



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:15 AM GMT

PDB ID : 2WIF  
Title : AGED FORM OF HUMAN BUTYRYLCHOLINESTERASE INHIBITED BY TABUN ANALOGUE TA1  
Authors : Carletti, E.; Aurbek, N.; Gillon, E.; Loiodice, M.; Nicolet, Y.; Fontecilla, J.; Masson, P.; Thiermann, H.; Nachon, F.; Worek, F.  
Deposited on : 2009-05-11  
Resolution : 2.25 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.

---

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

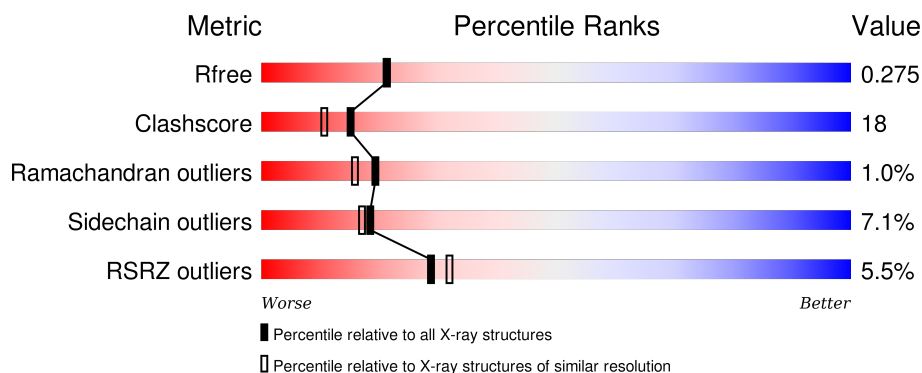
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	

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
7	FUL	A	1541	-	-	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	NAG	A	1543	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4747 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	7	2	0
			4213	2720	710	768	15			

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

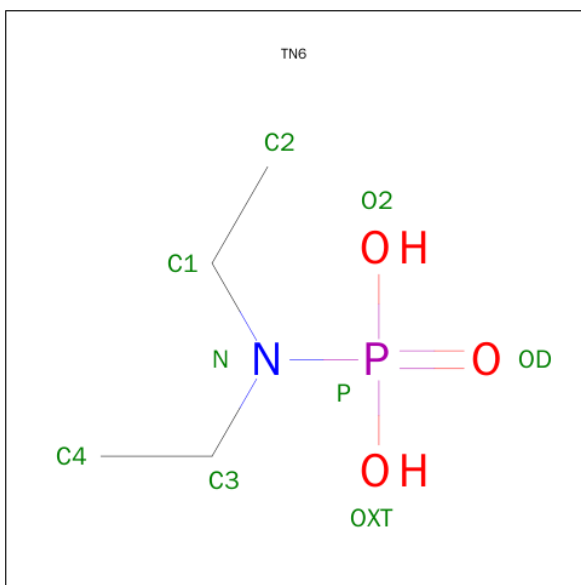
- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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

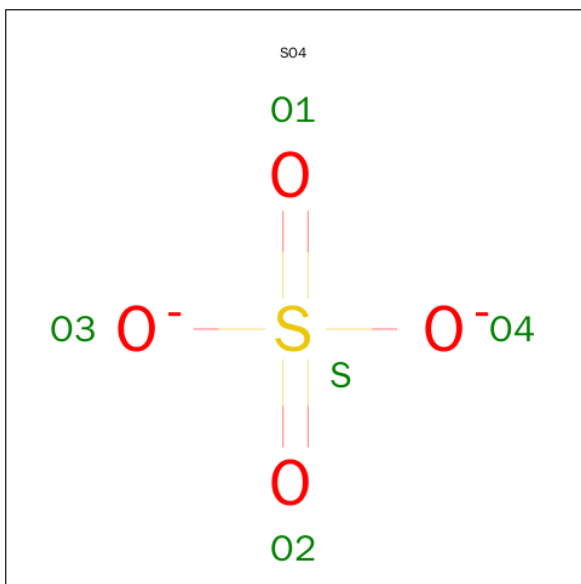
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Cl	0	0
			3	3		

