



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:34 PM GMT

PDB ID : 4TSM  
Title : MBP-fusion protein of PilA1 from *C. difficile* R20291 residues 26-166  
Authors : Piepenbrink, K.H.; Sundberg, E.J.  
Deposited on : 2014-06-19  
Resolution : 1.90 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

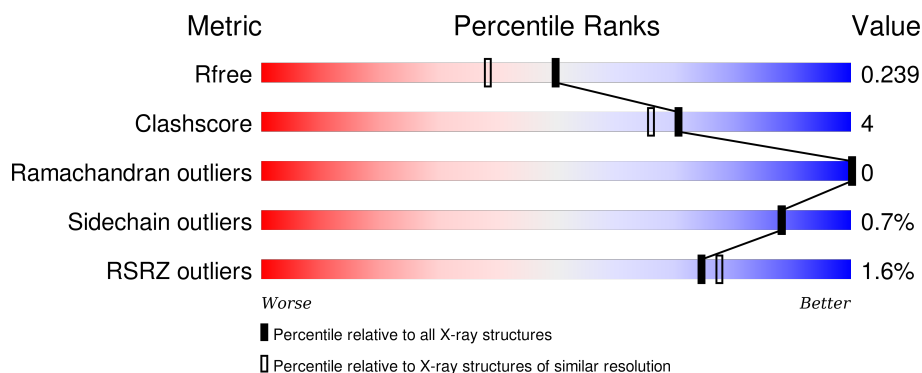
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	520	
1	B	520	
1	C	520	

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	TMO	A	1201	-	-	X	X
2	TMO	A	1207	-	-	-	X
2	TMO	C	1202	-	-	X	X
2	TMO	C	1203	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12717 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 maltose-binding protein, pilin chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	505	Total	C	N	O	S	0	2	0
			3861	2471	624	758	8			
1	B	512	Total	C	N	O	S	0	3	0
			3914	2503	633	768	10			
1	C	512	Total	C	N	O	S	0	4	0
			3915	2502	632	771	10			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP D8A942
A	82	ALA	ASP	engineered mutation	UNP D8A942
A	83	ALA	LYS	engineered mutation	UNP D8A942
A	172	ALA	GLU	engineered mutation	UNP D8A942
A	173	ALA	ASN	engineered mutation	UNP D8A942
A	239	ALA	LYS	engineered mutation	UNP D8A942
A	362	ALA	LYS	engineered mutation	UNP D8A942
A	363	ALA	ASP	engineered mutation	UNP D8A942
A	367	ASN	-	linker	UNP D8A942
A	368	ALA	-	linker	UNP D8A942
A	369	ALA	-	linker	UNP D8A942
A	370	ALA	-	linker	UNP D8A942
A	1165	GLY	-	expression tag	UNP C9YRY2
A	1166	SER	-	expression tag	UNP C9YRY2
A	1167	LEU	-	expression tag	UNP C9YRY2
A	1168	GLU	-	expression tag	UNP C9YRY2
A	1169	HIS	-	expression tag	UNP C9YRY2
A	1170	HIS	-	expression tag	UNP C9YRY2
A	1171	HIS	-	expression tag	UNP C9YRY2
A	1172	HIS	-	expression tag	UNP C9YRY2
A	1173	HIS	-	expression tag	UNP C9YRY2
A	1174	HIS	-	expression tag	UNP C9YRY2
B	0	MET	-	initiating methionine	UNP D8A942

