



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 20, 2016 – 08:21 PM EST

PDB ID : 4LZW  
Title : X-ray structure uridine phosphorylase from *Vibrio cholerae* in complex with thymidine at 1.29 Å resolution  
Authors : Prokofev, I.I.; Lashkov, A.A.; Gabdoulkhakov, A.G.; Betzel, C.; Mikhailov, A.M.  
Deposited on : 2013-08-01  
Resolution : 1.29 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	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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)	:	rb-20028442

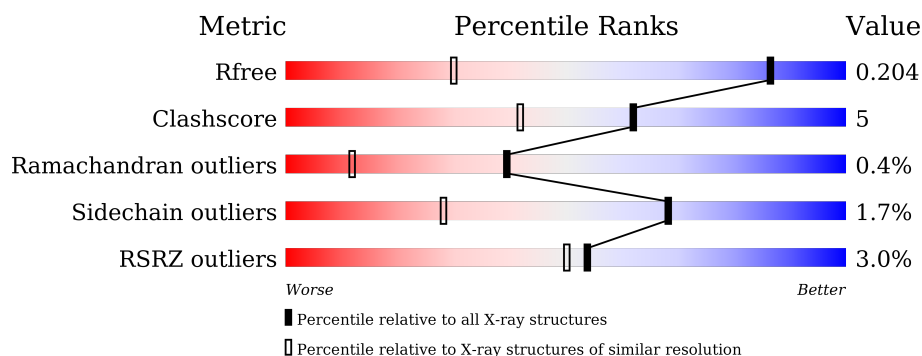
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.29 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	1475 (1.34-1.26)
Clashscore	102246	1031 (1.32-1.28)
Ramachandran outliers	100387	1504 (1.34-1.26)
Sidechain outliers	100360	1503 (1.34-1.26)
RSRZ outliers	91569	1476 (1.34-1.26)

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	253	<div> <div>2%</div> <div>87% 10% .</div> </div>
1	B	253	<div> <div>4%</div> <div>89% 11%</div> </div>
1	C	253	<div> <div>%</div> <div>87% 12% .</div> </div>
1	D	253	<div> <div>2%</div> <div>90% 9% .</div> </div>
1	E	253	<div> <div>6%</div> <div>85% 13% .</div> </div>
1	F	253	<div> <div>3%</div> <div>82% 15% .</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	THM	C	301	-	-	-	X
3	EOH	B	303	-	-	X	-
3	EOH	D	302	-	-	X	-
3	EOH	E	303	-	-	X	-
3	EOH	F	302	-	-	X	-
5	NA	A	305	-	-	-	X
5	NA	C	304	-	-	-	X
5	NA	F	304	-	-	-	X
6	MG	C	306	-	-	-	X
6	MG	D	305	-	-	-	X
7	EDO	E	302	-	-	-	X

## 2 Entry composition [i](#)

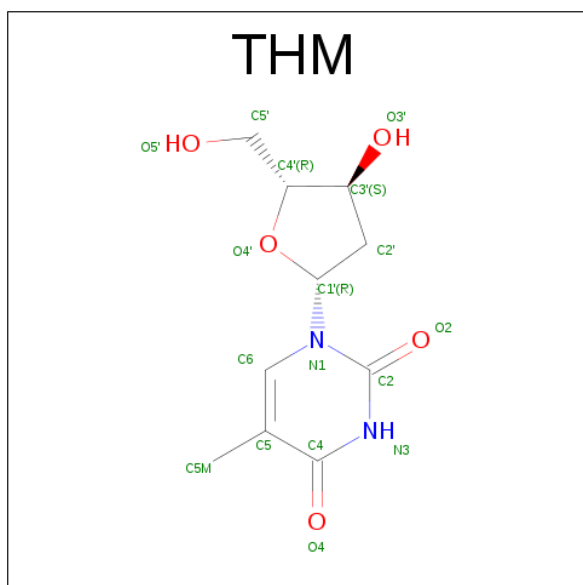
There are 8 unique types of molecules in this entry. The entry contains 14145 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uridine phosphorylase.

