



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 7, 2019 – 11:46 AM EDT

PDB ID : 2WSL
Title : Aged Form of Human Butyrylcholinesterase Inhibited by Tabun Analogue TA4
Authors : Carletti, E.; Aurbek, N.; Gillon, E.; Loiodice, M.; Nicolet, Y.; Fontecilla, J.; Masson, P.; Thiermann, H.; Nachon, F.; Worek, F.
Deposited on : 2009-09-08
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

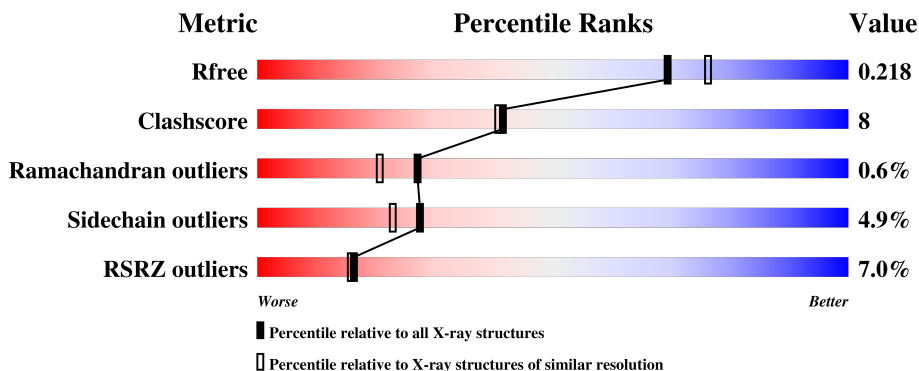
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	111664	7193 (2.00-2.00)
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)
RSRZ outliers	108989	7011 (2.00-2.00)

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. 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	529	<div> <div>7%</div> <div>84%</div> <div>13%</div> <div>.</div> </div>

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
2	NAG	A	1537	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	1539	-	-	-	X

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 4817 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.

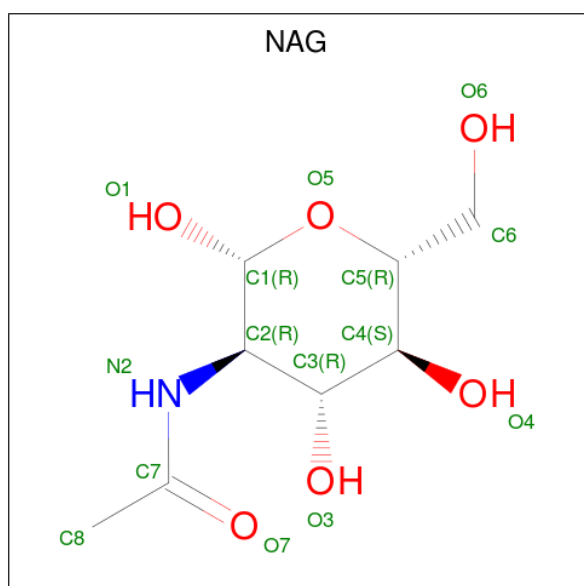
- Molecule 1 is a protein called CHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	527	4264	2756	714	777	17	0	10	0

There are 4 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	486	GLN	ASN	engineered mutation	UNP P06276

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



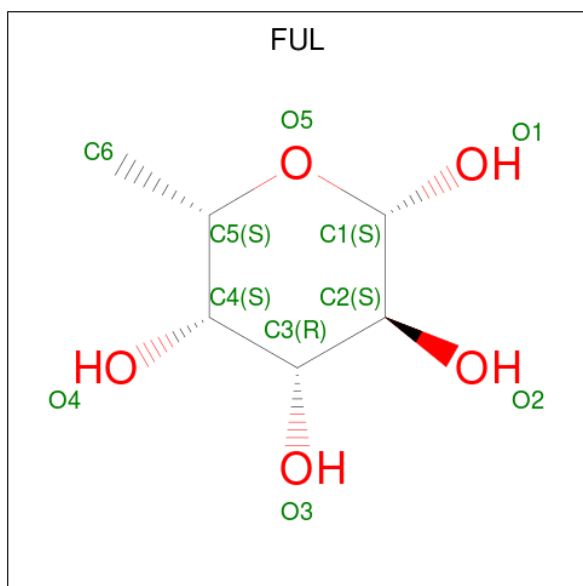
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0

