



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 3, 2023 – 01:28 PM EDT

PDB ID : 1HTQ
Title : Multicopy crystallographic structure of a relaxed glutamine synthetase from Mycobacterium tuberculosis
Authors : Gill, H.S.; Pfluegl, G.M.; Eisenberg, D.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2001-01-01
Resolution : 2.40 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.34
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.34

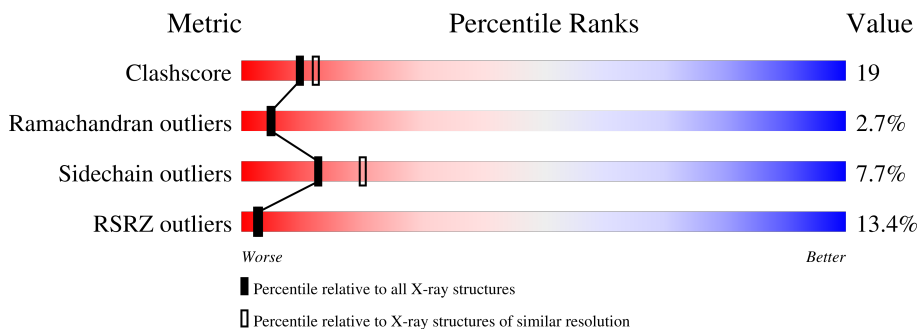
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-A	477	
1	1-B	477	
1	1-C	477	
1	1-D	477	
1	1-E	477	
1	1-F	477	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	1-G	477	13% 63% 31% 5%
1	1-H	477	14% 64% 31% 5%
1	1-I	477	17% 64% 31% 5%
1	1-J	477	12% 64% 31% 5%
1	1-K	477	14% 62% 32% 5%
1	1-L	477	13% 63% 31% 5%
1	1-M	477	15% 64% 31% 5%
1	1-N	477	14% 64% 30% 5%
1	1-O	477	16% 65% 30% 5%
1	1-P	477	15% 63% 31% 5%
1	1-Q	477	15% 62% 32% 5%
1	1-R	477	12% 64% 31% 5%
1	1-S	477	11% 64% 31% 5%
1	1-T	477	13% 64% 30% 5%
1	1-U	477	17% 65% 30% 5%
1	1-V	477	13% 64% 31% 5%
1	1-W	477	12% 63% 31% 5%
1	1-X	477	14% 63% 31% 5%
1	10-A	477	14% 64% 30% 6%
1	10-B	477	13% 65% 30% 5%
1	10-C	477	18% 65% 30% 5%
1	10-D	477	15% 64% 30% 6%
1	10-E	477	16% 62% 32% 5%
1	10-F	477	12% 63% 31% 6%
1	10-G	477	13% 64% 30% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain			
1	10-H	477	14%	64%	30%	6%
1	10-I	477	17%	65%	29%	5%
1	10-J	477	12%	65%	30%	5%
1	10-K	477	14%	62%	32%	6%
1	10-L	477	13%	62%	31%	6%
1	10-M	477	15%	65%	29%	5%
1	10-N	477	14%	63%	31%	5%
1	10-O	477	16%	65%	30%	5%
1	10-P	477	15%	63%	31%	6%
1	10-Q	477	15%	64%	31%	5%
1	10-R	477	12%	65%	29%	6%
1	10-S	477	11%	64%	31%	5%
1	10-T	477	13%	64%	30%	5%
1	10-U	477	17%	65%	29%	5%
1	10-V	477	13%	65%	30%	5%
1	10-W	477	12%	64%	31%	5%
1	10-X	477	14%	65%	29%	6%
1	2-A	477	14%	64%	30%	5% •
1	2-B	477	13%	66%	28%	5% •
1	2-C	477	18%	64%	30%	5% •
1	2-D	477	15%	64%	30%	5% •
1	2-E	477	16%	62%	31%	5% •
1	2-F	477	12%	65%	29%	5% •
1	2-G	477	13%	64%	29%	6% •
1	2-H	477	14%	65%	29%	5% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain			
1	2-I	477	17%	64%	30%	5%
1	2-J	477	12%	64%	30%	5%
1	2-K	477	14%	64%	30%	5%
1	2-L	477	13%	63%	30%	5%
1	2-M	477	15%	64%	30%	5%
1	2-N	477	14%	66%	28%	5%
1	2-O	477	16%	64%	30%	5%
1	2-P	477	15%	65%	29%	5%
1	2-Q	477	15%	64%	30%	5%
1	2-R	477	12%	65%	29%	5%
1	2-S	477	11%	65%	29%	5%
1	2-T	477	13%	65%	29%	5%
1	2-U	477	17%	64%	29%	5%
1	2-V	477	13%	63%	31%	5%
1	2-W	477	12%	65%	29%	5%
1	2-X	477	14%	65%	29%	6%
1	3-A	477	14%	70%	25%	5%
1	3-B	477	13%	69%	26%	5%
1	3-C	477	18%	71%	25%	5%
1	3-D	477	15%	70%	25%	5%
1	3-E	477	16%	69%	26%	5%
1	3-F	477	12%	70%	25%	5%
1	3-G	477	13%	70%	26%	5%
1	3-H	477	14%	70%	25%	5%
1	3-I	477	17%	71%	24%	5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
1	3-J	477	12%	69% 27% .
1	3-K	477	14%	69% 27% .
1	3-L	477	13%	70% 25% .
1	3-M	477	15%	70% 25% .
1	3-N	477	14%	70% 25% .
1	3-O	477	16%	70% 25% .
1	3-P	477	15%	70% 26% .
1	3-Q	477	15%	70% 25% 5%
1	3-R	477	12%	70% 25% .
1	3-S	477	11%	70% 26% .
1	3-T	477	13%	70% 25% .
1	3-U	477	17%	71% 24% .
1	3-V	477	13%	69% 26% .
1	3-W	477	12%	70% 25% .
1	3-X	477	14%	71% 25% .
1	4-A	477	14%	64% 31% . .
1	4-B	477	13%	65% 31% . .
1	4-C	477	18%	66% 30% . .
1	4-D	477	15%	65% 31% .
1	4-E	477	16%	65% 31% . .
1	4-F	477	12%	65% 31% . .
1	4-G	477	13%	64% 32% . .
1	4-H	477	14%	64% 32% . .
1	4-I	477	17%	65% 30% . .
1	4-J	477	12%	65% 31% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain			
1	4-K	477	14%	65%	31%	.
1	4-L	477	13%	65%	31%	..
1	4-M	477	15%	66%	30%	..
1	4-N	477	14%	64%	31%	..
1	4-O	477	16%	65%	31%	..
1	4-P	477	15%	64%	32%	.
1	4-Q	477	15%	64%	31%	..
1	4-R	477	12%	65%	30%	..
1	4-S	477	11%	65%	31%	..
1	4-T	477	13%	64%	31%	..
1	4-U	477	17%	66%	30%	..
1	4-V	477	13%	65%	30%	.
1	4-W	477	12%	64%	31%	..
1	4-X	477	14%	66%	30%	.
1	5-A	477	14%	63%	32%	.
1	5-B	477	13%	65%	31%	.
1	5-C	477	18%	65%	30%	..
1	5-D	477	15%	63%	33%	.
1	5-E	477	16%	62%	33%	.
1	5-F	477	12%	65%	30%	.
1	5-G	477	13%	64%	31%	.
1	5-H	477	14%	65%	30%	..
1	5-I	477	17%	65%	30%	.
1	5-J	477	12%	64%	31%	.
1	5-K	477	14%	63%	32%	.

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain			
1	5-L	477	13%	63%	32%	5%
1	5-M	477	15%	64%	31%	•
1	5-N	477	14%	63%	32%	•
1	5-O	477	16%	65%	30%	•
1	5-P	477	15%	63%	32%	•
1	5-Q	477	15%	62%	33%	•
1	5-R	477	12%	66%	30%	•
1	5-S	477	11%	65%	30%	•
1	5-T	477	13%	64%	31%	•
1	5-U	477	17%	66%	29%	•
1	5-V	477	13%	65%	30%	•
1	5-W	477	12%	64%	32%	•
1	5-X	477	14%	64%	31%	•
1	6-A	477	14%	61%	32%	7%
1	6-B	477	13%	63%	31%	6%
1	6-C	477	18%	62%	31%	6%
1	6-D	477	15%	62%	31%	6%
1	6-E	477	16%	61%	33%	6%
1	6-F	477	12%	62%	31%	6%
1	6-G	477	13%	62%	31%	6%
1	6-H	477	14%	62%	32%	6%
1	6-I	477	17%	63%	31%	6%
1	6-J	477	12%	61%	32%	6%
1	6-K	477	14%	62%	32%	6%
1	6-L	477	13%	61%	33%	6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain			
1	6-M	477	15%	62%	31%	7%
1	6-N	477	14%	62%	32%	6%
1	6-O	477	16%	62%	32%	6%
1	6-P	477	15%	62%	31%	6%
1	6-Q	477	15%	61%	32%	6%
1	6-R	477	12%	62%	32%	6%
1	6-S	477	11%	63%	31%	6%
1	6-T	477	13%	62%	31%	6%
1	6-U	477	17%	63%	31%	6%
1	6-V	477	13%	62%	32%	6%
1	6-W	477	12%	62%	31%	6%
1	6-X	477	14%	62%	31%	6%
1	7-A	477	14%	65%	30%	..
1	7-B	477	13%	67%	29%	..
1	7-C	477	18%	67%	28%	..
1	7-D	477	15%	66%	29%	..
1	7-E	477	16%	67%	29%	..
1	7-F	477	12%	67%	28%	..
1	7-G	477	13%	68%	28%	..
1	7-H	477	14%	68%	28%	..
1	7-I	477	17%	66%	29%	..
1	7-J	477	12%	67%	29%	..
1	7-K	477	14%	67%	29%	..
1	7-L	477	13%	66%	29%	..
1	7-M	477	15%	66%	29%	..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
1	7-N	477	14%	66% 29% ..
1	7-O	477	16%	67% 29% ..
1	7-P	477	15%	65% 30% ..
1	7-Q	477	15%	66% 29% ..
1	7-R	477	12%	68% 28% ..
1	7-S	477	11%	67% 28% ..
1	7-T	477	13%	68% 28% ..
1	7-U	477	17%	66% 29% ..
1	7-V	477	13%	67% 29% ..
1	7-W	477	12%	66% 29% ..
1	7-X	477	14%	67% 29% ..
1	8-A	477	14%	66% 30% .
1	8-B	477	13%	66% 30% .
1	8-C	477	18%	66% 29% .
1	8-D	477	15%	65% 30% .
1	8-E	477	16%	64% 32% 5%
1	8-F	477	12%	66% 30% 5%
1	8-G	477	13%	65% 30% .
1	8-H	477	14%	67% 29% .
1	8-I	477	17%	67% 29% .
1	8-J	477	12%	66% 30% .
1	8-K	477	14%	65% 30% 5%
1	8-L	477	13%	66% 30% .
1	8-M	477	15%	66% 29% .
1	8-N	477	14%	66% 29% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain			
1	8-O	477	16%	66%	29%	.
1	8-P	477	15%	66%	29%	5%
1	8-Q	477	15%	65%	30%	5%
1	8-R	477	12%	66%	30%	.
1	8-S	477	11%	66%	29%	5%
1	8-T	477	13%	67%	29%	.
1	8-U	477	17%	67%	29%	.
1	8-V	477	13%	66%	30%	.
1	8-W	477	12%	66%	29%	5%
1	8-X	477	14%	67%	29%	.
1	9-A	477	14%	62%	33%	..
1	9-B	477	13%	62%	33%	..
1	9-C	477	18%	63%	33%	..
1	9-D	477	15%	61%	34%	..
1	9-E	477	16%	61%	34%	..
1	9-F	477	12%	63%	32%	5% .
1	9-G	477	13%	61%	35%	..
1	9-H	477	14%	63%	32%	..
1	9-I	477	17%	63%	32%	..
1	9-J	477	12%	62%	33%	..
1	9-K	477	14%	61%	34%	..
1	9-L	477	13%	62%	33%	..
1	9-M	477	15%	63%	32%	..
1	9-N	477	14%	62%	33%	..
1	9-O	477	16%	63%	32%	..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
1	9-P	477	15%	61% 34%
1	9-Q	477	15%	63% 32%
1	9-R	477	12%	63% 32%
1	9-S	477	11%	62% 33%
1	9-T	477	13%	63% 32%
1	9-U	477	17%	64% 32%
1	9-V	477	13%	62% 33%
1	9-W	477	12%	62% 33%
1	9-X	477	14%	63% 32%

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	MN	1-A	470	-	-	-	X
2	MN	1-E	470	-	-	-	X
2	MN	1-I	470	-	-	-	X
2	MN	1-L	470	-	-	-	X
2	MN	1-N	470	-	-	-	X
2	MN	1-O	470	-	-	-	X
2	MN	1-R	470	-	-	-	X
2	MN	10-A	470	-	-	-	X
2	MN	10-E	470	-	-	-	X
2	MN	10-I	470	-	-	-	X
2	MN	10-L	470	-	-	-	X
2	MN	10-N	470	-	-	-	X
2	MN	10-O	470	-	-	-	X
2	MN	10-R	470	-	-	-	X
2	MN	2-A	470	-	-	-	X
2	MN	2-E	470	-	-	-	X
2	MN	2-I	470	-	-	-	X
2	MN	2-L	470	-	-	-	X
2	MN	2-N	470	-	-	-	X
2	MN	2-O	470	-	-	-	X
2	MN	2-R	470	-	-	-	X
2	MN	3-A	470	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MN	3-E	470	-	-	-	X
2	MN	3-I	470	-	-	-	X
2	MN	3-L	470	-	-	-	X
2	MN	3-N	470	-	-	-	X
2	MN	3-O	470	-	-	-	X
2	MN	3-R	470	-	-	-	X
2	MN	4-A	470	-	-	-	X
2	MN	4-E	470	-	-	-	X
2	MN	4-I	470	-	-	-	X
2	MN	4-L	470	-	-	-	X
2	MN	4-N	470	-	-	-	X
2	MN	4-O	470	-	-	-	X
2	MN	4-R	470	-	-	-	X
2	MN	5-A	470	-	-	-	X
2	MN	5-E	470	-	-	-	X
2	MN	5-I	470	-	-	-	X
2	MN	5-L	470	-	-	-	X
2	MN	5-N	470	-	-	-	X
2	MN	5-O	470	-	-	-	X
2	MN	5-R	470	-	-	-	X
2	MN	6-A	470	-	-	-	X
2	MN	6-E	470	-	-	-	X
2	MN	6-I	470	-	-	-	X
2	MN	6-L	470	-	-	-	X
2	MN	6-N	470	-	-	-	X
2	MN	6-O	470	-	-	-	X
2	MN	6-R	470	-	-	-	X
2	MN	7-A	470	-	-	-	X
2	MN	7-E	470	-	-	-	X
2	MN	7-I	470	-	-	-	X
2	MN	7-L	470	-	-	-	X
2	MN	7-N	470	-	-	-	X
2	MN	7-O	470	-	-	-	X
2	MN	7-R	470	-	-	-	X
2	MN	8-A	470	-	-	-	X
2	MN	8-E	470	-	-	-	X
2	MN	8-I	470	-	-	-	X
2	MN	8-L	470	-	-	-	X
2	MN	8-N	470	-	-	-	X
2	MN	8-O	470	-	-	-	X
2	MN	8-R	470	-	-	-	X
2	MN	9-A	470	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MN	9-E	470	-	-	-	X
2	MN	9-I	470	-	-	-	X
2	MN	9-L	470	-	-	-	X
2	MN	9-N	470	-	-	-	X
2	MN	9-O	470	-	-	-	X
2	MN	9-R	470	-	-	-	X
3	AMP	1-A	7475	-	-	-	X
3	AMP	1-B	7477	-	-	-	X
3	AMP	1-C	7479	-	-	-	X
3	AMP	1-D	7481	-	-	-	X
3	AMP	1-E	7483	-	-	-	X
3	AMP	1-F	7485	-	-	-	X
3	AMP	1-G	7487	-	-	-	X
3	AMP	1-H	7489	-	-	-	X
3	AMP	1-I	7491	-	-	-	X
3	AMP	1-J	7493	-	-	-	X
3	AMP	1-K	7495	-	-	-	X
3	AMP	1-L	7497	-	-	-	X
3	AMP	1-M	7499	-	-	-	X
3	AMP	1-N	7501	-	-	-	X
3	AMP	1-O	7503	-	-	-	X
3	AMP	1-P	7505	-	-	-	X
3	AMP	1-Q	7507	-	-	-	X
3	AMP	1-R	7509	-	-	-	X
3	AMP	1-S	7511	-	-	-	X
3	AMP	1-T	7513	-	-	-	X
3	AMP	1-U	7515	-	-	-	X
3	AMP	1-V	7517	-	-	-	X
3	AMP	1-W	7519	-	-	-	X
3	AMP	1-X	7521	-	-	-	X
3	AMP	10-A	7475	-	-	-	X
3	AMP	10-B	7477	-	-	-	X
3	AMP	10-C	7479	-	-	-	X
3	AMP	10-D	7481	-	-	-	X
3	AMP	10-E	7483	-	-	-	X
3	AMP	10-F	7485	-	-	-	X
3	AMP	10-G	7487	-	-	-	X
3	AMP	10-H	7489	-	-	-	X
3	AMP	10-I	7491	-	-	-	X
3	AMP	10-J	7493	-	-	-	X
3	AMP	10-K	7495	-	-	X	X
3	AMP	10-L	7497	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AMP	10-M	7499	-	-	-	X
3	AMP	10-N	7501	-	-	-	X
3	AMP	10-O	7503	-	-	-	X
3	AMP	10-P	7505	-	-	-	X
3	AMP	10-Q	7507	-	-	-	X
3	AMP	10-R	7509	-	-	-	X
3	AMP	10-S	7511	-	-	-	X
3	AMP	10-T	7513	-	-	-	X
3	AMP	10-U	7515	-	-	-	X
3	AMP	10-V	7517	-	-	-	X
3	AMP	10-W	7519	-	-	-	X
3	AMP	10-X	7521	-	-	-	X
3	AMP	2-A	7475	-	-	X	X
3	AMP	2-B	7477	-	-	-	X
3	AMP	2-C	7479	-	-	X	X
3	AMP	2-D	7481	-	-	X	X
3	AMP	2-E	7483	-	-	X	X
3	AMP	2-F	7485	-	-	X	X
3	AMP	2-G	7487	-	-	X	X
3	AMP	2-H	7489	-	-	X	X
3	AMP	2-I	7491	-	-	X	X
3	AMP	2-J	7493	-	-	-	X
3	AMP	2-K	7495	-	-	X	X
3	AMP	2-L	7497	-	-	X	X
3	AMP	2-M	7499	-	-	X	X
3	AMP	2-N	7501	-	-	-	X
3	AMP	2-O	7503	-	-	X	X
3	AMP	2-P	7505	-	-	X	X
3	AMP	2-Q	7507	-	-	X	X
3	AMP	2-R	7509	-	-	X	X
3	AMP	2-S	7511	-	-	-	X
3	AMP	2-T	7513	-	-	X	X
3	AMP	2-U	7515	-	-	-	X
3	AMP	2-V	7517	-	-	-	X
3	AMP	2-W	7519	-	-	-	X
3	AMP	2-X	7521	-	-	X	X
3	AMP	3-A	7475	-	-	X	X
3	AMP	3-B	7477	-	-	X	X
3	AMP	3-C	7479	-	-	X	X
3	AMP	3-D	7481	-	-	X	X
3	AMP	3-E	7483	-	-	X	X
3	AMP	3-F	7485	-	-	X	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AMP	3-G	7487	-	-	X	X
3	AMP	3-H	7489	-	-	X	X
3	AMP	3-I	7491	-	-	X	X
3	AMP	3-J	7493	-	-	X	X
3	AMP	3-K	7495	-	-	X	X
3	AMP	3-L	7497	-	-	X	X
3	AMP	3-M	7499	-	-	X	X
3	AMP	3-N	7501	-	-	X	X
3	AMP	3-O	7503	-	-	X	X
3	AMP	3-P	7505	-	-	X	X
3	AMP	3-Q	7507	-	-	X	X
3	AMP	3-R	7509	-	-	X	X
3	AMP	3-S	7511	-	-	X	X
3	AMP	3-T	7513	-	-	X	X
3	AMP	3-U	7515	-	-	X	X
3	AMP	3-V	7517	-	-	X	X
3	AMP	3-W	7519	-	-	X	X
3	AMP	3-X	7521	-	-	X	X
3	AMP	4-A	7475	-	-	X	X
3	AMP	4-B	7477	-	-	X	X
3	AMP	4-C	7479	-	-	X	X
3	AMP	4-D	7481	-	-	X	X
3	AMP	4-E	7483	-	-	X	X
3	AMP	4-F	7485	-	-	X	X
3	AMP	4-G	7487	-	-	X	X
3	AMP	4-H	7489	-	-	X	X
3	AMP	4-I	7491	-	-	X	X
3	AMP	4-J	7493	-	-	X	X
3	AMP	4-K	7495	-	-	X	X
3	AMP	4-L	7497	-	-	X	X
3	AMP	4-M	7499	-	-	X	X
3	AMP	4-N	7501	-	-	X	X
3	AMP	4-O	7503	-	-	X	X
3	AMP	4-P	7505	-	-	X	X
3	AMP	4-Q	7507	-	-	X	X
3	AMP	4-R	7509	-	-	X	X
3	AMP	4-S	7511	-	-	X	X
3	AMP	4-T	7513	-	-	X	X
3	AMP	4-U	7515	-	-	X	X
3	AMP	4-V	7517	-	-	X	X
3	AMP	4-W	7519	-	-	X	X
3	AMP	4-X	7521	-	-	X	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AMP	5-A	7475	-	-	X	X
3	AMP	5-B	7477	-	-	X	X
3	AMP	5-C	7479	-	-	X	X
3	AMP	5-D	7481	-	-	X	X
3	AMP	5-E	7483	-	-	X	X
3	AMP	5-F	7485	-	-	X	X
3	AMP	5-G	7487	-	-	X	X
3	AMP	5-H	7489	-	-	X	X
3	AMP	5-I	7491	-	-	X	X
3	AMP	5-J	7493	-	-	X	X
3	AMP	5-K	7495	-	-	X	X
3	AMP	5-L	7497	-	-	X	X
3	AMP	5-M	7499	-	-	X	X
3	AMP	5-N	7501	-	-	X	X
3	AMP	5-O	7503	-	-	X	X
3	AMP	5-P	7505	-	-	X	X
3	AMP	5-Q	7507	-	-	X	X
3	AMP	5-R	7509	-	-	X	X
3	AMP	5-S	7511	-	-	X	X
3	AMP	5-T	7513	-	-	X	X
3	AMP	5-U	7515	-	-	X	X
3	AMP	5-V	7517	-	-	X	X
3	AMP	5-W	7519	-	-	X	X
3	AMP	5-X	7521	-	-	X	X
3	AMP	6-A	7475	-	-	-	X
3	AMP	6-B	7477	-	-	X	X
3	AMP	6-C	7479	-	-	X	X
3	AMP	6-D	7481	-	-	X	X
3	AMP	6-E	7483	-	-	X	X
3	AMP	6-F	7485	-	-	X	X
3	AMP	6-G	7487	-	-	X	X
3	AMP	6-H	7489	-	-	X	X
3	AMP	6-I	7491	-	-	X	X
3	AMP	6-J	7493	-	-	X	X
3	AMP	6-K	7495	-	-	X	X
3	AMP	6-L	7497	-	-	X	X
3	AMP	6-M	7499	-	-	-	X
3	AMP	6-N	7501	-	-	X	X
3	AMP	6-O	7503	-	-	X	X
3	AMP	6-P	7505	-	-	X	X
3	AMP	6-Q	7507	-	-	X	X
3	AMP	6-R	7509	-	-	X	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AMP	6-S	7511	-	-	X	X
3	AMP	6-T	7513	-	-	X	X
3	AMP	6-U	7515	-	-	X	X
3	AMP	6-V	7517	-	-	X	X
3	AMP	6-W	7519	-	-	X	X
3	AMP	6-X	7521	-	-	X	X
3	AMP	7-A	7475	-	-	-	X
3	AMP	7-B	7477	-	-	-	X
3	AMP	7-C	7479	-	-	-	X
3	AMP	7-D	7481	-	-	-	X
3	AMP	7-E	7483	-	-	-	X
3	AMP	7-F	7485	-	-	-	X
3	AMP	7-G	7487	-	-	-	X
3	AMP	7-H	7489	-	-	-	X
3	AMP	7-I	7491	-	-	-	X
3	AMP	7-J	7493	-	-	-	X
3	AMP	7-K	7495	-	-	-	X
3	AMP	7-L	7497	-	-	-	X
3	AMP	7-M	7499	-	-	-	X
3	AMP	7-N	7501	-	-	-	X
3	AMP	7-O	7503	-	-	-	X
3	AMP	7-P	7505	-	-	-	X
3	AMP	7-Q	7507	-	-	-	X
3	AMP	7-R	7509	-	-	-	X
3	AMP	7-S	7511	-	-	-	X
3	AMP	7-T	7513	-	-	-	X
3	AMP	7-U	7515	-	-	-	X
3	AMP	7-V	7517	-	-	-	X
3	AMP	7-W	7519	-	-	-	X
3	AMP	7-X	7521	-	-	-	X
3	AMP	8-A	7475	-	-	-	X
3	AMP	8-B	7477	-	-	-	X
3	AMP	8-C	7479	-	-	-	X
3	AMP	8-D	7481	-	-	-	X
3	AMP	8-E	7483	-	-	-	X
3	AMP	8-F	7485	-	-	-	X
3	AMP	8-G	7487	-	-	-	X
3	AMP	8-H	7489	-	-	-	X
3	AMP	8-I	7491	-	-	-	X
3	AMP	8-J	7493	-	-	-	X
3	AMP	8-K	7495	-	-	X	X
3	AMP	8-L	7497	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AMP	8-M	7499	-	-	-	X
3	AMP	8-N	7501	-	-	-	X
3	AMP	8-O	7503	-	-	-	X
3	AMP	8-P	7505	-	-	-	X
3	AMP	8-Q	7507	-	-	-	X
3	AMP	8-R	7509	-	-	-	X
3	AMP	8-S	7511	-	-	-	X
3	AMP	8-T	7513	-	-	-	X
3	AMP	8-U	7515	-	-	-	X
3	AMP	8-V	7517	-	-	-	X
3	AMP	8-W	7519	-	-	-	X
3	AMP	8-X	7521	-	-	-	X
3	AMP	9-A	7475	-	-	X	X
3	AMP	9-B	7477	-	-	X	X
3	AMP	9-C	7479	-	-	X	X
3	AMP	9-D	7481	-	-	X	X
3	AMP	9-E	7483	-	-	X	X
3	AMP	9-F	7485	-	-	X	X
3	AMP	9-G	7487	-	-	X	X
3	AMP	9-H	7489	-	-	X	X
3	AMP	9-I	7491	-	-	X	X
3	AMP	9-J	7493	-	-	X	X
3	AMP	9-K	7495	-	-	X	X
3	AMP	9-L	7497	-	-	X	X
3	AMP	9-M	7499	-	-	X	X
3	AMP	9-N	7501	-	-	X	X
3	AMP	9-O	7503	-	-	X	X
3	AMP	9-P	7505	-	-	X	X
3	AMP	9-Q	7507	-	-	X	X
3	AMP	9-R	7509	-	-	X	X
3	AMP	9-S	7511	-	-	X	X
3	AMP	9-T	7513	-	-	X	X
3	AMP	9-U	7515	-	-	X	X
3	AMP	9-V	7517	-	-	X	X
3	AMP	9-W	7519	-	-	X	X
3	AMP	9-X	7521	-	-	X	X
4	CIT	1-A	7476	-	X	-	-
4	CIT	1-B	7478	-	X	-	-
4	CIT	1-C	7480	-	X	-	X
4	CIT	1-D	7482	-	X	-	X
4	CIT	1-E	7484	-	X	-	X
4	CIT	1-F	7486	-	X	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CIT	1-G	7488	-	X	-	X
4	CIT	1-H	7490	-	X	-	X
4	CIT	1-I	7492	-	X	-	-
4	CIT	1-J	7494	-	X	-	X
4	CIT	1-K	7496	-	X	-	X
4	CIT	1-L	7498	-	X	-	X
4	CIT	1-M	7500	-	X	-	X
4	CIT	1-N	7502	-	X	-	X
4	CIT	1-O	7504	-	X	-	X
4	CIT	1-P	7506	-	X	-	X
4	CIT	1-Q	7508	-	X	-	X
4	CIT	1-R	7510	-	X	-	X
4	CIT	1-S	7512	-	X	-	-
4	CIT	1-T	7514	-	X	-	X
4	CIT	1-U	7516	-	X	-	X
4	CIT	1-V	7518	-	X	-	X
4	CIT	1-W	7520	-	X	-	X
4	CIT	1-X	7522	-	X	-	-
4	CIT	10-A	7476	-	X	-	-
4	CIT	10-B	7478	-	X	-	-
4	CIT	10-C	7480	-	X	-	X
4	CIT	10-D	7482	-	X	-	X
4	CIT	10-E	7484	-	X	-	X
4	CIT	10-F	7486	-	X	-	X
4	CIT	10-G	7488	-	X	-	X
4	CIT	10-H	7490	-	X	-	X
4	CIT	10-I	7492	-	X	-	-
4	CIT	10-J	7494	-	X	-	X
4	CIT	10-K	7496	-	X	-	X
4	CIT	10-L	7498	-	X	-	X
4	CIT	10-M	7500	-	X	-	X
4	CIT	10-N	7502	-	X	-	X
4	CIT	10-O	7504	-	X	-	X
4	CIT	10-P	7506	-	X	-	X
4	CIT	10-Q	7508	-	X	-	X
4	CIT	10-R	7510	-	X	-	X
4	CIT	10-S	7512	-	X	-	-
4	CIT	10-T	7514	-	X	-	X
4	CIT	10-U	7516	-	X	-	X
4	CIT	10-V	7518	-	X	-	X
4	CIT	10-W	7520	-	X	-	X
4	CIT	10-X	7522	-	X	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CIT	2-A	7476	-	X	-	-
4	CIT	2-B	7478	-	X	-	-
4	CIT	2-C	7480	-	X	-	X
4	CIT	2-D	7482	-	X	-	X
4	CIT	2-E	7484	-	X	-	X
4	CIT	2-F	7486	-	X	-	X
4	CIT	2-G	7488	-	X	-	X
4	CIT	2-H	7490	-	X	-	X
4	CIT	2-I	7492	-	X	-	-
4	CIT	2-J	7494	-	X	-	X
4	CIT	2-K	7496	-	X	-	X
4	CIT	2-L	7498	-	X	-	X
4	CIT	2-M	7500	-	X	-	X
4	CIT	2-N	7502	-	X	-	X
4	CIT	2-O	7504	-	X	-	X
4	CIT	2-P	7506	-	X	-	X
4	CIT	2-Q	7508	-	X	-	X
4	CIT	2-R	7510	-	X	-	X
4	CIT	2-S	7512	-	X	-	-
4	CIT	2-T	7514	-	X	-	X
4	CIT	2-U	7516	-	X	-	X
4	CIT	2-V	7518	-	X	-	X
4	CIT	2-W	7520	-	X	-	X
4	CIT	2-X	7522	-	X	-	-
4	CIT	3-A	7476	-	X	-	-
4	CIT	3-B	7478	-	X	-	-
4	CIT	3-C	7480	-	X	-	X
4	CIT	3-D	7482	-	X	-	X
4	CIT	3-E	7484	-	X	-	X
4	CIT	3-F	7486	-	X	-	X
4	CIT	3-G	7488	-	X	-	X
4	CIT	3-H	7490	-	X	-	X
4	CIT	3-I	7492	-	X	-	-
4	CIT	3-J	7494	-	X	-	X
4	CIT	3-K	7496	-	X	-	X
4	CIT	3-L	7498	-	X	-	X
4	CIT	3-M	7500	-	X	-	X
4	CIT	3-N	7502	-	X	-	X
4	CIT	3-O	7504	-	X	-	X
4	CIT	3-P	7506	-	X	-	X
4	CIT	3-Q	7508	-	X	-	X
4	CIT	3-R	7510	-	X	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CIT	3-S	7512	-	X	-	-
4	CIT	3-T	7514	-	X	-	X
4	CIT	3-U	7516	-	X	-	X
4	CIT	3-V	7518	-	X	-	X
4	CIT	3-W	7520	-	X	-	X
4	CIT	3-X	7522	-	X	-	-
4	CIT	4-A	7476	-	X	-	-
4	CIT	4-B	7478	-	X	-	-
4	CIT	4-C	7480	-	X	-	X
4	CIT	4-D	7482	-	X	-	X
4	CIT	4-E	7484	-	X	-	X
4	CIT	4-F	7486	-	X	-	X
4	CIT	4-G	7488	-	X	-	X
4	CIT	4-H	7490	-	X	-	X
4	CIT	4-I	7492	-	X	-	-
4	CIT	4-J	7494	-	X	-	X
4	CIT	4-K	7496	-	X	-	X
4	CIT	4-L	7498	-	X	-	X
4	CIT	4-M	7500	-	X	-	X
4	CIT	4-N	7502	-	X	-	X
4	CIT	4-O	7504	-	X	-	X
4	CIT	4-P	7506	-	X	-	X
4	CIT	4-Q	7508	-	X	-	X
4	CIT	4-R	7510	-	X	-	X
4	CIT	4-S	7512	-	X	-	-
4	CIT	4-T	7514	-	X	-	X
4	CIT	4-U	7516	-	X	-	X
4	CIT	4-V	7518	-	X	-	X
4	CIT	4-W	7520	-	X	-	X
4	CIT	4-X	7522	-	X	-	-
4	CIT	5-A	7476	-	X	-	-
4	CIT	5-B	7478	-	X	-	-
4	CIT	5-C	7480	-	X	-	X
4	CIT	5-D	7482	-	X	-	X
4	CIT	5-E	7484	-	X	-	X
4	CIT	5-F	7486	-	X	-	X
4	CIT	5-G	7488	-	X	-	X
4	CIT	5-H	7490	-	X	-	X
4	CIT	5-I	7492	-	X	-	-
4	CIT	5-J	7494	-	X	-	X
4	CIT	5-K	7496	-	X	-	X
4	CIT	5-L	7498	-	X	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CIT	5-M	7500	-	X	-	X
4	CIT	5-N	7502	-	X	-	X
4	CIT	5-O	7504	-	X	-	X
4	CIT	5-P	7506	-	X	-	X
4	CIT	5-Q	7508	-	X	-	X
4	CIT	5-R	7510	-	X	-	X
4	CIT	5-S	7512	-	X	-	-
4	CIT	5-T	7514	-	X	-	X
4	CIT	5-U	7516	-	X	-	X
4	CIT	5-V	7518	-	X	-	X
4	CIT	5-W	7520	-	X	-	X
4	CIT	5-X	7522	-	X	-	-
4	CIT	6-A	7476	-	X	-	-
4	CIT	6-B	7478	-	X	-	-
4	CIT	6-C	7480	-	X	-	X
4	CIT	6-D	7482	-	X	-	X
4	CIT	6-E	7484	-	X	-	X
4	CIT	6-F	7486	-	X	-	X
4	CIT	6-G	7488	-	X	-	X
4	CIT	6-H	7490	-	X	-	X
4	CIT	6-I	7492	-	X	-	-
4	CIT	6-J	7494	-	X	-	X
4	CIT	6-K	7496	-	X	-	X
4	CIT	6-L	7498	-	X	-	X
4	CIT	6-M	7500	-	X	-	X
4	CIT	6-N	7502	-	X	-	X
4	CIT	6-O	7504	-	X	-	X
4	CIT	6-P	7506	-	X	-	X
4	CIT	6-Q	7508	-	X	-	X
4	CIT	6-R	7510	-	X	-	X
4	CIT	6-S	7512	-	X	-	-
4	CIT	6-T	7514	-	X	-	X
4	CIT	6-U	7516	-	X	-	X
4	CIT	6-V	7518	-	X	-	X
4	CIT	6-W	7520	-	X	-	X
4	CIT	6-X	7522	-	X	-	-
4	CIT	7-A	7476	-	X	X	-
4	CIT	7-B	7478	-	X	-	-
4	CIT	7-C	7480	-	X	X	X
4	CIT	7-D	7482	-	X	X	X
4	CIT	7-E	7484	-	X	X	X
4	CIT	7-F	7486	-	X	X	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CIT	7-G	7488	-	X	X	X
4	CIT	7-H	7490	-	X	X	X
4	CIT	7-I	7492	-	X	X	-
4	CIT	7-J	7494	-	X	X	X
4	CIT	7-K	7496	-	X	X	X
4	CIT	7-L	7498	-	X	-	X
4	CIT	7-M	7500	-	X	X	X
4	CIT	7-N	7502	-	X	-	X
4	CIT	7-O	7504	-	X	X	X
4	CIT	7-P	7506	-	X	X	X
4	CIT	7-Q	7508	-	X	X	X
4	CIT	7-R	7510	-	X	X	X
4	CIT	7-S	7512	-	X	X	-
4	CIT	7-T	7514	-	X	X	X
4	CIT	7-U	7516	-	X	X	X
4	CIT	7-V	7518	-	X	X	X
4	CIT	7-W	7520	-	X	X	X
4	CIT	7-X	7522	-	X	-	-
4	CIT	8-A	7476	-	X	-	-
4	CIT	8-B	7478	-	X	-	-
4	CIT	8-C	7480	-	X	-	X
4	CIT	8-D	7482	-	X	-	X
4	CIT	8-E	7484	-	X	-	X
4	CIT	8-F	7486	-	X	-	X
4	CIT	8-G	7488	-	X	-	X
4	CIT	8-H	7490	-	X	-	X
4	CIT	8-I	7492	-	X	-	-
4	CIT	8-J	7494	-	X	-	X
4	CIT	8-K	7496	-	X	-	X
4	CIT	8-L	7498	-	X	-	X
4	CIT	8-M	7500	-	X	-	X
4	CIT	8-N	7502	-	X	-	X
4	CIT	8-O	7504	-	X	-	X
4	CIT	8-P	7506	-	X	-	X
4	CIT	8-Q	7508	-	X	-	X
4	CIT	8-R	7510	-	X	-	X
4	CIT	8-S	7512	-	X	-	-
4	CIT	8-T	7514	-	X	-	X
4	CIT	8-U	7516	-	X	-	X
4	CIT	8-V	7518	-	X	-	X
4	CIT	8-W	7520	-	X	-	X
4	CIT	8-X	7522	-	X	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CIT	9-A	7476	-	X	-	-
4	CIT	9-B	7478	-	X	-	-
4	CIT	9-C	7480	-	X	-	X
4	CIT	9-D	7482	-	X	-	X
4	CIT	9-E	7484	-	X	-	X
4	CIT	9-F	7486	-	X	-	X
4	CIT	9-G	7488	-	X	-	X
4	CIT	9-H	7490	-	X	-	X
4	CIT	9-I	7492	-	X	-	-
4	CIT	9-J	7494	-	X	-	X
4	CIT	9-K	7496	-	X	-	X
4	CIT	9-L	7498	-	X	-	X
4	CIT	9-M	7500	-	X	-	X
4	CIT	9-N	7502	-	X	-	X
4	CIT	9-O	7504	-	X	-	X
4	CIT	9-P	7506	-	X	-	X
4	CIT	9-Q	7508	-	X	-	X
4	CIT	9-R	7510	-	X	-	X
4	CIT	9-S	7512	-	X	-	-
4	CIT	9-T	7514	-	X	-	X
4	CIT	9-U	7516	-	X	-	X
4	CIT	9-V	7518	-	X	-	X
4	CIT	9-W	7520	-	X	-	X
4	CIT	9-X	7522	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 978720 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 glutamine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1-A	477	3778	2406	633	727	12	0	0	0
1	2-A	477	3778	2406	633	727	12	0	0	0
1	3-A	477	3778	2406	633	727	12	0	0	0
1	4-A	477	3778	2406	633	727	12	0	0	0
1	5-A	477	3778	2406	633	727	12	0	0	0
1	6-A	477	3778	2406	633	727	12	0	0	0
1	7-A	477	3778	2406	633	727	12	0	0	0
1	8-A	477	3778	2406	633	727	12	0	0	0
1	9-A	477	3778	2406	633	727	12	0	0	0
1	10-A	477	3778	2406	633	727	12	0	0	0
1	1-B	477	3778	2406	633	727	12	0	0	0
1	2-B	477	3778	2406	633	727	12	0	0	0
1	3-B	477	3778	2406	633	727	12	0	0	0
1	4-B	477	3778	2406	633	727	12	0	0	0
1	5-B	477	3778	2406	633	727	12	0	0	0
1	6-B	477	3778	2406	633	727	12	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	7-B	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-B	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-B	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-B	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-C	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-C	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-C	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-C	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-C	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-C	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-C	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-C	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-C	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-C	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-D	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-D	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-D	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-D	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-D	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-D	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-D	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	8-D	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-D	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-D	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	9-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-G	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-G	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-G	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-G	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-G	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-G	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-G	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-G	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-G	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-G	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-H	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-H	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-H	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-H	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-H	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-H	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-H	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-H	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-H	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	10-H	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-I	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-I	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-I	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-I	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-I	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-I	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-I	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-I	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-I	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-I	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-J	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-J	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-J	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-J	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-J	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-J	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-J	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-J	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-J	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-J	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-K	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-K	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-K	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-K	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-K	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-K	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-K	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-K	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-K	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-K	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-L	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-L	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-L	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-L	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-L	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-L	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-L	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-L	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-L	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-L	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-M	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2-M	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-M	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-M	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-M	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-M	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-M	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-M	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-M	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-M	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-N	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-N	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-N	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-N	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-N	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-N	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-N	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-N	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-N	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-N	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	3-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-Q	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-Q	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-Q	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	4-Q	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-Q	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-Q	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-Q	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-Q	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-Q	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-Q	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-R	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-R	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-R	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-R	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-R	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-R	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-R	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-R	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-R	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-R	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-S	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-S	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-S	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-S	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	5-S	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-S	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-S	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-S	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-S	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-S	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-T	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-T	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-T	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-T	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-T	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-T	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-T	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-T	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-T	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-T	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-U	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-U	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-U	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-U	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-U	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	6-U	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-U	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-U	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-U	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-U	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-V	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-V	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-V	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-V	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-V	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-V	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-V	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-V	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-V	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-V	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-W	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-W	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-W	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-W	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-W	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-W	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	7-W	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-W	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-W	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-W	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-X	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-X	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-X	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-X	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-X	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-X	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-X	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-X	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-X	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-X	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1-A	1	Total 1	Mn 1	0	0
2	2-A	1	Total 1	Mn 1	0	0
2	3-A	1	Total 1	Mn 1	0	0
2	4-A	1	Total 1	Mn 1	0	0
2	5-A	1	Total 1	Mn 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	6-A	1	Total 1	Mn 1	0	0
2	7-A	1	Total 1	Mn 1	0	0
2	8-A	1	Total 1	Mn 1	0	0
2	9-A	1	Total 1	Mn 1	0	0
2	10-A	1	Total 1	Mn 1	0	0
2	1-B	1	Total 1	Mn 1	0	0
2	2-B	1	Total 1	Mn 1	0	0
2	3-B	1	Total 1	Mn 1	0	0
2	4-B	1	Total 1	Mn 1	0	0
2	5-B	1	Total 1	Mn 1	0	0
2	6-B	1	Total 1	Mn 1	0	0
2	7-B	1	Total 1	Mn 1	0	0
2	8-B	1	Total 1	Mn 1	0	0
2	9-B	1	Total 1	Mn 1	0	0
2	10-B	1	Total 1	Mn 1	0	0
2	1-C	1	Total 1	Mn 1	0	0
2	2-C	1	Total 1	Mn 1	0	0
2	3-C	1	Total 1	Mn 1	0	0
2	4-C	1	Total 1	Mn 1	0	0
2	5-C	1	Total 1	Mn 1	0	0
2	6-C	1	Total 1	Mn 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	7-C	1	Total 1	Mn 1	0	0
2	8-C	1	Total 1	Mn 1	0	0
2	9-C	1	Total 1	Mn 1	0	0
2	10-C	1	Total 1	Mn 1	0	0
2	1-D	1	Total 1	Mn 1	0	0
2	2-D	1	Total 1	Mn 1	0	0
2	3-D	1	Total 1	Mn 1	0	0
2	4-D	1	Total 1	Mn 1	0	0
2	5-D	1	Total 1	Mn 1	0	0
2	6-D	1	Total 1	Mn 1	0	0
2	7-D	1	Total 1	Mn 1	0	0
2	8-D	1	Total 1	Mn 1	0	0
2	9-D	1	Total 1	Mn 1	0	0
2	10-D	1	Total 1	Mn 1	0	0
2	1-E	1	Total 1	Mn 1	0	0
2	2-E	1	Total 1	Mn 1	0	0
2	3-E	1	Total 1	Mn 1	0	0
2	4-E	1	Total 1	Mn 1	0	0
2	5-E	1	Total 1	Mn 1	0	0
2	6-E	1	Total 1	Mn 1	0	0
2	7-E	1	Total 1	Mn 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	8-E	1	Total 1	Mn 1	0	0
2	9-E	1	Total 1	Mn 1	0	0
2	10-E	1	Total 1	Mn 1	0	0
2	1-F	1	Total 1	Mn 1	0	0
2	2-F	1	Total 1	Mn 1	0	0
2	3-F	1	Total 1	Mn 1	0	0
2	4-F	1	Total 1	Mn 1	0	0
2	5-F	1	Total 1	Mn 1	0	0
2	6-F	1	Total 1	Mn 1	0	0
2	7-F	1	Total 1	Mn 1	0	0
2	8-F	1	Total 1	Mn 1	0	0
2	9-F	1	Total 1	Mn 1	0	0
2	10-F	1	Total 1	Mn 1	0	0
2	1-G	1	Total 1	Mn 1	0	0
2	2-G	1	Total 1	Mn 1	0	0
2	3-G	1	Total 1	Mn 1	0	0
2	4-G	1	Total 1	Mn 1	0	0
2	5-G	1	Total 1	Mn 1	0	0
2	6-G	1	Total 1	Mn 1	0	0
2	7-G	1	Total 1	Mn 1	0	0
2	8-G	1	Total 1	Mn 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	9-G	1	Total 1	Mn 1	0	0
2	10-G	1	Total 1	Mn 1	0	0
2	1-H	1	Total 1	Mn 1	0	0
2	2-H	1	Total 1	Mn 1	0	0
2	3-H	1	Total 1	Mn 1	0	0
2	4-H	1	Total 1	Mn 1	0	0
2	5-H	1	Total 1	Mn 1	0	0
2	6-H	1	Total 1	Mn 1	0	0
2	7-H	1	Total 1	Mn 1	0	0
2	8-H	1	Total 1	Mn 1	0	0
2	9-H	1	Total 1	Mn 1	0	0
2	10-H	1	Total 1	Mn 1	0	0
2	1-I	1	Total 1	Mn 1	0	0
2	2-I	1	Total 1	Mn 1	0	0
2	3-I	1	Total 1	Mn 1	0	0
2	4-I	1	Total 1	Mn 1	0	0
2	5-I	1	Total 1	Mn 1	0	0
2	6-I	1	Total 1	Mn 1	0	0
2	7-I	1	Total 1	Mn 1	0	0
2	8-I	1	Total 1	Mn 1	0	0
2	9-I	1	Total 1	Mn 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	10-I	1	Total 1	Mn 1	0	0
2	1-J	1	Total 1	Mn 1	0	0
2	2-J	1	Total 1	Mn 1	0	0
2	3-J	1	Total 1	Mn 1	0	0
2	4-J	1	Total 1	Mn 1	0	0
2	5-J	1	Total 1	Mn 1	0	0
2	6-J	1	Total 1	Mn 1	0	0
2	7-J	1	Total 1	Mn 1	0	0
2	8-J	1	Total 1	Mn 1	0	0
2	9-J	1	Total 1	Mn 1	0	0
2	10-J	1	Total 1	Mn 1	0	0
2	1-K	1	Total 1	Mn 1	0	0
2	2-K	1	Total 1	Mn 1	0	0
2	3-K	1	Total 1	Mn 1	0	0
2	4-K	1	Total 1	Mn 1	0	0
2	5-K	1	Total 1	Mn 1	0	0
2	6-K	1	Total 1	Mn 1	0	0
2	7-K	1	Total 1	Mn 1	0	0
2	8-K	1	Total 1	Mn 1	0	0
2	9-K	1	Total 1	Mn 1	0	0
2	10-K	1	Total 1	Mn 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1-L	1	Total 1	Mn 1	0	0
2	2-L	1	Total 1	Mn 1	0	0
2	3-L	1	Total 1	Mn 1	0	0
2	4-L	1	Total 1	Mn 1	0	0
2	5-L	1	Total 1	Mn 1	0	0
2	6-L	1	Total 1	Mn 1	0	0
2	7-L	1	Total 1	Mn 1	0	0
2	8-L	1	Total 1	Mn 1	0	0
2	9-L	1	Total 1	Mn 1	0	0
2	10-L	1	Total 1	Mn 1	0	0
2	1-M	1	Total 1	Mn 1	0	0
2	2-M	1	Total 1	Mn 1	0	0
2	3-M	1	Total 1	Mn 1	0	0
2	4-M	1	Total 1	Mn 1	0	0
2	5-M	1	Total 1	Mn 1	0	0
2	6-M	1	Total 1	Mn 1	0	0
2	7-M	1	Total 1	Mn 1	0	0
2	8-M	1	Total 1	Mn 1	0	0
2	9-M	1	Total 1	Mn 1	0	0
2	10-M	1	Total 1	Mn 1	0	0
2	1-N	1	Total 1	Mn 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	2-N	1	Total 1	Mn 1	0	0
2	3-N	1	Total 1	Mn 1	0	0
2	4-N	1	Total 1	Mn 1	0	0
2	5-N	1	Total 1	Mn 1	0	0
2	6-N	1	Total 1	Mn 1	0	0
2	7-N	1	Total 1	Mn 1	0	0
2	8-N	1	Total 1	Mn 1	0	0
2	9-N	1	Total 1	Mn 1	0	0
2	10-N	1	Total 1	Mn 1	0	0
2	1-O	1	Total 1	Mn 1	0	0
2	2-O	1	Total 1	Mn 1	0	0
2	3-O	1	Total 1	Mn 1	0	0
2	4-O	1	Total 1	Mn 1	0	0
2	5-O	1	Total 1	Mn 1	0	0
2	6-O	1	Total 1	Mn 1	0	0
2	7-O	1	Total 1	Mn 1	0	0
2	8-O	1	Total 1	Mn 1	0	0
2	9-O	1	Total 1	Mn 1	0	0
2	10-O	1	Total 1	Mn 1	0	0
2	1-P	1	Total 1	Mn 1	0	0
2	2-P	1	Total 1	Mn 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	3-P	1	Total 1	Mn 1	0	0
2	4-P	1	Total 1	Mn 1	0	0
2	5-P	1	Total 1	Mn 1	0	0
2	6-P	1	Total 1	Mn 1	0	0
2	7-P	1	Total 1	Mn 1	0	0
2	8-P	1	Total 1	Mn 1	0	0
2	9-P	1	Total 1	Mn 1	0	0
2	10-P	1	Total 1	Mn 1	0	0
2	1-Q	1	Total 1	Mn 1	0	0
2	2-Q	1	Total 1	Mn 1	0	0
2	3-Q	1	Total 1	Mn 1	0	0
2	4-Q	1	Total 1	Mn 1	0	0
2	5-Q	1	Total 1	Mn 1	0	0
2	6-Q	1	Total 1	Mn 1	0	0
2	7-Q	1	Total 1	Mn 1	0	0
2	8-Q	1	Total 1	Mn 1	0	0
2	9-Q	1	Total 1	Mn 1	0	0
2	10-Q	1	Total 1	Mn 1	0	0
2	1-R	1	Total 1	Mn 1	0	0
2	2-R	1	Total 1	Mn 1	0	0
2	3-R	1	Total 1	Mn 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	4-R	1	Total 1	Mn 1	0	0
2	5-R	1	Total 1	Mn 1	0	0
2	6-R	1	Total 1	Mn 1	0	0
2	7-R	1	Total 1	Mn 1	0	0
2	8-R	1	Total 1	Mn 1	0	0
2	9-R	1	Total 1	Mn 1	0	0
2	10-R	1	Total 1	Mn 1	0	0
2	1-S	1	Total 1	Mn 1	0	0
2	2-S	1	Total 1	Mn 1	0	0
2	3-S	1	Total 1	Mn 1	0	0
2	4-S	1	Total 1	Mn 1	0	0
2	5-S	1	Total 1	Mn 1	0	0
2	6-S	1	Total 1	Mn 1	0	0
2	7-S	1	Total 1	Mn 1	0	0
2	8-S	1	Total 1	Mn 1	0	0
2	9-S	1	Total 1	Mn 1	0	0
2	10-S	1	Total 1	Mn 1	0	0
2	1-T	1	Total 1	Mn 1	0	0
2	2-T	1	Total 1	Mn 1	0	0
2	3-T	1	Total 1	Mn 1	0	0
2	4-T	1	Total 1	Mn 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	5-T	1	Total 1	Mn 1	0	0
2	6-T	1	Total 1	Mn 1	0	0
2	7-T	1	Total 1	Mn 1	0	0
2	8-T	1	Total 1	Mn 1	0	0
2	9-T	1	Total 1	Mn 1	0	0
2	10-T	1	Total 1	Mn 1	0	0
2	1-U	1	Total 1	Mn 1	0	0
2	2-U	1	Total 1	Mn 1	0	0
2	3-U	1	Total 1	Mn 1	0	0
2	4-U	1	Total 1	Mn 1	0	0
2	5-U	1	Total 1	Mn 1	0	0
2	6-U	1	Total 1	Mn 1	0	0
2	7-U	1	Total 1	Mn 1	0	0
2	8-U	1	Total 1	Mn 1	0	0
2	9-U	1	Total 1	Mn 1	0	0
2	10-U	1	Total 1	Mn 1	0	0
2	1-V	1	Total 1	Mn 1	0	0
2	2-V	1	Total 1	Mn 1	0	0
2	3-V	1	Total 1	Mn 1	0	0
2	4-V	1	Total 1	Mn 1	0	0
2	5-V	1	Total 1	Mn 1	0	0

Continued on next page...

Continued from previous page...

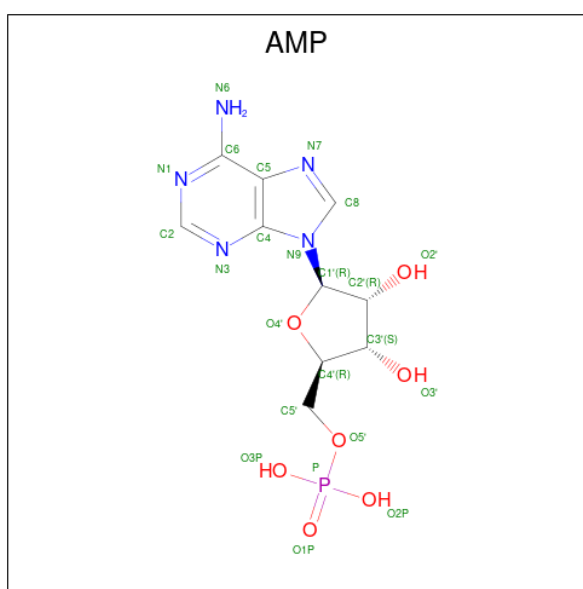
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	6-V	1	Total 1	Mn 1	0	0
2	7-V	1	Total 1	Mn 1	0	0
2	8-V	1	Total 1	Mn 1	0	0
2	9-V	1	Total 1	Mn 1	0	0
2	10-V	1	Total 1	Mn 1	0	0
2	1-W	1	Total 1	Mn 1	0	0
2	2-W	1	Total 1	Mn 1	0	0
2	3-W	1	Total 1	Mn 1	0	0
2	4-W	1	Total 1	Mn 1	0	0
2	5-W	1	Total 1	Mn 1	0	0
2	6-W	1	Total 1	Mn 1	0	0
2	7-W	1	Total 1	Mn 1	0	0
2	8-W	1	Total 1	Mn 1	0	0
2	9-W	1	Total 1	Mn 1	0	0
2	10-W	1	Total 1	Mn 1	0	0
2	1-X	1	Total 1	Mn 1	0	0
2	2-X	1	Total 1	Mn 1	0	0
2	3-X	1	Total 1	Mn 1	0	0
2	4-X	1	Total 1	Mn 1	0	0
2	5-X	1	Total 1	Mn 1	0	0
2	6-X	1	Total 1	Mn 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	7-X	1	Total	Mn	0	0
			1	1		
2	8-X	1	Total	Mn	0	0
			1	1		
2	9-X	1	Total	Mn	0	0
			1	1		
2	10-X	1	Total	Mn	0	0
			1	1		

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	1-A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	2-A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	3-A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	4-A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	5-A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	6-A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	7-A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	8-A	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-A	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-A	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-C	1	Total 23	C 10	N 5	O 7	P 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	9-C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-E	1	Total 23	C 10	N 5	O 7	P 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	10-E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-G	1	Total 23	C 10	N 5	O 7	P 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	1-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-J	1	Total 23	C 10	N 5	O 7	P 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	2-J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-L	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-L	1	Total 23	C 10	N 5	O 7	P 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	3-L	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	4-L	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	5-L	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	6-L	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	7-L	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	8-L	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	9-L	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	10-L	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	1-M	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	2-M	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	3-M	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	4-M	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	5-M	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	6-M	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	7-M	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	8-M	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	9-M	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	10-M	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	1-N	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	2-N	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	3-N	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	4-N	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-N	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-N	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-N	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-N	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-N	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-N	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-P	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-P	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-P	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-P	1	Total 23	C 10	N 5	O 7	P 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	5-P	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	6-P	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	7-P	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	8-P	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	9-P	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	10-P	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	1-Q	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	2-Q	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	3-Q	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	4-Q	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	5-Q	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	6-Q	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	7-Q	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	8-Q	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	9-Q	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	10-Q	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	1-R	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	2-R	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	3-R	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	4-R	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	5-R	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	6-R	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	7-R	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	8-R	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	9-R	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	10-R	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	1-S	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	2-S	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	3-S	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	4-S	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	5-S	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	6-S	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	7-S	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	8-S	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	9-S	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	10-S	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	1-T	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	2-T	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	3-T	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	4-T	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	5-T	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	6-T	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	7-T	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-T	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-T	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-T	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-V	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-V	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-V	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-V	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-V	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-V	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-V	1	Total 23	C 10	N 5	O 7	P 1	0	0

Continued on next page...

Continued from previous page...

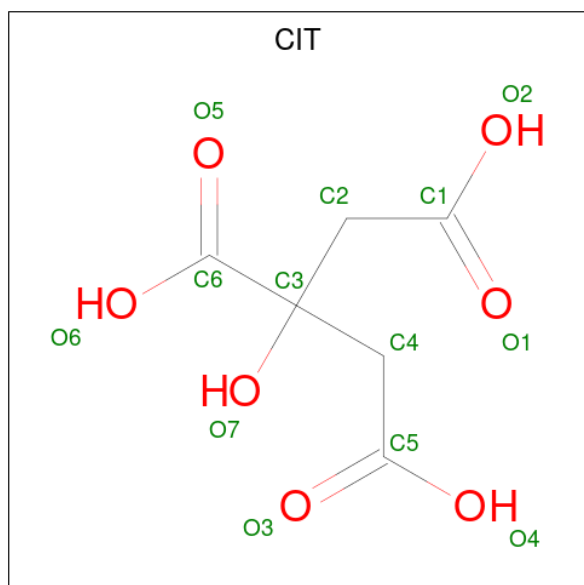
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	8-V	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-V	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-V	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-X	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-X	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-X	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-X	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-X	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-X	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-X	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-X	1	Total 23	C 10	N 5	O 7	P 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	9-X	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	10-X	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	1-A	1	Total	C	O	0	0
			13	6	7		
4	2-A	1	Total	C	O	0	0
			13	6	7		
4	3-A	1	Total	C	O	0	0
			13	6	7		
4	4-A	1	Total	C	O	0	0
			13	6	7		
4	5-A	1	Total	C	O	0	0
			13	6	7		
4	6-A	1	Total	C	O	0	0
			13	6	7		
4	7-A	1	Total	C	O	0	0
			13	6	7		
4	8-A	1	Total	C	O	0	0
			13	6	7		
4	9-A	1	Total	C	O	0	0
			13	6	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	10-A	1	13	6	7	0	0
4	1-B	1	13	6	7	0	0
4	2-B	1	13	6	7	0	0
4	3-B	1	13	6	7	0	0
4	4-B	1	13	6	7	0	0
4	5-B	1	13	6	7	0	0
4	6-B	1	13	6	7	0	0
4	7-B	1	13	6	7	0	0
4	8-B	1	13	6	7	0	0
4	9-B	1	13	6	7	0	0
4	10-B	1	13	6	7	0	0
4	1-C	1	13	6	7	0	0
4	2-C	1	13	6	7	0	0
4	3-C	1	13	6	7	0	0
4	4-C	1	13	6	7	0	0
4	5-C	1	13	6	7	0	0
4	6-C	1	13	6	7	0	0
4	7-C	1	13	6	7	0	0
4	8-C	1	13	6	7	0	0
4	9-C	1	13	6	7	0	0
4	10-C	1	13	6	7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	1-D	1	Total	C	O	0	0
			13	6	7		
4	2-D	1	Total	C	O	0	0
			13	6	7		
4	3-D	1	Total	C	O	0	0
			13	6	7		
4	4-D	1	Total	C	O	0	0
			13	6	7		
4	5-D	1	Total	C	O	0	0
			13	6	7		
4	6-D	1	Total	C	O	0	0
			13	6	7		
4	7-D	1	Total	C	O	0	0
			13	6	7		
4	8-D	1	Total	C	O	0	0
			13	6	7		
4	9-D	1	Total	C	O	0	0
			13	6	7		
4	10-D	1	Total	C	O	0	0
			13	6	7		
4	1-E	1	Total	C	O	0	0
			13	6	7		
4	2-E	1	Total	C	O	0	0
			13	6	7		
4	3-E	1	Total	C	O	0	0
			13	6	7		
4	4-E	1	Total	C	O	0	0
			13	6	7		
4	5-E	1	Total	C	O	0	0
			13	6	7		
4	6-E	1	Total	C	O	0	0
			13	6	7		
4	7-E	1	Total	C	O	0	0
			13	6	7		
4	8-E	1	Total	C	O	0	0
			13	6	7		
4	9-E	1	Total	C	O	0	0
			13	6	7		
4	10-E	1	Total	C	O	0	0
			13	6	7		
4	1-F	1	Total	C	O	0	0
			13	6	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	2-F	1	Total	C	O	0	0
			13	6	7		
4	3-F	1	Total	C	O	0	0
			13	6	7		
4	4-F	1	Total	C	O	0	0
			13	6	7		
4	5-F	1	Total	C	O	0	0
			13	6	7		
4	6-F	1	Total	C	O	0	0
			13	6	7		
4	7-F	1	Total	C	O	0	0
			13	6	7		
4	8-F	1	Total	C	O	0	0
			13	6	7		
4	9-F	1	Total	C	O	0	0
			13	6	7		
4	10-F	1	Total	C	O	0	0
			13	6	7		
4	1-G	1	Total	C	O	0	0
			13	6	7		
4	2-G	1	Total	C	O	0	0
			13	6	7		
4	3-G	1	Total	C	O	0	0
			13	6	7		
4	4-G	1	Total	C	O	0	0
			13	6	7		
4	5-G	1	Total	C	O	0	0
			13	6	7		
4	6-G	1	Total	C	O	0	0
			13	6	7		
4	7-G	1	Total	C	O	0	0
			13	6	7		
4	8-G	1	Total	C	O	0	0
			13	6	7		
4	9-G	1	Total	C	O	0	0
			13	6	7		
4	10-G	1	Total	C	O	0	0
			13	6	7		
4	1-H	1	Total	C	O	0	0
			13	6	7		
4	2-H	1	Total	C	O	0	0
			13	6	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	3-H	1	13	6	7	0	0
4	4-H	1	13	6	7	0	0
4	5-H	1	13	6	7	0	0
4	6-H	1	13	6	7	0	0
4	7-H	1	13	6	7	0	0
4	8-H	1	13	6	7	0	0
4	9-H	1	13	6	7	0	0
4	10-H	1	13	6	7	0	0
4	1-I	1	13	6	7	0	0
4	2-I	1	13	6	7	0	0
4	3-I	1	13	6	7	0	0
4	4-I	1	13	6	7	0	0
4	5-I	1	13	6	7	0	0
4	6-I	1	13	6	7	0	0
4	7-I	1	13	6	7	0	0
4	8-I	1	13	6	7	0	0
4	9-I	1	13	6	7	0	0
4	10-I	1	13	6	7	0	0
4	1-J	1	13	6	7	0	0
4	2-J	1	13	6	7	0	0
4	3-J	1	13	6	7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	4-J	1	13	6	7	0	0
4	5-J	1	13	6	7	0	0
4	6-J	1	13	6	7	0	0
4	7-J	1	13	6	7	0	0
4	8-J	1	13	6	7	0	0
4	9-J	1	13	6	7	0	0
4	10-J	1	13	6	7	0	0
4	1-K	1	13	6	7	0	0
4	2-K	1	13	6	7	0	0
4	3-K	1	13	6	7	0	0
4	4-K	1	13	6	7	0	0
4	5-K	1	13	6	7	0	0
4	6-K	1	13	6	7	0	0
4	7-K	1	13	6	7	0	0
4	8-K	1	13	6	7	0	0
4	9-K	1	13	6	7	0	0
4	10-K	1	13	6	7	0	0
4	1-L	1	13	6	7	0	0
4	2-L	1	13	6	7	0	0
4	3-L	1	13	6	7	0	0
4	4-L	1	13	6	7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	5-L	1	Total	C	O	0	0
			13	6	7		
4	6-L	1	Total	C	O	0	0
			13	6	7		
4	7-L	1	Total	C	O	0	0
			13	6	7		
4	8-L	1	Total	C	O	0	0
			13	6	7		
4	9-L	1	Total	C	O	0	0
			13	6	7		
4	10-L	1	Total	C	O	0	0
			13	6	7		
4	1-M	1	Total	C	O	0	0
			13	6	7		
4	2-M	1	Total	C	O	0	0
			13	6	7		
4	3-M	1	Total	C	O	0	0
			13	6	7		
4	4-M	1	Total	C	O	0	0
			13	6	7		
4	5-M	1	Total	C	O	0	0
			13	6	7		
4	6-M	1	Total	C	O	0	0
			13	6	7		
4	7-M	1	Total	C	O	0	0
			13	6	7		
4	8-M	1	Total	C	O	0	0
			13	6	7		
4	9-M	1	Total	C	O	0	0
			13	6	7		
4	10-M	1	Total	C	O	0	0
			13	6	7		
4	1-N	1	Total	C	O	0	0
			13	6	7		
4	2-N	1	Total	C	O	0	0
			13	6	7		
4	3-N	1	Total	C	O	0	0
			13	6	7		
4	4-N	1	Total	C	O	0	0
			13	6	7		
4	5-N	1	Total	C	O	0	0
			13	6	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	6-N	1	13	6	7	0	0
4	7-N	1	13	6	7	0	0
4	8-N	1	13	6	7	0	0
4	9-N	1	13	6	7	0	0
4	10-N	1	13	6	7	0	0
4	1-O	1	13	6	7	0	0
4	2-O	1	13	6	7	0	0
4	3-O	1	13	6	7	0	0
4	4-O	1	13	6	7	0	0
4	5-O	1	13	6	7	0	0
4	6-O	1	13	6	7	0	0
4	7-O	1	13	6	7	0	0
4	8-O	1	13	6	7	0	0
4	9-O	1	13	6	7	0	0
4	10-O	1	13	6	7	0	0
4	1-P	1	13	6	7	0	0
4	2-P	1	13	6	7	0	0
4	3-P	1	13	6	7	0	0
4	4-P	1	13	6	7	0	0
4	5-P	1	13	6	7	0	0
4	6-P	1	13	6	7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	7-P	1	Total	C	O	0	0
			13	6	7		
4	8-P	1	Total	C	O	0	0
			13	6	7		
4	9-P	1	Total	C	O	0	0
			13	6	7		
4	10-P	1	Total	C	O	0	0
			13	6	7		
4	1-Q	1	Total	C	O	0	0
			13	6	7		
4	2-Q	1	Total	C	O	0	0
			13	6	7		
4	3-Q	1	Total	C	O	0	0
			13	6	7		
4	4-Q	1	Total	C	O	0	0
			13	6	7		
4	5-Q	1	Total	C	O	0	0
			13	6	7		
4	6-Q	1	Total	C	O	0	0
			13	6	7		
4	7-Q	1	Total	C	O	0	0
			13	6	7		
4	8-Q	1	Total	C	O	0	0
			13	6	7		
4	9-Q	1	Total	C	O	0	0
			13	6	7		
4	10-Q	1	Total	C	O	0	0
			13	6	7		
4	1-R	1	Total	C	O	0	0
			13	6	7		
4	2-R	1	Total	C	O	0	0
			13	6	7		
4	3-R	1	Total	C	O	0	0
			13	6	7		
4	4-R	1	Total	C	O	0	0
			13	6	7		
4	5-R	1	Total	C	O	0	0
			13	6	7		
4	6-R	1	Total	C	O	0	0
			13	6	7		
4	7-R	1	Total	C	O	0	0
			13	6	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	8-R	1	13	6	7	0	0
4	9-R	1	13	6	7	0	0
4	10-R	1	13	6	7	0	0
4	1-S	1	13	6	7	0	0
4	2-S	1	13	6	7	0	0
4	3-S	1	13	6	7	0	0
4	4-S	1	13	6	7	0	0
4	5-S	1	13	6	7	0	0
4	6-S	1	13	6	7	0	0
4	7-S	1	13	6	7	0	0
4	8-S	1	13	6	7	0	0
4	9-S	1	13	6	7	0	0
4	10-S	1	13	6	7	0	0
4	1-T	1	13	6	7	0	0
4	2-T	1	13	6	7	0	0
4	3-T	1	13	6	7	0	0
4	4-T	1	13	6	7	0	0
4	5-T	1	13	6	7	0	0
4	6-T	1	13	6	7	0	0
4	7-T	1	13	6	7	0	0
4	8-T	1	13	6	7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	9-T	1	Total	C	O	0	0
			13	6	7		
4	10-T	1	Total	C	O	0	0
			13	6	7		
4	1-U	1	Total	C	O	0	0
			13	6	7		
4	2-U	1	Total	C	O	0	0
			13	6	7		
4	3-U	1	Total	C	O	0	0
			13	6	7		
4	4-U	1	Total	C	O	0	0
			13	6	7		
4	5-U	1	Total	C	O	0	0
			13	6	7		
4	6-U	1	Total	C	O	0	0
			13	6	7		
4	7-U	1	Total	C	O	0	0
			13	6	7		
4	8-U	1	Total	C	O	0	0
			13	6	7		
4	9-U	1	Total	C	O	0	0
			13	6	7		
4	10-U	1	Total	C	O	0	0
			13	6	7		
4	1-V	1	Total	C	O	0	0
			13	6	7		
4	2-V	1	Total	C	O	0	0
			13	6	7		
4	3-V	1	Total	C	O	0	0
			13	6	7		
4	4-V	1	Total	C	O	0	0
			13	6	7		
4	5-V	1	Total	C	O	0	0
			13	6	7		
4	6-V	1	Total	C	O	0	0
			13	6	7		
4	7-V	1	Total	C	O	0	0
			13	6	7		
4	8-V	1	Total	C	O	0	0
			13	6	7		
4	9-V	1	Total	C	O	0	0
			13	6	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	10-V	1	13	6	7	0	0
4	1-W	1	13	6	7	0	0
4	2-W	1	13	6	7	0	0
4	3-W	1	13	6	7	0	0
4	4-W	1	13	6	7	0	0
4	5-W	1	13	6	7	0	0
4	6-W	1	13	6	7	0	0
4	7-W	1	13	6	7	0	0
4	8-W	1	13	6	7	0	0
4	9-W	1	13	6	7	0	0
4	10-W	1	13	6	7	0	0
4	1-X	1	13	6	7	0	0
4	2-X	1	13	6	7	0	0
4	3-X	1	13	6	7	0	0
4	4-X	1	13	6	7	0	0
4	5-X	1	13	6	7	0	0
4	6-X	1	13	6	7	0	0
4	7-X	1	13	6	7	0	0
4	8-X	1	13	6	7	0	0
4	9-X	1	13	6	7	0	0
4	10-X	1	13	6	7	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	1-A	261	Total O 261 261	0	0
5	2-A	262	Total O 262 262	0	0
5	3-A	261	Total O 261 261	0	0
5	4-A	263	Total O 263 263	0	0
5	5-A	261	Total O 261 261	0	0
5	6-A	257	Total O 257 257	0	0
5	7-A	265	Total O 265 265	0	0
5	8-A	259	Total O 259 259	0	0
5	9-A	265	Total O 265 265	0	0
5	10-A	262	Total O 262 262	0	0
5	1-B	264	Total O 264 264	0	0
5	2-B	261	Total O 261 261	0	0
5	3-B	263	Total O 263 263	0	0
5	4-B	262	Total O 262 262	0	0
5	5-B	261	Total O 261 261	0	0
5	6-B	265	Total O 265 265	0	0
5	7-B	264	Total O 264 264	0	0
5	8-B	264	Total O 264 264	0	0
5	9-B	258	Total O 258 258	0	0
5	10-B	263	Total O 263 263	0	0
5	1-C	261	Total O 261 261	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	2-C	264	Total O 264 264	0	0
5	3-C	265	Total O 265 265	0	0
5	4-C	261	Total O 261 261	0	0
5	5-C	263	Total O 263 263	0	0
5	6-C	262	Total O 262 262	0	0
5	7-C	262	Total O 262 262	0	0
5	8-C	263	Total O 263 263	0	0
5	9-C	261	Total O 261 261	0	0
5	10-C	262	Total O 262 262	0	0
5	1-D	260	Total O 260 260	0	0
5	2-D	269	Total O 269 269	0	0
5	3-D	260	Total O 260 260	0	0
5	4-D	263	Total O 263 263	0	0
5	5-D	262	Total O 262 262	0	0
5	6-D	265	Total O 265 265	0	0
5	7-D	261	Total O 261 261	0	0
5	8-D	265	Total O 265 265	0	0
5	9-D	266	Total O 266 266	0	0
5	10-D	262	Total O 262 262	0	0
5	1-E	261	Total O 261 261	0	0
5	2-E	254	Total O 254 254	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	3-E	257	Total O 257 257	0	0
5	4-E	263	Total O 263 263	0	0
5	5-E	259	Total O 259 259	0	0
5	6-E	262	Total O 262 262	0	0
5	7-E	265	Total O 265 265	0	0
5	8-E	257	Total O 257 257	0	0
5	9-E	262	Total O 262 262	0	0
5	10-E	257	Total O 257 257	0	0
5	1-F	262	Total O 262 262	0	0
5	2-F	263	Total O 263 263	0	0
5	3-F	272	Total O 272 272	0	0
5	4-F	264	Total O 264 264	0	0
5	5-F	266	Total O 266 266	0	0
5	6-F	263	Total O 263 263	0	0
5	7-F	262	Total O 262 262	0	0
5	8-F	268	Total O 268 268	0	0
5	9-F	262	Total O 262 262	0	0
5	10-F	261	Total O 261 261	0	0
5	1-G	265	Total O 265 265	0	0
5	2-G	262	Total O 262 262	0	0
5	3-G	257	Total O 257 257	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	4-G	261	Total O 261 261	0	0
5	5-G	263	Total O 263 263	0	0
5	6-G	267	Total O 267 267	0	0
5	7-G	259	Total O 259 259	0	0
5	8-G	265	Total O 265 265	0	0
5	9-G	263	Total O 263 263	0	0
5	10-G	264	Total O 264 264	0	0
5	1-H	262	Total O 262 262	0	0
5	2-H	263	Total O 263 263	0	0
5	3-H	261	Total O 261 261	0	0
5	4-H	266	Total O 266 266	0	0
5	5-H	270	Total O 270 270	0	0
5	6-H	263	Total O 263 263	0	0
5	7-H	262	Total O 262 262	0	0
5	8-H	261	Total O 261 261	0	0
5	9-H	268	Total O 268 268	0	0
5	10-H	264	Total O 264 264	0	0
5	1-I	265	Total O 265 265	0	0
5	2-I	265	Total O 265 265	0	0
5	3-I	266	Total O 266 266	0	0
5	4-I	263	Total O 263 263	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	5-I	260	Total O 260 260	0	0
5	6-I	263	Total O 263 263	0	0
5	7-I	261	Total O 261 261	0	0
5	8-I	265	Total O 265 265	0	0
5	9-I	262	Total O 262 262	0	0
5	10-I	263	Total O 263 263	0	0
5	1-J	262	Total O 262 262	0	0
5	2-J	258	Total O 258 258	0	0
5	3-J	260	Total O 260 260	0	0
5	4-J	260	Total O 260 260	0	0
5	5-J	263	Total O 263 263	0	0
5	6-J	259	Total O 259 259	0	0
5	7-J	266	Total O 266 266	0	0
5	8-J	263	Total O 263 263	0	0
5	9-J	260	Total O 260 260	0	0
5	10-J	264	Total O 264 264	0	0
5	1-K	272	Total O 272 272	0	0
5	2-K	271	Total O 271 271	0	0
5	3-K	268	Total O 268 268	0	0
5	4-K	267	Total O 267 267	0	0
5	5-K	268	Total O 268 268	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	6-K	270	Total O 270 270	0	0
5	7-K	263	Total O 263 263	0	0
5	8-K	264	Total O 264 264	0	0
5	9-K	269	Total O 269 269	0	0
5	10-K	271	Total O 271 271	0	0
5	1-L	261	Total O 261 261	0	0
5	2-L	264	Total O 264 264	0	0
5	3-L	266	Total O 266 266	0	0
5	4-L	263	Total O 263 263	0	0
5	5-L	260	Total O 260 260	0	0
5	6-L	260	Total O 260 260	0	0
5	7-L	266	Total O 266 266	0	0
5	8-L	262	Total O 262 262	0	0
5	9-L	260	Total O 260 260	0	0
5	10-L	263	Total O 263 263	0	0
5	1-M	261	Total O 261 261	0	0
5	2-M	264	Total O 264 264	0	0
5	3-M	259	Total O 259 259	0	0
5	4-M	264	Total O 264 264	0	0
5	5-M	264	Total O 264 264	0	0
5	6-M	262	Total O 262 262	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	7-M	260	Total O 260 260	0	0
5	8-M	260	Total O 260 260	0	0
5	9-M	265	Total O 265 265	0	0
5	10-M	263	Total O 263 263	0	0
5	1-N	263	Total O 263 263	0	0
5	2-N	261	Total O 261 261	0	0
5	3-N	263	Total O 263 263	0	0
5	4-N	263	Total O 263 263	0	0
5	5-N	265	Total O 265 265	0	0
5	6-N	260	Total O 260 260	0	0
5	7-N	266	Total O 266 266	0	0
5	8-N	263	Total O 263 263	0	0
5	9-N	261	Total O 261 261	0	0
5	10-N	259	Total O 259 259	0	0
5	1-O	263	Total O 263 263	0	0
5	2-O	267	Total O 267 267	0	0
5	3-O	265	Total O 265 265	0	0
5	4-O	263	Total O 263 263	0	0
5	5-O	267	Total O 267 267	0	0
5	6-O	265	Total O 265 265	0	0
5	7-O	262	Total O 262 262	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	8-O	265	Total O 265 265	0	0
5	9-O	263	Total O 263 263	0	0
5	10-O	263	Total O 263 263	0	0
5	1-P	261	Total O 261 261	0	0
5	2-P	264	Total O 264 264	0	0
5	3-P	260	Total O 260 260	0	0
5	4-P	259	Total O 259 259	0	0
5	5-P	262	Total O 262 262	0	0
5	6-P	262	Total O 262 262	0	0
5	7-P	261	Total O 261 261	0	0
5	8-P	263	Total O 263 263	0	0
5	9-P	265	Total O 265 265	0	0
5	10-P	264	Total O 264 264	0	0
5	1-Q	260	Total O 260 260	0	0
5	2-Q	257	Total O 257 257	0	0
5	3-Q	259	Total O 259 259	0	0
5	4-Q	264	Total O 264 264	0	0
5	5-Q	261	Total O 261 261	0	0
5	6-Q	260	Total O 260 260	0	0
5	7-Q	264	Total O 264 264	0	0
5	8-Q	257	Total O 257 257	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	9-Q	263	Total O 263 263	0	0
5	10-Q	257	Total O 257 257	0	0
5	1-R	261	Total O 261 261	0	0
5	2-R	265	Total O 265 265	0	0
5	3-R	268	Total O 268 268	0	0
5	4-R	263	Total O 263 263	0	0
5	5-R	265	Total O 265 265	0	0
5	6-R	266	Total O 266 266	0	0
5	7-R	264	Total O 264 264	0	0
5	8-R	265	Total O 265 265	0	0
5	9-R	264	Total O 264 264	0	0
5	10-R	262	Total O 262 262	0	0
5	1-S	265	Total O 265 265	0	0
5	2-S	259	Total O 259 259	0	0
5	3-S	264	Total O 264 264	0	0
5	4-S	260	Total O 260 260	0	0
5	5-S	263	Total O 263 263	0	0
5	6-S	266	Total O 266 266	0	0
5	7-S	263	Total O 263 263	0	0
5	8-S	269	Total O 269 269	0	0
5	9-S	259	Total O 259 259	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	10-S	266	Total 266	O 266	0	0
5	1-T	261	Total 261	O 261	0	0
5	2-T	259	Total 259	O 259	0	0
5	3-T	262	Total 262	O 262	0	0
5	4-T	262	Total 262	O 262	0	0
5	5-T	258	Total 258	O 258	0	0
5	6-T	257	Total 257	O 257	0	0
5	7-T	263	Total 263	O 263	0	0
5	8-T	259	Total 259	O 259	0	0
5	9-T	265	Total 265	O 265	0	0
5	10-T	262	Total 262	O 262	0	0
5	1-U	263	Total 263	O 263	0	0
5	2-U	267	Total 267	O 267	0	0
5	3-U	267	Total 267	O 267	0	0
5	4-U	264	Total 264	O 264	0	0
5	5-U	263	Total 263	O 263	0	0
5	6-U	265	Total 265	O 265	0	0
5	7-U	262	Total 262	O 262	0	0
5	8-U	263	Total 263	O 263	0	0
5	9-U	265	Total 265	O 265	0	0
5	10-U	264	Total 264	O 264	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1-V	265	Total 265	O 265	0	0
5	2-V	260	Total 260	O 260	0	0
5	3-V	258	Total 258	O 258	0	0
5	4-V	266	Total 266	O 266	0	0
5	5-V	261	Total 261	O 261	0	0
5	6-V	265	Total 265	O 265	0	0
5	7-V	265	Total 265	O 265	0	0
5	8-V	264	Total 264	O 264	0	0
5	9-V	259	Total 259	O 259	0	0
5	10-V	265	Total 265	O 265	0	0
5	1-W	269	Total 269	O 269	0	0
5	2-W	266	Total 266	O 266	0	0
5	3-W	266	Total 266	O 266	0	0
5	4-W	263	Total 263	O 263	0	0
5	5-W	262	Total 262	O 262	0	0
5	6-W	264	Total 264	O 264	0	0
5	7-W	265	Total 265	O 265	0	0
5	8-W	263	Total 263	O 263	0	0
5	9-W	261	Total 261	O 261	0	0
5	10-W	265	Total 265	O 265	0	0
5	1-X	264	Total 264	O 264	0	0

Continued on next page...

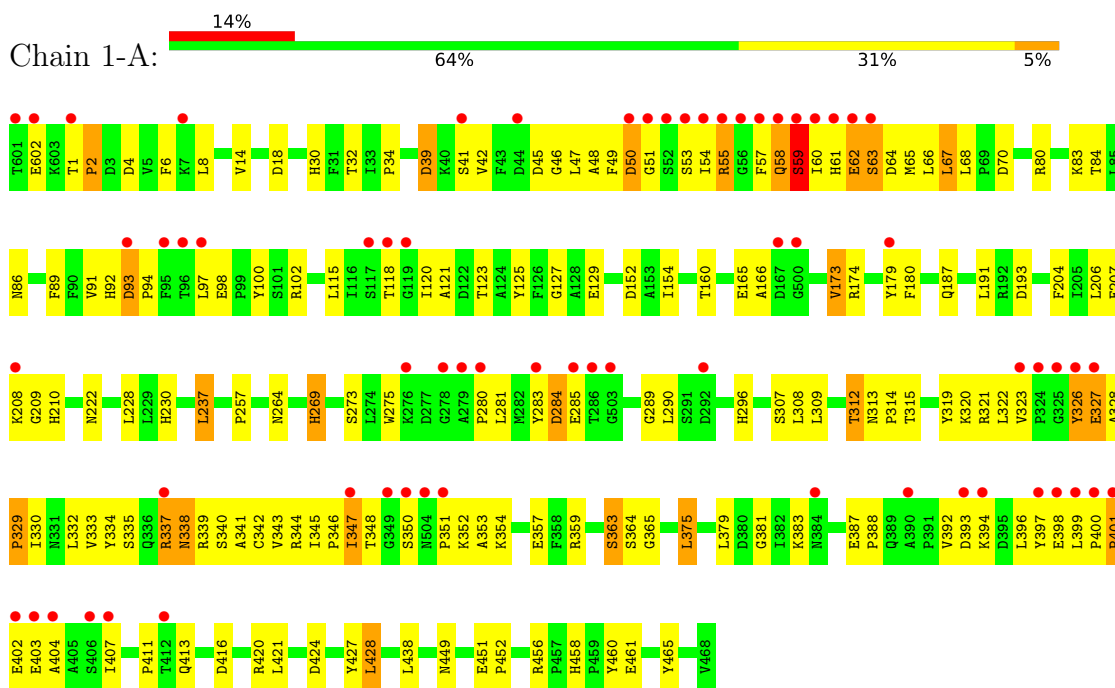
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	2-X	267	Total 267	O 267	0	0
5	3-X	265	Total 265	O 265	0	0
5	4-X	265	Total 265	O 265	0	0
5	5-X	265	Total 265	O 265	0	0
5	6-X	264	Total 264	O 264	0	0
5	7-X	261	Total 261	O 261	0	0
5	8-X	265	Total 265	O 265	0	0
5	9-X	266	Total 266	O 266	0	0
5	10-X	266	Total 266	O 266	0	0

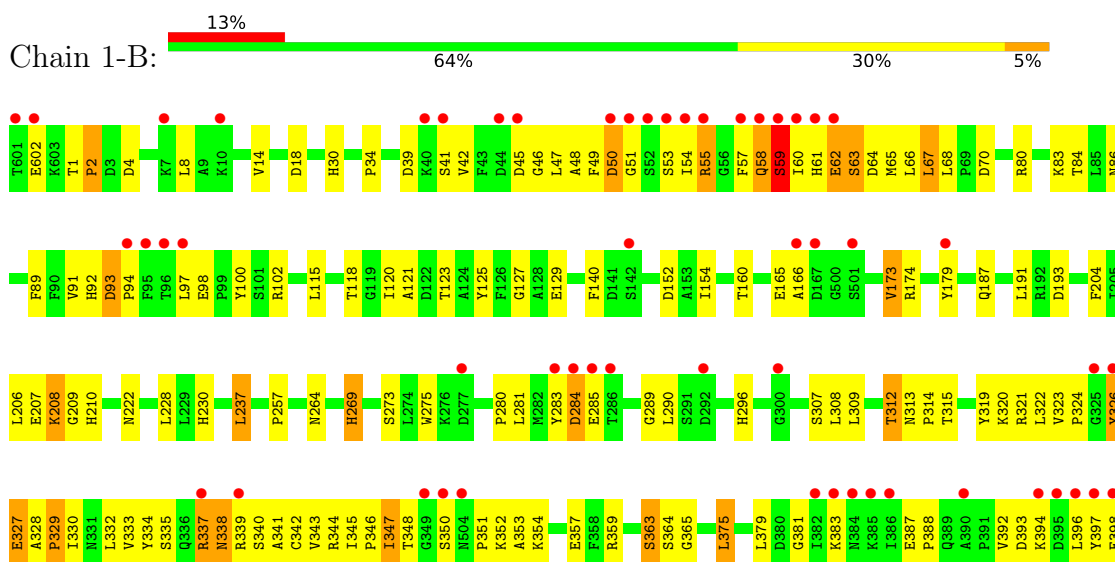
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: glutamine synthetase

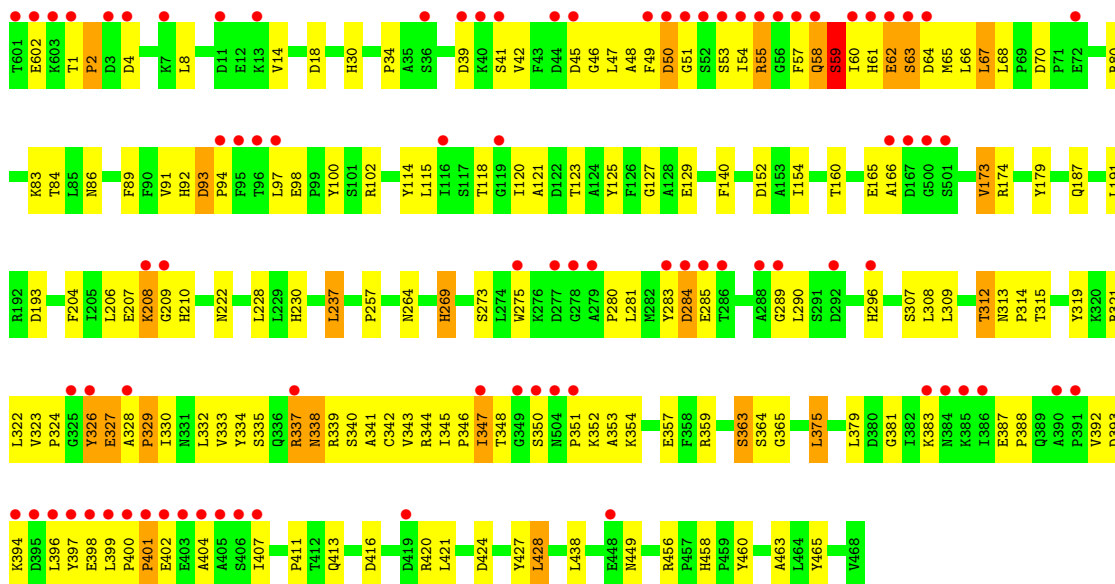


- Molecule 1: glutamine synthetase

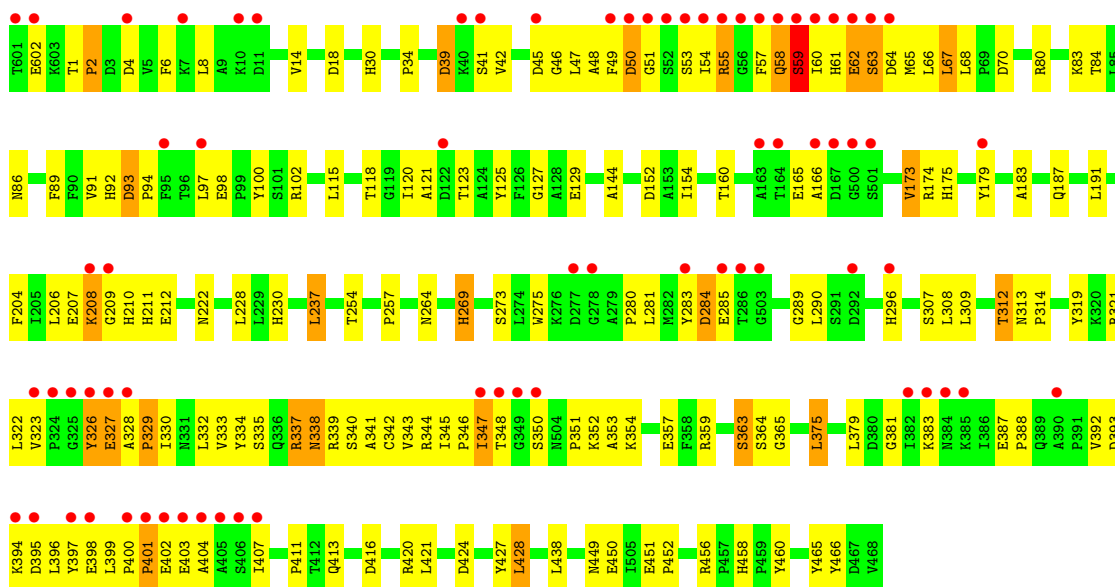




- Molecule 1: glutamine synthetase

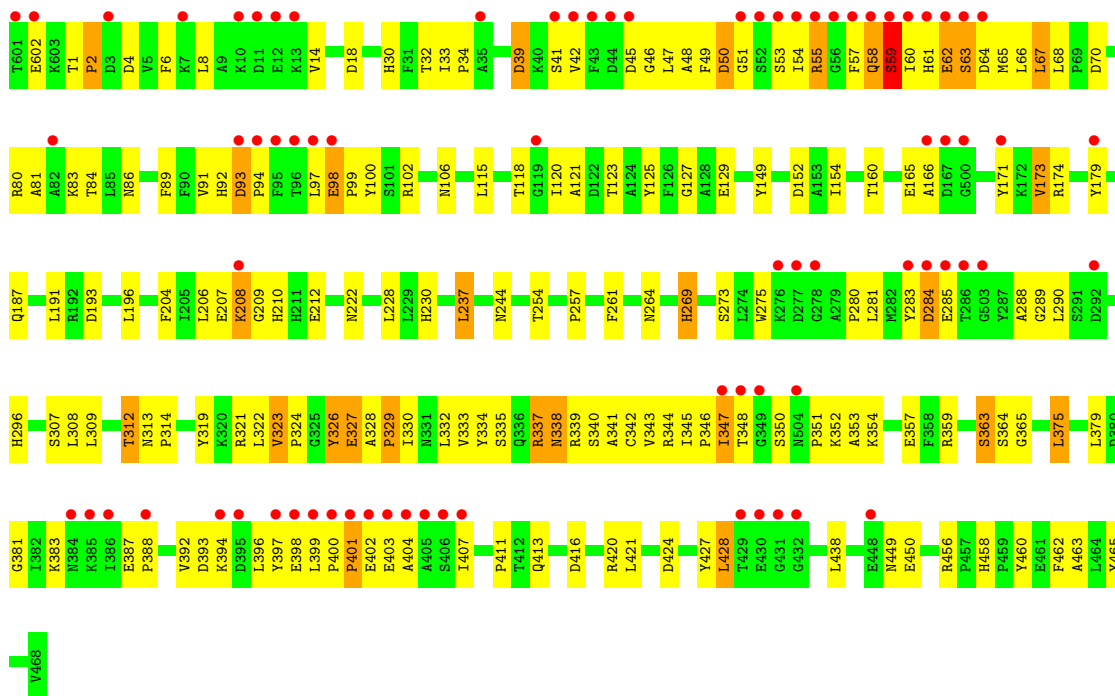


- Molecule 1: glutamine synthetase

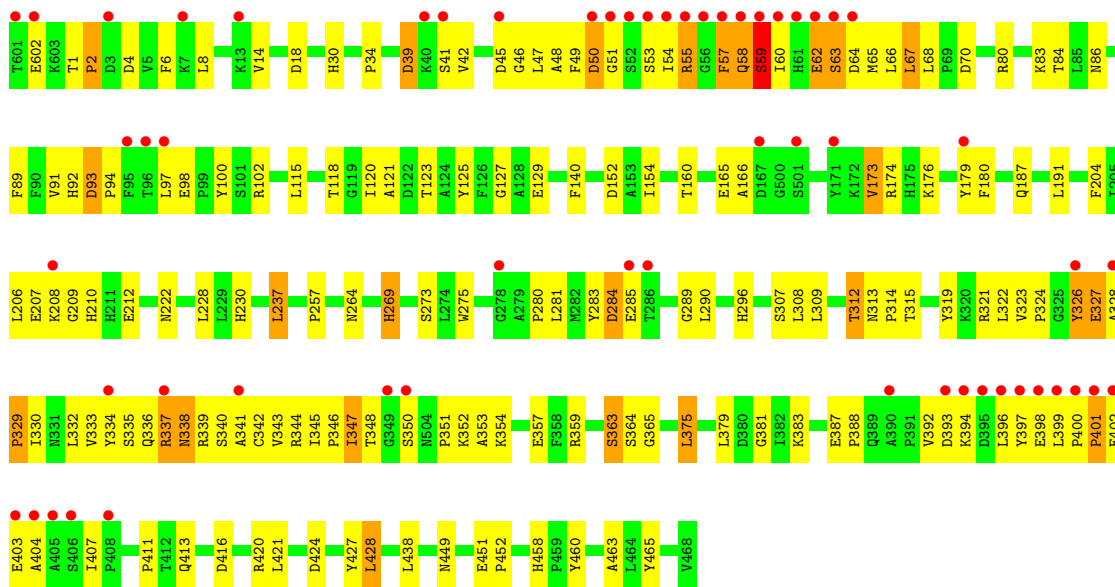


- Molecule 1: glutamine synthetase

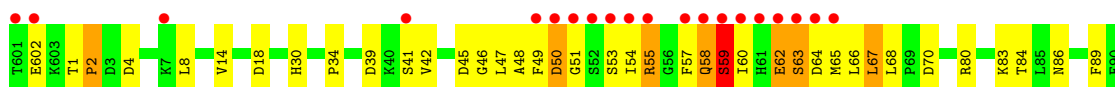


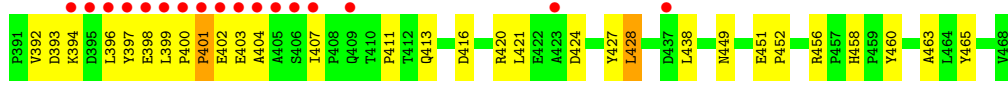
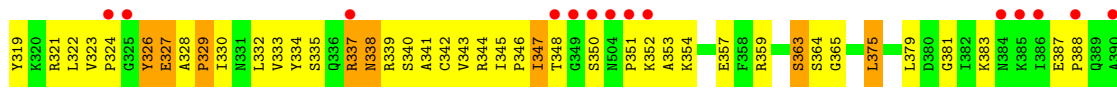


• Molecule 1: glutamine synthetase

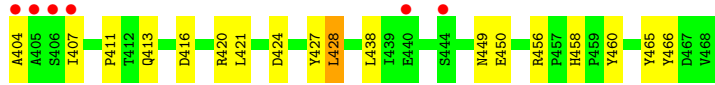
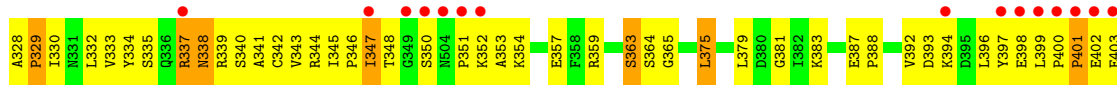
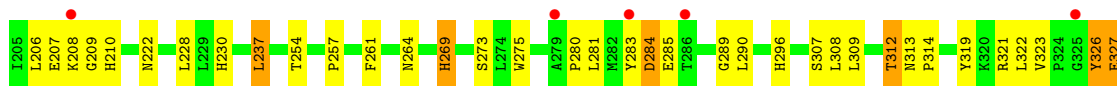
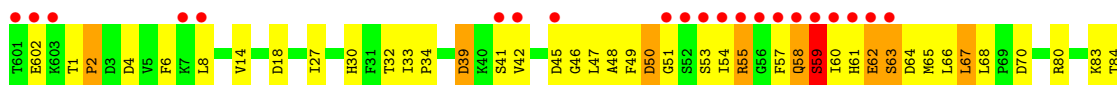


• Molecule 1: glutamine synthetase

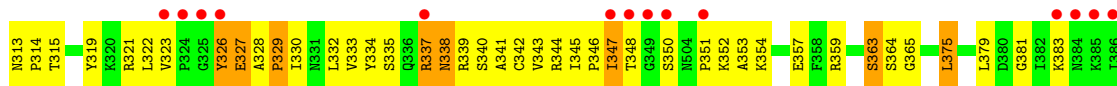
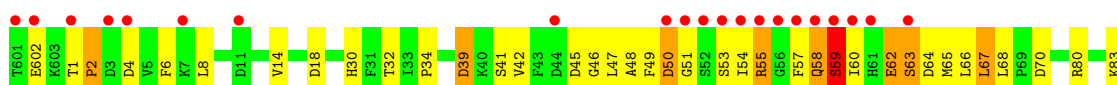




