



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 4, 2023 – 11:44 pm GMT

PDB ID : 2WG1
Title : TERNARY COMPLEX OF THE AGED CONJUGATE OF TORPEDO CALIFORNICA ACEYLCHOLINESTERASE WITH SOMAN AND 2-PAM
Authors : Sanson, B.; Nachon, F.; Colletier, J.P.; Froment, M.T.; Toker, L.; Greenblatt, H.M.; Sussman, J.L.; Ashani, Y.; Masson, P.; Silman, I.; Weik, M.
Deposited on : 2009-04-15
Resolution : 2.20 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

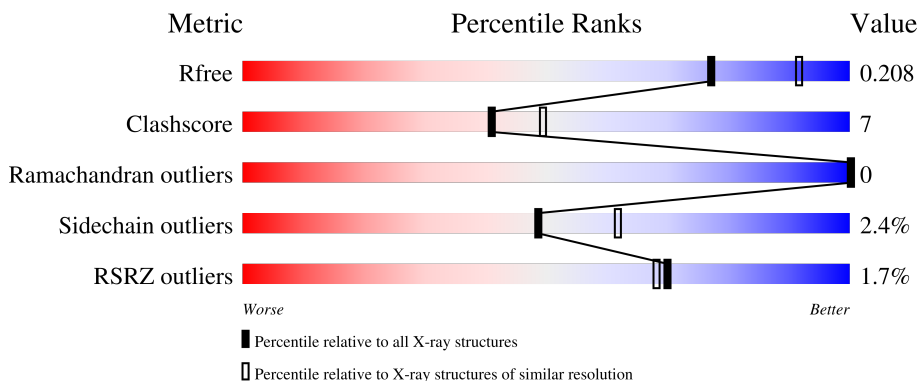
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


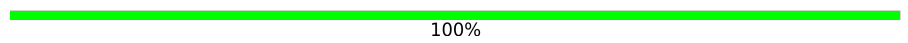
The reported resolution of this entry is 2.20 Å.

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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	537	 2% 86% 13% ..
2	B	2	 100%

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
6	MES	A	607	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 5221 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
			Total	C	N	O	S			
1	A	532	4449	2864	752	810	23	0	33	0

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



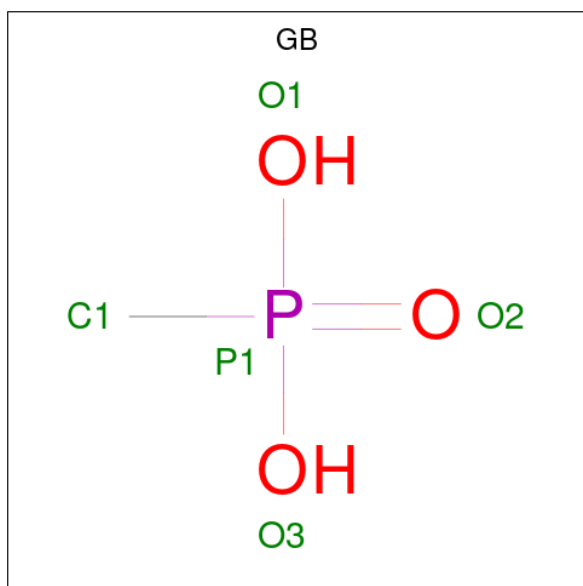
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	24	14	1	9	0	0	0

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



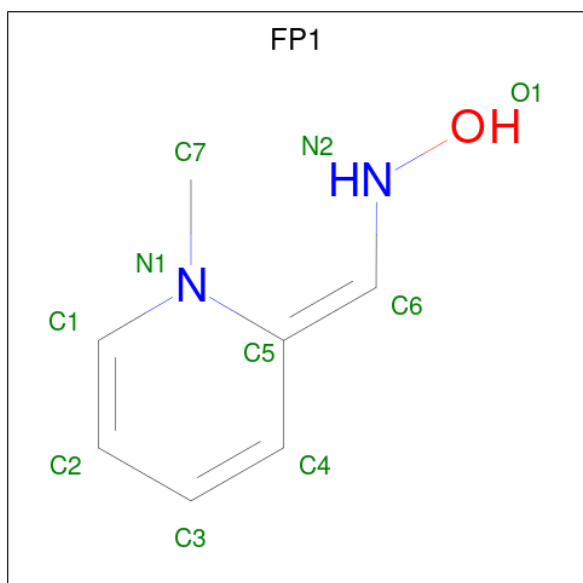
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	14	8	1	5	0	0

- Molecule 4 is METHYLPHOSPHONIC ACID ESTER GROUP (three-letter code: GB) (formula: $\text{CH}_5\text{O}_3\text{P}$).