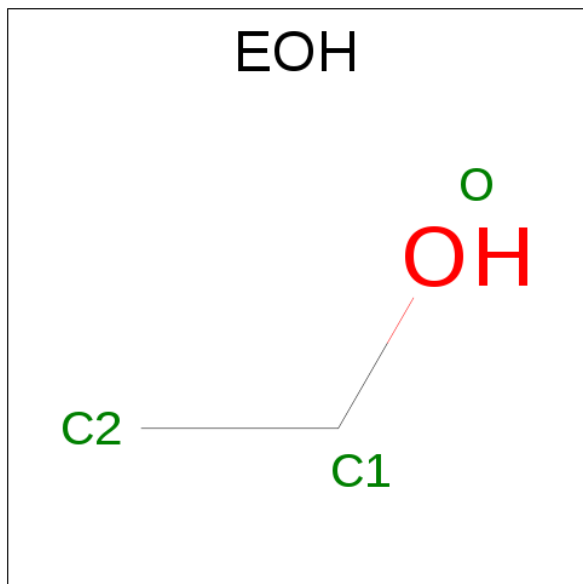
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	17	0
			1932	1217	331	368	16			
1	B	252	Total	C	N	O	S	0	22	0
			2014	1270	349	377	18			
1	C	251	Total	C	N	O	S	0	19	0
			1984	1255	338	374	17			
1	D	251	Total	C	N	O	S	0	16	0
			1973	1245	340	372	16			
1	E	251	Total	C	N	O	S	0	24	0
			2018	1274	349	378	17			
1	F	245	Total	C	N	O	S	0	21	0
			1945	1234	333	361	17			

- Molecule 2 is THYMIDINE (three-letter code: THM) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>2</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	10	2	5		
2	B	1	Total	C	N	O	0	0
			17	10	2	5		
2	C	1	Total	C	N	O	0	0
			17	10	2	5		
2	D	1	Total	C	N	O	0	0
			17	10	2	5		
2	E	1	Total	C	N	O	0	0
			17	10	2	5		
2	F	1	Total	C	N	O	0	0
			17	10	2	5		

- Molecule 3 is ETHANOL (three-letter code: EOH) (formula:  $C_2H_6O$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	2	1		
3	A	1	Total	C	O	0	0
			3	2	1		
3	B	1	Total	C	O	0	0
			3	2	1		
3	B	1	Total	C	O	0	0
			3	2	1		
3	D	1	Total	C	O	0	0
			3	2	1		
3	E	1	Total	C	O	0	0
			3	2	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			3	2	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		
4	A	2	Total	Cl	0	0
			2	2		
4	F	2	Total	Cl	0	0
			2	2		

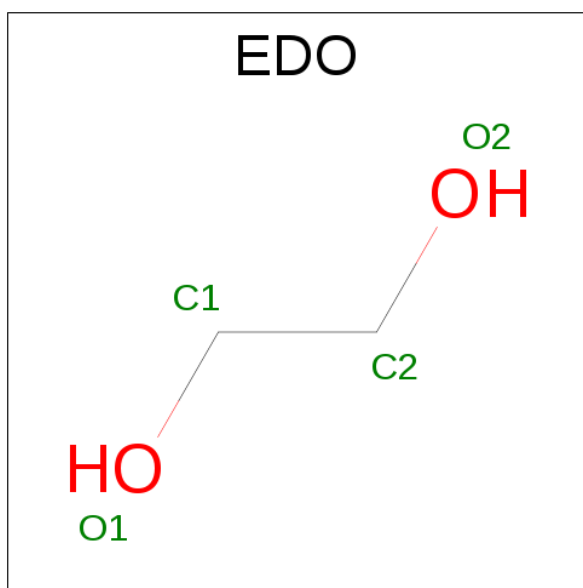
- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		
6	D	2	Total	Mg	0	0
			2	2		
6	C	2	Total	Mg	0	0
			2	2		
6	E	1	Total	Mg	0	0
			1	1		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	291	Total	O	0	23
			315	315		
8	B	335	Total	O	0	23
			359	359		
8	C	373	Total	O	0	24
			397	397		
8	D	350	Total	O	0	35
			385	385		
8	E	317	Total	O	0	27
			344	344		
8	F	301	Total	O	0	28
			330	330		