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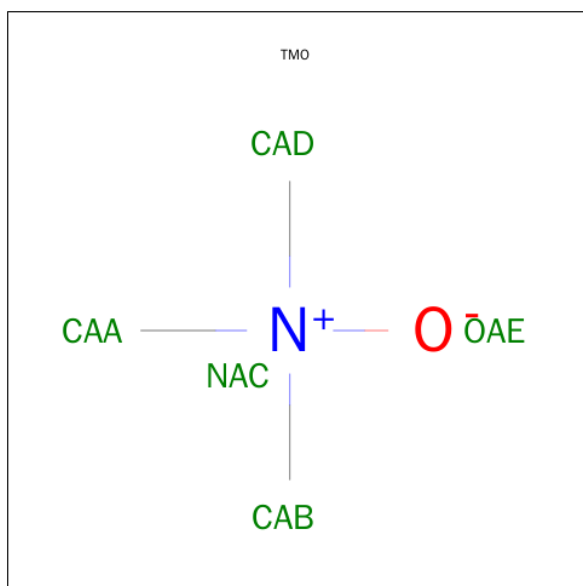
Chain	Residue	Modelled	Actual	Comment	Reference
B	82	ALA	ASP	engineered mutation	UNP D8A942
B	83	ALA	LYS	engineered mutation	UNP D8A942
B	172	ALA	GLU	engineered mutation	UNP D8A942
B	173	ALA	ASN	engineered mutation	UNP D8A942
B	239	ALA	LYS	engineered mutation	UNP D8A942
B	362	ALA	LYS	engineered mutation	UNP D8A942
B	363	ALA	ASP	engineered mutation	UNP D8A942
B	367	ASN	-	linker	UNP D8A942
B	368	ALA	-	linker	UNP D8A942
B	369	ALA	-	linker	UNP D8A942
B	370	ALA	-	linker	UNP D8A942
B	1165	GLY	-	expression tag	UNP C9YRY2
B	1166	SER	-	expression tag	UNP C9YRY2
B	1167	LEU	-	expression tag	UNP C9YRY2
B	1168	GLU	-	expression tag	UNP C9YRY2
B	1169	HIS	-	expression tag	UNP C9YRY2
B	1170	HIS	-	expression tag	UNP C9YRY2
B	1171	HIS	-	expression tag	UNP C9YRY2
B	1172	HIS	-	expression tag	UNP C9YRY2
B	1173	HIS	-	expression tag	UNP C9YRY2
B	1174	HIS	-	expression tag	UNP C9YRY2
C	0	MET	-	initiating methionine	UNP D8A942
C	82	ALA	ASP	engineered mutation	UNP D8A942
C	83	ALA	LYS	engineered mutation	UNP D8A942
C	172	ALA	GLU	engineered mutation	UNP D8A942
C	173	ALA	ASN	engineered mutation	UNP D8A942
C	239	ALA	LYS	engineered mutation	UNP D8A942
C	362	ALA	LYS	engineered mutation	UNP D8A942
C	363	ALA	ASP	engineered mutation	UNP D8A942
C	367	ASN	-	linker	UNP D8A942
C	368	ALA	-	linker	UNP D8A942
C	369	ALA	-	linker	UNP D8A942
C	370	ALA	-	linker	UNP D8A942
C	1165	GLY	-	expression tag	UNP C9YRY2
C	1166	SER	-	expression tag	UNP C9YRY2
C	1167	LEU	-	expression tag	UNP C9YRY2
C	1168	GLU	-	expression tag	UNP C9YRY2
C	1169	HIS	-	expression tag	UNP C9YRY2
C	1170	HIS	-	expression tag	UNP C9YRY2
C	1171	HIS	-	expression tag	UNP C9YRY2
C	1172	HIS	-	expression tag	UNP C9YRY2
C	1173	HIS	-	expression tag	UNP C9YRY2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1174	HIS	-	expression tag	UNP C9YRY2

- Molecule 2 is trimethylamine oxide (three-letter code: TMO) (formula: C<sub>3</sub>H<sub>9</sub>NO).



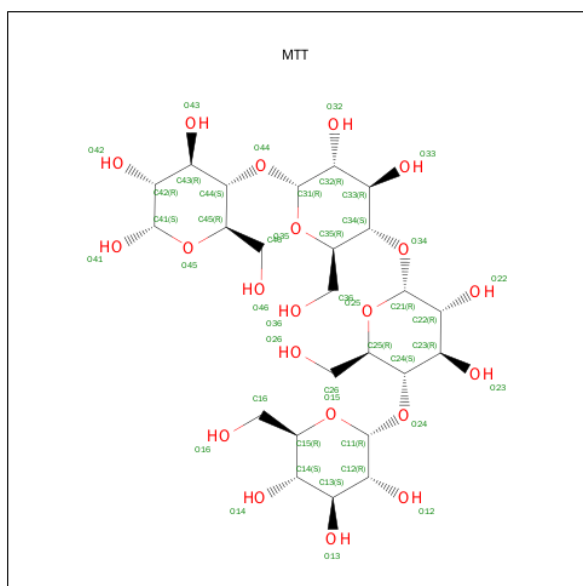
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			5	3	1	1		
2	A	1	Total	C	N	O	0	0
			5	3	1	1		
2	A	1	Total	C	N	O	0	0
			5	3	1	1		
2	A	1	Total	C	N	O	0	0
			5	3	1	1		
2	A	1	Total	C	N	O	0	0
			5	3	1	1		
2	A	1	Total	C	N	O	0	0
			5	3	1	1		
2	B	1	Total	C	N	O	0	0
			5	3	1	1		
2	B	1	Total	C	N	O	0	0
			5	3	1	1		
2	B	1	Total	C	N	O	0	0
			5	3	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			5	3	1	1		
2	B	1	Total	C	N	O	0	0
			5	3	1	1		
2	C	1	Total	C	N	O	0	0
			5	3	1	1		
2	C	1	Total	C	N	O	0	0
			5	3	1	1		
2	C	1	Total	C	N	O	0	0
			5	3	1	1		
2	C	1	Total	C	N	O	0	0
			5	3	1	1		
2	C	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 3 is MALTOTETRAOSE (three-letter code: MTT) (formula:  $C_{24}H_{42}O_{21}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			45	24	21		
3	B	1	Total	C	O	0	0
			45	24	21		
3	C	1	Total	C	O	0	0
			45	24	21		

- Molecule 4 is water.