- Molecule 4 is DIETHYLPHOSPHORAMIDIC ACID (three-letter code: TN6) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			8	4	1	2	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

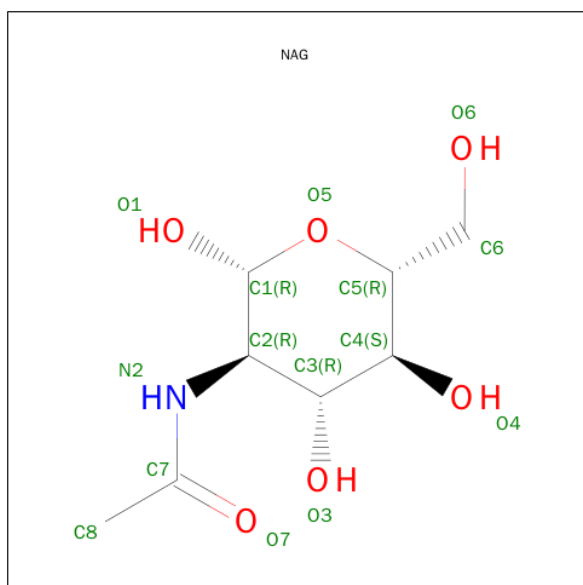
- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

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

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

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

- 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		

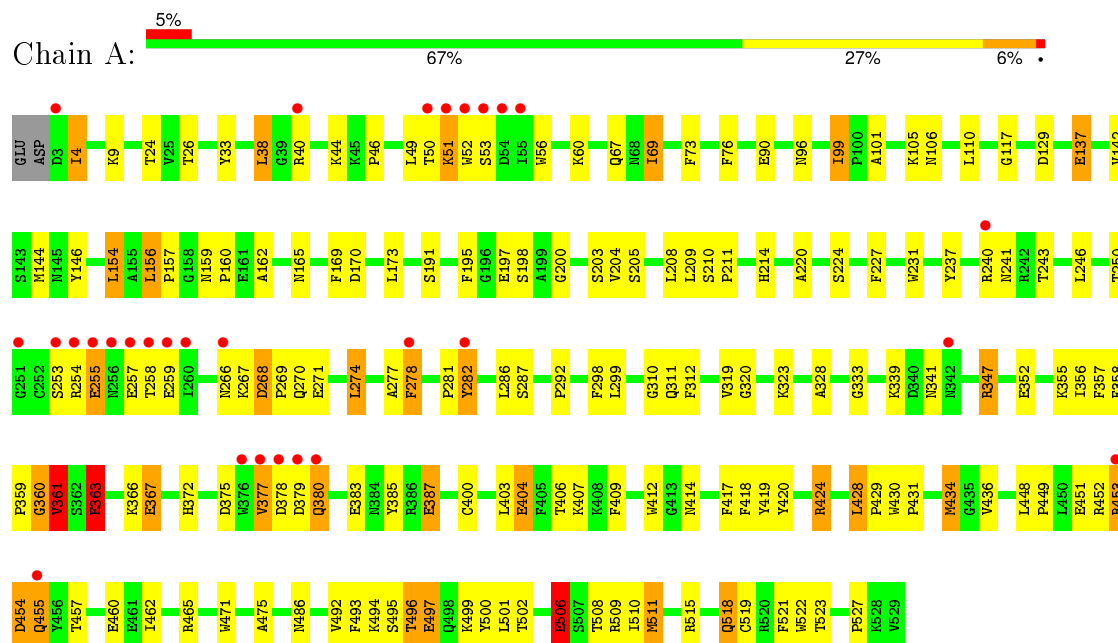
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	370	Total	O	0	0
			370	370		

### 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 ( $RSRZ > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	154.39 Å   154.39 Å   126.42 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	47.67 – 2.25 47.67 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.67-2.25) 96.8 (47.67-2.25)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.88 (at 2.24 Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, $R_{free}$	0.207   ,   0.275 0.206   ,   0.275	Depositor DCC
$R_{free}$ test set	1410 reflections (4.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.1	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 61.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 35241 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4747	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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: TN6, NAG, CL, NA, 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	1.21	12/4340 (0.3%)	1.03	9/5892 (0.2%)

