



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:20 AM GMT

PDB ID : 2WSL  
Title : AGED FORM OF HUMAN BUTYRYLCHOLINESTERASE INHIBITED BY TABUN ANALOGUE TA4  
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Deposited on : 2009-09-08  
Resolution : 2.00 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

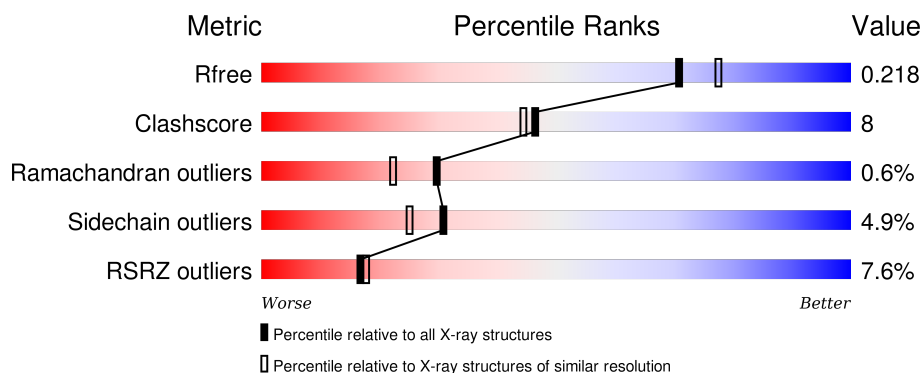
# 1 Overall quality at a glance

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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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  $\geq 3$ , 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>8%</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
3	FUC	A	1534	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	1536	-	-	-	X
4	NAG	A	1537	X	-	-	-
5	FUC	A	1540	-	-	-	X

## 2 Entry composition

There are 11 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
1	A	527	Total	C	N	O	S	0	10	0
			4264	2756	714	777	17			

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

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

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

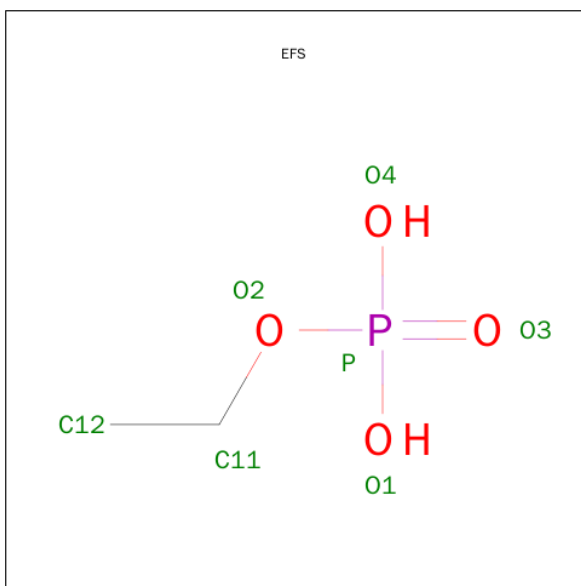
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Na	0	0
			1	1		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 9 is ETHYL DIHYDROGEN PHOSPHATE (three-letter code: EFS) (formula: C<sub>2</sub>H<sub>7</sub>O<sub>4</sub>P).



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

- Molecule 10 is FLUORIDE ION (three-letter code: F) (formula: F).

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

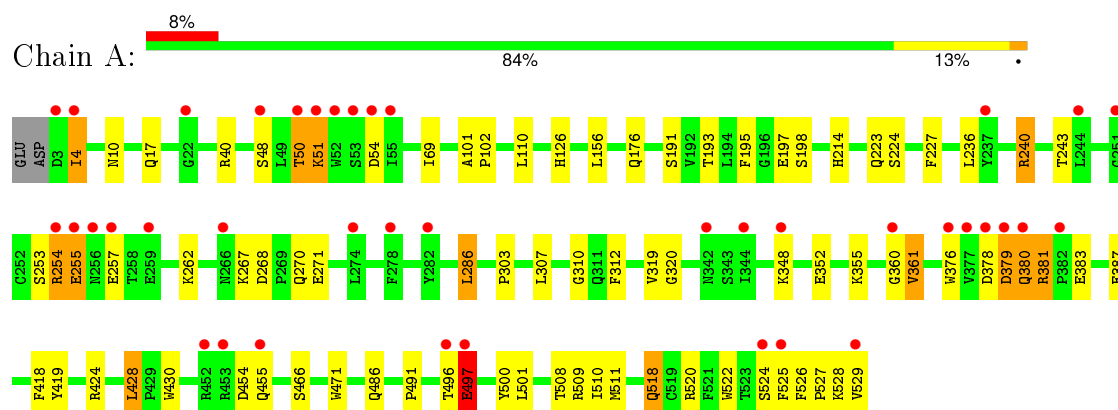
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	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 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 ( $\text{RSRZ} > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	154.86 Å   154.86 Å   126.01 Å 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.55 (at 2.00 Å)	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 (3.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.1	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 53.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 51413 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4817	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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

