



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:39 AM GMT

PDB ID : 2XUP  
Title : CRYSTAL STRUCTURE OF THE MACHE-Y337A MUTANT IN COMPLEX WITH SOAKED TZ2PA6 SYN INHIBITOR  
Authors : Bourne, Y.; Radic, Z.; Taylor, P.; Marchot, P.  
Deposited on : 2010-10-19  
Resolution : 2.70 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

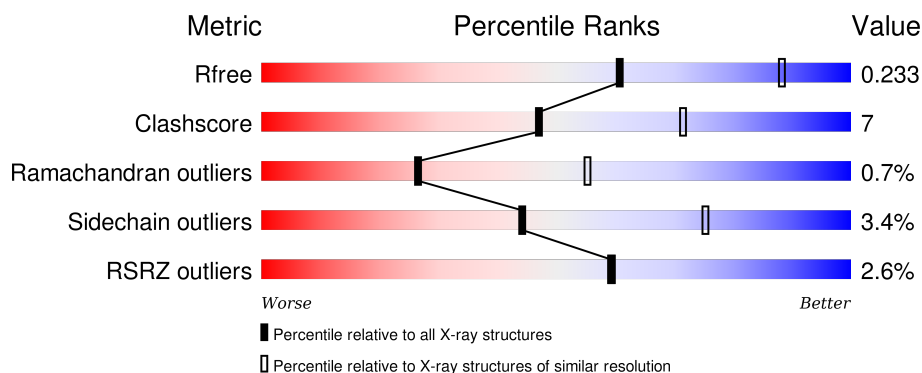
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	543	<div> <div>3%</div> <div>84%</div> <div>14%</div> <div>..</div> </div>
1	B	543	<div> <div>2%</div> <div>84%</div> <div>14%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	1544	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8693 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.

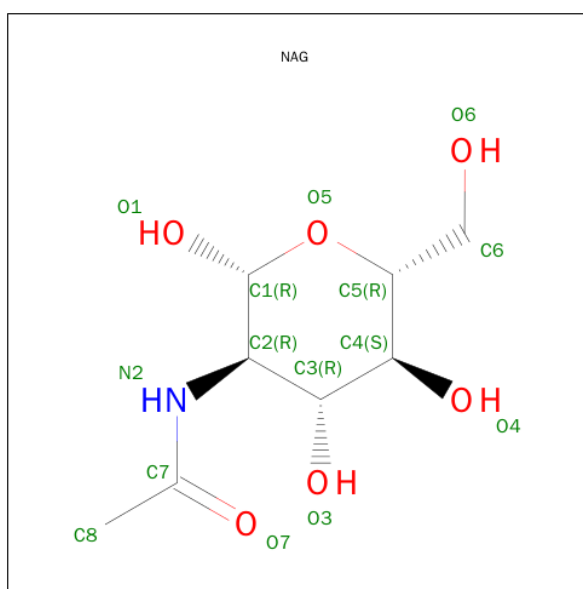
- Molecule 1 is a protein called ACETYLCHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	2	0
			4209	2701	731	763	14			
1	B	538	Total	C	N	O	S	0	3	0
			4203	2698	726	765	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	337	ALA	TYR	ENGINEERED MUTATION	UNP P21836
B	337	ALA	TYR	ENGINEERED MUTATION	UNP P21836

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



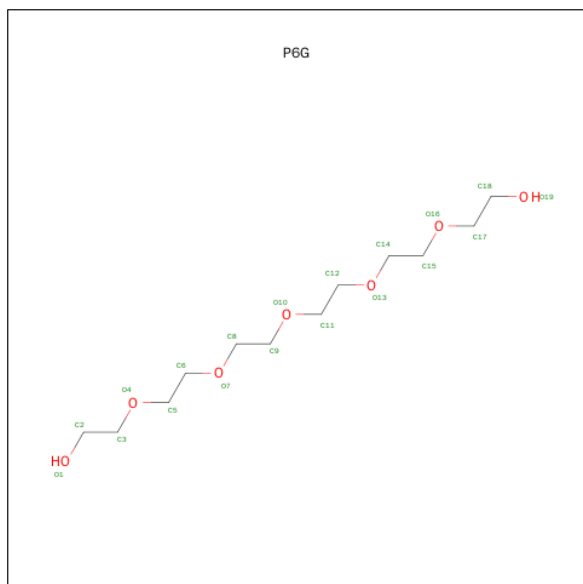
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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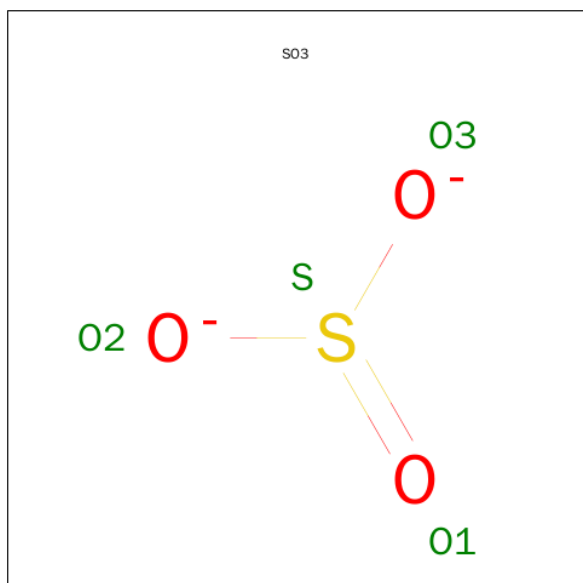
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			1	1		

