



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 04:46 PM BST

PDB ID : 1Q83
Title : Crystal structure of the mouse acetylcholinesterase-TZ2PA6 syn complex
Authors : Bourne, Y.; Kolb, H.C.; Radic, Z.; Sharpless, K.B.; Taylor, P.; Marchot, P.
Deposited on : 2003-08-20
Resolution : 2.65 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

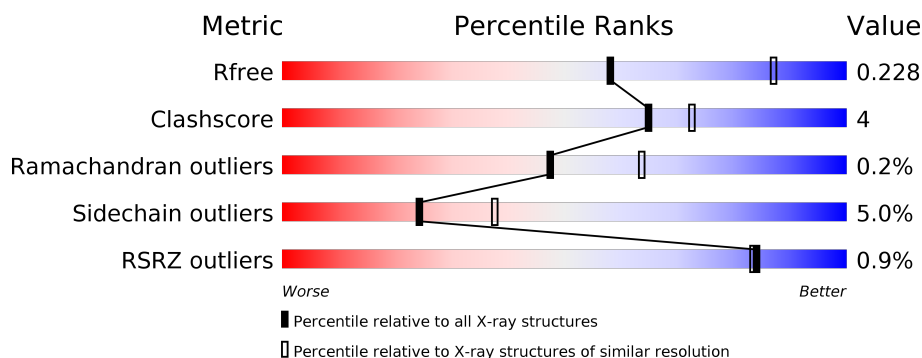
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	580	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 82% 9% 8% </div> </div>
1	B	580	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 79% 11% 8% </div> </div>
2	C	2	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow, green, grey);"></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	FUL	C	2	X	-	-	X
3	NAG	B	1601	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8768 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
			4182	2683	726	759	14			
1	B	531	Total	C	N	O	S	0	0	0
			4142	2662	715	751	14			

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



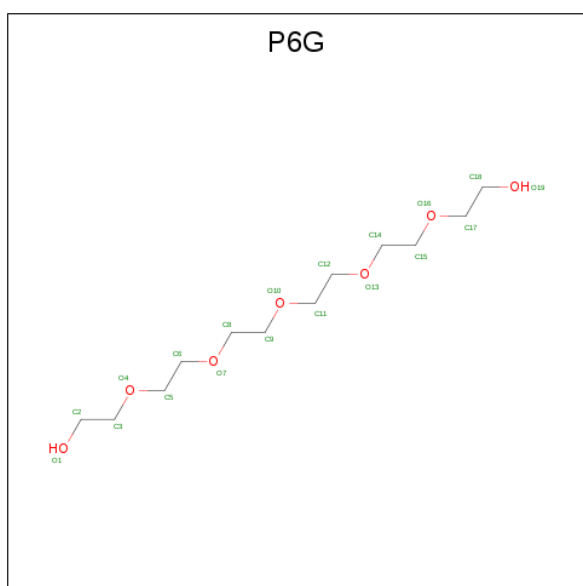
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			24	14	1	9			

- 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		

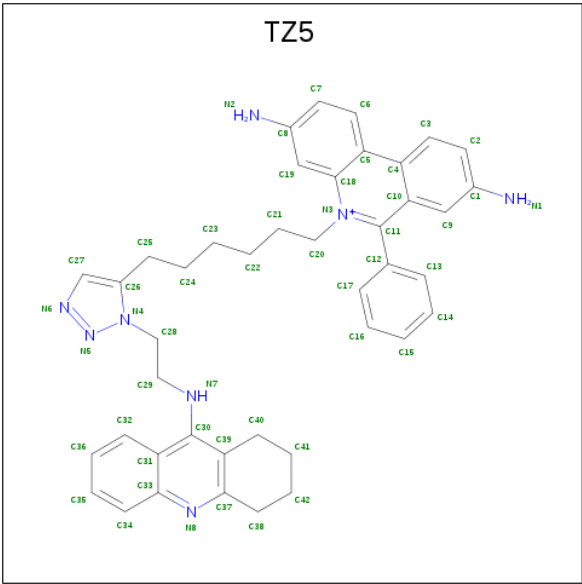
- Molecule 4 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



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

- Molecule 5 is 3,8-DIAMINO-6-PHENYL-5-[6-[1-[2-[(1,2,3,4-TETRAHYDRO-9-ACRI

DINYL)AMINO]ETHYL]-1H-1,2,3-TRIAZOL-5-YL]HEXYL]-PHENANTHRIDINIUM
(three-letter code: TZ5) (formula: C₄₂H₄₅N₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			50	42	8		
5	B	1	Total	C	N	0	0
			50	42	8		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	177	Total	O	0	0
			177	177		
6	B	96	Total	O	0	0
			96	96		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.74Å 111.95Å 226.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.65 29.83 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.65) 99.8 (29.83-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.182 , 0.221 0.195 , 0.228	Depositor DCC
R_{free} test set	1265 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	46.3	Xtriage
Anisotropy	0.735	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8768	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: FUL, TZ5, NAG, P6G

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	0.72	0/4306	0.89	13/5884 (0.2%)
1	B	0.68	0/4266	0.84	15/5833 (0.3%)
All	All	0.70	0/8572	0.87	28/11717 (0.2%)

