Full wwPDB X-ray Structure Validation Report (i)

Dec 13, 2016 – 04:26 AM EST

PDB ID	:	5TH3
Title	:	Restriction/modification system-Type II R.SwaI cleaved DNA complex
Authors	:	Shen, B.W.; Stoddard, B.L.
Deposited on	:	2016-09-29
Resolution	:	2.33 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*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

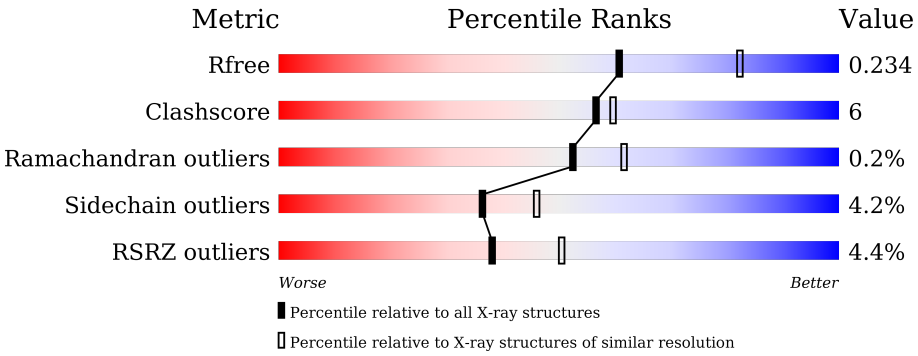
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (2.36-2.32)

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 >=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 <=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	226	2% 86% 11% ·
1	B	226	2% 88% 11% ·
1	C	226	4% 89% 10% ·
1	D	226	3% 85% 13% ·
2	H	14	21% 43% 43% 14%
2	J	14	29% 43% 50% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	h	13	15% 77% 23%
3	j	13	8% 85% 15%
4	I	14	14% 57% 36% 7%
4	K	14	7% 64% 29% 7%
5	i	13	15% 62% 31% 8%
5	k	13	23% 85% 15%

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
6	MG	A	301	-	-	-	X
6	MG	D	301	-	-	-	X
7	EDO	A	303	-	-	-	X
7	EDO	I	101	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9956 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 R-SwaI protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	Se	0	4	0
			1923	1237	317	359	1	9			
1	B	226	Total	C	N	O	S	Se	0	3	0
			1915	1232	316	358	1	8			
1	C	226	Total	C	N	O	S	Se	0	4	0
			1926	1236	319	363	1	7			
1	D	226	Total	C	N	O	S	Se	0	2	0
			1910	1228	316	358	1	7			

- Molecule 2 is a DNA chain called DNA (cleaved 25-MER, portion 1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	12	Total	C	N	O	P	0	0	0
			250	118	47	73	12			
2	J	14	Total	C	N	O	P	0	0	0
			291	138	57	83	13			

- Molecule 3 is a DNA chain called DNA (cleaved 25-MER, portion 2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	h	13	Total	C	N	O	P	0	0	0
			270	126	54	77	13			
3	j	13	Total	C	N	O	P	0	0	0
			270	126	54	77	13			

- Molecule 4 is a DNA chain called DNA (cleaved 26-MER, portion 1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	14	Total	C	N	O	P	0	0	0
			280	134	49	84	13			
4	K	13	Total	C	N	O	P	0	0	0
			261	125	46	78	12			

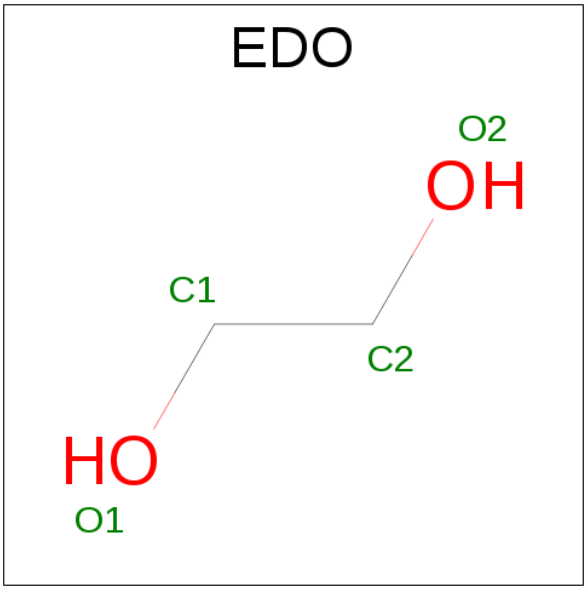
- Molecule 5 is a DNA chain called DNA (cleaved 26-MER, portion 2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	i	12	Total	C	N	O	P	0	0	0
			243	115	44	72	12			
5	k	13	Total	C	N	O	P	0	0	0
			262	124	47	78	13			

