	122.90
6	B	952	DCU	C21-C16-C17	2.20	124.81	121.63
6	A	951	DCU	C21-C16-C17	2.05	124.60	121.63

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	952	DCU	C3-C2-N23-C22
6	B	952	DCU	C3-C2-N23-C24
6	A	951	DCU	C3-C2-N23-C22
6	A	951	DCU	C3-C2-N23-C24
3	B	601	NAG	C8-C7-N2-C2
3	B	601	NAG	O7-C7-N2-C2
3	B	601	NAG	O5-C5-C6-O6
3	A	701	NAG	C8-C7-N2-C2
6	B	952	DCU	N23-C2-C3-C4
3	A	701	NAG	O7-C7-N2-C2
8	B	902	PG4	O2-C3-C4-O3
3	B	601	NAG	C4-C5-C6-O6
6	A	951	DCU	N23-C2-C3-C4
7	B	901	P6G	O1-C2-C3-O4
7	B	901	P6G	O16-C17-C18-O19
6	A	951	DCU	C9-C10-C11-N12
8	B	902	PG4	C4-C3-O2-C2
7	B	901	P6G	O13-C14-C15-O16
6	B	952	DCU	C9-C10-C11-N12
6	A	951	DCU	C3-C4-C5-C6
6	B	952	DCU	C6-C7-C8-C9
6	B	952	DCU	C3-C4-C5-C6
6	B	952	DCU	C11-C10-C9-C8
6	B	952	DCU	C7-C8-C9-C10
6	A	951	DCU	C7-C8-C9-C10
6	A	951	DCU	C11-C10-C9-C8
6	A	951	DCU	C6-C7-C8-C9