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 (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	A	390	ASP	CB-CG-OD2	8.20	125.68	118.30
1	B	396	ASP	CB-CG-OD2	7.38	124.95	118.30
1	A	74	ASP	CB-CG-OD2	7.20	124.78	118.30
1	A	396	ASP	CB-CG-OD2	7.10	124.69	118.30
1	B	175	ASP	CB-CG-OD2	7.00	124.60	118.30
1	B	323	ASP	CB-CG-OD2	7.00	124.60	118.30
1	B	74	ASP	CB-CG-OD2	6.93	124.54	118.30
1	B	5	ASP	CB-CG-OD2	6.57	124.22	118.30
1	A	246	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	B	349	ASP	CB-CG-OD2	6.48	124.13	118.30
1	B	274	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	B	424	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	18	ARG	NE-CZ-NH1	6.12	123.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	ASP	CB-CG-OD2	5.99	123.69	118.30
1	B	320	ASP	CB-CG-OD2	5.92	123.62	118.30
1	A	372	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	18	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	488	ASP	CB-CG-OD2	5.64	123.38	118.30
1	B	54	ARG	NE-CZ-NH1	-5.43	117.59	120.30
1	B	54	ARG	NE-CZ-NH2	5.37	122.99	120.30
1	A	404	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	193	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	390	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	404	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	306	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	161	LEU	CA-CB-CG	-5.02	103.76	115.30
1	A	349	ASP	CB-CG-OD2	5.02	122.82	118.30

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	4182	0	4065	34	0
1	B	4142	0	4022	35	0
2	C	24	0	22	0	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	19	0	26	5	0
5	A	50	0	45	2	0
5	B	50	0	45	2	0
6	A	177	0	0	3	0
6	B	96	0	0	2	0
All	All	8768	0	8251	69	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 4.

All (69) 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:369:GLN:HE21	1:B:369:GLN:H	0.99	0.91
1:B:245:ARG:O	1:B:249:THR:HG23	1.81	0.79
1:B:369:GLN:NE2	1:B:369:GLN:H	1.80	0.76
1:B:369:GLN:N	1:B:369:GLN:HE21	1.81	0.75
1:A:337:TYR:OH	1:A:341:TYR:CZ	2.40	0.73
1:A:381:HIS:HA	4:A:1901:P6G:H172	1.71	0.73
1:A:90:ARG:NE	6:A:2054:HOH:O	2.23	0.70
1:B:161:LEU:HD12	1:B:270:ILE:HD11	1.74	0.70
1:A:245:ARG:O	1:A:249:THR:HG23	1.96	0.66
1:B:161:LEU:HD12	1:B:270:ILE:CD1	2.25	0.66
1:A:4:GLU:OE2	1:A:18:ARG:HD3	1.95	0.65
4:A:1901:P6G:H51	1:B:381:HIS:HA	1.78	0.65
1:A:337:TYR:CE1	1:A:341:TYR:CE1	2.85	0.64
1:A:113:PRO:HG2	1:A:485:ARG:HG2	1.81	0.63
1:B:161:LEU:HD11	1:B:269:LEU:HD22	1.82	0.61
1:B:67:ASN:ND2	6:B:1991:HOH:O	2.35	0.59
1:B:497:SER:HB2	1:B:498:PRO:CA	2.36	0.56
1:A:197:VAL:H	1:A:223:HIS:HD2	1.55	0.55
1:A:535:PHE:CD2	4:A:1901:P6G:H92	2.43	0.54
1:B:328:VAL:O	1:B:427:ALA:HA	2.07	0.54
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.45	0.52
1:B:497:SER:HB2	1:B:498:PRO:HA	1.91	0.52
1:A:112:THR:HG21	1:A:143:GLY:O	2.10	0.52
1:A:257:CYS:HA	1:A:258:PRO:C	2.30	0.52
1:A:527:GLN:HG3	4:A:1901:P6G:H22	1.90	0.51
1:B:130:LEU:HD12	1:B:133:TYR:CE2	2.45	0.51
1:A:200:PHE:HB2	1:A:226:VAL:HB	1.93	0.51
1:B:353:LEU:HB3	1:B:391:PRO:HB2	1.93	0.51
1:A:424:ARG:HH11	1:A:424:ARG:HG2	1.76	0.51
1:A:245:ARG:O	1:A:249:THR:CG2	2.59	0.50
1:B:76:LEU:HD22	1:B:341:TYR:CD2	2.47	0.50
1:B:29:VAL:HG21	1:B:136:ARG:HB2	1.94	0.49
1:B:497:SER:HB2	1:B:498:PRO:C	2.32	0.49
1:A:286:TRP:CZ2	5:A:1951:TZ5:H17	2.48	0.49
1:A:337:TYR:HE1	1:A:341:TYR:CE1	2.31	0.49
1:B:58:GLY:O	6:B:2016:HOH:O	2.20	0.48
1:B:497:SER:CB	1:B:498:PRO:HA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLN:HG3	6:A:2099:HOH:O	2.14	0.47
1:A:535:PHE:CG	4:A:1901:P6G:H92	2.50	0.47
1:A:200:PHE:CB	1:A:226:VAL:HB	2.45	0.47
1:B:112:THR:HG21	1:B:143:GLY:O	2.16	0.46
1:A:90:ARG:CD	6:A:2054:HOH:O	2.63	0.46
1:B:4:GLU:OE1	1:B:18:ARG:NH1	2.48	0.46
1:A:369:GLN:H	1:A:369:GLN:HE21	1.64	0.45
1:A:286:TRP:HB2	5:A:1951:TZ5:C6	2.46	0.45
1:B:340:VAL:HG11	1:B:443:MET:CE	2.46	0.45
1:A:328:VAL:O	1:A:427:ALA:HA	2.16	0.45
1:B:76:LEU:HD13	5:B:1952:TZ5:H14	1.97	0.45
1:A:213:ILE:O	1:A:219:ARG:HD3	2.17	0.45
1:B:291:GLN:HE21	1:B:368:PRO:HB2	1.82	0.45
1:B:251:LEU:O	1:B:251:LEU:HG	2.17	0.45
1:A:68:VAL:HG23	1:A:90:ARG:HB2	2.00	0.43
1:A:376:GLU:O	1:A:380:LEU:HG	2.18	0.43
1:A:353:LEU:HB3	1:A:391:PRO:HB2	1.99	0.43
1:B:457:LEU:N	1:B:458:PRO:CD	2.81	0.43
1:A:369:GLN:H	1:A:369:GLN:NE2	2.18	0.42
1:B:300:VAL:HB	1:B:301:PRO:HD2	2.02	0.42
1:A:159:LEU:C	1:A:159:LEU:HD23	2.41	0.41
1:B:296:ARG:HH21	1:B:369:GLN:HE22	1.69	0.41
1:B:76:LEU:HD22	1:B:341:TYR:CE2	2.55	0.41
1:B:424:ARG:CG	1:B:424:ARG:HH11	2.34	0.41
1:B:497:SER:CB	1:B:498:PRO:CA	2.98	0.41
1:A:5:ASP:OD2	1:A:105:TYR:OH	2.21	0.41
1:A:116:ILE:HA	1:A:147:VAL:O	2.22	0.40
1:B:286:TRP:HB2	5:B:1952:TZ5:C6	2.51	0.40
1:A:395:ARG:HD2	1:A:396:ASP:OD1	2.22	0.40
1:A:457:LEU:N	1:A:458:PRO:CD	2.84	0.40
1:B:211:MET:HG2	1:B:308:LEU:HD21	2.03	0.40
1:B:224:ARG:HH11	1:B:325:GLN:HE22	1.70	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	532/580 (92%)	514 (97%)	18 (3%)	0	100	100
1	B	527/580 (91%)	512 (97%)	13 (2%)	2 (0%)	34	48
All	All	1059/1160 (91%)	1026 (97%)	31 (3%)	2 (0%)	47	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	497	SER
1	B	341	TYR