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

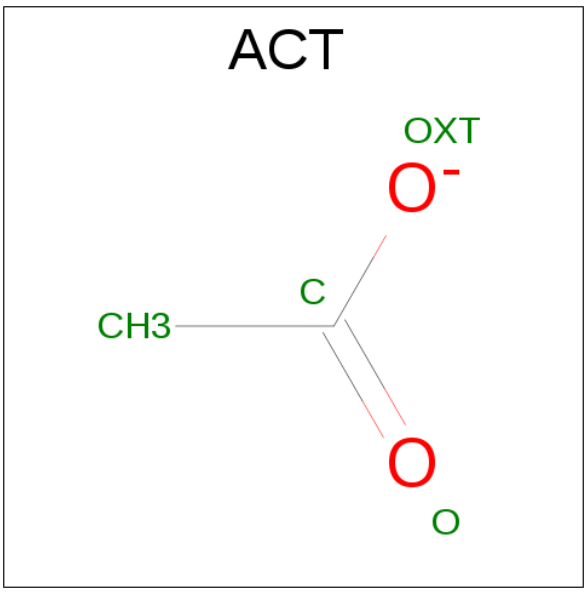
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	A	2	Total	Mg	0	0
			2	2		
6	D	2	Total	Mg	0	0
			2	2		
6	C	1	Total	Mg	0	0
			1	1		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		
7	I	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	31	Total O 31 31	0	0
9	B	27	Total O 27 27	0	0
9	C	16	Total O 16 16	0	0
9	D	23	Total O 23 23	0	0
9	H	4	Total O 4 4	0	0
9	h	6	Total O 6 6	0	0
9	I	7	Total O 7 7	0	0
9	i	6	Total O 6 6	0	0
9	J	2	Total O 2 2	0	0
9	j	4	Total O 4 4	0	0

Continued on next page...

Continued from previous page...

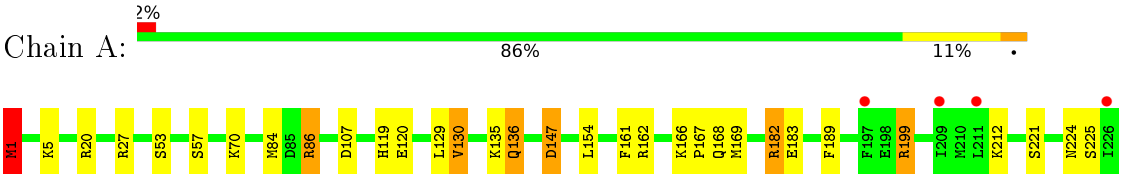
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	K	5	Total O 5 5	0	0
9	k	2	Total O 2 2	0	0

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.

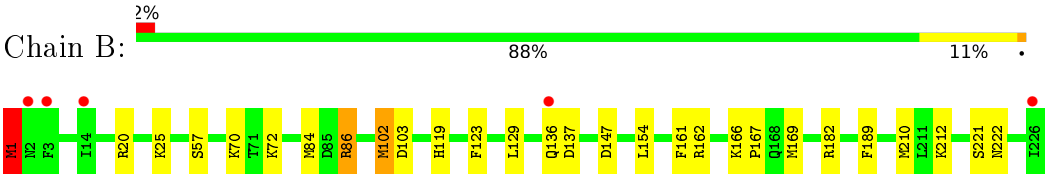
- Molecule 1: R-SwaI protein

Chain A:



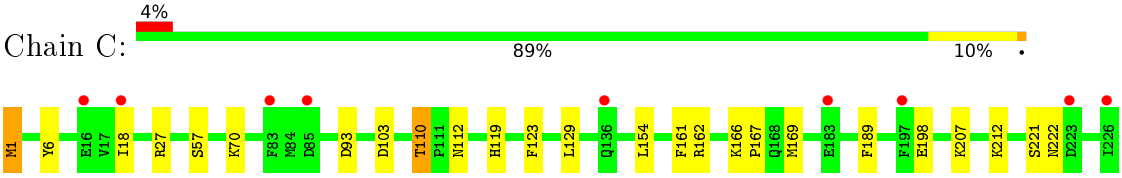
- Molecule 1: R-SwaI protein

Chain B:



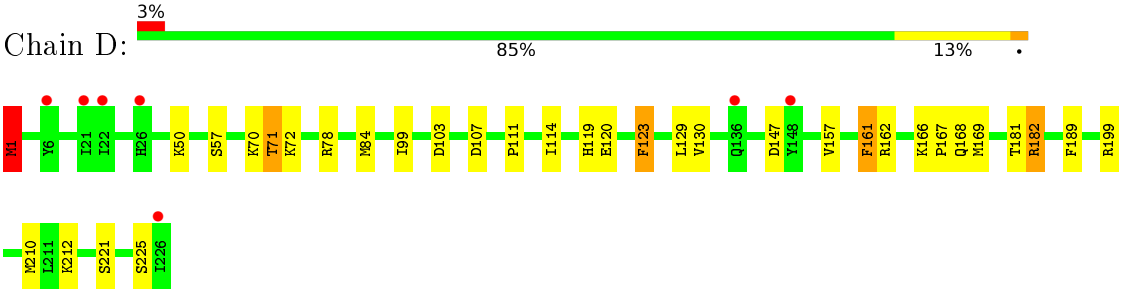
- Molecule 1: R-SwaI protein

Chain C:



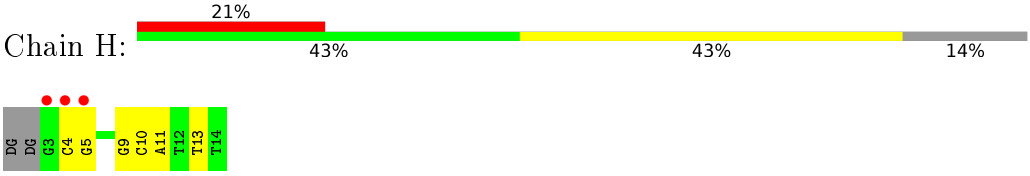
- Molecule 1: R-SwaI protein

Chain D:



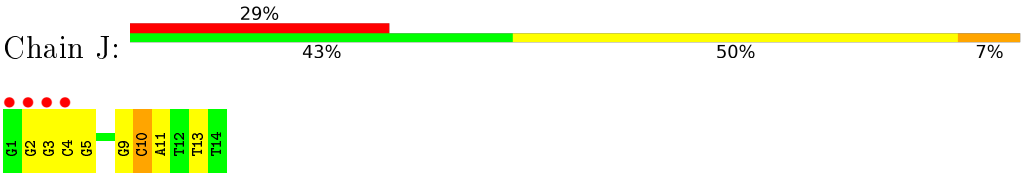
- Molecule 2: DNA (cleaved 25-MER, portion 1)

Chain H:



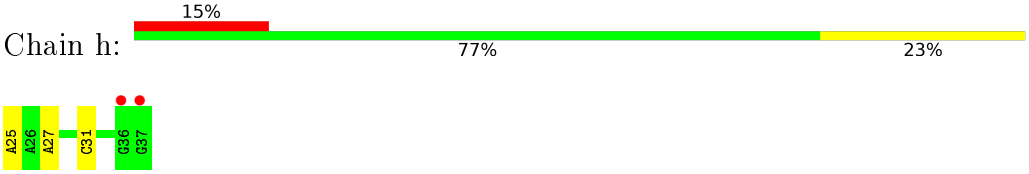
• Molecule 2: DNA (cleaved 25-MER, portion 1)

Chain J:



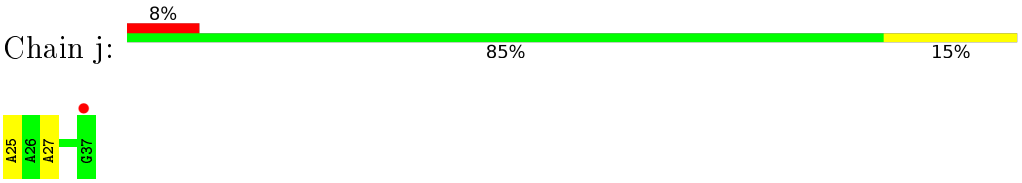
• Molecule 3: DNA (cleaved 25-MER, portion 2)

Chain h:



• Molecule 3: DNA (cleaved 25-MER, portion 2)

Chain j:

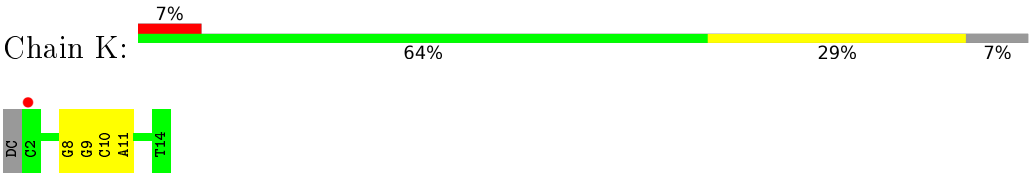


• Molecule 4: DNA (cleaved 26-MER, portion 1)

Chain I:

• Molecule 4: DNA (cleaved 26-MER, portion 1)