- Molecule 3 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula:  $C_{12}H_{26}O_7$ ).



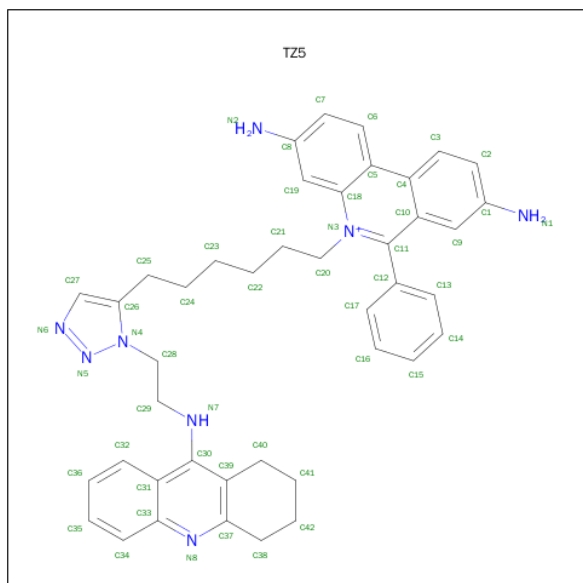
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			19	12	7		

- Molecule 4 is SULFITE ION (three-letter code: SO3) (formula:  $O_3S$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 4 3 1	0	0
4	B	1	Total O S 4 3 1	0	0

- Molecule 5 is 3,8-DIAMINO-6-PHENYL-5-[6-[1-[2-[(1,2,3,4-TETRAHYDRO-9-ACRIDINYL)AMINO]ETHYL]-1H-1,2,3-TRIAZOL-5-YL]HEXYL]-PHENANTHRIDINIUM (three-letter code: TZ5) (formula: C<sub>42</sub>H<sub>45</sub>N<sub>8</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N 100 84 16	0	1
5	B	1	Total C N 100 84 16	0	1

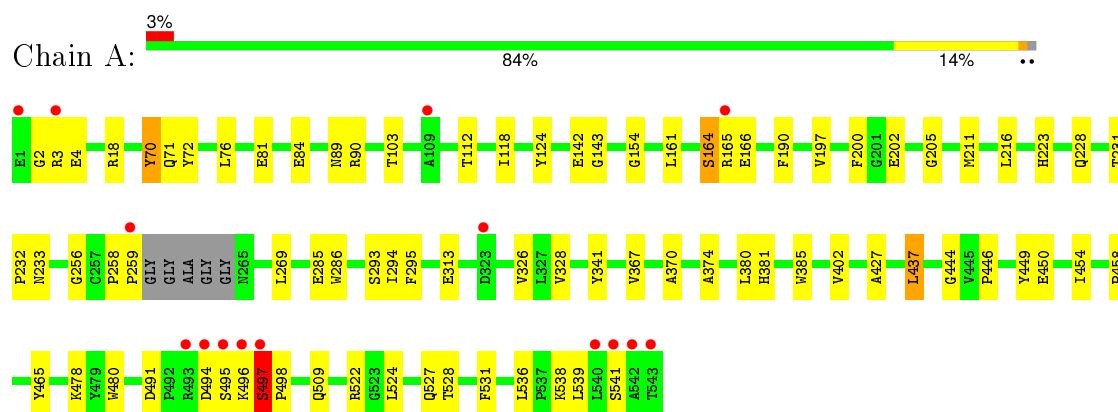
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	24	Total O 24 24	0	0
6	B	15	Total O 15 15	0	0