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	TYR	CB-CG	-10.71	1.35	1.51
1	A	497	GLU	CD-OE2	8.22	1.34	1.25
1	A	404	GLU	CG-CD	7.96	1.63	1.51
1	A	400	CYS	CB-SG	-7.70	1.69	1.82
1	A	367	GLU	CG-CD	6.02	1.60	1.51
1	A	137	GLU	CG-CD	5.97	1.60	1.51
1	A	471	TRP	CB-CG	5.84	1.60	1.50
1	A	146	TYR	CD1-CE1	5.56	1.47	1.39
1	A	521	PHE	CE1-CZ	5.49	1.47	1.37
1	A	363	GLU	CG-CD	5.35	1.59	1.51
1	A	420	TYR	CD1-CE1	-5.27	1.31	1.39
1	A	197	GLU	CD-OE2	5.24	1.31	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	515	ARG	NE-CZ-NH1	9.67	125.14	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	515	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	A	434	MET	CG-SD-CE	6.93	111.29	100.20
1	A	274	LEU	CA-CB-CG	6.05	129.21	115.30
1	A	424	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	360	GLY	C-N-CA	5.31	134.97	121.70
1	A	347	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	A	424	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	129	ASP	CB-CG-OD2	-5.04	113.77	118.30

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 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	4213	0	4110	146	0
2	A	1	0	0	0	0
3	A	3	0	0	1	0
4	A	8	0	11	3	0
5	A	10	0	0	0	0
6	A	76	0	68	1	0
7	A	24	0	22	2	0
8	A	42	0	39	5	0
9	A	370	0	0	25	0
All	All	4747	0	4250	151	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 18.