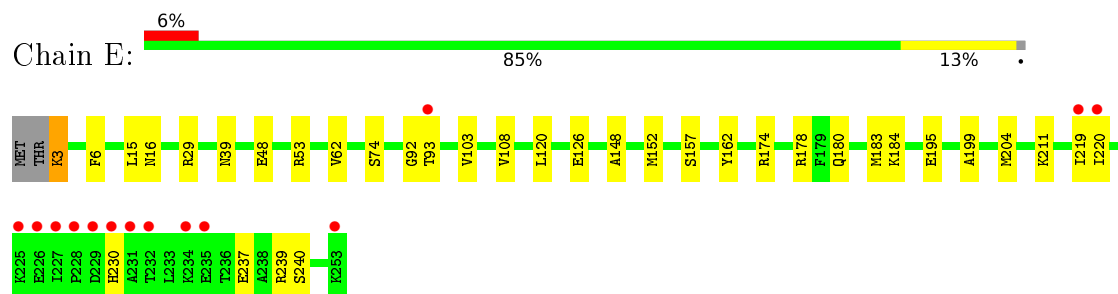


- Molecule 1: Uridine phosphorylase

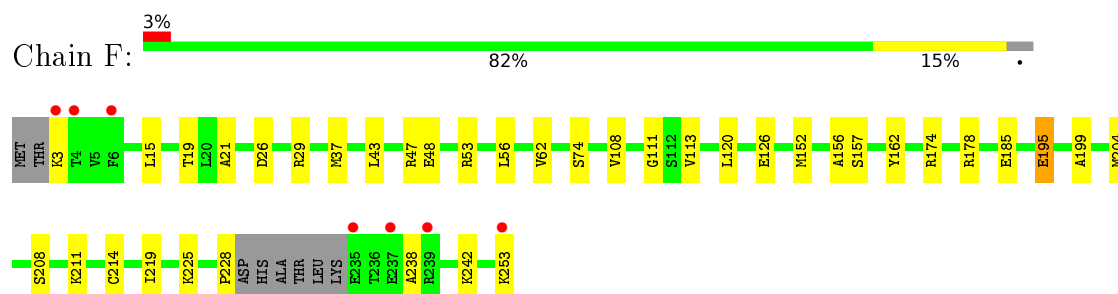




- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.74Å 95.85Å 91.83Å 90.00° 119.96° 90.00°	Depositor
Resolution (Å)	19.89 – 1.29 19.89 – 1.29	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.89-1.29) 99.4 (19.89-1.29)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 1.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.178 , 0.210 0.171 , 0.204	Depositor DCC
$R_{free}$ test set	17115 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	7.6	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.196 for -h-l,k,h 0.196 for l,k,-h-l 0.057 for h,-k,-h-l 0.067 for -h-l,-k,l 0.064 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14145	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, NA, EOH, EDO, THM

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	0.48	0/2003	0.64	0/2706
1	B	0.46	0/2103	0.62	0/2842
1	C	0.47	0/2073	0.65	0/2802
1	D	0.49	0/2053	0.63	0/2777
1	E	0.46	0/2113	0.61	0/2853
1	F	0.46	0/2034	0.65	0/2746
All	All	0.47	0/12379	0.63	0/16726

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1932	0	1973	20	0
1	B	2014	0	2076	24	0
1	C	1984	0	2052	21	0
1	D	1973	0	2026	14	0
1	E	2018	0	2091	26	0
1	F	1945	0	2032	32	0
2	A	17	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	17	0	13	2	0
2	C	17	0	13	0	0
2	D	17	0	13	0	0
2	E	17	0	12	0	0
2	F	17	0	12	2	0
3	A	6	0	12	1	0
3	B	6	0	12	6	0
3	D	3	0	6	2	0
3	E	3	0	6	3	0
3	F	3	0	6	3	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	1	0
4	F	2	0	0	2	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
6	E	1	0	0	0	0
7	C	4	0	6	2	0
7	E	4	0	6	1	0
8	A	315	0	0	7	0
8	B	359	0	0	11	0
8	C	397	0	0	7	0
8	D	385	0	0	4	0
8	E	344	0	0	9	0
8	F	330	0	0	8	0
All	All	14145	0	12379	131	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 5.

