



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 10:33 PM BST

PDB ID : 2GYW
Title : Crystal Structure of Mus musculus Acetylcholinesterase in Complex with Obidoxime
Authors : Pang, Y.P.; Boman, M.; Artursson, E.; Akfur, C.; Lundberg, S.
Deposited on : 2006-05-10
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

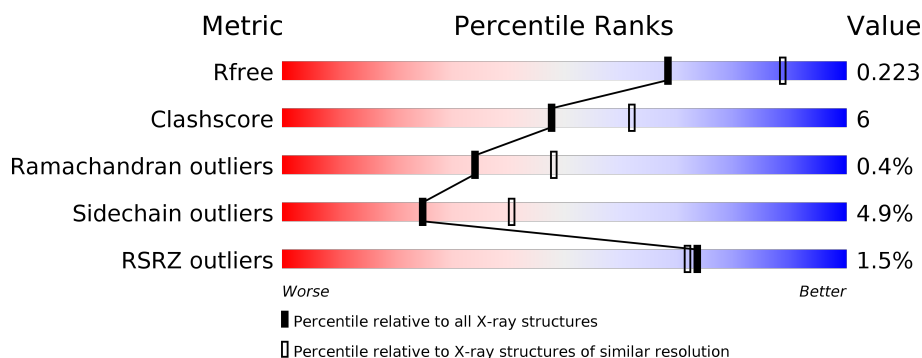
1 Overall quality at a glance

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 style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 82%; height: 10px; background-color: green;"></div> <div style="width: 15%; height: 10px; background-color: yellow;"></div> <div style="width: 3%; height: 10px; background-color: orange;"></div> <div style="width: 2%; height: 10px; background-color: red;"></div> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 82% 15% .. </div> </div>
1	B	543	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 84%; height: 10px; background-color: green;"></div> <div style="width: 13%; height: 10px; background-color: yellow;"></div> <div style="width: 3%; height: 10px; background-color: orange;"></div> <div style="width: 2%; height: 10px; background-color: red;"></div> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 84% 13% .. </div> </div>
2	C	2	<div> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <div style="text-align: center; margin-top: 5px;">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	NAG	C	1	-	-	-	X
2	FUC	C	2	-	-	-	X
3	NAG	B	601	-	-	-	X
4	CO3	A	951	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8825 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	535	Total	C	N	O	S	0	0	0
			4177	2679	725	759	14			
1	B	533	Total	C	N	O	S	0	0	0
			4159	2670	718	757	14			

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



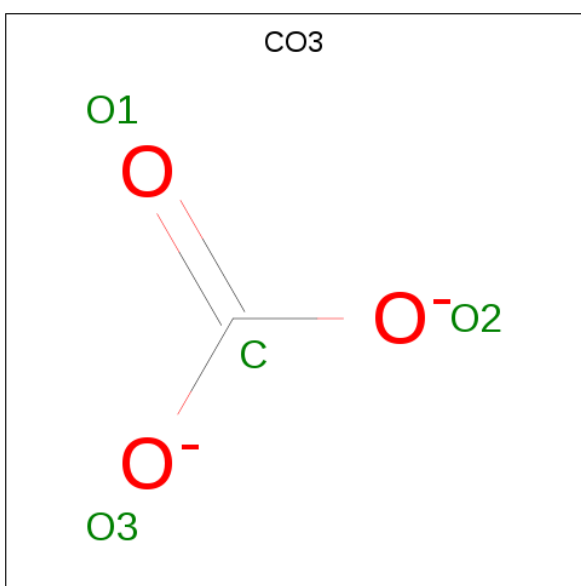
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



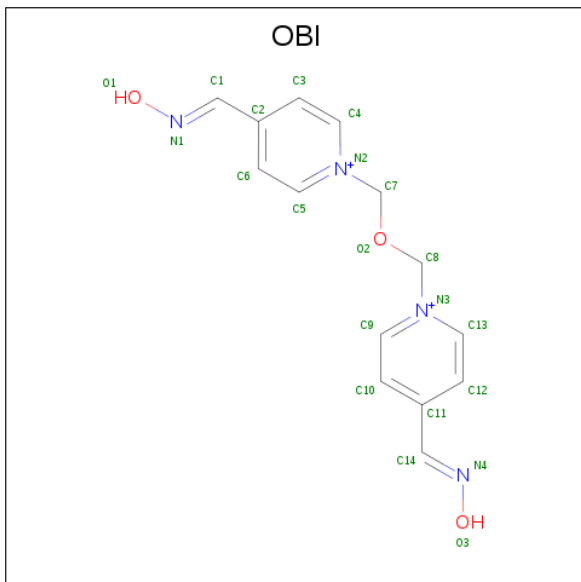
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



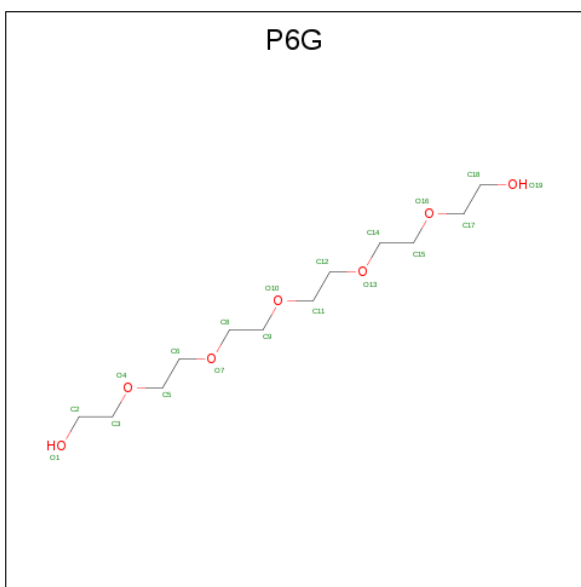
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	1	3		
4	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 5 is 1,1'-(OXYDIMETHYLENE)BIS(4-FORMYLPYRIDINIUM)DIOXIME (three-letter code: OBI) (formula: $C_{14}H_{16}N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			21	14	4	3		
5	B	1	Total	C	N	O	0	0
			21	14	4	3		

