Full wwPDB EM Validation Report ⓘ

May 20, 2024 – 05:11 AM EDT

PDB ID	:	7N61
EMDB ID	:	EMD-24191
Title	:	structure of C2 projections and MIPs
Authors	:	Han, L.; Zhang, K.
Deposited on	:	2021-06-07
Resolution	:	3.50 Å(reported)

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

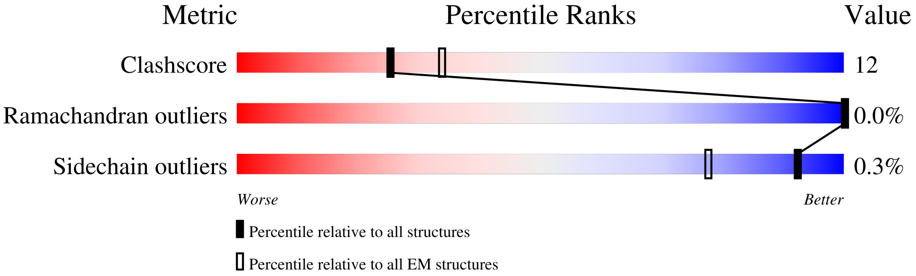
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

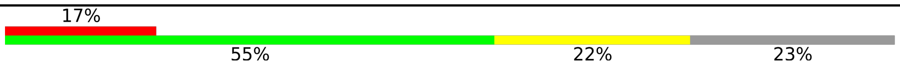
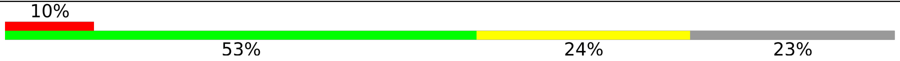
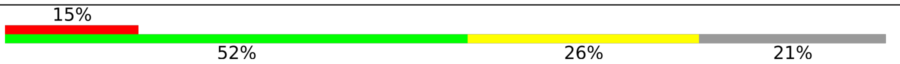
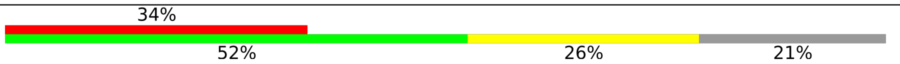
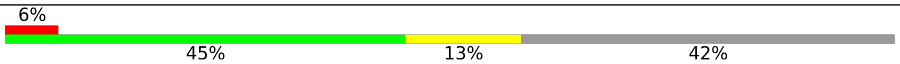
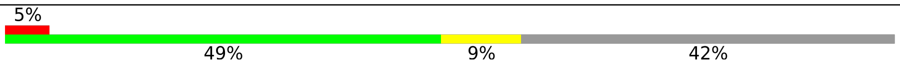
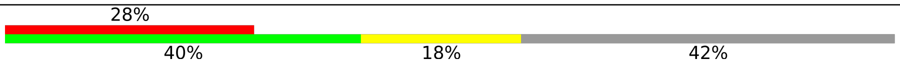
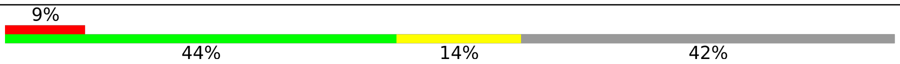
The reported resolution of this entry is 3.50 Å.

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.



