

Full wwPDB X-ray Structure Validation Report (i)

Apr 17, 2021 – 08:09 am BST

PDB ID : 7B8E

Title: Torpedo californica acetylcholinesterase complexed with Ca+2

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Deposited on : 2020-12-12

Resolution : 2.23 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 (i) symbol.

The following versions of software and data (see references (1)) 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 : 2.18 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)

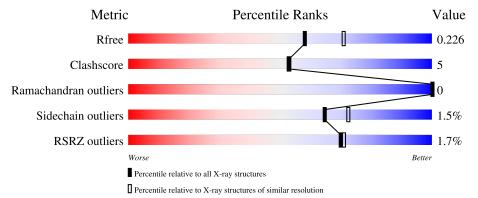
 $Validation\ Pipeline\ (wwPDB-VP) \quad : \quad 2.18$

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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	$egin{aligned} ext{Whole archive} \ (\# ext{Entries}) \end{aligned}$	Similar resolution $(\# \mathrm{Entries}, \mathrm{resolution} \mathrm{range}(\mathring{\mathrm{A}}))$
R_{free}	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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 <=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	Λ	537	2%		120/			
1	А	557	86%		12%	•		
2	E	2	50%	50%				
3	F	2	10	0%				



2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 4590 atoms, of which 6 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	${f Atoms}$			ZeroOcc	AltConf	Trace		
1	Λ	532	Total	С	N	О	S	0	9	0
1	A	952	4244	2725	717	779	23	0	3	0

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



Mol	Chain	Residues	${f Atoms}$				ZeroOcc	AltConf	Trace
2	Е	2	Total 28	C 16	N 2	O 10	0	0	0

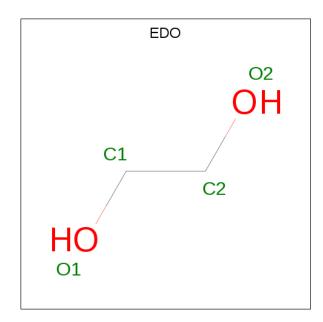
• Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-bet a-D-glucopyranose.



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

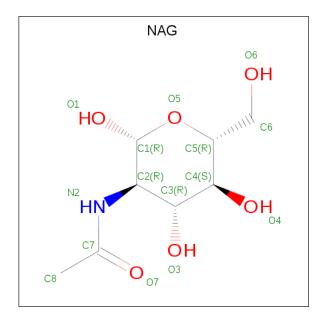
• Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C H O 10 2 6 2	0	0

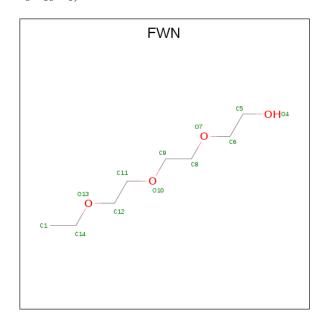
 \bullet Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $\rm C_8H_{15}NO_6).$





Mol	Chain	Residues	A	tor	ns		ZeroOcc	AltConf
5	Δ	1	Total	С	N	О	0	n
	11		14	8	1	5		

• Molecule 6 is 2-[2-(2-ethoxyethoxy)ethoxy]ethanol (three-letter code: FWN) (formula: $C_8H_{18}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 12 8 4	0	0

• Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0

• Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Zn 1 1	0	0

• Molecule 9 is water.



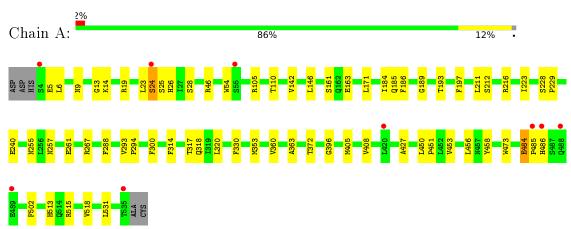
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	248	Total O 248 248	0	0



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

Chain E: 50% 50%

NAG1 NAG2

• Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants	139.07Å 139.07Å 71.32Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.96 - 2.23	Depositor
Resolution (A)	19.96 - 2.23	EDS
% Data completeness	99.5 (19.96-2.23)	Depositor
(in resolution range)	99.5 (19.96-2.23)	EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.32 (at 2.23Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472, REFMAC 5.8.0258	Depositor
P. P.	0.179 , 0.226	Depositor
R, R_{free}	0.179 , 0.226	DCC
R_{free} test set	1913 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33 , 41.3	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4590	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $< L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: EDO, NAG, FUC, FWN, ZN, CA

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).

Mal	Chain	Bond	lengths	Bond angles		
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.46	0/4373	0.57	0/5940	

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 (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	4244	0	4080	45	1
2	E	28	0	25	0	0
3	F	24	0	22	0	0
4	A	12	6	18	1	0
5	A	14	0	13	1	0
6	A	12	0	0	0	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	248	0	0	2	0
All	All	4584	6	4158	46	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.



