



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:39 AM GMT

PDB ID : 3MO0  
Title : Human G9a-like (GLP, also known as EHMT1) in complex with inhibitor E11  
Authors : Chang, Y.; Horton, J.R.; Cheng, X.  
Deposited on : 2010-04-22  
Resolution : 2.78 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

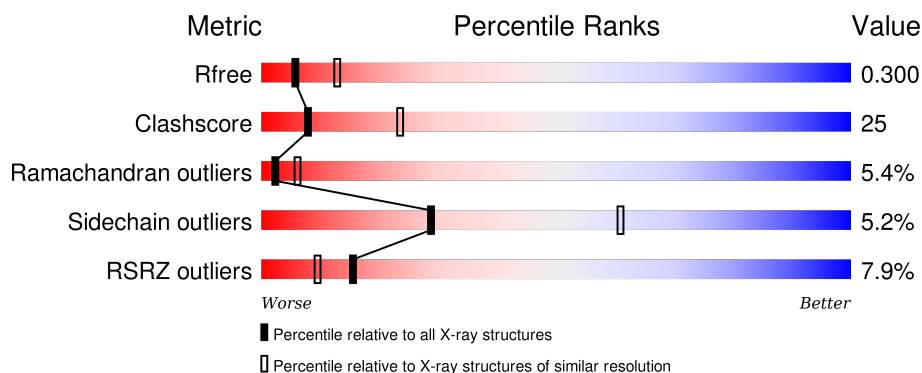
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.78 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	3004 (2.80-2.76)
Clashscore	102246	3480 (2.80-2.76)
Ramachandran outliers	100387	3423 (2.80-2.76)
Sidechain outliers	100360	3425 (2.80-2.76)
RSRZ outliers	91569	3016 (2.80-2.76)

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	285	<div> <div>6%</div> <div>55%</div> <div>29%</div> <div>•</div> <div>12%</div> </div>
1	B	285	<div> <div>8%</div> <div>48%</div> <div>31%</div> <div>6%</div> <div>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
3	E11	B	2003	-	-	-	X
5	EDO	B	1	-	-	-	X

## 2 Entry composition [i](#)

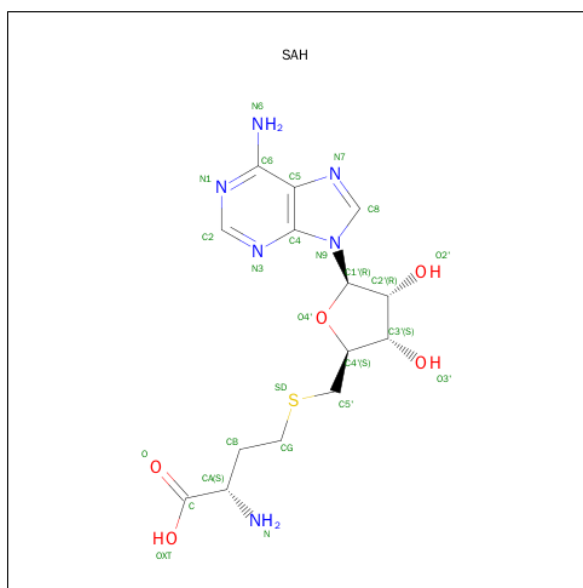
There are 6 unique types of molecules in this entry. The entry contains 4074 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Histone-lysine N-methyltransferase, H3 lysine-9 specific 5.

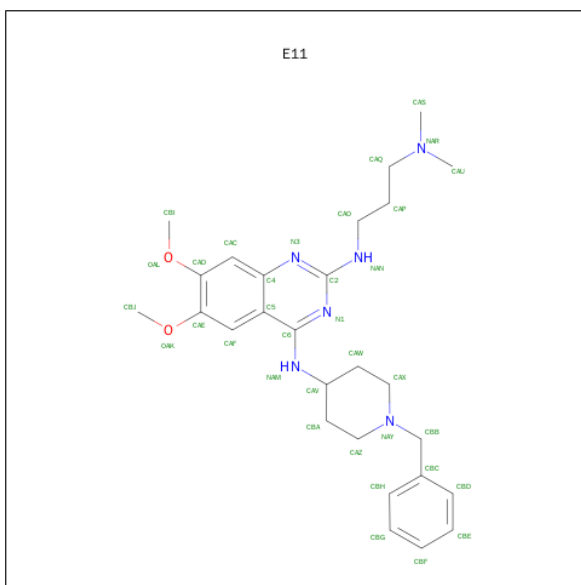
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	2	0
			2005	1250	366	365	24			
1	B	242	Total	C	N	O	S	0	0	0
			1850	1152	334	343	21			