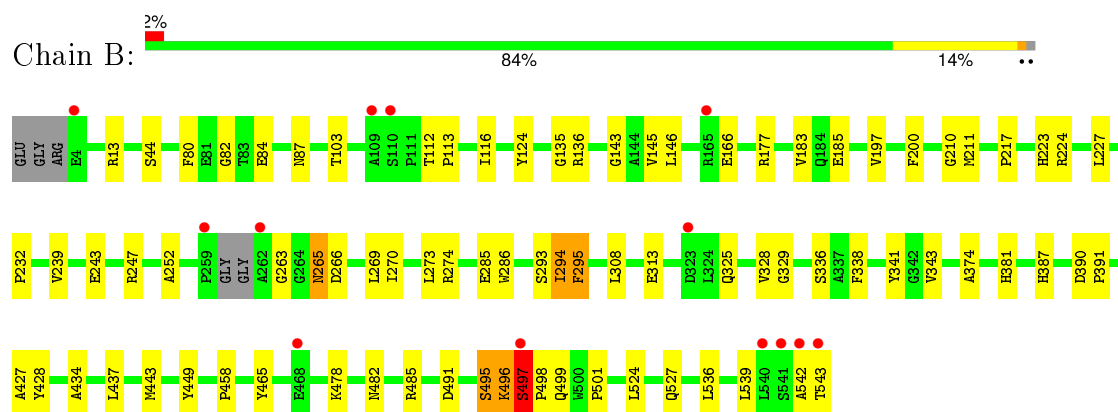
### 3 Residue-property plots

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: ACETYLCHOLINESTERASE



#### • Molecule 1: ACETYLCHOLINESTERASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.74Å 110.00Å 227.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 19.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.70) 99.8 (19.98-2.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.69 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.203 , 0.232 0.205 , 0.233	Depositor DCC
$R_{free}$ test set	1123 reflections (2.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.1	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 38.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 54932 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8693	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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: SO3, TZ5, NAG, P6G

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	0.54	0/4338	0.67	1/5930 (0.0%)
1	B	0.50	0/4337	0.62	0/5929
All	All	0.52	0/8675	0.64	1/11859 (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	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	71	GLN	N-CA-CB	-6.01	99.77	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	70	TYR	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	4093	53	0
1	B	4203	0	4083	48	0
2	A	15	0	13	0	0
3	A	19	0	26	6	0
4	A	4	0	0	1	0
4	B	4	0	0	0	0
5	A	100	0	90	22	0
5	B	100	0	90	27	0
6	A	24	0	0	0	0
6	B	15	0	0	0	0
All	All	8693	0	8395	127	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 7.

