



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:35 AM GMT

PDB ID : 2XMB  
Title : G117H MUTANT OF HUMAN BUTYRYLCHOLINESTERASE IN COMPLEX WITH SULFATE  
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Deposited on : 2010-07-27  
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 (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

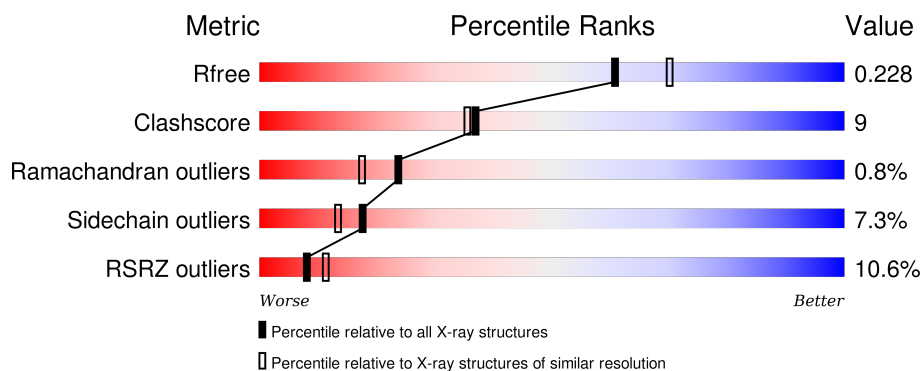
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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	

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	UNX	A	1556	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UNX	A	1563	-	-	-	X
2	UNX	A	1571	-	-	-	X
7	NAG	A	1547	X	-	-	-
7	FUL	A	1549	-	-	-	X
8	FUL	A	1543	-	-	-	X
9	NAG	A	1545	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 4778 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	0	0
			4209	2716	708	770	15			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	117	HIS	GLY	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 UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	23	Total	X	0	0
			23	23		

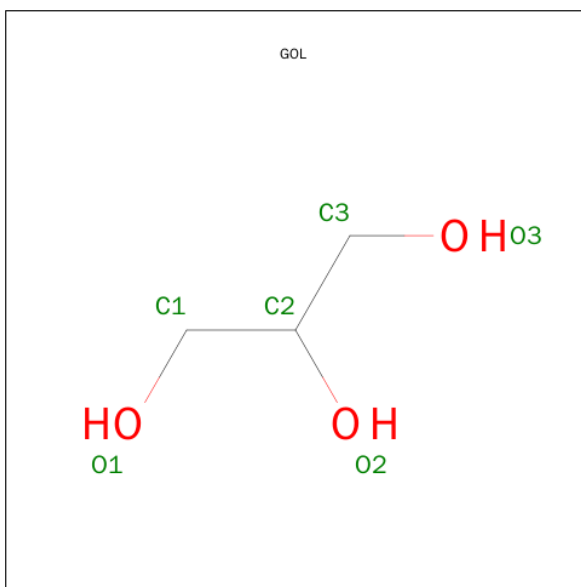
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	Cl	0	0
			7	7		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

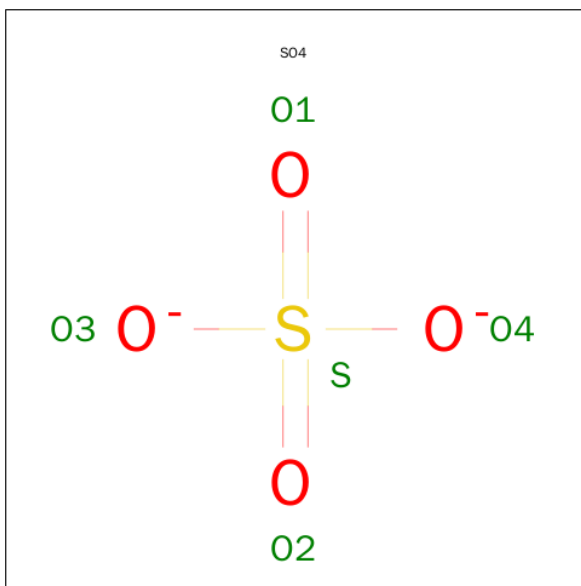
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