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	439/473 (93%)	417 (95%)	22 (5%)	24	38
1	B	435/473 (92%)	413 (95%)	22 (5%)	24	37
All	All	874/946 (92%)	830 (95%)	44 (5%)	24	38

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	4	GLU
1	A	18	ARG
1	A	21	ARG
1	A	45	ARG
1	A	165	ARG
1	A	200	PHE
1	A	216	LEU
1	A	246	ARG
1	A	249	THR

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Mol	Chain	Res	Type
1	A	258	PRO
1	A	291	GLN
1	A	295	PHE
1	A	325	GLN
1	A	369	GLN
1	A	424	ARG
1	A	433	ARG
1	A	470	ARG
1	A	524	LEU
1	A	525	ARG
1	A	536	LEU
1	A	539	LEU
1	B	115	LEU
1	B	136	ARG
1	B	165	ARG
1	B	181	GLN
1	B	200	PHE
1	B	246	ARG
1	B	265	ASN
1	B	281	LEU
1	B	291	GLN
1	B	295	PHE
1	B	323	ASP
1	B	325	GLN
1	B	337	TYR
1	B	369	GLN
1	B	386	LEU
1	B	424	ARG
1	B	478	LYS
1	B	485	ARG
1	B	525	ARG
1	B	536	LEU
1	B	539	LEU
1	B	540	LEU

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	291	GLN
1	A	325	GLN
1	A	369	GLN

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Mol	Chain	Res	Type
1	B	291	GLN
1	B	325	GLN
1	B	369	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	1.00	1 (7%)	17,19,21	1.61	2 (11%)
2	FUL	C	2	2	10,10,11	1.73	4 (40%)	14,14,16	1.24	1 (7%)

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	FUL	C	2	2	1/1/4/5	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	FUL	O5-C1	2.82	1.48	1.43
2	C	2	FUL	C6-C5	2.40	1.57	1.51
2	C	1	NAG	C1-C2	2.16	1.55	1.52
2	C	2	FUL	C2-C3	2.01	1.55	1.52
2	C	2	FUL	O5-C5	2.01	1.47	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C1-O5-C5	4.94	118.89	112.19
2	C	2	FUL	O5-C5-C6	3.33	114.49	107.33
2	C	1	NAG	O3-C3-C2	2.40	114.43	109.47

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	2	FUL	C1

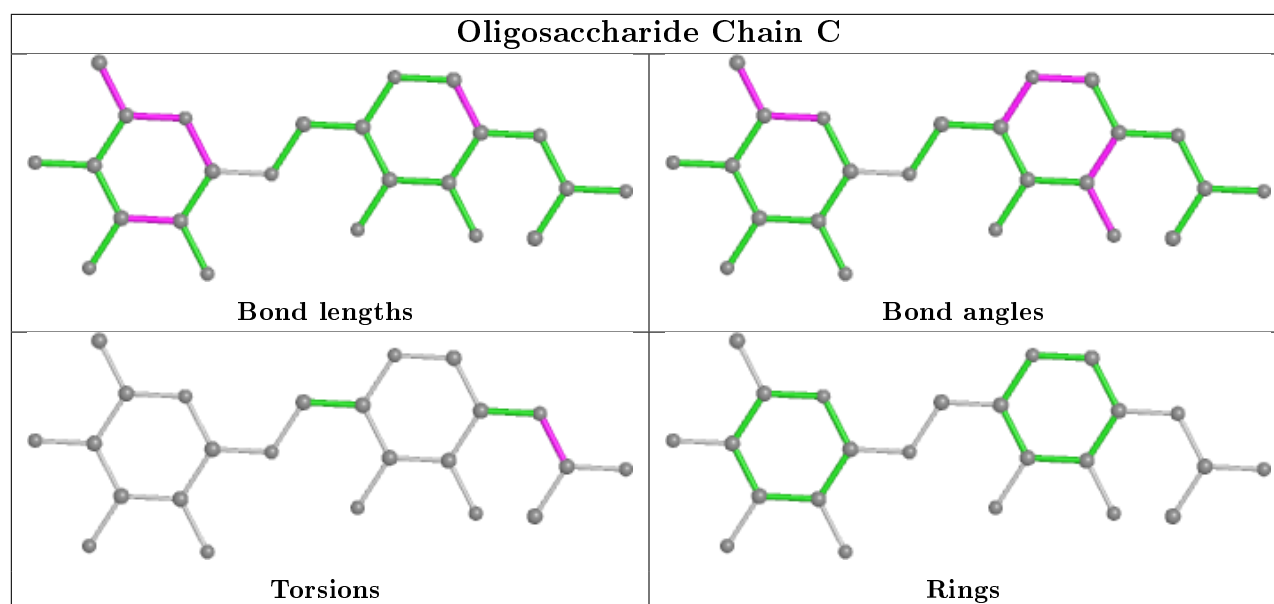
All (2) torsion outliers are listed below:

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](#)

5 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	$\# Z > 2$
5	TZ5	A	1951	-	54,57,57	1.64	12 (22%)	67,80,80	2.34	21 (31%)
5	TZ5	B	1952	-	54,57,57	1.58	8 (14%)	67,80,80	2.35	23 (34%)
4	P6G	A	1901	-	18,18,18	2.18	6 (33%)	17,17,17	1.50	2 (11%)
3	NAG	A	1701	1	14,14,15	1.59	2 (14%)	17,19,21	2.25	5 (29%)
3	NAG	B	1601	1	14,14,15	1.85	4 (28%)	17,19,21	2.10	5 (29%)

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	TZ5	A	1951	-	-	4/19/26/26	0/8/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TZ5	B	1952	-	-	6/19/26/26	0/8/8/8
4	P6G	A	1901	-	-	8/16/16/16	-
3	NAG	A	1701	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1601	1	-	2/6/23/26	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1952	TZ5	C40-C39	-4.55	1.44	1.51
4	A	1901	P6G	O10-C9	4.29	1.60	1.42
5	B	1952	TZ5	C41-C40	-4.07	1.36	1.51
5	A	1951	TZ5	C42-C38	-3.98	1.37	1.51
5	B	1952	TZ5	C42-C38	-3.97	1.37	1.51
4	A	1901	P6G	O13-C12	3.95	1.59	1.42
5	B	1952	TZ5	C38-C37	-3.80	1.44	1.50
5	A	1951	TZ5	C40-C39	-3.76	1.45	1.51
5	A	1951	TZ5	C41-C40	-3.75	1.37	1.51
4	A	1901	P6G	O16-C15	3.65	1.57	1.42
4	A	1901	P6G	O19-C18	3.51	1.60	1.42
5	A	1951	TZ5	C38-C37	-3.39	1.45	1.50
4	A	1901	P6G	O4-C3	3.32	1.56	1.42
3	A	1701	NAG	C1-C2	3.20	1.57	1.52
5	B	1952	TZ5	C30-C39	3.10	1.44	1.38
5	A	1951	TZ5	N6-N5	-2.97	1.30	1.34
5	B	1952	TZ5	N6-N5	-2.79	1.30	1.34
4	A	1901	P6G	O7-C6	2.79	1.54	1.42
3	A	1701	NAG	C3-C2	2.79	1.58	1.52
3	B	1601	NAG	C1-C2	2.67	1.56	1.52
3	B	1601	NAG	C4-C5	2.59	1.58	1.53
3	B	1601	NAG	C8-C7	2.58	1.55	1.50
3	B	1601	NAG	C3-C2	2.46	1.57	1.52
5	A	1951	TZ5	C37-N8	2.44	1.35	1.32
5	A	1951	TZ5	C10-C4	2.32	1.46	1.42
5	A	1951	TZ5	C6-C5	2.20	1.45	1.41
5	A	1951	TZ5	C42-C41	-2.20	1.42	1.51
5	B	1952	TZ5	C42-C41	-2.16	1.43	1.51
5	A	1951	TZ5	C9-C10	2.13	1.46	1.42
5	A	1951	TZ5	C3-C4	2.12	1.45	1.41
5	A	1951	TZ5	C30-C39	2.08	1.42	1.38
5	B	1952	TZ5	C39-C37	2.03	1.43	1.40