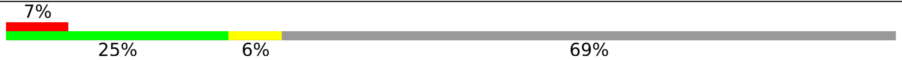
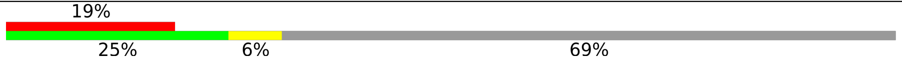
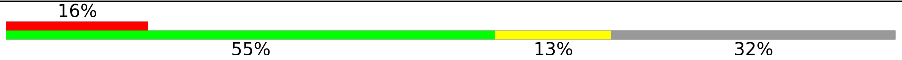
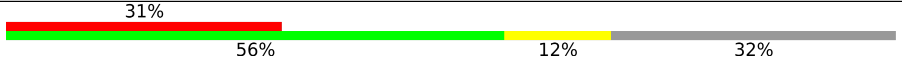
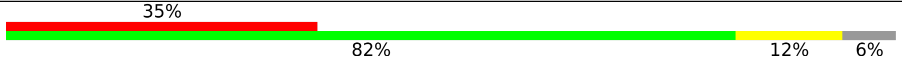
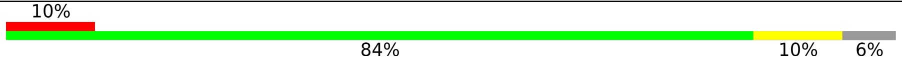
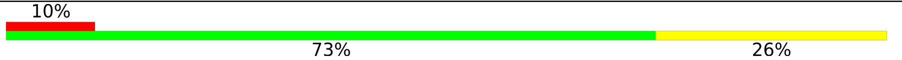
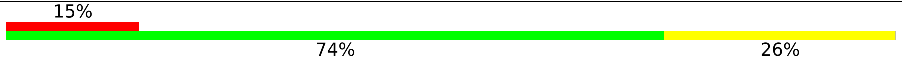
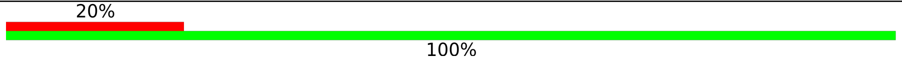
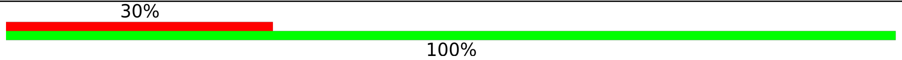
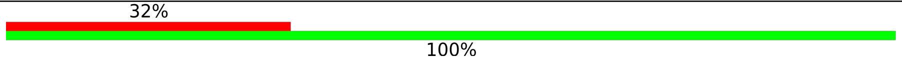
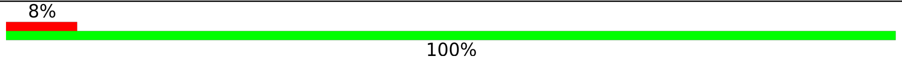
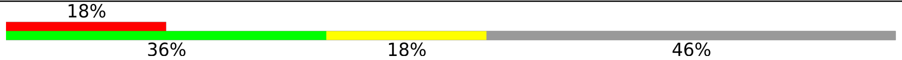
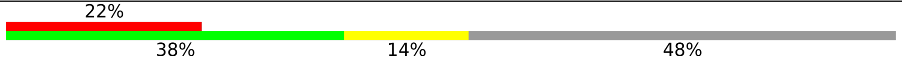
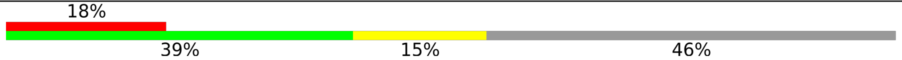
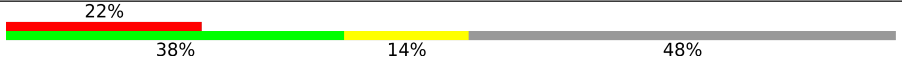
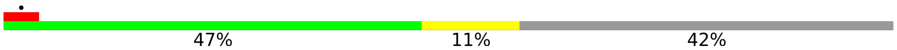
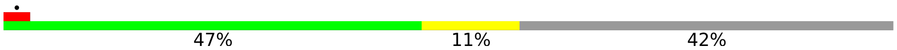
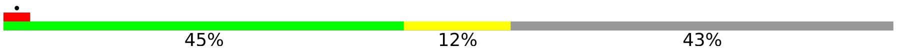
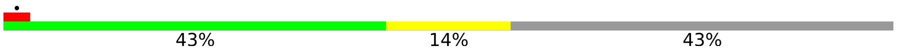
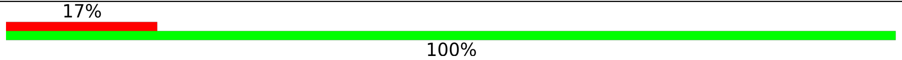
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0A	606	
1	0B	606	
1	0C	606	
1	0D	606	
2	0E	222	
2	0F	222	
2	0G	222	
2	0H	222	

