wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 12:43 AM GMT

PDB ID	:	2AAZ
Title	:	Cryptococcus neoformans thymidylate synthase complexed with substrate and an antifolate
Authors	:	Finer-Moore, J.S.; Anderson, A.C.; O'Neil, R.H.; Costi, M.P.; Ferrari, S.; Krucinski, J.; Stroud, R.M.
Deposited on	:	2005-07-14
Resolution	:	2.08 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

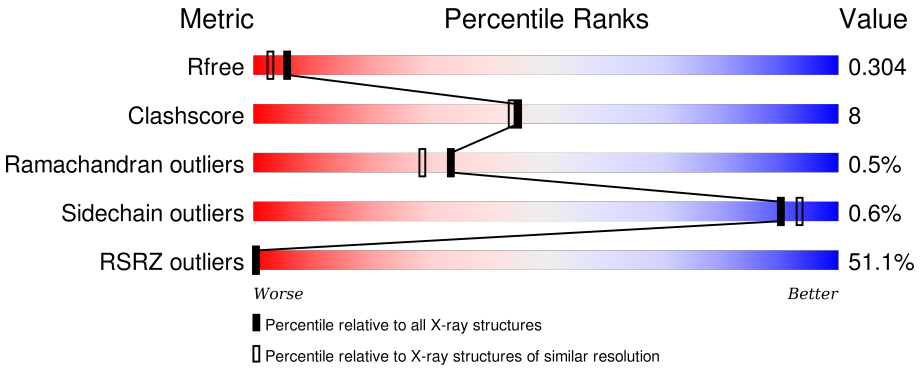
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.08 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	4546 (2.10-2.06)
Clashscore	102246	5101 (2.10-2.06)
Ramachandran outliers	100387	5048 (2.10-2.06)
Sidechain outliers	100360	5049 (2.10-2.06)
RSRZ outliers	91569	4556 (2.10-2.06)

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	1-A	317	4% 77% 18%
1	1-B	317	4% 81% 15%
1	1-C	317	4% 79% 17%
1	1-D	317	3% 79% 15%
1	1-E	317	4% 81% 14%

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Mol	Chain	Length	Quality of chain
1	1-F	317	5% 78% 16%
1	1-G	317	3% 83% 12%
1	1-H	317	3% 79% 16%
1	1-I	317	93% 80% 14% 6%
1	1-J	317	93% 78% 15% 6%
1	1-K	317	92% 78% 15% 6%
1	1-L	317	93% 78% 15% 6%
1	1-M	317	94% 79% 15% 6%
1	1-N	317	94% 78% 16% 6%
1	1-O	317	93% 80% 14% 6%
1	1-P	317	92% 79% 15% 6%
1	2-A	317	4% 78% 17%
1	2-B	317	4% 82% 15%
1	2-C	317	4% 80% 16%
1	2-D	317	3% 80% 15%
1	2-E	317	4% 82% 14%
1	2-F	317	5% 78% 18%
1	2-G	317	3% 85% 12%
1	2-H	317	3% 80% 16%
1	2-I	317	93% 79% 16% 6%
1	2-J	317	93% 78% 17% 6%
1	2-K	317	92% 77% 18% 6%
1	2-L	317	93% 78% 16% 6%
1	2-M	317	94% 78% 16% 6%
1	2-N	317	94% 76% 18% 6%

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Mol	Chain	Length	Quality of chain
1	2-O	317	93% 77% 17% 6%
1	2-P	317	92% 78% 16% 6%
1	3-A	317	4% 78% 17%
1	3-B	317	4% 82% 15%
1	3-C	317	4% 80% 16%
1	3-D	317	3% 80% 15%
1	3-E	317	4% 82% 14%
1	3-F	317	5% 78% 18%
1	3-G	317	3% 85% 12%
1	3-H	317	3% 80% 16%
1	3-I	317	93% 78% 16% 6%
1	3-J	317	93% 78% 16% 6%
1	3-K	317	92% 77% 17% 6%
1	3-L	317	93% 78% 16% 6%
1	3-M	317	94% 79% 15% 6%
1	3-N	317	94% 76% 18% 6%
1	3-O	317	93% 77% 17% 6%
1	3-P	317	92% 78% 16% 6%
1	4-A	317	4% 78% 17%
1	4-B	317	4% 82% 15%
1	4-C	317	4% 80% 16%
1	4-D	317	3% 80% 15%
1	4-E	317	4% 82% 14%
1	4-F	317	5% 78% 18%
1	4-G	317	3% 85% 12%

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Mol	Chain	Length	Quality of chain
1	4-H	317	3% 80% 16%
1	4-I	317	93% 79% 15% 6%
1	4-J	317	93% 78% 16% 6%
1	4-K	317	92% 76% 18% 6%
1	4-L	317	93% 78% 16% 6%
1	4-M	317	94% 78% 16% 6%
1	4-N	317	94% 78% 16% 6%
1	4-O	317	93% 77% 17% 6%
1	4-P	317	92% 78% 17% 6%

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	UMP	1-I	350[A]	-	-	-	X
2	UMP	1-J	400[A]	-	-	-	X
2	UMP	1-K	450[A]	-	-	-	X
2	UMP	1-M	550[A]	-	-	-	X
2	UMP	1-N	600[A]	-	-	-	X
2	UMP	1-O	650[A]	-	-	-	X
2	UMP	1-P	700[A]	-	-	-	X
2	UMP	2-I	350[B]	-	-	-	X
2	UMP	2-J	400[B]	-	-	-	X
2	UMP	2-K	450[B]	-	-	-	X
2	UMP	2-M	550[B]	-	-	-	X
2	UMP	2-N	600[B]	-	-	-	X
2	UMP	2-O	650[B]	-	-	-	X
2	UMP	2-P	700[B]	-	-	-	X
2	UMP	3-I	350[C]	-	-	-	X
2	UMP	3-J	400[C]	-	-	-	X
2	UMP	3-K	450[C]	-	-	-	X
2	UMP	3-M	550[C]	-	-	-	X
2	UMP	3-N	600[C]	-	-	-	X
2	UMP	3-O	650[C]	-	-	-	X
2	UMP	3-P	700[C]	-	-	-	X
2	UMP	4-I	350[D]	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UMP	4-J	400[D]	-	-	-	X
2	UMP	4-K	450[D]	-	-	-	X
2	UMP	4-M	550[D]	-	-	-	X
2	UMP	4-N	600[D]	-	-	-	X
2	UMP	4-O	650[D]	-	-	-	X
2	UMP	4-P	700[D]	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 161392 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 Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	305	Total	C	N	O	S	0	305	0
			2427	1553	419	442	13			
1	2-A	305	Total	C	N	O	S	0	305	0
			2427	1553	419	442	13			
1	3-A	305	Total	C	N	O	S	0	305	0
			2427	1553	419	442	13			
1	4-A	305	Total	C	N	O	S	0	305	0
			2427	1553	419	442	13			
1	1-B	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	2-B	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	3-B	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	4-B	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	1-C	305	Total	C	N	O	S	0	305	0
			2427	1553	419	442	13			
1	2-C	305	Total	C	N	O	S	0	305	0
			2427	1553	419	442	13			
1	3-C	305	Total	C	N	O	S	0	305	0
			2427	1553	419	442	13			
1	4-C	305	Total	C	N	O	S	0	305	0
			2427	1553	419	442	13			
1	1-D	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	2-D	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	3-D	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	4-D	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-E	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	2-E	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	3-E	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	4-E	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	1-F	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	2-F	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	3-F	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	4-F	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	1-G	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	2-G	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	3-G	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	4-G	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	1-H	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	2-H	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	3-H	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	4-H	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	1-I	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	2-I	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	3-I	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	4-I	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	1-J	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2-J	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	3-J	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	4-J	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	1-K	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	2-K	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	3-K	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	4-K	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	1-L	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	2-L	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	3-L	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	4-L	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	1-M	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	2-M	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	3-M	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	4-M	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	1-N	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	2-N	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	3-N	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	4-N	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	1-O	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	2-O	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			

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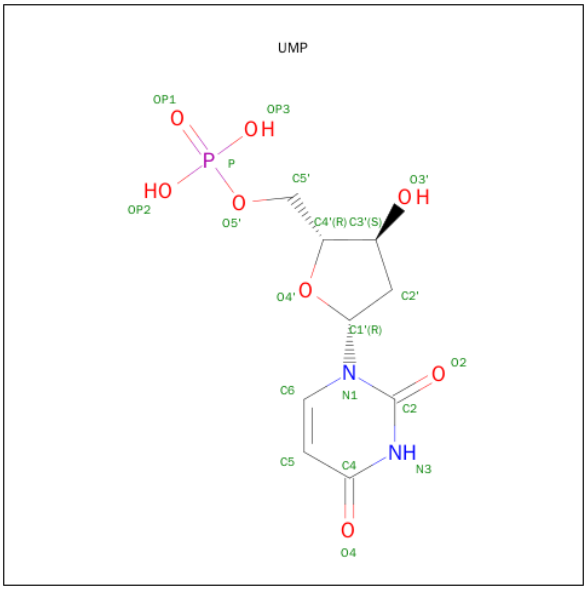
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	3-O	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	4-O	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	1-P	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	2-P	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	3-P	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	4-P	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	1-A	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	2-A	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	3-A	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	4-A	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	1-B	1	Total	C	N	O	P	0	1
			20	9	2	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	2-B	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	3-B	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	4-B	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	1-C	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	2-C	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	3-C	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	4-C	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	1-D	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	2-D	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	3-D	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	4-D	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	1-E	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	2-E	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	3-E	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	4-E	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	1-F	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	2-F	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	3-F	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	4-F	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	1-G	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	2-G	1	Total	C	N	O	P	0	1
			20	9	2	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	3-G	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	4-G	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	1-H	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	2-H	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	3-H	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	4-H	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	1-I	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	2-I	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	3-I	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	4-I	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	1-J	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	2-J	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	3-J	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	4-J	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	1-K	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	2-K	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	3-K	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	4-K	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	1-L	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	2-L	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	3-L	1	Total	C	N	O	P	0	1
			20	9	2	8	1		

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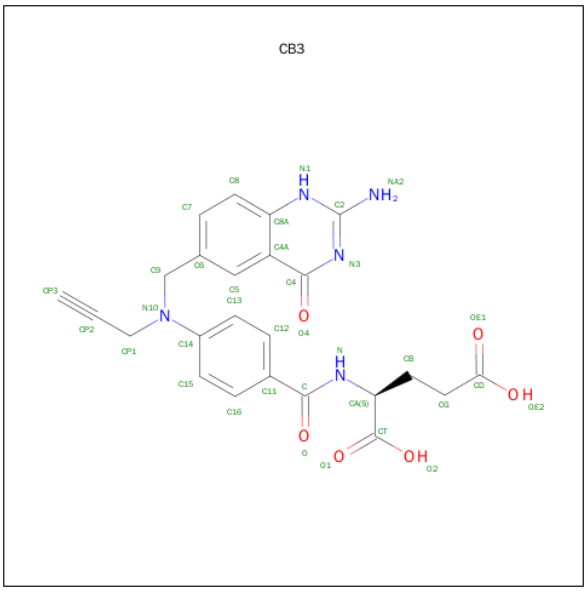
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	4-L	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	1-M	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	2-M	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	3-M	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	4-M	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	1-N	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	2-N	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	3-N	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	4-N	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	1-O	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	2-O	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	3-O	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	4-O	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	1-P	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	2-P	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	3-P	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	4-P	1	Total	C	N	O	P	0	1
			20	9	2	8	1		

- Molecule 3 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (three-letter code: CB3) (formula: $C_{24}H_{23}N_5O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	1-A	1	Total	C	N	O	0	1
			35	24	5	6		
3	2-A	1	Total	C	N	O	0	1
			35	24	5	6		
3	3-A	1	Total	C	N	O	0	1
			35	24	5	6		
3	4-A	1	Total	C	N	O	0	1
			35	24	5	6		
3	1-B	1	Total	C	N	O	0	1
			35	24	5	6		
3	2-B	1	Total	C	N	O	0	1
			35	24	5	6		
3	3-B	1	Total	C	N	O	0	1
			35	24	5	6		
3	4-B	1	Total	C	N	O	0	1
			35	24	5	6		
3	1-C	1	Total	C	N	O	0	1
			35	24	5	6		
3	2-C	1	Total	C	N	O	0	1
			35	24	5	6		
3	3-C	1	Total	C	N	O	0	1
			35	24	5	6		
3	4-C	1	Total	C	N	O	0	1
			35	24	5	6		
3	1-D	1	Total	C	N	O	0	1
			35	24	5	6		
3	2-D	1	Total	C	N	O	0	1
			35	24	5	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	3-D	1	Total C N O 35 24 5 6	0	1
3	4-D	1	Total C N O 35 24 5 6	0	1
3	1-E	1	Total C N O 35 24 5 6	0	1
3	2-E	1	Total C N O 35 24 5 6	0	1
3	3-E	1	Total C N O 35 24 5 6	0	1
3	4-E	1	Total C N O 35 24 5 6	0	1
3	1-F	1	Total C N O 35 24 5 6	0	1
3	2-F	1	Total C N O 35 24 5 6	0	1
3	3-F	1	Total C N O 35 24 5 6	0	1
3	4-F	1	Total C N O 35 24 5 6	0	1
3	1-G	1	Total C N O 35 24 5 6	0	1
3	2-G	1	Total C N O 35 24 5 6	0	1
3	3-G	1	Total C N O 35 24 5 6	0	1
3	4-G	1	Total C N O 35 24 5 6	0	1
3	1-H	1	Total C N O 35 24 5 6	0	1
3	2-H	1	Total C N O 35 24 5 6	0	1
3	3-H	1	Total C N O 35 24 5 6	0	1
3	4-H	1	Total C N O 35 24 5 6	0	1

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	1-A	185	Total O 185 185	0	185

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	2-A	185	Total O 185 185	0	185
4	3-A	185	Total O 185 185	0	185
4	4-A	185	Total O 185 185	0	185
4	1-B	143	Total O 143 143	0	143
4	2-B	143	Total O 143 143	0	143
4	3-B	143	Total O 143 143	0	143
4	4-B	143	Total O 143 143	0	143
4	1-C	151	Total O 151 151	0	151
4	2-C	151	Total O 151 151	0	151
4	3-C	151	Total O 151 151	0	151
4	4-C	151	Total O 151 151	0	151
4	1-D	148	Total O 148 148	0	148
4	2-D	148	Total O 148 148	0	148
4	3-D	148	Total O 148 148	0	148
4	4-D	148	Total O 148 148	0	148
4	1-E	155	Total O 155 155	0	155
4	2-E	155	Total O 155 155	0	155
4	3-E	155	Total O 155 155	0	155
4	4-E	155	Total O 155 155	0	155
4	1-F	138	Total O 138 138	0	138
4	2-F	138	Total O 138 138	0	138

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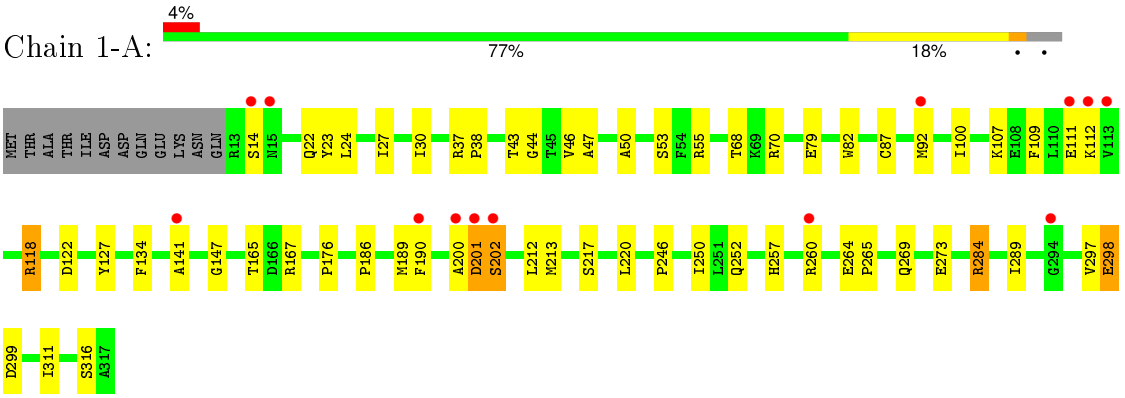
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	3-F	138	Total O 138 138	0	138
4	4-F	138	Total O 138 138	0	138
4	1-G	153	Total O 153 153	0	153
4	2-G	153	Total O 153 153	0	153
4	3-G	153	Total O 153 153	0	153
4	4-G	153	Total O 153 153	0	153
4	1-H	139	Total O 139 139	0	139
4	2-H	139	Total O 139 139	0	139
4	3-H	139	Total O 139 139	0	139
4	4-H	139	Total O 139 139	0	139

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.

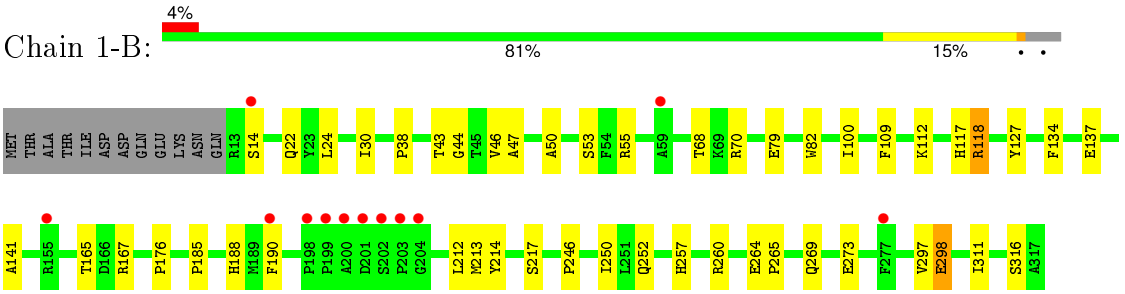
- Molecule 1: Thymidylate synthase

Chain 1-A:



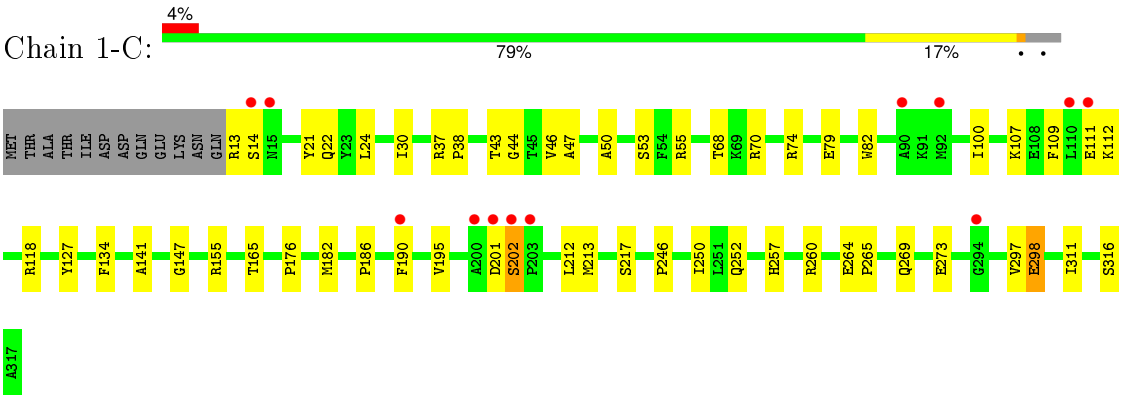
- Molecule 1: Thymidylate synthase

Chain 1-B:



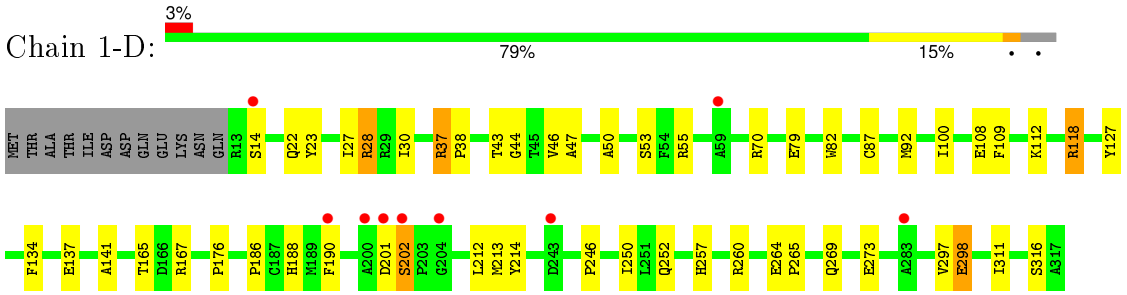
- Molecule 1: Thymidylate synthase

Chain 1-C:



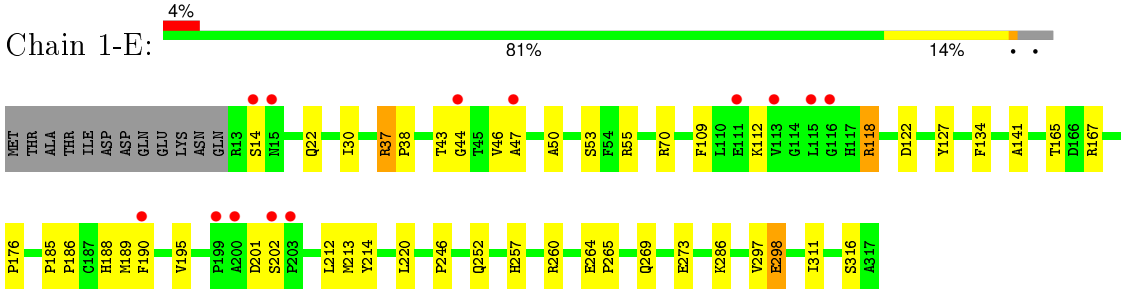
- Molecule 1: Thymidylate synthase

Chain 1-D:



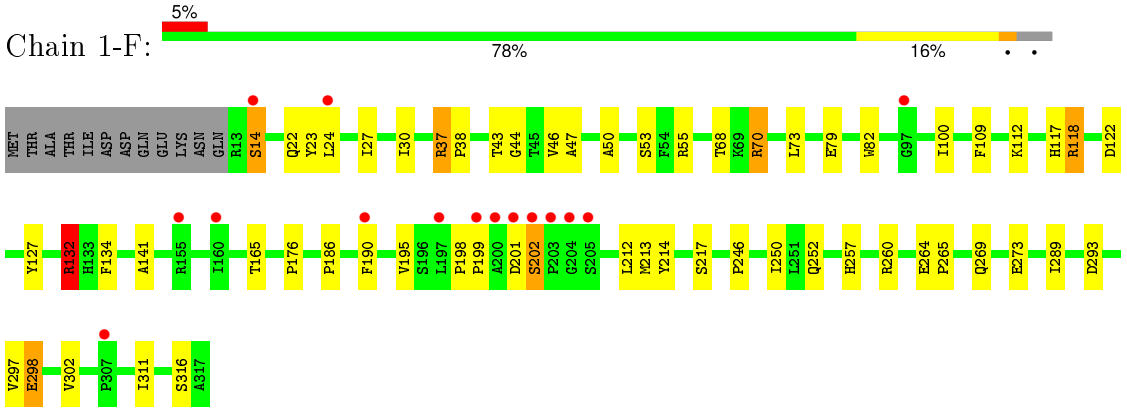
• Molecule 1: Thymidylate synthase

Chain 1-E:



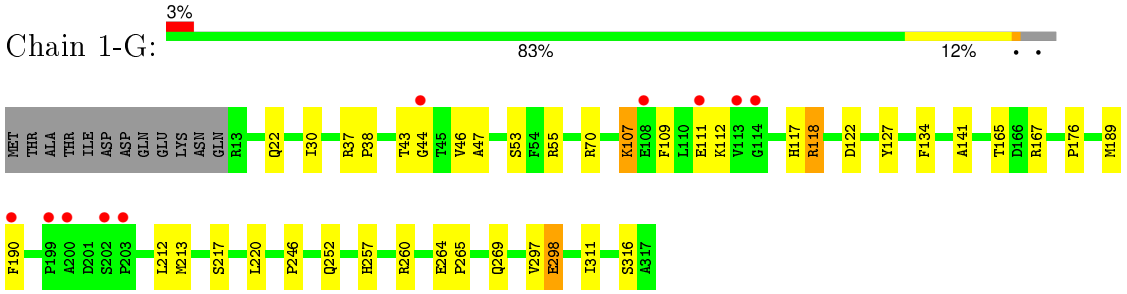
• Molecule 1: Thymidylate synthase

Chain 1-F:



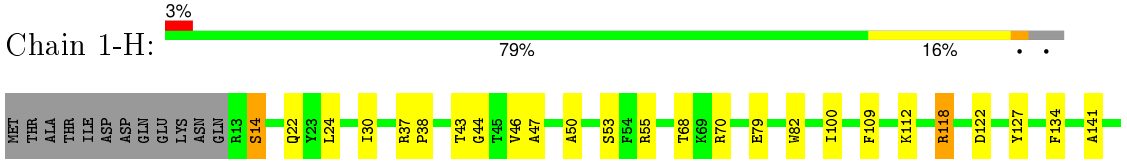
• Molecule 1: Thymidylate synthase

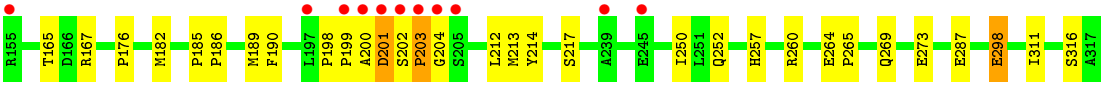
Chain 1-G:



• Molecule 1: Thymidylate synthase

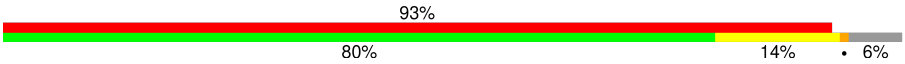
Chain 1-H:

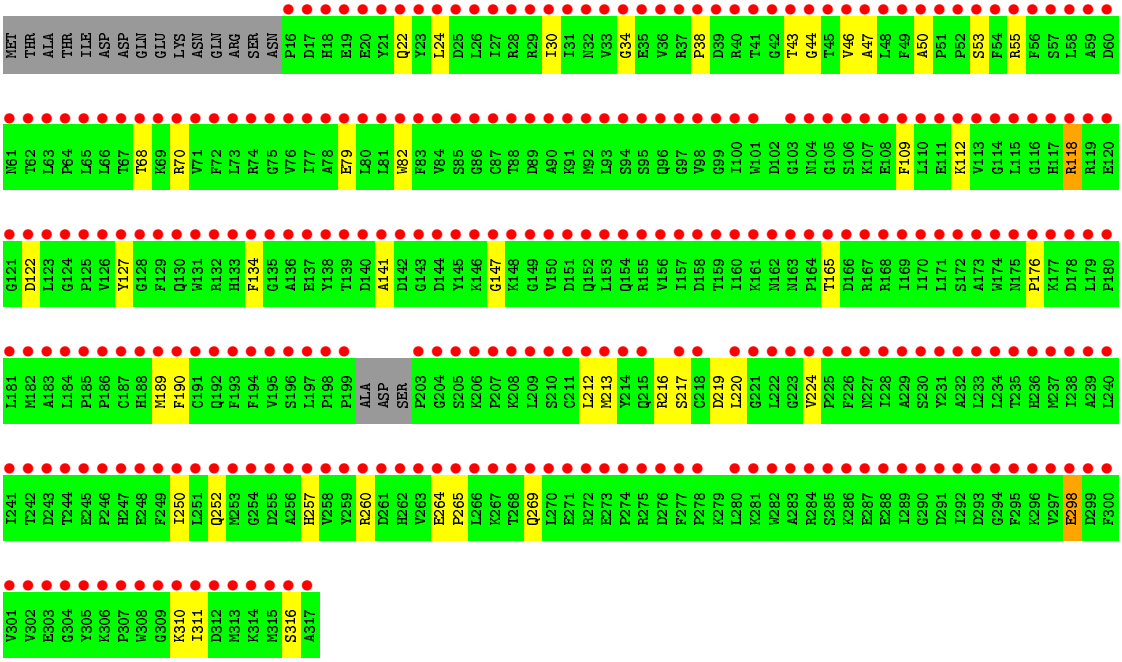




- Molecule 1: Thymidylate synthase

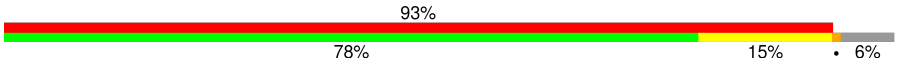
Chain 1-I:

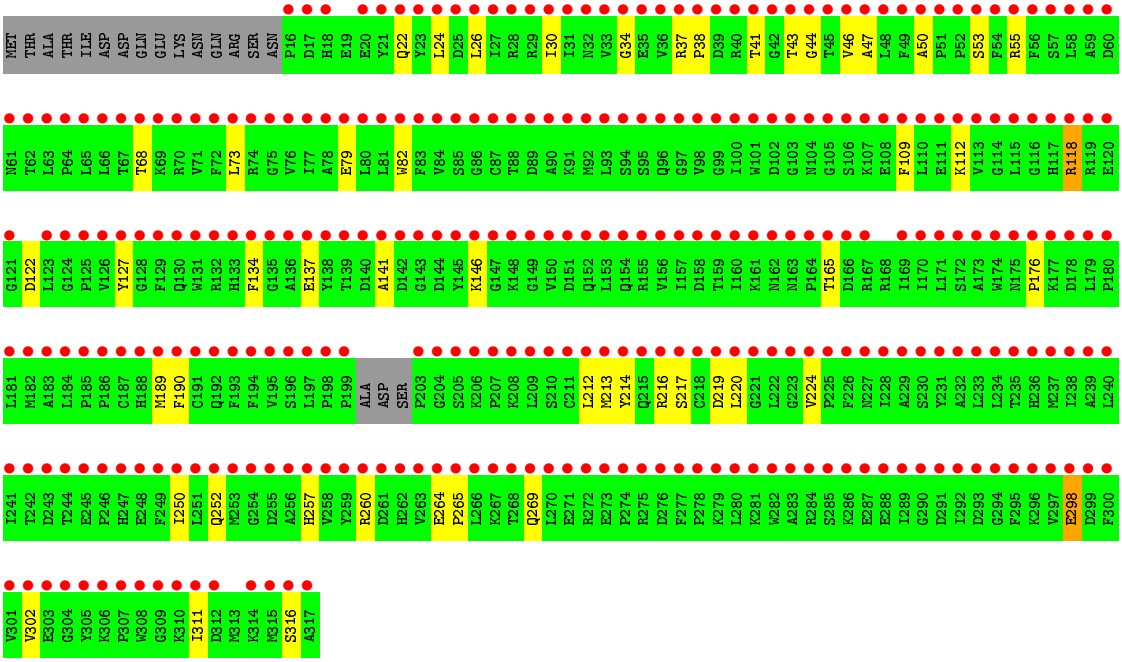




- Molecule 1: Thymidylate synthase

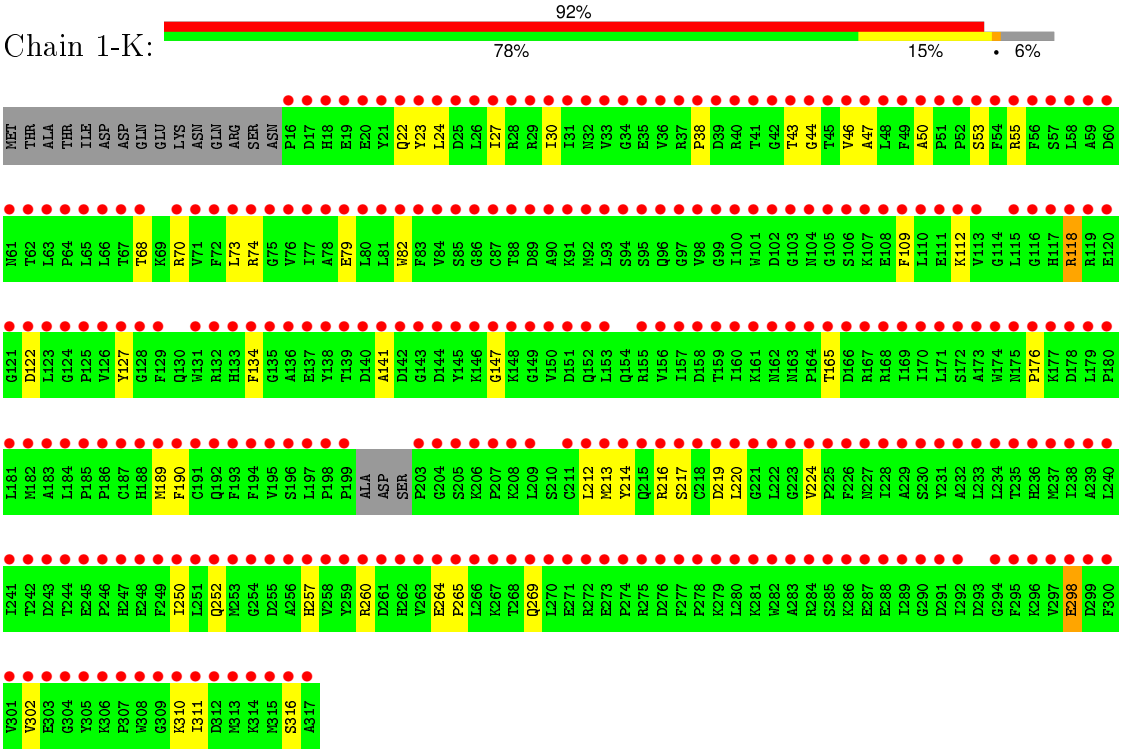
Chain 1-J:





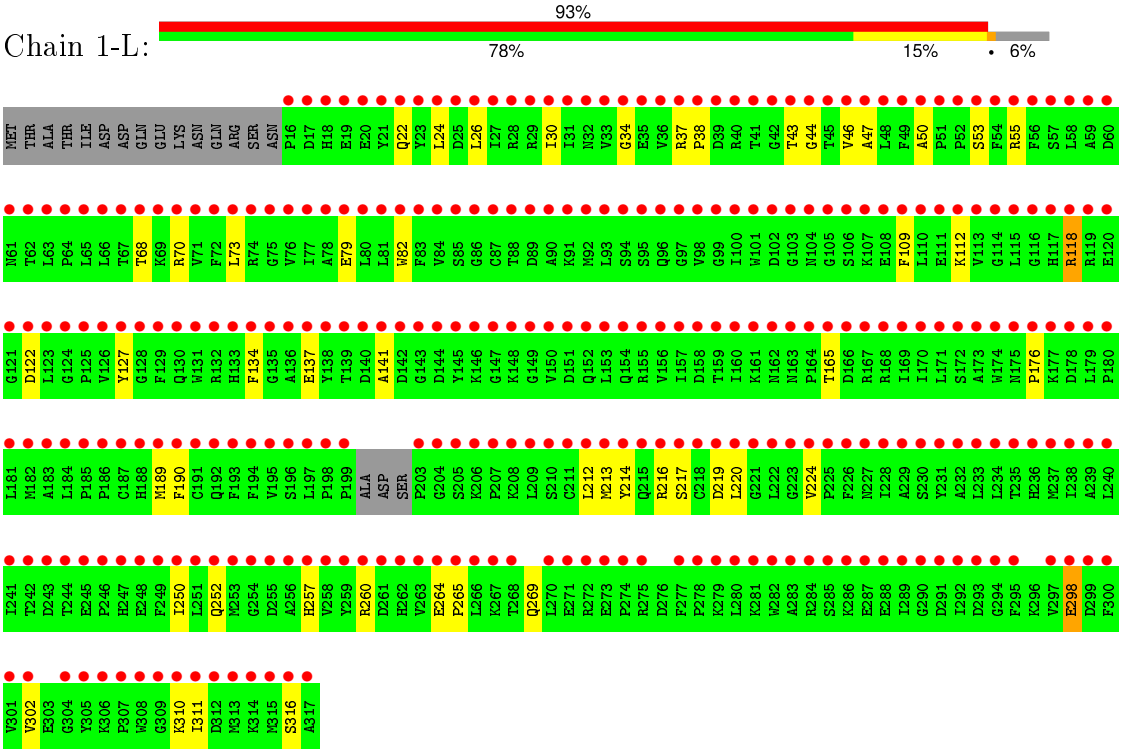
- Molecule 1: Thymidylate synthase

Chain 1-K:



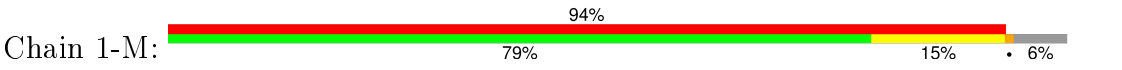
- Molecule 1: Thymidylate synthase

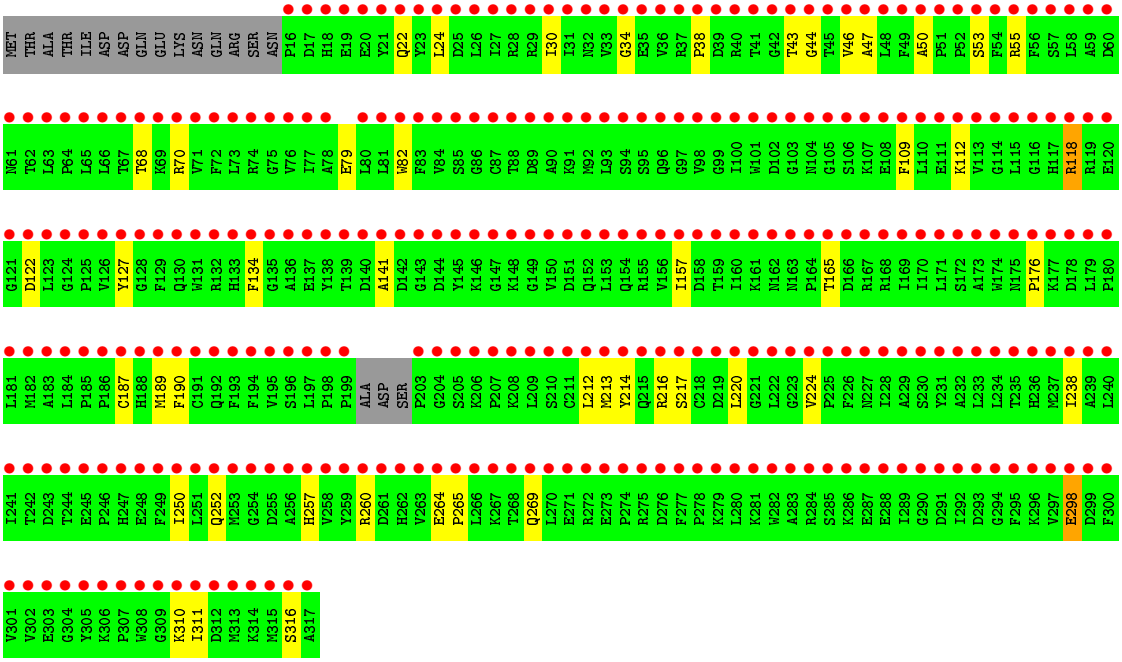
Chain 1-L:



- Molecule 1: Thymidylate synthase

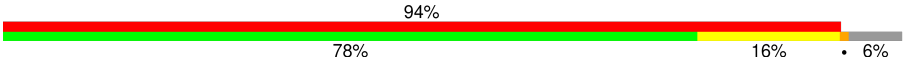
Chain 1-M:

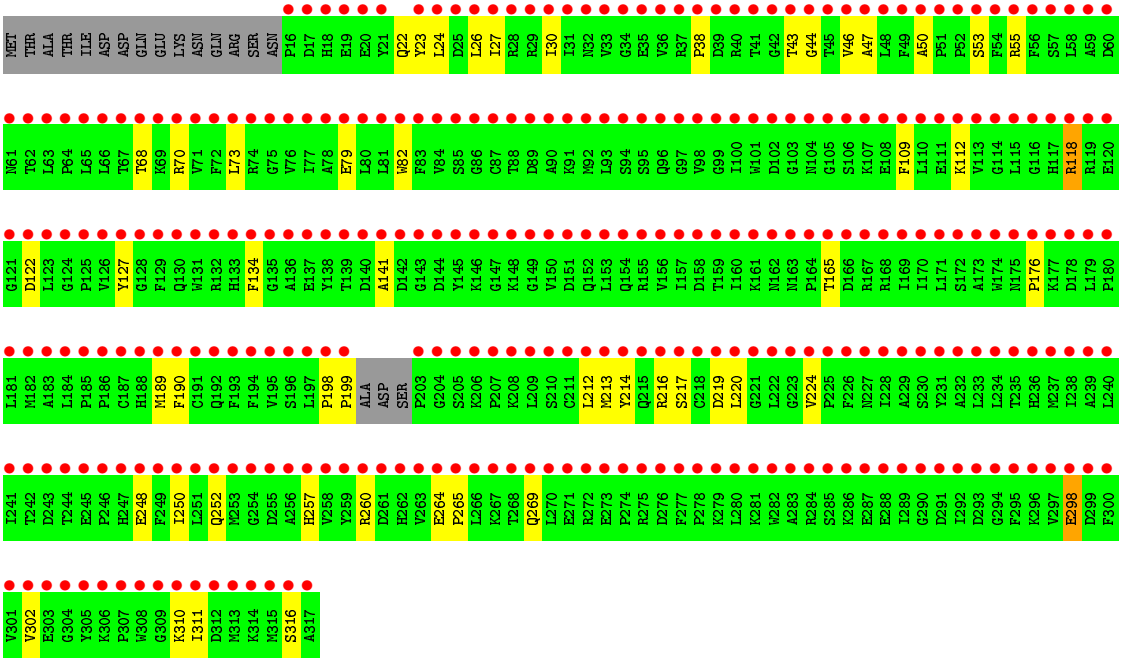




- Molecule 1: Thymidylate synthase

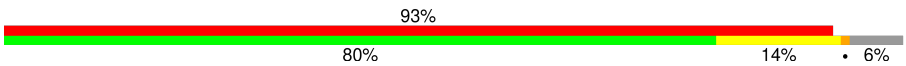
Chain 1-N:

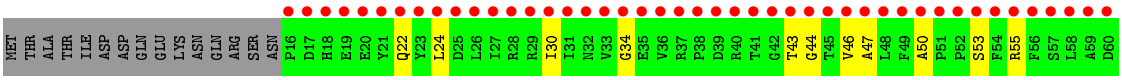


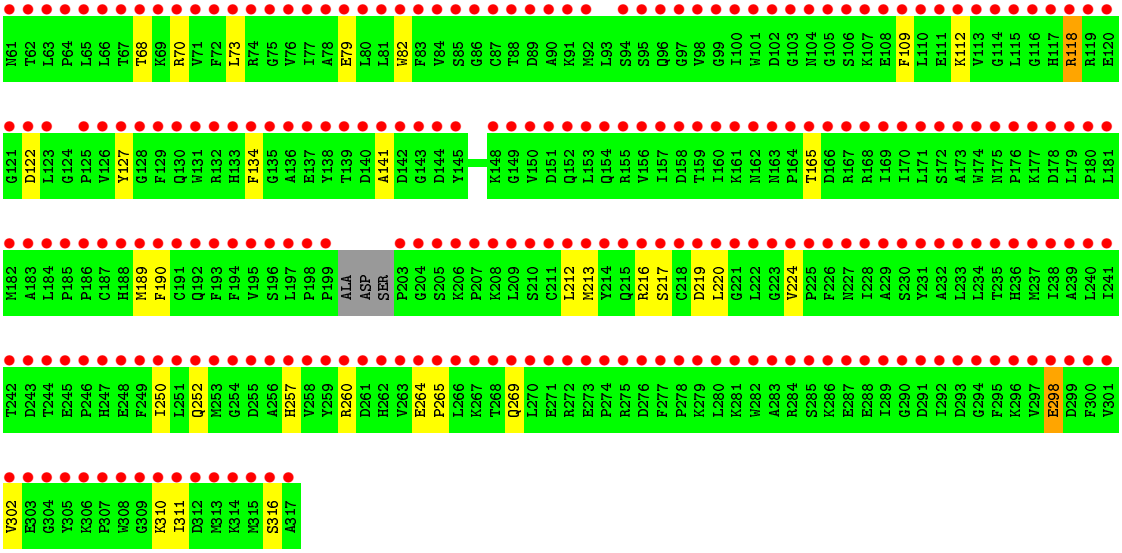


- Molecule 1: Thymidylate synthase

Chain 1-O:

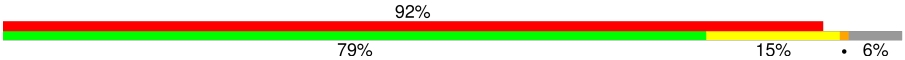


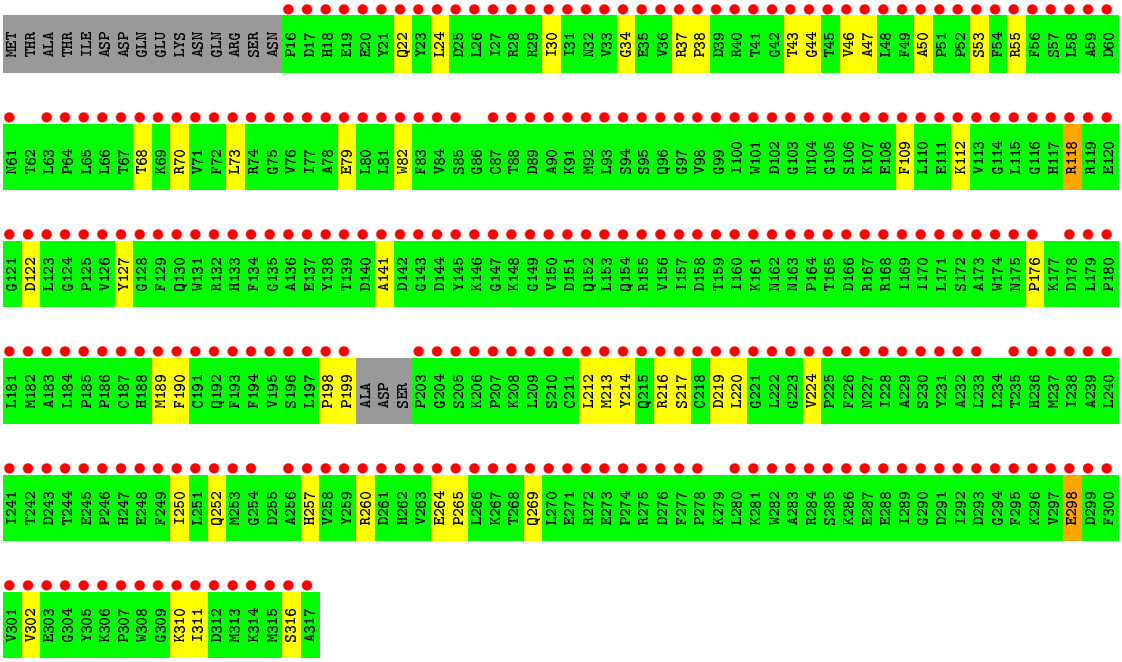




- Molecule 1: Thymidylate synthase

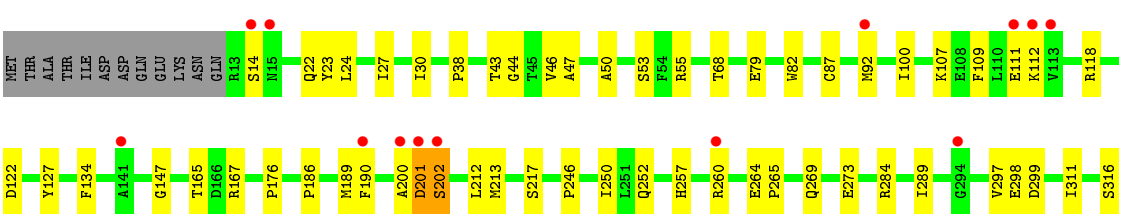
Chain 1-P:





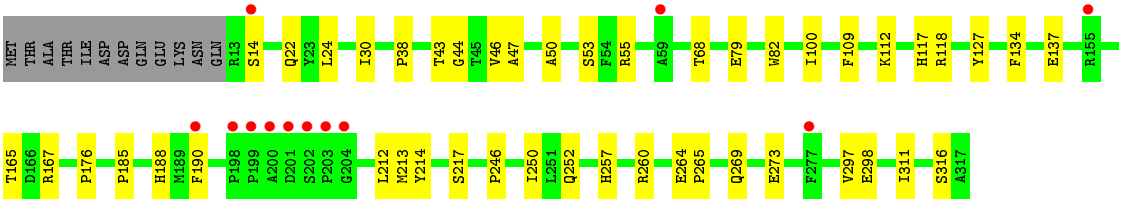
- Molecule 1: Thymidylate synthase

Chain 2-A:



