



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:05 AM UTC

PDB ID : 3ZV7 / pdb_00003zv7
Title : Torpedo californica Acetylcholinesterase Inhibition by Bisnorcymserine
Authors : Bartolucci, C.; Stojan, J.; Greig, N.H.; Lamba, D.
Deposited on : 2011-07-24
Resolution : 2.26 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
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

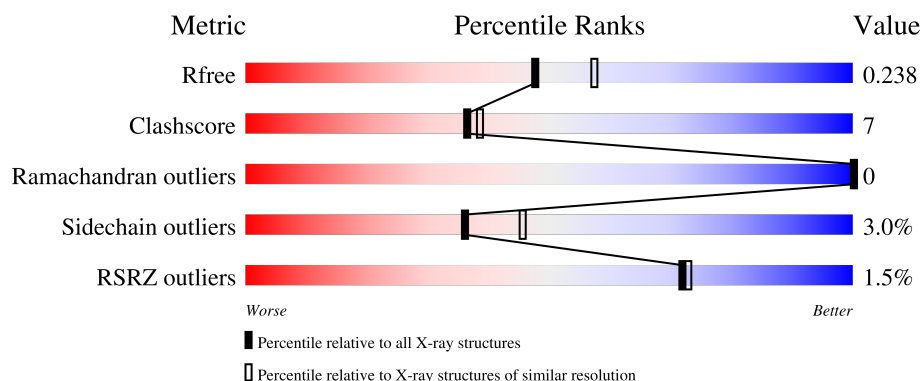
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	78% 19% ..
2	B	2	50% 50%

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
7	MES	A	1542	-	-	-	X
9	CL	A	1554	-	-	-	X

2 Entry composition [i](#)

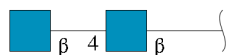
There are 10 unique types of molecules in this entry. The entry contains 4669 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

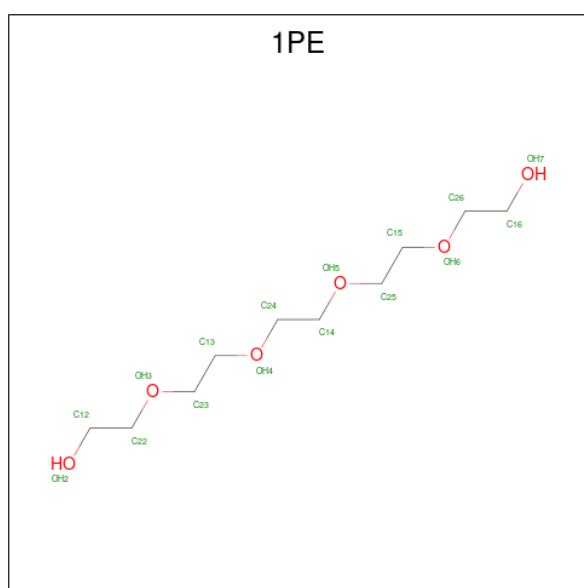
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	0	1
			4263	2731	725	785	22			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



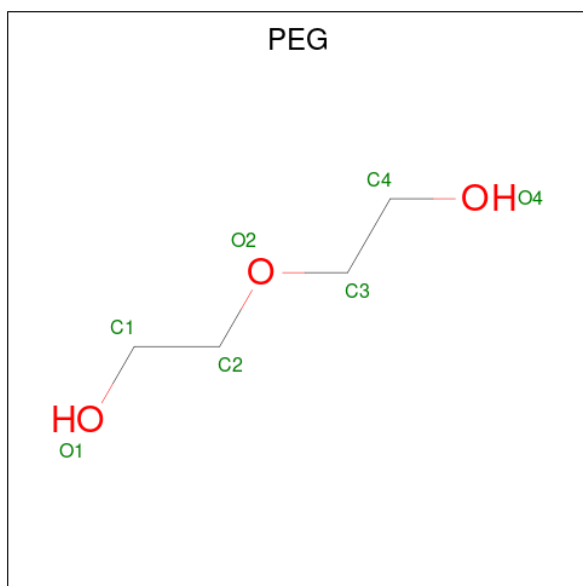
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