All (131) 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)
4:E:304:CL:CL	8:E:493:HOH:O	2.23	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180[A]:GLN:NE2	8:B:523:HOH:O	2.04	0.90
1:C:15:LEU:HG	1:C:62[B]:VAL:HG11	1.53	0.90
3:A:302:EOH:H12	1:B:120:LEU:HD22	1.59	0.84
1:C:106[B]:MET:SD	8:C:571:HOH:O	2.37	0.83
1:F:214[B]:CYS:SG	8:F:620:HOH:O	2.38	0.81
1:A:120:LEU:HD22	3:B:303:EOH:H12	1.64	0.80
1:B:185[B]:GLU:OE1	1:D:177:ARG:NH2	2.15	0.78
1:F:126[B]:GLU:OE1	8:F:495:HOH:O	2.02	0.76
1:B:53[B]:ARG:NH1	8:B:728:HOH:O	2.17	0.76
1:F:53[B]:ARG:NH1	8:F:695:HOH:O	2.18	0.76
7:C:302:EDO:H21	1:D:120:LEU:HD22	1.67	0.76
1:E:211[A]:LYS:NZ	8:E:499:HOH:O	2.20	0.73
1:E:126[A]:GLU:OE2	8:E:707:HOH:O	2.07	0.72
1:A:128:PRO:HB2	1:A:130[B]:VAL:HG23	1.72	0.71
1:A:47[A]:ARG:NH2	8:A:543:HOH:O	2.18	0.71
1:C:120:LEU:HD22	3:D:302:EOH:H12	1.71	0.70
1:A:126[A]:GLU:OE2	8:A:677:HOH:O	2.10	0.70
1:E:29[B]:ARG:NH2	1:E:240[B]:SER:OG	2.25	0.69
1:E:92[B]:GLY:O	8:E:433:HOH:O	2.10	0.69
1:F:15:LEU:HD22	1:F:62[B]:VAL:HG11	1.75	0.68
1:A:126[B]:GLU:OE1	8:A:535:HOH:O	2.11	0.68
1:B:16[A]:ASN:HB2	1:B:53[A]:ARG:HD2	1.76	0.67
1:E:16:ASN:HB2	1:E:53:ARG:HD2	1.77	0.67
1:B:177:ARG:NH2	1:F:185[B]:GLU:OE1	2.21	0.66
1:F:47[B]:ARG:NH2	8:F:700:HOH:O	2.29	0.66
1:B:126[B]:GLU:OE2	8:B:717:HOH:O	2.14	0.65
1:C:197:GLU:OE1	8:C:494:HOH:O	2.15	0.62
1:A:128:PRO:HB2	1:A:130[B]:VAL:CG2	2.29	0.62
1:E:120:LEU:HD22	3:F:302:EOH:H12	1.81	0.62
1:C:16:ASN:HB2	1:C:53:ARG:HD2	1.82	0.61
3:E:303:EOH:H12	1:F:120:LEU:HD22	1.84	0.60
1:F:19:THR:OG1	8:F:580:HOH:O	2.16	0.60
1:D:126[A]:GLU:OE2	8:D:538:HOH:O	2.17	0.60
1:F:3:LYS:N	8:F:646:HOH:O	2.35	0.59
1:A:26:ASP:HB3	1:A:29:ARG:HG2	1.84	0.59
1:E:15:LEU:HD22	1:E:62[B]:VAL:HG11	1.83	0.59
1:C:15:LEU:HG	1:C:62[B]:VAL:CG1	2.30	0.59
1:C:93[B]:THR:HG23	1:C:219:ILE:HG13	1.83	0.59
1:D:235[A]:GLU:OE1	8:D:661:HOH:O	2.17	0.59
1:E:3:LYS:NZ	8:E:498:HOH:O	2.31	0.59
1:B:220:ILE:HG12	2:B:301:THM:HM52	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:126[A]:GLU:OE2	8:F:684:HOH:O	2.17	0.59
1:E:184:LYS:NZ	8:E:658:HOH:O	2.36	0.58
1:F:26:ASP:HB3	1:F:29:ARG:HG2	1.86	0.58
1:B:126[A]:GLU:OE2	8:B:587:HOH:O	2.18	0.57
1:D:16:ASN:HB2	1:D:53:ARG:HD2	1.86	0.57
1:A:3:LYS:NZ	8:A:617:HOH:O	2.31	0.57
1:A:130[B]:VAL:HG21	1:F:111:GLY:HA3	1.85	0.57
1:F:157:SER:HB3	1:F:199:ALA:HB2	1.86	0.56
1:B:92[A]:GLY:O	8:B:402:HOH:O	2.18	0.56
1:A:188:ASP:HB3	1:E:174[A]:ARG:HD3	1.88	0.56
1:B:174[A]:ARG:NH1	8:B:727:HOH:O	2.15	0.56
1:A:246[B]:GLU:OE1	1:A:249:ARG:NE	2.34	0.56
1:A:16[B]:ASN:HB2	1:A:53:ARG:HD2	1.88	0.55
8:A:421:HOH:O	3:B:303:EOH:H21	2.05	0.55
1:F:238:ALA:O	1:F:242[A]:LYS:HG2	2.06	0.55
1:B:184:LYS:NZ	8:B:619[A]:HOH:O	2.27	0.55
1:F:225[A]:LYS:NZ	4:F:305:CL:CL	2.77	0.54
1:E:120:LEU:HB3	3:F:302:EOH:H11	1.88	0.54
1:F:211:LYS:NZ	8:F:596:HOH:O	2.30	0.54
1:D:32:LYS:NZ	8:D:743:HOH:O	2.31	0.54
1:E:157:SER:HB3	1:E:199:ALA:HB2	1.90	0.53
1:E:93[B]:THR:HG23	8:E:433:HOH:O	2.08	0.53
1:B:211[B]:LYS:HD2	8:B:475:HOH:O	2.08	0.52
1:E:148:ALA:HB2	1:E:239:ARG:HD2	1.91	0.52
1:C:74:SER:HA	1:C:204[B]:MET:HE1	1.93	0.51
1:E:74:SER:HA	1:E:204[B]:MET:HE1	1.93	0.51
8:A:417:HOH:O	3:B:303:EOH:H23	2.09	0.51