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1952	TZ5	C40-C39-C37	-7.70	113.89	121.08
5	A	1951	TZ5	C40-C39-C37	-7.63	113.95	121.08
5	B	1952	TZ5	C42-C38-C37	6.31	123.89	113.53
3	A	1701	NAG	O5-C5-C6	5.86	116.40	107.20
5	A	1951	TZ5	C25-C26-N4	5.78	135.41	122.34
5	A	1951	TZ5	C42-C38-C37	5.77	123.02	113.53
5	A	1951	TZ5	C27-C26-N4	-5.72	96.55	106.21
5	A	1951	TZ5	C1-C9-C10	5.53	125.70	120.90
5	B	1952	TZ5	C1-C9-C10	5.52	125.69	120.90
5	B	1952	TZ5	C25-C26-N4	5.42	134.59	122.34
5	B	1952	TZ5	C27-C26-N4	-5.38	97.13	106.21
5	B	1952	TZ5	C28-N4-C26	-5.24	121.82	128.48
5	B	1952	TZ5	C41-C40-C39	4.98	123.07	112.84
5	A	1951	TZ5	C41-C40-C39	4.82	122.74	112.84
3	B	1601	NAG	O5-C5-C6	4.73	114.62	107.20
5	A	1951	TZ5	C19-C18-C5	-4.29	115.17	120.61
5	A	1951	TZ5	C28-N4-C26	-4.01	123.38	128.48
3	B	1601	NAG	O5-C1-C2	-3.73	105.41	111.29
5	A	1951	TZ5	C27-N6-N5	-3.70	99.98	107.97
3	B	1601	NAG	C1-O5-C5	3.49	116.93	112.19
3	A	1701	NAG	O5-C5-C4	-3.47	102.39	110.83
5	B	1952	TZ5	C27-N6-N5	-3.38	100.67	107.97
5	B	1952	TZ5	C19-C18-C5	-3.35	116.37	120.61
4	A	1901	P6G	O1-C2-C3	3.19	130.32	111.81
4	A	1901	P6G	O13-C12-C11	2.94	123.67	110.39
3	A	1701	NAG	C3-C4-C5	-2.90	105.06	110.24
5	B	1952	TZ5	C13-C12-C11	2.72	124.25	120.24
5	A	1951	TZ5	C36-C32-C31	2.72	124.66	120.89
5	A	1951	TZ5	C38-C37-C39	-2.66	118.74	121.49
5	B	1952	TZ5	C28-N4-N5	2.59	127.04	119.93
3	A	1701	NAG	O4-C4-C5	2.57	115.69	109.30
5	A	1951	TZ5	C7-C6-C5	2.53	125.29	121.63
5	A	1951	TZ5	C32-C31-C33	-2.50	115.53	118.33
5	B	1952	TZ5	C12-C11-C10	-2.45	116.29	121.31
5	A	1951	TZ5	C24-C25-C26	2.42	120.20	113.82
5	B	1952	TZ5	C35-C34-C33	2.42	123.56	120.08
3	B	1601	NAG	C4-C3-C2	2.33	114.44	111.02
5	A	1951	TZ5	C3-C4-C10	-2.33	114.78	117.73
5	A	1951	TZ5	C39-C37-N8	-2.33	121.69	123.68
5	A	1951	TZ5	C35-C34-C33	2.32	123.42	120.08
5	B	1952	TZ5	C2-C1-C9	-2.31	114.82	119.65
5	A	1951	TZ5	C2-C3-C4	2.30	124.95	121.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1952	TZ5	C39-C37-N8	-2.30	121.72	123.68
5	B	1952	TZ5	C16-C17-C12	2.26	123.40	120.56
5	B	1952	TZ5	C36-C32-C31	2.25	124.01	120.89
5	B	1952	TZ5	C42-C41-C40	2.24	122.47	112.55
5	A	1951	TZ5	C7-C8-C19	-2.23	114.98	119.65
3	B	1601	NAG	O4-C4-C5	2.21	114.78	109.30
5	B	1952	TZ5	C7-C8-C19	-2.20	115.05	119.65
3	A	1701	NAG	O3-C3-C4	-2.18	105.31	110.35
5	A	1951	TZ5	C2-C1-C9	-2.18	115.09	119.65
5	B	1952	TZ5	C2-C3-C4	2.12	124.69	121.63
5	B	1952	TZ5	C26-N4-N5	-2.12	111.14	113.04
5	B	1952	TZ5	C3-C4-C10	-2.07	115.11	117.73
5	A	1951	TZ5	C37-N8-C33	2.06	120.21	117.67
5	B	1952	TZ5	C7-C6-C5	2.06	124.60	121.63

There are no chirality outliers.

All (22) torsion outliers are listed below:

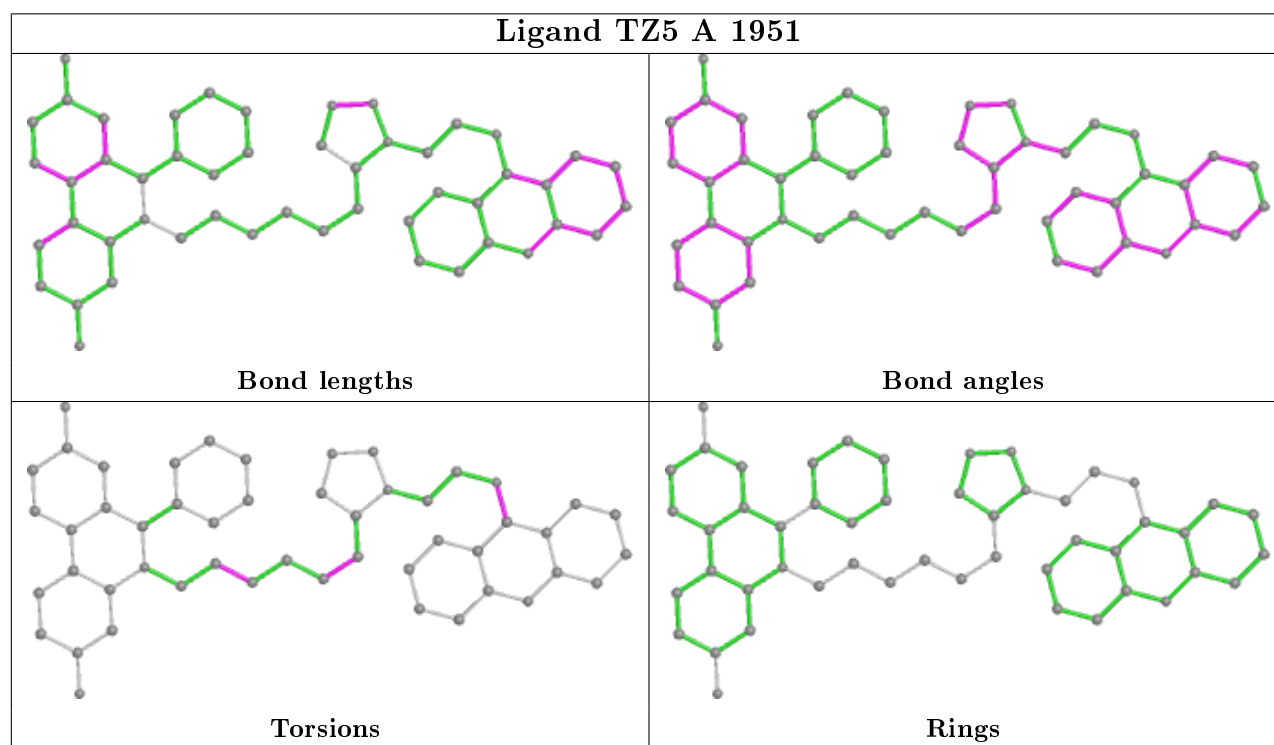
Mol	Chain	Res	Type	Atoms
3	A	1701	NAG	C8-C7-N2-C2
3	A	1701	NAG	O7-C7-N2-C2
5	A	1951	TZ5	C20-C21-C22-C23
3	B	1601	NAG	C4-C5-C6-O6
5	A	1951	TZ5	C23-C24-C25-C26
5	B	1952	TZ5	C23-C24-C25-C26
4	A	1901	P6G	O16-C17-C18-O19
4	A	1901	P6G	O7-C8-C9-O10
5	B	1952	TZ5	C22-C23-C24-C25
4	A	1901	P6G	O1-C2-C3-O4
5	B	1952	TZ5	N4-C28-C29-N7
5	A	1951	TZ5	C39-C30-N7-C29
4	A	1901	P6G	C5-C6-O7-C8
4	A	1901	P6G	C6-C5-O4-C3
5	A	1951	TZ5	C31-C30-N7-C29
5	B	1952	TZ5	C31-C30-N7-C29
3	B	1601	NAG	O5-C5-C6-O6
5	B	1952	TZ5	C39-C30-N7-C29
4	A	1901	P6G	C14-C15-O16-C17
4	A	1901	P6G	C2-C3-O4-C5
4	A	1901	P6G	C11-C12-O13-C14
5	B	1952	TZ5	C28-C29-N7-C30