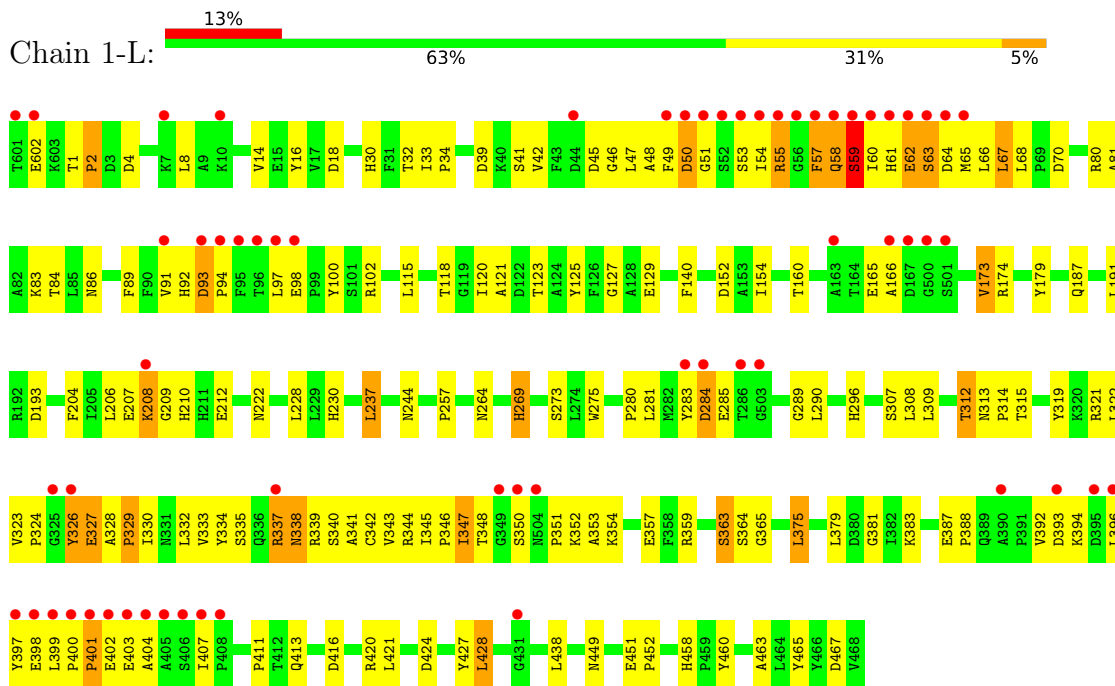
• Molecule 1: glutamine synthetase



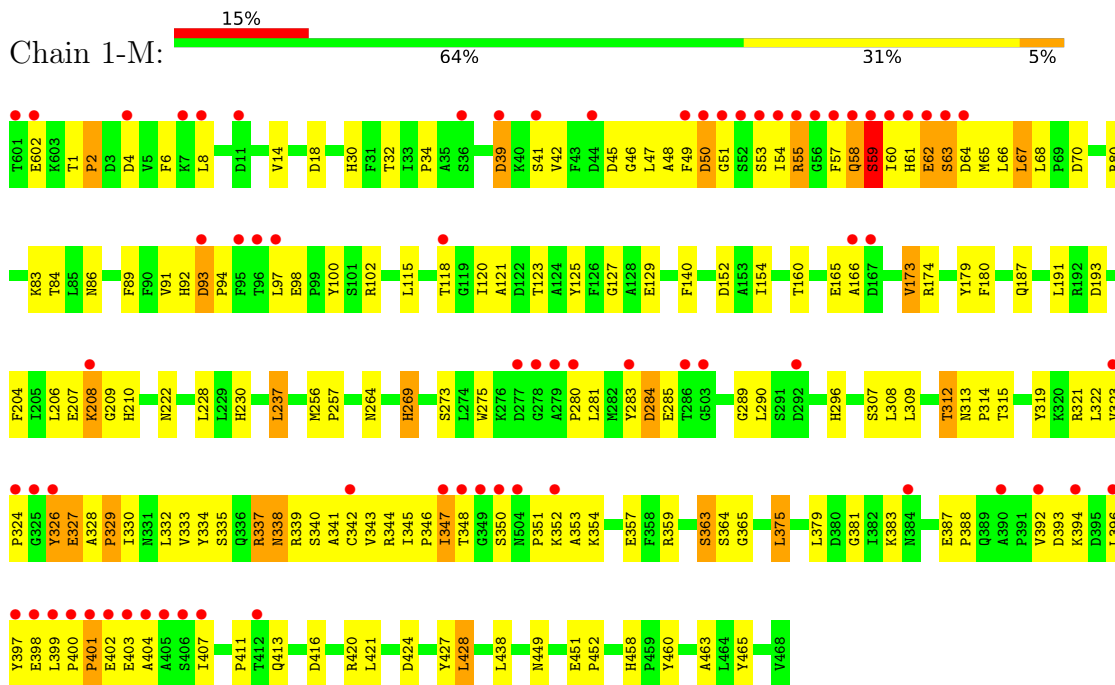
• Molecule 1: glutamine synthetase



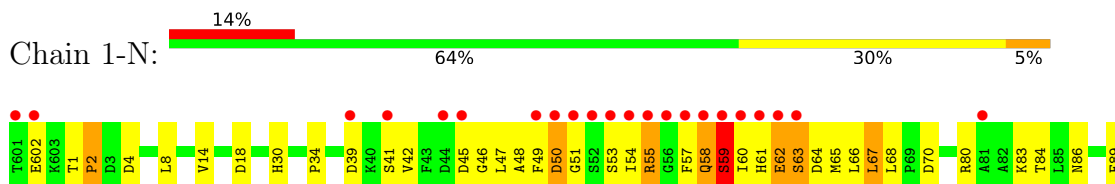
• Molecule 1: glutamine synthetase

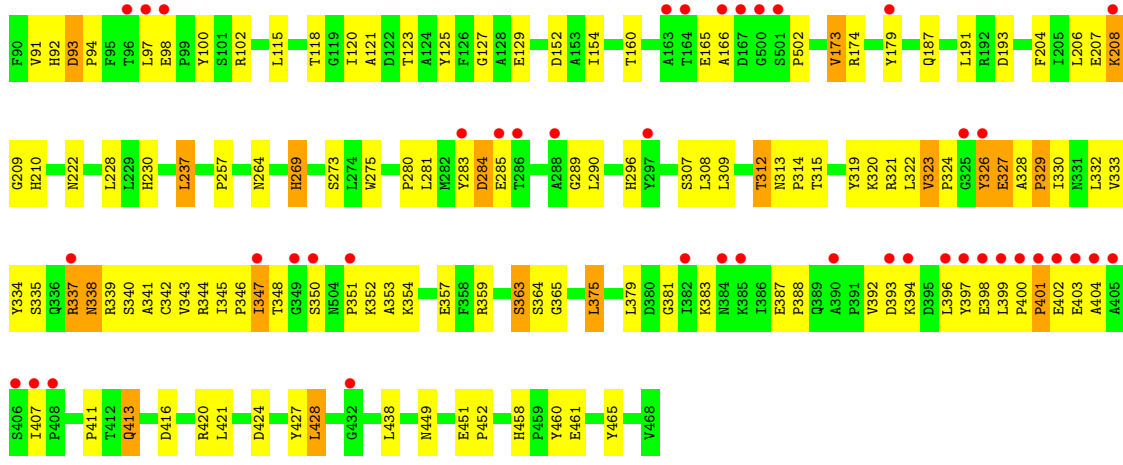


• Molecule 1: glutamine synthetase

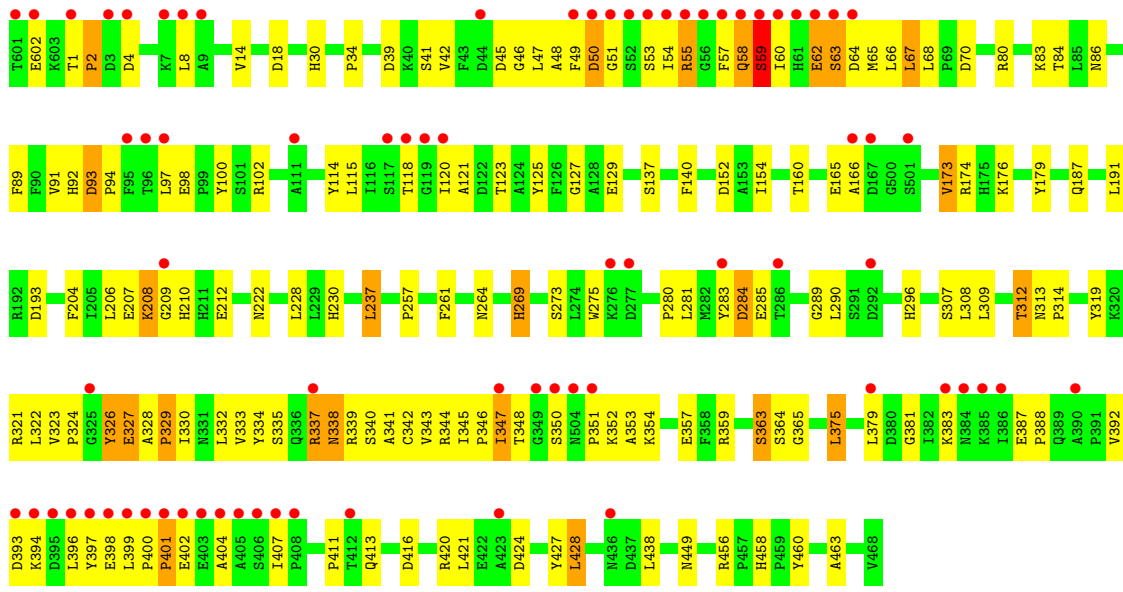


• Molecule 1: glutamine synthetase

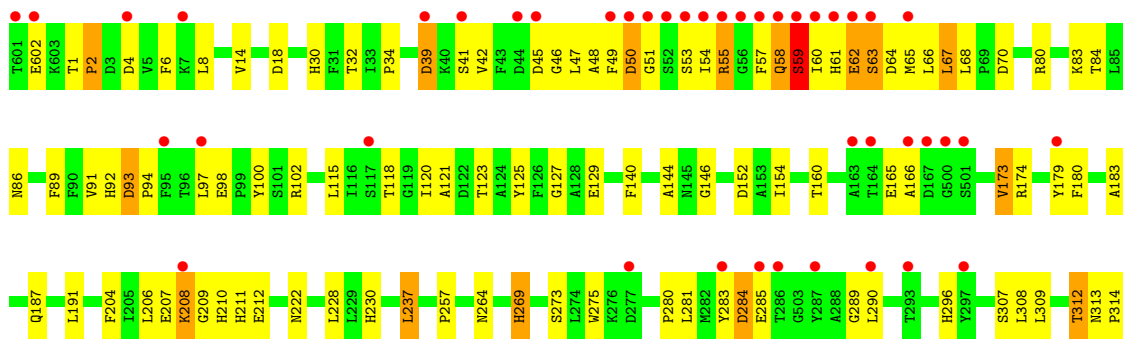


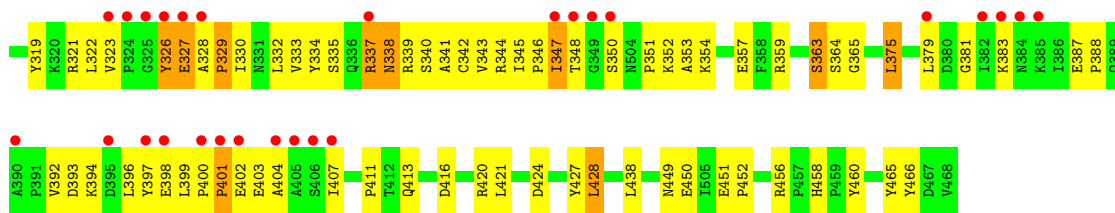


● Molecule 1: glutamine synthetase

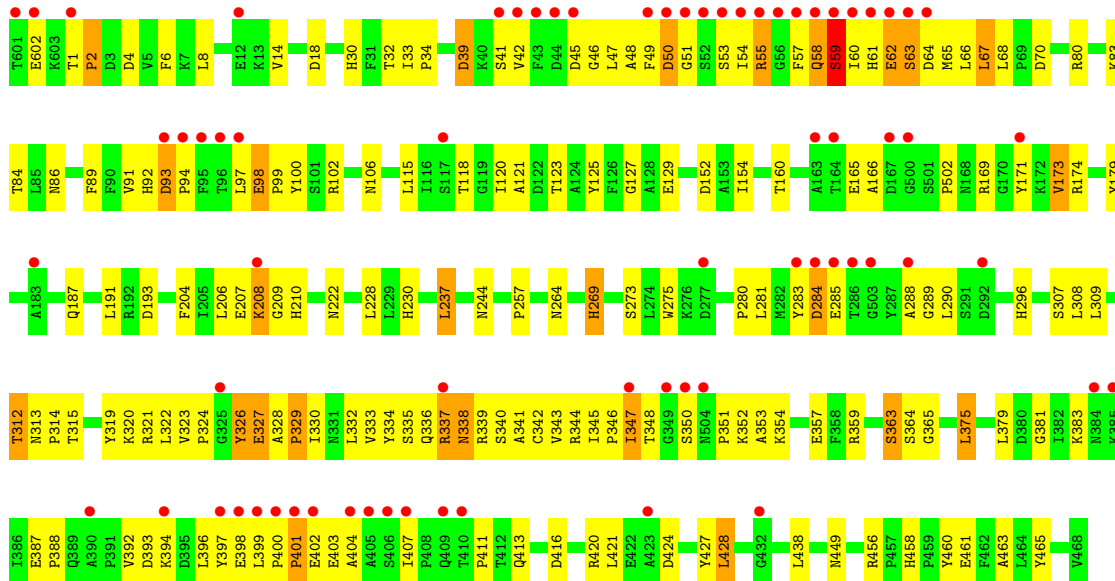


● Molecule 1: glutamine synthetase

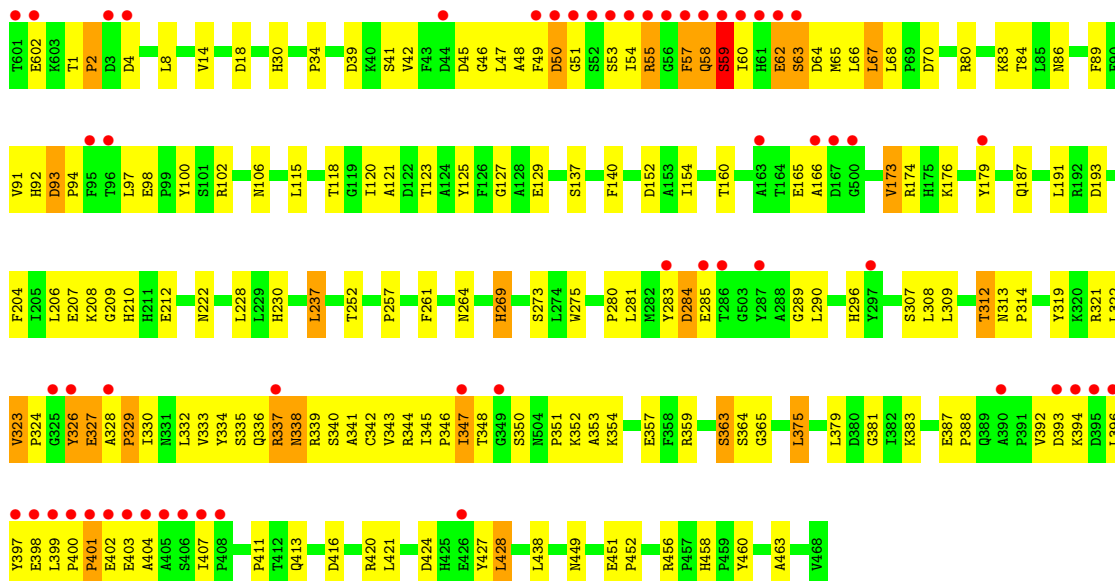


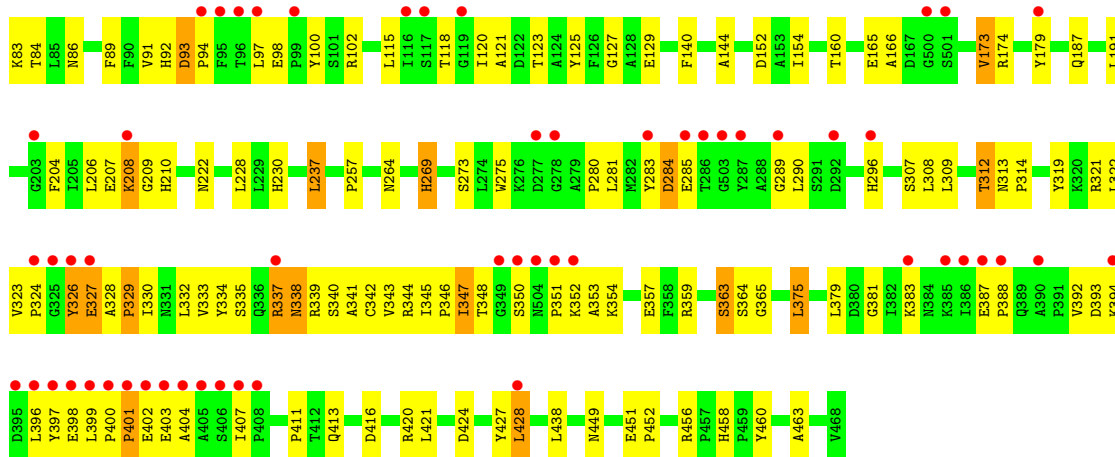


• Molecule 1: glutamine synthetase

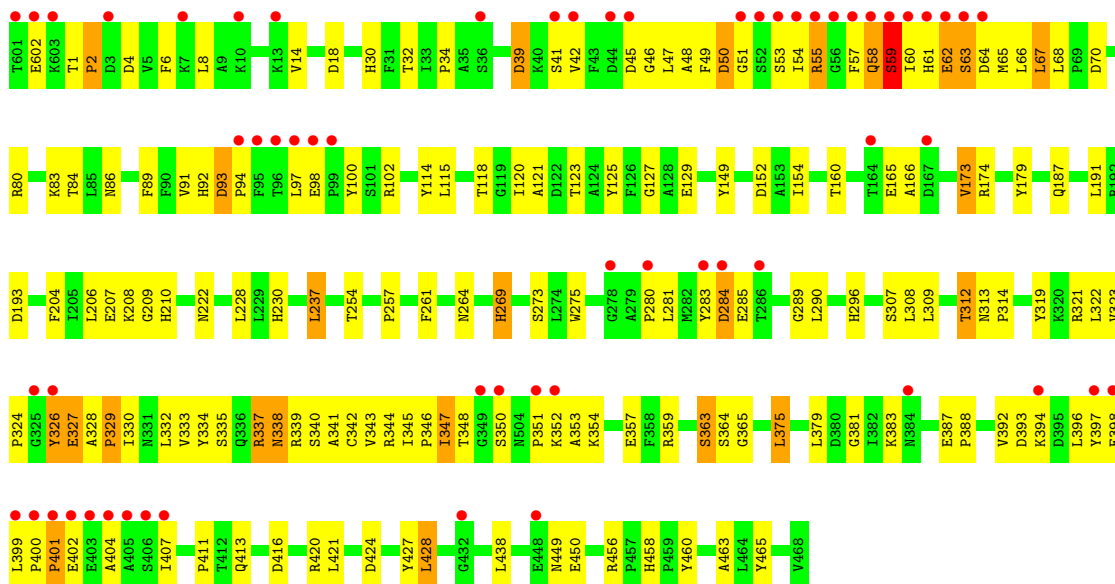


• Molecule 1: glutamine synthetase

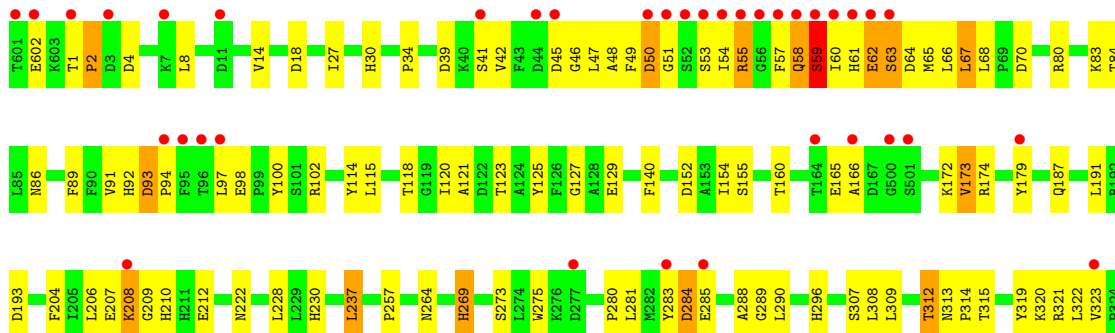


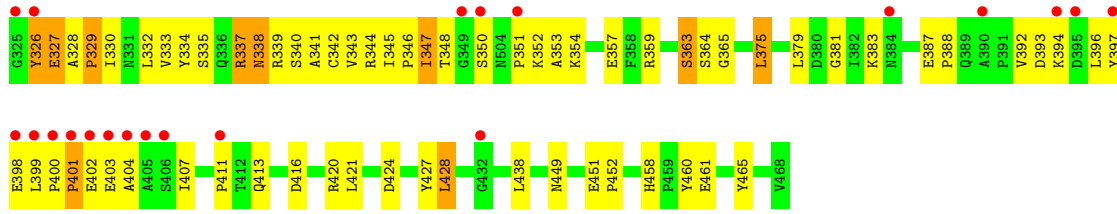


• Molecule 1: glutamine synthetase

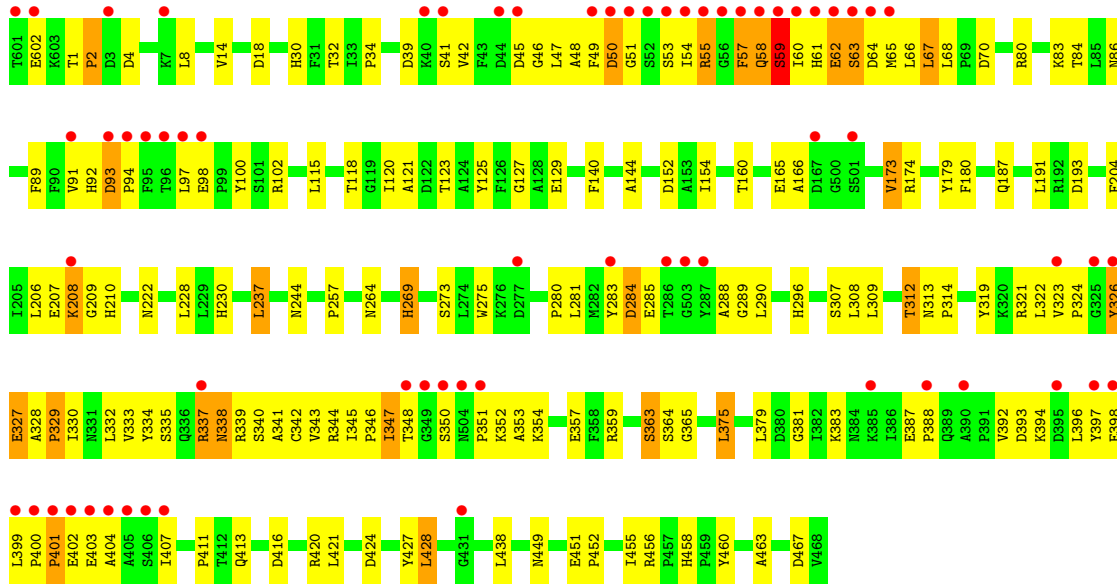


• Molecule 1: glutamine synthetase

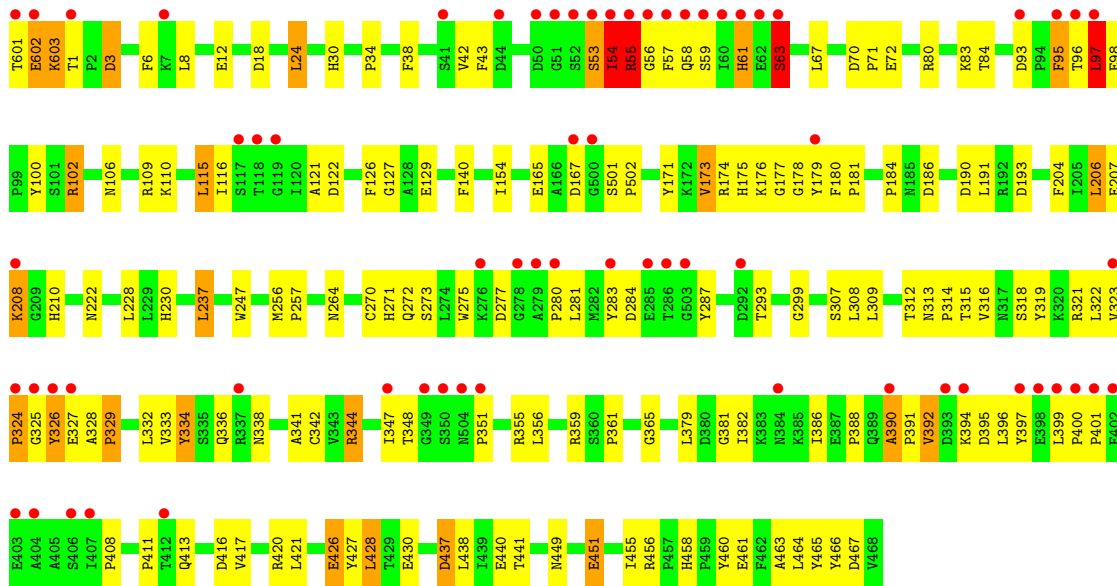


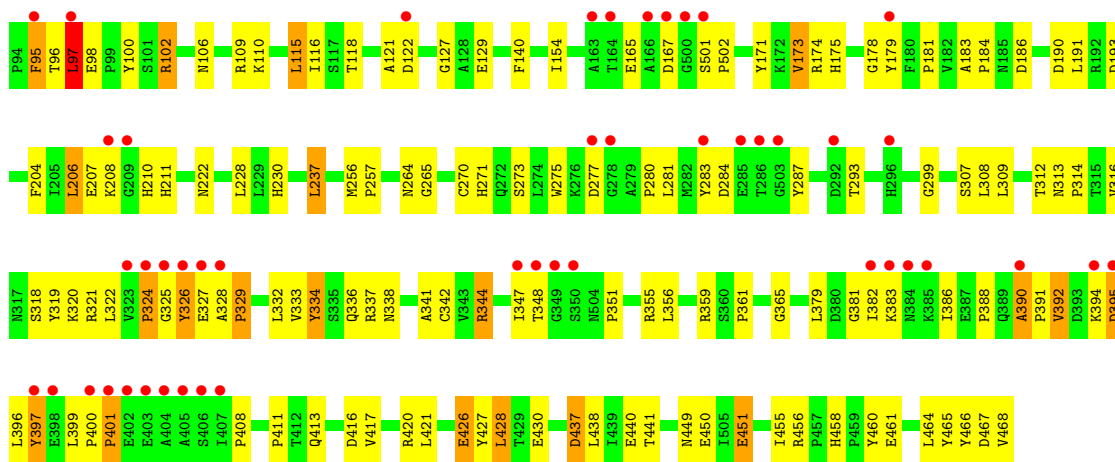


• Molecule 1: glutamine synthetase

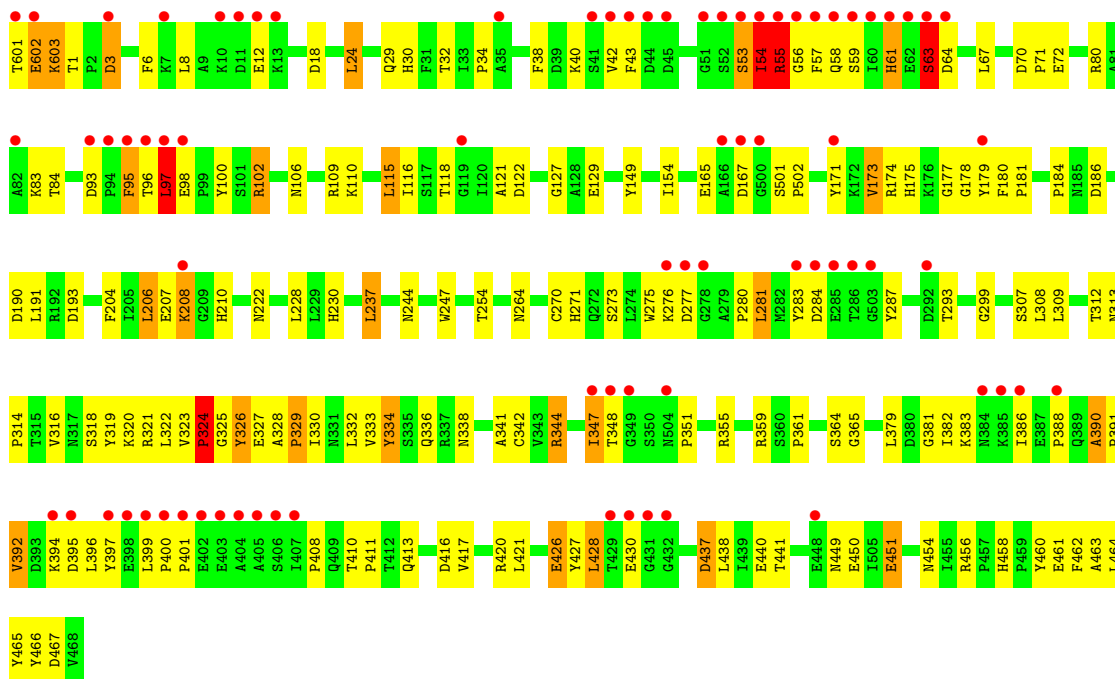


• Molecule 1: glutamine synthetase

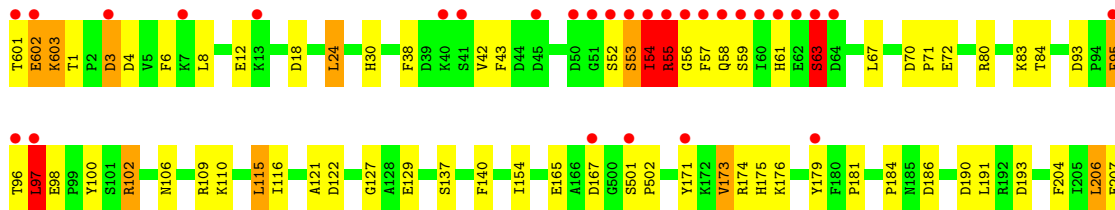


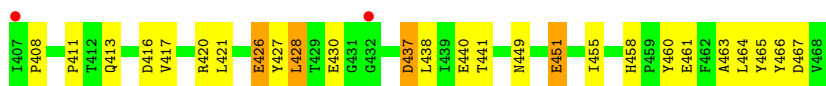


• Molecule 1: glutamine synthetase

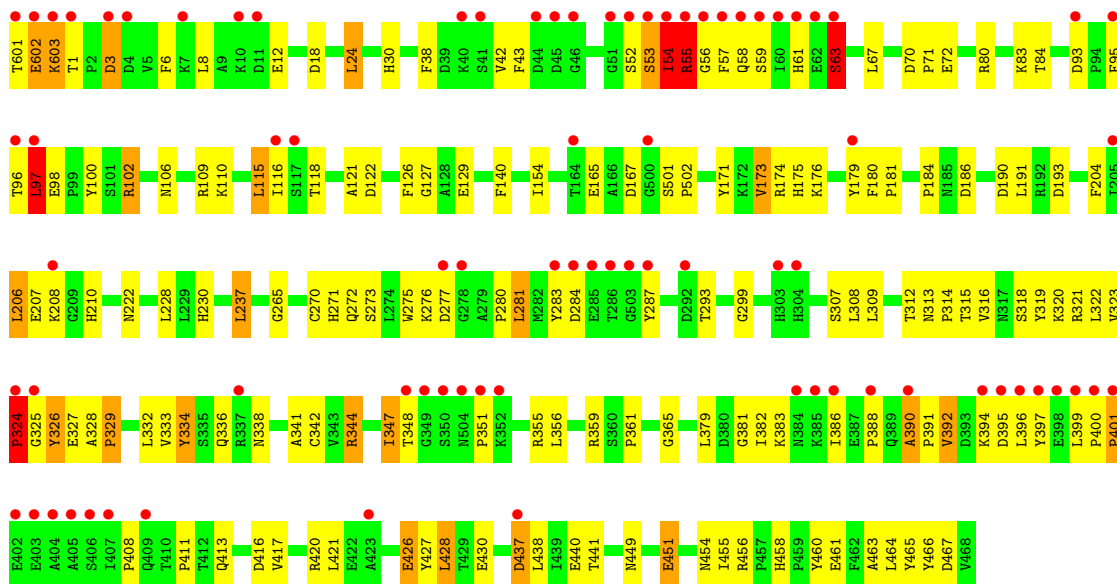


• Molecule 1: glutamine synthetase

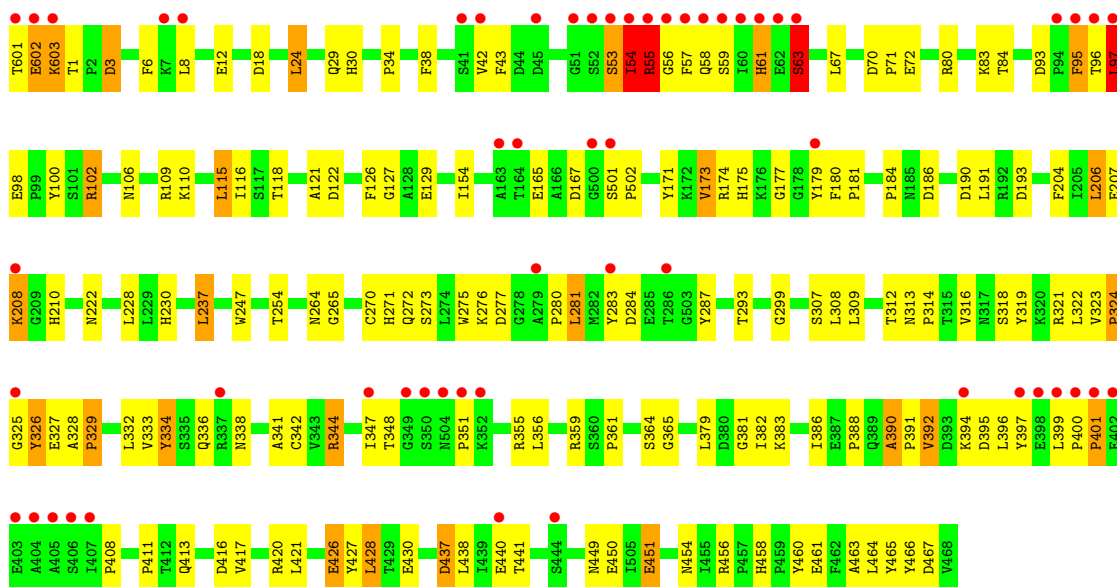




• Molecule 1: glutamine synthetase

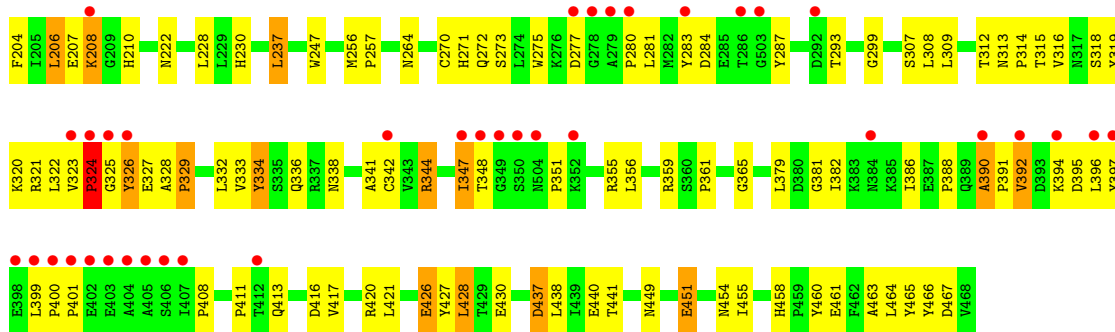


• Molecule 1: glutamine synthetase

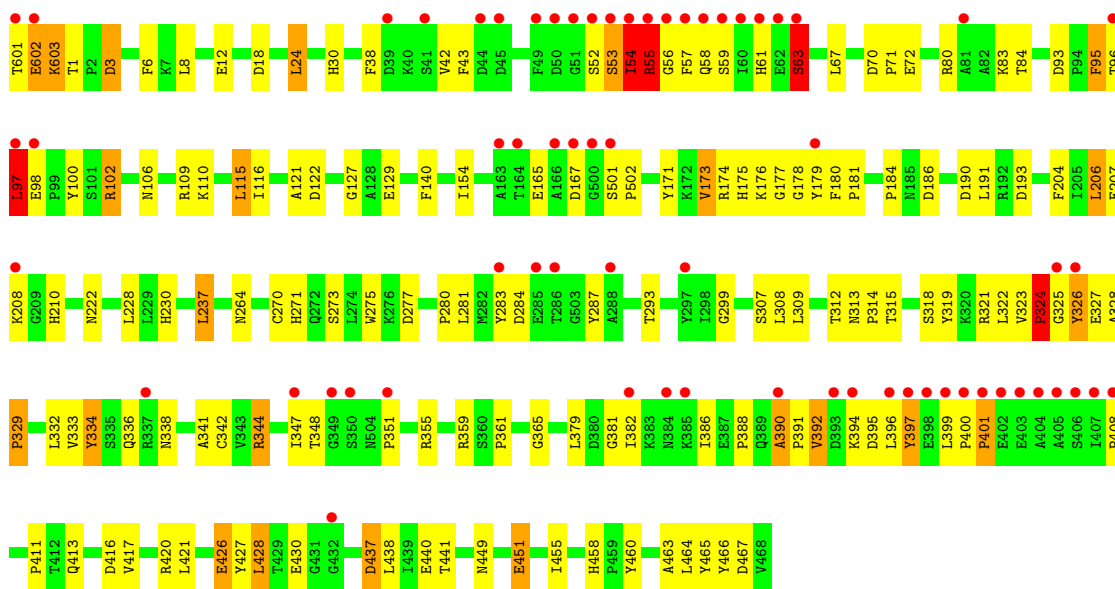


• Molecule 1: glutamine synthetase

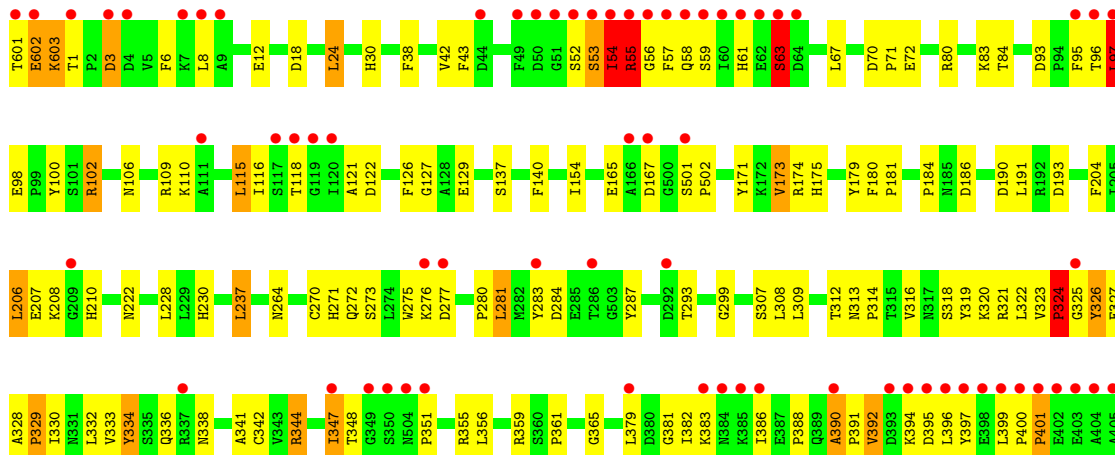


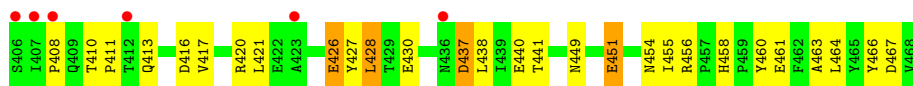


• Molecule 1: glutamine synthetase

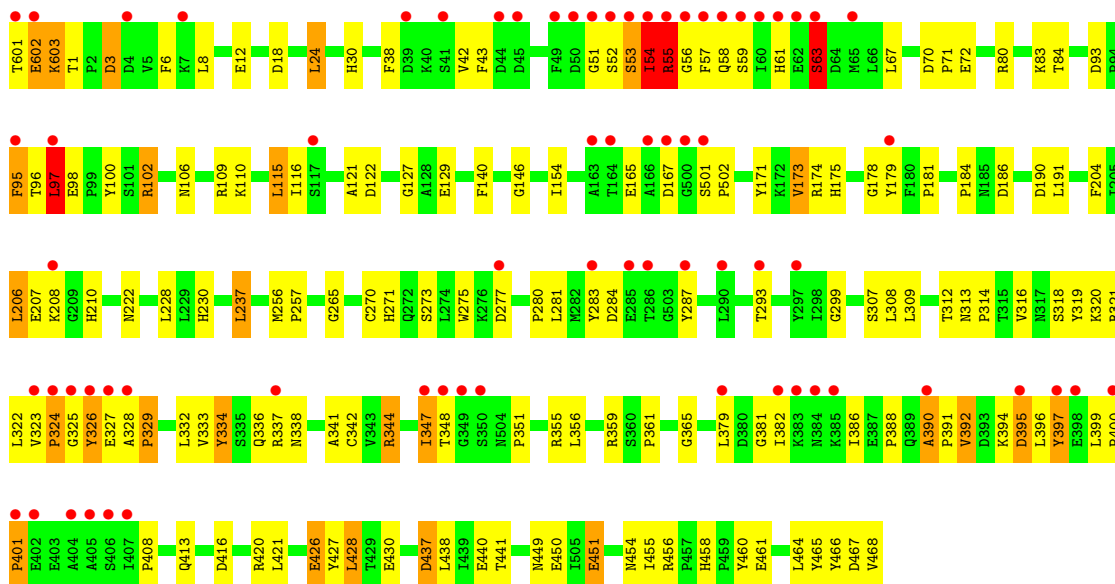


• Molecule 1: glutamine synthetase

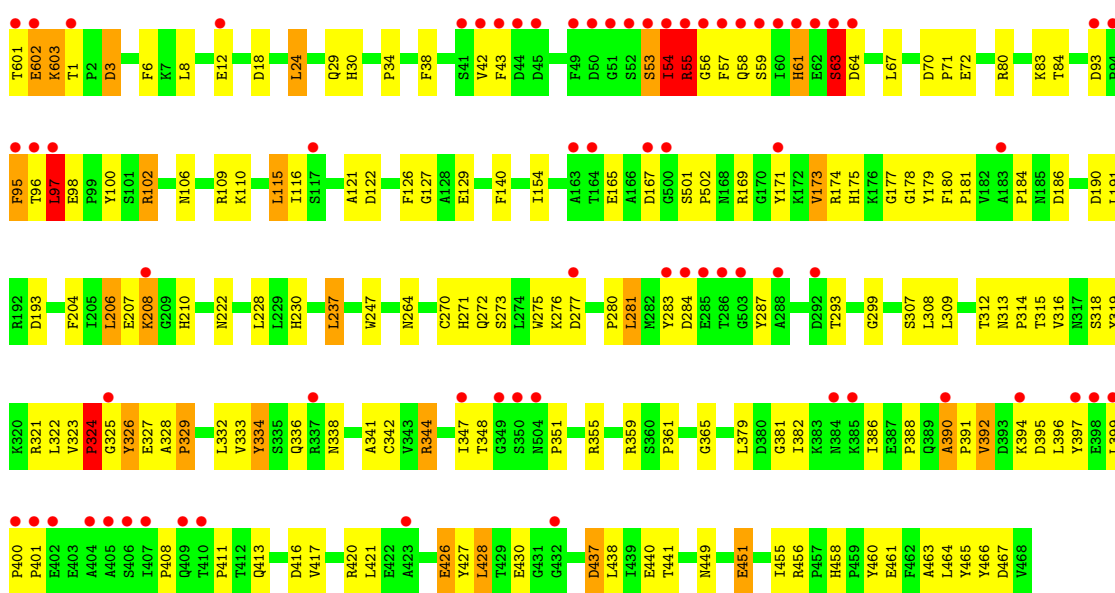




• Molecule 1: glutamine synthetase

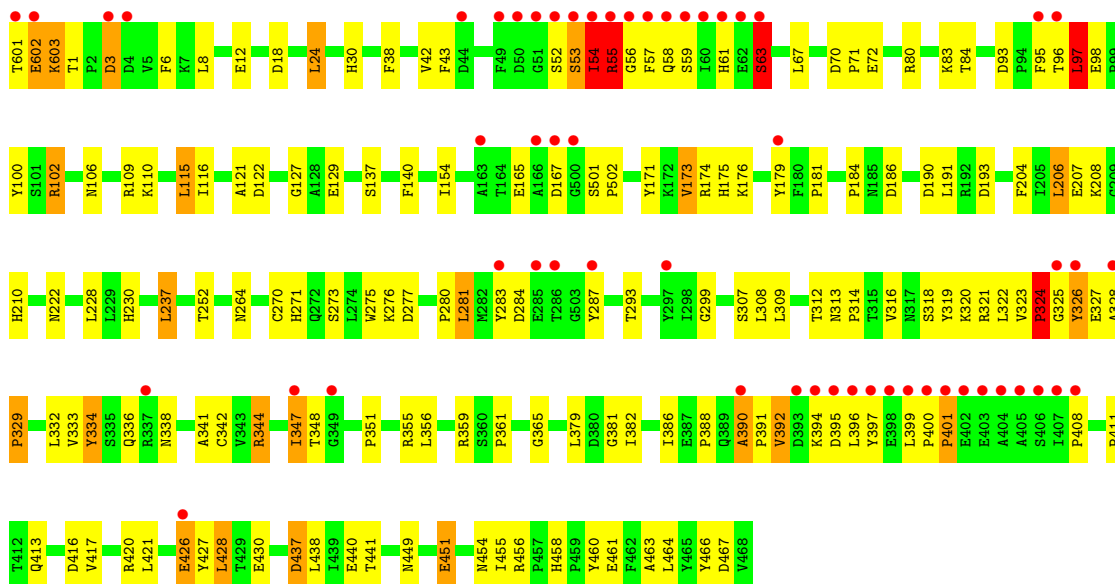


• Molecule 1: glutamine synthetase

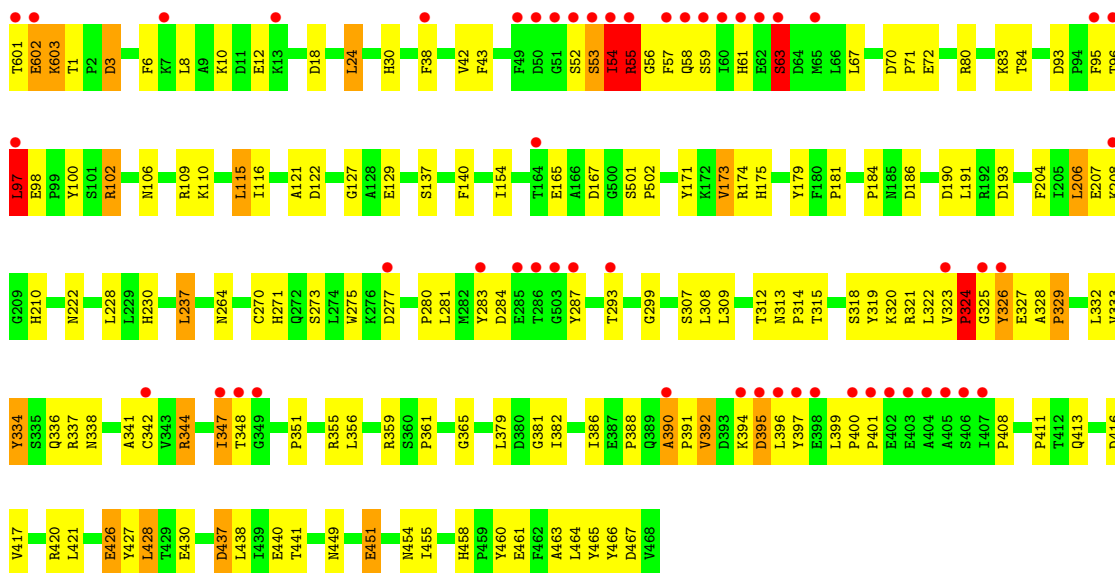


• Molecule 1: glutamine synthetase

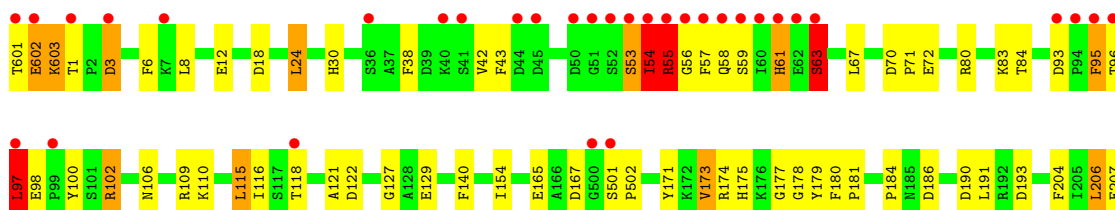


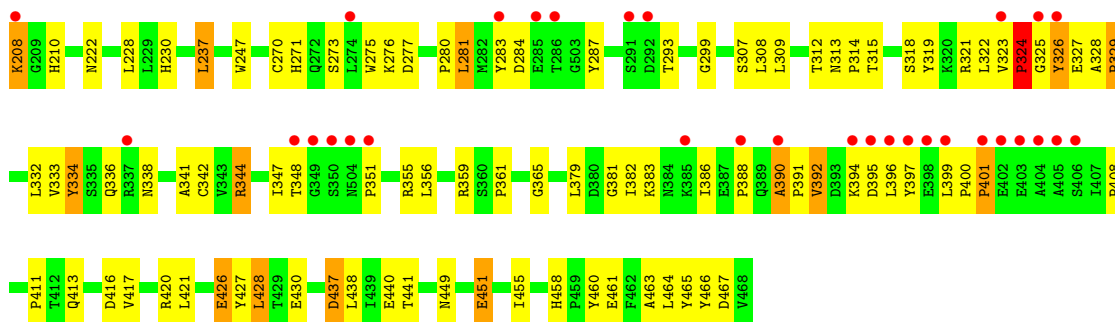


● Molecule 1: glutamine synthetase

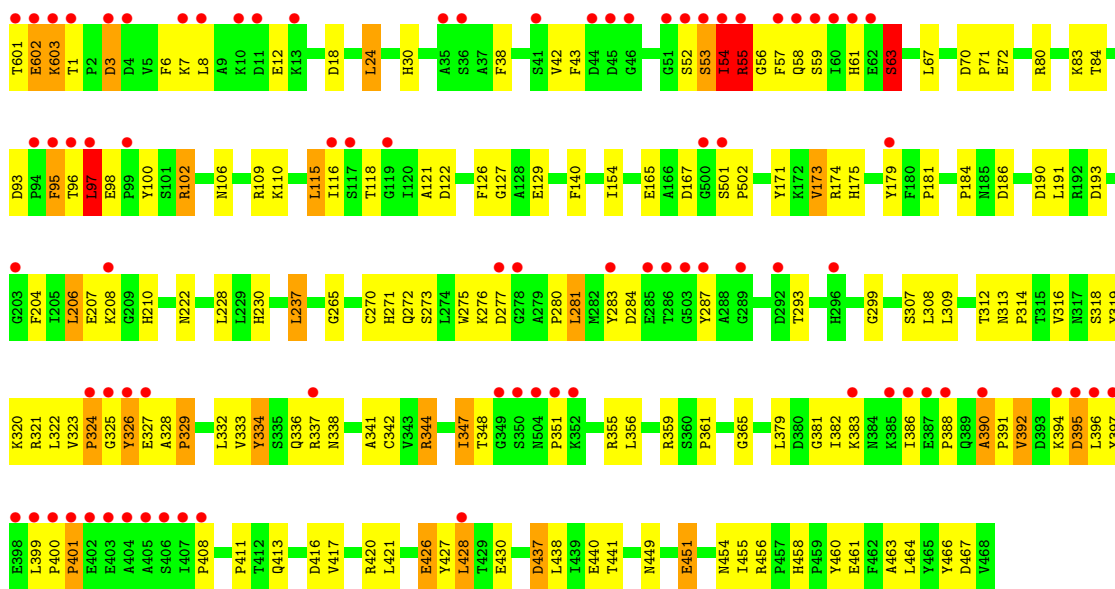


● Molecule 1: glutamine synthetase

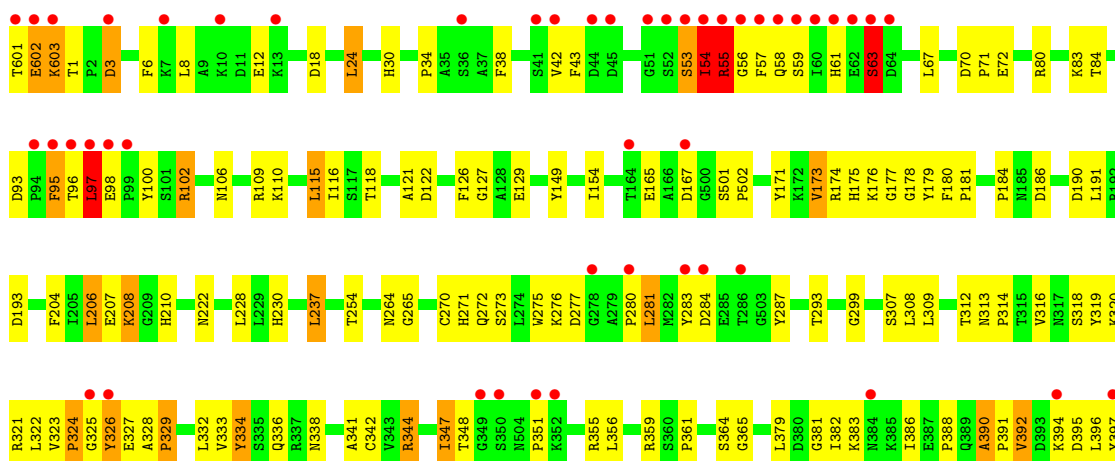


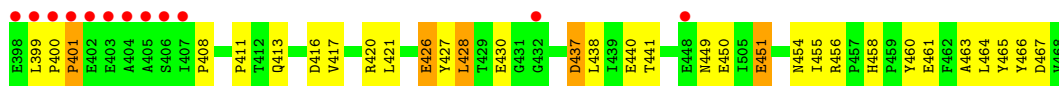


● Molecule 1: glutamine synthetase

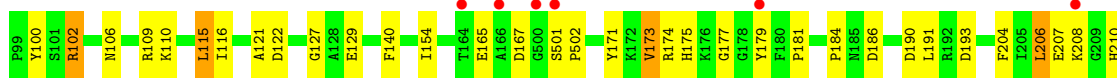
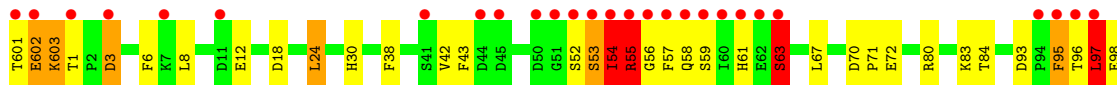


● Molecule 1: glutamine synthetase

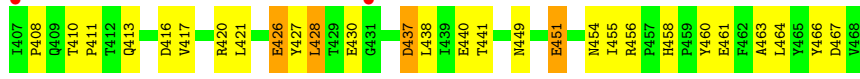
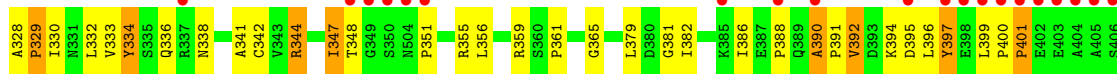
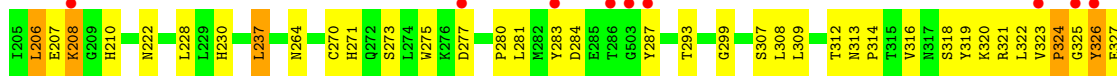
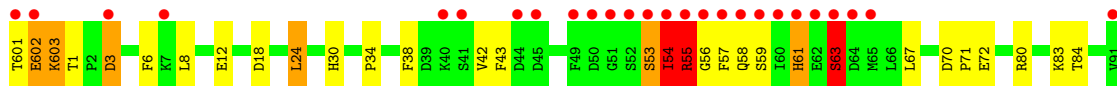




• Molecule 1: glutamine synthetase

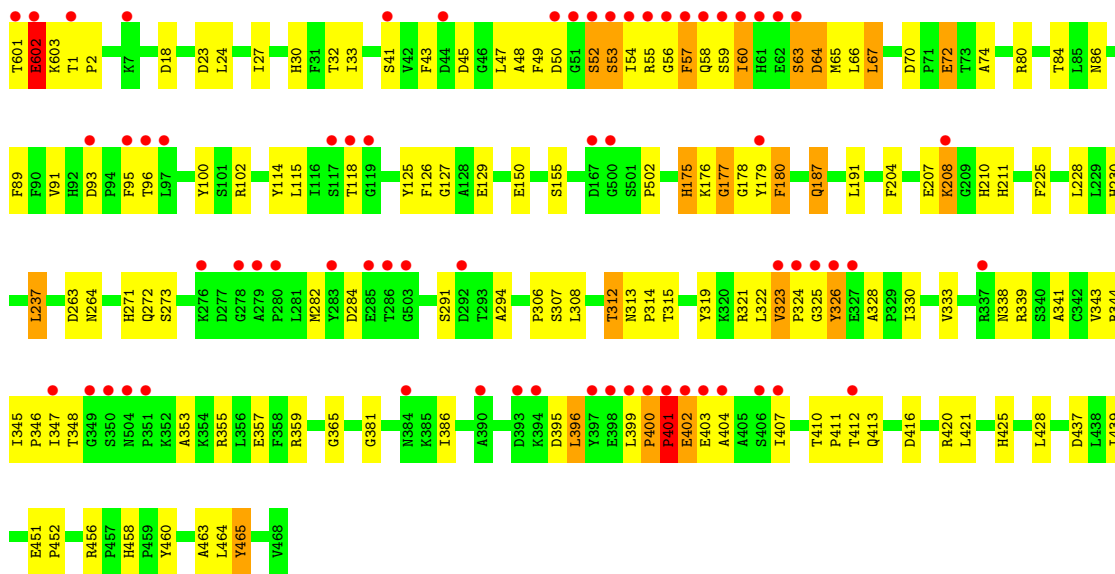


• Molecule 1: glutamine synthetase

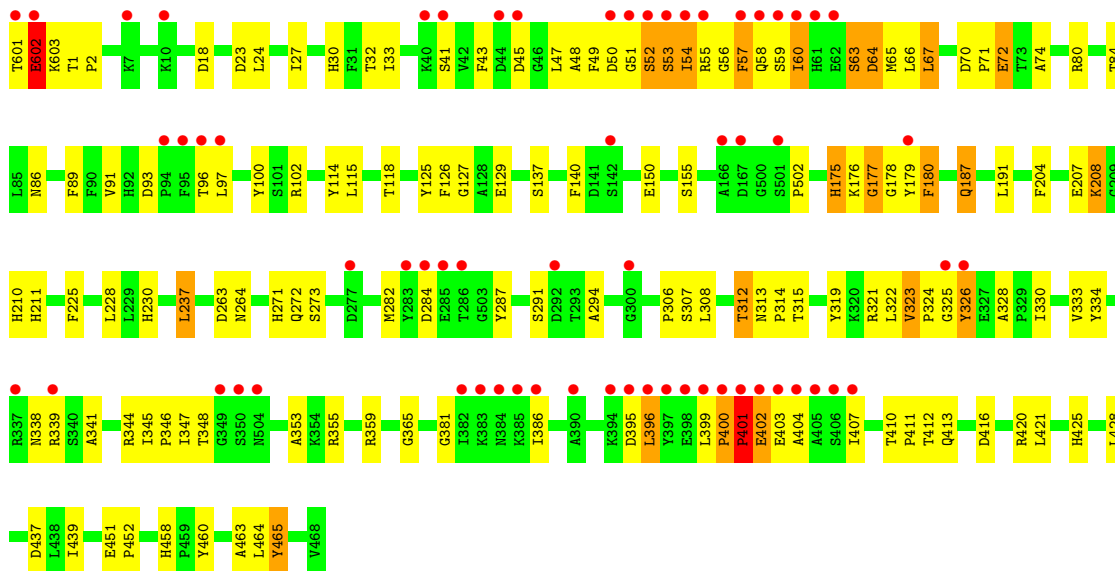


• Molecule 1: glutamine synthetase

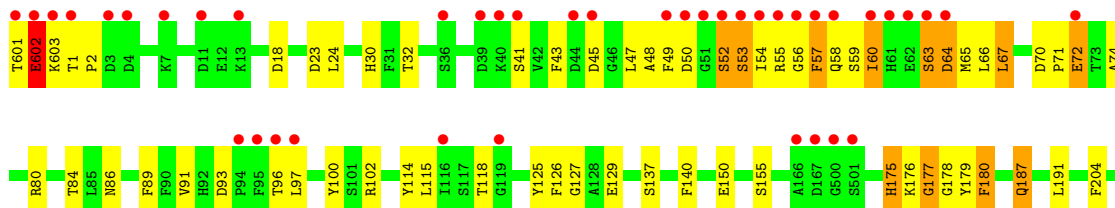
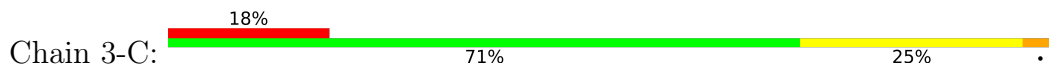


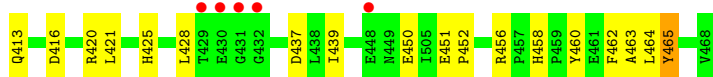


• Molecule 1: glutamine synthetase

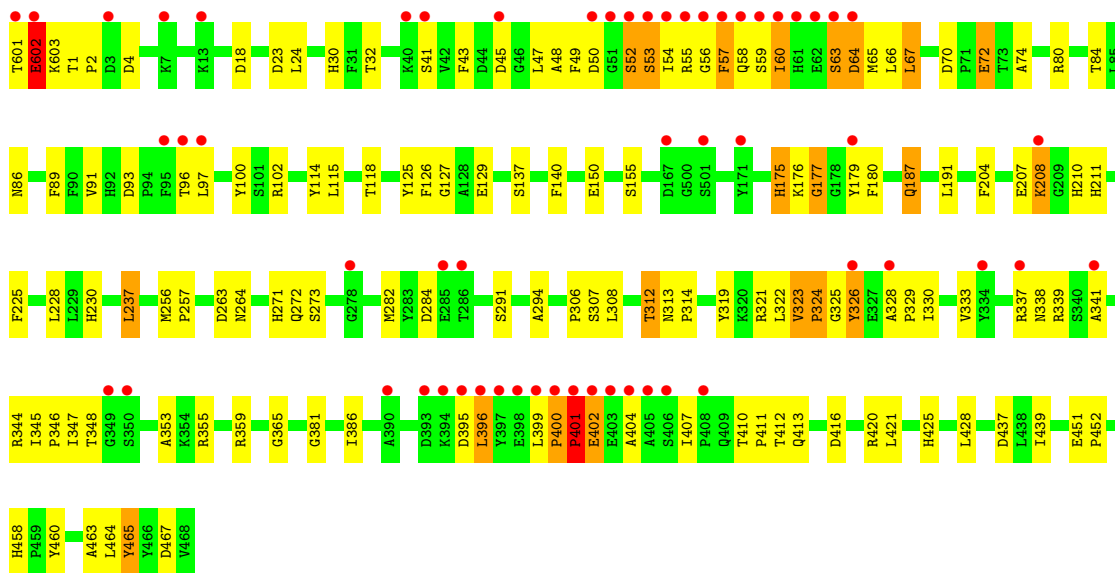
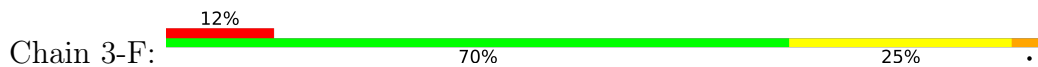


• Molecule 1: glutamine synthetase

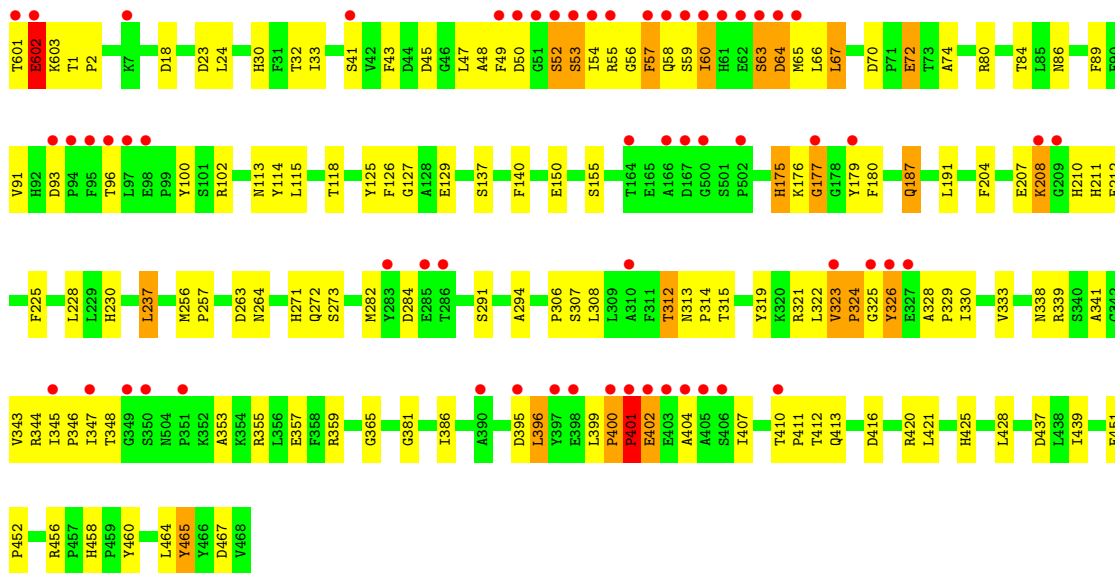
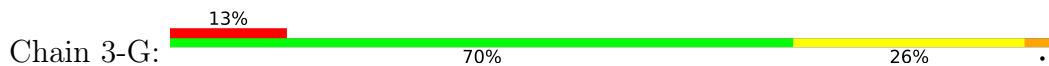




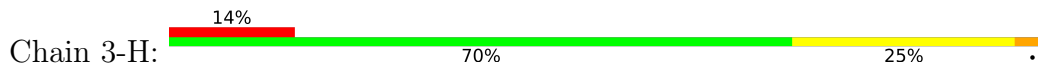
• Molecule 1: glutamine synthetase

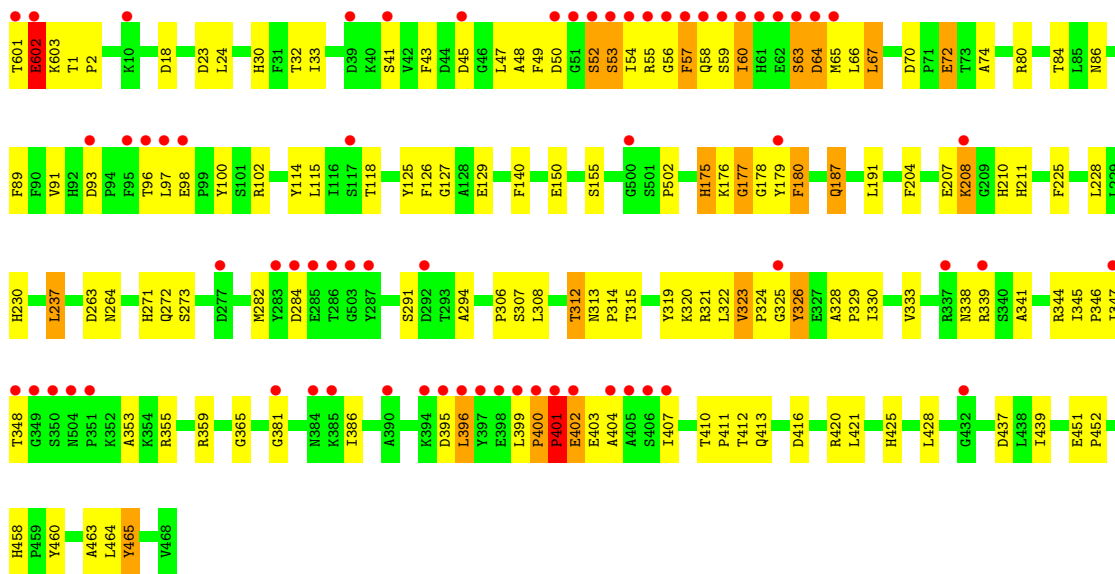


• Molecule 1: glutamine synthetase

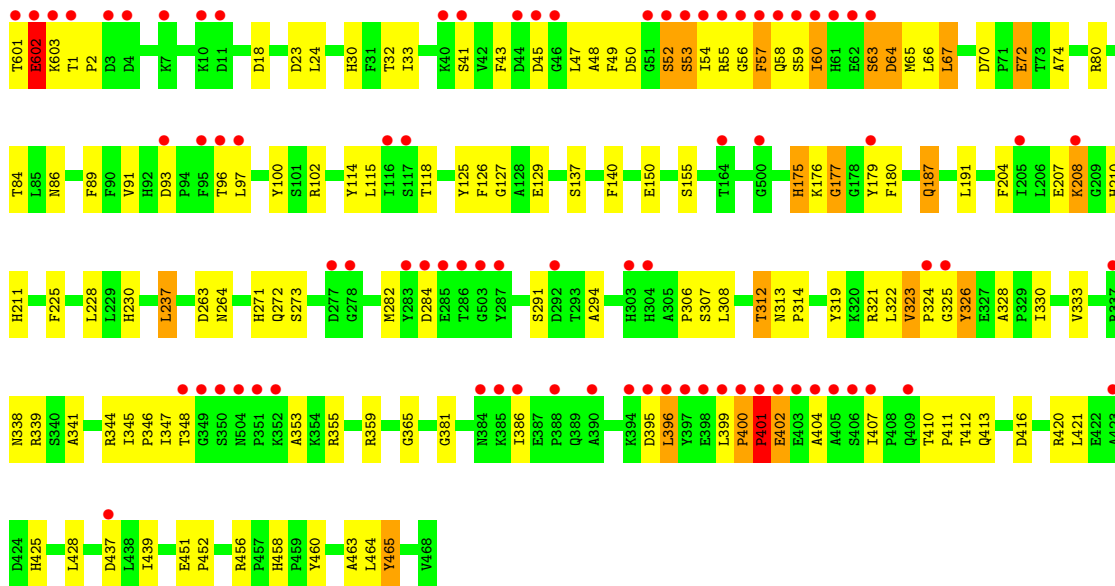
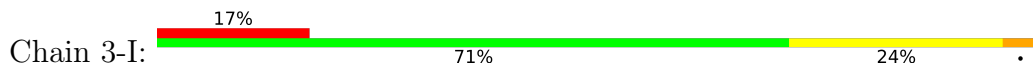


• Molecule 1: glutamine synthetase

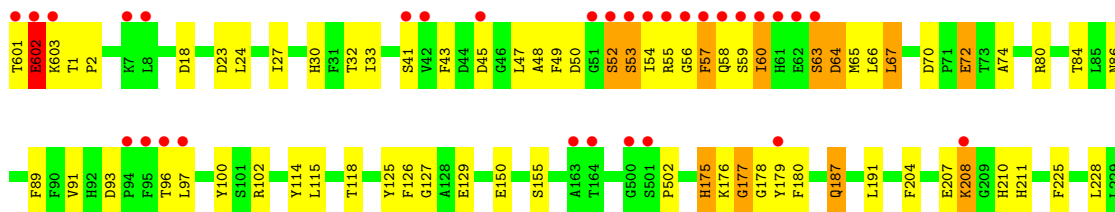




• Molecule 1: glutamine synthetase

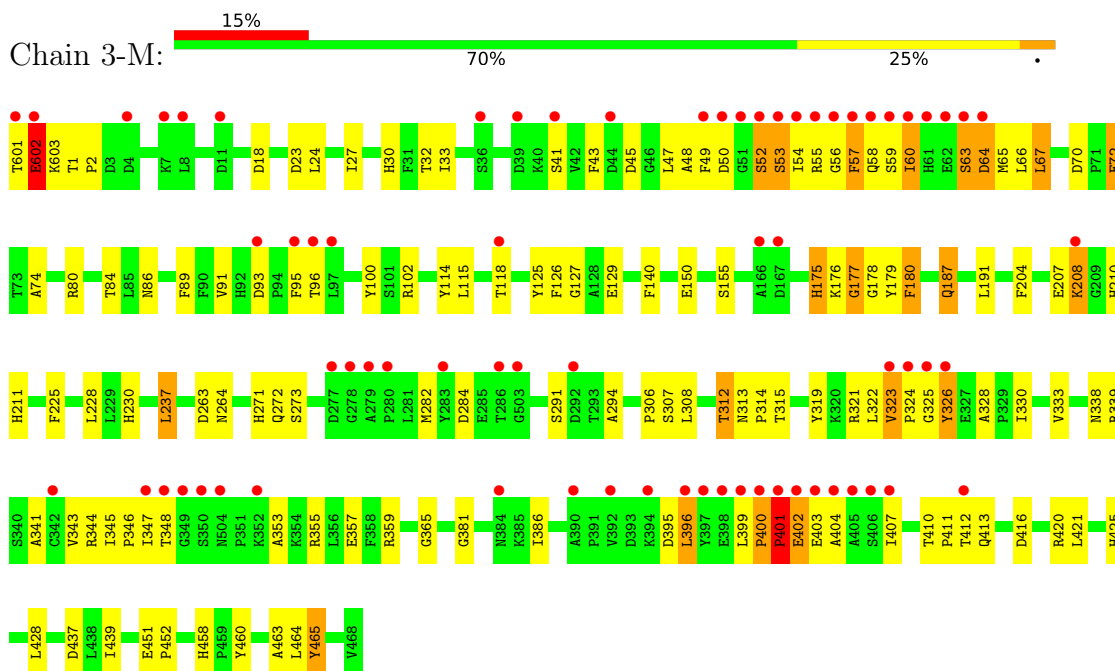


• Molecule 1: glutamine synthetase

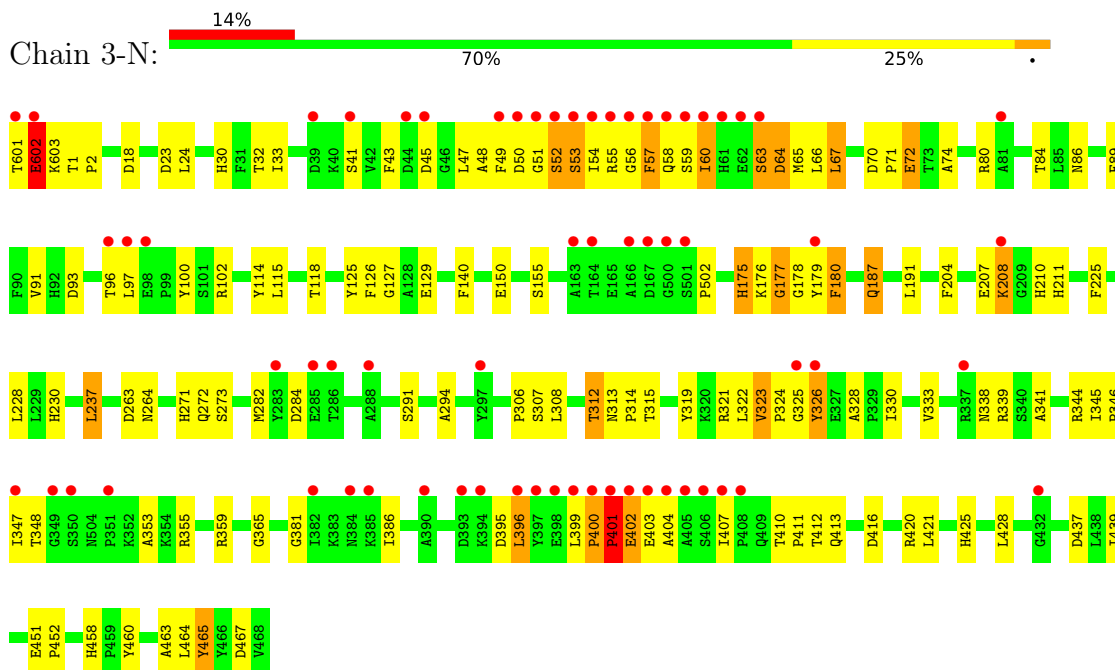




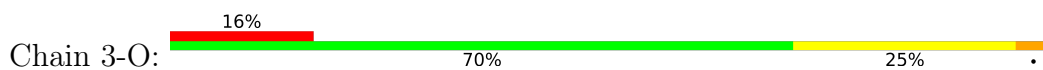
- Molecule 1: glutamine synthetase

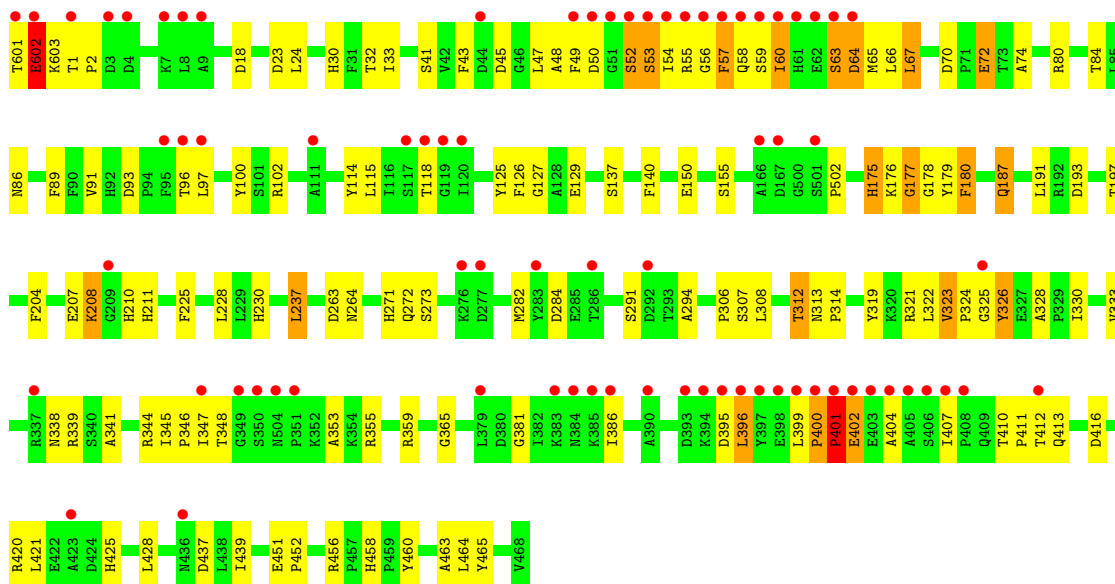


- Molecule 1: glutamine synthetase

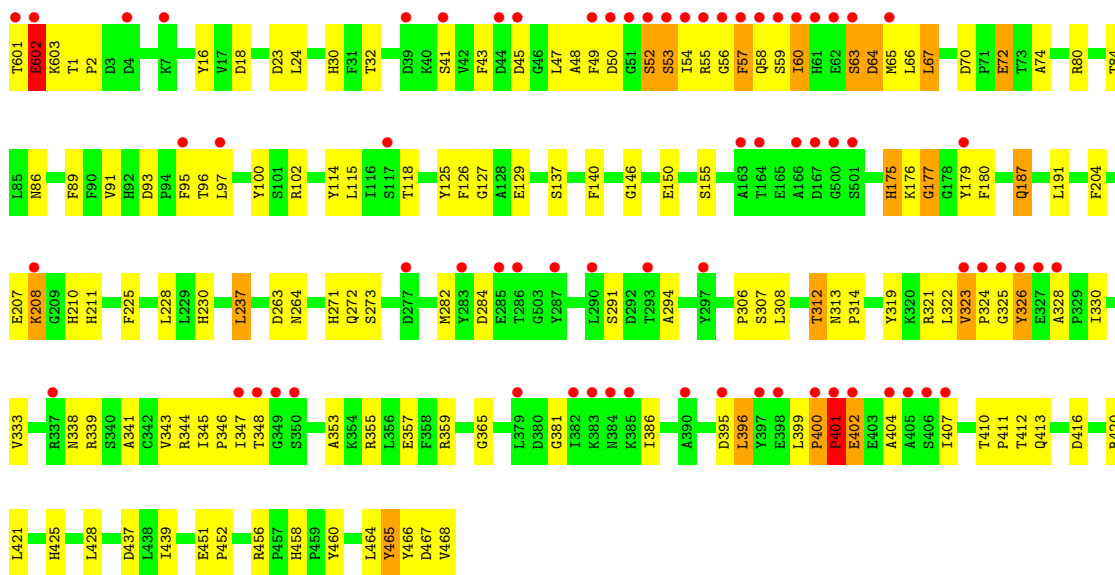
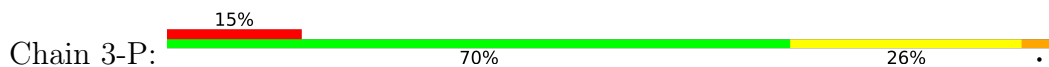


- Molecule 1: glutamine synthetase

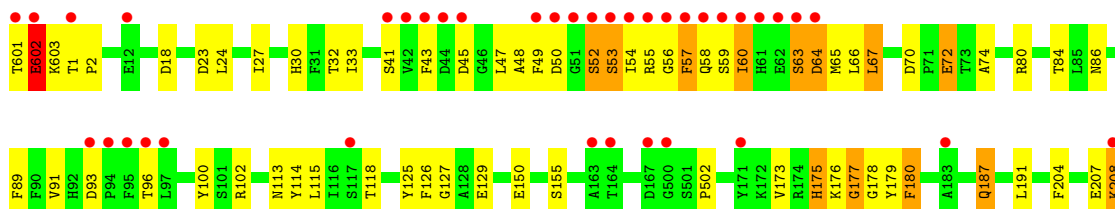
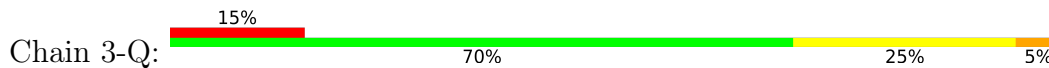


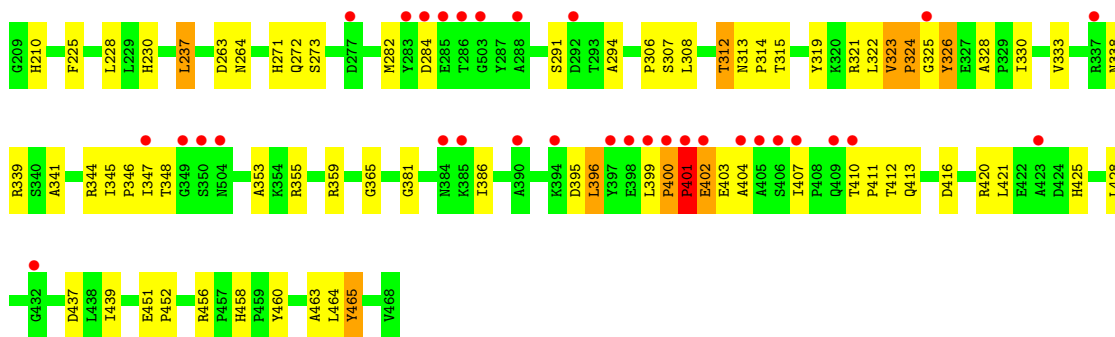


● Molecule 1: glutamine synthetase

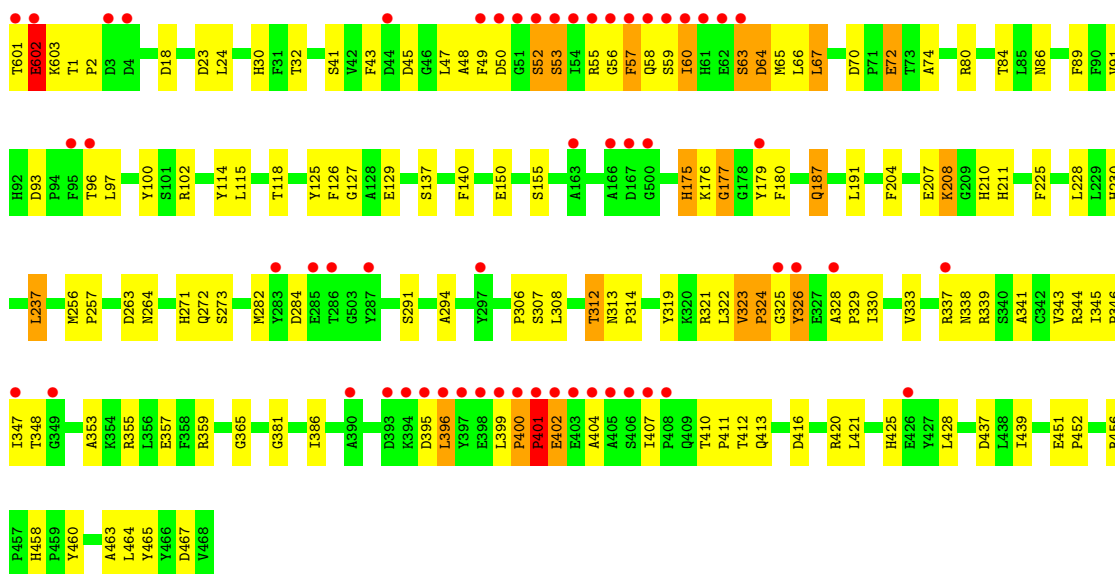
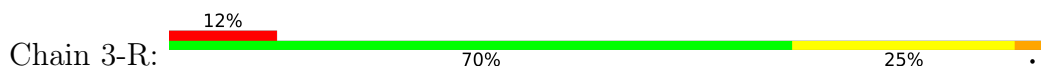


● Molecule 1: glutamine synthetase

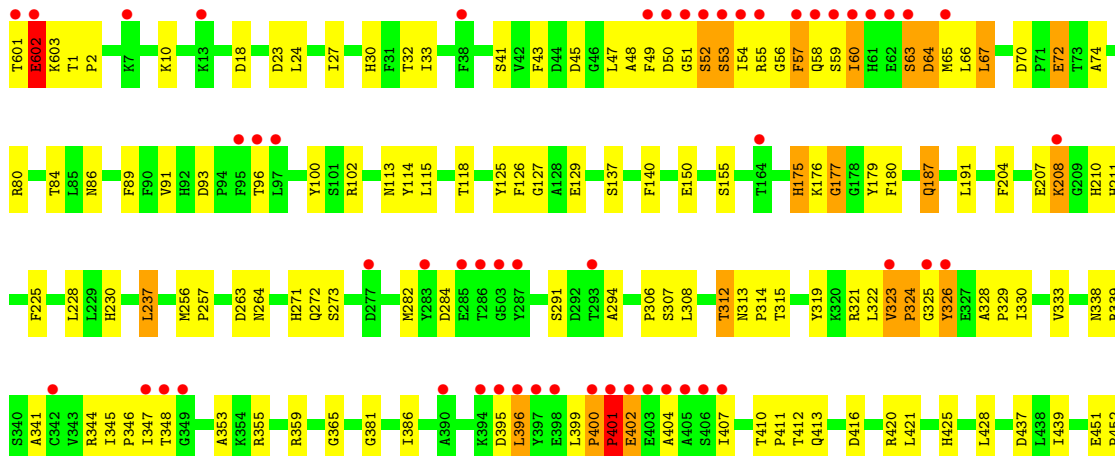
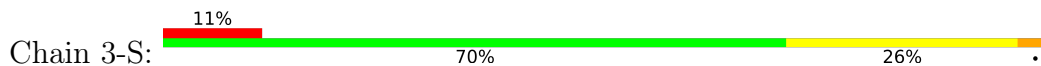




- Molecule 1: glutamine synthetase

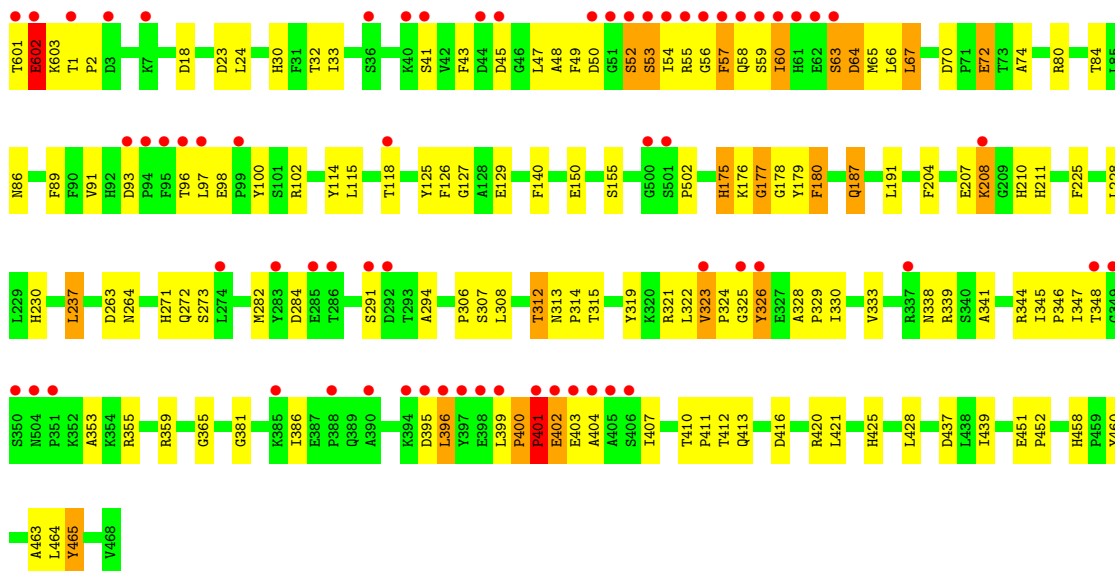
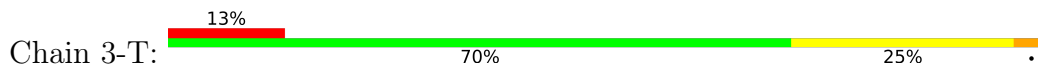


- Molecule 1: glutamine synthetase

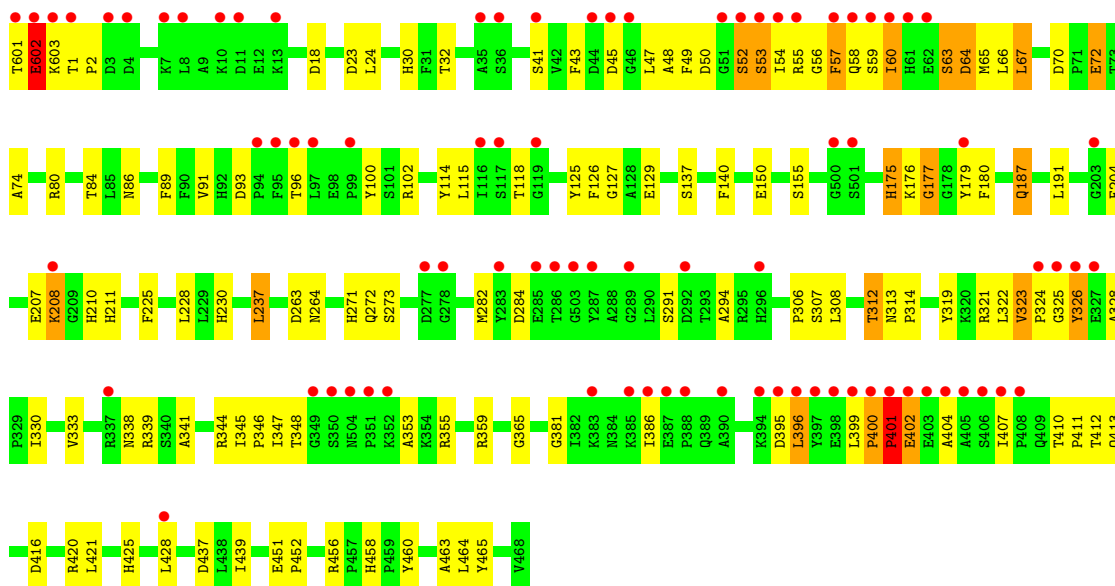
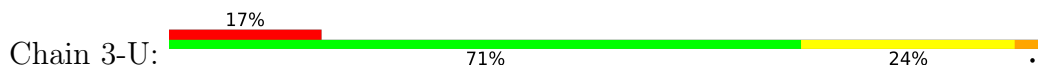




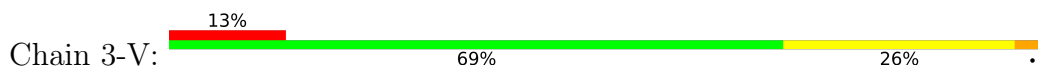
• Molecule 1: glutamine synthetase

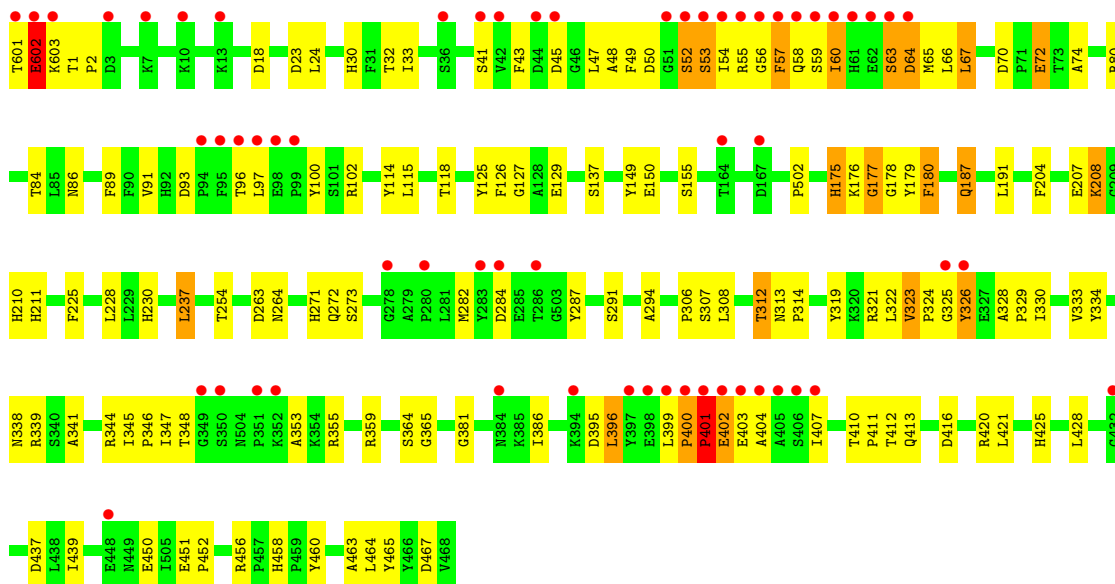


• Molecule 1: glutamine synthetase

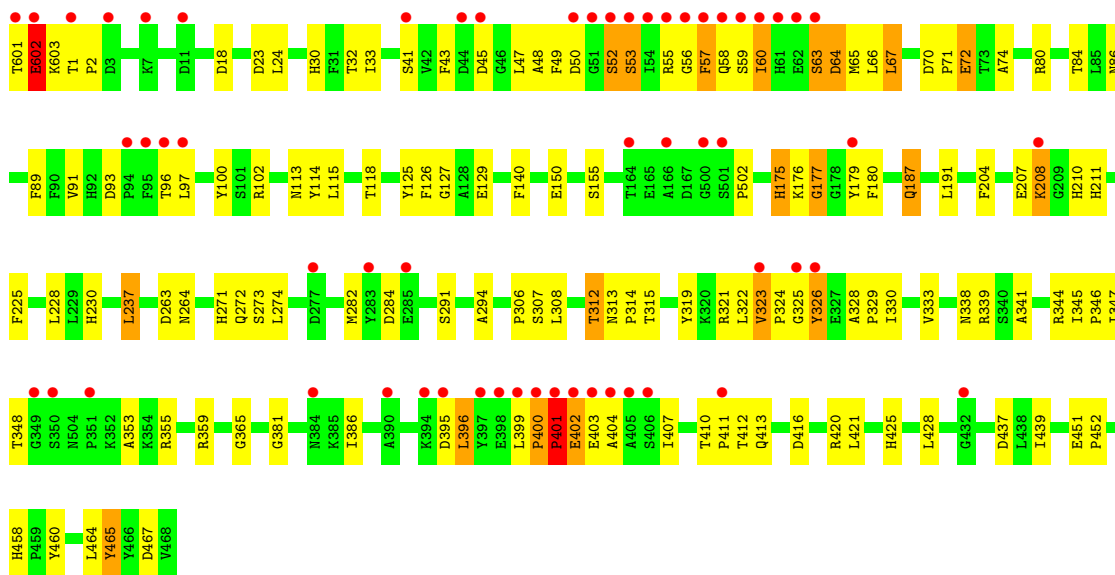
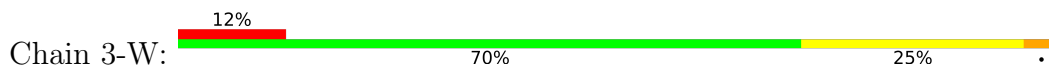


• Molecule 1: glutamine synthetase

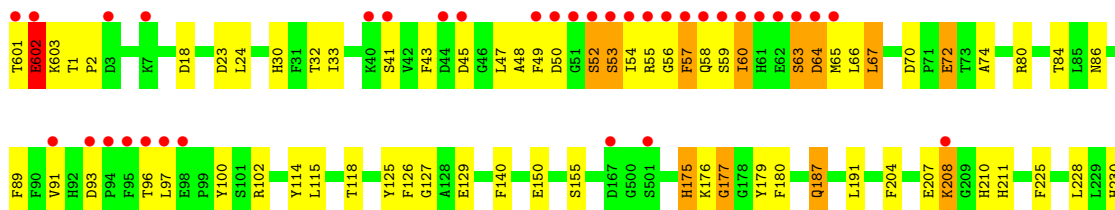
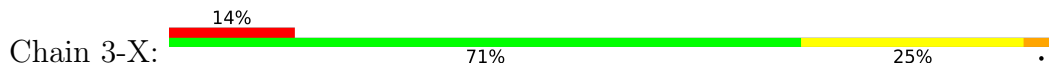


