



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 02:07 pm GMT

PDB ID : 3DJY  
Title : Nonaged Form of Human Butyrylcholinesterase Inhibited by Tabun  
Authors : Carletti, E.; Nachon, F.  
Deposited on : 2008-06-24  
Resolution : 2.10 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

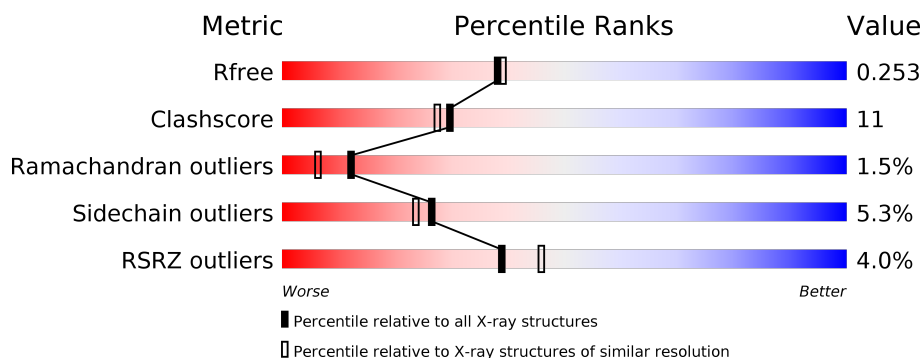
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (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  $\geq 3$ , 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>4%</div> <div>79%</div> <div>16%</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
4	NAG	A	536	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4656 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	P	S	0	1	0
			4221	2722	710	773	1	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	ENGINEERED	UNP P06276
A	455	GLN	ASN	ENGINEERED	UNP P06276
A	481	GLN	ASN	ENGINEERED	UNP P06276
A	486	GLN	ASN	ENGINEERED	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		
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 SODIUM ION (three-letter code: NA) (formula: Na).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Cl	0	0
			2	2		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

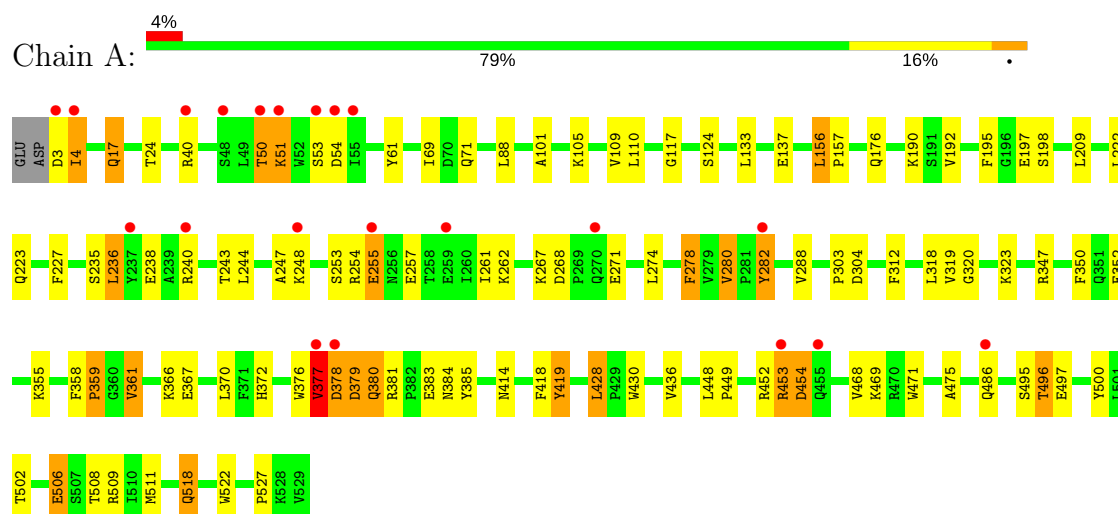
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	285	Total	O	0	0
			285	285		

### 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, $\alpha$ , $\beta$ , $\gamma$	156.58Å 156.58Å 127.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.38 – 2.10 55.36 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (55.38-2.10) 99.0 (55.36-2.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.61 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, $R_{free}$	0.211 , 0.249 0.211 , 0.253	Depositor DCC
$R_{free}$ test set	918 reflections (2.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.6	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 65.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4656	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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, 0.333 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: NAG, CL, SUN, PO4, NA, 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	0.82	2/4326 (0.0%)	0.78	1/5871 (0.0%)