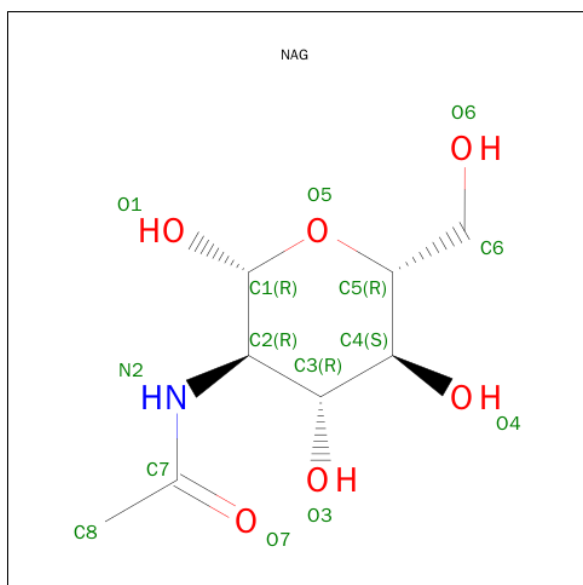
- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 9 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

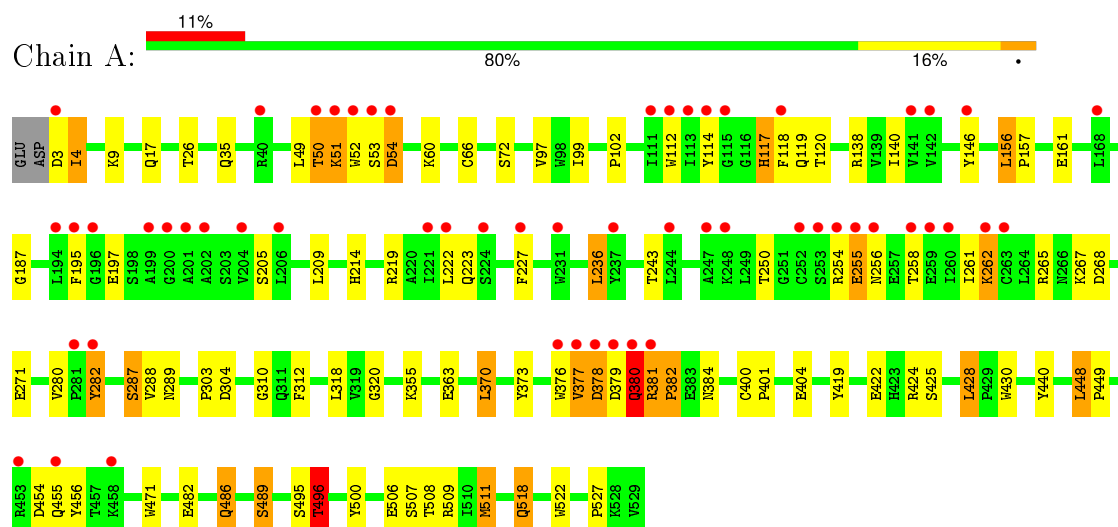
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	380	Total	O	0	0
			380	380		