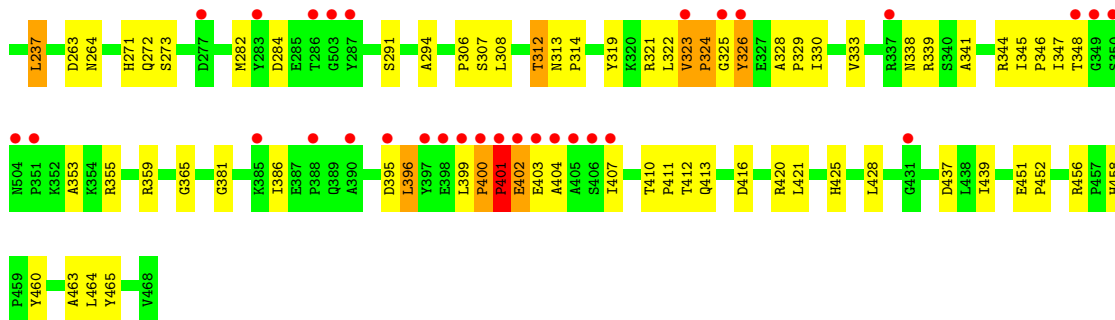


● Molecule 1: glutamine synthetase

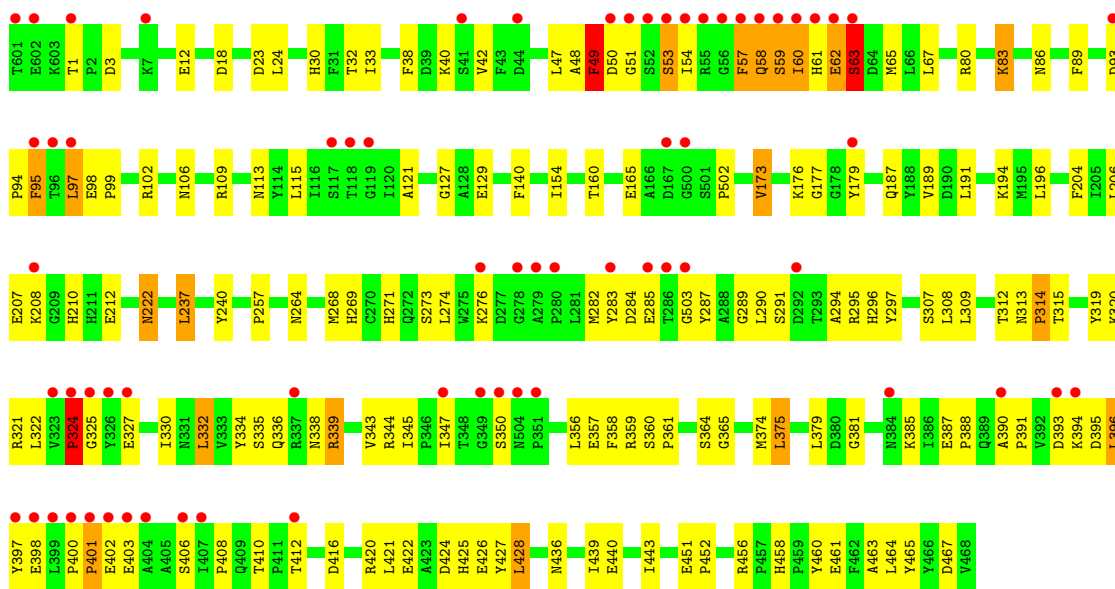


● Molecule 1: glutamine synthetase

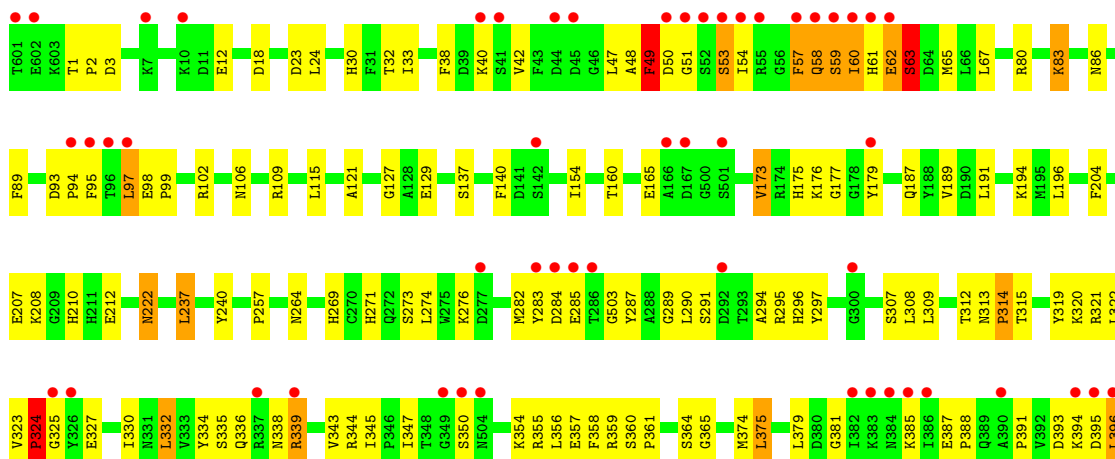


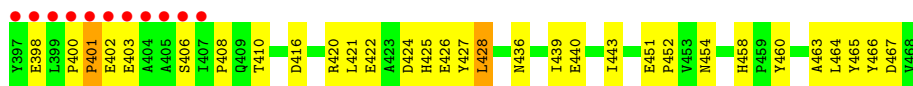


● Molecule 1: glutamine synthetase

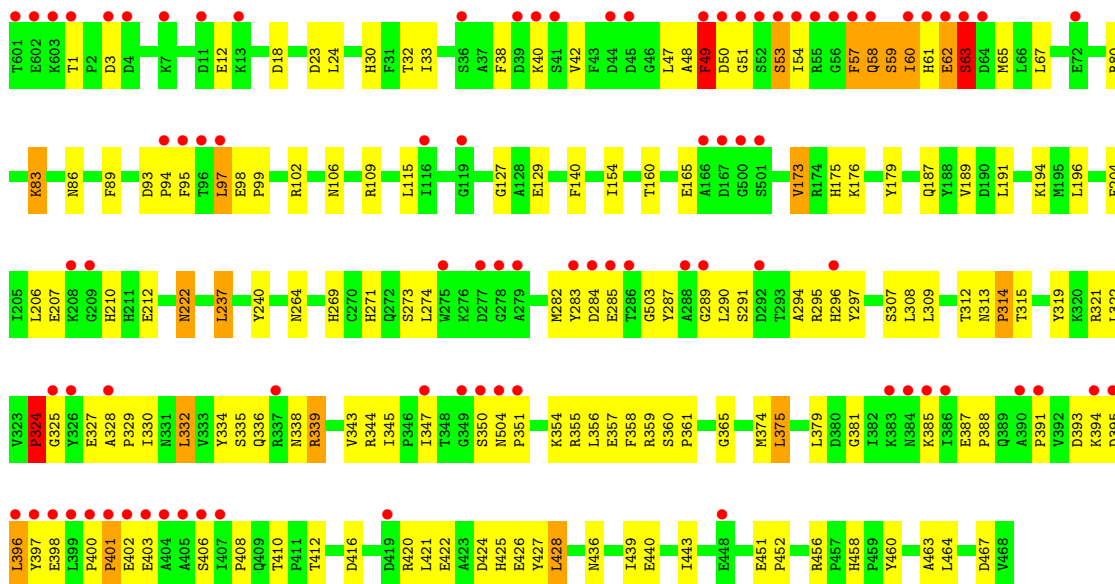


● Molecule 1: glutamine synthetase

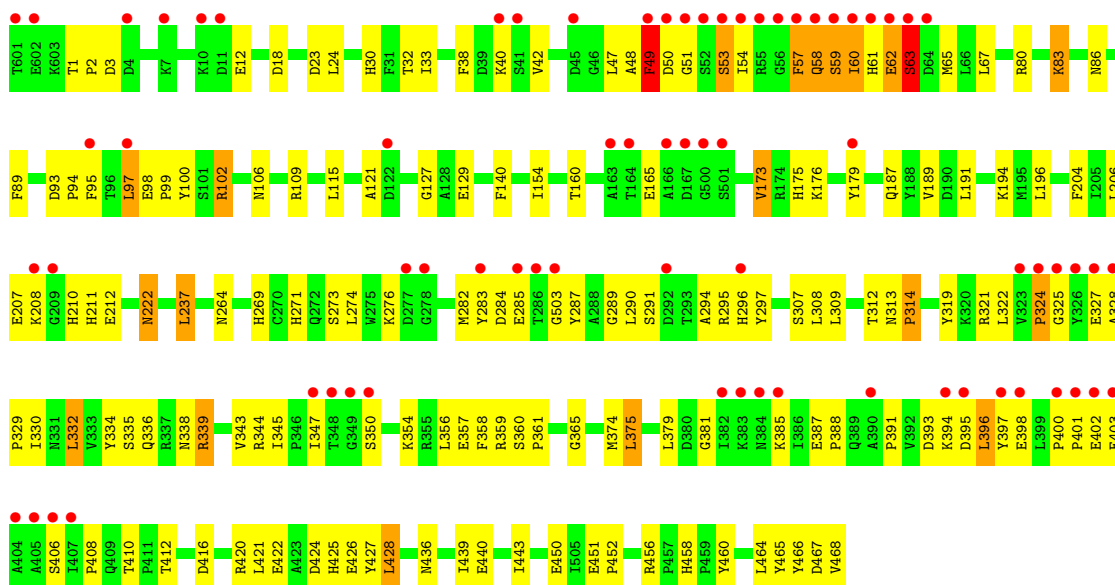




• Molecule 1: glutamine synthetase

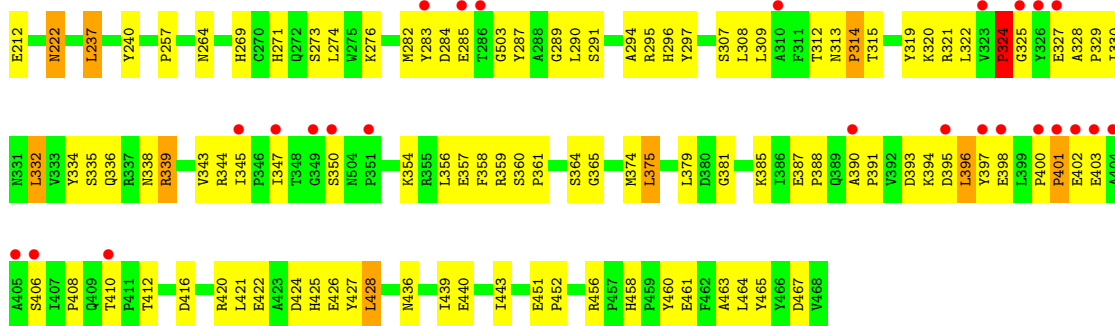


• Molecule 1: glutamine synthetase

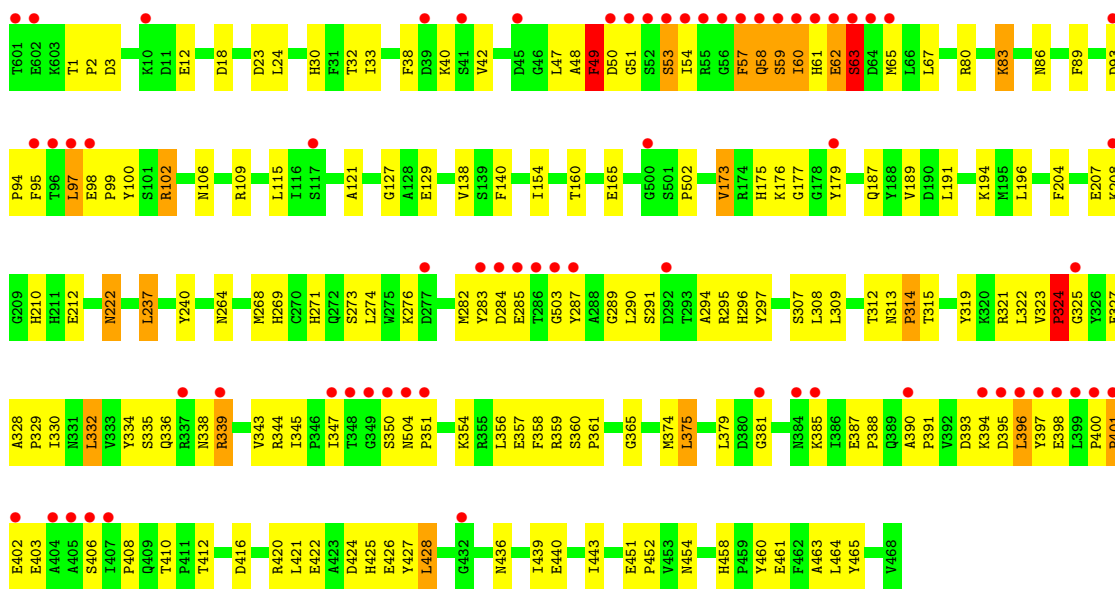


• Molecule 1: glutamine synthetase

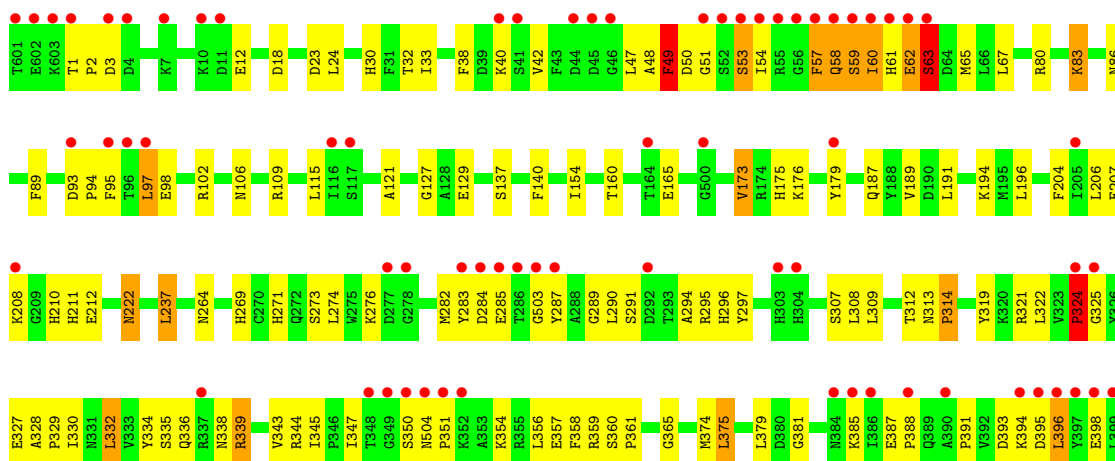


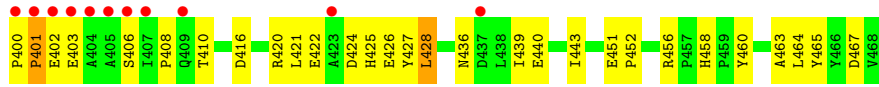


• Molecule 1: glutamine synthetase

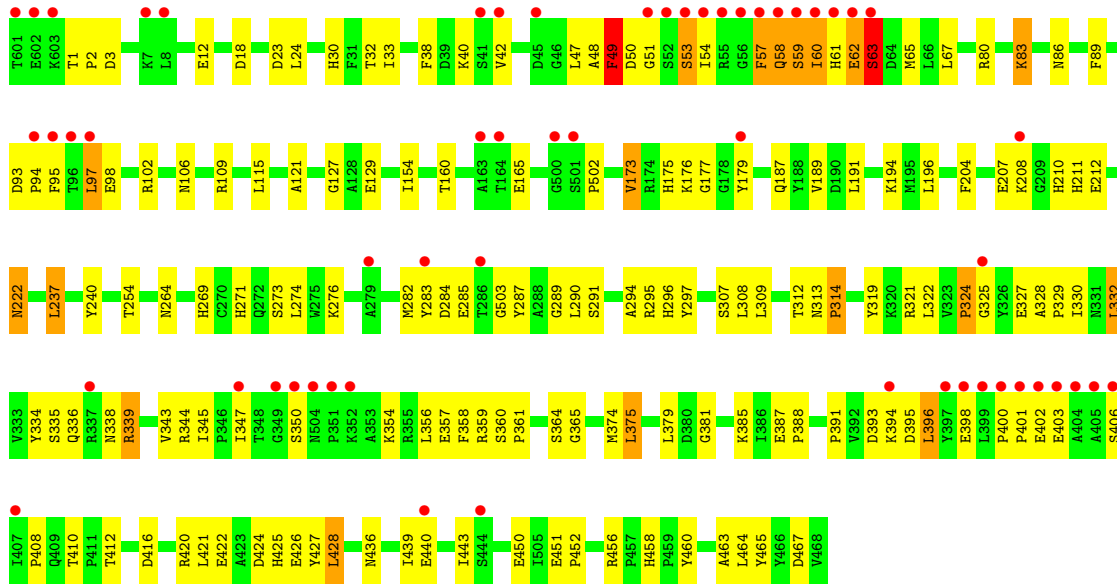


• Molecule 1: glutamine synthetase

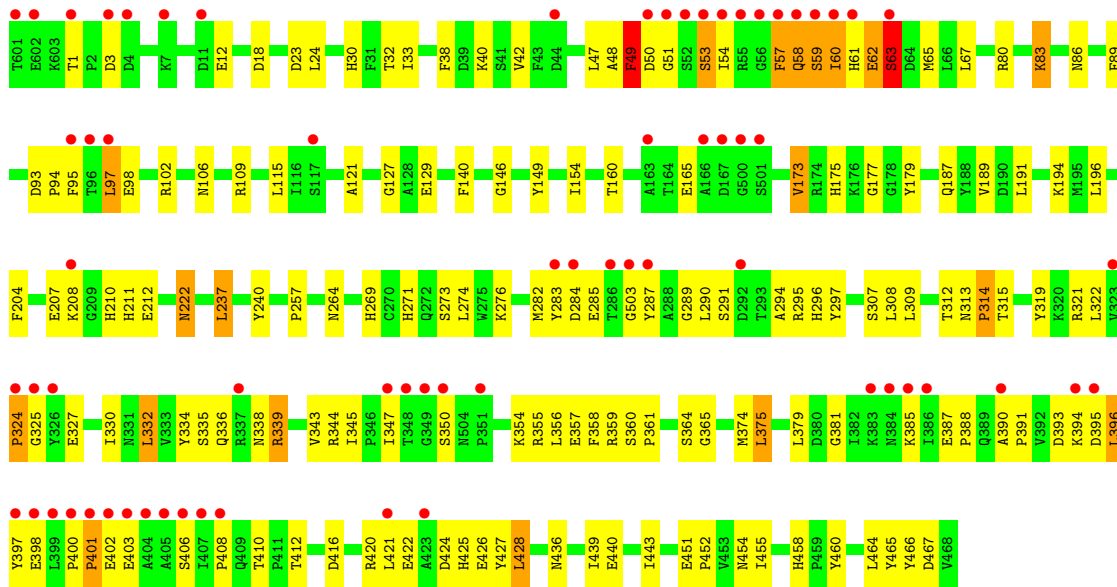




• Molecule 1: glutamine synthetase

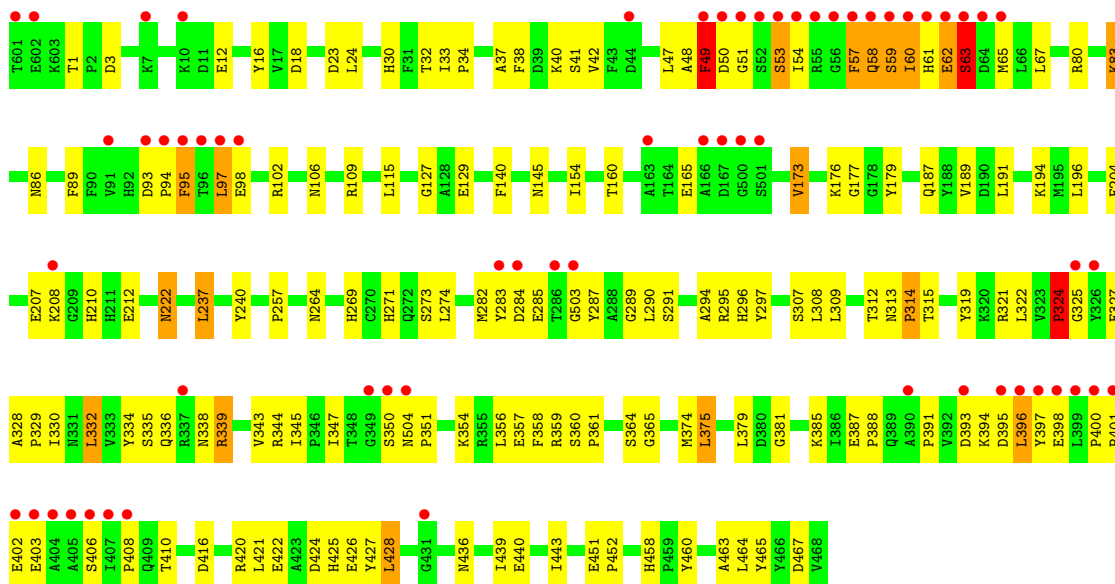


• Molecule 1: glutamine synthetase

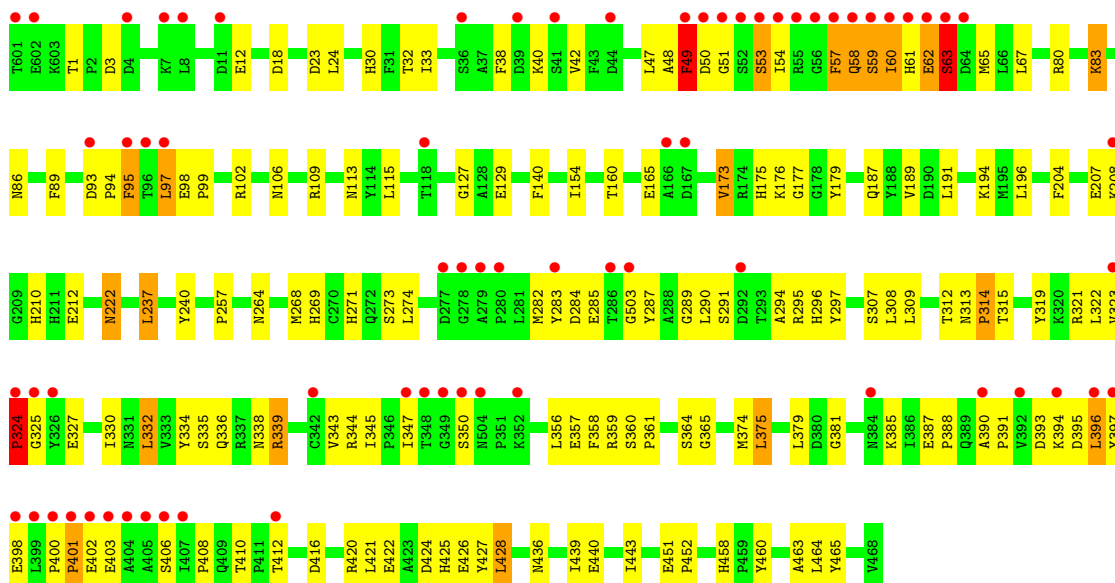


• Molecule 1: glutamine synthetase

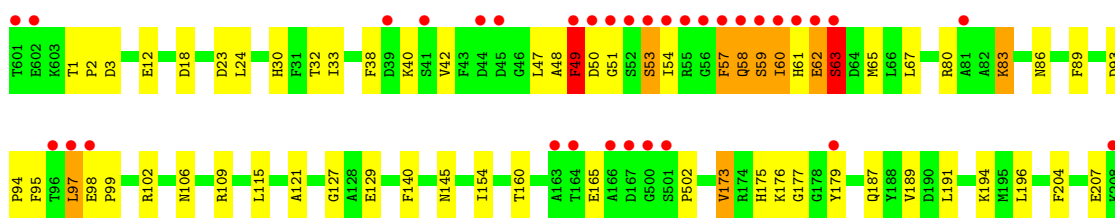


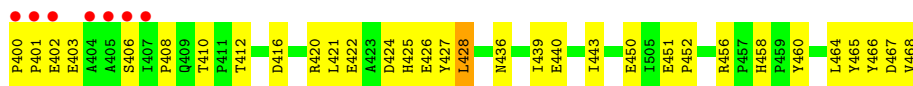


• Molecule 1: glutamine synthetase

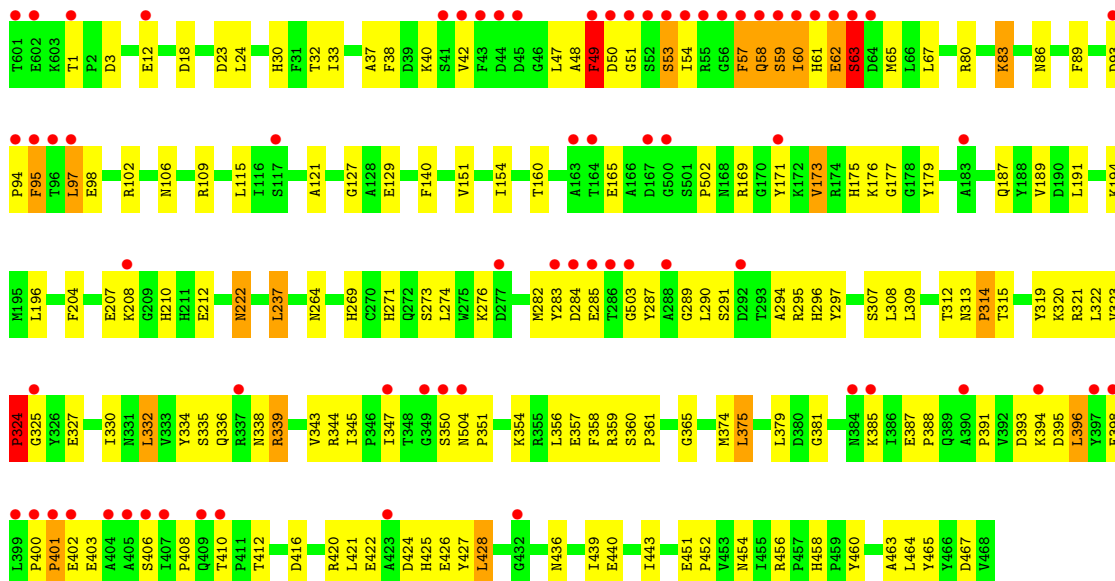


• Molecule 1: glutamine synthetase

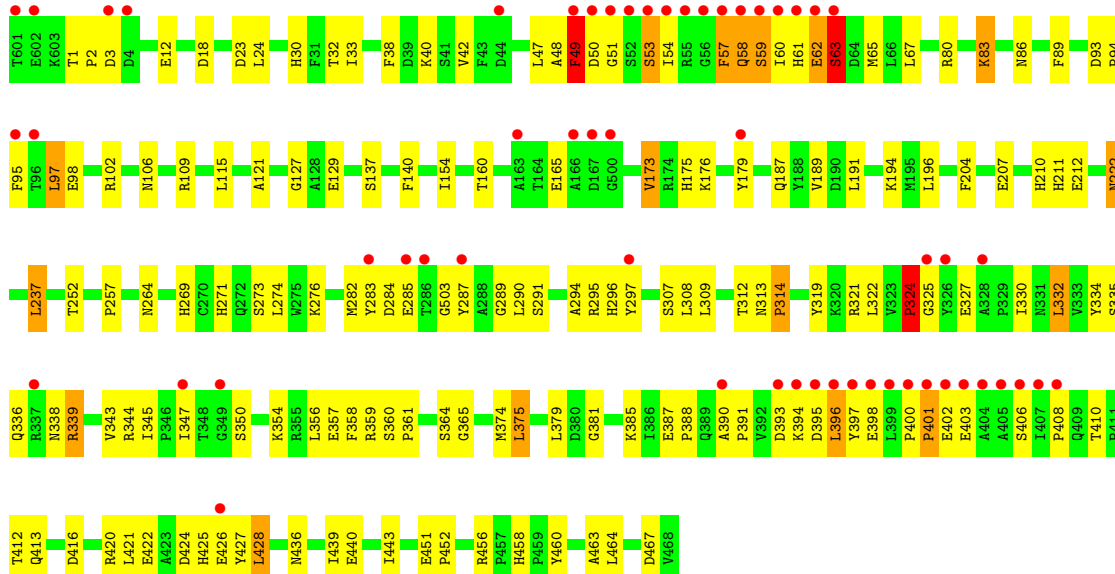




• Molecule 1: glutamine synthetase

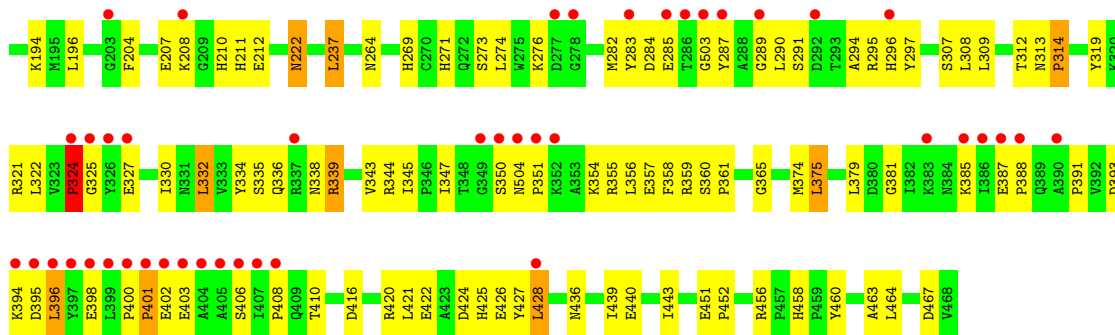


• Molecule 1: glutamine synthetase

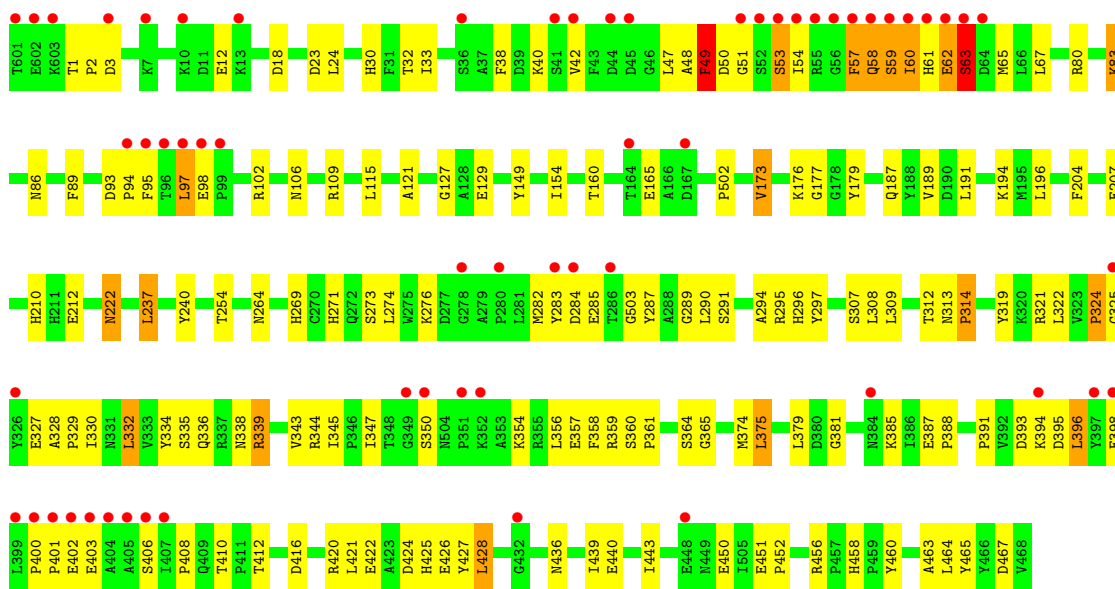


• Molecule 1: glutamine synthetase

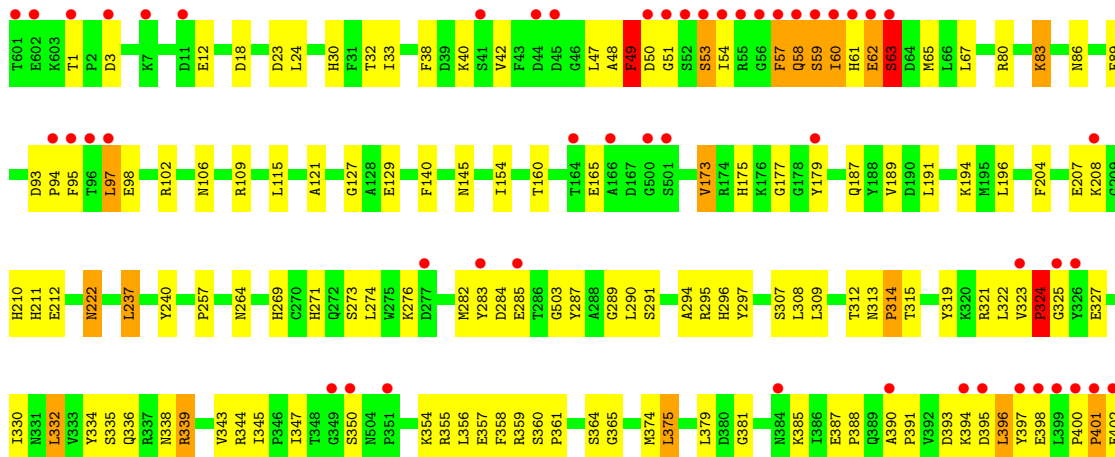


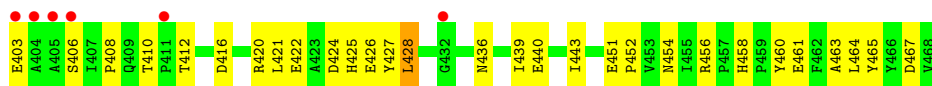


• Molecule 1: glutamine synthetase

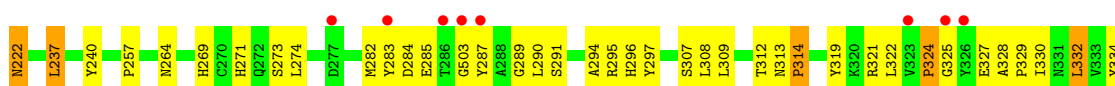
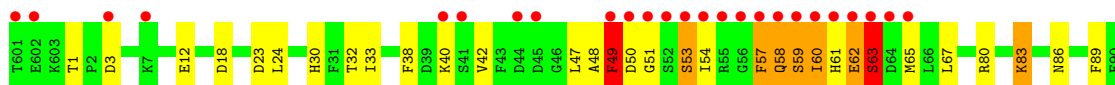


• Molecule 1: glutamine synthetase

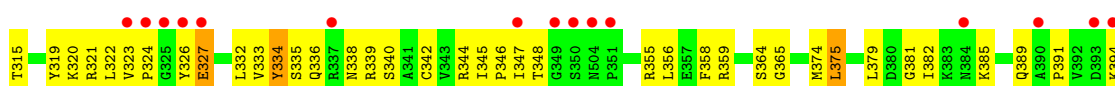
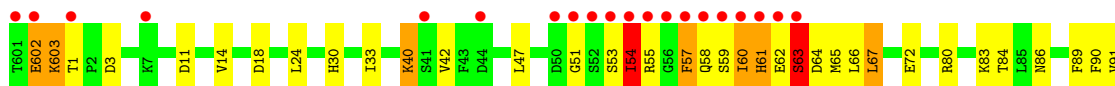




- Molecule 1: glutamine synthetase

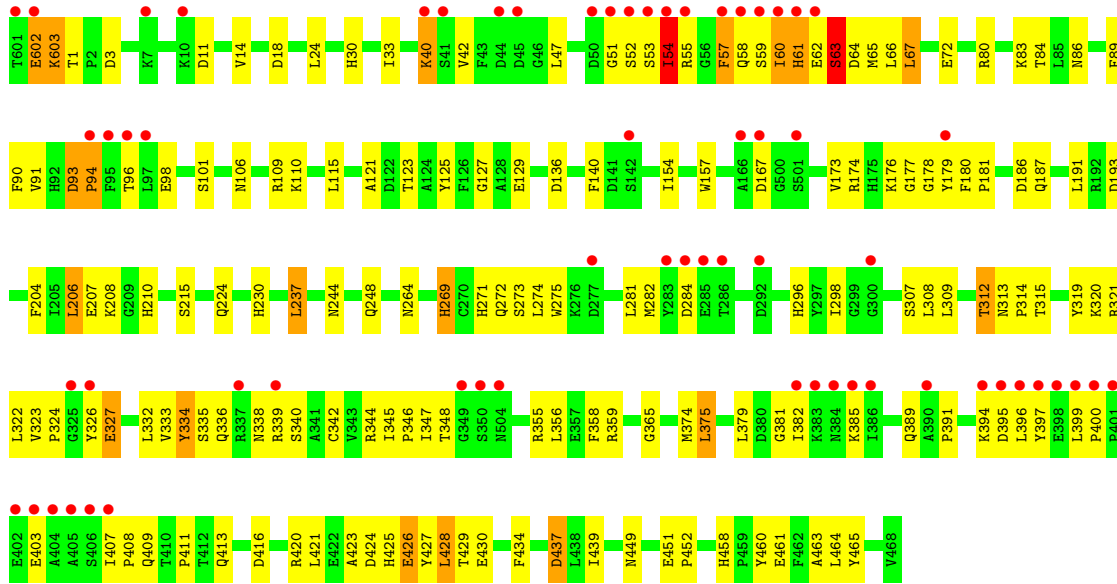


- Molecule 1: glutamine synthetase

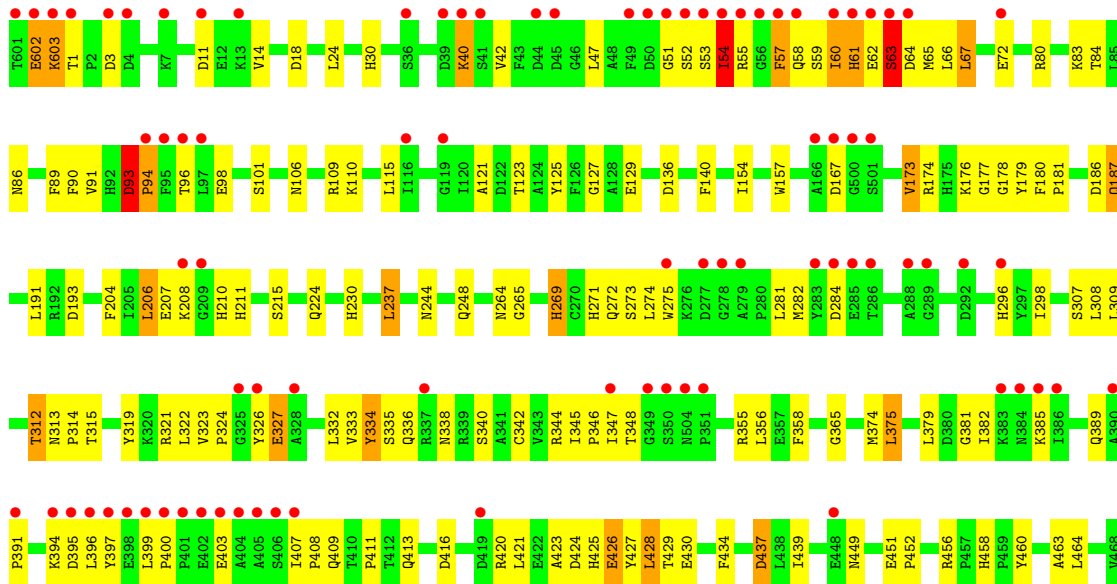


- Molecule 1: glutamine synthetase

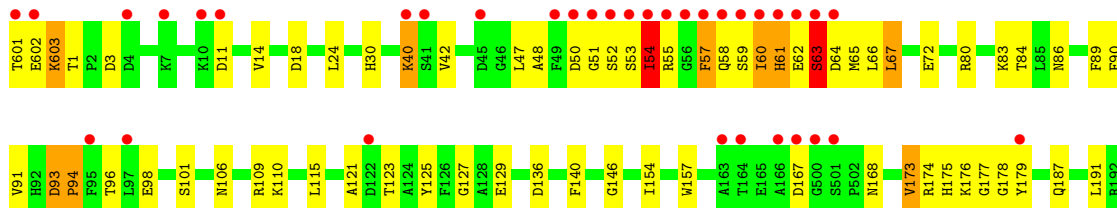


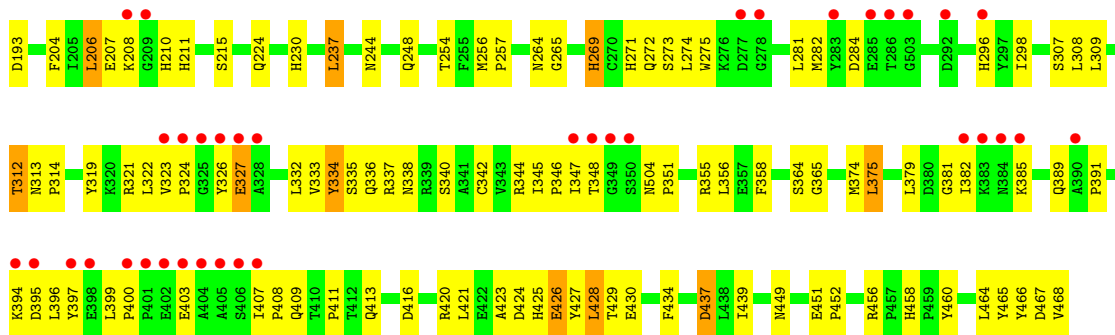


• Molecule 1: glutamine synthetase

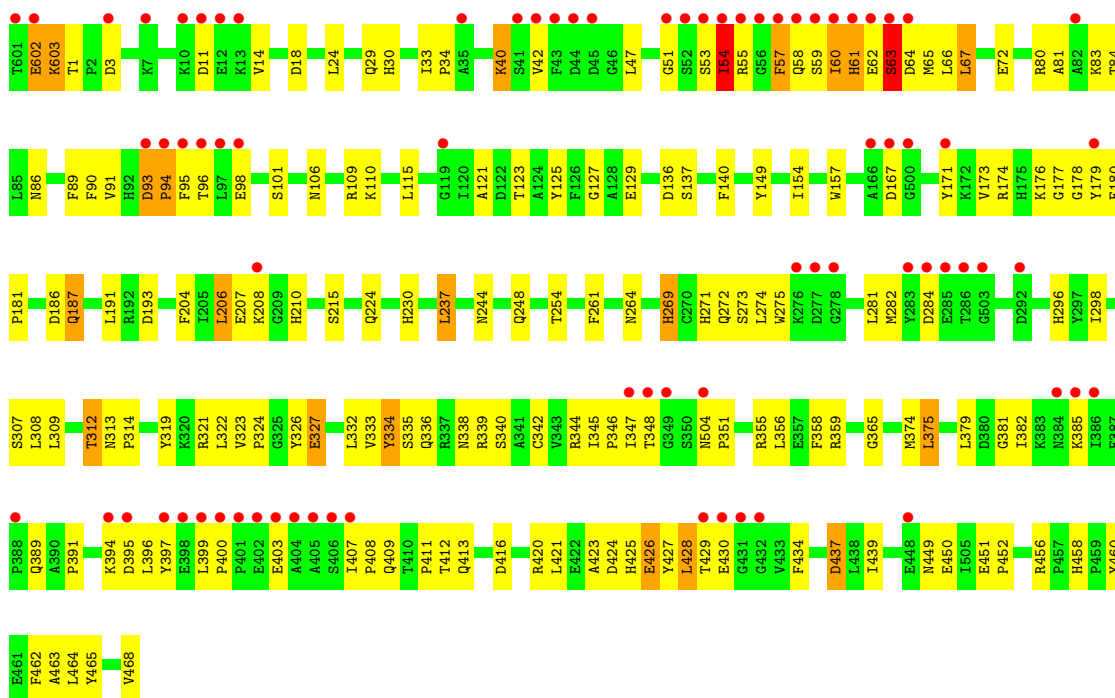


• Molecule 1: glutamine synthetase

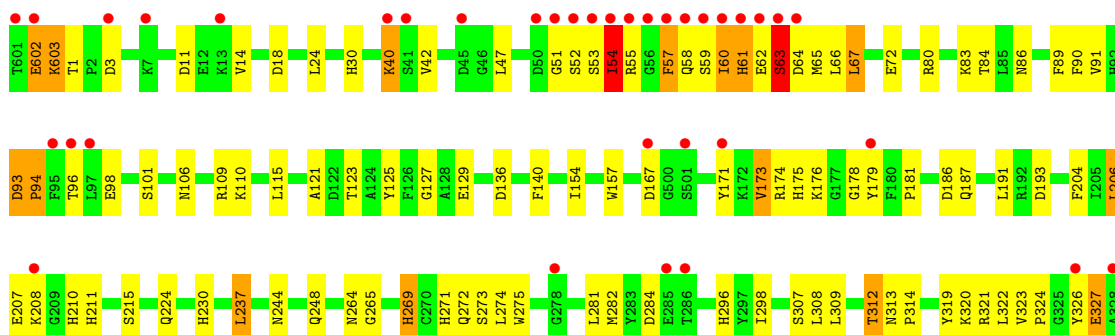


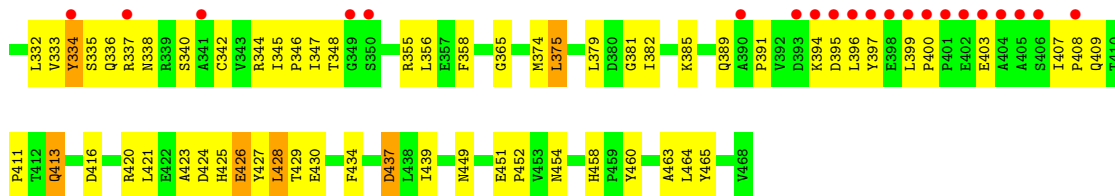


• Molecule 1: glutamine synthetase

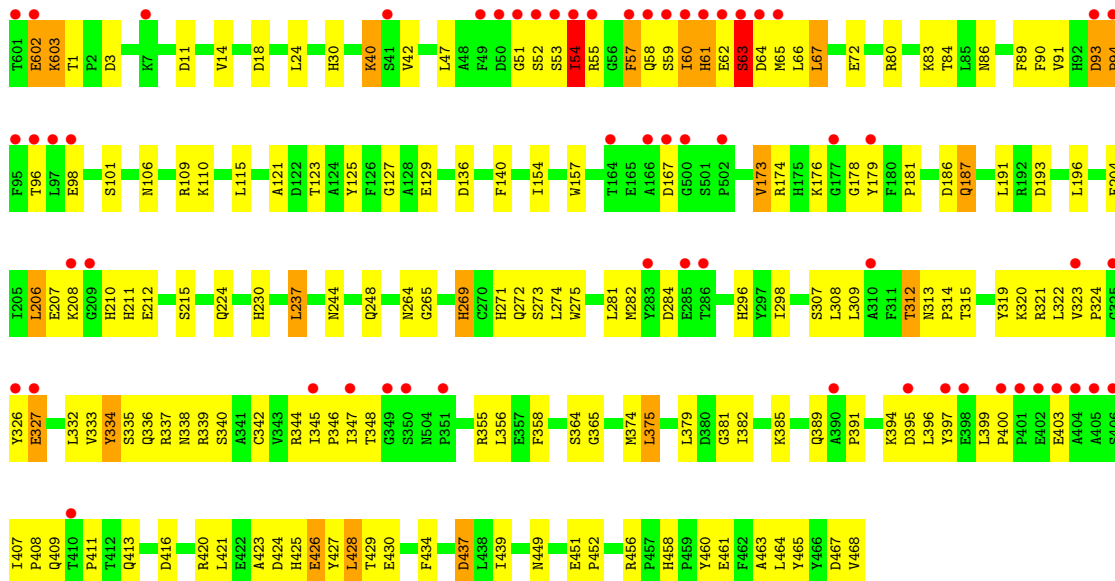


• Molecule 1: glutamine synthetase

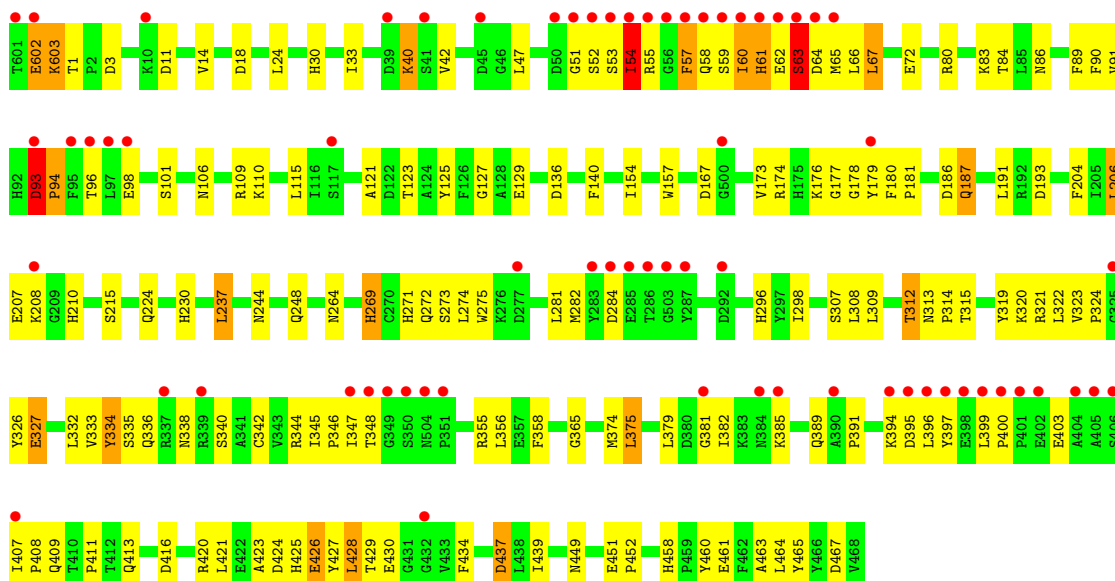




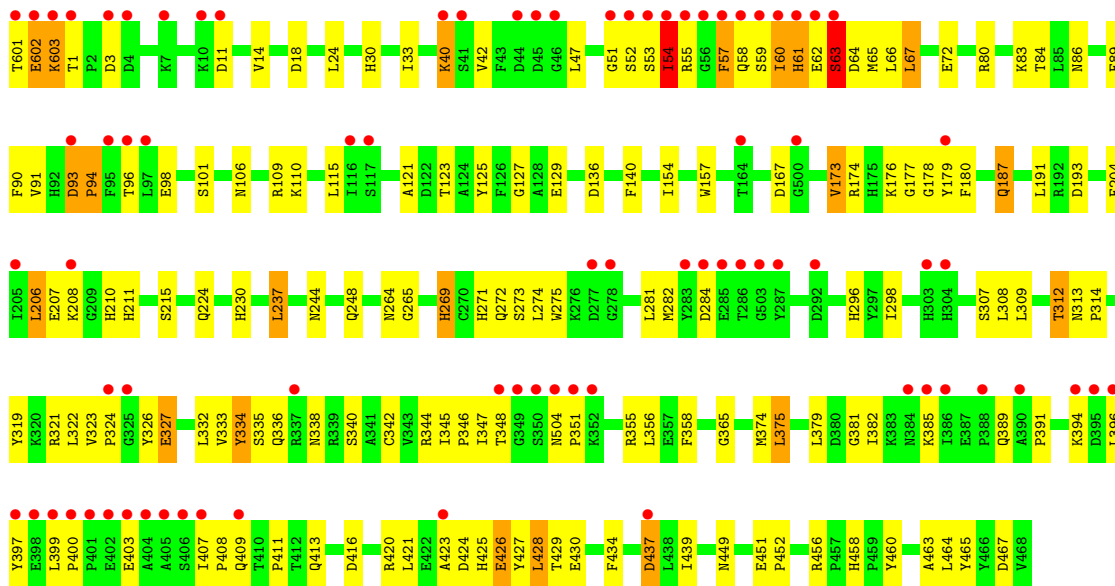
• Molecule 1: glutamine synthetase



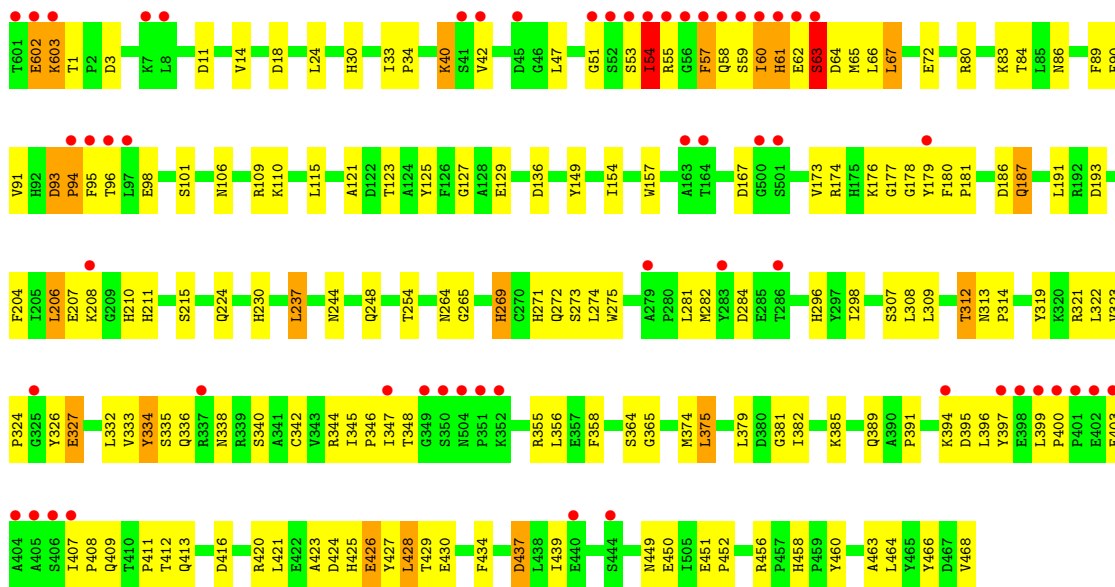
• Molecule 1: glutamine synthetase



• Molecule 1: glutamine synthetase

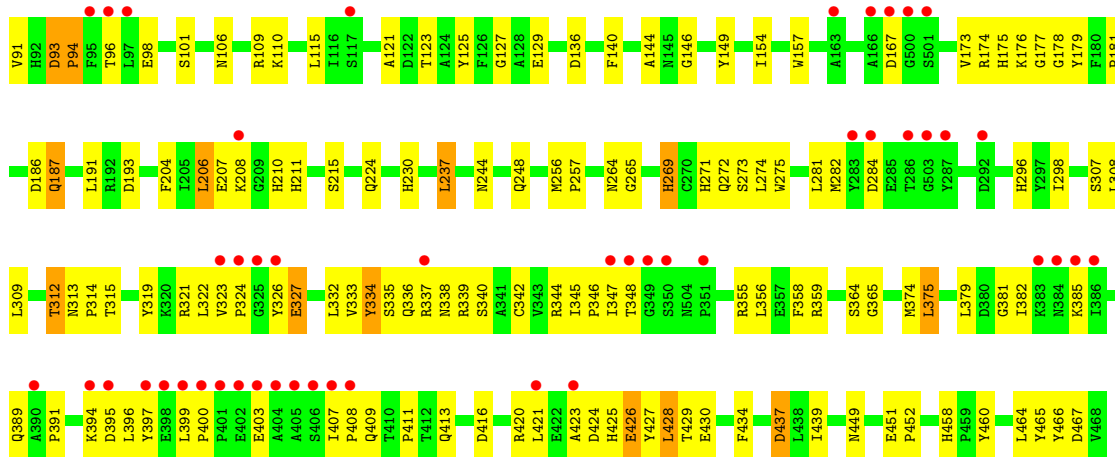


• Molecule 1: glutamine synthetase

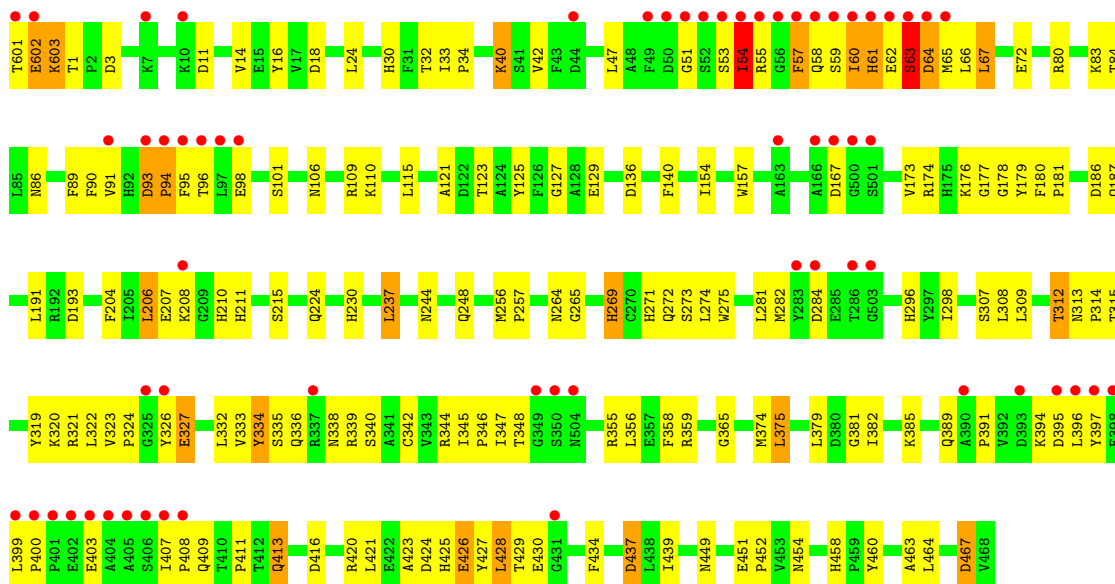


• Molecule 1: glutamine synthetase

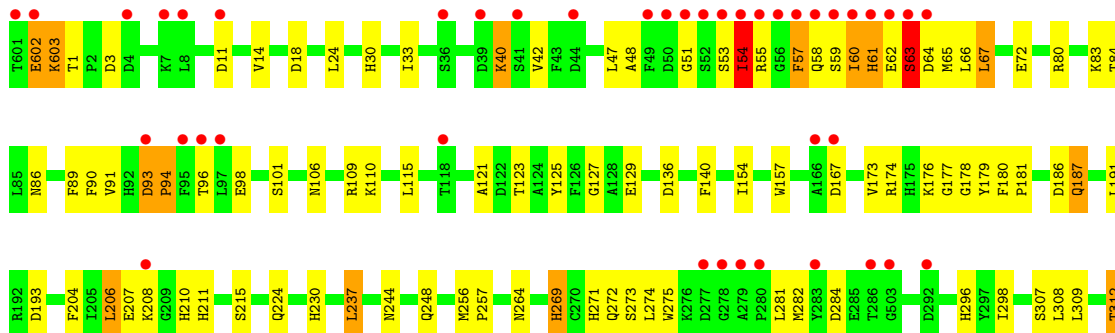


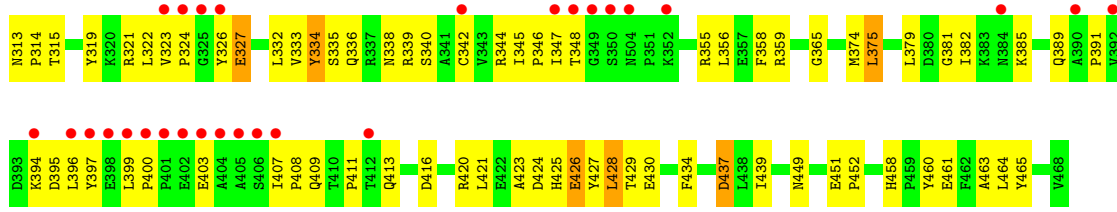


• Molecule 1: glutamine synthetase

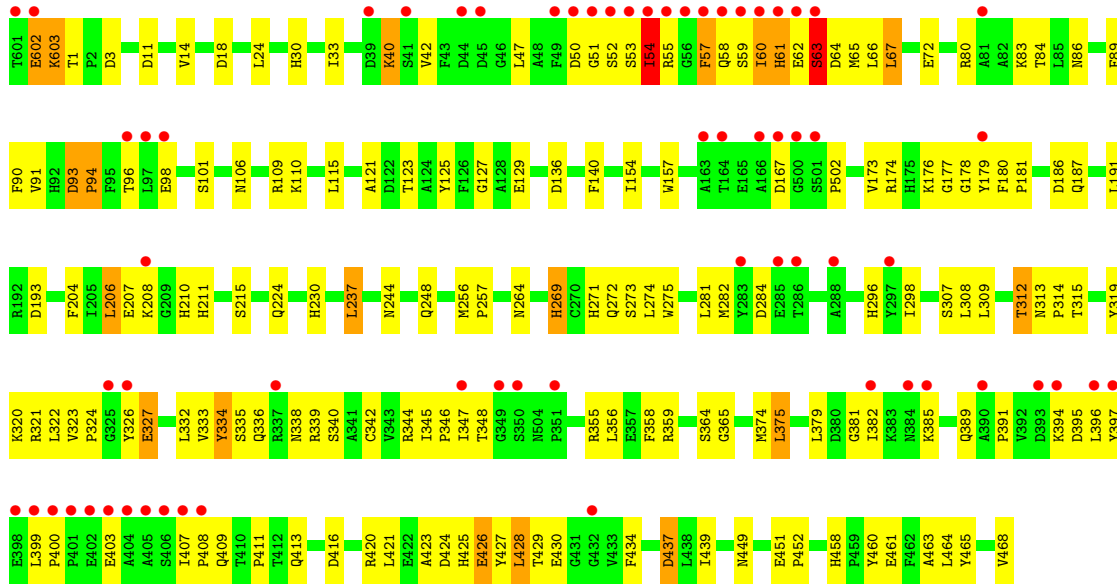


• Molecule 1: glutamine synthetase

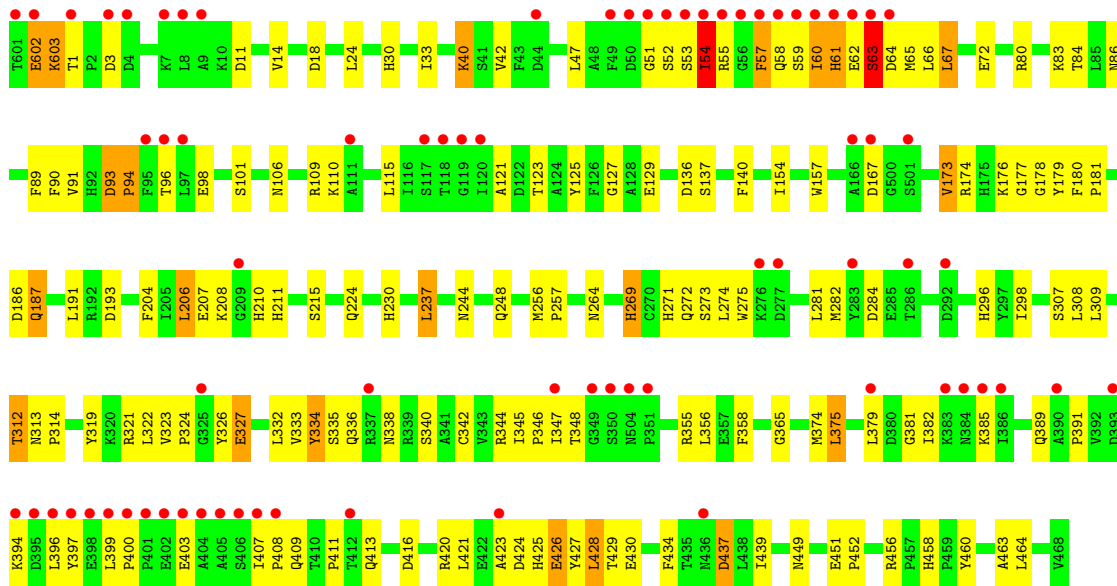




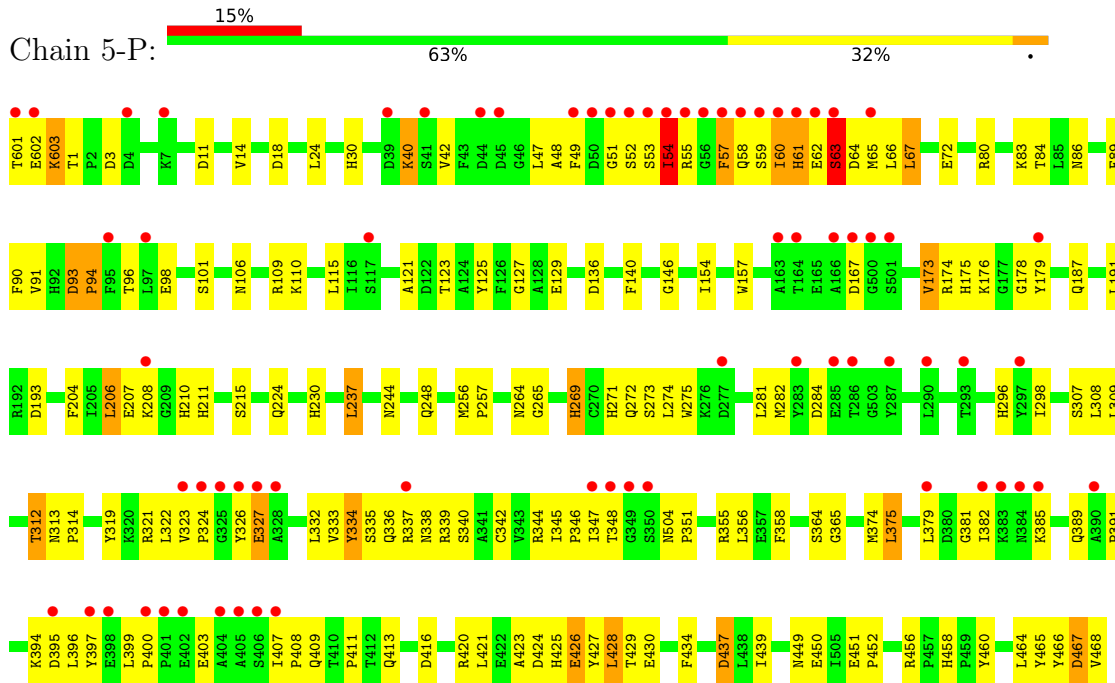
• Molecule 1: glutamine synthetase



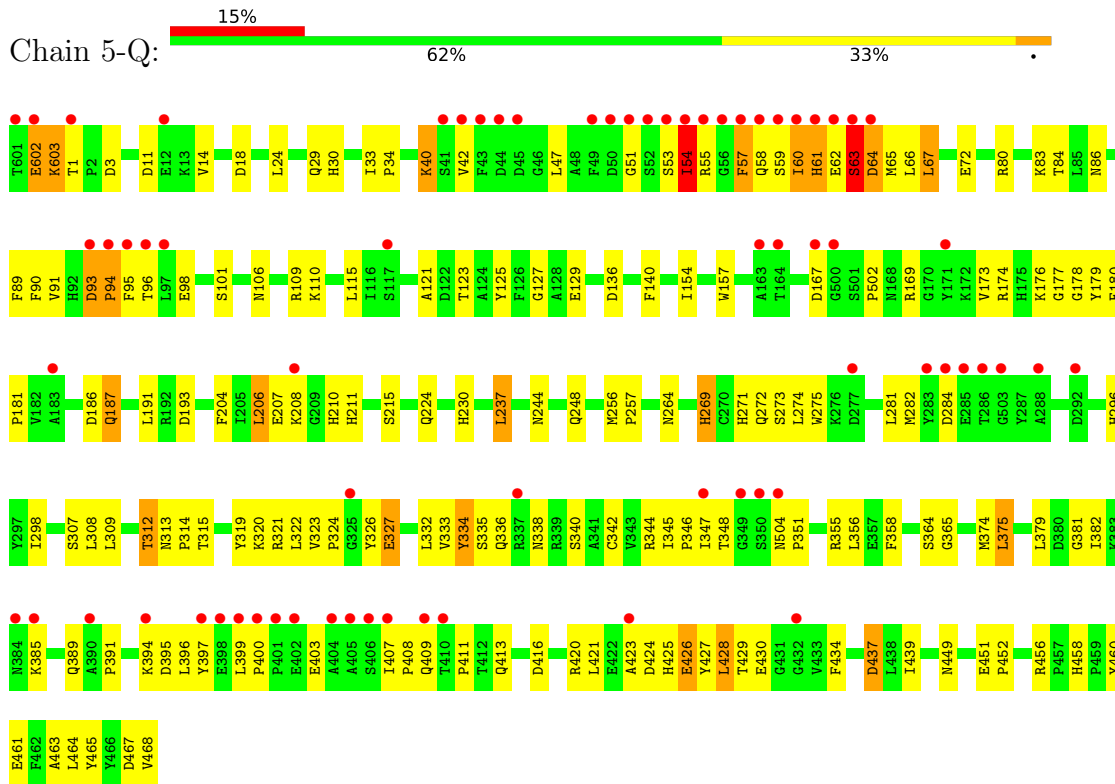
• Molecule 1: glutamine synthetase



- Molecule 1: glutamine synthetase

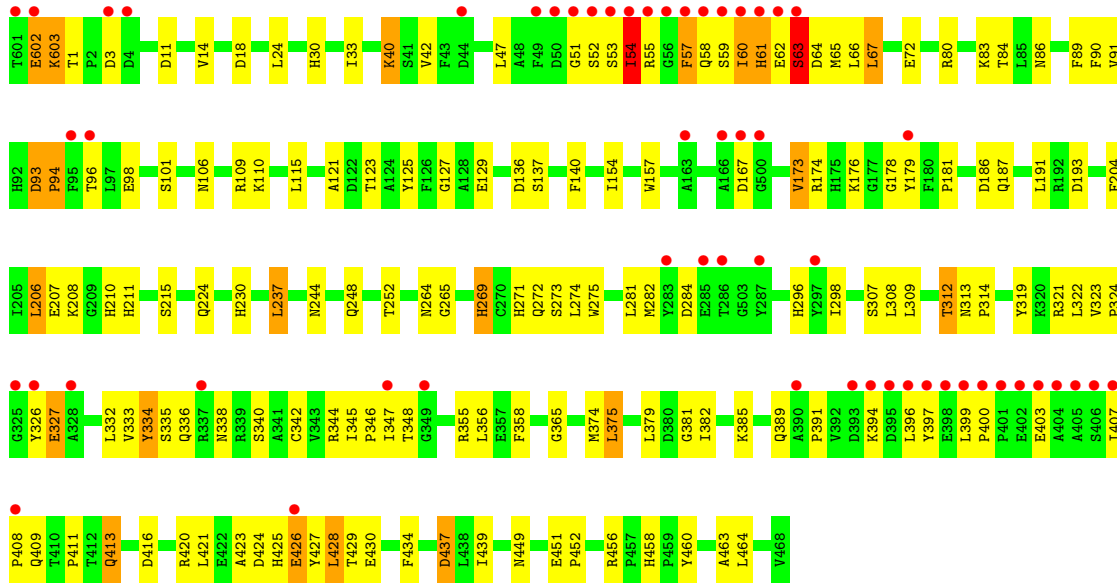


- Molecule 1: glutamine synthetase

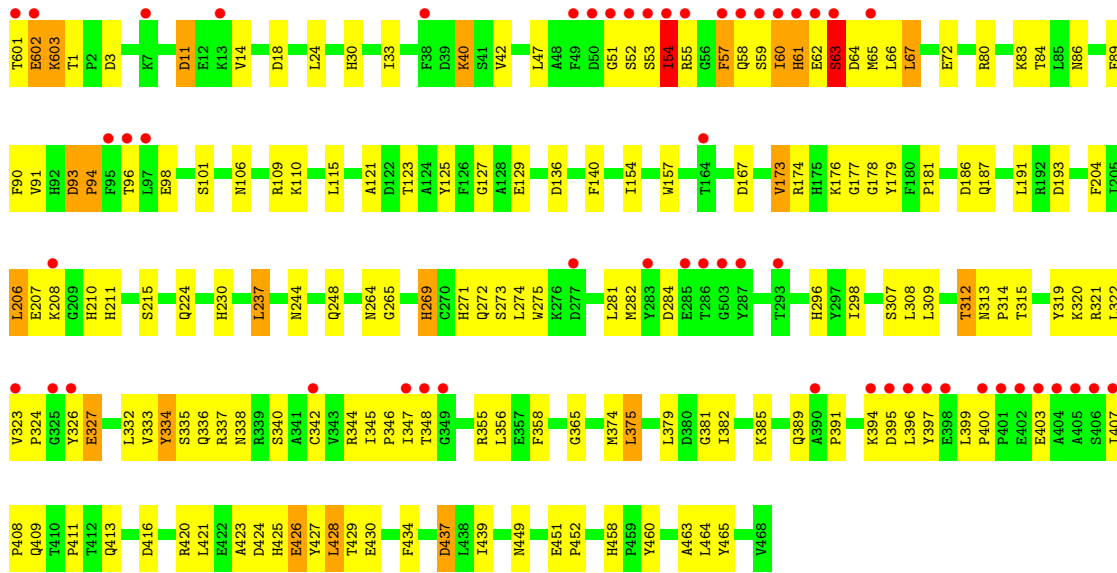


- Molecule 1: glutamine synthetase

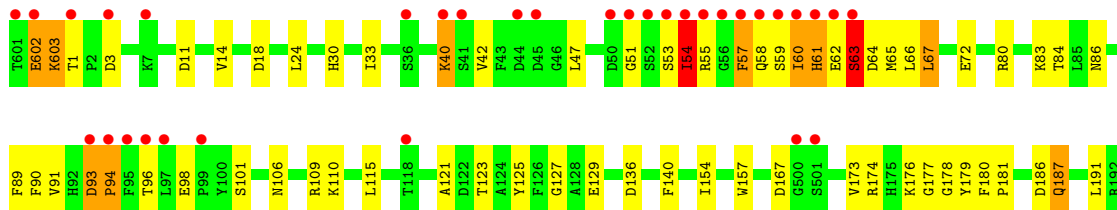


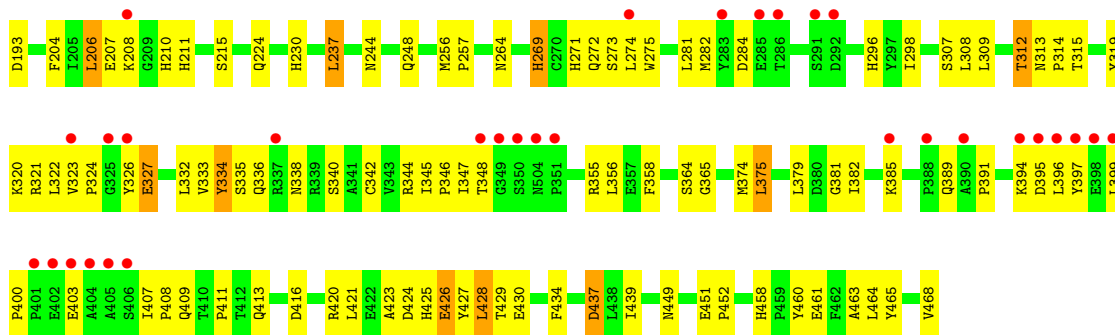


● Molecule 1: glutamine synthetase

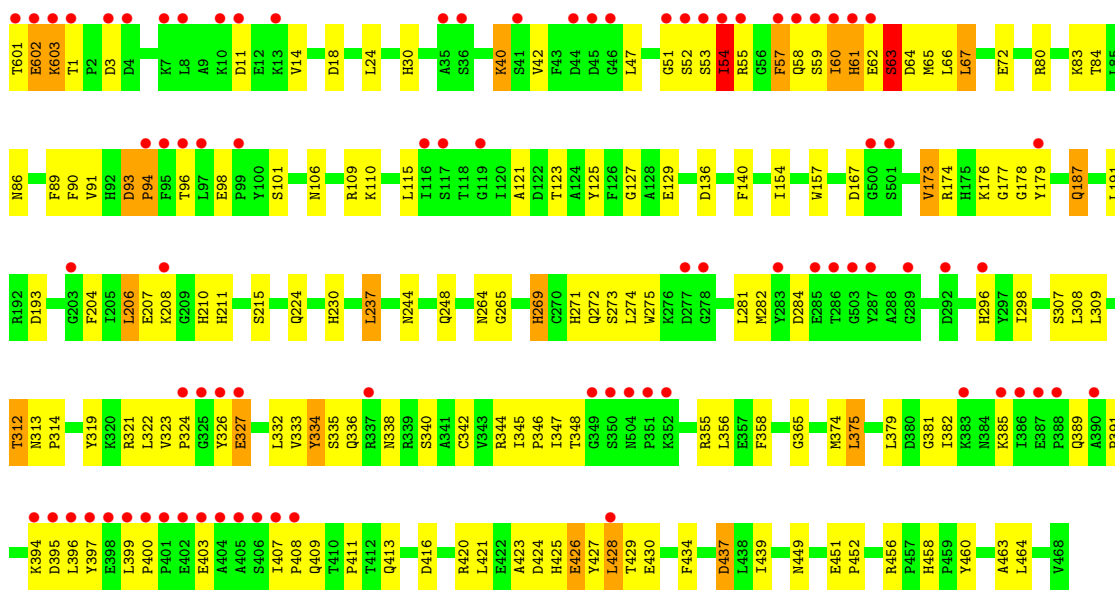


● Molecule 1: glutamine synthetase

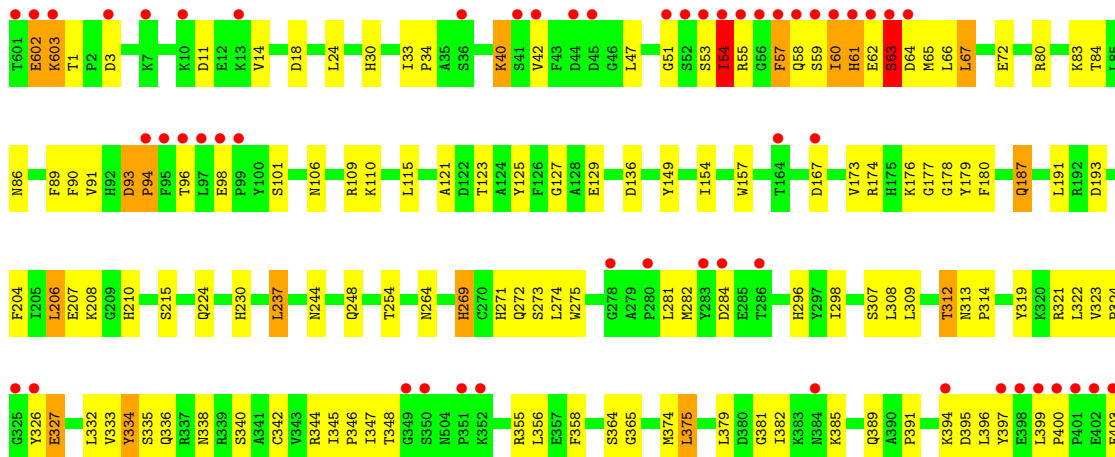


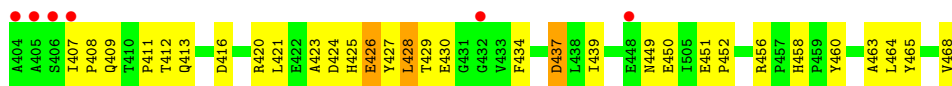


• Molecule 1: glutamine synthetase

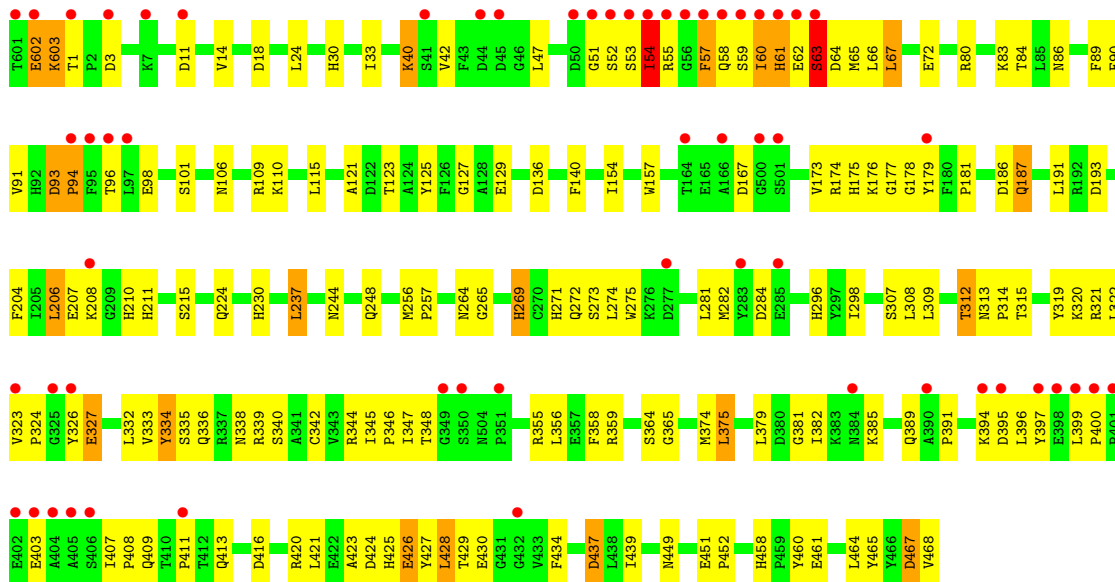


• Molecule 1: glutamine synthetase

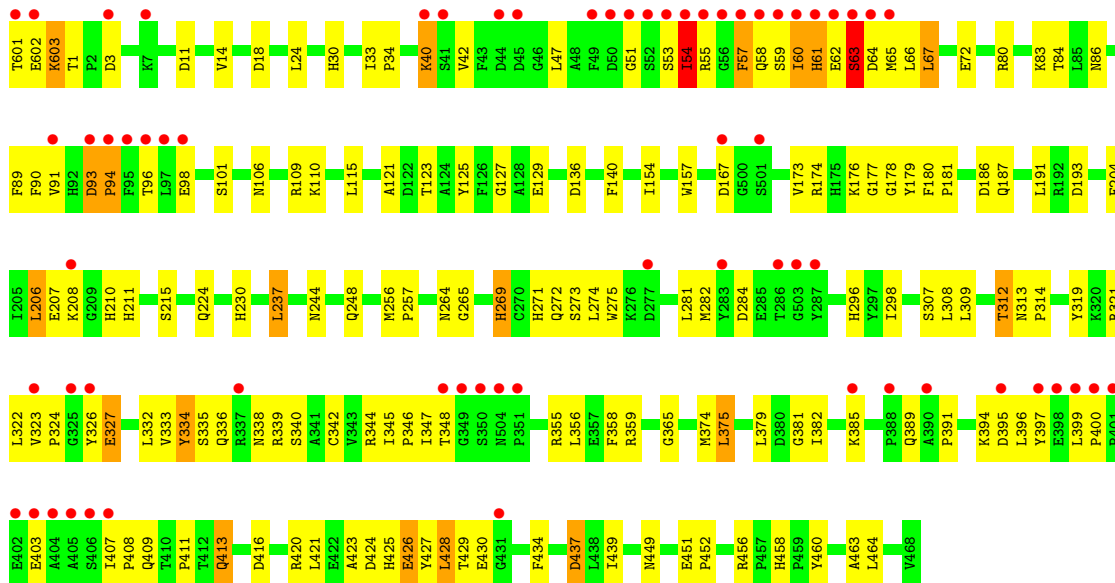




• Molecule 1: glutamine synthetase

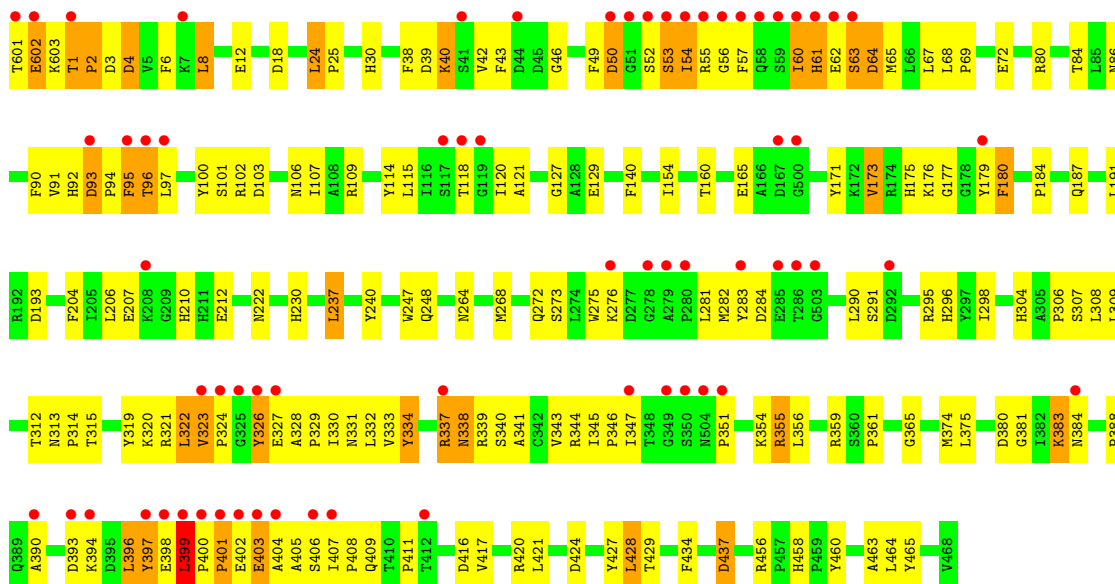


• Molecule 1: glutamine synthetase

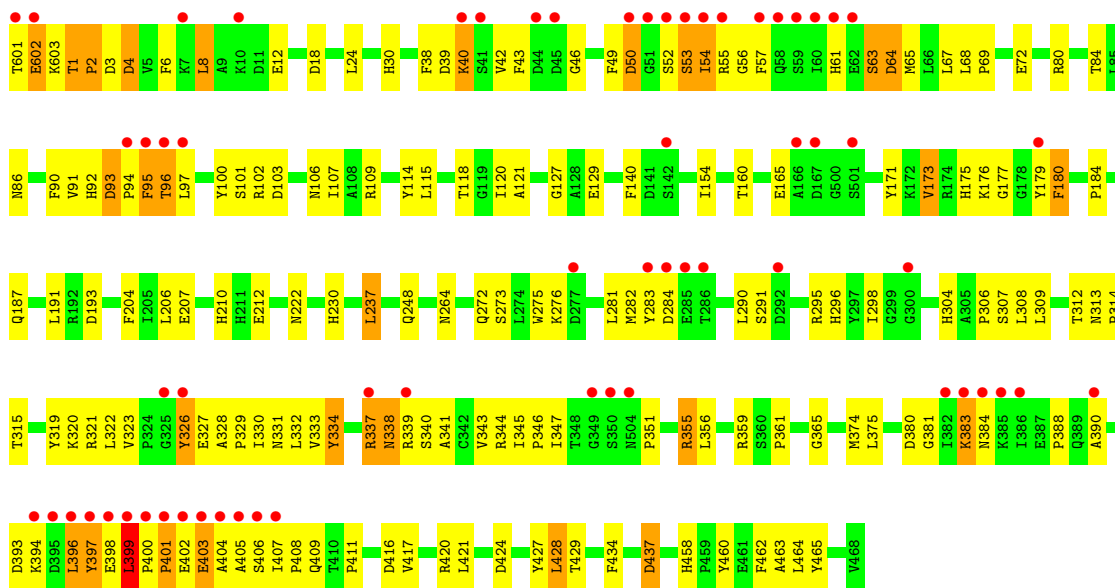


• Molecule 1: glutamine synthetase

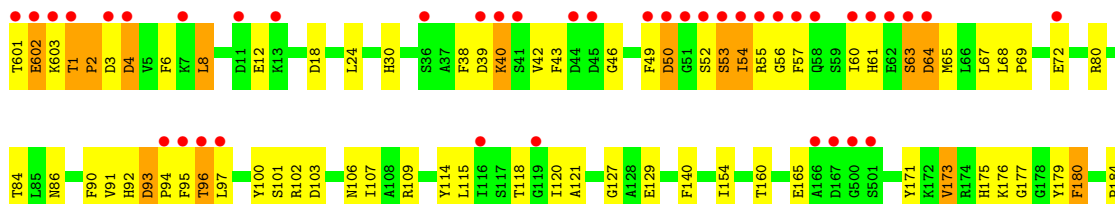


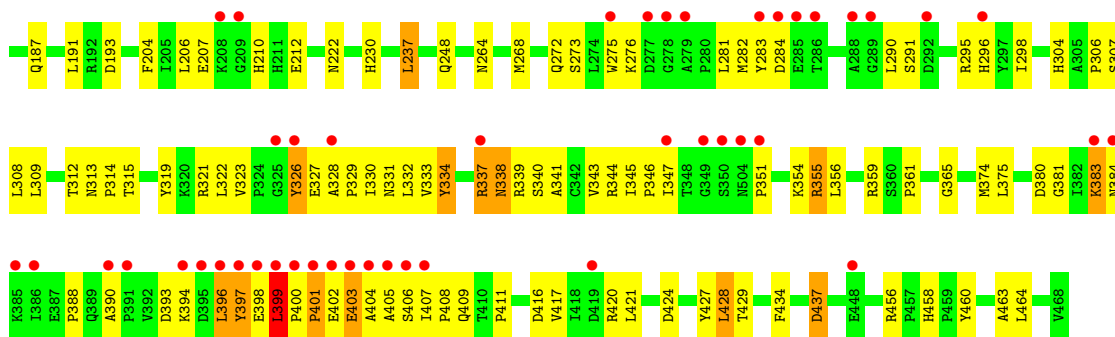


• Molecule 1: glutamine synthetase

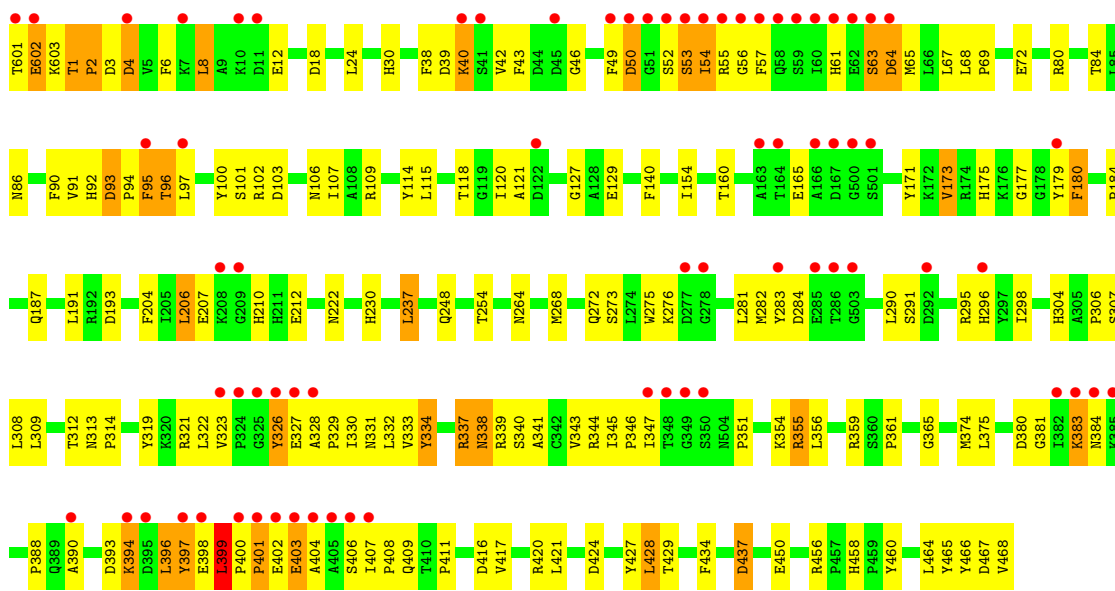


• Molecule 1: glutamine synthetase

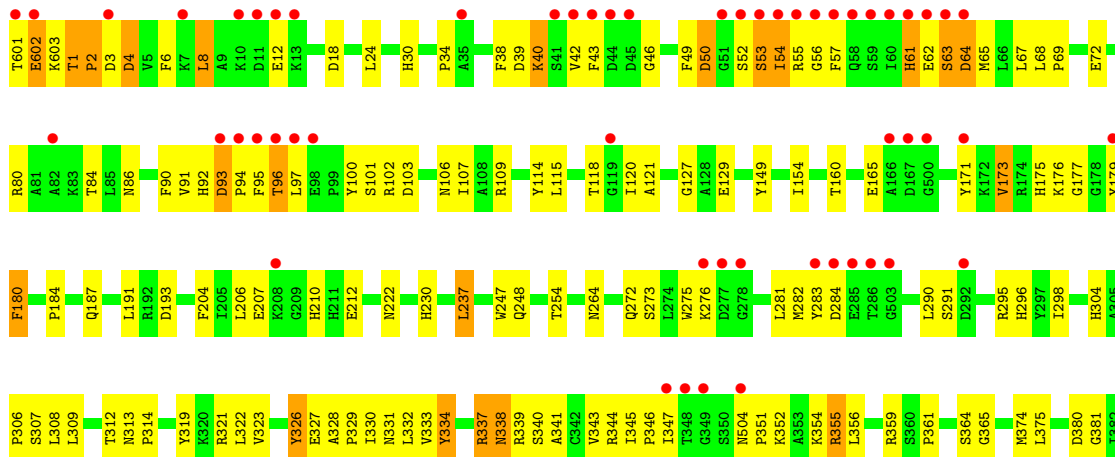


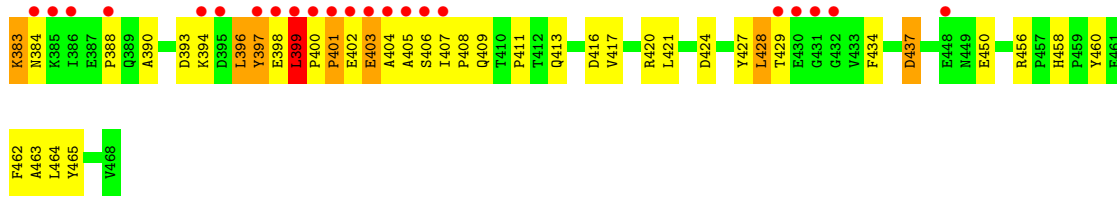


• Molecule 1: glutamine synthetase

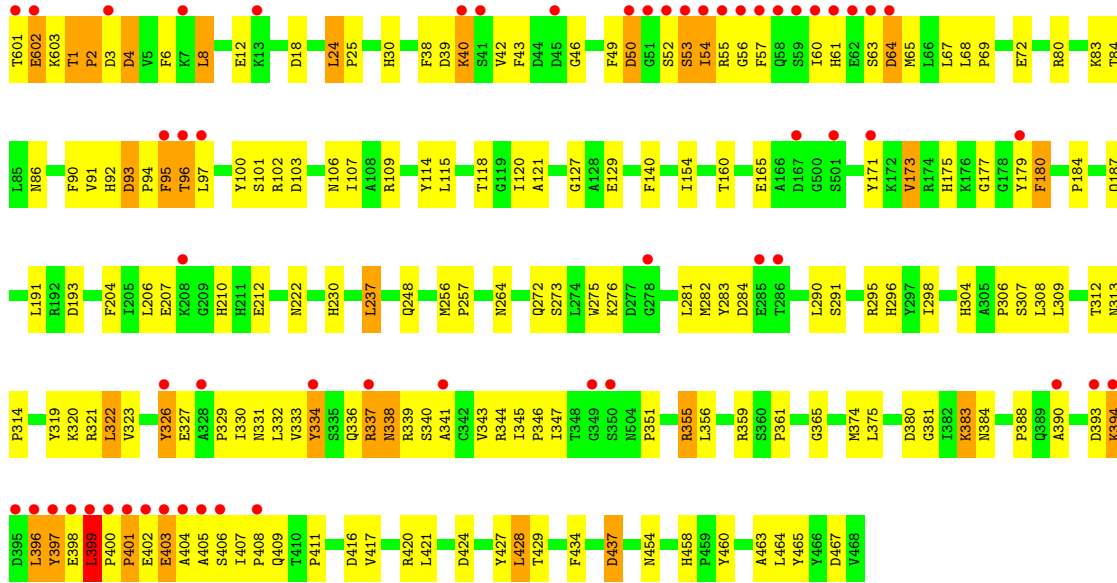


• Molecule 1: glutamine synthetase

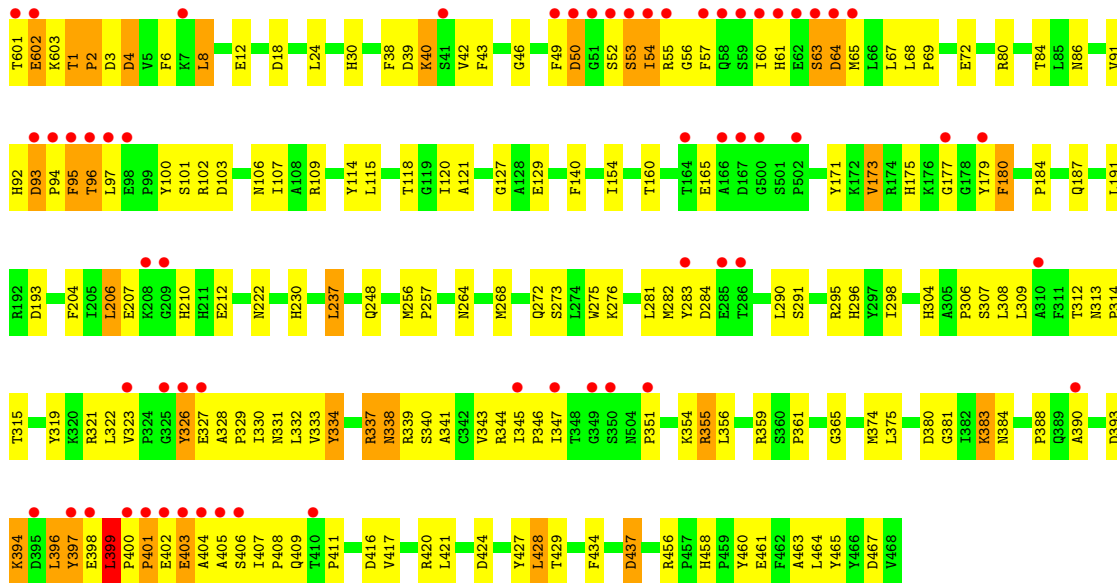




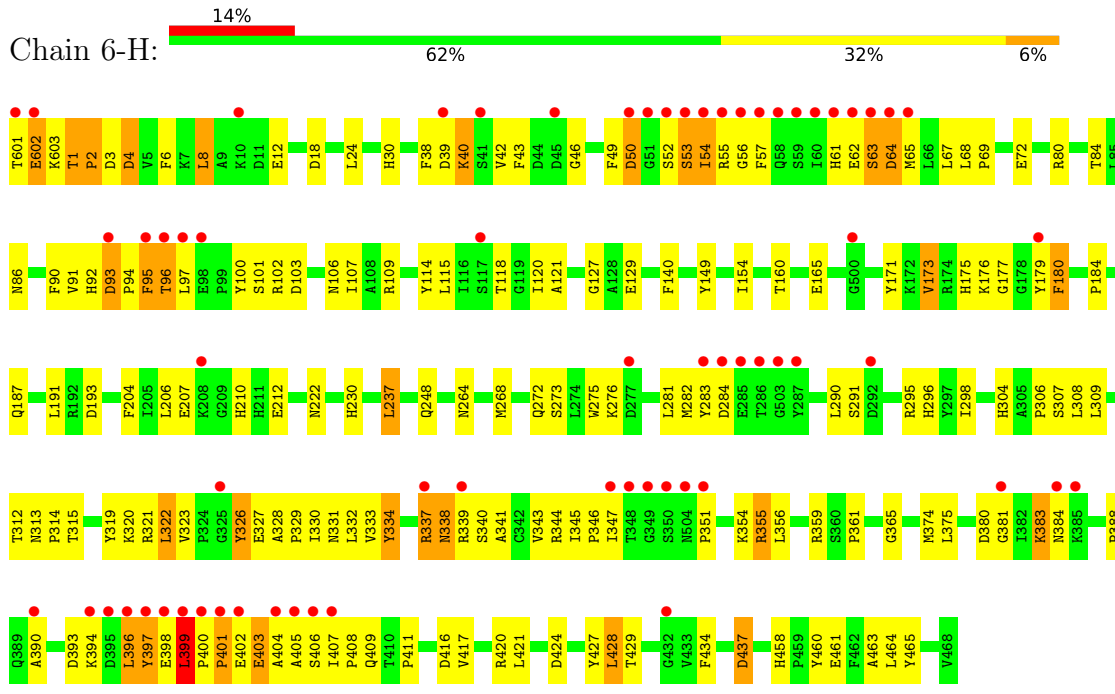
• Molecule 1: glutamine synthetase



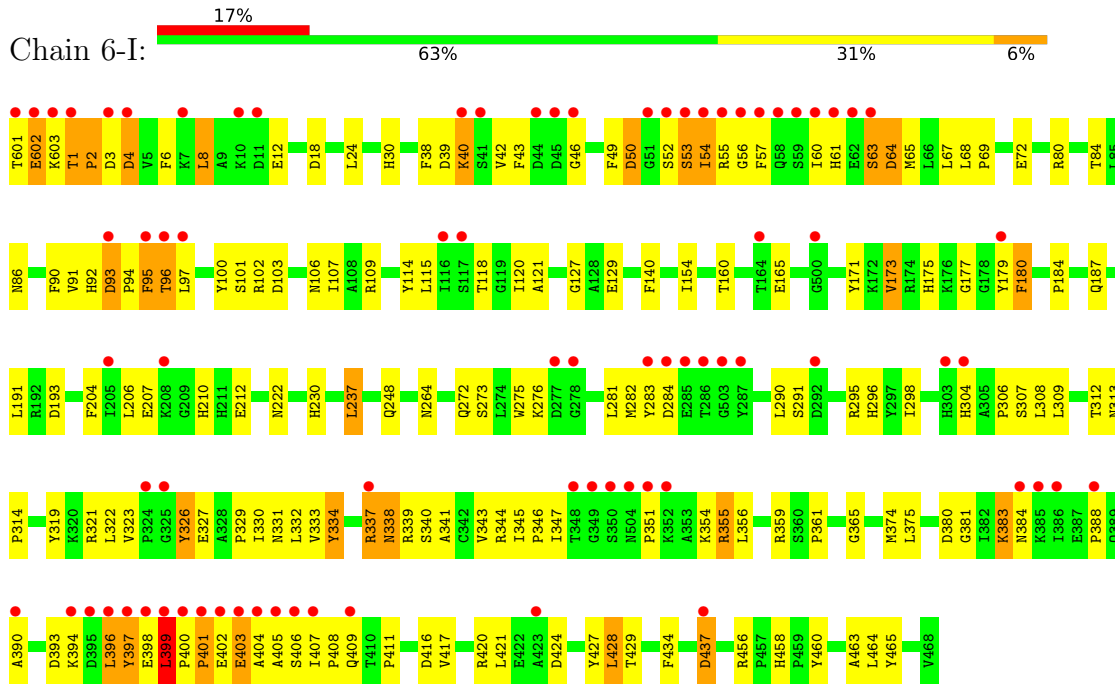
• Molecule 1: glutamine synthetase



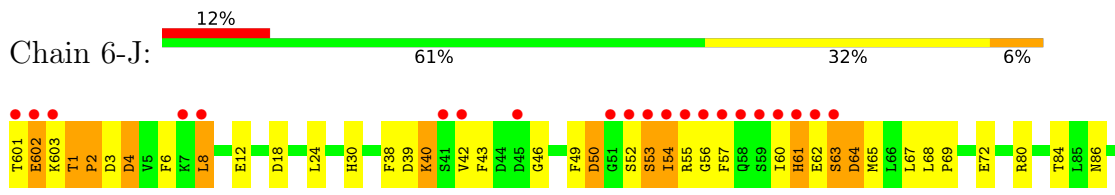
• Molecule 1: glutamine synthetase

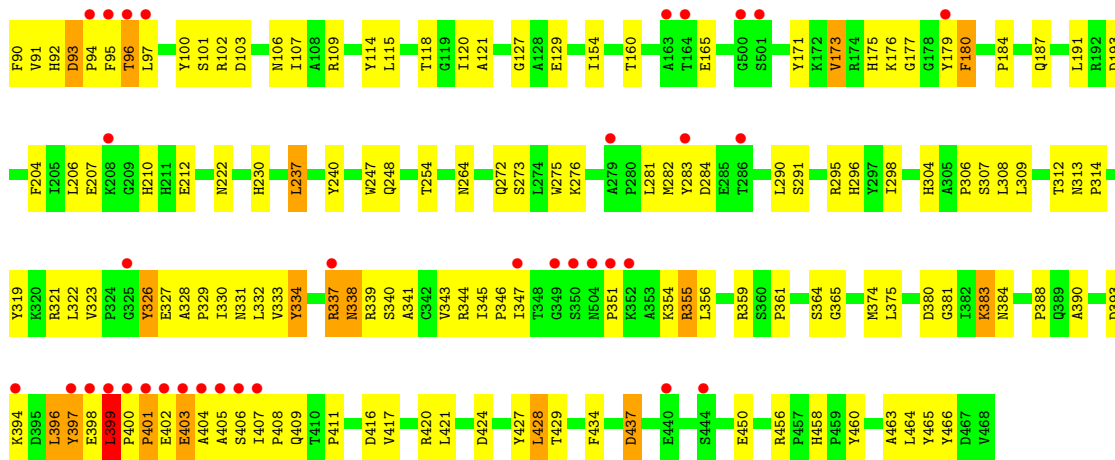


• Molecule 1: glutamine synthetase

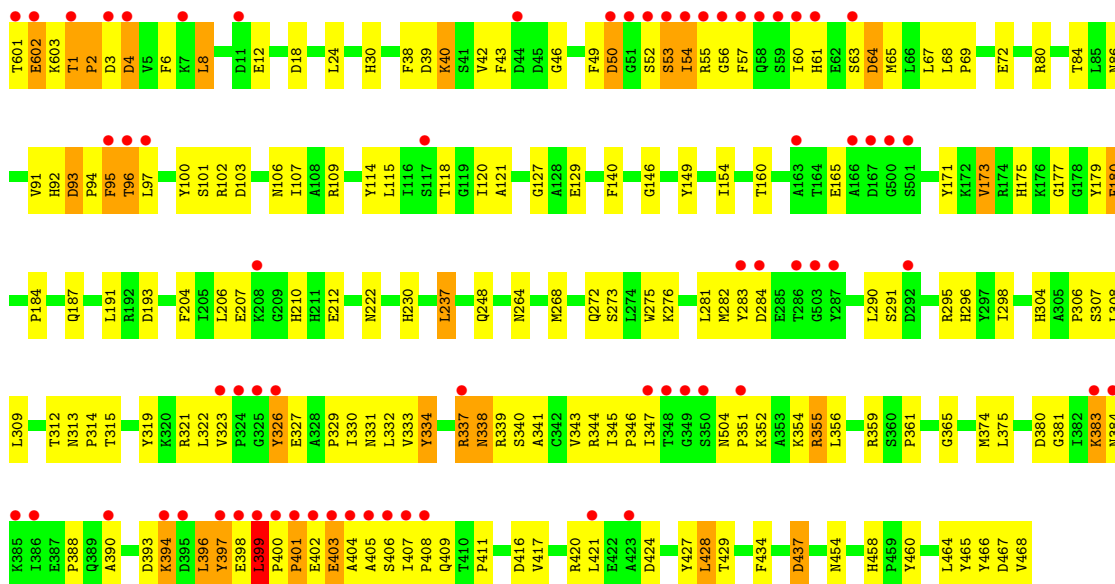


• Molecule 1: glutamine synthetase

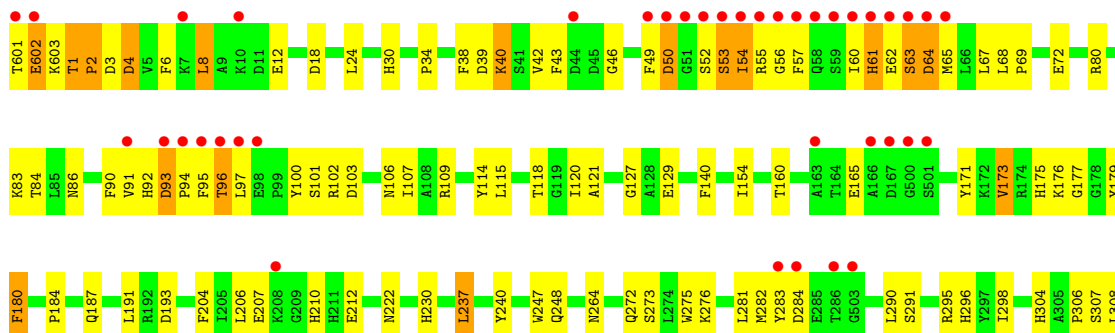


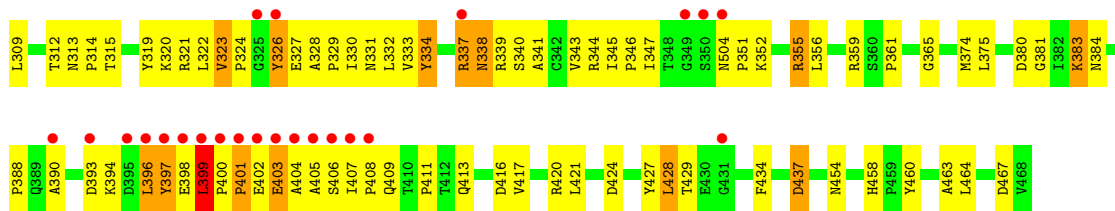


• Molecule 1: glutamine synthetase

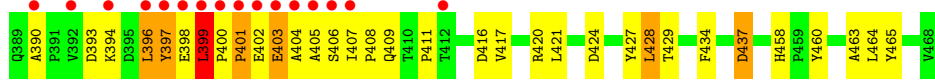
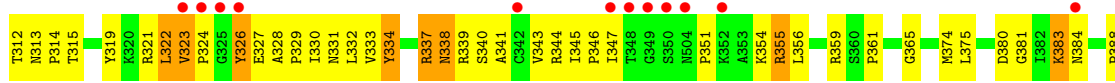
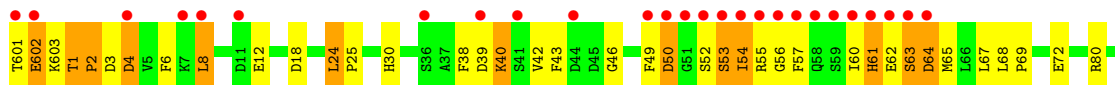


• Molecule 1: glutamine synthetase

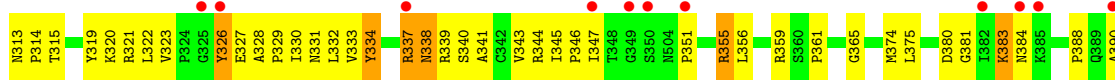
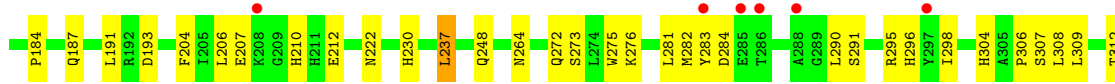