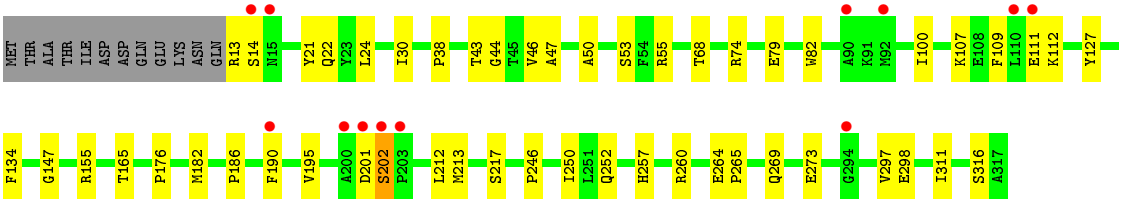
- Molecule 1: Thymidylate synthase

Chain 2-B:



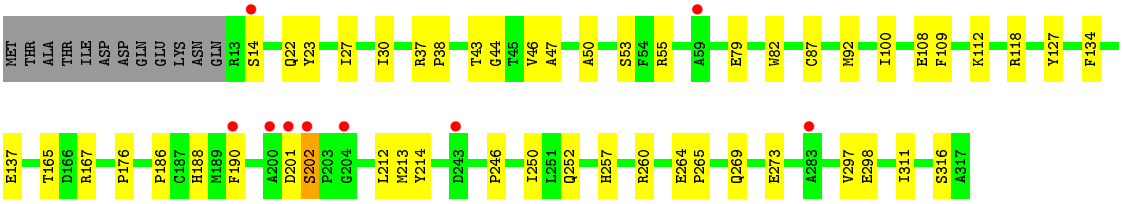
- Molecule 1: Thymidylate synthase

Chain 2-C:



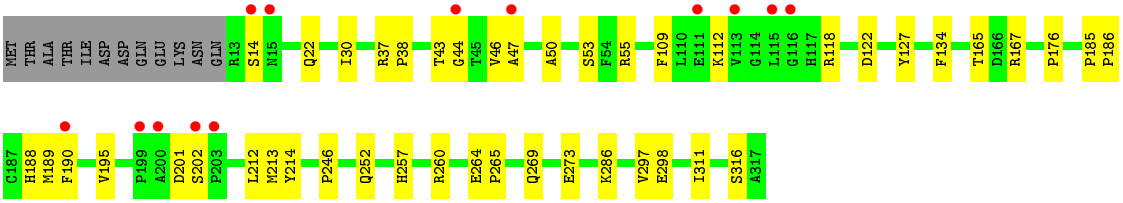
- Molecule 1: Thymidylate synthase

Chain 2-D:



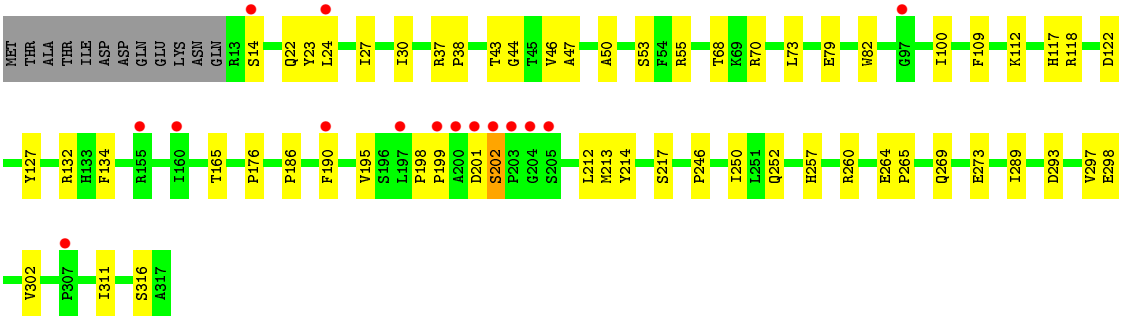
- Molecule 1: Thymidylate synthase

Chain 2-E:



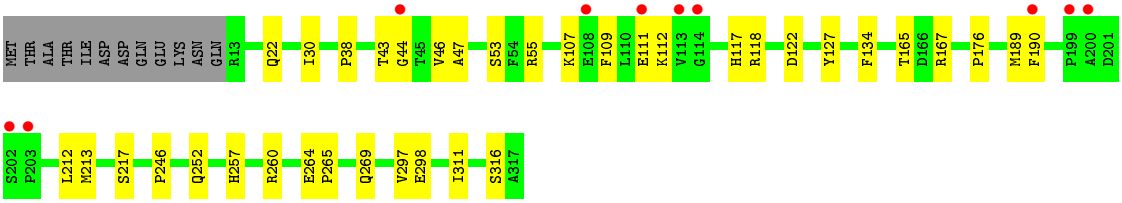
- Molecule 1: Thymidylate synthase

Chain 2-F:



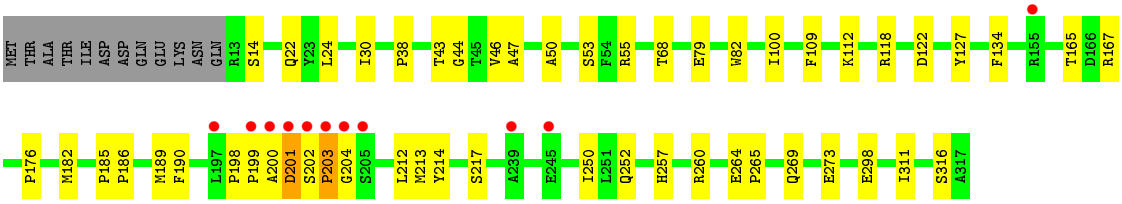
• Molecule 1: Thymidylate synthase

Chain 2-G:



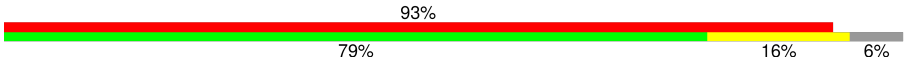
• Molecule 1: Thymidylate synthase

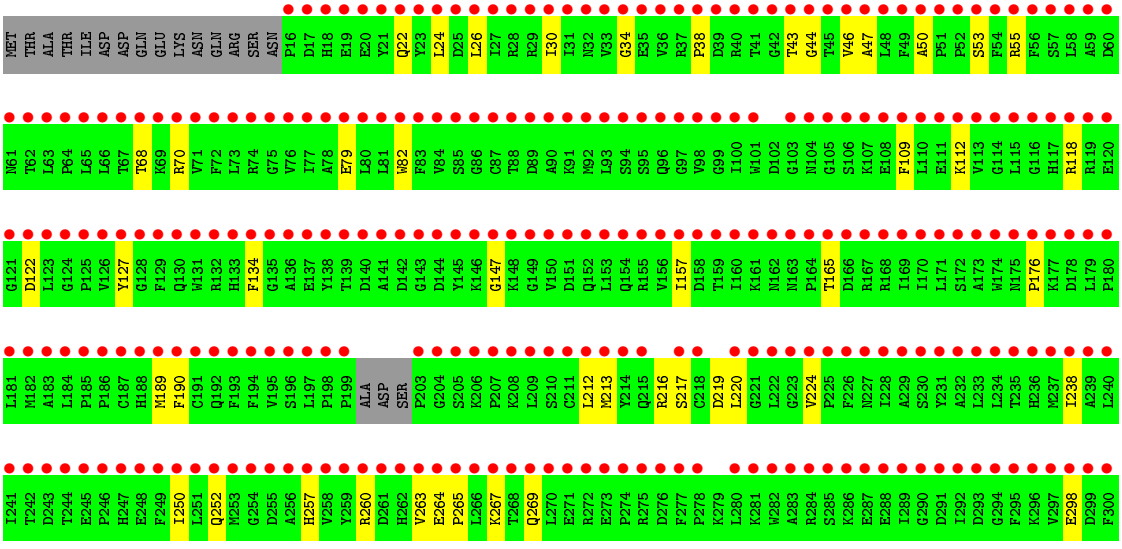
Chain 2-H:

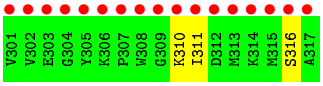


• Molecule 1: Thymidylate synthase

Chain 2-I:

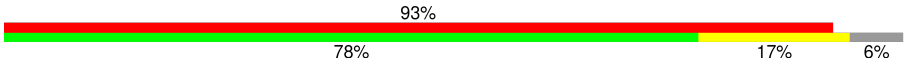


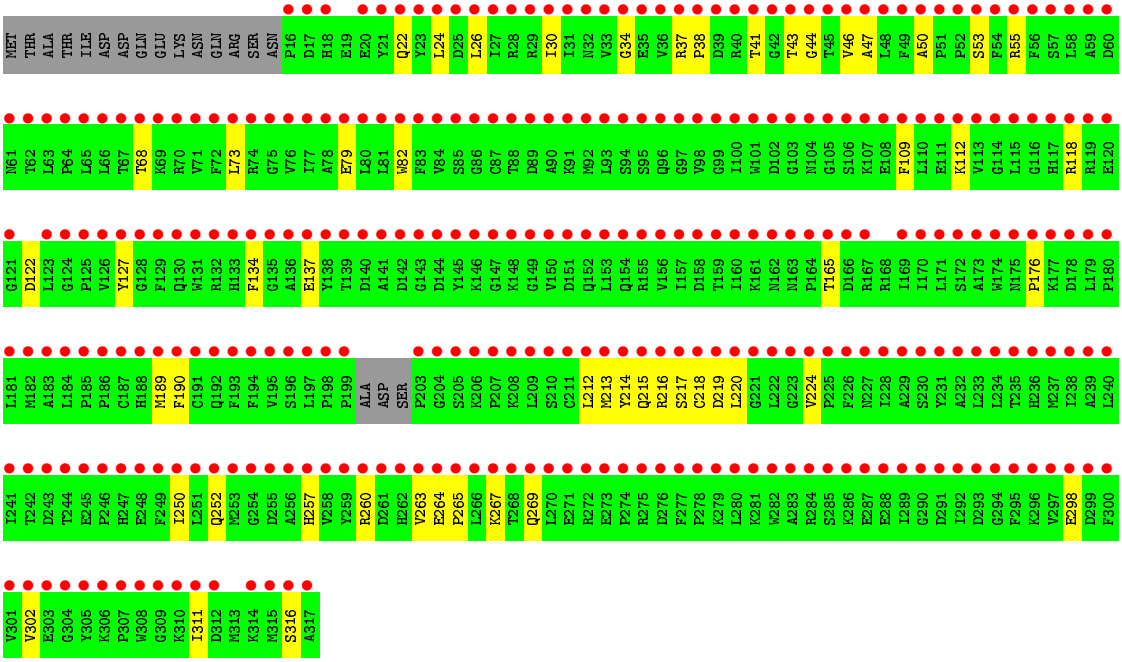




• Molecule 1: Thymidylate synthase

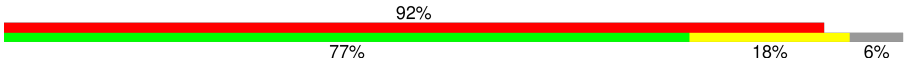
Chain 2-J:

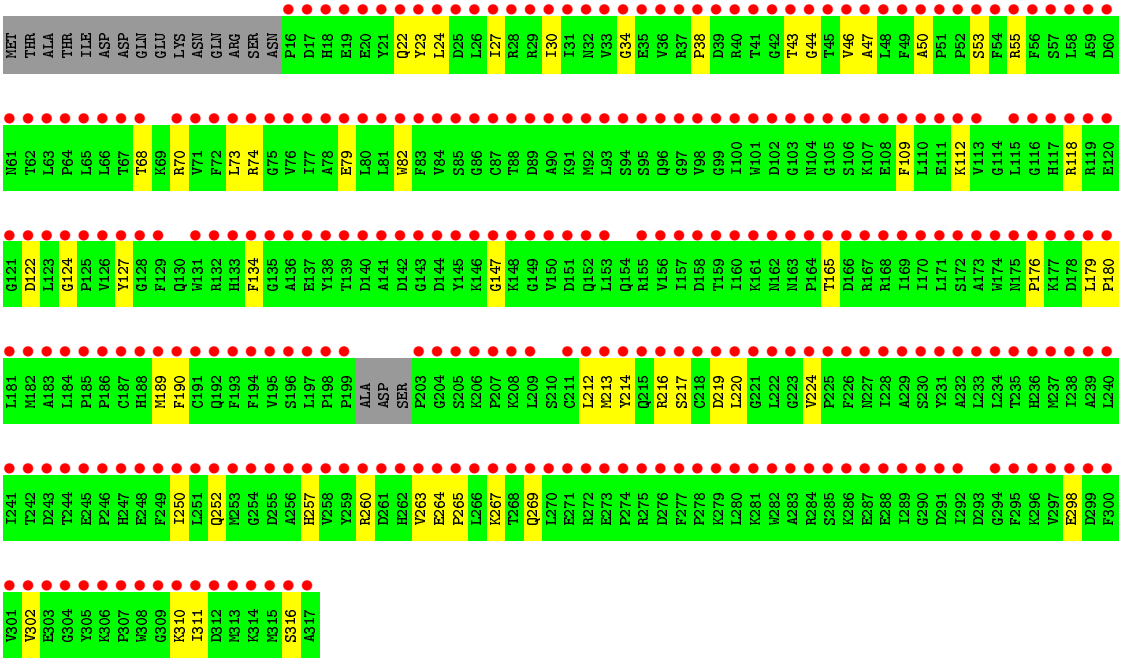




• Molecule 1: Thymidylate synthase

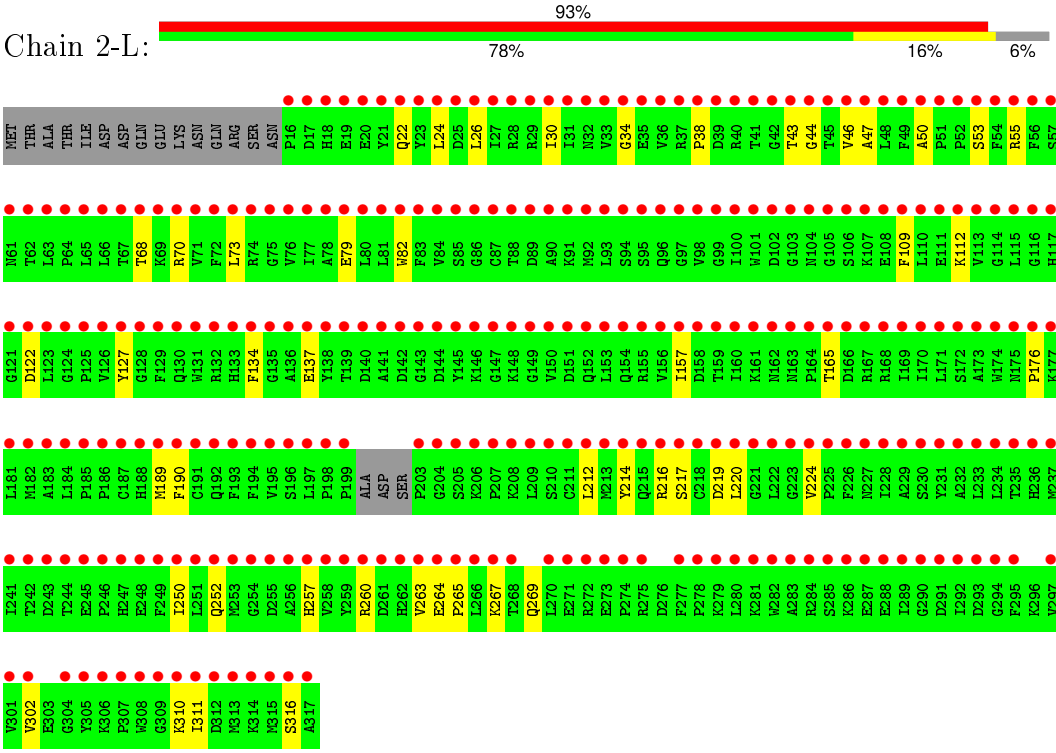
Chain 2-K:





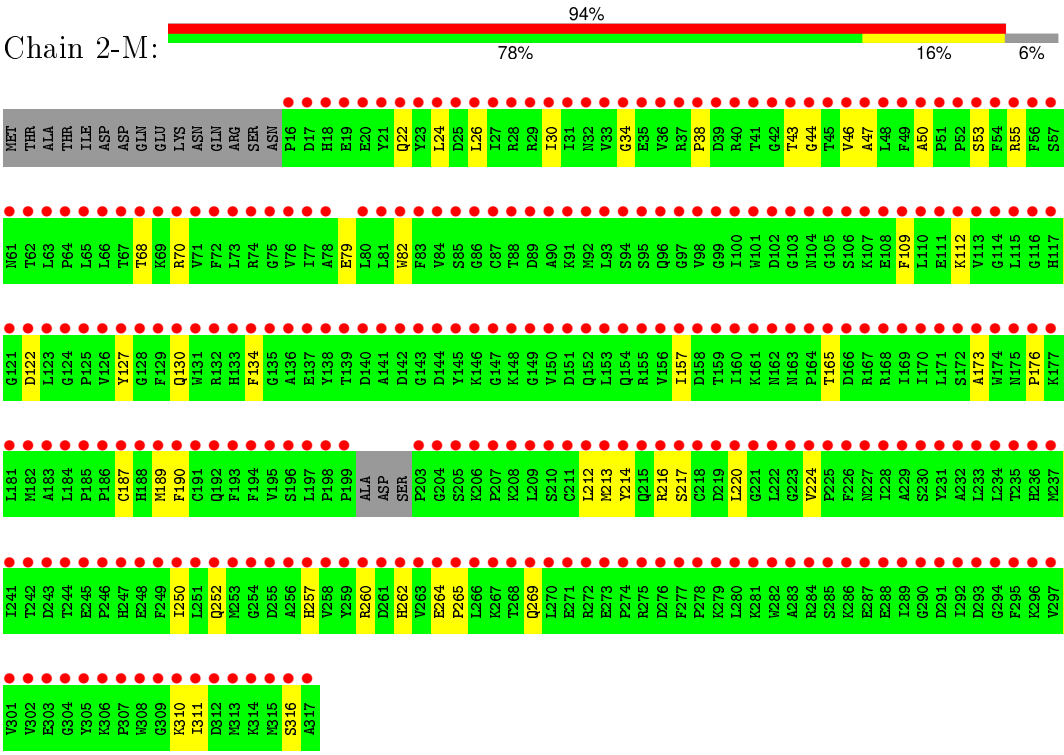
- Molecule 1: Thymidylate synthase

Chain 2-L:



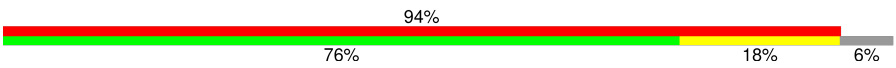
- Molecule 1: Thymidylate synthase

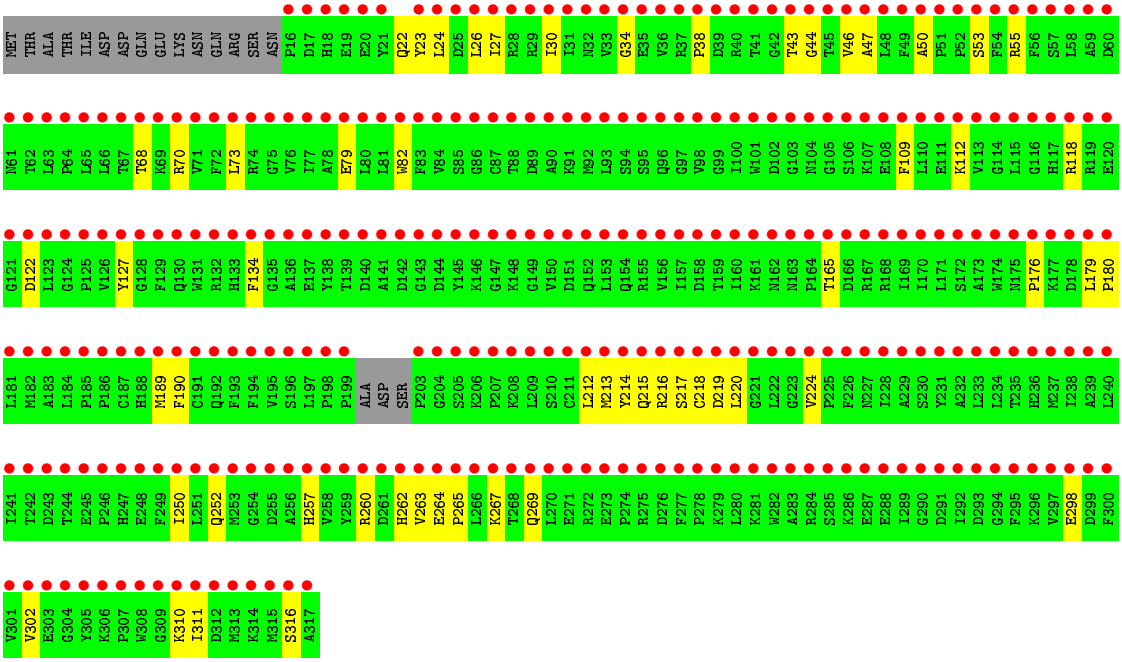
Chain 2-M:



- Molecule 1: Thymidylate synthase

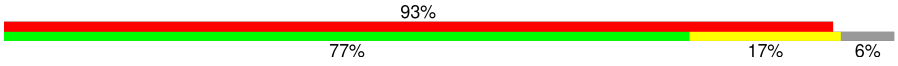
Chain 2-N:

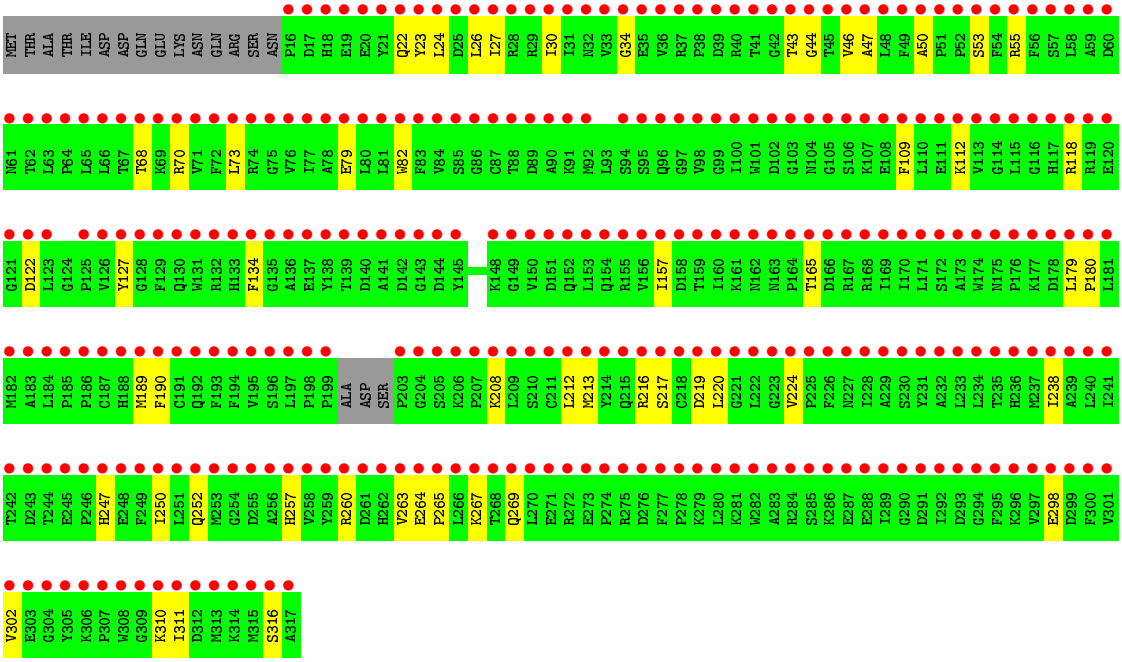




- Molecule 1: Thymidylate synthase

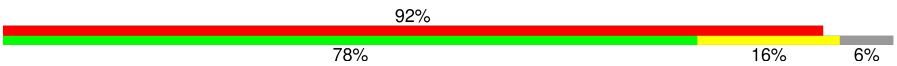
Chain 2-O:

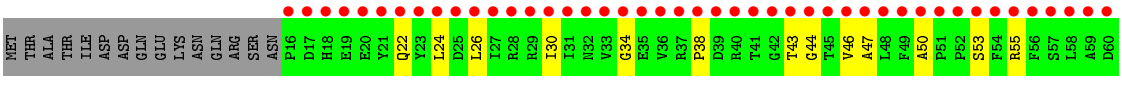


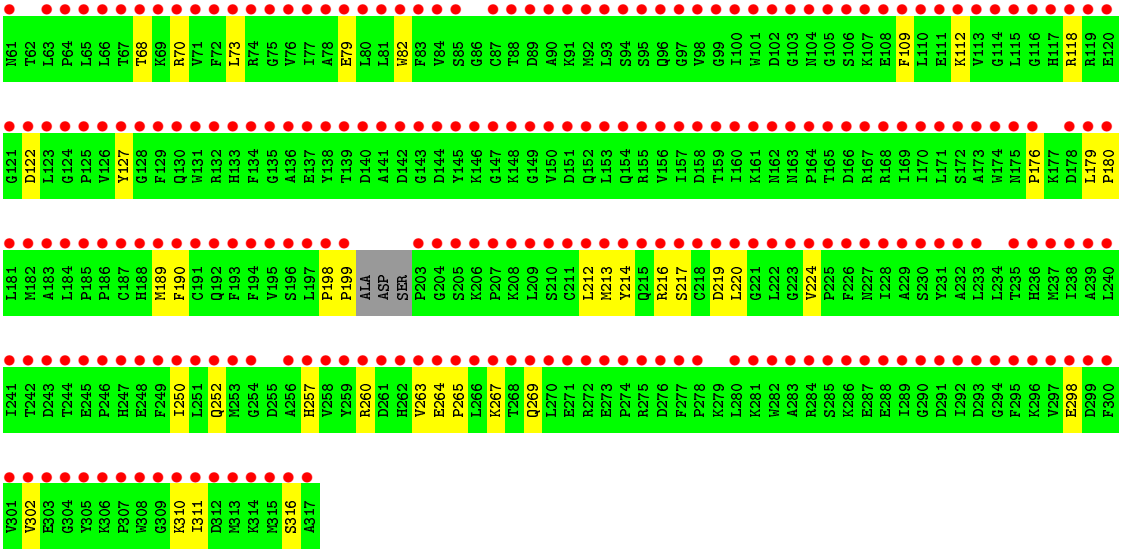


- Molecule 1: Thymidylate synthase

Chain 2-P:

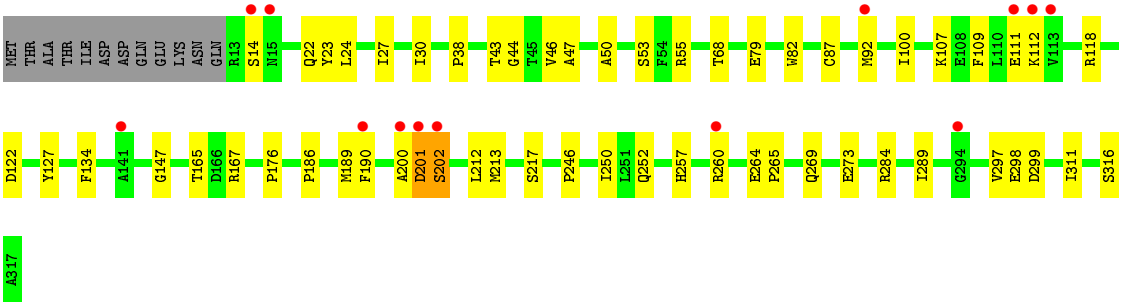






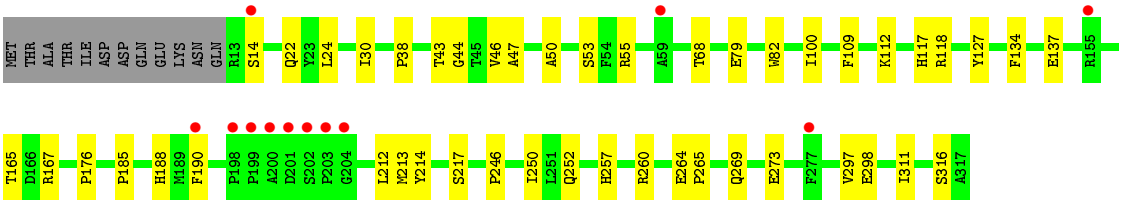
- Molecule 1: Thymidylate synthase

Chain 3-A:



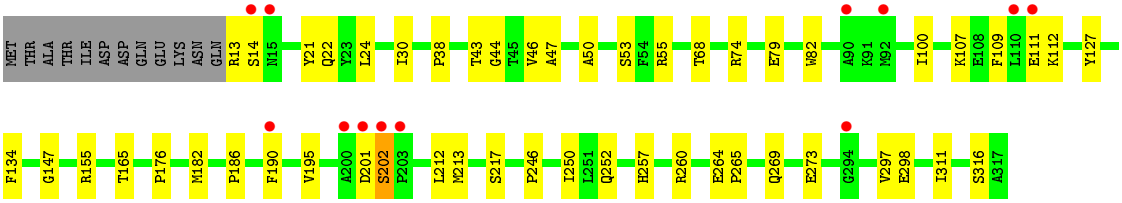
- Molecule 1: Thymidylate synthase

Chain 3-B:



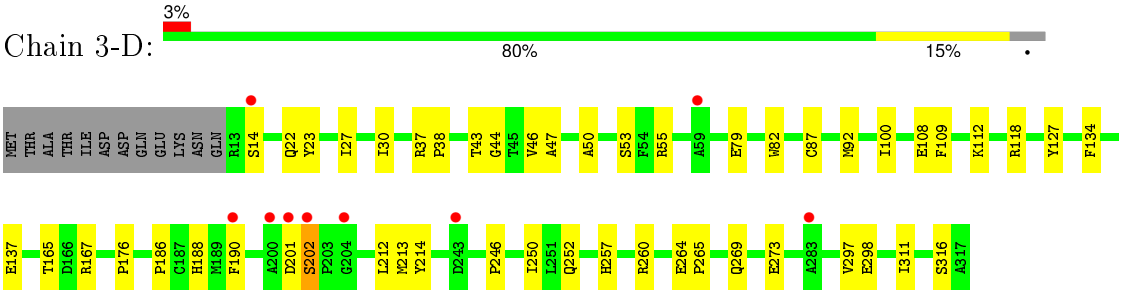
- Molecule 1: Thymidylate synthase

Chain 3-C:



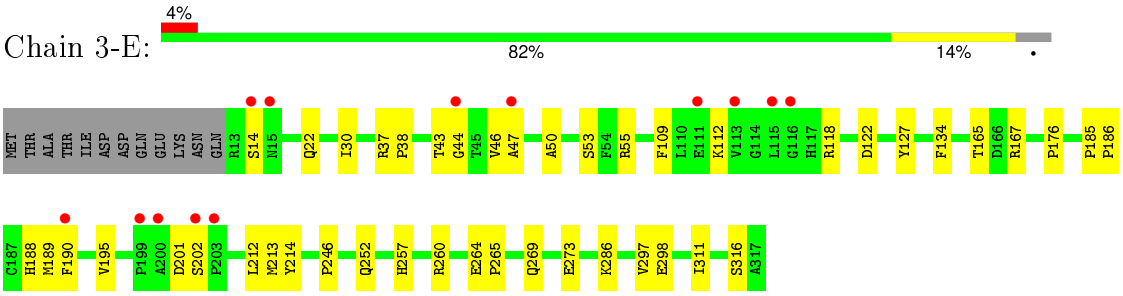
• Molecule 1: Thymidylate synthase

Chain 3-D:



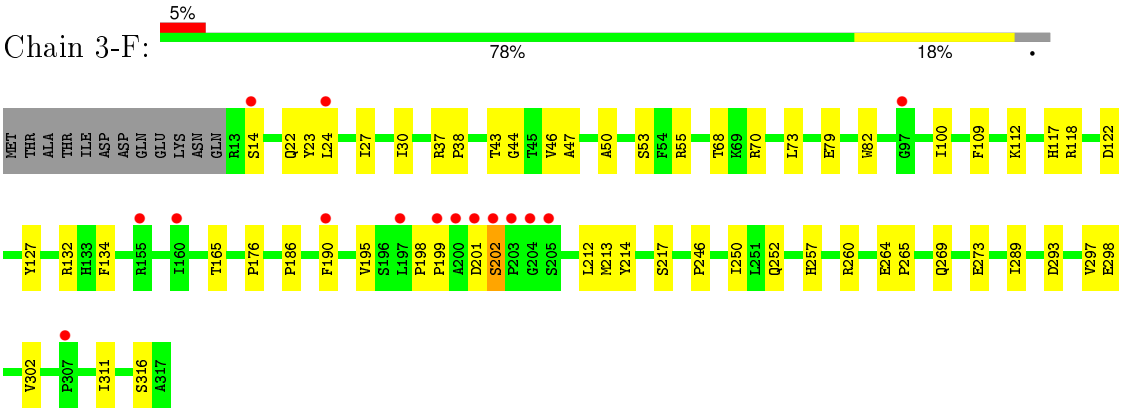
• Molecule 1: Thymidylate synthase

Chain 3-E:



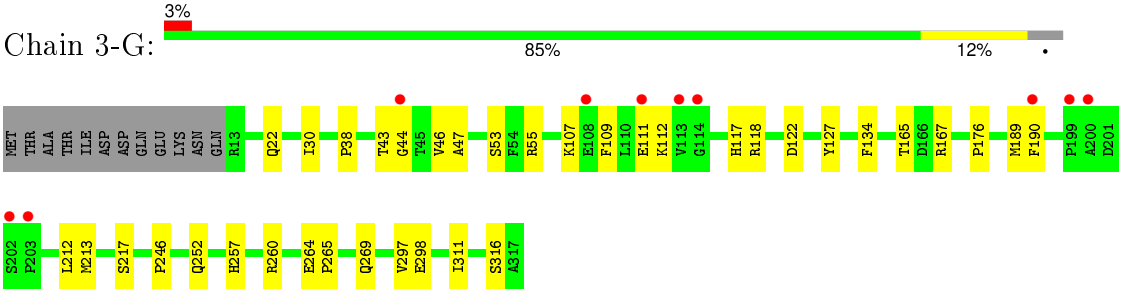
• Molecule 1: Thymidylate synthase

Chain 3-F:



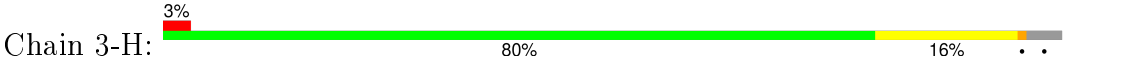
• Molecule 1: Thymidylate synthase

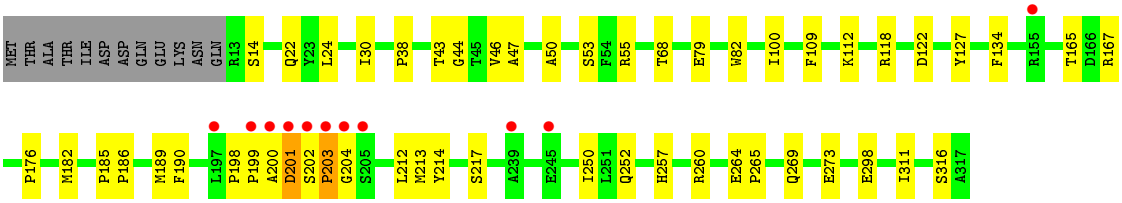
Chain 3-G:



• Molecule 1: Thymidylate synthase

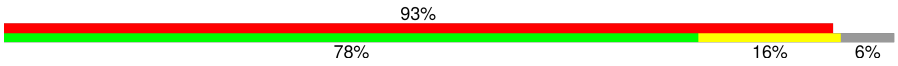
Chain 3-H:

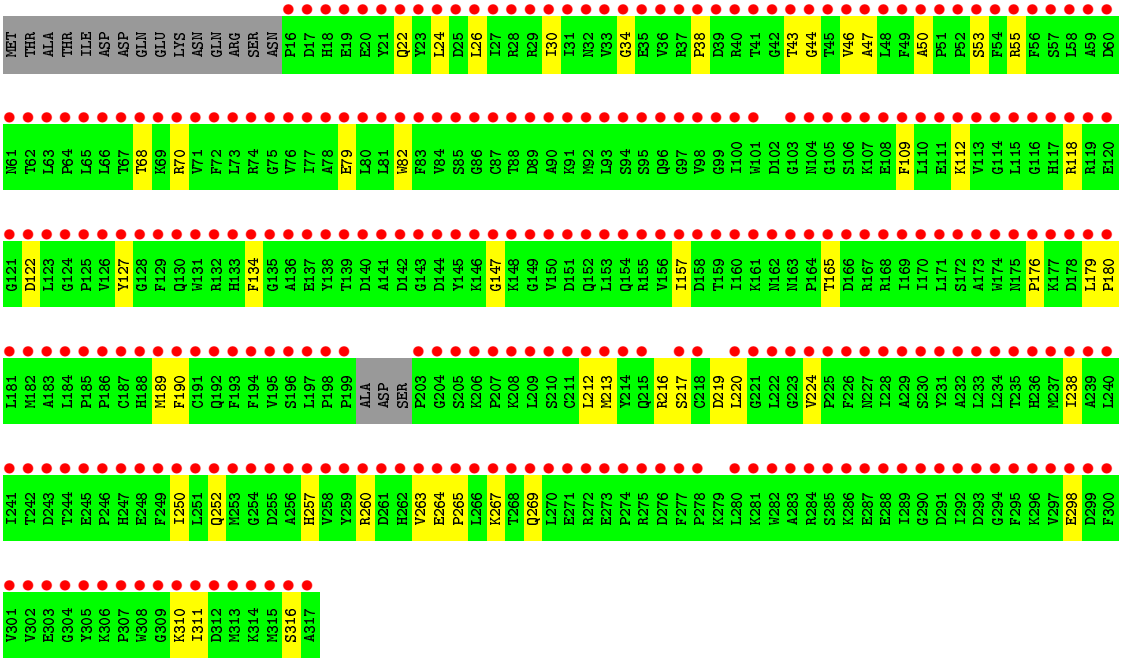




• Molecule 1: Thymidylate synthase

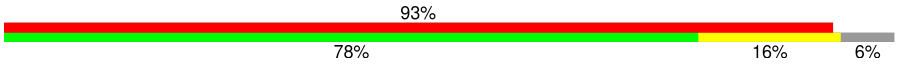
Chain 3-I:

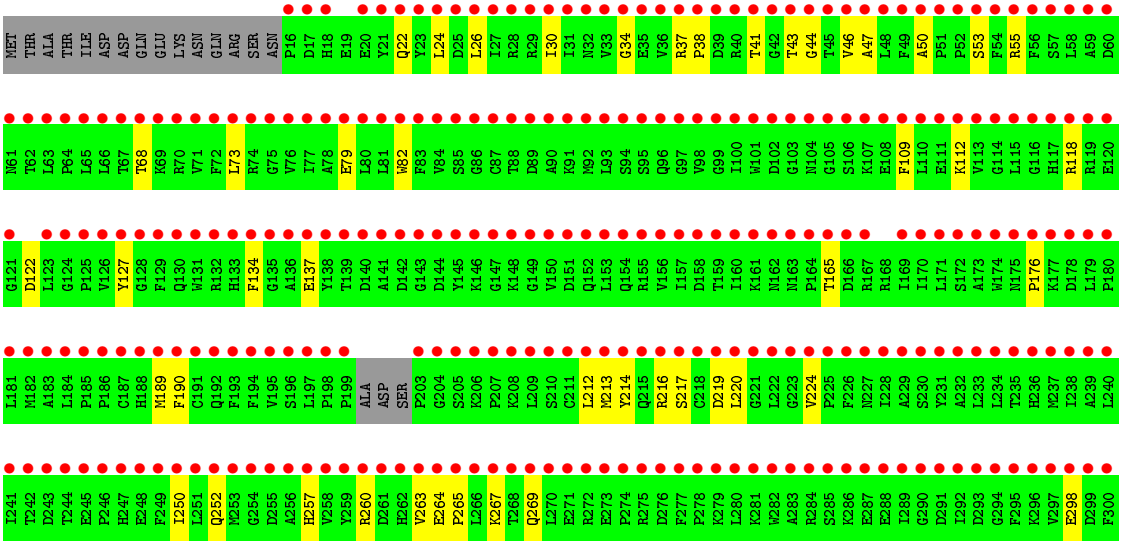


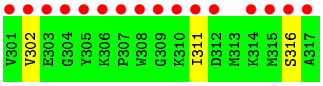


• Molecule 1: Thymidylate synthase

Chain 3-J:

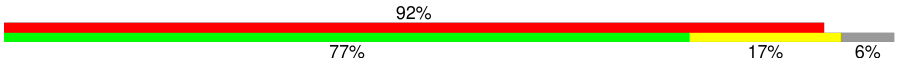


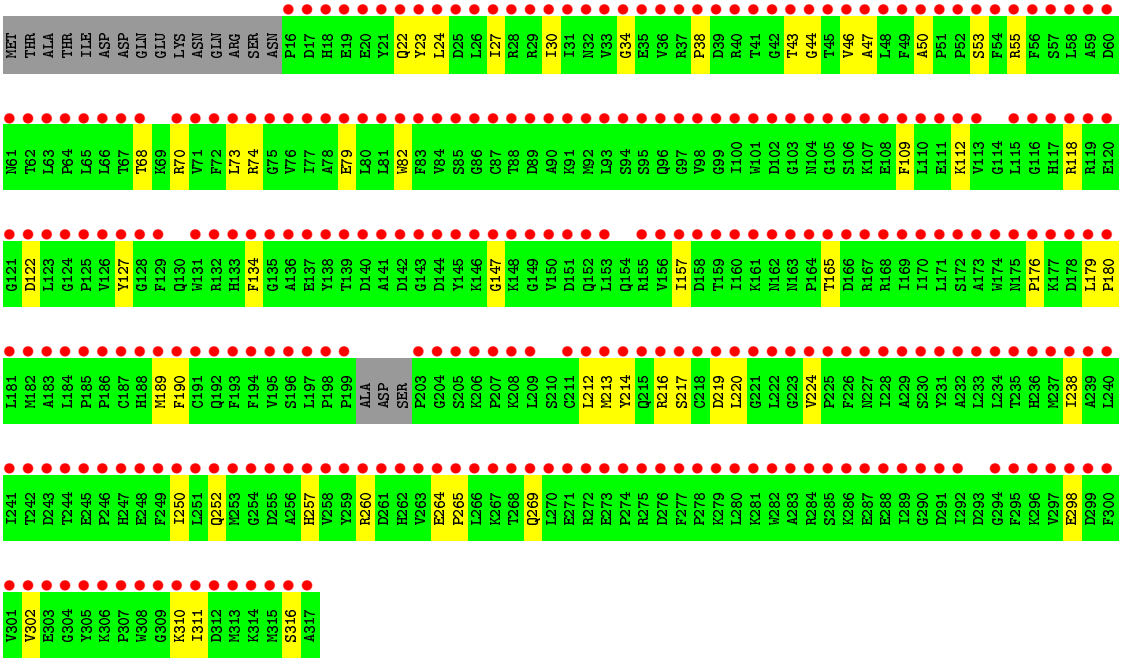




• Molecule 1: Thymidylate synthase

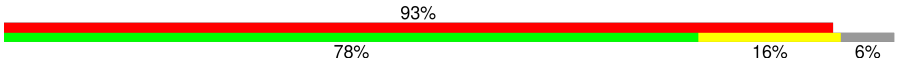
Chain 3-K:

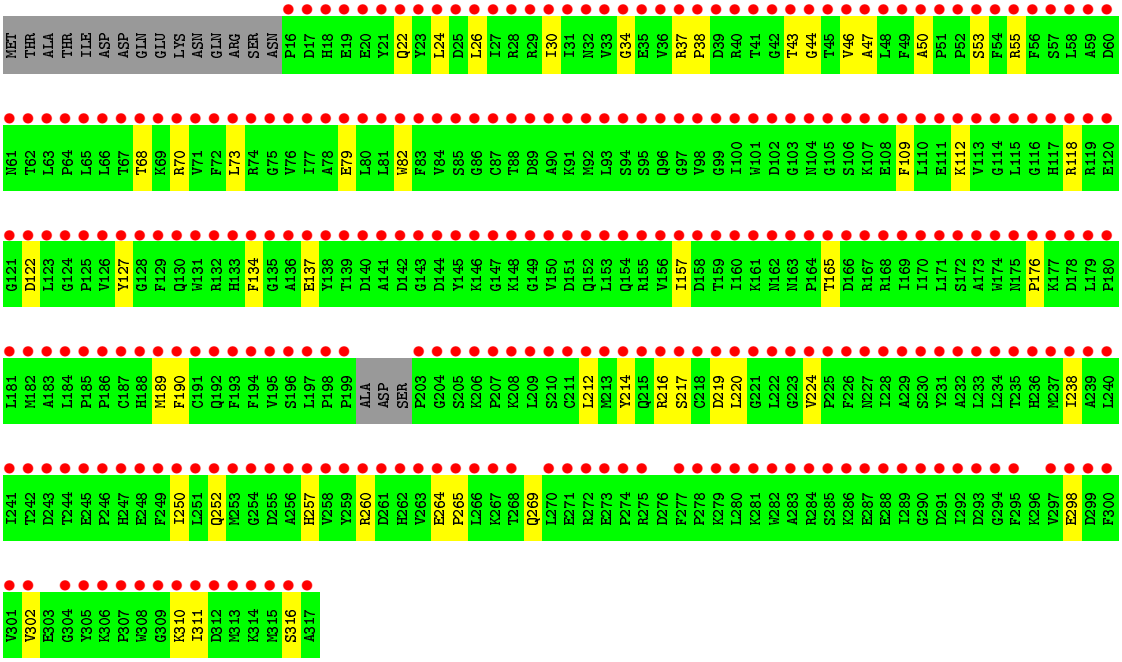




• Molecule 1: Thymidylate synthase

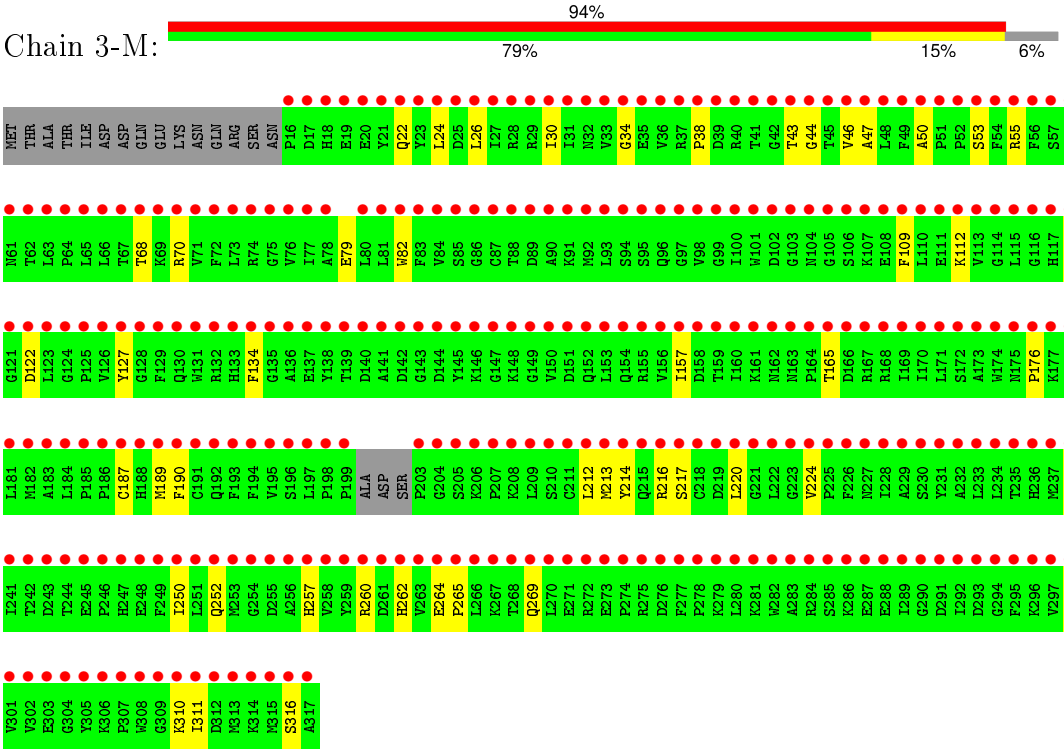
Chain 3-L:





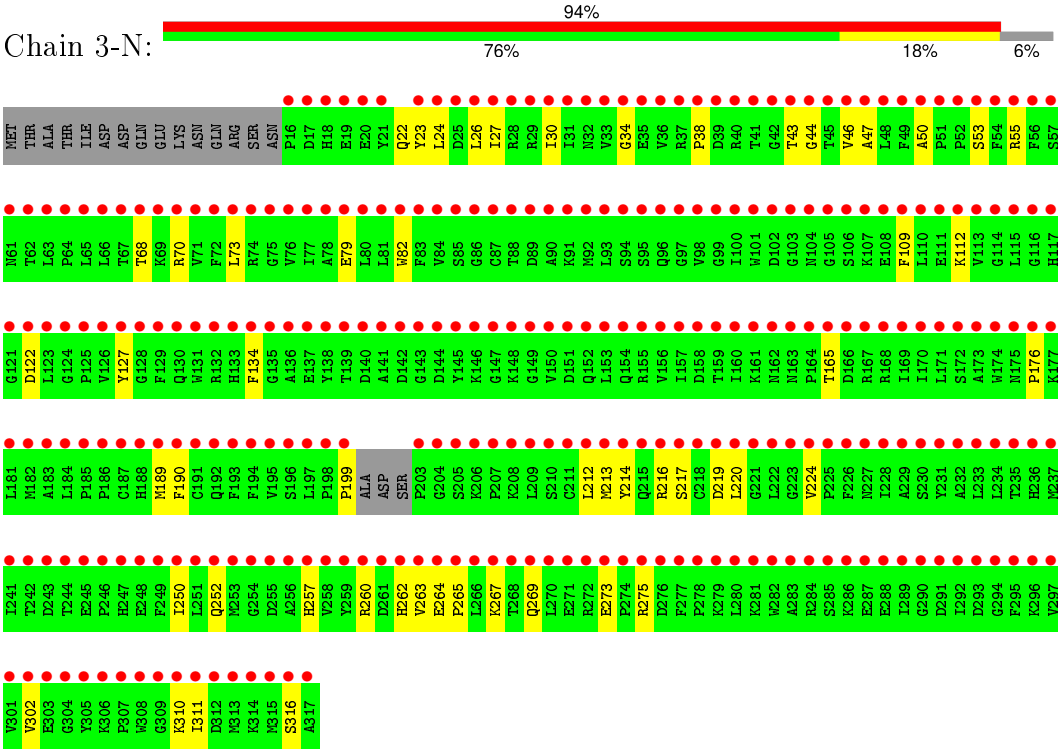
• Molecule 1: Thymidylate synthase

Chain 3-M:



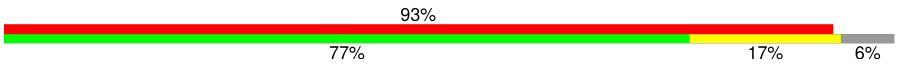
• Molecule 1: Thymidylate synthase

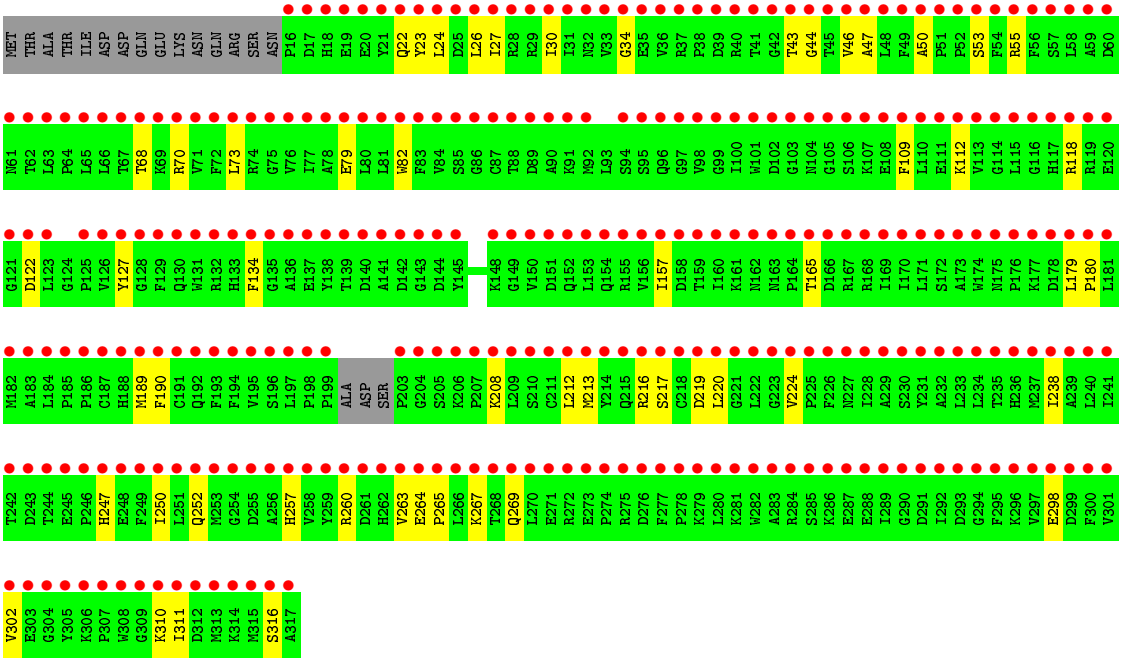
Chain 3-N:



• Molecule 1: Thymidylate synthase

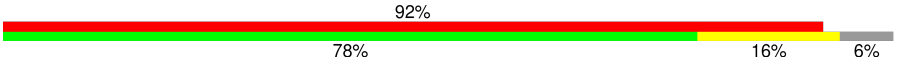
Chain 3-O:

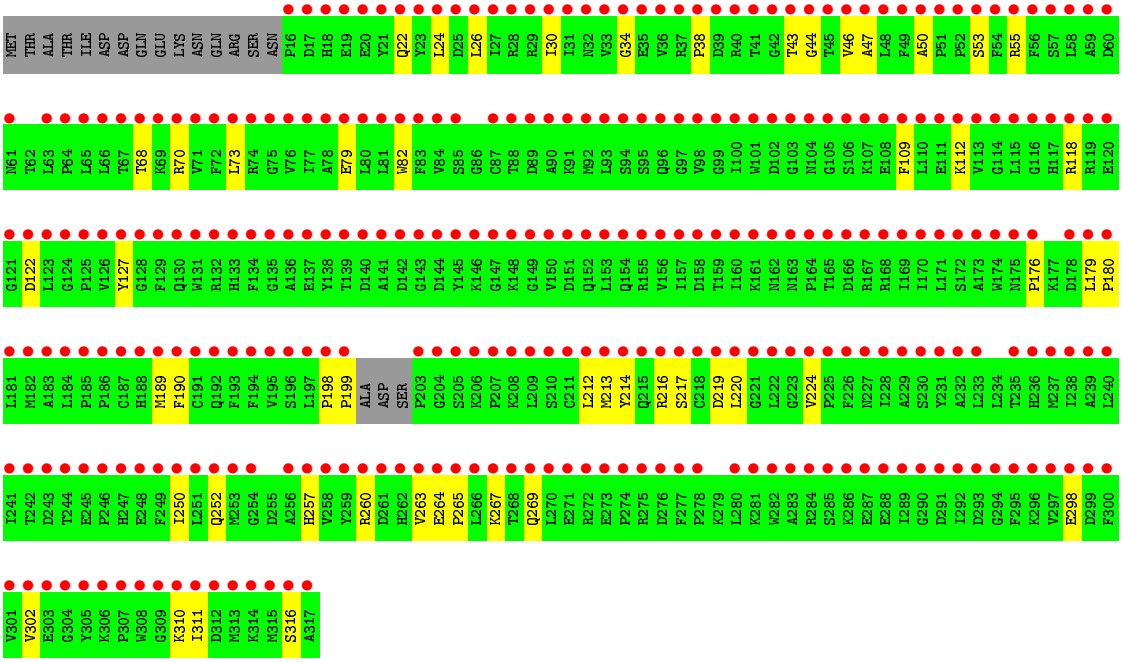




- Molecule 1: Thymidylate synthase

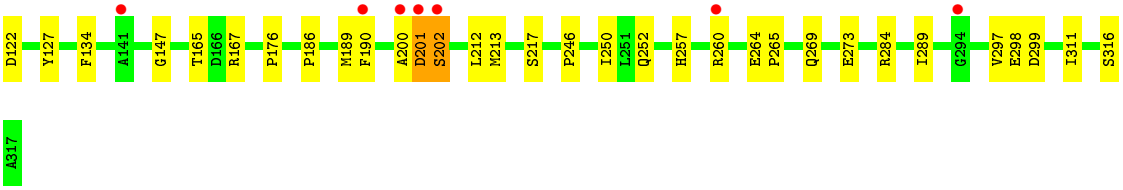
Chain 3-P:





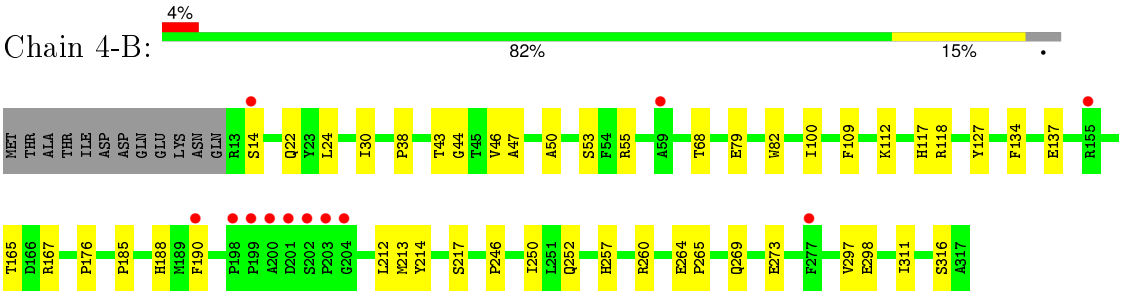
- Molecule 1: Thymidylate synthase

Chain 4-A:



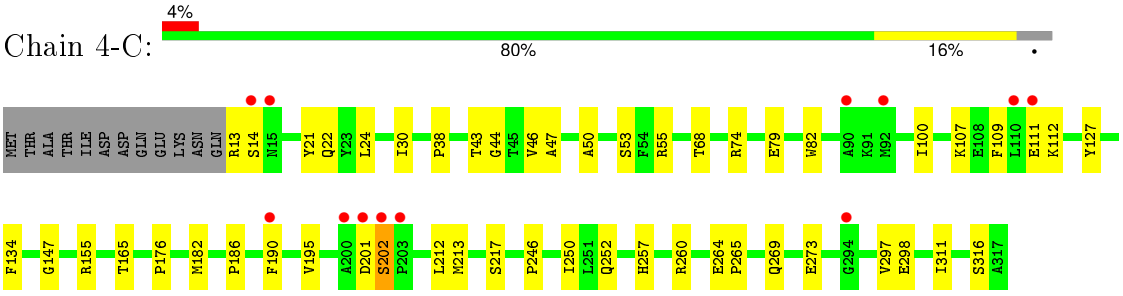
• Molecule 1: Thymidylate synthase

Chain 4-B:



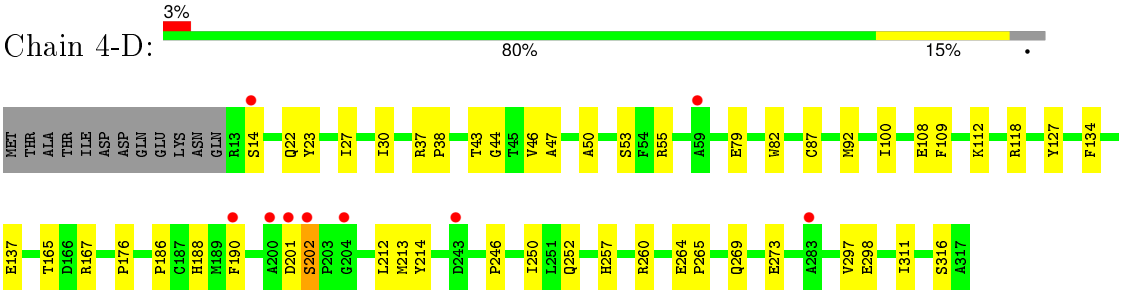
• Molecule 1: Thymidylate synthase

Chain 4-C:



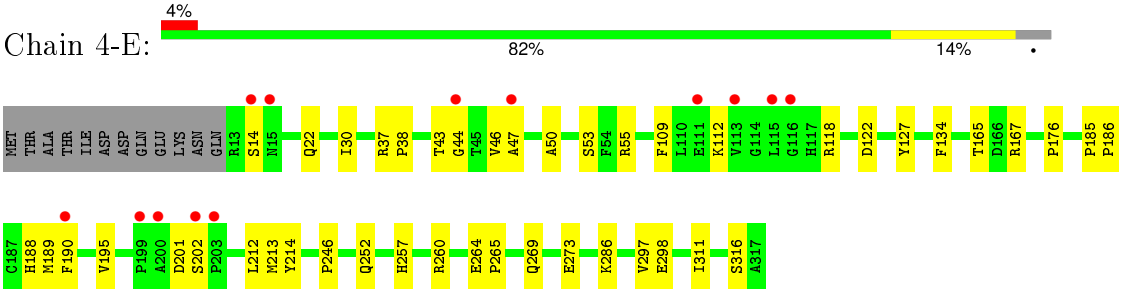
• Molecule 1: Thymidylate synthase

Chain 4-D:



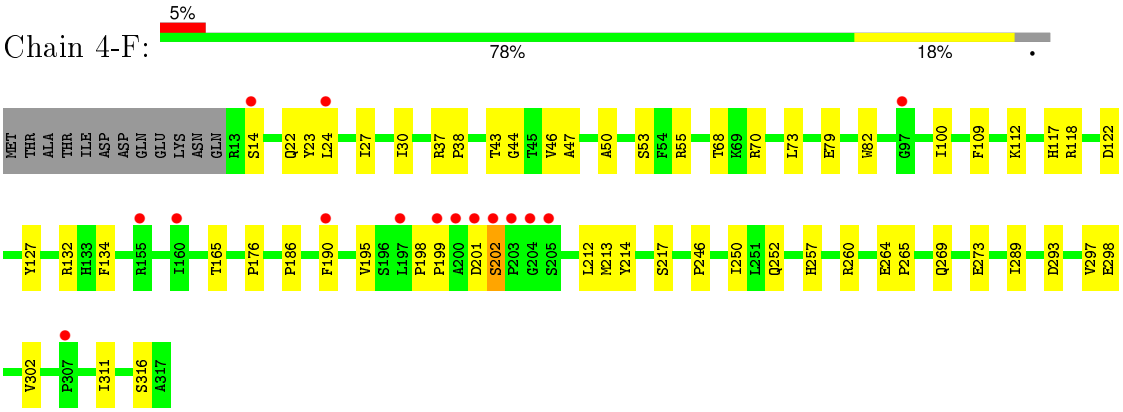
• Molecule 1: Thymidylate synthase

Chain 4-E:



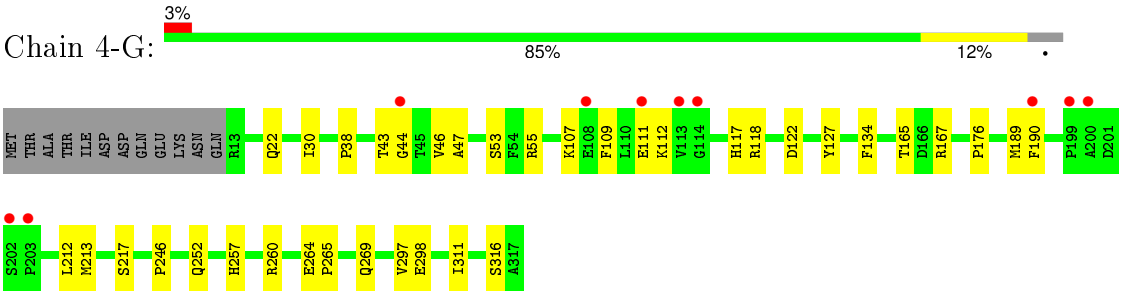
• Molecule 1: Thymidylate synthase

Chain 4-F:



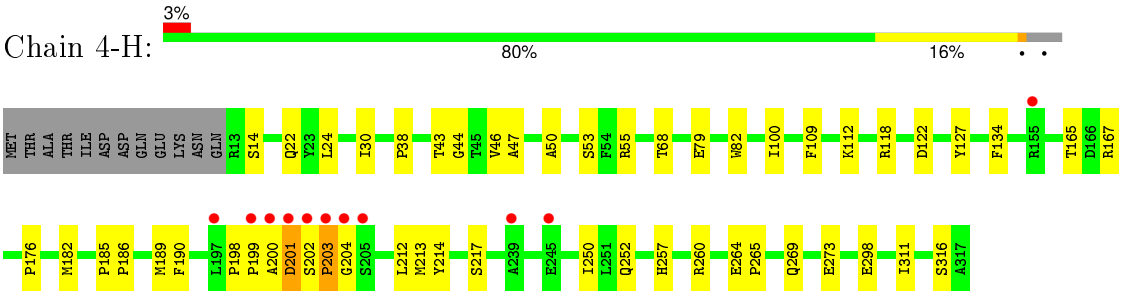
• Molecule 1: Thymidylate synthase

Chain 4-G:



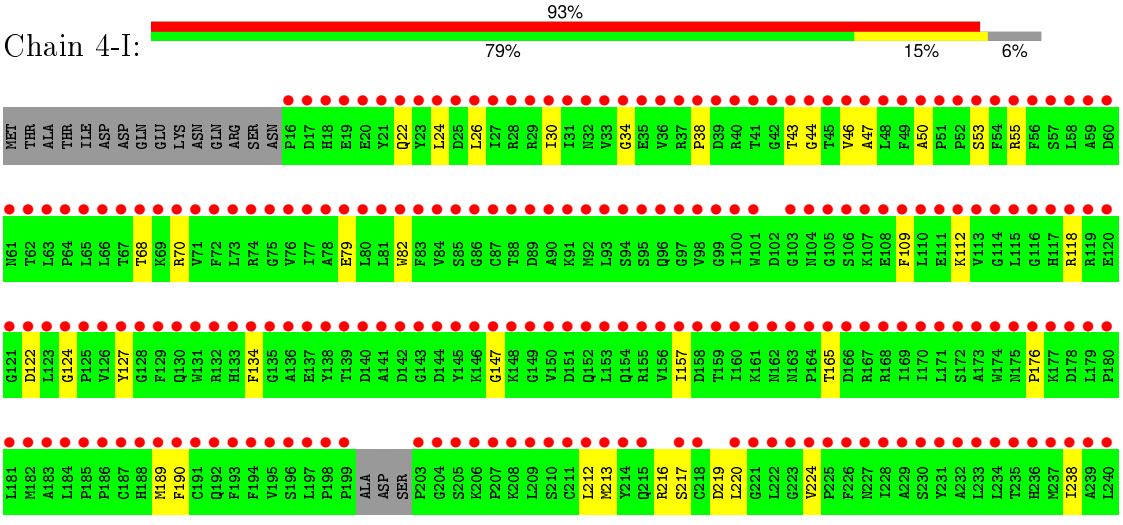
• Molecule 1: Thymidylate synthase

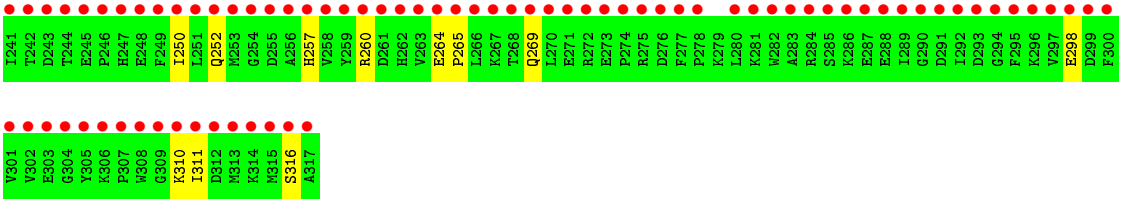
Chain 4-H:



• Molecule 1: Thymidylate synthase

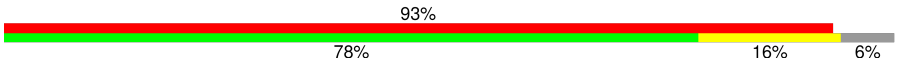
Chain 4-I:

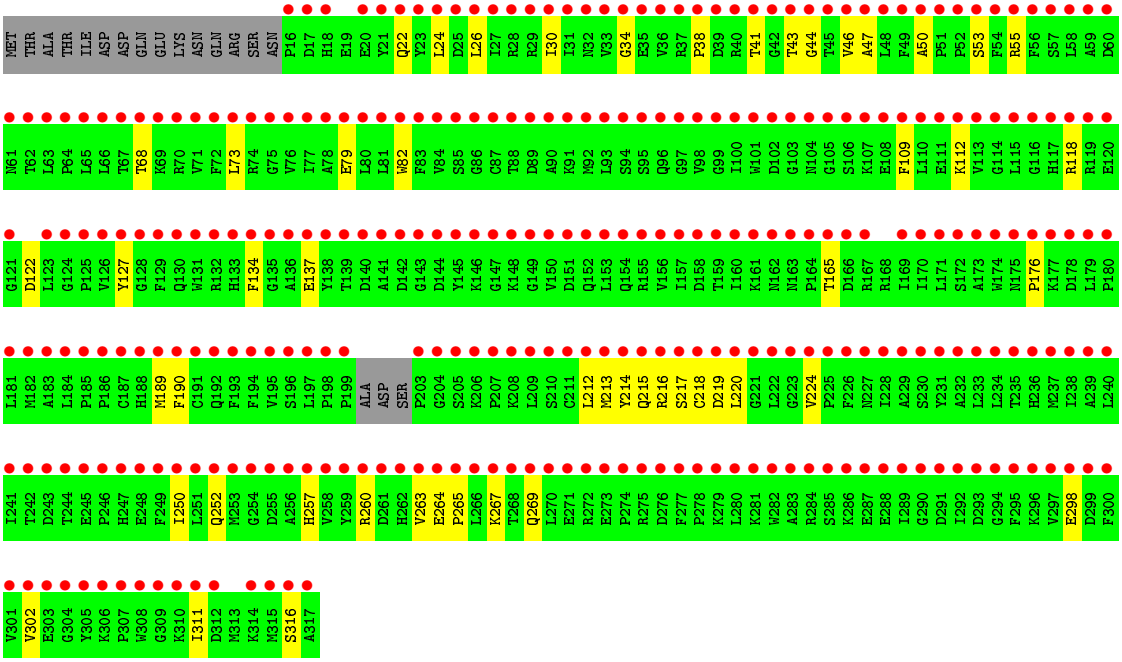




• Molecule 1: Thymidylate synthase

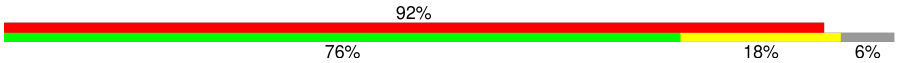
Chain 4-J:

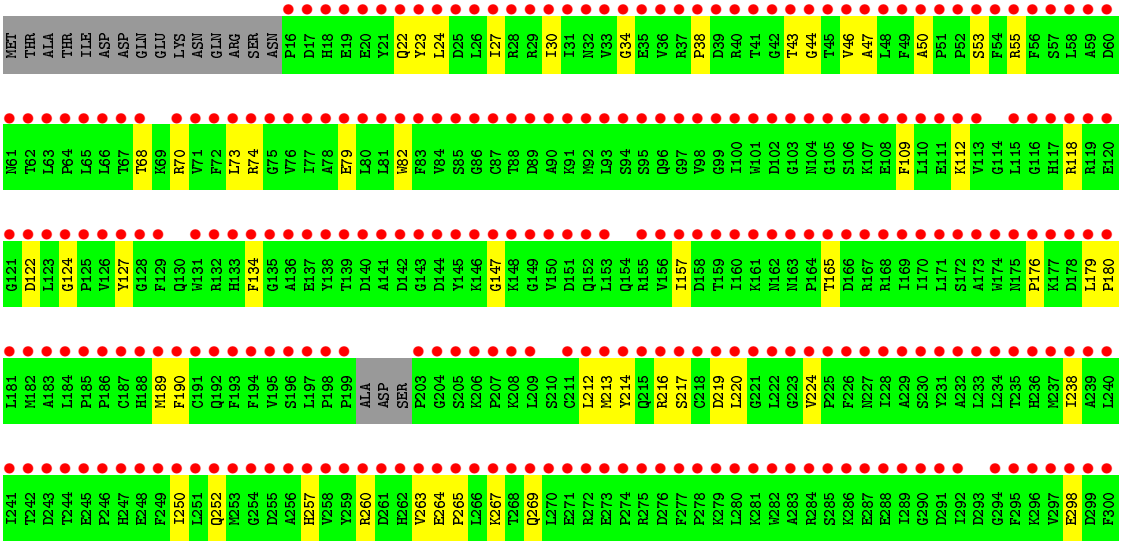


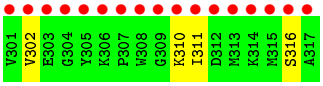


• Molecule 1: Thymidylate synthase

Chain 4-K:

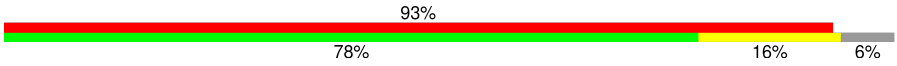


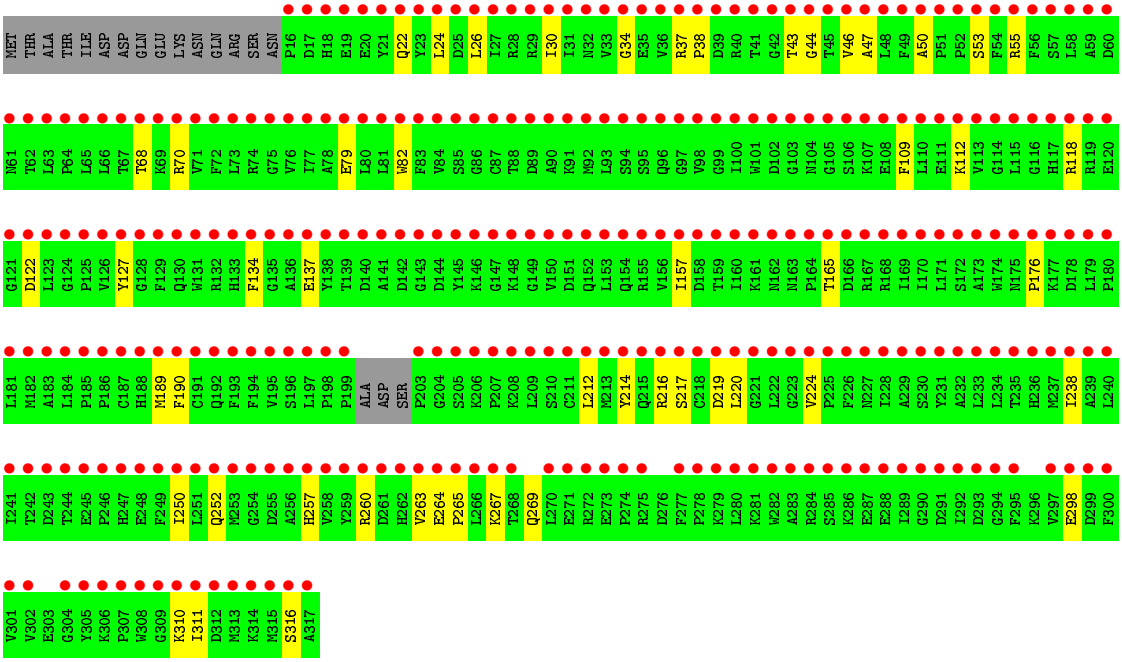




• Molecule 1: Thymidylate synthase

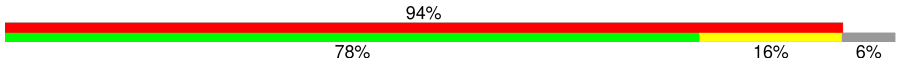
Chain 4-L:

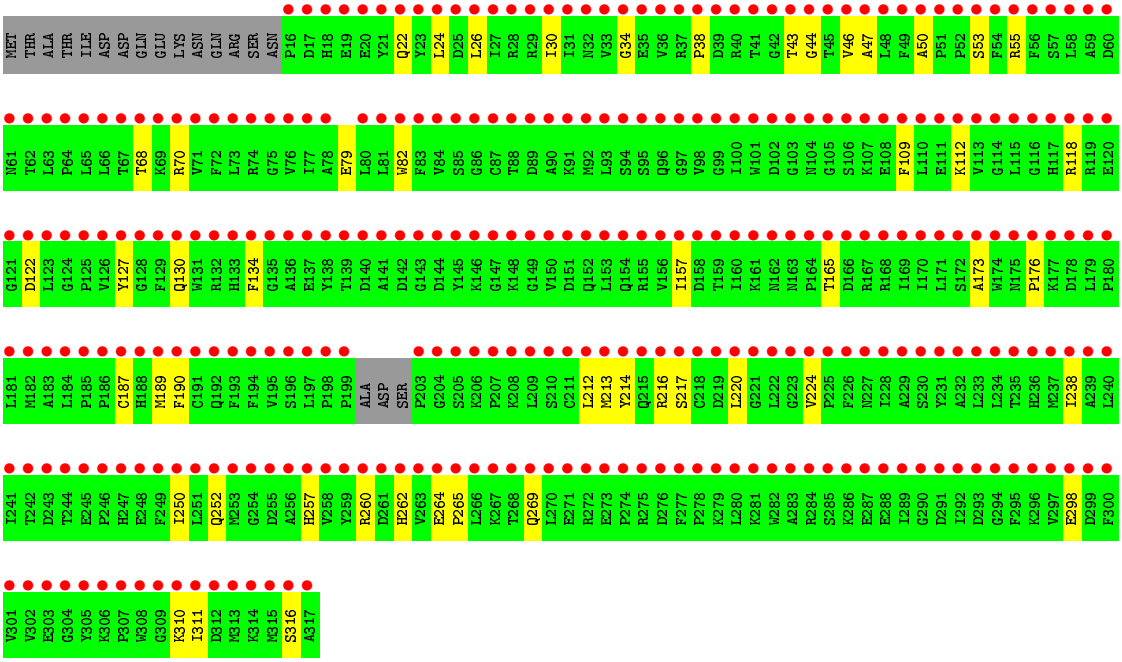




• Molecule 1: Thymidylate synthase

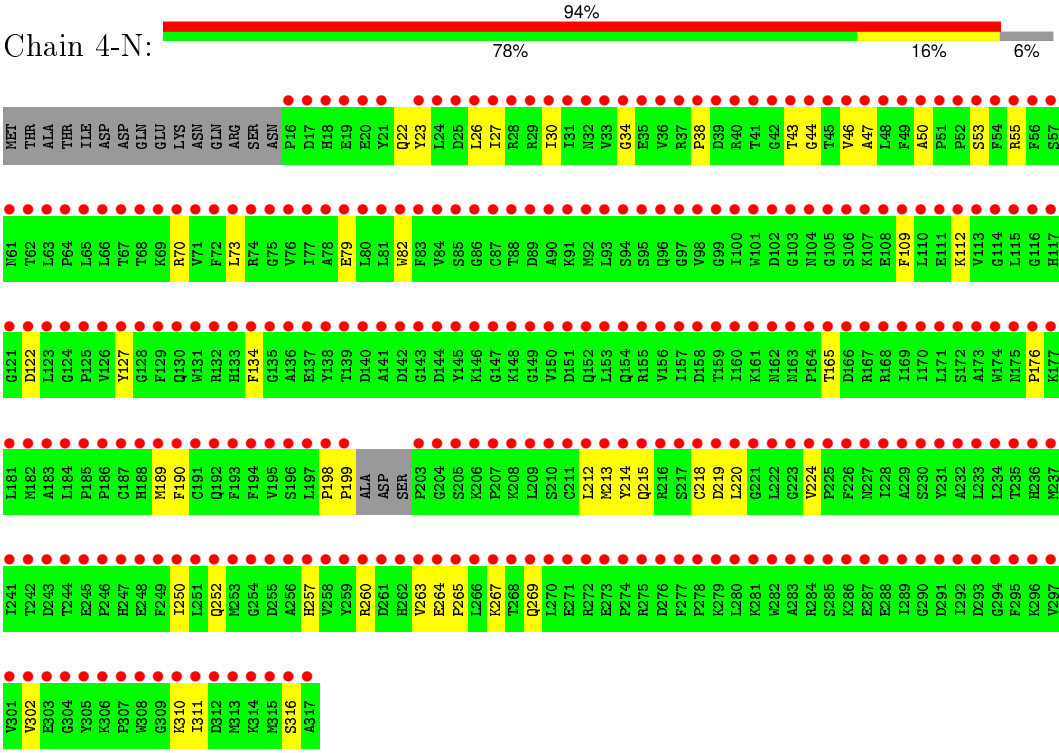
Chain 4-M:





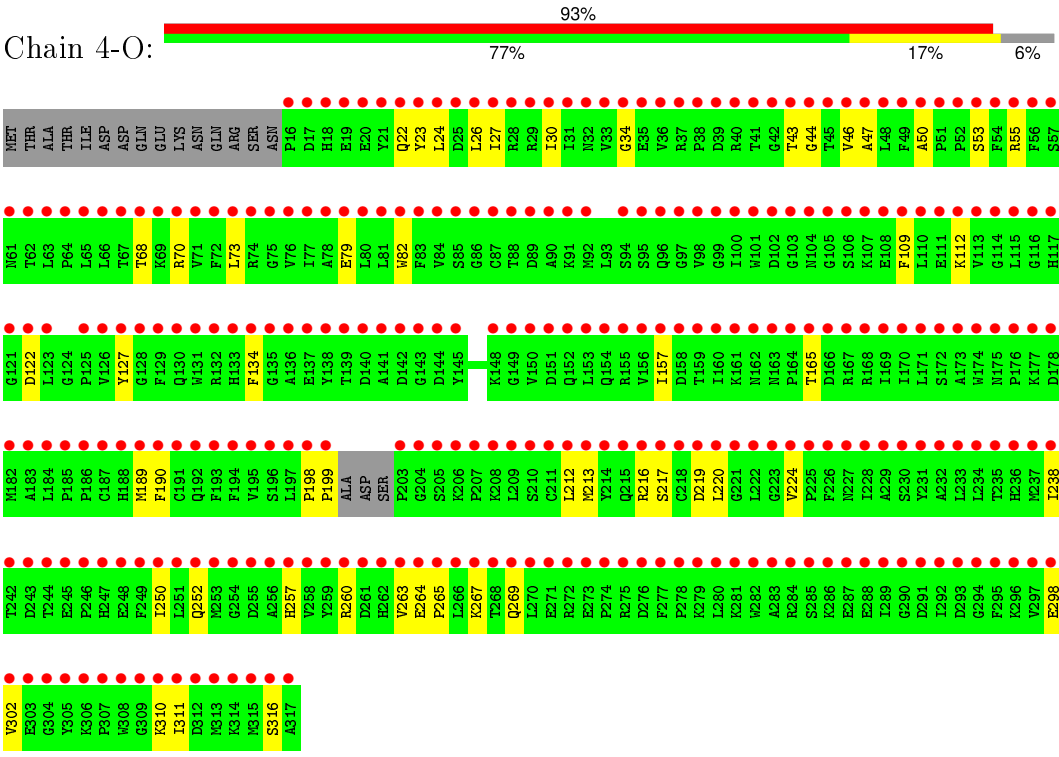
- Molecule 1: Thymidylate synthase

Chain 4-N:



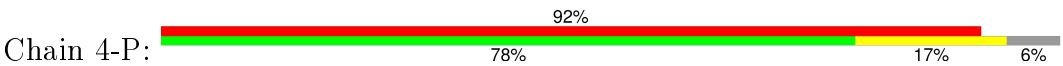
- Molecule 1: Thymidylate synthase

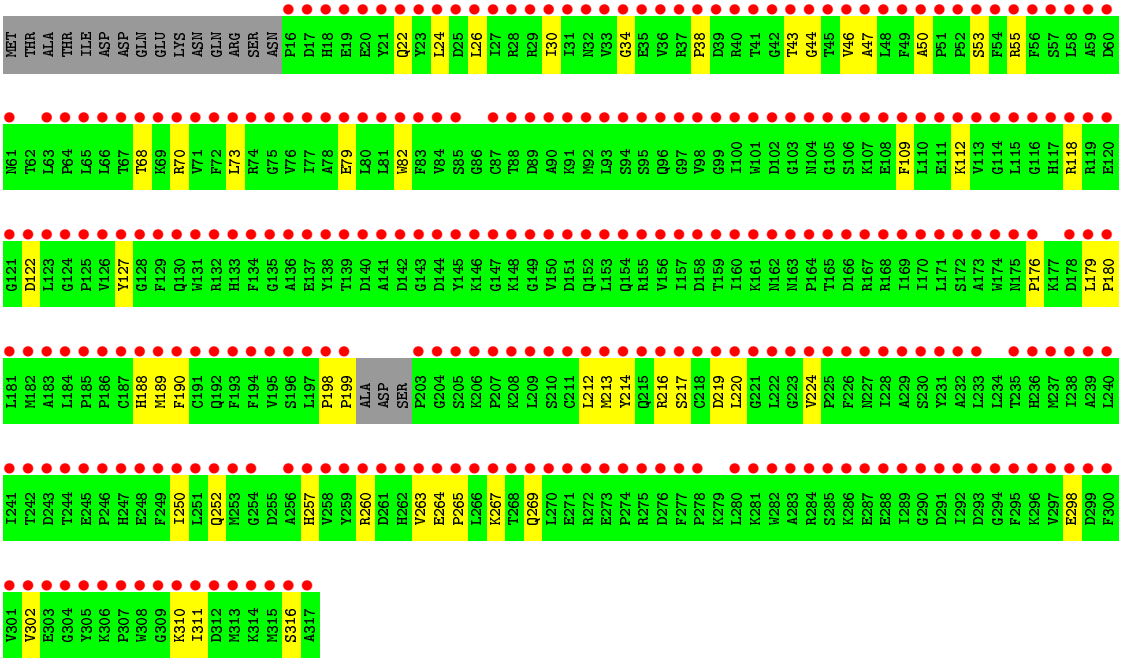
Chain 4-O:



- Molecule 1: Thymidylate synthase

Chain 4-P:

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N61 T62 L63 P64 L65 L66 T67 T68 K69 R70 V71 F72 L73 R74 G75 V76 I77 A78 E79 L80 L81 W82 F83 V84 S85 G86 C87 T88 D89 A90 K91 N92 L93 S94 S95 Q96 G97 V98 G99 I100 W101 D102 G103 N104 G105 S106 K107 E108 F109 L110 E111 K112 V113 G114 L115 G116 H117 R118 R119 E120
G121 D122 L123 G124 P125 V126 Y127 G128 F129 Q130 W131 R132 H133 F134 G135 A136 E137 Y138 T139 D140 A141 D142 G143 D144 Y145 K146 G147 K148 G149 V150 D151 Q152 L153 Q154 R155 V156 I157 D158 T159 I160 K161 N162 M163 P164 T165 D166 R167 R168 I169 I170 L171 S172 A173 W174 M175 P176 K177 D178 L179 P180
L181 M182 A183 L184 P185 P186 C187 H188 M189 F190 C191 Q192 F193 F194 V195 S196 L197 P198 P199 ALA ASP SER P203 G204 S205 K206 P207 K208 L209 S210 C211 L212 M213 Y214 Q215 R216 S217 C218 D219 L220 G221 L222 G223 V224 P225 F226 M227 I228 A229 S230 Y231 A232 L233 L234 T235 H236 M237 I238 A239 L240
I241 T242 D243 T244 E245 P246 H247 E248 F249 I250 L251 Q252 M253 G254 D255 A256 H257 V258 Y259 R260 D261 H262 V263 E264 P265 L266 K267 T268 Q269 L270 E271 R272 E273 P274 R275 D276 F277 P278 K279 L280 K281 W282 A283 R284 S285 K286 E287 E288 I289 G290 D291 I292 D293 G294 F295 K296 V297 E298 D299 F300
V301 V302 E303 G304 Y305 K306 P307 W308 G309 K310 I311 D312 M313 K314 M315 S316 A317

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	179.40Å 179.50Å 209.10Å 90.00° 89.80° 90.00°	Depositor
Resolution (Å)	49.91 – 2.08 89.75 – 2.07	Depositor EDS
% Data completeness (in resolution range)	88.1 (49.91-2.08) 88.0 (89.75-2.07)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 2.07Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.290 , 0.305 0.288 , 0.304	Depositor DCC
R_{free} test set	36675 reflections (11.70%)	DCC
Wilson B-factor (Å^2)	24.4	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 58.9	EDS
Estimated twinning fraction	0.206 for k,h,-l 0.198 for -k,-h,-l 0.349 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 371476 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	161392	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CB3, UMP

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	1-A	0.50	0/2492	1.21	11/3375 (0.3%)
1	1-B	0.47	0/2496	0.71	4/3380 (0.1%)
1	1-C	0.48	0/2492	1.03	8/3375 (0.2%)
1	1-D	0.51	0/2496	1.39	13/3380 (0.4%)
1	1-E	0.49	0/2496	1.01	8/3380 (0.2%)
1	1-F	0.50	1/2496 (0.0%)	1.28	12/3380 (0.4%)
1	1-G	0.49	0/2496	0.86	8/3380 (0.2%)
1	1-H	0.49	0/2496	0.85	7/3380 (0.2%)
1	1-I	0.28	0/2451	0.59	2/3316 (0.1%)
1	1-J	0.28	0/2451	0.59	3/3316 (0.1%)
1	1-K	0.28	0/2451	0.59	3/3316 (0.1%)
1	1-L	0.28	0/2451	0.59	2/3316 (0.1%)
1	1-M	0.28	0/2451	0.59	2/3316 (0.1%)
1	1-N	0.28	0/2451	0.59	2/3316 (0.1%)
1	1-O	0.28	0/2451	0.59	2/3316 (0.1%)
1	1-P	0.28	0/2451	0.59	3/3316 (0.1%)
All	All	0.40	1/39568 (0.0%)	0.86	90/53558 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-F	132[A]	ARG	CD-NE	-5.44	1.37	1.46

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1-D	37[A]	ARG	NE-CZ-NH1	-31.12	104.74	120.30
1	1-F	132[A]	ARG	NE-CZ-NH1	-30.91	104.84	120.30
1	1-F	132[A]	ARG	NE-CZ-NH2	30.10	135.35	120.30
1	1-E	37[A]	ARG	NE-CZ-NH1	-29.08	105.76	120.30
1	1-F	37[A]	ARG	NE-CZ-NH1	-28.95	105.82	120.30

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	1-A	2427	0	2393	50	0
1	1-B	2431	0	2397	45	0
1	1-C	2427	0	2393	49	0
1	1-D	2431	0	2397	48	0
1	1-E	2431	0	2397	43	0
1	1-F	2431	0	2397	53	0
1	1-G	2431	0	2397	35	0
1	1-H	2431	0	2397	51	0
1	1-I	2387	0	2360	40	0
1	1-J	2387	0	2360	47	0
1	1-K	2387	0	2360	47	0
1	1-L	2387	0	2360	46	0
1	1-M	2387	0	2360	41	0
1	1-N	2387	0	2360	46	0
1	1-O	2387	0	2360	37	0
1	1-P	2387	0	2360	38	0
1	2-A	2427	0	2393	50	0
1	2-B	2431	0	2397	45	0
1	2-C	2427	0	2393	49	0
1	2-D	2431	0	2397	48	0
1	2-E	2431	0	2397	43	0
1	2-F	2431	0	2397	53	0
1	2-G	2431	0	2397	35	0
1	2-H	2431	0	2397	47	0
1	2-I	2387	0	2360	45	0
1	2-J	2387	0	2360	46	0
1	2-K	2387	0	2360	51	0
1	2-L	2387	0	2360	46	0
1	2-M	2387	0	2360	46	0
1	2-N	2387	0	2360	49	0
1	2-O	2387	0	2360	45	0
1	2-P	2387	0	2360	45	0
1	3-A	2427	0	2393	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3-B	2431	0	2397	45	0
1	3-C	2427	0	2393	49	0
1	3-D	2431	0	2397	48	0
1	3-E	2431	0	2397	43	0
1	3-F	2431	0	2397	53	0
1	3-G	2431	0	2397	35	0
1	3-H	2431	0	2397	61	0
1	3-I	2387	0	2360	46	0
1	3-J	2387	0	2360	45	0
1	3-K	2387	0	2360	49	0
1	3-L	2387	0	2360	45	0
1	3-M	2387	0	2360	44	0
1	3-N	2387	0	2360	62	0
1	3-O	2387	0	2360	46	0
1	3-P	2387	0	2360	45	0
1	4-A	2427	0	2393	50	0
1	4-B	2431	0	2397	45	0
1	4-C	2427	0	2393	49	0
1	4-D	2431	0	2397	48	0
1	4-E	2431	0	2397	43	0
1	4-F	2431	0	2397	53	0
1	4-G	2431	0	2397	35	0
1	4-H	2431	0	2397	47	0
1	4-I	2387	0	2360	45	0
1	4-J	2387	0	2360	44	0
1	4-K	2387	0	2360	52	0
1	4-L	2387	0	2360	46	0
1	4-M	2387	0	2360	44	0
1	4-N	2387	0	2360	46	0
1	4-O	2387	0	2360	45	0
1	4-P	2387	0	2360	45	0
2	1-A	20	0	10	0	0
2	1-B	20	0	10	0	0
2	1-C	20	0	10	0	0
2	1-D	20	0	10	0	0
2	1-E	20	0	10	0	0
2	1-F	20	0	10	0	0
2	1-G	20	0	10	0	0
2	1-H	20	0	10	0	0
2	1-I	20	0	10	1	0
2	1-J	20	0	10	1	0
2	1-K	20	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1-L	20	0	10	1	0
2	1-M	20	0	10	1	0
2	1-N	20	0	10	1	0
2	1-O	20	0	10	1	0
2	1-P	20	0	10	1	0
2	2-A	20	0	10	0	0
2	2-B	20	0	10	0	0
2	2-C	20	0	10	0	0
2	2-D	20	0	10	0	0
2	2-E	20	0	10	0	0
2	2-F	20	0	10	0	0
2	2-G	20	0	10	0	0
2	2-H	20	0	10	0	0
2	2-I	20	0	10	1	0
2	2-J	20	0	10	1	0
2	2-K	20	0	10	1	0
2	2-L	20	0	10	1	0
2	2-M	20	0	10	1	0
2	2-N	20	0	10	1	0
2	2-O	20	0	10	1	0
2	2-P	20	0	10	1	0
2	3-A	20	0	10	0	0
2	3-B	20	0	10	0	0
2	3-C	20	0	10	0	0
2	3-D	20	0	10	0	0
2	3-E	20	0	10	0	0
2	3-F	20	0	10	0	0
2	3-G	20	0	10	0	0
2	3-H	20	0	10	0	0
2	3-I	20	0	10	1	0
2	3-J	20	0	10	1	0
2	3-K	20	0	10	1	0
2	3-L	20	0	10	1	0
2	3-M	20	0	10	1	0
2	3-N	20	0	10	1	0
2	3-O	20	0	10	1	0
2	3-P	20	0	10	1	0
2	4-A	20	0	10	0	0
2	4-B	20	0	10	0	0
2	4-C	20	0	10	0	0
2	4-D	20	0	10	0	0
2	4-E	20	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	4-F	20	0	10	0	0
2	4-G	20	0	10	0	0
2	4-H	20	0	10	0	0
2	4-I	20	0	10	1	0
2	4-J	20	0	10	1	0
2	4-K	20	0	10	1	0
2	4-L	20	0	10	1	0
2	4-M	20	0	10	1	0
2	4-N	20	0	10	1	0
2	4-O	20	0	10	1	0
2	4-P	20	0	10	1	0
3	1-A	35	0	21	1	0
3	1-B	35	0	21	1	0
3	1-C	35	0	21	1	0
3	1-D	35	0	21	1	0
3	1-E	35	0	21	0	0
3	1-F	35	0	21	1	0
3	1-G	35	0	21	0	0
3	1-H	35	0	21	1	0
3	2-A	35	0	21	1	0
3	2-B	35	0	21	1	0
3	2-C	35	0	21	1	0
3	2-D	35	0	21	1	0
3	2-E	35	0	21	0	0
3	2-F	35	0	21	1	0
3	2-G	35	0	21	0	0
3	2-H	35	0	21	1	0
3	3-A	35	0	21	1	0
3	3-B	35	0	21	1	0
3	3-C	35	0	21	1	0
3	3-D	35	0	21	1	0
3	3-E	35	0	21	0	0
3	3-F	35	0	21	1	0
3	3-G	35	0	21	0	0
3	3-H	35	0	21	1	0
3	4-A	35	0	21	1	0
3	4-B	35	0	21	1	0
3	4-C	35	0	21	1	0
3	4-D	35	0	21	1	0
3	4-E	35	0	21	0	0
3	4-F	35	0	21	1	0
3	4-G	35	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	4-H	35	0	21	1	0
4	1-A	185	0	0	4	0
4	1-B	143	0	0	7	0
4	1-C	151	0	0	4	0
4	1-D	148	0	0	5	0
4	1-E	155	0	0	6	0
4	1-F	138	0	0	6	0
4	1-G	153	0	0	3	0
4	1-H	139	0	0	2	0
4	2-A	185	0	0	4	0
4	2-B	143	0	0	7	0
4	2-C	151	0	0	4	0
4	2-D	148	0	0	5	0
4	2-E	155	0	0	6	0
4	2-F	138	0	0	6	0
4	2-G	153	0	0	3	0
4	2-H	139	0	0	2	0
4	3-A	185	0	0	4	0
4	3-B	143	0	0	7	0
4	3-C	151	0	0	4	0
4	3-D	148	0	0	5	0
4	3-E	155	0	0	6	0
4	3-F	138	0	0	6	0
4	3-G	153	0	0	3	0
4	3-H	139	0	0	2	0
4	4-A	185	0	0	4	0
4	4-B	143	0	0	7	0
4	4-C	151	0	0	4	0
4	4-D	148	0	0	5	0
4	4-E	155	0	0	6	0
4	4-F	138	0	0	6	0
4	4-G	153	0	0	3	0
4	4-H	139	0	0	2	0
All	All	161392	0	153504	2427	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 8.