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula:  $C_{14}H_{20}N_6O_5S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is N 4 -(1-BENZYLPIPERIDIN-4-YL)-N 2 -[3-(DIMETHYLAMINO)PROPYL]-6,7-DIMETHOXYQUINAZOLINE-2,4-DIAMINE (three-letter code: E11) (formula:  $C_{27}H_{38}N_6O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 35	C 27	N 6	O 2	0	1
3	A	1	Total 35	C 27	N 6	O 2	0	1
3	B	1	Total 35	C 27	N 6	O 2	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	5	Total Zn 5 5	0	0
4	A	5	Total Zn 5 5	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $\text{C}_2\text{H}_6\text{O}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

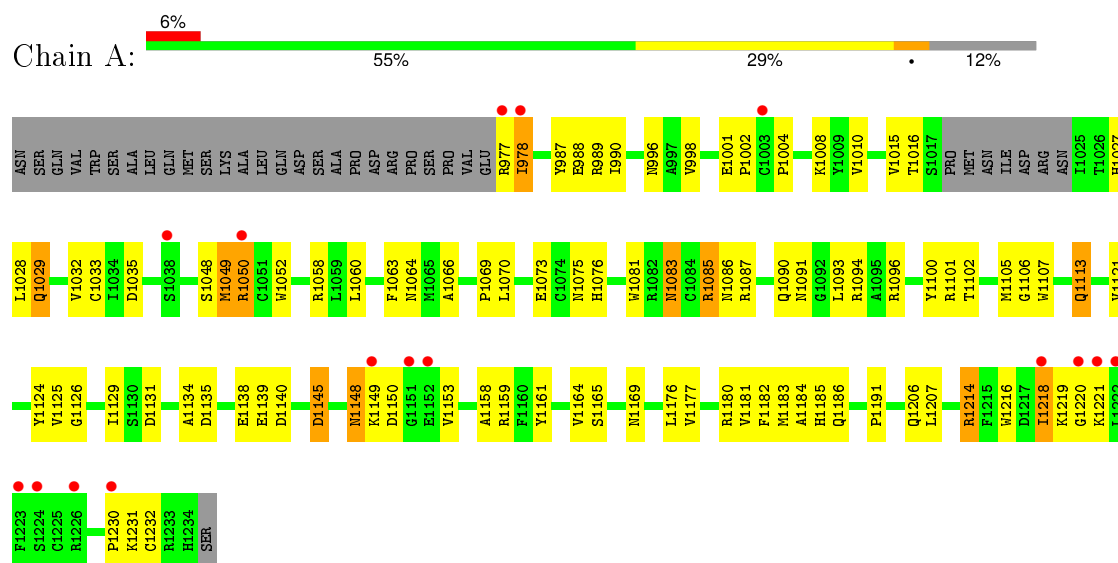
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	22	Total	O	0	0
			22	22		
6	B	22	Total	O	0	0
			22	22		

### 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: Histone-lysine N-methyltransferase, H3 lysine-9 specific 5



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.30 Å 94.50 Å 138.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.55 – 2.78 34.55 – 2.78	Depositor EDS
% Data completeness (in resolution range)	85.5 (34.55-2.78) 85.5 (34.55-2.78)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 2.76 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.225 , 0.306 0.225 , 0.300	Depositor DCC
$R_{free}$ test set	688 reflections (4.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.2	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 59.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 14872 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4074	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% 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: E11, ZN, SAH, EDO

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	0.41	0/2054	0.61	0/2781
1	B	0.39	0/1893	0.62	0/2570
All	All	0.40	0/3947	0.61	0/5351

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	2005	0	1845	91	0
1	B	1850	0	1676	97	0
2	A	26	0	19	0	0
2	B	26	0	19	1	0
3	A	70	0	76	24	0
3	B	35	0	38	13	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	B	8	0	12	0	0
6	A	22	0	0	0	0
6	B	22	0	0	1	0
All	All	4074	0	3685	192	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 25.