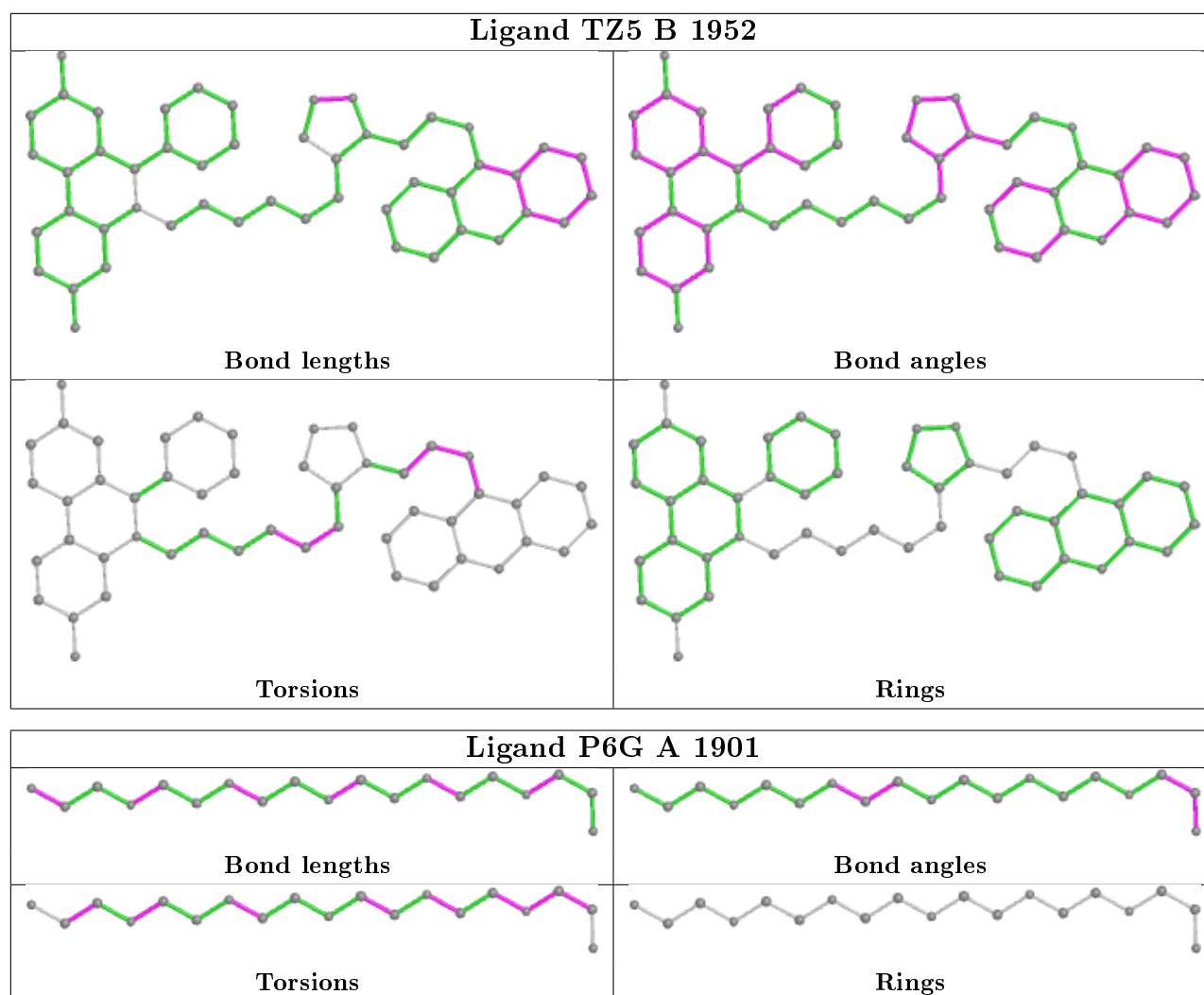
There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1951	TZ5	2	0
5	B	1952	TZ5	2	0
4	A	1901	P6G	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	536/580 (92%)	-0.46	7 (1%) 77 75	31, 46, 68, 102	0
1	B	531/580 (91%)	-0.35	3 (0%) 89 89	34, 51, 72, 91	0
All	All	1067/1160 (91%)	-0.40	10 (0%) 84 83	31, 48, 72, 102	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	496	LYS	2.9
1	A	540	LEU	2.6
1	A	493	ARG	2.6
1	B	109	ALA	2.4
1	A	494	ASP	2.4
1	A	495	SER	2.4
1	A	541	SER	2.3
1	A	497	SER	2.2
1	B	497	SER	2.2
1	B	393	HIS	2.2