- Molecule 6 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



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

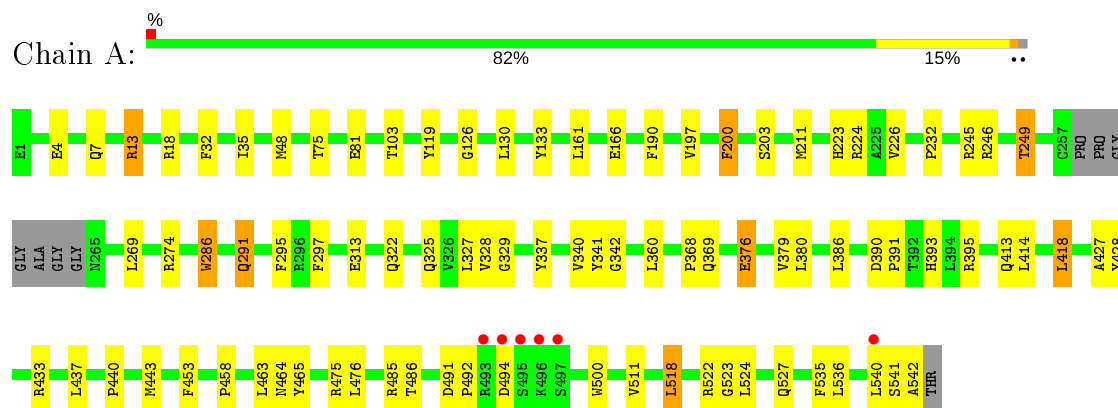
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	214	Total	O	0	0
			214	214		
7	B	154	Total	O	0	0
			154	154		

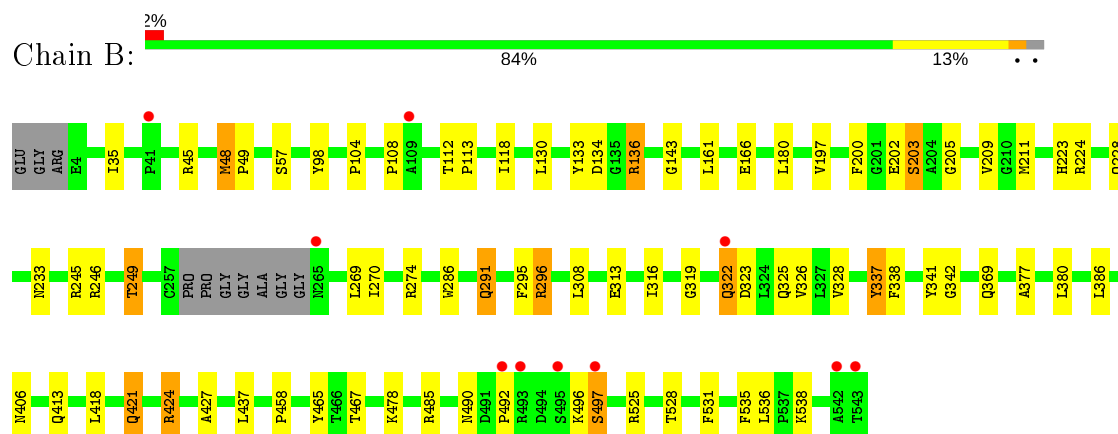
3 Residue-property plots [i](#)

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

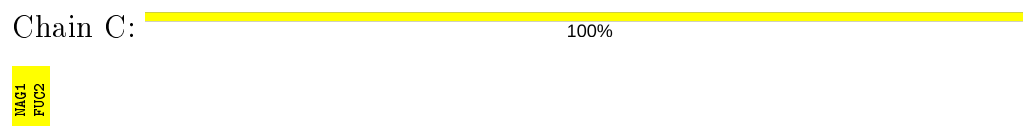
• Molecule 1: Acetylcholinesterase



• Molecule 1: Acetylcholinesterase



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.06Å 111.53Å 227.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.67 – 2.40 29.14 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.67-2.40) 100.0 (29.14-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.09 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.232 0.191 , 0.223	Depositor DCC
R_{free} test set	1568 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8825	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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: FUC, CO3, NAG, P6G, OBI

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	0.64	0/4300	0.72	3/5875 (0.1%)
1	B	0.58	0/4282	0.69	1/5851 (0.0%)
All	All	0.61	0/8582	0.71	4/11726 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	518	LEU	CA-CB-CG	5.55	128.06	115.30
1	B	296	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	395	ARG	NE-CZ-NH1	5.41	123.00	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4177	0	4063	56	1
1	B	4159	0	4046	50	1
2	C	24	0	22	0	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4	0	0	3	0
4	B	4	0	0	1	0
5	A	21	0	16	1	0
5	B	21	0	16	2	0
6	B	19	0	24	2	0
7	A	214	0	0	6	0
7	B	154	0	0	5	0
All	All	8825	0	8213	102	1

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 6.