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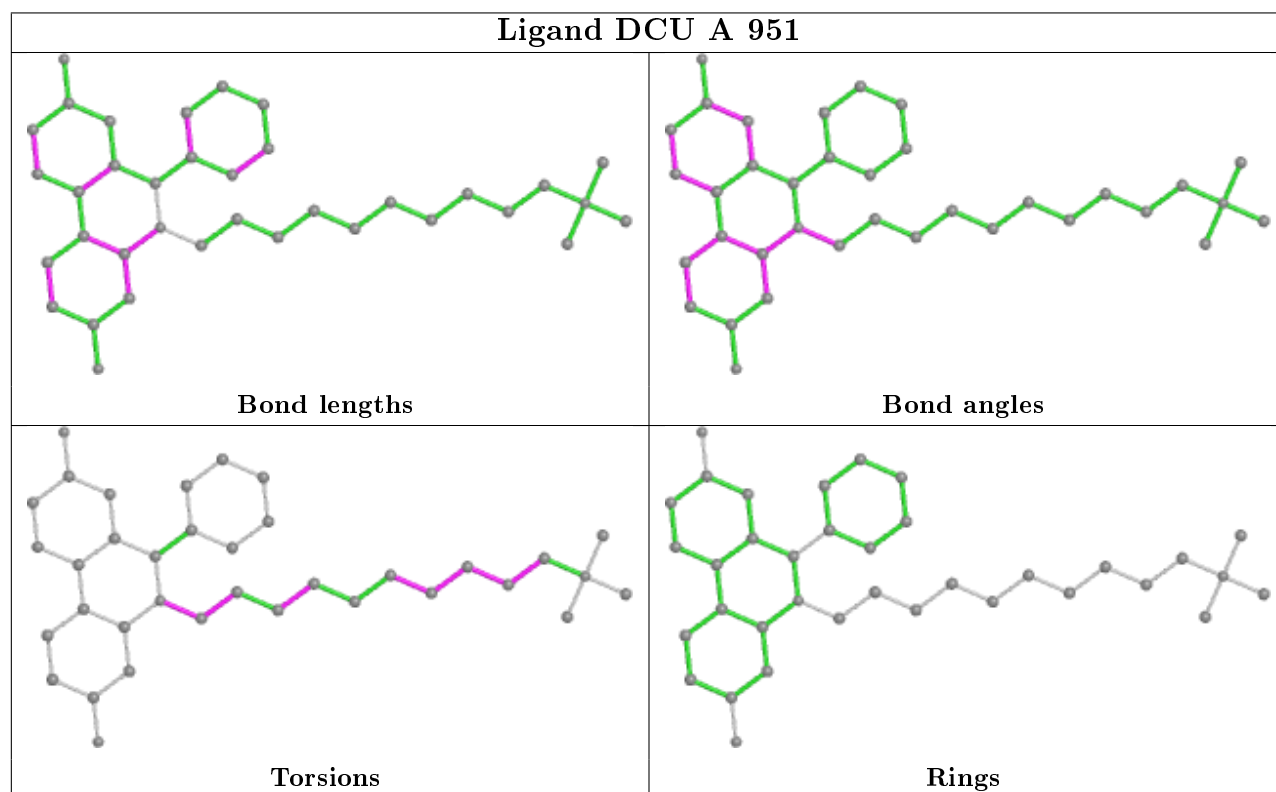
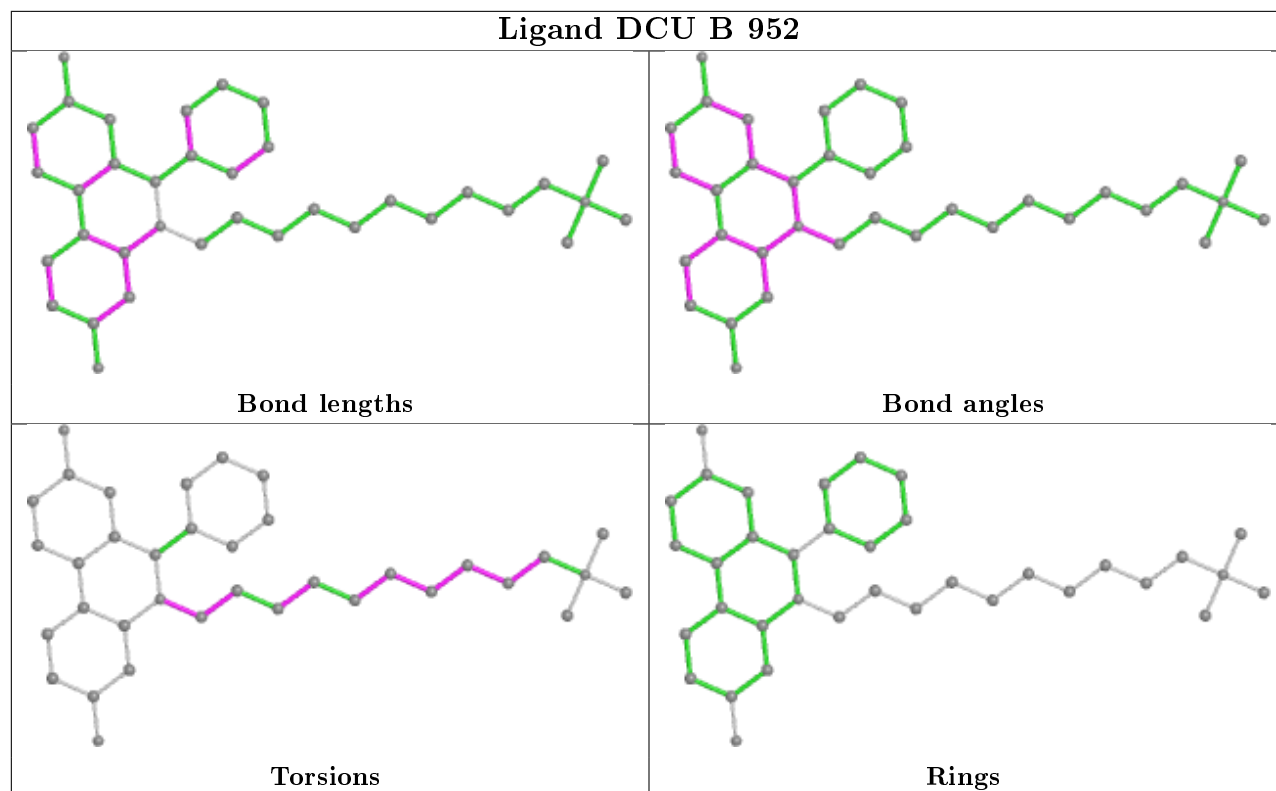
Mol	Chain	Res	Type	Atoms
6	B	952	DCU	C5-C6-C7-C8
7	B	901	P6G	C11-C12-O13-C14
7	B	901	P6G	C6-C5-O4-C3
8	B	902	PG4	C5-C6-O4-C7
7	B	901	P6G	O7-C8-C9-O10
8	B	902	PG4	O3-C5-C6-O4
7	B	901	P6G	C2-C3-O4-C5
7	B	901	P6G	C5-C6-O7-C8

