



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:15 AM UTC

PDB ID : 2HA5 / pdb_00002ha5
Title : Crystal structure of mutant S203A of acetylcholinesterase complexed with acetylthiocholine
Authors : Bourne, Y.; Radic, Z.; Sulzenbacher, G.; Kim, E.; Taylor, P.; Marchot, P.
Deposited on : 2006-06-12
Resolution : 2.15 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

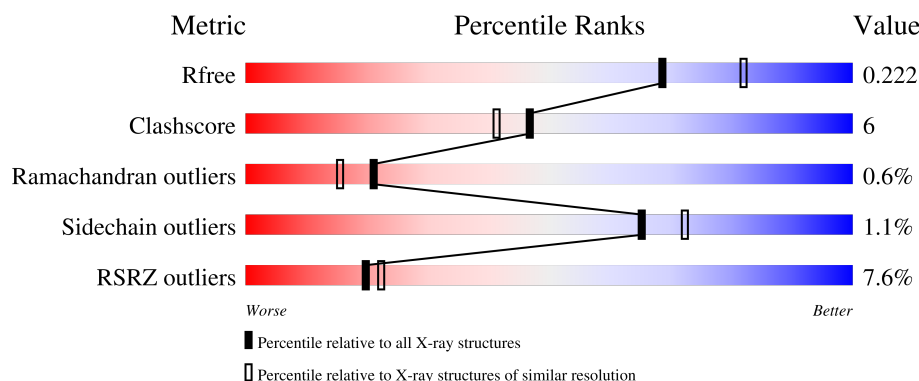
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

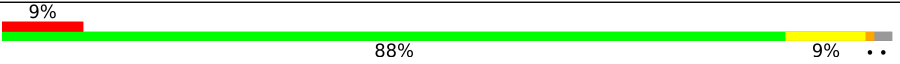
The reported resolution of this entry is 2.15 Å.

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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	543	
2	C	2	

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
4	ACT	A	1903	-	-	X	-
6	ETM	B	1955	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9414 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	1	7	0
			4211	2702	734	761	14			
1	B	533	Total	C	N	O	S	0	3	0
			4174	2681	722	757	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	ALA	SER	engineered mutation	UNP P21836
B	203	ALA	SER	engineered mutation	UNP P21836

- 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 (CCD ID: NAG) (formula: C₈H₁₅NO₆).



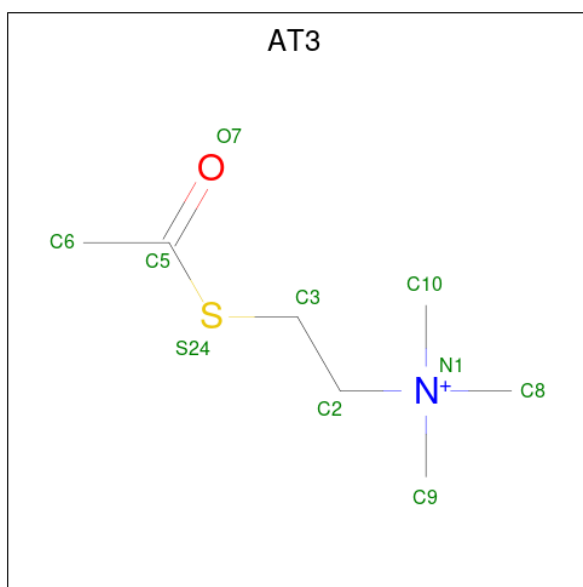
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



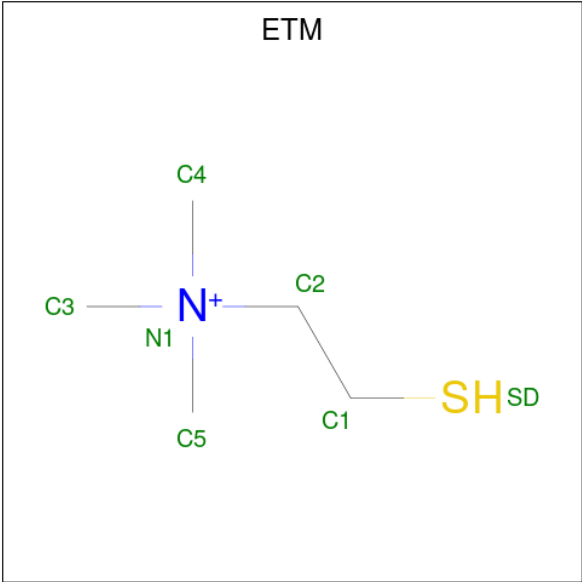
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is ACETYLTHIOCHOLINE (CCD ID: AT3) (formula: $C_7H_{16}NOS$).