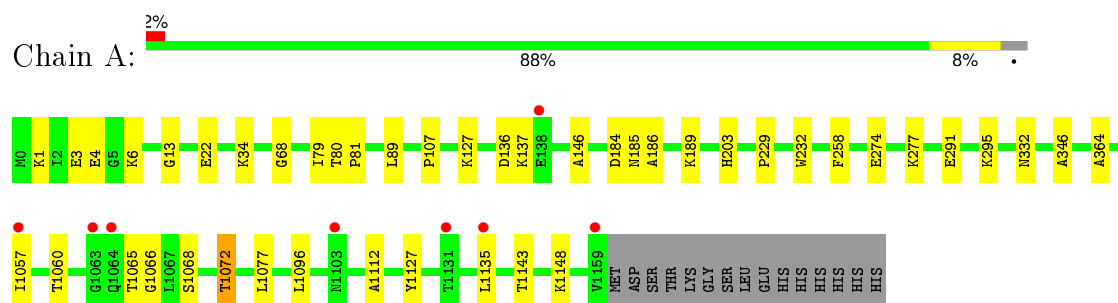
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	257	Total 257	O 257	0	0
4	B	261	Total 261	O 261	0	0
4	C	279	Total 279	O 279	0	0



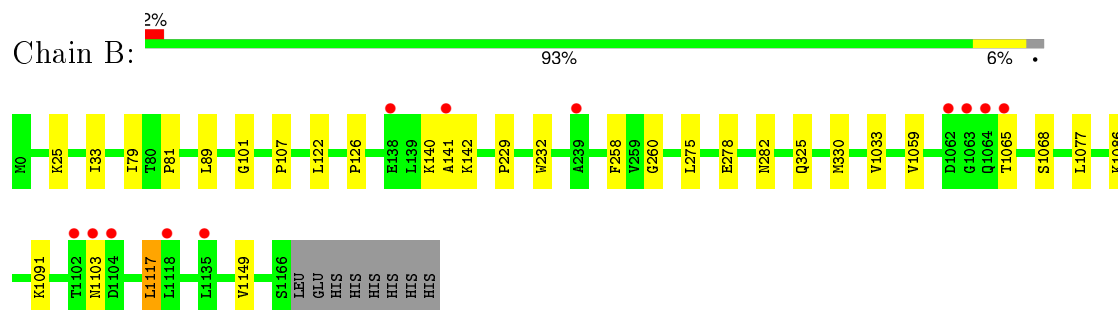
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

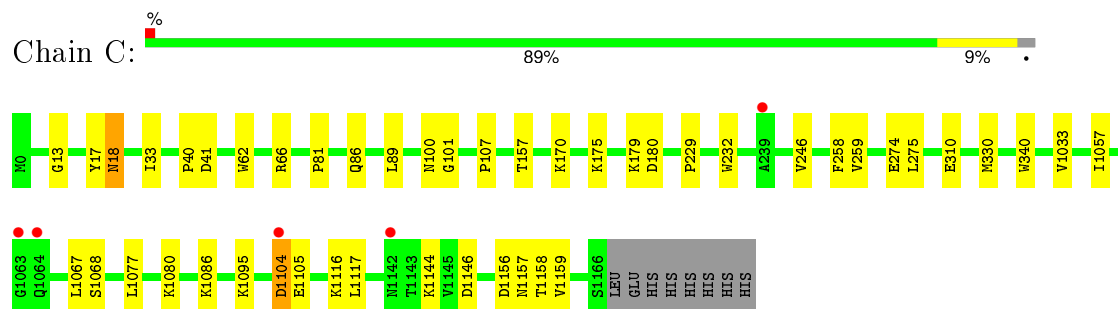
- Molecule 1: maltose-binding protein, pilin chimera



- Molecule 1: maltose-binding protein, pilin chimera



- Molecule 1: maltose-binding protein, pilin chimera



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.95Å 79.37Å 164.75Å 90.00° 90.23° 90.00°	Depositor
Resolution (Å)	38.58 – 1.90 38.58 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (38.58-1.90) 84.9 (38.58-1.90)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 1.89Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.197 , 0.233 0.202 , 0.239	Depositor DCC
$R_{free}$ test set	1999 reflections (1.63%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.6	Xtriage
Anisotropy	0.609	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 44.2	EDS
Estimated twinning fraction	0.014 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.014 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.086 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.099 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.017 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 139534 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12717	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MTT, TMO