All (127) 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:B:286[B]:TRP:HB2	5:B:1545[B]:TZ5:C6	1.79	1.13
5:B:1545[B]:TZ5:C19	5:B:1545[B]:TZ5:H211	1.77	1.06
5:B:1545[B]:TZ5:C21	5:B:1545[B]:TZ5:H19	1.86	1.03
1:A:286[B]:TRP:HB2	5:A:1548[B]:TZ5:C6	1.96	0.96
1:B:497:SER:HB2	1:B:498:PRO:C	1.87	0.95
1:A:72:TYR:CD1	5:A:1548[A]:TZ5:H16	2.04	0.93
5:B:1545[B]:TZ5:H19	5:B:1545[B]:TZ5:H211	0.94	0.93
5:B:1545[A]:TZ5:H201	5:B:1545[A]:TZ5:C13	2.00	0.91
1:B:286[B]:TRP:HB2	5:B:1545[B]:TZ5:C7	2.01	0.91
5:A:1548[B]:TZ5:H32	5:A:1548[B]:TZ5:H291	1.54	0.89
5:B:1545[A]:TZ5:H291	5:B:1545[A]:TZ5:H32	1.54	0.87
1:B:286[B]:TRP:CB	5:B:1545[B]:TZ5:C6	2.56	0.83
1:B:293:SER:O	5:B:1545[A]:TZ5:H7	1.77	0.83
1:A:527:GLN:HE21	3:A:1546:P6G:H171	1.45	0.82
1:A:161:LEU:O	1:A:164:SER:HB3	1.80	0.82
5:B:1545[A]:TZ5:H281	5:B:1545[A]:TZ5:H242	1.65	0.76
1:A:381:HIS:HA	3:A:1546:P6G:H31	1.68	0.76
1:A:385:TRP:HD1	1:B:527:GLN:OE1	1.71	0.73
1:A:4:GLU:OE1	1:A:18:ARG:HD3	1.89	0.72
1:B:497:SER:HB2	1:B:498:PRO:CA	2.20	0.72
1:B:285:GLU:HG3	5:B:1545[B]:TZ5:H7	1.73	0.71
1:A:496:LYS:HA	1:A:497:SER:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:THR:HG21	1:A:143:GLY:O	1.91	0.70
1:A:538:LYS:HA	1:A:541:SER:HB2	1.73	0.70
1:B:293:SER:O	5:B:1545[A]:TZ5:C7	2.41	0.69
1:A:285:GLU:HG3	5:A:1548[B]:TZ5:H7	1.74	0.68
1:A:496:LYS:HA	1:A:497:SER:C	2.15	0.67
1:A:197:VAL:H	1:A:223:HIS:HD2	1.43	0.67
5:A:1548[B]:TZ5:C32	5:A:1548[B]:TZ5:H291	2.22	0.65
1:A:286[B]:TRP:HB2	5:A:1548[B]:TZ5:H6	1.77	0.65
5:A:1548[A]:TZ5:H32	5:A:1548[A]:TZ5:H291	1.78	0.65
1:A:286[A]:TRP:CZ2	5:A:1548[A]:TZ5:H202	2.33	0.64
1:B:84:GLU:HG3	1:B:87:ASN:HD22	1.63	0.64
1:A:294:ILE:HD11	1:A:402:VAL:HG21	1.80	0.64
1:B:112:THR:HG21	1:B:143:GLY:O	1.99	0.63
5:A:1548[A]:TZ5:H291	5:A:1548[A]:TZ5:C32	2.29	0.62
1:B:113:PRO:HG2	1:B:485:ARG:HG3	1.80	0.61
1:A:326:VAL:HG12	1:A:328:VAL:HG13	1.84	0.59
1:A:76:LEU:HD13	5:A:1548[B]:TZ5:H16	1.85	0.58
5:B:1545[A]:TZ5:H291	5:B:1545[A]:TZ5:C32	2.31	0.58
1:B:197:VAL:H	1:B:223:HIS:HD2	1.51	0.58
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.38	0.57
1:A:374:ALA:HA	1:A:539:LEU:HD23	1.86	0.57
5:B:1545[A]:TZ5:H402	5:B:1545[A]:TZ5:N5	2.19	0.57
5:B:1545[A]:TZ5:H9	5:B:1545[A]:TZ5:C17	2.34	0.57
5:B:1545[A]:TZ5:C20	5:B:1545[A]:TZ5:C13	2.81	0.57
1:A:491:ASP:HB3	1:A:494:ASP:HB2	1.89	0.55
5:A:1548[A]:TZ5:C17	5:A:1548[A]:TZ5:H201	2.32	0.55
5:B:1545[A]:TZ5:H201	5:B:1545[A]:TZ5:H13	1.90	0.53
1:B:227:LEU:HB2	1:B:328:VAL:HG12	1.90	0.53
1:A:103:THR:HG21	1:A:190:PHE:HB3	1.89	0.53
1:B:210:GLY:HA3	1:B:232:PRO:HD3	1.91	0.53
1:A:72:TYR:CD1	5:A:1548[A]:TZ5:C16	2.87	0.52
1:B:224:ARG:HG2	1:B:325:GLN:HB2	1.92	0.52
1:A:367:VAL:HG12	1:A:370:ALA:HB2	1.92	0.52
1:A:380:LEU:HB3	3:A:1546:P6G:H51	1.91	0.51
1:B:243:GLU:O	1:B:247:ARG:HG3	2.10	0.51
1:B:286[B]:TRP:CG	1:B:286[B]:TRP:O	2.63	0.51
1:A:197:VAL:H	1:A:223:HIS:CD2	2.27	0.51
1:B:44:SER:HA	1:B:274:ARG:HD2	1.93	0.51
1:B:478:LYS:O	1:B:482:ASN:HB2	2.10	0.50
1:B:177:ARG:CZ	1:B:217:PRO:HB2	2.42	0.50
1:A:286[B]:TRP:CE3	5:A:1548[B]:TZ5:C3	2.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ILE:HD11	1:A:402:VAL:CG2	2.40	0.50
1:A:161:LEU:HD11	1:A:269:LEU:HD22	1.93	0.50
1:B:211:MET:HG2	1:B:308:LEU:HD21	1.94	0.50