All (192) 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:1131:ASP:O	3:A:2001[A]:E11:HAU	1.29	1.29
1:A:1131:ASP:OD2	3:A:2001[A]:E11:CAU	1.96	1.13
1:A:1131:ASP:O	3:A:2001[A]:E11:CAU	1.99	1.11
1:A:1131:ASP:OD2	3:A:2001[A]:E11:HAU	1.50	1.11
1:B:1013:ASN:HD22	1:B:1125:VAL:HG13	1.29	0.97
1:B:1096:ARG:H	1:B:1113:GLN:HE21	1.04	0.96
1:A:1214[A]:ARG:HH21	1:A:1214[A]:ARG:HB3	1.35	0.91
1:B:1146:LEU:HD13	1:B:1190:PHE:HA	1.56	0.85
1:A:1131:ASP:OD2	3:A:2001[A]:E11:HAUB	1.78	0.82
3:B:2003:E11:HAPA	3:B:2003:E11:N1	1.95	0.81
1:B:1096:ARG:H	1:B:1113:GLN:NE2	1.76	0.81
1:B:1029:GLN:HE21	1:B:1075:ASN:ND2	1.80	0.79
1:B:978:ILE:HG22	1:B:979:VAL:HG13	1.64	0.79
1:B:990:ILE:HD12	1:B:990:ILE:O	1.82	0.79
1:A:990:ILE:O	1:A:990:ILE:HD12	1.84	0.77
1:A:1131:ASP:C	3:A:2001[A]:E11:HAU	2.04	0.76
1:A:1048:SER:O	1:A:1049:MET:HB2	1.85	0.76
1:A:1138:GLU:HG2	3:A:2001[A]:E11:HBF	1.69	0.74
1:B:1182:PHE:CZ	1:B:1191:PRO:HB3	2.25	0.72
1:B:1013:ASN:HD21	1:B:1125:VAL:HA	1.55	0.71
1:B:1145:ASP:OD1	3:B:2003:E11:HAC	1.90	0.71
1:B:1017:SER:H	1:B:1018:PRO:CD	2.04	0.70
1:A:1138:GLU:HG2	3:A:2002[B]:E11:HBF	1.72	0.70
1:B:1013:ASN:ND2	1:B:1125:VAL:HG13	2.03	0.69
1:A:1131:ASP:OD2	3:A:2002[B]:E11:HAP	1.94	0.68
1:B:978:ILE:O	1:B:979:VAL:HG22	1.94	0.67
1:A:1073:GLU:HA	1:A:1086:ASN:ND2	2.09	0.67
1:B:1140:ASP:OD2	3:B:2003:E11:HAF	1.93	0.67
1:B:1221:LYS:O	1:B:1222:LEU:HD23	1.94	0.66
1:A:1214[A]:ARG:NH2	1:A:1214[A]:ARG:HB3	2.09	0.66
1:A:998:VAL:HG21	1:A:1101:ARG:O	1.95	0.66
1:A:1214[B]:ARG:HH21	3:A:2002[B]:E11:HBI	1.62	0.65
1:A:1070:LEU:HD22	1:A:1182:PHE:HE2	1.61	0.64
1:A:1214[B]:ARG:HB2	3:A:2002[B]:E11:HBIA	1.79	0.64
1:B:1140:ASP:HB2	1:B:1143:LEU:HD12	1.79	0.64
1:A:1016:THR:HA	1:B:1024:ASN:CB	2.27	0.64
1:B:1135:ASP:HA	3:B:2003:E11:HAZ	1.78	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1140:ASP:O	3:A:2002[B]:E11:HBJA	1.98	0.63
1:B:1153:VAL:HG12	1:B:1154:TYR:N	2.15	0.61
1:B:1068:PRO:N	1:B:1069:PRO:CD	2.63	0.61
1:A:1169:ASN:ND2	1:A:1206:GLN:OE1	2.32	0.61
1:A:1033:CYS:HB3	1:A:1035:ASP:OD1	2.01	0.60
1:B:1068:PRO:N	1:B:1069:PRO:HD2	2.15	0.60
1:A:1182:PHE:CZ	1:A:1191:PRO:HB3	2.36	0.60
1:A:1070:LEU:HD23	1:A:1180[A]:ARG:HB2	1.83	0.59
1:B:1029:GLN:HE21	1:B:1075:ASN:HD21	1.47	0.59
1:A:1214[B]:ARG:HH21	3:A:2002[B]:E11:CBI	2.13	0.59
1:A:1218:ILE:HG12	3:A:2001[A]:E11:HBJB	1.84	0.58
1:B:1178:PRO:HB3	1:B:1195:PHE:HE1	1.68	0.58
1:A:1129:ILE:HD11	1:A:1134:ALA:HB2	1.85	0.57
1:B:1029:GLN:NE2	1:B:1075:ASN:ND2	2.52	0.57
1:A:1140:ASP:O	3:A:2001[A]:E11:HBJA	2.04	0.57
1:B:978:ILE:HG12	1:B:1002:PRO:HA	1.87	0.57
1:A:1180[B]:ARG:N	1:A:1180[B]:ARG:HD2	2.20	0.56
1:B:1148:ASN:HB3	1:B:1189:ARG:HA	1.86	0.56
3:B:2003:E11:CAS	3:B:2003:E11:HAW	2.36	0.56
1:B:1146:LEU:HD12	1:B:1154:TYR:CB	2.35	0.55
1:B:1183:MET:HE1	1:B:1184:ALA:HB2	1.89	0.54
1:A:1063:PHE:CZ	1:A:1069:PRO:HD2	2.42	0.54
1:A:1096:ARG:HB2	1:A:1113:GLN:HG2	1.88	0.54
1:B:1123:GLU:HB2	1:B:1193:ILE:O	2.07	0.54
1:B:1158:ALA:HA	1:B:1161:TYR:O	2.09	0.53
1:A:1140:ASP:OD2	3:A:2002[B]:E11:HAF	2.09	0.53
