wwPDB X-ray Structure Validation Summary Report (i)

Feb 27, 2014 – 10:59 AM GMT

PDB ID	:	2WIK
Title	:	NONAGED FORM OF HUMAN BUTYRYLCHOLINESTERASEINHIB-ITED BY TABUN ANALOGUE TA6
Authors	:	Carletti, E.; Aurbek, N.; Gillon, E.; Loiodice, M.; Nicolet, Y.; Fontecilla, J.; Masson, P.; Thiermann, H.; Nachon, F.; Worek, F.
Deposited on	:	2009-05-12
Resolution	:	2.10 Å(reported)

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

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 2.10 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	Percentile Ranks	Value
Rfree		0.276
Clashscore		19
Ramachandran outliers		2.3%
Sidechain outliers		8.2%
RSRZ outliers		1.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
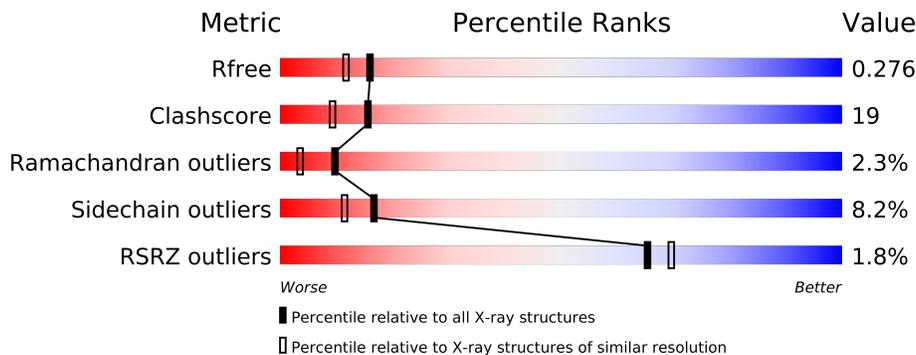
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	529	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	CL	A	1536	-	X
4	SO4	A	1532	-	X
4	SO4	A	1535	-	X
8	NAG	A	1542	-	X
8	NAG	A	1543	-	X
8	NAG	A	1544	-	X

WORLDWIDE wwPDB PROTEIN DATA BANK

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 4754 atoms, of which 0 are hydrogen and 0 are deuterium.

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 CHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total 4205	C 2713	N 709	O 768	S 15	0	2	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	455	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	481	GLN	ASN	ENGINEERED MUTATION	UNP P06276

- Molecule 2 is ETHYL HYDROGEN PROPYLAMIDOPHOSPHATE (three-letter code: TC5) (formula: $C_5H_{14}NO_3P$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 9	C 5	N 1	O 2	P 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	Cl 3	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
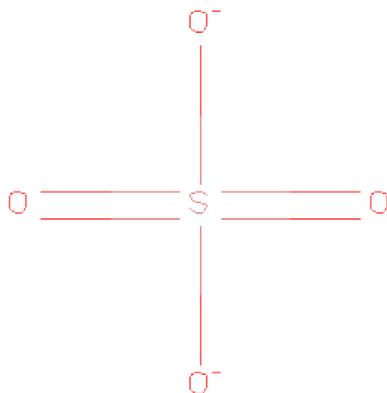
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	O 4	S 1	0	0
4	A	1	Total 5	O 4	S 1	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Na 1	0	0

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	3	Total 38	C 22	N 2	O 14	0	0
6	A	3	Total 38	C 22	N 2	O 14	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	455	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	481	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	17	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	455	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	481	GLN	ASN	ENGINEERED MUTATION	UNP P06276

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	455	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	481	GLN	ASN	ENGINEERED MUTATION	UNP P06276

- Molecule 8 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
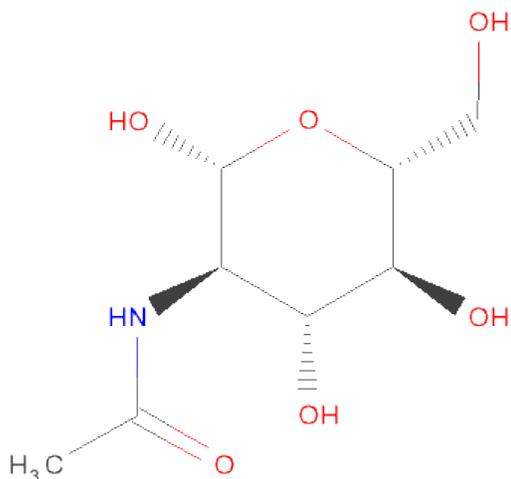
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	384	Total	O	0	0
			384	384		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: CHOLINESTERASE