All (46) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance}({f \AA})$	overlap (Å)
1:A:484:GLU:HG3	1:A:485:PRO:HD2	1.47	0.94
1:A:110:THR:HG23	1:A:193:THR:HG22	1.61	0.81
1:A:453:VAL:HB	1:A:456:LEU:HD12	1.81	0.62
1:A:228:SER:HB2	1:A:229:PRO:HD2	1.85	0.59
1:A:9:ASN:OD1	1:A:14:LYS:HG2	2.02	0.58
1:A:405:MET:HA	1:A:408:VAL:HG12	1.85	0.56
1:A:46:ARG:HD2	1:A:163:GLU:OE1	2.04	0.56
1:A:211:LEU:HD23	1:A:314:PHE:HB3	1.87	0.56
5:A:604:NAG:O7	5:A:604:NAG:O3	2.18	0.55
1:A:240:GLU:HB2	4:A:603:EDO:H21	1.88	0.54
1:A:257:ASN:OD1	1:A:261:GLU:HG3	2.07	0.54
1:A:142:VAL:HG11	1:A:184:ILE:HD11	1.89	0.54
1:A:451:PRO:HA	1:A:458:TYR:CD1	2.43	0.54
1:A:484:GLU:HG3	1:A:485:PRO:CD	2.32	0.52
1:A:502:PHE:CZ	1:A:513:HIS:HB2	2.45	0.51
1:A:185:GLN:HG2	1:A:186:PHE:H	1.75	0.51
1:A:531:LEU:C	1:A:531:LEU:HD23	2.33	0.49
1:A:450:LEU:O	1:A:456:LEU:HD12	2.12	0.49
1:A:110:THR:HG23	1:A:193:THR:CG2	2.38	0.48
1:A:163:GLU:HB3	1:A:267:ARG:HH22	1.79	0.48
1:A:23:LEU:O	1:A:24:SER:HB3	2.14	0.48
1:A:293:VAL:HB	1:A:294:PRO:HD2	1.97	0.47
1:A:515:ARG:HB3	1:A:518:VAL:HB	1.97	0.46
1:A:13:GLY:HA3	1:A:54:TRP:CE2	2.51	0.46
1:A:360:VAL:HG12	1:A:363:ALA:HB2	1.97	0.46
1:A:25:SER:OG	1:A:26:HIS:N	2.49	0.45
1:A:5:GLU:HA	1:A:105:ARG:HH21	1.82	0.45
1:A:257:ASN:ND2	1:A:257:ASN:H	2.15	0.45
1:A:212:SER:O	1:A:216:ARG:HG3	2.17	0.45
1:A:255:ASN:HB3	1:A:257:ASN:HD21	1.82	0.44
1:A:185:GLN:HA	1:A:189:GLY:O	2.18	0.44
1:A:257:ASN:H	1:A:257:ASN:HD22	1.65	0.44
1:A:212:SER:HB2	1:A:300:PHE:CE1	2.53	0.44
1:A:223:ILE:HA	1:A:320:LEU:O	2.18	0.44
1:A:453:VAL:HB	1:A:456:LEU:CD1	2.46	0.43
1:A:396:GLY:HA3	9:A:877:HOH:O	2.19	0.43
1:A:185:GLN:HG2	1:A:186:PHE:N	2.34	0.43
1:A:255:ASN:HB3	1:A:257:ASN:ND2	2.34	0.43
1:A:146:LEU:C	1:A:146:LEU:HD12	2.39	0.42
1:A:6:LEU:CD2	1:A:28:SER:HB3	2.49	0.41

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Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance} ({f \AA})$	overlap (Å)
1:A:171:LEU:HD23	1:A:171:LEU:HA	1.89	0.41
1:A:317:THR:OG1	1:A:318:GLN:N	2.54	0.41
1:A:6:LEU:HD11	1:A:19:ARG:HB2	2.03	0.41
1:A:427:ALA:HB2	9:A:844:HOH:O	2.20	0.41
1:A:353[B]:MET:HE1	1:A:372:THR:CG2	2.51	0.40
1:A:353[B]:MET:HE1	1:A:372:THR:HG21	2.04	0.40

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

Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{aligned}$	$egin{array}{c} { m Clash} \ { m overlap} \ ({ m \AA}) \end{array}$
1:A:484:GLU:OE1	1:A:486:HIS:CD2[4_556]	2.12	0.08

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	533/537 (99%)	506 (95%)	27 (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	Analysed Rotameric Ou		Percentiles
1	A	462/469 (98%)	455 (98%)	7 (2%)	65 72

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	SER
1	A	161	SER
1	A	197	PHE
1	A	288	PHE
1	A	330	PHE
1	A	473	TRP
1	A	484	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