### 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, $\alpha$ , $\beta$ , $\gamma$	154.80Å 154.80Å 134.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.66 – 2.10 37.66 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (37.66-2.10) 99.7 (37.66-2.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.92 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.168 , 0.208 0.200 , 0.228	Depositor DCC
$R_{free}$ test set	1422 reflections (3.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 47523 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4778	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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: GOL, NAG, CL, UNX, 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	1.15	9/4329 (0.2%)	0.97	9/5877 (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	0	1
7	A	1	0
All	All	1	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	TYR	CD1-CE1	7.86	1.51	1.39
1	A	146	TYR	CD1-CE1	5.84	1.48	1.39
1	A	377	VAL	CA-CB	5.80	1.67	1.54
1	A	404	GLU	CG-CD	5.45	1.60	1.51
1	A	373	TYR	CD2-CE2	5.43	1.47	1.39
1	A	496	THR	CA-CB	5.39	1.67	1.53
1	A	112	TRP	CE3-CZ3	5.38	1.47	1.38
1	A	52	TRP	CE3-CZ3	5.14	1.47	1.38
1	A	118	PHE	CD2-CE2	5.06	1.49	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	ARG	NE-CZ-NH1	-9.60	115.50	120.30
1	A	219	ARG	NE-CZ-NH2	9.06	124.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	254	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	448	LEU	CB-CG-CD2	6.14	121.44	111.00
1	A	496	THR	N-CA-CB	6.10	121.90	110.30
1	A	377	VAL	N-CA-C	-6.08	94.57	111.00
1	A	370	LEU	CA-CB-CG	5.85	128.76	115.30
1	A	66	CYS	CA-CB-SG	-5.09	104.84	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	1547	NAG	C1

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	376	TRP	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	4209	0	4103	78	0
2	A	23	0	0	0	0
3	A	7	0	0	0	0
4	A	1	0	0	0	0
5	A	6	0	8	0	0
6	A	10	0	0	1	0
7	A	76	0	68	1	0
8	A	24	0	22	1	0
9	A	42	0	39	1	0
10	A	380	0	0	18	0
All	All	4778	0	4240	81	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 9.