All (102) 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:424:ARG:HH11	1:B:424:ARG:HG3	1.07	1.08
1:B:48:MET:HE2	1:B:49:PRO:HD2	1.42	0.98
1:A:203:SER:OG	4:A:951:CO3:C	2.13	0.96
1:B:245:ARG:O	1:B:249:THR:HG22	1.66	0.96
1:A:48:MET:HE3	1:A:166:GLU:HA	1.48	0.95
1:B:424:ARG:HG3	1:B:424:ARG:NH1	1.83	0.89
1:B:323:ASP:HB3	7:B:1092:HOH:O	1.74	0.88
1:A:369:GLN:HB2	7:A:1027:HOH:O	1.74	0.86
1:B:197:VAL:H	1:B:223:HIS:HD2	1.24	0.84
1:A:245:ARG:O	1:A:249:THR:HG22	1.78	0.83
1:A:4:GLU:OE2	1:A:18:ARG:HD3	1.78	0.83
1:B:245:ARG:O	1:B:249:THR:CG2	2.30	0.80
1:B:197:VAL:H	1:B:223:HIS:CD2	2.04	0.75
1:B:203:SER:OG	4:B:952:CO3:C	2.38	0.72
1:B:161:LEU:HD11	1:B:269:LEU:HD22	1.74	0.69
1:B:369:GLN:HB2	7:B:988:HOH:O	1.92	0.69
1:B:322:GLN:HA	1:B:322:GLN:OE1	1.93	0.68
1:B:291:GLN:HE22	1:B:369:GLN:NE2	1.91	0.66
1:B:319:GLY:O	1:B:421:GLN:HG2	1.95	0.66
1:A:48:MET:HE3	1:A:166:GLU:CA	2.25	0.65
1:B:424:ARG:CG	1:B:424:ARG:HH11	1.97	0.64
1:A:485:ARG:HB3	1:A:486:THR:HG23	1.78	0.64
1:B:323:ASP:CB	7:B:1092:HOH:O	2.40	0.63
1:A:197:VAL:H	1:A:223:HIS:CD2	2.18	0.62
1:A:376:GLU:O	1:A:380:LEU:HG	1.99	0.61
1:B:104:PRO:HG2	1:B:108:PRO:HD3	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.37	0.59
1:A:527:GLN:HE21	6:B:901:P6G:H21	1.66	0.59
1:A:274:ARG:HD3	7:A:988:HOH:O	2.03	0.57
1:B:161:LEU:HD12	1:B:270:ILE:HD11	1.86	0.57
1:B:323:ASP:N	7:B:1101:HOH:O	2.30	0.57
1:A:211:MET:HG3	1:A:232:PRO:HB3	1.86	0.56
1:A:245:ARG:O	1:A:249:THR:CG2	2.51	0.56
1:B:341:TYR:CD2	5:B:953:OBI:H82	2.41	0.55
1:B:113:PRO:HG2	1:B:485:ARG:HG2	1.88	0.55
1:B:291:GLN:HE22	1:B:369:GLN:HE21	1.54	0.55
1:A:376:GLU:HG3	1:B:538:LYS:NZ	2.22	0.55
1:A:491:ASP:HB3	1:A:494:ASP:HB3	1.87	0.55
1:B:328:VAL:O	1:B:427:ALA:HA	2.07	0.55
1:B:48:MET:HA	1:B:48:MET:HE2	1.89	0.55
1:A:291:GLN:HE22	1:A:369:GLN:NE2	2.05	0.54
1:A:393:HIS:CD2	7:A:1138:HOH:O	2.62	0.53
1:A:393:HIS:HD2	7:A:1138:HOH:O	1.92	0.52
1:B:130:LEU:HD12	1:B:133:TYR:CE2	2.45	0.52
1:A:7:GLN:HG3	7:A:1134:HOH:O	2.10	0.51
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.46	0.51
1:A:226:VAL:HG22	1:A:327:LEU:HB3	1.93	0.51
1:A:224:ARG:HG2	1:A:325:GLN:HB2	1.93	0.51
1:B:224:ARG:HG2	1:B:325:GLN:HB2	1.93	0.51
1:A:197:VAL:H	1:A:223:HIS:HD2	1.57	0.50
1:A:328:VAL:O	1:A:427:ALA:HA	2.12	0.50
1:B:338:PHE:CD2	5:B:953:OBI:H12	2.46	0.50
1:A:376:GLU:HG3	1:B:538:LYS:HZ2	1.76	0.49
1:A:380:LEU:HD12	1:B:535:PHE:HB2	1.94	0.49
1:A:475:ARG:NH2	7:A:1017:HOH:O	2.32	0.49
1:A:414:LEU:HG	1:A:418:LEU:HD22	1.95	0.49
1:B:233:ASN:HD22	1:B:413:GLN:HE21	1.61	0.48
1:B:274:ARG:HD3	7:B:1085:HOH:O	2.14	0.48
1:B:35:ILE:O	1:B:98:TYR:HA	2.14	0.48
1:A:433:ARG:NH2	1:A:437:LEU:HD23	2.29	0.47
1:A:103:THR:HG21	1:A:190:PHE:HB3	1.96	0.47
1:B:166:GLU:HG2	1:B:270:ILE:HD13	1.95	0.47
1:B:296:ARG:NH2	1:B:406:ASN:OD1	2.48	0.47
1:B:205:GLY:O	1:B:209:VAL:HG23	2.15	0.46
1:A:341:TYR:CD2	5:A:952:OBI:H82	2.51	0.46
1:A:327:LEU:HD11	1:A:500:TRP:CH2	2.50	0.46
1:B:118:ILE:O	1:B:205:GLY:HA3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:VAL:HG21	1:B:418:LEU:HD13	1.97	0.45
1:B:490:ASN:O	1:B:492:PRO:HD3	2.17	0.45
1:A:161:LEU:HD11	1:A:269:LEU:HD22	1.98	0.45
1:A:541:SER:O	1:A:542:ALA:HB2	2.16	0.45
1:B:134:ASP:OD1	1:B:136:ARG:HD2	2.17	0.45
1:A:119:TYR:CD1	1:A:126:GLY:HA3	2.52	0.44
1:B:337:TYR:O	1:B:337:TYR:HD2	2.00	0.44
1:B:211:MET:HG2	1:B:308:LEU:HD21	1.98	0.44
1:A:291:GLN:HE22	1:A:369:GLN:HE22	1.65	0.44
1:B:380:LEU:C	6:B:901:P6G:H61	2.37	0.44
1:A:329:GLY:HA3	1:A:428:TYR:CE2	2.53	0.44
1:A:491:ASP:HA	1:A:492:PRO:HD3	1.84	0.44
1:A:463:LEU:O	1:A:464:ASN:HB2	2.18	0.43
1:A:32:PHE:HB3	1:A:35:ILE:HD11	2.00	0.43
1:A:453:PHE:HB3	1:A:476:LEU:HD12	2.00	0.43
1:B:528:THR:O	1:B:531:PHE:HB3	2.19	0.43
1:A:291:GLN:HB2	1:A:291:GLN:HE21	1.64	0.42
1:B:202:GLU:HA	1:B:228:GLN:O	2.20	0.42
1:A:340:VAL:HG11	1:A:443:MET:HE2	2.02	0.42
1:A:522:ARG:HE	1:A:522:ARG:HB3	1.71	0.42
1:A:203:SER:OG	4:A:951:CO3:O2	2.36	0.42
1:A:200:PHE:CB	1:A:226:VAL:HB	2.50	0.42
1:A:291:GLN:NE2	1:A:368:PRO:HB2	2.35	0.42
1:A:286:TRP:CH2	1:A:297:PHE:HA	2.55	0.41
1:A:535:PHE:CE1	1:B:377:ALA:HB2	2.54	0.41
1:A:200:PHE:HB3	1:A:226:VAL:HB	2.00	0.41
1:A:360:LEU:HD22	1:A:379:VAL:HG11	2.02	0.41
1:B:161:LEU:HD12	1:B:270:ILE:CD1	2.51	0.41
1:B:316:ILE:O	1:B:421:GLN:NE2	2.54	0.41
1:A:390:ASP:HA	1:A:391:PRO:HD3	1.83	0.40
1:A:130:LEU:HD12	1:A:133:TYR:CE2	2.57	0.40
1:A:440:PRO:CG	1:A:443:MET:HE3	2.52	0.40
1:A:203:SER:HG	4:A:951:CO3:C	2.26	0.40
1:B:112:THR:HG21	1:B:143:GLY:O	2.21	0.40
1:A:511:VAL:HG11	1:A:518:LEU:HD13	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ARG:NH1	1:B:57:SER:O[2_555]	2.09	0.11