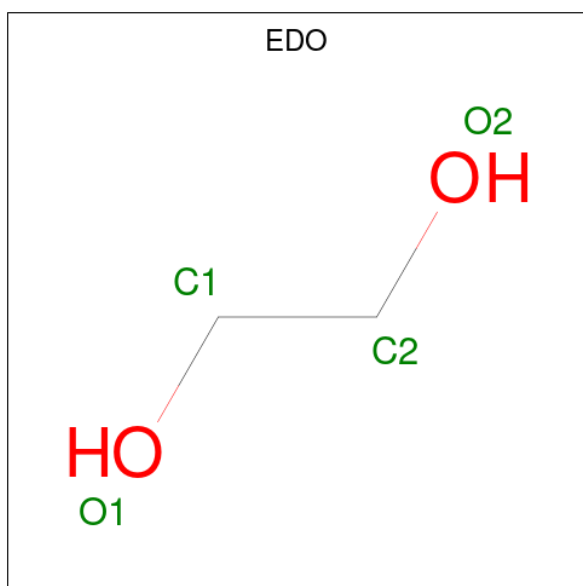
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



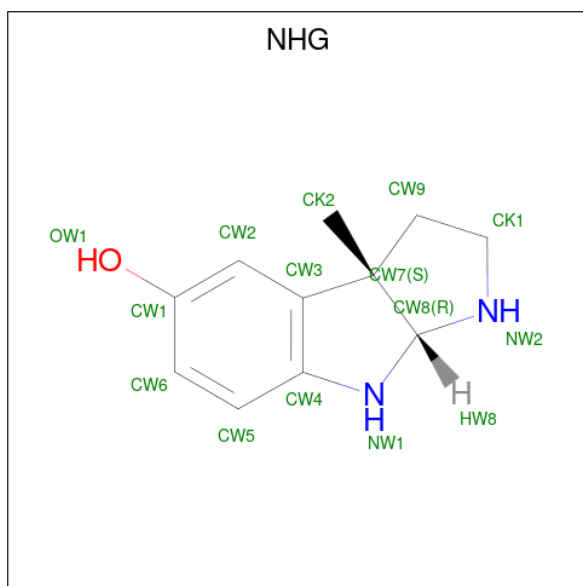
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



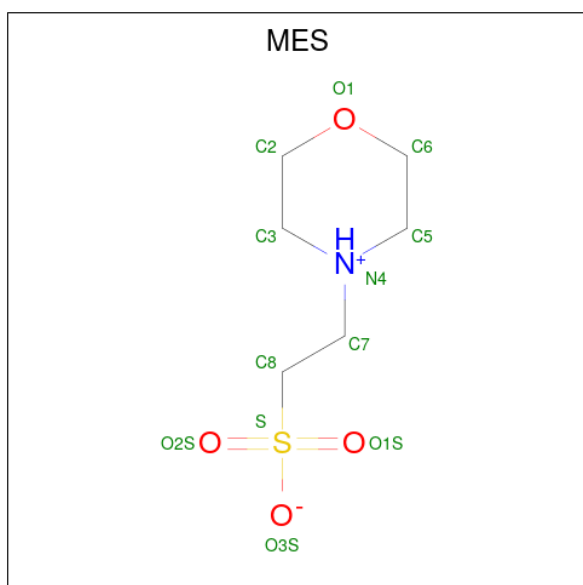
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is BIS-NORESEROLINE (CCD ID: NHG) (formula: $C_{11}H_{14}N_2O$).