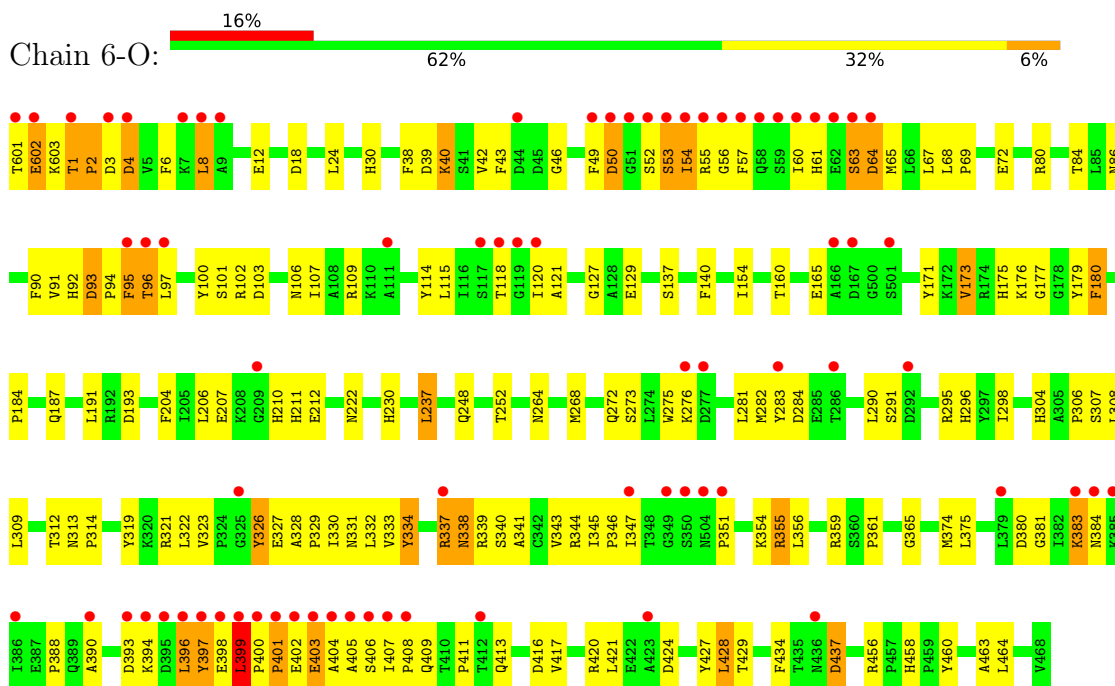
• Molecule 1: glutamine synthetase



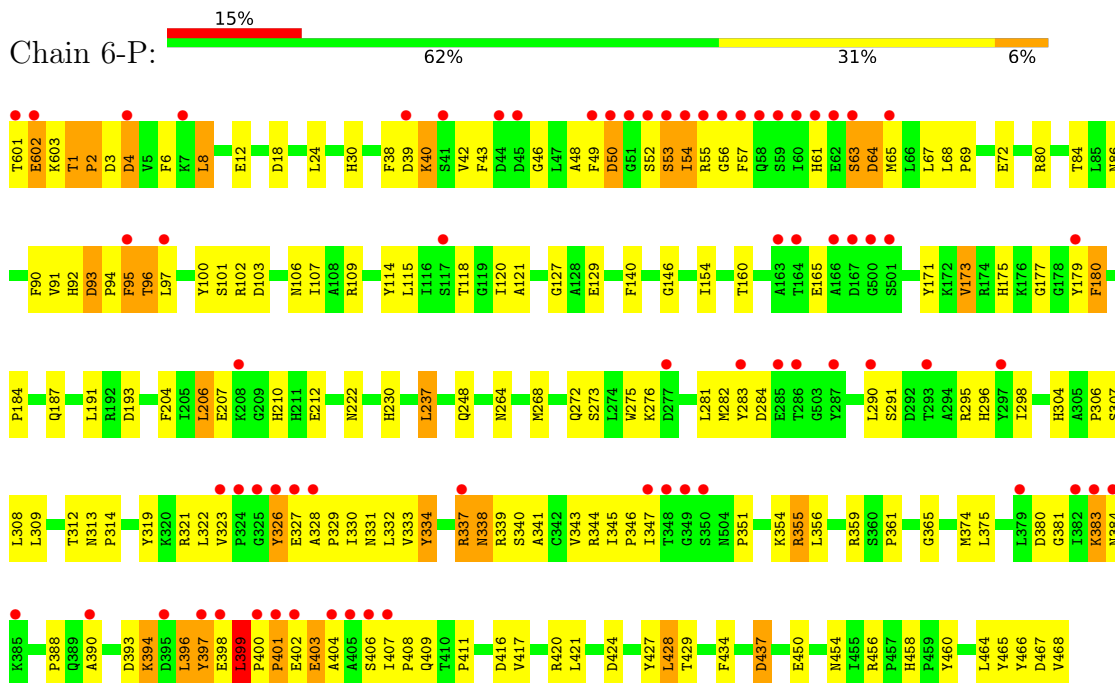
• Molecule 1: glutamine synthetase



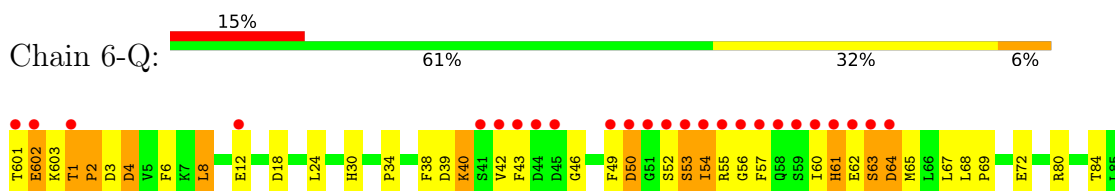
- Molecule 1: glutamine synthetase

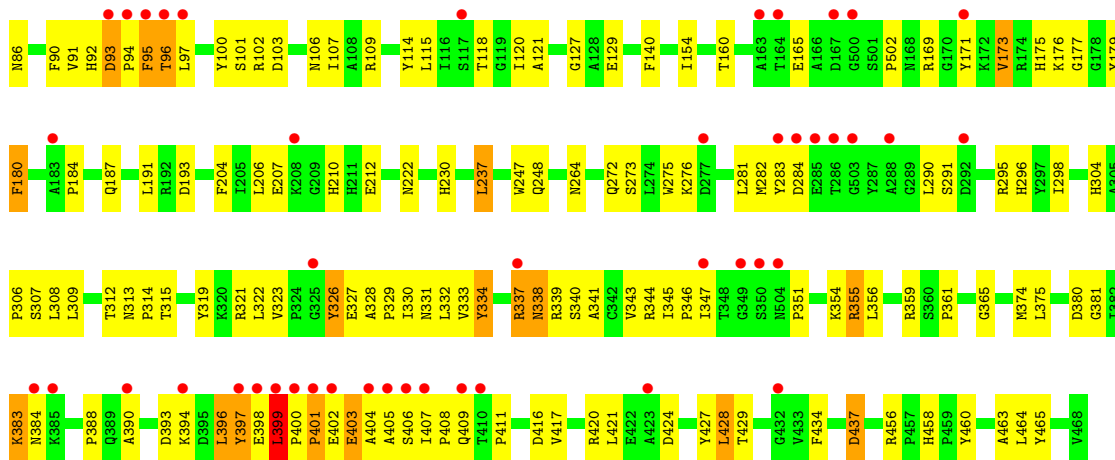


- Molecule 1: glutamine synthetase

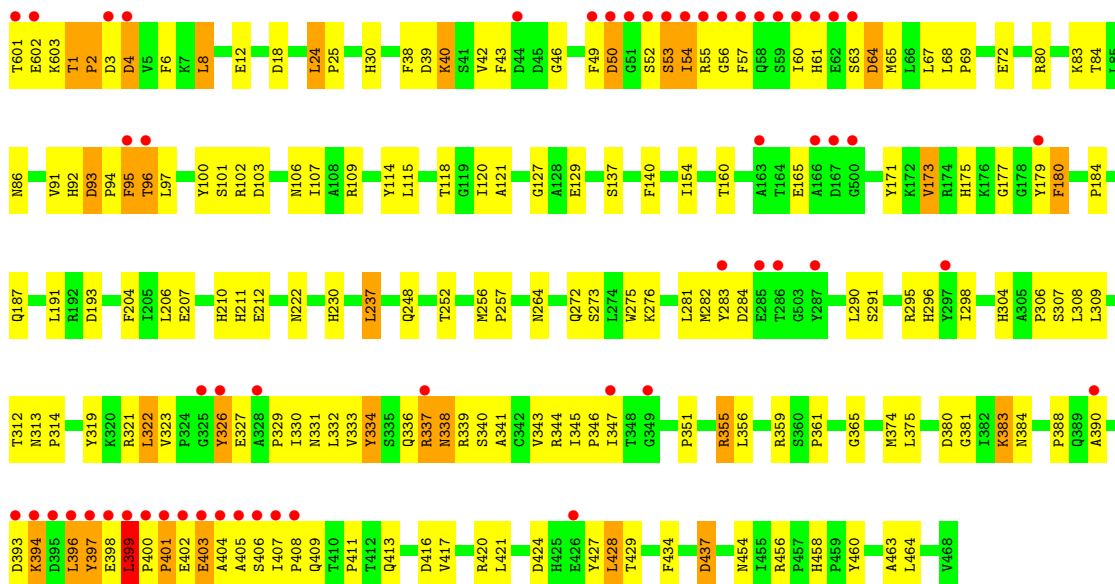


- Molecule 1: glutamine synthetase

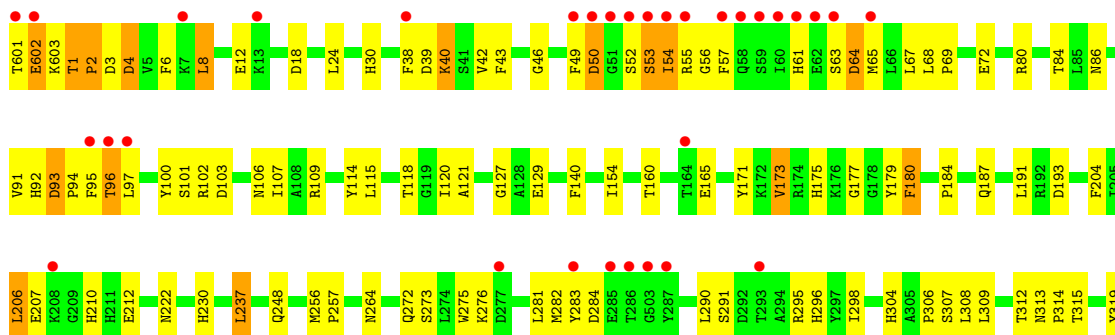


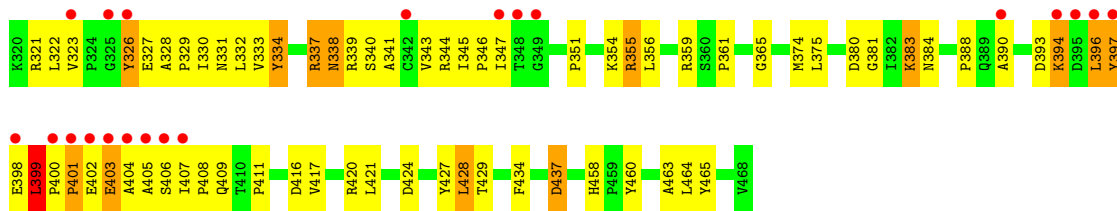


• Molecule 1: glutamine synthetase

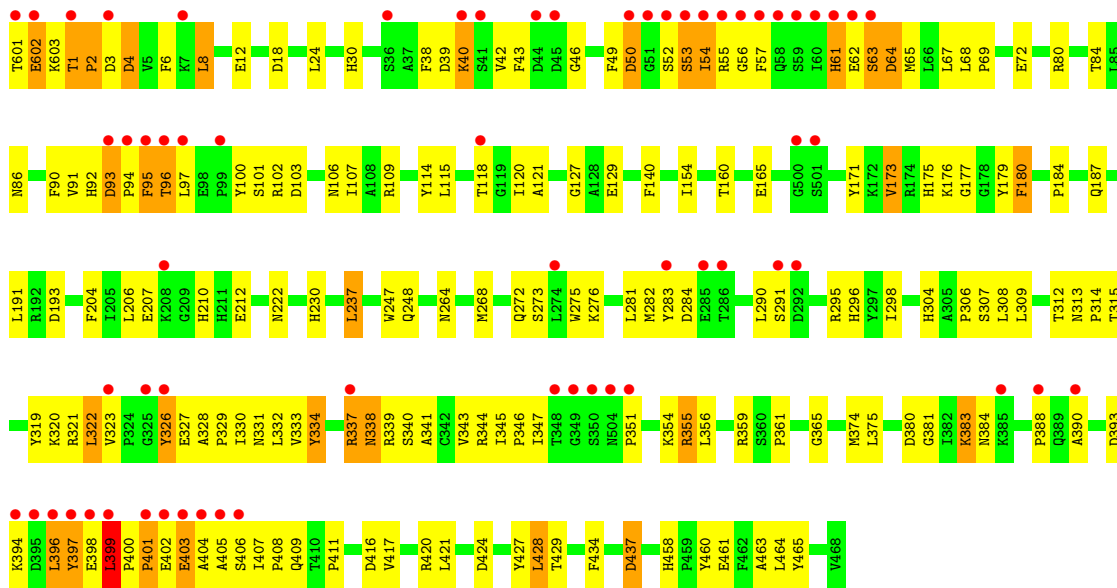


• Molecule 1: glutamine synthetase

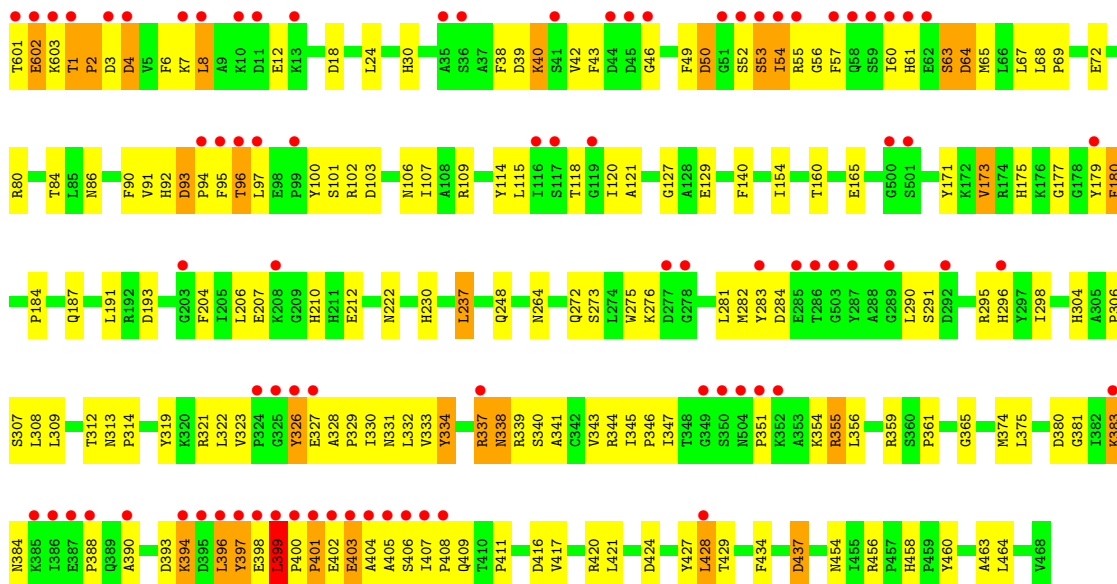




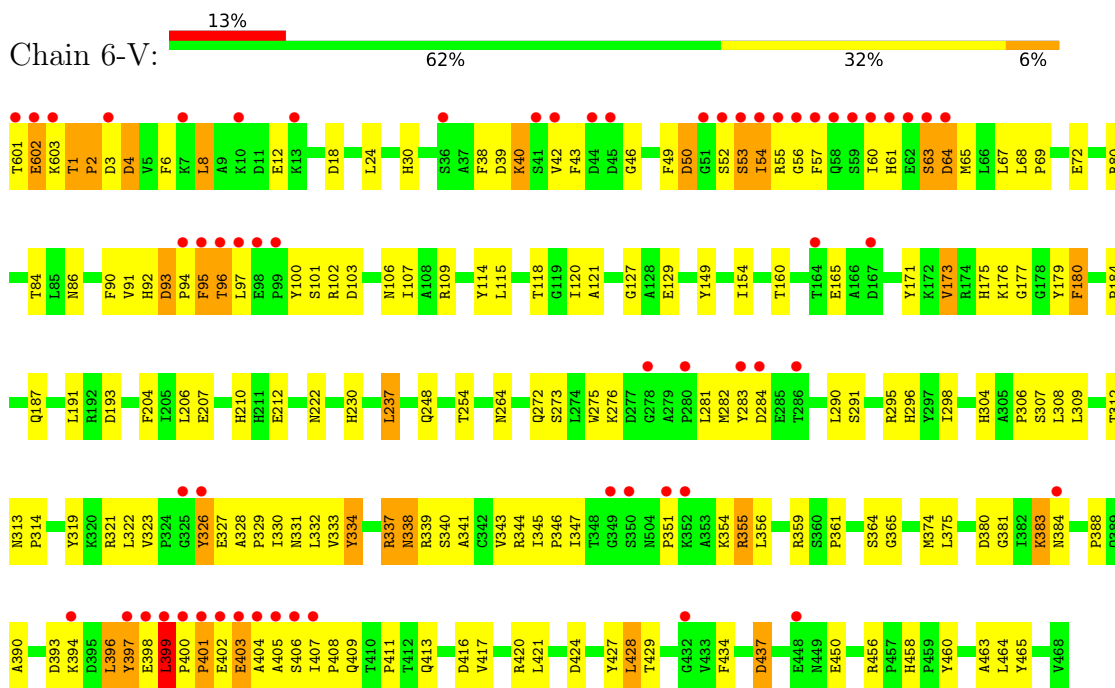
• Molecule 1: glutamine synthetase



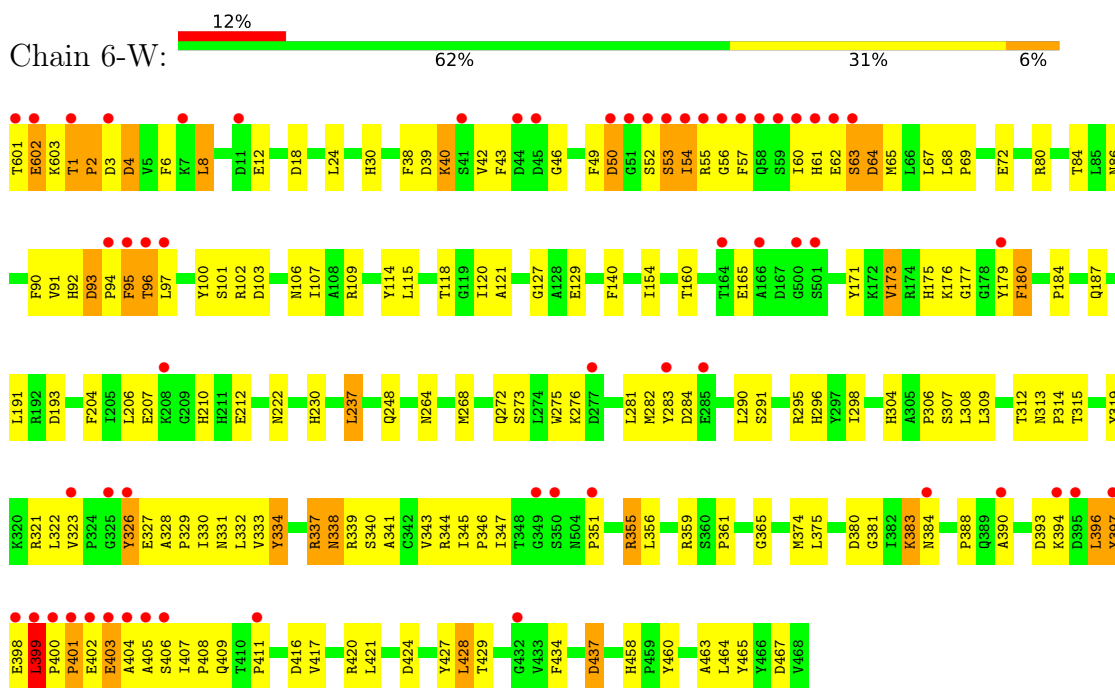
• Molecule 1: glutamine synthetase



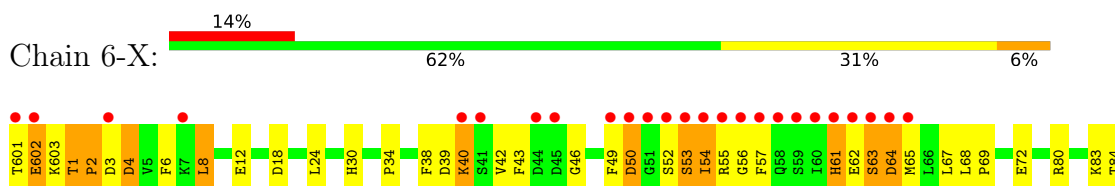
- Molecule 1: glutamine synthetase

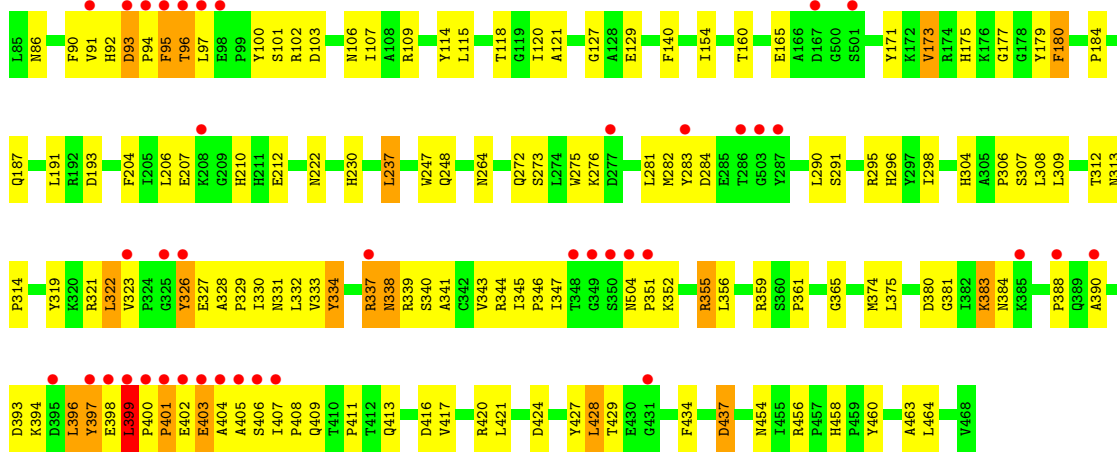


- Molecule 1: glutamine synthetase

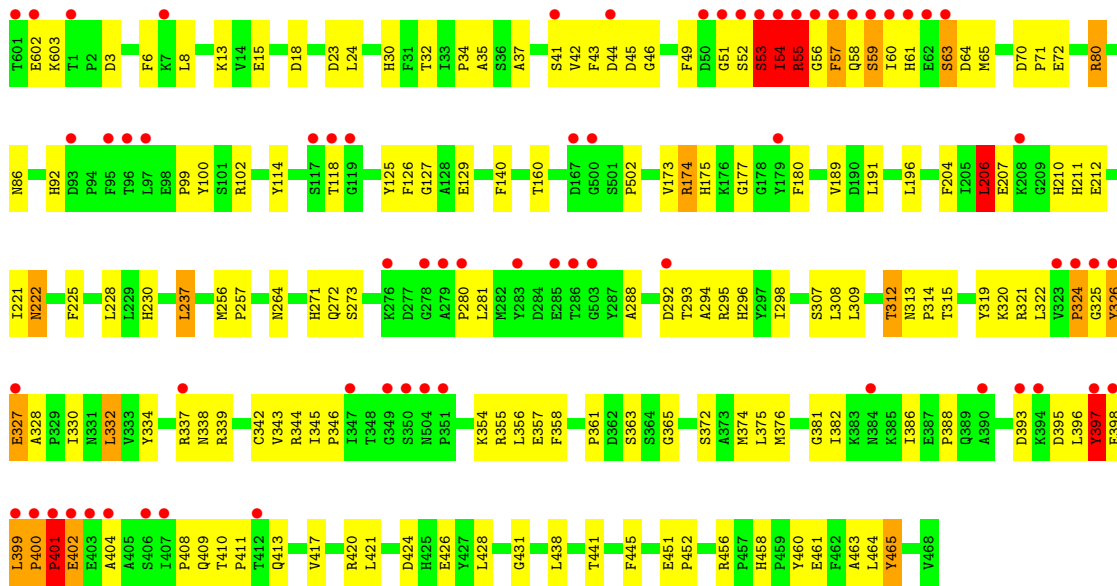


- Molecule 1: glutamine synthetase

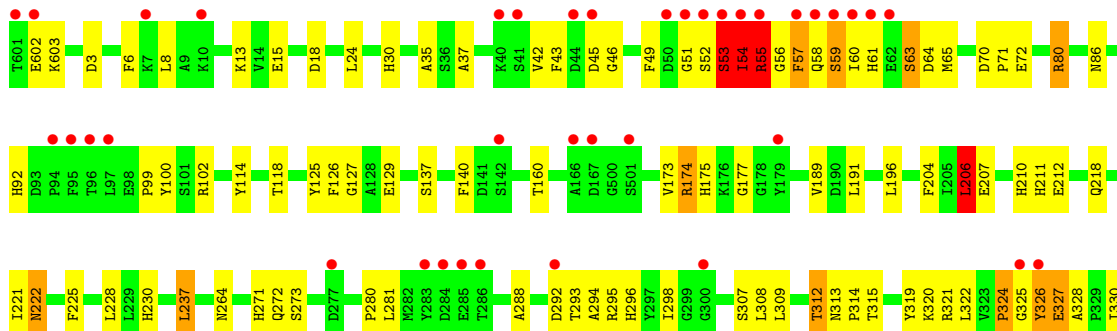


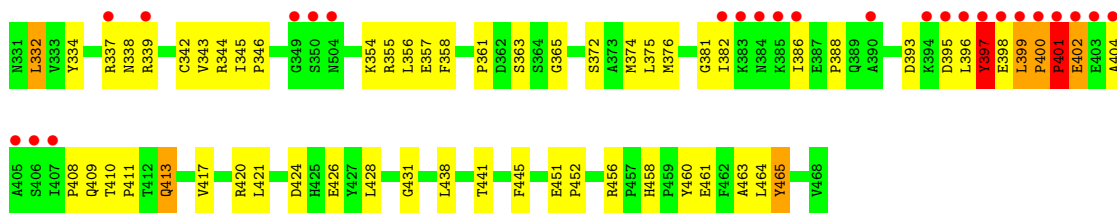


• Molecule 1: glutamine synthetase

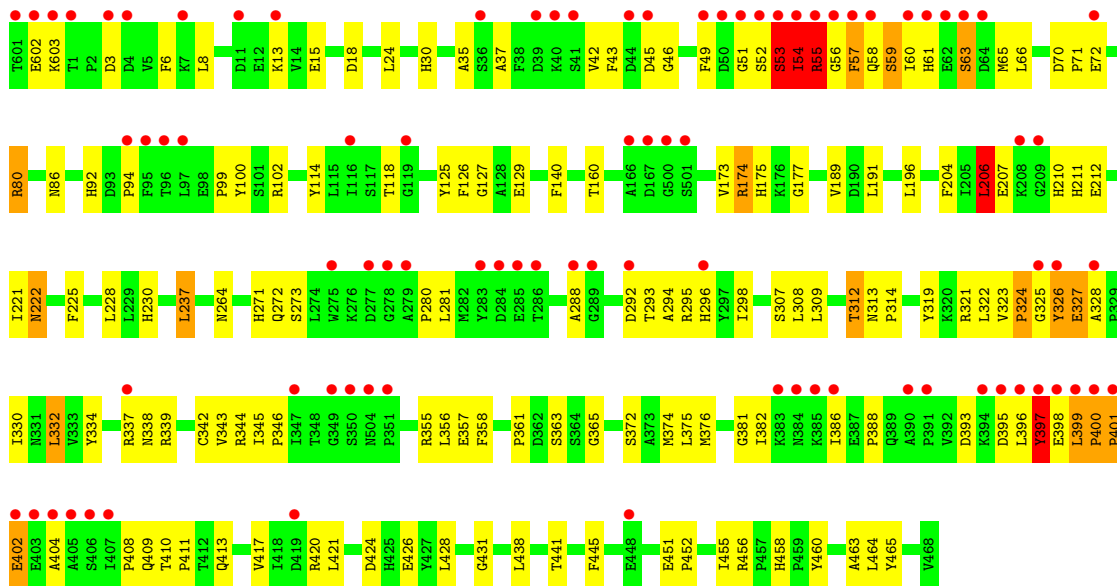


• Molecule 1: glutamine synthetase

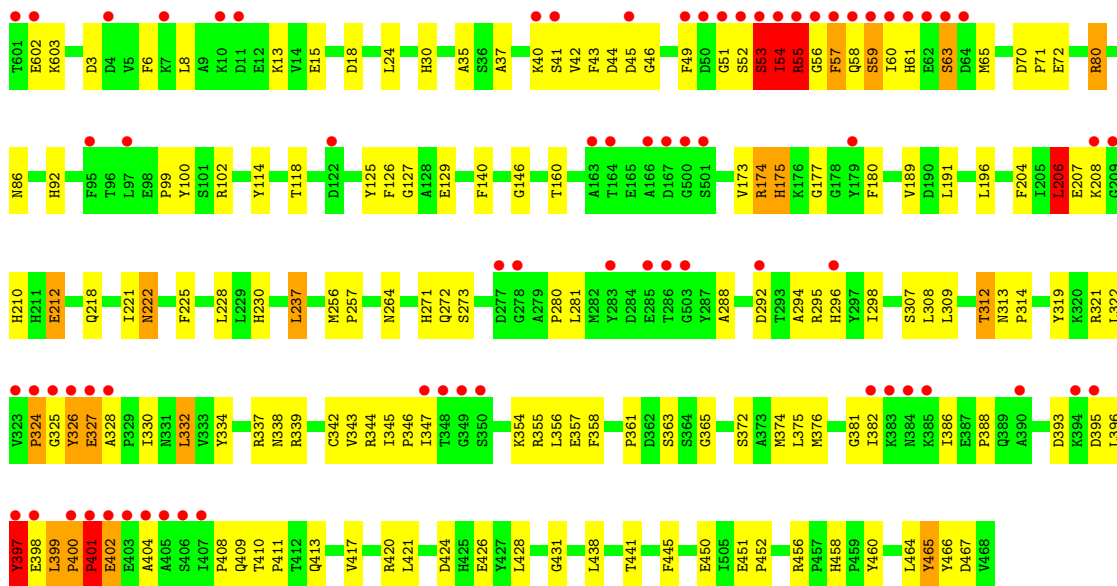




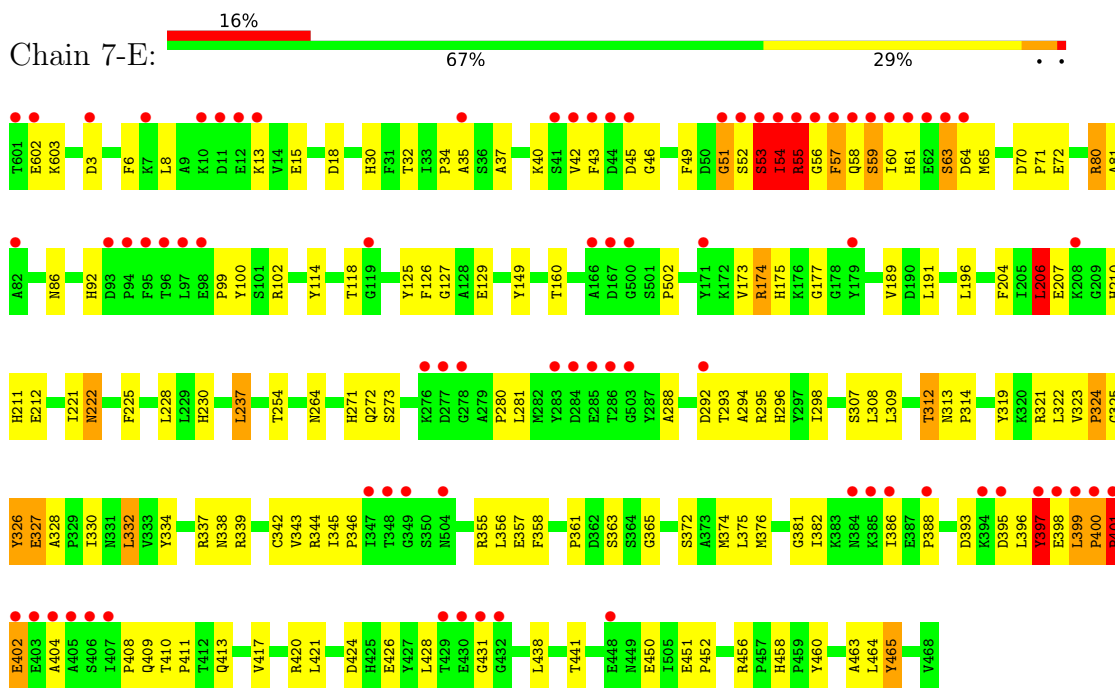
• Molecule 1: glutamine synthetase



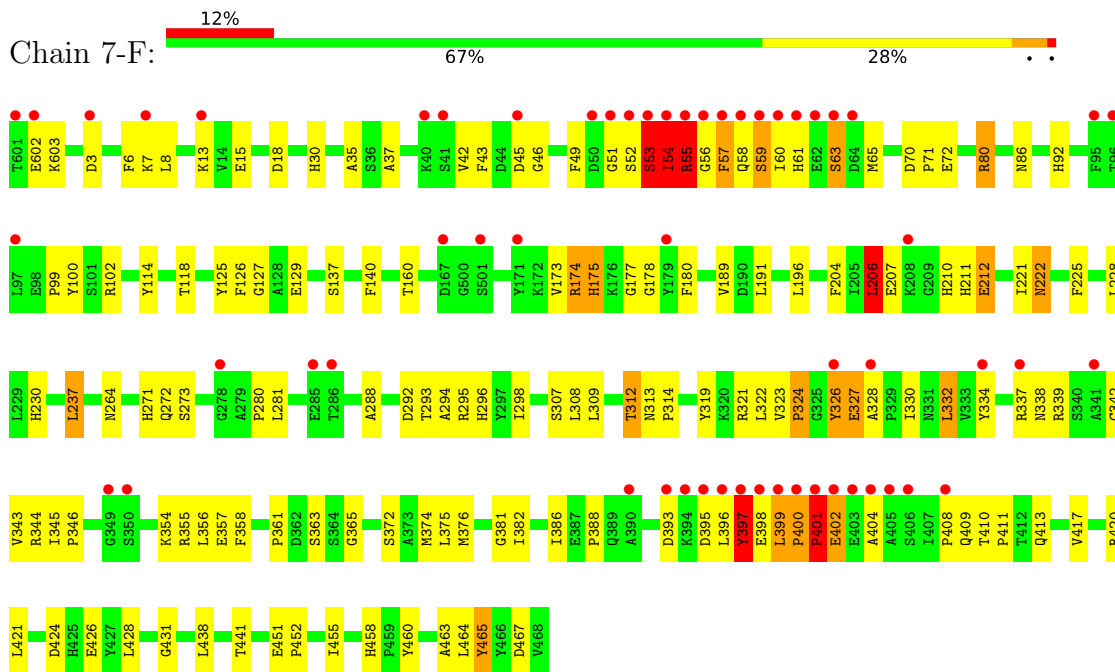
• Molecule 1: glutamine synthetase



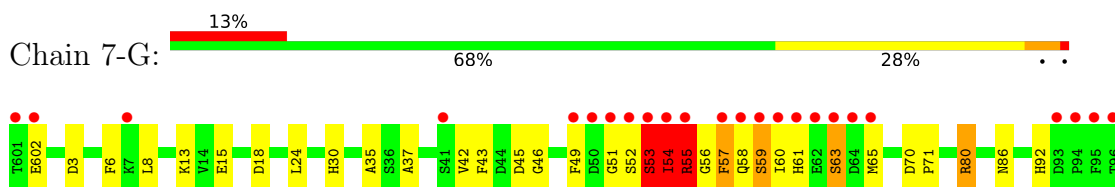
- Molecule 1: glutamine synthetase

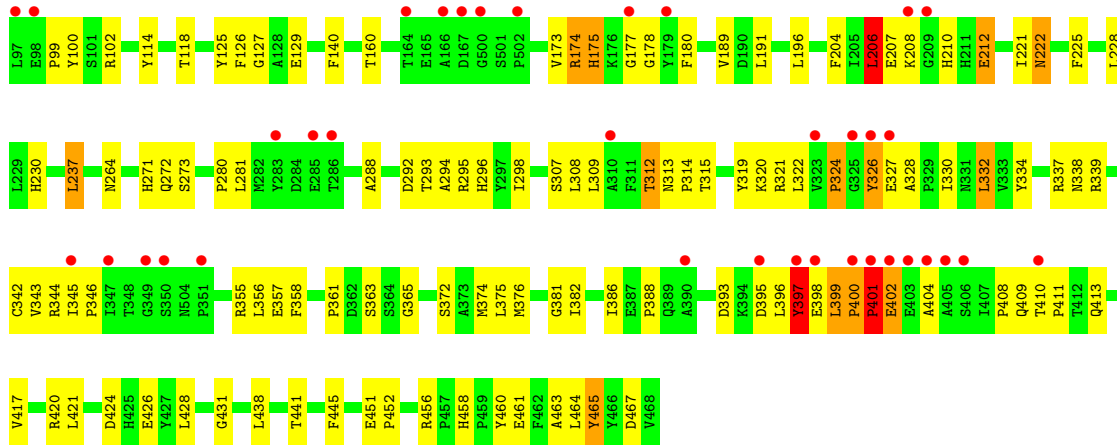


- Molecule 1: glutamine synthetase

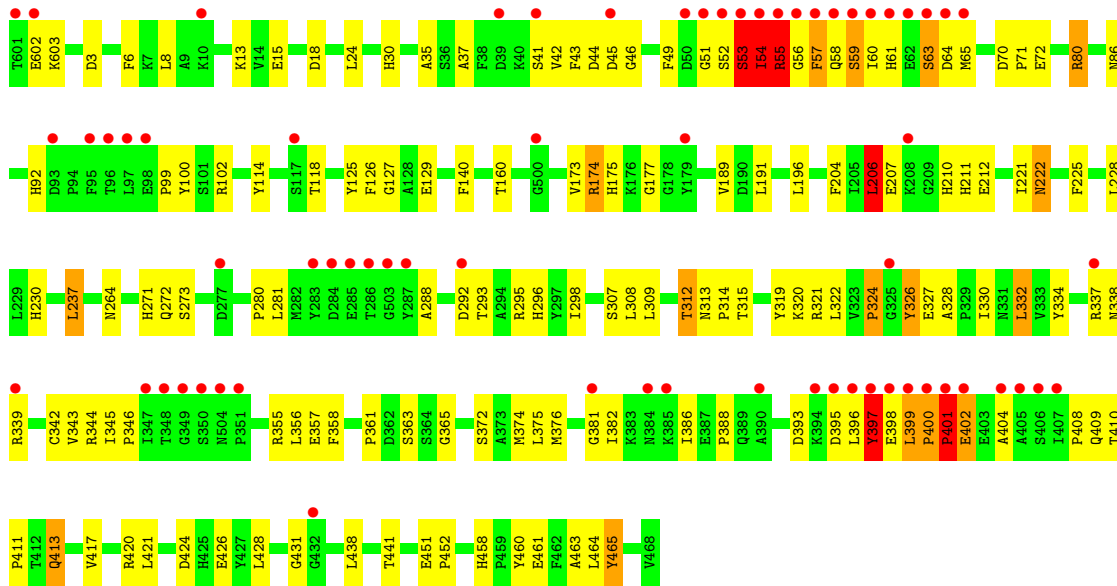


- Molecule 1: glutamine synthetase

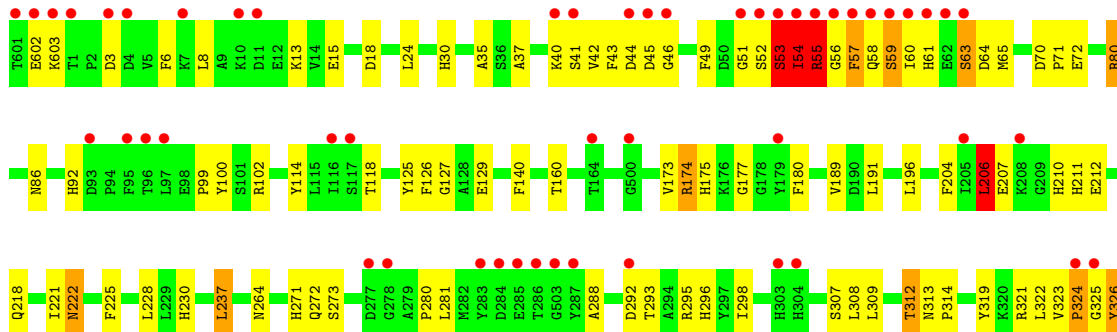


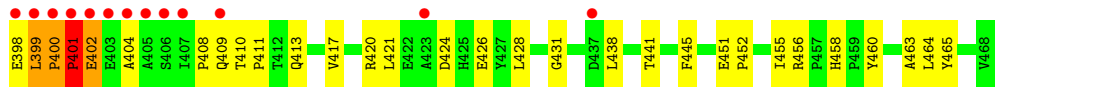


• Molecule 1: glutamine synthetase

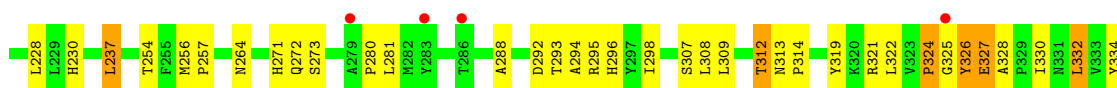
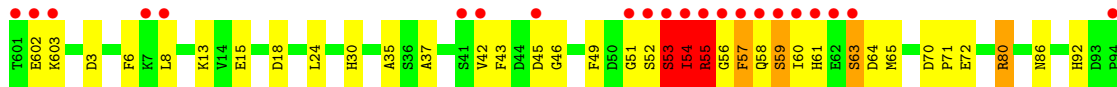


• Molecule 1: glutamine synthetase

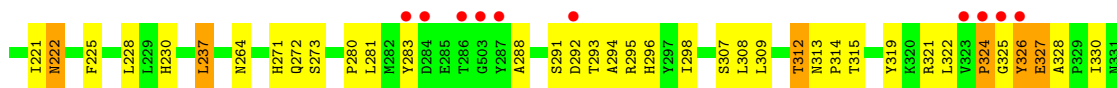
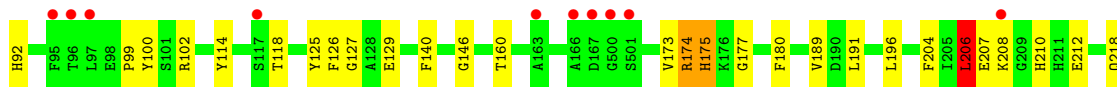
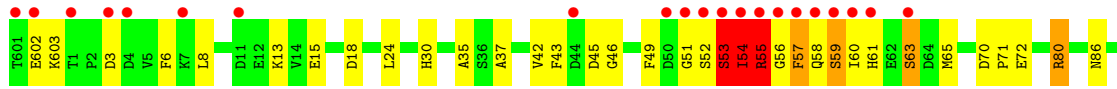




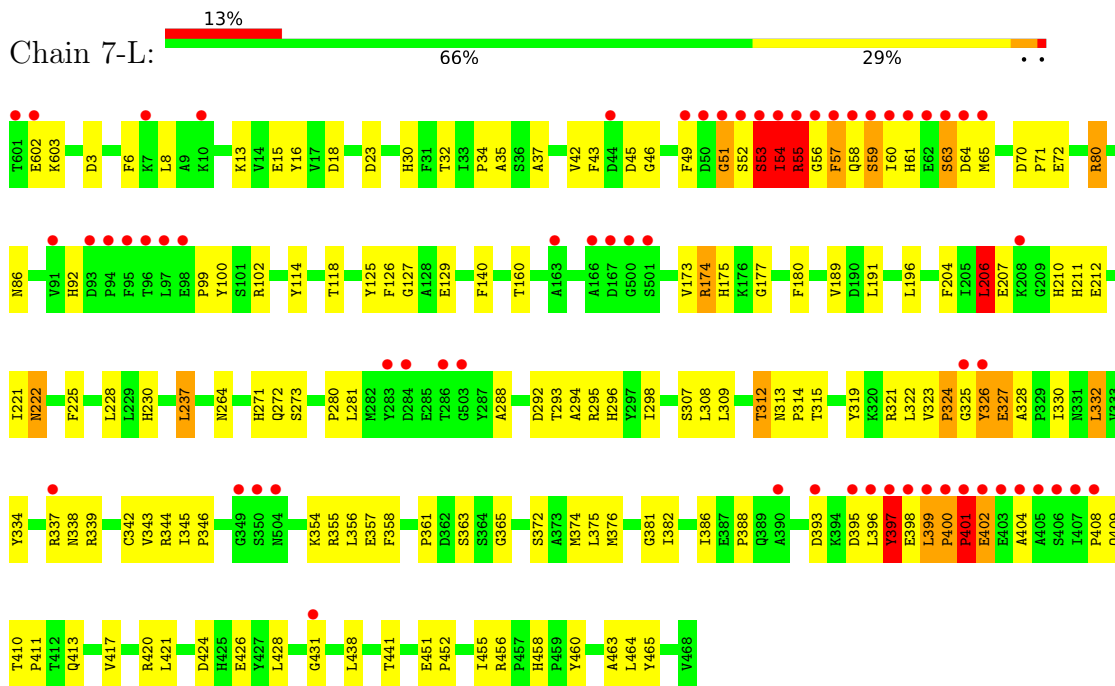
• Molecule 1: glutamine synthetase



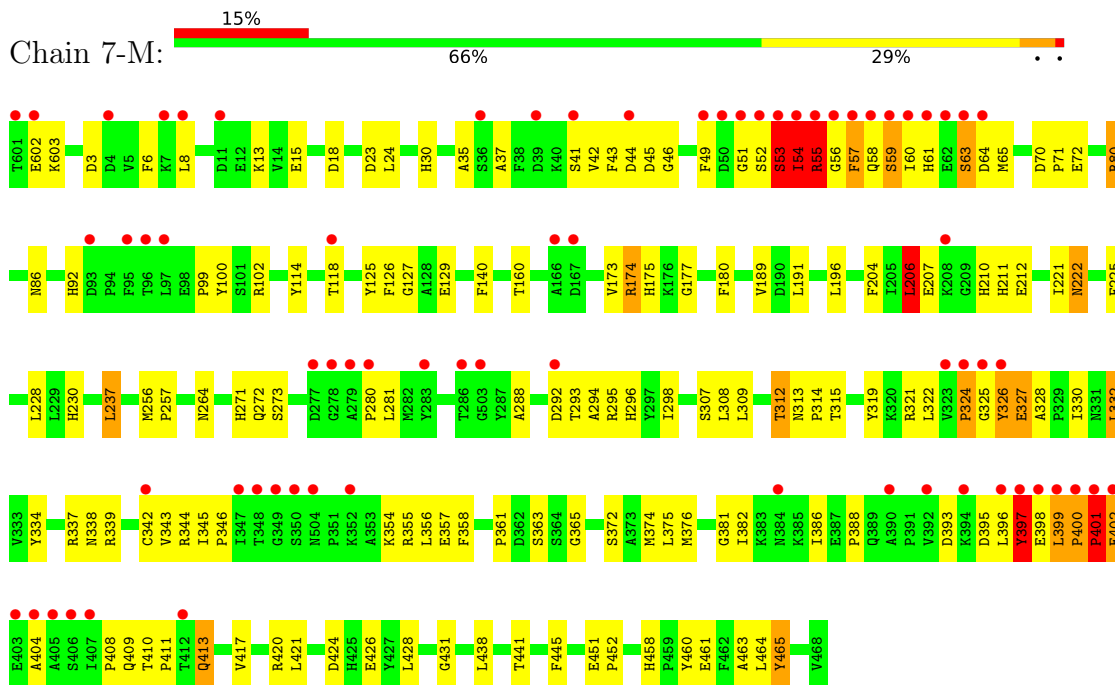
• Molecule 1: glutamine synthetase



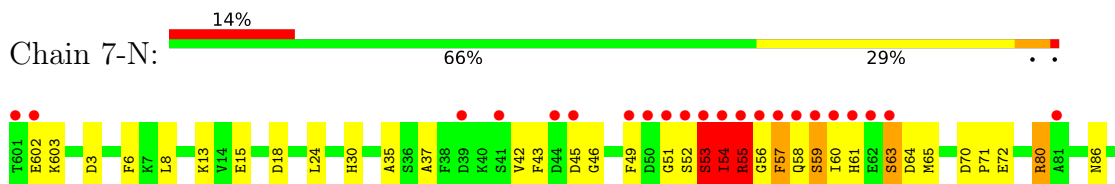
• Molecule 1: glutamine synthetase



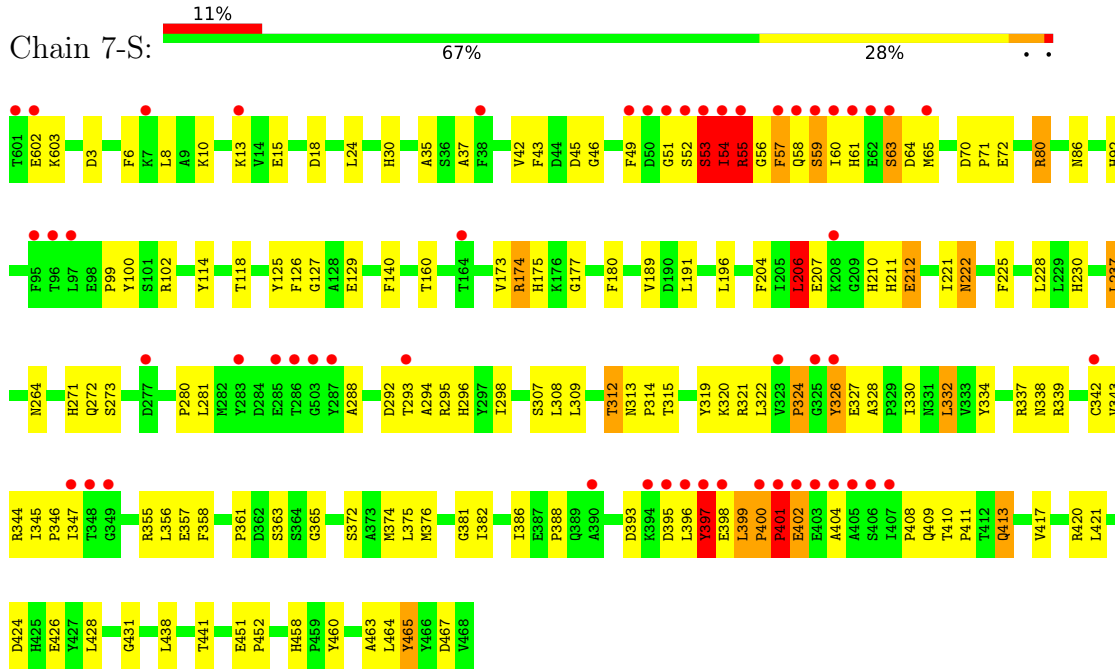
• Molecule 1: glutamine synthetase



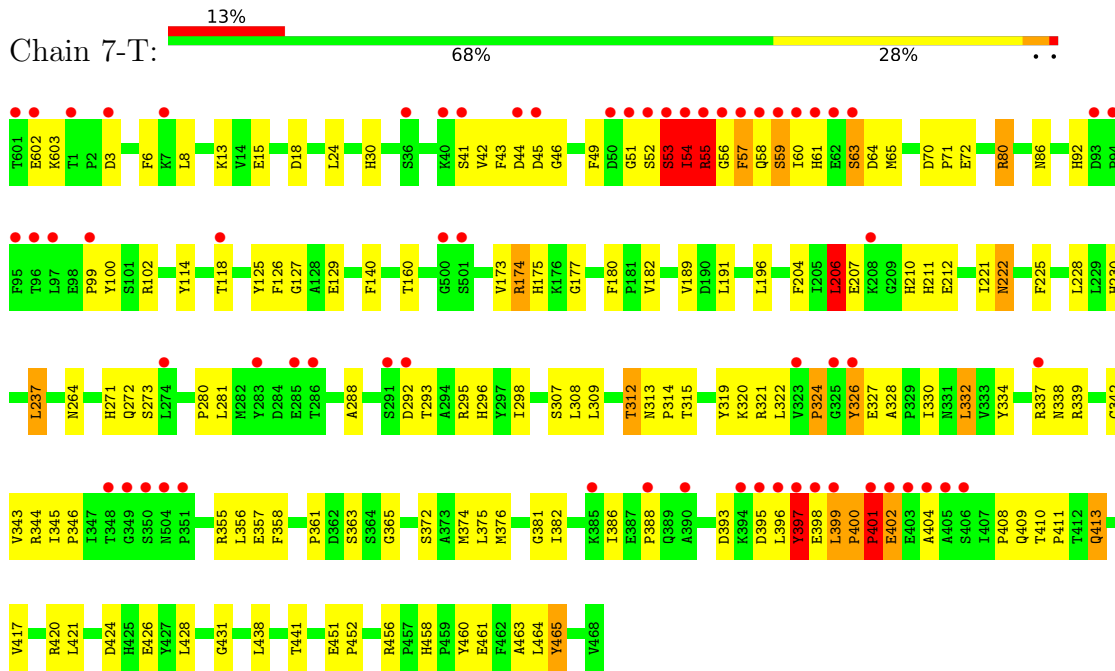
• Molecule 1: glutamine synthetase



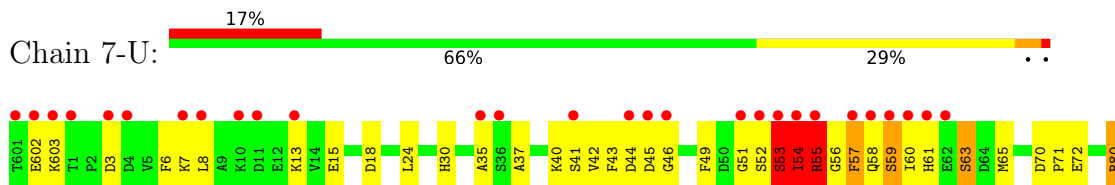
• Molecule 1: glutamine synthetase

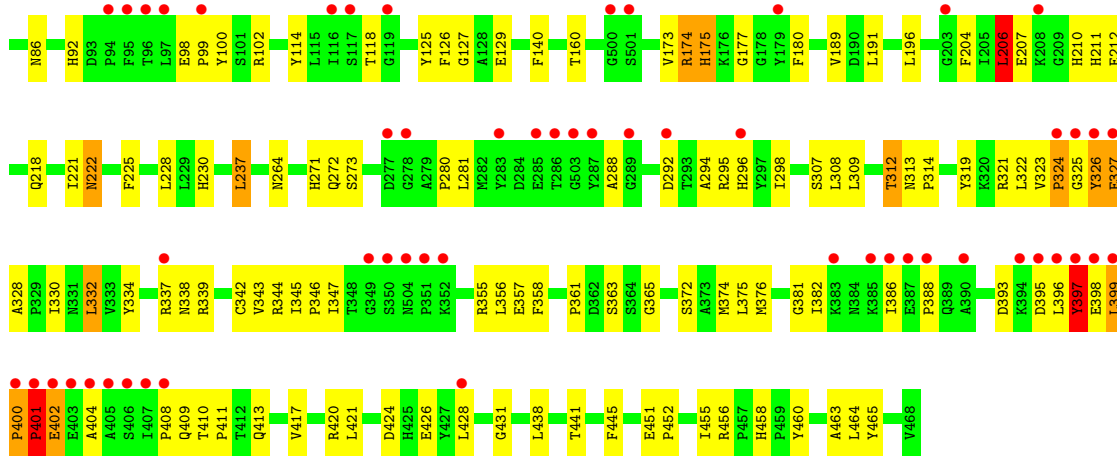


• Molecule 1: glutamine synthetase

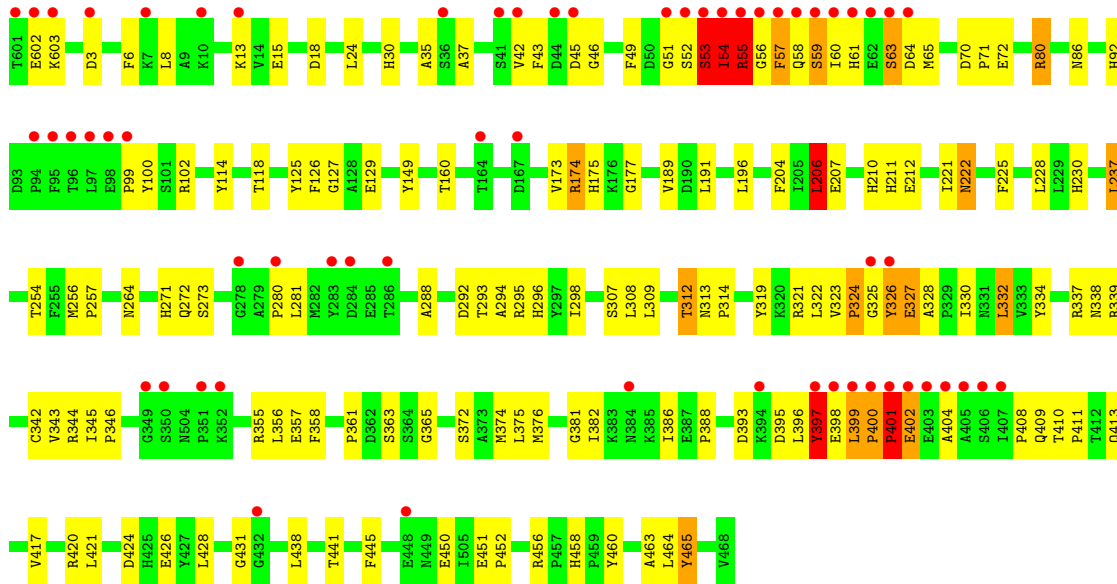


• Molecule 1: glutamine synthetase

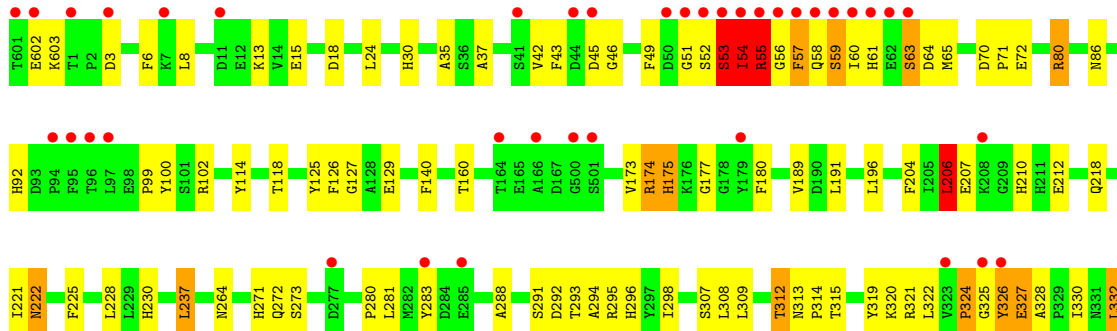


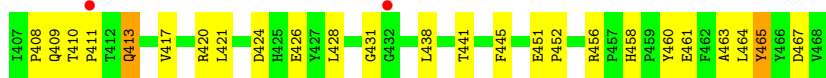
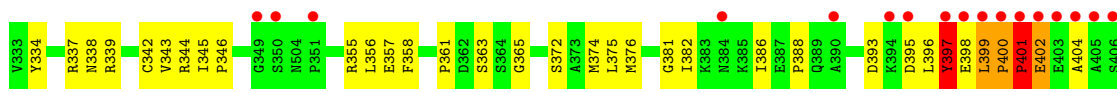


• Molecule 1: glutamine synthetase

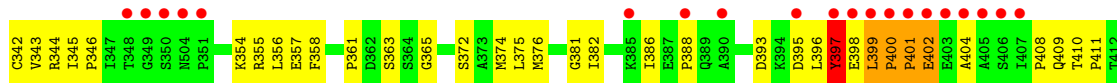
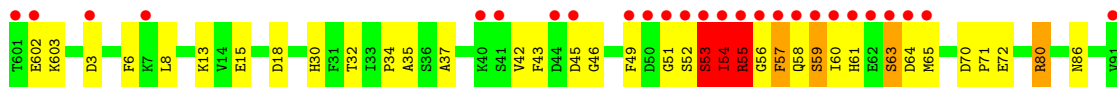


• Molecule 1: glutamine synthetase

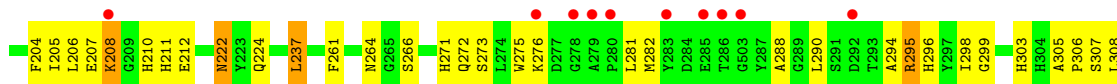
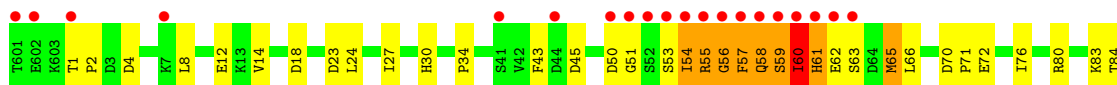