The worst 5 of 2427 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:H:201[C]:ASP:HB3	1:N:273[C]:GLU:CG	1.82	1.08
1:H:287[A]:GLU:HG2	1:J:146[A]:LYS:HZ3	1.25	0.99
1:H:287[A]:GLU:HG2	1:J:146[A]:LYS:NZ	1.78	0.98
1:H:201[C]:ASP:HB3	1:N:273[C]:GLU:HG2	1.45	0.93
1:H:202[C]:SER:HB3	1:N:275[C]:ARG:HG3	1.54	0.89

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	1-A	303/317 (96%)	293 (97%)	7 (2%)	3 (1%)	19	12
1	1-B	303/317 (96%)	293 (97%)	9 (3%)	1 (0%)	46	44
1	1-C	303/317 (96%)	293 (97%)	8 (3%)	2 (1%)	26	20
1	1-D	303/317 (96%)	293 (97%)	8 (3%)	2 (1%)	26	20
1	1-E	303/317 (96%)	292 (96%)	8 (3%)	3 (1%)	19	12
1	1-F	303/317 (96%)	292 (96%)	9 (3%)	2 (1%)	26	20
1	1-G	303/317 (96%)	294 (97%)	8 (3%)	1 (0%)	46	44
1	1-H	303/317 (96%)	291 (96%)	9 (3%)	3 (1%)	19	12
1	1-I	295/317 (93%)	287 (97%)	7 (2%)	1 (0%)	46	44
1	1-J	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	46	44
1	1-K	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	46	44
1	1-L	295/317 (93%)	285 (97%)	9 (3%)	1 (0%)	46	44
1	1-M	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	46	44
1	1-N	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	46	44
1	1-O	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	46	44
1	1-P	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	46	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2-A	303/317 (96%)	293 (97%)	7 (2%)	3 (1%)	19	12
1	2-B	303/317 (96%)	293 (97%)	9 (3%)	1 (0%)	46	44
1	2-C	303/317 (96%)	293 (97%)	8 (3%)	2 (1%)	26	20
1	2-D	303/317 (96%)	293 (97%)	8 (3%)	2 (1%)	26	20
1	2-E	303/317 (96%)	292 (96%)	8 (3%)	3 (1%)	19	12
1	2-F	303/317 (96%)	292 (96%)	9 (3%)	2 (1%)	26	20
1	2-G	303/317 (96%)	294 (97%)	8 (3%)	1 (0%)	46	44
1	2-H	303/317 (96%)	291 (96%)	9 (3%)	3 (1%)	19	12
1	2-I	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	46	44
1	2-J	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	46	44
1	2-K	295/317 (93%)	287 (97%)	7 (2%)	1 (0%)	46	44
1	2-L	295/317 (93%)	285 (97%)	9 (3%)	1 (0%)	46	44
1	2-M	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	46	44
1	2-N	295/317 (93%)	284 (96%)	10 (3%)	1 (0%)	46	44
1	2-O	295/317 (93%)	285 (97%)	9 (3%)	1 (0%)	46	44
1	2-P	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	46	44
1	3-A	303/317 (96%)	293 (97%)	7 (2%)	3 (1%)	19	12
1	3-B	303/317 (96%)	293 (97%)	9 (3%)	1 (0%)	46	44
1	3-C	303/317 (96%)	293 (97%)	8 (3%)	2 (1%)	26	20
1	3-D	303/317 (96%)	293 (97%)	8 (3%)	2 (1%)	26	20
1	3-E	303/317 (96%)	292 (96%)	8 (3%)	3 (1%)	19	12
1	3-F	303/317 (96%)	292 (96%)	9 (3%)	2 (1%)	26	20
1	3-G	303/317 (96%)	294 (97%)	8 (3%)	1 (0%)	46	44
1	3-H	303/317 (96%)	291 (96%)	9 (3%)	3 (1%)	19	12
1	3-I	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	46	44
1	3-J	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	46	44
1	3-K	295/317 (93%)	287 (97%)	7 (2%)	1 (0%)	46	44
1	3-L	295/317 (93%)	285 (97%)	9 (3%)	1 (0%)	46	44
1	3-M	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	46	44
1	3-N	295/317 (93%)	283 (96%)	11 (4%)	1 (0%)	46	44
1	3-O	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	46	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3-P	295/317 (93%)	285 (97%)	9 (3%)	1 (0%)	46	44
1	4-A	303/317 (96%)	293 (97%)	7 (2%)	3 (1%)	19	12
1	4-B	303/317 (96%)	293 (97%)	9 (3%)	1 (0%)	46	44
1	4-C	303/317 (96%)	293 (97%)	8 (3%)	2 (1%)	26	20
1	4-D	303/317 (96%)	293 (97%)	8 (3%)	2 (1%)	26	20
1	4-E	303/317 (96%)	292 (96%)	8 (3%)	3 (1%)	19	12
1	4-F	303/317 (96%)	292 (96%)	9 (3%)	2 (1%)	26	20
1	4-G	303/317 (96%)	294 (97%)	8 (3%)	1 (0%)	46	44
1	4-H	303/317 (96%)	291 (96%)	9 (3%)	3 (1%)	19	12
1	4-I	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	46	44
1	4-J	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	46	44
1	4-K	295/317 (93%)	287 (97%)	7 (2%)	1 (0%)	46	44
1	4-L	295/317 (93%)	285 (97%)	9 (3%)	1 (0%)	46	44
1	4-M	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	46	44
1	4-N	295/317 (93%)	283 (96%)	11 (4%)	1 (0%)	46	44
1	4-O	295/317 (93%)	285 (97%)	9 (3%)	1 (0%)	46	44
1	4-P	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	46	44
All	All	19136/20288 (94%)	18505 (97%)	531 (3%)	100 (0%)	34	29

5 of 100 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	127[A]	TYR
1	1-B	127[A]	TYR
1	1-C	127[A]	TYR
1	1-C	202[A]	SER
1	1-D	127[A]	TYR

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	1-A	262/274 (96%)	260 (99%)	2 (1%)	86	90
1	1-B	263/274 (96%)	262 (100%)	1 (0%)	93	96
1	1-C	262/274 (96%)	261 (100%)	1 (0%)	93	96
1	1-D	263/274 (96%)	261 (99%)	2 (1%)	86	90
1	1-E	263/274 (96%)	261 (99%)	2 (1%)	86	90
1	1-F	263/274 (96%)	260 (99%)	3 (1%)	80	84
1	1-G	263/274 (96%)	260 (99%)	3 (1%)	80	84
1	1-H	263/274 (96%)	261 (99%)	2 (1%)	86	90
1	1-I	258/274 (94%)	257 (100%)	1 (0%)	93	96
1	1-J	258/274 (94%)	257 (100%)	1 (0%)	93	96
1	1-K	258/274 (94%)	257 (100%)	1 (0%)	93	96
1	1-L	258/274 (94%)	257 (100%)	1 (0%)	93	96
1	1-M	258/274 (94%)	257 (100%)	1 (0%)	93	96
1	1-N	258/274 (94%)	257 (100%)	1 (0%)	93	96
1	1-O	258/274 (94%)	257 (100%)	1 (0%)	93	96
1	1-P	258/274 (94%)	257 (100%)	1 (0%)	93	96
All	All	4166/4384 (95%)	4142 (99%)	24 (1%)	90	93

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-F	298[A]	GLU
1	1-G	298[A]	GLU
1	1-O	298[A]	GLU
1	1-G	107[A]	LYS
1	1-G	220[A]	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
1	1-H	96[A]	GLN
1	1-J	22[A]	GLN
1	1-O	252[A]	GLN
1	1-H	154[A]	GLN
1	1-I	32[A]	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

96 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	$\#\|Z\| > 2$
3	CB3	1-A	2351[A]	-	31,37,37	2.81	14 (45%)	35,51,51	2.37	9 (25%)
2	UMP	1-A	350[A]	1	16,21,21	3.35	4 (25%)	23,31,31	2.30	3 (13%)
3	CB3	1-B	2401[A]	-	31,37,37	2.50	15 (48%)	35,51,51	2.19	13 (37%)
2	UMP	1-B	400[A]	1	16,21,21	3.13	3 (18%)	23,31,31	3.11	5 (21%)
3	CB3	1-C	2451[A]	-	31,37,37	2.36	13 (41%)	35,51,51	2.09	8 (22%)
2	UMP	1-C	450[A]	1	16,21,21	3.22	4 (25%)	23,31,31	2.43	7 (30%)
3	CB3	1-D	2501[A]	-	31,37,37	2.43	14 (45%)	35,51,51	1.89	12 (34%)
2	UMP	1-D	500[A]	1	16,21,21	2.74	3 (18%)	23,31,31	2.85	3 (13%)
3	CB3	1-E	2551[A]	-	31,37,37	2.59	15 (48%)	35,51,51	2.17	10 (28%)
2	UMP	1-E	550[A]	1	16,21,21	2.91	2 (12%)	23,31,31	2.63	8 (34%)
3	CB3	1-F	2601[A]	-	31,37,37	2.61	14 (45%)	35,51,51	2.09	11 (31%)
2	UMP	1-F	600[A]	1	16,21,21	2.93	3 (18%)	23,31,31	2.62	6 (26%)
3	CB3	1-G	2651[A]	-	31,37,37	2.60	13 (41%)	35,51,51	2.31	12 (34%)
2	UMP	1-G	650[A]	1	16,21,21	2.98	2 (12%)	23,31,31	2.51	5 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	CB3	1-H	2701[A]	-	31,37,37	2.12	13 (41%)	35,51,51	2.43	12 (34%)
2	UMP	1-H	700[A]	1	16,21,21	3.85	7 (43%)	23,31,31	2.59	7 (30%)
2	UMP	1-I	350[A]	1	16,21,21	3.27	5 (31%)	23,31,31	3.26	5 (21%)
2	UMP	1-J	400[A]	1	16,21,21	3.25	5 (31%)	23,31,31	3.23	6 (26%)
2	UMP	1-K	450[A]	1	16,21,21	3.25	5 (31%)	23,31,31	3.22	5 (21%)
2	UMP	1-L	500[A]	1	16,21,21	3.29	5 (31%)	23,31,31	3.22	5 (21%)
2	UMP	1-M	550[A]	1	16,21,21	3.18	5 (31%)	23,31,31	3.19	5 (21%)
2	UMP	1-N	600[A]	1	16,21,21	3.27	5 (31%)	23,31,31	3.27	5 (21%)
2	UMP	1-O	650[A]	1	16,21,21	3.20	5 (31%)	23,31,31	3.13	5 (21%)
2	UMP	1-P	700[A]	1	16,21,21	3.30	5 (31%)	23,31,31	3.21	5 (21%)
3	CB3	2-A	2351[B]	-	31,37,37	2.81	14 (45%)	35,51,51	2.37	9 (25%)
2	UMP	2-A	350[B]	-	16,21,21	3.35	4 (25%)	23,31,31	2.30	3 (13%)
3	CB3	2-B	2401[B]	-	31,37,37	2.50	15 (48%)	35,51,51	2.19	13 (37%)
2	UMP	2-B	400[B]	-	16,21,21	3.13	3 (18%)	23,31,31	3.11	5 (21%)
3	CB3	2-C	2451[B]	-	31,37,37	2.36	13 (41%)	35,51,51	2.09	8 (22%)
2	UMP	2-C	450[B]	-	16,21,21	3.22	4 (25%)	23,31,31	2.43	7 (30%)
3	CB3	2-D	2501[B]	-	31,37,37	2.43	14 (45%)	35,51,51	1.89	12 (34%)
2	UMP	2-D	500[B]	-	16,21,21	2.74	3 (18%)	23,31,31	2.85	3 (13%)
3	CB3	2-E	2551[B]	-	31,37,37	2.59	15 (48%)	35,51,51	2.17	10 (28%)
2	UMP	2-E	550[B]	-	16,21,21	2.91	2 (12%)	23,31,31	2.63	8 (34%)
3	CB3	2-F	2601[B]	-	31,37,37	2.61	14 (45%)	35,51,51	2.09	11 (31%)
2	UMP	2-F	600[B]	-	16,21,21	2.93	3 (18%)	23,31,31	2.62	6 (26%)
3	CB3	2-G	2651[B]	-	31,37,37	2.60	13 (41%)	35,51,51	2.31	12 (34%)
2	UMP	2-G	650[B]	-	16,21,21	2.98	2 (12%)	23,31,31	2.51	5 (21%)
3	CB3	2-H	2701[B]	-	31,37,37	2.12	13 (41%)	35,51,51	2.43	12 (34%)
2	UMP	2-H	700[B]	-	16,21,21	3.85	7 (43%)	23,31,31	2.59	7 (30%)
2	UMP	2-I	350[B]	-	16,21,21	3.18	5 (31%)	23,31,31	3.25	5 (21%)
2	UMP	2-J	400[B]	-	16,21,21	3.25	5 (31%)	23,31,31	3.22	5 (21%)
2	UMP	2-K	450[B]	-	16,21,21	3.24	5 (31%)	23,31,31	3.24	5 (21%)
2	UMP	2-L	500[B]	-	16,21,21	3.28	5 (31%)	23,31,31	3.22	5 (21%)
2	UMP	2-M	550[B]	-	16,21,21	3.21	5 (31%)	23,31,31	3.19	5 (21%)
2	UMP	2-N	600[B]	-	16,21,21	3.27	5 (31%)	23,31,31	3.26	5 (21%)
2	UMP	2-O	650[B]	-	16,21,21	3.24	4 (25%)	23,31,31	3.08	5 (21%)
2	UMP	2-P	700[B]	-	16,21,21	3.24	5 (31%)	23,31,31	3.17	5 (21%)
3	CB3	3-A	2351[C]	-	31,37,37	2.81	14 (45%)	35,51,51	2.37	9 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	UMP	3-A	350[C]	-	16,21,21	3.35	4 (25%)	23,31,31	2.30	3 (13%)
3	CB3	3-B	2401[C]	-	31,37,37	2.50	15 (48%)	35,51,51	2.19	13 (37%)
2	UMP	3-B	400[C]	-	16,21,21	3.13	3 (18%)	23,31,31	3.11	5 (21%)
3	CB3	3-C	2451[C]	-	31,37,37	2.36	13 (41%)	35,51,51	2.09	8 (22%)
2	UMP	3-C	450[C]	-	16,21,21	3.22	4 (25%)	23,31,31	2.43	7 (30%)
3	CB3	3-D	2501[C]	-	31,37,37	2.43	14 (45%)	35,51,51	1.89	12 (34%)
2	UMP	3-D	500[C]	-	16,21,21	2.74	3 (18%)	23,31,31	2.85	3 (13%)
3	CB3	3-E	2551[C]	-	31,37,37	2.59	15 (48%)	35,51,51	2.17	10 (28%)
2	UMP	3-E	550[C]	-	16,21,21	2.91	2 (12%)	23,31,31	2.63	8 (34%)
3	CB3	3-F	2601[C]	-	31,37,37	2.61	14 (45%)	35,51,51	2.09	11 (31%)
2	UMP	3-F	600[C]	-	16,21,21	2.93	3 (18%)	23,31,31	2.62	6 (26%)
3	CB3	3-G	2651[C]	-	31,37,37	2.60	13 (41%)	35,51,51	2.31	12 (34%)
2	UMP	3-G	650[C]	-	16,21,21	2.98	2 (12%)	23,31,31	2.51	5 (21%)
3	CB3	3-H	2701[C]	-	31,37,37	2.12	13 (41%)	35,51,51	2.43	12 (34%)
2	UMP	3-H	700[C]	-	16,21,21	3.85	7 (43%)	23,31,31	2.59	7 (30%)
2	UMP	3-I	350[C]	-	16,21,21	3.24	5 (31%)	23,31,31	3.28	5 (21%)
2	UMP	3-J	400[C]	-	16,21,21	3.25	5 (31%)	23,31,31	3.25	5 (21%)
2	UMP	3-K	450[C]	-	16,21,21	3.29	5 (31%)	23,31,31	3.22	5 (21%)
2	UMP	3-L	500[C]	-	16,21,21	3.28	5 (31%)	23,31,31	3.20	5 (21%)
2	UMP	3-M	550[C]	-	16,21,21	3.21	5 (31%)	23,31,31	3.19	5 (21%)
2	UMP	3-N	600[C]	-	16,21,21	3.31	5 (31%)	23,31,31	3.26	5 (21%)
2	UMP	3-O	650[C]	-	16,21,21	3.22	5 (31%)	23,31,31	3.15	5 (21%)
2	UMP	3-P	700[C]	-	16,21,21	3.29	5 (31%)	23,31,31	3.21	5 (21%)
3	CB3	4-A	2351[D]	-	31,37,37	2.81	14 (45%)	35,51,51	2.37	9 (25%)
2	UMP	4-A	350[D]	-	16,21,21	3.35	4 (25%)	23,31,31	2.30	3 (13%)
3	CB3	4-B	2401[D]	-	31,37,37	2.50	15 (48%)	35,51,51	2.19	13 (37%)
2	UMP	4-B	400[D]	-	16,21,21	3.13	3 (18%)	23,31,31	3.11	5 (21%)
3	CB3	4-C	2451[D]	-	31,37,37	2.36	13 (41%)	35,51,51	2.09	8 (22%)
2	UMP	4-C	450[D]	-	16,21,21	3.22	4 (25%)	23,31,31	2.43	7 (30%)
3	CB3	4-D	2501[D]	-	31,37,37	2.43	14 (45%)	35,51,51	1.89	12 (34%)
2	UMP	4-D	500[D]	-	16,21,21	2.74	3 (18%)	23,31,31	2.85	3 (13%)
3	CB3	4-E	2551[D]	-	31,37,37	2.59	15 (48%)	35,51,51	2.17	10 (28%)
2	UMP	4-E	550[D]	-	16,21,21	2.91	2 (12%)	23,31,31	2.63	8 (34%)
3	CB3	4-F	2601[D]	-	31,37,37	2.61	14 (45%)	35,51,51	2.09	11 (31%)
2	UMP	4-F	600[D]	-	16,21,21	2.93	3 (18%)	23,31,31	2.62	6 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	CB3	4-G	2651[D]	-	31,37,37	2.60	13 (41%)	35,51,51	2.31	12 (34%)
2	UMP	4-G	650[D]	-	16,21,21	2.98	2 (12%)	23,31,31	2.51	5 (21%)
3	CB3	4-H	2701[D]	-	31,37,37	2.12	13 (41%)	35,51,51	2.43	12 (34%)
2	UMP	4-H	700[D]	-	16,21,21	3.85	7 (43%)	23,31,31	2.59	7 (30%)
2	UMP	4-I	350[D]	-	16,21,21	3.22	5 (31%)	23,31,31	3.26	5 (21%)
2	UMP	4-J	400[D]	-	16,21,21	3.26	5 (31%)	23,31,31	3.22	5 (21%)
2	UMP	4-K	450[D]	-	16,21,21	3.26	5 (31%)	23,31,31	3.26	5 (21%)
2	UMP	4-L	500[D]	-	16,21,21	3.29	5 (31%)	23,31,31	3.21	5 (21%)
2	UMP	4-M	550[D]	-	16,21,21	3.16	5 (31%)	23,31,31	3.20	5 (21%)
2	UMP	4-N	600[D]	-	16,21,21	3.30	5 (31%)	23,31,31	3.26	5 (21%)
2	UMP	4-O	650[D]	-	16,21,21	3.26	5 (31%)	23,31,31	3.02	5 (21%)
2	UMP	4-P	700[D]	-	16,21,21	3.28	5 (31%)	23,31,31	3.17	5 (21%)

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
3	CB3	1-A	2351[A]	-	-	0/21/28/28	0/3/3/3
2	UMP	1-A	350[A]	1	-	0/6/22/22	0/2/2/2
3	CB3	1-B	2401[A]	-	-	0/21/28/28	0/3/3/3
2	UMP	1-B	400[A]	1	-	0/6/22/22	0/2/2/2
3	CB3	1-C	2451[A]	-	-	0/21/28/28	0/3/3/3
2	UMP	1-C	450[A]	1	-	0/6/22/22	0/2/2/2
3	CB3	1-D	2501[A]	-	-	0/21/28/28	0/3/3/3
2	UMP	1-D	500[A]	1	-	0/6/22/22	0/2/2/2
3	CB3	1-E	2551[A]	-	-	0/21/28/28	0/3/3/3
2	UMP	1-E	550[A]	1	-	0/6/22/22	0/2/2/2
3	CB3	1-F	2601[A]	-	-	0/21/28/28	0/3/3/3
2	UMP	1-F	600[A]	1	-	0/6/22/22	0/2/2/2
3	CB3	1-G	2651[A]	-	-	0/21/28/28	0/3/3/3
2	UMP	1-G	650[A]	1	-	0/6/22/22	0/2/2/2
3	CB3	1-H	2701[A]	-	-	0/21/28/28	0/3/3/3
2	UMP	1-H	700[A]	1	-	0/6/22/22	0/2/2/2
2	UMP	1-I	350[A]	1	-	0/6/22/22	0/2/2/2
2	UMP	1-J	400[A]	1	-	0/6/22/22	0/2/2/2
2	UMP	1-K	450[A]	1	-	0/6/22/22	0/2/2/2
2	UMP	1-L	500[A]	1	-	0/6/22/22	0/2/2/2
2	UMP	1-M	550[A]	1	-	0/6/22/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UMP	1-N	600[A]	1	-	0/6/22/22	0/2/2/2
2	UMP	1-O	650[A]	1	-	0/6/22/22	0/2/2/2
2	UMP	1-P	700[A]	1	-	0/6/22/22	0/2/2/2
3	CB3	2-A	2351[B]	-	-	0/21/28/28	0/3/3/3
2	UMP	2-A	350[B]	-	-	0/6/22/22	0/2/2/2
3	CB3	2-B	2401[B]	-	-	0/21/28/28	0/3/3/3
2	UMP	2-B	400[B]	-	-	0/6/22/22	0/2/2/2
3	CB3	2-C	2451[B]	-	-	0/21/28/28	0/3/3/3
2	UMP	2-C	450[B]	-	-	0/6/22/22	0/2/2/2
3	CB3	2-D	2501[B]	-	-	0/21/28/28	0/3/3/3
2	UMP	2-D	500[B]	-	-	0/6/22/22	0/2/2/2
3	CB3	2-E	2551[B]	-	-	0/21/28/28	0/3/3/3
2	UMP	2-E	550[B]	-	-	0/6/22/22	0/2/2/2
3	CB3	2-F	2601[B]	-	-	0/21/28/28	0/3/3/3
2	UMP	2-F	600[B]	-	-	0/6/22/22	0/2/2/2
3	CB3	2-G	2651[B]	-	-	0/21/28/28	0/3/3/3
2	UMP	2-G	650[B]	-	-	0/6/22/22	0/2/2/2
3	CB3	2-H	2701[B]	-	-	0/21/28/28	0/3/3/3
2	UMP	2-H	700[B]	-	-	0/6/22/22	0/2/2/2
2	UMP	2-I	350[B]	-	-	0/6/22/22	0/2/2/2
2	UMP	2-J	400[B]	-	-	0/6/22/22	0/2/2/2
2	UMP	2-K	450[B]	-	-	0/6/22/22	0/2/2/2
2	UMP	2-L	500[B]	-	-	0/6/22/22	0/2/2/2
2	UMP	2-M	550[B]	-	-	0/6/22/22	0/2/2/2
2	UMP	2-N	600[B]	-	-	0/6/22/22	0/2/2/2
2	UMP	2-O	650[B]	-	-	0/6/22/22	0/2/2/2
2	UMP	2-P	700[B]	-	-	0/6/22/22	0/2/2/2
3	CB3	3-A	2351[C]	-	-	0/21/28/28	0/3/3/3
2	UMP	3-A	350[C]	-	-	0/6/22/22	0/2/2/2
3	CB3	3-B	2401[C]	-	-	0/21/28/28	0/3/3/3
2	UMP	3-B	400[C]	-	-	0/6/22/22	0/2/2/2
3	CB3	3-C	2451[C]	-	-	0/21/28/28	0/3/3/3
2	UMP	3-C	450[C]	-	-	0/6/22/22	0/2/2/2
3	CB3	3-D	2501[C]	-	-	0/21/28/28	0/3/3/3
2	UMP	3-D	500[C]	-	-	0/6/22/22	0/2/2/2
3	CB3	3-E	2551[C]	-	-	0/21/28/28	0/3/3/3
2	UMP	3-E	550[C]	-	-	0/6/22/22	0/2/2/2
3	CB3	3-F	2601[C]	-	-	0/21/28/28	0/3/3/3
2	UMP	3-F	600[C]	-	-	0/6/22/22	0/2/2/2
3	CB3	3-G	2651[C]	-	-	0/21/28/28	0/3/3/3
2	UMP	3-G	650[C]	-	-	0/6/22/22	0/2/2/2
3	CB3	3-H	2701[C]	-	-	0/21/28/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UMP	3-H	700[C]	-	-	0/6/22/22	0/2/2/2
2	UMP	3-I	350[C]	-	-	0/6/22/22	0/2/2/2
2	UMP	3-J	400[C]	-	-	0/6/22/22	0/2/2/2
2	UMP	3-K	450[C]	-	-	0/6/22/22	0/2/2/2
2	UMP	3-L	500[C]	-	-	0/6/22/22	0/2/2/2
2	UMP	3-M	550[C]	-	-	0/6/22/22	0/2/2/2
2	UMP	3-N	600[C]	-	-	0/6/22/22	0/2/2/2
2	UMP	3-O	650[C]	-	-	0/6/22/22	0/2/2/2
2	UMP	3-P	700[C]	-	-	0/6/22/22	0/2/2/2
3	CB3	4-A	2351[D]	-	-	0/21/28/28	0/3/3/3
2	UMP	4-A	350[D]	-	-	0/6/22/22	0/2/2/2
3	CB3	4-B	2401[D]	-	-	0/21/28/28	0/3/3/3
2	UMP	4-B	400[D]	-	-	0/6/22/22	0/2/2/2
3	CB3	4-C	2451[D]	-	-	0/21/28/28	0/3/3/3
2	UMP	4-C	450[D]	-	-	0/6/22/22	0/2/2/2
3	CB3	4-D	2501[D]	-	-	0/21/28/28	0/3/3/3
2	UMP	4-D	500[D]	-	-	0/6/22/22	0/2/2/2
3	CB3	4-E	2551[D]	-	-	0/21/28/28	0/3/3/3
2	UMP	4-E	550[D]	-	-	0/6/22/22	0/2/2/2
3	CB3	4-F	2601[D]	-	-	0/21/28/28	0/3/3/3
2	UMP	4-F	600[D]	-	-	0/6/22/22	0/2/2/2
3	CB3	4-G	2651[D]	-	-	0/21/28/28	0/3/3/3
2	UMP	4-G	650[D]	-	-	0/6/22/22	0/2/2/2
3	CB3	4-H	2701[D]	-	-	0/21/28/28	0/3/3/3
2	UMP	4-H	700[D]	-	-	0/6/22/22	0/2/2/2
2	UMP	4-I	350[D]	-	-	0/6/22/22	0/2/2/2
2	UMP	4-J	400[D]	-	-	0/6/22/22	0/2/2/2
2	UMP	4-K	450[D]	-	-	0/6/22/22	0/2/2/2
2	UMP	4-L	500[D]	-	-	0/6/22/22	0/2/2/2
2	UMP	4-M	550[D]	-	-	0/6/22/22	0/2/2/2
2	UMP	4-N	600[D]	-	-	0/6/22/22	0/2/2/2
2	UMP	4-O	650[D]	-	-	0/6/22/22	0/2/2/2
2	UMP	4-P	700[D]	-	-	0/6/22/22	0/2/2/2