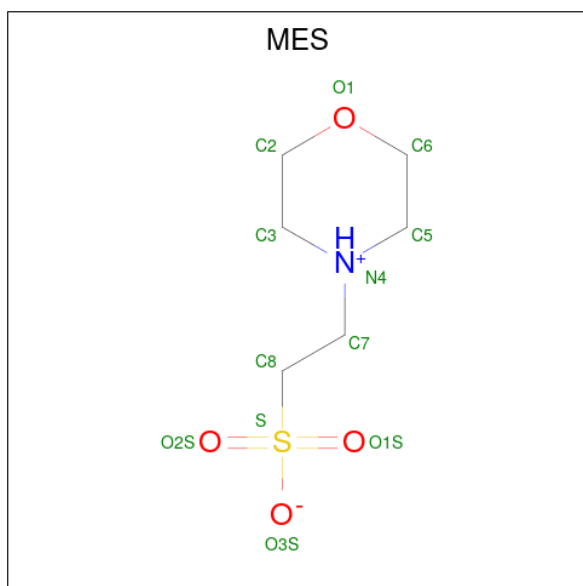
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
4	A	1	4	1	2	1	0	0

- Molecule 5 is N-hydroxy-1-(1-methylpyridin-2(1H)-ylidene)methanamine (three-letter code: FP1) (formula: $\text{C}_7\text{H}_{10}\text{N}_2\text{O}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	10	7	2	1	0	0

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



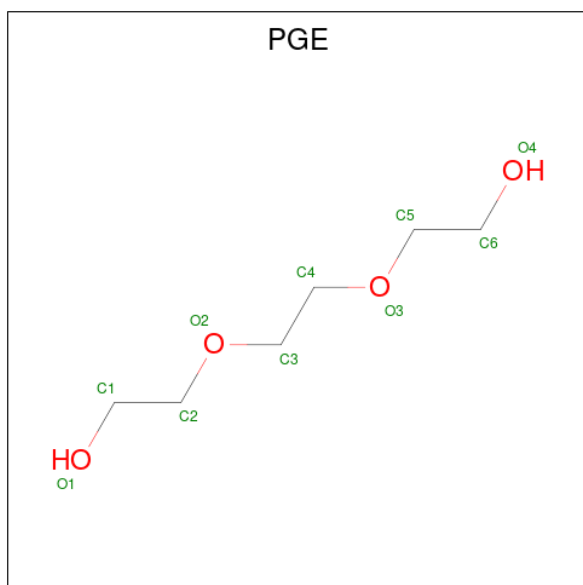
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	A	1	12	6	1	4	1	0	0
6	A	1	12	6	1	4	1	0	0
6	A	1	12	6	1	4	1	0	0
6	A	1	12	6	1	4	1	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



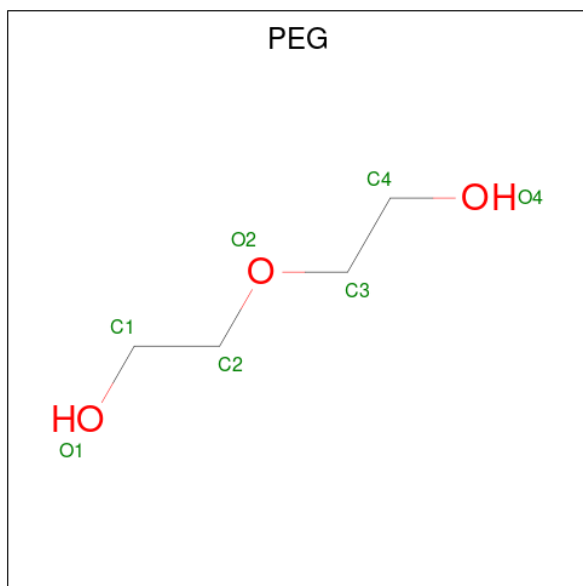
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 13 8 5	0	0
7	A	1	Total C O 13 8 5	0	0
7	A	1	Total C O 13 8 5	0	0
7	A	1	Total C O 13 8 5	0	0