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	38	0	34	0	0
3	A	24	0	22	1	0
4	A	42	0	39	0	0
5	A	38	0	34	0	0
6	A	1	0	0	1	0
7	A	1	0	0	0	0
8	A	5	0	0	0	0
9	A	6	0	5	1	0
10	A	1	0	0	1	0
11	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.

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:48:SER:HB3	11: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
1:A:509[B]:ARG:HH11	1:A:509[B]:ARG:HG3	1.37	0.86
1:A:518:GLN:H	1:A:518:GLN:HE21	1.25	0.84
6:A:1541:CL:CL	11:A:2241:HOH:O	2.32	0.84
1:A:509[B]:ARG:NH1	1:A:509[B]:ARG:CG	2.42	0.78
1:A:501:LEU:HD11	1:A:508:THR:HG23	1.66	0.77
1:A:509[B]:ARG:NH1	1:A:509[B]:ARG:HG3	1.97	0.77
1:A:509[B]:ARG:HH11	1:A:509[B]:ARG:HG2	1.51	0.76
1:A:522:TRP:O	1:A:527:PRO:HD3	1.88	0.73
1:A:253:SER:O	1:A:254:ARG:HD3	1.97	0.64
1:A:497:GLU:HG2	11:A:2351:HOH:O	1.96	0.63
1:A:240:ARG:NH1	1:A:257:GLU:OE2	2.32	0.62
1:A:54:ASP:HB2	11:A:2046:HOH:O	1.99	0.62
1:A:176:GLN:NE2	11:A:2145:HOH:O	2.31	0.61
1:A:268[A]:ASP:OD2	1:A:270:GLN:HB3	2.00	0.61
1:A:255:GLU:CD	1:A:255:GLU:H	2.06	0.59
1:A:267:LYS:HE3	1:A:271:GLU:OE1	2.01	0.59
1:A:156:LEU:HD13	1:A:243:THR:HG21	1.84	0.58
1:A:227[A]:PHE:CE1	1:A:303:PRO:HB2	2.41	0.56
1:A:379:ASP:CG	11:A:2254:HOH:O	2.44	0.56
1:A:520:ARG:NH2	11:A:2381:HOH:O	2.39	0.55
1:A:126:HIS:HE1	11:A:2309:HOH:O	1.89	0.55
1:A:428:LEU:HD13	1:A:430:TRP:HB2	1.89	0.55
1:A:380:GLN:N	1:A:381:ARG:HB2	2.21	0.54
1:A:320:GLY:HA3	1:A:419:TYR:CE1	2.43	0.53
1:A:526:PHE:HA	1:A:529:VAL:HG22	1.90	0.53
1:A:352:GLU:HA	1:A:355:LYS:HE3	1.91	0.52
1:A:4:ILE:HD12	1:A:4:ILE:H	1.75	0.51
1:A:491:PRO:CD	1:A:510[B]:ILE:HD12	2.41	0.51
1:A:518:GLN:H	1:A:518:GLN:NE2	2.02	0.50
1:A:50:THR:O	1:A:51:LYS:HG2	2.12	0.50
1:A:520:ARG:NH1	11:A:2382:HOH:O	2.45	0.49
1:A:424:ARG:NH1	1:A:428:LEU:HD12	2.28	0.48
1:A:497:GLU:HA	11:A:2349:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ALA:HA	1:A:102:PRO:C	2.34	0.47
1:A:466:SER:OG	10:A:1546:F:F	2.16	0.47
1:A:268[A]:ASP:OD2	1:A:270:GLN:CB	2.61	0.46
1:A:191:SER:HB2	3:A:1534:FUC:H3	1.96	0.46
1:A:319:VAL:O	1:A:418:PHE:HA	2.15	0.46
1:A:198:SER:HA	1:A:224:SER:O	2.16	0.45
1:A:380:GLN:N	1:A:380:GLN:HE21	2.14	0.45
1:A:491:PRO:HD3	1:A:510[B]:ILE:HD12	1.99	0.45
1:A:500:TYR:CZ	1:A:511[A]:MET:HB2	2.52	0.45
1:A:509[B]:ARG:NH1	11:A:2367:HOH:O	2.50	0.45
1:A:227[B]:PHE:HZ	1:A:307:LEU:HB2	1.82	0.44
1:A:214:HIS:HE1	11:A:2216:HOH:O	2.01	0.44
1:A:320:GLY:HA3	1:A:419:TYR:CZ	2.53	0.44
1:A:4:ILE:N	1:A:4:ILE:HD12	2.34	0.42
1:A:197:GLU:HA	1:A:223:GLN:O	2.19	0.42
1:A:360:GLY:HA2	1:A:361:VAL:O	2.20	0.42
1:A:383:GLU:O	1:A:387:GLU:HG3	2.19	0.42
1:A:376:TRP:C	1:A:378:ASP:HA	2.40	0.42
1:A:286:LEU:HD23	9:A:1544:EFS:H123	2.02	0.42
1:A:509[A]:ARG:HA	1:A:509[A]:ARG:HD2	1.82	0.42
1:A:227[A]:PHE:CD1	1:A:303:PRO:HB2	2.55	0.41
1:A:4:ILE:HD11	1:A:17:GLN:HG2	2.03	0.40
1:A:10:ASN:ND2	11:A:2002:HOH:O	2.55	0.40
1:A:525:PHE:CE2	1:A:529:VAL:HG21	2.57	0.40
1:A:110:LEU:HD23	1:A:193:THR:HB	2.03	0.40
1:A:310:GLY:HA2	1:A:312:PHE:CE2	2.57	0.40
1:A:524:SER:O	1:A:528:LYS:HE3	2.21	0.40