5:A:1548[A]:TZ5:H32	5:A:1548[A]:TZ5:C29	2.41	0.50
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.47	0.50
1:A:285:GLU:CG	5:A:1548[B]:TZ5:H7	2.43	0.49
1:B:328:VAL:O	1:B:427:ALA:HA	2.12	0.49
1:A:293:SER:O	5:A:1548[A]:TZ5:H7	2.12	0.49
5:B:1545[B]:TZ5:C21	5:B:1545[B]:TZ5:C19	2.62	0.49
1:A:286[A]:TRP:CH2	5:A:1548[A]:TZ5:H202	2.47	0.49
1:A:341:TYR:CD2	5:A:1548[A]:TZ5:H13	2.48	0.49
5:B:1545[A]:TZ5:N4	5:B:1545[A]:TZ5:C30	2.76	0.49
5:B:1545[B]:TZ5:C29	5:B:1545[B]:TZ5:H32	2.44	0.48
1:B:135:GLY:HA3	1:B:146:LEU:HD22	1.96	0.48
1:B:197:VAL:H	1:B:223:HIS:CD2	2.31	0.48
3:A:1546:P6G:H182	1:B:381:HIS:CE1	2.49	0.48
1:A:528:THR:O	1:A:531:PHE:HB3	2.14	0.47
1:B:103:THR:HG22	1:B:145:VAL:HG22	1.96	0.47
1:A:211:MET:HG3	1:A:232:PRO:HB3	1.96	0.47
1:B:437:LEU:HD11	1:B:449:TYR:CD2	2.49	0.47
1:A:286[B]:TRP:CZ3	5:A:1548[B]:TZ5:C1	2.98	0.47
5:A:1548[B]:TZ5:C29	5:A:1548[B]:TZ5:H32	2.37	0.47
1:A:286[B]:TRP:CE3	5:A:1548[B]:TZ5:C2	2.98	0.47
1:B:499:GLN:O	1:B:501:PRO:HD3	2.15	0.47
1:B:13:ARG:HH12	1:B:185:GLU:CD	2.19	0.46
3:A:1546:P6G:H142	1:B:381:HIS:HA	1.97	0.46
1:A:89:ASN:O	1:A:90:ARG:NH1	2.46	0.45
5:B:1545[B]:TZ5:C13	5:B:1545[B]:TZ5:H201	2.45	0.45
1:A:509:GLN:HE21	1:A:522:ARG:NH2	2.14	0.45
1:A:450:GLU:HG2	1:A:454:ILE:HD12	1.99	0.45
1:B:374:ALA:HA	1:B:539:LEU:HD23	1.97	0.45
1:A:118:ILE:O	1:A:205:GLY:HA3	2.16	0.45
1:B:124:TYR:OH	5:B:1545[B]:TZ5:H281	2.17	0.45
1:A:328:VAL:O	1:A:427:ALA:HA	2.17	0.45
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.51	0.44
1:B:495:SER:OG	1:B:496:LYS:N	2.49	0.44
1:A:124:TYR:HA	1:A:154:GLY:H	1.82	0.44
1:A:444:GLY:O	1:A:446:PRO:HD3	2.17	0.44
1:B:295:PHE:CE2	1:B:338:PHE:CZ	3.05	0.44
1:B:116:ILE:HD11	1:B:183:VAL:HG11	1.99	0.44
1:B:341:TYR:HD2	5:B:1545[A]:TZ5:H17	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:PRO:HA	1:A:259:PRO:HD2	1.80	0.43
1:A:202:GLU:HA	1:A:228:GLN:O	2.18	0.43
1:A:81:GLU:HG2	4:A:1547:SO3:O1	2.19	0.42
1:B:252:ALA:HB2	1:B:269:LEU:HD21	2.01	0.42
1:A:142:GLU:OE1	1:A:478:LYS:HE3	2.18	0.42
1:B:329:GLY:HA3	1:B:428:TYR:CE2	2.55	0.42
1:B:336:SER:HB2	1:B:443:MET:HG2	2.02	0.42
5:B:1545[A]:TZ5:N5	5:B:1545[A]:TZ5:C30	2.83	0.42
5:B:1545[A]:TZ5:C39	5:B:1545[A]:TZ5:N5	2.83	0.42
5:B:1545[A]:TZ5:C9	5:B:1545[A]:TZ5:C17	2.97	0.41
1:B:80:PHE:CE2	1:B:82:GLY:HA3	2.55	0.41
1:A:437:LEU:HD11	1:A:449:TYR:CD2	2.55	0.41
1:A:231:THR:HB	1:A:233:ASN:OD1	2.20	0.41
5:A:1548[A]:TZ5:H212	5:A:1548[A]:TZ5:H19	2.02	0.41
1:B:252:ALA:HA	1:B:273:LEU:HD21	2.03	0.41
5:B:1545[B]:TZ5:H32	5:B:1545[B]:TZ5:H291	2.03	0.40
1:B:166:GLU:HB2	1:B:270:ILE:HD13	2.03	0.40
1:B:294:ILE:HD13	1:B:343:VAL:CG2	2.51	0.40
1:A:497:SER:HA	1:A:498:PRO:HD3	1.96	0.40
1:B:434:ALA:HB3	1:B:437:LEU:HD13	2.02	0.40
1:B:390:ASP:HA	1:B:391:PRO:HD3	1.82	0.40
1:A:380:LEU:CB	3:A:1546:P6G:H51	2.52	0.40
1:A:256:GLY:O	1:A:258:PRO:HD3	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	536/543 (99%)	513 (96%)	21 (4%)	2 (0%)	39 69
1	B	537/543 (99%)	503 (94%)	28 (5%)	6 (1%)	17 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1073/1086 (99%)	1016 (95%)	49 (5%)	8 (1%)	26	55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	496	LYS
1	B	497	SER
1	A	2	GLY
1	B	265	ASN
1	B	495	SER
1	B	542	ALA
1	A	497	SER
1	B	263	GLY