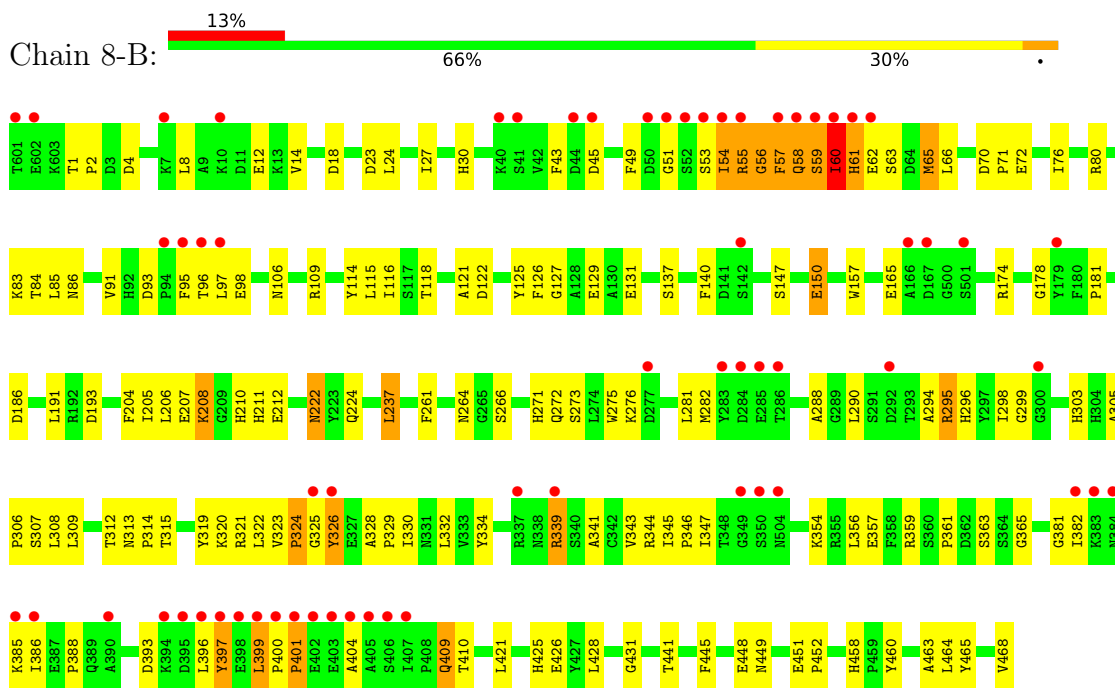
• Molecule 1: glutamine synthetase



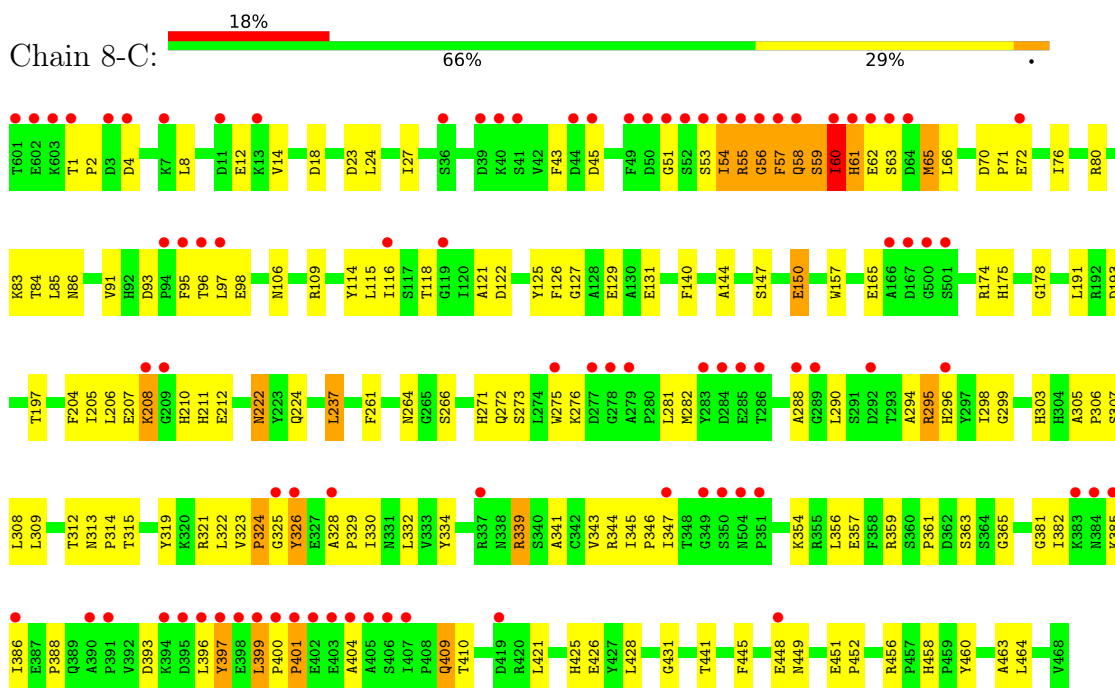
• Molecule 1: glutamine synthetase



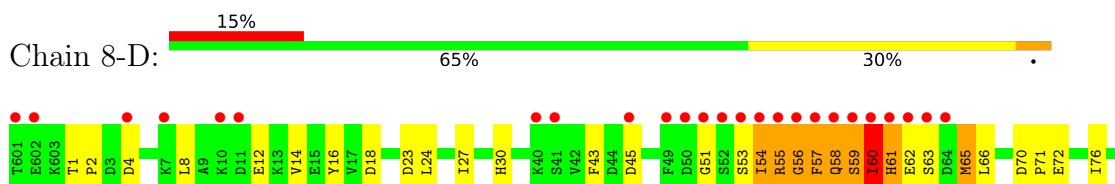
- Molecule 1: glutamine synthetase

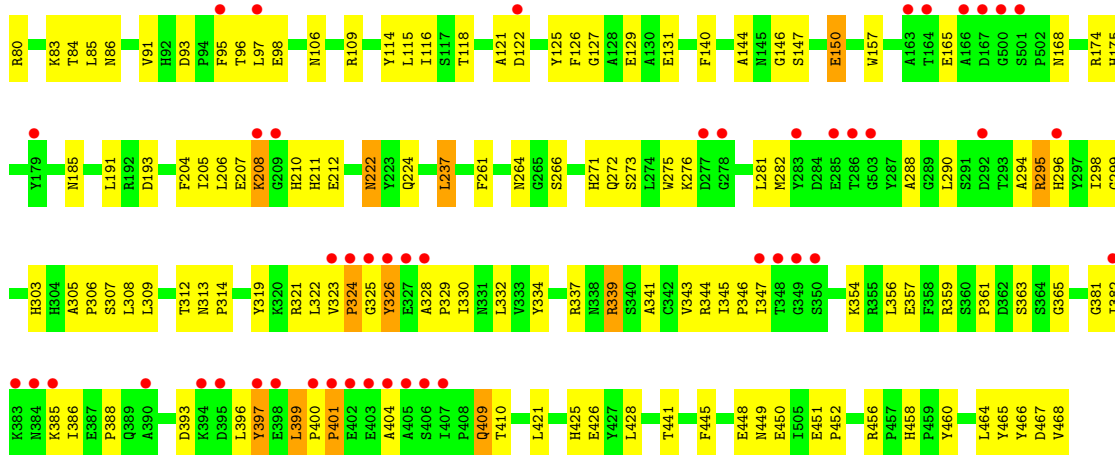


- Molecule 1: glutamine synthetase

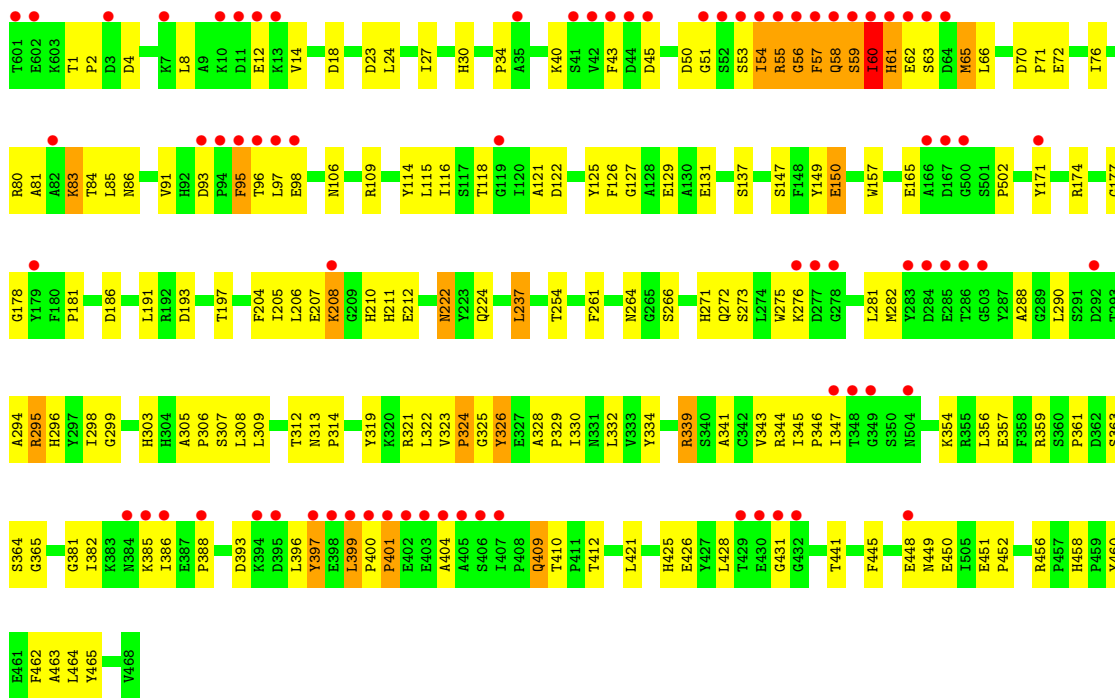


- Molecule 1: glutamine synthetase

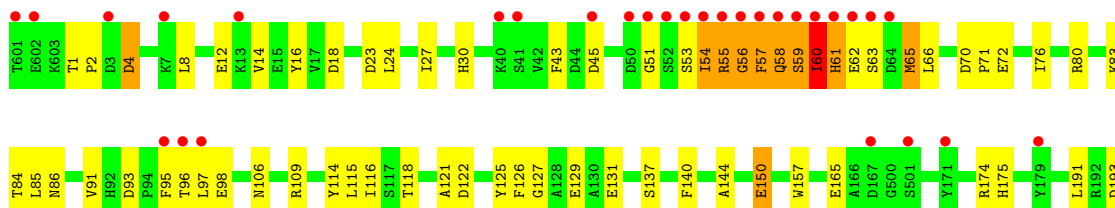


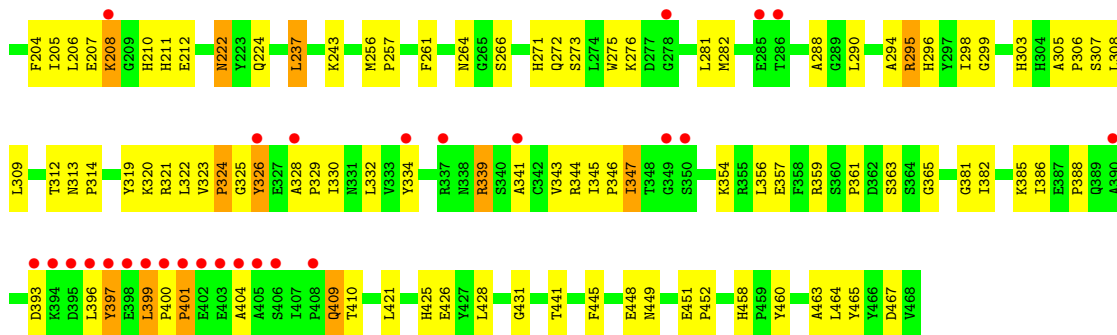


• Molecule 1: glutamine synthetase

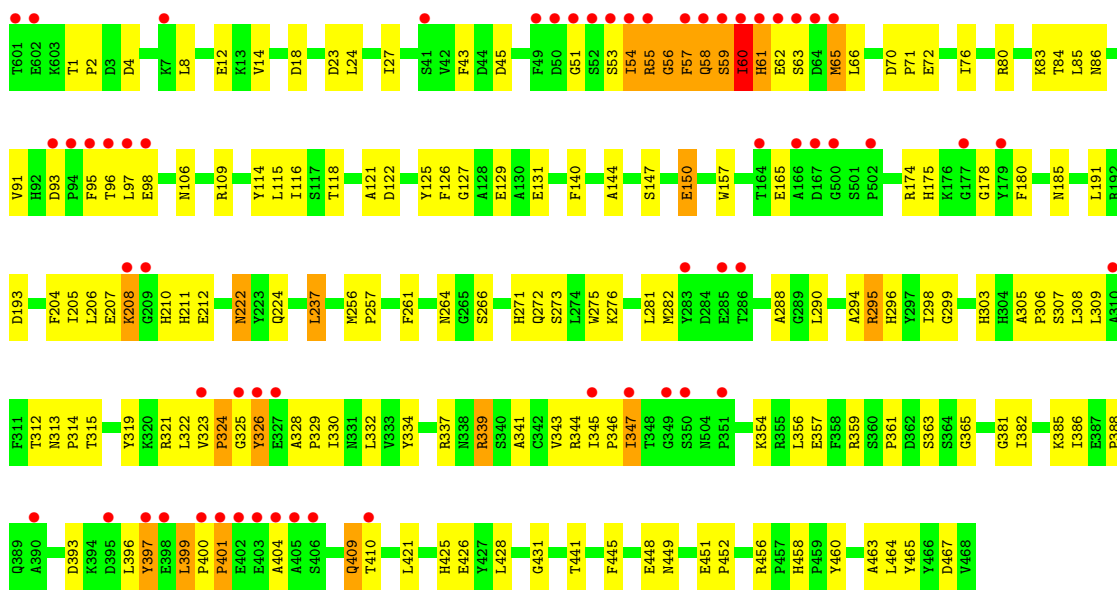


• Molecule 1: glutamine synthetase

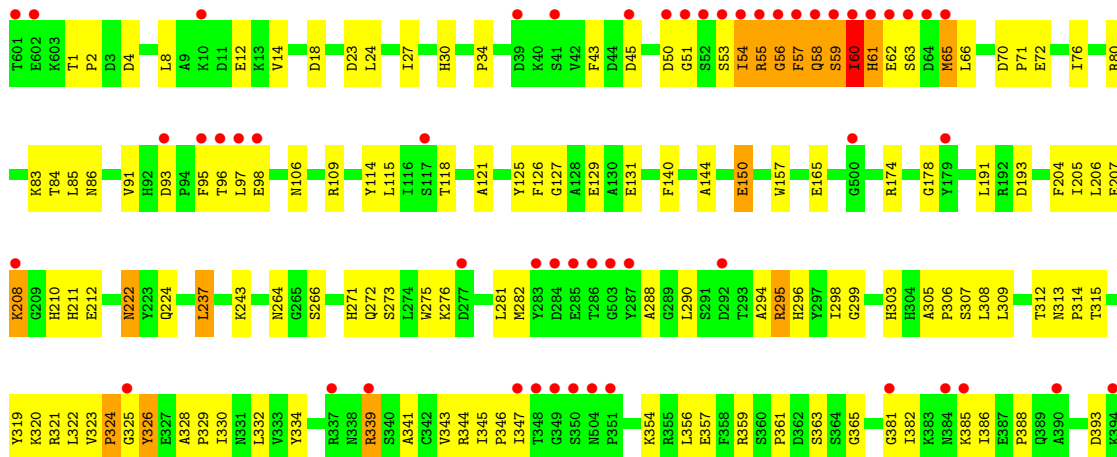


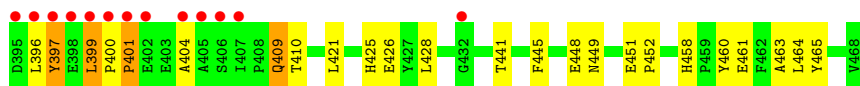


• Molecule 1: glutamine synthetase

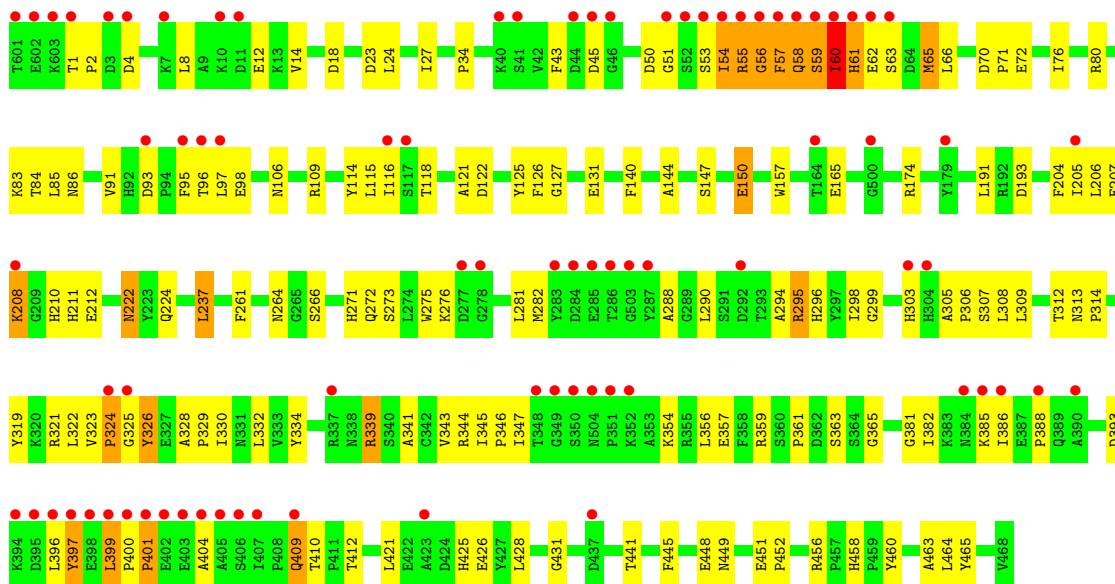


• Molecule 1: glutamine synthetase

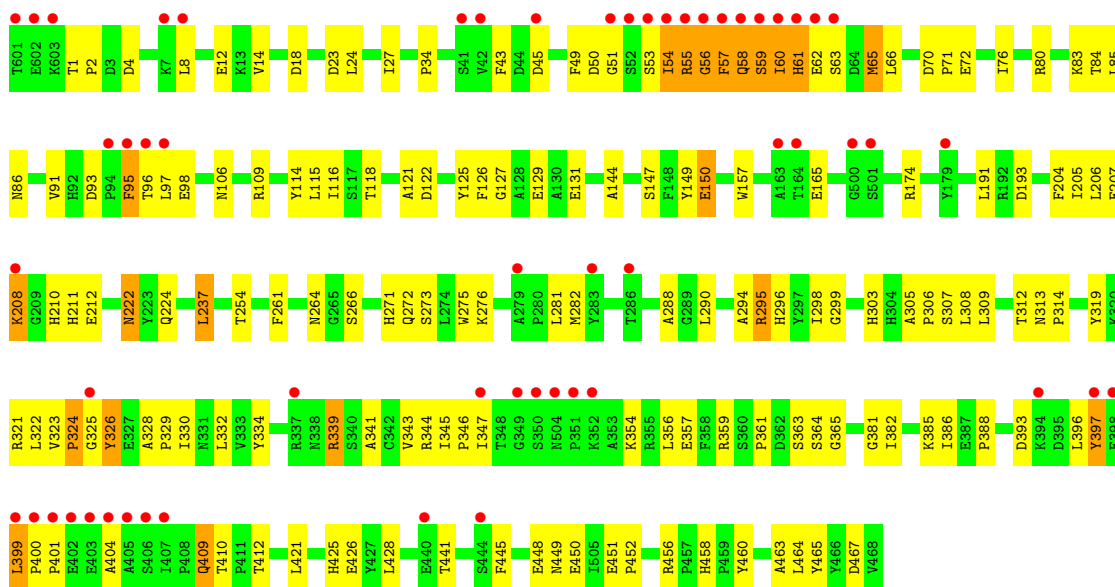




• Molecule 1: glutamine synthetase

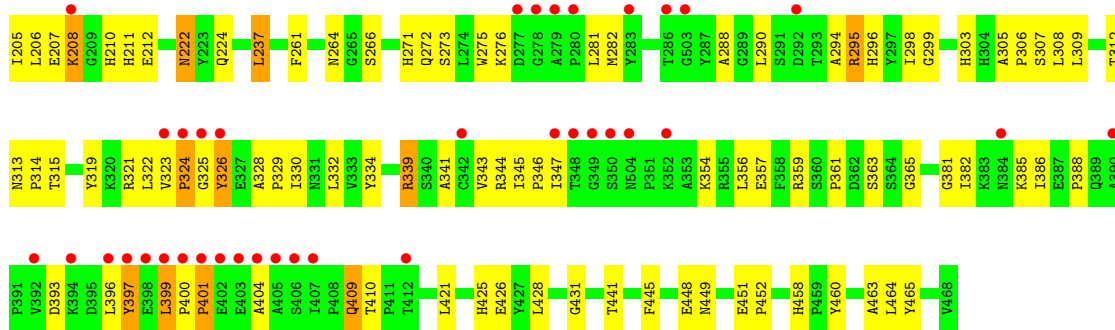


• Molecule 1: glutamine synthetase

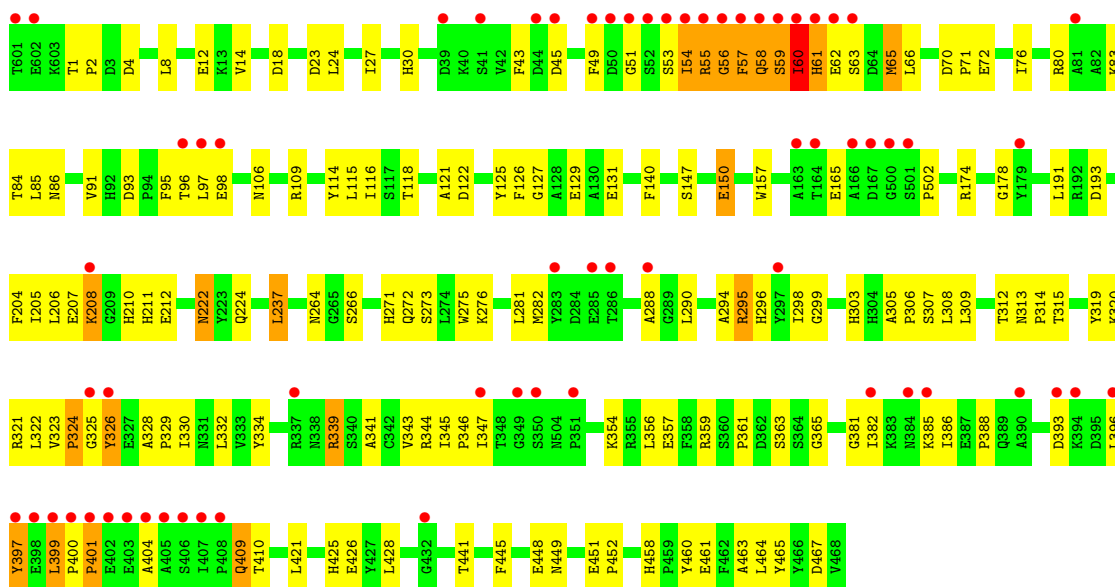


• Molecule 1: glutamine synthetase

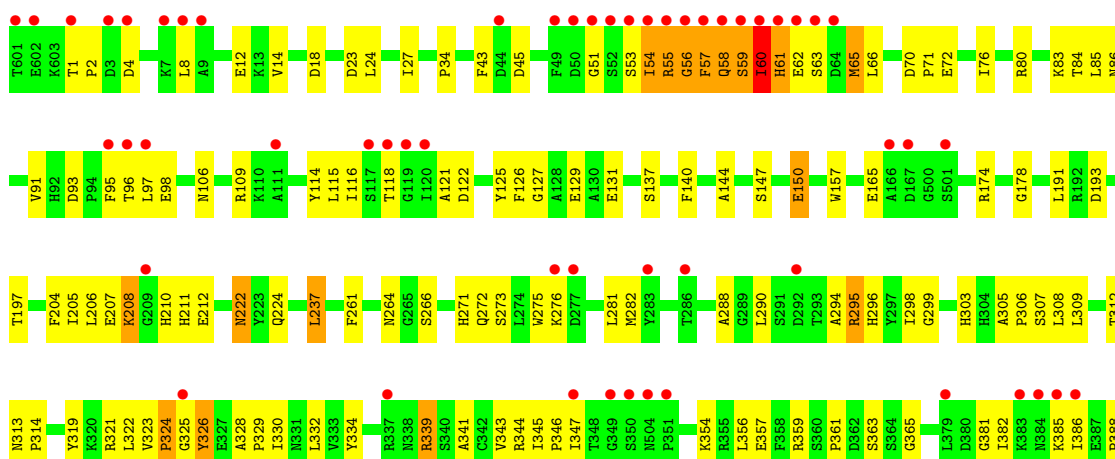


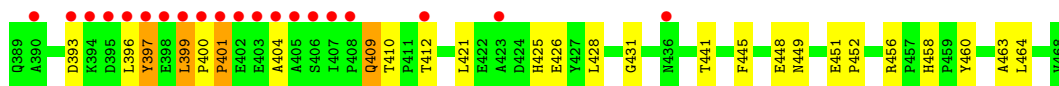


• Molecule 1: glutamine synthetase

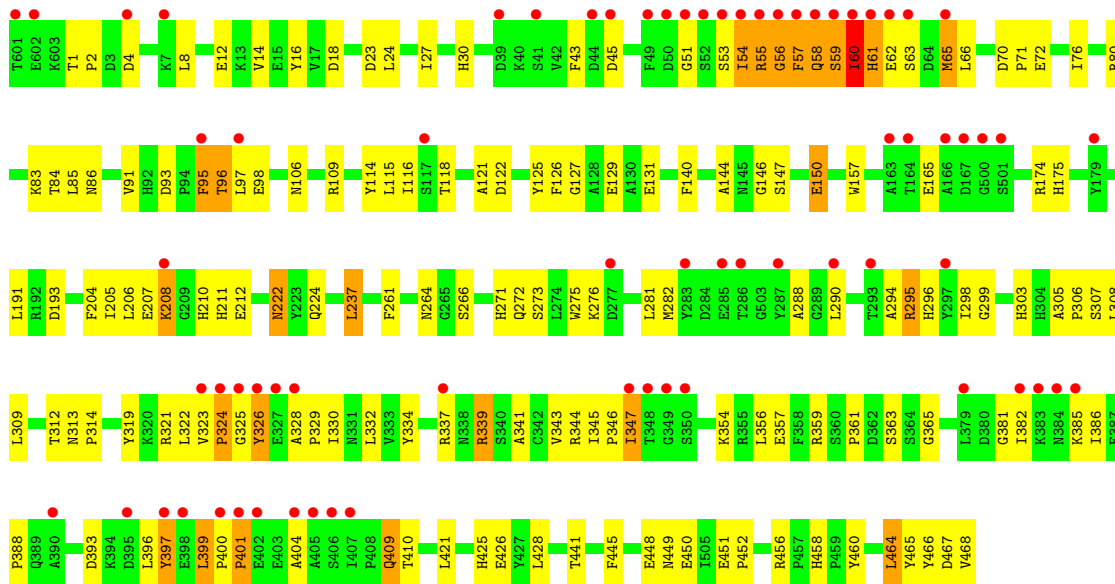


• Molecule 1: glutamine synthetase

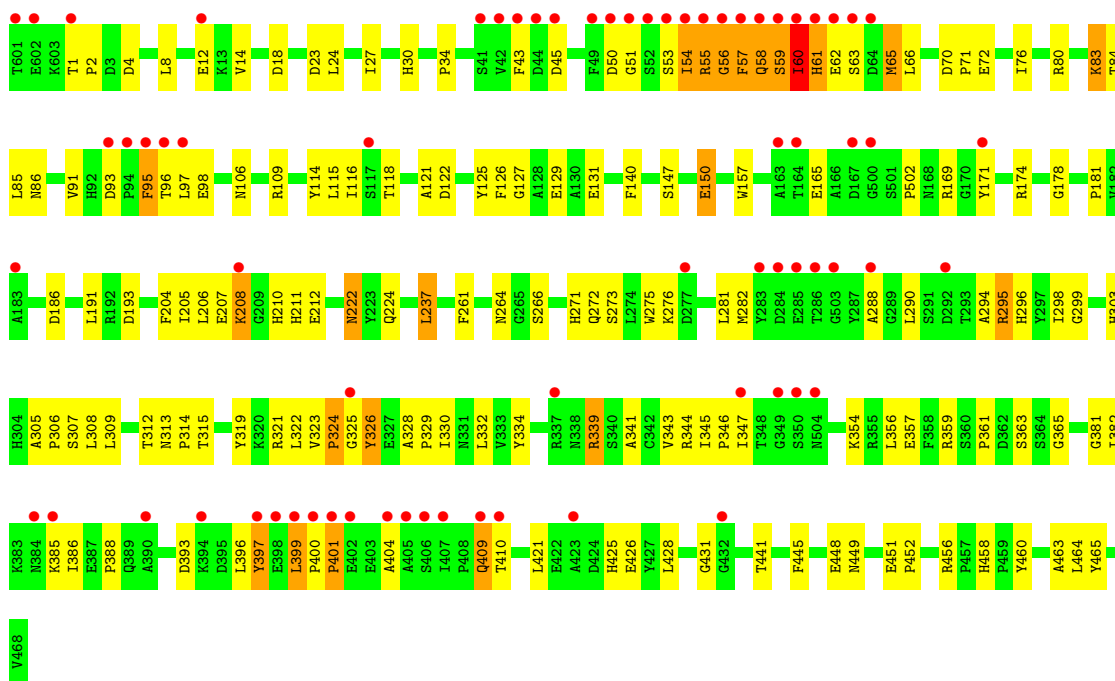




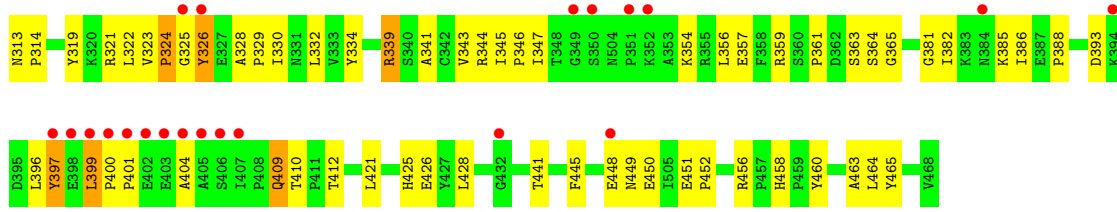
• Molecule 1: glutamine synthetase



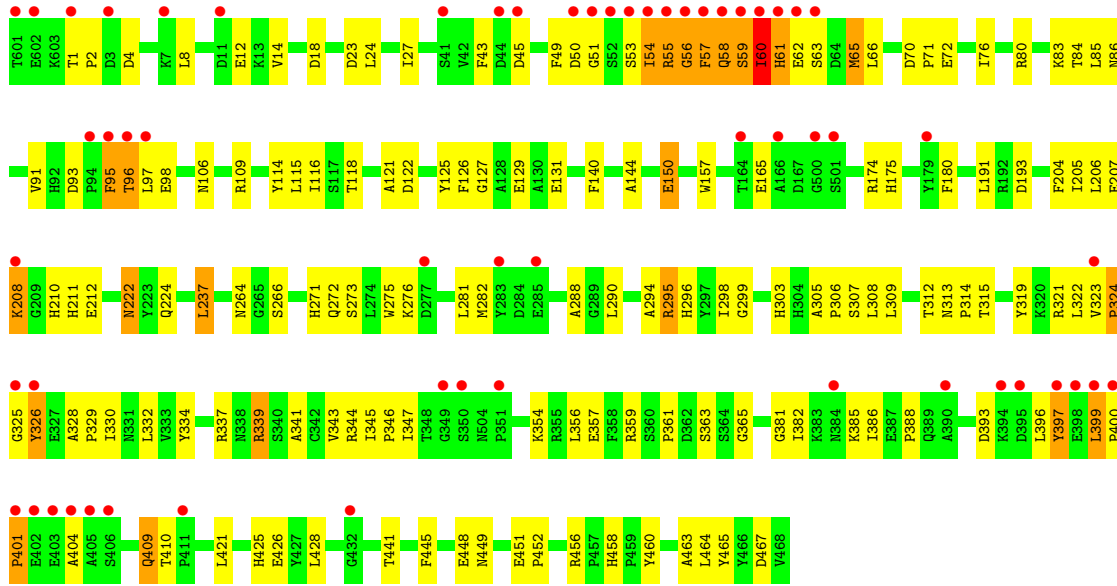
• Molecule 1: glutamine synthetase



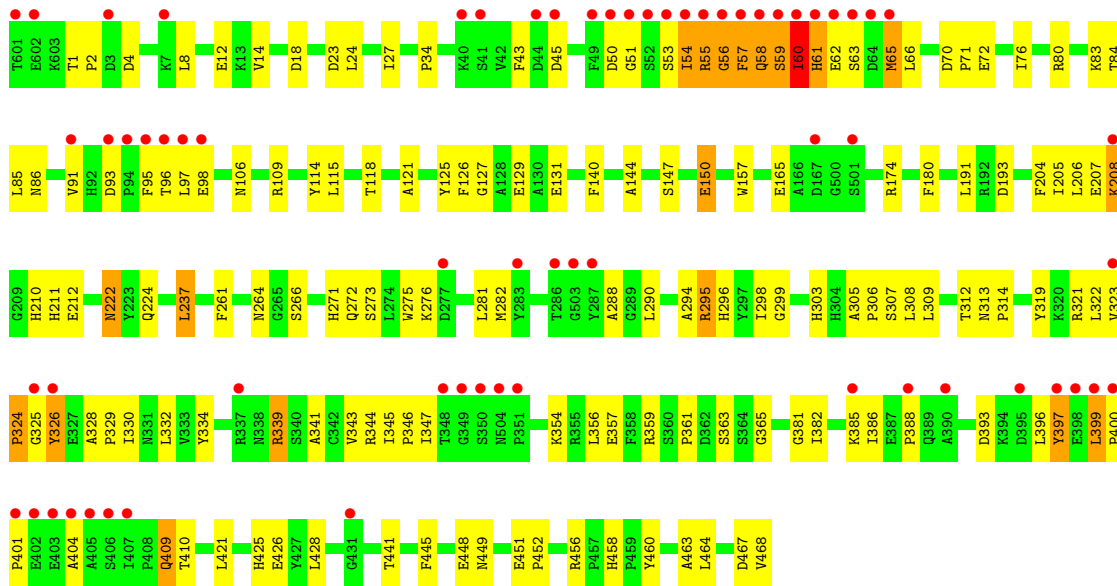
• Molecule 1: glutamine synthetase



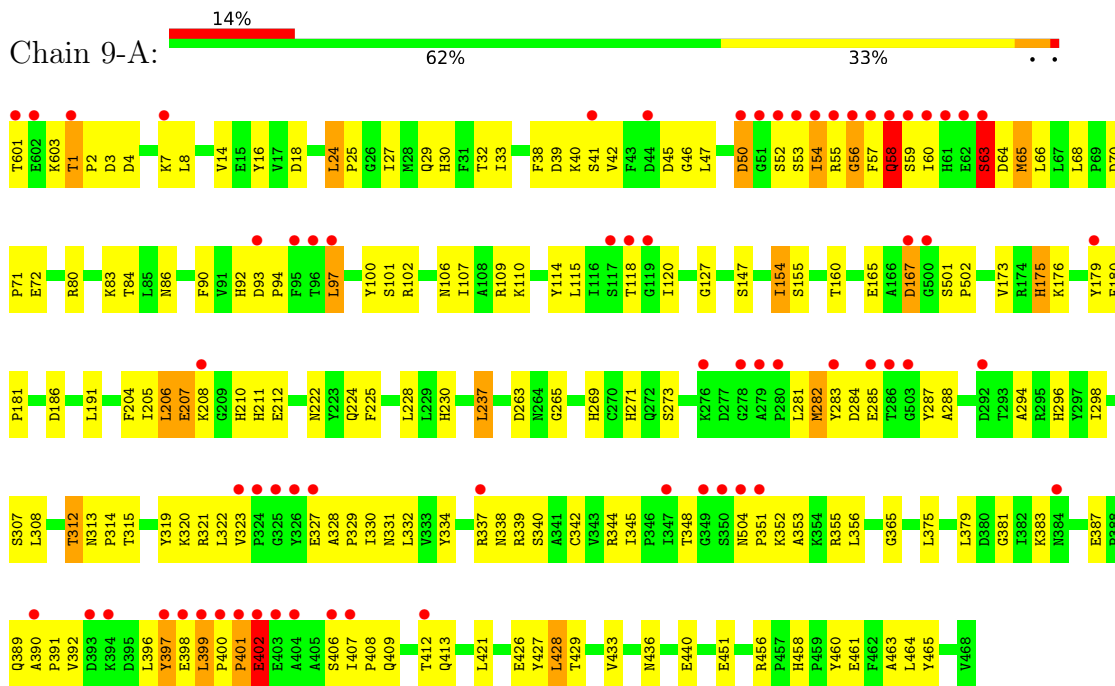
• Molecule 1: glutamine synthetase



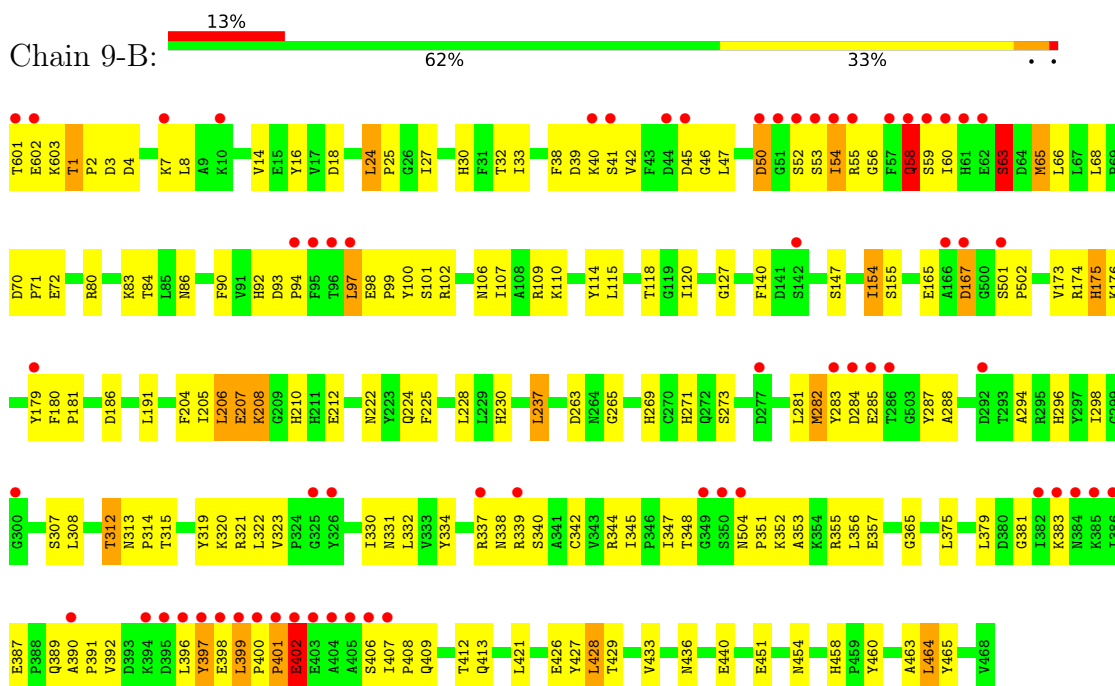
• Molecule 1: glutamine synthetase



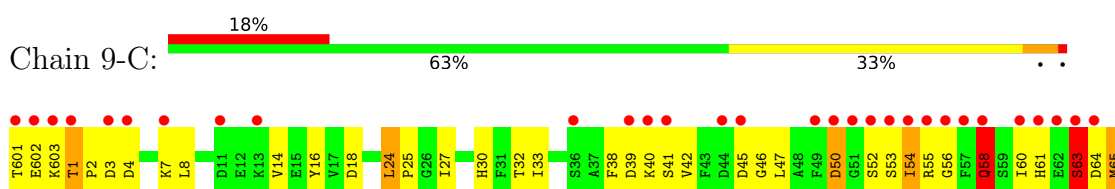
• Molecule 1: glutamine synthetase

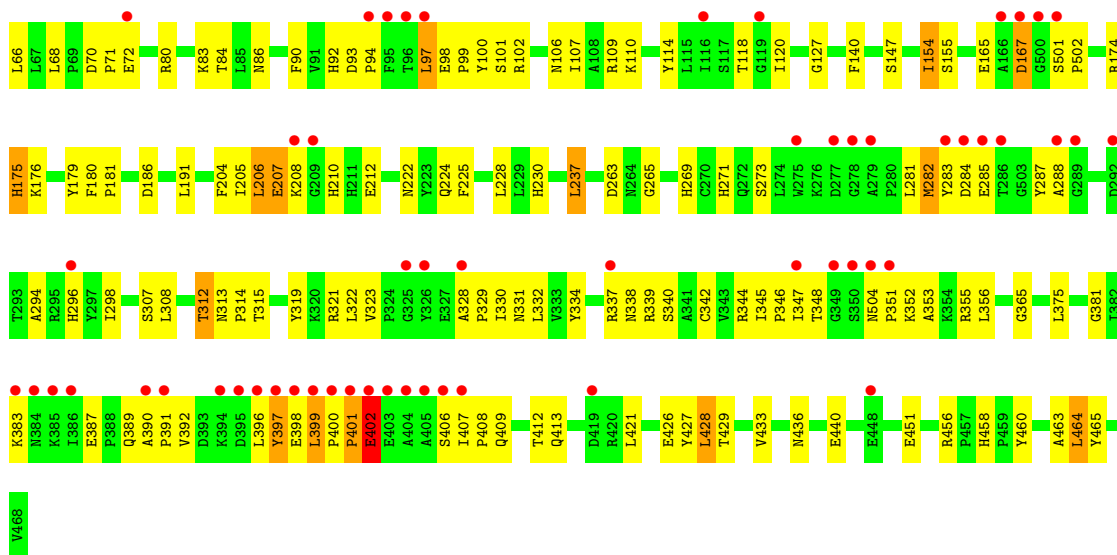


• Molecule 1: glutamine synthetase

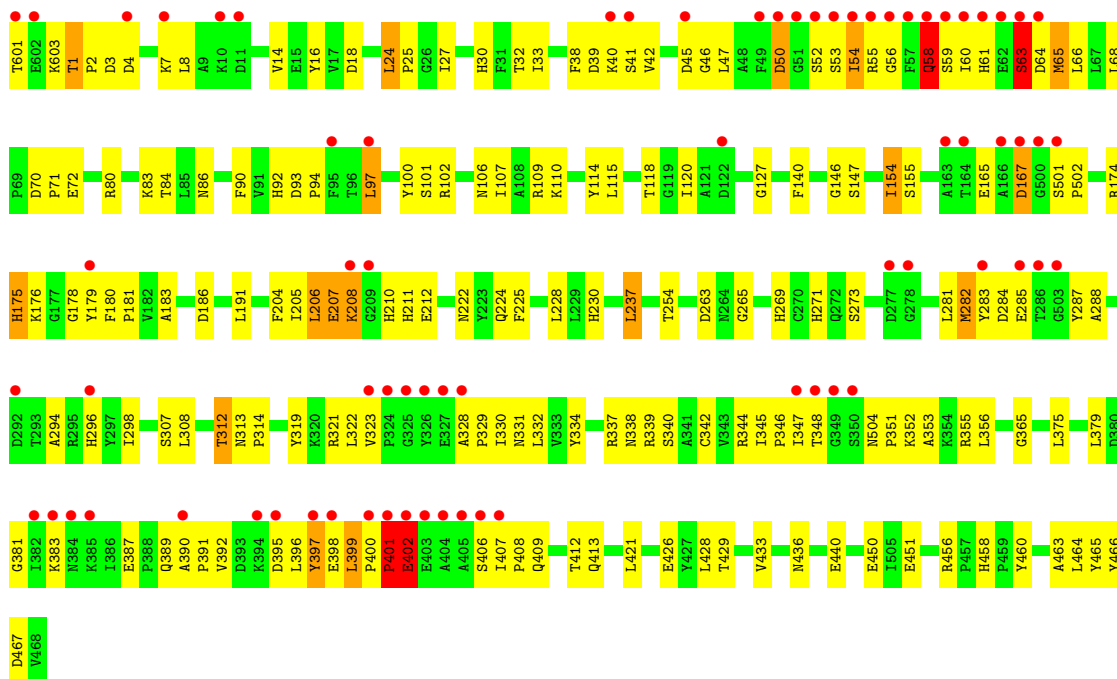


• Molecule 1: glutamine synthetase



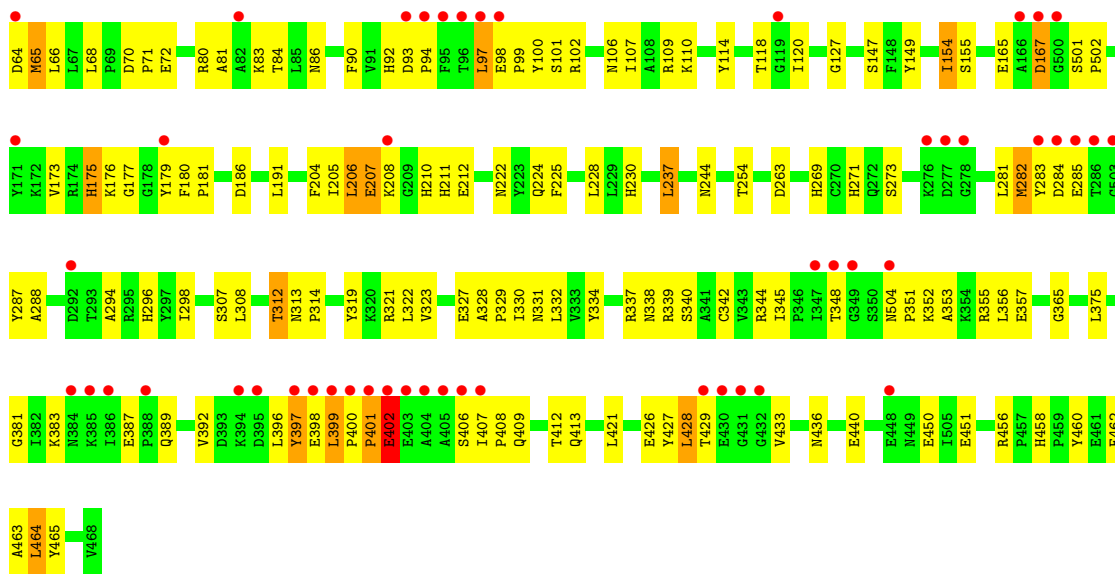


• Molecule 1: glutamine synthetase

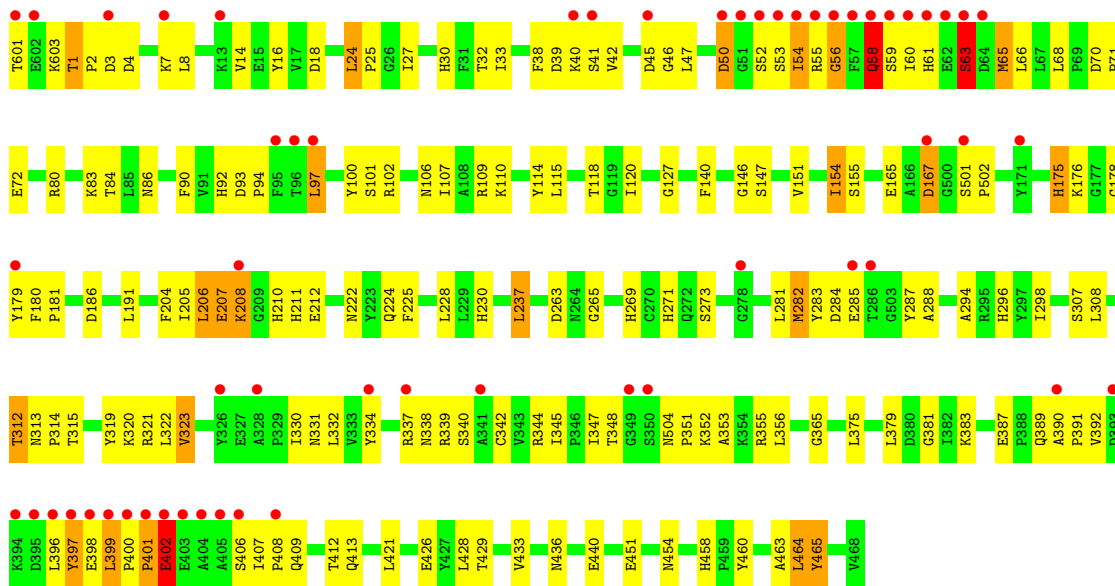


• Molecule 1: glutamine synthetase

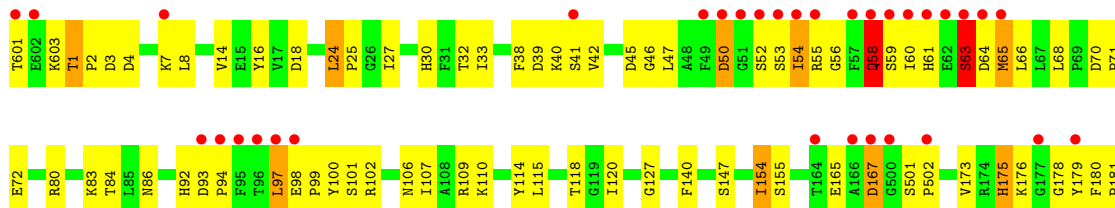




• Molecule 1: glutamine synthetase

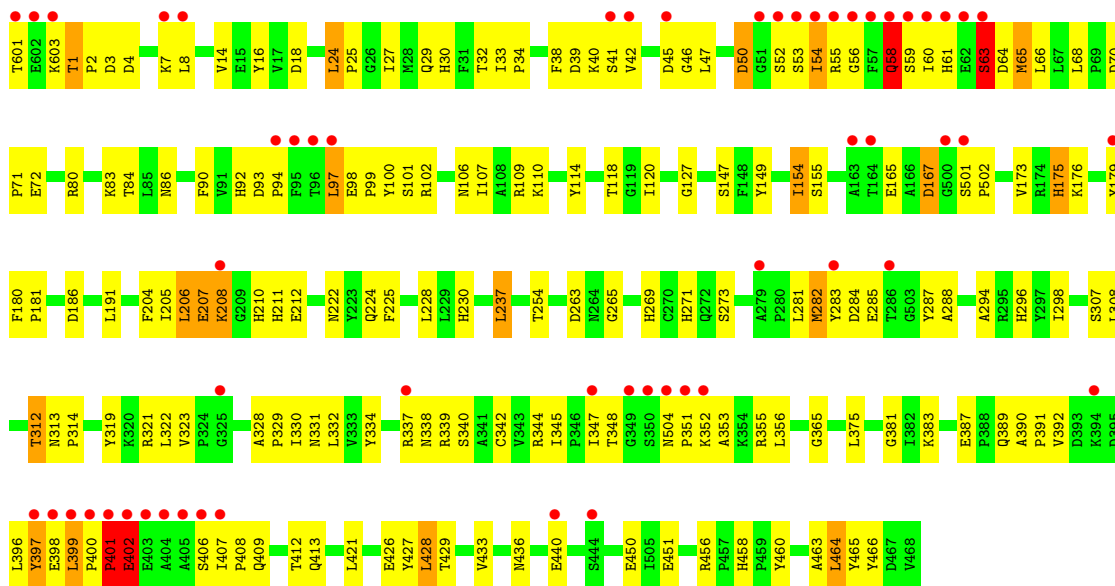


• Molecule 1: glutamine synthetase

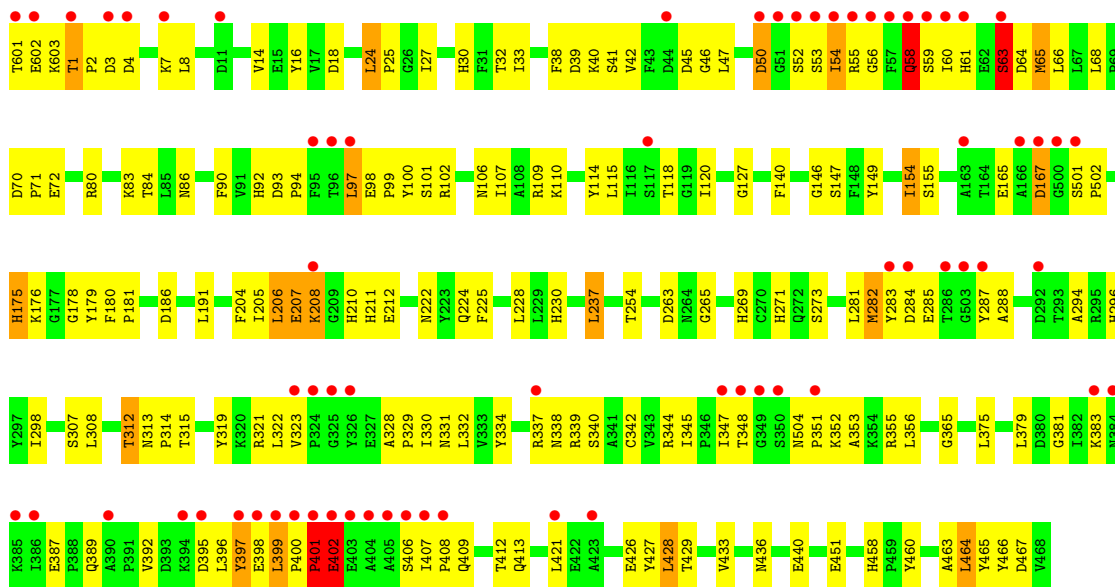




• Molecule 1: glutamine synthetase

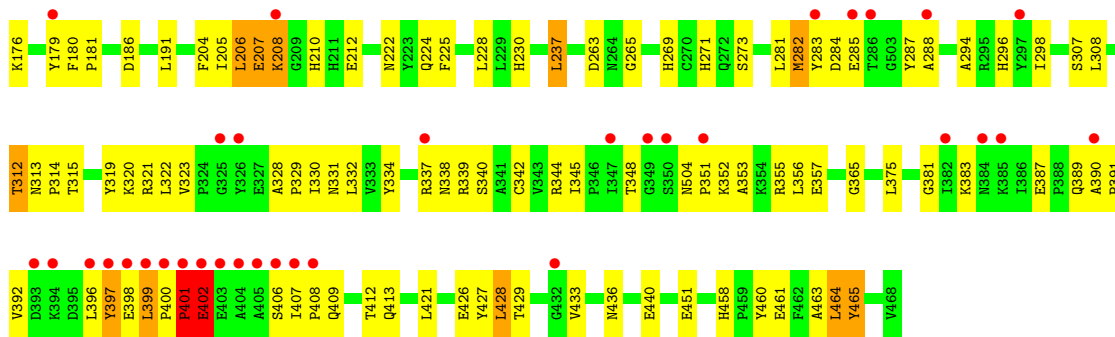


• Molecule 1: glutamine synthetase

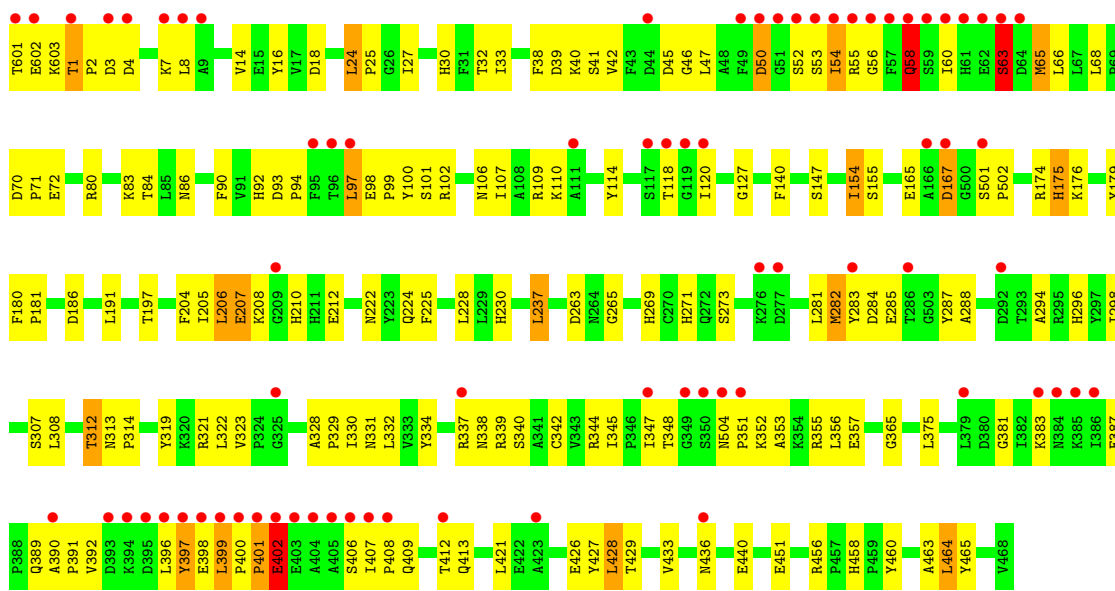


• Molecule 1: glutamine synthetase

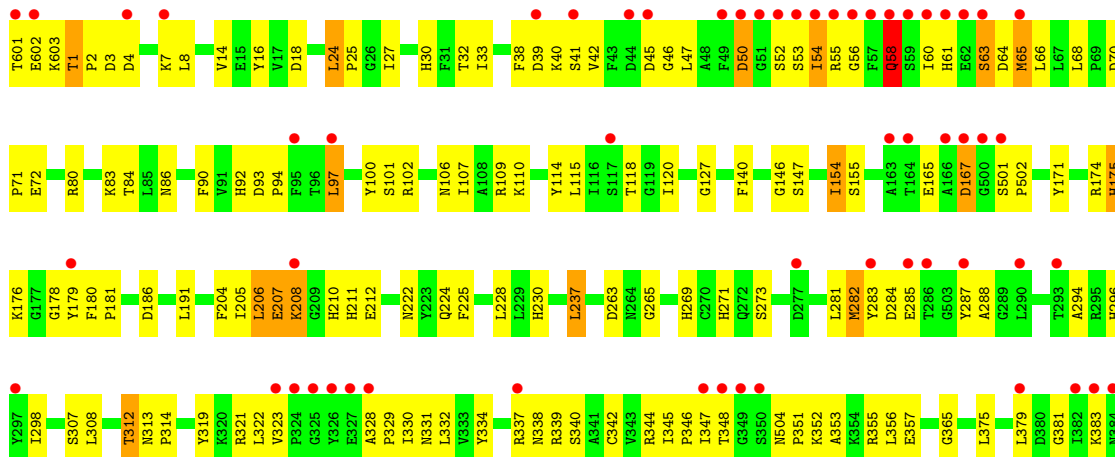


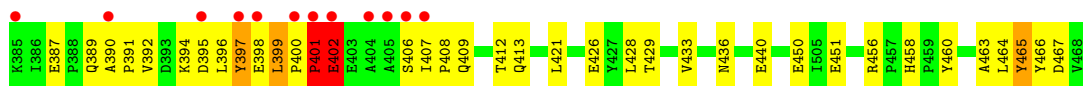


• Molecule 1: glutamine synthetase

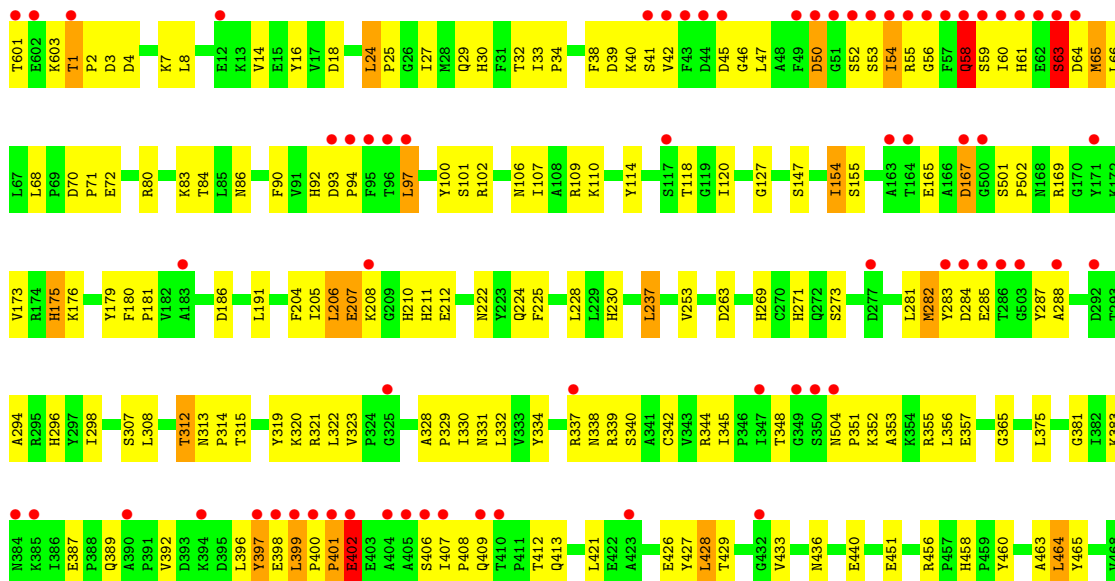


• Molecule 1: glutamine synthetase

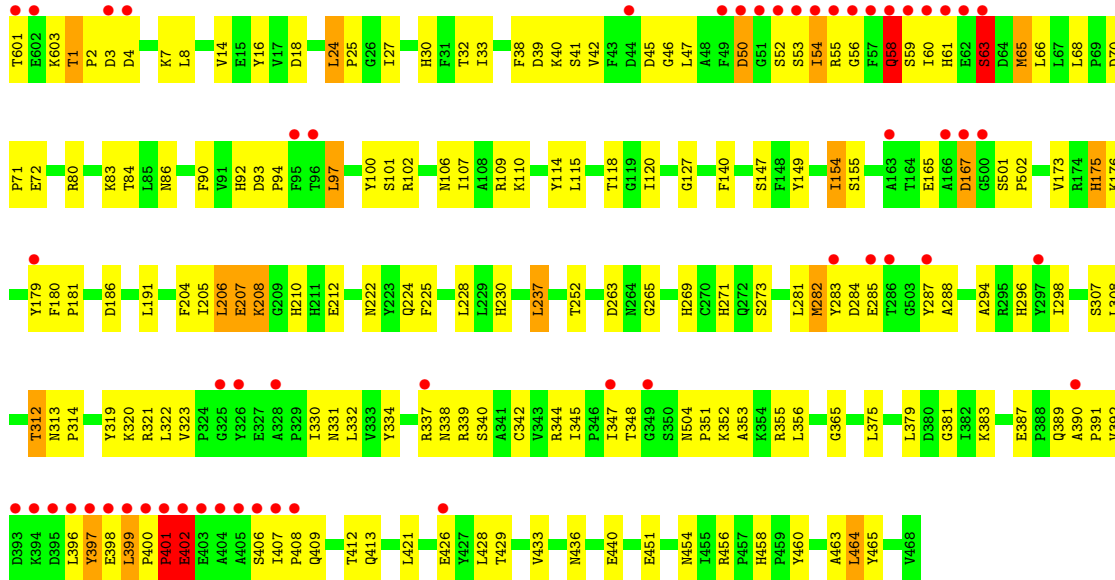




• Molecule 1: glutamine synthetase

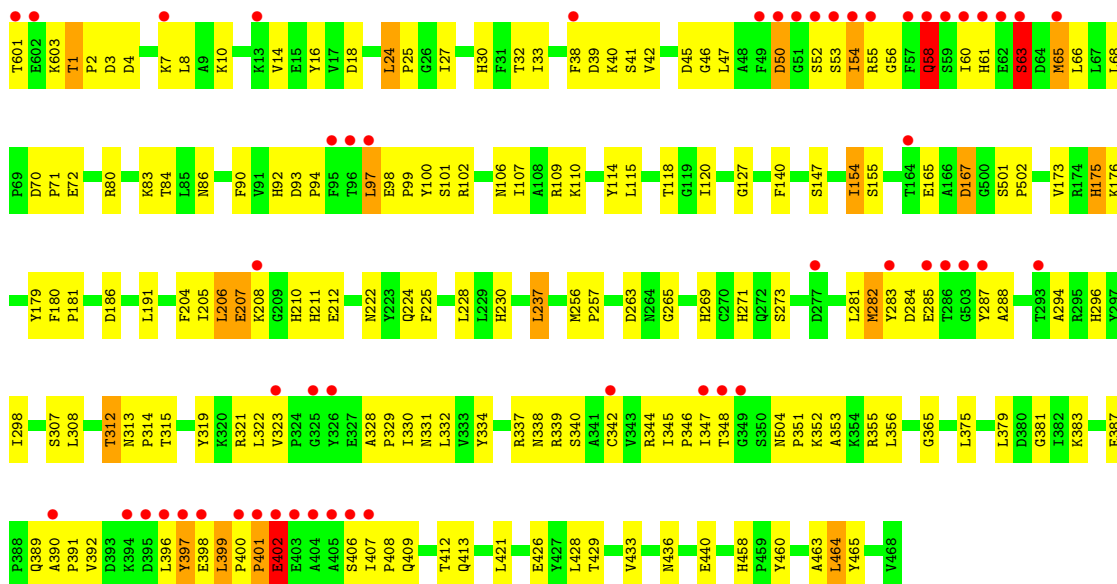


• Molecule 1: glutamine synthetase

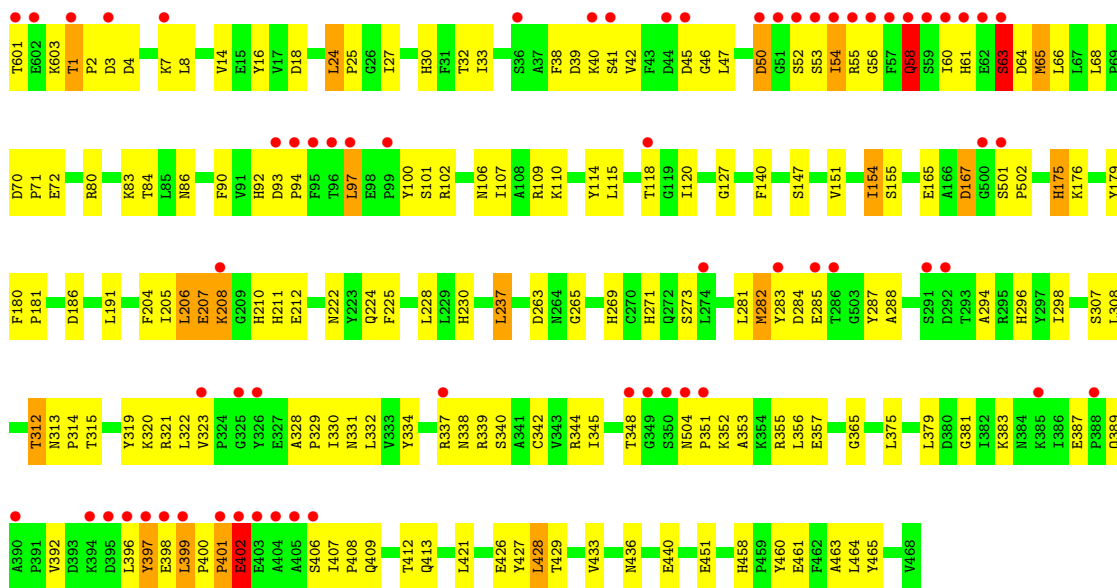


• Molecule 1: glutamine synthetase

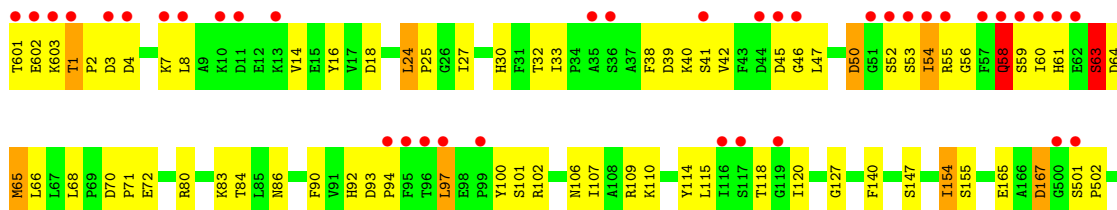


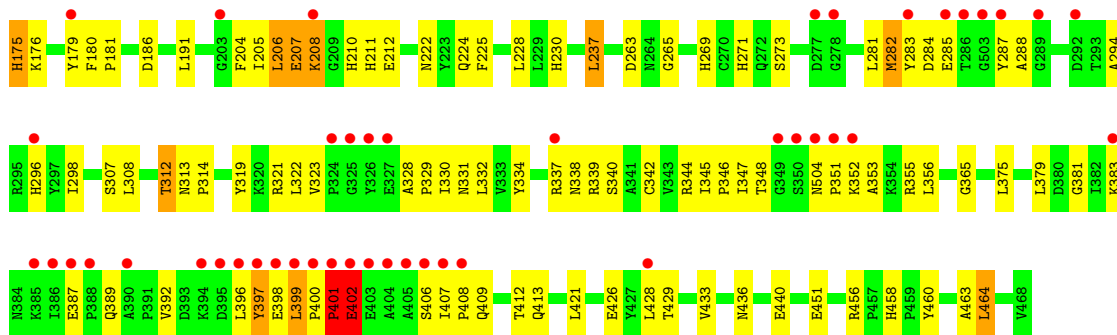


• Molecule 1: glutamine synthetase

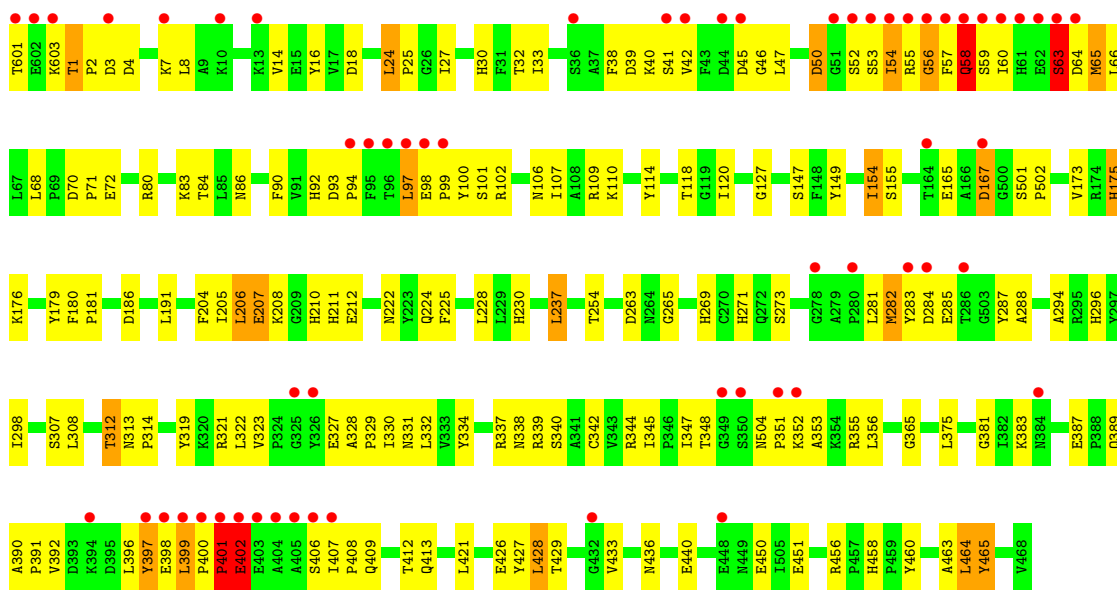


• Molecule 1: glutamine synthetase

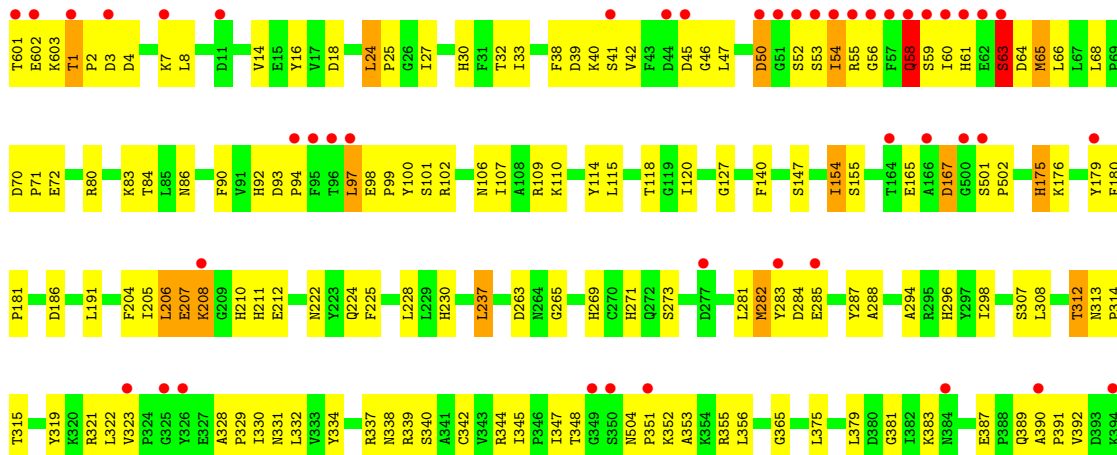




• Molecule 1: glutamine synthetase

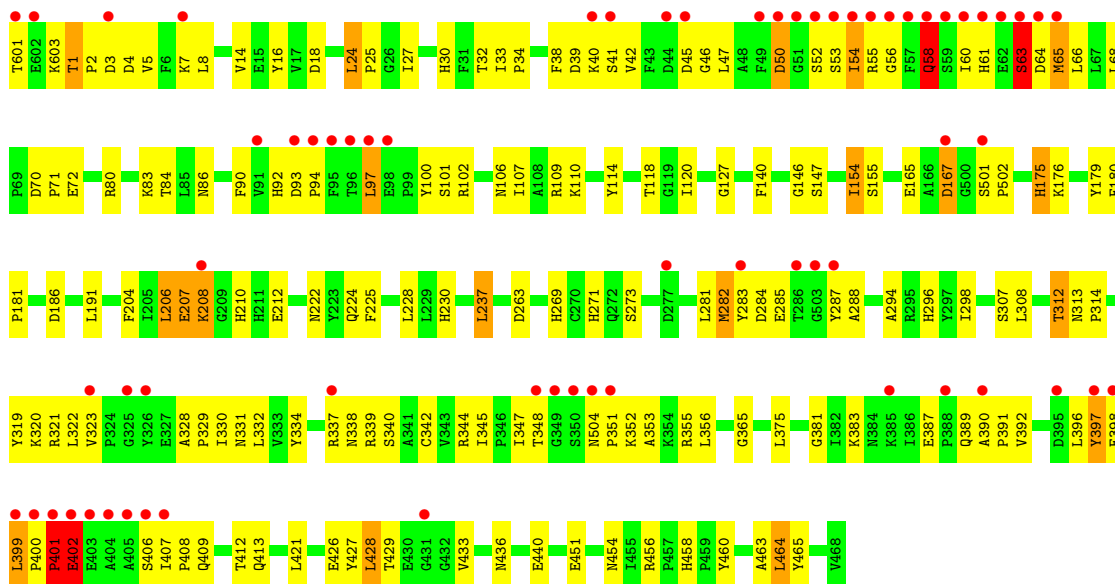


• Molecule 1: glutamine synthetase

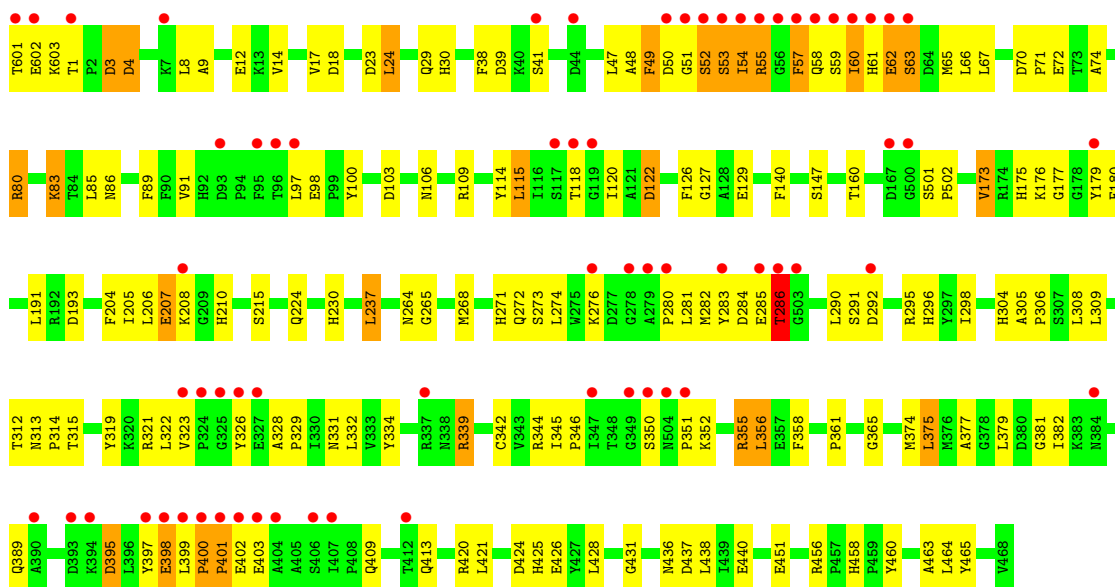




• Molecule 1: glutamine synthetase

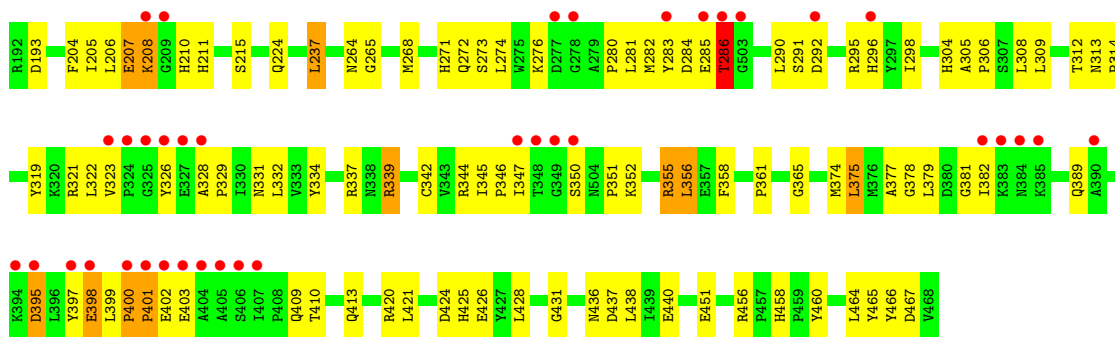


• Molecule 1: glutamine synthetase

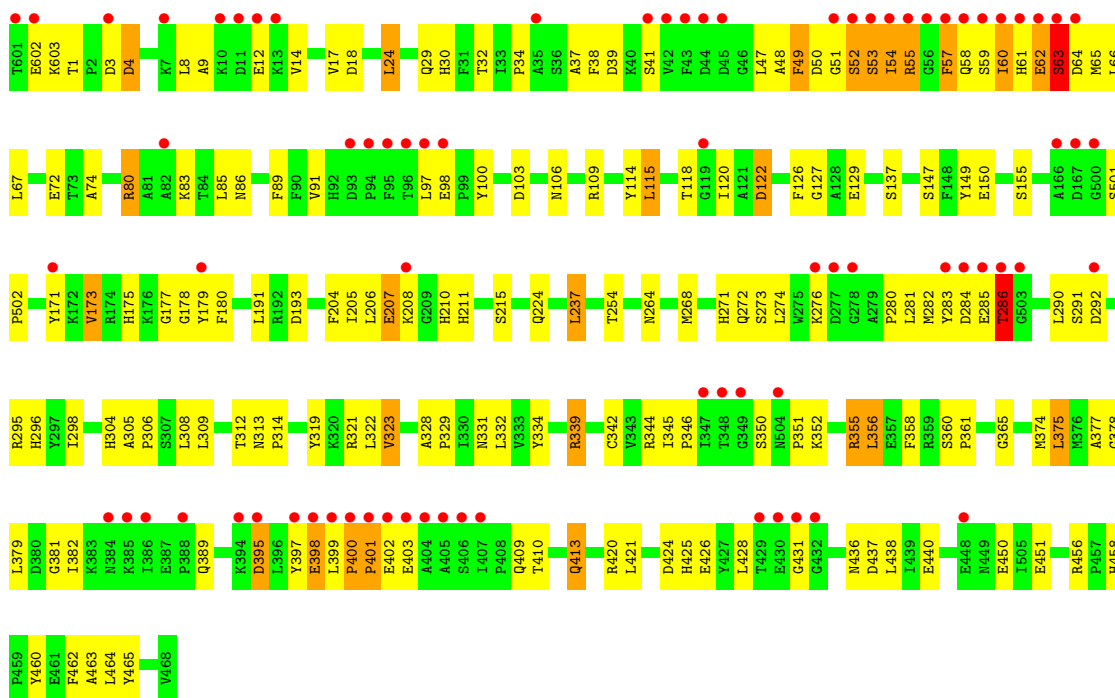


• Molecule 1: glutamine synthetase

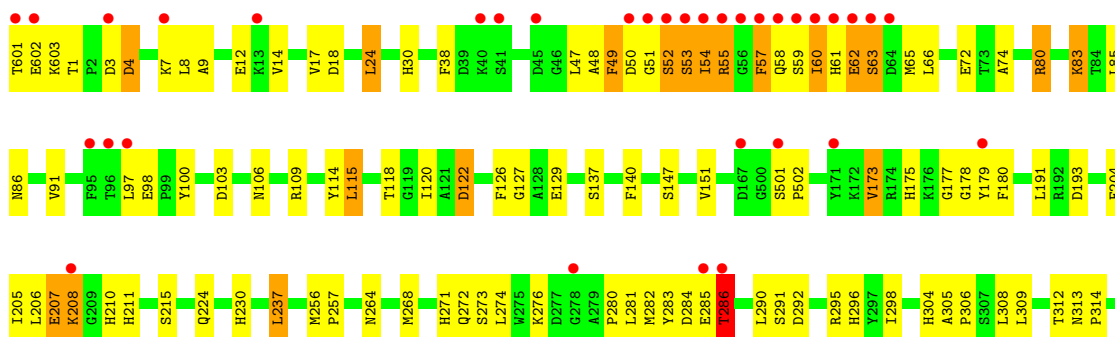


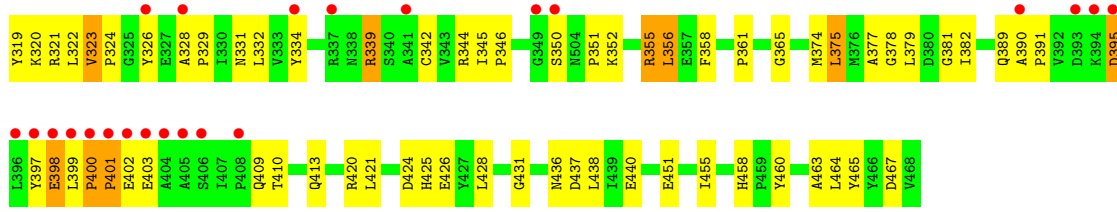


• Molecule 1: glutamine synthetase

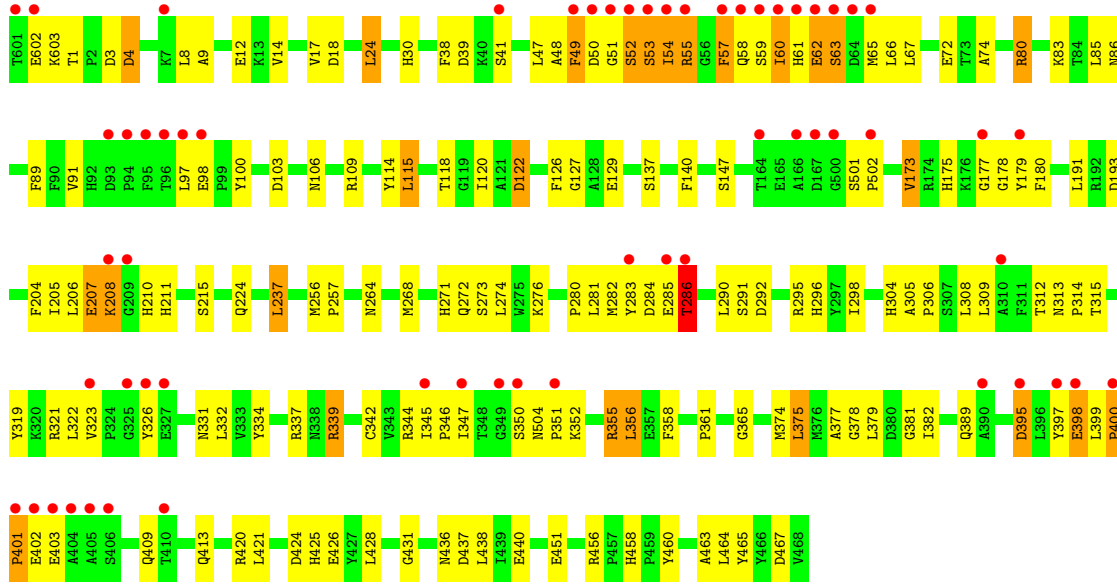


• Molecule 1: glutamine synthetase

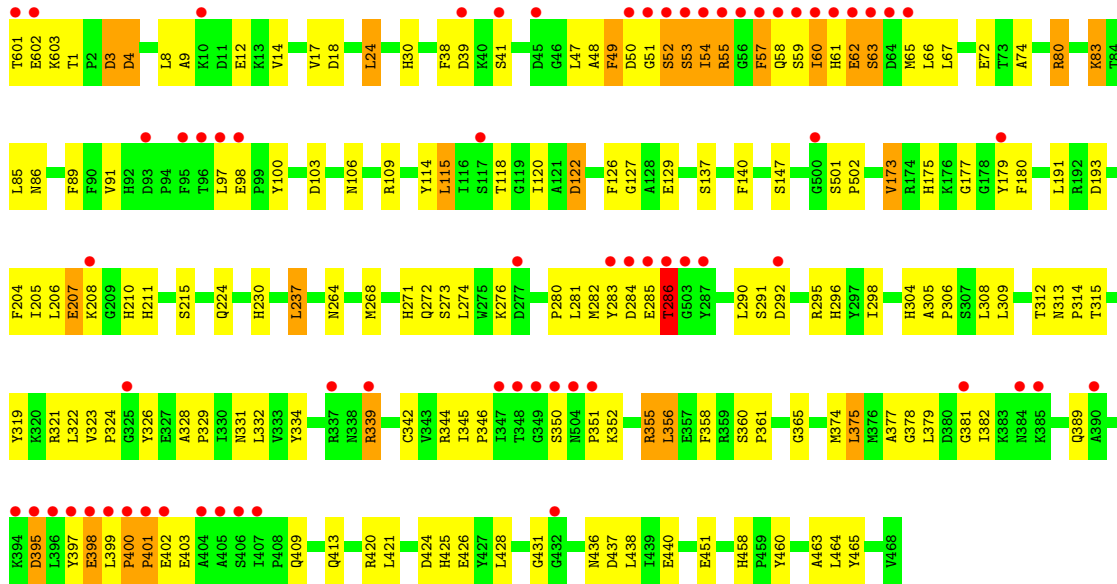


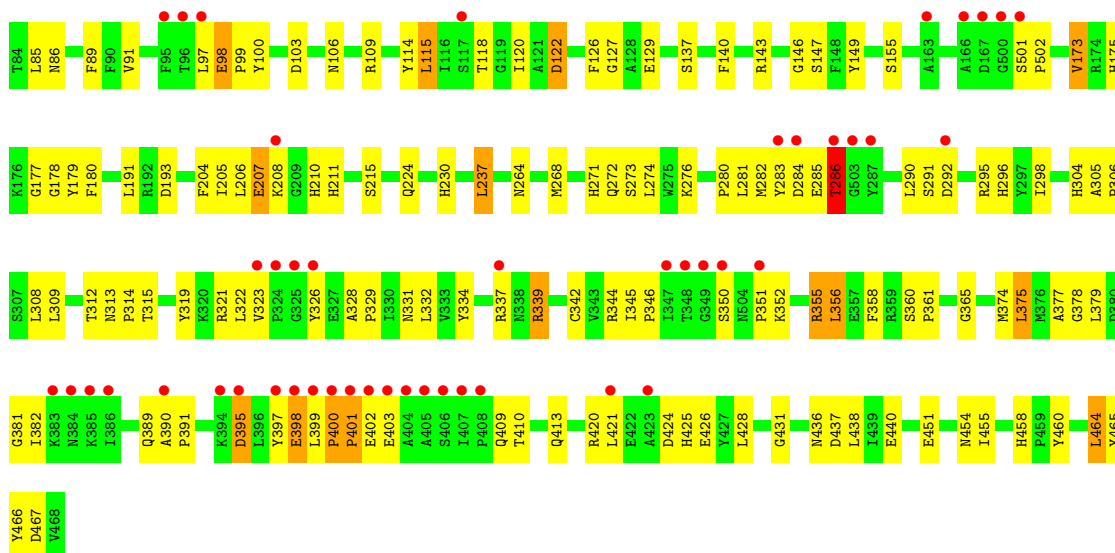


● Molecule 1: glutamine synthetase

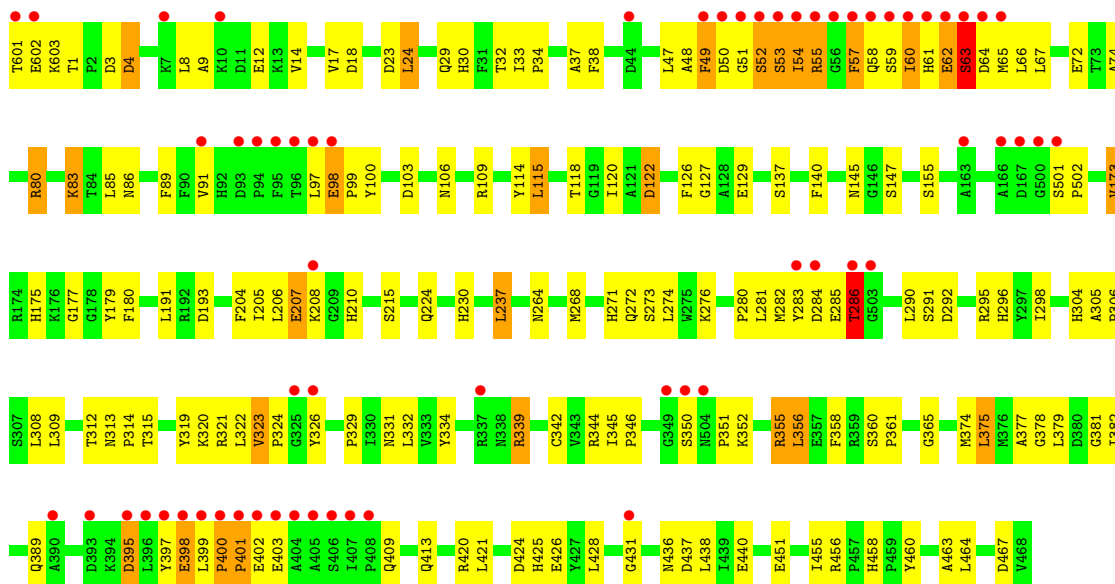


● Molecule 1: glutamine synthetase

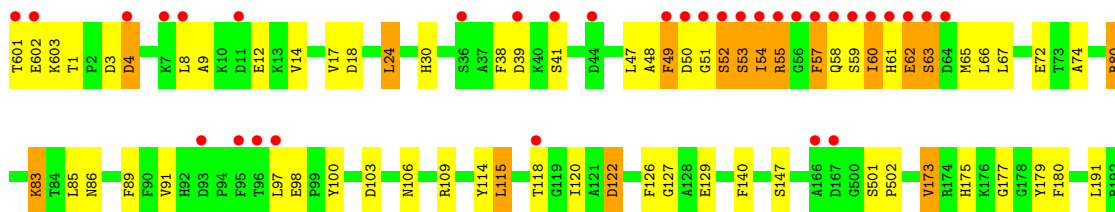


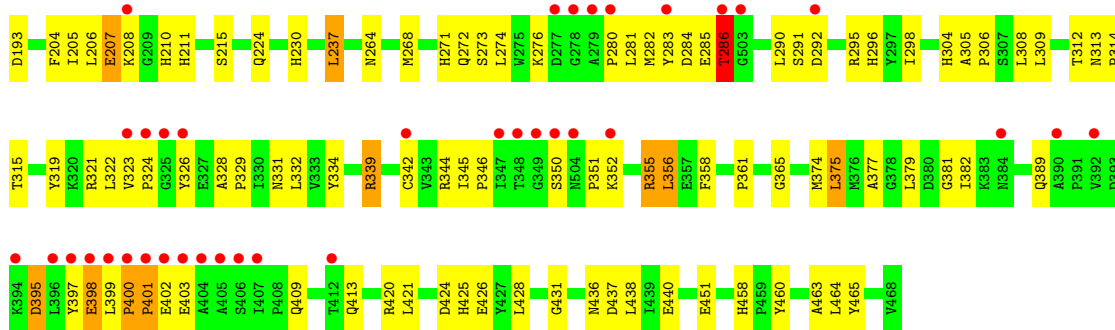


• Molecule 1: glutamine synthetase

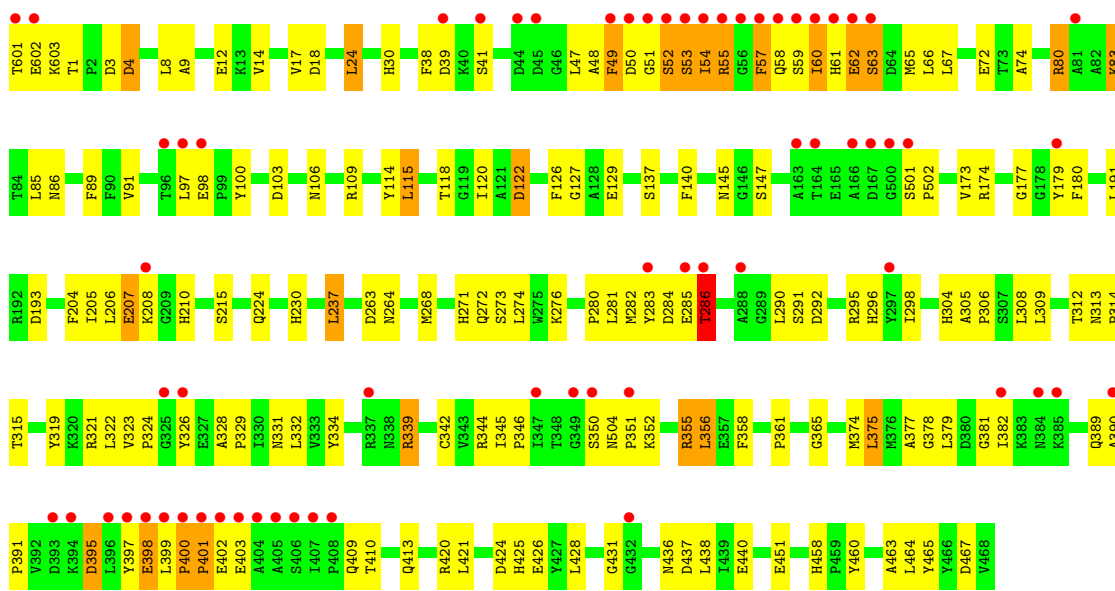


• Molecule 1: glutamine synthetase

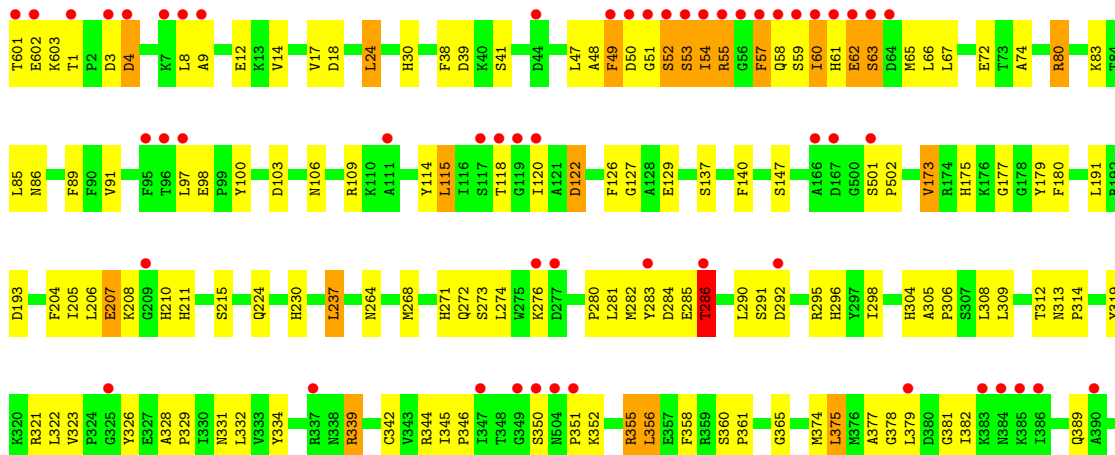




• Molecule 1: glutamine synthetase

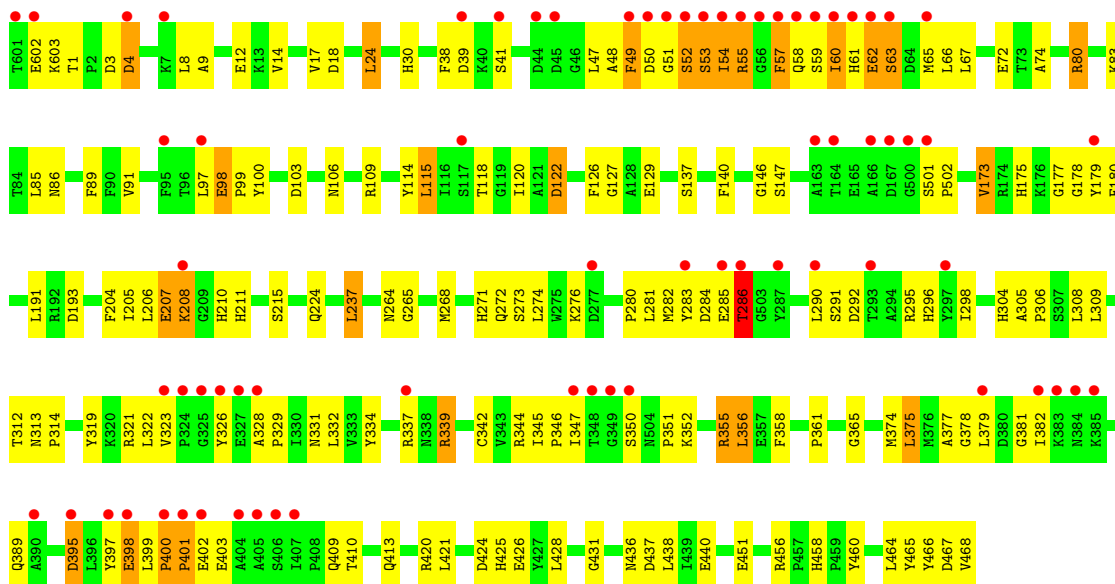


• Molecule 1: glutamine synthetase

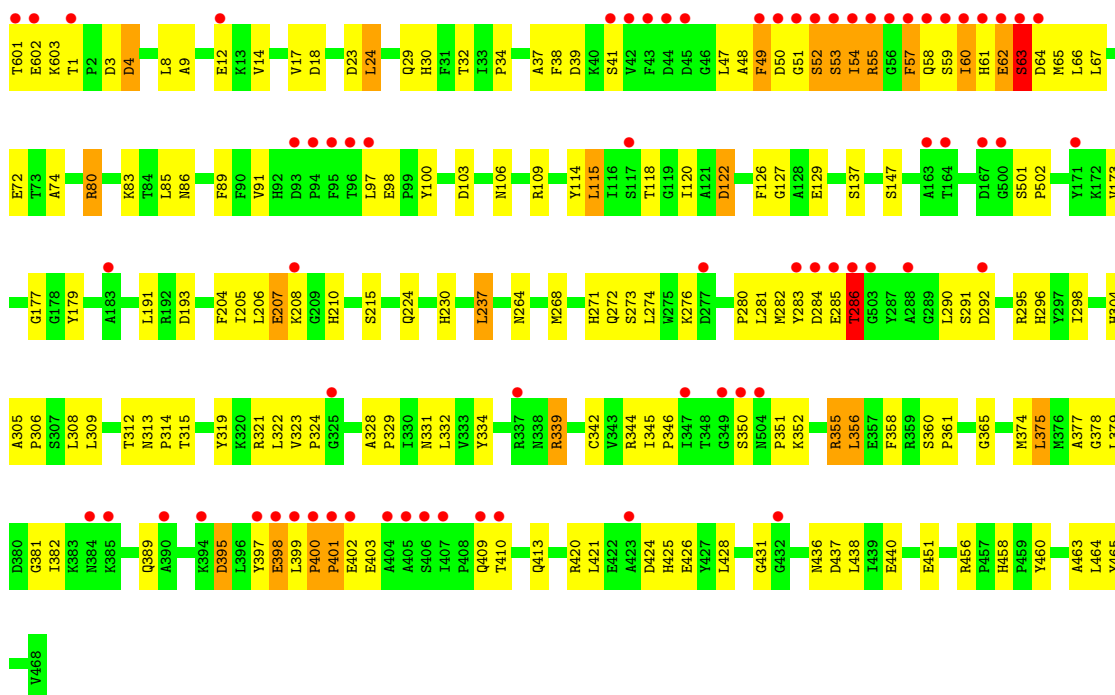




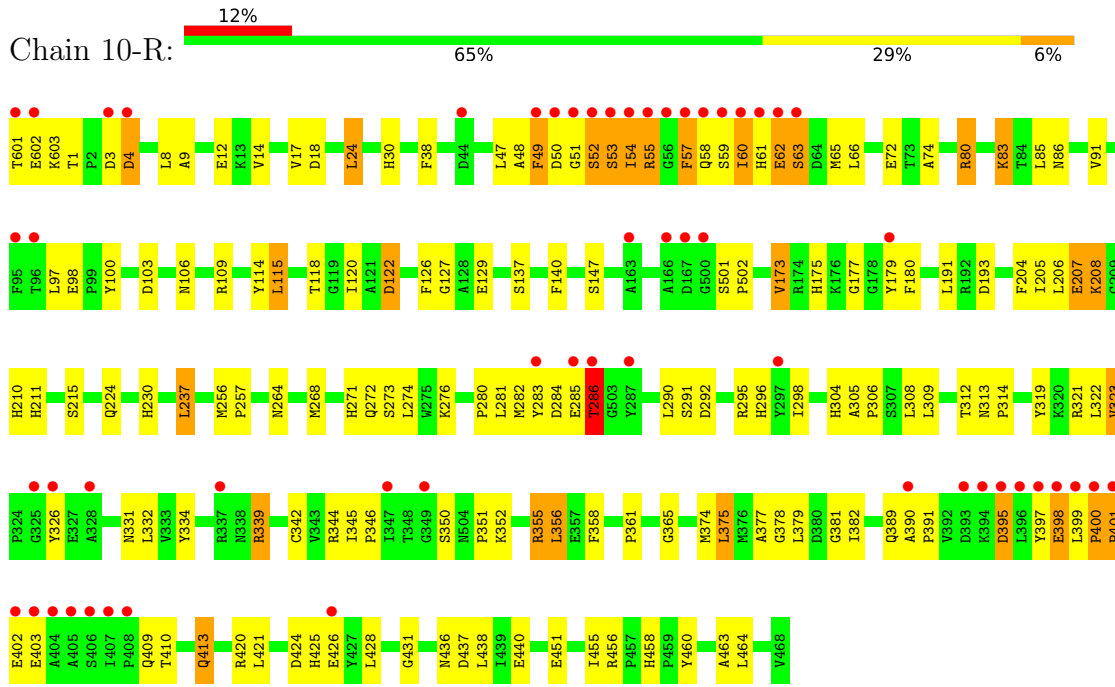
• Molecule 1: glutamine synthetase



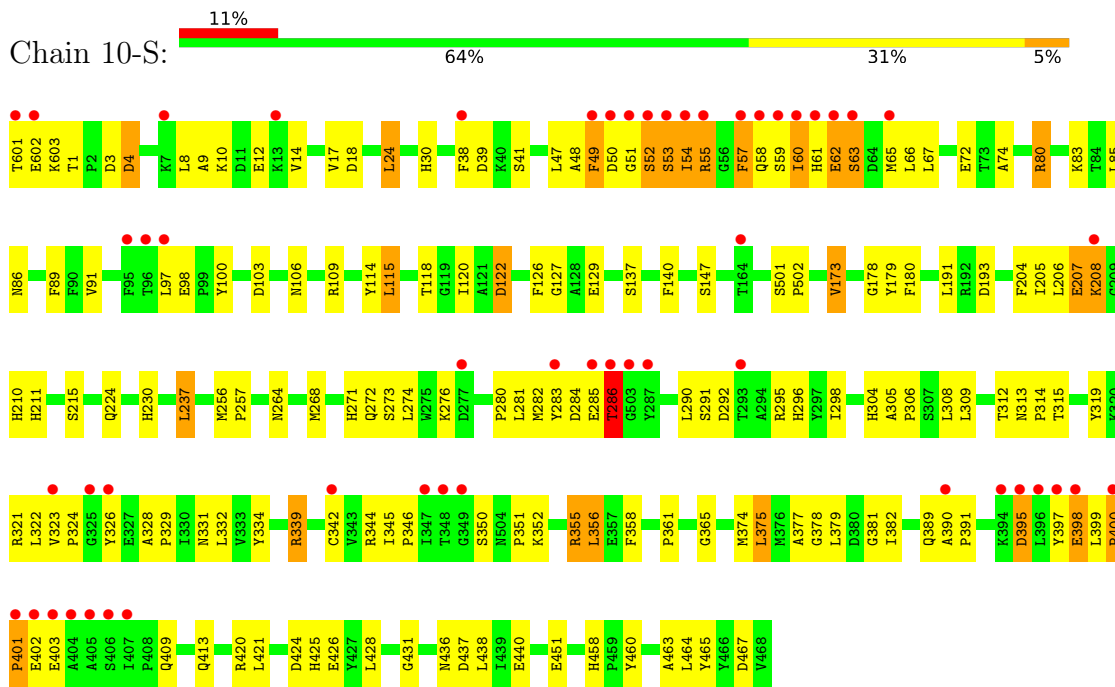
• Molecule 1: glutamine synthetase



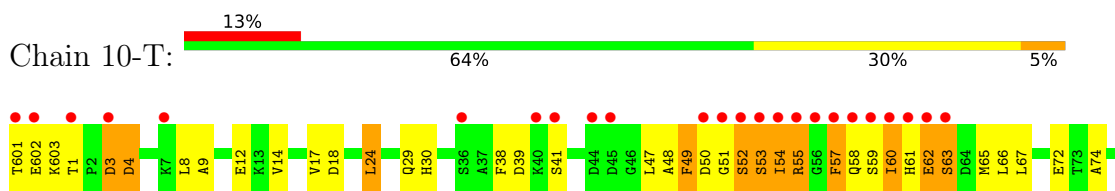
• Molecule 1: glutamine synthetase

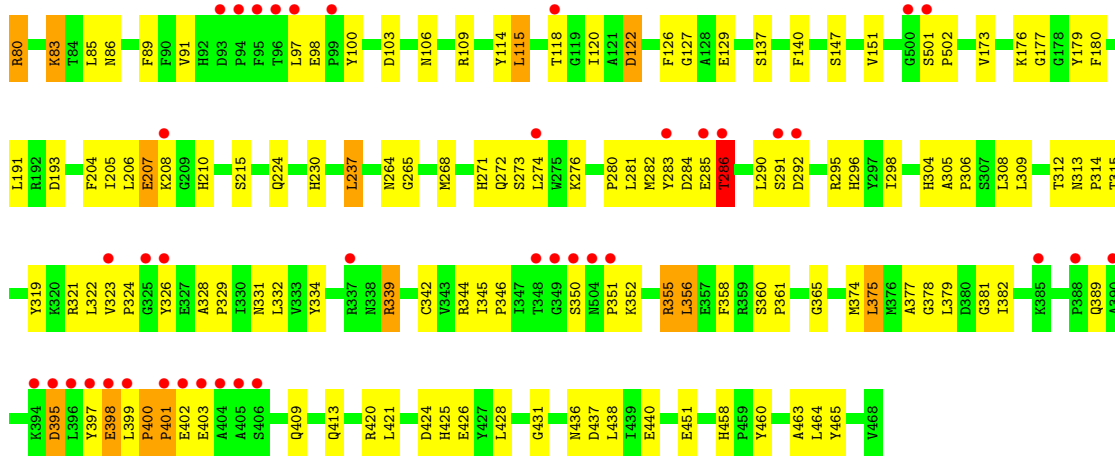


• Molecule 1: glutamine synthetase

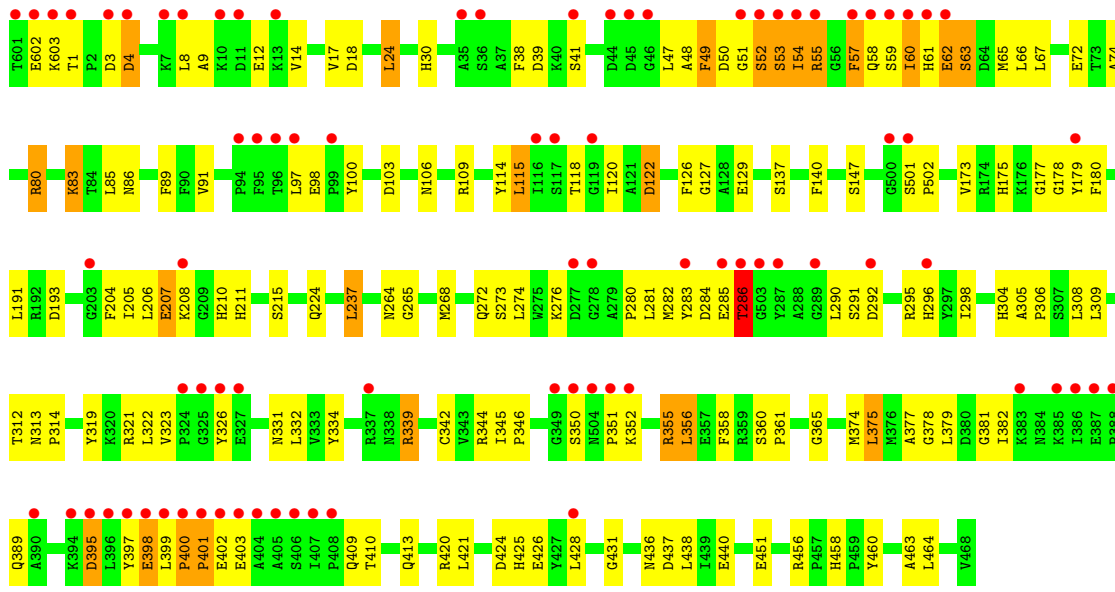


• Molecule 1: glutamine synthetase

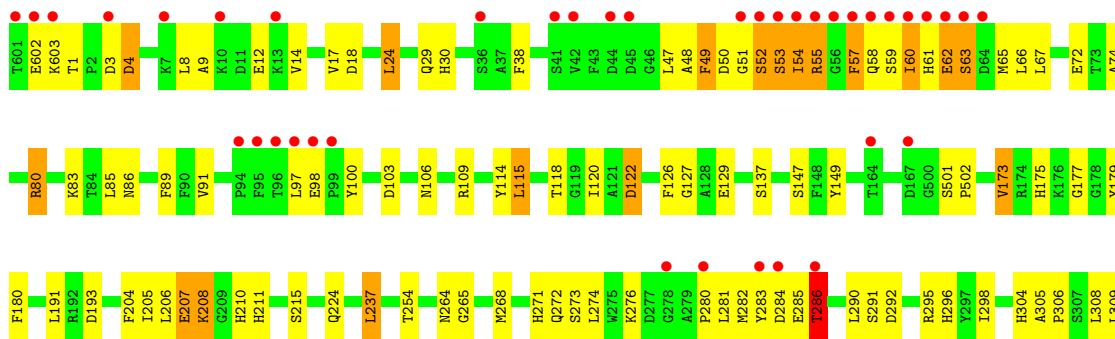


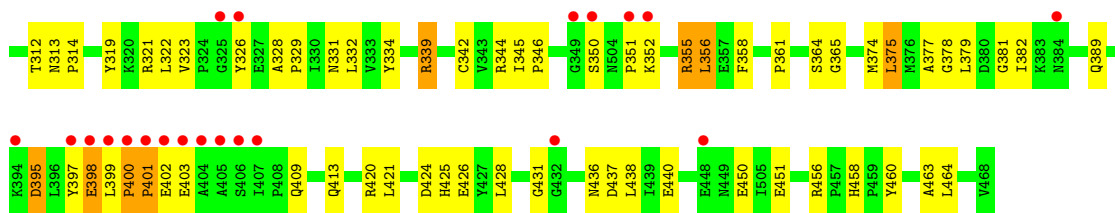


• Molecule 1: glutamine synthetase

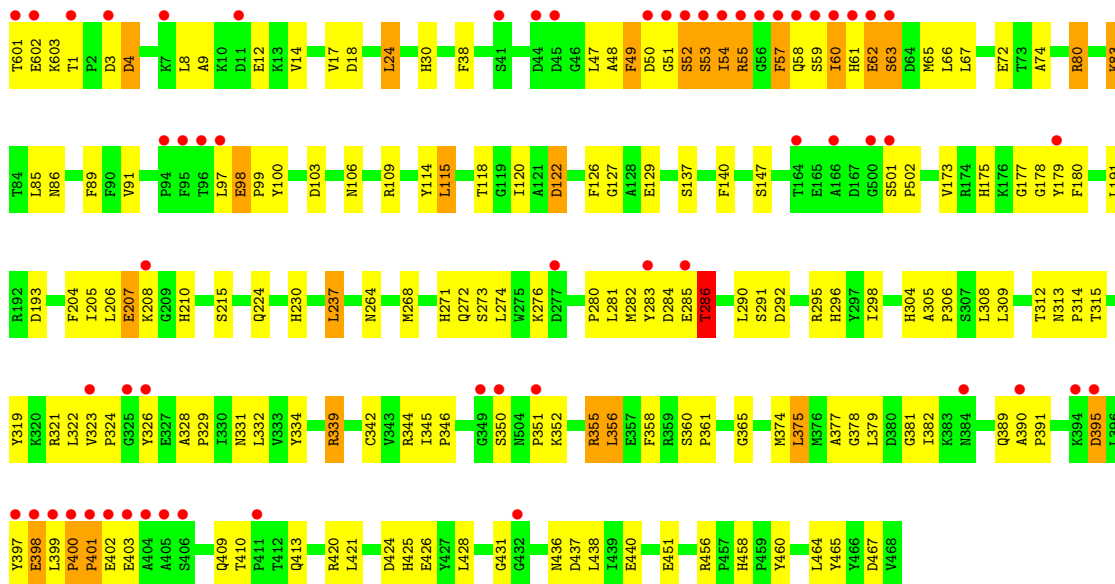


• Molecule 1: glutamine synthetase

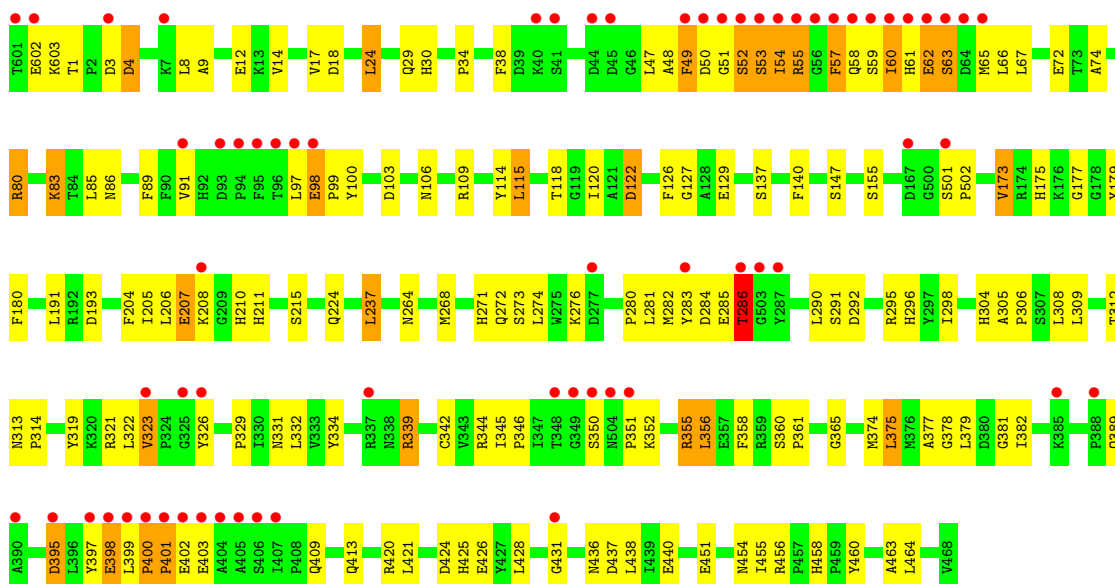




● Molecule 1: glutamine synthetase



● Molecule 1: glutamine synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	207.72Å 257.69Å 274.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.40) 99.7 (20.00-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.38 (at 2.41Å)	Xtrriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.204 , 0.223 0.219 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtrriage
Anisotropy	0.287	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 91.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	978720	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.31 % 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 5.0949e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, AMP, CIT

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	0.45	0/3884	0.71	1/5279 (0.0%)
1	1-B	0.45	0/3884	0.71	1/5279 (0.0%)
1	1-C	0.45	0/3884	0.71	1/5279 (0.0%)
1	1-D	0.45	0/3884	0.71	1/5279 (0.0%)
1	1-E	0.45	0/3884	0.71	1/5279 (0.0%)
1	1-F	0.45	0/3884	0.71	1/5279 (0.0%)
1	1-G	0.45	0/3884	0.71	1/5279 (0.0%)
1	1-H	0.45	0/3884	0.71	1/5279 (0.0%)
1	1-I	0.45	0/3884	0.71	1/5279 (0.0%)
1	1-J	0.45	0/3884	0.71	1/5279 (0.0%)
1	1-K	0.45	0/3884	0.71	1/5279 (0.0%)
1	1-L	0.45	0/3884	0.71	1/5279 (0.0%)
1	1-M	0.45	0/3884	0.71	1/5279 (0.0%)
1	1-N	0.45	0/3884	0.71	1/5279 (0.0%)
1	1-O	0.45	0/3884	0.71	1/5279 (0.0%)
1	1-P	0.45	0/3884	0.71	1/5279 (0.0%)
1	1-Q	0.45	0/3884	0.71	1/5279 (0.0%)
1	1-R	0.45	0/3884	0.71	1/5279 (0.0%)
1	1-S	0.45	0/3884	0.71	1/5279 (0.0%)
1	1-T	0.45	0/3884	0.71	1/5279 (0.0%)
1	1-U	0.45	0/3884	0.71	1/5279 (0.0%)
1	1-V	0.45	0/3884	0.71	1/5279 (0.0%)
1	1-W	0.45	0/3884	0.71	1/5279 (0.0%)
1	1-X	0.45	0/3884	0.71	1/5279 (0.0%)
1	2-A	0.46	0/3884	0.72	3/5279 (0.1%)
1	2-B	0.46	0/3884	0.72	3/5279 (0.1%)
1	2-C	0.46	0/3884	0.72	3/5279 (0.1%)
1	2-D	0.46	0/3884	0.72	3/5279 (0.1%)
1	2-E	0.46	0/3884	0.72	3/5279 (0.1%)
1	2-F	0.46	0/3884	0.72	3/5279 (0.1%)
1	2-G	0.46	0/3884	0.72	3/5279 (0.1%)
1	2-H	0.46	0/3884	0.72	3/5279 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	2-I	0.46	0/3884	0.72	3/5279 (0.1%)
1	2-J	0.46	0/3884	0.72	3/5279 (0.1%)
1	2-K	0.46	0/3884	0.72	3/5279 (0.1%)
1	2-L	0.46	0/3884	0.72	3/5279 (0.1%)
1	2-M	0.46	0/3884	0.72	3/5279 (0.1%)
1	2-N	0.46	0/3884	0.72	3/5279 (0.1%)
1	2-O	0.46	0/3884	0.72	3/5279 (0.1%)
1	2-P	0.46	0/3884	0.72	3/5279 (0.1%)
1	2-Q	0.46	0/3884	0.72	3/5279 (0.1%)
1	2-R	0.46	0/3884	0.72	3/5279 (0.1%)
1	2-S	0.46	0/3884	0.72	3/5279 (0.1%)
1	2-T	0.46	0/3884	0.72	3/5279 (0.1%)
1	2-U	0.46	0/3884	0.72	3/5279 (0.1%)
1	2-V	0.46	0/3884	0.72	3/5279 (0.1%)
1	2-W	0.46	0/3884	0.72	3/5279 (0.1%)
1	2-X	0.46	0/3884	0.72	3/5279 (0.1%)
1	3-A	0.46	0/3884	0.71	3/5279 (0.1%)
1	3-B	0.46	0/3884	0.71	3/5279 (0.1%)
1	3-C	0.46	0/3884	0.71	3/5279 (0.1%)
1	3-D	0.46	0/3884	0.71	3/5279 (0.1%)
1	3-E	0.46	0/3884	0.71	3/5279 (0.1%)
1	3-F	0.46	0/3884	0.71	3/5279 (0.1%)
1	3-G	0.46	0/3884	0.71	3/5279 (0.1%)
1	3-H	0.46	0/3884	0.71	3/5279 (0.1%)
1	3-I	0.46	0/3884	0.71	3/5279 (0.1%)
1	3-J	0.46	0/3884	0.71	3/5279 (0.1%)
1	3-K	0.46	0/3884	0.71	3/5279 (0.1%)
1	3-L	0.46	0/3884	0.71	3/5279 (0.1%)
1	3-M	0.46	0/3884	0.71	3/5279 (0.1%)
1	3-N	0.46	0/3884	0.71	3/5279 (0.1%)
1	3-O	0.46	0/3884	0.71	3/5279 (0.1%)
1	3-P	0.46	0/3884	0.71	3/5279 (0.1%)
1	3-Q	0.46	0/3884	0.71	3/5279 (0.1%)
1	3-R	0.46	0/3884	0.71	3/5279 (0.1%)
1	3-S	0.46	0/3884	0.71	3/5279 (0.1%)
1	3-T	0.46	0/3884	0.71	3/5279 (0.1%)
1	3-U	0.46	0/3884	0.71	3/5279 (0.1%)
1	3-V	0.46	0/3884	0.71	3/5279 (0.1%)
1	3-W	0.46	0/3884	0.71	3/5279 (0.1%)
1	3-X	0.46	0/3884	0.71	3/5279 (0.1%)
1	4-A	0.46	0/3884	0.71	1/5279 (0.0%)
1	4-B	0.46	0/3884	0.71	1/5279 (0.0%)
1	4-C	0.46	0/3884	0.71	1/5279 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	4-D	0.46	0/3884	0.71	1/5279 (0.0%)
1	4-E	0.46	0/3884	0.71	1/5279 (0.0%)
1	4-F	0.46	0/3884	0.71	1/5279 (0.0%)
1	4-G	0.46	0/3884	0.71	1/5279 (0.0%)
1	4-H	0.46	0/3884	0.71	1/5279 (0.0%)
1	4-I	0.46	0/3884	0.71	1/5279 (0.0%)
1	4-J	0.46	0/3884	0.71	1/5279 (0.0%)
1	4-K	0.46	0/3884	0.71	1/5279 (0.0%)
1	4-L	0.46	0/3884	0.71	1/5279 (0.0%)
1	4-M	0.46	0/3884	0.71	1/5279 (0.0%)
1	4-N	0.46	0/3884	0.71	1/5279 (0.0%)
1	4-O	0.46	0/3884	0.71	1/5279 (0.0%)
1	4-P	0.46	0/3884	0.71	1/5279 (0.0%)
1	4-Q	0.46	0/3884	0.71	1/5279 (0.0%)
1	4-R	0.46	0/3884	0.71	1/5279 (0.0%)
1	4-S	0.46	0/3884	0.71	1/5279 (0.0%)
1	4-T	0.46	0/3884	0.71	1/5279 (0.0%)
1	4-U	0.46	0/3884	0.71	1/5279 (0.0%)
1	4-V	0.46	0/3884	0.71	1/5279 (0.0%)
1	4-W	0.46	0/3884	0.71	1/5279 (0.0%)
1	4-X	0.46	0/3884	0.71	1/5279 (0.0%)
1	5-A	0.46	0/3884	0.71	2/5279 (0.0%)
1	5-B	0.46	0/3884	0.71	2/5279 (0.0%)
1	5-C	0.46	0/3884	0.71	2/5279 (0.0%)
1	5-D	0.46	0/3884	0.71	2/5279 (0.0%)
1	5-E	0.46	0/3884	0.71	2/5279 (0.0%)
1	5-F	0.46	0/3884	0.71	2/5279 (0.0%)
1	5-G	0.46	0/3884	0.71	2/5279 (0.0%)
1	5-H	0.46	0/3884	0.71	2/5279 (0.0%)
1	5-I	0.46	0/3884	0.71	2/5279 (0.0%)
1	5-J	0.46	0/3884	0.71	2/5279 (0.0%)
1	5-K	0.46	0/3884	0.71	2/5279 (0.0%)
1	5-L	0.46	0/3884	0.71	2/5279 (0.0%)
1	5-M	0.46	0/3884	0.71	2/5279 (0.0%)
1	5-N	0.46	0/3884	0.71	2/5279 (0.0%)
1	5-O	0.46	0/3884	0.71	2/5279 (0.0%)
1	5-P	0.46	0/3884	0.71	2/5279 (0.0%)
1	5-Q	0.46	0/3884	0.71	2/5279 (0.0%)
1	5-R	0.46	0/3884	0.71	2/5279 (0.0%)
1	5-S	0.46	0/3884	0.71	2/5279 (0.0%)
1	5-T	0.46	0/3884	0.71	2/5279 (0.0%)
1	5-U	0.46	0/3884	0.71	2/5279 (0.0%)
1	5-V	0.46	0/3884	0.71	2/5279 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	5-W	0.46	0/3884	0.71	2/5279 (0.0%)
1	5-X	0.46	0/3884	0.71	2/5279 (0.0%)
1	6-A	0.45	0/3884	0.72	3/5279 (0.1%)
1	6-B	0.46	0/3884	0.72	3/5279 (0.1%)
1	6-C	0.46	0/3884	0.72	3/5279 (0.1%)
1	6-D	0.46	0/3884	0.72	3/5279 (0.1%)
1	6-E	0.46	0/3884	0.72	3/5279 (0.1%)
1	6-F	0.46	0/3884	0.72	3/5279 (0.1%)
1	6-G	0.46	0/3884	0.72	3/5279 (0.1%)
1	6-H	0.45	0/3884	0.72	3/5279 (0.1%)
1	6-I	0.45	0/3884	0.72	3/5279 (0.1%)
1	6-J	0.46	0/3884	0.72	3/5279 (0.1%)
1	6-K	0.46	0/3884	0.72	3/5279 (0.1%)
1	6-L	0.45	0/3884	0.72	3/5279 (0.1%)
1	6-M	0.45	0/3884	0.72	3/5279 (0.1%)
1	6-N	0.46	0/3884	0.72	3/5279 (0.1%)
1	6-O	0.46	0/3884	0.72	3/5279 (0.1%)
1	6-P	0.46	0/3884	0.72	3/5279 (0.1%)
1	6-Q	0.46	0/3884	0.72	3/5279 (0.1%)
1	6-R	0.45	0/3884	0.72	3/5279 (0.1%)
1	6-S	0.46	0/3884	0.72	3/5279 (0.1%)
1	6-T	0.46	0/3884	0.72	3/5279 (0.1%)
1	6-U	0.46	0/3884	0.72	3/5279 (0.1%)
1	6-V	0.46	0/3884	0.72	3/5279 (0.1%)
1	6-W	0.45	0/3884	0.72	3/5279 (0.1%)
1	6-X	0.45	0/3884	0.72	3/5279 (0.1%)
1	7-A	0.47	0/3884	0.74	5/5279 (0.1%)
1	7-B	0.47	0/3884	0.74	5/5279 (0.1%)
1	7-C	0.47	0/3884	0.74	5/5279 (0.1%)
1	7-D	0.47	0/3884	0.74	5/5279 (0.1%)
1	7-E	0.47	0/3884	0.74	5/5279 (0.1%)
1	7-F	0.47	0/3884	0.74	5/5279 (0.1%)
1	7-G	0.47	0/3884	0.74	5/5279 (0.1%)
1	7-H	0.47	0/3884	0.74	5/5279 (0.1%)
1	7-I	0.47	0/3884	0.74	5/5279 (0.1%)
1	7-J	0.47	0/3884	0.74	6/5279 (0.1%)
1	7-K	0.47	0/3884	0.74	5/5279 (0.1%)
1	7-L	0.47	0/3884	0.74	5/5279 (0.1%)
1	7-M	0.47	0/3884	0.74	5/5279 (0.1%)
1	7-N	0.47	0/3884	0.74	5/5279 (0.1%)
1	7-O	0.47	0/3884	0.74	5/5279 (0.1%)
1	7-P	0.47	0/3884	0.74	5/5279 (0.1%)
1	7-Q	0.47	0/3884	0.74	5/5279 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	7-R	0.47	0/3884	0.74	5/5279 (0.1%)
1	7-S	0.47	0/3884	0.74	5/5279 (0.1%)
1	7-T	0.47	0/3884	0.74	5/5279 (0.1%)
1	7-U	0.47	0/3884	0.74	5/5279 (0.1%)
1	7-V	0.47	0/3884	0.74	5/5279 (0.1%)
1	7-W	0.47	0/3884	0.74	5/5279 (0.1%)
1	7-X	0.47	0/3884	0.74	5/5279 (0.1%)
1	8-A	0.46	0/3884	0.69	0/5279
1	8-B	0.46	0/3884	0.69	0/5279
1	8-C	0.46	0/3884	0.69	0/5279
1	8-D	0.46	0/3884	0.69	0/5279
1	8-E	0.46	0/3884	0.69	0/5279
1	8-F	0.46	0/3884	0.69	0/5279
1	8-G	0.46	0/3884	0.69	0/5279
1	8-H	0.46	0/3884	0.69	0/5279
1	8-I	0.46	0/3884	0.69	0/5279
1	8-J	0.46	0/3884	0.69	0/5279
1	8-K	0.46	0/3884	0.69	0/5279
1	8-L	0.46	0/3884	0.69	0/5279
1	8-M	0.46	0/3884	0.69	0/5279
1	8-N	0.46	0/3884	0.69	0/5279
1	8-O	0.46	0/3884	0.69	0/5279
1	8-P	0.46	0/3884	0.69	0/5279
1	8-Q	0.46	0/3884	0.69	0/5279
1	8-R	0.46	0/3884	0.69	0/5279
1	8-S	0.46	0/3884	0.69	0/5279
1	8-T	0.46	0/3884	0.69	0/5279
1	8-U	0.46	0/3884	0.69	0/5279
1	8-V	0.46	0/3884	0.69	0/5279
1	8-W	0.46	0/3884	0.69	0/5279
1	8-X	0.46	0/3884	0.69	0/5279
1	9-A	0.46	0/3884	0.74	2/5279 (0.0%)
1	9-B	0.46	0/3884	0.74	2/5279 (0.0%)
1	9-C	0.46	0/3884	0.74	2/5279 (0.0%)
1	9-D	0.46	0/3884	0.74	2/5279 (0.0%)
1	9-E	0.46	0/3884	0.74	2/5279 (0.0%)
1	9-F	0.46	0/3884	0.74	3/5279 (0.1%)
1	9-G	0.46	0/3884	0.74	2/5279 (0.0%)
1	9-H	0.46	0/3884	0.74	2/5279 (0.0%)
1	9-I	0.46	0/3884	0.74	2/5279 (0.0%)
1	9-J	0.46	0/3884	0.74	2/5279 (0.0%)
1	9-K	0.46	0/3884	0.74	2/5279 (0.0%)
1	9-L	0.46	0/3884	0.74	2/5279 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	9-M	0.46	0/3884	0.74	2/5279 (0.0%)
1	9-N	0.46	0/3884	0.74	3/5279 (0.1%)
1	9-O	0.46	0/3884	0.74	3/5279 (0.1%)
1	9-P	0.46	0/3884	0.74	3/5279 (0.1%)
1	9-Q	0.46	0/3884	0.74	2/5279 (0.0%)
1	9-R	0.46	0/3884	0.74	3/5279 (0.1%)
1	9-S	0.46	0/3884	0.74	2/5279 (0.0%)
1	9-T	0.46	0/3884	0.74	2/5279 (0.0%)
1	9-U	0.46	0/3884	0.74	2/5279 (0.0%)
1	9-V	0.46	0/3884	0.74	3/5279 (0.1%)
1	9-W	0.46	0/3884	0.74	3/5279 (0.1%)
1	9-X	0.46	0/3884	0.74	3/5279 (0.1%)
1	10-A	0.46	0/3884	0.71	2/5279 (0.0%)
1	10-B	0.46	0/3884	0.71	2/5279 (0.0%)
1	10-C	0.46	0/3884	0.71	2/5279 (0.0%)
1	10-D	0.46	0/3884	0.71	2/5279 (0.0%)
1	10-E	0.46	0/3884	0.71	2/5279 (0.0%)
1	10-F	0.46	0/3884	0.71	2/5279 (0.0%)
1	10-G	0.46	0/3884	0.71	2/5279 (0.0%)
1	10-H	0.46	0/3884	0.71	2/5279 (0.0%)
1	10-I	0.46	0/3884	0.71	2/5279 (0.0%)
1	10-J	0.46	0/3884	0.71	2/5279 (0.0%)
1	10-K	0.46	0/3884	0.71	2/5279 (0.0%)
1	10-L	0.46	0/3884	0.71	2/5279 (0.0%)
1	10-M	0.46	0/3884	0.71	2/5279 (0.0%)
1	10-N	0.46	0/3884	0.71	2/5279 (0.0%)
1	10-O	0.46	0/3884	0.71	2/5279 (0.0%)
1	10-P	0.46	0/3884	0.71	2/5279 (0.0%)
1	10-Q	0.46	0/3884	0.71	2/5279 (0.0%)
1	10-R	0.46	0/3884	0.71	2/5279 (0.0%)
1	10-S	0.46	0/3884	0.71	2/5279 (0.0%)
1	10-T	0.46	0/3884	0.71	2/5279 (0.0%)
1	10-U	0.46	0/3884	0.71	2/5279 (0.0%)
1	10-V	0.46	0/3884	0.71	2/5279 (0.0%)
1	10-W	0.46	0/3884	0.71	2/5279 (0.0%)
1	10-X	0.46	0/3884	0.71	2/5279 (0.0%)
All	All	0.46	0/932160	0.72	537/1266960 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-A	0	1
1	1-B	0	1
1	1-C	0	1
1	1-D	0	1
1	1-E	0	1
1	1-F	0	1
1	1-G	0	1
1	1-H	0	1
1	1-I	0	1
1	1-J	0	1
1	1-K	0	1
1	1-L	0	1
1	1-M	0	1
1	1-N	0	1
1	1-O	0	1
1	1-P	0	1
1	1-Q	0	1
1	1-R	0	1
1	1-S	0	1
1	1-T	0	1
1	1-U	0	1
1	1-V	0	1
1	1-W	0	1
1	1-X	0	1
1	2-A	0	1
1	2-B	0	1
1	2-C	0	1
1	2-D	0	1
1	2-E	0	1
1	2-F	0	1
1	2-G	0	1
1	2-H	0	1
1	2-I	0	1
1	2-J	0	1
1	2-K	0	1
1	2-L	0	1
1	2-M	0	1
1	2-N	0	1
1	2-O	0	1
1	2-P	0	1
1	2-Q	0	1
1	2-R	0	1
1	2-S	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2-T	0	1
1	2-U	0	1
1	2-V	0	1
1	2-W	0	1
1	2-X	0	1
1	3-A	0	1
1	3-B	0	1
1	3-C	0	1
1	3-D	0	1
1	3-E	0	1
1	3-F	0	1
1	3-G	0	1
1	3-H	0	1
1	3-I	0	1
1	3-J	0	1
1	3-K	0	1
1	3-L	0	1
1	3-M	0	1
1	3-N	0	1
1	3-O	0	1
1	3-P	0	1
1	3-Q	0	1
1	3-R	0	1
1	3-S	0	1
1	3-T	0	1
1	3-U	0	1
1	3-V	0	1
1	3-W	0	1
1	3-X	0	1
1	4-A	0	1
1	4-B	0	1
1	4-C	0	1
1	4-D	0	1
1	4-E	0	1
1	4-F	0	1
1	4-G	0	1
1	4-H	0	1
1	4-I	0	1
1	4-J	0	1
1	4-K	0	1
1	4-L	0	1
1	4-M	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	4-N	0	1
1	4-O	0	1
1	4-P	0	1
1	4-Q	0	1
1	4-R	0	1
1	4-S	0	1
1	4-T	0	1
1	4-U	0	1
1	4-V	0	1
1	4-W	0	1
1	4-X	0	1
1	5-A	0	1
1	5-B	0	1
1	5-C	0	1
1	5-D	0	1
1	5-E	0	1
1	5-F	0	1
1	5-G	0	1
1	5-H	0	1
1	5-I	0	1
1	5-J	0	1
1	5-K	0	1
1	5-L	0	1
1	5-M	0	1
1	5-N	0	1
1	5-O	0	1
1	5-P	0	1
1	5-Q	0	1
1	5-R	0	1
1	5-S	0	1
1	5-T	0	1
1	5-U	0	1
1	5-V	0	1
1	5-W	0	1
1	5-X	0	1
1	6-A	0	1
1	6-B	0	1
1	6-C	0	1
1	6-D	0	1
1	6-E	0	1
1	6-F	0	1
1	6-G	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	6-H	0	1
1	6-I	0	1
1	6-J	0	1
1	6-K	0	1
1	6-L	0	1
1	6-M	0	1
1	6-N	0	1
1	6-O	0	1
1	6-P	0	1
1	6-Q	0	1
1	6-R	0	1
1	6-S	0	1
1	6-T	0	1
1	6-U	0	1
1	6-V	0	1
1	6-W	0	1
1	6-X	0	1
1	7-A	0	1
1	7-B	0	1
1	7-C	0	1
1	7-D	0	1
1	7-E	0	1
1	7-F	0	1
1	7-G	0	1
1	7-H	0	1
1	7-I	0	1
1	7-J	0	1
1	7-K	0	1
1	7-L	0	1
1	7-M	0	1
1	7-N	0	1
1	7-O	0	1
1	7-P	0	1
1	7-Q	0	1
1	7-R	0	1
1	7-S	0	1
1	7-T	0	1
1	7-U	0	1
1	7-V	0	1
1	7-W	0	1
1	7-X	0	1
1	8-A	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	8-B	0	1
1	8-C	0	1
1	8-D	0	1
1	8-E	0	1
1	8-F	0	1
1	8-G	0	1
1	8-H	0	1
1	8-I	0	1
1	8-J	0	1
1	8-K	0	1
1	8-L	0	1
1	8-M	0	1
1	8-N	0	1
1	8-O	0	1
1	8-P	0	1
1	8-Q	0	1
1	8-R	0	1
1	8-S	0	1
1	8-T	0	1
1	8-U	0	1
1	8-V	0	1
1	8-W	0	1
1	8-X	0	1
1	9-A	0	1
1	9-B	0	1
1	9-C	0	1
1	9-D	0	1
1	9-E	0	1
1	9-F	0	1
1	9-G	0	1
1	9-H	0	1
1	9-I	0	1
1	9-J	0	1
1	9-K	0	1
1	9-L	0	1
1	9-M	0	1
1	9-N	0	1
1	9-O	0	1
1	9-P	0	1
1	9-Q	0	1
1	9-R	0	1
1	9-S	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	9-T	0	1
1	9-U	0	1
1	9-V	0	1
1	9-W	0	1
1	9-X	0	1
1	10-A	0	1
1	10-B	0	1
1	10-C	0	1
1	10-D	0	1
1	10-E	0	1
1	10-F	0	1
1	10-G	0	1
1	10-H	0	1
1	10-I	0	1
1	10-J	0	1
1	10-K	0	1
1	10-L	0	1
1	10-M	0	1
1	10-N	0	1
1	10-O	0	1
1	10-P	0	1
1	10-Q	0	1
1	10-R	0	1
1	10-S	0	1
1	10-T	0	1
1	10-U	0	1
1	10-V	0	1
1	10-W	0	1
1	10-X	0	1
All	All	0	240

There are no bond length outliers.

The worst 5 of 537 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-P	402	GLU	N-CA-C	6.62	128.89	111.00
1	9-B	402	GLU	N-CA-C	6.62	128.88	111.00
1	9-F	402	GLU	N-CA-C	6.62	128.88	111.00
1	9-N	402	GLU	N-CA-C	6.62	128.88	111.00
1	9-T	402	GLU	N-CA-C	6.62	128.87	111.00

There are no chirality outliers.