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%)	30 22

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 ⓘ

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%)	31 26

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	40	ARG
1	A	50	THR
1	A	51	LYS
1	A	69	ILE
1	A	195	PHE
1	A	236	LEU
1	A	240	ARG
1	A	254	ARG
1	A	255	GLU
1	A	262	LYS
1	A	286	LEU
1	A	348	LYS
1	A	380	GLN
1	A	381	ARG
1	A	428	LEU
1	A	454	ASP
1	A	455	GLN

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Mol	Chain	Res	Type
1	A	471	TRP
1	A	486	GLN
1	A	497	GLU
1	A	518	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	126	HIS
1	A	172	GLN
1	A	214	HIS
1	A	275	ASN
1	A	289	ASN
1	A	380	GLN
1	A	517	GLN
1	A	518	GLN

### 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	4,6,7	1.02	0	3,6,8	1.09	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	0/0/0/0

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

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	$\# Z  > 2$
2	NAG	A	1530	1,2	14,14,15	0.70	0	15,19,21	1.69	2 (13%)
2	NAG	A	1531	2	14,14,15	0.45	0	15,19,21	0.97	0
2	FUL	A	1532	2	10,10,11	0.74	0	14,14,16	1.85	4 (28%)
3	NAG	A	1533	1,3	14,14,15	0.70	0	15,19,21	1.14	0
3	FUC	A	1534	3	10,10,11	0.62	0	14,14,16	1.22	1 (7%)
5	NAG	A	1538	1,5	14,14,15	0.43	0	15,19,21	0.90	0
5	NAG	A	1539	5	14,14,15	0.47	0	15,19,21	1.21	1 (6%)
5	FUC	A	1540	5	10,10,11	0.59	0	14,14,16	0.80	1 (7%)

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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1531	2	-	0/6/23/26	0/1/1/1
2	FUL	A	1532	2	-	0/0/17/20	0/1/1/1
3	NAG	A	1533	1,3	-	0/6/23/26	0/1/1/1
3	FUC	A	1534	3	-	0/0/17/20	0/1/1/1
5	NAG	A	1538	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1539	5	-	0/6/23/26	0/1/1/1
5	FUC	A	1540	5	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1532	FUL	C1-C2-C3	-4.48	104.25	109.54
2	A	1532	FUL	C1-O5-C5	-2.65	108.29	112.38
2	A	1532	FUL	O5-C1-C2	-2.60	106.64	110.86
5	A	1540	FUC	O5-C5-C6	2.03	109.48	106.13
2	A	1530	NAG	C8-C7-N2	2.53	120.94	116.11
2	A	1532	FUL	O5-C5-C6	2.60	110.43	106.13
3	A	1534	FUC	C1-C2-C3	3.40	113.56	109.54
5	A	1539	NAG	C1-O5-C5	3.90	117.19	112.25
2	A	1530	NAG	C2-N2-C7	4.15	128.37	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1534	FUC	1	0