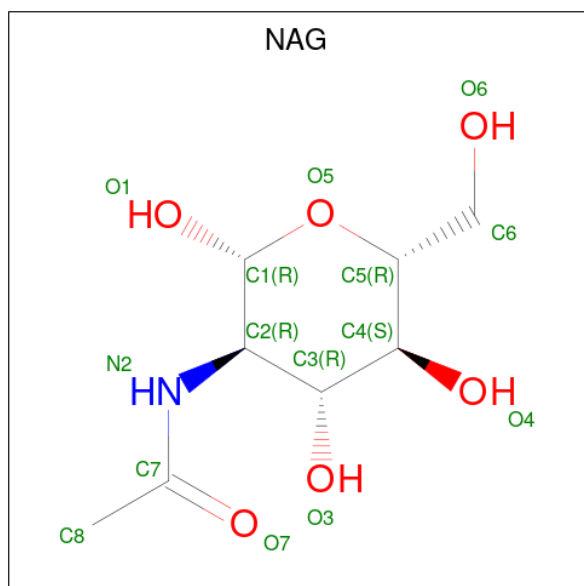
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	11	2	1		

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	11	Total	Cl	0	0
			11	11		

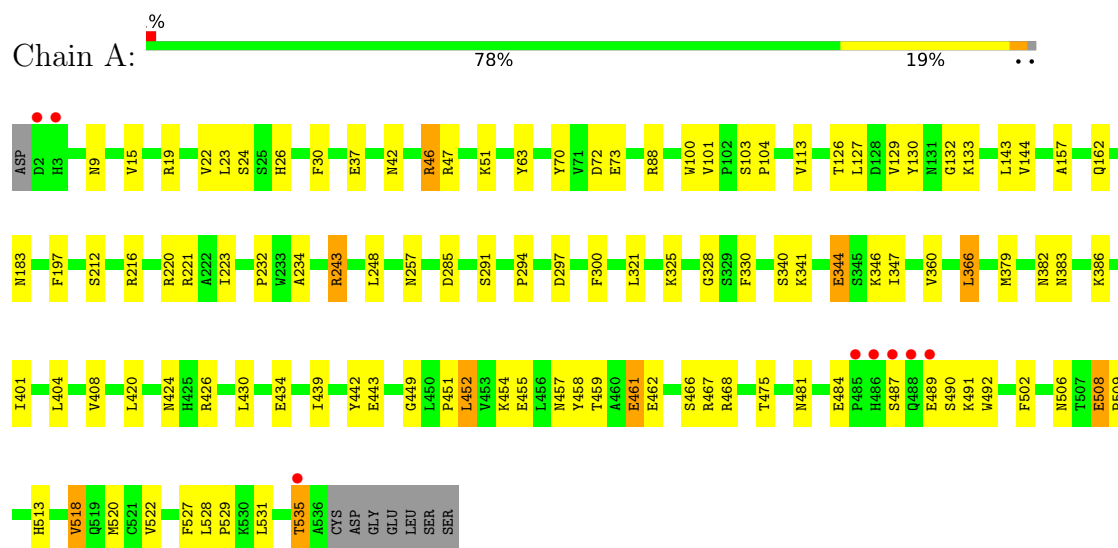
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	300	Total	O	0	0
			300	300		

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 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	111.01Å 111.01Å 137.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.21 – 2.26 29.21 – 2.26	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.21-2.26) 98.7 (29.21-2.26)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.26Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.206 , 0.247 0.201 , 0.238	Depositor DCC
R_{free} test set	4611 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.646	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4669	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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: EDO, CL, MES, 1PE, PEG, NHG, NAG

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	0.57	1/4387 (0.0%)	1.03	27/5957 (0.5%)