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

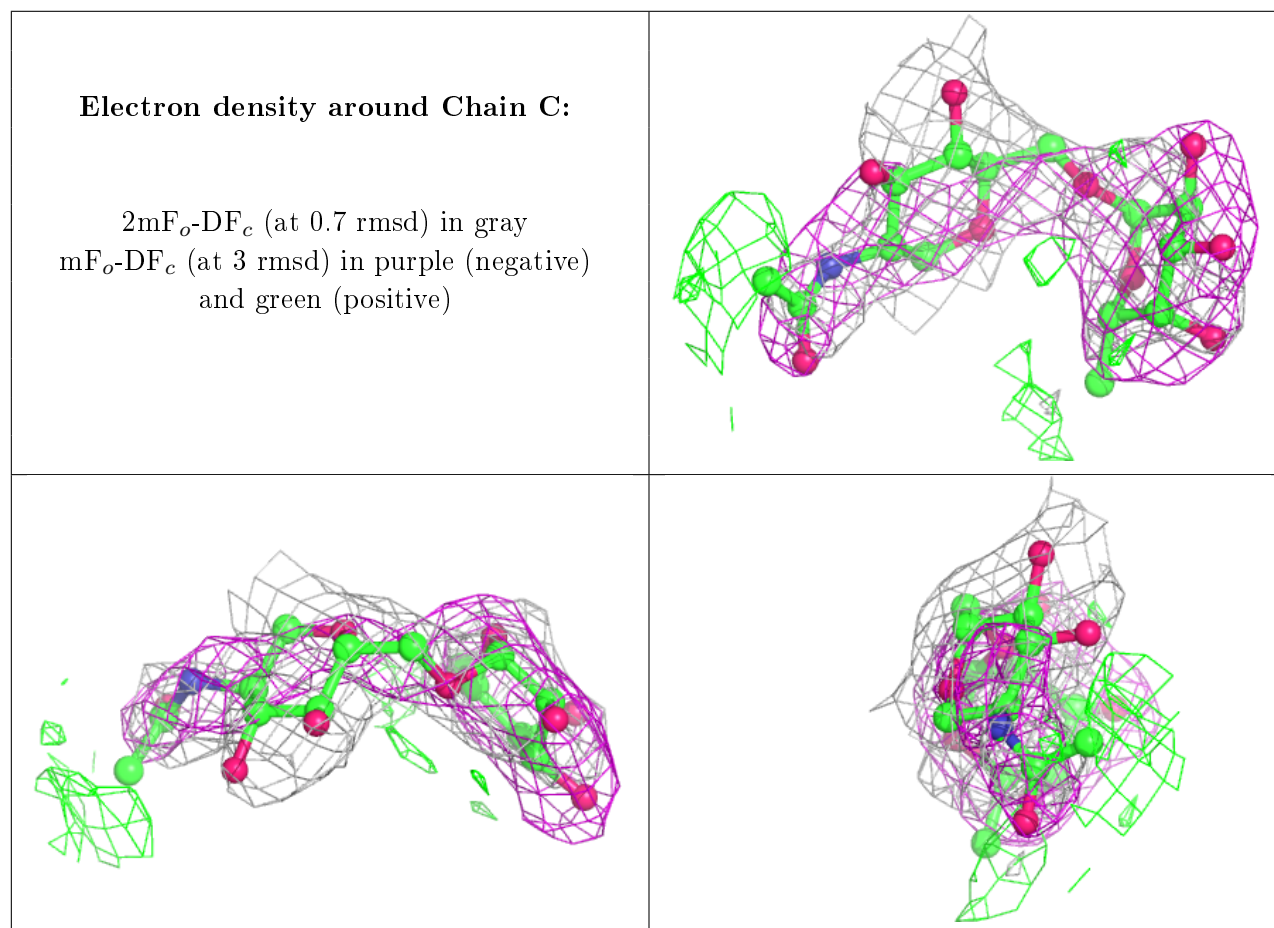
There are no non-standard protein/DNA/RNA residues in this entry.

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(\AA^2)	Q<0.9
2	FUL	C	2	10/11	0.75	0.69	52,54,58,59	0
2	NAG	C	1	14/15	0.83	0.46	63,75,79,81	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](#)

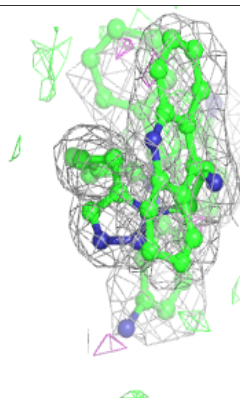
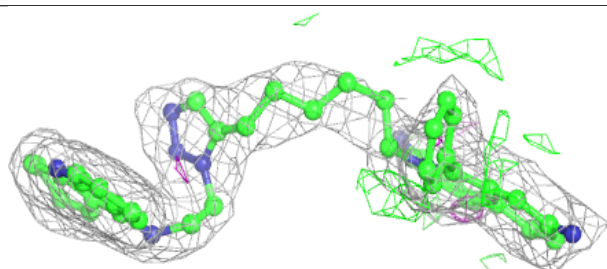
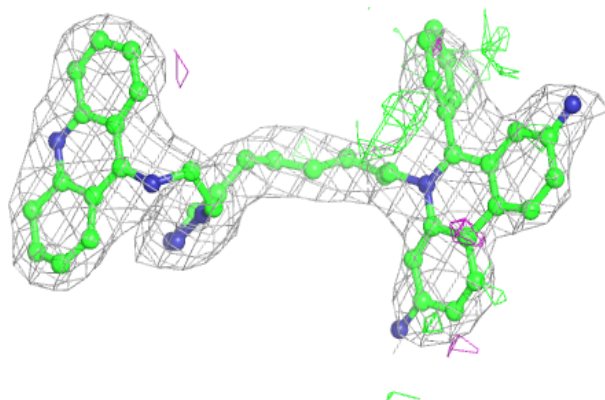
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	1601	14/15	0.62	0.52	56,62,65,66	0
3	NAG	A	1701	14/15	0.82	0.51	49,55,58,58	0
5	TZ5	A	1951	50/50	0.88	0.20	42,62,84,85	0
5	TZ5	B	1952	50/50	0.90	0.18	50,72,83,84	0
4	P6G	A	1901	19/19	0.94	0.16	57,66,75,76	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.