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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	419	TYR	CD1-CE1	6.33	1.48	1.39
1	A	367	GLU	CG-CD	5.76	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	VAL	CB-CA-C	-5.03	101.84	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	359	PRO	Peptide
1	A	380	GLN	Peptide



## 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	4221	0	4116	89	0
2	A	76	0	68	1	0
3	A	24	0	22	1	0
4	A	42	0	39	1	0
5	A	1	0	0	0	0
6	A	2	0	0	1	0
7	A	5	0	0	0	0
8	A	285	0	0	9	0
All	All	4656	0	4245	92	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 11.

All (92) 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:4:ILE:H	1:A:4:ILE:HD12	1.12	1.06
1:A:4:ILE:N	1:A:4:ILE:HD12	1.67	1.03
1:A:518:GLN:H	1:A:518:GLN:HE21	1.02	1.00
1:A:50:THR:O	1:A:51:LYS:HB3	1.63	0.95
1:A:17:GLN:HE21	1:A:17:GLN:HA	1.32	0.93
6:A:543:CL:CL	8:A:733:HOH:O	2.24	0.91
1:A:377:VAL:O	1:A:377:VAL:HG23	1.71	0.89
1:A:378:ASP:O	1:A:380:GLN:N	2.08	0.86
1:A:378:ASP:OD1	1:A:380:GLN:OE1	1.95	0.83
1:A:518:GLN:HE21	1:A:518:GLN:N	1.81	0.77
1:A:4:ILE:CD1	1:A:4:ILE:H	1.95	0.74
1:A:377:VAL:HA	1:A:378:ASP:HB2	1.71	0.72
1:A:50:THR:O	1:A:51:LYS:CB	2.37	0.72
1:A:253:SER:O	1:A:254:ARG:HD3	1.93	0.68
1:A:282:TYR:HD2	1:A:282:TYR:O	1.82	0.63
1:A:379:ASP:HB2	1:A:381:ARG:HG3	1.80	0.63
1:A:320:GLY:HA3	1:A:419:TYR:CZ	2.35	0.62
1:A:453:ARG:HG3	8:A:721:HOH:O	2.00	0.62
1:A:379:ASP:O	1:A:380:GLN:HB2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:GLY:HA3	1:A:419:TYR:CE1	2.35	0.61
4:A:535:NAG:O6	8:A:611:HOH:O	2.16	0.60
1:A:500:TYR:CZ	1:A:511:MET:HB2	2.37	0.60
1:A:414:ASN:HB2	8:A:624:HOH:O	2.04	0.58
1:A:61:TYR:CD1	1:A:124:SER:HB3	2.38	0.58
1:A:500:TYR:CE1	1:A:511:MET:HB2	2.40	0.57
1:A:4:ILE:N	1:A:4:ILE:CD1	2.40	0.56
1:A:502:THR:O	1:A:508:THR:HB	2.06	0.56
1:A:304:ASP:N	1:A:304:ASP:OD1	2.40	0.55
1:A:379:ASP:CB	1:A:381:ARG:HG3	2.38	0.54
1:A:117:GLY:HA2	1:A:198:SUN:C2	2.38	0.54
1:A:17:GLN:NE2	1:A:17:GLN:HA	2.13	0.54
1:A:190:LYS:HB3	3:A:534:FUL:H5	1.91	0.53
1:A:109:VAL:HB	1:A:192:VAL:HG22	1.90	0.53
1:A:495:SER:O	1:A:496:THR:OG1	2.17	0.53
1:A:235:SER:OG	1:A:238:GLU:HG3	2.09	0.52
1:A:267:LYS:HE3	1:A:271:GLU:OE1	2.10	0.52
1:A:377:VAL:CG2	1:A:377:VAL:O	2.39	0.52
1:A:53:SER:O	1:A:54:ASP:HB2	2.09	0.51
1:A:378:ASP:O	1:A:379:ASP:C	2.49	0.51
1:A:378:ASP:O	1:A:378:ASP:OD1	2.29	0.50