1:B:979:VAL:HG23	1:B:979:VAL:O	2.06	0.53
1:A:1216:TRP:O	1:A:1220:GLY:HA3	2.08	0.53
1:B:1089:VAL:HG21	1:B:1181:VAL:HG21	1.91	0.53
1:A:1073:GLU:OE1	1:A:1090:GLN:HG2	2.09	0.53
1:B:1098:GLN:HB2	1:B:1112:LEU:HD11	1.90	0.52
1:A:1070:LEU:HD23	1:A:1180[B]:ARG:HB2	1.91	0.52
1:A:1058:ARG:NH1	1:A:1058:ARG:HG3	2.24	0.52
1:A:1058:ARG:HH11	1:A:1058:ARG:HG3	1.75	0.52
1:B:1070:LEU:HD23	1:B:1180:ARG:HB2	1.91	0.52
1:B:1133:GLU:O	1:B:1136:VAL:HB	2.11	0.51
3:B:2003:E11:HAS	3:B:2003:E11:HAW	1.93	0.51
1:A:977:ARG:HG3	1:A:978:ILE:N	2.25	0.51
1:B:1166:ARG:NH1	1:B:1167:PHE:CZ	2.79	0.51
1:A:1218:ILE:HG12	3:A:2002[B]:E11:HBJB	1.92	0.51
3:B:2003:E11:N1	3:B:2003:E11:CAP	2.64	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1064:ASN:OD1	1:A:1066:ALA:HB3	2.11	0.51
1:A:1001:GLU:HG3	1:A:1002:PRO:HD2	1.92	0.51
1:A:1124:TYR:CD1	1:A:1165:SER:HB3	2.46	0.51
1:A:1131:ASP:HB2	1:A:1153:VAL:O	2.11	0.50
1:B:978:ILE:HG12	1:B:1002:PRO:CA	2.41	0.50
1:B:990:ILE:HD12	1:B:990:ILE:C	2.31	0.50
1:B:1127:GLU:OE2	1:B:1137:ARG:NH2	2.43	0.50
1:A:1010:VAL:HG12	1:B:1076:HIS:HB2	1.94	0.50
1:B:1026:THR:OG1	1:B:1185:HIS:HA	2.11	0.50
1:A:1048:SER:O	1:A:1049:MET:CB	2.59	0.50
1:A:1083:ASN:HD22	1:A:1083:ASN:H	1.58	0.50
1:B:1153:VAL:CG1	1:B:1154:TYR:N	2.74	0.50
1:B:1176:LEU:HB2	1:B:1208:GLY:O	2.11	0.50
1:A:1131:ASP:O	3:A:2001[A]:E11:HAUA	2.04	0.50
1:A:1086:ASN:O	1:A:1087:ARG:HG2	2.11	0.49
1:B:1001:GLU:OE2	1:B:1002:PRO:HD2	2.12	0.49
1:B:978:ILE:HG12	1:B:1002:PRO:HB3	1.95	0.49
1:A:1135:ASP:HB2	3:A:2001[A]:E11:NAR	2.28	0.48
3:B:2003:E11:HAV	3:B:2003:E11:HASB	1.95	0.48
1:B:1178:PRO:HB3	1:B:1195:PHE:CE1	2.46	0.48
1:A:1148:ASN:O	1:A:1150:ASP:N	2.43	0.48
1:A:1145:ASP:OD2	3:A:2002[B]:E11:HBIB	2.13	0.48
1:A:1081:TRP:CH2	1:B:981:ARG:NH2	2.80	0.48
1:A:977:ARG:O	1:A:978:ILE:HB	2.14	0.48
1:A:1085:ARG:NH1	1:A:1085:ARG:HG2	2.29	0.48
1:A:1158:ALA:HA	1:A:1161:TYR:O	2.14	0.47
1:B:1148:ASN:CB	1:B:1189:ARG:HA	2.44	0.47
1:B:1071:ILE:HD12	1:B:1179:VAL:HG11	1.96	0.47
1:A:988:GLU:OE2	1:A:988:GLU:HA	2.15	0.47
1:B:1096:ARG:N	1:B:1113:GLN:HE21	1.89	0.47
1:B:1140:ASP:OD2	3:B:2003:E11:HBJB	2.15	0.47
1:B:1017:SER:H	1:B:1018:PRO:HD3	1.76	0.47
1:B:1157:ASP:OD1	1:B:1159:ARG:HB3	2.15	0.47
1:A:1148:ASN:C	1:A:1150:ASP:H	2.18	0.46
1:B:981:ARG:O	1:B:982:ASP:HB2	2.14	0.46
1:A:1093:LEU:HD12	1:A:1121:VAL:O	2.15	0.46
1:A:996:ASN:ND2	1:A:1001:GLU:O	2.48	0.46
1:A:1176:LEU:HD11	1:A:1207:LEU:HB3	1.98	0.46
1:A:1004:PRO:HD3	1:A:1107:TRP:CZ2	2.51	0.46
1:B:1129:ILE:HG13	1:B:1130:SER:N	2.31	0.46
1:A:1008:LYS:HB3	1:A:1161:TYR:CD1	2.51	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1181:VAL:HG12	1:A:1183:MET:HE2	1.98	0.46
1:A:1214[B]:ARG:NH2	3:A:2002[B]:E11:HBI	2.29	0.45
1:A:1214[A]:ARG:HB2	3:A:2001[A]:E11:HBIA	1.97	0.45
1:A:1076:HIS:HD1	1:A:1076:HIS:H	1.63	0.45
1:B:1182:PHE:CE1	1:B:1191:PRO:HB3	2.50	0.45
1:A:1073:GLU:HA	1:A:1086:ASN:HD21	1.80	0.45
1:A:989:ARG:NH2	1:A:1094:ARG:HE	2.15	0.45
1:B:1171:HIS:CE1	1:B:1229:SER:HB2	2.52	0.45
1:B:1176:LEU:HA	1:B:1196:PHE:O	2.17	0.45
1:B:1026:THR:C	1:B:1028:LEU:H	2.18	0.45