All (81) 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)
8:A:1543:FUL:O3	10:A:2370:HOH:O	1.63	1.15
1:A:282:TYR:HD2	1:A:282:TYR:O	1.34	1.06
1:A:379:ASP:HB3	1:A:381:ARG:HB2	1.43	1.00
1:A:282:TYR:O	1:A:282:TYR:CD2	2.23	0.92
1:A:518:GLN:H	1:A:518:GLN:NE2	1.70	0.89
1:A:518:GLN:H	1:A:518:GLN:HE21	0.90	0.89
1:A:156:LEU:HD13	1:A:243:THR:HG21	1.56	0.85
1:A:363:GLU:HG2	10:A:2247:HOH:O	1.76	0.84
1:A:518:GLN:HE21	1:A:518:GLN:N	1.74	0.84
1:A:267:LYS:HE3	1:A:271:GLU:OE1	1.79	0.82
1:A:379:ASP:CB	1:A:381:ARG:HB2	2.12	0.80
1:A:262:LYS:HE3	10:A:2183:HOH:O	1.80	0.79
1:A:156:LEU:CD1	1:A:243:THR:HG21	2.16	0.74
1:A:156:LEU:HD22	1:A:261:ILE:HD11	1.67	0.74
1:A:255:GLU:CD	1:A:255:GLU:H	1.93	0.72
1:A:4:ILE:H	1:A:4:ILE:HD12	1.57	0.70
1:A:4:ILE:N	1:A:4:ILE:HD12	2.08	0.68
1:A:304:ASP:OD1	10:A:2207:HOH:O	2.12	0.68
1:A:50:THR:O	1:A:51:LYS:HE2	1.99	0.62
1:A:3:ASP:N	10:A:2001:HOH:O	2.33	0.61
1:A:119:GLN:NE2	1:A:288:VAL:HG13	2.16	0.60
1:A:428:LEU:HD21	1:A:440:TYR:CD2	2.38	0.59
1:A:522:TRP:O	1:A:527:PRO:HD3	2.03	0.58
1:A:486:GLN:NE2	1:A:486:GLN:HA	2.18	0.58
1:A:508:THR:HG21	10:A:2145:HOH:O	2.03	0.58
9:A:1545:NAG:H62	10:A:2376:HOH:O	2.03	0.57
1:A:377:VAL:HA	1:A:378:ASP:HB2	1.86	0.57
1:A:428:LEU:HD21	1:A:440:TYR:CG	2.39	0.56
1:A:209:LEU:HD23	1:A:312:PHE:HB3	1.87	0.56
7:A:1540:NAG:H4	10:A:2364:HOH:O	2.05	0.56
1:A:377:VAL:HA	1:A:378:ASP:CB	2.37	0.55
1:A:262:LYS:CE	10:A:2183:HOH:O	2.46	0.54
1:A:120:THR:HG21	10:A:2107:HOH:O	2.08	0.54
1:A:320:GLY:HA3	1:A:419:TYR:CE1	2.43	0.54
1:A:161:GLU:OE1	1:A:265:ARG:NH1	2.40	0.54
1:A:54:ASP:HB3	10:A:2035:HOH:O	2.07	0.54
1:A:50:THR:O	1:A:51:LYS:CE	2.57	0.53
1:A:53:SER:O	1:A:54:ASP:OD2	2.28	0.52
1:A:214:HIS:HE1	10:A:2216:HOH:O	1.92	0.50
1:A:495:SER:O	1:A:496:THR:CB	2.60	0.50
1:A:489:SER:HB3	10:A:2322:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:PHE:CD2	1:A:227:PHE:C	2.85	0.49
1:A:157:PRO:HG2	1:A:236:LEU:HG	1.94	0.49
1:A:255:GLU:OE1	1:A:256:ASN:N	2.47	0.48
1:A:197:GLU:HA	1:A:223:GLN:O	2.14	0.48
1:A:250:THR:HB	1:A:267:LYS:HE2	1.94	0.47
1:A:289:ASN:ND2	10:A:2196:HOH:O	2.46	0.47
1:A:280:VAL:HG23	1:A:289:ASN:HD22	1.81	0.46
1:A:310:GLY:HA2	1:A:312:PHE:CE2	2.51	0.46
1:A:495:SER:O	1:A:496:THR:OG1	2.30	0.46
1:A:303:PRO:HD2	10:A:2207:HOH:O	2.16	0.45
1:A:400:CYS:N	1:A:401:PRO:CD	2.80	0.45
1:A:255:GLU:CD	1:A:255:GLU:N	2.63	0.45
1:A:320:GLY:HA3	1:A:419:TYR:CD1	2.51	0.45
1:A:500:TYR:CZ	1:A:511:MET:HB2	2.51	0.45
1:A:507:SER:O	1:A:507:SER:OG	2.27	0.45
1:A:51:LYS:HB3	1:A:51:LYS:HE2	1.77	0.44
1:A:4:ILE:N	1:A:4:ILE:CD1	2.76	0.44
1:A:428:LEU:CD2	1:A:440:TYR:CD2	3.01	0.44
1:A:17:GLN:NE2	1:A:26:THR:OG1	2.50	0.44
1:A:227:PHE:CE2	1:A:303:PRO:HB2	2.52	0.44
1:A:54:ASP:C	1:A:54:ASP:OD2	2.56	0.44
1:A:449:PRO:HA	1:A:456:TYR:CD1	2.53	0.43
1:A:140:ILE:HD12	1:A:187:GLY:CA	2.48	0.43
1:A:117:HIS:ND1	6:A:1538:SO4:O3	2.51	0.43
1:A:102:PRO:O	1:A:138:ARG:NH2	2.48	0.43
1:A:318:LEU:HD23	1:A:318:LEU:C	2.40	0.43
1:A:500:TYR:CE1	1:A:511:MET:HB2	2.54	0.42
1:A:205:SER:HB3	1:A:222:LEU:HD21	2.01	0.42
1:A:428:LEU:HD12	1:A:430:TRP:HB2	2.02	0.42
1:A:380:GLN:HA	1:A:384:ASN:ND2	2.34	0.42
1:A:267:LYS:HD2	1:A:267:LYS:HA	1.92	0.42
1:A:49:LEU:HD12	1:A:50:THR:H	1.84	0.42
1:A:486:GLN:HE21	1:A:486:GLN:HA	1.85	0.41
1:A:378:ASP:O	1:A:379:ASP:HB2	2.20	0.41
1:A:509:ARG:HB2	10:A:2340:HOH:O	2.19	0.41
1:A:287:SER:HB3	10:A:2196:HOH:O	2.21	0.41
1:A:97:VAL:CG1	1:A:99:ILE:HD11	2.51	0.41
1:A:425:SER:HB3	1:A:428:LEU:HD23	2.03	0.40
1:A:381:ARG:HA	1:A:382:PRO:HD2	1.90	0.40
1:A:355:LYS:HE2	10:A:2245:HOH:O	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	525/529 (99%)	502 (96%)	19 (4%)	4 (1%)	24 17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	496	THR
1	A	378	ASP
1	A	380	GLN
1	A	381	ARG