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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	535	THR	C-N	-5.28	1.25	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	439	ILE	N-CA-C	9.87	122.93	109.80
1	A	291	SER	N-CA-C	7.97	119.66	110.97
1	A	285	ASP	N-CA-C	-7.48	97.80	109.25
1	A	216	ARG	N-CA-C	6.78	119.25	111.11
1	A	522	VAL	N-CA-C	-6.70	103.96	110.72
1	A	457	ASN	N-CA-C	6.65	120.84	111.92
1	A	527	PHE	N-CA-C	6.50	118.24	111.03
1	A	443	GLU	N-CA-C	-6.45	105.56	113.50
1	A	401	ILE	N-CA-C	6.32	116.43	110.30
1	A	157	ALA	N-CA-C	6.28	119.20	108.02
1	A	360	VAL	CA-C-N	6.06	126.50	119.47
1	A	360	VAL	C-N-CA	6.06	126.50	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	GLY	N-CA-C	5.87	121.93	114.66
1	A	347	ILE	N-CA-C	5.82	117.39	108.71
1	A	492	TRP	N-CA-C	-5.78	97.97	109.60
1	A	297	ASP	N-CA-C	5.70	120.23	113.28
1	A	344	GLU	N-CA-C	-5.48	106.43	113.01
1	A	379	MET	N-CA-C	-5.48	106.60	113.28
1	A	101	VAL	N-CA-C	5.47	113.85	107.89
1	A	341	LYS	N-CA-C	5.47	117.24	111.28
1	A	325	LYS	N-CA-C	5.43	117.20	111.28
1	A	257	ASN	N-CA-C	5.22	117.71	111.71
1	A	248	LEU	N-CA-C	-5.18	105.53	111.07
1	A	424	ASN	N-CA-C	5.14	116.61	110.44
1	A	72	ASP	N-CA-C	5.10	116.57	108.67
1	A	518	VAL	CB-CA-C	-5.07	105.39	111.88
1	A	183	ASN	N-CA-C	5.04	121.17	113.61