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			10	6	4		
8	A	1	Total	C	O	0	0
			10	6	4		
8	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	555	Total	O	0	0
			555	555		

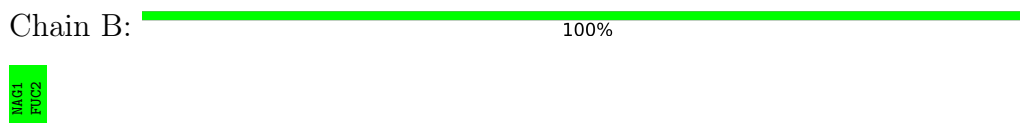
3 Residue-property plots [i](#)

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



4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	111.91Å 111.91Å 137.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.20) 98.8 (20.00-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.19Å)	Xtrriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.166 , 0.212 0.162 , 0.208	Depositor DCC
R_{free} test set	2462 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtrriage
Anisotropy	0.616	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5221	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: PGE, FP1, PG4, GB, PEG, NAG, FUC, MES

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	0.65	0/4663	0.65	3/6323 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	494	LEU	CA-CB-CG	5.80	128.63	115.30
1	A	388	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	388	ARG	NE-CZ-NH1	5.31	122.95	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	4449	0	4389	63	0
2	B	24	0	22	0	0
3	A	14	0	13	0	0
4	A	4	0	3	0	0
5	A	10	0	8	2	0
6	A	48	0	52	8	0
7	A	52	0	72	8	0
8	A	30	0	42	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	35	0	50	1	0
10	A	555	0	0	21	0
All	All	5221	0	4651	66	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 7.