1:A:495:SER:O	1:A:496:THR:CB	2.60	0.50
1:A:255:GLU:H	1:A:255:GLU:CD	2.14	0.50
1:A:227:PHE:CD2	1:A:227:PHE:C	2.84	0.50
1:A:3:ASP:N	8:A:725:HOH:O	2.44	0.50
1:A:110:LEU:HD11	1:A:475:ALA:CB	2.42	0.49
2:A:531:NAG:H61	8:A:641:HOH:O	2.11	0.49
1:A:518:GLN:H	1:A:518:GLN:NE2	1.88	0.49
1:A:278:PHE:C	1:A:280:VAL:H	2.17	0.48
1:A:157:PRO:HD2	1:A:240:ARG:CD	2.44	0.48
1:A:156:LEU:HD13	1:A:243:THR:HG21	1.95	0.48
1:A:361:VAL:O	1:A:366:LYS:NZ	2.47	0.47
1:A:240:ARG:NH1	1:A:257:GLU:OE2	2.47	0.47
1:A:267:LYS:HD2	1:A:267:LYS:HA	1.76	0.47
1:A:282:TYR:O	1:A:282:TYR:CD2	2.67	0.47
1:A:381:ARG:NH1	1:A:384:ASN:OD1	2.47	0.47
1:A:378:ASP:OD1	1:A:378:ASP:C	2.54	0.46
1:A:253:SER:O	1:A:254:ARG:CD	2.63	0.45
1:A:117:GLY:HA2	1:A:198:SUN:H2C2	1.99	0.45
1:A:377:VAL:N	1:A:378:ASP:HA	2.30	0.45
1:A:452:ARG:C	1:A:454:ASP:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:GLU:HA	1:A:223:GLN:O	2.17	0.45
1:A:236:LEU:HA	1:A:236:LEU:HD12	1.71	0.45
1:A:318:LEU:HD23	1:A:318:LEU:C	2.37	0.45
1:A:352:GLU:HA	1:A:355:LYS:HE3	1.98	0.45
1:A:448:LEU:N	1:A:449:PRO:CD	2.80	0.45
1:A:452:ARG:HG2	8:A:612:HOH:O	2.17	0.45
1:A:71:GLN:HG2	8:A:826:HOH:O	2.16	0.44
1:A:372[B]:HIS:CD2	8:A:803:HOH:O	2.70	0.44
1:A:24:THR:O	1:A:101:ALA:HB3	2.18	0.43
1:A:448:LEU:HB2	1:A:449:PRO:HD3	2.00	0.43
1:A:156:LEU:HD22	1:A:261:ILE:HD11	2.01	0.43
1:A:381:ARG:NH2	1:A:383:GLU:OE1	2.51	0.43
1:A:133:LEU:HD23	1:A:468:VAL:HG13	2.00	0.43
1:A:253:SER:C	1:A:254:ARG:HD3	2.38	0.43
1:A:319:VAL:O	1:A:418:PHE:HA	2.19	0.43
1:A:350:PHE:CE2	1:A:370:LEU:HD12	2.54	0.42
1:A:247:ALA:O	1:A:248:LYS:C	2.58	0.42
1:A:358:PHE:N	1:A:359:PRO:HD3	2.34	0.42
1:A:347:ARG:HB2	1:A:385:TYR:CZ	2.55	0.42
1:A:222:LEU:N	1:A:222:LEU:HD12	2.34	0.42
1:A:69:ILE:HD11	1:A:88:LEU:HD11	2.02	0.42
1:A:428:LEU:CD1	1:A:430:TRP:HB2	2.49	0.42
1:A:137:GLU:OE2	1:A:469:LYS:HE2	2.20	0.42
1:A:117:GLY:HA2	1:A:198:SUN:H2C3	2.01	0.41
1:A:376:TRP:CD1	1:A:380:GLN:NE2	2.89	0.41
1:A:227:PHE:CE2	1:A:303:PRO:HB2	2.56	0.41
1:A:209:LEU:HD23	1:A:312:PHE:HB3	2.03	0.41
1:A:255:GLU:CD	1:A:255:GLU:N	2.74	0.40
1:A:244:LEU:O	1:A:247:ALA:HB3	2.21	0.40
1:A:323:LYS:HB3	1:A:436:VAL:HB	2.02	0.40
1:A:288:VAL:HG12	1:A:288:VAL:O	2.21	0.40
1:A:522:TRP:O	1:A:527:PRO:HD3	2.22	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	525/529 (99%)	491 (94%)	26 (5%)	8 (2%)	12 6