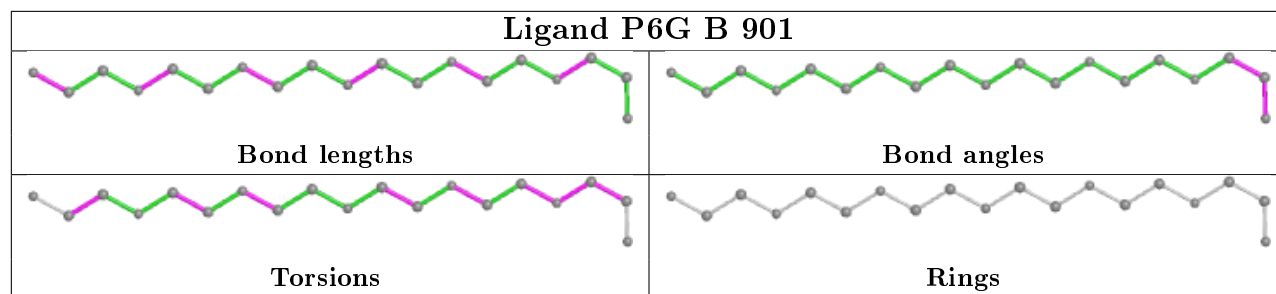
There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	952	DCU	3	0
6	A	951	DCU	4	0
4	B	904	CO3	1	0
4	A	903	CO3	1	0
7	B	901	P6G	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	536/543 (98%)	0.07	35 (6%)	18 27	32, 47, 69, 98	0
1	B	534/543 (98%)	0.18	37 (6%)	16 24	36, 52, 75, 99	0
All	All	1070/1086 (98%)	0.12	72 (6%)	17 26	32, 49, 72, 99	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	543	THR	6.5
1	B	542	ALA	5.0
1	A	495	SER	4.5
1	B	118	ILE	4.5
1	A	497	SER	4.4
1	B	207	ALA	4.3
1	B	204	ALA	4.0
1	A	496	LYS	4.0
1	B	541	SER	3.8
1	A	118	ILE	3.8
1	A	117	TRP	3.8
1	B	117	TRP	3.8
1	A	493	ARG	3.7
1	A	206	ALA	3.6
1	A	207	ALA	3.5
1	A	204	ALA	3.5
1	B	497	SER	3.4
1	B	123	PHE	3.2
1	A	201	GLY	3.2
1	B	206	ALA	3.1
1	B	495	SER	3.1
1	A	541	SER	3.0
1	B	258	PRO	3.0
1	A	494	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	119	TYR	3.0
1	B	208	SER	2.9
1	A	236	TRP	2.9
1	A	542	ALA	2.9
1	B	201	GLY	2.9
1	B	227	LEU	2.9
1	A	203	SER	2.9
1	A	205	GLY	2.9
1	B	4	GLU	2.9
1	A	123	PHE	2.8
1	B	268	GLU	2.7
1	A	540	LEU	2.6
1	A	208	SER	2.6
1	B	121	GLY	2.6
1	B	205	GLY	2.6
1	A	209	VAL	2.6
1	B	200	PHE	2.6
1	A	498	PRO	2.5
1	A	120	GLY	2.5
1	A	119	TYR	2.5
1	B	540	LEU	2.5
1	B	349	ASP	2.5
1	B	78	PRO	2.4
1	A	230	GLY	2.4
1	A	122	GLY	2.3
1	B	116	ILE	2.3
1	B	467	THR	2.3
1	A	295	PHE	2.3
1	B	132	VAL	2.3
1	B	133	TYR	2.3
1	A	268	GLU	2.3
1	A	492	PRO	2.2
1	B	493	ARG	2.2
1	B	228	GLN	2.2
1	B	236	TRP	2.2
1	A	226	VAL	2.2
1	B	122	GLY	2.2
1	A	300	VAL	2.1
1	B	226	VAL	2.1
1	B	79	GLY	2.1
1	B	257	CYS	2.1
1	A	202	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	228	GLN	2.1
1	A	451	ILE	2.1
1	B	229	SER	2.1
1	A	229	SER	2.1
1	B	120	GLY	2.1
1	A	116	ILE	2.0