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	531/543 (98%)	507 (96%)	22 (4%)	2 (0%)	34	48
1	B	529/543 (97%)	506 (96%)	21 (4%)	2 (0%)	34	48
All	All	1060/1086 (98%)	1013 (96%)	43 (4%)	4 (0%)	34	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	342	GLY
1	A	342	GLY
1	A	523	GLY
1	B	497	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	439/443 (99%)	420 (96%)	19 (4%)	29	46
1	B	438/443 (99%)	414 (94%)	24 (6%)	21	35
All	All	877/886 (99%)	834 (95%)	43 (5%)	25	40

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	75	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	81	GLU
1	A	200	PHE
1	A	246	ARG
1	A	249	THR
1	A	286	TRP
1	A	291	GLN
1	A	295	PHE
1	A	313	GLU
1	A	322	GLN
1	A	337	TYR
1	A	376	GLU
1	A	386	LEU
1	A	413	GLN
1	A	418	LEU
1	A	524	LEU
1	A	536	LEU
1	A	540	LEU
1	B	45	ARG
1	B	48	MET
1	B	136	ARG
1	B	180	LEU
1	B	200	PHE
1	B	203	SER
1	B	246	ARG
1	B	249	THR
1	B	286	TRP
1	B	291	GLN
1	B	295	PHE
1	B	313	GLU
1	B	322	GLN
1	B	337	TYR
1	B	386	LEU
1	B	421	GLN
1	B	424	ARG
1	B	437	LEU
1	B	467	THR
1	B	478	LYS
1	B	496	LYS
1	B	497	SER
1	B	525	ARG
1	B	536	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	HIS
1	A	291	GLN
1	A	322	GLN
1	B	223	HIS
1	B	291	GLN
1	B	413	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	0.81	1 (7%)	17,19,21	1.93	1 (5%)
2	FUC	C	2	2	10,10,11	0.93	0	14,14,16	1.92	4 (28%)

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	2.26	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C1-O5-C5	6.96	121.62	112.19
2	C	2	FUC	C3-C4-C5	4.49	116.76	109.77
2	C	2	FUC	C1-C2-C3	2.84	113.16	109.67
2	C	2	FUC	O5-C5-C4	2.73	114.43	109.52
2	C	2	FUC	C2-C3-C4	2.69	115.55	110.89

There are no chirality outliers.