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	379	ASP
1	A	496	THR
1	A	453	ARG
1	A	378	ASP
1	A	506	GLU
1	A	361	VAL
1	A	377	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	452/453 (100%)	428 (95%)	24 (5%)	26 24

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	17	GLN
1	A	40	ARG
1	A	50	THR
1	A	105	LYS
1	A	156	LEU
1	A	176	GLN
1	A	195	PHE
1	A	236	LEU

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Mol	Chain	Res	Type
1	A	255	GLU
1	A	262	LYS
1	A	268	ASP
1	A	274	LEU
1	A	278	PHE
1	A	280	VAL
1	A	282	TYR
1	A	428	LEU
1	A	454	ASP
1	A	471	TRP
1	A	486	GLN
1	A	497	GLU
1	A	506	GLU
1	A	509	ARG
1	A	518	GLN

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

Mol	Chain	Res	Type
1	A	17	GLN
1	A	172	GLN
1	A	275	ASN
1	A	289	ASN
1	A	380	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	SUN	A	198	1	12,13,14	1.85	3 (25%)	12,17,19	2.57	6 (50%)

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	SUN	A	198	1	-	0/15/18/20	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SUN	P1-O1	2.19	1.48	1.46
1	A	198	SUN	P1-OG	2.87	1.65	1.57
1	A	198	SUN	CA-C	4.94	1.56	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SUN	P1-O2-C3	-4.57	108.42	120.61
1	A	198	SUN	OG-P1-O1	-3.91	108.33	115.84
1	A	198	SUN	C1-N1-C2	-2.68	103.94	113.62
1	A	198	SUN	P1-OG-CB	2.17	126.40	120.61
1	A	198	SUN	O2-P1-OG	3.69	109.36	100.02
1	A	198	SUN	OG-CB-CA	3.72	111.84	108.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SUN	3	0

## 5.5 Carbohydrates [i](#)

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	530	1,2	14,14,15	1.10	1 (7%)	15,19,21	1.70	2 (13%)
2	NAG	A	531	2	14,14,15	0.65	0	15,19,21	1.05	1 (6%)
2	FUL	A	532	2	9,10,11	0.91	0	13,14,16	2.85	5 (38%)
3	NAG	A	533	1,3	14,14,15	0.77	1 (7%)	15,19,21	1.41	1 (6%)
3	FUL	A	534	3	9,10,11	0.77	0	13,14,16	1.87	2 (15%)
2	NAG	A	538	1,2	14,14,15	0.53	0	15,19,21	1.53	3 (20%)
2	NAG	A	539	2	14,14,15	0.55	0	15,19,21	1.01	1 (6%)
2	FUL	A	540	2	9,10,11	0.70	0	13,14,16	2.73	4 (30%)

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	530	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	531	2	-	0/6/23/26	0/1/1/1
2	FUL	A	532	2	-	0/0/17/20	0/1/1/1
3	NAG	A	533	1,3	-	0/6/23/26	0/1/1/1
3	FUL	A	534	3	-	0/0/17/20	0/1/1/1
2	NAG	A	538	1,2	-	2/6/23/26	0/1/1/1
2	NAG	A	539	2	-	0/6/23/26	0/1/1/1
2	FUL	A	540	2	-	0/0/17/20	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	530	NAG	O5-C1	-2.57	1.39	1.43
3	A	533	NAG	C1-C2	2.37	1.55	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	532	FUL	C1-C2-C3	-8.08	99.41	109.65
2	A	540	FUL	C1-C2-C3	-7.41	100.26	109.65
3	A	534	FUL	C1-C2-C3	-4.54	103.90	109.65
2	A	540	FUL	C1-O5-C5	-3.95	103.66	112.39
2	A	530	NAG	O5-C1-C2	-3.91	106.04	111.47
2	A	532	FUL	O5-C1-C2	-3.69	105.00	110.79
3	A	534	FUL	C2-C3-C4	-3.60	104.59	110.88
2	A	538	NAG	O5-C1-C2	-3.40	106.73	111.47
2	A	538	NAG	C2-N2-C7	-3.14	118.36	122.94
3	A	533	NAG	C3-C4-C5	-2.98	104.96	110.22
2	A	540	FUL	O5-C1-C2	-2.68	106.58	110.79
2	A	538	NAG	O4-C4-C3	-2.50	104.92	110.36
2	A	531	NAG	C1-O5-C5	-2.45	108.79	112.17
2	A	532	FUL	C2-C3-C4	-2.13	107.17	110.88
2	A	532	FUL	O2-C2-C1	2.25	113.75	109.18
2	A	532	FUL	O2-C2-C3	2.61	115.31	110.17
2	A	539	NAG	C1-O5-C5	2.62	115.78	112.17
2	A	530	NAG	C2-N2-C7	3.36	127.84	122.94
2	A	540	FUL	C3-C4-C5	3.76	115.59	109.68