All (151) 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:377:VAL:O	1:A:377:VAL:HG23	1.62	0.99
1:A:320:GLY:HA3	1:A:419:TYR:CE1	1.96	0.99
1:A:282:TYR:HD1	1:A:282:TYR:O	1.45	0.97
1:A:51:LYS:N	9:A:2044:HOH:O	1.96	0.96
1:A:518:GLN:H	1:A:518:GLN:HE21	1.00	0.96
1:A:320:GLY:HA3	1:A:419:TYR:CZ	2.06	0.91
1:A:509:ARG:HH11	1:A:509:ARG:HG2	1.36	0.88
1:A:361:VAL:O	1:A:366:LYS:NZ	2.11	0.83
1:A:380:GLN:HB2	3:A:1533:CL:CL	2.16	0.83
1:A:367:GLU:HB3	9:A:2240:HOH:O	1.79	0.83
1:A:518:GLN:H	1:A:518:GLN:NE2	1.77	0.81
1:A:328:ALA:HA	1:A:434:MET:CE	2.13	0.79
1:A:377:VAL:CG2	1:A:377:VAL:O	2.31	0.77
1:A:282:TYR:CD1	1:A:282:TYR:O	2.37	0.76
1:A:509:ARG:NH1	1:A:509:ARG:HG2	1.97	0.76
1:A:117:GLY:HA2	4:A:1532:TN6:H22C	1.68	0.76
1:A:250:THR:HB	1:A:267:LYS:HE2	1.67	0.76
1:A:454:ASP:O	1:A:455:GLN:HB2	1.85	0.75
1:A:495:SER:HA	9:A:2319:HOH:O	1.87	0.75
1:A:50:THR:O	1:A:51:LYS:HG2	1.88	0.74
1:A:452:ARG:HD2	9:A:2289:HOH:O	1.88	0.74
1:A:4:ILE:N	1:A:4:ILE:HD12	2.04	0.73
1:A:156:LEU:HD13	1:A:243:THR:HG21	1.72	0.72
1:A:494:LYS:NZ	9:A:2317:HOH:O	2.22	0.71
1:A:267:LYS:HE3	1:A:271:GLU:OE1	1.89	0.71
1:A:270:GLN:O	1:A:274:LEU:HB2	1.91	0.71
1:A:424:ARG:NH1	1:A:428:LEU:HD12	2.05	0.70
1:A:451:GLU:OE1	1:A:453:ARG:HG2	1.92	0.70
1:A:24:THR:O	1:A:101:ALA:HB3	1.92	0.70
1:A:428:LEU:HD13	1:A:430:TRP:HB2	1.73	0.69
1:A:518:GLN:HE21	1:A:518:GLN:N	1.83	0.69
1:A:257:GLU:OE1	9:A:2168:HOH:O	2.14	0.66
1:A:452:ARG:C	1:A:454:ASP:H	1.99	0.65
1:A:522:TRP:O	1:A:527:PRO:HD3	1.96	0.65
1:A:4:ILE:H	1:A:4:ILE:HD12	1.63	0.63
1:A:277:ALA:HB2	9:A:2180:HOH:O	1.98	0.63
1:A:191:SER:HB2	7:A:1541:FUL:H3	1.82	0.62
1:A:495:SER:CA	9:A:2319:HOH:O	2.46	0.61
1:A:320:GLY:HA3	1:A:419:TYR:CD1	2.36	0.61
1:A:383:GLU:O	1:A:387:GLU:HG2	2.01	0.60
1:A:452:ARG:O	1:A:454:ASP:N	2.34	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LEU:HD23	1:A:162:ALA:HB1	1.84	0.60
1:A:403:LEU:O	1:A:407:LYS:HG3	2.02	0.60
1:A:404:GLU:HG2	9:A:2160:HOH:O	2.01	0.59
1:A:496:THR:N	9:A:2319:HOH:O	2.21	0.59
1:A:198:SER:HA	1:A:224:SER:O	2.03	0.59
1:A:428:LEU:CD1	1:A:430:TRP:HB2	2.32	0.58
1:A:500:TYR:CZ	1:A:511:MET:HB2	2.38	0.58
1:A:358:PHE:N	1:A:359:PRO:HD3	2.19	0.58
8:A:1544:NAG:H62	9:A:2361:HOH:O	2.03	0.57