1:B:1159:ARG:HH11	1:B:1159:ARG:HG3	1.82	0.45
1:B:1218:ILE:O	1:B:1218:ILE:HG22	2.16	0.45
1:B:1133:GLU:HA	1:B:1136:VAL:CG2	2.46	0.45
1:A:1015:VAL:HG23	1:A:1015:VAL:O	2.17	0.45
1:A:1129:ILE:CD1	1:A:1134:ALA:HB2	2.47	0.44
1:B:1147:ASP:HB2	1:B:1180:ARG:HH22	1.82	0.44
1:A:989:ARG:CZ	1:A:1094:ARG:HE	2.31	0.44
3:B:2003:E11:CAV	3:B:2003:E11:HASB	2.48	0.44
1:B:1094:ARG:HG3	6:B:39:HOH:O	2.16	0.44
1:B:1148:ASN:OD1	1:B:1153:VAL:N	2.50	0.44
1:B:990:ILE:HD11	1:B:1093:LEU:HD21	1.99	0.44
1:A:1085:ARG:HH11	1:A:1085:ARG:HG2	1.81	0.44
1:B:1213:GLU:O	1:B:1214:ARG:C	2.54	0.44
1:B:1029:GLN:HG3	1:B:1029:GLN:O	2.18	0.44
1:B:1170:HIS:CG	1:B:1171:HIS:N	2.86	0.43
3:B:2003:E11:CBH	3:B:2003:E11:HAXA	2.48	0.43
1:A:1052:TRP:O	1:A:1060:LEU:HG	2.18	0.43
1:A:1184:ALA:O	1:A:1185:HIS:HB2	2.19	0.43
1:B:1009:TYR:HA	1:B:1162:GLY:O	2.18	0.43
1:B:1013:ASN:ND2	1:B:1125:VAL:HA	2.29	0.43
1:B:1035:ASP:HB2	1:B:1036:ASP:H	1.65	0.43
1:A:989:ARG:NH2	1:A:1091:ASN:O	2.32	0.43
1:B:1002:PRO:O	1:B:1003:CYS:C	2.57	0.43
1:B:1090:GLN:OE1	1:B:1183:MET:CE	2.67	0.43
1:B:1082:ARG:HG3	1:B:1082:ARG:O	2.18	0.43
1:B:1164:VAL:HG22	1:B:1164:VAL:O	2.19	0.43
1:B:1146:LEU:O	1:B:1180:ARG:NH2	2.52	0.43
1:B:1133:GLU:HA	1:B:1136:VAL:HG23	2.01	0.43
1:B:1159:ARG:NH1	1:B:1159:ARG:HG3	2.34	0.43
1:B:1175:ASN:O	1:B:1197:SER:HA	2.19	0.42
1:B:1101:ARG:HB2	1:B:1107:TRP:CZ3	2.53	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1145:ASP:OD2	3:A:2001[A]:E11:HBIB	2.19	0.42
1:A:1010:VAL:HG11	1:B:1076:HIS:HD2	1.83	0.42
1:A:1131:ASP:OD2	3:A:2001[A]:E11:CAS	2.68	0.42
3:B:2003:E11:HAPA	3:B:2003:E11:HASB	1.60	0.42
1:B:1029:GLN:HE21	1:B:1075:ASN:HD22	1.65	0.42
1:B:1094:ARG:HD3	1:B:1095:ALA:N	2.34	0.42
1:A:1177:VAL:HG13	1:A:1177:VAL:O	2.20	0.42
1:B:1183:MET:HE1	1:B:1184:ALA:N	2.34	0.42
1:A:1139:GLU:HG2	1:A:1159:ARG:HD3	2.01	0.42
1:B:1229:SER:C	1:B:1231:LYS:H	2.22	0.42
1:B:1226:ARG:H	2:B:102:SAH:HN62	1.68	0.42
1:B:979:VAL:O	1:B:979:VAL:CG2	2.68	0.41
1:A:1048:SER:C	1:A:1050:ARG:H	2.24	0.41
3:B:2003:E11:HAW	3:B:2003:E11:HASB	2.02	0.41
1:A:1028:LEU:O	1:A:1029:GLN:CB	2.67	0.41
1:A:1139:GLU:OE1	1:A:1139:GLU:HA	2.20	0.41
1:A:1125:VAL:HG12	1:A:1126:GLY:N	2.36	0.41
1:B:1017:SER:H	1:B:1018:PRO:HD2	1.83	0.41
1:A:1100:TYR:OH	1:A:1206:GLN:HG3	2.20	0.41
1:A:1102:THR:OG1	1:A:1106:GLY:N	2.54	0.41
1:B:1097:LEU:HD22	1:B:1207:LEU:HD11	2.03	0.41
1:B:1123:GLU:HG3	1:B:1125:VAL:HG23	2.03	0.41
1:A:1075:ASN:CB	1:A:1184:ALA:HB2	2.51	0.41
1:B:1216:TRP:C	1:B:1218:ILE:N	2.72	0.40
1:A:1105:MET:CE	1:A:1206:GLN:HE22	2.34	0.40
1:A:1094:ARG:HD3	1:A:1094:ARG:HA	1.81	0.40
1:B:1004:PRO:HD3	1:B:1107:TRP:CE2	2.56	0.40
1:B:1146:LEU:O	1:B:1147:ASP:CB	2.70	0.40
1:A:1219:LYS:C	1:A:1221:LYS:H	2.24	0.40
1:B:1121:VAL:O	1:B:1122:CYS:HB3	2.22	0.40
1:B:1083:ASN:HD22	1:B:1083:ASN:H	1.70	0.40
1:A:987:TYR:CD1	1:B:1082:ARG:HB2	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	249/285 (87%)	205 (82%)	36 (14%)	8 (3%)	5	15
1	B	238/285 (84%)	188 (79%)	32 (13%)	18 (8%)	1	2
All	All	487/570 (85%)	393 (81%)	68 (14%)	26 (5%)	2	6