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

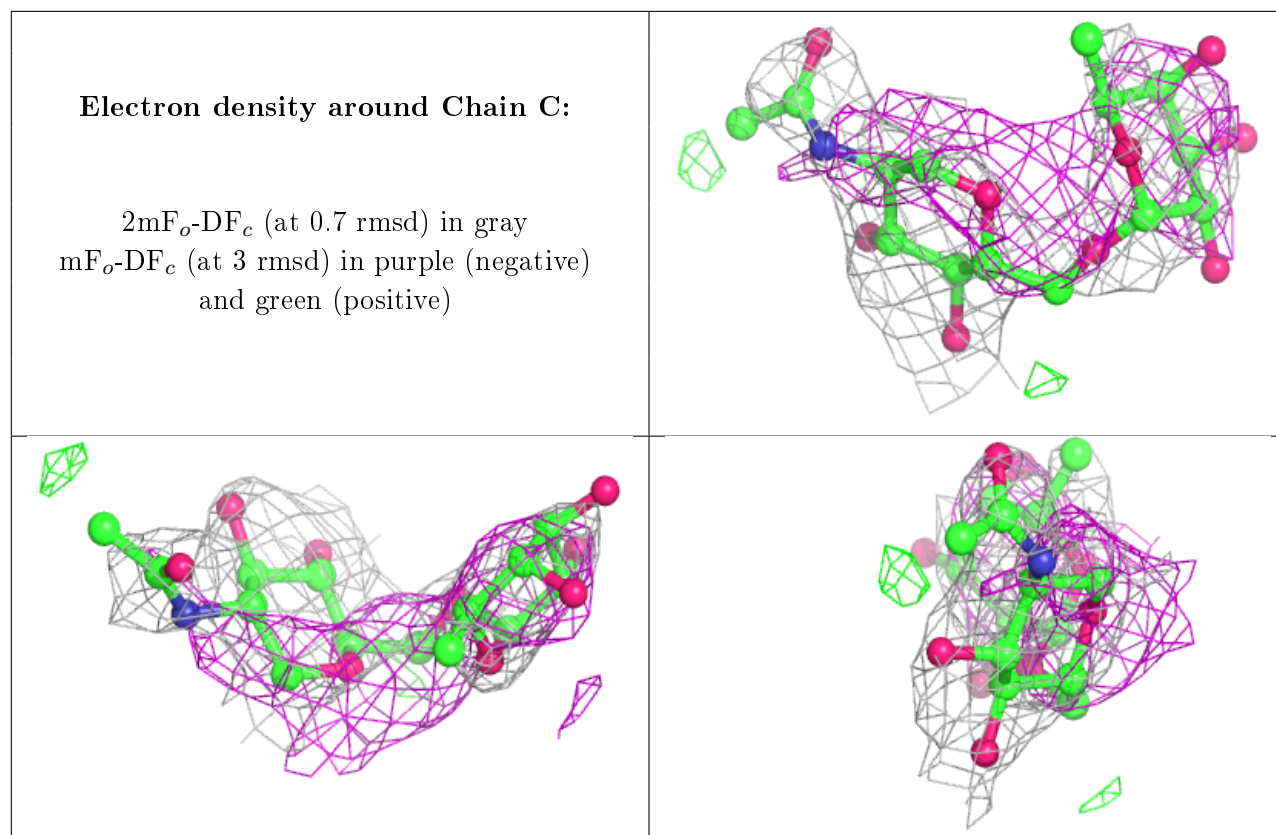
There are no non-standard protein/DNA/RNA residues in this entry.