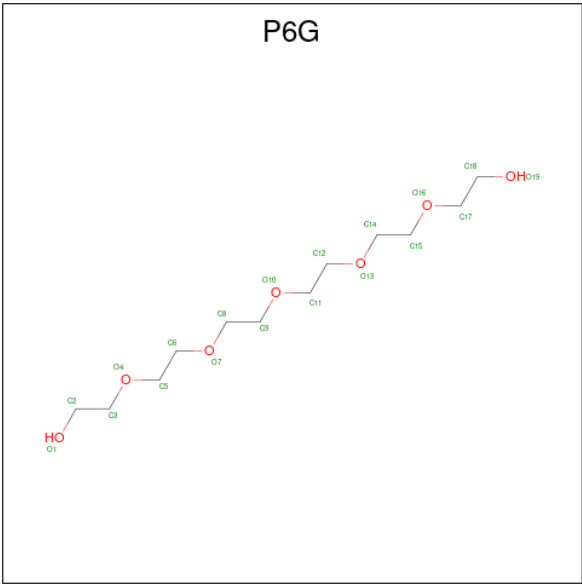
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	1
			10	7	1	1	1		
5	A	1	Total	C	N	O	S	0	0
			10	7	1	1	1		
5	B	1	Total	C	N	O	S	0	1
			10	7	1	1	1		
5	B	1	Total	C	N	O	S	0	0
			10	7	1	1	1		
5	B	1	Total	C	N	O	S	0	0
			10	7	1	1	1		

- Molecule 6 is 2-(TRIMETHYLAMMONIUM)ETHYL THIOL (CCD ID: ETM) (formula: $C_5H_{14}NS$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	S	0	1
			7	5	1	1		
6	A	1	Total	C	N	S	0	0
			7	5	1	1		
6	B	1	Total	C	N	S	0	1
			7	5	1	1		
6	B	1	Total	C	N	S	0	0
			7	5	1	1		

- Molecule 7 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C₁₂H₂₆O₇).



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

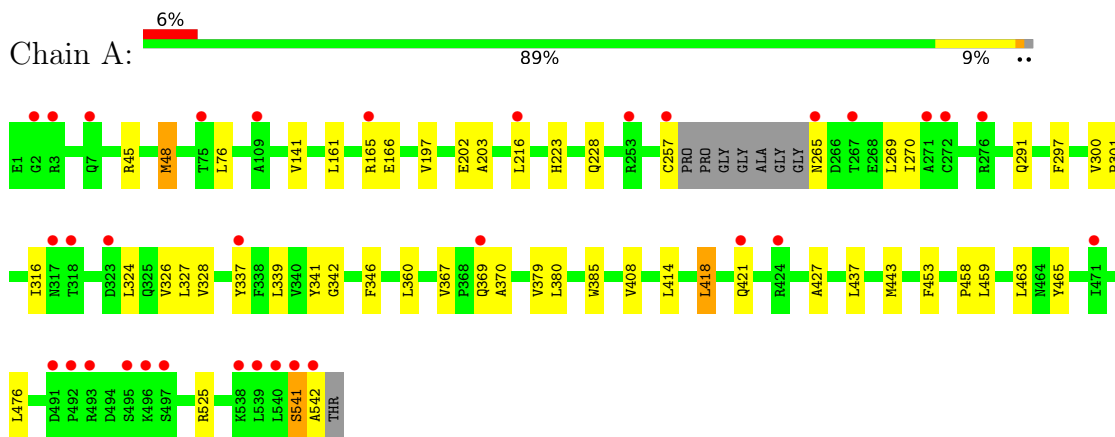
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	485	Total	O	0	0
			485	485		
8	B	401	Total	O	0	0
			401	401		

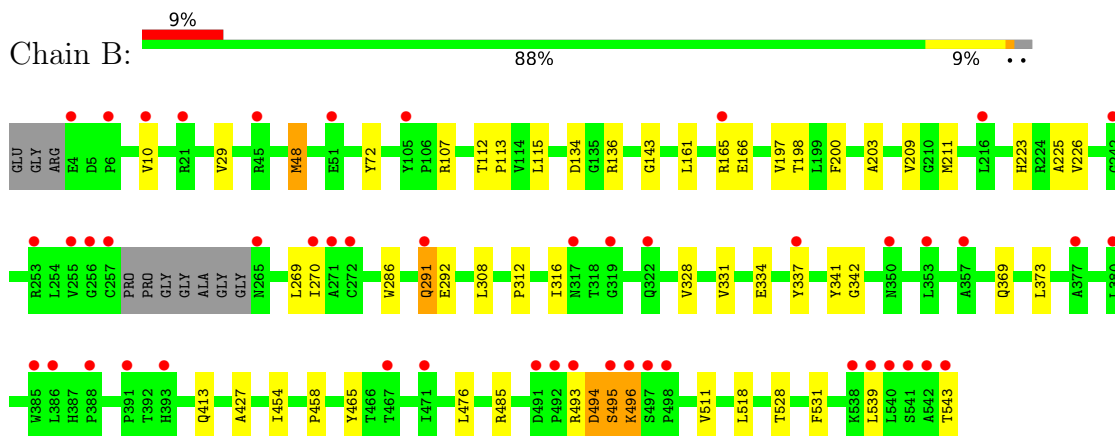
3 Residue-property plots

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

• Molecule 1: Acetylcholinesterase



• Molecule 1: Acetylcholinesterase



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.48Å 109.84Å 227.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.15 30.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.6 (30.00-2.15) 86.5 (30.00-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.177 , 0.210 0.187 , 0.222	Depositor DCC
R_{free} test set	2062 reflections (1.93%)	wwPDB-VP
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.772	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9414	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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: NAG, ETM, FUC, AT3, ACT, 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	0.61	0/4365	0.77	0/5961
1	B	0.57	0/4309	0.76	0/5888
All	All	0.59	0/8674	0.77	0/11849

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4211	0	4102	43	0
1	B	4174	0	4067	48	0
2	C	24	0	22	0	0
3	A	14	0	13	1	0
4	A	4	0	3	2	0
4	B	4	0	3	1	0
5	A	20	0	32	1	0
5	B	30	0	48	6	0
6	A	14	0	28	3	0
6	B	14	0	28	8	0
7	B	19	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	485	0	0	3	0
8	B	401	0	0	2	0
All	All	9414	0	8372	96	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 6.