All (66) 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:A:220[B]:ARG:NH1	10:A:702:HOH:O	1.62	1.19
1:A:181[B]:HIS:ND1	10:A:703:HOH:O	1.90	1.04
1:A:353[A]:MET:HE2	10:A:1104:HOH:O	1.70	0.90
1:A:19[B]:ARG:NH1	10:A:705:HOH:O	1.99	0.89
1:A:504[B]:ASP:OD2	10:A:704:HOH:O	1.91	0.87
1:A:110:THR:OG1	1:A:478[B]:LYS:HG2	1.76	0.86
1:A:526[B]:GLN:CG	10:A:832:HOH:O	2.28	0.82
1:A:19[B]:ARG:NH2	10:A:705:HOH:O	2.01	0.81
1:A:526[B]:GLN:HG3	10:A:832:HOH:O	1.79	0.81
1:A:431:VAL:HG22	6:A:609:MES:O3S	1.84	0.78
1:A:190:ASP:OD1	1:A:192:LYS:HG2	1.87	0.73
1:A:42[A]:ASN:OD1	10:A:706:HOH:O	2.07	0.72
1:A:491:LYS:HE2	10:A:764:HOH:O	1.90	0.69
1:A:19[B]:ARG:CZ	10:A:705:HOH:O	2.30	0.69
1:A:404:LEU:O	1:A:408[B]:VAL:HG23	1.92	0.68
1:A:321:LEU:HD11	1:A:408[A]:VAL:HG12	1.74	0.68
1:A:520:MET:SD	10:A:1076:HOH:O	2.51	0.67
1:A:346:LYS:HG2	1:A:385:ILE:HD13	1.81	0.63
1:A:455:GLU:OE2	6:A:607:MES:H52	1.98	0.62
1:A:23:LEU:HA	6:A:607:MES:H31	1.81	0.61
1:A:454[B]:LYS:H	6:A:607:MES:H61	1.69	0.58
7:A:613:PG4:H11	10:A:928:HOH:O	2.03	0.58
1:A:454[A]:LYS:H	6:A:607:MES:H61	1.69	0.57
1:A:107:LYS:HA	7:A:611:PG4:H81	1.88	0.56
1:A:321:LEU:HD11	1:A:408[A]:VAL:CG1	2.35	0.56
1:A:419:TYR:CZ	1:A:494:LEU:HD13	2.40	0.56
1:A:440:HIS:O	5:A:605:FP1:O1	2.24	0.55
1:A:313:ASN:OD1	9:A:620:PEG:H11	2.06	0.55
1:A:357[A]:LYS:HD3	10:A:1175:HOH:O	2.06	0.54
1:A:211[B]:LEU:HD23	1:A:305:LEU:HD22	1.91	0.53
1:A:223:ILE:HA	1:A:320:LEU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:MET:CE	10:A:1002:HOH:O	2.58	0.52
1:A:9[B]:ASN:H	7:A:611:PG4:H32	1.74	0.52
1:A:453:VAL:HG13	6:A:607:MES:H82	1.93	0.51
5:A:605:FP1:HB	10:A:871:HOH:O	2.10	0.50
1:A:9[A]:ASN:H	7:A:611:PG4:H32	1.74	0.50
1:A:454[A]:LYS:HA	1:A:454[A]:LYS:HE2	1.93	0.49
1:A:451:PRO:HA	1:A:458:TYR:CD1	2.48	0.49
1:A:408[B]:VAL:CG1	1:A:418:THR:HG21	2.43	0.49
1:A:20:VAL:HG11	8:A:616:PGE:H52	1.95	0.48
1:A:186:PHE:O	7:A:611:PG4:H51	2.14	0.48
1:A:186:PHE:HA	7:A:611:PG4:H51	1.96	0.47
1:A:31:LEU:HD11	8:A:616:PGE:H5	1.95	0.47
1:A:504[B]:ASP:CG	10:A:704:HOH:O	2.45	0.47
1:A:260[A]:GLU:H	1:A:260[A]:GLU:CD	2.18	0.46
1:A:413[A]:LYS:O	1:A:413[A]:LYS:HG2	2.14	0.46
1:A:321:LEU:HD11	1:A:408[B]:VAL:HG22	1.98	0.46
1:A:449:GLY:HA2	1:A:466:SER:OG	2.15	0.46
1:A:531:LEU:C	1:A:531:LEU:HD23	2.36	0.46
7:A:612:PG4:H22	10:A:1024:HOH:O	2.15	0.46
1:A:468[B]:ARG:NH2	10:A:709:HOH:O	2.29	0.45
1:A:518:VAL:HG23	6:A:608:MES:H72	1.99	0.45
1:A:78:PHE:CZ	1:A:431:VAL:HG23	2.52	0.45
1:A:405:MET:HA	1:A:408[A]:VAL:HG22	2.00	0.43
1:A:526[B]:GLN:NE2	10:A:714:HOH:O	2.42	0.43
1:A:350[B]:GLU:HG2	10:A:1104:HOH:O	2.17	0.43
1:A:207:GLY:HA3	1:A:229:PRO:HD3	2.01	0.43
1:A:158:LEU:O	1:A:161:SER:HB3	2.19	0.42
1:A:197:PHE:CB	1:A:223:ILE:HB	2.49	0.42
1:A:502:PHE:CZ	1:A:513:HIS:HB2	2.53	0.42
1:A:366:LEU:HD23	1:A:535:THR:HG21	2.02	0.42
1:A:185:GLN:HA	1:A:189:GLY:O	2.20	0.41
1:A:105:ARG:NH1	7:A:611:PG4:H52	2.35	0.41
1:A:454[B]:LYS:HD3	6:A:607:MES:H61	2.01	0.41

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	563/537 (105%)	537 (95%)	26 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	498/469 (106%)	486 (98%)	12 (2%)	49	62