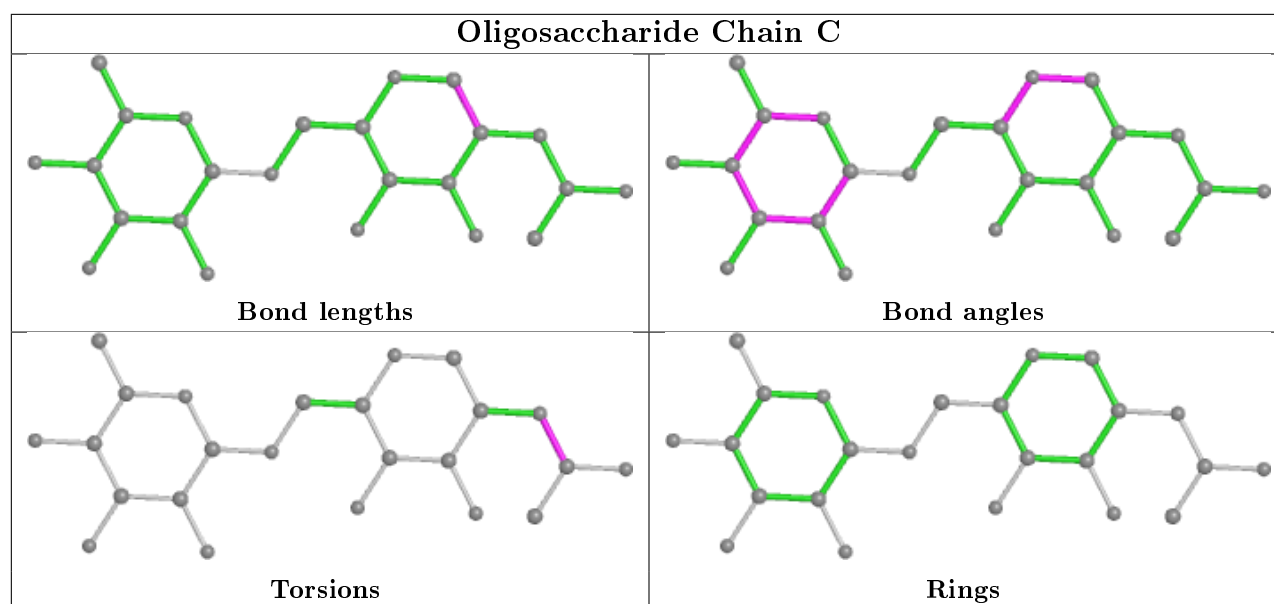
All (2) torsion outliers are listed below:

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](#)

7 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	$\# Z > 2$
4	CO3	A	951	-	0,3,3	0.00	-	0,3,3	0.00	-
5	OBI	A	952	-	18,22,22	0.57	0	20,27,27	1.63	2 (10%)
3	NAG	B	601	1	14,14,15	0.85	1 (7%)	17,19,21	1.74	4 (23%)
3	NAG	A	701	1	14,14,15	0.79	1 (7%)	17,19,21	1.52	3 (17%)
6	P6G	B	901	-	18,18,18	1.76	5 (27%)	17,17,17	2.13	9 (52%)
4	CO3	B	952	-	0,3,3	0.00	-	0,3,3	0.00	-
5	OBI	B	953	-	18,22,22	0.50	0	20,27,27	2.01	2 (10%)

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
5	OBI	A	952	-	-	3/12/12/12	0/2/2/2
3	NAG	B	601	1	-	4/6/23/26	0/1/1/1
5	OBI	B	953	-	-	3/12/12/12	0/2/2/2
6	P6G	B	901	-	-	6/16/16/16	-
3	NAG	A	701	1	-	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	901	P6G	C3-C2	-3.06	1.33	1.49
6	B	901	P6G	C17-C18	-2.90	1.34	1.49
6	B	901	P6G	C12-C11	-2.87	1.34	1.49
6	B	901	P6G	C6-C5	-2.85	1.34	1.49
6	B	901	P6G	C15-C14	-2.63	1.35	1.49
3	A	701	NAG	C1-C2	2.08	1.55	1.52
3	B	601	NAG	C1-C2	2.01	1.55	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	953	OBI	O3-N4-C14	6.83	123.92	111.86
5	A	952	OBI	O3-N4-C14	5.12	120.90	111.86
5	B	953	OBI	O1-N1-C1	4.90	120.51	111.86
3	B	601	NAG	C1-O5-C5	4.65	118.49	112.19
5	A	952	OBI	O1-N1-C1	3.52	118.08	111.86
3	A	701	NAG	O5-C5-C6	3.25	112.29	107.20
6	B	901	P6G	O13-C12-C11	3.02	124.01	110.39
6	B	901	P6G	O4-C5-C6	2.82	123.09	110.39
3	B	601	NAG	O5-C5-C6	2.75	111.52	107.20
6	B	901	P6G	O7-C6-C5	2.73	122.72	110.39
3	B	601	NAG	C4-C3-C2	2.73	115.02	111.02
6	B	901	P6G	O16-C15-C14	2.66	122.38	110.39
6	B	901	P6G	O10-C11-C12	2.65	122.35	110.39
3	A	701	NAG	O5-C1-C2	2.64	115.46	111.29
3	B	601	NAG	C2-N2-C7	2.60	126.60	122.90
6	B	901	P6G	O13-C14-C15	2.43	121.33	110.39
6	B	901	P6G	C14-O13-C12	2.23	122.97	113.29
6	B	901	P6G	O16-C17-C18	2.21	119.77	110.07
6	B	901	P6G	O4-C3-C2	2.06	119.10	110.07
3	A	701	NAG	C3-C4-C5	-2.02	106.63	110.24

There are no chirality outliers.