All (96) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LEU:HD11	1:B:269:LEU:HD22	1.59	0.85
1:B:48:MET:HA	1:B:48:MET:HE2	1.58	0.84
1:B:543:THR:HG23	8:B:3179:HOH:O	1.78	0.83
1:A:48:MET:HE1	1:A:165:ARG:O	1.79	0.82
1:B:286:TRP:CZ2	6:B:1955:ETM:H53	2.15	0.81
1:A:337:TYR:OH	6:A:1909[B]:ETM:SD	2.43	0.76
1:B:341:TYR:CE2	6:B:1955:ETM:H42	2.24	0.72
1:B:286:TRP:CZ2	6:B:1955:ETM:C5	2.73	0.72
1:B:72:TYR:CE1	6:B:1955:ETM:H52	2.25	0.72
1:A:380:LEU:HD23	1:A:385:TRP:HZ2	1.57	0.69
5:B:1951[A]:AT3:S24	5:B:1951[A]:AT3:C9	2.81	0.69
5:B:1951[A]:AT3:S24	5:B:1951[A]:AT3:H9C2	2.33	0.68
1:B:48:MET:HE1	1:B:165:ARG:O	1.94	0.67
1:B:203:ALA:HB1	4:B:1953:ACT:C	2.25	0.67
1:A:203:ALA:HB1	4:A:1903:ACT:C	2.29	0.63
1:A:161:LEU:HD11	1:A:269:LEU:HD22	1.81	0.62
1:B:286:TRP:CE2	6:B:1955:ETM:H53	2.33	0.62
1:A:380:LEU:HD23	1:A:385:TRP:CZ2	2.36	0.61
1:B:48:MET:HA	1:B:48:MET:CE	2.31	0.61
1:B:495:SER:OG	1:B:496:LYS:N	2.33	0.60
1:B:465:TYR:OH	5:B:1952:AT3:H9C1	2.02	0.60
1:A:414:LEU:HG	1:A:418:LEU:HD22	1.84	0.59
1:B:341:TYR:CD2	6:B:1955:ETM:H42	2.37	0.59
1:B:291:GLN:HE22	1:B:369:GLN:NE2	2.01	0.58
1:A:541:SER:O	1:A:542:ALA:HB3	2.05	0.57
1:A:316:ILE:O	1:A:421:GLN:NE2	2.25	0.56
1:B:291:GLN:HE22	1:B:369:GLN:HE21	1.52	0.56
1:B:134:ASP:OD1	1:B:136:ARG:HD2	2.06	0.55
1:A:48:MET:HA	1:A:48:MET:HE2	1.89	0.54
1:A:291:GLN:NE2	1:A:369[B]:GLN:HE21	2.05	0.54
1:B:197:VAL:H	1:B:223:HIS:CD2	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:ARG:O	1:B:494:ASP:HB3	2.09	0.53
1:A:337:TYR:HA	1:A:443[A]:MET:CE	2.39	0.53
1:A:541:SER:O	1:A:542:ALA:CB	2.57	0.52
1:A:360:LEU:HD22	1:A:379:VAL:HG21	1.91	0.52
1:B:161:LEU:HD12	1:B:270:ILE:CG1	2.39	0.52
1:B:493:ARG:O	1:B:494:ASP:CB	2.59	0.51
1:A:48:MET:HE3	1:A:166:GLU:O	2.10	0.51
1:B:10:VAL:HG22	1:B:107:ARG:NH1	2.26	0.50
1:A:76:LEU:HD22	1:A:341:TYR:CE2	2.46	0.50
1:A:324:LEU:HG	1:A:326:VAL:HG13	1.94	0.50
1:A:463:LEU:HA	3:A:701:NAG:H82	1.94	0.49
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.48	0.49
1:A:48:MET:HE3	1:A:166:GLU:C	2.38	0.49
1:B:48:MET:HE3	1:B:166:GLU:O	2.13	0.49
1:B:291:GLN:NE2	1:B:369:GLN:HE21	2.11	0.49
1:A:291:GLN:NE2	1:A:369[B]:GLN:NE2	2.60	0.48
1:B:197:VAL:H	1:B:223:HIS:HD2	1.61	0.48
1:B:328:VAL:O	1:B:427:ALA:HA	2.13	0.48
1:B:291:GLN:NE2	1:B:369:GLN:NE2	2.62	0.48
1:B:48:MET:HE3	1:B:166:GLU:C	2.38	0.47
1:A:166:GLU:HB2	1:A:270:ILE:HD13	1.95	0.47
1:A:291:GLN:NE2	8:A:2368:HOH:O	2.35	0.47
1:A:76:LEU:HD22	1:A:341:TYR:CD2	2.49	0.47
1:A:465:TYR:OH	5:A:1902:AT3:H9C1	2.15	0.47
1:B:115:LEU:HD23	1:B:198:THR:HB	1.97	0.47
1:B:312:PRO:O	1:B:316:ILE:HG23	2.15	0.46
1:A:197:VAL:H	1:A:223:HIS:HD2	1.63	0.46
1:B:286:TRP:CZ2	6:B:1955:ETM:H51	2.51	0.46
1:B:511:VAL:HB	1:B:518:LEU:HD22	1.98	0.46
1:A:337:TYR:HA	1:A:443[A]:MET:HE3	1.98	0.45
1:B:454:ILE:HD13	1:B:476:LEU:HB3	1.98	0.45
1:A:141:VAL:HG21	1:A:459:LEU:CD2	2.45	0.45
1:A:257:CYS:C	8:A:2019:HOH:O	2.60	0.45
1:A:453:PHE:HB3	1:A:476:LEU:HD12	1.98	0.45
1:B:200:PHE:CB	1:B:226:VAL:HB	2.47	0.45
1:B:209:VAL:CG1	1:B:225:ALA:HB1	2.47	0.45
1:B:539:LEU:O	1:B:543:THR:N	2.50	0.44
1:A:367:VAL:HG12	1:A:370:ALA:HB2	1.99	0.44
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.53	0.44
1:A:300:VAL:HB	1:A:301:PRO:HD2	2.01	0.43
1:B:29:VAL:HG21	1:B:136:ARG:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1959[B]:ETM:H33	6:B:1959[B]:ETM:H12	1.86	0.43
1:A:141:VAL:HG21	1:A:459:LEU:HD23	2.01	0.42
1:A:408:VAL:HG11	1:A:525:ARG:HG3	2.01	0.42
1:A:202:GLU:OE1	6:A:1909[B]:ETM:H41	2.20	0.42
1:B:200:PHE:HB2	1:B:226:VAL:HB	2.01	0.42
1:A:339:LEU:HD13	1:A:346:PHE:CE2	2.54	0.42
1:B:166:GLU:HB2	1:B:270:ILE:HD13	2.02	0.42
1:B:211:MET:HG2	1:B:308:LEU:HD21	2.00	0.42
1:A:337:TYR:HA	1:A:443[A]:MET:HE1	2.01	0.42
1:A:297:PHE:CZ	4:A:1903:ACT:H2	2.55	0.41
1:B:112:THR:HG21	1:B:143:GLY:O	2.20	0.41
5:B:1951[A]:AT3:S24	5:B:1951[A]:AT3:H9C3	2.61	0.41
1:B:161:LEU:HD12	1:B:270:ILE:HD11	2.03	0.41
5:B:1952:AT3:H9C2	8:B:3066:HOH:O	2.19	0.41
1:A:265:ASN:ND2	8:A:2302:HOH:O	2.53	0.41
1:A:328:VAL:O	1:A:427:ALA:HA	2.20	0.41
1:A:337:TYR:CZ	6:A:1909[B]:ETM:SD	3.11	0.41
1:B:113:PRO:HG2	1:B:485:ARG:HG2	2.03	0.41
1:B:337:TYR:CE2	5:B:1951[A]:AT3:H6C1	2.56	0.41
1:B:373:LEU:HD23	1:B:539:LEU:HD11	2.03	0.40
1:B:528:THR:O	1:B:531:PHE:HB3	2.21	0.40
1:A:197:VAL:H	1:A:223:HIS:CD2	2.39	0.40
1:A:202:GLU:HA	1:A:228:GLN:O	2.21	0.40
1:B:331:VAL:HG22	1:B:334:GLU:CD	2.46	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	538/543 (99%)	519 (96%)	17 (3%)	2 (0%)	30 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	532/543 (98%)	513 (96%)	15 (3%)	4 (1%)	16	10
All	All	1070/1086 (98%)	1032 (96%)	32 (3%)	6 (1%)	21	15