1:E:103:VAL:HG13	1:E:219:ILE:HA	1.92	0.51
1:D:37:MET:HG2	1:D:56:LEU:HD13	1.92	0.50
3:B:303:EOH:H22	8:B:539:HOH:O	2.12	0.50
1:E:180[A]:GLN:OE1	8:E:622:HOH:O	2.19	0.50
1:B:157:SER:HB3	1:B:199:ALA:HB2	1.95	0.49
1:C:57:ASP:OD2	1:C:249[A]:ARG:HG3	2.12	0.49
3:E:303:EOH:H11	1:F:120:LEU:HB3	1.94	0.49
1:E:6:PHE:CZ	1:F:228:PRO:HG2	2.49	0.48
1:A:31:GLN:NE2	1:A:35[A]:GLU:OE1	2.41	0.48
1:D:104:GLY:O	1:D:239[B]:ARG:NH1	2.47	0.47
1:A:57:ASP:OD2	1:A:249:ARG:HG3	2.14	0.47
1:A:157:SER:HB3	1:A:199:ALA:HB2	1.95	0.47
1:C:157:SER:HB3	1:C:199:ALA:HB2	1.97	0.47
1:E:183[A]:MET:HG3	7:E:302:EDO:H22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:219:ILE:HD11	2:F:301:THM:HM51	1.97	0.47
1:B:106[A]:MET:SD	8:B:490:HOH:O	2.60	0.46
1:B:178:ARG:HH11	3:B:303:EOH:H11	1.79	0.46
1:C:211:LYS:NZ	8:C:540:HOH:O	2.31	0.46
1:B:185[B]:GLU:OE2	8:B:444:HOH:O	2.21	0.46
1:B:228:PRO:HB2	1:B:233:LEU:HD11	1.98	0.46
1:A:188:ASP:HB3	1:E:174[A]:ARG:CD	2.45	0.46
1:D:157:SER:HB3	1:D:199:ALA:HB2	1.98	0.46
1:F:74:SER:HA	1:F:204[B]:MET:HE1	1.97	0.46
1:F:238:ALA:O	1:F:242[B]:LYS:HG2	2.16	0.46
1:F:21:ALA:HB2	1:F:62[B]:VAL:HG23	1.96	0.46
1:B:101:VAL:O	1:B:221:ASN:ND2	2.50	0.45
1:D:57:ASP:OD2	1:D:249[A]:ARG:HG3	2.16	0.45
1:F:37:MET:HG2	1:F:56:LEU:HD13	1.98	0.45
1:E:39:ASN:OD1	8:E:576:HOH:O	2.21	0.45
1:D:15:LEU:HG	1:D:62[B]:VAL:CG2	2.47	0.45
1:F:113:VAL:HB	1:F:156:ALA:HA	1.99	0.45
1:F:29:ARG:HG3	4:F:303:CL:CL	2.55	0.44
1:C:178:ARG:HD2	7:C:302:EDO:H22	2.00	0.43
1:E:108:VAL:HB	1:E:152:MET:SD	2.58	0.43
1:E:6:PHE:CE1	1:F:228:PRO:HG2	2.54	0.43
1:C:235[B]:GLU:HG3	8:C:576:HOH:O	2.18	0.43
1:C:48:GLU:HB3	1:D:48:GLU:HB3	2.00	0.43
1:A:219:ILE:HD11	2:A:301:THM:HM51	2.01	0.42
1:D:235[B]:GLU:HG3	8:D:557:HOH:O	2.19	0.42
1:A:108:VAL:HB	1:A:152:MET:SD	2.59	0.42
1:C:124:PRO:HB2	1:C:126[B]:GLU:OE1	2.19	0.42
1:E:174[A]:ARG:HH22	1:F:208:SER:HA	1.85	0.42
1:A:25:GLY:HA3	8:A:476[A]:HOH:O	2.19	0.42
1:C:234:LYS:HD2	8:C:576:HOH:O	2.20	0.42
1:F:43:LEU:HD21	1:F:53[B]:ARG:HH11	1.85	0.42
1:B:74:SER:HA	1:B:204[B]:MET:HE1	2.02	0.41
8:C:761:HOH:O	3:D:302:EOH:H21	2.21	0.41
1:F:178:ARG:HD2	3:F:302:EOH:H22	2.01	0.41
1:C:31:GLN:O	1:C:35[B]:GLU:HG2	2.21	0.41
3:B:302:EOH:H12	1:C:125:MET:HB3	2.00	0.41
1:E:48:GLU:HB3	1:F:48:GLU:HB3	2.03	0.41
1:F:108:VAL:HB	1:F:152:MET:SD	2.61	0.41
1:C:235[A]:GLU:OE2	1:C:239:ARG:NH2	2.53	0.41
1:B:219:ILE:HD11	2:B:301:THM:HM51	2.02	0.41
1:C:180:GLN:NE2	8:C:666:HOH:O	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:VAL:HB	1:C:152:MET:SD	2.61	0.41
1:D:108:VAL:HB	1:D:152:MET:SD	2.61	0.41
1:E:178:ARG:HH11	3:E:303:EOH:H11	1.86	0.40
1:F:195:GLU:HA	2:F:301:THM:O2	2.22	0.40
1:B:204[B]:MET:HE3	1:B:204[B]:MET:HB3	1.88	0.40
1:A:48:GLU:HB3	1:B:48:GLU:HB3	2.03	0.40
1:B:47[B]:ARG:HB3	1:B:48:GLU:OE1	2.20	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	258/253 (102%)	253 (98%)	4 (2%)	1 (0%)	39	12
1	B	272/253 (108%)	267 (98%)	4 (2%)	1 (0%)	39	12
1	C	268/253 (106%)	264 (98%)	3 (1%)	1 (0%)	39	12
1	D	265/253 (105%)	260 (98%)	4 (2%)	1 (0%)	39	12
1	E	273/253 (108%)	267 (98%)	5 (2%)	1 (0%)	39	12
1	F	262/253 (104%)	258 (98%)	3 (1%)	1 (0%)	39	12
All	All	1598/1518 (105%)	1569 (98%)	23 (1%)	6 (0%)	39	12