5 of 240 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	319	TYR	Sidechain
1	1-B	319	TYR	Sidechain
1	1-C	319	TYR	Sidechain
1	1-D	319	TYR	Sidechain
1	1-E	319	TYR	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	3778	0	3604	158	0
1	1-B	3778	0	3604	152	0
1	1-C	3778	0	3604	150	0
1	1-D	3778	0	3604	159	0
1	1-E	3778	0	3604	165	0
1	1-F	3778	0	3604	153	0
1	1-G	3778	0	3604	162	0
1	1-H	3778	0	3604	150	0
1	1-I	3778	0	3604	153	0
1	1-J	3778	0	3604	154	0
1	1-K	3778	0	3604	161	0
1	1-L	3778	0	3604	157	0
1	1-M	3778	0	3604	159	0
1	1-N	3778	0	3604	152	0
1	1-O	3778	0	3604	148	0
1	1-P	3778	0	3604	164	0
1	1-Q	3778	0	3604	164	0
1	1-R	3778	0	3604	157	0
1	1-S	3778	0	3604	153	0
1	1-T	3778	0	3604	150	0
1	1-U	3778	0	3604	152	0
1	1-V	3778	0	3604	151	0
1	1-W	3778	0	3604	155	0
1	1-X	3778	0	3604	159	0
1	2-A	3778	0	3604	142	0
1	2-B	3778	0	3604	130	0
1	2-C	3778	0	3604	133	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2-D	3778	0	3604	142	0
1	2-E	3778	0	3604	152	0
1	2-F	3778	0	3604	149	0
1	2-G	3778	0	3604	144	0
1	2-H	3778	0	3604	132	0
1	2-I	3778	0	3604	135	0
1	2-J	3778	0	3604	140	0
1	2-K	3778	0	3604	143	0
1	2-L	3778	0	3604	150	0
1	2-M	3778	0	3604	136	0
1	2-N	3778	0	3604	129	0
1	2-O	3778	0	3604	140	0
1	2-P	3778	0	3604	147	0
1	2-Q	3778	0	3604	145	0
1	2-R	3778	0	3604	141	0
1	2-S	3778	0	3604	132	0
1	2-T	3778	0	3604	132	0
1	2-U	3778	0	3604	136	0
1	2-V	3778	0	3604	146	0
1	2-W	3778	0	3604	130	0
1	2-X	3778	0	3604	136	0
1	3-A	3778	0	3604	149	0
1	3-B	3778	0	3604	157	0
1	3-C	3778	0	3604	150	0
1	3-D	3778	0	3604	153	0
1	3-E	3778	0	3604	150	0
1	3-F	3778	0	3604	155	0
1	3-G	3778	0	3604	153	0
1	3-H	3778	0	3604	147	0
1	3-I	3778	0	3604	134	0
1	3-J	3778	0	3604	147	0
1	3-K	3778	0	3604	158	0
1	3-L	3778	0	3604	141	0
1	3-M	3778	0	3604	148	0
1	3-N	3778	0	3604	152	0
1	3-O	3778	0	3604	154	0
1	3-P	3778	0	3604	161	0
1	3-Q	3778	0	3604	140	0
1	3-R	3778	0	3604	149	0
1	3-S	3778	0	3604	152	0
1	3-T	3778	0	3604	144	0
1	3-U	3778	0	3602	135	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3-V	3778	0	3604	152	0
1	3-W	3778	0	3604	146	0
1	3-X	3778	0	3604	138	0
1	4-A	3778	0	3604	165	0
1	4-B	3778	0	3604	149	0
1	4-C	3778	0	3604	146	0
1	4-D	3778	0	3604	165	0
1	4-E	3778	0	3604	159	0
1	4-F	3778	0	3604	157	0
1	4-G	3778	0	3604	175	0
1	4-H	3778	0	3604	160	0
1	4-I	3778	0	3604	145	0
1	4-J	3778	0	3604	158	0
1	4-K	3778	0	3604	167	0
1	4-L	3778	0	3604	159	0
1	4-M	3778	0	3604	151	0
1	4-N	3778	0	3604	152	0
1	4-O	3778	0	3604	150	0
1	4-P	3778	0	3604	171	0
1	4-Q	3778	0	3604	167	0
1	4-R	3778	0	3604	148	0
1	4-S	3778	0	3602	153	0
1	4-T	3778	0	3604	154	0
1	4-U	3778	0	3604	148	0
1	4-V	3778	0	3604	149	0
1	4-W	3778	0	3604	159	0
1	4-X	3778	0	3604	145	0
1	5-A	3778	0	3604	187	0
1	5-B	3778	0	3604	187	0
1	5-C	3778	0	3604	173	0
1	5-D	3778	0	3604	191	0
1	5-E	3778	0	3604	200	0
1	5-F	3778	0	3604	183	0
1	5-G	3778	0	3604	194	0
1	5-H	3778	0	3604	173	0
1	5-I	3778	0	3604	177	0
1	5-J	3778	0	3604	185	0
1	5-K	3778	0	3604	195	0
1	5-L	3778	0	3604	193	0
1	5-M	3778	0	3604	168	0
1	5-N	3778	0	3604	191	0
1	5-O	3778	0	3604	190	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5-P	3778	0	3604	202	0
1	5-Q	3778	0	3604	194	0
1	5-R	3778	0	3604	173	0
1	5-S	3778	0	3604	181	0
1	5-T	3778	0	3604	185	0
1	5-U	3778	0	3604	172	0
1	5-V	3778	0	3604	183	0
1	5-W	3778	0	3604	188	0
1	5-X	3778	0	3604	174	0
1	6-A	3778	0	3604	196	0
1	6-B	3778	0	3604	183	0
1	6-C	3778	0	3604	182	0
1	6-D	3778	0	3604	198	0
1	6-E	3778	0	3604	212	0
1	6-F	3778	0	3604	197	0
1	6-G	3778	0	3604	196	0
1	6-H	3778	0	3604	184	0
1	6-I	3778	0	3604	179	0
1	6-J	3778	0	3604	188	0
1	6-K	3778	0	3604	198	0
1	6-L	3778	0	3604	192	0
1	6-M	3778	0	3604	189	0
1	6-N	3778	0	3604	186	0
1	6-O	3778	0	3604	189	0
1	6-P	3778	0	3604	211	0
1	6-Q	3778	0	3604	196	0
1	6-R	3778	0	3604	193	0
1	6-S	3778	0	3604	182	0
1	6-T	3778	0	3604	184	0
1	6-U	3778	0	3604	202	0
1	6-V	3778	0	3604	188	0
1	6-W	3778	0	3604	187	0
1	6-X	3778	0	3604	188	0
1	7-A	3778	0	3604	146	0
1	7-B	3778	0	3604	143	0
1	7-C	3778	0	3604	134	0
1	7-D	3778	0	3604	157	0
1	7-E	3778	0	3604	160	0
1	7-F	3778	0	3604	149	0
1	7-G	3778	0	3604	147	0
1	7-H	3778	0	3604	138	0
1	7-I	3778	0	3604	138	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	7-J	3778	0	3604	137	0
1	7-K	3778	0	3604	152	0
1	7-L	3778	0	3604	144	0
1	7-M	3778	0	3604	141	0
1	7-N	3778	0	3604	148	0
1	7-O	3778	0	3604	146	0
1	7-P	3778	0	3604	161	0
1	7-Q	3778	0	3604	148	0
1	7-R	3778	0	3604	141	0
1	7-S	3778	0	3601	143	0
1	7-T	3778	0	3604	143	0
1	7-U	3778	0	3604	150	0
1	7-V	3778	0	3604	142	0
1	7-W	3778	0	3604	148	0
1	7-X	3778	0	3604	133	0
1	8-A	3778	0	3604	162	0
1	8-B	3778	0	3604	154	0
1	8-C	3778	0	3604	153	0
1	8-D	3778	0	3604	182	0
1	8-E	3778	0	3604	201	0
1	8-F	3778	0	3604	166	0
1	8-G	3778	0	3604	174	0
1	8-H	3778	0	3604	152	0
1	8-I	3778	0	3604	154	0
1	8-J	3778	0	3604	171	0
1	8-K	3778	0	3604	180	0
1	8-L	3778	0	3604	168	0
1	8-M	3778	0	3604	159	0
1	8-N	3778	0	3604	154	0
1	8-O	3778	0	3604	154	0
1	8-P	3778	0	3604	181	0
1	8-Q	3778	0	3604	175	0
1	8-R	3778	0	3604	163	0
1	8-S	3778	0	3604	159	0
1	8-T	3778	0	3604	150	0
1	8-U	3778	0	3604	169	0
1	8-V	3778	0	3604	160	0
1	8-W	3778	0	3604	163	0
1	8-X	3778	0	3604	154	0
1	9-A	3778	0	3604	144	0
1	9-B	3778	0	3604	145	0
1	9-C	3778	0	3604	141	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	9-D	3778	0	3604	162	0
1	9-E	3778	0	3604	161	0
1	9-F	3778	0	3604	159	0
1	9-G	3778	0	3604	162	0
1	9-H	3778	0	3604	137	0
1	9-I	3778	0	3604	143	0
1	9-J	3778	0	3604	154	0
1	9-K	3778	0	3604	152	0
1	9-L	3778	0	3604	157	0
1	9-M	3778	0	3604	138	0
1	9-N	3778	0	3604	146	0
1	9-O	3778	0	3604	144	0
1	9-P	3778	0	3604	169	0
1	9-Q	3778	0	3604	157	0
1	9-R	3778	0	3604	149	0
1	9-S	3778	0	3602	162	0
1	9-T	3778	0	3604	144	0
1	9-U	3778	0	3604	145	0
1	9-V	3778	0	3604	152	0
1	9-W	3778	0	3604	148	0
1	9-X	3778	0	3604	147	0
1	10-A	3778	0	3604	156	0
1	10-B	3778	0	3604	159	0
1	10-C	3778	0	3604	153	0
1	10-D	3778	0	3604	165	0
1	10-E	3778	0	3604	169	0
1	10-F	3778	0	3604	169	0
1	10-G	3778	0	3604	167	0
1	10-H	3778	0	3604	159	0
1	10-I	3778	0	3604	154	0
1	10-J	3778	0	3604	157	0
1	10-K	3778	0	3604	178	0
1	10-L	3778	0	3604	172	0
1	10-M	3778	0	3604	149	0
1	10-N	3778	0	3604	165	0
1	10-O	3778	0	3604	157	0
1	10-P	3778	0	3604	168	0
1	10-Q	3778	0	3604	162	0
1	10-R	3778	0	3604	159	0
1	10-S	3778	0	3604	157	0
1	10-T	3778	0	3604	161	0
1	10-U	3778	0	3604	154	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	10-V	3778	0	3604	156	0
1	10-W	3778	0	3604	163	0
1	10-X	3778	0	3604	152	0
2	1-A	1	0	0	0	0
2	1-B	1	0	0	0	0
2	1-C	1	0	0	0	0
2	1-D	1	0	0	0	0
2	1-E	1	0	0	0	0
2	1-F	1	0	0	0	0
2	1-G	1	0	0	0	0
2	1-H	1	0	0	0	0
2	1-I	1	0	0	0	0
2	1-J	1	0	0	0	0
2	1-K	1	0	0	0	0
2	1-L	1	0	0	0	0
2	1-M	1	0	0	0	0
2	1-N	1	0	0	0	0
2	1-O	1	0	0	0	0
2	1-P	1	0	0	0	0
2	1-Q	1	0	0	0	0
2	1-R	1	0	0	0	0
2	1-S	1	0	0	0	0
2	1-T	1	0	0	0	0
2	1-U	1	0	0	0	0
2	1-V	1	0	0	0	0
2	1-W	1	0	0	0	0
2	1-X	1	0	0	0	0
2	2-A	1	0	0	0	0
2	2-B	1	0	0	0	0
2	2-C	1	0	0	0	0
2	2-D	1	0	0	0	0
2	2-E	1	0	0	0	0
2	2-F	1	0	0	0	0
2	2-G	1	0	0	0	0
2	2-H	1	0	0	0	0
2	2-I	1	0	0	0	0
2	2-J	1	0	0	0	0
2	2-K	1	0	0	0	0
2	2-L	1	0	0	0	0
2	2-M	1	0	0	0	0
2	2-N	1	0	0	0	0
2	2-O	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2-P	1	0	0	0	0
2	2-Q	1	0	0	0	0
2	2-R	1	0	0	0	0
2	2-S	1	0	0	0	0
2	2-T	1	0	0	0	0
2	2-U	1	0	0	0	0
2	2-V	1	0	0	0	0
2	2-W	1	0	0	0	0
2	2-X	1	0	0	0	0
2	3-A	1	0	0	0	0
2	3-B	1	0	0	0	0
2	3-C	1	0	0	0	0
2	3-D	1	0	0	0	0
2	3-E	1	0	0	0	0
2	3-F	1	0	0	0	0
2	3-G	1	0	0	0	0
2	3-H	1	0	0	0	0
2	3-I	1	0	0	0	0
2	3-J	1	0	0	0	0
2	3-K	1	0	0	0	0
2	3-L	1	0	0	0	0
2	3-M	1	0	0	0	0
2	3-N	1	0	0	0	0
2	3-O	1	0	0	0	0
2	3-P	1	0	0	0	0
2	3-Q	1	0	0	0	0
2	3-R	1	0	0	0	0
2	3-S	1	0	0	0	0
2	3-T	1	0	0	0	0
2	3-U	1	0	0	0	0
2	3-V	1	0	0	0	0
2	3-W	1	0	0	0	0
2	3-X	1	0	0	0	0
2	4-A	1	0	0	0	0
2	4-B	1	0	0	0	0
2	4-C	1	0	0	0	0
2	4-D	1	0	0	0	0
2	4-E	1	0	0	0	0
2	4-F	1	0	0	0	0
2	4-G	1	0	0	0	0
2	4-H	1	0	0	0	0
2	4-I	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	4-J	1	0	0	0	0
2	4-K	1	0	0	0	0
2	4-L	1	0	0	0	0
2	4-M	1	0	0	0	0
2	4-N	1	0	0	0	0
2	4-O	1	0	0	0	0
2	4-P	1	0	0	0	0
2	4-Q	1	0	0	0	0
2	4-R	1	0	0	0	0
2	4-S	1	0	0	0	0
2	4-T	1	0	0	0	0
2	4-U	1	0	0	0	0
2	4-V	1	0	0	0	0
2	4-W	1	0	0	0	0
2	4-X	1	0	0	0	0
2	5-A	1	0	0	0	0
2	5-B	1	0	0	0	0
2	5-C	1	0	0	0	0
2	5-D	1	0	0	0	0
2	5-E	1	0	0	0	0
2	5-F	1	0	0	0	0
2	5-G	1	0	0	0	0
2	5-H	1	0	0	0	0
2	5-I	1	0	0	0	0
2	5-J	1	0	0	0	0
2	5-K	1	0	0	0	0
2	5-L	1	0	0	0	0
2	5-M	1	0	0	0	0
2	5-N	1	0	0	0	0
2	5-O	1	0	0	0	0
2	5-P	1	0	0	0	0
2	5-Q	1	0	0	0	0
2	5-R	1	0	0	0	0
2	5-S	1	0	0	0	0
2	5-T	1	0	0	0	0
2	5-U	1	0	0	0	0
2	5-V	1	0	0	0	0
2	5-W	1	0	0	0	0
2	5-X	1	0	0	0	0
2	6-A	1	0	0	0	0
2	6-B	1	0	0	0	0
2	6-C	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	6-D	1	0	0	0	0
2	6-E	1	0	0	0	0
2	6-F	1	0	0	0	0
2	6-G	1	0	0	0	0
2	6-H	1	0	0	0	0
2	6-I	1	0	0	0	0
2	6-J	1	0	0	0	0
2	6-K	1	0	0	0	0
2	6-L	1	0	0	0	0
2	6-M	1	0	0	0	0
2	6-N	1	0	0	0	0
2	6-O	1	0	0	0	0
2	6-P	1	0	0	0	0
2	6-Q	1	0	0	0	0
2	6-R	1	0	0	0	0
2	6-S	1	0	0	0	0
2	6-T	1	0	0	0	0
2	6-U	1	0	0	0	0
2	6-V	1	0	0	0	0
2	6-W	1	0	0	0	0
2	6-X	1	0	0	0	0
2	7-A	1	0	0	0	0
2	7-B	1	0	0	0	0
2	7-C	1	0	0	0	0
2	7-D	1	0	0	0	0
2	7-E	1	0	0	0	0
2	7-F	1	0	0	0	0
2	7-G	1	0	0	0	0
2	7-H	1	0	0	0	0
2	7-I	1	0	0	0	0
2	7-J	1	0	0	0	0
2	7-K	1	0	0	0	0
2	7-L	1	0	0	0	0
2	7-M	1	0	0	0	0
2	7-N	1	0	0	0	0
2	7-O	1	0	0	0	0
2	7-P	1	0	0	0	0
2	7-Q	1	0	0	0	0
2	7-R	1	0	0	0	0
2	7-S	1	0	0	0	0
2	7-T	1	0	0	0	0
2	7-U	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	7-V	1	0	0	0	0
2	7-W	1	0	0	0	0
2	7-X	1	0	0	0	0
2	8-A	1	0	0	0	0
2	8-B	1	0	0	0	0
2	8-C	1	0	0	0	0
2	8-D	1	0	0	0	0
2	8-E	1	0	0	0	0
2	8-F	1	0	0	0	0
2	8-G	1	0	0	0	0
2	8-H	1	0	0	0	0
2	8-I	1	0	0	0	0
2	8-J	1	0	0	0	0
2	8-K	1	0	0	0	0
2	8-L	1	0	0	0	0
2	8-M	1	0	0	0	0
2	8-N	1	0	0	0	0
2	8-O	1	0	0	0	0
2	8-P	1	0	0	0	0
2	8-Q	1	0	0	0	0
2	8-R	1	0	0	0	0
2	8-S	1	0	0	0	0
2	8-T	1	0	0	0	0
2	8-U	1	0	0	0	0
2	8-V	1	0	0	0	0
2	8-W	1	0	0	0	0
2	8-X	1	0	0	0	0
2	9-A	1	0	0	0	0
2	9-B	1	0	0	0	0
2	9-C	1	0	0	0	0
2	9-D	1	0	0	0	0
2	9-E	1	0	0	0	0
2	9-F	1	0	0	0	0
2	9-G	1	0	0	0	0
2	9-H	1	0	0	0	0
2	9-I	1	0	0	0	0
2	9-J	1	0	0	0	0
2	9-K	1	0	0	0	0
2	9-L	1	0	0	0	0
2	9-M	1	0	0	0	0
2	9-N	1	0	0	0	0
2	9-O	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	9-P	1	0	0	0	0
2	9-Q	1	0	0	0	0
2	9-R	1	0	0	0	0
2	9-S	1	0	0	0	0
2	9-T	1	0	0	0	0
2	9-U	1	0	0	0	0
2	9-V	1	0	0	0	0
2	9-W	1	0	0	0	0
2	9-X	1	0	0	0	0
2	10-A	1	0	0	0	0
2	10-B	1	0	0	0	0
2	10-C	1	0	0	0	0
2	10-D	1	0	0	0	0
2	10-E	1	0	0	0	0
2	10-F	1	0	0	0	0
2	10-G	1	0	0	0	0
2	10-H	1	0	0	0	0
2	10-I	1	0	0	0	0
2	10-J	1	0	0	0	0
2	10-K	1	0	0	0	0
2	10-L	1	0	0	0	0
2	10-M	1	0	0	0	0
2	10-N	1	0	0	0	0
2	10-O	1	0	0	0	0
2	10-P	1	0	0	0	0
2	10-Q	1	0	0	0	0
2	10-R	1	0	0	0	0
2	10-S	1	0	0	0	0
2	10-T	1	0	0	0	0
2	10-U	1	0	0	0	0
2	10-V	1	0	0	0	0
2	10-W	1	0	0	0	0
2	10-X	1	0	0	0	0
3	1-A	23	0	10	4	0
3	1-B	23	0	10	4	0
3	1-C	23	0	10	4	0
3	1-D	23	0	10	4	0
3	1-E	23	0	10	4	0
3	1-F	23	0	10	4	0
3	1-G	23	0	10	4	0
3	1-H	23	0	10	4	0
3	1-I	23	0	10	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	1-J	23	0	10	4	0
3	1-K	23	0	10	5	0
3	1-L	23	0	10	4	0
3	1-M	23	0	10	4	0
3	1-N	23	0	10	4	0
3	1-O	23	0	10	4	0
3	1-P	23	0	10	4	0
3	1-Q	23	0	10	4	0
3	1-R	23	0	10	4	0
3	1-S	23	0	10	4	0
3	1-T	23	0	10	4	0
3	1-U	23	0	10	4	0
3	1-V	23	0	10	4	0
3	1-W	23	0	10	4	0
3	1-X	23	0	10	4	0
3	2-A	23	0	10	7	0
3	2-B	23	0	10	6	0
3	2-C	23	0	10	7	0
3	2-D	23	0	10	7	0
3	2-E	23	0	10	7	0
3	2-F	23	0	10	7	0
3	2-G	23	0	10	7	0
3	2-H	23	0	10	7	0
3	2-I	23	0	10	7	0
3	2-J	23	0	10	6	0
3	2-K	23	0	10	7	0
3	2-L	23	0	10	7	0
3	2-M	23	0	10	7	0
3	2-N	23	0	10	6	0
3	2-O	23	0	10	7	0
3	2-P	23	0	10	7	0
3	2-Q	23	0	10	7	0
3	2-R	23	0	10	7	0
3	2-S	23	0	10	6	0
3	2-T	23	0	10	7	0
3	2-U	23	0	10	6	0
3	2-V	23	0	10	6	0
3	2-W	23	0	10	6	0
3	2-X	23	0	10	7	0
3	3-A	23	0	10	10	0
3	3-B	23	0	10	10	0
3	3-C	23	0	10	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	3-D	23	0	10	10	0
3	3-E	23	0	10	10	0
3	3-F	23	0	10	10	0
3	3-G	23	0	10	10	0
3	3-H	23	0	10	10	0
3	3-I	23	0	10	10	0
3	3-J	23	0	10	10	0
3	3-K	23	0	10	11	0
3	3-L	23	0	10	10	0
3	3-M	23	0	10	10	0
3	3-N	23	0	10	10	0
3	3-O	23	0	10	10	0
3	3-P	23	0	10	10	0
3	3-Q	23	0	10	10	0
3	3-R	23	0	10	10	0
3	3-S	23	0	10	10	0
3	3-T	23	0	10	10	0
3	3-U	23	0	10	10	0
3	3-V	23	0	10	10	0
3	3-W	23	0	10	10	0
3	3-X	23	0	10	10	0
3	4-A	23	0	10	10	0
3	4-B	23	0	10	9	0
3	4-C	23	0	10	10	0
3	4-D	23	0	10	10	0
3	4-E	23	0	10	10	0
3	4-F	23	0	10	9	0
3	4-G	23	0	10	10	0
3	4-H	23	0	10	10	0
3	4-I	23	0	10	9	0
3	4-J	23	0	10	9	0
3	4-K	23	0	10	10	0
3	4-L	23	0	10	9	0
3	4-M	23	0	10	10	0
3	4-N	23	0	10	10	0
3	4-O	23	0	10	10	0
3	4-P	23	0	10	10	0
3	4-Q	23	0	10	10	0
3	4-R	23	0	10	9	0
3	4-S	23	0	10	10	0
3	4-T	23	0	10	10	0
3	4-U	23	0	10	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	4-V	23	0	10	9	0
3	4-W	23	0	10	10	0
3	4-X	23	0	10	9	0
3	5-A	23	0	10	7	0
3	5-B	23	0	10	8	0
3	5-C	23	0	10	7	0
3	5-D	23	0	10	7	0
3	5-E	23	0	10	7	0
3	5-F	23	0	10	7	0
3	5-G	23	0	10	7	0
3	5-H	23	0	10	7	0
3	5-I	23	0	10	7	0
3	5-J	23	0	10	7	0
3	5-K	23	0	10	8	0
3	5-L	23	0	10	7	0
3	5-M	23	0	10	7	0
3	5-N	23	0	10	7	0
3	5-O	23	0	10	7	0
3	5-P	23	0	10	7	0
3	5-Q	23	0	10	7	0
3	5-R	23	0	10	7	0
3	5-S	23	0	10	7	0
3	5-T	23	0	10	7	0
3	5-U	23	0	10	7	0
3	5-V	23	0	10	7	0
3	5-W	23	0	10	7	0
3	5-X	23	0	10	7	0
3	6-A	23	0	10	6	0
3	6-B	23	0	10	7	0
3	6-C	23	0	10	7	0
3	6-D	23	0	10	7	0
3	6-E	23	0	10	7	0
3	6-F	23	0	10	7	0
3	6-G	23	0	10	7	0
3	6-H	23	0	10	7	0
3	6-I	23	0	10	7	0
3	6-J	23	0	10	7	0
3	6-K	23	0	10	8	0
3	6-L	23	0	10	7	0
3	6-M	23	0	10	6	0
3	6-N	23	0	10	7	0
3	6-O	23	0	10	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	6-P	23	0	10	7	0
3	6-Q	23	0	10	7	0
3	6-R	23	0	10	7	0
3	6-S	23	0	10	7	0
3	6-T	23	0	10	7	0
3	6-U	23	0	10	7	0
3	6-V	23	0	10	7	0
3	6-W	23	0	10	7	0
3	6-X	23	0	10	7	0
3	7-A	23	0	10	5	0
3	7-B	23	0	10	5	0
3	7-C	23	0	10	5	0
3	7-D	23	0	10	5	0
3	7-E	23	0	10	5	0
3	7-F	23	0	10	5	0
3	7-G	23	0	10	5	0
3	7-H	23	0	10	5	0
3	7-I	23	0	10	5	0
3	7-J	23	0	10	5	0
3	7-K	23	0	10	6	0
3	7-L	23	0	10	5	0
3	7-M	23	0	10	5	0
3	7-N	23	0	10	5	0
3	7-O	23	0	10	5	0
3	7-P	23	0	10	5	0
3	7-Q	23	0	10	5	0
3	7-R	23	0	10	5	0
3	7-S	23	0	10	5	0
3	7-T	23	0	10	5	0
3	7-U	23	0	10	5	0
3	7-V	23	0	10	5	0
3	7-W	23	0	10	5	0
3	7-X	23	0	10	5	0
3	8-A	23	0	10	6	0
3	8-B	23	0	10	6	0
3	8-C	23	0	10	6	0
3	8-D	23	0	10	5	0
3	8-E	23	0	10	6	0
3	8-F	23	0	10	5	0
3	8-G	23	0	10	5	0
3	8-H	23	0	10	5	0
3	8-I	23	0	10	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	8-J	23	0	10	6	0
3	8-K	23	0	10	7	0
3	8-L	23	0	10	6	0
3	8-M	23	0	10	6	0
3	8-N	23	0	10	6	0
3	8-O	23	0	10	6	0
3	8-P	23	0	10	5	0
3	8-Q	23	0	10	6	0
3	8-R	23	0	10	5	0
3	8-S	23	0	10	5	0
3	8-T	23	0	10	5	0
3	8-U	23	0	10	5	0
3	8-V	23	0	10	6	0
3	8-W	23	0	10	6	0
3	8-X	23	0	10	6	0
3	9-A	23	0	10	7	0
3	9-B	23	0	10	8	0
3	9-C	23	0	10	8	0
3	9-D	23	0	10	8	0
3	9-E	23	0	10	8	0
3	9-F	23	0	10	8	0
3	9-G	23	0	10	8	0
3	9-H	23	0	10	8	0
3	9-I	23	0	10	8	0
3	9-J	23	0	10	8	0
3	9-K	23	0	10	9	0
3	9-L	23	0	10	7	0
3	9-M	23	0	10	7	0
3	9-N	23	0	10	7	0
3	9-O	23	0	10	7	0
3	9-P	23	0	10	8	0
3	9-Q	23	0	10	8	0
3	9-R	23	0	10	8	0
3	9-S	23	0	10	8	0
3	9-T	23	0	10	8	0
3	9-U	23	0	10	8	0
3	9-V	23	0	10	8	0
3	9-W	23	0	10	8	0
3	9-X	23	0	10	7	0
3	10-A	23	0	10	6	0
3	10-B	23	0	10	6	0
3	10-C	23	0	10	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	10-D	23	0	10	6	0
3	10-E	23	0	10	6	0
3	10-F	23	0	10	6	0
3	10-G	23	0	10	6	0
3	10-H	23	0	10	6	0
3	10-I	23	0	10	6	0
3	10-J	23	0	10	6	0
3	10-K	23	0	10	7	0
3	10-L	23	0	10	6	0
3	10-M	23	0	10	6	0
3	10-N	23	0	10	6	0
3	10-O	23	0	10	6	0
3	10-P	23	0	10	6	0
3	10-Q	23	0	10	6	0
3	10-R	23	0	10	6	0
3	10-S	23	0	10	6	0
3	10-T	23	0	10	6	0
3	10-U	23	0	10	5	0
3	10-V	23	0	10	6	0
3	10-W	23	0	10	6	0
3	10-X	23	0	10	6	0
4	1-A	13	0	5	5	0
4	1-B	13	0	5	5	0
4	1-C	13	0	5	5	0
4	1-D	13	0	5	5	0
4	1-E	13	0	5	5	0
4	1-F	13	0	5	5	0
4	1-G	13	0	5	5	0
4	1-H	13	0	5	5	0
4	1-I	13	0	5	5	0
4	1-J	13	0	5	5	0
4	1-K	13	0	5	5	0
4	1-L	13	0	5	5	0
4	1-M	13	0	5	5	0
4	1-N	13	0	5	5	0
4	1-O	13	0	5	5	0
4	1-P	13	0	5	5	0
4	1-Q	13	0	5	5	0
4	1-R	13	0	5	5	0
4	1-S	13	0	5	5	0
4	1-T	13	0	5	5	0
4	1-U	13	0	5	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	1-V	13	0	5	5	0
4	1-W	13	0	5	5	0
4	1-X	13	0	5	5	0
4	2-A	13	0	5	3	0
4	2-B	13	0	5	3	0
4	2-C	13	0	5	3	0
4	2-D	13	0	5	3	0
4	2-E	13	0	5	3	0
4	2-F	13	0	5	2	0
4	2-G	13	0	5	2	0
4	2-H	13	0	5	2	0
4	2-I	13	0	5	3	0
4	2-J	13	0	5	4	0
4	2-K	13	0	5	3	0
4	2-L	13	0	5	2	0
4	2-M	13	0	5	3	0
4	2-N	13	0	5	3	0
4	2-O	13	0	5	3	0
4	2-P	13	0	5	2	0
4	2-Q	13	0	5	3	0
4	2-R	13	0	5	2	0
4	2-S	13	0	5	2	0
4	2-T	13	0	5	1	0
4	2-U	13	0	5	3	0
4	2-V	13	0	5	4	0
4	2-W	13	0	5	3	0
4	2-X	13	0	5	3	0
4	3-A	13	0	5	4	0
4	3-B	13	0	5	4	0
4	3-C	13	0	5	4	0
4	3-D	13	0	5	4	0
4	3-E	13	0	5	4	0
4	3-F	13	0	5	4	0
4	3-G	13	0	5	4	0
4	3-H	13	0	5	4	0
4	3-I	13	0	5	4	0
4	3-J	13	0	5	4	0
4	3-K	13	0	5	4	0
4	3-L	13	0	5	4	0
4	3-M	13	0	5	4	0
4	3-N	13	0	5	4	0
4	3-O	13	0	5	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	3-P	13	0	5	4	0
4	3-Q	13	0	5	4	0
4	3-R	13	0	5	4	0
4	3-S	13	0	5	4	0
4	3-T	13	0	5	4	0
4	3-U	13	0	5	4	0
4	3-V	13	0	5	4	0
4	3-W	13	0	5	4	0
4	3-X	13	0	5	4	0
4	4-A	13	0	5	5	0
4	4-B	13	0	5	4	0
4	4-C	13	0	5	4	0
4	4-D	13	0	5	3	0
4	4-E	13	0	5	5	0
4	4-F	13	0	5	3	0
4	4-G	13	0	5	4	0
4	4-H	13	0	5	4	0
4	4-I	13	0	5	5	0
4	4-J	13	0	5	4	0
4	4-K	13	0	5	3	0
4	4-L	13	0	5	3	0
4	4-M	13	0	5	5	0
4	4-N	13	0	5	4	0
4	4-O	13	0	5	4	0
4	4-P	13	0	5	4	0
4	4-Q	13	0	5	5	0
4	4-R	13	0	5	3	0
4	4-S	13	0	5	4	0
4	4-T	13	0	5	4	0
4	4-U	13	0	5	5	0
4	4-V	13	0	5	4	0
4	4-W	13	0	5	3	0
4	4-X	13	0	5	3	0
4	5-A	13	0	5	4	0
4	5-B	13	0	5	3	0
4	5-C	13	0	5	4	0
4	5-D	13	0	5	3	0
4	5-E	13	0	5	3	0
4	5-F	13	0	5	4	0
4	5-G	13	0	5	4	0
4	5-H	13	0	5	3	0
4	5-I	13	0	5	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	5-J	13	0	5	4	0
4	5-K	13	0	5	4	0
4	5-L	13	0	5	4	0
4	5-M	13	0	5	3	0
4	5-N	13	0	5	3	0
4	5-O	13	0	5	3	0
4	5-P	13	0	5	3	0
4	5-Q	13	0	5	3	0
4	5-R	13	0	5	4	0
4	5-S	13	0	5	4	0
4	5-T	13	0	5	3	0
4	5-U	13	0	5	4	0
4	5-V	13	0	5	3	0
4	5-W	13	0	5	4	0
4	5-X	13	0	5	4	0
4	6-A	13	0	5	3	0
4	6-B	13	0	5	2	0
4	6-C	13	0	5	3	0
4	6-D	13	0	5	2	0
4	6-E	13	0	5	3	0
4	6-F	13	0	5	2	0
4	6-G	13	0	5	2	0
4	6-H	13	0	5	2	0
4	6-I	13	0	5	3	0
4	6-J	13	0	5	3	0
4	6-K	13	0	5	3	0
4	6-L	13	0	5	3	0
4	6-M	13	0	5	3	0
4	6-N	13	0	5	2	0
4	6-O	13	0	5	3	0
4	6-P	13	0	5	2	0
4	6-Q	13	0	5	3	0
4	6-R	13	0	5	2	0
4	6-S	13	0	5	2	0
4	6-T	13	0	5	2	0
4	6-U	13	0	5	3	0
4	6-V	13	0	5	3	0
4	6-W	13	0	5	3	0
4	6-X	13	0	5	3	0
4	7-A	13	0	5	6	0
4	7-B	13	0	5	5	0
4	7-C	13	0	5	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	7-D	13	0	5	6	0
4	7-E	13	0	5	6	0
4	7-F	13	0	5	6	0
4	7-G	13	0	5	6	0
4	7-H	13	0	5	6	0
4	7-I	13	0	5	6	0
4	7-J	13	0	5	6	0
4	7-K	13	0	5	6	0
4	7-L	13	0	5	5	0
4	7-M	13	0	5	6	0
4	7-N	13	0	5	5	0
4	7-O	13	0	5	6	0
4	7-P	13	0	5	6	0
4	7-Q	13	0	5	6	0
4	7-R	13	0	5	6	0
4	7-S	13	0	5	6	0
4	7-T	13	0	5	6	0
4	7-U	13	0	5	6	0
4	7-V	13	0	5	6	0
4	7-W	13	0	5	6	0
4	7-X	13	0	5	5	0
4	8-A	13	0	5	4	0
4	8-B	13	0	5	4	0
4	8-C	13	0	5	4	0
4	8-D	13	0	5	4	0
4	8-E	13	0	5	4	0
4	8-F	13	0	5	4	0
4	8-G	13	0	5	4	0
4	8-H	13	0	5	4	0
4	8-I	13	0	5	4	0
4	8-J	13	0	5	4	0
4	8-K	13	0	5	4	0
4	8-L	13	0	5	4	0
4	8-M	13	0	5	4	0
4	8-N	13	0	5	4	0
4	8-O	13	0	5	4	0
4	8-P	13	0	5	4	0
4	8-Q	13	0	5	4	0
4	8-R	13	0	5	4	0
4	8-S	13	0	5	4	0
4	8-T	13	0	5	4	0
4	8-U	13	0	5	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	8-V	13	0	5	4	0
4	8-W	13	0	5	4	0
4	8-X	13	0	5	4	0
4	9-A	13	0	5	3	0
4	9-B	13	0	5	3	0
4	9-C	13	0	5	3	0
4	9-D	13	0	5	3	0
4	9-E	13	0	5	1	0
4	9-F	13	0	5	3	0
4	9-G	13	0	5	3	0
4	9-H	13	0	5	3	0
4	9-I	13	0	5	3	0
4	9-J	13	0	5	2	0
4	9-K	13	0	5	3	0
4	9-L	13	0	5	1	0
4	9-M	13	0	5	2	0
4	9-N	13	0	5	3	0
4	9-O	13	0	5	3	0
4	9-P	13	0	5	3	0
4	9-Q	13	0	5	1	0
4	9-R	13	0	5	3	0
4	9-S	13	0	5	3	0
4	9-T	13	0	5	3	0
4	9-U	13	0	5	3	0
4	9-V	13	0	5	2	0
4	9-W	13	0	5	3	0
4	9-X	13	0	5	1	0
4	10-A	13	0	5	5	0
4	10-B	13	0	5	4	0
4	10-C	13	0	5	4	0
4	10-D	13	0	5	4	0
4	10-E	13	0	5	3	0
4	10-F	13	0	5	4	0
4	10-G	13	0	5	4	0
4	10-H	13	0	5	3	0
4	10-I	13	0	5	5	0
4	10-J	13	0	5	4	0
4	10-K	13	0	5	4	0
4	10-L	13	0	5	3	0
4	10-M	13	0	5	4	0
4	10-N	13	0	5	4	0
4	10-O	13	0	5	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	10-P	13	0	5	4	0
4	10-Q	13	0	5	3	0
4	10-R	13	0	5	3	0
4	10-S	13	0	5	3	0
4	10-T	13	0	5	5	0
4	10-U	13	0	5	5	0
4	10-V	13	0	5	4	0
4	10-W	13	0	5	4	0
4	10-X	13	0	5	3	0
5	1-A	261	0	0	6	0
5	1-B	264	0	0	5	0
5	1-C	261	0	0	5	0
5	1-D	260	0	0	5	0
5	1-E	261	0	0	4	0
5	1-F	262	0	0	5	0
5	1-G	265	0	0	5	0
5	1-H	262	0	0	5	0
5	1-I	265	0	0	5	0
5	1-J	262	0	0	4	0
5	1-K	272	0	0	6	0
5	1-L	261	0	0	5	0
5	1-M	261	0	0	6	0
5	1-N	263	0	0	7	0
5	1-O	263	0	0	5	0
5	1-P	261	0	0	6	0
5	1-Q	260	0	0	4	0
5	1-R	261	0	0	5	0
5	1-S	265	0	0	5	0
5	1-T	261	0	0	5	0
5	1-U	263	0	0	5	0
5	1-V	265	0	0	4	0
5	1-W	269	0	0	5	0
5	1-X	264	0	0	6	0
5	2-A	262	0	0	7	0
5	2-B	261	0	0	6	0
5	2-C	264	0	0	5	0
5	2-D	269	0	0	6	0
5	2-E	254	0	0	4	0
5	2-F	263	0	0	6	0
5	2-G	262	0	0	4	0
5	2-H	263	0	0	6	0
5	2-I	265	0	0	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	2-J	258	0	0	5	0
5	2-K	271	0	0	6	0
5	2-L	264	0	0	7	0
5	2-M	264	0	0	8	0
5	2-N	261	0	0	6	0
5	2-O	267	0	0	5	0
5	2-P	264	0	0	5	0
5	2-Q	257	0	0	5	0
5	2-R	265	0	0	4	0
5	2-S	259	0	0	6	0
5	2-T	259	0	0	6	0
5	2-U	267	0	0	5	0
5	2-V	260	0	0	5	0
5	2-W	266	0	0	7	0
5	2-X	267	0	0	6	0
5	3-A	261	0	0	2	0
5	3-B	263	0	0	3	0
5	3-C	265	0	0	2	0
5	3-D	260	0	0	4	0
5	3-E	257	0	0	2	0
5	3-F	272	0	0	3	0
5	3-G	257	0	0	2	0
5	3-H	261	0	0	3	0
5	3-I	266	0	0	1	0
5	3-J	260	0	0	2	0
5	3-K	268	0	0	3	0
5	3-L	266	0	0	2	0
5	3-M	259	0	0	3	0
5	3-N	263	0	0	2	0
5	3-O	265	0	0	2	0
5	3-P	260	0	0	3	0
5	3-Q	259	0	0	2	0
5	3-R	268	0	0	3	0
5	3-S	264	0	0	2	0
5	3-T	262	0	0	2	0
5	3-U	267	0	0	1	0
5	3-V	258	0	0	2	0
5	3-W	266	0	0	2	0
5	3-X	265	0	0	1	0
5	4-A	263	0	0	11	0
5	4-B	262	0	0	12	0
5	4-C	261	0	0	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	4-D	263	0	0	9	0
5	4-E	263	0	0	11	0
5	4-F	264	0	0	14	0
5	4-G	261	0	0	11	0
5	4-H	266	0	0	13	0
5	4-I	263	0	0	11	0
5	4-J	260	0	0	9	0
5	4-K	267	0	0	12	0
5	4-L	263	0	0	12	0
5	4-M	264	0	0	12	0
5	4-N	263	0	0	12	0
5	4-O	263	0	0	12	0
5	4-P	259	0	0	10	0
5	4-Q	264	0	0	13	0
5	4-R	263	0	0	12	0
5	4-S	260	0	0	12	0
5	4-T	262	0	0	13	0
5	4-U	264	0	0	10	0
5	4-V	266	0	0	9	0
5	4-W	263	0	0	13	0
5	4-X	265	0	0	11	0
5	5-A	261	0	0	7	0
5	5-B	261	0	0	9	0
5	5-C	263	0	0	7	0
5	5-D	262	0	0	11	0
5	5-E	259	0	0	10	0
5	5-F	266	0	0	7	0
5	5-G	263	0	0	8	0
5	5-H	270	0	0	9	0
5	5-I	260	0	0	7	0
5	5-J	263	0	0	8	0
5	5-K	268	0	0	10	0
5	5-L	260	0	0	9	0
5	5-M	264	0	0	7	0
5	5-N	265	0	0	7	0
5	5-O	267	0	0	8	0
5	5-P	262	0	0	9	0
5	5-Q	261	0	0	7	0
5	5-R	265	0	0	9	0
5	5-S	263	0	0	7	0
5	5-T	258	0	0	8	0
5	5-U	263	0	0	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	5-V	261	0	0	9	0
5	5-W	262	0	0	6	0
5	5-X	265	0	0	8	0
5	6-A	257	0	0	4	0
5	6-B	265	0	0	6	0
5	6-C	262	0	0	4	0
5	6-D	265	0	0	6	0
5	6-E	262	0	0	4	0
5	6-F	263	0	0	7	0
5	6-G	267	0	0	7	0
5	6-H	263	0	0	5	0
5	6-I	263	0	0	4	0
5	6-J	259	0	0	4	0
5	6-K	270	0	0	7	0
5	6-L	260	0	0	5	0
5	6-M	262	0	0	4	0
5	6-N	260	0	0	4	0
5	6-O	265	0	0	5	0
5	6-P	262	0	0	9	0
5	6-Q	260	0	0	4	0
5	6-R	266	0	0	5	0
5	6-S	266	0	0	5	0
5	6-T	257	0	0	4	0
5	6-U	265	0	0	5	0
5	6-V	265	0	0	4	0
5	6-W	264	0	0	4	0
5	6-X	264	0	0	4	0
5	7-A	265	0	0	2	0
5	7-B	264	0	0	3	0
5	7-C	262	0	0	1	0
5	7-D	261	0	0	4	0
5	7-E	265	0	0	1	0
5	7-F	262	0	0	2	0
5	7-G	259	0	0	2	0
5	7-H	262	0	0	2	0
5	7-I	261	0	0	2	0
5	7-J	266	0	0	1	0
5	7-K	263	0	0	2	0
5	7-L	266	0	0	2	0
5	7-M	260	0	0	3	0
5	7-N	266	0	0	3	0
5	7-O	262	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	7-P	261	0	0	4	0
5	7-Q	264	0	0	2	0
5	7-R	264	0	0	3	0
5	7-S	263	0	0	2	0
5	7-T	263	0	0	2	0
5	7-U	262	0	0	1	0
5	7-V	265	0	0	1	0
5	7-W	265	0	0	3	0
5	7-X	261	0	0	2	0
5	8-A	259	0	0	3	0
5	8-B	264	0	0	3	0
5	8-C	263	0	0	3	0
5	8-D	265	0	0	6	0
5	8-E	257	0	0	4	0
5	8-F	268	0	0	4	0
5	8-G	265	0	0	4	0
5	8-H	261	0	0	3	0
5	8-I	265	0	0	4	0
5	8-J	263	0	0	4	0
5	8-K	264	0	0	4	0
5	8-L	262	0	0	5	0
5	8-M	260	0	0	3	0
5	8-N	263	0	0	3	0
5	8-O	265	0	0	4	0
5	8-P	263	0	0	4	0
5	8-Q	257	0	0	3	0
5	8-R	265	0	0	5	0
5	8-S	269	0	0	3	0
5	8-T	259	0	0	2	0
5	8-U	263	0	0	3	0
5	8-V	264	0	0	4	0
5	8-W	263	0	0	3	0
5	8-X	265	0	0	3	0
5	9-A	265	0	0	8	0
5	9-B	258	0	0	11	0
5	9-C	261	0	0	9	0
5	9-D	266	0	0	11	0
5	9-E	262	0	0	9	0
5	9-F	262	0	0	10	0
5	9-G	263	0	0	11	0
5	9-H	268	0	0	9	0
5	9-I	262	0	0	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	9-J	260	0	0	8	0
5	9-K	269	0	0	10	0
5	9-L	260	0	0	11	0
5	9-M	265	0	0	8	0
5	9-N	261	0	0	8	0
5	9-O	263	0	0	10	0
5	9-P	265	0	0	10	0
5	9-Q	263	0	0	8	0
5	9-R	264	0	0	11	0
5	9-S	259	0	0	8	0
5	9-T	265	0	0	8	0
5	9-U	265	0	0	9	0
5	9-V	259	0	0	9	0
5	9-W	261	0	0	8	0
5	9-X	266	0	0	9	0
5	10-A	262	0	0	4	0
5	10-B	263	0	0	5	0
5	10-C	262	0	0	5	0
5	10-D	262	0	0	6	0
5	10-E	257	0	0	5	0
5	10-F	261	0	0	9	0
5	10-G	264	0	0	5	0
5	10-H	264	0	0	5	0
5	10-I	263	0	0	4	0
5	10-J	264	0	0	4	0
5	10-K	271	0	0	7	0
5	10-L	263	0	0	8	0
5	10-M	263	0	0	6	0
5	10-N	259	0	0	5	0
5	10-O	263	0	0	5	0
5	10-P	264	0	0	6	0
5	10-Q	257	0	0	5	0
5	10-R	262	0	0	6	0
5	10-S	266	0	0	6	0
5	10-T	262	0	0	5	0
5	10-U	264	0	0	5	0
5	10-V	265	0	0	4	0
5	10-W	265	0	0	6	0
5	10-X	266	0	0	6	0
All	All	978720	0	868551	34637	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 19.

The worst 5 of 34637 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:E:40:LYS:HG2	1:U:7:LYS:CE	1.19	1.55
3:L:7497:AMP:N9	3:L:7497:AMP:C1'	1.76	1.49
3:X:7521:AMP:N9	3:X:7521:AMP:C1'	1.76	1.49
3:L:7497:AMP:N9	3:L:7497:AMP:C1'	1.76	1.49
3:X:7521:AMP:N9	3:X:7521:AMP:C1'	1.76	1.49

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	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	3	3
1	1-B	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	3	3
1	1-C	475/477 (100%)	430 (90%)	28 (6%)	17 (4%)	3	3
1	1-D	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	3	3
1	1-E	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	3	3
1	1-F	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	3	3
1	1-G	475/477 (100%)	430 (90%)	28 (6%)	17 (4%)	3	3
1	1-H	475/477 (100%)	430 (90%)	28 (6%)	17 (4%)	3	3
1	1-I	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	3	3
1	1-J	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	3	3
1	1-K	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	3	3
1	1-L	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	3	3
1	1-M	475/477 (100%)	430 (90%)	28 (6%)	17 (4%)	3	3
1	1-N	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	3	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-O	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	3	3
1	1-P	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	3	3
1	1-Q	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	3	3
1	1-R	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	3	3
1	1-S	475/477 (100%)	430 (90%)	28 (6%)	17 (4%)	3	3
1	1-T	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	3	3
1	1-U	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	3	3
1	1-V	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	3	3
1	1-W	475/477 (100%)	429 (90%)	29 (6%)	17 (4%)	3	3
1	1-X	475/477 (100%)	430 (90%)	28 (6%)	17 (4%)	3	3
1	2-A	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	3	2
1	2-B	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	3	2
1	2-C	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	3	2
1	2-D	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	3	2
1	2-E	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	3	2
1	2-F	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	3	2
1	2-G	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	3	2
1	2-H	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	3	2
1	2-I	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	3	2
1	2-J	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	3	2
1	2-K	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	3	2
1	2-L	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	3	2
1	2-M	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	3	2
1	2-N	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	3	2
1	2-O	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	3	2
1	2-P	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	3	2
1	2-Q	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	3	2
1	2-R	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	3	2
1	2-S	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	3	2
1	2-T	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	3	2
1	2-U	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	3	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2-V	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	3	2
1	2-W	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	3	2
1	2-X	475/477 (100%)	429 (90%)	28 (6%)	18 (4%)	3	2
1	3-A	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	5	6
1	3-B	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	5	6
1	3-C	475/477 (100%)	432 (91%)	31 (6%)	12 (2%)	5	6
1	3-D	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	5	6
1	3-E	475/477 (100%)	432 (91%)	31 (6%)	12 (2%)	5	6
1	3-F	475/477 (100%)	432 (91%)	31 (6%)	12 (2%)	5	6
1	3-G	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	5	6
1	3-H	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	5	6
1	3-I	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	5	6
1	3-J	475/477 (100%)	432 (91%)	31 (6%)	12 (2%)	5	6
1	3-K	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	5	6
1	3-L	475/477 (100%)	432 (91%)	31 (6%)	12 (2%)	5	6
1	3-M	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	5	6
1	3-N	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	5	6
1	3-O	475/477 (100%)	432 (91%)	31 (6%)	12 (2%)	5	6
1	3-P	475/477 (100%)	432 (91%)	31 (6%)	12 (2%)	5	6
1	3-Q	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	5	6
1	3-R	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	5	6
1	3-S	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	5	6
1	3-T	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	5	6
1	3-U	475/477 (100%)	432 (91%)	31 (6%)	12 (2%)	5	6
1	3-V	475/477 (100%)	433 (91%)	30 (6%)	12 (2%)	5	6
1	3-W	475/477 (100%)	432 (91%)	31 (6%)	12 (2%)	5	6
1	3-X	475/477 (100%)	432 (91%)	31 (6%)	12 (2%)	5	6
1	4-A	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	4	4
1	4-B	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	4	4
1	4-C	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	4	4
1	4-D	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	4	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4-E	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	4	4
1	4-F	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	4	4
1	4-G	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	4	4
1	4-H	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	4	4
1	4-I	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	4	4
1	4-J	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	4	4
1	4-K	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	4	4
1	4-L	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	4	4
1	4-M	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	4	4
1	4-N	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	4	4
1	4-O	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	4	4
1	4-P	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	4	4
1	4-Q	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	4	4
1	4-R	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	4	4
1	4-S	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	4	4
1	4-T	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	4	4
1	4-U	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	4	4
1	4-V	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	4	4
1	4-W	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	4	4
1	4-X	475/477 (100%)	428 (90%)	33 (7%)	14 (3%)	4	4
1	5-A	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	8	10
1	5-B	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	8	10
1	5-C	475/477 (100%)	423 (89%)	43 (9%)	9 (2%)	8	10
1	5-D	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	8	10
1	5-E	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	8	10
1	5-F	475/477 (100%)	423 (89%)	43 (9%)	9 (2%)	8	10
1	5-G	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	8	10
1	5-H	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	8	10
1	5-I	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	8	10
1	5-J	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	8	10
1	5-K	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	8	10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5-L	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	8	10
1	5-M	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	8	10
1	5-N	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	8	10
1	5-O	475/477 (100%)	423 (89%)	43 (9%)	9 (2%)	8	10
1	5-P	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	8	10
1	5-Q	475/477 (100%)	423 (89%)	43 (9%)	9 (2%)	8	10
1	5-R	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	8	10
1	5-S	475/477 (100%)	423 (89%)	43 (9%)	9 (2%)	8	10
1	5-T	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	8	10
1	5-U	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	8	10
1	5-V	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	8	10
1	5-W	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	8	10
1	5-X	475/477 (100%)	424 (89%)	42 (9%)	9 (2%)	8	10
1	6-A	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	5	5
1	6-B	475/477 (100%)	423 (89%)	40 (8%)	12 (2%)	5	6
1	6-C	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	5	5
1	6-D	475/477 (100%)	423 (89%)	40 (8%)	12 (2%)	5	6
1	6-E	475/477 (100%)	423 (89%)	40 (8%)	12 (2%)	5	6
1	6-F	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	5	5
1	6-G	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	5	5
1	6-H	475/477 (100%)	423 (89%)	40 (8%)	12 (2%)	5	6
1	6-I	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	5	5
1	6-J	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	5	5
1	6-K	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	5	5
1	6-L	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	5	5
1	6-M	475/477 (100%)	423 (89%)	40 (8%)	12 (2%)	5	6
1	6-N	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	5	5
1	6-O	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	5	5
1	6-P	475/477 (100%)	423 (89%)	40 (8%)	12 (2%)	5	6
1	6-Q	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	5	5
1	6-R	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	5	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	6-S	475/477 (100%)	423 (89%)	40 (8%)	12 (2%)	5	6
1	6-T	475/477 (100%)	423 (89%)	40 (8%)	12 (2%)	5	6
1	6-U	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	5	5
1	6-V	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	5	5
1	6-W	475/477 (100%)	423 (89%)	39 (8%)	13 (3%)	5	5
1	6-X	475/477 (100%)	423 (89%)	40 (8%)	12 (2%)	5	6
1	7-A	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	3
1	7-B	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	3
1	7-C	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	3
1	7-D	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	3
1	7-E	475/477 (100%)	424 (89%)	35 (7%)	16 (3%)	3	3
1	7-F	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	3
1	7-G	475/477 (100%)	424 (89%)	35 (7%)	16 (3%)	3	3
1	7-H	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	3
1	7-I	475/477 (100%)	424 (89%)	35 (7%)	16 (3%)	3	3
1	7-J	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	3
1	7-K	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	3
1	7-L	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	3
1	7-M	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	3
1	7-N	475/477 (100%)	424 (89%)	35 (7%)	16 (3%)	3	3
1	7-O	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	3
1	7-P	475/477 (100%)	424 (89%)	35 (7%)	16 (3%)	3	3
1	7-Q	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	3
1	7-R	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	3
1	7-S	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	3
1	7-T	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	3
1	7-U	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	3
1	7-V	475/477 (100%)	424 (89%)	35 (7%)	16 (3%)	3	3
1	7-W	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	3
1	7-X	475/477 (100%)	423 (89%)	36 (8%)	16 (3%)	3	3
1	8-A	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	8	10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	8-B	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	8	10
1	8-C	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	8	10
1	8-D	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	8	10
1	8-E	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	8	10
1	8-F	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	8	10
1	8-G	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	8	10
1	8-H	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	8	10
1	8-I	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	8	10
1	8-J	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	8	10
1	8-K	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	8	10
1	8-L	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	8	10
1	8-M	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	8	10
1	8-N	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	8	10
1	8-O	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	8	10
1	8-P	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	8	10
1	8-Q	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	8	10
1	8-R	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	8	10
1	8-S	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	8	10
1	8-T	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	8	10
1	8-U	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	8	10
1	8-V	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	8	10
1	8-W	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	8	10
1	8-X	475/477 (100%)	434 (91%)	32 (7%)	9 (2%)	8	10
1	9-A	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	8	10
1	9-B	475/477 (100%)	425 (90%)	41 (9%)	9 (2%)	8	10
1	9-C	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	8	10
1	9-D	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	8	10
1	9-E	475/477 (100%)	425 (90%)	41 (9%)	9 (2%)	8	10
1	9-F	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	8	10
1	9-G	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	8	10
1	9-H	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	8	10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	9-I	475/477 (100%)	425 (90%)	41 (9%)	9 (2%)	8	10
1	9-J	475/477 (100%)	425 (90%)	41 (9%)	9 (2%)	8	10
1	9-K	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	8	10
1	9-L	475/477 (100%)	425 (90%)	41 (9%)	9 (2%)	8	10
1	9-M	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	8	10
1	9-N	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	8	10
1	9-O	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	8	10
1	9-P	475/477 (100%)	425 (90%)	41 (9%)	9 (2%)	8	10
1	9-Q	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	8	10
1	9-R	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	8	10
1	9-S	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	8	10
1	9-T	475/477 (100%)	425 (90%)	41 (9%)	9 (2%)	8	10
1	9-U	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	8	10
1	9-V	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	8	10
1	9-W	475/477 (100%)	425 (90%)	41 (9%)	9 (2%)	8	10
1	9-X	475/477 (100%)	426 (90%)	40 (8%)	9 (2%)	8	10
1	10-A	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	5	5
1	10-B	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	5	5
1	10-C	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	5	5
1	10-D	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	5	5
1	10-E	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	5	5
1	10-F	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	5	5
1	10-G	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	5	5
1	10-H	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	5	5
1	10-I	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	5	5
1	10-J	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	5	5
1	10-K	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	5	5
1	10-L	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	5	5
1	10-M	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	5	5
1	10-N	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	5	5
1	10-O	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	5	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	10-P	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	5	5
1	10-Q	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	5	5
1	10-R	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	5	5
1	10-S	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	5	5
1	10-T	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	5	5
1	10-U	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	5	5
1	10-V	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	5	5
1	10-W	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	5	5
1	10-X	475/477 (100%)	421 (89%)	41 (9%)	13 (3%)	5	5
All	All	114000/114480 (100%)	102469 (90%)	8420 (7%)	3111 (3%)	5	5

5 of 3111 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	57	PHE
1	1-A	59	SER
1	1-A	63	SER
1	1-A	327	GLU
1	1-B	57	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	1-A	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	1-B	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	1-C	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	1-D	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	1-E	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	1-F	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	1-G	404/404 (100%)	374 (93%)	30 (7%)	13	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-H	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	1-I	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	1-J	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	1-K	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	1-L	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	1-M	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	1-N	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	1-O	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	1-P	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	1-Q	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	1-R	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	1-S	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	1-T	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	1-U	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	1-V	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	1-W	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	1-X	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	2-A	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	2-B	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	2-C	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	2-D	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	2-E	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	2-F	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	2-G	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	2-H	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	2-I	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	2-J	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	2-K	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	2-L	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	2-M	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	2-N	404/404 (100%)	372 (92%)	32 (8%)	12	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2-O	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	2-P	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	2-Q	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	2-R	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	2-S	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	2-T	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	2-U	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	2-V	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	2-W	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	2-X	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	3-A	404/404 (100%)	377 (93%)	27 (7%)	16	26
1	3-B	404/404 (100%)	377 (93%)	27 (7%)	16	26
1	3-C	404/404 (100%)	377 (93%)	27 (7%)	16	26
1	3-D	404/404 (100%)	377 (93%)	27 (7%)	16	26
1	3-E	404/404 (100%)	377 (93%)	27 (7%)	16	26
1	3-F	404/404 (100%)	377 (93%)	27 (7%)	16	26
1	3-G	404/404 (100%)	377 (93%)	27 (7%)	16	26
1	3-H	404/404 (100%)	377 (93%)	27 (7%)	16	26
1	3-I	404/404 (100%)	377 (93%)	27 (7%)	16	26
1	3-J	404/404 (100%)	377 (93%)	27 (7%)	16	26
1	3-K	404/404 (100%)	377 (93%)	27 (7%)	16	26
1	3-L	404/404 (100%)	377 (93%)	27 (7%)	16	26
1	3-M	404/404 (100%)	377 (93%)	27 (7%)	16	26
1	3-N	404/404 (100%)	377 (93%)	27 (7%)	16	26
1	3-O	404/404 (100%)	377 (93%)	27 (7%)	16	26
1	3-P	404/404 (100%)	377 (93%)	27 (7%)	16	26
1	3-Q	404/404 (100%)	377 (93%)	27 (7%)	16	26
1	3-R	404/404 (100%)	378 (94%)	26 (6%)	17	28
1	3-S	404/404 (100%)	377 (93%)	27 (7%)	16	26
1	3-T	404/404 (100%)	377 (93%)	27 (7%)	16	26
1	3-U	404/404 (100%)	377 (93%)	27 (7%)	16	26

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3-V	404/404 (100%)	377 (93%)	27 (7%)	16	26
1	3-W	404/404 (100%)	378 (94%)	26 (6%)	17	28
1	3-X	404/404 (100%)	377 (93%)	27 (7%)	16	26
1	4-A	404/404 (100%)	379 (94%)	25 (6%)	18	29
1	4-B	404/404 (100%)	379 (94%)	25 (6%)	18	29
1	4-C	404/404 (100%)	379 (94%)	25 (6%)	18	29
1	4-D	404/404 (100%)	379 (94%)	25 (6%)	18	29
1	4-E	404/404 (100%)	379 (94%)	25 (6%)	18	29
1	4-F	404/404 (100%)	379 (94%)	25 (6%)	18	29
1	4-G	404/404 (100%)	379 (94%)	25 (6%)	18	29
1	4-H	404/404 (100%)	379 (94%)	25 (6%)	18	29
1	4-I	404/404 (100%)	379 (94%)	25 (6%)	18	29
1	4-J	404/404 (100%)	379 (94%)	25 (6%)	18	29
1	4-K	404/404 (100%)	379 (94%)	25 (6%)	18	29
1	4-L	404/404 (100%)	379 (94%)	25 (6%)	18	29
1	4-M	404/404 (100%)	379 (94%)	25 (6%)	18	29
1	4-N	404/404 (100%)	379 (94%)	25 (6%)	18	29
1	4-O	404/404 (100%)	379 (94%)	25 (6%)	18	29
1	4-P	404/404 (100%)	379 (94%)	25 (6%)	18	29
1	4-Q	404/404 (100%)	379 (94%)	25 (6%)	18	29
1	4-R	404/404 (100%)	379 (94%)	25 (6%)	18	29
1	4-S	404/404 (100%)	379 (94%)	25 (6%)	18	29
1	4-T	404/404 (100%)	379 (94%)	25 (6%)	18	29
1	4-U	404/404 (100%)	379 (94%)	25 (6%)	18	29
1	4-V	404/404 (100%)	379 (94%)	25 (6%)	18	29
1	4-W	404/404 (100%)	379 (94%)	25 (6%)	18	29
1	4-X	404/404 (100%)	379 (94%)	25 (6%)	18	29
1	5-A	404/404 (100%)	375 (93%)	29 (7%)	14	23
1	5-B	404/404 (100%)	375 (93%)	29 (7%)	14	23
1	5-C	404/404 (100%)	375 (93%)	29 (7%)	14	23
1	5-D	404/404 (100%)	375 (93%)	29 (7%)	14	23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5-E	404/404 (100%)	375 (93%)	29 (7%)	14	23
1	5-F	404/404 (100%)	375 (93%)	29 (7%)	14	23
1	5-G	404/404 (100%)	375 (93%)	29 (7%)	14	23
1	5-H	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	5-I	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	5-J	404/404 (100%)	375 (93%)	29 (7%)	14	23
1	5-K	404/404 (100%)	375 (93%)	29 (7%)	14	23
1	5-L	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	5-M	404/404 (100%)	375 (93%)	29 (7%)	14	23
1	5-N	404/404 (100%)	375 (93%)	29 (7%)	14	23
1	5-O	404/404 (100%)	375 (93%)	29 (7%)	14	23
1	5-P	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	5-Q	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	5-R	404/404 (100%)	375 (93%)	29 (7%)	14	23
1	5-S	404/404 (100%)	375 (93%)	29 (7%)	14	23
1	5-T	404/404 (100%)	375 (93%)	29 (7%)	14	23
1	5-U	404/404 (100%)	375 (93%)	29 (7%)	14	23
1	5-V	404/404 (100%)	375 (93%)	29 (7%)	14	23
1	5-W	404/404 (100%)	374 (93%)	30 (7%)	13	22
1	5-X	404/404 (100%)	375 (93%)	29 (7%)	14	23
1	6-A	404/404 (100%)	368 (91%)	36 (9%)	9	14
1	6-B	404/404 (100%)	368 (91%)	36 (9%)	9	14
1	6-C	404/404 (100%)	369 (91%)	35 (9%)	10	15
1	6-D	404/404 (100%)	368 (91%)	36 (9%)	9	14
1	6-E	404/404 (100%)	369 (91%)	35 (9%)	10	15
1	6-F	404/404 (100%)	368 (91%)	36 (9%)	9	14
1	6-G	404/404 (100%)	368 (91%)	36 (9%)	9	14
1	6-H	404/404 (100%)	368 (91%)	36 (9%)	9	14
1	6-I	404/404 (100%)	368 (91%)	36 (9%)	9	14
1	6-J	404/404 (100%)	369 (91%)	35 (9%)	10	15
1	6-K	404/404 (100%)	368 (91%)	36 (9%)	9	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	6-L	404/404 (100%)	369 (91%)	35 (9%)	10	15
1	6-M	404/404 (100%)	368 (91%)	36 (9%)	9	14
1	6-N	404/404 (100%)	369 (91%)	35 (9%)	10	15
1	6-O	404/404 (100%)	368 (91%)	36 (9%)	9	14
1	6-P	404/404 (100%)	368 (91%)	36 (9%)	9	14
1	6-Q	404/404 (100%)	368 (91%)	36 (9%)	9	14
1	6-R	404/404 (100%)	368 (91%)	36 (9%)	9	14
1	6-S	404/404 (100%)	369 (91%)	35 (9%)	10	15
1	6-T	404/404 (100%)	368 (91%)	36 (9%)	9	14
1	6-U	404/404 (100%)	369 (91%)	35 (9%)	10	15
1	6-V	404/404 (100%)	368 (91%)	36 (9%)	9	14
1	6-W	404/404 (100%)	368 (91%)	36 (9%)	9	14
1	6-X	404/404 (100%)	368 (91%)	36 (9%)	9	14
1	7-A	404/404 (100%)	373 (92%)	31 (8%)	13	20
1	7-B	404/404 (100%)	373 (92%)	31 (8%)	13	20
1	7-C	404/404 (100%)	373 (92%)	31 (8%)	13	20
1	7-D	404/404 (100%)	373 (92%)	31 (8%)	13	20
1	7-E	404/404 (100%)	373 (92%)	31 (8%)	13	20
1	7-F	404/404 (100%)	373 (92%)	31 (8%)	13	20
1	7-G	404/404 (100%)	373 (92%)	31 (8%)	13	20
1	7-H	404/404 (100%)	373 (92%)	31 (8%)	13	20
1	7-I	404/404 (100%)	373 (92%)	31 (8%)	13	20
1	7-J	404/404 (100%)	373 (92%)	31 (8%)	13	20
1	7-K	404/404 (100%)	373 (92%)	31 (8%)	13	20
1	7-L	404/404 (100%)	373 (92%)	31 (8%)	13	20
1	7-M	404/404 (100%)	373 (92%)	31 (8%)	13	20
1	7-N	404/404 (100%)	373 (92%)	31 (8%)	13	20
1	7-O	404/404 (100%)	373 (92%)	31 (8%)	13	20
1	7-P	404/404 (100%)	373 (92%)	31 (8%)	13	20
1	7-Q	404/404 (100%)	373 (92%)	31 (8%)	13	20
1	7-R	404/404 (100%)	373 (92%)	31 (8%)	13	20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	7-S	404/404 (100%)	373 (92%)	31 (8%)	13	20
1	7-T	404/404 (100%)	373 (92%)	31 (8%)	13	20
1	7-U	404/404 (100%)	373 (92%)	31 (8%)	13	20
1	7-V	404/404 (100%)	373 (92%)	31 (8%)	13	20
1	7-W	404/404 (100%)	373 (92%)	31 (8%)	13	20
1	7-X	404/404 (100%)	373 (92%)	31 (8%)	13	20
1	8-A	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	8-B	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	8-C	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	8-D	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	8-E	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	8-F	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	8-G	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	8-H	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	8-I	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	8-J	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	8-K	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	8-L	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	8-M	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	8-N	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	8-O	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	8-P	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	8-Q	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	8-R	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	8-S	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	8-T	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	8-U	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	8-V	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	8-W	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	8-X	404/404 (100%)	372 (92%)	32 (8%)	12	19
1	9-A	404/404 (100%)	370 (92%)	34 (8%)	11	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	9-B	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	9-C	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	9-D	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	9-E	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	9-F	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	9-G	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	9-H	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	9-I	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	9-J	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	9-K	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	9-L	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	9-M	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	9-N	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	9-O	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	9-P	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	9-Q	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	9-R	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	9-S	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	9-T	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	9-U	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	9-V	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	9-W	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	9-X	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	10-A	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	10-B	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	10-C	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	10-D	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	10-E	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	10-F	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	10-G	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	10-H	404/404 (100%)	370 (92%)	34 (8%)	11	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	10-I	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	10-J	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	10-K	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	10-L	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	10-M	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	10-N	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	10-O	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	10-P	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	10-Q	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	10-R	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	10-S	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	10-T	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	10-U	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	10-V	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	10-W	404/404 (100%)	370 (92%)	34 (8%)	11	16
1	10-X	404/404 (100%)	370 (92%)	34 (8%)	11	16
All	All	96960/96960 (100%)	89523 (92%)	7437 (8%)	13	20

5 of 7437 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	6-H	248	GLN
1	10-N	413	GLN
1	7-J	237	LEU
1	10-L	356	LEU
1	9-R	237	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 3688 such sidechains are listed below:

Mol	Chain	Res	Type
1	6-G	30	HIS
1	10-O	211	HIS
1	7-J	248	GLN
1	10-M	86	ASN
1	9-Q	248	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 720 ligands modelled in this entry, 240 are monoatomic - leaving 480 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$
3	AMP	2-N	7501	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	9-B	7478	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	8-W	7520	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	3-P	7505	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	4-M	7500	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	5-N	7502	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	1-X	7522	-	12,12,12	3.37	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	1-P	7506	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	9-L	7498	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	3-N	7502	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	2-G	7488	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	7-W	7519	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	2-G	7487	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	8-U	7516	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CIT	7-Q	7508	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	9-C	7479	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	10-B	7477	-	22,25,25	3.47	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	1-N	7501	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	9-C	7480	-	12,12,12	3.41	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	8-C	7480	-	12,12,12	3.41	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	1-T	7514	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	4-V	7518	-	12,12,12	3.41	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	9-T	7514	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	3-X	7521	-	22,25,25	3.47	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	4-M	7499	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	8-E	7483	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	2-T	7514	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	5-T	7513	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	1-F	7486	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	7-L	7497	-	22,25,25	3.46	13 (59%)	25,38,38	4.15	10 (40%)
4	CIT	5-F	7486	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	8-H	7489	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	1-X	7521	-	22,25,25	3.47	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	9-M	7499	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	4-C	7479	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	6-H	7490	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	9-I	7491	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	10-O	7504	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	4-X	7522	-	12,12,12	3.37	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	4-N	7501	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	9-L	7497	-	22,25,25	3.46	13 (59%)	25,38,38	4.15	10 (40%)
4	CIT	6-Q	7508	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	2-Q	7507	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	7-P	7506	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	2-Q	7508	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	5-O	7504	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	5-P	7506	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	6-I	7491	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	5-U	7516	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AMP	2-U	7515	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	8-V	7517	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	3-E	7483	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	9-X	7521	-	22,25,25	3.47	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	3-S	7512	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	8-P	7505	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	5-N	7501	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	10-T	7513	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	1-E	7484	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	9-H	7489	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	10-M	7500	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	6-J	7494	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	1-Q	7507	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	1-C	7479	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	1-O	7503	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	9-H	7490	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	5-C	7479	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	1-S	7512	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	6-A	7475	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	1-E	7483	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	2-X	7522	-	12,12,12	3.37	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	9-E	7483	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	7-E	7484	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	10-F	7485	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	1-W	7519	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	5-X	7521	-	22,25,25	3.47	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	5-S	7512	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	6-K	7496	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	1-G	7487	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	2-X	7521	-	22,25,25	3.47	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	7-L	7498	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	8-T	7513	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	3-Q	7508	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	9-D	7482	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	7-I	7492	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CIT	3-W	7520	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	4-I	7492	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	7-C	7479	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	7-H	7489	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	5-F	7485	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	10-W	7519	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	9-W	7520	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	9-O	7504	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	2-A	7476	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	6-B	7477	-	22,25,25	3.47	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	6-I	7492	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	2-B	7477	-	22,25,25	3.47	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	2-I	7491	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	5-J	7494	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	2-L	7497	-	22,25,25	3.46	13 (59%)	25,38,38	4.15	10 (40%)
4	CIT	8-D	7482	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	8-X	7521	-	22,25,25	3.47	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	3-L	7497	-	22,25,25	3.46	13 (59%)	25,38,38	4.15	10 (40%)
3	AMP	6-C	7479	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	9-V	7517	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	9-N	7501	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	7-A	7476	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	8-B	7478	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	2-F	7486	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	10-R	7510	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	7-B	7477	-	22,25,25	3.47	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	10-P	7506	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	5-G	7488	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	3-E	7484	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	6-O	7504	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	6-L	7498	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	3-I	7491	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	2-R	7509	-	22,25,25	3.46	13 (59%)	25,38,38	4.15	10 (40%)
4	CIT	5-I	7492	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	8-L	7497	-	22,25,25	3.46	13 (59%)	25,38,38	4.15	10 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CIT	3-F	7486	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	7-F	7485	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	4-J	7494	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	10-T	7514	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	6-T	7514	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	2-K	7496	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	4-T	7513	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	5-O	7503	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	10-P	7505	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	2-J	7494	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	8-N	7501	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	4-F	7486	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	6-U	7515	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	7-N	7501	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	2-O	7503	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	8-Q	7508	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	1-P	7505	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	3-B	7477	-	22,25,25	3.47	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	7-J	7494	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	6-M	7500	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	6-R	7510	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	6-M	7499	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	2-H	7490	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	4-O	7504	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	9-J	7494	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	8-K	7496	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	4-S	7511	-	22,25,25	3.45	13 (59%)	25,38,38	4.15	10 (40%)
3	AMP	7-A	7475	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	2-J	7493	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	2-R	7510	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	2-S	7511	-	22,25,25	3.45	13 (59%)	25,38,38	4.15	10 (40%)
3	AMP	3-J	7493	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	6-D	7482	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	8-C	7479	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	10-Q	7507	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AMP	8-O	7503	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	1-K	7496	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	6-O	7503	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	7-O	7504	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	2-D	7481	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	7-R	7510	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	3-O	7504	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	10-J	7493	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	1-H	7490	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	6-E	7484	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	2-V	7517	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	8-F	7485	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	5-A	7476	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	4-R	7509	-	22,25,25	3.46	13 (59%)	25,38,38	4.15	10 (40%)
4	CIT	4-S	7512	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	5-H	7490	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	5-X	7522	-	12,12,12	3.37	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	5-Q	7508	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	10-D	7482	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	9-F	7486	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	7-P	7505	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	4-Q	7508	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	5-K	7495	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	4-F	7485	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	1-J	7493	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	6-T	7513	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	9-O	7503	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	10-E	7483	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	3-C	7480	-	12,12,12	3.41	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	9-X	7522	-	12,12,12	3.37	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	1-Q	7508	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	7-U	7515	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	8-J	7494	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	9-M	7500	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	10-A	7476	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CIT	8-E	7484	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	6-P	7506	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	1-B	7478	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	10-I	7491	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	2-S	7512	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	10-L	7497	-	22,25,25	3.46	13 (59%)	25,38,38	4.15	10 (40%)
3	AMP	5-Q	7507	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	2-N	7502	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	6-D	7481	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	3-S	7511	-	22,25,25	3.45	13 (59%)	25,38,38	4.15	10 (40%)
3	AMP	8-Q	7507	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	6-N	7501	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	5-R	7509	-	22,25,25	3.46	13 (59%)	25,38,38	4.15	10 (40%)
3	AMP	1-I	7491	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	7-T	7514	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	1-L	7497	-	22,25,25	3.46	13 (59%)	25,38,38	4.15	10 (40%)
3	AMP	4-P	7505	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	2-B	7478	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	8-F	7486	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	3-I	7492	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	7-I	7491	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	4-P	7506	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	1-W	7520	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	7-M	7499	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	2-V	7518	-	12,12,12	3.41	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	10-N	7501	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	10-K	7496	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	3-F	7485	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	2-K	7495	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	1-S	7511	-	22,25,25	3.45	13 (59%)	25,38,38	4.15	10 (40%)
4	CIT	9-G	7488	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	1-U	7516	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	2-O	7504	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	3-K	7495	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	2-W	7519	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AMP	10-M	7499	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	1-V	7518	-	12,12,12	3.41	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	3-R	7510	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	8-M	7499	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	4-Q	7507	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	10-X	7521	-	22,25,25	3.47	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	6-F	7485	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	10-A	7475	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	3-U	7515	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	7-V	7517	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	7-B	7478	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	10-S	7511	-	22,25,25	3.45	13 (59%)	25,38,38	4.15	10 (40%)
3	AMP	5-W	7519	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	10-S	7512	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	5-R	7510	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	4-A	7475	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	9-A	7476	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	5-L	7497	-	22,25,25	3.46	13 (59%)	25,38,38	4.15	10 (40%)
4	CIT	7-F	7486	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	3-K	7496	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	1-H	7489	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	7-Q	7507	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	4-U	7516	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	9-R	7509	-	22,25,25	3.46	13 (59%)	25,38,38	4.15	10 (40%)
4	CIT	3-A	7476	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	3-A	7475	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	7-R	7509	-	22,25,25	3.46	13 (59%)	25,38,38	4.15	10 (40%)
4	CIT	8-H	7490	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	5-J	7493	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	7-M	7500	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	7-D	7482	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	10-E	7484	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	7-K	7496	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	5-D	7482	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	2-I	7492	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CIT	8-M	7500	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	3-V	7517	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	1-R	7510	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	10-Q	7508	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	6-S	7511	-	22,25,25	3.45	13 (59%)	25,38,38	4.15	10 (40%)
4	CIT	10-G	7488	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	9-K	7496	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	5-A	7475	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	3-H	7489	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	10-F	7486	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	7-V	7518	-	12,12,12	3.41	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	5-G	7487	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	6-F	7486	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	8-A	7476	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	3-Q	7507	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	8-B	7477	-	22,25,25	3.47	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	1-O	7504	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	7-E	7483	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	5-H	7489	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	9-R	7510	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	9-S	7511	-	22,25,25	3.45	13 (59%)	25,38,38	4.15	10 (40%)
3	AMP	10-O	7503	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	9-V	7518	-	12,12,12	3.41	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	4-K	7496	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	9-Q	7508	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	9-D	7481	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	3-P	7506	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	10-N	7502	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	5-V	7517	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	3-M	7500	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	5-E	7484	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	1-T	7513	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	4-C	7480	-	12,12,12	3.41	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	10-W	7520	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	5-U	7515	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CIT	3-B	7478	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	5-M	7499	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	8-G	7487	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	5-W	7520	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	1-R	7509	-	22,25,25	3.46	13 (59%)	25,38,38	4.15	10 (40%)
4	CIT	1-C	7480	-	12,12,12	3.41	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	6-S	7512	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	6-G	7487	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	6-N	7502	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	4-W	7520	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	5-V	7518	-	12,12,12	3.41	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	6-K	7495	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	6-P	7505	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	4-N	7502	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	4-B	7478	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	2-T	7513	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	7-X	7521	-	22,25,25	3.47	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	1-K	7495	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	3-V	7518	-	12,12,12	3.41	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	8-D	7481	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	9-A	7475	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	10-U	7516	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	10-D	7481	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	9-S	7512	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	9-G	7487	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	4-L	7497	-	22,25,25	3.46	13 (59%)	25,38,38	4.15	10 (40%)
4	CIT	9-N	7502	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	3-W	7519	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	1-B	7477	-	22,25,25	3.47	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	7-S	7512	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	10-H	7490	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	8-W	7519	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	8-A	7475	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	7-N	7502	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	10-K	7495	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AMP	8-J	7493	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	6-Q	7507	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	4-X	7521	-	22,25,25	3.47	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	8-S	7511	-	22,25,25	3.45	13 (59%)	25,38,38	4.15	10 (40%)
3	AMP	4-W	7519	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	4-G	7487	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	4-J	7493	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	7-O	7503	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	6-A	7476	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	4-L	7498	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	6-R	7509	-	22,25,25	3.46	13 (59%)	25,38,38	4.15	10 (40%)
3	AMP	6-L	7497	-	22,25,25	3.46	13 (59%)	25,38,38	4.15	10 (40%)
4	CIT	1-M	7500	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	1-F	7485	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	4-D	7482	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	6-X	7522	-	12,12,12	3.37	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	3-M	7499	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	9-Q	7507	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	2-C	7480	-	12,12,12	3.41	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	10-C	7479	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	7-G	7487	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	7-J	7493	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	1-A	7476	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	9-W	7519	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	2-W	7520	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	10-R	7509	-	22,25,25	3.46	13 (59%)	25,38,38	4.15	10 (40%)
4	CIT	2-M	7500	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	4-O	7503	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	9-J	7493	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	1-D	7481	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	10-X	7522	-	12,12,12	3.37	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	9-U	7516	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	8-L	7498	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	8-R	7510	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	4-G	7488	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CIT	8-S	7512	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	8-R	7509	-	22,25,25	3.46	13 (59%)	25,38,38	4.15	10 (40%)
3	AMP	1-A	7475	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	9-P	7505	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	6-X	7521	-	22,25,25	3.47	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	2-L	7498	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	6-W	7519	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	3-H	7490	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	2-M	7499	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	5-L	7498	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	2-P	7505	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	2-A	7475	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	5-B	7477	-	22,25,25	3.47	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	7-G	7488	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	9-K	7495	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	6-U	7516	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	1-V	7517	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	10-V	7517	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	4-T	7514	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	3-G	7487	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	3-D	7482	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	8-V	7518	-	12,12,12	3.41	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	5-T	7514	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	6-V	7517	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	1-J	7494	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	8-K	7495	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	8-O	7504	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	9-E	7484	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	7-K	7495	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	1-U	7515	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	4-K	7495	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	5-S	7511	-	22,25,25	3.45	13 (59%)	25,38,38	4.15	10 (40%)
4	CIT	1-L	7498	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	5-I	7491	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	2-P	7506	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CIT	8-I	7492	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	1-G	7488	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	10-I	7492	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	10-U	7515	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	4-B	7477	-	22,25,25	3.47	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	6-H	7489	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	2-D	7482	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	9-I	7492	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	8-X	7522	-	12,12,12	3.37	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	1-N	7502	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	10-G	7487	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	9-B	7477	-	22,25,25	3.47	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	10-L	7498	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	8-P	7506	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	3-N	7501	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	7-U	7516	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	3-T	7513	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	9-T	7513	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	10-H	7489	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	6-W	7520	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	4-E	7483	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	3-J	7494	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	9-F	7485	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	6-J	7493	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	1-M	7499	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	6-V	7518	-	12,12,12	3.41	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	4-A	7476	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	7-X	7522	-	12,12,12	3.37	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	4-I	7491	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	4-D	7481	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	9-U	7515	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	2-E	7483	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	2-C	7479	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	5-B	7478	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	1-I	7492	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AMP	5-D	7481	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	7-S	7511	-	22,25,25	3.45	13 (59%)	25,38,38	4.15	10 (40%)
4	CIT	4-H	7490	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	3-L	7498	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	10-V	7518	-	12,12,12	3.41	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	3-G	7488	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	3-U	7516	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	8-G	7488	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	10-B	7478	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	5-E	7483	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	5-C	7480	-	12,12,12	3.41	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	3-T	7514	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	4-R	7510	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	6-E	7483	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	7-T	7513	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	8-T	7514	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	7-H	7490	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	1-D	7482	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	6-C	7480	-	12,12,12	3.41	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	3-X	7522	-	12,12,12	3.37	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	3-C	7479	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	3-O	7503	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	4-V	7517	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	3-R	7509	-	22,25,25	3.46	13 (59%)	25,38,38	4.15	10 (40%)
4	CIT	4-E	7484	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	6-G	7488	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	8-I	7491	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	2-H	7489	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	10-J	7494	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	6-B	7478	-	12,12,12	3.39	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	8-N	7502	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
4	CIT	7-W	7520	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	2-F	7485	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	7-D	7481	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	9-P	7506	-	12,12,12	3.40	9 (75%)	17,17,17	1.96	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CIT	7-C	7480	-	12,12,12	3.41	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	8-U	7515	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	5-K	7496	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
4	CIT	10-C	7480	-	12,12,12	3.41	9 (75%)	17,17,17	1.96	8 (47%)
3	AMP	4-H	7489	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	2-U	7516	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	4-U	7515	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	2-E	7484	-	12,12,12	3.40	9 (75%)	17,17,17	1.97	8 (47%)
3	AMP	5-P	7505	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	3-D	7481	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	5-M	7500	-	12,12,12	3.39	9 (75%)	17,17,17	1.97	8 (47%)

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	AMP	2-N	7501	-	-	3/6/26/26	0/3/3/3
4	CIT	9-B	7478	-	-	3/16/16/16	-
4	CIT	8-W	7520	-	-	3/16/16/16	-
3	AMP	3-P	7505	-	-	3/6/26/26	0/3/3/3
4	CIT	4-M	7500	-	-	3/16/16/16	-
4	CIT	5-N	7502	-	-	3/16/16/16	-
4	CIT	1-X	7522	-	-	3/16/16/16	-
4	CIT	1-P	7506	-	-	3/16/16/16	-
4	CIT	9-L	7498	-	-	3/16/16/16	-
4	CIT	3-N	7502	-	-	3/16/16/16	-
4	CIT	2-G	7488	-	-	3/16/16/16	-
3	AMP	7-W	7519	-	-	3/6/26/26	0/3/3/3
3	AMP	2-G	7487	-	-	3/6/26/26	0/3/3/3
4	CIT	8-U	7516	-	-	3/16/16/16	-
4	CIT	7-Q	7508	-	-	3/16/16/16	-
3	AMP	9-C	7479	-	-	3/6/26/26	0/3/3/3
3	AMP	10-B	7477	-	-	3/6/26/26	0/3/3/3
3	AMP	1-N	7501	-	-	3/6/26/26	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	9-C	7480	-	-	3/16/16/16	-
4	CIT	8-C	7480	-	-	3/16/16/16	-
4	CIT	1-T	7514	-	-	3/16/16/16	-
4	CIT	4-V	7518	-	-	3/16/16/16	-
4	CIT	9-T	7514	-	-	3/16/16/16	-
3	AMP	3-X	7521	-	-	3/6/26/26	0/3/3/3
3	AMP	4-M	7499	-	-	3/6/26/26	0/3/3/3
3	AMP	8-E	7483	-	-	3/6/26/26	0/3/3/3
4	CIT	2-T	7514	-	-	3/16/16/16	-
3	AMP	5-T	7513	-	-	3/6/26/26	0/3/3/3
4	CIT	1-F	7486	-	-	3/16/16/16	-
3	AMP	7-L	7497	-	-	3/6/26/26	0/3/3/3
4	CIT	5-F	7486	-	-	3/16/16/16	-
3	AMP	8-H	7489	-	-	3/6/26/26	0/3/3/3
3	AMP	1-X	7521	-	-	3/6/26/26	0/3/3/3
3	AMP	9-M	7499	-	-	3/6/26/26	0/3/3/3
3	AMP	4-C	7479	-	-	3/6/26/26	0/3/3/3
4	CIT	6-H	7490	-	-	3/16/16/16	-
3	AMP	9-I	7491	-	-	3/6/26/26	0/3/3/3
4	CIT	10-O	7504	-	-	3/16/16/16	-
4	CIT	4-X	7522	-	-	3/16/16/16	-
3	AMP	4-N	7501	-	-	3/6/26/26	0/3/3/3
3	AMP	9-L	7497	-	-	3/6/26/26	0/3/3/3
4	CIT	6-Q	7508	-	-	3/16/16/16	-
3	AMP	2-Q	7507	-	-	3/6/26/26	0/3/3/3
4	CIT	7-P	7506	-	-	3/16/16/16	-
4	CIT	2-Q	7508	-	-	3/16/16/16	-
4	CIT	5-O	7504	-	-	3/16/16/16	-
4	CIT	5-P	7506	-	-	3/16/16/16	-
3	AMP	6-I	7491	-	-	3/6/26/26	0/3/3/3
4	CIT	5-U	7516	-	-	3/16/16/16	-
3	AMP	2-U	7515	-	-	3/6/26/26	0/3/3/3
3	AMP	8-V	7517	-	-	3/6/26/26	0/3/3/3
3	AMP	3-E	7483	-	-	3/6/26/26	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	9-X	7521	-	-	3/6/26/26	0/3/3/3
4	CIT	3-S	7512	-	-	3/16/16/16	-
3	AMP	8-P	7505	-	-	3/6/26/26	0/3/3/3
3	AMP	5-N	7501	-	-	3/6/26/26	0/3/3/3
3	AMP	10-T	7513	-	-	3/6/26/26	0/3/3/3
4	CIT	1-E	7484	-	-	3/16/16/16	-
3	AMP	9-H	7489	-	-	3/6/26/26	0/3/3/3
4	CIT	10-M	7500	-	-	3/16/16/16	-
4	CIT	6-J	7494	-	-	3/16/16/16	-
3	AMP	1-Q	7507	-	-	3/6/26/26	0/3/3/3
3	AMP	1-C	7479	-	-	3/6/26/26	0/3/3/3
3	AMP	1-O	7503	-	-	3/6/26/26	0/3/3/3
4	CIT	9-H	7490	-	-	3/16/16/16	-
3	AMP	5-C	7479	-	-	3/6/26/26	0/3/3/3
4	CIT	1-S	7512	-	-	3/16/16/16	-
3	AMP	6-A	7475	-	-	3/6/26/26	0/3/3/3
3	AMP	1-E	7483	-	-	3/6/26/26	0/3/3/3
4	CIT	2-X	7522	-	-	3/16/16/16	-
3	AMP	9-E	7483	-	-	3/6/26/26	0/3/3/3
4	CIT	7-E	7484	-	-	3/16/16/16	-
3	AMP	10-F	7485	-	-	3/6/26/26	0/3/3/3
3	AMP	1-W	7519	-	-	3/6/26/26	0/3/3/3
3	AMP	5-X	7521	-	-	3/6/26/26	0/3/3/3
4	CIT	5-S	7512	-	-	3/16/16/16	-
4	CIT	6-K	7496	-	-	3/16/16/16	-
3	AMP	1-G	7487	-	-	3/6/26/26	0/3/3/3
3	AMP	2-X	7521	-	-	3/6/26/26	0/3/3/3
4	CIT	7-L	7498	-	-	3/16/16/16	-
3	AMP	8-T	7513	-	-	3/6/26/26	0/3/3/3
4	CIT	3-Q	7508	-	-	3/16/16/16	-
4	CIT	9-D	7482	-	-	3/16/16/16	-
4	CIT	7-I	7492	-	-	3/16/16/16	-
4	CIT	3-W	7520	-	-	3/16/16/16	-
4	CIT	4-I	7492	-	-	3/16/16/16	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	7-C	7479	-	-	3/6/26/26	0/3/3/3
3	AMP	7-H	7489	-	-	3/6/26/26	0/3/3/3
3	AMP	5-F	7485	-	-	3/6/26/26	0/3/3/3
3	AMP	10-W	7519	-	-	3/6/26/26	0/3/3/3
4	CIT	9-W	7520	-	-	3/16/16/16	-
4	CIT	9-O	7504	-	-	3/16/16/16	-
4	CIT	2-A	7476	-	-	3/16/16/16	-
3	AMP	6-B	7477	-	-	3/6/26/26	0/3/3/3
4	CIT	6-I	7492	-	-	3/16/16/16	-
3	AMP	2-B	7477	-	-	3/6/26/26	0/3/3/3
3	AMP	2-I	7491	-	-	3/6/26/26	0/3/3/3
4	CIT	5-J	7494	-	-	3/16/16/16	-
3	AMP	2-L	7497	-	-	3/6/26/26	0/3/3/3
4	CIT	8-D	7482	-	-	3/16/16/16	-
3	AMP	8-X	7521	-	-	3/6/26/26	0/3/3/3
3	AMP	3-L	7497	-	-	3/6/26/26	0/3/3/3
3	AMP	6-C	7479	-	-	3/6/26/26	0/3/3/3
3	AMP	9-V	7517	-	-	3/6/26/26	0/3/3/3
3	AMP	9-N	7501	-	-	3/6/26/26	0/3/3/3
4	CIT	7-A	7476	-	-	3/16/16/16	-
4	CIT	8-B	7478	-	-	3/16/16/16	-
4	CIT	2-F	7486	-	-	3/16/16/16	-
4	CIT	10-R	7510	-	-	3/16/16/16	-
3	AMP	7-B	7477	-	-	3/6/26/26	0/3/3/3
4	CIT	10-P	7506	-	-	3/16/16/16	-
4	CIT	5-G	7488	-	-	3/16/16/16	-
4	CIT	3-E	7484	-	-	3/16/16/16	-
4	CIT	6-O	7504	-	-	3/16/16/16	-
4	CIT	6-L	7498	-	-	3/16/16/16	-
3	AMP	3-I	7491	-	-	3/6/26/26	0/3/3/3
3	AMP	2-R	7509	-	-	3/6/26/26	0/3/3/3
4	CIT	5-I	7492	-	-	3/16/16/16	-
3	AMP	8-L	7497	-	-	3/6/26/26	0/3/3/3
4	CIT	3-F	7486	-	-	3/16/16/16	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	7-F	7485	-	-	3/6/26/26	0/3/3/3
4	CIT	4-J	7494	-	-	3/16/16/16	-
4	CIT	10-T	7514	-	-	3/16/16/16	-
4	CIT	6-T	7514	-	-	3/16/16/16	-
4	CIT	2-K	7496	-	-	3/16/16/16	-
3	AMP	4-T	7513	-	-	3/6/26/26	0/3/3/3
3	AMP	5-O	7503	-	-	3/6/26/26	0/3/3/3
3	AMP	10-P	7505	-	-	3/6/26/26	0/3/3/3
4	CIT	2-J	7494	-	-	3/16/16/16	-
3	AMP	8-N	7501	-	-	3/6/26/26	0/3/3/3
4	CIT	4-F	7486	-	-	3/16/16/16	-
3	AMP	6-U	7515	-	-	3/6/26/26	0/3/3/3
3	AMP	7-N	7501	-	-	3/6/26/26	0/3/3/3
3	AMP	2-O	7503	-	-	3/6/26/26	0/3/3/3
4	CIT	8-Q	7508	-	-	3/16/16/16	-
3	AMP	1-P	7505	-	-	3/6/26/26	0/3/3/3
3	AMP	3-B	7477	-	-	3/6/26/26	0/3/3/3
4	CIT	7-J	7494	-	-	3/16/16/16	-
4	CIT	6-M	7500	-	-	3/16/16/16	-
4	CIT	6-R	7510	-	-	3/16/16/16	-
3	AMP	6-M	7499	-	-	3/6/26/26	0/3/3/3
4	CIT	2-H	7490	-	-	3/16/16/16	-
4	CIT	4-O	7504	-	-	3/16/16/16	-
4	CIT	9-J	7494	-	-	3/16/16/16	-
4	CIT	8-K	7496	-	-	3/16/16/16	-
3	AMP	4-S	7511	-	-	3/6/26/26	0/3/3/3
3	AMP	7-A	7475	-	-	3/6/26/26	0/3/3/3
3	AMP	2-J	7493	-	-	3/6/26/26	0/3/3/3
4	CIT	2-R	7510	-	-	3/16/16/16	-
3	AMP	2-S	7511	-	-	3/6/26/26	0/3/3/3
3	AMP	3-J	7493	-	-	3/6/26/26	0/3/3/3
4	CIT	6-D	7482	-	-	3/16/16/16	-
3	AMP	8-C	7479	-	-	3/6/26/26	0/3/3/3
3	AMP	10-Q	7507	-	-	3/6/26/26	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	8-O	7503	-	-	3/6/26/26	0/3/3/3
4	CIT	1-K	7496	-	-	3/16/16/16	-
3	AMP	6-O	7503	-	-	3/6/26/26	0/3/3/3
4	CIT	7-O	7504	-	-	3/16/16/16	-
3	AMP	2-D	7481	-	-	3/6/26/26	0/3/3/3
4	CIT	7-R	7510	-	-	3/16/16/16	-
4	CIT	3-O	7504	-	-	3/16/16/16	-
3	AMP	10-J	7493	-	-	3/6/26/26	0/3/3/3
4	CIT	1-H	7490	-	-	3/16/16/16	-
4	CIT	6-E	7484	-	-	3/16/16/16	-
3	AMP	2-V	7517	-	-	3/6/26/26	0/3/3/3
3	AMP	8-F	7485	-	-	3/6/26/26	0/3/3/3
4	CIT	5-A	7476	-	-	3/16/16/16	-
3	AMP	4-R	7509	-	-	3/6/26/26	0/3/3/3
4	CIT	4-S	7512	-	-	3/16/16/16	-
4	CIT	5-H	7490	-	-	3/16/16/16	-
4	CIT	5-X	7522	-	-	3/16/16/16	-
4	CIT	5-Q	7508	-	-	3/16/16/16	-
4	CIT	10-D	7482	-	-	3/16/16/16	-
4	CIT	9-F	7486	-	-	3/16/16/16	-
3	AMP	7-P	7505	-	-	3/6/26/26	0/3/3/3
4	CIT	4-Q	7508	-	-	3/16/16/16	-
3	AMP	5-K	7495	-	-	3/6/26/26	0/3/3/3
3	AMP	4-F	7485	-	-	3/6/26/26	0/3/3/3
3	AMP	1-J	7493	-	-	3/6/26/26	0/3/3/3
3	AMP	6-T	7513	-	-	3/6/26/26	0/3/3/3
3	AMP	9-O	7503	-	-	3/6/26/26	0/3/3/3
3	AMP	10-E	7483	-	-	3/6/26/26	0/3/3/3
4	CIT	3-C	7480	-	-	3/16/16/16	-
4	CIT	9-X	7522	-	-	3/16/16/16	-
4	CIT	1-Q	7508	-	-	3/16/16/16	-
3	AMP	7-U	7515	-	-	3/6/26/26	0/3/3/3
4	CIT	8-J	7494	-	-	3/16/16/16	-
4	CIT	9-M	7500	-	-	3/16/16/16	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	10-A	7476	-	-	3/16/16/16	-
4	CIT	8-E	7484	-	-	3/16/16/16	-
4	CIT	6-P	7506	-	-	3/16/16/16	-
4	CIT	1-B	7478	-	-	3/16/16/16	-
3	AMP	10-I	7491	-	-	3/6/26/26	0/3/3/3
4	CIT	2-S	7512	-	-	3/16/16/16	-
3	AMP	10-L	7497	-	-	3/6/26/26	0/3/3/3
3	AMP	5-Q	7507	-	-	3/6/26/26	0/3/3/3
4	CIT	2-N	7502	-	-	3/16/16/16	-
3	AMP	6-D	7481	-	-	3/6/26/26	0/3/3/3
3	AMP	3-S	7511	-	-	3/6/26/26	0/3/3/3
3	AMP	8-Q	7507	-	-	3/6/26/26	0/3/3/3
3	AMP	6-N	7501	-	-	3/6/26/26	0/3/3/3
3	AMP	5-R	7509	-	-	3/6/26/26	0/3/3/3
3	AMP	1-I	7491	-	-	3/6/26/26	0/3/3/3
4	CIT	7-T	7514	-	-	3/16/16/16	-
3	AMP	1-L	7497	-	-	3/6/26/26	0/3/3/3
3	AMP	4-P	7505	-	-	3/6/26/26	0/3/3/3
4	CIT	2-B	7478	-	-	3/16/16/16	-
4	CIT	8-F	7486	-	-	3/16/16/16	-
4	CIT	3-I	7492	-	-	3/16/16/16	-
3	AMP	7-I	7491	-	-	3/6/26/26	0/3/3/3
4	CIT	4-P	7506	-	-	3/16/16/16	-
4	CIT	1-W	7520	-	-	3/16/16/16	-
3	AMP	7-M	7499	-	-	3/6/26/26	0/3/3/3
4	CIT	2-V	7518	-	-	3/16/16/16	-
3	AMP	10-N	7501	-	-	3/6/26/26	0/3/3/3
4	CIT	10-K	7496	-	-	3/16/16/16	-
3	AMP	3-F	7485	-	-	3/6/26/26	0/3/3/3
3	AMP	2-K	7495	-	-	3/6/26/26	0/3/3/3
3	AMP	1-S	7511	-	-	3/6/26/26	0/3/3/3
4	CIT	9-G	7488	-	-	3/16/16/16	-
4	CIT	1-U	7516	-	-	3/16/16/16	-
4	CIT	2-O	7504	-	-	3/16/16/16	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	3-K	7495	-	-	3/6/26/26	0/3/3/3
3	AMP	2-W	7519	-	-	3/6/26/26	0/3/3/3
3	AMP	10-M	7499	-	-	3/6/26/26	0/3/3/3
4	CIT	1-V	7518	-	-	3/16/16/16	-
4	CIT	3-R	7510	-	-	3/16/16/16	-
3	AMP	8-M	7499	-	-	3/6/26/26	0/3/3/3
3	AMP	4-Q	7507	-	-	3/6/26/26	0/3/3/3
3	AMP	10-X	7521	-	-	3/6/26/26	0/3/3/3
3	AMP	6-F	7485	-	-	3/6/26/26	0/3/3/3
3	AMP	10-A	7475	-	-	3/6/26/26	0/3/3/3
3	AMP	3-U	7515	-	-	3/6/26/26	0/3/3/3
3	AMP	7-V	7517	-	-	3/6/26/26	0/3/3/3
4	CIT	7-B	7478	-	-	3/16/16/16	-
3	AMP	10-S	7511	-	-	3/6/26/26	0/3/3/3
3	AMP	5-W	7519	-	-	3/6/26/26	0/3/3/3
4	CIT	10-S	7512	-	-	3/16/16/16	-
4	CIT	5-R	7510	-	-	3/16/16/16	-
3	AMP	4-A	7475	-	-	3/6/26/26	0/3/3/3
4	CIT	9-A	7476	-	-	3/16/16/16	-
3	AMP	5-L	7497	-	-	3/6/26/26	0/3/3/3
4	CIT	7-F	7486	-	-	3/16/16/16	-
4	CIT	3-K	7496	-	-	3/16/16/16	-
3	AMP	1-H	7489	-	-	3/6/26/26	0/3/3/3
3	AMP	7-Q	7507	-	-	3/6/26/26	0/3/3/3
4	CIT	4-U	7516	-	-	3/16/16/16	-
3	AMP	9-R	7509	-	-	3/6/26/26	0/3/3/3
4	CIT	3-A	7476	-	-	3/16/16/16	-
3	AMP	3-A	7475	-	-	3/6/26/26	0/3/3/3
3	AMP	7-R	7509	-	-	3/6/26/26	0/3/3/3
4	CIT	8-H	7490	-	-	3/16/16/16	-
3	AMP	5-J	7493	-	-	3/6/26/26	0/3/3/3
4	CIT	7-M	7500	-	-	3/16/16/16	-
4	CIT	7-D	7482	-	-	3/16/16/16	-
4	CIT	10-E	7484	-	-	3/16/16/16	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	7-K	7496	-	-	3/16/16/16	-
4	CIT	5-D	7482	-	-	3/16/16/16	-
4	CIT	2-I	7492	-	-	3/16/16/16	-
4	CIT	8-M	7500	-	-	3/16/16/16	-
3	AMP	3-V	7517	-	-	3/6/26/26	0/3/3/3
4	CIT	1-R	7510	-	-	3/16/16/16	-
4	CIT	10-Q	7508	-	-	3/16/16/16	-
3	AMP	6-S	7511	-	-	3/6/26/26	0/3/3/3
4	CIT	10-G	7488	-	-	3/16/16/16	-
4	CIT	9-K	7496	-	-	3/16/16/16	-
3	AMP	5-A	7475	-	-	3/6/26/26	0/3/3/3
3	AMP	3-H	7489	-	-	3/6/26/26	0/3/3/3
4	CIT	10-F	7486	-	-	3/16/16/16	-
4	CIT	7-V	7518	-	-	3/16/16/16	-
3	AMP	5-G	7487	-	-	3/6/26/26	0/3/3/3
4	CIT	6-F	7486	-	-	3/16/16/16	-
4	CIT	8-A	7476	-	-	3/16/16/16	-
3	AMP	3-Q	7507	-	-	3/6/26/26	0/3/3/3
3	AMP	8-B	7477	-	-	3/6/26/26	0/3/3/3
4	CIT	1-O	7504	-	-	3/16/16/16	-
3	AMP	7-E	7483	-	-	3/6/26/26	0/3/3/3
3	AMP	5-H	7489	-	-	3/6/26/26	0/3/3/3
4	CIT	9-R	7510	-	-	3/16/16/16	-
3	AMP	9-S	7511	-	-	3/6/26/26	0/3/3/3
3	AMP	10-O	7503	-	-	3/6/26/26	0/3/3/3
4	CIT	9-V	7518	-	-	3/16/16/16	-
4	CIT	4-K	7496	-	-	3/16/16/16	-
4	CIT	9-Q	7508	-	-	3/16/16/16	-
3	AMP	9-D	7481	-	-	3/6/26/26	0/3/3/3
4	CIT	3-P	7506	-	-	3/16/16/16	-
4	CIT	10-N	7502	-	-	3/16/16/16	-
3	AMP	5-V	7517	-	-	3/6/26/26	0/3/3/3
4	CIT	3-M	7500	-	-	3/16/16/16	-
4	CIT	5-E	7484	-	-	3/16/16/16	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	1-T	7513	-	-	3/6/26/26	0/3/3/3
4	CIT	4-C	7480	-	-	3/16/16/16	-
4	CIT	10-W	7520	-	-	3/16/16/16	-
3	AMP	5-U	7515	-	-	3/6/26/26	0/3/3/3
4	CIT	3-B	7478	-	-	3/16/16/16	-
3	AMP	5-M	7499	-	-	3/6/26/26	0/3/3/3
3	AMP	8-G	7487	-	-	3/6/26/26	0/3/3/3
4	CIT	5-W	7520	-	-	3/16/16/16	-
3	AMP	1-R	7509	-	-	3/6/26/26	0/3/3/3
4	CIT	1-C	7480	-	-	3/16/16/16	-
4	CIT	6-S	7512	-	-	3/16/16/16	-
3	AMP	6-G	7487	-	-	3/6/26/26	0/3/3/3
4	CIT	6-N	7502	-	-	3/16/16/16	-
4	CIT	4-W	7520	-	-	3/16/16/16	-
4	CIT	5-V	7518	-	-	3/16/16/16	-
3	AMP	6-K	7495	-	-	3/6/26/26	0/3/3/3
3	AMP	6-P	7505	-	-	3/6/26/26	0/3/3/3
4	CIT	4-N	7502	-	-	3/16/16/16	-
4	CIT	4-B	7478	-	-	3/16/16/16	-
3	AMP	2-T	7513	-	-	3/6/26/26	0/3/3/3
3	AMP	7-X	7521	-	-	3/6/26/26	0/3/3/3
3	AMP	1-K	7495	-	-	3/6/26/26	0/3/3/3
4	CIT	3-V	7518	-	-	3/16/16/16	-
3	AMP	8-D	7481	-	-	3/6/26/26	0/3/3/3
3	AMP	9-A	7475	-	-	3/6/26/26	0/3/3/3
4	CIT	10-U	7516	-	-	3/16/16/16	-
3	AMP	10-D	7481	-	-	3/6/26/26	0/3/3/3
4	CIT	9-S	7512	-	-	3/16/16/16	-
3	AMP	9-G	7487	-	-	3/6/26/26	0/3/3/3
3	AMP	4-L	7497	-	-	3/6/26/26	0/3/3/3
4	CIT	9-N	7502	-	-	3/16/16/16	-
3	AMP	3-W	7519	-	-	3/6/26/26	0/3/3/3
3	AMP	1-B	7477	-	-	3/6/26/26	0/3/3/3
4	CIT	7-S	7512	-	-	3/16/16/16	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	10-H	7490	-	-	3/16/16/16	-
3	AMP	8-W	7519	-	-	3/6/26/26	0/3/3/3
3	AMP	8-A	7475	-	-	3/6/26/26	0/3/3/3
4	CIT	7-N	7502	-	-	3/16/16/16	-
3	AMP	10-K	7495	-	-	3/6/26/26	0/3/3/3
3	AMP	8-J	7493	-	-	3/6/26/26	0/3/3/3
3	AMP	6-Q	7507	-	-	3/6/26/26	0/3/3/3
3	AMP	4-X	7521	-	-	3/6/26/26	0/3/3/3
3	AMP	8-S	7511	-	-	3/6/26/26	0/3/3/3
3	AMP	4-W	7519	-	-	3/6/26/26	0/3/3/3
3	AMP	4-G	7487	-	-	3/6/26/26	0/3/3/3
3	AMP	4-J	7493	-	-	3/6/26/26	0/3/3/3
3	AMP	7-O	7503	-	-	3/6/26/26	0/3/3/3
4	CIT	6-A	7476	-	-	3/16/16/16	-
4	CIT	4-L	7498	-	-	3/16/16/16	-
3	AMP	6-R	7509	-	-	3/6/26/26	0/3/3/3
3	AMP	6-L	7497	-	-	3/6/26/26	0/3/3/3
4	CIT	1-M	7500	-	-	3/16/16/16	-
3	AMP	1-F	7485	-	-	3/6/26/26	0/3/3/3
4	CIT	4-D	7482	-	-	3/16/16/16	-
4	CIT	6-X	7522	-	-	3/16/16/16	-
3	AMP	3-M	7499	-	-	3/6/26/26	0/3/3/3
3	AMP	9-Q	7507	-	-	3/6/26/26	0/3/3/3
4	CIT	2-C	7480	-	-	3/16/16/16	-
3	AMP	10-C	7479	-	-	3/6/26/26	0/3/3/3
3	AMP	7-G	7487	-	-	3/6/26/26	0/3/3/3
3	AMP	7-J	7493	-	-	3/6/26/26	0/3/3/3
4	CIT	1-A	7476	-	-	3/16/16/16	-
3	AMP	9-W	7519	-	-	3/6/26/26	0/3/3/3
4	CIT	2-W	7520	-	-	3/16/16/16	-
3	AMP	10-R	7509	-	-	3/6/26/26	0/3/3/3
4	CIT	2-M	7500	-	-	3/16/16/16	-
3	AMP	4-O	7503	-	-	3/6/26/26	0/3/3/3
3	AMP	9-J	7493	-	-	3/6/26/26	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	1-D	7481	-	-	3/6/26/26	0/3/3/3
4	CIT	10-X	7522	-	-	3/16/16/16	-
4	CIT	9-U	7516	-	-	3/16/16/16	-
4	CIT	8-L	7498	-	-	3/16/16/16	-
4	CIT	8-R	7510	-	-	3/16/16/16	-
4	CIT	4-G	7488	-	-	3/16/16/16	-
4	CIT	8-S	7512	-	-	3/16/16/16	-
3	AMP	8-R	7509	-	-	3/6/26/26	0/3/3/3
3	AMP	1-A	7475	-	-	3/6/26/26	0/3/3/3
3	AMP	9-P	7505	-	-	3/6/26/26	0/3/3/3
3	AMP	6-X	7521	-	-	3/6/26/26	0/3/3/3
4	CIT	2-L	7498	-	-	3/16/16/16	-
3	AMP	6-W	7519	-	-	3/6/26/26	0/3/3/3
4	CIT	3-H	7490	-	-	3/16/16/16	-
3	AMP	2-M	7499	-	-	3/6/26/26	0/3/3/3
4	CIT	5-L	7498	-	-	3/16/16/16	-
3	AMP	2-P	7505	-	-	3/6/26/26	0/3/3/3
3	AMP	2-A	7475	-	-	3/6/26/26	0/3/3/3
3	AMP	5-B	7477	-	-	3/6/26/26	0/3/3/3
4	CIT	7-G	7488	-	-	3/16/16/16	-
3	AMP	9-K	7495	-	-	3/6/26/26	0/3/3/3
4	CIT	6-U	7516	-	-	3/16/16/16	-
3	AMP	1-V	7517	-	-	3/6/26/26	0/3/3/3
3	AMP	10-V	7517	-	-	3/6/26/26	0/3/3/3
4	CIT	4-T	7514	-	-	3/16/16/16	-
3	AMP	3-G	7487	-	-	3/6/26/26	0/3/3/3
4	CIT	3-D	7482	-	-	3/16/16/16	-
4	CIT	8-V	7518	-	-	3/16/16/16	-
4	CIT	5-T	7514	-	-	3/16/16/16	-
3	AMP	6-V	7517	-	-	3/6/26/26	0/3/3/3
4	CIT	1-J	7494	-	-	3/16/16/16	-
3	AMP	8-K	7495	-	-	3/6/26/26	0/3/3/3
4	CIT	8-O	7504	-	-	3/16/16/16	-
4	CIT	9-E	7484	-	-	3/16/16/16	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	7-K	7495	-	-	3/6/26/26	0/3/3/3
3	AMP	1-U	7515	-	-	3/6/26/26	0/3/3/3
3	AMP	4-K	7495	-	-	3/6/26/26	0/3/3/3
3	AMP	5-S	7511	-	-	3/6/26/26	0/3/3/3
4	CIT	1-L	7498	-	-	3/16/16/16	-
3	AMP	5-I	7491	-	-	3/6/26/26	0/3/3/3
4	CIT	2-P	7506	-	-	3/16/16/16	-
4	CIT	8-I	7492	-	-	3/16/16/16	-
4	CIT	1-G	7488	-	-	3/16/16/16	-
4	CIT	10-I	7492	-	-	3/16/16/16	-
3	AMP	10-U	7515	-	-	3/6/26/26	0/3/3/3
3	AMP	4-B	7477	-	-	3/6/26/26	0/3/3/3
3	AMP	6-H	7489	-	-	3/6/26/26	0/3/3/3
4	CIT	2-D	7482	-	-	3/16/16/16	-
4	CIT	9-I	7492	-	-	3/16/16/16	-
4	CIT	8-X	7522	-	-	3/16/16/16	-
4	CIT	1-N	7502	-	-	3/16/16/16	-
3	AMP	10-G	7487	-	-	3/6/26/26	0/3/3/3
3	AMP	9-B	7477	-	-	3/6/26/26	0/3/3/3
4	CIT	10-L	7498	-	-	3/16/16/16	-
4	CIT	8-P	7506	-	-	3/16/16/16	-
3	AMP	3-N	7501	-	-	3/6/26/26	0/3/3/3
4	CIT	7-U	7516	-	-	3/16/16/16	-
3	AMP	3-T	7513	-	-	3/6/26/26	0/3/3/3
3	AMP	9-T	7513	-	-	3/6/26/26	0/3/3/3
3	AMP	10-H	7489	-	-	3/6/26/26	0/3/3/3
4	CIT	6-W	7520	-	-	3/16/16/16	-
3	AMP	4-E	7483	-	-	3/6/26/26	0/3/3/3
4	CIT	3-J	7494	-	-	3/16/16/16	-
3	AMP	9-F	7485	-	-	3/6/26/26	0/3/3/3
3	AMP	6-J	7493	-	-	3/6/26/26	0/3/3/3
3	AMP	1-M	7499	-	-	3/6/26/26	0/3/3/3
4	CIT	6-V	7518	-	-	3/16/16/16	-
4	CIT	4-A	7476	-	-	3/16/16/16	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	7-X	7522	-	-	3/16/16/16	-
3	AMP	4-I	7491	-	-	3/6/26/26	0/3/3/3
3	AMP	4-D	7481	-	-	3/6/26/26	0/3/3/3
3	AMP	9-U	7515	-	-	3/6/26/26	0/3/3/3
3	AMP	2-E	7483	-	-	3/6/26/26	0/3/3/3
3	AMP	2-C	7479	-	-	3/6/26/26	0/3/3/3
4	CIT	5-B	7478	-	-	3/16/16/16	-
4	CIT	1-I	7492	-	-	3/16/16/16	-
3	AMP	5-D	7481	-	-	3/6/26/26	0/3/3/3
3	AMP	7-S	7511	-	-	3/6/26/26	0/3/3/3
4	CIT	4-H	7490	-	-	3/16/16/16	-
4	CIT	3-L	7498	-	-	3/16/16/16	-
4	CIT	10-V	7518	-	-	3/16/16/16	-
4	CIT	3-G	7488	-	-	3/16/16/16	-
4	CIT	3-U	7516	-	-	3/16/16/16	-
4	CIT	8-G	7488	-	-	3/16/16/16	-
4	CIT	10-B	7478	-	-	3/16/16/16	-
3	AMP	5-E	7483	-	-	3/6/26/26	0/3/3/3
4	CIT	5-C	7480	-	-	3/16/16/16	-
4	CIT	3-T	7514	-	-	3/16/16/16	-
4	CIT	4-R	7510	-	-	3/16/16/16	-
3	AMP	6-E	7483	-	-	3/6/26/26	0/3/3/3
3	AMP	7-T	7513	-	-	3/6/26/26	0/3/3/3
4	CIT	8-T	7514	-	-	3/16/16/16	-
4	CIT	7-H	7490	-	-	3/16/16/16	-
4	CIT	1-D	7482	-	-	3/16/16/16	-
4	CIT	6-C	7480	-	-	3/16/16/16	-
4	CIT	3-X	7522	-	-	3/16/16/16	-
3	AMP	3-C	7479	-	-	3/6/26/26	0/3/3/3
3	AMP	3-O	7503	-	-	3/6/26/26	0/3/3/3
3	AMP	4-V	7517	-	-	3/6/26/26	0/3/3/3
3	AMP	3-R	7509	-	-	3/6/26/26	0/3/3/3
4	CIT	4-E	7484	-	-	3/16/16/16	-
4	CIT	6-G	7488	-	-	3/16/16/16	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	8-I	7491	-	-	3/6/26/26	0/3/3/3
3	AMP	2-H	7489	-	-	3/6/26/26	0/3/3/3
4	CIT	10-J	7494	-	-	3/16/16/16	-
4	CIT	6-B	7478	-	-	3/16/16/16	-
4	CIT	8-N	7502	-	-	3/16/16/16	-
4	CIT	7-W	7520	-	-	3/16/16/16	-
3	AMP	2-F	7485	-	-	3/6/26/26	0/3/3/3
3	AMP	7-D	7481	-	-	3/6/26/26	0/3/3/3
4	CIT	9-P	7506	-	-	3/16/16/16	-
4	CIT	7-C	7480	-	-	3/16/16/16	-
3	AMP	8-U	7515	-	-	3/6/26/26	0/3/3/3
4	CIT	5-K	7496	-	-	3/16/16/16	-
4	CIT	10-C	7480	-	-	3/16/16/16	-
3	AMP	4-H	7489	-	-	3/6/26/26	0/3/3/3
4	CIT	2-U	7516	-	-	3/16/16/16	-
3	AMP	4-U	7515	-	-	3/6/26/26	0/3/3/3
4	CIT	2-E	7484	-	-	3/16/16/16	-
3	AMP	5-P	7505	-	-	3/6/26/26	0/3/3/3
3	AMP	3-D	7481	-	-	3/6/26/26	0/3/3/3
4	CIT	5-M	7500	-	-	3/16/16/16	-

The worst 5 of 5280 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-X	7521	AMP	O4'-C1'	8.64	1.53	1.41
3	2-X	7521	AMP	O4'-C1'	8.64	1.53	1.41
3	3-X	7521	AMP	O4'-C1'	8.64	1.53	1.41
3	4-X	7521	AMP	O4'-C1'	8.64	1.53	1.41
3	5-X	7521	AMP	O4'-C1'	8.64	1.53	1.41

The worst 5 of 4320 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-P	7505	AMP	O4'-C1'-C2'	-13.64	87.00	106.93
3	2-P	7505	AMP	O4'-C1'-C2'	-13.64	87.00	106.93
3	3-P	7505	AMP	O4'-C1'-C2'	-13.64	87.00	106.93
3	4-P	7505	AMP	O4'-C1'-C2'	-13.64	87.00	106.93
3	5-P	7505	AMP	O4'-C1'-C2'	-13.64	87.00	106.93

There are no chirality outliers.

5 of 1440 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	1-A	7475	AMP	C5'-O5'-P-O2P
3	1-A	7475	AMP	C5'-O5'-P-O3P
3	2-A	7475	AMP	C5'-O5'-P-O2P
3	2-A	7475	AMP	C5'-O5'-P-O3P
3	3-A	7475	AMP	C5'-O5'-P-O2P

There are no ring outliers.