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	494	ASP
1	B	495	SER
1	A	541	SER
1	B	496	LYS
1	A	342	GLY
1	B	342	GLY

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	445/442 (101%)	439 (99%)	6 (1%)	61	68
1	B	440/442 (100%)	436 (99%)	4 (1%)	70	77
All	All	885/884 (100%)	875 (99%)	10 (1%)	65	72

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
1	A	48	MET
1	A	216	LEU
1	A	327	LEU
1	A	418	LEU
1	A	437	LEU
1	B	48	MET
1	B	291	GLN
1	B	292	GLU
1	B	413	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	223	HIS
1	A	291	GLN
1	A	317	ASN
1	A	325	GLN
1	B	223	HIS
1	B	291	GLN
1	B	317	ASN
1	B	474	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	2,1	14,14,15	0.67	0	17,19,21	1.24	2 (11%)
2	FUC	C	2	2	10,10,11	0.62	0	14,14,16	1.03	2 (14%)

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

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C1-O5-C5	3.19	116.46	112.19
2	C	1	NAG	O5-C1-C2	-2.36	107.64	111.29
2	C	2	FUC	C3-C4-C5	2.32	113.34	109.81
2	C	2	FUC	O5-C5-C4	2.02	113.19	109.55

There are no chirality outliers.