Chain A:
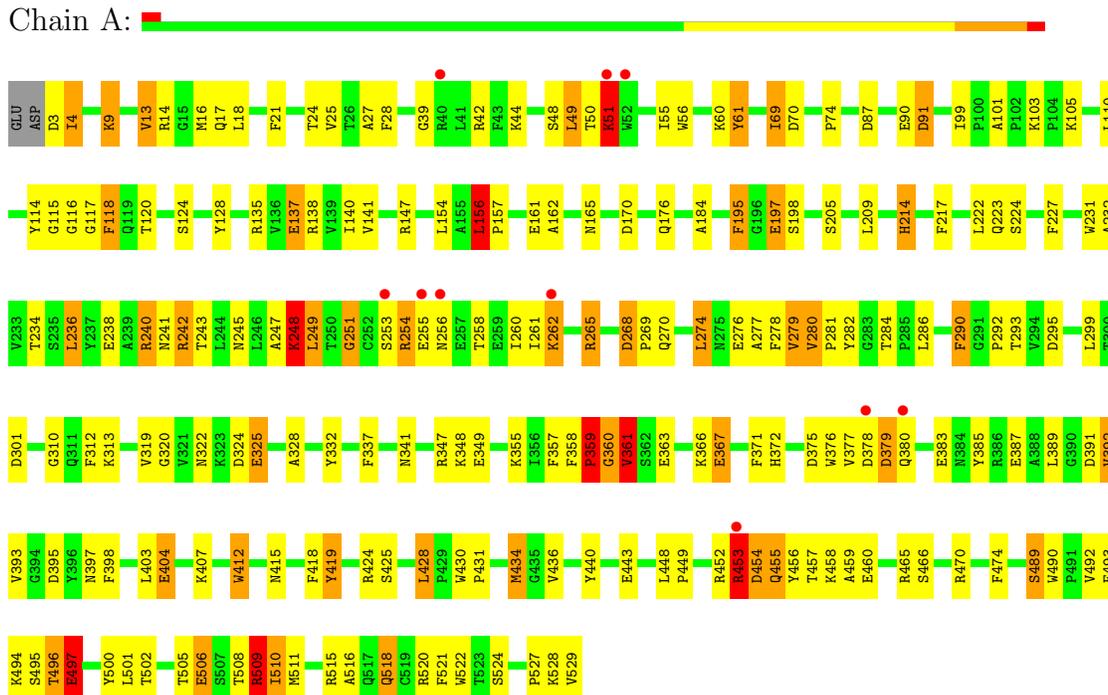
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	155.24Å 155.24Å 127.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.05 – 2.10 55.05 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (55.05-2.10) 99.7 (55.05-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.213 , 0.276 0.213 , 0.276	Depositor DCC
R_{free} test set	1358 reflections (3.09%)	DCC
Wilson B-factor (Å^2)	27.3	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 55.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Outliers	0 of 45255 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4754	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CL, NA, TC5, SO4, FUL

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	1.59	45/4330 (1.0%)	1.36	36/5879 (0.6%)

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	1	1

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	367	GLU	CG-CD	10.03	1.67	1.51
1	A	398	PHE	CE2-CZ	9.74	1.55	1.37
1	A	419	TYR	CD1-CE1	8.64	1.52	1.39
1	A	371	PHE	CE1-CZ	8.53	1.53	1.37
1	A	118	PHE	CE2-CZ	7.85	1.52	1.37

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	A	509	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	A	170	ASP	CB-CG-OD1	8.33	125.80	118.30
1	A	520	ARG	NE-CZ-NH1	-8.18	116.21	120.30
1	A	242	ARG	NE-CZ-NH2	-8.11	116.25	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	361	VAL	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	GLY	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4205	0	4104	158	1
2	A	9	0	13	2	0
3	A	3	0	0	1	0
4	A	10	0	0	1	0
5	A	1	0	0	0	0
6	A	76	0	68	0	0
7	A	24	0	22	0	0
8	A	42	0	39	1	0
9	A	384	0	0	37	0
All	All	4754	0	4246	160	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

The worst 5 of 160 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:495:SER:HA	9:A:2331:HOH:O	1.36	1.21
1:A:176:GLN:HB3	9:A:2147:HOH:O	1.01	1.16
1:A:50:THR:HG21	9:A:2053:HOH:O	1.41	1.16
1:A:4:ILE:N	1:A:4:ILE:HD12	1.51	1.14
1:A:4:ILE:H	1:A:4:ILE:HD12	0.92	1.07

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	Distance(Å)	Clash(Å)
1:A:367:GLU:OE1	1:A:367:GLU:OE1[5_555]	2.17	0.03

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	527/529 (100%)	475 (90%)	40 (8%)	12 (2%)	10	3

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	248	LYS
1	A	379	ASP
1	A	496	THR
1	A	249	LEU

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	452/454 (100%)	415 (92%)	37 (8%)	17	11

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	265	ARG
1	A	299	LEU
1	A	509	ARG
1	A	274	LEU
1	A	280	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	289	ASN
1	A	380	GLN
1	A	518	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

8 carbohydrates 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	NAG	A	1537	1,6	12,14,15	1.56	2 (16%)	15,19,21	2.84	10 (66%)
6	NAG	A	1538	6	12,14,15	0.65	0	15,19,21	3.28	8 (53%)
6	FUL	A	1539	6	9,10,11	1.47	2 (22%)	10,14,16	3.17	4 (40%)
7	NAG	A	1540	1,7	12,14,15	1.36	2 (16%)	15,19,21	3.35	7 (46%)
7	FUL	A	1541	7	9,10,11	1.06	1 (11%)	10,14,16	2.22	3 (30%)
6	NAG	A	1545	1,6	12,14,15	1.25	1 (8%)	15,19,21	2.47	5 (33%)
6	NAG	A	1546	6	12,14,15	1.33	2 (16%)	15,19,21	1.88	4 (26%)
6	FUL	A	1547	6	9,10,11	1.24	1 (11%)	10,14,16	2.54	4 (40%)