480 monomers are involved in 2567 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	2-N	7501	AMP	6	0
4	9-B	7478	CIT	3	0
4	8-W	7520	CIT	4	0
3	3-P	7505	AMP	10	0
4	4-M	7500	CIT	5	0
4	5-N	7502	CIT	3	0
4	1-X	7522	CIT	5	0
4	1-P	7506	CIT	5	0
4	9-L	7498	CIT	1	0
4	3-N	7502	CIT	4	0
4	2-G	7488	CIT	2	0
3	7-W	7519	AMP	5	0
3	2-G	7487	AMP	7	0
4	8-U	7516	CIT	4	0
4	7-Q	7508	CIT	6	0
3	9-C	7479	AMP	8	0
3	10-B	7477	AMP	6	0
3	1-N	7501	AMP	4	0
4	9-C	7480	CIT	3	0
4	8-C	7480	CIT	4	0
4	1-T	7514	CIT	5	0
4	4-V	7518	CIT	4	0
4	9-T	7514	CIT	3	0
3	3-X	7521	AMP	10	0
3	4-M	7499	AMP	10	0
3	8-E	7483	AMP	6	0
4	2-T	7514	CIT	1	0
3	5-T	7513	AMP	7	0
4	1-F	7486	CIT	5	0
3	7-L	7497	AMP	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	5-F	7486	CIT	4	0
3	8-H	7489	AMP	5	0
3	1-X	7521	AMP	4	0
3	9-M	7499	AMP	7	0
3	4-C	7479	AMP	10	0
4	6-H	7490	CIT	2	0
3	9-I	7491	AMP	8	0
4	10-O	7504	CIT	4	0
4	4-X	7522	CIT	3	0
3	4-N	7501	AMP	10	0
3	9-L	7497	AMP	7	0
4	6-Q	7508	CIT	3	0
3	2-Q	7507	AMP	7	0
4	7-P	7506	CIT	6	0
4	2-Q	7508	CIT	3	0
4	5-O	7504	CIT	3	0
4	5-P	7506	CIT	3	0
3	6-I	7491	AMP	7	0
4	5-U	7516	CIT	4	0
3	2-U	7515	AMP	6	0
3	8-V	7517	AMP	6	0
3	3-E	7483	AMP	10	0
3	9-X	7521	AMP	7	0
4	3-S	7512	CIT	4	0
3	8-P	7505	AMP	5	0
3	5-N	7501	AMP	7	0
3	10-T	7513	AMP	6	0
4	1-E	7484	CIT	5	0
3	9-H	7489	AMP	8	0
4	10-M	7500	CIT	4	0
4	6-J	7494	CIT	3	0
3	1-Q	7507	AMP	4	0
3	1-C	7479	AMP	4	0
3	1-O	7503	AMP	4	0
4	9-H	7490	CIT	3	0
3	5-C	7479	AMP	7	0
4	1-S	7512	CIT	5	0
3	6-A	7475	AMP	6	0
3	1-E	7483	AMP	4	0
4	2-X	7522	CIT	3	0
3	9-E	7483	AMP	8	0
4	7-E	7484	CIT	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	10-F	7485	AMP	6	0
3	1-W	7519	AMP	4	0
3	5-X	7521	AMP	7	0
4	5-S	7512	CIT	4	0
4	6-K	7496	CIT	3	0
3	1-G	7487	AMP	4	0
3	2-X	7521	AMP	7	0
4	7-L	7498	CIT	5	0
3	8-T	7513	AMP	5	0
4	3-Q	7508	CIT	4	0
4	9-D	7482	CIT	3	0
4	7-I	7492	CIT	6	0
4	3-W	7520	CIT	4	0
4	4-I	7492	CIT	5	0
3	7-C	7479	AMP	5	0
3	7-H	7489	AMP	5	0
3	5-F	7485	AMP	7	0
3	10-W	7519	AMP	6	0
4	9-W	7520	CIT	3	0
4	9-O	7504	CIT	3	0
4	2-A	7476	CIT	3	0
3	6-B	7477	AMP	7	0
4	6-I	7492	CIT	3	0
3	2-B	7477	AMP	6	0
3	2-I	7491	AMP	7	0
4	5-J	7494	CIT	4	0
3	2-L	7497	AMP	7	0
4	8-D	7482	CIT	4	0
3	8-X	7521	AMP	6	0
3	3-L	7497	AMP	10	0
3	6-C	7479	AMP	7	0
3	9-V	7517	AMP	8	0
3	9-N	7501	AMP	7	0
4	7-A	7476	CIT	6	0
4	8-B	7478	CIT	4	0
4	2-F	7486	CIT	2	0
4	10-R	7510	CIT	3	0
3	7-B	7477	AMP	5	0
4	10-P	7506	CIT	4	0
4	5-G	7488	CIT	4	0
4	3-E	7484	CIT	4	0
4	6-O	7504	CIT	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	6-L	7498	CIT	3	0
3	3-I	7491	AMP	10	0
3	2-R	7509	AMP	7	0
4	5-I	7492	CIT	4	0
3	8-L	7497	AMP	6	0
4	3-F	7486	CIT	4	0
3	7-F	7485	AMP	5	0
4	4-J	7494	CIT	4	0
4	10-T	7514	CIT	5	0
4	6-T	7514	CIT	2	0
4	2-K	7496	CIT	3	0
3	4-T	7513	AMP	10	0
3	5-O	7503	AMP	7	0
3	10-P	7505	AMP	6	0
4	2-J	7494	CIT	4	0
3	8-N	7501	AMP	6	0
4	4-F	7486	CIT	3	0
3	6-U	7515	AMP	7	0
3	7-N	7501	AMP	5	0
3	2-O	7503	AMP	7	0
4	8-Q	7508	CIT	4	0
3	1-P	7505	AMP	4	0
3	3-B	7477	AMP	10	0
4	7-J	7494	CIT	6	0
4	6-M	7500	CIT	3	0
4	6-R	7510	CIT	2	0
3	6-M	7499	AMP	6	0
4	2-H	7490	CIT	2	0
4	4-O	7504	CIT	4	0
4	9-J	7494	CIT	2	0
4	8-K	7496	CIT	4	0
3	4-S	7511	AMP	10	0
3	7-A	7475	AMP	5	0
3	2-J	7493	AMP	6	0
4	2-R	7510	CIT	2	0
3	2-S	7511	AMP	6	0
3	3-J	7493	AMP	10	0
4	6-D	7482	CIT	2	0
3	8-C	7479	AMP	6	0
3	10-Q	7507	AMP	6	0
3	8-O	7503	AMP	6	0
4	1-K	7496	CIT	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	6-O	7503	AMP	7	0
4	7-O	7504	CIT	6	0
3	2-D	7481	AMP	7	0
4	7-R	7510	CIT	6	0
4	3-O	7504	CIT	4	0
3	10-J	7493	AMP	6	0
4	1-H	7490	CIT	5	0
4	6-E	7484	CIT	3	0
3	2-V	7517	AMP	6	0
3	8-F	7485	AMP	5	0
4	5-A	7476	CIT	4	0
3	4-R	7509	AMP	9	0
4	4-S	7512	CIT	4	0
4	5-H	7490	CIT	3	0
4	5-X	7522	CIT	4	0
4	5-Q	7508	CIT	3	0
4	10-D	7482	CIT	4	0
4	9-F	7486	CIT	3	0
3	7-P	7505	AMP	5	0
4	4-Q	7508	CIT	5	0
3	5-K	7495	AMP	8	0
3	4-F	7485	AMP	9	0
3	1-J	7493	AMP	4	0
3	6-T	7513	AMP	7	0
3	9-O	7503	AMP	7	0
3	10-E	7483	AMP	6	0
4	3-C	7480	CIT	4	0
4	9-X	7522	CIT	1	0
4	1-Q	7508	CIT	5	0
3	7-U	7515	AMP	5	0
4	8-J	7494	CIT	4	0
4	9-M	7500	CIT	2	0
4	10-A	7476	CIT	5	0
4	8-E	7484	CIT	4	0
4	6-P	7506	CIT	2	0
4	1-B	7478	CIT	5	0
3	10-I	7491	AMP	6	0
4	2-S	7512	CIT	2	0
3	10-L	7497	AMP	6	0
3	5-Q	7507	AMP	7	0
4	2-N	7502	CIT	3	0
3	6-D	7481	AMP	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	3-S	7511	AMP	10	0
3	8-Q	7507	AMP	6	0
3	6-N	7501	AMP	7	0
3	5-R	7509	AMP	7	0
3	1-I	7491	AMP	4	0
4	7-T	7514	CIT	6	0
3	1-L	7497	AMP	4	0
3	4-P	7505	AMP	10	0
4	2-B	7478	CIT	3	0
4	8-F	7486	CIT	4	0
4	3-I	7492	CIT	4	0
3	7-I	7491	AMP	5	0
4	4-P	7506	CIT	4	0
4	1-W	7520	CIT	5	0
3	7-M	7499	AMP	5	0
4	2-V	7518	CIT	4	0
3	10-N	7501	AMP	6	0
4	10-K	7496	CIT	4	0
3	3-F	7485	AMP	10	0
3	2-K	7495	AMP	7	0
3	1-S	7511	AMP	4	0
4	9-G	7488	CIT	3	0
4	1-U	7516	CIT	5	0
4	2-O	7504	CIT	3	0
3	3-K	7495	AMP	11	0
3	2-W	7519	AMP	6	0
3	10-M	7499	AMP	6	0
4	1-V	7518	CIT	5	0
4	3-R	7510	CIT	4	0
3	8-M	7499	AMP	6	0
3	4-Q	7507	AMP	10	0
3	10-X	7521	AMP	6	0
3	6-F	7485	AMP	7	0
3	10-A	7475	AMP	6	0
3	3-U	7515	AMP	10	0
3	7-V	7517	AMP	5	0
4	7-B	7478	CIT	5	0
3	10-S	7511	AMP	6	0
3	5-W	7519	AMP	7	0
4	10-S	7512	CIT	3	0
4	5-R	7510	CIT	4	0
3	4-A	7475	AMP	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	9-A	7476	CIT	3	0
3	5-L	7497	AMP	7	0
4	7-F	7486	CIT	6	0
4	3-K	7496	CIT	4	0
3	1-H	7489	AMP	4	0
3	7-Q	7507	AMP	5	0
4	4-U	7516	CIT	5	0
3	9-R	7509	AMP	8	0
4	3-A	7476	CIT	4	0
3	3-A	7475	AMP	10	0
3	7-R	7509	AMP	5	0
4	8-H	7490	CIT	4	0
3	5-J	7493	AMP	7	0
4	7-M	7500	CIT	6	0
4	7-D	7482	CIT	6	0
4	10-E	7484	CIT	3	0
4	7-K	7496	CIT	6	0
4	5-D	7482	CIT	3	0
4	2-I	7492	CIT	3	0
4	8-M	7500	CIT	4	0
3	3-V	7517	AMP	10	0
4	1-R	7510	CIT	5	0
4	10-Q	7508	CIT	3	0
3	6-S	7511	AMP	7	0
4	10-G	7488	CIT	4	0
4	9-K	7496	CIT	3	0
3	5-A	7475	AMP	7	0
3	3-H	7489	AMP	10	0
4	10-F	7486	CIT	4	0
4	7-V	7518	CIT	6	0
3	5-G	7487	AMP	7	0
4	6-F	7486	CIT	2	0
4	8-A	7476	CIT	4	0
3	3-Q	7507	AMP	10	0
3	8-B	7477	AMP	6	0
4	1-O	7504	CIT	5	0
3	7-E	7483	AMP	5	0
3	5-H	7489	AMP	7	0
4	9-R	7510	CIT	3	0
3	9-S	7511	AMP	8	0
3	10-O	7503	AMP	6	0
4	9-V	7518	CIT	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	4-K	7496	CIT	3	0
4	9-Q	7508	CIT	1	0
3	9-D	7481	AMP	8	0
4	3-P	7506	CIT	4	0
4	10-N	7502	CIT	4	0
3	5-V	7517	AMP	7	0
4	3-M	7500	CIT	4	0
4	5-E	7484	CIT	3	0
3	1-T	7513	AMP	4	0
4	4-C	7480	CIT	4	0
4	10-W	7520	CIT	4	0
3	5-U	7515	AMP	7	0
4	3-B	7478	CIT	4	0
3	5-M	7499	AMP	7	0
3	8-G	7487	AMP	5	0
4	5-W	7520	CIT	4	0
3	1-R	7509	AMP	4	0
4	1-C	7480	CIT	5	0
4	6-S	7512	CIT	2	0
3	6-G	7487	AMP	7	0
4	6-N	7502	CIT	2	0
4	4-W	7520	CIT	3	0
4	5-V	7518	CIT	3	0
3	6-K	7495	AMP	8	0
3	6-P	7505	AMP	7	0
4	4-N	7502	CIT	4	0
4	4-B	7478	CIT	4	0
3	2-T	7513	AMP	7	0
3	7-X	7521	AMP	5	0
3	1-K	7495	AMP	5	0
4	3-V	7518	CIT	4	0
3	8-D	7481	AMP	5	0
3	9-A	7475	AMP	7	0
4	10-U	7516	CIT	5	0
3	10-D	7481	AMP	6	0
4	9-S	7512	CIT	3	0
3	9-G	7487	AMP	8	0
3	4-L	7497	AMP	9	0
4	9-N	7502	CIT	3	0
3	3-W	7519	AMP	10	0
3	1-B	7477	AMP	4	0
4	7-S	7512	CIT	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	10-H	7490	CIT	3	0
3	8-W	7519	AMP	6	0
3	8-A	7475	AMP	6	0
4	7-N	7502	CIT	5	0
3	10-K	7495	AMP	7	0
3	8-J	7493	AMP	6	0
3	6-Q	7507	AMP	7	0
3	4-X	7521	AMP	9	0
3	8-S	7511	AMP	5	0
3	4-W	7519	AMP	10	0
3	4-G	7487	AMP	10	0
3	4-J	7493	AMP	9	0
3	7-O	7503	AMP	5	0
4	6-A	7476	CIT	3	0
4	4-L	7498	CIT	3	0
3	6-R	7509	AMP	7	0
3	6-L	7497	AMP	7	0
4	1-M	7500	CIT	5	0
3	1-F	7485	AMP	4	0
4	4-D	7482	CIT	3	0
4	6-X	7522	CIT	3	0
3	3-M	7499	AMP	10	0
3	9-Q	7507	AMP	8	0
4	2-C	7480	CIT	3	0
3	10-C	7479	AMP	6	0
3	7-G	7487	AMP	5	0
3	7-J	7493	AMP	5	0
4	1-A	7476	CIT	5	0
3	9-W	7519	AMP	8	0
4	2-W	7520	CIT	3	0
3	10-R	7509	AMP	6	0
4	2-M	7500	CIT	3	0
3	4-O	7503	AMP	10	0
3	9-J	7493	AMP	8	0
3	1-D	7481	AMP	4	0
4	10-X	7522	CIT	3	0
4	9-U	7516	CIT	3	0
4	8-L	7498	CIT	4	0
4	8-R	7510	CIT	4	0
4	4-G	7488	CIT	4	0
4	8-S	7512	CIT	4	0
3	8-R	7509	AMP	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	1-A	7475	AMP	4	0
3	9-P	7505	AMP	8	0
3	6-X	7521	AMP	7	0
4	2-L	7498	CIT	2	0
3	6-W	7519	AMP	7	0
4	3-H	7490	CIT	4	0
3	2-M	7499	AMP	7	0
4	5-L	7498	CIT	4	0
3	2-P	7505	AMP	7	0
3	2-A	7475	AMP	7	0
3	5-B	7477	AMP	8	0
4	7-G	7488	CIT	6	0
3	9-K	7495	AMP	9	0
4	6-U	7516	CIT	3	0
3	1-V	7517	AMP	4	0
3	10-V	7517	AMP	6	0
4	4-T	7514	CIT	4	0
3	3-G	7487	AMP	10	0
4	3-D	7482	CIT	4	0
4	8-V	7518	CIT	4	0
4	5-T	7514	CIT	3	0
3	6-V	7517	AMP	7	0
4	1-J	7494	CIT	5	0
3	8-K	7495	AMP	7	0
4	8-O	7504	CIT	4	0
4	9-E	7484	CIT	1	0
3	7-K	7495	AMP	6	0
3	1-U	7515	AMP	4	0
3	4-K	7495	AMP	10	0
3	5-S	7511	AMP	7	0
4	1-L	7498	CIT	5	0
3	5-I	7491	AMP	7	0
4	2-P	7506	CIT	2	0
4	8-I	7492	CIT	4	0
4	1-G	7488	CIT	5	0
4	10-I	7492	CIT	5	0
3	10-U	7515	AMP	5	0
3	4-B	7477	AMP	9	0
3	6-H	7489	AMP	7	0
4	2-D	7482	CIT	3	0
4	9-I	7492	CIT	3	0
4	8-X	7522	CIT	4	0

Continued on next page...

Continued from previous page...

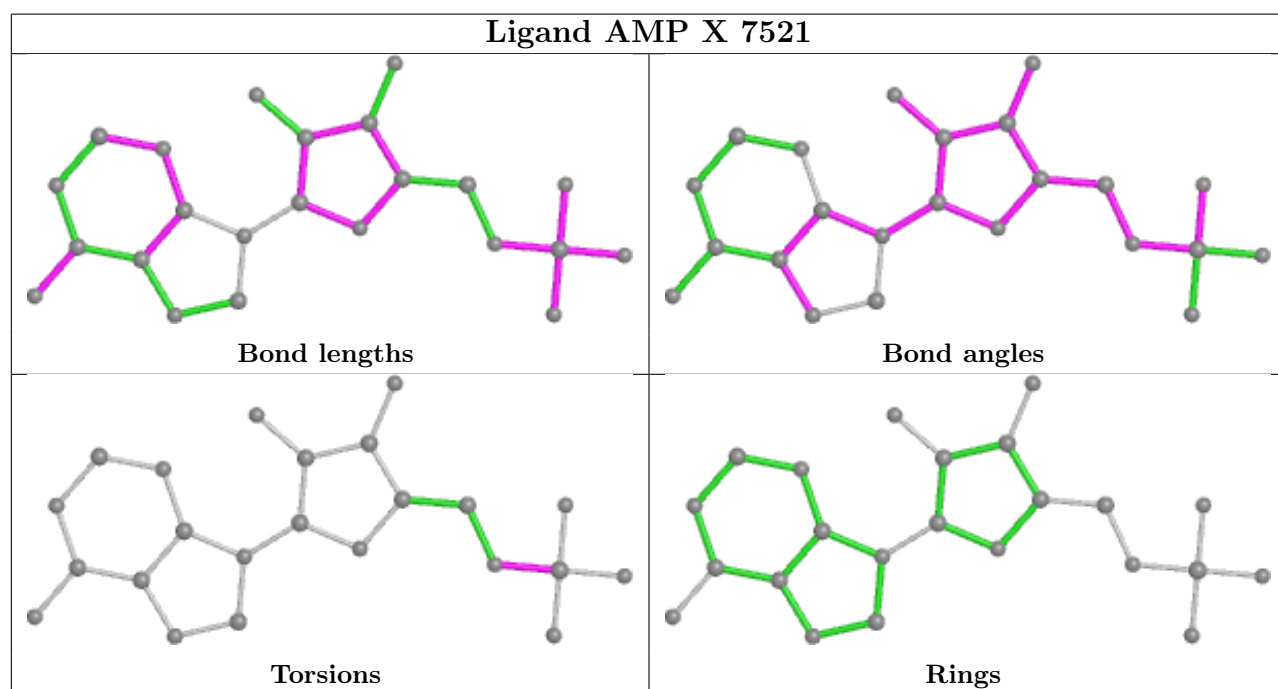
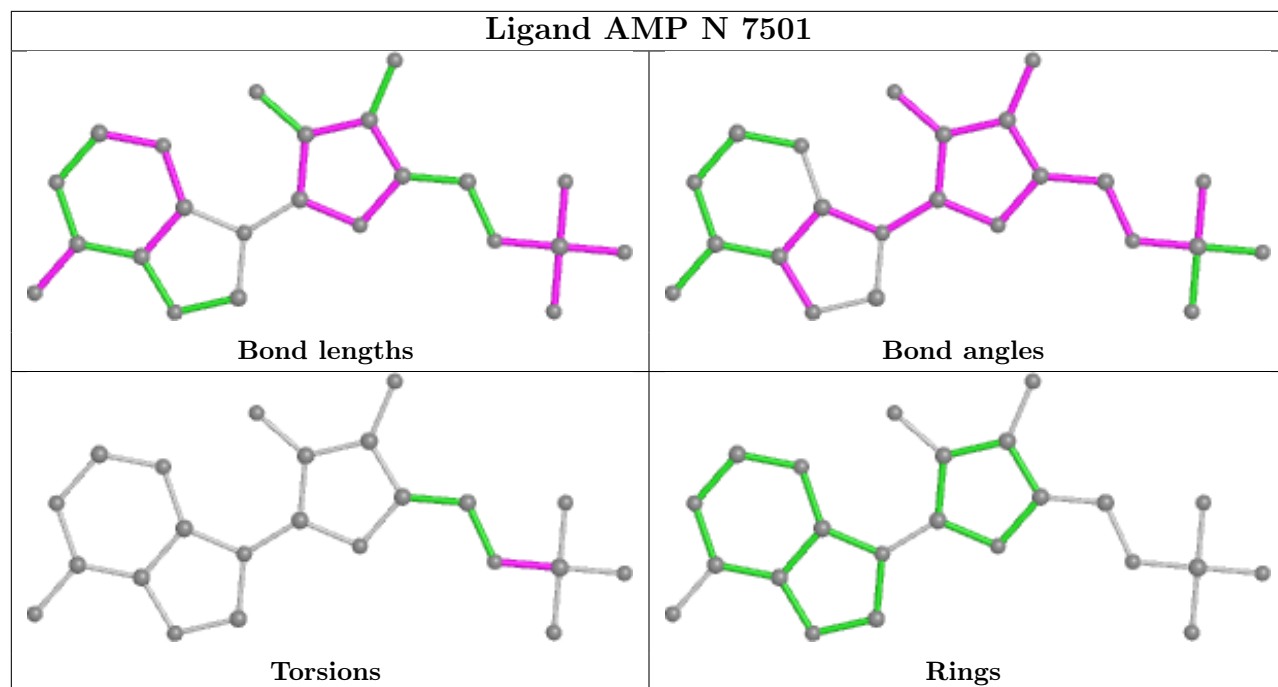
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	1-N	7502	CIT	5	0
3	10-G	7487	AMP	6	0
3	9-B	7477	AMP	8	0
4	10-L	7498	CIT	3	0
4	8-P	7506	CIT	4	0
3	3-N	7501	AMP	10	0
4	7-U	7516	CIT	6	0
3	3-T	7513	AMP	10	0
3	9-T	7513	AMP	8	0
3	10-H	7489	AMP	6	0
4	6-W	7520	CIT	3	0
3	4-E	7483	AMP	10	0
4	3-J	7494	CIT	4	0
3	9-F	7485	AMP	8	0
3	6-J	7493	AMP	7	0
3	1-M	7499	AMP	4	0
4	6-V	7518	CIT	3	0
4	4-A	7476	CIT	5	0
4	7-X	7522	CIT	5	0
3	4-I	7491	AMP	9	0
3	4-D	7481	AMP	10	0
3	9-U	7515	AMP	8	0
3	2-E	7483	AMP	7	0
3	2-C	7479	AMP	7	0
4	5-B	7478	CIT	3	0
4	1-I	7492	CIT	5	0
3	5-D	7481	AMP	7	0
3	7-S	7511	AMP	5	0
4	4-H	7490	CIT	4	0
4	3-L	7498	CIT	4	0
4	10-V	7518	CIT	4	0
4	3-G	7488	CIT	4	0
4	3-U	7516	CIT	4	0
4	8-G	7488	CIT	4	0
4	10-B	7478	CIT	4	0
3	5-E	7483	AMP	7	0
4	5-C	7480	CIT	4	0
4	3-T	7514	CIT	4	0
4	4-R	7510	CIT	3	0
3	6-E	7483	AMP	7	0
3	7-T	7513	AMP	5	0
4	8-T	7514	CIT	4	0

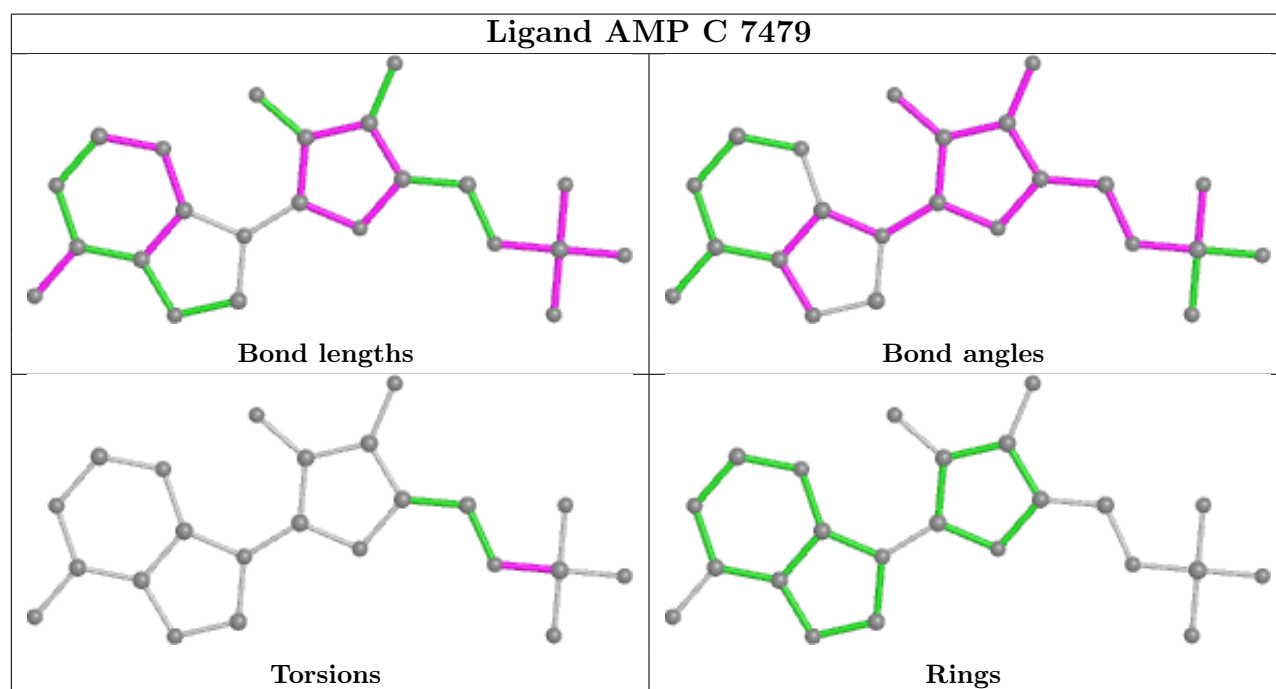
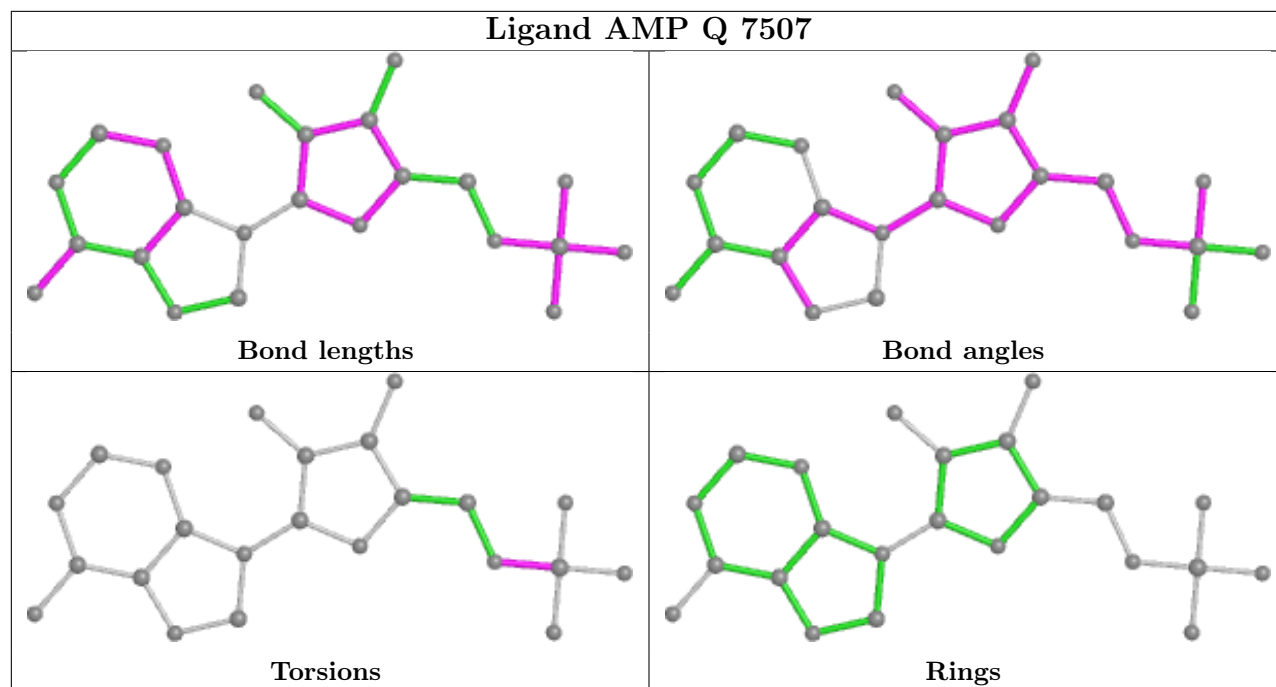
Continued on next page...

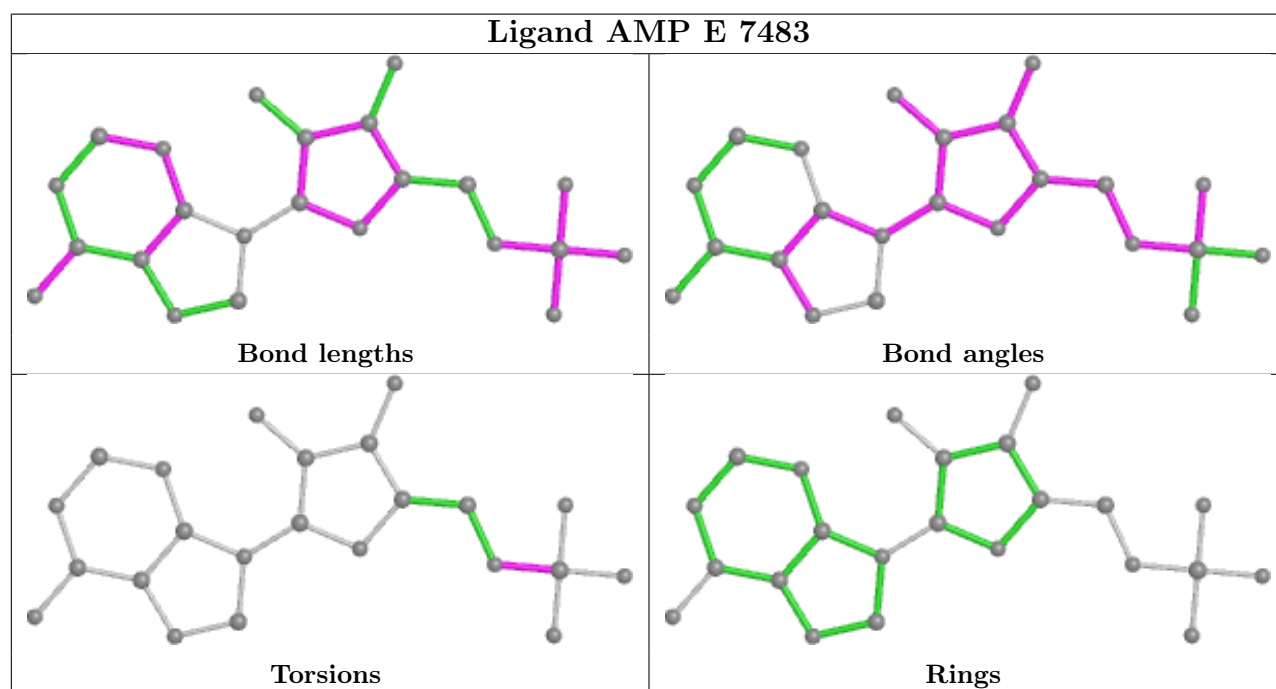
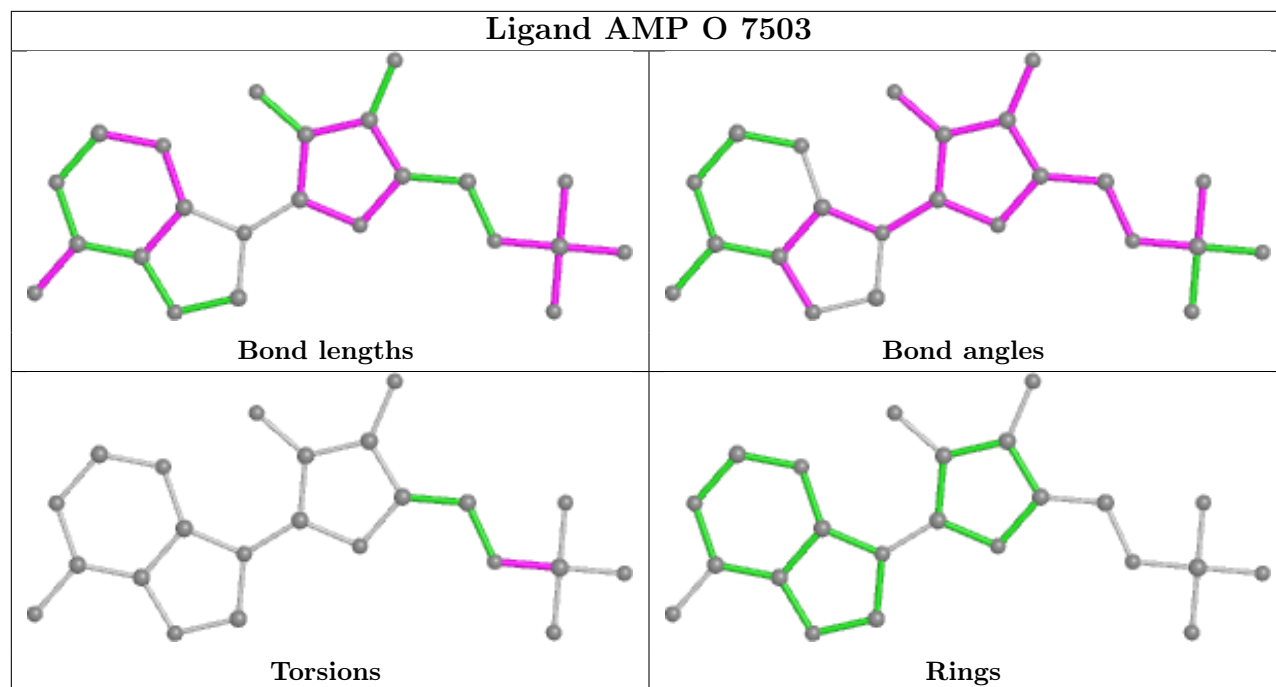
Continued from previous page...

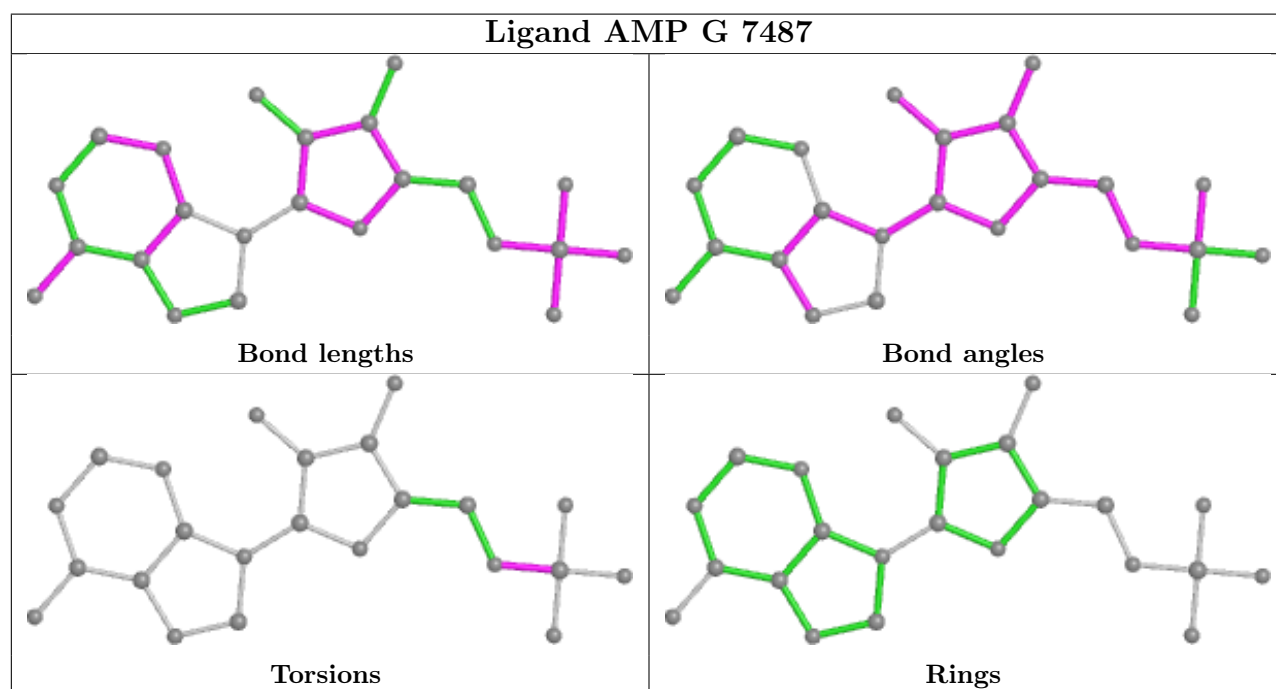
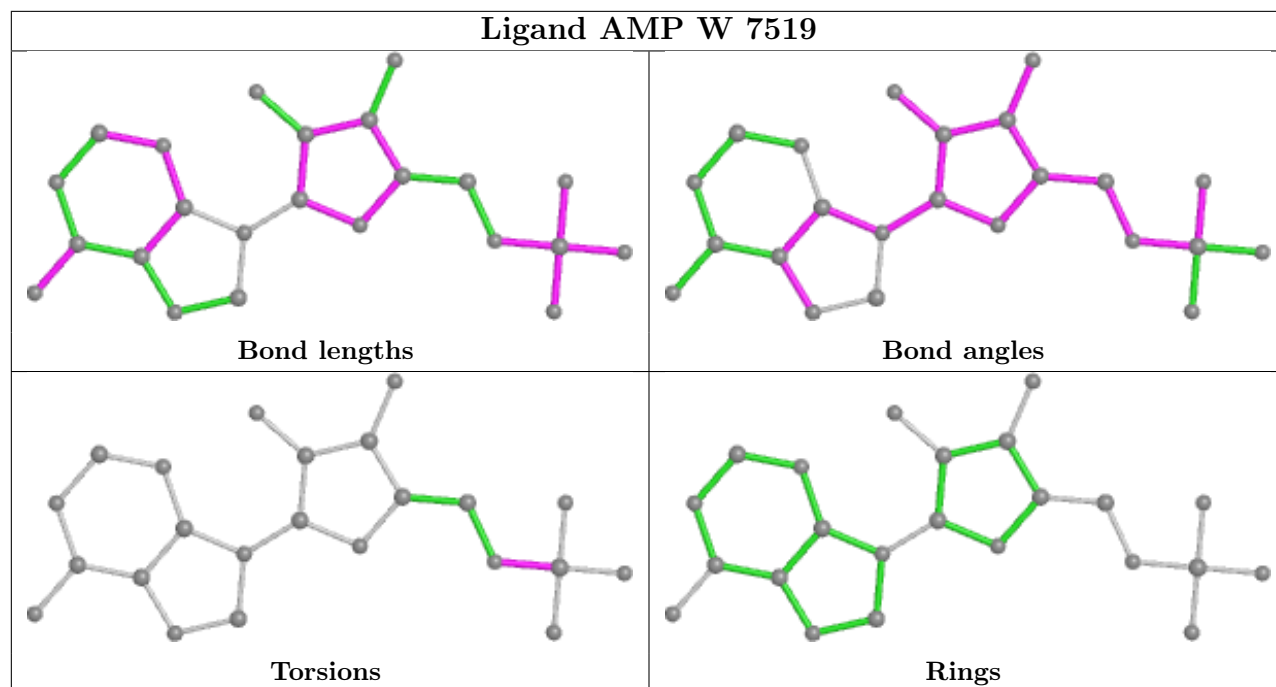
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	7-H	7490	CIT	6	0
4	1-D	7482	CIT	5	0
4	6-C	7480	CIT	3	0
4	3-X	7522	CIT	4	0
3	3-C	7479	AMP	10	0
3	3-O	7503	AMP	10	0
3	4-V	7517	AMP	9	0
3	3-R	7509	AMP	10	0
4	4-E	7484	CIT	5	0
4	6-G	7488	CIT	2	0
3	8-I	7491	AMP	5	0
3	2-H	7489	AMP	7	0
4	10-J	7494	CIT	4	0
4	6-B	7478	CIT	2	0
4	8-N	7502	CIT	4	0
4	7-W	7520	CIT	6	0
3	2-F	7485	AMP	7	0
3	7-D	7481	AMP	5	0
4	9-P	7506	CIT	3	0
4	7-C	7480	CIT	6	0
3	8-U	7515	AMP	5	0
4	5-K	7496	CIT	4	0
4	10-C	7480	CIT	4	0
3	4-H	7489	AMP	10	0
4	2-U	7516	CIT	3	0
3	4-U	7515	AMP	9	0
4	2-E	7484	CIT	3	0
3	5-P	7505	AMP	7	0
3	3-D	7481	AMP	10	0
4	5-M	7500	CIT	3	0

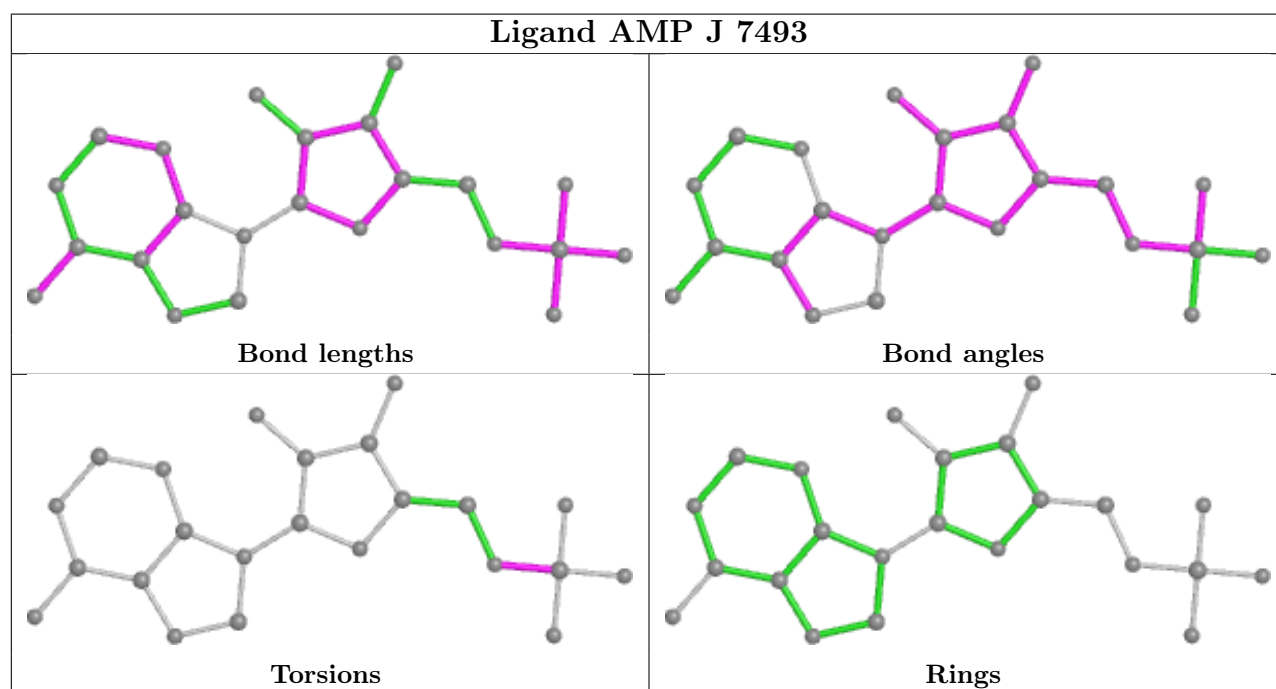
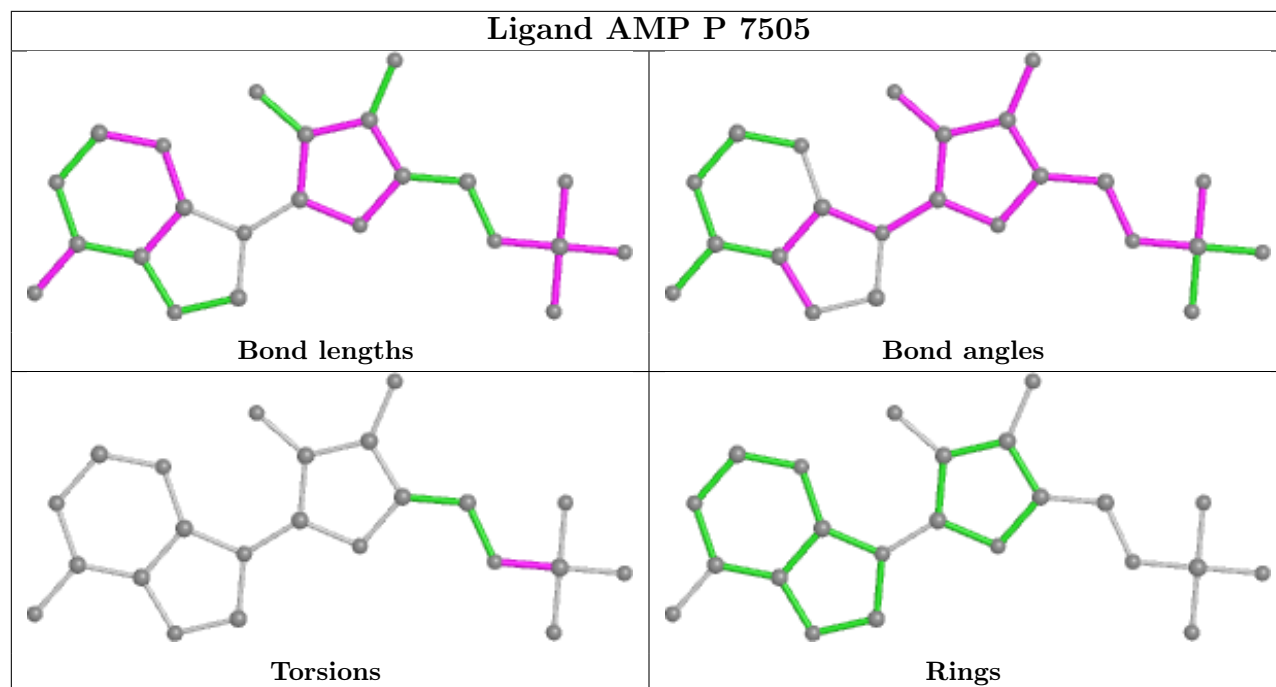
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

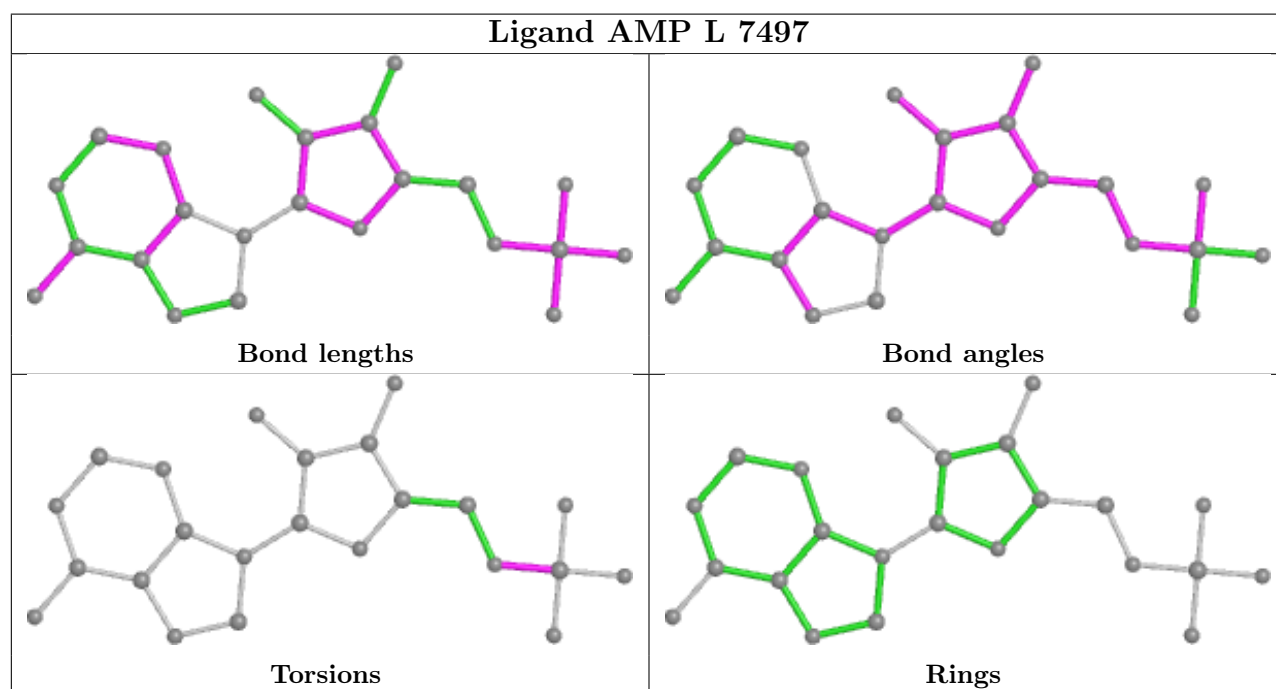
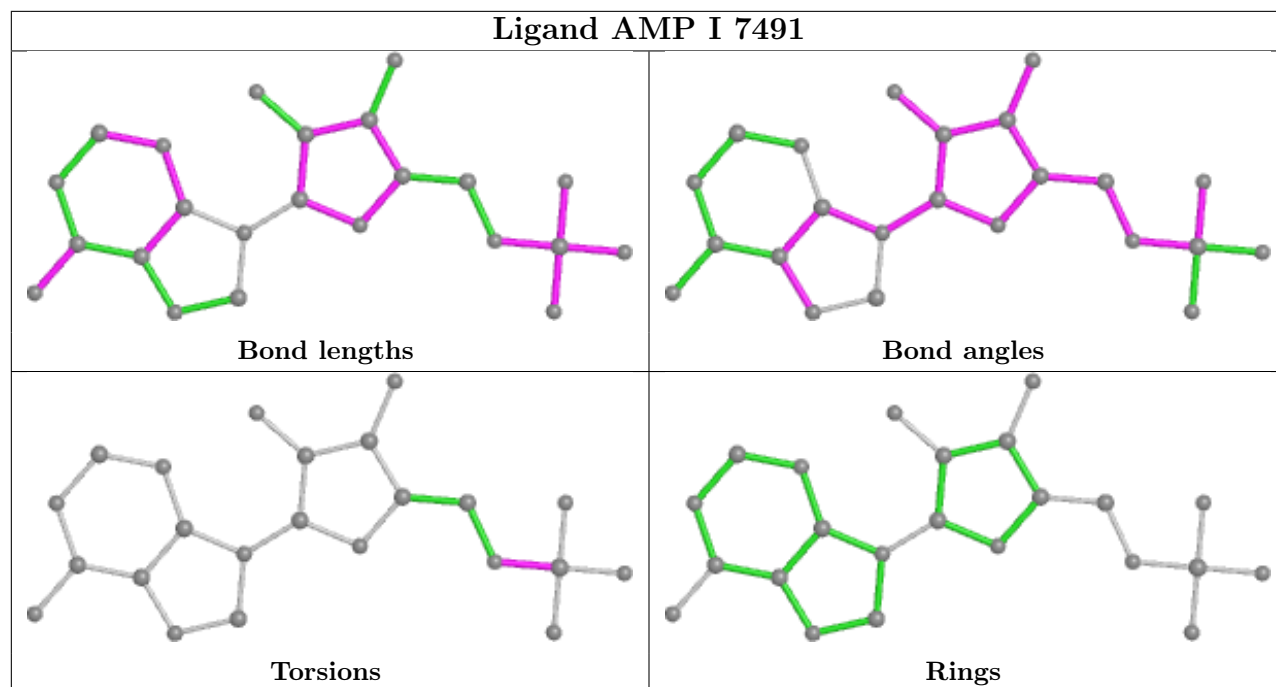


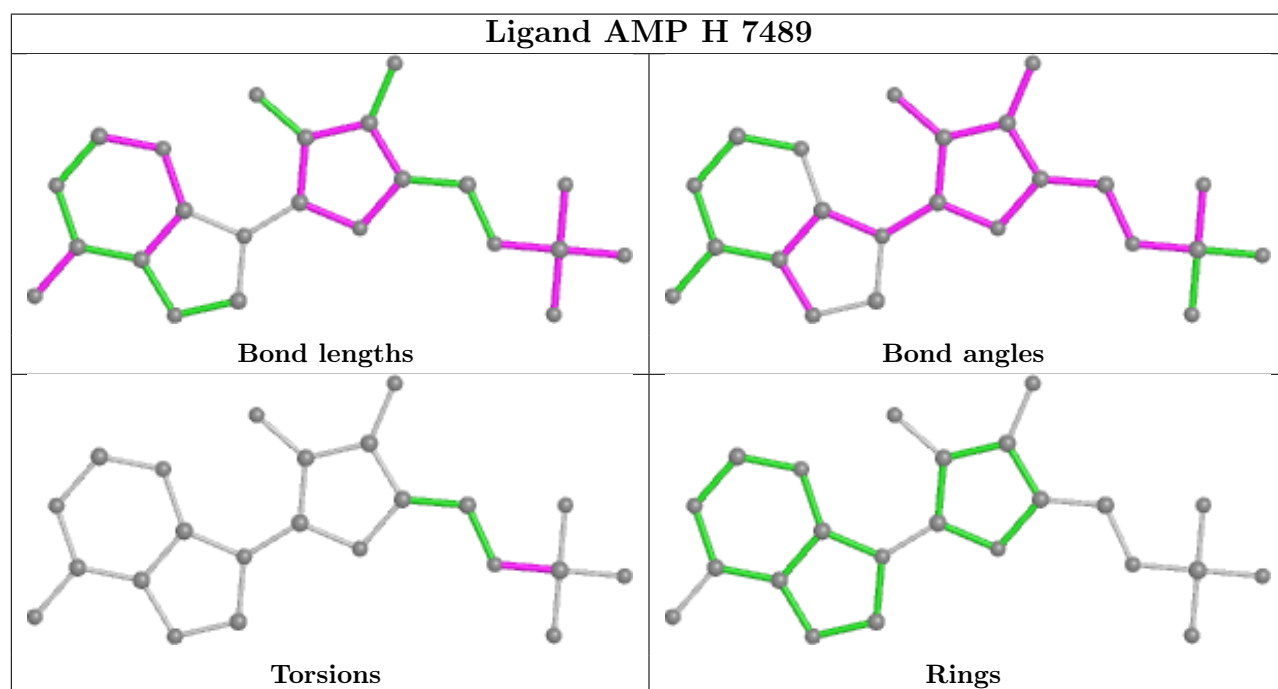
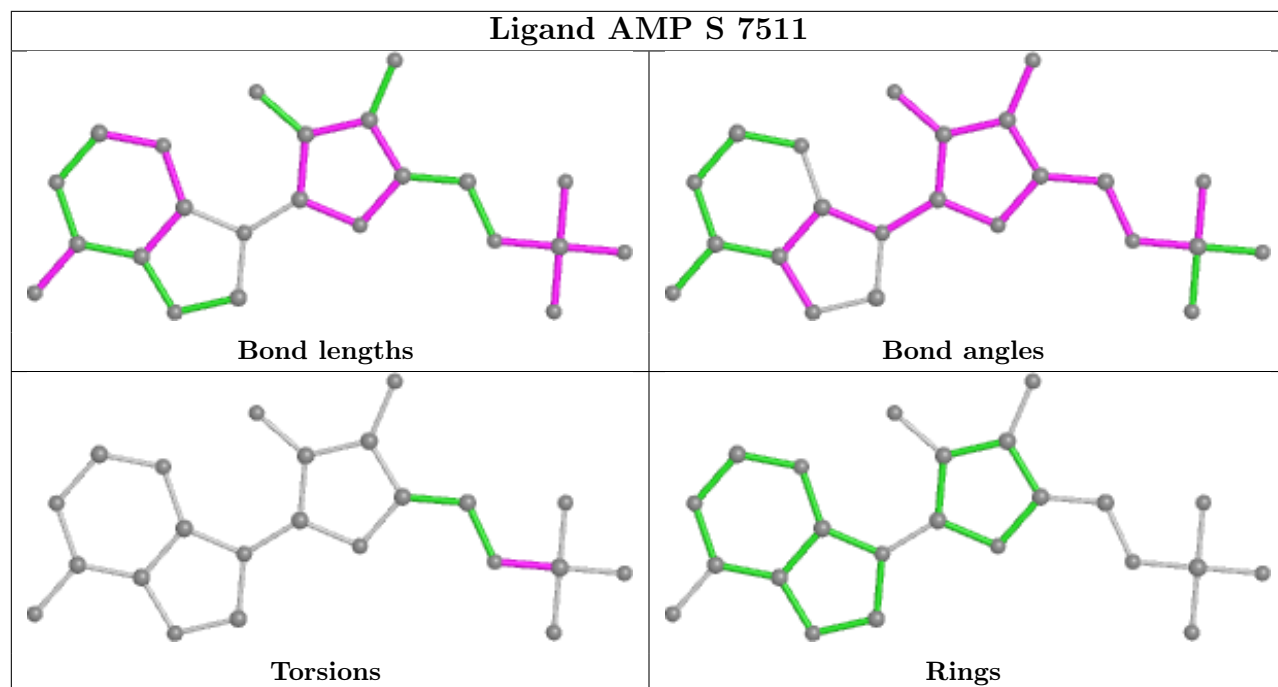


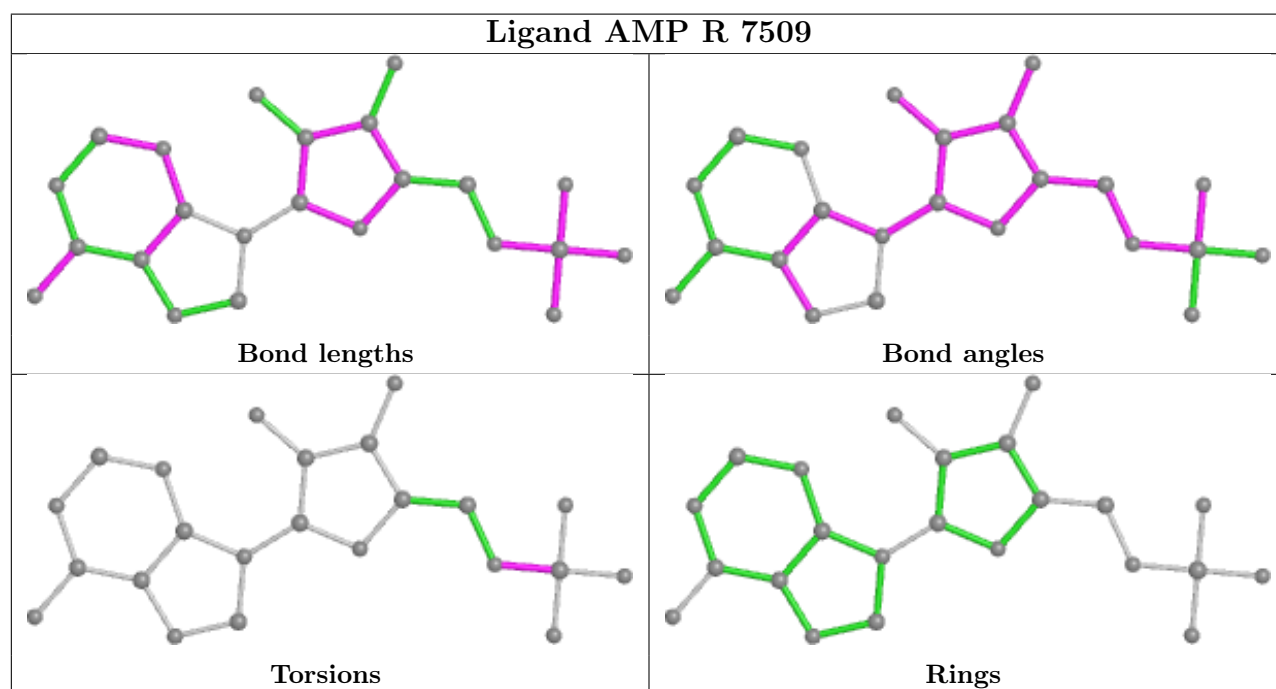
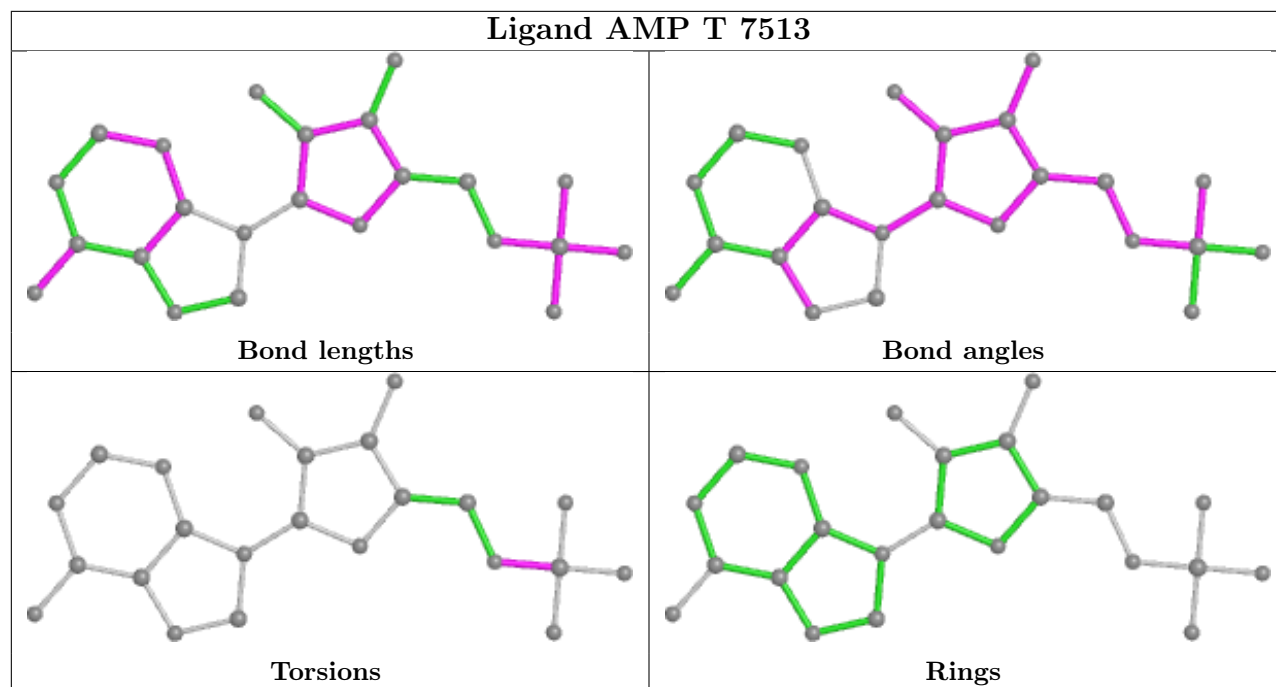


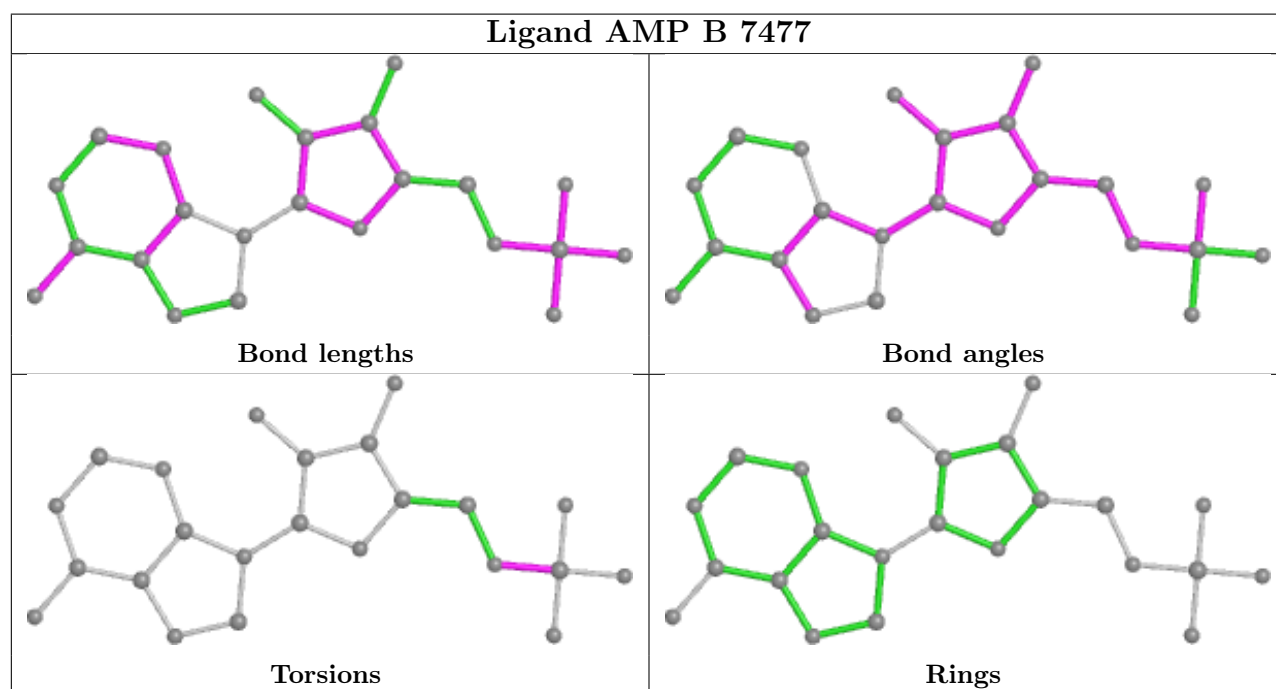
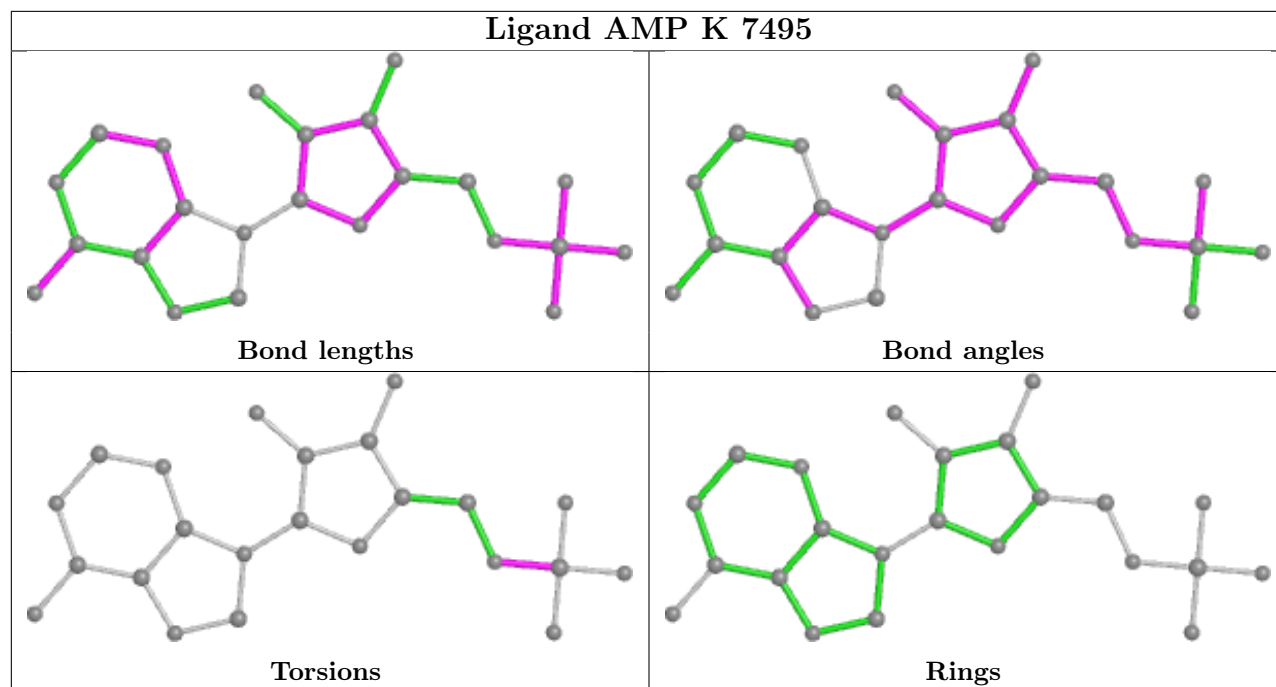


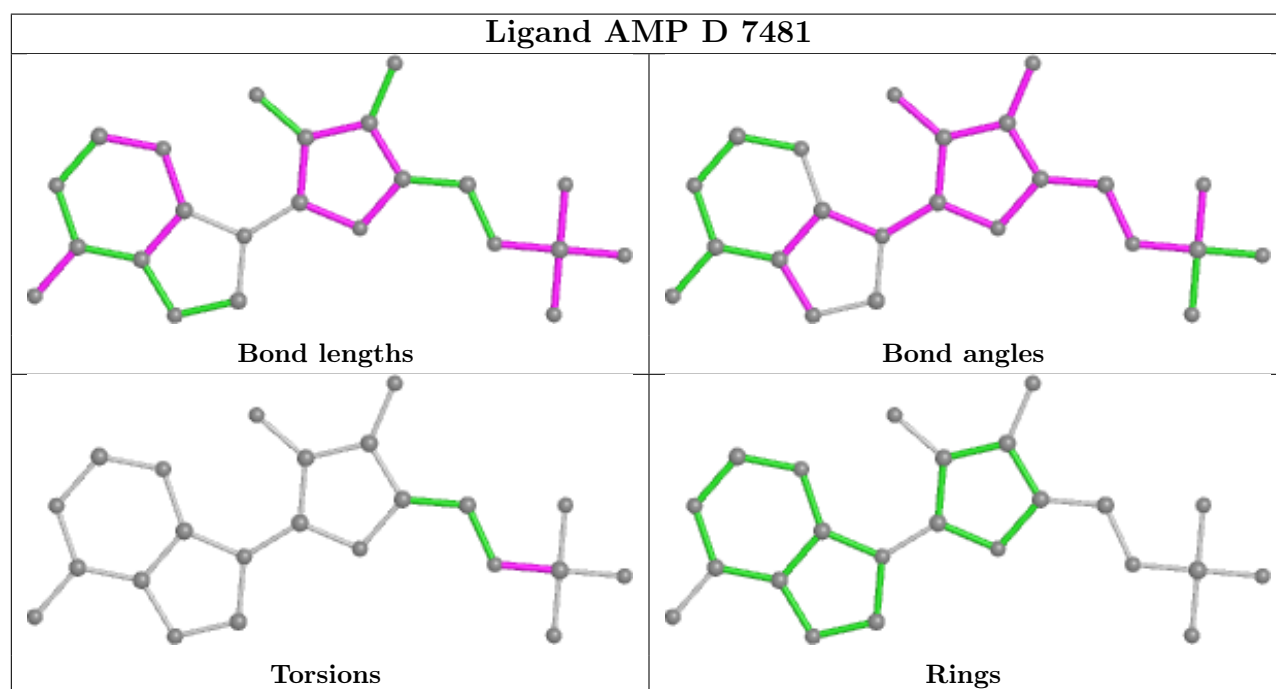
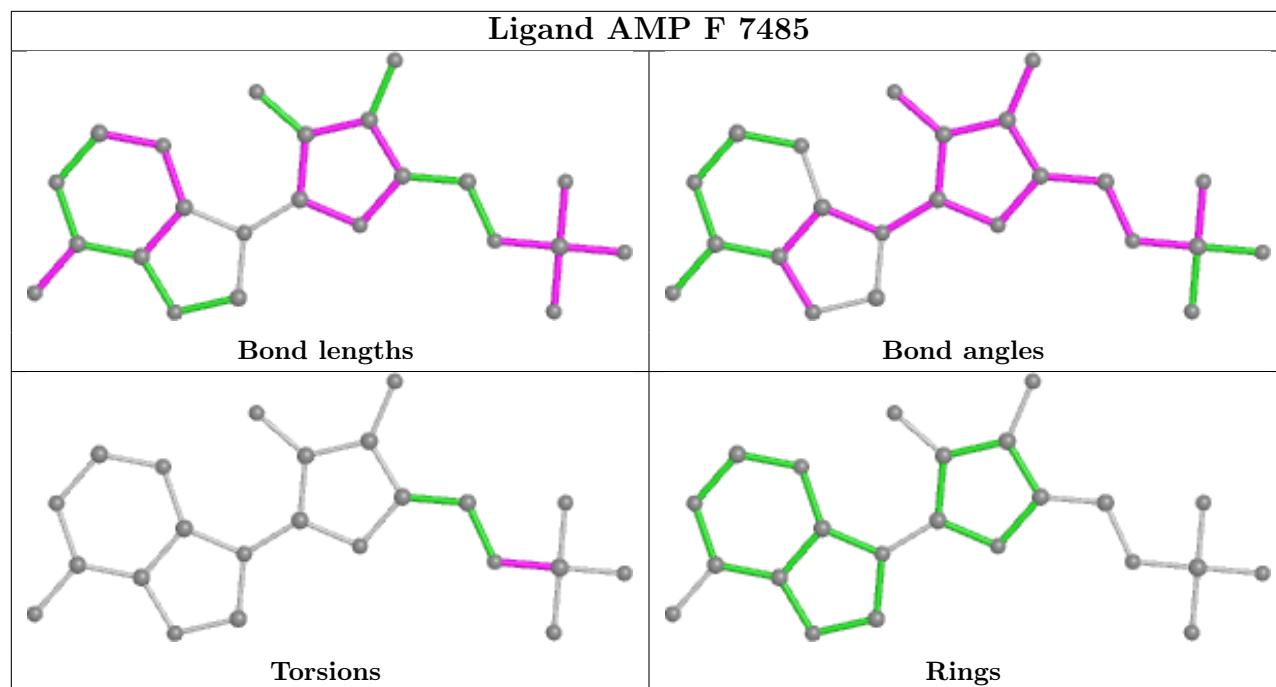


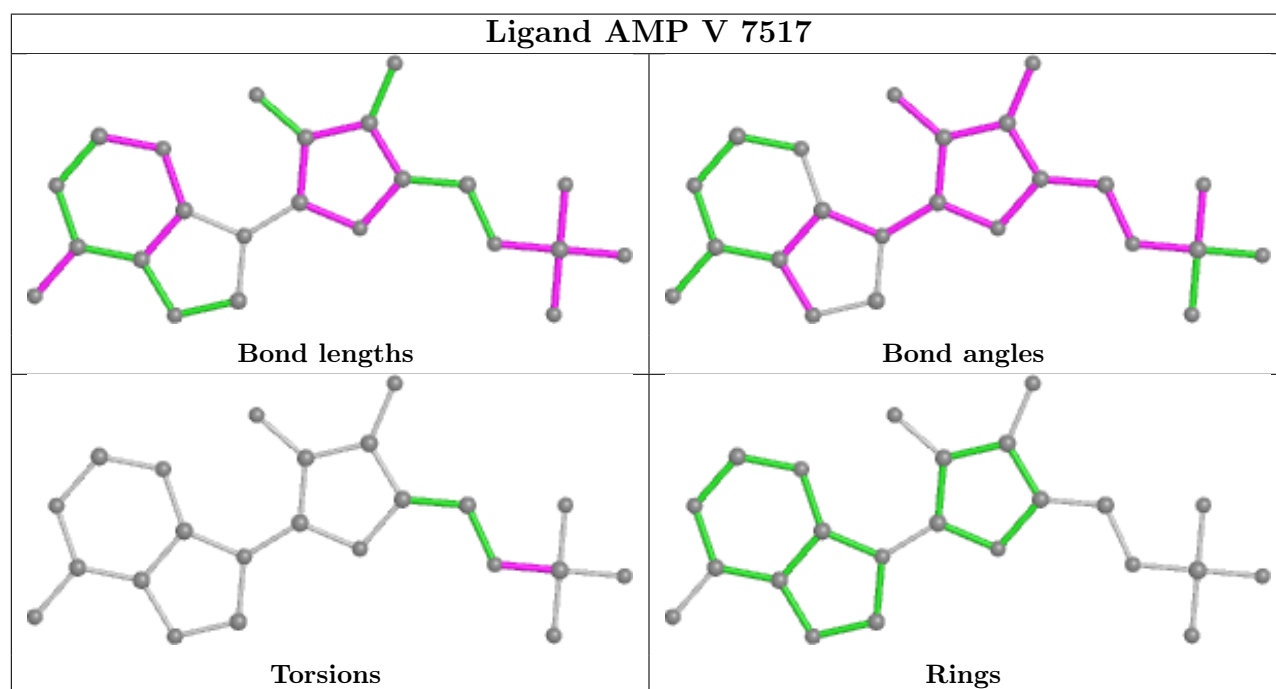
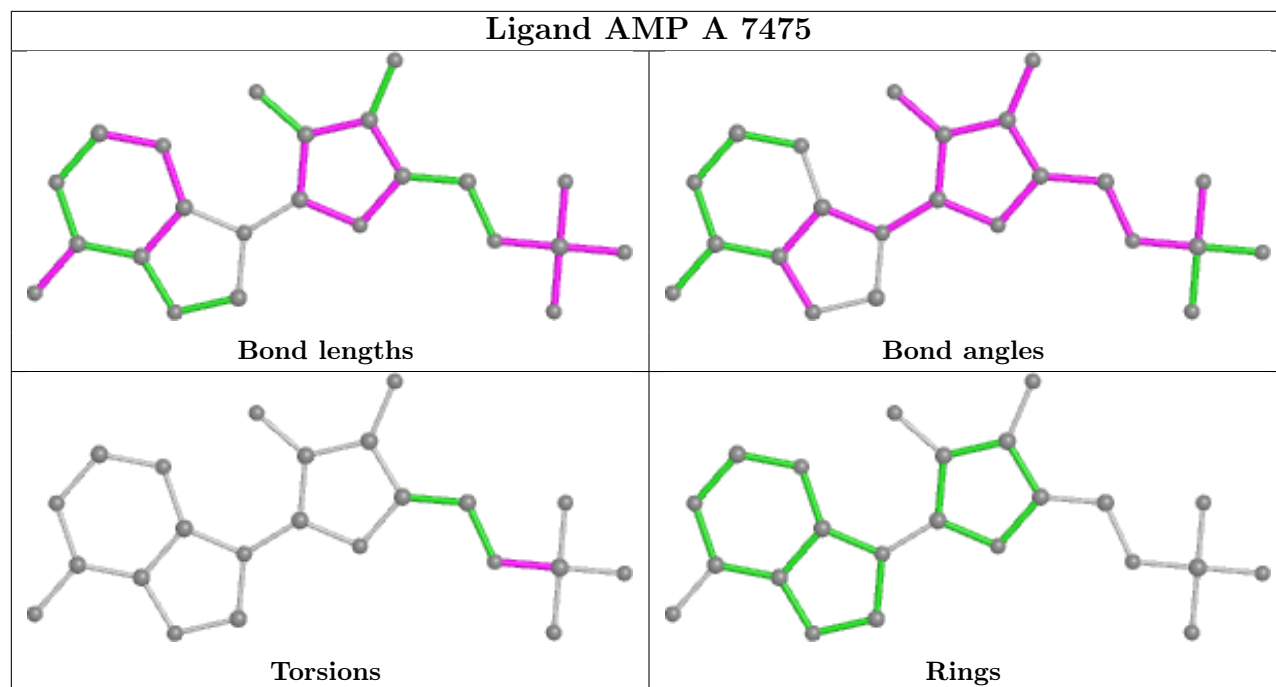


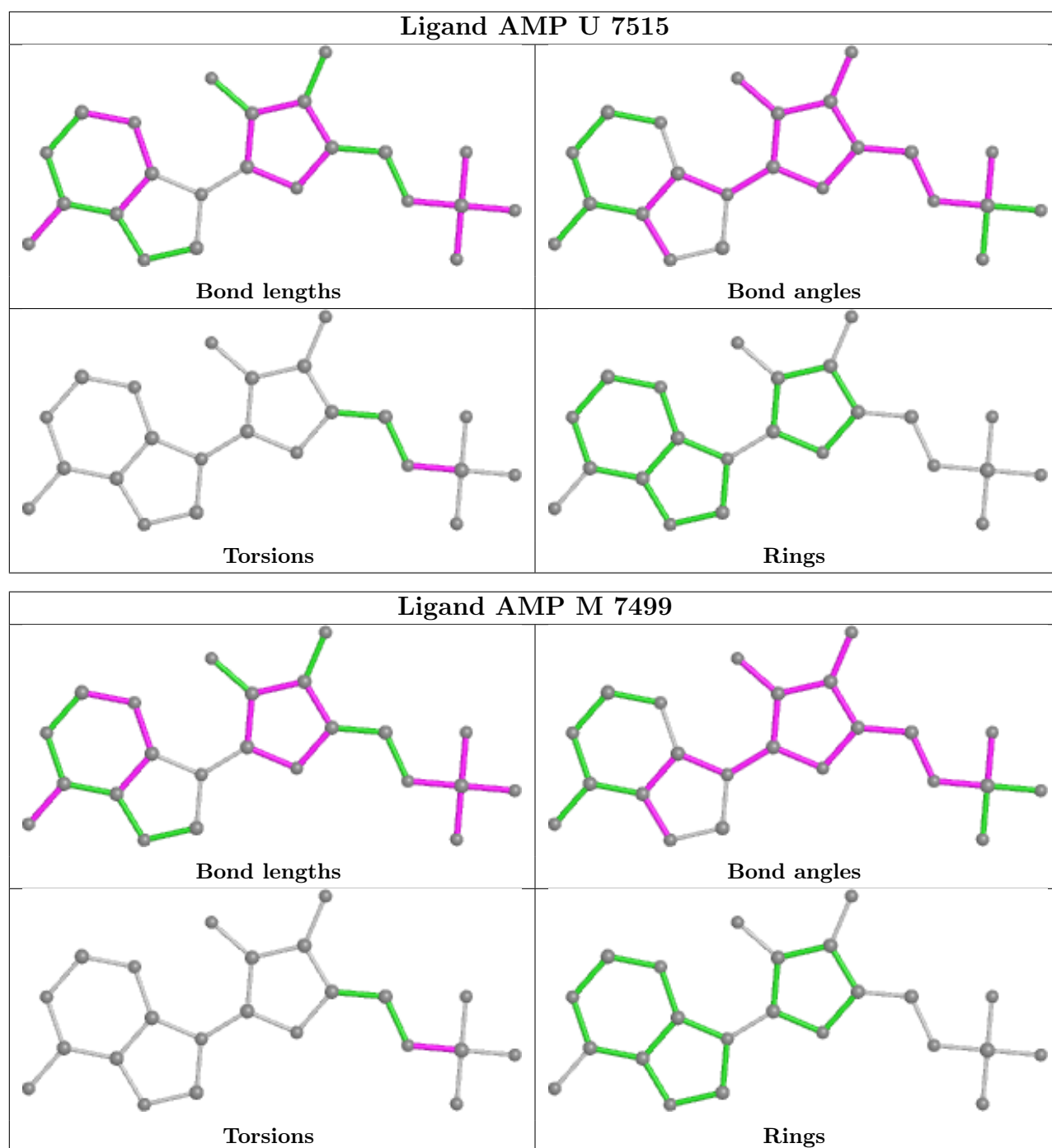












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	477/477 (100%)	0.55	66 (13%) 2 2	11, 24, 38, 60	477 (100%)
1	1-B	477/477 (100%)	0.66	63 (13%) 3 3	11, 24, 38, 60	477 (100%)
1	1-C	477/477 (100%)	0.86	86 (18%) 1 1	11, 24, 38, 60	477 (100%)
1	1-D	477/477 (100%)	0.61	72 (15%) 2 1	11, 24, 38, 60	477 (100%)
1	1-E	477/477 (100%)	0.69	77 (16%) 1 1	11, 24, 38, 60	477 (100%)
1	1-F	477/477 (100%)	0.60	57 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	1-G	477/477 (100%)	0.67	60 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	1-H	477/477 (100%)	0.66	66 (13%) 2 2	11, 24, 38, 60	477 (100%)
1	1-I	477/477 (100%)	0.89	80 (16%) 1 1	11, 24, 38, 60	477 (100%)
1	1-J	477/477 (100%)	0.52	56 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	1-K	477/477 (100%)	0.68	68 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	1-L	477/477 (100%)	0.80	62 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	1-M	477/477 (100%)	0.70	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	1-N	477/477 (100%)	0.79	65 (13%) 3 2	11, 24, 38, 60	477 (100%)
1	1-O	477/477 (100%)	0.88	74 (15%) 2 1	11, 24, 38, 60	477 (100%)
1	1-P	477/477 (100%)	0.79	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	1-Q	477/477 (100%)	0.86	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	1-R	477/477 (100%)	0.76	56 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	1-S	477/477 (100%)	0.57	53 (11%) 5 4	11, 24, 38, 60	477 (100%)
1	1-T	477/477 (100%)	0.59	64 (13%) 3 2	11, 24, 38, 60	477 (100%)
1	1-U	477/477 (100%)	0.83	83 (17%) 1 1	11, 24, 38, 60	477 (100%)
1	1-V	477/477 (100%)	0.55	60 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	1-W	477/477 (100%)	0.49	58 (12%) 4 3	11, 24, 38, 60	477 (100%)
1	1-X	477/477 (100%)	0.64	65 (13%) 3 2	11, 24, 38, 60	477 (100%)

Continued on next page..

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	2-A	477/477 (100%)	0.55	66 (13%) 2 2	11, 24, 38, 60	477 (100%)
1	2-B	477/477 (100%)	0.66	63 (13%) 3 3	11, 24, 38, 60	477 (100%)
1	2-C	477/477 (100%)	0.86	86 (18%) 1 1	11, 24, 38, 60	477 (100%)
1	2-D	477/477 (100%)	0.61	72 (15%) 2 1	11, 24, 38, 60	477 (100%)
1	2-E	477/477 (100%)	0.69	77 (16%) 1 1	11, 24, 38, 60	477 (100%)
1	2-F	477/477 (100%)	0.60	57 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	2-G	477/477 (100%)	0.67	60 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	2-H	477/477 (100%)	0.66	66 (13%) 2 2	11, 24, 38, 60	477 (100%)
1	2-I	477/477 (100%)	0.89	80 (16%) 1 1	11, 24, 38, 60	477 (100%)
1	2-J	477/477 (100%)	0.52	56 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	2-K	477/477 (100%)	0.68	68 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	2-L	477/477 (100%)	0.80	62 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	2-M	477/477 (100%)	0.70	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	2-N	477/477 (100%)	0.79	65 (13%) 3 2	11, 24, 38, 60	477 (100%)
1	2-O	477/477 (100%)	0.88	74 (15%) 2 1	11, 24, 38, 60	477 (100%)
1	2-P	477/477 (100%)	0.79	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	2-Q	477/477 (100%)	0.86	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	2-R	477/477 (100%)	0.76	56 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	2-S	477/477 (100%)	0.57	53 (11%) 5 4	11, 24, 38, 60	477 (100%)
1	2-T	477/477 (100%)	0.59	64 (13%) 3 2	11, 24, 38, 60	477 (100%)
1	2-U	477/477 (100%)	0.83	83 (17%) 1 1	11, 24, 38, 60	477 (100%)
1	2-V	477/477 (100%)	0.55	60 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	2-W	477/477 (100%)	0.49	58 (12%) 4 3	11, 24, 38, 60	477 (100%)
1	2-X	477/477 (100%)	0.64	65 (13%) 3 2	11, 24, 38, 60	477 (100%)
1	3-A	477/477 (100%)	0.55	66 (13%) 2 2	11, 24, 38, 60	477 (100%)
1	3-B	477/477 (100%)	0.66	63 (13%) 3 3	11, 24, 38, 60	477 (100%)
1	3-C	477/477 (100%)	0.86	86 (18%) 1 1	11, 24, 38, 60	477 (100%)
1	3-D	477/477 (100%)	0.61	72 (15%) 2 1	11, 24, 38, 60	477 (100%)
1	3-E	477/477 (100%)	0.69	77 (16%) 1 1	11, 24, 38, 60	477 (100%)
1	3-F	477/477 (100%)	0.60	57 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	3-G	477/477 (100%)	0.67	60 (12%) 3 3	11, 24, 38, 60	477 (100%)

Continued on next page..

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	3-H	477/477 (100%)	0.66	66 (13%) 2 2	11, 24, 38, 60	477 (100%)
1	3-I	477/477 (100%)	0.89	80 (16%) 1 1	11, 24, 38, 60	477 (100%)
1	3-J	477/477 (100%)	0.52	56 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	3-K	477/477 (100%)	0.68	68 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	3-L	477/477 (100%)	0.80	62 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	3-M	477/477 (100%)	0.70	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	3-N	477/477 (100%)	0.79	65 (13%) 3 2	11, 24, 38, 60	477 (100%)
1	3-O	477/477 (100%)	0.88	74 (15%) 2 1	11, 24, 38, 60	477 (100%)
1	3-P	477/477 (100%)	0.79	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	3-Q	477/477 (100%)	0.86	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	3-R	477/477 (100%)	0.76	56 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	3-S	477/477 (100%)	0.57	53 (11%) 5 4	11, 24, 38, 60	477 (100%)
1	3-T	477/477 (100%)	0.59	64 (13%) 3 2	11, 24, 38, 60	477 (100%)
1	3-U	477/477 (100%)	0.83	83 (17%) 1 1	11, 24, 38, 60	477 (100%)
1	3-V	477/477 (100%)	0.55	60 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	3-W	477/477 (100%)	0.49	58 (12%) 4 3	11, 24, 38, 60	477 (100%)
1	3-X	477/477 (100%)	0.64	65 (13%) 3 2	11, 24, 38, 60	477 (100%)
1	4-A	477/477 (100%)	0.55	66 (13%) 2 2	11, 24, 38, 60	477 (100%)
1	4-B	477/477 (100%)	0.66	63 (13%) 3 3	11, 24, 38, 60	477 (100%)
1	4-C	477/477 (100%)	0.86	86 (18%) 1 1	11, 24, 38, 60	477 (100%)
1	4-D	477/477 (100%)	0.61	72 (15%) 2 1	11, 24, 38, 60	477 (100%)
1	4-E	477/477 (100%)	0.69	77 (16%) 1 1	11, 24, 38, 60	477 (100%)
1	4-F	477/477 (100%)	0.60	57 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	4-G	477/477 (100%)	0.67	60 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	4-H	477/477 (100%)	0.66	66 (13%) 2 2	11, 24, 38, 60	477 (100%)
1	4-I	477/477 (100%)	0.89	80 (16%) 1 1	11, 24, 38, 60	477 (100%)
1	4-J	477/477 (100%)	0.52	56 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	4-K	477/477 (100%)	0.68	68 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	4-L	477/477 (100%)	0.80	62 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	4-M	477/477 (100%)	0.70	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	4-N	477/477 (100%)	0.79	65 (13%) 3 2	11, 24, 38, 60	477 (100%)

Continued on next page..

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	4-O	477/477 (100%)	0.88	74 (15%) 2 1	11, 24, 38, 60	477 (100%)
1	4-P	477/477 (100%)	0.79	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	4-Q	477/477 (100%)	0.86	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	4-R	477/477 (100%)	0.76	56 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	4-S	477/477 (100%)	0.57	53 (11%) 5 4	11, 24, 38, 60	477 (100%)
1	4-T	477/477 (100%)	0.59	64 (13%) 3 2	11, 24, 38, 60	477 (100%)
1	4-U	477/477 (100%)	0.83	83 (17%) 1 1	11, 24, 38, 60	477 (100%)
1	4-V	477/477 (100%)	0.55	60 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	4-W	477/477 (100%)	0.49	58 (12%) 4 3	11, 24, 38, 60	477 (100%)
1	4-X	477/477 (100%)	0.64	65 (13%) 3 2	11, 24, 38, 60	477 (100%)
1	5-A	477/477 (100%)	0.55	66 (13%) 2 2	11, 24, 38, 60	477 (100%)
1	5-B	477/477 (100%)	0.66	63 (13%) 3 3	11, 24, 38, 60	477 (100%)
1	5-C	477/477 (100%)	0.86	86 (18%) 1 1	11, 24, 38, 60	477 (100%)
1	5-D	477/477 (100%)	0.61	72 (15%) 2 1	11, 24, 38, 60	477 (100%)
1	5-E	477/477 (100%)	0.69	77 (16%) 1 1	11, 24, 38, 60	477 (100%)
1	5-F	477/477 (100%)	0.60	57 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	5-G	477/477 (100%)	0.67	60 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	5-H	477/477 (100%)	0.66	66 (13%) 2 2	11, 24, 38, 60	477 (100%)
1	5-I	477/477 (100%)	0.89	80 (16%) 1 1	11, 24, 38, 60	477 (100%)
1	5-J	477/477 (100%)	0.52	56 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	5-K	477/477 (100%)	0.68	68 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	5-L	477/477 (100%)	0.80	62 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	5-M	477/477 (100%)	0.70	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	5-N	477/477 (100%)	0.79	65 (13%) 3 2	11, 24, 38, 60	477 (100%)
1	5-O	477/477 (100%)	0.88	74 (15%) 2 1	11, 24, 38, 60	477 (100%)
1	5-P	477/477 (100%)	0.79	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	5-Q	477/477 (100%)	0.86	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	5-R	477/477 (100%)	0.76	56 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	5-S	477/477 (100%)	0.57	53 (11%) 5 4	11, 24, 38, 60	477 (100%)
1	5-T	477/477 (100%)	0.59	64 (13%) 3 2	11, 24, 38, 60	477 (100%)
1	5-U	477/477 (100%)	0.83	83 (17%) 1 1	11, 24, 38, 60	477 (100%)

Continued on next page..

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	5-V	477/477 (100%)	0.55	60 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	5-W	477/477 (100%)	0.49	58 (12%) 4 3	11, 24, 38, 60	477 (100%)
1	5-X	477/477 (100%)	0.64	65 (13%) 3 2	11, 24, 38, 60	477 (100%)
1	6-A	477/477 (100%)	0.55	66 (13%) 2 2	11, 24, 38, 60	477 (100%)
1	6-B	477/477 (100%)	0.66	63 (13%) 3 3	11, 24, 38, 60	477 (100%)
1	6-C	477/477 (100%)	0.86	86 (18%) 1 1	11, 24, 38, 60	477 (100%)
1	6-D	477/477 (100%)	0.61	72 (15%) 2 1	11, 24, 38, 60	477 (100%)
1	6-E	477/477 (100%)	0.69	77 (16%) 1 1	11, 24, 38, 60	477 (100%)
1	6-F	477/477 (100%)	0.60	57 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	6-G	477/477 (100%)	0.67	60 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	6-H	477/477 (100%)	0.66	66 (13%) 2 2	11, 24, 38, 60	477 (100%)
1	6-I	477/477 (100%)	0.89	80 (16%) 1 1	11, 24, 38, 60	477 (100%)
1	6-J	477/477 (100%)	0.52	56 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	6-K	477/477 (100%)	0.68	68 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	6-L	477/477 (100%)	0.80	62 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	6-M	477/477 (100%)	0.70	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	6-N	477/477 (100%)	0.79	65 (13%) 3 2	11, 24, 38, 60	477 (100%)
1	6-O	477/477 (100%)	0.88	74 (15%) 2 1	11, 24, 38, 60	477 (100%)
1	6-P	477/477 (100%)	0.79	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	6-Q	477/477 (100%)	0.86	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	6-R	477/477 (100%)	0.76	56 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	6-S	477/477 (100%)	0.57	53 (11%) 5 4	11, 24, 38, 60	477 (100%)
1	6-T	477/477 (100%)	0.59	64 (13%) 3 2	11, 24, 38, 60	477 (100%)
1	6-U	477/477 (100%)	0.83	83 (17%) 1 1	11, 24, 38, 60	477 (100%)
1	6-V	477/477 (100%)	0.55	60 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	6-W	477/477 (100%)	0.49	58 (12%) 4 3	11, 24, 38, 60	477 (100%)
1	6-X	477/477 (100%)	0.64	65 (13%) 3 2	11, 24, 38, 60	477 (100%)
1	7-A	477/477 (100%)	0.55	66 (13%) 2 2	11, 24, 38, 60	477 (100%)
1	7-B	477/477 (100%)	0.66	63 (13%) 3 3	11, 24, 38, 60	477 (100%)
1	7-C	477/477 (100%)	0.86	86 (18%) 1 1	11, 24, 38, 60	477 (100%)
1	7-D	477/477 (100%)	0.61	72 (15%) 2 1	11, 24, 38, 60	477 (100%)

Continued on next page..

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	7-E	477/477 (100%)	0.69	77 (16%) 1 1	11, 24, 38, 60	477 (100%)
1	7-F	477/477 (100%)	0.60	57 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	7-G	477/477 (100%)	0.67	60 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	7-H	477/477 (100%)	0.66	66 (13%) 2 2	11, 24, 38, 60	477 (100%)
1	7-I	477/477 (100%)	0.89	80 (16%) 1 1	11, 24, 38, 60	477 (100%)
1	7-J	477/477 (100%)	0.52	56 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	7-K	477/477 (100%)	0.68	68 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	7-L	477/477 (100%)	0.80	62 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	7-M	477/477 (100%)	0.70	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	7-N	477/477 (100%)	0.79	65 (13%) 3 2	11, 24, 38, 60	477 (100%)
1	7-O	477/477 (100%)	0.88	74 (15%) 2 1	11, 24, 38, 60	477 (100%)
1	7-P	477/477 (100%)	0.79	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	7-Q	477/477 (100%)	0.86	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	7-R	477/477 (100%)	0.76	56 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	7-S	477/477 (100%)	0.57	53 (11%) 5 4	11, 24, 38, 60	477 (100%)
1	7-T	477/477 (100%)	0.59	64 (13%) 3 2	11, 24, 38, 60	477 (100%)
1	7-U	477/477 (100%)	0.83	83 (17%) 1 1	11, 24, 38, 60	477 (100%)
1	7-V	477/477 (100%)	0.55	60 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	7-W	477/477 (100%)	0.49	58 (12%) 4 3	11, 24, 38, 60	477 (100%)
1	7-X	477/477 (100%)	0.64	65 (13%) 3 2	11, 24, 38, 60	477 (100%)
1	8-A	477/477 (100%)	0.55	66 (13%) 2 2	11, 24, 38, 60	477 (100%)
1	8-B	477/477 (100%)	0.66	63 (13%) 3 3	11, 24, 38, 60	477 (100%)
1	8-C	477/477 (100%)	0.86	86 (18%) 1 1	11, 24, 38, 60	477 (100%)
1	8-D	477/477 (100%)	0.61	72 (15%) 2 1	11, 24, 38, 60	477 (100%)
1	8-E	477/477 (100%)	0.69	77 (16%) 1 1	11, 24, 38, 60	477 (100%)
1	8-F	477/477 (100%)	0.60	57 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	8-G	477/477 (100%)	0.67	60 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	8-H	477/477 (100%)	0.66	66 (13%) 2 2	11, 24, 38, 60	477 (100%)
1	8-I	477/477 (100%)	0.89	80 (16%) 1 1	11, 24, 38, 60	477 (100%)
1	8-J	477/477 (100%)	0.52	56 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	8-K	477/477 (100%)	0.68	68 (14%) 2 2	11, 24, 38, 60	477 (100%)

Continued on next page..

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	8-L	477/477 (100%)	0.80	62 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	8-M	477/477 (100%)	0.70	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	8-N	477/477 (100%)	0.79	65 (13%) 3 2	11, 24, 38, 60	477 (100%)
1	8-O	477/477 (100%)	0.88	74 (15%) 2 1	11, 24, 38, 60	477 (100%)
1	8-P	477/477 (100%)	0.79	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	8-Q	477/477 (100%)	0.86	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	8-R	477/477 (100%)	0.76	56 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	8-S	477/477 (100%)	0.57	53 (11%) 5 4	11, 24, 38, 60	477 (100%)
1	8-T	477/477 (100%)	0.59	64 (13%) 3 2	11, 24, 38, 60	477 (100%)
1	8-U	477/477 (100%)	0.83	83 (17%) 1 1	11, 24, 38, 60	477 (100%)
1	8-V	477/477 (100%)	0.55	60 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	8-W	477/477 (100%)	0.49	58 (12%) 4 3	11, 24, 38, 60	477 (100%)
1	8-X	477/477 (100%)	0.64	65 (13%) 3 2	11, 24, 38, 60	477 (100%)
1	9-A	477/477 (100%)	0.55	66 (13%) 2 2	11, 24, 38, 60	477 (100%)
1	9-B	477/477 (100%)	0.66	63 (13%) 3 3	11, 24, 38, 60	477 (100%)
1	9-C	477/477 (100%)	0.86	86 (18%) 1 1	11, 24, 38, 60	477 (100%)
1	9-D	477/477 (100%)	0.61	72 (15%) 2 1	11, 24, 38, 60	477 (100%)
1	9-E	477/477 (100%)	0.69	77 (16%) 1 1	11, 24, 38, 60	477 (100%)
1	9-F	477/477 (100%)	0.60	57 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	9-G	477/477 (100%)	0.67	60 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	9-H	477/477 (100%)	0.66	66 (13%) 2 2	11, 24, 38, 60	477 (100%)
1	9-I	477/477 (100%)	0.89	80 (16%) 1 1	11, 24, 38, 60	477 (100%)
1	9-J	477/477 (100%)	0.52	56 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	9-K	477/477 (100%)	0.68	68 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	9-L	477/477 (100%)	0.80	62 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	9-M	477/477 (100%)	0.70	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	9-N	477/477 (100%)	0.79	65 (13%) 3 2	11, 24, 38, 60	477 (100%)
1	9-O	477/477 (100%)	0.88	74 (15%) 2 1	11, 24, 38, 60	477 (100%)
1	9-P	477/477 (100%)	0.79	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	9-Q	477/477 (100%)	0.86	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	9-R	477/477 (100%)	0.76	56 (11%) 4 4	11, 24, 38, 60	477 (100%)

Continued on next page..