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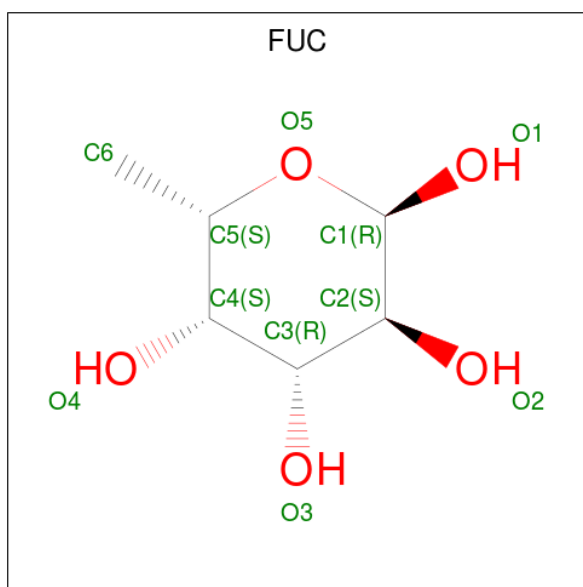
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is BETA-L-FUCOSE (three-letter code: FUL) (formula: C₆H₁₂O₅).



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

- Molecule 4 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C₆H₁₂O₅).



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

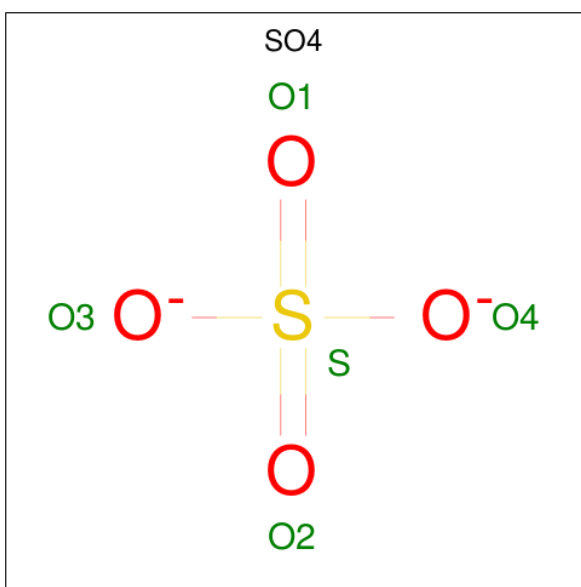
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

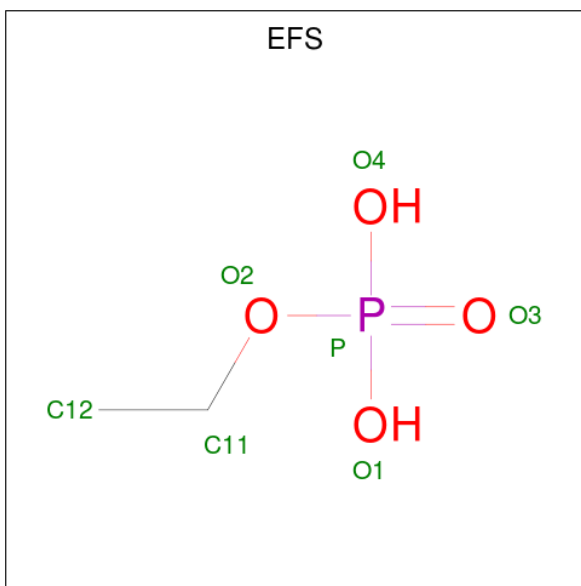
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is ETHYL DIHYDROGEN PHOSPHATE (three-letter code: EFS) (formula: C₂H₇O₄P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	O	P	0	0
			6	2	3	1		