1:A:417:PHE:CE2	1:A:492:VAL:HG12	2.38	0.57
1:A:372[A]:HIS:CE1	9:A:2241:HOH:O	2.58	0.56
1:A:319:VAL:O	1:A:418:PHE:HA	2.06	0.56
1:A:500:TYR:CE1	1:A:511:MET:HB2	2.41	0.55
1:A:495:SER:O	1:A:496:THR:OG1	2.19	0.55
1:A:110:LEU:HD21	1:A:475:ALA:CB	2.36	0.55
1:A:452:ARG:C	1:A:454:ASP:N	2.58	0.55
1:A:4:ILE:N	1:A:4:ILE:CD1	2.67	0.55
1:A:274:LEU:O	1:A:278:PHE:CE2	2.61	0.54
1:A:383:GLU:N	1:A:383:GLU:OE2	2.39	0.54
1:A:357:PHE:C	1:A:359:PRO:HD3	2.28	0.53
1:A:204:VAL:CG1	1:A:220:ALA:HB1	2.38	0.53
1:A:208:LEU:O	1:A:214[B]:HIS:HE1	1.91	0.53
1:A:428:LEU:HD22	1:A:429:PRO:HD2	1.92	0.52
8:A:1542:NAG:C6	9:A:2358:HOH:O	2.56	0.52
8:A:1542:NAG:H61	9:A:2358:HOH:O	2.08	0.52
1:A:497:GLU:CD	1:A:499:LYS:HE3	2.30	0.52
1:A:96:ASN:O	1:A:142:VAL:HA	2.10	0.52
1:A:209:LEU:HD23	1:A:312:PHE:HB3	1.92	0.52
1:A:277:ALA:CB	9:A:2180:HOH:O	2.55	0.51
1:A:378:ASP:C	1:A:380:GLN:H	2.13	0.51
1:A:157:PRO:HD2	1:A:240:ARG:HD3	1.92	0.51
1:A:60:LYS:HE3	9:A:2051:HOH:O	2.09	0.51
1:A:255:GLU:CD	1:A:255:GLU:N	2.64	0.51
1:A:208:LEU:O	1:A:214[B]:HIS:CE1	2.64	0.50
1:A:378:ASP:CG	1:A:379:ASP:H	2.14	0.50
1:A:414:ASN:HB2	9:A:2272:HOH:O	2.12	0.50
1:A:40:ARG:NH1	9:A:2031:HOH:O	2.33	0.50
1:A:110:LEU:HD21	1:A:475:ALA:HB2	1.94	0.50
1:A:383:GLU:O	1:A:387:GLU:CG	2.60	0.49
1:A:406:THR:HG22	1:A:493:PHE:CD1	2.48	0.49
1:A:339:LYS:O	1:A:431:PRO:HG3	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:TRP:O	1:A:52:TRP:CD1	2.66	0.48
1:A:40:ARG:HB2	9:A:2032:HOH:O	2.13	0.48
1:A:231:TRP:CE3	4:A:1532:TN6:H21C	2.48	0.48
8:A:1542:NAG:H83	9:A:2050:HOH:O	2.14	0.48
1:A:352:GLU:HA	1:A:355:LYS:HE3	1.95	0.48
1:A:253:SER:O	1:A:254:ARG:HD3	2.13	0.47
1:A:26:THR:HB	1:A:99:ILE:HG12	1.95	0.47
1:A:448:LEU:N	1:A:449:PRO:CD	2.77	0.47
1:A:50:THR:O	1:A:51:LYS:CG	2.60	0.47
1:A:377:VAL:N	1:A:378:ASP:HA	2.29	0.47
1:A:355:LYS:HD3	9:A:2234:HOH:O	2.15	0.47
1:A:378:ASP:O	1:A:380:GLN:N	2.48	0.47
1:A:496:THR:OG1	9:A:2320:HOH:O	2.20	0.47
1:A:347:ARG:HB2	1:A:385:TYR:CZ	2.50	0.46
1:A:495:SER:O	1:A:496:THR:CB	2.64	0.46
1:A:424:ARG:CZ	1:A:428:LEU:HD12	2.46	0.46
1:A:205:SER:O	1:A:208:LEU:HB2	2.15	0.46
1:A:267:LYS:HD2	1:A:267:LYS:HA	1.60	0.46
1:A:38:LEU:HD23	1:A:90:GLU:HB2	1.97	0.45
1:A:67:GLN:O	1:A:69:ILE:HD12	2.16	0.45