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	162	TYR
1	C	162	TYR
1	D	162	TYR
1	E	162	TYR
1	F	162	TYR
1	A	162	TYR



### 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	212/203 (104%)	208 (98%)	4 (2%)	65	23
1	B	223/203 (110%)	221 (99%)	2 (1%)	84	55
1	C	220/203 (108%)	217 (99%)	3 (1%)	74	36
1	D	217/203 (107%)	212 (98%)	5 (2%)	58	16
1	E	224/203 (110%)	219 (98%)	5 (2%)	60	17
1	F	216/203 (106%)	213 (99%)	3 (1%)	74	36
All	All	1312/1218 (108%)	1290 (98%)	22 (2%)	68	28

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16[A]	ASN
1	A	16[B]	ASN
1	A	195	GLU
1	A	227	ILE
1	B	195	GLU
1	B	253	LYS
1	C	3	LYS
1	C	195	GLU
1	C	234	LYS
1	D	3	LYS
1	D	62[A]	VAL
1	D	62[B]	VAL
1	D	195	GLU
1	D	253	LYS
1	E	3	LYS
1	E	195	GLU
1	E	220	ILE
1	E	230	HIS
1	E	237	GLU
1	F	174	ARG
1	F	195	GLU
1	F	253	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 33 ligands modelled in this entry, 18 are monoatomic - leaving 15 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	THM	A	301	-	13,18,18	1.89	4 (30%)	16,26,26	2.67	4 (25%)
3	EOH	A	302	-	2,2,2	0.44	0	1,1,1	0.36	0
3	EOH	A	303	-	2,2,2	0.44	0	1,1,1	0.12	0
2	THM	B	301	-	13,18,18	2.04	3 (23%)	16,26,26	2.67	3 (18%)
3	EOH	B	302	-	2,2,2	0.44	0	1,1,1	0.06	0
3	EOH	B	303	-	2,2,2	0.39	0	1,1,1	0.26	0
2	THM	C	301	-	13,18,18	2.03	4 (30%)	16,26,26	2.98	3 (18%)
7	EDO	C	302	-	3,3,3	0.37	0	2,2,2	0.37	0
2	THM	D	301	-	13,18,18	1.98	4 (30%)	16,26,26	2.93	3 (18%)
3	EOH	D	302	-	2,2,2	0.40	0	1,1,1	0.18	0
2	THM	E	301	-	13,18,18	2.11	4 (30%)	16,26,26	2.79	3 (18%)
7	EDO	E	302	-	3,3,3	0.37	0	2,2,2	0.43	0
3	EOH	E	303	-	2,2,2	0.40	0	1,1,1	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	THM	F	301	-	13,18,18	1.95	3 (23%)	16,26,26	3.23	3 (18%)
3	EOH	F	302	-	2,2,2	0.42	0	1,1,1	0.05	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	THM	A	301	-	-	0/2/18/18	0/2/2/2
3	EOH	A	302	-	-	0/0/0/0	0/0/0/0
3	EOH	A	303	-	-	0/0/0/0	0/0/0/0
2	THM	B	301	-	-	0/2/18/18	0/2/2/2
3	EOH	B	302	-	-	0/0/0/0	0/0/0/0
3	EOH	B	303	-	-	0/0/0/0	0/0/0/0
2	THM	C	301	-	-	0/2/18/18	0/2/2/2
7	EDO	C	302	-	-	0/1/1/1	0/0/0/0
2	THM	D	301	-	-	0/2/18/18	0/2/2/2
3	EOH	D	302	-	-	0/0/0/0	0/0/0/0
2	THM	E	301	-	-	0/2/18/18	0/2/2/2
7	EDO	E	302	-	-	0/1/1/1	0/0/0/0
3	EOH	E	303	-	-	0/0/0/0	0/0/0/0
2	THM	F	301	-	-	0/2/18/18	0/2/2/2
3	EOH	F	302	-	-	0/0/0/0	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	THM	O3'-C3'	-4.13	1.34	1.43
2	E	301	THM	O3'-C3'	-4.10	1.34	1.43
2	C	301	THM	O3'-C3'	-4.06	1.34	1.43
2	D	301	THM	O3'-C3'	-3.89	1.34	1.43
2	F	301	THM	O3'-C3'	-3.61	1.35	1.43
2	A	301	THM	O3'-C3'	-3.58	1.35	1.43
2	B	301	THM	C2'-C3'	-2.62	1.45	1.52
2	E	301	THM	C2'-C3'	-2.60	1.45	1.52
2	F	301	THM	C2'-C3'	-2.59	1.45	1.52
2	C	301	THM	C2'-C3'	-2.32	1.46	1.52
2	D	301	THM	C2-N3	-2.27	1.33	1.38
2	C	301	THM	C2-N3	-2.23	1.33	1.38
2	D	301	THM	C2'-C3'	-2.20	1.46	1.52
2	A	301	THM	C2-N3	-2.17	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	THM	C2'-C3'	-2.14	1.47	1.52
2	E	301	THM	O4'-C4'	-2.09	1.40	1.45
2	C	301	THM	O4-C4	2.94	1.32	1.24
2	A	301	THM	O4-C4	3.02	1.32	1.24
2	D	301	THM	O4-C4	3.08	1.32	1.24
2	B	301	THM	O4-C4	3.26	1.32	1.24
2	F	301	THM	O4-C4	3.30	1.32	1.24
2	E	301	THM	O4-C4	3.58	1.33	1.24