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	442	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4263	0	4107	61	0
2	B	28	0	25	0	0
3	A	16	0	22	2	0
4	A	7	0	10	1	0
5	A	4	0	6	0	0
6	A	14	0	13	0	0
7	A	12	0	13	1	0
8	A	14	0	13	0	0
9	A	11	0	0	3	0
10	A	300	0	0	6	0
All	All	4669	0	4209	62	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 (62) 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:46:ARG:HH11	1:A:46:ARG:HB3	1.29	0.96
1:A:46:ARG:HB3	1:A:46:ARG:NH1	2.00	0.76
1:A:243:ARG:NH2	9:A:1552:CL:CL	2.60	0.72
1:A:455:GLU:CD	1:A:455:GLU:H	2.00	0.70
1:A:484:GLU:HB3	1:A:487:SER:HB2	1.73	0.70
1:A:37:GLU:OE2	1:A:51:LYS:HD2	1.93	0.68
1:A:88:ARG:HH11	1:A:88:ARG:HG2	1.60	0.66
1:A:9:ASN:ND2	7:A:1542:MES:H72	2.10	0.66
1:A:46:ARG:HH11	1:A:46:ARG:CB	2.08	0.64
1:A:19:ARG:HH21	1:A:26:HIS:HB2	1.64	0.63
1:A:19:ARG:NH2	1:A:26:HIS:HB2	2.17	0.60
1:A:366:LEU:HD12	1:A:535:THR:HG21	1.83	0.59
1:A:127:LEU:HD12	1:A:130:TYR:CE2	2.38	0.59
1:A:88:ARG:HG2	1:A:88:ARG:NH1	2.20	0.57
1:A:452:LEU:HD13	1:A:467:ARG:NH2	2.19	0.57
1:A:19:ARG:HD2	10:A:2010:HOH:O	2.05	0.56
1:A:487:SER:HB3	1:A:491:LYS:NZ	2.21	0.56
1:A:426:ARG:CZ	1:A:430:LEU:HD23	2.36	0.56
1:A:434:GLU:HG2	10:A:2257:HOH:O	2.08	0.54
1:A:63:TYR:CD1	1:A:126:THR:HG22	2.43	0.54
1:A:531:LEU:C	1:A:531:LEU:HD23	2.33	0.53
1:A:404:LEU:O	1:A:408:VAL:HG23	2.08	0.53
1:A:42:ASN:O	1:A:46:ARG:HD2	2.08	0.53
1:A:22:VAL:HG22	1:A:133:LYS:HD2	1.90	0.53
1:A:508:GLU:HG3	1:A:509:PRO:HD2	1.91	0.52
1:A:47:ARG:NH1	1:A:162:GLN:OE1	2.36	0.52
1:A:344:GLU:OE1	1:A:346:LYS:HE3	2.09	0.51
1:A:232:PRO:HA	4:A:1538:PEG:H31	1.93	0.51
1:A:430:LEU:HD12	9:A:1553:CL:CL	2.50	0.49
1:A:426:ARG:NH2	1:A:430:LEU:HD23	2.28	0.48
1:A:234:ALA:O	1:A:294:PRO:HD2	2.13	0.48
1:A:321:LEU:HD11	1:A:408:VAL:HG22	1.95	0.48
1:A:197:PHE:HB3	1:A:223:ILE:HB	1.96	0.48
1:A:197:PHE:CB	1:A:223:ILE:HB	2.44	0.48
1:A:451:PRO:HA	1:A:458:TYR:CD1	2.49	0.48
1:A:70:TYR:HE1	3:A:1537:1PE:H122	1.79	0.48
1:A:113:VAL:HG22	1:A:144:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:SER:HB2	1:A:300:PHE:CE1	2.50	0.47
9:A:1555:CL:CL	10:A:2083:HOH:O	2.58	0.47
1:A:420:LEU:HD23	1:A:502:PHE:HB3	1.98	0.46
1:A:487:SER:HB3	1:A:491:LYS:HZ1	1.81	0.46
1:A:502:PHE:CZ	1:A:513:HIS:HB2	2.50	0.46
1:A:452:LEU:HD13	1:A:467:ARG:CZ	2.46	0.45
1:A:383:ASN:HB3	1:A:386:LYS:HB2	2.00	0.44
1:A:19:ARG:HE	1:A:26:HIS:CB	2.31	0.43
1:A:23:LEU:O	1:A:24:SER:HB2	2.19	0.43
1:A:220:ARG:HG3	1:A:221:ARG:HG3	2.01	0.43
1:A:70:TYR:CE1	3:A:1537:1PE:H122	2.53	0.43
1:A:132:GLY:HA3	1:A:143:LEU:HD12	2.00	0.42
1:A:449:GLY:HA2	1:A:466:SER:OG	2.18	0.42
1:A:468:ARG:HD3	10:A:2269:HOH:O	2.20	0.42
1:A:506:ASN:HB2	10:A:2254:HOH:O	2.18	0.42
1:A:520:MET:HG2	10:A:2292:HOH:O	2.20	0.42
1:A:475:THR:HG22	1:A:481:ASN:O	2.19	0.42
1:A:455:GLU:CD	1:A:455:GLU:N	2.74	0.42
1:A:461:GLU:CD	1:A:461:GLU:H	2.28	0.41
1:A:528:LEU:N	1:A:529:PRO:HD2	2.36	0.41
1:A:15:VAL:HG12	1:A:30:PHE:HD2	1.86	0.40
1:A:100:TRP:CE3	1:A:143:LEU:HD12	2.56	0.40
1:A:459:THR:OG1	1:A:462:GLU:HG3	2.20	0.40
1:A:103:SER:HA	1:A:104:PRO:C	2.46	0.40
1:A:454:LYS:HB3	1:A:455:GLU:OE2	2.21	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	533/543 (98%)	502 (94%)	31 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	467/474 (98%)	453 (97%)	14 (3%)	36 45

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ARG
1	A	73	GLU
1	A	129	VAL
1	A	243	ARG
1	A	330	PHE
1	A	340	SER
1	A	366	LEU
1	A	382	ASN
1	A	452	LEU
1	A	461	GLU
1	A	489	GLU
1	A	490	SER
1	A	508	GLU
1	A	518	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	66	ASN
1	A	131	ASN
1	A	374	GLN
1	A	500	GLN
1	A	519	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	B	1	2,1	14,14,15	0.68	0	17,19,21	0.62	0
2	NAG	B	2	2	14,14,15	0.64	0	17,19,21	1.03	1 (5%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C2-N2-C7	-2.59	119.42	122.90

There are no chirality outliers.