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 3 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	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	1535	1	14,14,15	0.40	0	15,19,21	1.39	1 (6%)
4	NAG	A	1536	1	14,14,15	0.54	0	15,19,21	1.30	1 (6%)
4	NAG	A	1537	1	14,14,15	0.66	0	15,19,21	1.51	2 (13%)
8	SO4	A	1543	-	4,4,4	0.24	0	6,6,6	0.34	0
9	EFS	A	1544	1	1,5,6	0.64	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
4	NAG	A	1535	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1536	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1537	1	1/1/5/7	0/6/23/26	0/1/1/1
8	SO4	A	1543	-	-	0/0/0/0	0/0/0/0
9	EFS	A	1544	1	-	0/1/3/4	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1537	NAG	C3-C4-C5	2.84	115.15	110.20
4	A	1535	NAG	C1-O5-C5	3.47	116.65	112.25
4	A	1536	NAG	C1-O5-C5	3.50	116.69	112.25
4	A	1537	NAG	C4-C3-C2	4.08	117.57	111.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1537	NAG	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	526/529 (99%)	0.23	40 (7%) 17 18	16, 24, 42, 55	6 (1%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	377	VAL	5.0
1	A	379	ASP	5.0
1	A	3	ASP	4.8
1	A	255	GLU	4.8
1	A	50	THR	4.4
1	A	529	VAL	4.4
1	A	54	ASP	4.2
1	A	282	TYR	4.1
1	A	453	ARG	4.0
1	A	380	GLN	3.6
1	A	53	SER	3.5
1	A	378	ASP	3.4
1	A	525	PHE	3.4
1	A	259	GLU	3.3
1	A	455	GLN	3.2
1	A	51	LYS	2.8
1	A	254	ARG	2.8
1	A	360	GLY	2.7
1	A	376	TRP	2.7
1	A	237	TYR	2.7
1	A	496	THR	2.6
1	A	342	ASN	2.5
1	A	452	ARG	2.5
1	A	256	ASN	2.5
1	A	274	LEU	2.5
1	A	524	SER	2.4
1	A	4	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	251	GLY	2.4
1	A	344	ILE	2.4
1	A	278	PHE	2.3
1	A	22	GLY	2.3
1	A	55	ILE	2.3
1	A	382	PRO	2.3
1	A	257	GLU	2.3
1	A	244	LEU	2.1
1	A	48	SER	2.1
1	A	266	ASN	2.1
1	A	52	TRP	2.1
1	A	497	GLU	2.1
1	A	348	LYS	2.1

## 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. 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, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CSS	A	66	7/8	0.97	0.11	-	20,21,25,28	1

## 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. 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, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	FUC	A	1534	10/11	0.86	0.25	4.19	27,29,31,31	10
5	FUC	A	1540	10/11	0.91	0.42	3.98	56,56,56,57	0
2	NAG	A	1530	14/15	0.93	0.16	-0.07	36,40,49,50	0
2	NAG	A	1531	14/15	0.85	0.48	-	53,57,58,58	0
2	FUL	A	1532	10/11	0.78	0.35	-	52,53,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	A	1538	14/15	0.89	0.28	-	52,57,60,60	0
3	NAG	A	1533	14/15	0.92	0.17	-	33,37,39,41	0
5	NAG	A	1539	14/15	0.79	0.47	-	63,64,65,66	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. 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, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	1536	14/15	0.69	0.27	3.81	43,45,49,51	0
9	EFS	A	1544	6/7	0.99	0.20	1.70	21,24,25,25	0
4	NAG	A	1535	14/15	0.71	0.30	-	48,52,53,53	0
7	NA	A	1542	1/1	0.93	0.33	-	47,47,47,47	1
10	F	A	1546	1/1	0.85	0.34	-	46,46,46,46	0
4	NAG	A	1537	14/15	0.43	0.58	-	58,61,62,62	0
6	CL	A	1541	1/1	0.92	0.06	-	52,52,52,52	0
8	SO4	A	1543	5/5	0.97	0.17	-	27,31,32,33	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.