### 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	442/442 (100%)	426 (96%)	16 (4%)	42	73
1	B	442/442 (100%)	428 (97%)	14 (3%)	46	77
All	All	884/884 (100%)	854 (97%)	30 (3%)	44	75

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	70	TYR
1	A	84	GLU
1	A	164	SER
1	A	165	ARG
1	A	166	GLU
1	A	200	PHE
1	A	216	LEU
1	A	295	PHE
1	A	313	GLU

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Mol	Chain	Res	Type
1	A	437	LEU
1	A	480	TRP
1	A	495	SER
1	A	497	SER
1	A	524	LEU
1	A	536	LEU
1	B	136	ARG
1	B	200	PHE
1	B	239	VAL
1	B	265	ASN
1	B	266	ASP
1	B	294	ILE
1	B	295	PHE
1	B	313	GLU
1	B	387	HIS
1	B	491	ASP
1	B	497	SER
1	B	524	LEU
1	B	536	LEU
1	B	543	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	HIS
1	A	509	GLN
1	A	527	GLN
1	B	223	HIS
1	B	287	HIS
1	B	322	GLN
1	B	381	HIS
1	B	387	HIS

### 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

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 9 ligands modelled in this entry, 1 is modelled with single atom - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	A	1544	1	14,14,15	0.98	1 (7%)	15,19,21	1.35	1 (6%)
3	P6G	A	1546	-	18,18,18	2.24	6 (33%)	17,17,17	1.30	1 (5%)
4	SO3	A	1547	-	1,3,3	0.37	0	0,3,3	0.00	-
5	TZ5	A	1548[A]	-	55,57,57	1.44	8 (14%)	68,80,80	1.95	11 (16%)
5	TZ5	A	1548[B]	-	55,57,57	1.40	7 (12%)	68,80,80	2.40	13 (19%)
4	SO3	B	1544	-	1,3,3	0.57	0	0,3,3	0.00	-
5	TZ5	B	1545[A]	-	55,57,57	1.43	7 (12%)	68,80,80	1.93	10 (14%)
5	TZ5	B	1545[B]	-	55,57,57	1.44	8 (14%)	68,80,80	2.05	11 (16%)

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	1544	1	-	0/6/23/26	0/1/1/1
3	P6G	A	1546	-	-	0/16/16/16	0/0/0/0
4	SO3	A	1547	-	-	0/0/0/0	0/0/0/0
5	TZ5	A	1548[A]	-	-	0/19/26/26	0/8/8/8
5	TZ5	A	1548[B]	-	-	0/19/26/26	0/8/8/8
4	SO3	B	1544	-	-	0/0/0/0	0/0/0/0
5	TZ5	B	1545[A]	-	-	0/19/26/26	0/8/8/8
5	TZ5	B	1545[B]	-	-	0/19/26/26	0/8/8/8