### 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	453/455 (100%)	420 (93%)	33 (7%)	17 13

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	9	LYS
1	A	35	GLN
1	A	50	THR
1	A	51	LYS
1	A	54	ASP
1	A	60	LYS

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Mol	Chain	Res	Type
1	A	72	SER
1	A	117	HIS
1	A	156	LEU
1	A	195	PHE
1	A	236	LEU
1	A	255	GLU
1	A	258	THR
1	A	262	LYS
1	A	268	ASP
1	A	282	TYR
1	A	287	SER
1	A	370	LEU
1	A	380	GLN
1	A	382	PRO
1	A	422	GLU
1	A	428	LEU
1	A	448	LEU
1	A	454	ASP
1	A	455	GLN
1	A	471	TRP
1	A	482	GLU
1	A	486	GLN
1	A	489	SER
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 (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	172	GLN
1	A	289	ASN
1	A	311	GLN
1	A	380	GLN
1	A	455	GLN
1	A	486	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 ⓘ

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$
7	NAG	A	1539	1,7	14,14,15	1.54	2 (14%)	15,19,21	2.72	8 (53%)
7	NAG	A	1540	7	14,14,15	0.50	0	15,19,21	2.03	5 (33%)
7	FUL	A	1541	7	10,10,11	1.11	1 (10%)	14,14,16	3.90	8 (57%)
8	NAG	A	1542	1,8	14,14,15	1.30	1 (7%)	15,19,21	2.16	4 (26%)
8	FUL	A	1543	8	10,10,11	1.08	0	14,14,16	3.92	6 (42%)
7	NAG	A	1547	1,7	14,14,15	0.98	1 (7%)	15,19,21	2.28	5 (33%)
7	NAG	A	1548	7	14,14,15	1.46	2 (14%)	15,19,21	2.91	6 (40%)
7	FUL	A	1549	7	10,10,11	0.72	0	14,14,16	1.22	2 (14%)