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, 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	0.75	0.69	97,99,99,99	0
2	NAG	C	1	14/15	0.77	0.51	84,88,92,95	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 ⓘ

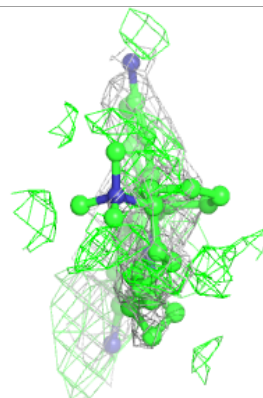
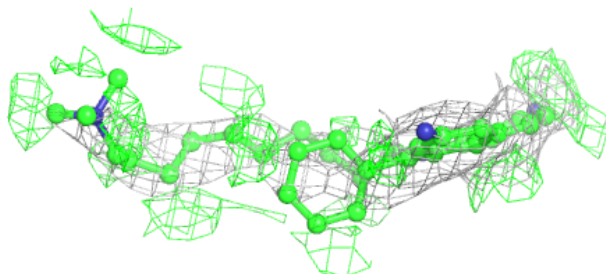
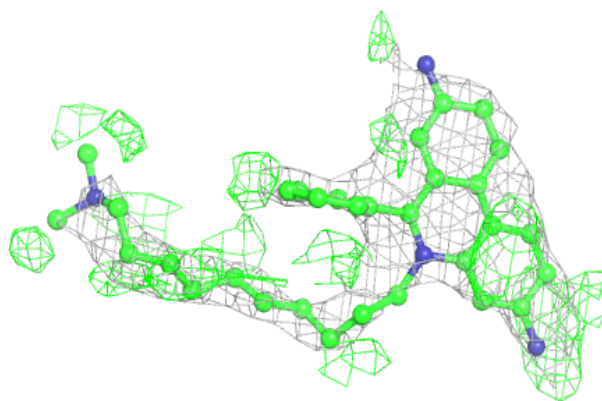
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	DCU	B	952	36/36	0.62	0.30	88,90,94,94	36
8	PG4	B	902	11/13	0.68	0.22	95,97,98,98	0
3	NAG	B	601	14/15	0.73	0.51	94,97,99,99	0
6	DCU	A	951	36/36	0.74	0.24	87,91,99,99	0
5	CL	A	999	1/1	0.75	0.34	85,85,85,85	0
3	NAG	A	701	14/15	0.87	0.42	90,94,96,97	0
4	CO3	B	904	4/4	0.88	0.28	74,75,76,76	0
4	CO3	A	903	4/4	0.89	0.31	61,62,64,66	0
5	CL	A	1867	1/1	0.90	0.24	90,90,90,90	1
7	P6G	B	901	19/19	0.92	0.16	59,67,75,77	0