The worst 5 of 715 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3-H	700[C]	UMP	P-OP2	-4.92	1.37	1.54
2	4-H	700[D]	UMP	P-OP2	-4.92	1.37	1.54
2	1-H	700[A]	UMP	P-OP2	-4.92	1.37	1.54
2	2-H	700[B]	UMP	P-OP2	-4.92	1.37	1.54
2	3-H	700[C]	UMP	P-OP3	-4.69	1.37	1.54

The worst 5 of 685 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	4-H	2701[D]	CB3	N1-C2-N3	-8.01	115.25	127.44
3	3-H	2701[C]	CB3	N1-C2-N3	-8.01	115.25	127.44
3	2-H	2701[B]	CB3	N1-C2-N3	-8.01	115.25	127.44
3	1-H	2701[A]	CB3	N1-C2-N3	-8.01	115.25	127.44
3	3-G	2651[C]	CB3	CP1-CP2-CP3	-7.86	167.56	177.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

56 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	1-A	2351[A]	CB3	1	0
3	1-B	2401[A]	CB3	1	0
3	1-C	2451[A]	CB3	1	0
3	1-D	2501[A]	CB3	1	0
3	1-F	2601[A]	CB3	1	0
3	1-H	2701[A]	CB3	1	0
2	1-I	350[A]	UMP	1	0
2	1-J	400[A]	UMP	1	0
2	1-K	450[A]	UMP	1	0
2	1-L	500[A]	UMP	1	0
2	1-M	550[A]	UMP	1	0
2	1-N	600[A]	UMP	1	0
2	1-O	650[A]	UMP	1	0
2	1-P	700[A]	UMP	1	0
3	2-A	2351[B]	CB3	1	0
3	2-B	2401[B]	CB3	1	0
3	2-C	2451[B]	CB3	1	0
3	2-D	2501[B]	CB3	1	0
3	2-F	2601[B]	CB3	1	0
3	2-H	2701[B]	CB3	1	0
2	2-I	350[B]	UMP	1	0
2	2-J	400[B]	UMP	1	0
2	2-K	450[B]	UMP	1	0
2	2-L	500[B]	UMP	1	0
2	2-M	550[B]	UMP	1	0
2	2-N	600[B]	UMP	1	0
2	2-O	650[B]	UMP	1	0
2	2-P	700[B]	UMP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	3-A	2351[C]	CB3	1	0
3	3-B	2401[C]	CB3	1	0
3	3-C	2451[C]	CB3	1	0
3	3-D	2501[C]	CB3	1	0
3	3-F	2601[C]	CB3	1	0
3	3-H	2701[C]	CB3	1	0
2	3-I	350[C]	UMP	1	0
2	3-J	400[C]	UMP	1	0
2	3-K	450[C]	UMP	1	0
2	3-L	500[C]	UMP	1	0
2	3-M	550[C]	UMP	1	0
2	3-N	600[C]	UMP	1	0
2	3-O	650[C]	UMP	1	0
2	3-P	700[C]	UMP	1	0
3	4-A	2351[D]	CB3	1	0
3	4-B	2401[D]	CB3	1	0
3	4-C	2451[D]	CB3	1	0
3	4-D	2501[D]	CB3	1	0
3	4-F	2601[D]	CB3	1	0
3	4-H	2701[D]	CB3	1	0
2	4-I	350[D]	UMP	1	0
2	4-J	400[D]	UMP	1	0
2	4-K	450[D]	UMP	1	0
2	4-L	500[D]	UMP	1	0
2	4-M	550[D]	UMP	1	0
2	4-N	600[D]	UMP	1	0
2	4-O	650[D]	UMP	1	0
2	4-P	700[D]	UMP	1	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	1-A	305/317 (96%)	0.33	13 (4%) 39 47	18, 26, 41, 61	305 (100%)
1	1-B	305/317 (96%)	0.29	12 (3%) 43 51	18, 27, 42, 63	305 (100%)
1	1-C	305/317 (96%)	0.30	12 (3%) 43 51	17, 26, 41, 61	305 (100%)
1	1-D	305/317 (96%)	0.28	9 (2%) 54 61	18, 27, 42, 63	305 (100%)
1	1-E	305/317 (96%)	0.31	13 (4%) 39 47	17, 26, 43, 63	305 (100%)
1	1-F	305/317 (96%)	0.31	15 (4%) 33 41	18, 27, 42, 64	305 (100%)
1	1-G	305/317 (96%)	0.33	10 (3%) 50 58	18, 26, 41, 62	305 (100%)
1	1-H	305/317 (96%)	0.35	11 (3%) 46 55	17, 27, 41, 64	305 (100%)
1	1-I	299/317 (94%)	6.97	295 (98%) 0 0	18, 26, 38, 56	299 (100%)
1	1-J	299/317 (94%)	7.28	295 (98%) 0 0	18, 26, 37, 56	299 (100%)
1	1-K	299/317 (94%)	6.54	293 (97%) 0 0	17, 26, 37, 56	299 (100%)
1	1-L	299/317 (94%)	6.78	295 (98%) 0 0	17, 26, 37, 56	299 (100%)
1	1-M	299/317 (94%)	6.89	298 (99%) 0 0	17, 26, 37, 56	299 (100%)
1	1-N	299/317 (94%)	7.14	298 (99%) 0 0	18, 26, 37, 56	299 (100%)
1	1-O	299/317 (94%)	7.05	295 (98%) 0 0	17, 26, 37, 56	299 (100%)
1	1-P	299/317 (94%)	6.74	293 (97%) 0 0	18, 26, 37, 56	299 (100%)
1	2-A	305/317 (96%)	0.33	13 (4%) 39 47	18, 26, 41, 61	305 (100%)
1	2-B	305/317 (96%)	0.29	12 (3%) 43 51	18, 27, 42, 63	305 (100%)
1	2-C	305/317 (96%)	0.30	12 (3%) 43 51	17, 26, 41, 61	305 (100%)
1	2-D	305/317 (96%)	0.28	9 (2%) 54 61	18, 27, 42, 63	305 (100%)
1	2-E	305/317 (96%)	0.31	13 (4%) 39 47	17, 26, 43, 63	305 (100%)
1	2-F	305/317 (96%)	0.31	15 (4%) 33 41	18, 27, 42, 64	305 (100%)
1	2-G	305/317 (96%)	0.33	10 (3%) 50 58	18, 26, 41, 62	305 (100%)
1	2-H	305/317 (96%)	0.35	11 (3%) 46 55	17, 27, 41, 64	305 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	2-I	299/317 (94%)	6.97	295 (98%)	0	0	18, 26, 38, 56	299 (100%)
1	2-J	299/317 (94%)	7.28	295 (98%)	0	0	18, 26, 37, 56	299 (100%)
1	2-K	299/317 (94%)	6.54	293 (97%)	0	0	17, 26, 37, 56	299 (100%)
1	2-L	299/317 (94%)	6.78	295 (98%)	0	0	17, 26, 37, 56	299 (100%)
1	2-M	299/317 (94%)	6.89	298 (99%)	0	0	17, 26, 37, 56	299 (100%)
1	2-N	299/317 (94%)	7.14	298 (99%)	0	0	18, 26, 37, 56	299 (100%)
1	2-O	299/317 (94%)	7.05	295 (98%)	0	0	17, 26, 37, 56	299 (100%)
1	2-P	299/317 (94%)	6.74	293 (97%)	0	0	18, 26, 37, 56	299 (100%)
1	3-A	305/317 (96%)	0.33	13 (4%)	39	47	18, 26, 41, 61	305 (100%)
1	3-B	305/317 (96%)	0.29	12 (3%)	43	51	18, 27, 42, 63	305 (100%)
1	3-C	305/317 (96%)	0.30	12 (3%)	43	51	17, 26, 41, 61	305 (100%)
1	3-D	305/317 (96%)	0.28	9 (2%)	54	61	18, 27, 42, 63	305 (100%)
1	3-E	305/317 (96%)	0.31	13 (4%)	39	47	17, 26, 43, 63	305 (100%)
1	3-F	305/317 (96%)	0.31	15 (4%)	33	41	18, 27, 42, 64	305 (100%)
1	3-G	305/317 (96%)	0.33	10 (3%)	50	58	18, 26, 41, 62	305 (100%)
1	3-H	305/317 (96%)	0.35	11 (3%)	46	55	17, 27, 41, 64	305 (100%)
1	3-I	299/317 (94%)	6.97	295 (98%)	0	0	18, 26, 38, 56	299 (100%)
1	3-J	299/317 (94%)	7.28	295 (98%)	0	0	18, 26, 37, 56	299 (100%)
1	3-K	299/317 (94%)	6.54	293 (97%)	0	0	17, 26, 37, 56	299 (100%)
1	3-L	299/317 (94%)	6.78	295 (98%)	0	0	17, 26, 37, 56	299 (100%)
1	3-M	299/317 (94%)	6.89	298 (99%)	0	0	17, 26, 37, 56	299 (100%)
1	3-N	299/317 (94%)	7.14	298 (99%)	0	0	18, 26, 37, 56	299 (100%)
1	3-O	299/317 (94%)	7.05	295 (98%)	0	0	17, 26, 37, 56	299 (100%)
1	3-P	299/317 (94%)	6.74	293 (97%)	0	0	18, 26, 37, 56	299 (100%)
1	4-A	305/317 (96%)	0.33	13 (4%)	39	47	18, 26, 41, 61	305 (100%)
1	4-B	305/317 (96%)	0.29	12 (3%)	43	51	18, 27, 42, 63	305 (100%)
1	4-C	305/317 (96%)	0.30	12 (3%)	43	51	17, 26, 41, 61	305 (100%)
1	4-D	305/317 (96%)	0.28	9 (2%)	54	61	18, 27, 42, 63	305 (100%)
1	4-E	305/317 (96%)	0.31	13 (4%)	39	47	17, 26, 43, 63	305 (100%)
1	4-F	305/317 (96%)	0.31	15 (4%)	33	41	18, 27, 42, 64	305 (100%)
1	4-G	305/317 (96%)	0.33	10 (3%)	50	58	18, 26, 41, 62	305 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	4-H	305/317 (96%)	0.35	11 (3%) 46 55	17, 27, 41, 64	305 (100%)
1	4-I	299/317 (94%)	6.97	295 (98%) 0 0	18, 26, 38, 56	299 (100%)
1	4-J	299/317 (94%)	7.28	295 (98%) 0 0	18, 26, 37, 56	299 (100%)
1	4-K	299/317 (94%)	6.54	293 (97%) 0 0	17, 26, 37, 56	299 (100%)
1	4-L	299/317 (94%)	6.78	295 (98%) 0 0	17, 26, 37, 56	299 (100%)
1	4-M	299/317 (94%)	6.89	298 (99%) 0 0	17, 26, 37, 56	299 (100%)
1	4-N	299/317 (94%)	7.14	298 (99%) 0 0	18, 26, 37, 56	299 (100%)
1	4-O	299/317 (94%)	7.05	295 (98%) 0 0	17, 26, 37, 56	299 (100%)
1	4-P	299/317 (94%)	6.74	293 (97%) 0 0	18, 26, 37, 56	299 (100%)
All	All	19328/20288 (95%)	3.59	9828 (50%) 0 0	17, 26, 40, 64	19328 (100%)

The worst 5 of 9828 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-P	211[A]	CYS	25.3
1	2-P	211[B]	CYS	25.3
1	3-P	211[C]	CYS	25.3
1	4-P	211[D]	CYS	25.3
1	1-K	153[A]	LEU	22.5

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, 95th 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
2	UMP	4-J	400[D]	20/20	0.47	0.59	0.80	49,61,70,70	20
2	UMP	1-J	400[A]	20/20	0.47	0.59	0.80	48,61,70,71	20
2	UMP	3-J	400[C]	20/20	0.47	0.59	0.80	49,60,70,70	20
2	UMP	2-J	400[B]	20/20	0.47	0.59	0.80	49,61,71,71	20
2	UMP	3-A	350[C]	20/20	0.96	0.15	0.74	18,23,27,29	20
2	UMP	4-A	350[D]	20/20	0.96	0.15	0.74	18,23,27,29	20
2	UMP	2-A	350[B]	20/20	0.96	0.15	0.74	18,23,27,29	20
2	UMP	1-A	350[A]	20/20	0.96	0.15	0.74	18,23,27,29	20
2	UMP	3-I	350[C]	20/20	0.56	0.55	0.68	50,62,74,74	20
2	UMP	2-I	350[B]	20/20	0.56	0.55	0.68	50,62,74,74	20
2	UMP	1-I	350[A]	20/20	0.56	0.55	0.68	50,62,74,74	20
2	UMP	4-I	350[D]	20/20	0.56	0.55	0.68	50,62,74,74	20
3	CB3	3-F	2601[C]	35/35	0.94	0.14	0.61	16,23,32,39	35
3	CB3	2-F	2601[B]	35/35	0.94	0.14	0.61	16,23,32,39	35
3	CB3	1-F	2601[A]	35/35	0.94	0.14	0.61	16,23,32,39	35
3	CB3	4-F	2601[D]	35/35	0.94	0.14	0.61	16,23,32,39	35
2	UMP	2-C	450[B]	20/20	0.96	0.16	0.57	17,21,27,27	20
2	UMP	4-C	450[D]	20/20	0.96	0.16	0.57	17,21,27,27	20
2	UMP	1-C	450[A]	20/20	0.96	0.16	0.57	17,21,27,27	20
2	UMP	3-C	450[C]	20/20	0.96	0.16	0.57	17,21,27,27	20
3	CB3	2-B	2401[B]	35/35	0.94	0.13	0.50	18,22,38,40	35
3	CB3	4-B	2401[D]	35/35	0.94	0.13	0.50	18,22,38,40	35
3	CB3	3-B	2401[C]	35/35	0.94	0.13	0.50	18,22,38,40	35
3	CB3	1-B	2401[A]	35/35	0.94	0.13	0.50	18,22,38,40	35
2	UMP	3-N	600[C]	20/20	0.45	0.62	0.43	48,60,72,72	20
2	UMP	4-N	600[D]	20/20	0.45	0.62	0.43	48,60,72,72	20
2	UMP	2-N	600[B]	20/20	0.45	0.62	0.35	49,61,72,72	20
2	UMP	1-N	600[A]	20/20	0.45	0.62	0.32	48,61,72,72	20
3	CB3	1-D	2501[A]	35/35	0.94	0.13	0.28	14,23,41,44	35
3	CB3	4-D	2501[D]	35/35	0.94	0.13	0.28	14,23,41,44	35
3	CB3	3-D	2501[C]	35/35	0.94	0.13	0.28	14,23,41,44	35
3	CB3	2-D	2501[B]	35/35	0.94	0.13	0.28	14,23,41,44	35
2	UMP	2-G	650[B]	20/20	0.96	0.14	0.25	18,21,23,26	20
2	UMP	1-G	650[A]	20/20	0.96	0.14	0.25	18,21,23,26	20
2	UMP	3-G	650[C]	20/20	0.96	0.14	0.25	18,21,23,26	20
2	UMP	4-G	650[D]	20/20	0.96	0.14	0.25	18,21,23,26	20
2	UMP	1-H	700[A]	20/20	0.97	0.14	0.14	13,19,30,56	20
2	UMP	3-H	700[C]	20/20	0.97	0.14	0.14	13,19,30,56	20
2	UMP	4-H	700[D]	20/20	0.97	0.14	0.14	13,19,30,56	20
2	UMP	2-H	700[B]	20/20	0.97	0.14	0.14	13,19,30,56	20
2	UMP	1-P	700[A]	20/20	0.69	0.52	0.13	48,60,70,70	20
2	UMP	2-P	700[B]	20/20	0.69	0.52	0.13	48,60,70,70	20
2	UMP	4-P	700[D]	20/20	0.69	0.52	0.10	49,60,70,70	20

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	UMP	3-P	700[C]	20/20	0.69	0.52	0.07	49,60,70,70	20
2	UMP	4-K	450[D]	20/20	0.55	0.48	0.06	50,62,73,73	20
2	UMP	2-K	450[B]	20/20	0.55	0.48	0.06	49,62,73,73	20
2	UMP	1-K	450[A]	20/20	0.55	0.48	0.06	49,62,73,73	20
2	UMP	3-K	450[C]	20/20	0.55	0.48	0.06	49,62,73,73	20
2	UMP	1-D	500[A]	20/20	0.97	0.12	0.02	14,19,22,25	20
2	UMP	2-D	500[B]	20/20	0.97	0.12	0.02	14,19,22,25	20
2	UMP	4-D	500[D]	20/20	0.97	0.12	0.02	14,19,22,25	20
2	UMP	3-D	500[C]	20/20	0.97	0.12	0.02	14,19,22,25	20
3	CB3	1-E	2551[A]	35/35	0.92	0.14	-0.13	15,23,37,37	35
3	CB3	4-E	2551[D]	35/35	0.92	0.14	-0.13	15,23,37,37	35
3	CB3	2-E	2551[B]	35/35	0.92	0.14	-0.13	15,23,37,37	35
3	CB3	3-E	2551[C]	35/35	0.92	0.14	-0.13	15,23,37,37	35
3	CB3	1-H	2701[A]	35/35	0.94	0.13	-0.14	14,22,31,36	35
3	CB3	2-H	2701[B]	35/35	0.94	0.13	-0.14	14,22,31,36	35
3	CB3	3-H	2701[C]	35/35	0.94	0.13	-0.14	14,22,31,36	35
3	CB3	4-H	2701[D]	35/35	0.94	0.13	-0.14	14,22,31,36	35
2	UMP	1-E	550[A]	20/20	0.97	0.13	-0.19	20,22,24,24	20
2	UMP	2-E	550[B]	20/20	0.97	0.13	-0.19	20,22,24,24	20
2	UMP	4-E	550[D]	20/20	0.97	0.13	-0.19	20,22,24,24	20
2	UMP	3-E	550[C]	20/20	0.97	0.13	-0.19	20,22,24,24	20
3	CB3	1-C	2451[A]	35/35	0.94	0.13	-0.32	20,26,32,37	35
3	CB3	4-C	2451[D]	35/35	0.94	0.13	-0.32	20,26,32,37	35
3	CB3	2-C	2451[B]	35/35	0.94	0.13	-0.32	20,26,32,37	35
3	CB3	3-C	2451[C]	35/35	0.94	0.13	-0.32	20,26,32,37	35
2	UMP	4-O	650[D]	20/20	0.79	0.42	-0.46	17,18,19,20	20
2	UMP	3-O	650[C]	20/20	0.79	0.42	-0.46	17,19,20,22	20
2	UMP	2-O	650[B]	20/20	0.79	0.42	-0.46	17,19,19,19	20
2	UMP	1-O	650[A]	20/20	0.79	0.42	-0.46	17,18,19,19	20
3	CB3	2-G	2651[B]	35/35	0.95	0.13	-0.47	18,24,32,37	35
3	CB3	3-G	2651[C]	35/35	0.95	0.13	-0.47	18,24,32,37	35
3	CB3	4-G	2651[D]	35/35	0.95	0.13	-0.47	18,24,32,37	35
3	CB3	1-G	2651[A]	35/35	0.95	0.13	-0.47	18,24,32,37	35
2	UMP	1-B	400[A]	20/20	0.98	0.11	-0.51	13,17,22,22	20
2	UMP	2-B	400[B]	20/20	0.98	0.11	-0.51	13,17,22,22	20
2	UMP	4-B	400[D]	20/20	0.98	0.11	-0.51	13,17,22,22	20
2	UMP	3-B	400[C]	20/20	0.98	0.11	-0.51	13,17,22,22	20
2	UMP	2-F	600[B]	20/20	0.98	0.12	-0.74	15,18,22,22	20
2	UMP	4-F	600[D]	20/20	0.98	0.12	-0.74	15,18,22,22	20
2	UMP	1-F	600[A]	20/20	0.98	0.12	-0.74	15,18,22,22	20
2	UMP	3-F	600[C]	20/20	0.98	0.12	-0.74	15,18,22,22	20
3	CB3	4-A	2351[D]	35/35	0.96	0.11	-0.97	16,24,31,35	35

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CB3	3-A	2351[C]	35/35	0.96	0.11	-0.97	16,24,31,35	35
3	CB3	2-A	2351[B]	35/35	0.96	0.11	-0.97	16,24,31,35	35
3	CB3	1-A	2351[A]	35/35	0.96	0.11	-0.97	16,24,31,35	35
2	UMP	4-L	500[D]	20/20	0.69	0.37	-0.99	49,61,71,71	20
2	UMP	3-L	500[C]	20/20	0.69	0.37	-0.99	49,61,71,71	20
2	UMP	1-L	500[A]	20/20	0.69	0.37	-0.99	49,61,71,71	20
2	UMP	2-L	500[B]	20/20	0.69	0.37	-0.99	49,61,71,71	20
2	UMP	2-M	550[B]	20/20	0.58	0.41	-1.00	50,62,73,73	20
2	UMP	4-M	550[D]	20/20	0.58	0.41	-1.00	50,61,73,73	20
2	UMP	1-M	550[A]	20/20	0.58	0.41	-1.00	49,62,73,73	20
2	UMP	3-M	550[C]	20/20	0.58	0.41	-1.00	49,62,72,72	20

6.5 Other polymers (i)

There are no such residues in this entry.