Chain K:

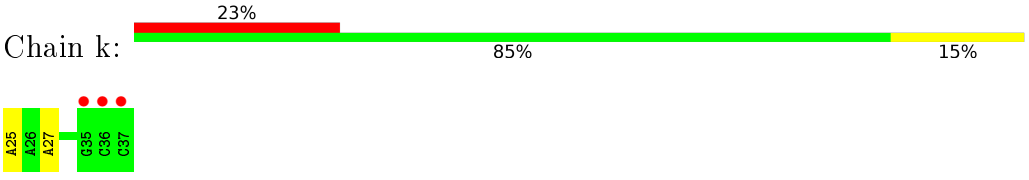


• Molecule 5: DNA (cleaved 26-MER, portion 2)

Chain i:

• Molecule 5: DNA (cleaved 26-MER, portion 2)

Chain k:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	109.75Å 57.07Å 113.44Å 90.00° 107.60° 90.00°	Depositor
Resolution (Å)	50.01 – 2.33 48.20 – 2.33	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.01-2.33) 98.0 (48.20-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	9.50	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.198 , 0.239 0.200 , 0.234	Depositor DCC
R_{free} test set	2894 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	53.9	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 43.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9956	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.58 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2769e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: MG, EDO, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.07	2/1964 (0.1%)	1.05	11/2626 (0.4%)
1	B	0.97	0/1956	1.07	10/2616 (0.4%)
1	C	0.99	2/1964 (0.1%)	1.09	8/2628 (0.3%)
1	D	0.97	2/1948 (0.1%)	1.02	6/2606 (0.2%)
2	H	0.89	0/280	1.29	4/431 (0.9%)
2	J	0.76	0/327	1.38	6/505 (1.2%)
3	h	0.96	1/303 (0.3%)	1.52	5/464 (1.1%)
3	j	0.96	1/303 (0.3%)	1.48	2/464 (0.4%)
4	I	0.81	0/312	1.37	7/479 (1.5%)
4	K	0.81	0/291	1.31	7/447 (1.6%)
5	i	0.99	1/271 (0.4%)	1.62	4/413 (1.0%)
5	k	0.90	1/292 (0.3%)	1.53	3/445 (0.7%)
All	All	0.97	10/10211 (0.1%)	1.17	73/14124 (0.5%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	j	25	DA	OP3-P	-8.88	1.50	1.61
5	i	25	DA	OP3-P	-8.07	1.51	1.61
3	h	25	DA	OP3-P	-7.97	1.51	1.61
5	k	25	DA	OP3-P	-7.79	1.51	1.61
1	C	198	GLU	CG-CD	6.33	1.61	1.51
1	D	120	GLU	CD-OE1	6.17	1.32	1.25
1	C	93	ASP	CB-CG	5.43	1.63	1.51
1	A	120	GLU	CD-OE1	5.32	1.31	1.25
1	A	225	SER	CB-OG	-5.25	1.35	1.42
1	D	225	SER	CB-OG	-5.06	1.35	1.42