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	MET
1	A	28	SER
1	A	161	SER
1	A	197	PHE
1	A	288	PHE
1	A	430	LEU
1	A	454[A]	LYS
1	A	454[B]	LYS
1	A	473	TRP
1	A	487	SER
1	A	490	SER
1	A	494	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	B	1	1,2	14,14,15	0.63	0	17,19,21	1.03	0
2	FUC	B	2	2	10,10,11	0.68	0	14,14,16	0.70	0

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

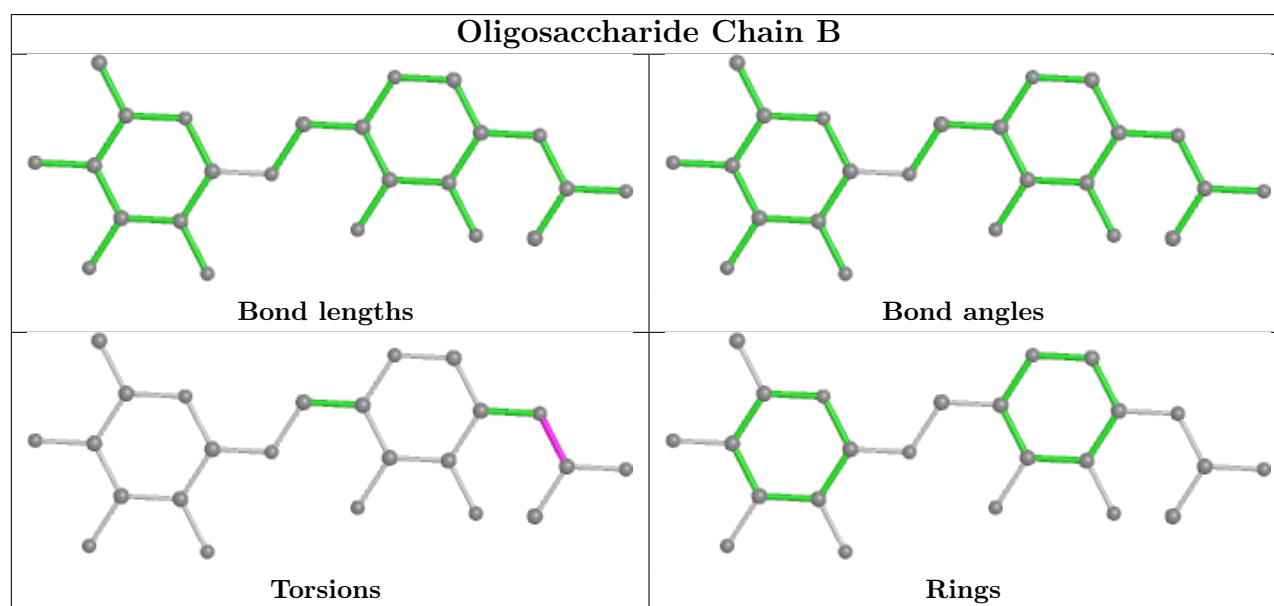
All (2) torsion outliers are listed below:

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

19 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	$\# Z > 2$
9	PEG	A	619	-	6,6,6	0.62	0	5,5,5	0.31	0
7	PG4	A	612	-	12,12,12	0.71	0	11,11,11	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PEG	A	617	-	6,6,6	0.60	0	5,5,5	0.44	0
6	MES	A	607	-	12,12,12	1.83	1 (8%)	14,16,16	1.70	2 (14%)
9	PEG	A	618	-	6,6,6	0.60	0	5,5,5	0.33	0
8	PGE	A	615	-	9,9,9	0.76	0	8,8,8	0.77	0
9	PEG	A	621	-	6,6,6	0.84	0	5,5,5	0.26	0
7	PG4	A	613	-	12,12,12	0.69	0	11,11,11	0.44	0
8	PGE	A	616	-	9,9,9	0.59	0	8,8,8	0.42	0
4	GB	A	604	1	0,3,4	-	-	0,3,6	-	-
5	FP1	A	605	-	9,10,10	4.72	4 (44%)	8,12,12	9.22	2 (25%)
7	PG4	A	611	-	12,12,12	0.68	0	11,11,11	1.01	0
6	MES	A	608	-	12,12,12	1.96	1 (8%)	14,16,16	1.36	2 (14%)
3	NAG	A	601	1	14,14,15	0.60	0	17,19,21	0.93	1 (5%)
6	MES	A	609	-	12,12,12	1.72	1 (8%)	14,16,16	1.41	3 (21%)
9	PEG	A	620	-	6,6,6	0.49	0	5,5,5	1.05	1 (20%)
7	PG4	A	610	-	12,12,12	0.74	0	11,11,11	0.76	0
8	PGE	A	614	-	9,9,9	0.70	0	8,8,8	0.51	0
6	MES	A	606	-	12,12,12	1.33	2 (16%)	14,16,16	1.48	3 (21%)