All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1545[A]	TZ5	C40-C39	-4.17	1.44	1.51
5	B	1545[B]	TZ5	C40-C39	-4.12	1.44	1.51
5	B	1545[B]	TZ5	C38-C37	-4.09	1.44	1.50
5	B	1545[A]	TZ5	C38-C37	-4.08	1.44	1.50
5	A	1548[A]	TZ5	C42-C38	-4.06	1.36	1.51
5	B	1545[B]	TZ5	C42-C38	-4.05	1.36	1.51
5	B	1545[A]	TZ5	C42-C38	-4.04	1.36	1.51
5	A	1548[A]	TZ5	C38-C37	-3.97	1.44	1.50
5	A	1548[B]	TZ5	C42-C38	-3.94	1.36	1.51
5	B	1545[A]	TZ5	C41-C40	-3.79	1.37	1.51
5	A	1548[B]	TZ5	C40-C39	-3.76	1.45	1.51
5	A	1548[A]	TZ5	C41-C40	-3.73	1.37	1.51
5	B	1545[B]	TZ5	C41-C40	-3.69	1.37	1.51
5	A	1548[B]	TZ5	C38-C37	-3.67	1.45	1.50
5	A	1548[A]	TZ5	C40-C39	-3.66	1.45	1.51
5	A	1548[B]	TZ5	C41-C40	-3.66	1.37	1.51
5	A	1548[A]	TZ5	N6-N5	-2.37	1.31	1.34
5	A	1548[B]	TZ5	N6-N5	-2.25	1.31	1.34
5	B	1545[A]	TZ5	N6-N5	-2.15	1.31	1.34
5	B	1545[B]	TZ5	N6-N5	-2.15	1.31	1.34
5	B	1545[B]	TZ5	C42-C41	-2.14	1.42	1.51
5	B	1545[A]	TZ5	C42-C41	-2.13	1.42	1.51
5	A	1548[A]	TZ5	C42-C41	-2.10	1.42	1.51
5	A	1548[B]	TZ5	C36-C35	2.14	1.43	1.38
5	A	1548[A]	TZ5	C36-C35	2.18	1.43	1.38
5	B	1545[B]	TZ5	C30-C39	2.22	1.42	1.39
5	B	1545[B]	TZ5	C37-N8	2.37	1.35	1.32
5	B	1545[A]	TZ5	C37-N8	2.37	1.35	1.32
5	A	1548[B]	TZ5	C37-N8	2.49	1.35	1.32
5	A	1548[A]	TZ5	C37-N8	2.52	1.35	1.32
2	A	1544	NAG	C1-C2	2.59	1.56	1.52
3	A	1546	P6G	O13-C14	2.77	1.53	1.42
3	A	1546	P6G	O1-C2	3.41	1.60	1.42
3	A	1546	P6G	O4-C5	3.62	1.57	1.42
3	A	1546	P6G	O7-C8	3.72	1.57	1.42
3	A	1546	P6G	O16-C17	3.73	1.57	1.42
3	A	1546	P6G	O10-C11	4.63	1.61	1.42