All (18) torsion outliers are listed below:

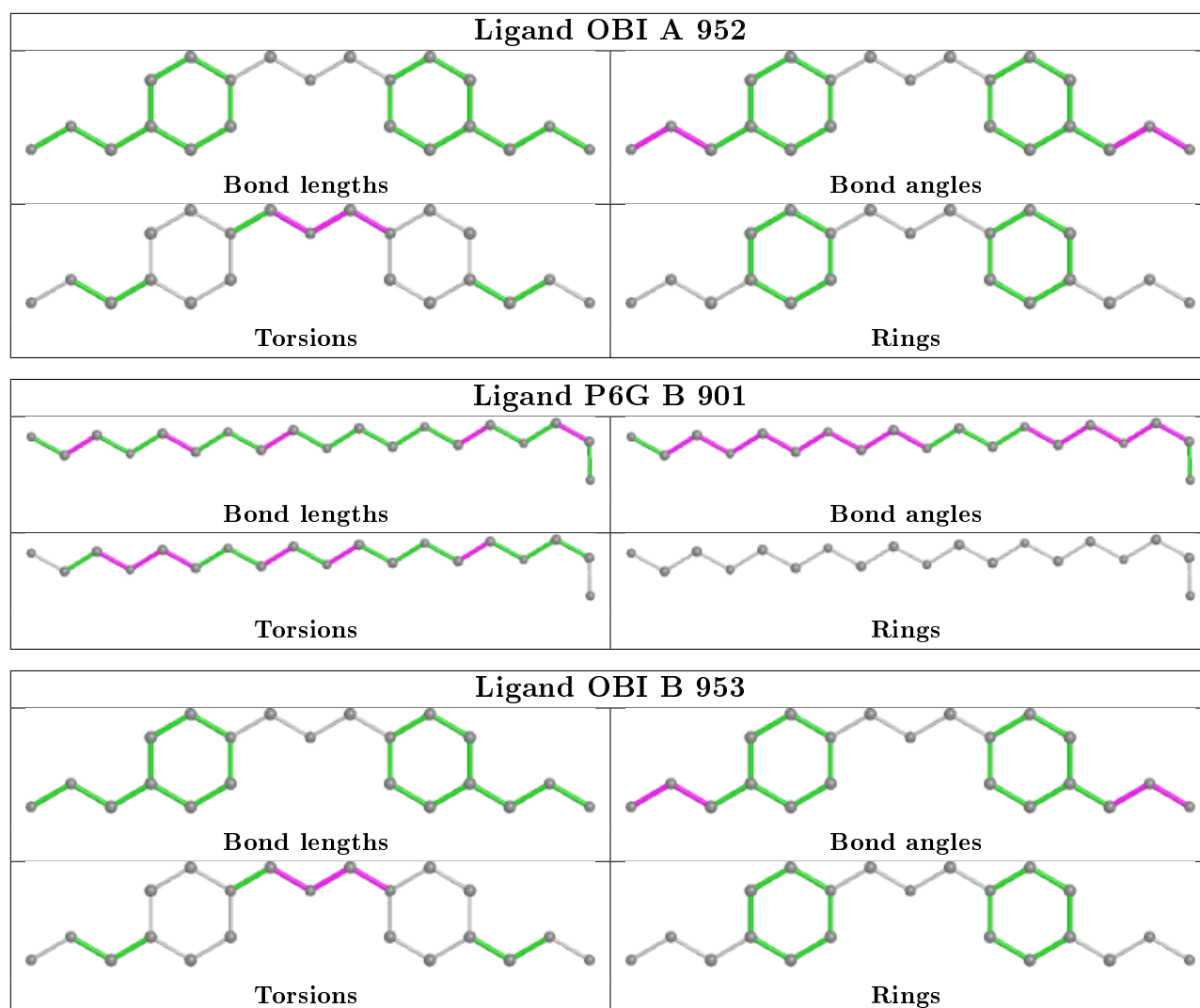
Mol	Chain	Res	Type	Atoms
5	A	952	OBI	O2-C8-N3-C9
5	B	953	OBI	O2-C8-N3-C13
3	B	601	NAG	O5-C5-C6-O6
3	B	601	NAG	C8-C7-N2-C2
3	B	601	NAG	O7-C7-N2-C2
3	B	601	NAG	C4-C5-C6-O6
3	A	701	NAG	C8-C7-N2-C2
3	A	701	NAG	O7-C7-N2-C2
6	B	901	P6G	O10-C11-C12-O13
6	B	901	P6G	O13-C14-C15-O16
6	B	901	P6G	O4-C5-C6-O7
5	A	952	OBI	N3-C8-O2-C7
5	B	953	OBI	N3-C8-O2-C7
6	B	901	P6G	C18-C17-O16-C15
6	B	901	P6G	C8-C9-O10-C11
5	B	953	OBI	N2-C7-O2-C8
6	B	901	P6G	C14-C15-O16-C17
5	A	952	OBI	N2-C7-O2-C8