1:A:227:PHE:CD2	1:A:227:PHE:C	2.89	0.45
1:A:49:LEU:HD12	1:A:49:LEU:HA	1.75	0.45
1:A:519:CYS:O	1:A:523:THR:HB	2.16	0.45
1:A:282:TYR:CD1	1:A:282:TYR:C	2.83	0.45
1:A:333:GLY:O	1:A:356:ILE:HG13	2.17	0.45
1:A:363:GLU:O	1:A:367:GLU:HG3	2.17	0.45
1:A:320:GLY:CA	1:A:419:TYR:CE1	2.86	0.44
1:A:159:ASN:HA	1:A:160:PRO:HD3	1.89	0.44
8:A:1542:NAG:H2	8:A:1542:NAG:H83	1.78	0.44
1:A:246:LEU:HD12	1:A:246:LEU:HA	1.80	0.44
1:A:311:GLN:NE2	9:A:2200:HOH:O	2.44	0.43
1:A:462:ILE:HD12	1:A:462:ILE:HG23	1.80	0.43
1:A:38:LEU:CD2	1:A:90:GLU:HB2	2.48	0.43
1:A:323:LYS:HB3	1:A:436:VAL:HB	1.99	0.43
1:A:106:ASN:HB2	7:A:1540:NAG:H83	1.99	0.43
1:A:240:ARG:O	1:A:241:ASN:C	2.54	0.43
1:A:274:LEU:O	1:A:278:PHE:HE2	1.97	0.43
1:A:46:PRO:HB2	1:A:173:LEU:HD23	2.01	0.43
1:A:281:PRO:HG3	6:A:1545:NAG:H83	2.00	0.43
1:A:231:TRP:CD2	4:A:1532:TN6:H21C	2.54	0.43
1:A:502:THR:O	1:A:508:THR:HB	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:SER:HA	1:A:211:PRO:HD2	1.70	0.43
1:A:457:THR:OG1	1:A:460:GLU:HG3	2.19	0.42
1:A:209:LEU:HD23	1:A:209:LEU:HA	1.80	0.42
1:A:341:ASN:C	1:A:341:ASN:OD1	2.57	0.42
1:A:44:LYS:HB3	1:A:44:LYS:HE3	1.93	0.42
1:A:200:GLY:O	1:A:203:SER:HB2	2.20	0.42
1:A:266:ASN:HB3	9:A:2173:HOH:O	2.19	0.42
1:A:159:ASN:OD1	1:A:159:ASN:C	2.58	0.42
1:A:33:TYR:OH	1:A:170:ASP:HB3	2.20	0.42
1:A:157:PRO:HD2	1:A:240:ARG:CD	2.49	0.42
1:A:501:LEU:HD12	1:A:510:ILE:HD13	2.02	0.42
1:A:169:PHE:CE1	1:A:298:PHE:HB2	2.55	0.41
1:A:56:TRP:C	1:A:56:TRP:CD1	2.93	0.41
1:A:137:GLU:OE2	1:A:465:ARG:NH2	2.51	0.41
1:A:328:ALA:HA	1:A:434:MET:HE3	1.97	0.41
1:A:253:SER:C	1:A:254:ARG:HD3	2.41	0.41
1:A:506:GLU:H	1:A:506:GLU:HG3	1.66	0.41
1:A:299:LEU:HD23	1:A:299:LEU:HA	1.68	0.41
1:A:358:PHE:N	1:A:359:PRO:CD	2.84	0.41
1:A:452:ARG:O	1:A:453:ARG:C	2.58	0.41
1:A:214[A]:HIS:NE2	9:A:2154:HOH:O	2.37	0.41
1:A:268:ASP:O	1:A:269:PRO:C	2.59	0.40
1:A:73:PHE:O	1:A:76:PHE:HB3	2.21	0.40
1:A:310:GLY:HA3	1:A:412:TRP:CE2	2.56	0.40
1:A:255:GLU:CD	1:A:255:GLU:H	2.25	0.40
1:A:169:PHE:CZ	1:A:298:PHE:HB2	2.57	0.40
1:A:312:PHE:CD1	1:A:409:PHE:CE1	3.10	0.40
1:A:165:ASN:OD1	1:A:292:PRO:HA	2.22	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	527/529 (100%)	489 (93%)	33 (6%)	5 (1%)	21 18