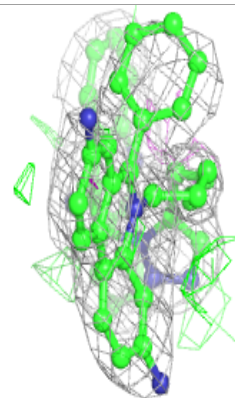
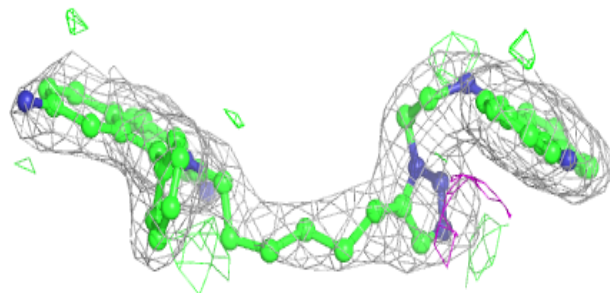
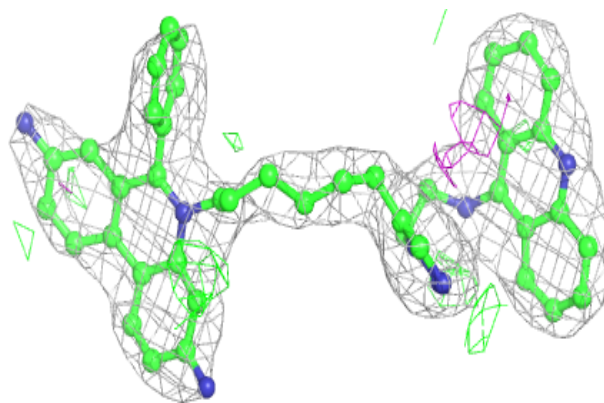
Electron density around TZ5 A 1951:

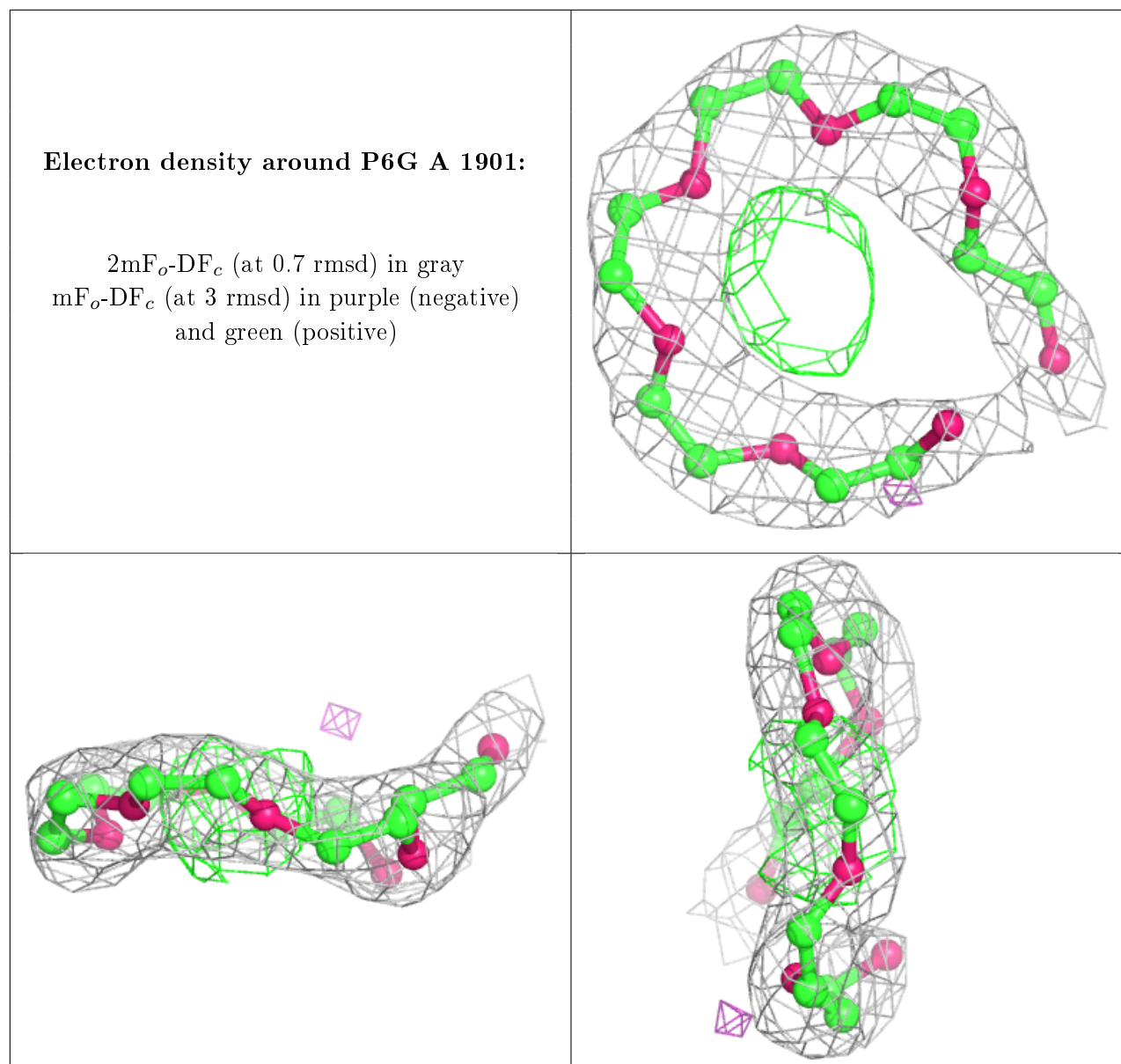
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around TZ5 B 1952:

$2mF_o-DF_c$ (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.