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
8	PGE	A	615	-	-	4/7/7/7	-
9	PEG	A	619	-	-	3/4/4/4	-
6	MES	A	608	-	-	5/6/14/14	0/1/1/1
7	PG4	A	613	-	-	7/10/10/10	-
7	PG4	A	612	-	-	6/10/10/10	-
8	PGE	A	616	-	-	5/7/7/7	-
3	NAG	A	601	1	-	1/6/23/26	0/1/1/1
6	MES	A	607	-	-	0/6/14/14	0/1/1/1
9	PEG	A	617	-	-	2/4/4/4	-
9	PEG	A	618	-	-	1/4/4/4	-
9	PEG	A	621	-	-	2/4/4/4	-
6	MES	A	609	-	-	0/6/14/14	0/1/1/1
5	FP1	A	605	-	-	0/0/3/3	0/1/1/1
7	PG4	A	611	-	-	4/10/10/10	-
9	PEG	A	620	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PG4	A	610	-	-	5/10/10/10	-
8	PGE	A	614	-	-	3/7/7/7	-
6	MES	A	606	-	-	1/6/14/14	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	605	FP1	C6-C5	-9.48	1.24	1.40
5	A	605	FP1	C6-N2	-9.19	1.18	1.30
6	A	608	MES	C8-S	5.70	1.85	1.77
6	A	607	MES	C8-S	4.97	1.84	1.77
6	A	609	MES	C8-S	4.74	1.84	1.77
5	A	605	FP1	C5-N1	3.47	1.41	1.37
6	A	606	MES	C8-S	3.35	1.82	1.77
5	A	605	FP1	C1-C2	2.02	1.40	1.35
6	A	606	MES	O1S-S	2.00	1.50	1.45

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	605	FP1	C5-C6-N2	25.29	179.71	126.76
5	A	605	FP1	C4-C5-N1	6.12	121.63	116.68
6	A	607	MES	O1S-S-C8	4.27	112.06	106.92
6	A	609	MES	O3S-S-C8	3.36	111.20	105.77
6	A	606	MES	C2-C3-N4	-2.67	106.06	110.10
6	A	609	MES	O1S-S-C8	2.55	109.99	106.92
3	A	601	NAG	O5-C5-C6	2.43	111.02	107.20
6	A	606	MES	O1-C6-C5	-2.40	106.51	111.80
6	A	608	MES	C5-N4-C3	2.39	114.21	108.83
6	A	606	MES	C5-N4-C3	2.39	114.20	108.83
6	A	609	MES	O3S-S-O1S	-2.28	105.71	111.27
6	A	607	MES	C2-C3-N4	2.09	113.28	110.10
9	A	620	PEG	C3-O2-C2	-2.08	104.26	113.29
6	A	608	MES	O3S-S-C8	2.00	109.01	105.77

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	608	MES	C8-C7-N4-C5
6	A	608	MES	C7-C8-S-O1S