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
7	NAG	A	1539	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1540	7	-	0/6/23/26	0/1/1/1
7	FUL	A	1541	7	-	0/0/17/20	0/1/1/1
8	NAG	A	1542	1,8	-	0/6/23/26	0/1/1/1
8	FUL	A	1543	8	-	0/0/17/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	1547	1,7	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	A	1548	7	-	0/6/23/26	0/1/1/1
7	FUL	A	1549	7	-	0/0/17/20	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1539	NAG	O5-C1	-3.46	1.37	1.43
7	A	1539	NAG	C2-N2	-3.15	1.40	1.46
7	A	1547	NAG	C4-C5	2.01	1.57	1.53
7	A	1541	FUL	C4-C3	2.15	1.58	1.52
7	A	1548	NAG	C2-N2	2.24	1.50	1.46
8	A	1542	NAG	C1-C2	3.63	1.57	1.52
7	A	1548	NAG	C1-C2	4.02	1.58	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1543	FUL	C1-C2-C3	-13.32	93.78	109.54
7	A	1541	FUL	C1-C2-C3	-8.97	98.93	109.54
7	A	1541	FUL	C1-O5-C5	-6.38	102.53	112.38
7	A	1539	NAG	C3-C4-C5	-5.56	100.51	110.20
7	A	1541	FUL	O5-C1-C2	-4.35	103.79	110.86
8	A	1542	NAG	O7-C7-C8	-3.81	115.07	122.06
7	A	1539	NAG	C3-C2-N2	-3.59	101.97	110.56
7	A	1540	NAG	O6-C6-C5	-3.21	100.73	111.33
7	A	1540	NAG	C6-C5-C4	-2.80	106.11	113.02
8	A	1543	FUL	O4-C4-C3	-2.64	104.39	110.34
7	A	1539	NAG	O7-C7-N2	-2.60	116.55	121.86
7	A	1539	NAG	O4-C4-C3	-2.56	104.57	110.34
8	A	1542	NAG	C3-C4-C5	-2.25	106.27	110.20
7	A	1548	NAG	O7-C7-C8	-2.23	117.97	122.06
8	A	1543	FUL	C2-C3-C4	-2.23	107.26	111.04
7	A	1540	NAG	O7-C7-C8	-2.18	118.06	122.06
8	A	1543	FUL	C6-C5-C4	-2.09	108.97	113.08
7	A	1541	FUL	O4-C4-C3	2.03	114.91	110.34
7	A	1548	NAG	O7-C7-N2	2.10	126.15	121.86
7	A	1548	NAG	C4-C3-C2	2.15	114.57	111.23
7	A	1541	FUL	C2-C3-C4	2.16	114.70	111.04
8	A	1543	FUL	O2-C2-C1	2.23	113.69	109.21
7	A	1547	NAG	C3-C2-N2	2.31	116.09	110.56
7	A	1540	NAG	O3-C3-C2	2.38	113.82	109.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1547	NAG	O4-C4-C5	2.43	115.69	109.24
7	A	1549	FUL	C3-C4-C5	2.45	113.85	109.72
7	A	1549	FUL	O5-C5-C4	2.76	114.31	109.53
7	A	1547	NAG	C1-O5-C5	2.83	115.84	112.25
7	A	1547	NAG	O4-C4-C3	2.90	116.87	110.34
8	A	1543	FUL	C3-C4-C5	3.05	114.87	109.72
7	A	1539	NAG	C1-O5-C5	3.14	116.23	112.25
7	A	1539	NAG	O6-C6-C5	3.24	122.02	111.33
7	A	1548	NAG	C3-C4-C5	3.33	116.01	110.20
7	A	1541	FUL	O2-C2-C1	3.44	116.09	109.21
7	A	1539	NAG	C2-N2-C7	3.48	127.51	123.04
7	A	1539	NAG	C6-C5-C4	3.67	122.06	113.02
8	A	1542	NAG	C8-C7-N2	3.86	123.50	116.11
7	A	1541	FUL	O5-C5-C6	4.29	113.23	106.13
8	A	1542	NAG	O5-C5-C6	4.68	117.47	107.35
7	A	1541	FUL	C3-C4-C5	4.80	117.80	109.72
7	A	1540	NAG	C1-O5-C5	4.92	118.49	112.25
7	A	1547	NAG	C2-N2-C7	6.07	130.84	123.04
7	A	1548	NAG	C1-O5-C5	6.07	119.95	112.25
7	A	1548	NAG	C2-N2-C7	7.80	133.06	123.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	1547	NAG	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1540	NAG	1	0
8	A	1543	FUL	1	0