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	0.40	0/3947	0.54	0/5366
1	B	0.39	0/4003	0.55	0/5438
1	C	0.40	0/4007	0.56	0/5445
All	All	0.40	0/11957	0.55	0/16249

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	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	18	ASN	Sidechain

### 5.2 Too-close contacts [i](#)

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	3861	0	3858	38	0
1	B	3914	0	3920	22	0
1	C	3915	0	3914	42	0
2	A	40	0	72	16	0
2	B	25	0	45	3	0
2	C	30	0	54	9	0
3	A	45	0	42	1	0
3	B	45	0	42	0	0
3	C	45	0	42	2	0
4	A	257	0	0	9	1
4	B	261	0	0	5	2
4	C	279	0	0	7	2
All	All	12717	0	11989	106	3

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 4.

All (106) 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:274:GLU:H	2:A:1201:TMO:HAA	1.43	0.83
1:B:101:GLY:H	2:B:1201:TMO:HABA	1.42	0.81
1:B:79:ILE:HG22	1:B:81:PRO:HD3	1.62	0.81
1:A:79:ILE:HD12	1:A:81:PRO:HD3	1.62	0.80
1:C:41:ASP:H	2:C:1203:TMO:HAB	1.47	0.78
1:C:274:GLU:H	2:C:1202:TMO:HADB	1.48	0.78
1:B:278:GLU:OE2	1:B:282:ASN:ND2	2.18	0.74
1:B:142:LYS:O	4:B:1542:HOH:O	2.11	0.68
1:B:1065:THR:O	4:B:1524:HOH:O	2.11	0.67
1:A:3[A]:GLU:OE1	4:A:1526:HOH:O	2.14	0.65
1:C:17:TYR:CD1	1:C:18:ASN:ND2	2.65	0.65
2:A:1201:TMO:HADB	1:C:179:LYS:NZ	2.13	0.63
1:A:1057:ILE:HD11	1:A:1096:LEU:HB2	1.82	0.62
3:C:1207:MTT:O14	4:C:1573:HOH:O	2.16	0.61
1:B:1033:VAL:HG13	1:B:1117:LEU:HD13	1.81	0.61
1:B:325:GLN:OE1	4:B:1400:HOH:O	2.16	0.61
1:C:1104:ASP:HB3	1:C:1105:GLU:HG3	1.84	0.60
1:A:1065:THR:OG1	1:A:1066:GLY:N	2.33	0.59
1:C:1116:LYS:NZ	4:C:1510:HOH:O	2.22	0.59
1:C:157:THR:HG23	4:C:1534:HOH:O	2.02	0.59
1:A:137:LYS:HE2	1:A:203:HIS:HE1	1.67	0.59
1:B:101:GLY:N	2:B:1201:TMO:HABA	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:GLY:H	2:B:1201:TMO:CAB	2.14	0.57
1:C:274:GLU:H	2:C:1202:TMO:CAD	2.16	0.56
1:A:4[B]:GLU:OE1	1:C:179:LYS:HB2	2.06	0.55
1:A:1148:LYS:HD3	4:A:1303:HOH:O	2.07	0.54
1:A:137:LYS:HE2	1:A:203:HIS:CE1	2.42	0.54
1:A:291:GLU:OE2	1:A:295:LYS:HE2	2.07	0.54
1:A:274:GLU:H	2:A:1201:TMO:CAA	2.14	0.54
1:C:62:TRP:CD1	1:C:66:ARG:HG2	2.42	0.54
1:B:25:LYS:NZ	4:B:1548:HOH:O	2.38	0.54
1:A:184:ASP:O	1:A:189:LYS:NZ	2.41	0.54
1:A:1112:ALA:HB1	2:A:1207:TMO:HADB	1.90	0.52
1:A:186:ALA:N	2:A:1206:TMO:OAE	2.42	0.52
1:A:277:LYS:NZ	4:A:1545:HOH:O	2.42	0.51
1:B:1103:ASN:OD1	1:B:1149:VAL:HG23	2.11	0.51
2:C:1202:TMO:HAD	4:C:1357:HOH:O	2.09	0.51
2:A:1201:TMO:HADB	1:C:179:LYS:HZ3	1.74	0.50
1:C:33:ILE:HD13	1:C:275:LEU:HD22	1.93	0.50
1:B:1068:SER:HA	1:B:1077:LEU:HD21	1.94	0.50
1:C:17:TYR:CE1	1:C:18:ASN:ND2	2.80	0.50
1:C:1144:LYS:HE3	1:C:1146[A]:ASP:OD2	2.12	0.49
1:B:260:GLY:HA2	1:B:330:MET:HE2	1.95	0.49
1:C:18:ASN:HD22	1:C:18:ASN:N	2.11	0.49
1:B:89:LEU:HD23	1:B:107:PRO:HG2	1.95	0.49
1:C:41:ASP:N	2:C:1203:TMO:HAB	2.23	0.48