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1029	GLN
1	A	1231	LYS
1	B	1017	SER
1	B	1023	ARG
1	B	1069	PRO
1	B	1070	LEU
1	B	1153	VAL
1	B	1184	ALA
1	A	1149	LYS
1	B	982	ASP
1	B	998	VAL
1	B	1024	ASN
1	B	1147	ASP
1	B	1183	MET
1	A	978	ILE
1	A	1049	MET
1	A	1232	CYS
1	B	1016	THR
1	B	979	VAL
1	B	1004	PRO
1	B	1013	ASN
1	B	1018	PRO
1	A	1164	VAL
1	B	1088	VAL
1	B	1190	PHE
1	A	1230	PRO

### 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	214/257 (83%)	202 (94%)	12 (6%)	26	57
1	B	194/257 (76%)	184 (95%)	10 (5%)	29	61
All	All	408/514 (79%)	386 (95%)	22 (5%)	29	59

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

Mol	Chain	Res	Type
1	A	1027	HIS
1	A	1032	VAL
1	A	1050	ARG
1	A	1083	ASN
1	A	1085	ARG
1	A	1113	GLN
1	A	1145	ASP
1	A	1148	ASN
1	A	1186	GLN
1	A	1214[A]	ARG
1	A	1214[B]	ARG
1	A	1218	ILE
1	B	1008	LYS
1	B	1010	VAL
1	B	1029	GLN
1	B	1035	ASP
1	B	1083	ASN
1	B	1094	ARG
1	B	1110	ARG
1	B	1114	ASP
1	B	1183	MET
1	B	1227	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1027	HIS
1	A	1083	ASN
1	B	1013	ASN
1	B	1029	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	1083	ASN
1	B	1113	GLN
1	B	1186	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 10 are monoatomic - leaving 7 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	SAH	A	101	-	20,28,28	1.89	5 (25%)	19,40,40	2.93	7 (36%)
3	E11	A	2001[A]	-	37,38,38	1.09	2 (5%)	48,51,51	1.93	10 (20%)
3	E11	A	2002[B]	-	37,38,38	1.12	2 (5%)	48,51,51	1.97	11 (22%)
5	EDO	B	1	-	3,3,3	0.53	0	2,2,2	0.35	0
2	SAH	B	102	-	20,28,28	1.98	5 (25%)	19,40,40	3.09	7 (36%)
5	EDO	B	2	-	3,3,3	0.58	0	2,2,2	0.26	0
3	E11	B	2003	-	37,38,38	1.11	2 (5%)	48,51,51	1.98	12 (25%)