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	NAG	A	1537	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1538	6	-	0/6/23/26	0/1/1/1
6	FUL	A	1539	6	-	0/0/17/20	0/1/1/1
7	NAG	A	1540	1,7	-	0/6/23/26	0/1/1/1
7	FUL	A	1541	7	-	0/0/17/20	0/1/1/1
6	NAG	A	1545	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1546	6	-	0/6/23/26	0/1/1/1
6	FUL	A	1547	6	-	0/0/17/20	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1537	NAG	C2-N2	-3.93	1.41	1.46
6	A	1547	FUL	O5-C5	-2.97	1.39	1.45
6	A	1545	NAG	C2-N2	2.71	1.49	1.46
7	A	1540	NAG	C3-C2	2.69	1.58	1.52
6	A	1539	FUL	C4-C5	2.67	1.58	1.52

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1540	NAG	O5-C5-C6	8.82	116.23	106.98
6	A	1538	NAG	C3-C4-C5	-7.81	96.26	110.20
6	A	1539	FUL	C6-C5-C4	6.04	122.87	113.06
6	A	1539	FUL	C3-C4-C5	5.94	119.74	109.84
6	A	1538	NAG	O6-C6-C5	-5.77	91.49	111.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 4 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	#$|Z| > 2$
2	TC5	A	1530	1	5,8,9	0.82	0	5,8,11	1.70	1 (20%)
4	SO4	A	1532	-	4,4,4	0.26	0	6,6,6	0.38	0
4	SO4	A	1535	-	4,4,4	0.42	0	6,6,6	0.91	1 (16%)
8	NAG	A	1542	1	12,14,15	0.93	0	15,19,21	2.28	5 (33%)
8	NAG	A	1543	1	12,14,15	1.83	2 (16%)	15,19,21	3.08	7 (46%)
8	NAG	A	1544	1	12,14,15	1.14	1 (8%)	15,19,21	2.29	5 (33%)

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	TC5	A	1530	1	-	0/3/7/9	0/0/0/0
4	SO4	A	1532	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1535	-	-	0/0/0/0	0/0/0/0
8	NAG	A	1542	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1543	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1544	1	1/1/5/7	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1543	NAG	C3-C2	3.89	1.60	1.52
8	A	1543	NAG	C2-N2	3.47	1.50	1.46
8	A	1544	NAG	C2-N2	2.43	1.49	1.46

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1543	NAG	C3-C2-N2	6.19	121.18	111.76
8	A	1543	NAG	O7-C7-C8	-5.52	111.27	122.04
8	A	1544	NAG	O5-C5-C4	4.78	116.72	110.65
8	A	1544	NAG	C3-C2-N2	4.55	118.69	111.76
8	A	1542	NAG	O5-C5-C6	4.45	111.65	106.98

All (1) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
8	A	1544	NAG	C1

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	527/529 (99%)	-0.11	10 (1%)	64	68	17, 32, 59, 80	11 (2%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	380	GLN	3.3
1	A	40	ARG	2.8
1	A	453	ARG	2.7
1	A	51	LYS	2.5
1	A	253	SER	2.5

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

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors($Å^2$)	Q<0.9
6	NAG	A	1538	14/15	0.19	16.80	65,72,75,75	0
7	FUL	A	1541	10/11	0.26	14.33	39,44,49,50	10
7	NAG	A	1540	14/15	0.23	4.38	59,66,68,69	0
6	NAG	A	1545	14/15	0.19	0.98	70,74,83,84	0
6	FUL	A	1547	10/11	0.18	0.90	64,70,74,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	FUL	A	1539	10/11	0.15	0.33	72,76,78,79	0
6	NAG	A	1537	14/15	0.10	0.08	43,47,61,69	0
6	NAG	A	1546	14/15	0.28	-	70,79,81,82	0

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	SO4	A	1535	5/5	0.11	9.48	39,41,45,48	5
8	NAG	A	1542	14/15	0.30	6.82	81,87,89,90	0
3	CL	A	1536	1/1	0.12	5.49	73,73,73,73	0
8	NAG	A	1544	14/15	0.40	5.31	89,91,97,98	0
8	NAG	A	1543	14/15	0.20	4.31	53,73,80,81	0
4	SO4	A	1532	5/5	0.12	3.80	51,57,59,60	5
3	CL	A	1531	1/1	0.16	1.15	51,51,51,51	0
2	TC5	A	1530	9/10	0.14	0.76	27,32,45,51	0
5	NA	A	1533	1/1	0.12	-0.07	43,43,43,43	1
3	CL	A	1534	1/1	0.13	-1.08	81,81,81,81	0

6.5 Other polymers ⓘ

There are no such residues in this entry.