## 5.6 Ligand geometry

Of 37 ligands modelled in this entry, 23 are unknown and 8 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
5	GOL	A	1536	-	5,5,5	0.58	0	5,5,5	0.94	0
6	SO4	A	1537	-	4,4,4	1.32	0	6,6,6	0.83	0
6	SO4	A	1538	-	4,4,4	0.53	0	6,6,6	1.11	0
9	NAG	A	1544	1	14,14,15	1.17	1 (7%)	15,19,21	4.17	8 (53%)
9	NAG	A	1545	1	14,14,15	0.54	0	15,19,21	3.01	1 (6%)
9	NAG	A	1546	1	14,14,15	1.11	1 (7%)	15,19,21	2.21	5 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	1536	-	-	0/4/4/4	0/0/0/0
6	SO4	A	1537	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1538	-	-	0/0/0/0	0/0/0/0
9	NAG	A	1544	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1545	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1546	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1546	NAG	C1-C2	2.43	1.55	1.52
9	A	1544	NAG	O5-C1	2.78	1.48	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1544	NAG	C2-N2-C7	-4.91	116.73	123.04
9	A	1544	NAG	O3-C3-C2	-3.44	102.30	109.11
9	A	1544	NAG	O7-C7-C8	-2.31	117.82	122.06
9	A	1546	NAG	C3-C4-C5	-2.10	106.53	110.20
9	A	1544	NAG	C8-C7-N2	2.11	120.14	116.11
9	A	1546	NAG	O4-C4-C5	2.36	115.50	109.24
9	A	1544	NAG	C4-C3-C2	2.38	114.93	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1546	NAG	O5-C5-C6	3.12	114.11	107.35
9	A	1544	NAG	C3-C4-C5	3.43	116.18	110.20
9	A	1544	NAG	C3-C2-N2	3.60	119.17	110.56
9	A	1546	NAG	C2-N2-C7	3.90	128.05	123.04
9	A	1546	NAG	C1-O5-C5	5.34	119.03	112.25
9	A	1545	NAG	C1-O5-C5	11.10	126.34	112.25
9	A	1544	NAG	C1-O5-C5	13.30	129.13	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1538	SO4	1	0
9	A	1545	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%)	0.39	56 (10%) 8 11	21, 37, 71, 110	5 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	377	VAL	7.9
1	A	379	ASP	6.0
1	A	282	TYR	5.6
1	A	50	THR	4.6
1	A	281	PRO	4.4
1	A	112	TRP	3.9
1	A	113	ILE	3.9
1	A	378	ASP	3.8
1	A	255	GLU	3.7
1	A	111	ILE	3.5
1	A	453	ARG	3.4
1	A	199	ALA	3.3
1	A	260	ILE	3.2
1	A	194	LEU	3.1
1	A	195	PHE	3.1
1	A	455	GLN	3.0
1	A	196	GLY	2.9
1	A	201	ALA	2.9
1	A	259	GLU	2.9
1	A	244	LEU	2.9
1	A	258	THR	2.8
1	A	204	VAL	2.8
1	A	202	ALA	2.7
1	A	52	TRP	2.7
1	A	231	TRP	2.7
1	A	222	LEU	2.7
1	A	53	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	206	LEU	2.7
1	A	380	GLN	2.7
1	A	168	LEU	2.6
1	A	221	ILE	2.6
1	A	262	LYS	2.6
1	A	142	VAL	2.6
1	A	54	ASP	2.6
1	A	237	TYR	2.6
1	A	40	ARG	2.5
1	A	227	PHE	2.5
1	A	114	TYR	2.5
1	A	247	ALA	2.5
1	A	200	GLY	2.5
1	A	115	GLY	2.4
1	A	146	TYR	2.4
1	A	51	LYS	2.4
1	A	252	CYS	2.4
1	A	254	ARG	2.4
1	A	376	TRP	2.4
1	A	256	ASN	2.3
1	A	224	SER	2.3
1	A	253	SER	2.2
1	A	263	CYS	2.2
1	A	381	ARG	2.2
1	A	458	LYS	2.2
1	A	141	VAL	2.1
1	A	118	PHE	2.1
1	A	3	ASP	2.1
1	A	248	LYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
8	FUL	A	1543	10/11	0.86	0.24	4.86	38,45,47,47	10
7	FUL	A	1549	10/11	0.79	0.48	3.48	105,106,107,109	0
7	NAG	A	1539	14/15	0.96	0.12	0.22	41,54,60,70	0
7	FUL	A	1541	10/11	0.83	0.31	-	76,80,83,84	0
7	NAG	A	1548	14/15	0.54	0.50	-	107,110,111,112	0
8	NAG	A	1542	14/15	0.88	0.12	-	50,56,58,65	0
7	NAG	A	1540	14/15	0.92	0.20	-	68,74,77,78	0
7	NAG	A	1547	14/15	0.85	0.36	-	80,95,102,102	0