1:C:89:LEU:HD23	1:C:107:PRO:HG2	1.95	0.48
1:A:1068:SER:HA	1:A:1077:LEU:HD21	1.95	0.48
1:A:80:THR:OG1	4:A:1545:HOH:O	2.21	0.47
1:C:1033:VAL:HG13	1:C:1117:LEU:HD13	1.96	0.47
1:A:1060:THR:HG21	1:A:1065:THR:HA	1.96	0.47
1:C:41:ASP:H	2:C:1203:TMO:CAB	2.23	0.47
2:A:1207:TMO:HABA	4:A:1510:HOH:O	2.14	0.47
1:B:33:ILE:HD12	1:B:275:LEU:HD22	1.97	0.46
1:C:175:LYS:NZ	4:C:1577:HOH:O	2.49	0.46
2:A:1201:TMO:HADB	1:C:179:LYS:HZ1	1.81	0.46
1:C:229:PRO:HA	1:C:232:TRP:CE2	2.51	0.46
1:B:122:LEU:HD21	1:B:126:PRO:HD3	1.96	0.46
2:A:1201:TMO:HABA	4:A:1503:HOH:O	2.15	0.46
1:B:1059:VAL:HG11	1:B:1091:LYS:HG3	1.98	0.46
2:A:1201:TMO:HAAA	4:A:1367:HOH:O	2.15	0.46
1:A:185:ASN:HB2	2:A:1206:TMO:HABA	1.98	0.46
1:A:6:LYS:HD2	1:A:34:LYS:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LYS:CD	1:A:34:LYS:HD3	2.47	0.45
1:C:1157:ASN:OD1	1:C:1159:VAL:HG22	2.17	0.45
1:A:137:LYS:HD3	1:A:137:LYS:HA	1.67	0.44
1:A:1127:TYR:CE1	1:A:1135:LEU:HD13	2.52	0.44
1:C:310:GLU:OE1	4:C:1301:HOH:O	2.21	0.44
1:C:1095:LYS:HG2	1:C:1156:ASP:O	2.16	0.44
1:A:89:LEU:HD23	1:A:107:PRO:HG2	2.00	0.44
1:A:3[B]:GLU:OE2	1:B:141:ALA:HA	2.18	0.43
1:C:18:ASN:ND2	1:C:18:ASN:N	2.66	0.43
1:C:1067:LEU:HB2	1:C:1077:LEU:HD22	1.99	0.43
1:C:170:LYS:HD2	1:C:180:ASP:OD2	2.19	0.43
1:A:1:LYS:HG3	2:A:1208:TMO:HABA	2.01	0.43
1:C:66:ARG:HD3	3:C:1207:MTT:O22	2.19	0.43
1:A:79:ILE:HD12	1:A:81:PRO:CD	2.41	0.43
1:B:33:ILE:CD1	1:B:275:LEU:HD13	2.49	0.43
1:C:274:GLU:N	2:C:1202:TMO:HADB	2.26	0.43
2:A:1208:TMO:HAD	1:C:101:GLY:HA2	2.01	0.43
1:C:40:PRO:HA	2:C:1203:TMO:HAD	2.01	0.42
1:A:136:ASP:HA	1:A:146:ALA:HB2	2.01	0.42
1:C:13:GLY:HA3	2:C:1205:TMO:HAD	2.01	0.42
1:A:68:GLY:HA3	1:A:332:ASN:O	2.19	0.42
1:C:1080:LYS:HG2	1:C:1086:LYS:HG2	2.01	0.42
1:C:1068:SER:HA	1:C:1077:LEU:HD11	2.01	0.42
1:B:1086:LYS:HD3	4:B:1556:HOH:O	2.19	0.42
1:C:330:MET:CE	1:C:340:TRP:HZ2	2.32	0.42
1:A:22:GLU:HG2	4:A:1548:HOH:O	2.20	0.42
1:A:346:ALA:HB2	1:A:364:ALA:HB2	2.00	0.42
1:A:229:PRO:HA	1:A:232:TRP:CE2	2.55	0.42
3:A:1209:MTT:H262	3:A:1209:MTT:H151	2.02	0.42
1:C:330:MET:HE3	1:C:340:TRP:HZ2	1.84	0.41
1:A:1072:THR:HB	4:A:1437:HOH:O	2.20	0.41
1:A:13:GLY:HA3	2:A:1203:TMO:HADB	2.01	0.41
1:A:1:LYS:HG2	1:C:100:ASN:HA	2.02	0.41
1:C:330:MET:CE	1:C:340:TRP:HE1	2.33	0.41
1:C:259:VAL:O	1:C:330:MET:HG3	2.20	0.41
1:C:81:PRO:HG2	1:C:86:GLN:HG2	2.03	0.41
1:B:229:PRO:HA	1:B:232:TRP:CE2	2.56	0.40
1:A:127:LYS:HA	1:A:127:LYS:HD2	1.89	0.40
1:B:140:LYS:C	1:B:142:LYS:H	2.25	0.40
1:A:1112:ALA:CB	2:A:1207:TMO:HADB	2.52	0.40
2:A:1205:TMO:HAB	4:C:1389:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1057:ILE:CD1	1:C:1158:THR:HB	2.51	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1324:HOH:O	4:C:1377:HOH:O[2_758]	2.11	0.09
4:A:1346:HOH:O	4:C:1350:HOH:O[2_757]	2.13	0.07
4:B:1362:HOH:O	4:B:1365:HOH:O[4_758]	2.15	0.05