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1545[B]	TZ5	C40-C39-C37	-5.88	116.59	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1545[A]	TZ5	C40-C39-C37	-5.46	116.92	121.05
5	A	1548[A]	TZ5	C40-C39-C37	-5.33	117.01	121.05
5	A	1548[B]	TZ5	C40-C39-C37	-4.37	117.74	121.05
5	A	1548[A]	TZ5	C27-C26-N4	-3.85	100.25	106.20
5	A	1548[B]	TZ5	C27-C26-N4	-3.63	100.59	106.20
5	B	1545[B]	TZ5	C27-C26-N4	-3.60	100.63	106.20
5	B	1545[A]	TZ5	C27-C26-N4	-3.48	100.83	106.20
5	A	1548[B]	TZ5	C12-C11-C10	-3.36	113.98	122.53
5	B	1545[B]	TZ5	C39-C30-C31	-3.30	118.02	120.38
5	B	1545[A]	TZ5	C39-C30-C31	-3.19	118.10	120.38
5	B	1545[B]	TZ5	C28-C29-N7	-3.06	107.36	113.01
5	A	1548[A]	TZ5	C39-C30-C31	-3.02	118.22	120.38
5	A	1548[A]	TZ5	C12-C11-N3	-3.02	116.84	120.46
5	A	1548[B]	TZ5	C39-C30-C31	-2.63	118.50	120.38
5	B	1545[A]	TZ5	C25-C26-C27	-2.62	125.44	129.48
5	B	1545[B]	TZ5	C25-C26-C27	-2.55	125.54	129.48
5	A	1548[B]	TZ5	C39-C30-N7	-2.47	114.48	119.56
5	A	1548[B]	TZ5	C28-C29-N7	-2.44	108.50	113.01
5	A	1548[A]	TZ5	C25-C26-C27	-2.36	125.83	129.48
5	A	1548[A]	TZ5	C38-C37-C39	-2.31	119.27	121.69
5	B	1545[B]	TZ5	C12-C11-C10	-2.20	116.94	122.53
5	B	1545[A]	TZ5	C38-C37-C39	-2.19	119.40	121.69
5	B	1545[A]	TZ5	C28-C29-N7	-2.06	109.21	113.01
5	A	1548[A]	TZ5	C39-C30-N7	-2.03	115.38	119.56
5	A	1548[B]	TZ5	C25-C26-C27	-2.01	126.38	129.48
5	A	1548[B]	TZ5	C37-N8-C33	2.12	119.96	117.64
5	B	1545[B]	TZ5	C12-C11-N3	2.24	123.14	120.46
5	A	1548[A]	TZ5	C42-C38-C37	2.86	118.30	113.48
3	A	1546	P6G	O19-C18-C17	3.35	132.71	112.03
5	A	1548[B]	TZ5	C41-C40-C39	3.51	120.19	113.02
5	A	1548[A]	TZ5	C41-C40-C39	3.56	120.30	113.02
5	A	1548[B]	TZ5	C42-C38-C37	3.56	119.48	113.48
5	B	1545[A]	TZ5	C42-C38-C37	3.65	119.62	113.48
5	A	1548[B]	TZ5	C12-C11-N3	3.79	125.00	120.46
5	B	1545[B]	TZ5	C42-C38-C37	3.83	119.94	113.48
5	B	1545[A]	TZ5	C41-C40-C39	3.97	121.14	113.02
5	B	1545[B]	TZ5	C41-C40-C39	3.99	121.18	113.02
2	A	1544	NAG	C1-O5-C5	4.01	117.34	112.25
5	B	1545[A]	TZ5	C21-C20-N3	7.15	118.33	112.29
5	A	1548[A]	TZ5	C21-C20-N3	7.40	118.54	112.29
5	A	1548[B]	TZ5	C25-C26-N4	7.88	133.02	121.95
5	B	1545[B]	TZ5	C21-C20-N3	7.91	118.97	112.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1545[A]	TZ5	C25-C26-N4	8.38	133.72	121.95
5	B	1545[B]	TZ5	C25-C26-N4	8.45	133.83	121.95
5	A	1548[A]	TZ5	C25-C26-N4	8.51	133.91	121.95
5	A	1548[B]	TZ5	C21-C20-N3	13.09	123.34	112.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1546	P6G	6	0
4	A	1547	SO3	1	0
5	A	1548[A]	TZ5	11	0
5	A	1548[B]	TZ5	11	0
5	B	1545[A]	TZ5	15	0
5	B	1545[B]	TZ5	12	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	538/543 (99%)	-0.34	15 (2%) 56 57	33, 51, 75, 106	0
1	B	538/543 (99%)	-0.29	13 (2%) 62 62	37, 58, 86, 128	0
All	All	1076/1086 (99%)	-0.31	28 (2%) 59 59	33, 54, 83, 128	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	542	ALA	7.3
1	A	541	SER	5.2
1	A	493	ARG	5.0
1	B	542	ALA	4.5
1	B	259	PRO	4.2
1	B	497	SER	3.8
1	B	540	LEU	3.7
1	B	541	SER	3.6
1	B	543	THR	3.5
1	A	496	LYS	3.4
1	A	497	SER	3.3
1	A	259	PRO	3.2
1	B	262	ALA	3.1
1	A	495	SER	3.0
1	A	165	ARG	3.0
1	B	110	SER	2.9
1	A	494	ASP	2.7
1	B	165	ARG	2.7
1	A	3	ARG	2.7
1	B	109	ALA	2.7
1	B	4	GLU	2.5
1	A	540	LEU	2.4
1	A	323	ASP	2.4
1	A	1	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	323	ASP	2.2
1	A	109	ALA	2.2
1	A	543	THR	2.2
1	B	468	GLU	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](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	NAG	A	1544	14/15	0.55	0.63	9.26	68,76,79,79	0
5	TZ5	B	1545[A]	50/50	0.92	0.21	1.93	50,65,77,78	50
5	TZ5	B	1545[B]	50/50	0.92	0.21	1.90	37,51,65,65	50
3	P6G	A	1546	19/19	0.89	0.23	1.84	59,64,77,78	0
5	TZ5	A	1548[A]	50/50	0.93	0.19	1.43	32,43,55,55	50
4	SO3	A	1547	4/4	0.94	0.18	1.25	79,79,79,81	0
5	TZ5	A	1548[B]	50/50	0.93	0.19	1.19	28,39,43,44	50
4	SO3	B	1544	4/4	0.96	0.10	-1.91	74,75,76,76	0
2	NAG	A	1545	1/15	0.81	0.30	-	125,125,125,125	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.