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	VAL
1	A	453	ARG
1	A	496	THR
1	A	506	GLU
1	A	51	LYS

### 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	453/454 (100%)	421 (93%)	32 (7%)	18 17

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	9	LYS
1	A	38	LEU
1	A	53	SER
1	A	69	ILE
1	A	99	ILE
1	A	105	LYS
1	A	144	MET
1	A	154	LEU
1	A	156	LEU
1	A	195	PHE
1	A	255	GLU
1	A	258	THR
1	A	259	GLU
1	A	268	ASP
1	A	278	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	282	TYR
1	A	286	LEU
1	A	287	SER
1	A	361	VAL
1	A	363	GLU
1	A	375	ASP
1	A	377	VAL
1	A	380	GLN
1	A	387	GLU
1	A	428	LEU
1	A	454	ASP
1	A	455	GLN
1	A	486	ASN
1	A	506	GLU
1	A	511	MET
1	A	518	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	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 ⓘ

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	14,14,15	1.19	2 (14%)	15,19,21	1.60	3 (20%)
6	NAG	A	1538	6	14,14,15	0.86	1 (7%)	15,19,21	1.95	5 (33%)
6	FUL	A	1539	6	10,10,11	0.91	0	14,14,16	4.31	6 (42%)
7	NAG	A	1540	1,7	14,14,15	0.84	1 (7%)	15,19,21	2.39	7 (46%)
7	FUL	A	1541	7	10,10,11	0.81	0	14,14,16	2.77	7 (50%)
6	NAG	A	1545	1,6	14,14,15	0.78	0	15,19,21	1.87	2 (13%)
6	NAG	A	1546	6	14,14,15	0.41	0	15,19,21	1.96	4 (26%)
6	FUL	A	1547	6	10,10,11	0.71	0	14,14,16	3.23	7 (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
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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1537	NAG	O5-C1	-2.81	1.39	1.43
6	A	1538	NAG	O5-C1	-2.38	1.39	1.43
6	A	1537	NAG	C2-N2	-2.27	1.42	1.46
7	A	1540	NAG	C1-C2	2.38	1.55	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1539	FUL	C1-C2-C3	-12.98	94.19	109.54
6	A	1547	FUL	C1-C2-C3	-7.05	101.20	109.54
6	A	1547	FUL	C1-O5-C5	-6.72	102.00	112.38
6	A	1539	FUL	C1-O5-C5	-6.00	103.11	112.38
7	A	1541	FUL	C1-O5-C5	-5.98	103.14	112.38
6	A	1538	NAG	C1-O5-C5	-4.97	105.95	112.25
7	A	1541	FUL	C1-C2-C3	-4.54	104.17	109.54
6	A	1537	NAG	C3-C2-N2	-4.28	100.31	110.56
7	A	1540	NAG	C3-C4-C5	-4.13	103.00	110.20
6	A	1547	FUL	O5-C1-C2	-3.78	104.73	110.86
7	A	1541	FUL	C2-C3-C4	-3.45	105.18	111.04
6	A	1539	FUL	O5-C1-C2	-3.07	105.87	110.86
7	A	1540	NAG	O7-C7-C8	-2.45	117.57	122.06
6	A	1537	NAG	C3-C4-C5	-2.42	105.99	110.20
6	A	1545	NAG	O7-C7-C8	-2.34	117.76	122.06
7	A	1541	FUL	O5-C1-C2	-2.28	107.17	110.86
6	A	1538	NAG	O6-C6-C5	-2.25	103.91	111.33
6	A	1538	NAG	C3-C2-N2	-2.02	105.73	110.56
6	A	1546	NAG	C6-C5-C4	-2.01	108.06	113.02
6	A	1547	FUL	O2-C2-C1	2.11	113.44	109.21
7	A	1541	FUL	O2-C2-C3	2.24	114.63	110.12
7	A	1541	FUL	O3-C3-C2	2.25	114.07	110.00
6	A	1547	FUL	C3-C4-C5	2.30	113.59	109.72
6	A	1538	NAG	C2-N2-C7	2.45	126.19	123.04
6	A	1538	NAG	O5-C5-C6	2.46	112.68	107.35
6	A	1547	FUL	O2-C2-C3	2.49	115.12	110.12
7	A	1540	NAG	C6-C5-C4	2.49	119.15	113.02
6	A	1546	NAG	O3-C3-C2	2.54	114.15	109.11
6	A	1539	FUL	O5-C5-C6	2.67	110.54	106.13
6	A	1537	NAG	C2-N2-C7	2.72	126.53	123.04
6	A	1539	FUL	C6-C5-C4	2.84	118.67	113.08
6	A	1546	NAG	C2-N2-C7	2.86	126.72	123.04
6	A	1547	FUL	O5-C5-C6	3.02	111.12	106.13
7	A	1540	NAG	O5-C5-C6	3.09	114.05	107.35
7	A	1540	NAG	O4-C4-C5	3.36	118.14	109.24
7	A	1540	NAG	C2-N2-C7	3.43	127.44	123.04
7	A	1541	FUL	C3-C4-C5	3.75	116.04	109.72
7	A	1540	NAG	C8-C7-N2	3.76	123.29	116.11
6	A	1539	FUL	O2-C2-C1	3.89	117.01	109.21
6	A	1546	NAG	C1-O5-C5	4.97	118.56	112.25
6	A	1545	NAG	C1-O5-C5	5.85	119.67	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1540	NAG	1	0
7	A	1541	FUL	1	0
6	A	1545	NAG	1	0