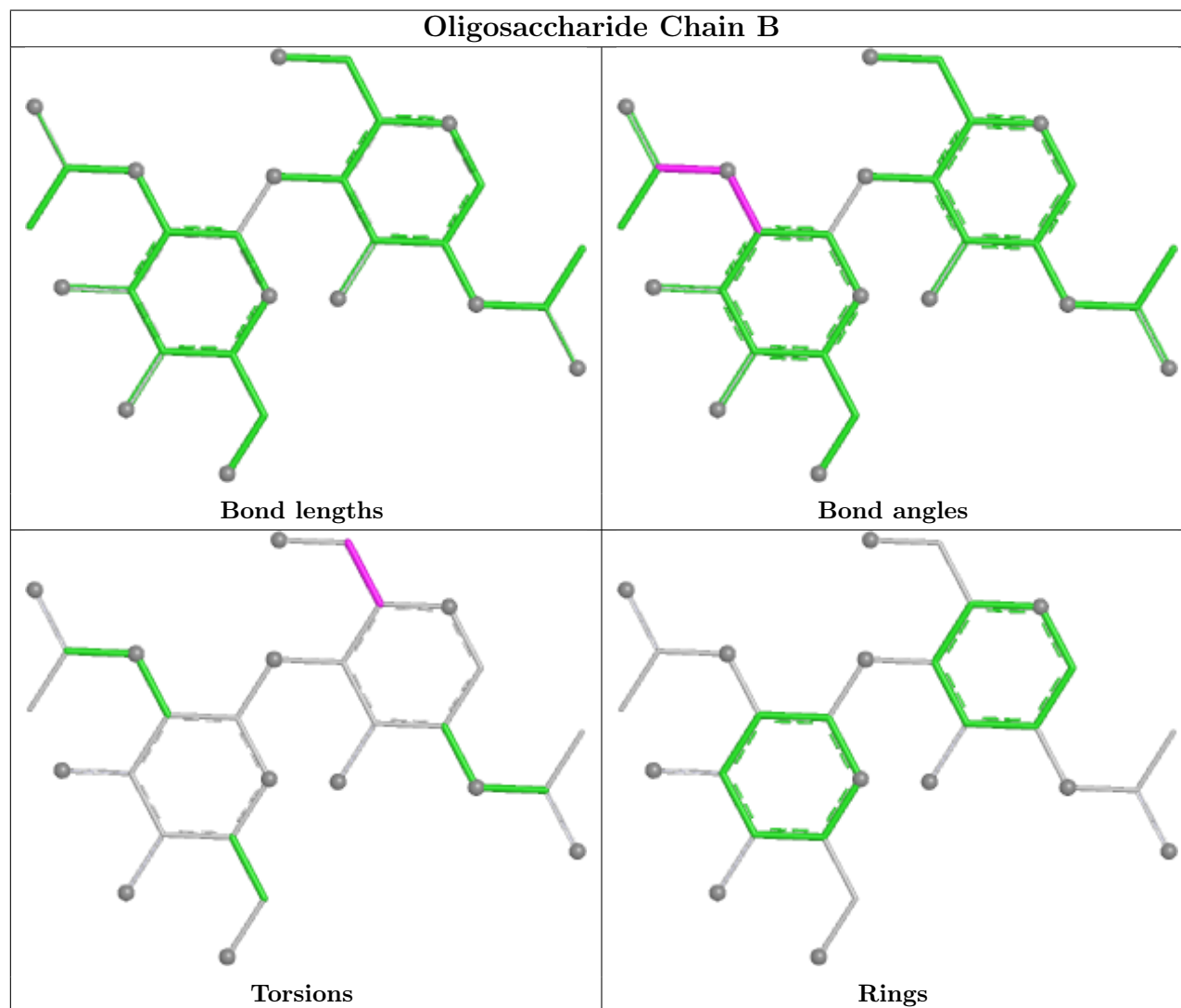
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6