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	h	27	DA	O5'-P-OP1	16.71	130.75	110.70
3	j	27	DA	O5'-P-OP1	15.76	129.62	110.70
5	i	27	DA	O5'-P-OP2	-15.73	91.54	105.70
5	k	27	DA	O5'-P-OP1	15.27	129.02	110.70
5	k	27	DA	O5'-P-OP2	-15.14	92.07	105.70
3	j	27	DA	O5'-P-OP2	-14.58	92.58	105.70
3	h	27	DA	O5'-P-OP2	-14.56	92.60	105.70
5	i	27	DA	O5'-P-OP1	14.53	128.14	110.70
2	J	10	DC	O5'-P-OP2	-14.02	93.08	105.70
1	C	27	ARG	NE-CZ-NH1	-13.91	113.34	120.30
4	I	10	DC	O5'-P-OP2	-12.39	94.55	105.70
1	C	27	ARG	NE-CZ-NH2	12.35	126.47	120.30
1	B	84[A]	MSE	CA-CB-CG	-8.56	98.75	113.30
1	B	84[B]	MSE	CA-CB-CG	-8.56	98.75	113.30
4	I	10	DC	O5'-P-OP1	8.25	120.61	110.70
1	A	182	ARG	NE-CZ-NH1	7.88	124.24	120.30
2	H	10	DC	O5'-P-OP2	7.81	120.08	110.70
2	H	9	DG	O5'-P-OP2	-7.77	98.70	105.70
1	B	102	MSE	CG-SE-CE	7.74	115.92	98.90
2	J	10	DC	O5'-P-OP1	7.73	119.97	110.70
5	i	35	DG	O5'-P-OP2	-7.61	98.86	105.70
1	B	182	ARG	NE-CZ-NH1	7.55	124.07	120.30
4	K	10	DC	O5'-P-OP1	7.48	119.68	110.70
1	C	18	ILE	CA-CB-CG1	-7.43	96.88	111.00
1	D	182	ARG	NE-CZ-NH1	7.39	123.99	120.30
1	A	182	ARG	NE-CZ-NH2	-7.29	116.65	120.30
4	I	11	DA	O5'-P-OP2	-7.29	99.14	105.70
4	K	11	DA	O5'-P-OP2	-7.26	99.16	105.70
4	K	10	DC	O5'-P-OP2	-7.25	99.17	105.70
1	C	198	GLU	CA-CB-CG	7.18	129.19	113.40
4	I	9	DG	O5'-P-OP2	-6.83	99.55	105.70
2	H	11	DA	O5'-P-OP2	-6.80	99.58	105.70
4	I	10	DC	O4'-C4'-C3'	-6.77	101.79	104.50
2	J	11	DA	O5'-P-OP2	-6.75	99.62	105.70
4	I	10	DC	C1'-O4'-C4'	-6.71	103.39	110.10
2	J	9	DG	O5'-P-OP2	-6.70	99.67	105.70
1	B	210[A]	MSE	CG-SE-CE	6.70	113.64	98.90
1	B	210[B]	MSE	CG-SE-CE	6.70	113.64	98.90
1	B	20	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	D	182	ARG	NE-CZ-NH2	-6.54	117.03	120.30
2	J	10	DC	C1'-O4'-C4'	-6.52	103.58	110.10
1	A	224	ASN	CB-CA-C	-6.50	97.39	110.40
4	K	10	DC	C1'-O4'-C4'	-6.43	103.67	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1	MSE	CG-SE-CE	-6.33	84.97	98.90
1	D	103	ASP	CB-CG-OD1	6.10	123.79	118.30
5	i	28	DT	O5'-P-OP2	-5.93	100.36	105.70
1	A	86	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	199	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	C	207	LYS	CB-CG-CD	5.75	126.56	111.60
1	C	18	ILE	CG1-CB-CG2	-5.62	99.04	111.40
1	A	1	MSE	CA-CB-CG	5.59	122.81	113.30
1	D	1	MSE	CB-CA-C	5.48	121.36	110.40
1	C	110	THR	CB-CA-C	-5.47	96.83	111.60
4	I	10	DC	C5'-C4'-O4'	5.44	119.64	109.30
5	k	25	DA	O5'-P-OP1	5.41	117.19	110.70
4	K	8	DG	O5'-P-OP1	-5.32	100.91	105.70
1	B	103	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	130	VAL	N-CA-CB	-5.30	99.83	111.50
1	D	78	ARG	NE-CZ-NH2	-5.29	117.66	120.30
2	J	10	DC	O4'-C4'-C3'	-5.29	102.39	104.50
1	A	147	ASP	CB-CG-OD2	-5.25	113.57	118.30
4	K	10	DC	O4'-C4'-C3'	-5.18	102.43	104.50
1	D	78	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	B	86	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	27	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	130	VAL	CB-CA-C	5.15	121.18	111.40
1	A	136	GLN	N-CA-C	-5.13	97.16	111.00
1	C	103	ASP	CB-CG-OD1	5.11	122.89	118.30
4	K	9	DG	O5'-P-OP2	-5.09	101.12	105.70
2	H	13	DT	C1'-O4'-C4'	-5.09	105.01	110.10
3	h	27	DA	P-O5'-C5'	5.08	129.03	120.90
3	h	31	DC	O5'-P-OP2	-5.03	101.17	105.70
3	h	25	DA	O4'-C1'-N9	-5.00	104.50	108.00

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	1923	0	1915	18	0
1	B	1915	0	1907	15	0
1	C	1926	0	1906	19	0
1	D	1910	0	1898	27	0
2	H	250	0	136	1	0
2	J	291	0	159	7	0
3	h	270	0	145	0	0
3	j	270	0	145	0	0
4	I	280	0	159	8	0
4	K	261	0	148	0	0
5	i	243	0	135	0	0
5	k	262	0	146	0	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
7	A	4	0	6	0	0
7	D	4	0	6	3	0
7	I	4	0	6	0	0
8	B	4	0	3	0	0
9	A	31	0	0	0	0
9	B	27	0	0	1	0
9	C	16	0	0	0	0
9	D	23	0	0	0	0
9	H	4	0	0	0	0
9	I	7	0	0	0	0
9	J	2	0	0	0	0
9	K	5	0	0	0	0
9	h	6	0	0	0	0
9	i	6	0	0	0	0
9	j	4	0	0	0	0
9	k	2	0	0	0	0
All	All	9956	0	8820	84	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 6.