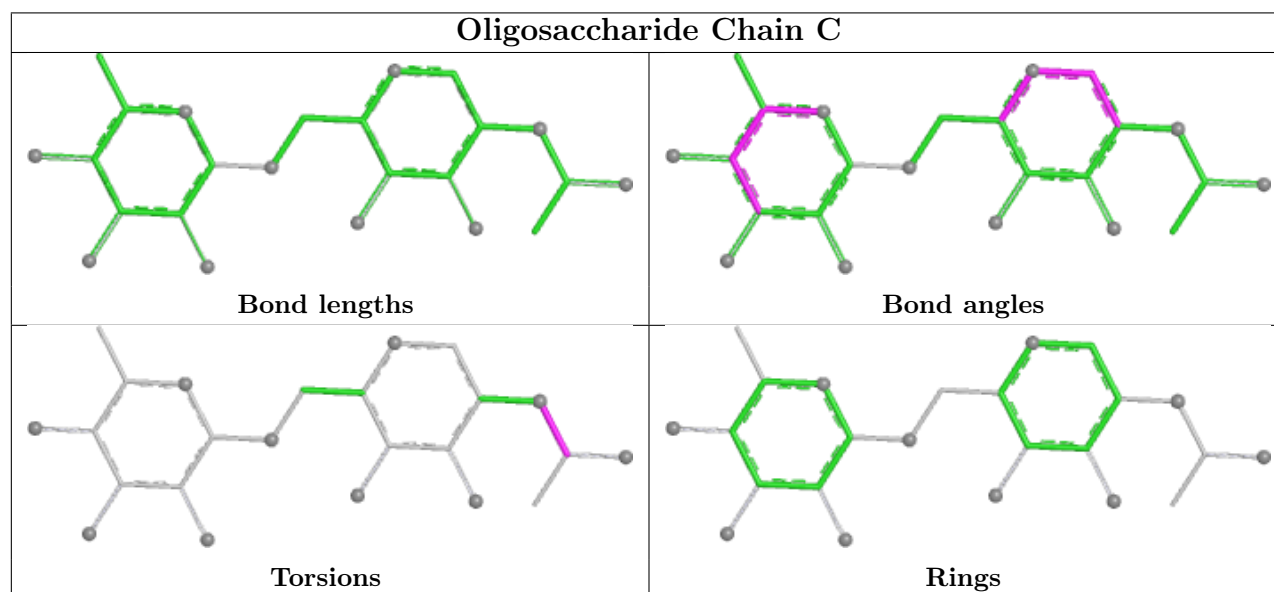
All (2) torsion outliers are listed below:

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

13 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
6	ETM	B	1959[B]	-	6,6,6	1.05	0	8,8,8	1.01	1 (12%)
6	ETM	A	1905	-	6,6,6	0.61	0	8,8,8	1.29	1 (12%)
6	ETM	B	1955	-	6,6,6	0.71	0	8,8,8	0.95	0
5	AT3	A	1901[A]	-	9,9,9	1.21	0	12,12,12	0.80	0
7	P6G	B	2901	-	18,18,18	2.20	6 (33%)	17,17,17	1.27	1 (5%)
5	AT3	B	1951[A]	-	9,9,9	1.22	0	12,12,12	0.55	0
6	ETM	A	1909[B]	-	6,6,6	1.02	0	8,8,8	1.10	1 (12%)
3	NAG	A	701	1	14,14,15	0.51	0	17,19,21	0.83	0
5	AT3	A	1902	-	9,9,9	0.81	0	12,12,12	0.50	0
5	AT3	B	1961	-	9,9,9	0.83	0	12,12,12	0.90	1 (8%)
4	ACT	B	1953	-	3,3,3	0.69	0	3,3,3	1.28	0
5	AT3	B	1952	-	9,9,9	0.89	0	12,12,12	0.66	0
4	ACT	A	1903	-	3,3,3	0.68	0	3,3,3	1.15	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
6	ETM	B	1959[B]	-	-	4/4/4/4	-
6	ETM	A	1905	-	-	4/4/4/4	-
6	ETM	B	1955	-	-	1/4/4/4	-
5	AT3	A	1901[A]	-	-	5/7/7/7	-
7	P6G	B	2901	-	-	8/16/16/16	-
5	AT3	B	1951[A]	-	-	7/7/7/7	-
6	ETM	A	1909[B]	-	-	1/4/4/4	-
3	NAG	A	701	1	-	0/6/23/26	0/1/1/1
5	AT3	A	1902	-	-	0/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	AT3	B	1961	-	-	0/7/7/7	-
5	AT3	B	1952	-	-	3/7/7/7	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	2901	P6G	O10-C9	4.33	1.60	1.42
7	B	2901	P6G	O13-C12	3.76	1.58	1.42
7	B	2901	P6G	O16-C15	3.55	1.57	1.42
7	B	2901	P6G	O19-C18	3.54	1.60	1.42
7	B	2901	P6G	O4-C3	3.45	1.57	1.42
7	B	2901	P6G	O7-C6	2.83	1.54	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	2901	P6G	O1-C2-C3	3.27	131.09	111.82
5	B	1961	AT3	C3-S24-C5	2.53	113.61	101.42
6	A	1905	ETM	C3-N1-C2	2.37	119.34	109.91
6	B	1959[B]	ETM	C2-C1-SD	-2.21	105.26	114.08
6	A	1909[B]	ETM	C3-N1-C2	2.09	118.21	109.91