4 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		Bo	Bond lengths			ond ang	les
MIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	Е	1	2,1	14,14,15	0.72	1 (7%)	17,19,21	0.51	0
2	NAG	E	2	2	14,14,15	0.35	0	17,19,21	0.43	0
3	NAG	F	1	3,1	14,14,15	0.58	0	17,19,21	0.52	0
3	FUC	F	2	3	10,10,11	0.90	0	14,14,16	0.84	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	Ε	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Ε	2	2	-	0/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	FUC	F	2	3	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\mathbf{Ideal}(exttt{\AA})$
2	Ε	1	NAG	O5-C1	2.31	1.47	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	${f Bond\ lengths}$			Bond angles		
				nes	LIIIK	Counts	RMSZ	RMSZ	# Z > 2		
	4	EDO	A	603	_	3,3,3	0.69	0	2,2,2	0.23	0
	6	FWN	A	605	_	11,11,11	0.19	0	10,10,10	0.25	0



Mol	Type	Chain	Res	Link	Bo	Bond lengths			Bond angles		
			nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
4	EDO	A	601	_	3,3,3	0.58	0	2,2,2	0.14	0	
5	NAG	A	604	1	14,14,15	0.54	0	17,19,21	0.45	0	
4	EDO	A	602	-	3,3,3	0.57	0	2,2,2	0.22	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
4	EDO	A	603	_	-	1/1/1/1	-
6	FWN	A	605	_	-	1/9/9/9	-
4	EDO	A	601	_	-	0/1/1/1	-
5	NAG	A	604	1	-	2/6/23/26	0/1/1/1
4	EDO	A	602	_	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	604	NAG	C1-C2-N2-C7
4	A	603	EDO	O1-C1-C2-O2
5	A	604	NAG	C3-C2-N2-C7
6	A	605	FWN	O10-C11-C12-O13

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	EDO	1	0
5	A	604	NAG	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, 95^{th} 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 $>$	$\#\mathrm{RSRZ}{>}2$		$OWAB(A^2)$	Q < 0.9	
1	A	532/537 (99%)	-0.28	9 (1%)	70	71	26, 41, 62, 79	0

All (9) RSRZ outliers are listed below:

Mol	Chain	$f hain \mid Res \mid Type$		RSRZ	
1	A	535	THR	4.4	
1	A	489	GLU	3.4	
1	A	24	SER	3.0	
1	A	4	SER	3.0	
1	A	486	HIS	2.7	
1	A	55	SER	2.5	
1	A	420	LEU	2.3	
1	A	488	GLN	2.2	
1	A	485	PRO	2.1	

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	${f B-factors}({f \AA}^2)$	Q<0.9
2	NAG	Ε	2	14/15	0.85	0.52	84,90,93,93	0
3	NAG	F	1	14/15	0.88	0.28	62,73,81,82	0
2	NAG	Ε	1	14/15	0.91	0.25	47,62,72,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B\text{-factors}}({f \AA}^2)$	Q < 0.9
3	FUC	F	2	10/11	0.92	0.36	80,90,91,94	0

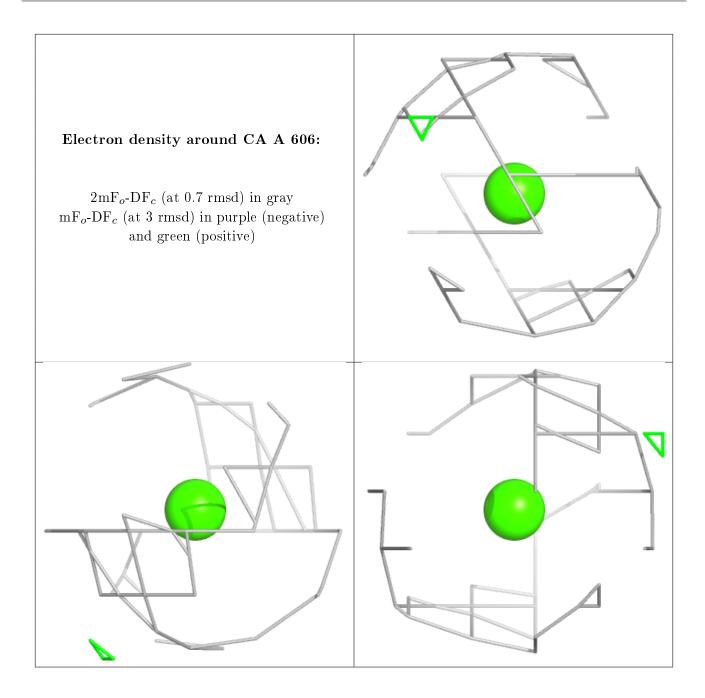
6.4 Ligands (i)

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, 95^{th} 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	$ extbf{B-factors}(extbf{A}^2)$	Q < 0.9
4	EDO	A	603	4/4	0.69	0.39	50,60,66,71	0
4	EDO	A	602	4/4	0.81	0.29	58,60,66,69	0
4	EDO	A	601	4/4	0.85	0.34	52,53,56,58	0
6	FWN	A	605	12/12	0.88	0.15	45,51,54,62	0
5	NAG	A	604	14/15	0.90	0.43	82,89,93,95	0
8	ZN	A	607	1/1	0.98	0.04	65,65,65,65	0
7	CA	A	606	1/1	0.99	0.03	46,46,46,46	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.