All (84) 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:I:2:DC:H2"	4:I:3:DC:C6	1.76	1.21
1:D:111:PRO:HA	1:D:169[B]:MSE:CE	1.89	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:THR:HG22	1:C:112:ASN:H	1.29	0.97
4:I:2:DC:C2'	4:I:3:DC:C6	2.49	0.95
4:I:2:DC:H2'	4:I:3:DC:C5	2.11	0.85
1:A:154:LEU:HD21	1:A:169[B]:MSE:HE1	1.61	0.81
4:I:2:DC:C2'	4:I:3:DC:C5	2.64	0.80
1:D:111:PRO:HA	1:D:169[B]:MSE:HE3	1.64	0.78
1:C:169[B]:MSE:HE3	1:C:189:PHE:CE1	2.19	0.77
1:D:114:ILE:CG1	1:D:169[B]:MSE:HE1	2.16	0.76
1:C:161:PHE:CZ	1:C:169[B]:MSE:HE2	2.24	0.71
1:B:169[B]:MSE:HE3	1:B:189:PHE:CE1	2.27	0.69
1:D:107:ASP:HB3	1:D:168:GLN:HE21	1.57	0.69
1:D:1:MSE:CE	1:D:84:MSE:HE3	2.25	0.67
4:I:2:DC:H5"	4:I:2:DC:C6	2.29	0.67
1:D:114:ILE:HG12	1:D:169[B]:MSE:HE1	1.77	0.66
1:A:107:ASP:HB3	1:A:168:GLN:HE21	1.61	0.66
1:D:111:PRO:HA	1:D:169[B]:MSE:HE2	1.77	0.66
1:B:161:PHE:CZ	1:B:169[B]:MSE:HE2	2.32	0.65
1:D:1:MSE:HE3	1:D:84:MSE:HE3	1.78	0.64
1:D:114:ILE:HG13	1:D:169[B]:MSE:HE1	1.78	0.63
1:B:169[B]:MSE:HE3	1:B:189:PHE:CD1	2.35	0.62
1:B:154:LEU:HD21	1:B:169[B]:MSE:HE1	1.83	0.60
1:C:169[B]:MSE:HE3	1:C:189:PHE:HE1	1.65	0.60
4:I:2:DC:H6	4:I:2:DC:H5"	1.65	0.60
1:C:169[B]:MSE:HE3	1:C:189:PHE:CD1	2.36	0.59
1:A:221:SER:OG	1:B:119:HIS:HD2	1.85	0.59
2:J:4:DC:H2'	2:J:5:DG:C8	2.38	0.59
1:C:110:THR:HG22	1:C:112:ASN:N	2.10	0.58
1:C:154:LEU:HD21	1:C:169[B]:MSE:HE1	1.85	0.57
1:D:182:ARG:H	7:D:303:EDO:H11	1.68	0.57
1:B:161:PHE:CE2	1:B:169[B]:MSE:HE2	2.41	0.56
1:D:111:PRO:CA	1:D:169[B]:MSE:HE3	2.34	0.55
1:C:119:HIS:HD2	1:D:221:SER:OG	1.90	0.55
1:C:110:THR:HG21	2:J:13:DT:OP2	2.07	0.55
1:A:182:ARG:NH1	1:B:222:ASN:OD1	2.36	0.55
1:C:1:MSE:HE1	1:C:6:TYR:HB2	1.89	0.54
1:A:119:HIS:HD2	1:B:221:SER:OG	1.90	0.53
1:A:161:PHE:CE2	1:A:169[B]:MSE:HE2	2.44	0.52
1:A:169[B]:MSE:HE3	1:A:189:PHE:CD1	2.44	0.52
1:D:71:THR:HG22	1:D:72:LYS:HG3	1.91	0.52
1:D:181:THR:HA	7:D:303:EDO:H12	1.93	0.51
1:A:169[B]:MSE:HE3	1:A:189:PHE:CE1	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:ARG:N	7:D:303:EDO:H11	2.26	0.50