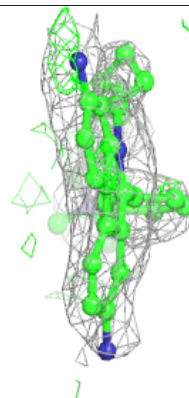
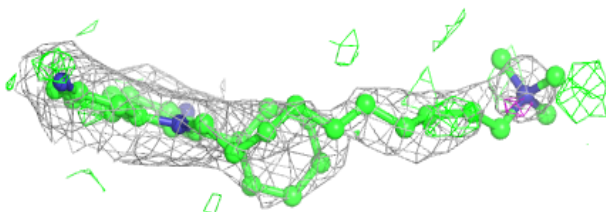
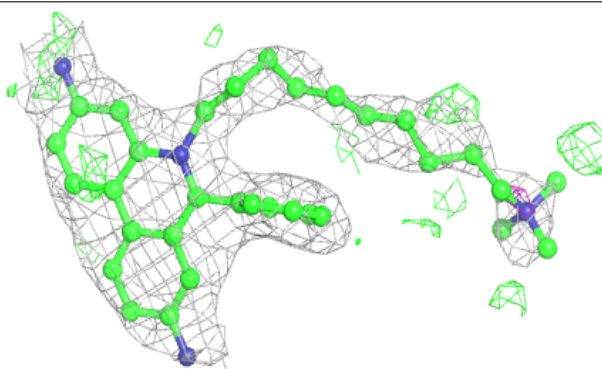
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DCU 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)

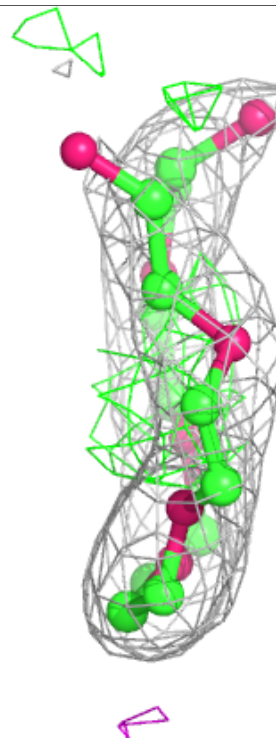
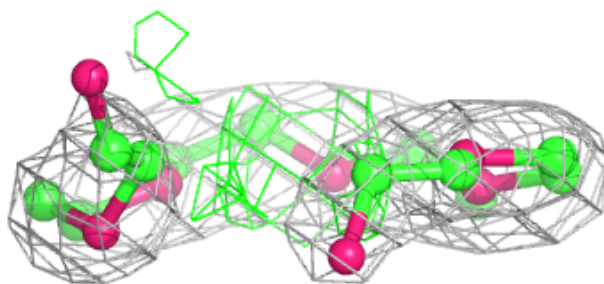
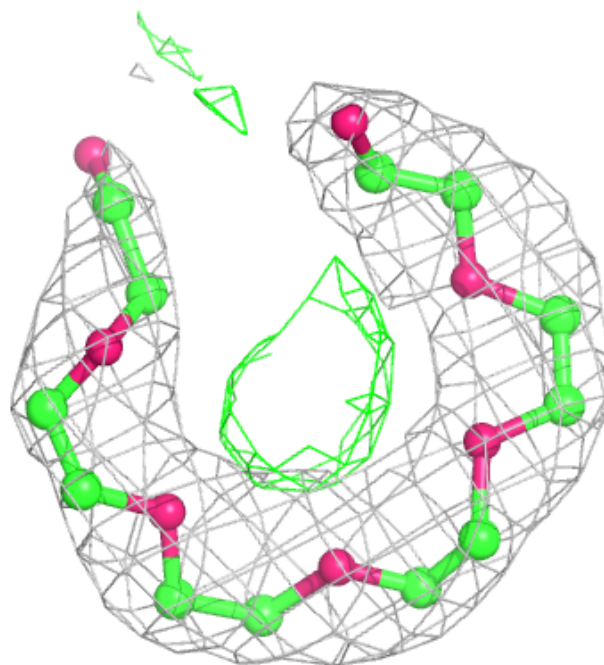
**Electron density around DCU A 951:**

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



Electron density around P6G B 901:

$2mF_o-DF_c$ (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.