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Mol	Chain	Res	Type	Atoms
6	A	608	MES	C7-C8-S-O2S
6	A	608	MES	C7-C8-S-O3S
8	A	615	PGE	O2-C3-C4-O3
7	A	612	PG4	O3-C5-C6-O4
8	A	616	PGE	O3-C5-C6-O4
7	A	610	PG4	O1-C1-C2-O2
9	A	617	PEG	O2-C3-C4-O4
7	A	610	PG4	O3-C5-C6-O4
7	A	613	PG4	O2-C3-C4-O3
8	A	615	PGE	O3-C5-C6-O4
8	A	616	PGE	O1-C1-C2-O2
7	A	611	PG4	O3-C5-C6-O4
7	A	612	PG4	O4-C7-C8-O5
9	A	621	PEG	O2-C3-C4-O4
7	A	612	PG4	O1-C1-C2-O2
9	A	619	PEG	O2-C3-C4-O4
7	A	611	PG4	O1-C1-C2-O2
9	A	617	PEG	O1-C1-C2-O2
7	A	612	PG4	O2-C3-C4-O3
7	A	610	PG4	O4-C7-C8-O5
7	A	613	PG4	O1-C1-C2-O2
8	A	614	PGE	O1-C1-C2-O2
8	A	615	PGE	C6-C5-O3-C4
7	A	613	PG4	O4-C7-C8-O5
8	A	616	PGE	C1-C2-O2-C3
9	A	619	PEG	C4-C3-O2-C2
7	A	613	PG4	C1-C2-O2-C3
8	A	614	PGE	C1-C2-O2-C3
9	A	620	PEG	O1-C1-C2-O2
8	A	616	PGE	C3-C4-O3-C5
9	A	618	PEG	C4-C3-O2-C2
9	A	619	PEG	C1-C2-O2-C3
8	A	614	PGE	C4-C3-O2-C2
8	A	616	PGE	O2-C3-C4-O3
7	A	613	PG4	C8-C7-O4-C6
7	A	610	PG4	C3-C4-O3-C5
7	A	613	PG4	C4-C3-O2-C2
7	A	611	PG4	C3-C4-O3-C5
7	A	612	PG4	C1-C2-O2-C3
6	A	608	MES	C8-C7-N4-C3
9	A	621	PEG	C4-C3-O2-C2
7	A	611	PG4	O4-C7-C8-O5

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Mol	Chain	Res	Type	Atoms
7	A	613	PG4	O3-C5-C6-O4
3	A	601	NAG	C4-C5-C6-O6
8	A	615	PGE	O1-C1-C2-O2
7	A	610	PG4	C4-C3-O2-C2
7	A	612	PG4	C3-C4-O3-C5
6	A	606	MES	C8-C7-N4-C3

There are no ring outliers.

9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	612	PG4	1	0
6	A	607	MES	6	0
7	A	613	PG4	1	0
8	A	616	PGE	2	0
5	A	605	FP1	2	0
7	A	611	PG4	6	0
6	A	608	MES	1	0
6	A	609	MES	1	0
9	A	620	PEG	1	0

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	532/537 (99%)	-0.68	9 (1%) 70 68	17, 27, 41, 61	5 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	486	HIS	5.1
1	A	485	PRO	4.6
1	A	488	GLN	4.3
1	A	55	SER	3.4
1	A	535	THR	2.8
1	A	487	SER	2.6
1	A	42[A]	ASN	2.6
1	A	489	GLU	2.4
1	A	257	ASN	2.3