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	9-S	477/477 (100%)	0.57	53 (11%) 5 4	11, 24, 38, 60	477 (100%)
1	9-T	477/477 (100%)	0.59	64 (13%) 3 2	11, 24, 38, 60	477 (100%)
1	9-U	477/477 (100%)	0.83	83 (17%) 1 1	11, 24, 38, 60	477 (100%)
1	9-V	477/477 (100%)	0.55	60 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	9-W	477/477 (100%)	0.49	58 (12%) 4 3	11, 24, 38, 60	477 (100%)
1	9-X	477/477 (100%)	0.64	65 (13%) 3 2	11, 24, 38, 60	477 (100%)
1	10-A	477/477 (100%)	0.55	66 (13%) 2 2	11, 24, 38, 60	477 (100%)
1	10-B	477/477 (100%)	0.66	63 (13%) 3 3	11, 24, 38, 60	477 (100%)
1	10-C	477/477 (100%)	0.86	86 (18%) 1 1	11, 24, 38, 60	477 (100%)
1	10-D	477/477 (100%)	0.61	72 (15%) 2 1	11, 24, 38, 60	477 (100%)
1	10-E	477/477 (100%)	0.69	77 (16%) 1 1	11, 24, 38, 60	477 (100%)
1	10-F	477/477 (100%)	0.60	57 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	10-G	477/477 (100%)	0.67	60 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	10-H	477/477 (100%)	0.66	66 (13%) 2 2	11, 24, 38, 60	477 (100%)
1	10-I	477/477 (100%)	0.89	80 (16%) 1 1	11, 24, 38, 60	477 (100%)
1	10-J	477/477 (100%)	0.52	56 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	10-K	477/477 (100%)	0.68	68 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	10-L	477/477 (100%)	0.80	62 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	10-M	477/477 (100%)	0.70	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	10-N	477/477 (100%)	0.79	65 (13%) 3 2	11, 24, 38, 60	477 (100%)
1	10-O	477/477 (100%)	0.88	74 (15%) 2 1	11, 24, 38, 60	477 (100%)
1	10-P	477/477 (100%)	0.79	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	10-Q	477/477 (100%)	0.86	70 (14%) 2 2	11, 24, 38, 60	477 (100%)
1	10-R	477/477 (100%)	0.76	56 (11%) 4 4	11, 24, 38, 60	477 (100%)
1	10-S	477/477 (100%)	0.57	53 (11%) 5 4	11, 24, 38, 60	477 (100%)
1	10-T	477/477 (100%)	0.59	64 (13%) 3 2	11, 24, 38, 60	477 (100%)
1	10-U	477/477 (100%)	0.83	83 (17%) 1 1	11, 24, 38, 60	477 (100%)
1	10-V	477/477 (100%)	0.55	60 (12%) 3 3	11, 24, 38, 60	477 (100%)
1	10-W	477/477 (100%)	0.49	58 (12%) 4 3	11, 24, 38, 60	477 (100%)
1	10-X	477/477 (100%)	0.64	65 (13%) 3 2	11, 24, 38, 60	477 (100%)
All	All	114480/114480 (100%)	0.69	16010 (13%) 3 2	11, 24, 38, 60	114480 (100%)

The worst 5 of 16010 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-R	61	HIS	40.7
1	2-R	61	HIS	40.7
1	3-R	61	HIS	40.7
1	4-R	61	HIS	40.7
1	5-R	61	HIS	40.7

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 monosaccharides 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. 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	B-factors(\AA^2)	Q<0.9
3	AMP	1-A	7475	23/23	0.37	0.57	24,24,24,24	23
3	AMP	2-A	7475	23/23	0.37	0.57	24,24,24,24	23
3	AMP	3-A	7475	23/23	0.37	0.57	24,24,24,24	23
3	AMP	4-A	7475	23/23	0.37	0.57	24,24,24,24	23
3	AMP	5-A	7475	23/23	0.37	0.57	24,24,24,24	23
3	AMP	6-A	7475	23/23	0.37	0.57	24,24,24,24	23
3	AMP	7-A	7475	23/23	0.37	0.57	24,24,24,24	23
3	AMP	8-A	7475	23/23	0.37	0.57	24,24,24,24	23
3	AMP	9-A	7475	23/23	0.37	0.57	24,24,24,24	23
3	AMP	10-A	7475	23/23	0.37	0.57	24,24,24,24	23
3	AMP	1-L	7497	23/23	0.41	0.55	24,24,24,24	23
3	AMP	2-L	7497	23/23	0.41	0.55	24,24,24,24	23
3	AMP	3-L	7497	23/23	0.41	0.55	24,24,24,24	23
3	AMP	4-L	7497	23/23	0.41	0.55	24,24,24,24	23
3	AMP	5-L	7497	23/23	0.41	0.55	24,24,24,24	23
3	AMP	6-L	7497	23/23	0.41	0.55	24,24,24,24	23
3	AMP	7-L	7497	23/23	0.41	0.55	24,24,24,24	23

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	AMP	8-L	7497	23/23	0.41	0.55	24,24,24,24	23
3	AMP	9-L	7497	23/23	0.41	0.55	24,24,24,24	23
3	AMP	10-L	7497	23/23	0.41	0.55	24,24,24,24	23
3	AMP	1-J	7493	23/23	0.44	0.62	24,24,24,24	23
3	AMP	2-J	7493	23/23	0.44	0.62	24,24,24,24	23
3	AMP	3-J	7493	23/23	0.44	0.62	24,24,24,24	23
3	AMP	4-J	7493	23/23	0.44	0.62	24,24,24,24	23
3	AMP	5-J	7493	23/23	0.44	0.62	24,24,24,24	23
3	AMP	6-J	7493	23/23	0.44	0.62	24,24,24,24	23
3	AMP	7-J	7493	23/23	0.44	0.62	24,24,24,24	23
3	AMP	8-J	7493	23/23	0.44	0.62	24,24,24,24	23
3	AMP	9-J	7493	23/23	0.44	0.62	24,24,24,24	23
3	AMP	10-J	7493	23/23	0.44	0.62	24,24,24,24	23
3	AMP	1-R	7509	23/23	0.44	0.59	24,24,24,24	23
3	AMP	2-R	7509	23/23	0.44	0.59	24,24,24,24	23
3	AMP	3-R	7509	23/23	0.44	0.59	24,24,24,24	23
3	AMP	4-R	7509	23/23	0.44	0.59	24,24,24,24	23
3	AMP	5-R	7509	23/23	0.44	0.59	24,24,24,24	23
3	AMP	6-R	7509	23/23	0.44	0.59	24,24,24,24	23
3	AMP	7-R	7509	23/23	0.44	0.59	24,24,24,24	23
3	AMP	8-R	7509	23/23	0.44	0.59	24,24,24,24	23
3	AMP	9-R	7509	23/23	0.44	0.59	24,24,24,24	23
3	AMP	10-R	7509	23/23	0.44	0.59	24,24,24,24	23
3	AMP	1-S	7511	23/23	0.44	0.53	24,24,24,24	23
3	AMP	2-S	7511	23/23	0.44	0.53	24,24,24,24	23
3	AMP	3-S	7511	23/23	0.44	0.53	24,24,24,24	23
3	AMP	4-S	7511	23/23	0.44	0.53	24,24,24,24	23
3	AMP	5-S	7511	23/23	0.44	0.53	24,24,24,24	23
3	AMP	6-S	7511	23/23	0.44	0.53	24,24,24,24	23
3	AMP	7-S	7511	23/23	0.44	0.53	24,24,24,24	23
3	AMP	8-S	7511	23/23	0.44	0.53	24,24,24,24	23
3	AMP	9-S	7511	23/23	0.44	0.53	24,24,24,24	23
3	AMP	10-S	7511	23/23	0.44	0.53	24,24,24,24	23
3	AMP	1-D	7481	23/23	0.45	0.74	24,24,24,24	23
3	AMP	2-D	7481	23/23	0.45	0.74	24,24,24,24	23
3	AMP	3-D	7481	23/23	0.45	0.74	24,24,24,24	23
3	AMP	4-D	7481	23/23	0.45	0.74	24,24,24,24	23
3	AMP	5-D	7481	23/23	0.45	0.74	24,24,24,24	23
3	AMP	6-D	7481	23/23	0.45	0.74	24,24,24,24	23
3	AMP	7-D	7481	23/23	0.45	0.74	24,24,24,24	23
3	AMP	8-D	7481	23/23	0.45	0.74	24,24,24,24	23

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	AMP	9-D	7481	23/23	0.45	0.74	24,24,24,24	23
3	AMP	10-D	7481	23/23	0.45	0.74	24,24,24,24	23
3	AMP	1-E	7483	23/23	0.45	0.65	24,24,24,24	23
3	AMP	2-E	7483	23/23	0.45	0.65	24,24,24,24	23
3	AMP	3-E	7483	23/23	0.45	0.65	24,24,24,24	23
3	AMP	4-E	7483	23/23	0.45	0.65	24,24,24,24	23
3	AMP	5-E	7483	23/23	0.45	0.65	24,24,24,24	23
3	AMP	6-E	7483	23/23	0.45	0.65	24,24,24,24	23
3	AMP	7-E	7483	23/23	0.45	0.65	24,24,24,24	23
3	AMP	8-E	7483	23/23	0.45	0.65	24,24,24,24	23
3	AMP	9-E	7483	23/23	0.45	0.65	24,24,24,24	23
3	AMP	10-E	7483	23/23	0.45	0.65	24,24,24,24	23
3	AMP	1-O	7503	23/23	0.46	0.73	24,24,24,24	23
3	AMP	2-O	7503	23/23	0.46	0.73	24,24,24,24	23
3	AMP	3-O	7503	23/23	0.46	0.73	24,24,24,24	23
3	AMP	4-O	7503	23/23	0.46	0.73	24,24,24,24	23
3	AMP	5-O	7503	23/23	0.46	0.73	24,24,24,24	23
3	AMP	6-O	7503	23/23	0.46	0.73	24,24,24,24	23
3	AMP	7-O	7503	23/23	0.46	0.73	24,24,24,24	23
3	AMP	8-O	7503	23/23	0.46	0.73	24,24,24,24	23
3	AMP	9-O	7503	23/23	0.46	0.73	24,24,24,24	23
3	AMP	10-O	7503	23/23	0.46	0.73	24,24,24,24	23
3	AMP	1-P	7505	23/23	0.47	0.68	24,24,24,24	23
3	AMP	2-P	7505	23/23	0.47	0.68	24,24,24,24	23
3	AMP	3-P	7505	23/23	0.47	0.68	24,24,24,24	23
3	AMP	4-P	7505	23/23	0.47	0.68	24,24,24,24	23
3	AMP	5-P	7505	23/23	0.47	0.68	24,24,24,24	23
3	AMP	6-P	7505	23/23	0.47	0.68	24,24,24,24	23
3	AMP	7-P	7505	23/23	0.47	0.68	24,24,24,24	23
3	AMP	8-P	7505	23/23	0.47	0.68	24,24,24,24	23
3	AMP	9-P	7505	23/23	0.47	0.68	24,24,24,24	23
3	AMP	10-P	7505	23/23	0.47	0.68	24,24,24,24	23
3	AMP	1-G	7487	23/23	0.49	0.53	24,24,24,24	23
3	AMP	2-G	7487	23/23	0.49	0.53	24,24,24,24	23
3	AMP	3-G	7487	23/23	0.49	0.53	24,24,24,24	23
3	AMP	4-G	7487	23/23	0.49	0.53	24,24,24,24	23
3	AMP	5-G	7487	23/23	0.49	0.53	24,24,24,24	23
3	AMP	6-G	7487	23/23	0.49	0.53	24,24,24,24	23
3	AMP	7-G	7487	23/23	0.49	0.53	24,24,24,24	23
3	AMP	8-G	7487	23/23	0.49	0.53	24,24,24,24	23
3	AMP	9-G	7487	23/23	0.49	0.53	24,24,24,24	23

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	AMP	10-G	7487	23/23	0.49	0.53	24,24,24,24	23
3	AMP	1-I	7491	23/23	0.50	0.59	24,24,24,24	23
3	AMP	2-I	7491	23/23	0.50	0.59	24,24,24,24	23
3	AMP	3-I	7491	23/23	0.50	0.59	24,24,24,24	23
3	AMP	4-I	7491	23/23	0.50	0.59	24,24,24,24	23
3	AMP	5-I	7491	23/23	0.50	0.59	24,24,24,24	23
3	AMP	6-I	7491	23/23	0.50	0.59	24,24,24,24	23
3	AMP	7-I	7491	23/23	0.50	0.59	24,24,24,24	23
3	AMP	8-I	7491	23/23	0.50	0.59	24,24,24,24	23
3	AMP	9-I	7491	23/23	0.50	0.59	24,24,24,24	23
3	AMP	10-I	7491	23/23	0.50	0.59	24,24,24,24	23
3	AMP	1-U	7515	23/23	0.50	0.74	24,24,24,24	23
3	AMP	2-U	7515	23/23	0.50	0.74	24,24,24,24	23
3	AMP	3-U	7515	23/23	0.50	0.74	24,24,24,24	23
3	AMP	4-U	7515	23/23	0.50	0.74	24,24,24,24	23
3	AMP	5-U	7515	23/23	0.50	0.74	24,24,24,24	23
3	AMP	6-U	7515	23/23	0.50	0.74	24,24,24,24	23
3	AMP	7-U	7515	23/23	0.50	0.74	24,24,24,24	23
3	AMP	8-U	7515	23/23	0.50	0.74	24,24,24,24	23
3	AMP	9-U	7515	23/23	0.50	0.74	24,24,24,24	23
3	AMP	10-U	7515	23/23	0.50	0.74	24,24,24,24	23
3	AMP	1-W	7519	23/23	0.50	0.64	24,24,24,24	23
3	AMP	2-W	7519	23/23	0.50	0.64	24,24,24,24	23
3	AMP	3-W	7519	23/23	0.50	0.64	24,24,24,24	23
3	AMP	4-W	7519	23/23	0.50	0.64	24,24,24,24	23
3	AMP	5-W	7519	23/23	0.50	0.64	24,24,24,24	23
3	AMP	6-W	7519	23/23	0.50	0.64	24,24,24,24	23
3	AMP	7-W	7519	23/23	0.50	0.64	24,24,24,24	23
3	AMP	8-W	7519	23/23	0.50	0.64	24,24,24,24	23
3	AMP	9-W	7519	23/23	0.50	0.64	24,24,24,24	23
3	AMP	10-W	7519	23/23	0.50	0.64	24,24,24,24	23
3	AMP	1-K	7495	23/23	0.53	0.60	24,24,24,24	23
3	AMP	2-K	7495	23/23	0.53	0.60	24,24,24,24	23
3	AMP	3-K	7495	23/23	0.53	0.60	24,24,24,24	23
3	AMP	4-K	7495	23/23	0.53	0.60	24,24,24,24	23
3	AMP	5-K	7495	23/23	0.53	0.60	24,24,24,24	23
3	AMP	6-K	7495	23/23	0.53	0.60	24,24,24,24	23
3	AMP	7-K	7495	23/23	0.53	0.60	24,24,24,24	23
3	AMP	8-K	7495	23/23	0.53	0.60	24,24,24,24	23
3	AMP	9-K	7495	23/23	0.53	0.60	24,24,24,24	23
3	AMP	10-K	7495	23/23	0.53	0.60	24,24,24,24	23

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	AMP	1-V	7517	23/23	0.53	0.64	24,24,24,24	23
3	AMP	2-V	7517	23/23	0.53	0.64	24,24,24,24	23
3	AMP	3-V	7517	23/23	0.53	0.64	24,24,24,24	23
3	AMP	4-V	7517	23/23	0.53	0.64	24,24,24,24	23
3	AMP	5-V	7517	23/23	0.53	0.64	24,24,24,24	23
3	AMP	6-V	7517	23/23	0.53	0.64	24,24,24,24	23
3	AMP	7-V	7517	23/23	0.53	0.64	24,24,24,24	23
3	AMP	8-V	7517	23/23	0.53	0.64	24,24,24,24	23
3	AMP	9-V	7517	23/23	0.53	0.64	24,24,24,24	23
3	AMP	10-V	7517	23/23	0.53	0.64	24,24,24,24	23
3	AMP	1-H	7489	23/23	0.53	0.57	24,24,24,24	23
3	AMP	2-H	7489	23/23	0.53	0.57	24,24,24,24	23
3	AMP	3-H	7489	23/23	0.53	0.57	24,24,24,24	23
3	AMP	4-H	7489	23/23	0.53	0.57	24,24,24,24	23
3	AMP	5-H	7489	23/23	0.53	0.57	24,24,24,24	23
3	AMP	6-H	7489	23/23	0.53	0.57	24,24,24,24	23
3	AMP	7-H	7489	23/23	0.53	0.57	24,24,24,24	23
3	AMP	8-H	7489	23/23	0.53	0.57	24,24,24,24	23
3	AMP	9-H	7489	23/23	0.53	0.57	24,24,24,24	23
3	AMP	10-H	7489	23/23	0.53	0.57	24,24,24,24	23
3	AMP	1-X	7521	23/23	0.53	0.64	24,24,24,24	23
3	AMP	2-X	7521	23/23	0.53	0.64	24,24,24,24	23
3	AMP	3-X	7521	23/23	0.53	0.64	24,24,24,24	23
3	AMP	4-X	7521	23/23	0.53	0.64	24,24,24,24	23
3	AMP	5-X	7521	23/23	0.53	0.64	24,24,24,24	23
3	AMP	6-X	7521	23/23	0.53	0.64	24,24,24,24	23
3	AMP	7-X	7521	23/23	0.53	0.64	24,24,24,24	23
3	AMP	8-X	7521	23/23	0.53	0.64	24,24,24,24	23
3	AMP	9-X	7521	23/23	0.53	0.64	24,24,24,24	23
3	AMP	10-X	7521	23/23	0.53	0.64	24,24,24,24	23
3	AMP	1-F	7485	23/23	0.54	0.62	24,24,24,24	23
3	AMP	2-F	7485	23/23	0.54	0.62	24,24,24,24	23
3	AMP	3-F	7485	23/23	0.54	0.62	24,24,24,24	23
3	AMP	4-F	7485	23/23	0.54	0.62	24,24,24,24	23
3	AMP	5-F	7485	23/23	0.54	0.62	24,24,24,24	23
3	AMP	6-F	7485	23/23	0.54	0.62	24,24,24,24	23
3	AMP	7-F	7485	23/23	0.54	0.62	24,24,24,24	23
3	AMP	8-F	7485	23/23	0.54	0.62	24,24,24,24	23
3	AMP	9-F	7485	23/23	0.54	0.62	24,24,24,24	23
3	AMP	10-F	7485	23/23	0.54	0.62	24,24,24,24	23
3	AMP	1-N	7501	23/23	0.55	0.59	24,24,24,24	23

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	AMP	2-N	7501	23/23	0.55	0.59	24,24,24,24	23
3	AMP	3-N	7501	23/23	0.55	0.59	24,24,24,24	23
3	AMP	4-N	7501	23/23	0.55	0.59	24,24,24,24	23
3	AMP	5-N	7501	23/23	0.55	0.59	24,24,24,24	23
3	AMP	6-N	7501	23/23	0.55	0.59	24,24,24,24	23
3	AMP	7-N	7501	23/23	0.55	0.59	24,24,24,24	23
3	AMP	8-N	7501	23/23	0.55	0.59	24,24,24,24	23
3	AMP	9-N	7501	23/23	0.55	0.59	24,24,24,24	23
3	AMP	10-N	7501	23/23	0.55	0.59	24,24,24,24	23
3	AMP	1-Q	7507	23/23	0.55	0.54	24,24,24,24	23
3	AMP	2-Q	7507	23/23	0.55	0.54	24,24,24,24	23
3	AMP	3-Q	7507	23/23	0.55	0.54	24,24,24,24	23
3	AMP	4-Q	7507	23/23	0.55	0.54	24,24,24,24	23
3	AMP	5-Q	7507	23/23	0.55	0.54	24,24,24,24	23
3	AMP	6-Q	7507	23/23	0.55	0.54	24,24,24,24	23
3	AMP	7-Q	7507	23/23	0.55	0.54	24,24,24,24	23
3	AMP	8-Q	7507	23/23	0.55	0.54	24,24,24,24	23
3	AMP	9-Q	7507	23/23	0.55	0.54	24,24,24,24	23
3	AMP	10-Q	7507	23/23	0.55	0.54	24,24,24,24	23
3	AMP	1-B	7477	23/23	0.56	0.60	24,24,24,24	23
3	AMP	2-B	7477	23/23	0.56	0.60	24,24,24,24	23
3	AMP	3-B	7477	23/23	0.56	0.60	24,24,24,24	23
3	AMP	4-B	7477	23/23	0.56	0.60	24,24,24,24	23
3	AMP	5-B	7477	23/23	0.56	0.60	24,24,24,24	23
3	AMP	6-B	7477	23/23	0.56	0.60	24,24,24,24	23
3	AMP	7-B	7477	23/23	0.56	0.60	24,24,24,24	23
3	AMP	8-B	7477	23/23	0.56	0.60	24,24,24,24	23
3	AMP	9-B	7477	23/23	0.56	0.60	24,24,24,24	23
3	AMP	10-B	7477	23/23	0.56	0.60	24,24,24,24	23
3	AMP	1-M	7499	23/23	0.56	0.64	24,24,24,24	23
3	AMP	2-M	7499	23/23	0.56	0.64	24,24,24,24	23
3	AMP	3-M	7499	23/23	0.56	0.64	24,24,24,24	23
3	AMP	4-M	7499	23/23	0.56	0.64	24,24,24,24	23
3	AMP	5-M	7499	23/23	0.56	0.64	24,24,24,24	23
3	AMP	6-M	7499	23/23	0.56	0.64	24,24,24,24	23
3	AMP	7-M	7499	23/23	0.56	0.64	24,24,24,24	23
3	AMP	8-M	7499	23/23	0.56	0.64	24,24,24,24	23
3	AMP	9-M	7499	23/23	0.56	0.64	24,24,24,24	23
3	AMP	10-M	7499	23/23	0.56	0.64	24,24,24,24	23
2	MN	1-R	470	1/1	0.57	0.65	24,24,24,24	1
2	MN	2-R	470	1/1	0.57	0.65	24,24,24,24	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MN	3-R	470	1/1	0.57	0.65	24,24,24,24	1
2	MN	4-R	470	1/1	0.57	0.65	24,24,24,24	1
2	MN	5-R	470	1/1	0.57	0.65	24,24,24,24	1
2	MN	6-R	470	1/1	0.57	0.65	24,24,24,24	1
2	MN	7-R	470	1/1	0.57	0.65	24,24,24,24	1
2	MN	8-R	470	1/1	0.57	0.65	24,24,24,24	1
2	MN	9-R	470	1/1	0.57	0.65	24,24,24,24	1
2	MN	10-R	470	1/1	0.57	0.65	24,24,24,24	1
3	AMP	1-C	7479	23/23	0.57	0.73	24,24,24,24	23
3	AMP	2-C	7479	23/23	0.57	0.73	24,24,24,24	23
3	AMP	3-C	7479	23/23	0.57	0.73	24,24,24,24	23
3	AMP	4-C	7479	23/23	0.57	0.73	24,24,24,24	23
3	AMP	5-C	7479	23/23	0.57	0.73	24,24,24,24	23
3	AMP	6-C	7479	23/23	0.57	0.73	24,24,24,24	23
3	AMP	7-C	7479	23/23	0.57	0.73	24,24,24,24	23
3	AMP	8-C	7479	23/23	0.57	0.73	24,24,24,24	23
3	AMP	9-C	7479	23/23	0.57	0.73	24,24,24,24	23
3	AMP	10-C	7479	23/23	0.57	0.73	24,24,24,24	23
3	AMP	1-T	7513	23/23	0.58	0.68	24,24,24,24	23
3	AMP	2-T	7513	23/23	0.58	0.68	24,24,24,24	23
3	AMP	3-T	7513	23/23	0.58	0.68	24,24,24,24	23
3	AMP	4-T	7513	23/23	0.58	0.68	24,24,24,24	23
3	AMP	5-T	7513	23/23	0.58	0.68	24,24,24,24	23
3	AMP	6-T	7513	23/23	0.58	0.68	24,24,24,24	23
3	AMP	7-T	7513	23/23	0.58	0.68	24,24,24,24	23
3	AMP	8-T	7513	23/23	0.58	0.68	24,24,24,24	23
3	AMP	9-T	7513	23/23	0.58	0.68	24,24,24,24	23
3	AMP	10-T	7513	23/23	0.58	0.68	24,24,24,24	23
4	CIT	1-R	7510	13/13	0.62	0.48	24,24,24,24	13
4	CIT	2-R	7510	13/13	0.62	0.48	24,24,24,24	13
4	CIT	3-R	7510	13/13	0.62	0.48	24,24,24,24	13
4	CIT	4-R	7510	13/13	0.62	0.48	24,24,24,24	13
4	CIT	5-R	7510	13/13	0.62	0.48	24,24,24,24	13
4	CIT	6-R	7510	13/13	0.62	0.48	24,24,24,24	13
4	CIT	7-R	7510	13/13	0.62	0.48	24,24,24,24	13
4	CIT	8-R	7510	13/13	0.62	0.48	24,24,24,24	13
4	CIT	9-R	7510	13/13	0.62	0.48	24,24,24,24	13
4	CIT	10-R	7510	13/13	0.62	0.48	24,24,24,24	13
4	CIT	1-F	7486	13/13	0.63	0.51	24,24,24,24	13
4	CIT	2-F	7486	13/13	0.63	0.51	24,24,24,24	13
4	CIT	3-F	7486	13/13	0.63	0.51	24,24,24,24	13

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CIT	4-F	7486	13/13	0.63	0.51	24,24,24,24	13
4	CIT	5-F	7486	13/13	0.63	0.51	24,24,24,24	13
4	CIT	6-F	7486	13/13	0.63	0.51	24,24,24,24	13
4	CIT	7-F	7486	13/13	0.63	0.51	24,24,24,24	13
4	CIT	8-F	7486	13/13	0.63	0.51	24,24,24,24	13
4	CIT	9-F	7486	13/13	0.63	0.51	24,24,24,24	13
4	CIT	10-F	7486	13/13	0.63	0.51	24,24,24,24	13
4	CIT	1-H	7490	13/13	0.64	0.61	24,24,24,24	13
4	CIT	2-H	7490	13/13	0.64	0.61	24,24,24,24	13
4	CIT	3-H	7490	13/13	0.64	0.61	24,24,24,24	13
4	CIT	4-H	7490	13/13	0.64	0.61	24,24,24,24	13
4	CIT	5-H	7490	13/13	0.64	0.61	24,24,24,24	13
4	CIT	6-H	7490	13/13	0.64	0.61	24,24,24,24	13
4	CIT	7-H	7490	13/13	0.64	0.61	24,24,24,24	13
4	CIT	8-H	7490	13/13	0.64	0.61	24,24,24,24	13
4	CIT	9-H	7490	13/13	0.64	0.61	24,24,24,24	13
4	CIT	10-H	7490	13/13	0.64	0.61	24,24,24,24	13
2	MN	1-N	470	1/1	0.65	0.45	24,24,24,24	1
2	MN	2-N	470	1/1	0.65	0.45	24,24,24,24	1
2	MN	3-N	470	1/1	0.65	0.45	24,24,24,24	1
2	MN	4-N	470	1/1	0.65	0.45	24,24,24,24	1
2	MN	5-N	470	1/1	0.65	0.45	24,24,24,24	1
2	MN	6-N	470	1/1	0.65	0.45	24,24,24,24	1
2	MN	7-N	470	1/1	0.65	0.45	24,24,24,24	1
2	MN	8-N	470	1/1	0.65	0.45	24,24,24,24	1
2	MN	9-N	470	1/1	0.65	0.45	24,24,24,24	1
2	MN	10-N	470	1/1	0.65	0.45	24,24,24,24	1
4	CIT	1-Q	7508	13/13	0.66	0.52	24,24,24,24	13
4	CIT	2-Q	7508	13/13	0.66	0.52	24,24,24,24	13
4	CIT	3-Q	7508	13/13	0.66	0.52	24,24,24,24	13
4	CIT	4-Q	7508	13/13	0.66	0.52	24,24,24,24	13
4	CIT	5-Q	7508	13/13	0.66	0.52	24,24,24,24	13
4	CIT	6-Q	7508	13/13	0.66	0.52	24,24,24,24	13
4	CIT	7-Q	7508	13/13	0.66	0.52	24,24,24,24	13
4	CIT	8-Q	7508	13/13	0.66	0.52	24,24,24,24	13
4	CIT	9-Q	7508	13/13	0.66	0.52	24,24,24,24	13
4	CIT	10-Q	7508	13/13	0.66	0.52	24,24,24,24	13
4	CIT	1-N	7502	13/13	0.66	0.45	24,24,24,24	13
4	CIT	2-N	7502	13/13	0.66	0.45	24,24,24,24	13
4	CIT	3-N	7502	13/13	0.66	0.45	24,24,24,24	13
4	CIT	4-N	7502	13/13	0.66	0.45	24,24,24,24	13

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CIT	5-N	7502	13/13	0.66	0.45	24,24,24,24	13
4	CIT	6-N	7502	13/13	0.66	0.45	24,24,24,24	13
4	CIT	7-N	7502	13/13	0.66	0.45	24,24,24,24	13
4	CIT	8-N	7502	13/13	0.66	0.45	24,24,24,24	13
4	CIT	9-N	7502	13/13	0.66	0.45	24,24,24,24	13
4	CIT	10-N	7502	13/13	0.66	0.45	24,24,24,24	13
4	CIT	1-T	7514	13/13	0.66	0.47	24,24,24,24	13
4	CIT	2-T	7514	13/13	0.66	0.47	24,24,24,24	13
4	CIT	3-T	7514	13/13	0.66	0.47	24,24,24,24	13
4	CIT	4-T	7514	13/13	0.66	0.47	24,24,24,24	13
4	CIT	5-T	7514	13/13	0.66	0.47	24,24,24,24	13
4	CIT	6-T	7514	13/13	0.66	0.47	24,24,24,24	13
4	CIT	7-T	7514	13/13	0.66	0.47	24,24,24,24	13
4	CIT	8-T	7514	13/13	0.66	0.47	24,24,24,24	13
4	CIT	9-T	7514	13/13	0.66	0.47	24,24,24,24	13
4	CIT	10-T	7514	13/13	0.66	0.47	24,24,24,24	13
4	CIT	1-G	7488	13/13	0.67	0.44	24,24,24,24	13
4	CIT	2-G	7488	13/13	0.67	0.44	24,24,24,24	13
4	CIT	3-G	7488	13/13	0.67	0.44	24,24,24,24	13
4	CIT	4-G	7488	13/13	0.67	0.44	24,24,24,24	13
4	CIT	5-G	7488	13/13	0.67	0.44	24,24,24,24	13
4	CIT	6-G	7488	13/13	0.67	0.44	24,24,24,24	13
4	CIT	7-G	7488	13/13	0.67	0.44	24,24,24,24	13
4	CIT	8-G	7488	13/13	0.67	0.44	24,24,24,24	13
4	CIT	9-G	7488	13/13	0.67	0.44	24,24,24,24	13
4	CIT	10-G	7488	13/13	0.67	0.44	24,24,24,24	13
4	CIT	1-K	7496	13/13	0.67	0.52	24,24,24,24	13
4	CIT	2-K	7496	13/13	0.67	0.52	24,24,24,24	13
4	CIT	3-K	7496	13/13	0.67	0.52	24,24,24,24	13
4	CIT	4-K	7496	13/13	0.67	0.52	24,24,24,24	13
4	CIT	5-K	7496	13/13	0.67	0.52	24,24,24,24	13
4	CIT	6-K	7496	13/13	0.67	0.52	24,24,24,24	13
4	CIT	7-K	7496	13/13	0.67	0.52	24,24,24,24	13
4	CIT	8-K	7496	13/13	0.67	0.52	24,24,24,24	13
4	CIT	9-K	7496	13/13	0.67	0.52	24,24,24,24	13
4	CIT	10-K	7496	13/13	0.67	0.52	24,24,24,24	13
4	CIT	1-U	7516	13/13	0.67	0.46	24,24,24,24	13
4	CIT	2-U	7516	13/13	0.67	0.46	24,24,24,24	13
4	CIT	3-U	7516	13/13	0.67	0.46	24,24,24,24	13
4	CIT	4-U	7516	13/13	0.67	0.46	24,24,24,24	13
4	CIT	5-U	7516	13/13	0.67	0.46	24,24,24,24	13

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CIT	6-U	7516	13/13	0.67	0.46	24,24,24,24	13
4	CIT	7-U	7516	13/13	0.67	0.46	24,24,24,24	13
4	CIT	8-U	7516	13/13	0.67	0.46	24,24,24,24	13
4	CIT	9-U	7516	13/13	0.67	0.46	24,24,24,24	13
4	CIT	10-U	7516	13/13	0.67	0.46	24,24,24,24	13
2	MN	1-O	470	1/1	0.68	0.77	24,24,24,24	1
2	MN	2-O	470	1/1	0.68	0.77	24,24,24,24	1
2	MN	3-O	470	1/1	0.68	0.77	24,24,24,24	1
2	MN	4-O	470	1/1	0.68	0.77	24,24,24,24	1
2	MN	5-O	470	1/1	0.68	0.77	24,24,24,24	1
2	MN	6-O	470	1/1	0.68	0.77	24,24,24,24	1
2	MN	7-O	470	1/1	0.68	0.77	24,24,24,24	1
2	MN	8-O	470	1/1	0.68	0.77	24,24,24,24	1
2	MN	9-O	470	1/1	0.68	0.77	24,24,24,24	1
2	MN	10-O	470	1/1	0.68	0.77	24,24,24,24	1
4	CIT	1-V	7518	13/13	0.68	0.43	24,24,24,24	13
4	CIT	2-V	7518	13/13	0.68	0.43	24,24,24,24	13
4	CIT	3-V	7518	13/13	0.68	0.43	24,24,24,24	13
4	CIT	4-V	7518	13/13	0.68	0.43	24,24,24,24	13
4	CIT	5-V	7518	13/13	0.68	0.43	24,24,24,24	13
4	CIT	6-V	7518	13/13	0.68	0.43	24,24,24,24	13
4	CIT	7-V	7518	13/13	0.68	0.43	24,24,24,24	13
4	CIT	8-V	7518	13/13	0.68	0.43	24,24,24,24	13
4	CIT	9-V	7518	13/13	0.68	0.43	24,24,24,24	13
4	CIT	10-V	7518	13/13	0.68	0.43	24,24,24,24	13
4	CIT	1-P	7506	13/13	0.69	0.41	24,24,24,24	13
4	CIT	2-P	7506	13/13	0.69	0.41	24,24,24,24	13
4	CIT	3-P	7506	13/13	0.69	0.41	24,24,24,24	13
4	CIT	4-P	7506	13/13	0.69	0.41	24,24,24,24	13
4	CIT	5-P	7506	13/13	0.69	0.41	24,24,24,24	13
4	CIT	6-P	7506	13/13	0.69	0.41	24,24,24,24	13
4	CIT	7-P	7506	13/13	0.69	0.41	24,24,24,24	13
4	CIT	8-P	7506	13/13	0.69	0.41	24,24,24,24	13
4	CIT	9-P	7506	13/13	0.69	0.41	24,24,24,24	13
4	CIT	10-P	7506	13/13	0.69	0.41	24,24,24,24	13
4	CIT	1-L	7498	13/13	0.69	0.47	24,24,24,24	13
4	CIT	2-L	7498	13/13	0.69	0.47	24,24,24,24	13
4	CIT	3-L	7498	13/13	0.69	0.47	24,24,24,24	13
4	CIT	4-L	7498	13/13	0.69	0.47	24,24,24,24	13
4	CIT	5-L	7498	13/13	0.69	0.47	24,24,24,24	13
4	CIT	6-L	7498	13/13	0.69	0.47	24,24,24,24	13

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CIT	7-L	7498	13/13	0.69	0.47	24,24,24,24	13
4	CIT	8-L	7498	13/13	0.69	0.47	24,24,24,24	13
4	CIT	9-L	7498	13/13	0.69	0.47	24,24,24,24	13
4	CIT	10-L	7498	13/13	0.69	0.47	24,24,24,24	13
4	CIT	1-E	7484	13/13	0.69	0.50	24,24,24,24	13
4	CIT	2-E	7484	13/13	0.69	0.50	24,24,24,24	13
4	CIT	3-E	7484	13/13	0.69	0.50	24,24,24,24	13
4	CIT	4-E	7484	13/13	0.69	0.50	24,24,24,24	13
4	CIT	5-E	7484	13/13	0.69	0.50	24,24,24,24	13
4	CIT	6-E	7484	13/13	0.69	0.50	24,24,24,24	13
4	CIT	7-E	7484	13/13	0.69	0.50	24,24,24,24	13
4	CIT	8-E	7484	13/13	0.69	0.50	24,24,24,24	13
4	CIT	9-E	7484	13/13	0.69	0.50	24,24,24,24	13
4	CIT	10-E	7484	13/13	0.69	0.50	24,24,24,24	13
4	CIT	1-D	7482	13/13	0.70	0.46	24,24,24,24	13
4	CIT	2-D	7482	13/13	0.70	0.46	24,24,24,24	13
4	CIT	3-D	7482	13/13	0.70	0.46	24,24,24,24	13
4	CIT	4-D	7482	13/13	0.70	0.46	24,24,24,24	13
4	CIT	5-D	7482	13/13	0.70	0.46	24,24,24,24	13
4	CIT	6-D	7482	13/13	0.70	0.46	24,24,24,24	13
4	CIT	7-D	7482	13/13	0.70	0.46	24,24,24,24	13
4	CIT	8-D	7482	13/13	0.70	0.46	24,24,24,24	13
4	CIT	9-D	7482	13/13	0.70	0.46	24,24,24,24	13
4	CIT	10-D	7482	13/13	0.70	0.46	24,24,24,24	13
2	MN	1-E	470	1/1	0.72	0.54	24,24,24,24	1
2	MN	2-E	470	1/1	0.72	0.54	24,24,24,24	1
2	MN	3-E	470	1/1	0.72	0.54	24,24,24,24	1
2	MN	4-E	470	1/1	0.72	0.54	24,24,24,24	1
2	MN	5-E	470	1/1	0.72	0.54	24,24,24,24	1
2	MN	6-E	470	1/1	0.72	0.54	24,24,24,24	1
2	MN	7-E	470	1/1	0.72	0.54	24,24,24,24	1
2	MN	8-E	470	1/1	0.72	0.54	24,24,24,24	1
2	MN	9-E	470	1/1	0.72	0.54	24,24,24,24	1
2	MN	10-E	470	1/1	0.72	0.54	24,24,24,24	1
4	CIT	1-I	7492	13/13	0.73	0.35	24,24,24,24	13
4	CIT	2-I	7492	13/13	0.73	0.35	24,24,24,24	13
4	CIT	3-I	7492	13/13	0.73	0.35	24,24,24,24	13
4	CIT	4-I	7492	13/13	0.73	0.35	24,24,24,24	13
4	CIT	5-I	7492	13/13	0.73	0.35	24,24,24,24	13
4	CIT	6-I	7492	13/13	0.73	0.35	24,24,24,24	13
4	CIT	7-I	7492	13/13	0.73	0.35	24,24,24,24	13

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CIT	8-I	7492	13/13	0.73	0.35	24,24,24,24	13
4	CIT	9-I	7492	13/13	0.73	0.35	24,24,24,24	13
4	CIT	10-I	7492	13/13	0.73	0.35	24,24,24,24	13
4	CIT	1-J	7494	13/13	0.74	0.51	24,24,24,24	13
4	CIT	2-J	7494	13/13	0.74	0.51	24,24,24,24	13
4	CIT	3-J	7494	13/13	0.74	0.51	24,24,24,24	13
4	CIT	4-J	7494	13/13	0.74	0.51	24,24,24,24	13
4	CIT	5-J	7494	13/13	0.74	0.51	24,24,24,24	13
4	CIT	6-J	7494	13/13	0.74	0.51	24,24,24,24	13
4	CIT	7-J	7494	13/13	0.74	0.51	24,24,24,24	13
4	CIT	8-J	7494	13/13	0.74	0.51	24,24,24,24	13
4	CIT	9-J	7494	13/13	0.74	0.51	24,24,24,24	13
4	CIT	10-J	7494	13/13	0.74	0.51	24,24,24,24	13
4	CIT	1-A	7476	13/13	0.75	0.39	24,24,24,24	13
4	CIT	2-A	7476	13/13	0.75	0.39	24,24,24,24	13
4	CIT	3-A	7476	13/13	0.75	0.39	24,24,24,24	13
4	CIT	4-A	7476	13/13	0.75	0.39	24,24,24,24	13
4	CIT	5-A	7476	13/13	0.75	0.39	24,24,24,24	13
4	CIT	6-A	7476	13/13	0.75	0.39	24,24,24,24	13
4	CIT	7-A	7476	13/13	0.75	0.39	24,24,24,24	13
4	CIT	8-A	7476	13/13	0.75	0.39	24,24,24,24	13
4	CIT	9-A	7476	13/13	0.75	0.39	24,24,24,24	13
4	CIT	10-A	7476	13/13	0.75	0.39	24,24,24,24	13
4	CIT	1-B	7478	13/13	0.75	0.38	24,24,24,24	13
4	CIT	2-B	7478	13/13	0.75	0.38	24,24,24,24	13
4	CIT	3-B	7478	13/13	0.75	0.38	24,24,24,24	13
4	CIT	4-B	7478	13/13	0.75	0.38	24,24,24,24	13
4	CIT	5-B	7478	13/13	0.75	0.38	24,24,24,24	13
4	CIT	6-B	7478	13/13	0.75	0.38	24,24,24,24	13
4	CIT	7-B	7478	13/13	0.75	0.38	24,24,24,24	13
4	CIT	8-B	7478	13/13	0.75	0.38	24,24,24,24	13
4	CIT	9-B	7478	13/13	0.75	0.38	24,24,24,24	13
4	CIT	10-B	7478	13/13	0.75	0.38	24,24,24,24	13
4	CIT	1-X	7522	13/13	0.75	0.37	24,24,24,24	13
4	CIT	2-X	7522	13/13	0.75	0.37	24,24,24,24	13
4	CIT	3-X	7522	13/13	0.75	0.37	24,24,24,24	13
4	CIT	4-X	7522	13/13	0.75	0.37	24,24,24,24	13
4	CIT	5-X	7522	13/13	0.75	0.37	24,24,24,24	13
4	CIT	6-X	7522	13/13	0.75	0.37	24,24,24,24	13
4	CIT	7-X	7522	13/13	0.75	0.37	24,24,24,24	13
4	CIT	8-X	7522	13/13	0.75	0.37	24,24,24,24	13
4	CIT	9-X	7522	13/13	0.75	0.37	24,24,24,24	13

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CIT	10-X	7522	13/13	0.75	0.37	24,24,24,24	13
4	CIT	1-O	7504	13/13	0.76	0.42	24,24,24,24	13
4	CIT	2-O	7504	13/13	0.76	0.42	24,24,24,24	13
4	CIT	3-O	7504	13/13	0.76	0.42	24,24,24,24	13
4	CIT	4-O	7504	13/13	0.76	0.42	24,24,24,24	13
4	CIT	5-O	7504	13/13	0.76	0.42	24,24,24,24	13
4	CIT	6-O	7504	13/13	0.76	0.42	24,24,24,24	13
4	CIT	7-O	7504	13/13	0.76	0.42	24,24,24,24	13
4	CIT	8-O	7504	13/13	0.76	0.42	24,24,24,24	13
4	CIT	9-O	7504	13/13	0.76	0.42	24,24,24,24	13
4	CIT	10-O	7504	13/13	0.76	0.42	24,24,24,24	13
4	CIT	1-W	7520	13/13	0.77	0.42	24,24,24,24	13
4	CIT	2-W	7520	13/13	0.77	0.42	24,24,24,24	13
4	CIT	3-W	7520	13/13	0.77	0.42	24,24,24,24	13
4	CIT	4-W	7520	13/13	0.77	0.42	24,24,24,24	13
4	CIT	5-W	7520	13/13	0.77	0.42	24,24,24,24	13
4	CIT	6-W	7520	13/13	0.77	0.42	24,24,24,24	13
4	CIT	7-W	7520	13/13	0.77	0.42	24,24,24,24	13
4	CIT	8-W	7520	13/13	0.77	0.42	24,24,24,24	13
4	CIT	9-W	7520	13/13	0.77	0.42	24,24,24,24	13
4	CIT	10-W	7520	13/13	0.77	0.42	24,24,24,24	13
4	CIT	1-S	7512	13/13	0.77	0.38	24,24,24,24	13
4	CIT	2-S	7512	13/13	0.77	0.38	24,24,24,24	13
4	CIT	3-S	7512	13/13	0.77	0.38	24,24,24,24	13
4	CIT	4-S	7512	13/13	0.77	0.38	24,24,24,24	13
4	CIT	5-S	7512	13/13	0.77	0.38	24,24,24,24	13
4	CIT	6-S	7512	13/13	0.77	0.38	24,24,24,24	13
4	CIT	7-S	7512	13/13	0.77	0.38	24,24,24,24	13
4	CIT	8-S	7512	13/13	0.77	0.38	24,24,24,24	13
4	CIT	9-S	7512	13/13	0.77	0.38	24,24,24,24	13
4	CIT	10-S	7512	13/13	0.77	0.38	24,24,24,24	13
4	CIT	1-M	7500	13/13	0.78	0.43	24,24,24,24	13
4	CIT	2-M	7500	13/13	0.78	0.43	24,24,24,24	13
4	CIT	3-M	7500	13/13	0.78	0.43	24,24,24,24	13
4	CIT	4-M	7500	13/13	0.78	0.43	24,24,24,24	13
4	CIT	5-M	7500	13/13	0.78	0.43	24,24,24,24	13
4	CIT	6-M	7500	13/13	0.78	0.43	24,24,24,24	13
4	CIT	7-M	7500	13/13	0.78	0.43	24,24,24,24	13
4	CIT	8-M	7500	13/13	0.78	0.43	24,24,24,24	13
4	CIT	9-M	7500	13/13	0.78	0.43	24,24,24,24	13
4	CIT	10-M	7500	13/13	0.78	0.43	24,24,24,24	13

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CIT	1-C	7480	13/13	0.78	0.41	24,24,24,24	13
4	CIT	2-C	7480	13/13	0.78	0.41	24,24,24,24	13
4	CIT	3-C	7480	13/13	0.78	0.41	24,24,24,24	13
4	CIT	4-C	7480	13/13	0.78	0.41	24,24,24,24	13
4	CIT	5-C	7480	13/13	0.78	0.41	24,24,24,24	13
4	CIT	6-C	7480	13/13	0.78	0.41	24,24,24,24	13
4	CIT	7-C	7480	13/13	0.78	0.41	24,24,24,24	13
4	CIT	8-C	7480	13/13	0.78	0.41	24,24,24,24	13
4	CIT	9-C	7480	13/13	0.78	0.41	24,24,24,24	13
4	CIT	10-C	7480	13/13	0.78	0.41	24,24,24,24	13
2	MN	1-L	470	1/1	0.78	0.58	24,24,24,24	1
2	MN	2-L	470	1/1	0.78	0.58	24,24,24,24	1
2	MN	3-L	470	1/1	0.78	0.58	24,24,24,24	1
2	MN	4-L	470	1/1	0.78	0.58	24,24,24,24	1
2	MN	5-L	470	1/1	0.78	0.58	24,24,24,24	1
2	MN	6-L	470	1/1	0.78	0.58	24,24,24,24	1
2	MN	7-L	470	1/1	0.78	0.58	24,24,24,24	1
2	MN	8-L	470	1/1	0.78	0.58	24,24,24,24	1
2	MN	9-L	470	1/1	0.78	0.58	24,24,24,24	1
2	MN	10-L	470	1/1	0.78	0.58	24,24,24,24	1
2	MN	1-A	470	1/1	0.79	0.50	24,24,24,24	1
2	MN	2-A	470	1/1	0.79	0.50	24,24,24,24	1
2	MN	3-A	470	1/1	0.79	0.50	24,24,24,24	1
2	MN	4-A	470	1/1	0.79	0.50	24,24,24,24	1
2	MN	5-A	470	1/1	0.79	0.50	24,24,24,24	1
2	MN	6-A	470	1/1	0.79	0.50	24,24,24,24	1
2	MN	7-A	470	1/1	0.79	0.50	24,24,24,24	1
2	MN	8-A	470	1/1	0.79	0.50	24,24,24,24	1
2	MN	9-A	470	1/1	0.79	0.50	24,24,24,24	1
2	MN	10-A	470	1/1	0.79	0.50	24,24,24,24	1
2	MN	1-I	470	1/1	0.80	0.55	24,24,24,24	1
2	MN	2-I	470	1/1	0.80	0.55	24,24,24,24	1
2	MN	3-I	470	1/1	0.80	0.55	24,24,24,24	1
2	MN	4-I	470	1/1	0.80	0.55	24,24,24,24	1
2	MN	5-I	470	1/1	0.80	0.55	24,24,24,24	1
2	MN	6-I	470	1/1	0.80	0.55	24,24,24,24	1
2	MN	7-I	470	1/1	0.80	0.55	24,24,24,24	1
2	MN	8-I	470	1/1	0.80	0.55	24,24,24,24	1
2	MN	9-I	470	1/1	0.80	0.55	24,24,24,24	1
2	MN	10-I	470	1/1	0.80	0.55	24,24,24,24	1
2	MN	1-M	470	1/1	0.81	0.52	24,24,24,24	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MN	2-M	470	1/1	0.81	0.52	24,24,24,24	1
2	MN	3-M	470	1/1	0.81	0.52	24,24,24,24	1
2	MN	4-M	470	1/1	0.81	0.52	24,24,24,24	1
2	MN	5-M	470	1/1	0.81	0.52	24,24,24,24	1
2	MN	6-M	470	1/1	0.81	0.52	24,24,24,24	1
2	MN	7-M	470	1/1	0.81	0.52	24,24,24,24	1
2	MN	8-M	470	1/1	0.81	0.52	24,24,24,24	1
2	MN	9-M	470	1/1	0.81	0.52	24,24,24,24	1
2	MN	10-M	470	1/1	0.81	0.52	24,24,24,24	1
2	MN	1-Q	470	1/1	0.82	0.61	24,24,24,24	1
2	MN	2-Q	470	1/1	0.82	0.61	24,24,24,24	1
2	MN	3-Q	470	1/1	0.82	0.61	24,24,24,24	1
2	MN	4-Q	470	1/1	0.82	0.61	24,24,24,24	1
2	MN	5-Q	470	1/1	0.82	0.61	24,24,24,24	1
2	MN	6-Q	470	1/1	0.82	0.61	24,24,24,24	1
2	MN	7-Q	470	1/1	0.82	0.61	24,24,24,24	1
2	MN	8-Q	470	1/1	0.82	0.61	24,24,24,24	1
2	MN	9-Q	470	1/1	0.82	0.61	24,24,24,24	1
2	MN	10-Q	470	1/1	0.82	0.61	24,24,24,24	1
2	MN	1-D	470	1/1	0.82	0.60	24,24,24,24	1
2	MN	2-D	470	1/1	0.82	0.60	24,24,24,24	1
2	MN	3-D	470	1/1	0.82	0.60	24,24,24,24	1
2	MN	4-D	470	1/1	0.82	0.60	24,24,24,24	1
2	MN	5-D	470	1/1	0.82	0.60	24,24,24,24	1
2	MN	6-D	470	1/1	0.82	0.60	24,24,24,24	1
2	MN	7-D	470	1/1	0.82	0.60	24,24,24,24	1
2	MN	8-D	470	1/1	0.82	0.60	24,24,24,24	1
2	MN	9-D	470	1/1	0.82	0.60	24,24,24,24	1
2	MN	10-D	470	1/1	0.82	0.60	24,24,24,24	1
2	MN	1-W	470	1/1	0.82	0.51	24,24,24,24	1
2	MN	2-W	470	1/1	0.82	0.51	24,24,24,24	1
2	MN	3-W	470	1/1	0.82	0.51	24,24,24,24	1
2	MN	4-W	470	1/1	0.82	0.51	24,24,24,24	1
2	MN	5-W	470	1/1	0.82	0.51	24,24,24,24	1
2	MN	6-W	470	1/1	0.82	0.51	24,24,24,24	1
2	MN	7-W	470	1/1	0.82	0.51	24,24,24,24	1
2	MN	8-W	470	1/1	0.82	0.51	24,24,24,24	1
2	MN	9-W	470	1/1	0.82	0.51	24,24,24,24	1
2	MN	10-W	470	1/1	0.82	0.51	24,24,24,24	1
2	MN	1-G	470	1/1	0.83	0.57	24,24,24,24	1
2	MN	2-G	470	1/1	0.83	0.57	24,24,24,24	1
2	MN	3-G	470	1/1	0.83	0.57	24,24,24,24	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MN	4-G	470	1/1	0.83	0.57	24,24,24,24	1
2	MN	5-G	470	1/1	0.83	0.57	24,24,24,24	1
2	MN	6-G	470	1/1	0.83	0.57	24,24,24,24	1
2	MN	7-G	470	1/1	0.83	0.57	24,24,24,24	1
2	MN	8-G	470	1/1	0.83	0.57	24,24,24,24	1
2	MN	9-G	470	1/1	0.83	0.57	24,24,24,24	1
2	MN	10-G	470	1/1	0.83	0.57	24,24,24,24	1
2	MN	1-F	470	1/1	0.88	0.59	24,24,24,24	1
2	MN	2-F	470	1/1	0.88	0.59	24,24,24,24	1
2	MN	3-F	470	1/1	0.88	0.59	24,24,24,24	1
2	MN	4-F	470	1/1	0.88	0.59	24,24,24,24	1
2	MN	5-F	470	1/1	0.88	0.59	24,24,24,24	1
2	MN	6-F	470	1/1	0.88	0.59	24,24,24,24	1
2	MN	7-F	470	1/1	0.88	0.59	24,24,24,24	1
2	MN	8-F	470	1/1	0.88	0.59	24,24,24,24	1
2	MN	9-F	470	1/1	0.88	0.59	24,24,24,24	1
2	MN	10-F	470	1/1	0.88	0.59	24,24,24,24	1
2	MN	1-P	470	1/1	0.89	0.51	24,24,24,24	1
2	MN	2-P	470	1/1	0.89	0.51	24,24,24,24	1
2	MN	3-P	470	1/1	0.89	0.51	24,24,24,24	1
2	MN	4-P	470	1/1	0.89	0.51	24,24,24,24	1
2	MN	5-P	470	1/1	0.89	0.51	24,24,24,24	1
2	MN	6-P	470	1/1	0.89	0.51	24,24,24,24	1
2	MN	7-P	470	1/1	0.89	0.51	24,24,24,24	1
2	MN	8-P	470	1/1	0.89	0.51	24,24,24,24	1
2	MN	9-P	470	1/1	0.89	0.51	24,24,24,24	1
2	MN	10-P	470	1/1	0.89	0.51	24,24,24,24	1
2	MN	1-K	470	1/1	0.89	0.53	24,24,24,24	1
2	MN	2-K	470	1/1	0.89	0.53	24,24,24,24	1
2	MN	3-K	470	1/1	0.89	0.53	24,24,24,24	1
2	MN	4-K	470	1/1	0.89	0.53	24,24,24,24	1
2	MN	5-K	470	1/1	0.89	0.53	24,24,24,24	1
2	MN	6-K	470	1/1	0.89	0.53	24,24,24,24	1
2	MN	7-K	470	1/1	0.89	0.53	24,24,24,24	1
2	MN	8-K	470	1/1	0.89	0.53	24,24,24,24	1
2	MN	9-K	470	1/1	0.89	0.53	24,24,24,24	1
2	MN	10-K	470	1/1	0.89	0.53	24,24,24,24	1
2	MN	1-J	470	1/1	0.90	0.56	24,24,24,24	1
2	MN	2-J	470	1/1	0.90	0.56	24,24,24,24	1
2	MN	3-J	470	1/1	0.90	0.56	24,24,24,24	1
2	MN	4-J	470	1/1	0.90	0.56	24,24,24,24	1
2	MN	5-J	470	1/1	0.90	0.56	24,24,24,24	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MN	6-J	470	1/1	0.90	0.56	24,24,24,24	1
2	MN	7-J	470	1/1	0.90	0.56	24,24,24,24	1
2	MN	8-J	470	1/1	0.90	0.56	24,24,24,24	1
2	MN	9-J	470	1/1	0.90	0.56	24,24,24,24	1
2	MN	10-J	470	1/1	0.90	0.56	24,24,24,24	1
2	MN	1-C	470	1/1	0.90	0.55	24,24,24,24	1
2	MN	2-C	470	1/1	0.90	0.55	24,24,24,24	1
2	MN	3-C	470	1/1	0.90	0.55	24,24,24,24	1
2	MN	4-C	470	1/1	0.90	0.55	24,24,24,24	1
2	MN	5-C	470	1/1	0.90	0.55	24,24,24,24	1
2	MN	6-C	470	1/1	0.90	0.55	24,24,24,24	1
2	MN	7-C	470	1/1	0.90	0.55	24,24,24,24	1
2	MN	8-C	470	1/1	0.90	0.55	24,24,24,24	1
2	MN	9-C	470	1/1	0.90	0.55	24,24,24,24	1
2	MN	10-C	470	1/1	0.90	0.55	24,24,24,24	1
2	MN	1-H	470	1/1	0.91	0.58	24,24,24,24	1
2	MN	2-H	470	1/1	0.91	0.58	24,24,24,24	1
2	MN	3-H	470	1/1	0.91	0.58	24,24,24,24	1
2	MN	4-H	470	1/1	0.91	0.58	24,24,24,24	1
2	MN	5-H	470	1/1	0.91	0.58	24,24,24,24	1
2	MN	6-H	470	1/1	0.91	0.58	24,24,24,24	1
2	MN	7-H	470	1/1	0.91	0.58	24,24,24,24	1
2	MN	8-H	470	1/1	0.91	0.58	24,24,24,24	1
2	MN	9-H	470	1/1	0.91	0.58	24,24,24,24	1
2	MN	10-H	470	1/1	0.91	0.58	24,24,24,24	1
2	MN	1-X	470	1/1	0.91	0.60	24,24,24,24	1
2	MN	2-X	470	1/1	0.91	0.60	24,24,24,24	1
2	MN	3-X	470	1/1	0.91	0.60	24,24,24,24	1
2	MN	4-X	470	1/1	0.91	0.60	24,24,24,24	1
2	MN	5-X	470	1/1	0.91	0.60	24,24,24,24	1
2	MN	6-X	470	1/1	0.91	0.60	24,24,24,24	1
2	MN	7-X	470	1/1	0.91	0.60	24,24,24,24	1
2	MN	8-X	470	1/1	0.91	0.60	24,24,24,24	1
2	MN	9-X	470	1/1	0.91	0.60	24,24,24,24	1
2	MN	10-X	470	1/1	0.91	0.60	24,24,24,24	1
2	MN	1-T	470	1/1	0.92	0.39	24,24,24,24	1
2	MN	2-T	470	1/1	0.92	0.39	24,24,24,24	1
2	MN	3-T	470	1/1	0.92	0.39	24,24,24,24	1
2	MN	4-T	470	1/1	0.92	0.39	24,24,24,24	1
2	MN	5-T	470	1/1	0.92	0.39	24,24,24,24	1
2	MN	6-T	470	1/1	0.92	0.39	24,24,24,24	1
2	MN	7-T	470	1/1	0.92	0.39	24,24,24,24	1

Continued on next page...

Continued from previous page...

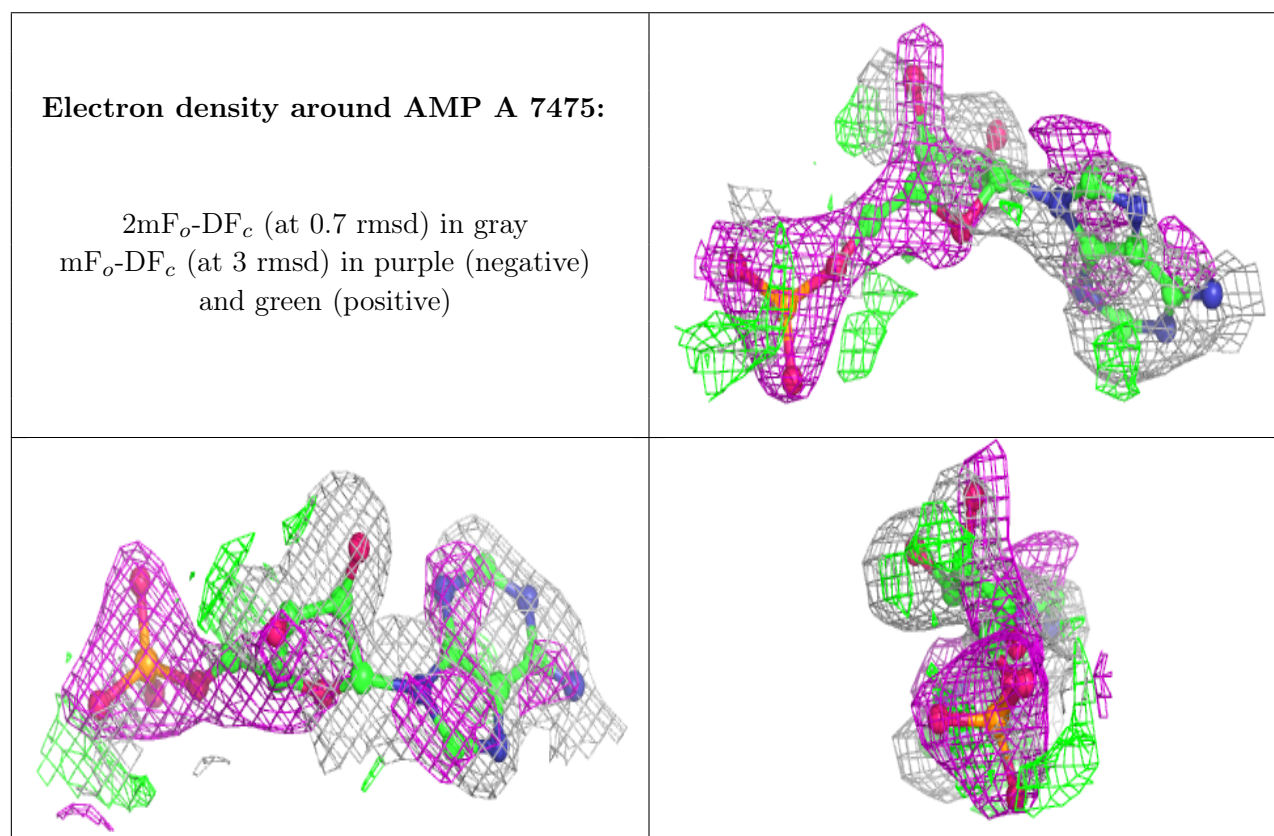
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MN	8-T	470	1/1	0.92	0.39	24,24,24,24	1
2	MN	9-T	470	1/1	0.92	0.39	24,24,24,24	1
2	MN	10-T	470	1/1	0.92	0.39	24,24,24,24	1
2	MN	1-V	470	1/1	0.94	0.46	24,24,24,24	1
2	MN	2-V	470	1/1	0.94	0.46	24,24,24,24	1
2	MN	3-V	470	1/1	0.94	0.46	24,24,24,24	1
2	MN	4-V	470	1/1	0.94	0.46	24,24,24,24	1
2	MN	5-V	470	1/1	0.94	0.46	24,24,24,24	1
2	MN	6-V	470	1/1	0.94	0.46	24,24,24,24	1
2	MN	7-V	470	1/1	0.94	0.46	24,24,24,24	1
2	MN	8-V	470	1/1	0.94	0.46	24,24,24,24	1
2	MN	9-V	470	1/1	0.94	0.46	24,24,24,24	1
2	MN	10-V	470	1/1	0.94	0.46	24,24,24,24	1
2	MN	1-B	470	1/1	0.94	0.52	24,24,24,24	1
2	MN	2-B	470	1/1	0.94	0.52	24,24,24,24	1
2	MN	3-B	470	1/1	0.94	0.52	24,24,24,24	1
2	MN	4-B	470	1/1	0.94	0.52	24,24,24,24	1
2	MN	5-B	470	1/1	0.94	0.52	24,24,24,24	1
2	MN	6-B	470	1/1	0.94	0.52	24,24,24,24	1
2	MN	7-B	470	1/1	0.94	0.52	24,24,24,24	1
2	MN	8-B	470	1/1	0.94	0.52	24,24,24,24	1
2	MN	9-B	470	1/1	0.94	0.52	24,24,24,24	1
2	MN	10-B	470	1/1	0.94	0.52	24,24,24,24	1
2	MN	1-U	470	1/1	0.94	0.56	24,24,24,24	1
2	MN	2-U	470	1/1	0.94	0.56	24,24,24,24	1
2	MN	3-U	470	1/1	0.94	0.56	24,24,24,24	1
2	MN	4-U	470	1/1	0.94	0.56	24,24,24,24	1
2	MN	5-U	470	1/1	0.94	0.56	24,24,24,24	1
2	MN	6-U	470	1/1	0.94	0.56	24,24,24,24	1
2	MN	7-U	470	1/1	0.94	0.56	24,24,24,24	1
2	MN	8-U	470	1/1	0.94	0.56	24,24,24,24	1
2	MN	9-U	470	1/1	0.94	0.56	24,24,24,24	1
2	MN	10-U	470	1/1	0.94	0.56	24,24,24,24	1
2	MN	1-S	470	1/1	0.96	0.50	24,24,24,24	1
2	MN	2-S	470	1/1	0.96	0.50	24,24,24,24	1
2	MN	3-S	470	1/1	0.96	0.50	24,24,24,24	1
2	MN	4-S	470	1/1	0.96	0.50	24,24,24,24	1
2	MN	5-S	470	1/1	0.96	0.50	24,24,24,24	1
2	MN	6-S	470	1/1	0.96	0.50	24,24,24,24	1
2	MN	7-S	470	1/1	0.96	0.50	24,24,24,24	1
2	MN	8-S	470	1/1	0.96	0.50	24,24,24,24	1
2	MN	9-S	470	1/1	0.96	0.50	24,24,24,24	1

Continued on next page...

Continued from previous page...

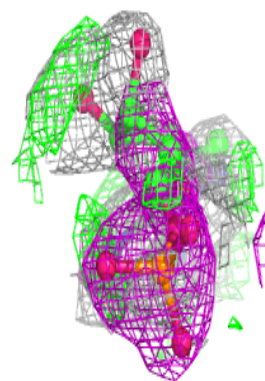
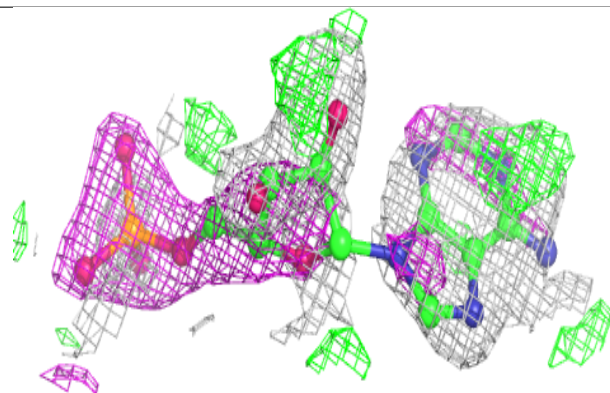
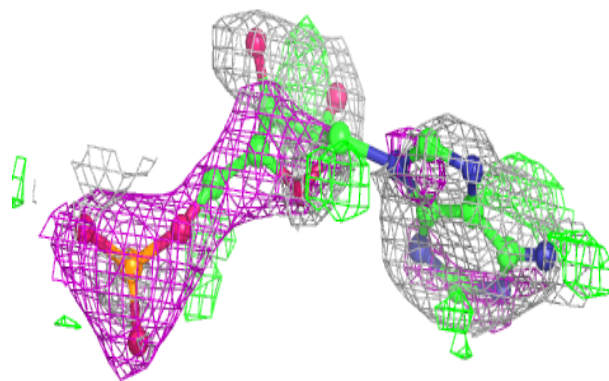
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MN	10-S	470	1/1	0.96	0.50	24,24,24,24	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

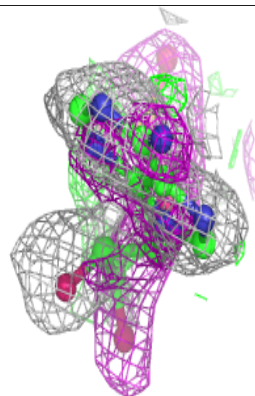
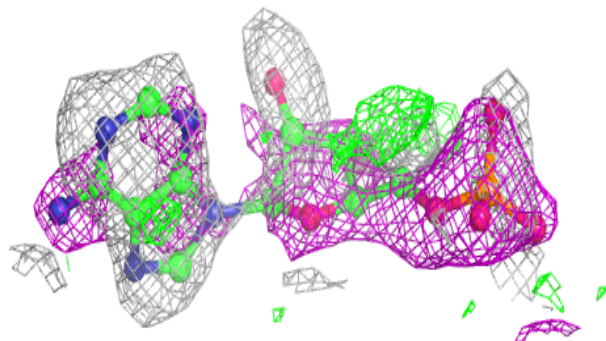
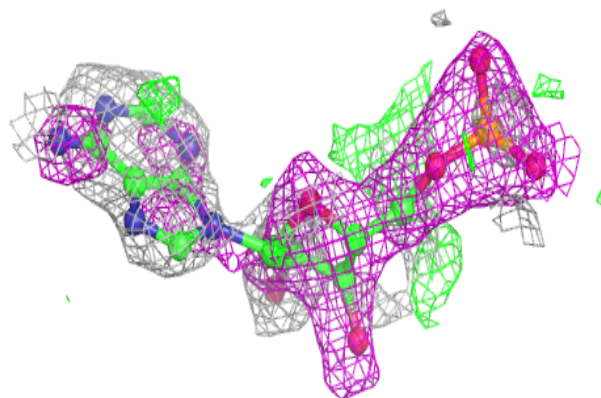


Electron density around AMP L 7497:

$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)

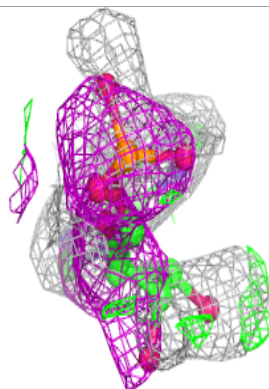
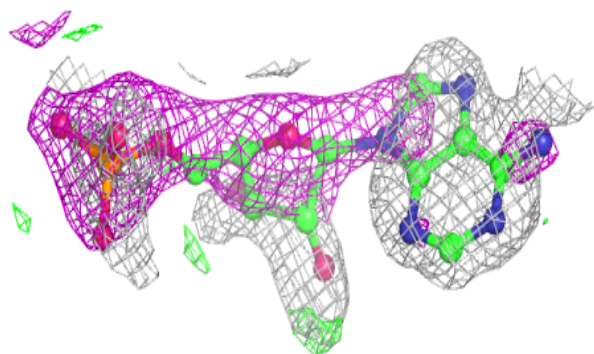
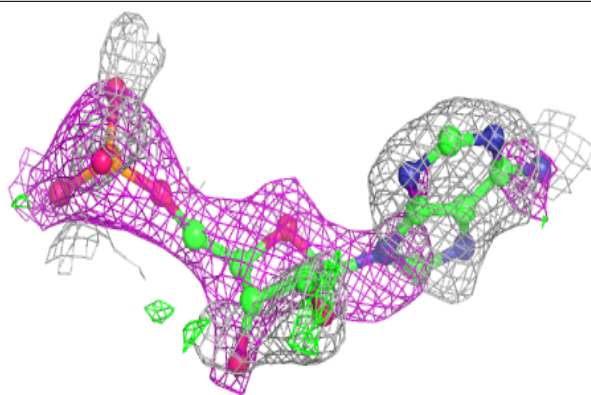
**Electron density around AMP J 7493:**

$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)

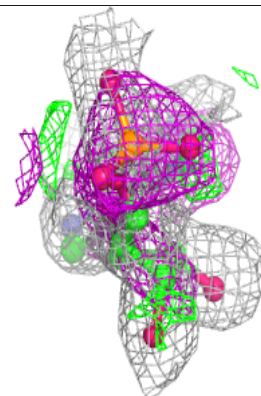
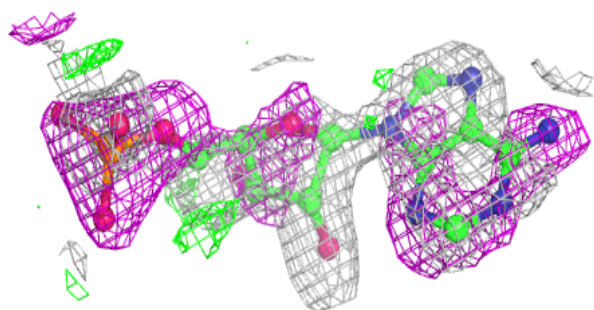
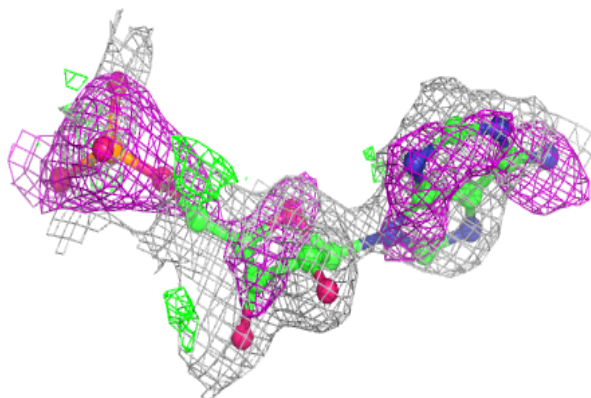


Electron density around AMP R 7509:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

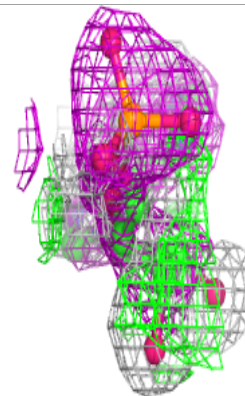
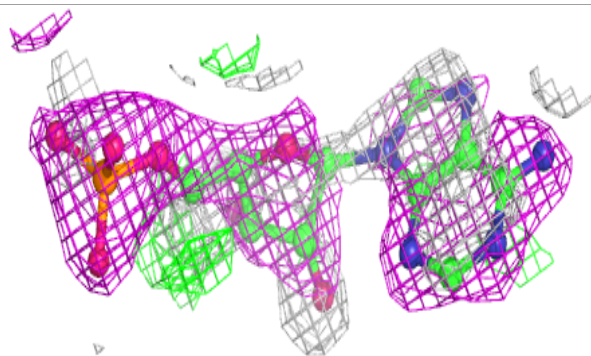
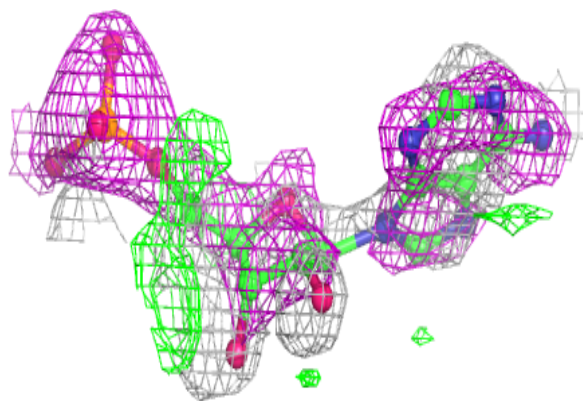
**Electron density around AMP S 7511:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

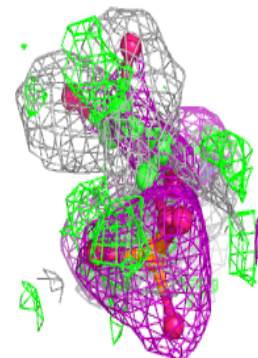
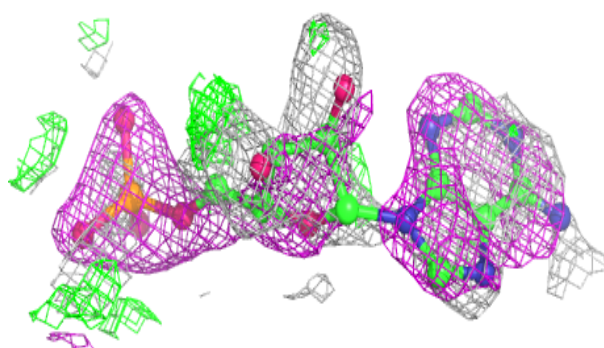
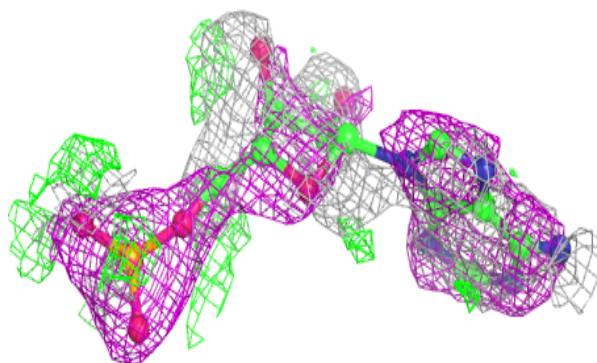


Electron density around AMP D 7481:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

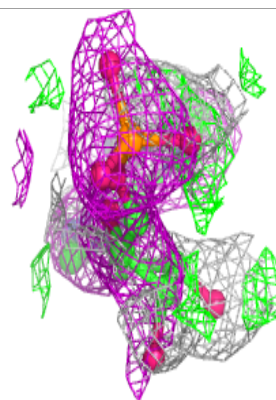
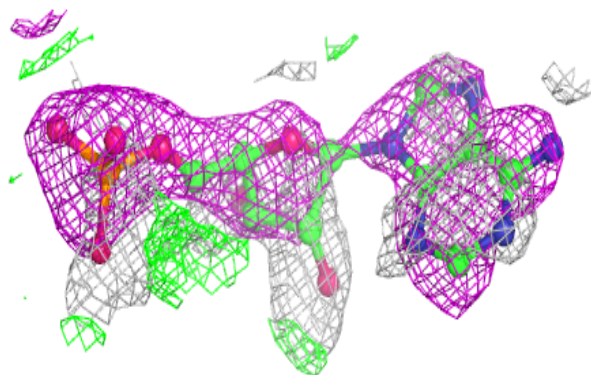
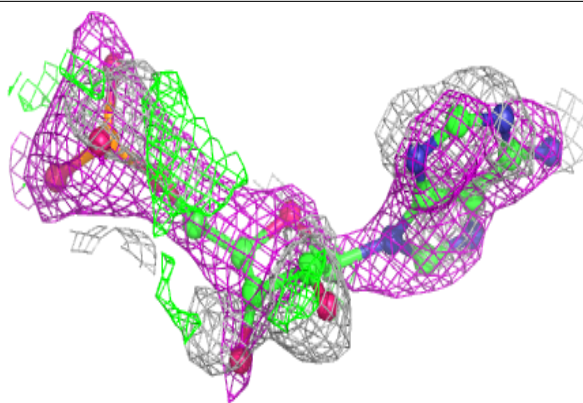
**Electron density around AMP E 7483:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

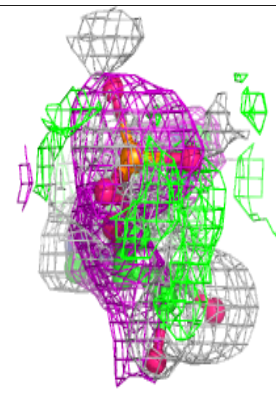
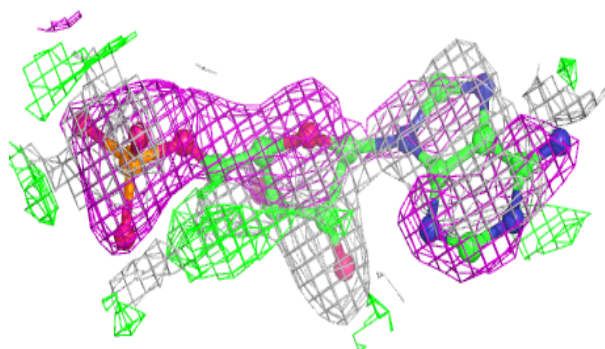
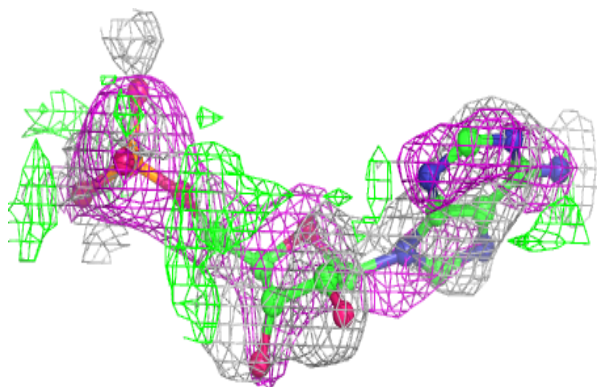


Electron density around AMP O 7503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

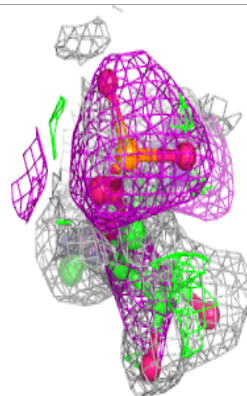
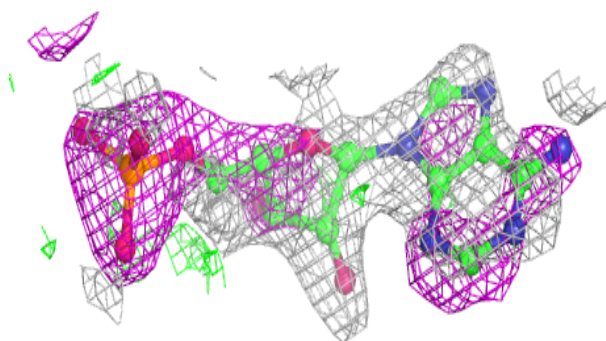
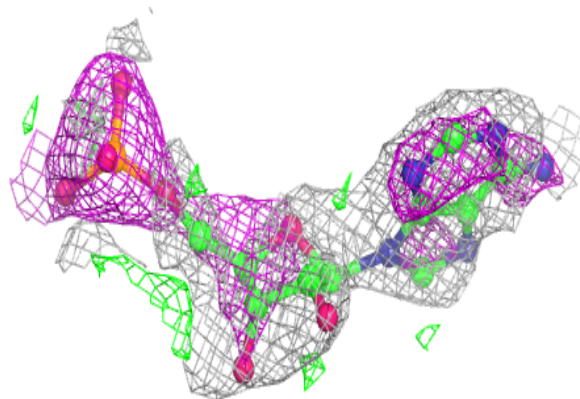
**Electron density around AMP P 7505:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

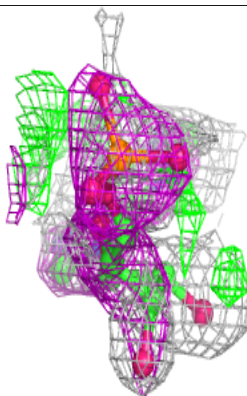
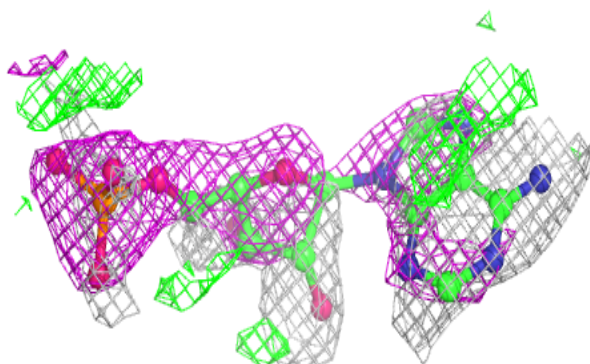
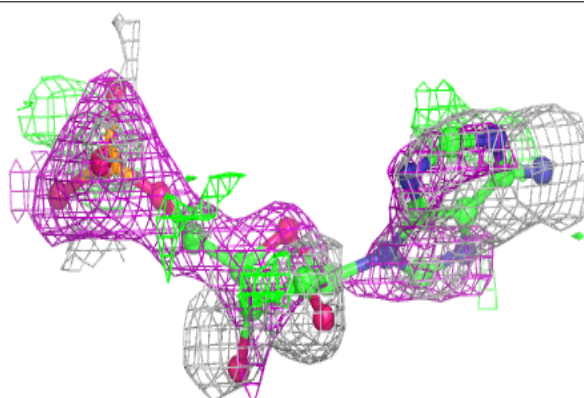


Electron density around AMP G 7487:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

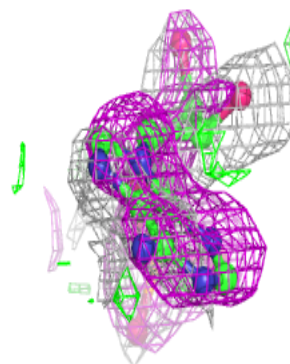
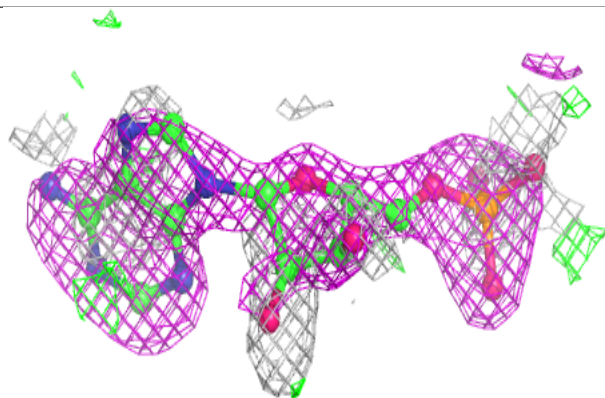
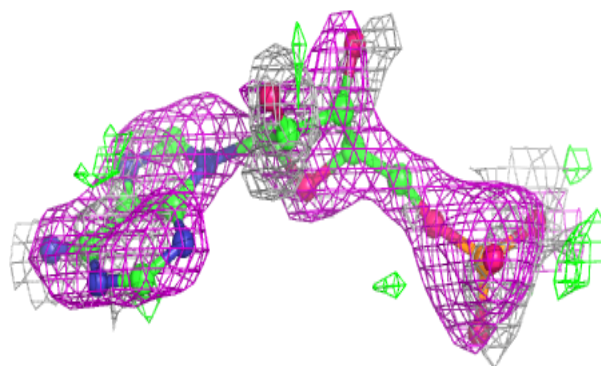
**Electron density around AMP I 7491:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

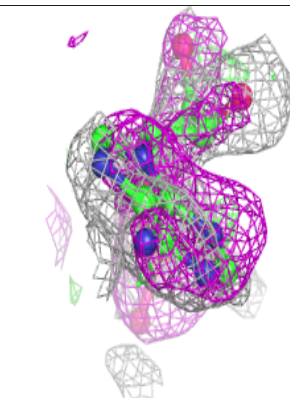
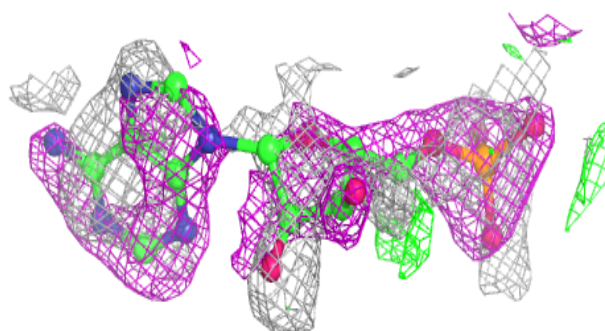
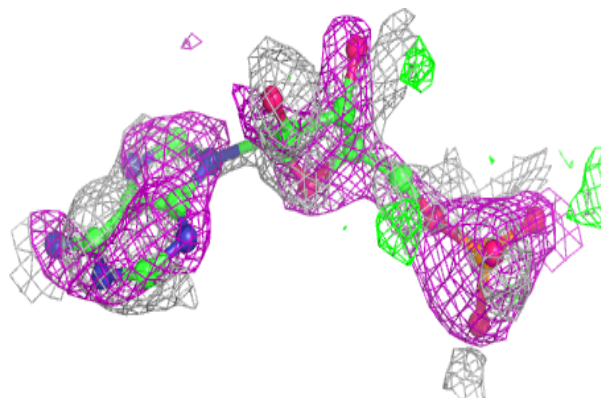


Electron density around AMP U 7515:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

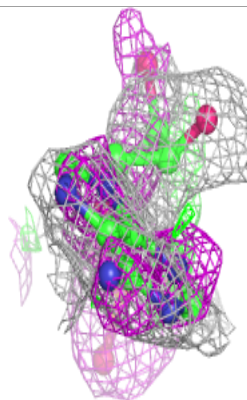
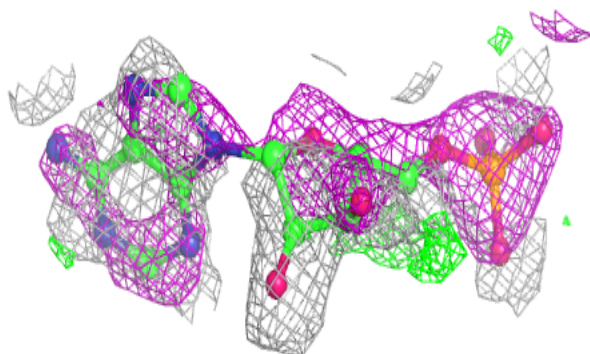
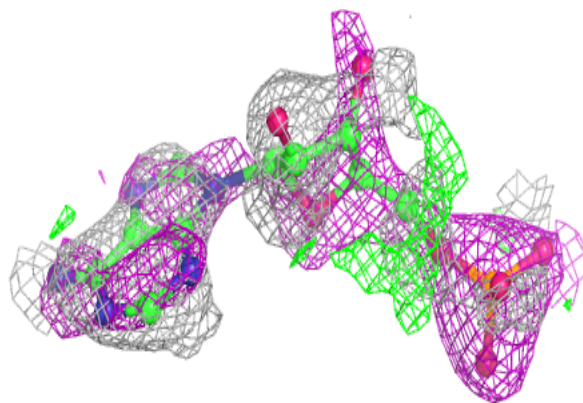
**Electron density around AMP W 7519:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

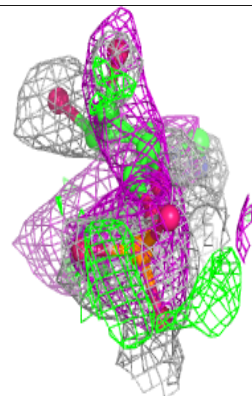
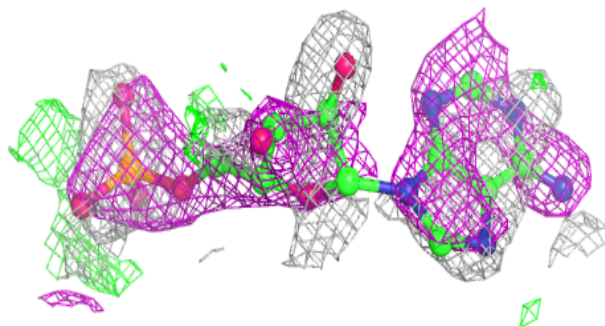
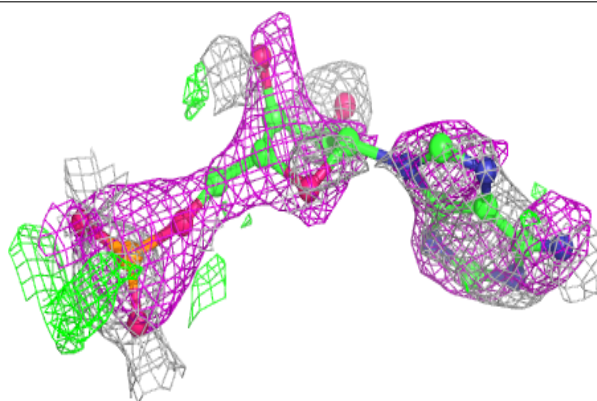


Electron density around AMP K 7495:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

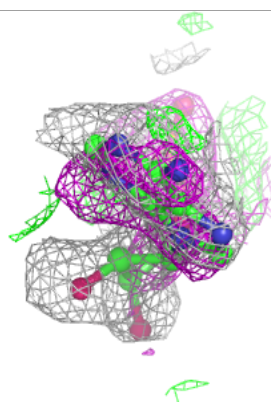
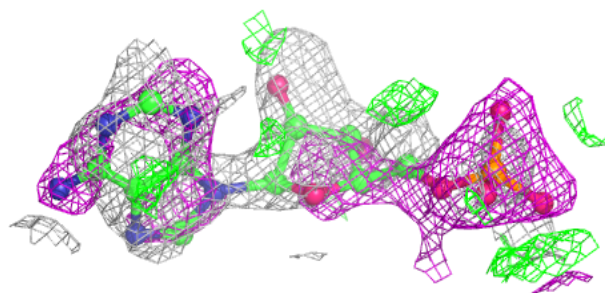
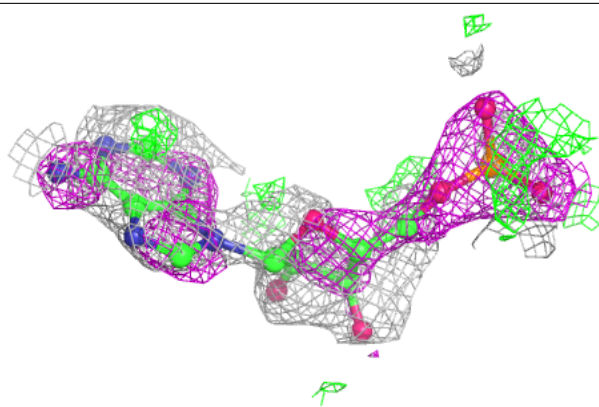
**Electron density around AMP V 7517:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

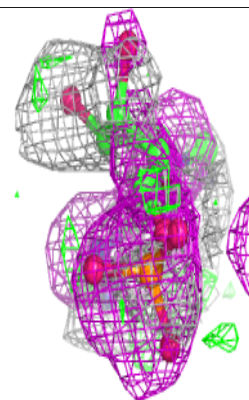
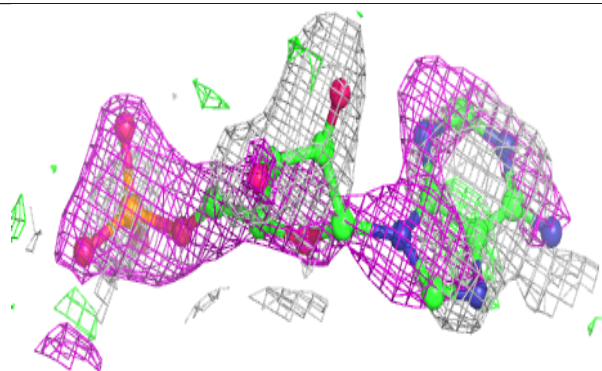
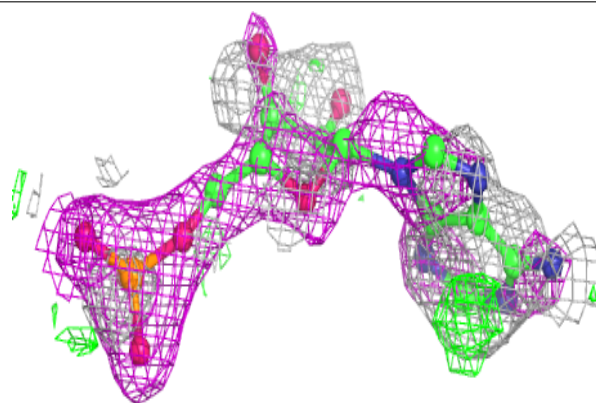


Electron density around AMP H 7489:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

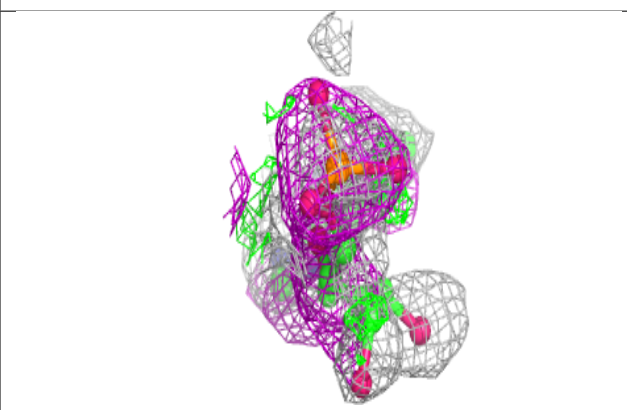
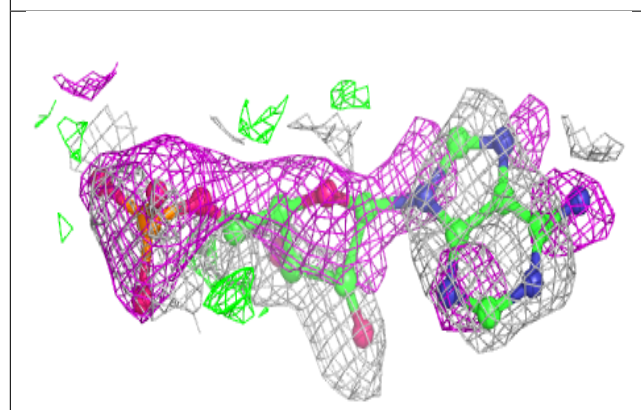
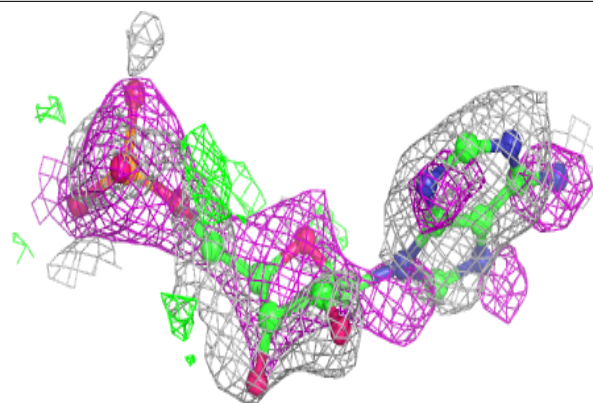
**Electron density around AMP X 7521:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

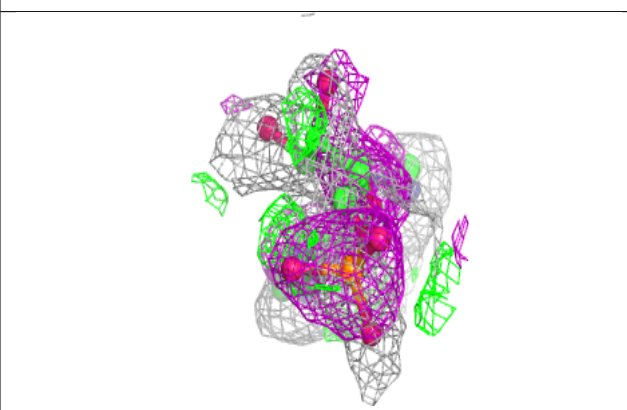
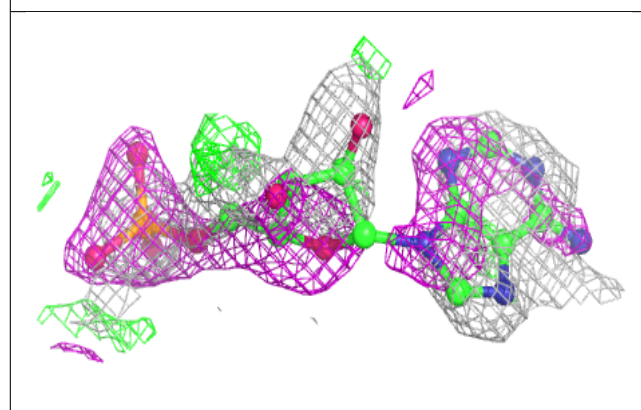
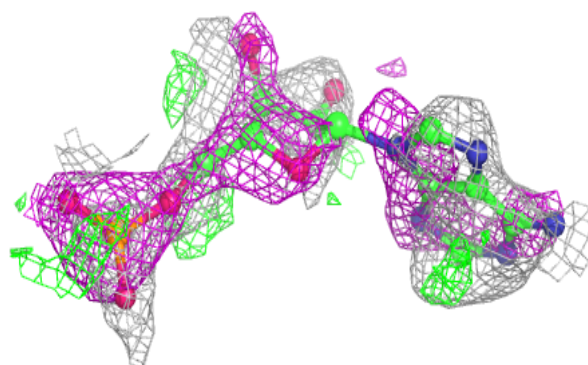


Electron density around AMP F 7485:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

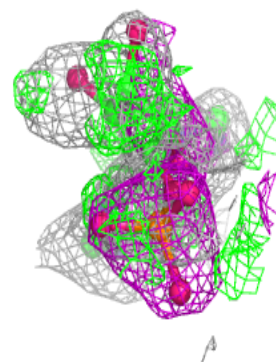
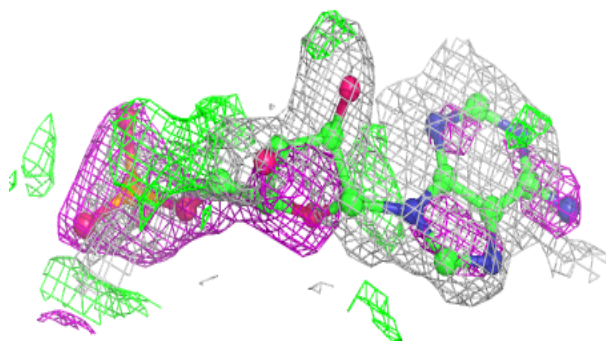
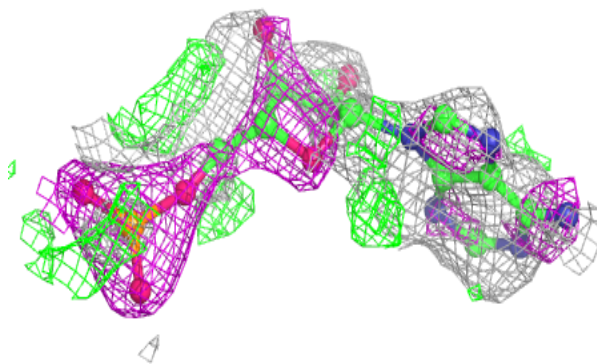
**Electron density around AMP N 7501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

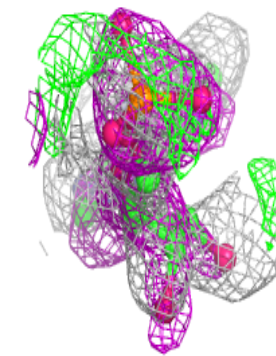
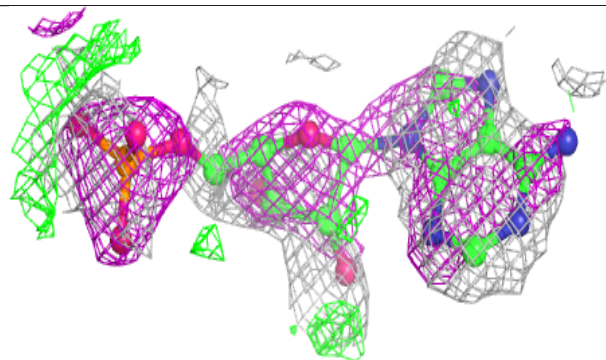
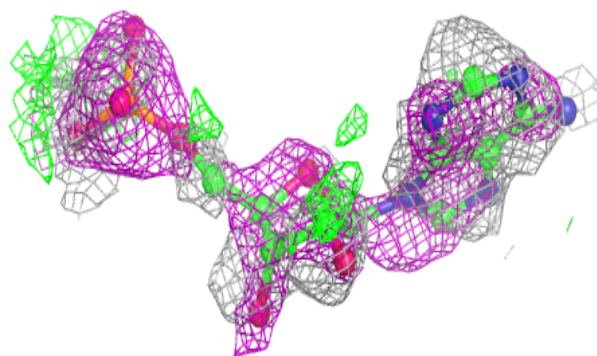


Electron density around AMP Q 7507:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

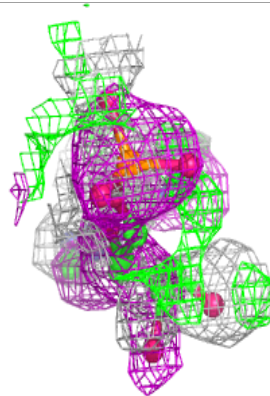
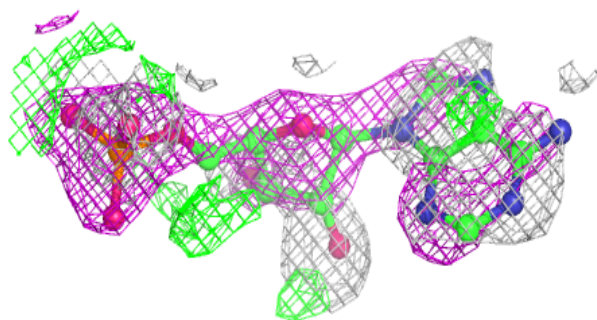
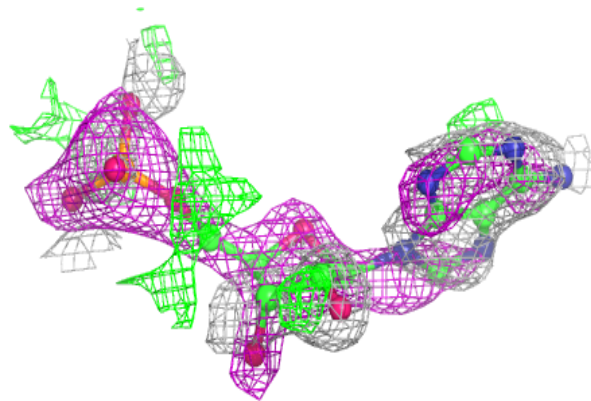
**Electron density around AMP B 7477:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

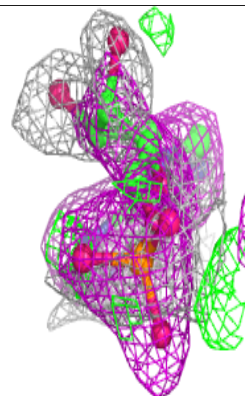
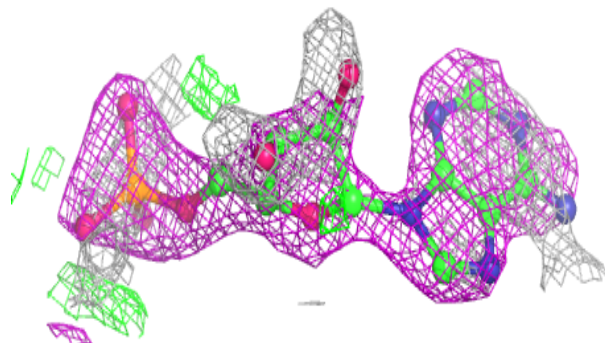
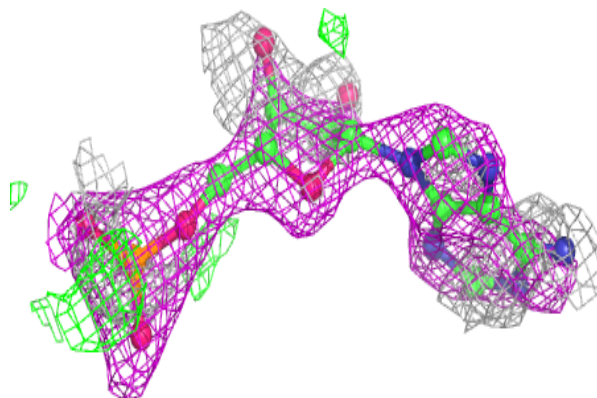


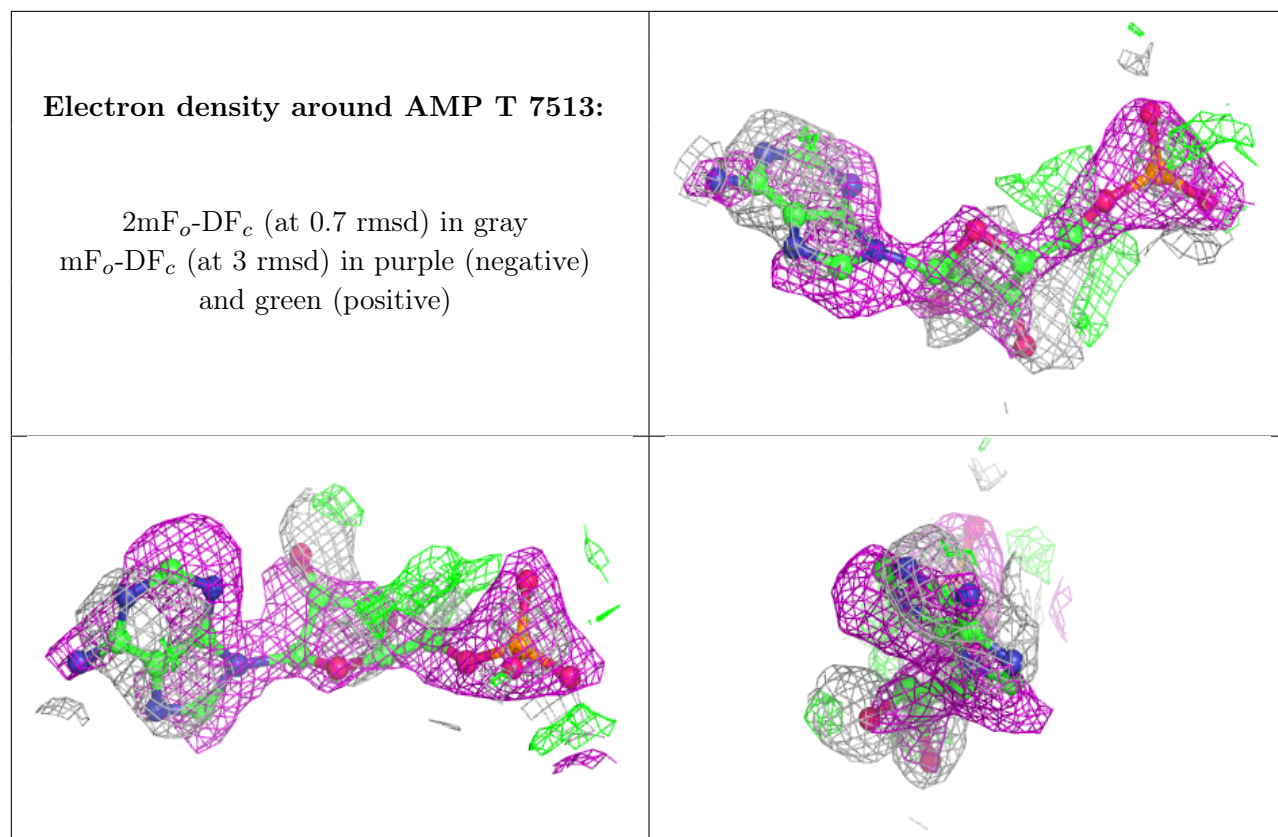
Electron density around AMP M 7499:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around AMP C 7479:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.