- Molecule 9 is FLUORIDE ION (three-letter code: F) (formula: F).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total F 1 1	0	0

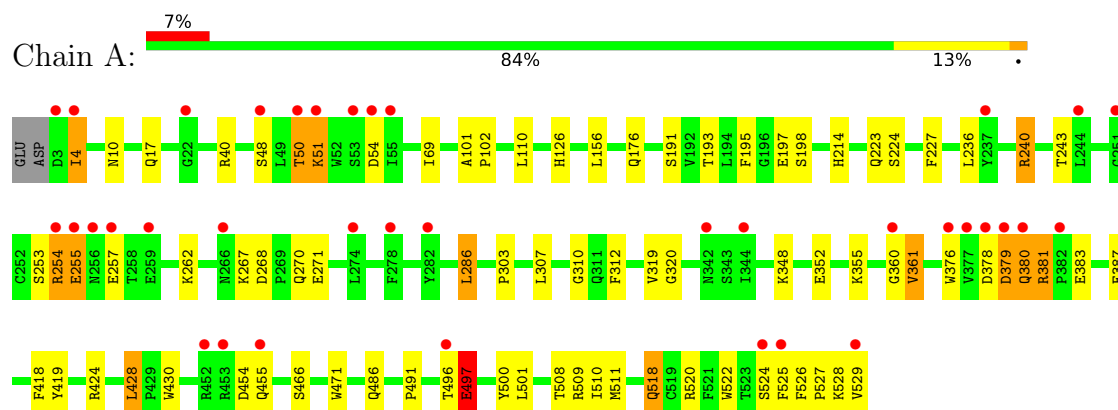
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	397	Total O 397 397	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: CHOLINESTERASE



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	154.86Å 154.86Å 126.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.87 – 2.00 48.87 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.87-2.00) 99.8 (48.87-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.55 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0044	Depositor
R, R_{free}	0.184 , 0.220 0.183 , 0.218	Depositor DCC
R_{free} test set	1543 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4817	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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: CL, NAG, F, NA, EFS, FUC, FUL, CSS, SO4

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	0.58	0/4408	0.62	0/5982

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	4264	0	4173	65	0
2	A	112	0	99	0	0
3	A	10	0	10	0	0
4	A	20	0	20	1	0
5	A	1	0	0	1	0
6	A	1	0	0	0	0
7	A	5	0	0	0	0
8	A	6	0	5	1	0
9	A	1	0	0	1	0
10	A	397	0	0	13	0
All	All	4817	0	4307	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 8.

The worst 5 of 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:48:SER:HB3	10:A:2041:HOH:O	1.44	1.18
1:A:496:THR:O	1:A:497:GLU:HB2	1.37	1.14
1:A:509[B]:ARG:HH11	1:A:509[B]:ARG:CG	1.71	1.03
1:A:496:THR:O	1:A:497:GLU:CB	2.19	0.90
1:A:501:LEU:HD11	1:A:508:THR:CG2	2.04	0.88

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	534/529 (101%)	515 (96%)	16 (3%)	3 (1%)	27 21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	497	GLU
1	A	379	ASP
1	A	361	VAL

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	461/453 (102%)	439 (95%)	22 (5%)	28 24