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1901[A]	AT3	C2-C3-S24-C5
5	B	1951[A]	AT3	N1-C2-C3-S24
5	B	1951[A]	AT3	C2-C3-S24-C5
5	B	1951[A]	AT3	O7-C5-S24-C3
5	B	1951[A]	AT3	C6-C5-S24-C3
5	B	1952	AT3	C2-C3-S24-C5
5	B	1952	AT3	O7-C5-S24-C3
6	A	1905	ETM	SD-C1-C2-N1
6	B	1959[B]	ETM	SD-C1-C2-N1
7	B	2901	P6G	O16-C17-C18-O19
7	B	2901	P6G	O7-C8-C9-O10
5	B	1952	AT3	C6-C5-S24-C3
7	B	2901	P6G	O13-C14-C15-O16
6	B	1959[B]	ETM	C1-C2-N1-C3
6	B	1959[B]	ETM	C1-C2-N1-C5

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Mol	Chain	Res	Type	Atoms
5	A	1901[A]	AT3	N1-C2-C3-S24
7	B	2901	P6G	C2-C3-O4-C5
7	B	2901	P6G	C8-C9-O10-C11
6	B	1955	ETM	SD-C1-C2-N1
7	B	2901	P6G	C11-C12-O13-C14
5	A	1901[A]	AT3	C3-C2-N1-C9
5	A	1901[A]	AT3	C3-C2-N1-C10
5	B	1951[A]	AT3	C3-C2-N1-C9
5	B	1951[A]	AT3	C3-C2-N1-C10
6	A	1909[B]	ETM	C1-C2-N1-C3
6	A	1905	ETM	C1-C2-N1-C3
6	B	1959[B]	ETM	C1-C2-N1-C4
7	B	2901	P6G	O4-C5-C6-O7
7	B	2901	P6G	C6-C5-O4-C3
5	A	1901[A]	AT3	C3-C2-N1-C8
5	B	1951[A]	AT3	C3-C2-N1-C8
6	A	1905	ETM	C1-C2-N1-C4
6	A	1905	ETM	C1-C2-N1-C5

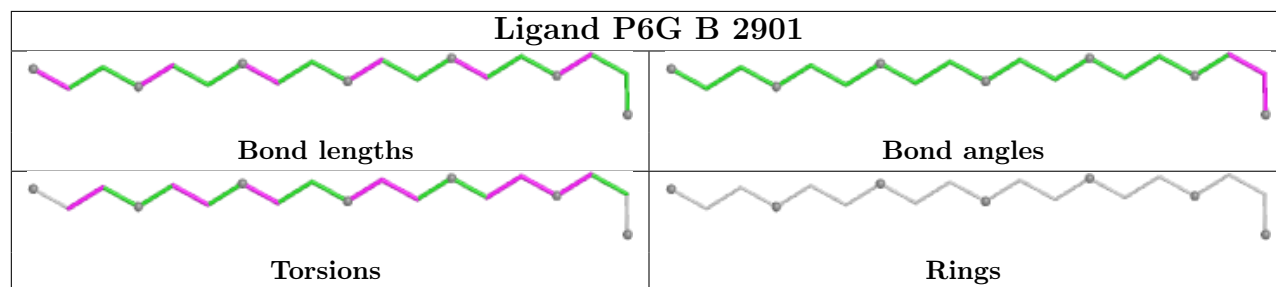
There are no ring outliers.

9 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1959[B]	ETM	1	0
6	B	1955	ETM	7	0
5	B	1951[A]	AT3	4	0
6	A	1909[B]	ETM	3	0
3	A	701	NAG	1	0
5	A	1902	AT3	1	0
4	B	1953	ACT	1	0
5	B	1952	AT3	2	0
4	A	1903	ACT	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