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	951	CO3	3	0
5	A	952	OBI	1	0
6	B	901	P6G	2	0
4	B	952	CO3	1	0
5	B	953	OBI	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	535/543 (98%)	-0.31	6 (1%) 80 79	33, 42, 54, 73	0
1	B	533/543 (98%)	-0.22	10 (1%) 66 64	35, 42, 52, 70	0
All	All	1068/1086 (98%)	-0.27	16 (1%) 73 72	33, 42, 53, 73	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	495	SER	5.3
1	B	497	SER	5.0
1	A	493	ARG	4.3
1	B	543	THR	4.1
1	A	494	ASP	3.8
1	A	540	LEU	3.4
1	B	322	GLN	3.0
1	B	493	ARG	3.0
1	A	497	SER	2.9
1	A	496	LYS	2.9
1	B	492	PRO	2.6
1	B	265	ASN	2.5
1	B	41	PRO	2.4
1	B	542	ALA	2.1
1	B	109	ALA	2.1
1	B	495	SER	2.1

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

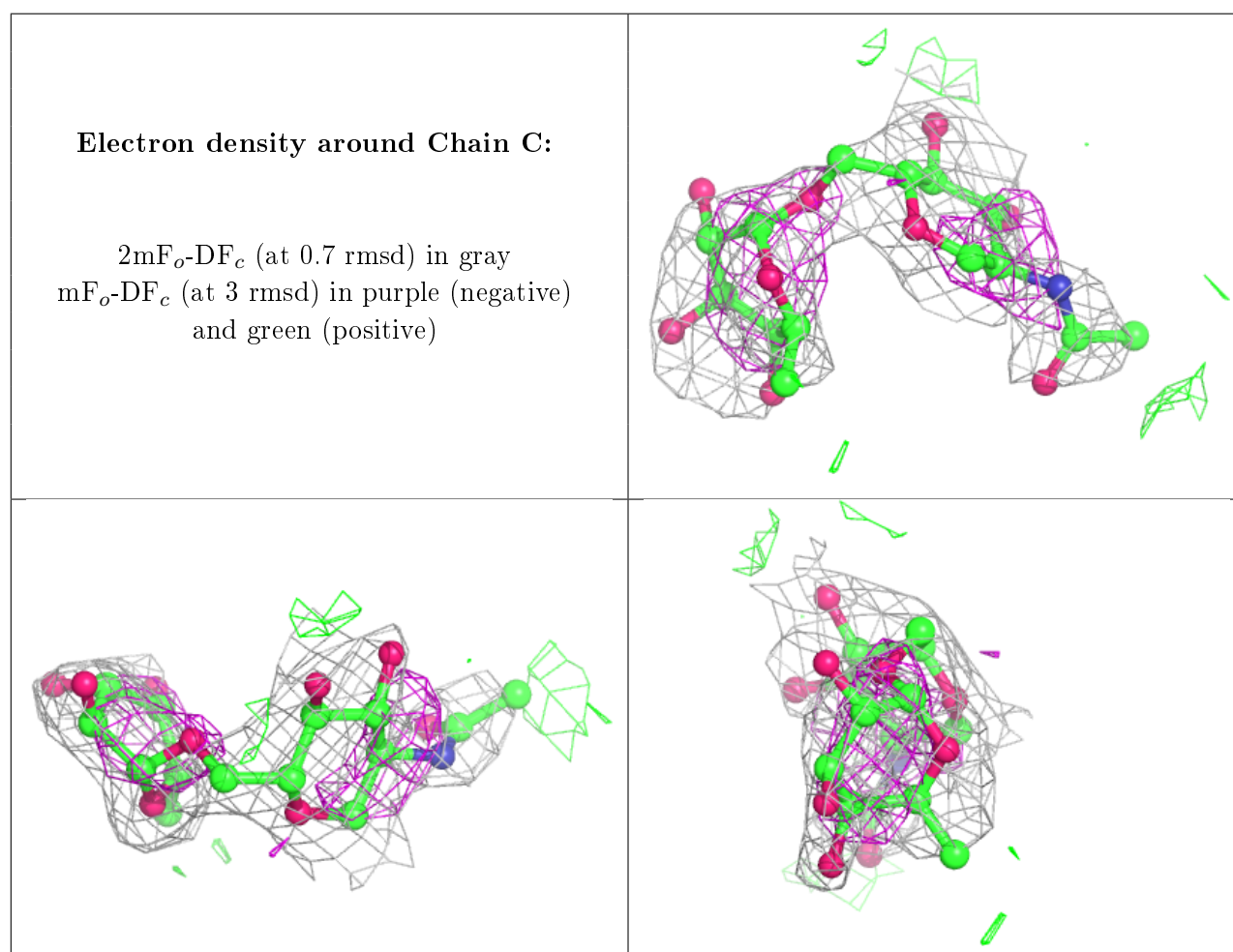
There are no non-standard protein/DNA/RNA residues in this entry.

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	0.74	0.54	94,95,96,96	0
2	NAG	C	1	14/15	0.80	0.42	74,81,86,91	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