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	GLU
1	A	348	LYS
1	A	497	GLU
1	A	262	LYS
1	A	286	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	275	ASN
1	A	518	GLN
1	A	380	GLN
1	A	172	GLN
1	A	289	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	CSS	A	66	1	5,6,7	1.02	0	2,6,8	1.17	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
1	CSS	A	66	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 3 are monoatomic - leaving 13 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	NAG	A	1530	1,3,2	14,14,15	0.72	0	17,19,21	1.72	4 (23%)
2	NAG	A	1531	2	14,14,15	0.45	0	17,19,21	0.99	0
3	FUL	A	1532	2	9,10,11	0.80	0	13,14,16	1.72	2 (15%)
2	NAG	A	1533	1,4	14,14,15	0.71	0	17,19,21	1.31	3 (17%)
4	FUC	A	1534	2	9,10,11	0.67	0	13,14,16	1.13	1 (7%)
2	NAG	A	1535	1	14,14,15	0.42	0	17,19,21	1.36	3 (17%)
2	NAG	A	1536	1	14,14,15	0.56	0	17,19,21	1.44	2 (11%)
2	NAG	A	1537	1	14,14,15	0.68	0	17,19,21	1.55	2 (11%)
2	NAG	A	1538	1,2,4	14,14,15	0.45	0	17,19,21	1.04	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	1539	2	14,14,15	0.48	0	17,19,21	1.15	1 (5%)
4	FUC	A	1540	2	9,10,11	0.63	0	13,14,16	0.55	0
7	SO4	A	1543	-	4,4,4	0.23	0	6,6,6	0.26	0
8	EFS	A	1544	1	1,5,6	0.63	0	0,5,8	0.00	-

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	A	1530	1,3,2	-	3/6/23/26	0/1/1/1
2	NAG	A	1531	2	-	2/6/23/26	0/1/1/1
3	FUL	A	1532	2	-	-	0/1/1/1
2	NAG	A	1533	1,4	-	2/6/23/26	0/1/1/1
4	FUC	A	1534	2	-	-	0/1/1/1
2	NAG	A	1535	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1536	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1537	1	1/1/5/7	1/6/23/26	0/1/1/1
2	NAG	A	1538	1,2,4	-	2/6/23/26	0/1/1/1
2	NAG	A	1539	2	-	2/6/23/26	0/1/1/1
4	FUC	A	1540	2	-	-	0/1/1/1
8	EFS	A	1544	1	-	0/1/3/4	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1537	NAG	C4-C3-C2	4.47	117.57	111.02
3	A	1532	FUL	C1-C2-C3	-4.40	104.25	109.66
2	A	1530	NAG	C2-N2-C7	3.81	128.37	122.92
2	A	1539	NAG	C1-O5-C5	3.67	117.19	112.20
2	A	1536	NAG	C1-O5-C5	3.30	116.69	112.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1537	NAG	C1

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1539	NAG	O5-C5-C6-O6
2	A	1535	NAG	O5-C5-C6-O6
2	A	1531	NAG	O5-C5-C6-O6
2	A	1539	NAG	C4-C5-C6-O6
2	A	1535	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1534	FUC	1	0
8	A	1544	EFS	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	526/529 (99%)	0.17	37 (7%) 16 16	16, 24, 42, 55	6 (1%)

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	379	ASP	4.8
1	A	377	VAL	4.7
1	A	255	GLU	4.6
1	A	3	ASP	4.6
1	A	50	THR	4.2

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSS	A	66	7/8	0.97	0.11	20,21,25,28	1

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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
2	NAG	A	1537	14/15	0.43	0.58	58,61,62,62	0
2	NAG	A	1536	14/15	0.69	0.27	43,45,49,51	0
2	NAG	A	1535	14/15	0.71	0.30	48,52,53,53	0
3	FUL	A	1532	10/11	0.78	0.35	52,53,54,54	0
2	NAG	A	1539	14/15	0.79	0.47	63,64,65,66	0
9	F	A	1546	1/1	0.85	0.34	46,46,46,46	0
2	NAG	A	1531	14/15	0.85	0.48	53,57,58,58	0
4	FUC	A	1534	10/11	0.86	0.24	27,29,31,31	10
2	NAG	A	1538	14/15	0.89	0.28	52,57,60,60	0
4	FUC	A	1540	10/11	0.91	0.42	56,56,56,57	0
2	NAG	A	1533	14/15	0.92	0.17	33,37,39,41	0
5	CL	A	1541	1/1	0.92	0.06	52,52,52,52	0
6	NA	A	1542	1/1	0.93	0.33	47,47,47,47	1
2	NAG	A	1530	14/15	0.93	0.16	36,40,49,50	0
7	SO4	A	1543	5/5	0.97	0.17	27,31,32,33	5
8	EFS	A	1544	6/7	0.99	0.20	21,24,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.