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

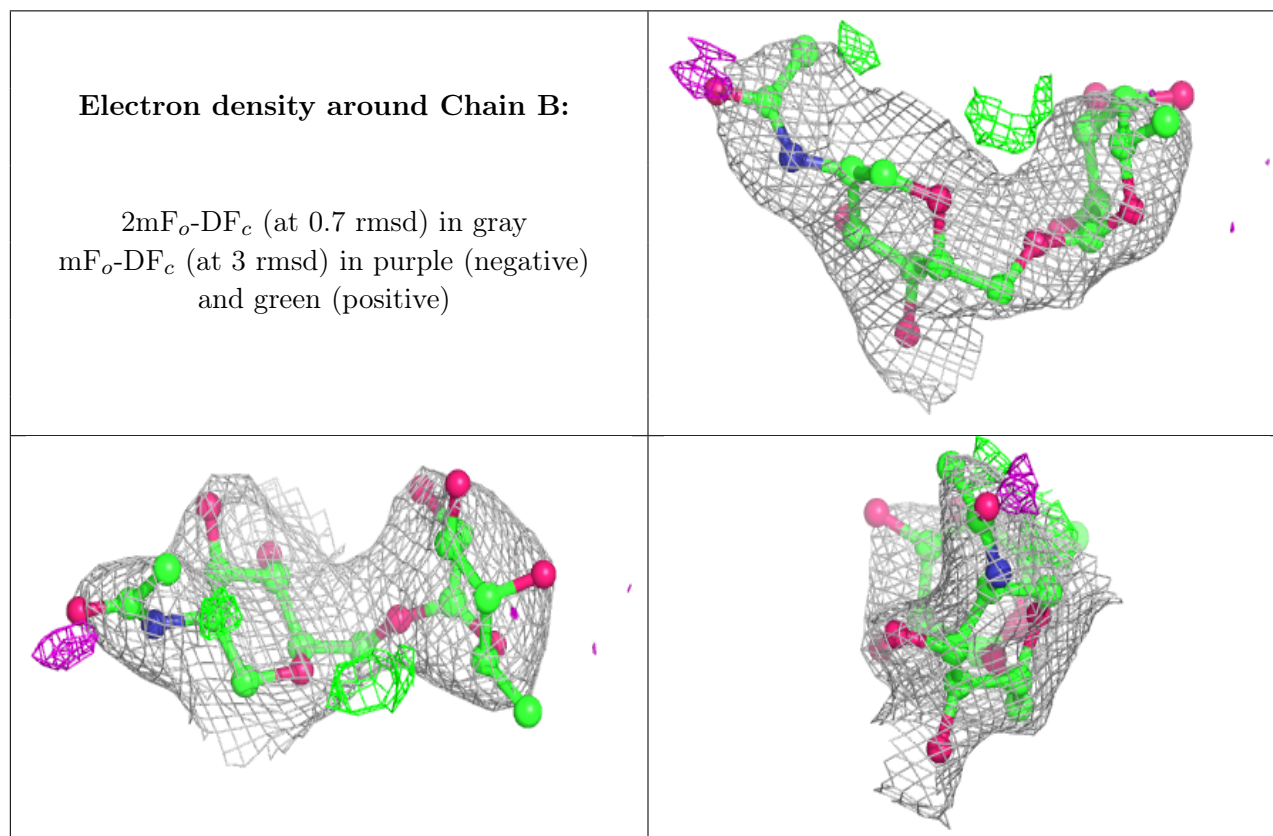
There are no non-standard protein/DNA/RNA residues in this entry.

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	B	2	10/11	0.85	0.36	85,87,88,89	0
2	NAG	B	1	14/15	0.88	0.26	59,66,68,75	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
8	PGE	A	614	10/10	0.68	0.28	60,63,69,69	0
9	PEG	A	621	7/7	0.69	0.28	64,68,73,74	0
9	PEG	A	617	7/7	0.71	0.26	68,69,71,71	0
7	PG4	A	611	13/13	0.72	0.32	61,64,69,69	0
8	PGE	A	616	10/10	0.72	0.29	70,78,82,82	0
7	PG4	A	613	13/13	0.73	0.25	85,88,91,91	0
7	PG4	A	612	13/13	0.74	0.27	69,70,75,75	0
9	PEG	A	619	7/7	0.76	0.24	97,98,99,99	0
6	MES	A	606	12/12	0.77	0.24	56,59,62,63	12
7	PG4	A	610	13/13	0.79	0.21	60,62,64,65	0
6	MES	A	607	12/12	0.87	0.27	54,62,67,67	12
9	PEG	A	618	7/7	0.88	0.20	72,72,74,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	PGE	A	615	10/10	0.89	0.22	56,57,58,58	0
9	PEG	A	620	7/7	0.90	0.27	58,59,60,60	0
3	NAG	A	601	14/15	0.90	0.26	40,44,49,50	0
6	MES	A	609	12/12	0.91	0.17	52,57,59,60	12
5	FP1	A	605	10/10	0.95	0.13	28,30,43,45	0
6	MES	A	608	12/12	0.96	0.12	41,46,48,49	12
4	GB	A	604	4/5	1.00	0.08	19,20,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.