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 ⓘ

Of 17 ligands modelled in this entry, 11 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	A	1544	1	14,14,15	0.84	0	17,19,21	1.05	1 (5%)
4	PEG	A	1538	-	6,6,6	0.54	0	5,5,5	0.42	0
7	MES	A	1542	-	12,12,12	1.47	1 (8%)	15,16,16	1.16	0
5	EDO	A	1540	-	3,3,3	0.44	0	2,2,2	0.39	0
3	1PE	A	1537	-	15,15,15	0.54	0	14,14,14	0.41	0
6	NHG	A	1541	-	15,16,16	1.27	2 (13%)	21,25,25	1.56	3 (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
8	NAG	A	1544	1	-	1/6/23/26	0/1/1/1
4	PEG	A	1538	-	-	0/4/4/4	-
7	MES	A	1542	-	-	0/6/14/14	0/1/1/1
5	EDO	A	1540	-	-	0/1/1/1	-
3	1PE	A	1537	-	-	1/13/13/13	-
6	NHG	A	1541	-	-	-	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1542	MES	C8-S	4.05	1.83	1.77
6	A	1541	NHG	CW4-NW1	-3.73	1.33	1.39
6	A	1541	NHG	CW8-NW1	2.35	1.47	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1541	NHG	NW1-CW8-NW2	-4.96	110.61	114.39
6	A	1541	NHG	CW5-CW4-CW3	-3.10	119.02	121.92
8	A	1544	NAG	C2-N2-C7	-2.83	119.11	122.90
6	A	1541	NHG	CW4-NW1-CW8	2.38	112.22	108.92

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1544	NAG	O5-C5-C6-O6
3	A	1537	1PE	OH5-C14-C24-OH4

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1538	PEG	1	0
7	A	1542	MES	1	0
3	A	1537	1PE	2	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	535/543 (98%)	-0.17	8 (1%) 72 73	27, 44, 65, 85	7 (1%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	HIS	10.5
1	A	485	PRO	9.8
1	A	487	SER	9.4
1	A	486	HIS	8.1
1	A	488	GLN	7.4
1	A	489	GLU	7.3
1	A	2	ASP	6.6
1	A	535	THR	3.3