## 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	505/520 (97%)	496 (98%)	9 (2%)	0	100	100
1	B	513/520 (99%)	503 (98%)	10 (2%)	0	100	100
1	C	514/520 (99%)	505 (98%)	9 (2%)	0	100	100
All	All	1532/1560 (98%)	1504 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	406/418 (97%)	403 (99%)	3 (1%)	88	88
1	B	413/418 (99%)	411 (100%)	2 (0%)	92	92
1	C	414/418 (99%)	411 (99%)	3 (1%)	88	88
All	All	1233/1254 (98%)	1225 (99%)	8 (1%)	88	90

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	PHE
1	A	1072	THR
1	A	1143	THR
1	B	258	PHE
1	B	1117	LEU
1	C	246	VAL
1	C	258	PHE
1	C	1104	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	241	ASN
1	B	325	GLN
1	B	1064	GLN
1	C	18	ASN

### 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

22 ligands 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	TMO	A	1201	-	0,4,4	0.00	-	6,6,6	0.79	0
2	TMO	A	1202	-	0,4,4	0.00	-	6,6,6	0.30	0
2	TMO	A	1203	-	0,4,4	0.00	-	6,6,6	0.30	0
2	TMO	A	1204	-	0,4,4	0.00	-	6,6,6	0.29	0
2	TMO	A	1205	-	0,4,4	0.00	-	6,6,6	0.43	0
2	TMO	A	1206	-	0,4,4	0.00	-	6,6,6	0.45	0
2	TMO	A	1207	-	0,4,4	0.00	-	6,6,6	0.55	0
2	TMO	A	1208	-	0,4,4	0.00	-	6,6,6	0.51	0
3	MTT	A	1209	-	48,48,48	2.06	15 (31%)	71,71,71	1.04	5 (7%)
2	TMO	B	1201	-	0,4,4	0.00	-	6,6,6	0.29	0
2	TMO	B	1202	-	0,4,4	0.00	-	6,6,6	0.60	0
2	TMO	B	1203	-	0,4,4	0.00	-	6,6,6	0.36	0
2	TMO	B	1204	-	0,4,4	0.00	-	6,6,6	0.35	0
2	TMO	B	1205	-	0,4,4	0.00	-	6,6,6	0.56	0
3	MTT	B	1206	-	48,48,48	2.08	15 (31%)	71,71,71	1.12	7 (9%)
2	TMO	C	1201	-	0,4,4	0.00	-	6,6,6	0.33	0
2	TMO	C	1202	-	0,4,4	0.00	-	6,6,6	0.37	0
2	TMO	C	1203	-	0,4,4	0.00	-	6,6,6	0.36	0
2	TMO	C	1204	-	0,4,4	0.00	-	6,6,6	0.35	0
2	TMO	C	1205	-	0,4,4	0.00	-	6,6,6	0.33	0
2	TMO	C	1206	-	0,4,4	0.00	-	6,6,6	0.37	0
3	MTT	C	1207	-	48,48,48	2.11	13 (27%)	71,71,71	1.13	6 (8%)