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	THM	C5-C4-N3	-7.78	118.82	125.35
2	E	301	THM	C5-C4-N3	-6.71	119.71	125.35
2	C	301	THM	C5-C4-N3	-6.70	119.72	125.35
2	D	301	THM	C5-C4-N3	-6.47	119.92	125.35
2	B	301	THM	C5-C4-N3	-6.31	120.05	125.35
2	A	301	THM	C5-C4-N3	-5.58	120.67	125.35
2	A	301	THM	C5M-C5-C6	2.05	122.79	118.63
2	C	301	THM	O5'-C5'-C4'	2.06	118.17	111.30
2	F	301	THM	O5'-C5'-C4'	2.14	118.44	111.30
2	A	301	THM	O5'-C5'-C4'	2.43	119.43	111.30
2	B	301	THM	O5'-C5'-C4'	2.55	119.81	111.30
2	E	301	THM	O5'-C5'-C4'	2.68	120.25	111.30
2	D	301	THM	O5'-C5'-C4'	2.68	120.26	111.30
2	B	301	THM	C4-N3-C2	7.48	121.40	115.16
2	E	301	THM	C4-N3-C2	7.91	121.75	115.16
2	A	301	THM	C4-N3-C2	7.96	121.80	115.16
2	D	301	THM	C4-N3-C2	8.87	122.56	115.16
2	C	301	THM	C4-N3-C2	8.99	122.66	115.16
2	F	301	THM	C4-N3-C2	9.31	122.92	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	THM	1	0
3	A	302	EOH	1	0
2	B	301	THM	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	EOH	1	0
3	B	303	EOH	5	0
7	C	302	EDO	2	0
3	D	302	EOH	2	0
7	E	302	EDO	1	0
3	E	303	EOH	3	0
2	F	301	THM	2	0
3	F	302	EOH	3	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	245/253 (96%)	-0.01	6 (2%) 62 59	4, 8, 18, 39	1 (0%)
1	B	252/253 (99%)	0.05	11 (4%) 38 34	4, 8, 24, 39	0
1	C	251/253 (99%)	-0.16	3 (1%) 81 80	4, 7, 14, 37	0
1	D	251/253 (99%)	-0.16	4 (1%) 74 72	4, 7, 14, 34	0
1	E	251/253 (99%)	0.11	14 (5%) 28 24	4, 8, 23, 42	1 (0%)
1	F	245/253 (96%)	-0.03	7 (2%) 55 51	4, 9, 19, 40	1 (0%)
All	All	1495/1518 (98%)	-0.03	45 (3%) 54 50	4, 8, 18, 42	3 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	THR	8.2
1	E	227	ILE	7.5
1	C	4	THR	7.1
1	B	2	THR	5.8
1	B	227	ILE	5.7
1	E	230	HIS	5.6
1	B	230	HIS	5.4
1	A	3	LYS	5.3
1	F	253	LYS	5.2
1	E	253	LYS	5.0
1	E	225	LYS	4.9
1	D	4	THR	4.4
1	E	231	ALA	4.3
1	B	225	LYS	4.0
1	E	226	GLU	3.8
1	B	229	ASP	3.7
1	B	231	ALA	3.7
1	F	6	PHE	3.7
1	B	226	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	253	LYS	3.6
1	D	3	LYS	3.5
1	C	3	LYS	3.5
1	E	229	ASP	3.4
1	F	235	GLU	3.4
1	A	253	LYS	3.3
1	C	253	LYS	3.2
1	D	253	LYS	3.1
1	A	6	PHE	2.9
1	A	227	ILE	2.9
1	D	62[A]	VAL	2.9
1	E	228	PRO	2.9
1	E	93[A]	THR	2.7
1	B	234	LYS	2.7
1	A	235	GLU	2.6
1	B	228	PRO	2.5
1	E	235	GLU	2.4
1	B	252	LEU	2.4
1	E	232	THR	2.4
1	E	234	LYS	2.3
1	F	237	GLU	2.3
1	E	219	ILE	2.2
1	F	4	THR	2.1
1	F	3	LYS	2.1
1	E	220	ILE	2.1
1	F	239	ARG	2.0