1:D:107:ASP:HB3	1:D:168:GLN:NE2	2.26	0.50
1:C:221:SER:OG	1:D:119:HIS:HD2	1.93	0.50
1:D:111:PRO:CA	1:D:169[B]:MSE:CE	2.78	0.49
1:C:161:PHE:CE1	1:C:169[B]:MSE:HE2	2.48	0.49
1:A:1:MSE:HE1	1:A:86:ARG:HB2	1.94	0.49
1:B:169[B]:MSE:HE3	1:B:189:PHE:HE1	1.77	0.49
1:C:110:THR:CG2	2:J:13:DT:OP2	2.62	0.47
2:J:2:DG:H4'	2:J:3:DG:OP1	2.14	0.47
1:A:53:SER:O	1:D:50:LYS:HG3	2.15	0.47
1:A:161:PHE:CZ	1:A:169[B]:MSE:HE2	2.50	0.46
1:B:1:MSE:HE1	1:B:86:ARG:HB2	1.97	0.46
1:A:107:ASP:HB3	1:A:168:GLN:NE2	2.29	0.46
4:I:1:DC:H2'	4:I:2:DC:C5	2.50	0.46
1:D:1:MSE:CE	1:D:84:MSE:CE	2.93	0.46
1:B:72:LYS:NZ	9:B:403:HOH:O	2.49	0.46
1:D:166:LYS:N	1:D:167:PRO:HA	2.31	0.46
1:B:129:LEU:N	1:B:129:LEU:HD12	2.31	0.45
1:C:222:ASN:OD1	1:D:182:ARG:NH1	2.47	0.45
1:A:135:LYS:HB2	1:A:136:GLN:O	2.16	0.45
1:A:166:LYS:N	1:A:167:PRO:HA	2.32	0.45
1:B:136:GLN:HG3	1:B:137:ASP:N	2.32	0.44
1:C:129:LEU:N	1:C:129:LEU:HD12	2.32	0.44
1:C:166:LYS:N	1:C:167:PRO:HA	2.33	0.44
2:J:2:DG:H1'	2:J:3:DG:N7	2.33	0.44
1:D:169[B]:MSE:HE2	1:D:189:PHE:HE1	1.82	0.43
1:C:161:PHE:HZ	1:C:169[B]:MSE:HE2	1.81	0.43
1:C:161:PHE:CZ	1:C:169[B]:MSE:CE	3.00	0.43
1:B:166:LYS:N	1:B:167:PRO:HA	2.34	0.42
1:A:199:ARG:CZ	4:I:10:DC:H5"	2.50	0.42
1:A:1:MSE:HE1	1:A:86:ARG:CB	2.50	0.42
1:D:199:ARG:CZ	2:J:10:DC:H5"	2.50	0.41
2:H:4:DC:H2'	2:H:5:DG:C8	2.56	0.41
1:D:157:VAL:HG11	1:D:161:PHE:CD2	2.56	0.41
1:C:161:PHE:HZ	1:C:169[B]:MSE:CE	2.34	0.41
1:D:99:ILE:HA	1:D:99:ILE:HD12	1.93	0.41
1:A:129:LEU:HD12	1:A:129:LEU:N	2.36	0.41
1:D:129:LEU:N	1:D:129:LEU:HD12	2.36	0.41
1:B:161:PHE:CZ	1:B:169[B]:MSE:CE	3.02	0.40
2:J:2:DG:H1'	2:J:3:DG:C8	2.56	0.40
1:A:1:MSE:HB2	1:A:84[A]:MSE:HE3	2.03	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	228/226 (101%)	219 (96%)	9 (4%)	0	100	100
1	B	227/226 (100%)	221 (97%)	6 (3%)	0	100	100
1	C	228/226 (101%)	220 (96%)	8 (4%)	0	100	100
1	D	226/226 (100%)	216 (96%)	8 (4%)	2 (1%)	21	21
All	All	909/904 (101%)	876 (96%)	31 (3%)	2 (0%)	52	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	161	PHE
1	D	123	PHE