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	TMO	A	1201	-	-	0/0/0/0	0/0/0/0
2	TMO	A	1202	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TMO	A	1203	-	-	0/0/0/0	0/0/0/0
2	TMO	A	1204	-	-	0/0/0/0	0/0/0/0
2	TMO	A	1205	-	-	0/0/0/0	0/0/0/0
2	TMO	A	1206	-	-	0/0/0/0	0/0/0/0
2	TMO	A	1207	-	-	0/0/0/0	0/0/0/0
2	TMO	A	1208	-	-	0/0/0/0	0/0/0/0
3	MTT	A	1209	-	-	0/20/100/100	0/4/4/4
2	TMO	B	1201	-	-	0/0/0/0	0/0/0/0
2	TMO	B	1202	-	-	0/0/0/0	0/0/0/0
2	TMO	B	1203	-	-	0/0/0/0	0/0/0/0
2	TMO	B	1204	-	-	0/0/0/0	0/0/0/0
2	TMO	B	1205	-	-	0/0/0/0	0/0/0/0
3	MTT	B	1206	-	-	0/20/100/100	0/4/4/4
2	TMO	C	1201	-	-	0/0/0/0	0/0/0/0
2	TMO	C	1202	-	-	0/0/0/0	0/0/0/0
2	TMO	C	1203	-	-	0/0/0/0	0/0/0/0
2	TMO	C	1204	-	-	0/0/0/0	0/0/0/0
2	TMO	C	1205	-	-	0/0/0/0	0/0/0/0
2	TMO	C	1206	-	-	0/0/0/0	0/0/0/0
3	MTT	C	1207	-	-	0/20/100/100	0/4/4/4

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1206	MTT	C36-C35	-3.87	1.38	1.51
3	A	1209	MTT	C36-C35	-3.71	1.38	1.51
3	C	1207	MTT	C36-C35	-3.70	1.38	1.51
3	A	1209	MTT	C46-C45	-3.17	1.40	1.51
3	C	1207	MTT	C46-C45	-3.08	1.41	1.51
3	B	1206	MTT	C46-C45	-2.94	1.41	1.51
3	A	1209	MTT	C26-C25	-2.80	1.42	1.51
3	C	1207	MTT	C26-C25	-2.71	1.42	1.51
3	B	1206	MTT	C26-C25	-2.42	1.43	1.51
3	C	1207	MTT	C12-C13	-2.15	1.46	1.52
3	B	1206	MTT	C42-C43	-2.13	1.46	1.52
3	B	1206	MTT	C12-C13	-2.11	1.46	1.52
3	A	1209	MTT	C16-C15	-2.08	1.44	1.51
3	B	1206	MTT	O35-C31	2.10	1.47	1.41
3	B	1206	MTT	O42-C42	2.11	1.48	1.43
3	A	1209	MTT	O13-C13	2.17	1.48	1.43
3	A	1209	MTT	O35-C31	2.25	1.47	1.41
3	A	1209	MTT	O42-C42	2.27	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1209	MTT	O45-C41	2.28	1.47	1.43
3	C	1207	MTT	O35-C31	2.36	1.47	1.41
3	C	1207	MTT	O45-C41	2.37	1.47	1.43
3	A	1209	MTT	O25-C21	2.49	1.48	1.41
3	C	1207	MTT	O25-C21	2.68	1.48	1.41
3	B	1206	MTT	O25-C21	2.83	1.49	1.41
3	A	1209	MTT	O15-C11	2.85	1.49	1.41
3	B	1206	MTT	O15-C11	2.96	1.49	1.41
3	B	1206	MTT	O45-C41	2.99	1.48	1.43
3	B	1206	MTT	O12-C12	3.09	1.50	1.43
3	C	1207	MTT	O12-C12	3.14	1.50	1.43
3	C	1207	MTT	O15-C11	3.25	1.50	1.41
3	A	1209	MTT	O12-C12	3.31	1.50	1.43
3	A	1209	MTT	O15-C15	3.63	1.53	1.44
3	C	1207	MTT	O45-C45	4.04	1.54	1.44
3	B	1206	MTT	O45-C45	4.06	1.54	1.44
3	B	1206	MTT	O15-C15	4.07	1.54	1.44
3	A	1209	MTT	O45-C45	4.08	1.54	1.44
3	C	1207	MTT	O15-C15	4.71	1.56	1.44
3	C	1207	MTT	O35-C35	4.83	1.56	1.44
3	A	1209	MTT	O35-C35	4.83	1.56	1.44
3	B	1206	MTT	O25-C25	4.93	1.56	1.44
3	C	1207	MTT	O25-C25	5.03	1.56	1.44
3	B	1206	MTT	O35-C35	5.18	1.57	1.44
3	A	1209	MTT	O25-C25	5.32	1.57	1.44