## 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	$\# Z  > 2$
4	TN6	A	1532	1	2,7,8	1.79	1 (50%)	1,8,11	0.70	0
5	SO4	A	1534	-	4,4,4	0.24	0	6,6,6	0.33	0
5	SO4	A	1536	-	4,4,4	0.21	0	6,6,6	0.73	0
8	NAG	A	1542	1	14,14,15	0.57	0	15,19,21	1.81	3 (20%)
8	NAG	A	1543	1	14,14,15	0.82	0	15,19,21	2.06	2 (13%)
8	NAG	A	1544	1	14,14,15	0.47	0	15,19,21	1.82	3 (20%)

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	TN6	A	1532	1	-	0/4/8/10	0/0/0/0
5	SO4	A	1534	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1536	-	-	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	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1532	TN6	C4-C3	2.33	1.63	1.49

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1542	NAG	C2-N2-C7	-4.36	117.44	123.04
8	A	1544	NAG	C1-O5-C5	-4.17	106.96	112.25
8	A	1543	NAG	C4-C3-C2	2.27	114.76	111.23
8	A	1542	NAG	C4-C3-C2	2.61	115.29	111.23
8	A	1544	NAG	O5-C5-C6	2.83	113.48	107.35
8	A	1542	NAG	C3-C4-C5	3.60	116.48	110.20
8	A	1544	NAG	C3-C4-C5	3.81	116.84	110.20
8	A	1543	NAG	C1-O5-C5	6.72	120.78	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1532	TN6	3	0
8	A	1542	NAG	4	0
8	A	1544	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 ⓘ

### 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	527/529 (99%)	0.20	29 (5%)	29 32	17, 34, 58, 76	9 (1%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	378	ASP	5.6
1	A	50	THR	5.2
1	A	379	ASP	5.2
1	A	3	ASP	4.8
1	A	282	TYR	4.4
1	A	380	GLN	4.2
1	A	453	ARG	4.0
1	A	255	GLU	4.0
1	A	256	ASN	3.6
1	A	55	ILE	3.1
1	A	342	ASN	3.1
1	A	51	LYS	3.1
1	A	455	GLN	3.0
1	A	377	VAL	2.9
1	A	40	ARG	2.6
1	A	260	ILE	2.6
1	A	376	TRP	2.5
1	A	266	ASN	2.4
1	A	259	GLU	2.4
1	A	254	ARG	2.4
1	A	240	ARG	2.4
1	A	253	SER	2.3
1	A	278	PHE	2.2
1	A	257	GLU	2.2
1	A	258	THR	2.1
1	A	54	ASP	2.1
1	A	251	GLY	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	52	TRP	2.1
1	A	53	SER	2.1

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

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

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
7	FUL	A	1541	10/11	0.71	0.32	4.89	40,46,47,49	10
6	FUL	A	1547	10/11	0.77	0.29	1.80	71,73,75,77	0
6	NAG	A	1537	14/15	0.95	0.17	-0.13	46,52,58,64	0
6	NAG	A	1545	14/15	0.87	0.25	-	67,72,79,79	0
7	NAG	A	1540	14/15	0.79	0.24	-	54,59,61,64	0
6	FUL	A	1539	10/11	0.73	0.31	-	65,69,73,73	0
6	NAG	A	1546	14/15	0.76	0.39	-	65,76,78,78	0
6	NAG	A	1538	14/15	0.79	0.22	-	62,67,70,70	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
8	NAG	A	1543	14/15	0.70	0.21	4.19	45,60,64,66	0
4	TN6	A	1532	8/9	0.98	0.15	0.22	24,27,28,29	0
3	CL	A	1533	1/1	0.94	0.18	-1.09	71,71,71,71	0
5	SO4	A	1534	5/5	0.96	0.09	-	52,52,57,58	5
3	CL	A	1531	1/1	0.94	0.18	-	58,58,58,58	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	NAG	A	1544	14/15	0.82	0.50	-	82,85,88,88	0
3	CL	A	1535	1/1	0.92	0.11	-	62,62,62,62	0
2	NA	A	1530	1/1	0.99	0.24	-	41,41,41,41	1
5	SO4	A	1536	5/5	0.98	0.20	-	40,42,43,45	5
8	NAG	A	1542	14/15	0.57	0.37	-	73,77,79,82	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.