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
2	UNX	A	1571	1/1	0.94	0.48	7.31	39,39,39,39	0
2	UNX	A	1563	1/1	0.82	0.56	4.51	28,28,28,28	0
2	UNX	A	1556	1/1	0.90	0.27	2.98	40,40,40,40	0
9	NAG	A	1545	14/15	0.83	0.14	2.78	42,58,68,73	0
5	GOL	A	1536	6/6	0.95	0.12	1.31	42,44,50,51	0
2	UNX	A	1558	1/1	0.72	0.21	1.00	45,45,45,45	0
6	SO4	A	1538	5/5	0.96	0.24	0.49	34,41,44,45	5
2	UNX	A	1568	1/1	0.93	0.17	0.17	58,58,58,58	0
2	UNX	A	1575	1/1	0.81	0.31	-	31,31,31,31	0
2	UNX	A	1562	1/1	0.73	0.56	-	57,57,57,57	0
2	UNX	A	1550	1/1	0.81	0.21	-	35,35,35,35	0
3	CL	A	1564	1/1	0.79	0.23	-	77,77,77,77	0
2	UNX	A	1560	1/1	0.52	0.81	-	47,47,47,47	0
2	UNX	A	1574	1/1	0.87	0.17	-	41,41,41,41	0
3	CL	A	1565	1/1	0.77	0.24	-	82,82,82,82	0
2	UNX	A	1570	1/1	0.98	0.46	-	39,39,39,39	0
2	UNX	A	1572	1/1	0.95	0.31	-	37,37,37,37	0
3	CL	A	1532	1/1	0.71	0.07	-	81,81,81,81	0
2	UNX	A	1559	1/1	0.89	0.44	-	33,33,33,33	0
9	NAG	A	1544	14/15	0.72	0.33	-	63,71,73,74	0
2	UNX	A	1557	1/1	0.64	0.46	-	49,49,49,49	0
3	CL	A	1531	1/1	0.76	0.06	-	78,78,78,78	0
2	UNX	A	1554	1/1	0.67	0.33	-	45,45,45,45	0
2	UNX	A	1561	1/1	0.97	0.33	-	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	A	1534	1/1	0.92	0.22	-	60,60,60,60	0
3	CL	A	1530	1/1	0.93	0.08	-	76,76,76,76	0
2	UNX	A	1569	1/1	0.89	0.51	-	48,48,48,48	0
4	NA	A	1533	1/1	0.30	0.52	-	93,93,93,93	0
6	SO4	A	1537	5/5	0.97	0.14	-	20,26,29,32	5
2	UNX	A	1555	1/1	0.94	0.11	-	37,37,37,37	0
2	UNX	A	1566	1/1	0.78	0.59	-	40,40,40,40	0
3	CL	A	1535	1/1	0.95	0.16	-	60,60,60,60	0
9	NAG	A	1546	14/15	0.68	0.48	-	78,89,91,92	0
2	UNX	A	1567	1/1	0.35	0.47	-	35,35,35,35	0
2	UNX	A	1552	1/1	0.91	0.25	-	47,47,47,47	0
2	UNX	A	1553	1/1	0.79	0.44	-	38,38,38,38	0
2	UNX	A	1551	1/1	0.65	0.68	-	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.