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	538	NAG	C8-C7-N2-C2
2	A	538	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	531	NAG	1	0
3	A	534	FUL	1	0

## 5.6 Ligand geometry

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	535	1	14,14,15	0.43	0	15,19,21	2.38	5 (33%)
4	NAG	A	536	1	14,14,15	0.49	0	15,19,21	1.38	1 (6%)
4	NAG	A	537	1	14,14,15	0.47	0	15,19,21	0.86	0
7	PO4	A	544	-	4,4,4	0.80	0	6,6,6	0.32	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	NAG	A	535	1	-	0/6/23/26	0/1/1/1
4	NAG	A	536	1	-	0/6/23/26	0/1/1/1
4	NAG	A	537	1	-	0/6/23/26	0/1/1/1
7	PO4	A	544	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	535	NAG	C4-C3-C2	-4.55	104.35	111.02
4	A	535	NAG	O5-C1-C2	-4.00	105.91	111.47
4	A	536	NAG	C4-C3-C2	-3.03	106.58	111.02
4	A	535	NAG	C2-N2-C7	-2.66	119.07	122.94
4	A	535	NAG	C1-C2-N2	2.32	114.45	110.49
4	A	535	NAG	C1-O5-C5	5.22	119.37	112.17

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
4	A	535	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<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%)	-0.03	21 (3%)	39 46	21, 35, 60, 73	10 (1%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	54	ASP	4.6
1	A	50	THR	3.9
1	A	453	ARG	3.6
1	A	3	ASP	3.5
1	A	255	GLU	3.2
1	A	377	VAL	3.2
1	A	51	LYS	3.0
1	A	282	TYR	2.8
1	A	378	ASP	2.8
1	A	55	ILE	2.8
1	A	40	ARG	2.7
1	A	53	SER	2.6
1	A	259	GLU	2.5
1	A	248	LYS	2.4
1	A	486	GLN	2.3
1	A	270	GLN	2.3
1	A	455	GLN	2.2
1	A	48	SER	2.1
1	A	4	ILE	2.0
1	A	240	ARG	2.0
1	A	237	TYR	2.0

### 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	SUN	A	198	14/15	0.96	0.12	-	25,32,41,44	0

### 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
2	FUL	A	540	10/11	0.94	0.20	0.66	70,71,72,73	0
2	NAG	A	530	14/15	0.95	0.10	-0.26	47,52,58,62	0
2	NAG	A	531	14/15	0.83	0.20	-	63,65,71,73	0
2	NAG	A	538	14/15	0.91	0.22	-	67,71,74,75	0
2	FUL	A	532	10/11	0.76	0.22	-	67,69,71,72	0
3	FUL	A	534	10/11	0.74	0.25	-	54,56,57,58	10
2	NAG	A	539	14/15	0.85	0.29	-	71,76,79,79	0
3	NAG	A	533	14/15	0.64	0.25	-	61,65,66,68	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(Å <sup>2</sup> )	Q<0.9
4	NAG	A	536	14/15	0.77	0.21	5.04	53,66,69,70	0
7	PO4	A	544	5/5	0.97	0.11	-	51,53,55,56	0
4	NAG	A	535	14/15	0.78	0.25	-	73,77,78,78	0
6	CL	A	542	1/1	0.87	0.15	-	58,58,58,58	0
5	NA	A	541	1/1	0.92	0.11	-	57,57,57,57	1
4	NAG	A	537	14/15	0.80	0.47	-	83,87,89,89	0
6	CL	A	543	1/1	0.97	0.04	-	70,70,70,70	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.