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	214/206 (104%)	204 (95%)	10 (5%)	32	40
1	B	213/206 (103%)	204 (96%)	9 (4%)	36	46
1	C	214/206 (104%)	208 (97%)	6 (3%)	51	64
1	D	212/206 (103%)	201 (95%)	11 (5%)	29	35
All	All	853/824 (104%)	817 (96%)	36 (4%)	36	46

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	5	LYS
1	A	20	ARG
1	A	57	SER
1	A	70	LYS
1	A	130	VAL
1	A	147	ASP
1	A	162	ARG
1	A	183	GLU
1	A	212	LYS
1	B	1	MSE
1	B	25	LYS
1	B	57	SER
1	B	70	LYS
1	B	102	MSE
1	B	123	PHE
1	B	147	ASP
1	B	162	ARG
1	B	212	LYS
1	C	1	MSE
1	C	57	SER
1	C	70	LYS
1	C	123	PHE
1	C	162	ARG
1	C	212	LYS
1	D	1	MSE
1	D	57	SER
1	D	70	LYS
1	D	71	THR
1	D	123	PHE
1	D	130	VAL
1	D	147	ASP
1	D	162	ARG
1	D	210[A]	MSE
1	D	210[B]	MSE
1	D	212	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	119	HIS
1	A	168	GLN
1	A	200	GLN
1	B	101	ASN
1	B	119	HIS
1	C	101	ASN
1	C	119	HIS
1	C	200	GLN
1	D	101	ASN
1	D	119	HIS
1	D	168	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
7	EDO	A	303	-	3,3,3	0.76	0	2,2,2	0.80	0
8	ACT	B	302	-	0,3,3	0.00	-	0,3,3	0.00	-
7	EDO	D	303	-	3,3,3	0.54	0	2,2,2	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	EDO	I	101	-	3,3,3	0.52	0	2,2,2	0.34	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
7	EDO	A	303	-	-	0/1/1/1	0/0/0/0
8	ACT	B	302	-	-	0/0/0/0	0/0/0/0
7	EDO	D	303	-	-	0/1/1/1	0/0/0/0
7	EDO	I	101	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	303	EDO	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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^2)	Q<0.9
1	A	221/226 (97%)	0.20	4 (1%) 71 80	35, 61, 100, 130	0
1	B	221/226 (97%)	0.24	5 (2%) 64 75	46, 70, 100, 122	0
1	C	221/226 (97%)	0.31	9 (4%) 41 53	41, 71, 102, 134	0
1	D	221/226 (97%)	0.33	7 (3%) 51 62	39, 70, 113, 151	0
2	H	12/14 (85%)	1.08	3 (25%) 1 2	39, 69, 211, 213	0
2	J	14/14 (100%)	1.22	4 (28%) 1 1	46, 90, 181, 216	0
3	h	13/13 (100%)	0.63	2 (15%) 3 5	43, 70, 169, 202	0
3	j	13/13 (100%)	0.46	1 (7%) 16 25	45, 71, 155, 181	0
4	I	14/14 (100%)	0.72	2 (14%) 4 6	43, 80, 164, 183	0
4	K	13/14 (92%)	0.31	1 (7%) 16 25	39, 61, 163, 197	0
5	i	12/13 (92%)	0.62	2 (16%) 2 4	45, 75, 178, 202	0
5	k	13/13 (100%)	0.53	3 (23%) 1 2	53, 74, 162, 183	0
All	All	988/1012 (97%)	0.31	43 (4%) 38 50	35, 70, 119, 216	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	1	DG	7.3
2	H	3	DG	6.9
4	I	1	DC	5.4
1	A	226	ILE	4.9
2	H	4	DC	4.6
1	B	3	PHE	4.2
1	C	226	ILE	4.1
2	J	2	DG	3.8
3	j	37	DG	3.8
5	k	37	DC	3.6
3	h	37	DG	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	226	ILE	3.4
1	D	226	ILE	3.1
1	C	223[A]	ASP	3.1
2	J	3	DG	3.0
4	I	2	DC	2.9
1	D	148	TYR	2.9
1	D	6	TYR	2.8
1	C	136	GLN	2.8
4	K	2	DC	2.7
1	C	85	ASP	2.7
5	k	36	DC	2.7
5	k	35	DG	2.6
1	A	211	LEU	2.6
1	C	197	PHE	2.4
1	B	136	GLN	2.4
1	D	136	GLN	2.4
1	A	197	PHE	2.4
1	C	18	ILE	2.4
5	i	36	DC	2.3
1	A	209	ILE	2.3
1	C	83	PHE	2.3
3	h	36	DG	2.3
1	C	16	GLU	2.3
1	B	14	ILE	2.3
1	D	22	ILE	2.2
2	H	5	DG	2.2
1	D	21	ILE	2.1
2	J	4	DC	2.1
1	D	26	HIS	2.1
5	i	33	DC	2.0
1	C	183	GLU	2.0
1	B	2	ASN	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

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^{th} 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^2)	Q<0.9
7	EDO	A	303	4/4	0.83	0.41	14.71	60,62,71,74	0
6	MG	D	301	1/1	0.91	0.24	3.59	52,52,52,52	0
7	EDO	I	101	4/4	0.88	0.17	2.28	74,88,91,92	0
6	MG	A	301	1/1	0.97	0.23	2.03	42,42,42,42	0
7	EDO	D	303	4/4	0.82	0.32	1.99	62,65,68,69	0
6	MG	A	302	1/1	0.96	0.22	1.71	56,56,56,56	0
6	MG	B	301	1/1	0.97	0.20	1.21	51,51,51,51	0
6	MG	C	301	1/1	0.96	0.20	1.18	50,50,50,50	0
6	MG	D	302	1/1	0.94	0.18	0.59	63,63,63,63	0
8	ACT	B	302	4/4	0.82	0.19	0.37	93,96,98,105	0

6.5 Other polymers

There are no such residues in this entry.