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	535/543 (98%)	0.49	33 (6%) 26 30	27, 52, 70, 98	7 (1%)
1	B	533/543 (98%)	0.83	48 (9%) 15 16	35, 59, 78, 99	3 (0%)
All	All	1068/1086 (98%)	0.66	81 (7%) 20 22	27, 55, 76, 99	10 (0%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	542	ALA	6.2
1	B	540	LEU	6.1
1	B	542	ALA	6.0
1	B	495	SER	5.3
1	B	543	THR	5.2
1	B	498	PRO	5.0
1	B	497	SER	4.9
1	B	496	LYS	4.5
1	B	492	PRO	4.5
1	B	272	CYS	4.1
1	A	492	PRO	4.0
1	A	496	LYS	3.9
1	B	257	CYS	3.9
1	B	493	ARG	3.6
1	A	497	SER	3.6
1	B	467	THR	3.4
1	B	4	GLU	3.4
1	A	424[A]	ARG	3.4
1	B	353	LEU	3.3
1	A	257	CYS	3.2
1	A	2	GLY	3.2
1	A	541	SER	3.2
1	B	539	LEU	3.1
1	A	495	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	322	GLN	3.1
1	B	541	SER	3.1
1	B	216[A]	LEU	2.9
1	B	255	VAL	2.9
1	A	421	GLN	2.9
1	A	272	CYS	2.9
1	B	51	GLU	2.9
1	A	471	ILE	2.8
1	B	357	ALA	2.8
1	A	75	THR	2.7
1	B	242	GLY	2.7
1	A	165	ARG	2.7
1	A	539	LEU	2.6
1	A	3	ARG	2.6
1	B	265	ASN	2.6
1	B	393	HIS	2.6
1	B	377	ALA	2.6
1	B	491	ASP	2.6
1	A	540	LEU	2.6
1	B	380	LEU	2.6
1	B	291	GLN	2.5
1	B	319	GLY	2.5
1	B	256	GLY	2.5
1	B	270	ILE	2.5
1	A	216	LEU	2.5
1	B	388	PRO	2.4
1	B	350	ASN	2.4
1	A	109	ALA	2.4
1	B	317	ASN	2.4
1	A	491	ASP	2.4
1	B	271	ALA	2.4
1	B	386	LEU	2.3
1	B	538	LYS	2.3
1	A	265	ASN	2.3
1	B	45[A]	ARG	2.3
1	A	538	LYS	2.3
1	A	7	GLN	2.2
1	A	267	THR	2.2
1	A	317	ASN	2.2
1	A	493	ARG	2.2
1	B	165	ARG	2.2
1	B	253	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	385	TRP	2.2
1	B	21	ARG	2.1
1	B	337	TYR	2.1
1	B	6	PRO	2.1
1	A	369[A]	GLN	2.1
1	A	253	ARG	2.1
1	A	337	TYR	2.1
1	A	318	THR	2.1
1	B	105	TYR	2.1
1	A	271	ALA	2.1
1	B	391	PRO	2.0
1	B	471	ILE	2.0
1	B	10	VAL	2.0
1	A	323[A]	ASP	2.0
1	A	276	ARG	2.0

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

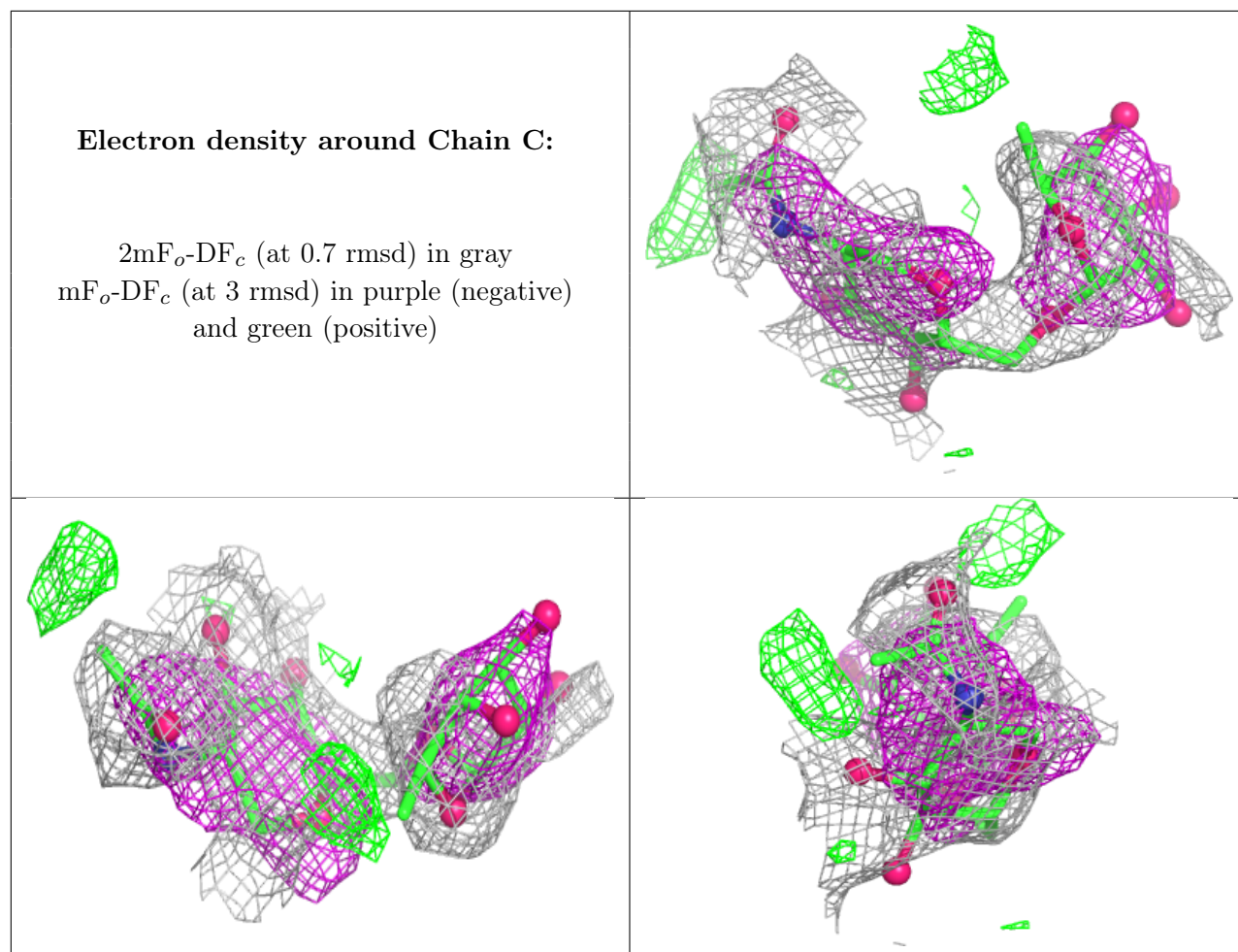
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FUC	C	2	10/11	0.24	0.25	102,104,105,105	0
2	NAG	C	1	14/15	0.62	0.22	83,90,94,98	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.