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	SAH	A	101	-	-	0/7/31/31	0/3/3/3
3	E11	A	2001[A]	-	-	0/19/29/29	0/4/4/4
3	E11	A	2002[B]	-	-	0/19/29/29	0/4/4/4
5	EDO	B	1	-	-	0/1/1/1	0/0/0/0
2	SAH	B	102	-	-	0/7/31/31	0/3/3/3
5	EDO	B	2	-	-	0/1/1/1	0/0/0/0
3	E11	B	2003	-	-	0/19/29/29	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2002[B]	E11	C6-C5	-4.73	1.39	1.44
3	B	2003	E11	C6-C5	-4.59	1.39	1.44
3	A	2001[A]	E11	C6-C5	-4.43	1.39	1.44
2	A	101	SAH	C5'-SD	-3.10	1.75	1.81
2	B	102	SAH	C5'-SD	-3.03	1.75	1.81
2	B	102	SAH	C8-N7	-2.42	1.30	1.34
2	A	101	SAH	C8-N7	-2.39	1.30	1.34
3	B	2003	E11	C5-C4	-2.12	1.39	1.42
3	A	2001[A]	E11	C5-C4	-2.03	1.39	1.42
3	A	2002[B]	E11	C5-C4	-2.00	1.39	1.42
2	A	101	SAH	C5'-C4'	2.30	1.58	1.52
2	B	102	SAH	C5'-C4'	2.38	1.59	1.52
2	B	102	SAH	C2-N3	3.29	1.38	1.32
2	A	101	SAH	C2-N3	3.47	1.38	1.32
2	A	101	SAH	O4'-C1'	4.71	1.47	1.41
2	B	102	SAH	O4'-C1'	5.81	1.48	1.41

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	102	SAH	N3-C2-N1	-8.81	122.15	128.89
2	A	101	SAH	N3-C2-N1	-8.61	122.30	128.89
3	A	2002[B]	E11	CAF-C5-C6	-7.05	121.13	124.89
3	B	2003	E11	CAF-C5-C6	-6.97	121.17	124.89
3	A	2001[A]	E11	CAF-C5-C6	-6.89	121.22	124.89
2	A	101	SAH	CB-CG-SD	-4.82	104.28	113.57
2	B	102	SAH	CB-CG-SD	-4.37	105.15	113.57
3	A	2002[B]	E11	CBJ-OAK-CAE	-3.87	111.68	117.54