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1207	MTT	C16-C15-C14	-3.65	104.02	113.02
3	A	1209	MTT	O15-C15-C14	-3.01	104.04	109.68
3	B	1206	MTT	O24-C24-C25	-2.78	102.00	109.32
3	C	1207	MTT	O13-C13-C14	-2.53	104.64	110.34
3	A	1209	MTT	O32-C32-C31	-2.36	104.85	110.02
3	B	1206	MTT	C16-C15-C14	-2.19	107.60	113.02
3	A	1209	MTT	C31-O44-C44	-2.16	112.35	118.01
3	A	1209	MTT	C21-O34-C34	-2.12	112.46	118.01
3	B	1206	MTT	C21-O34-C34	-2.09	112.54	118.01
3	B	1206	MTT	C11-O24-C24	-2.08	112.56	118.01
3	B	1206	MTT	O13-C13-C14	-2.06	105.70	110.34
3	A	1209	MTT	O24-C24-C25	-2.04	103.96	109.32
3	C	1207	MTT	C31-O44-C44	-2.04	112.68	118.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1206	MTT	C41-C42-C43	2.26	113.80	110.43
3	C	1207	MTT	O15-C11-C12	2.35	115.10	110.28
3	C	1207	MTT	C11-O15-C15	2.63	118.84	113.75
3	B	1206	MTT	C11-O15-C15	2.68	118.95	113.75
3	C	1207	MTT	C13-C14-C15	2.79	115.07	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	TMO	7	0
2	A	1203	TMO	1	0
2	A	1205	TMO	1	0
2	A	1206	TMO	2	0
2	A	1207	TMO	3	0
2	A	1208	TMO	2	0
3	A	1209	MTT	1	0
2	B	1201	TMO	3	0
2	C	1202	TMO	4	0
2	C	1203	TMO	4	0
2	C	1205	TMO	1	0
3	C	1207	MTT	2	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	505/520 (97%)	-0.03	8 (1%) 74 78	15, 24, 41, 60	0
1	B	512/520 (98%)	0.01	12 (2%) 64 67	15, 24, 41, 59	0
1	C	512/520 (98%)	-0.10	5 (0%) 84 86	14, 23, 37, 55	0
All	All	1529/1560 (98%)	-0.04	25 (1%) 74 78	14, 23, 40, 60	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1063	GLY	5.9
1	A	1063	GLY	4.6
1	B	141	ALA	4.0
1	B	1063	GLY	3.6
1	B	1103	ASN	3.5
1	B	1064	GLN	3.5
1	C	1104	ASP	3.4
1	A	1159	VAL	3.3
1	A	1135	LEU	3.2
1	C	239	ALA	3.1
1	B	1102	THR	2.9
1	A	1057	ILE	2.8
1	A	1064	GLN	2.6
1	C	1142	ASN	2.5
1	B	138	GLU	2.5
1	B	239	ALA	2.5
1	B	1104	ASP	2.5
1	A	1131	THR	2.5
1	B	1135	LEU	2.4
1	B	1062	ASP	2.4
1	B	1065	THR	2.4
1	A	138	GLU	2.3
1	A	1103	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1118	LEU	2.1
1	C	1064	GLN	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	TMO	C	1202	5/5	0.97	0.15	4.36	13,15,17,18	0
2	TMO	A	1201	5/5	0.95	0.17	4.19	12,13,18,20	0
2	TMO	A	1207	5/5	0.86	0.18	2.83	29,32,36,40	0
2	TMO	B	1202	5/5	0.97	0.14	1.66	10,12,17,22	0
2	TMO	A	1208	5/5	0.97	0.15	0.66	18,24,28,33	0
3	MTT	B	1206	45/45	0.93	0.12	0.50	15,22,37,44	0
3	MTT	C	1207	45/45	0.93	0.13	0.43	16,21,37,46	0
2	TMO	C	1201	5/5	0.98	0.14	0.18	15,19,22,26	0
2	TMO	B	1201	5/5	0.95	0.13	-0.05	19,21,30,40	0
3	MTT	A	1209	45/45	0.95	0.10	-0.51	15,20,35,39	0
2	TMO	B	1204	5/5	0.97	0.12	-	28,31,33,36	0
2	TMO	B	1205	5/5	0.94	0.14	-	31,31,32,33	0
2	TMO	A	1203	5/5	0.93	0.15	-	33,33,37,39	0
2	TMO	C	1203	5/5	0.97	0.11	-	23,29,40,44	0
2	TMO	B	1203	5/5	0.96	0.12	-	28,35,37,38	0
2	TMO	C	1205	5/5	0.95	0.16	-	34,38,41,44	0
2	TMO	A	1206	5/5	0.92	0.16	-	40,43,50,50	0
2	TMO	C	1206	5/5	0.91	0.18	-	36,43,45,48	0
2	TMO	A	1204	5/5	0.90	0.26	-	33,34,35,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	TMO	C	1204	5/5	0.89	0.13	-	31,33,41,45	0
2	TMO	A	1205	5/5	0.92	0.14	-	27,30,32,33	0
2	TMO	A	1202	5/5	0.97	0.11	-	30,30,34,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.