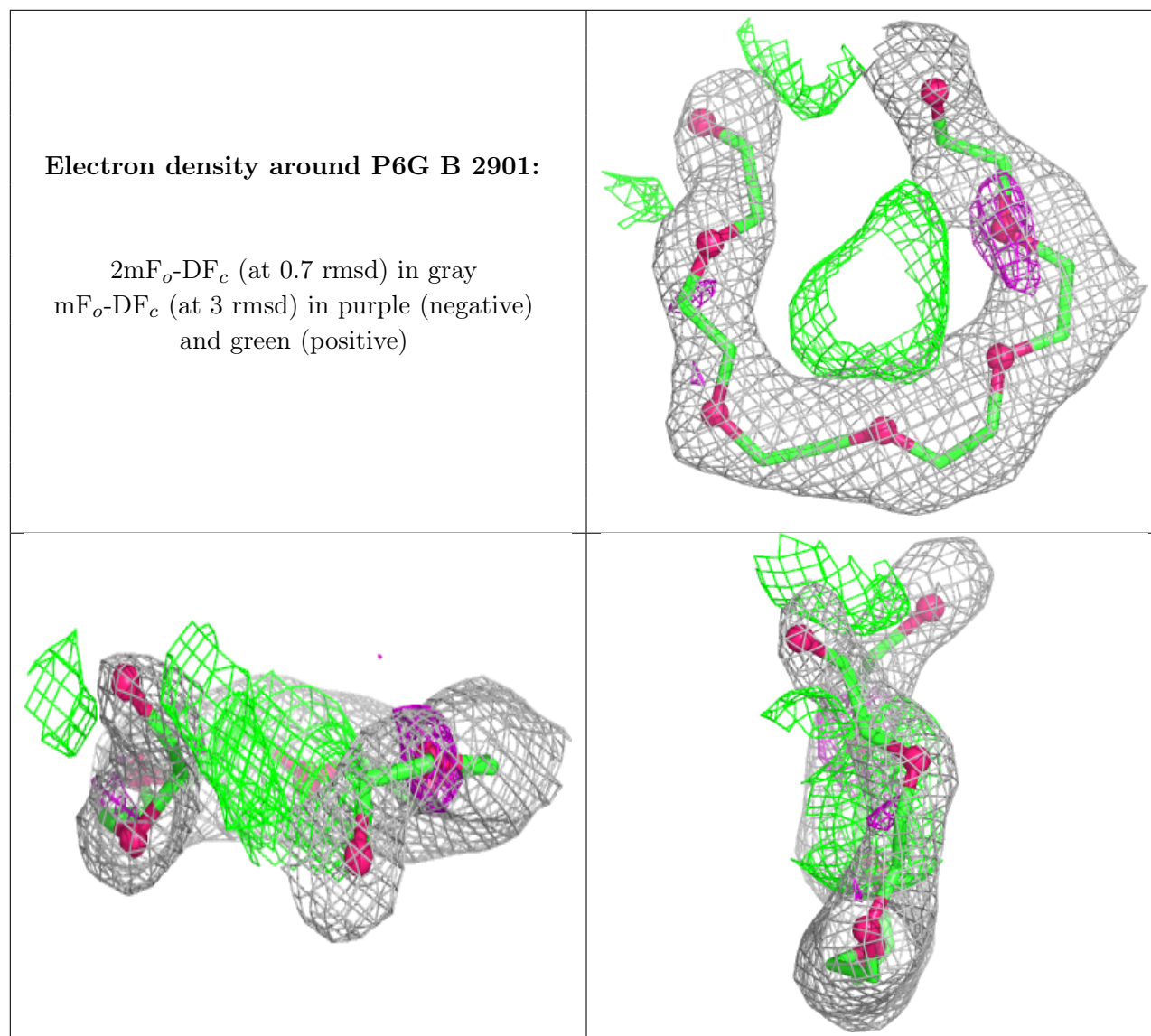
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	A	701	14/15	0.72	0.17	81,86,89,90	0
6	ETM	B	1955	7/7	0.79	0.31	93,93,95,97	7
6	ETM	A	1905	7/7	0.81	0.26	94,95,96,98	0
5	AT3	A	1902	10/10	0.84	0.22	78,80,81,81	0
5	AT3	B	1952	10/10	0.84	0.26	86,90,91,91	0
5	AT3	B	1951[A]	10/10	0.85	0.27	78,79,83,84	10
4	ACT	B	1953	4/4	0.86	0.27	62,64,64,64	0
4	ACT	A	1903	4/4	0.88	0.19	59,60,61,61	0
7	P6G	B	2901	19/19	0.88	0.17	67,72,77,77	0
6	ETM	A	1909[B]	7/7	0.91	0.18	58,58,60,62	7
5	AT3	A	1901[A]	10/10	0.91	0.23	80,81,83,84	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	ETM	B	1959[B]	7/7	0.94	0.15	73,74,75,77	7
5	AT3	B	1961	10/10	0.95	0.16	68,70,71,73	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.