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2002[B]	E11	CBI-OAL-CAD	-3.86	111.68	117.54
3	A	2001[A]	E11	CBJ-OAK-CAE	-3.80	111.77	117.54
3	B	2003	E11	CBI-OAL-CAD	-3.69	111.94	117.54
3	B	2003	E11	N3-C2-N1	-3.68	120.57	126.22
3	A	2001[A]	E11	N3-C2-N1	-3.60	120.69	126.22
3	B	2003	E11	CBJ-OAK-CAE	-3.60	112.08	117.54
3	A	2002[B]	E11	N3-C2-N1	-3.52	120.82	126.22
3	A	2001[A]	E11	CBI-OAL-CAD	-3.48	112.26	117.54
3	A	2002[B]	E11	C5-C4-N3	-3.45	119.53	122.90
3	B	2003	E11	C5-C4-N3	-3.44	119.54	122.90
3	A	2001[A]	E11	C5-C4-N3	-3.43	119.55	122.90
3	B	2003	E11	OAL-CAD-CAC	-3.34	120.77	125.25
3	B	2003	E11	OAK-CAE-CAF	-3.32	120.80	125.25
3	A	2002[B]	E11	OAK-CAE-CAF	-3.17	121.01	125.25
2	B	102	SAH	C1'-N9-C4	-3.14	122.20	126.94
3	A	2001[A]	E11	OAK-CAE-CAF	-3.14	121.05	125.25
3	A	2001[A]	E11	OAL-CAD-CAC	-3.11	121.08	125.25
2	A	101	SAH	C1'-N9-C4	-3.11	122.25	126.94
3	A	2002[B]	E11	OAL-CAD-CAC	-3.04	121.17	125.25
3	A	2002[B]	E11	CAO-NAN-C2	-2.12	119.78	123.80
3	B	2003	E11	CAO-NAN-C2	-2.04	119.94	123.80
3	B	2003	E11	C2-N1-C6	2.03	121.08	116.92
3	A	2002[B]	E11	OAL-CAD-CAE	2.19	118.52	115.40
2	A	101	SAH	O4'-C1'-N9	2.20	112.71	108.10
3	A	2001[A]	E11	OAL-CAD-CAE	2.41	118.84	115.40
2	A	101	SAH	C2-N1-C6	2.45	123.15	118.77
3	A	2001[A]	E11	OAK-CAE-CAD	2.47	118.93	115.40
3	B	2003	E11	OAK-CAE-CAD	2.54	119.02	115.40
2	B	102	SAH	O4'-C1'-N9	2.56	113.46	108.10
3	A	2002[B]	E11	OAK-CAE-CAD	2.65	119.18	115.40
2	B	102	SAH	C2-N1-C6	2.70	123.60	118.77
3	B	2003	E11	OAL-CAD-CAE	2.78	119.36	115.40
2	A	101	SAH	CB-CA-N	3.30	119.90	110.52
2	B	102	SAH	CB-CA-N	3.40	120.18	110.52
3	A	2002[B]	E11	C6-C5-C4	4.76	118.48	115.77
3	A	2001[A]	E11	C6-C5-C4	4.89	118.56	115.77
3	B	2003	E11	C6-C5-C4	4.98	118.61	115.77
2	A	101	SAH	C4'-O4'-C1'	5.14	115.37	109.72
2	B	102	SAH	C4'-O4'-C1'	6.46	116.82	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001[A]	E11	14	0
3	A	2002[B]	E11	10	0
2	B	102	SAH	1	0
3	B	2003	E11	13	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	251/285 (88%)	0.37	16 (6%)	23 16	23, 46, 88, 96	0
1	B	242/285 (84%)	0.37	23 (9%)	10 6	28, 53, 105, 113	0
All	All	493/570 (86%)	0.37	39 (7%)	15 9	23, 50, 95, 113	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1051	CYS	8.1
1	B	1017	SER	4.9
1	B	978	ILE	4.8
1	B	1152	GLU	4.3
1	A	1151	GLY	3.9
1	A	978	ILE	3.8
1	B	1068	PRO	3.7
1	B	1050	ARG	3.6
1	A	1226	ARG	3.6
1	B	1151	GLY	3.5
1	B	1018	PRO	3.5
1	B	1069	PRO	3.4
1	A	1223	PHE	3.3
1	B	1025	ILE	3.3
1	A	1230	PRO	3.2
1	B	1016	THR	3.2
1	B	1000	SER	3.1
1	B	1070	LEU	3.0
1	A	1224	SER	2.9
1	A	1149	LYS	2.8
1	B	1150	ASP	2.7
1	B	1085	ARG	2.7
1	B	1048	SER	2.6
1	B	1134	ALA	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	1218	ILE	2.6
1	A	1222	LEU	2.5
1	B	1149	LYS	2.5
1	A	977	ARG	2.5
1	B	1049	MET	2.4
1	A	1221	LYS	2.4
1	B	1147	ASP	2.3
1	A	1050	ARG	2.2
1	B	1148	ASN	2.2
1	A	1152	GLU	2.2
1	B	1217	ASP	2.2
1	B	1023	ARG	2.2
1	A	1038	SER	2.1
1	A	1220	GLY	2.1
1	A	1003	CYS	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
5	EDO	B	1	4/4	0.87	0.27	4.07	55,59,60,61	0
3	E11	B	2003	35/35	0.77	0.36	2.53	83,91,101,101	0
5	EDO	B	2	4/4	0.90	0.23	1.08	60,61,61,63	0
2	SAH	B	102	26/26	0.93	0.18	0.51	57,64,65,68	0
3	E11	A	2001[A]	35/35	0.84	0.23	0.09	62,66,72,72	35
2	SAH	A	101	26/26	0.85	0.23	0.05	72,78,79,79	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	E11	A	2002[B]	35/35	0.85	0.21	-0.14	59,64,71,71	35
4	ZN	A	2	1/1	0.99	0.15	-0.24	35,35,35,35	0
4	ZN	A	3	1/1	0.99	0.13	-0.44	36,36,36,36	0
4	ZN	A	1236	1/1	1.00	0.13	-0.75	35,35,35,35	0
4	ZN	B	7	1/1	0.99	0.10	-0.94	35,35,35,35	0
4	ZN	B	5	1/1	0.99	0.11	-1.12	40,40,40,40	0
4	ZN	B	8	1/1	0.99	0.11	-1.41	51,51,51,51	0
4	ZN	B	6	1/1	0.99	0.09	-1.43	37,37,37,37	0
4	ZN	A	4	1/1	0.98	0.07	-2.79	70,70,70,70	0
4	ZN	A	10	1/1	0.93	0.14	-	91,91,91,91	0
4	ZN	B	9	1/1	0.99	0.13	-	53,53,53,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.