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

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

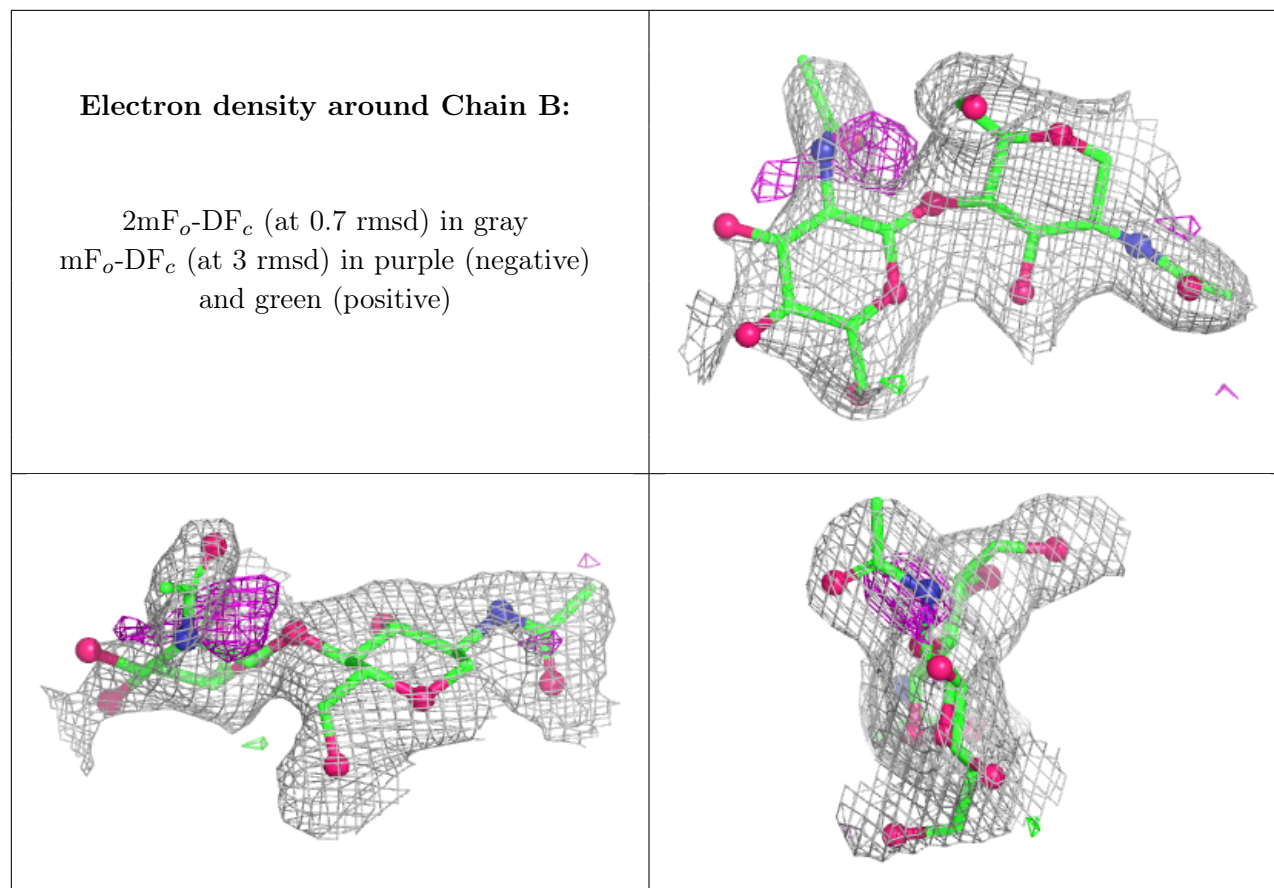
6.3 Carbohydrates [i](#)

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	NAG	B	2	14/15	0.70	0.14	65,88,98,99	0
2	NAG	B	1	14/15	0.89	0.09	46,62,71,81	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. 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
7	MES	A	1542	12/12	0.72	0.46	40,49,64,71	12
8	NAG	A	1544	14/15	0.73	0.16	70,83,91,94	0
9	CL	A	1554	1/1	0.79	0.52	73,73,73,73	1
9	CL	A	1553	1/1	0.83	0.25	59,59,59,59	1
9	CL	A	1552	1/1	0.83	0.13	48,48,48,48	1
3	1PE	A	1537	16/16	0.86	0.20	59,77,82,84	0
4	PEG	A	1538	7/7	0.86	0.14	58,62,66,70	0
9	CL	A	1547	1/1	0.86	0.33	56,56,56,56	1
9	CL	A	1548	1/1	0.87	0.31	58,58,58,58	1
9	CL	A	1551	1/1	0.89	0.35	64,64,64,64	1
5	EDO	A	1540	4/4	0.89	0.20	53,55,55,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	CL	A	1550	1/1	0.90	0.31	52,52,52,52	1
9	CL	A	1549	1/1	0.91	0.46	64,64,64,64	1
9	CL	A	1545	1/1	0.93	0.39	42,42,42,42	1
9	CL	A	1555	1/1	0.93	0.25	63,63,63,63	1
9	CL	A	1546	1/1	0.95	0.12	47,47,47,47	1
6	NHG	A	1541	14/14	0.96	0.07	34,43,45,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.