## 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
6	MG	C	306	1/1	0.61	0.32	20.60	17,17,17,17	1
7	EDO	E	302	4/4	0.93	0.22	16.73	22,23,24,24	0
5	NA	F	304	1/1	0.82	0.28	16.65	7,7,7,7	1
6	MG	D	305	1/1	0.80	0.43	16.30	15,15,15,15	1
5	NA	A	305	1/1	0.98	0.13	5.92	5,5,5,5	1
2	THM	C	301	17/17	0.97	0.12	2.76	2,5,12,12	17
5	NA	C	304	1/1	0.99	0.08	2.39	7,7,7,7	1
2	THM	E	301	17/17	0.92	0.12	0.56	8,12,19,20	17
2	THM	B	301	17/17	0.95	0.09	0.40	7,12,18,19	0
2	THM	D	301	17/17	0.97	0.07	0.17	5,6,13,13	0
2	THM	F	301	17/17	0.97	0.07	-0.11	5,7,13,14	0
2	THM	A	301	17/17	0.97	0.07	-0.32	6,8,14,14	0
4	CL	F	303	1/1	0.97	0.07	-0.47	28,28,28,28	0
4	CL	A	304	1/1	0.97	0.07	-0.66	31,31,31,31	0
4	CL	B	304	1/1	1.00	0.05	-1.13	13,13,13,13	0
4	CL	A	306	1/1	1.00	0.04	-1.45	11,11,11,11	0
4	CL	E	304	1/1	0.98	0.04	-1.58	18,18,18,18	1
4	CL	C	303	1/1	1.00	0.04	-1.63	4,4,4,4	1
4	CL	F	305	1/1	1.00	0.04	-2.32	10,10,10,10	1
4	CL	D	303	1/1	1.00	0.03	-3.31	9,9,9,9	0
3	EOH	D	302	3/3	0.89	0.14	-	12,12,12,16	3
6	MG	D	304	1/1	0.98	0.18	-	15,15,15,15	1
3	EOH	E	303	3/3	0.90	0.14	-	13,13,13,16	3
6	MG	C	305	1/1	0.84	0.15	-	17,17,17,17	1
7	EDO	C	302	4/4	0.89	0.17	-	17,17,21,23	4
3	EOH	F	302	3/3	0.87	0.13	-	13,13,14,17	3
3	EOH	A	303	3/3	0.85	0.18	-	22,22,22,22	3
3	EOH	B	303	3/3	0.85	0.18	-	16,16,17,21	0
6	MG	A	307	1/1	0.94	0.16	-	19,19,19,19	1
6	MG	B	305	1/1	0.89	0.13	-	15,15,15,15	1
6	MG	E	305	1/1	0.97	0.15	-	18,18,18,18	1
3	EOH	A	302	3/3	0.85	0.17	-	10,10,11,14	3
3	EOH	B	302	3/3	0.75	0.20	-	26,26,26,26	3

## 6.5 Other polymers ⓘ

There are no such residues in this entry.