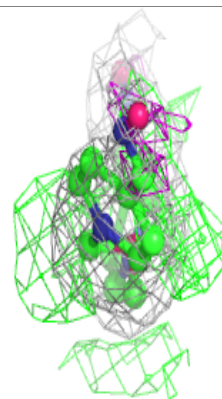
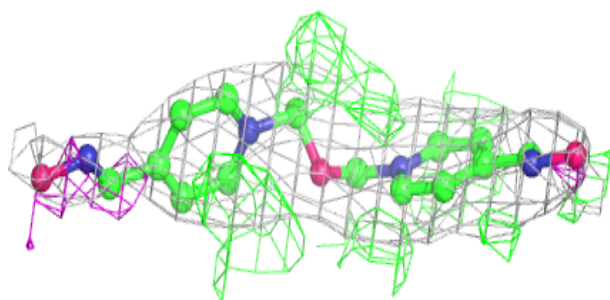
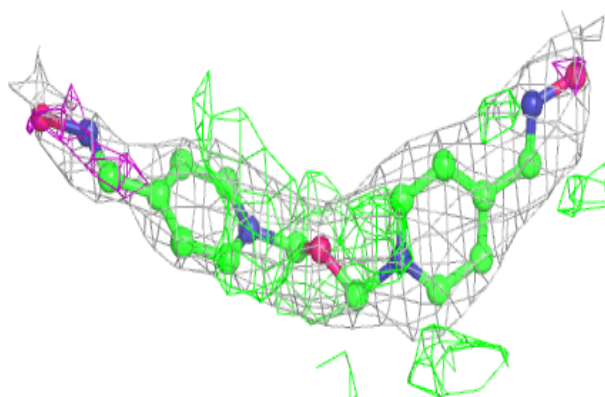
labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	B	601	14/15	0.66	0.47	72,79,83,84	0
3	NAG	A	701	14/15	0.87	0.42	74,79,81,81	0
5	OBI	A	952	21/21	0.89	0.19	49,53,54,57	21
5	OBI	B	953	21/21	0.89	0.16	53,55,57,60	21
6	P6G	B	901	19/19	0.90	0.16	51,56,62,63	0
4	CO3	B	952	4/4	0.96	0.12	75,75,75,75	0
4	CO3	A	951	4/4	0.97	0.10	57,58,58,58	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.

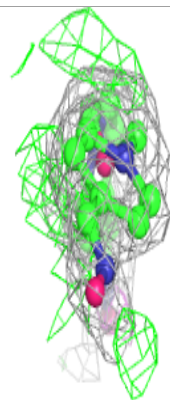
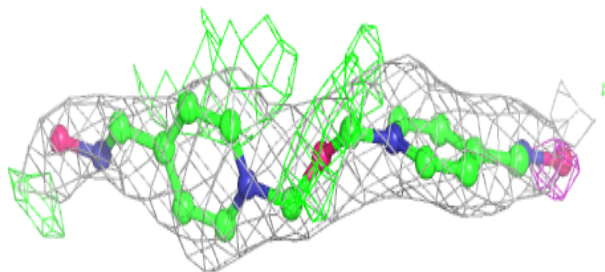
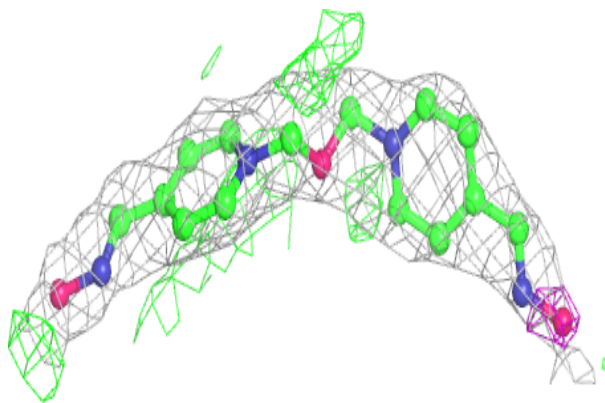
Electron density around OBI A 952:

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



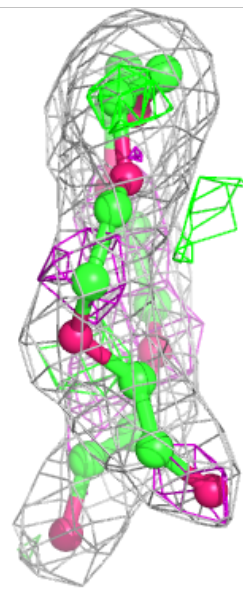
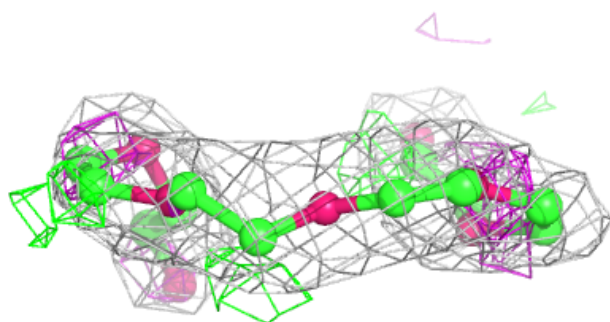
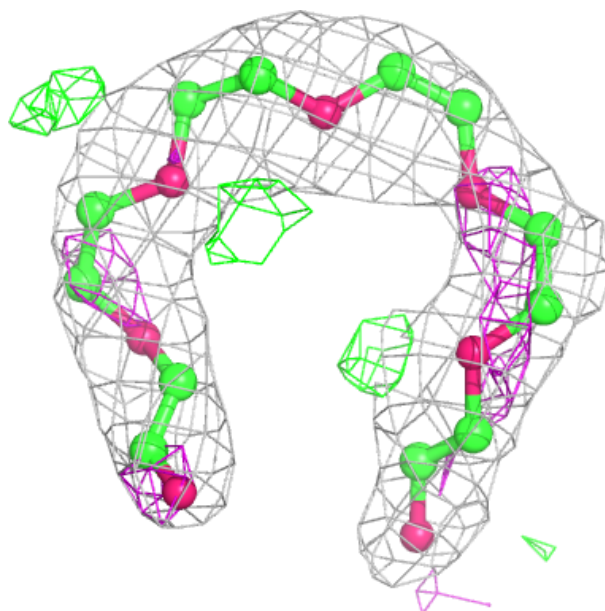
Electron density around OBI B 953:

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.