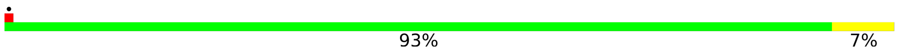
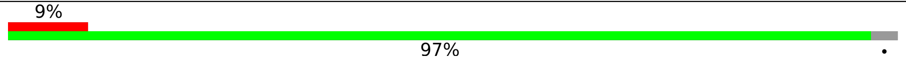
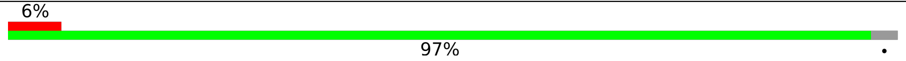
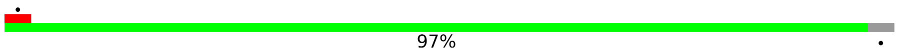
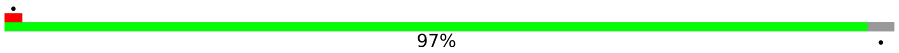
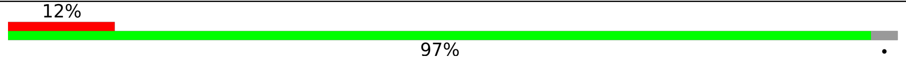
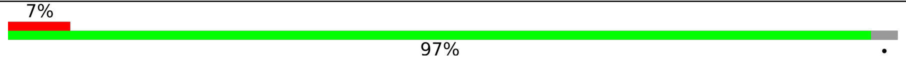
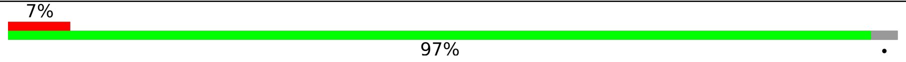
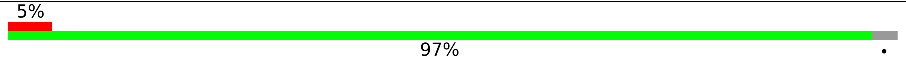
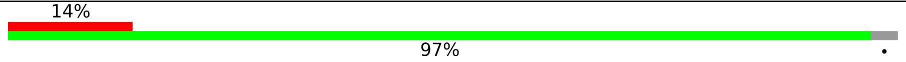
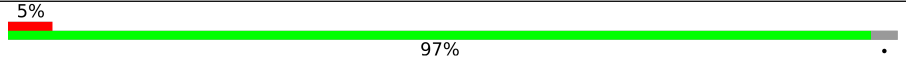
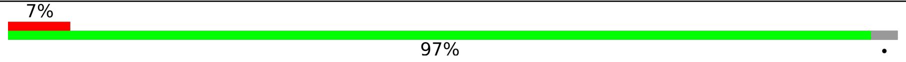
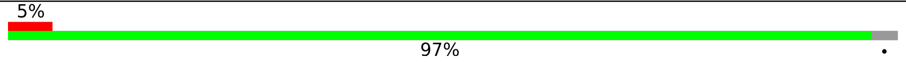
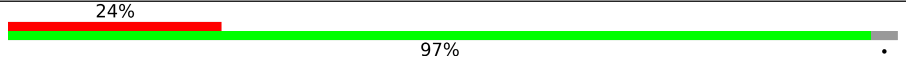
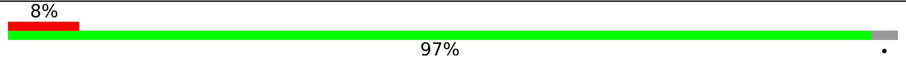
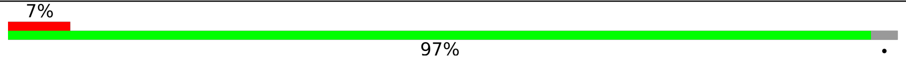
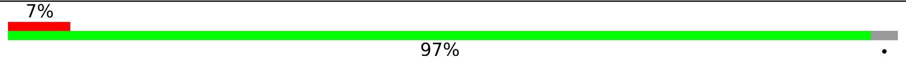
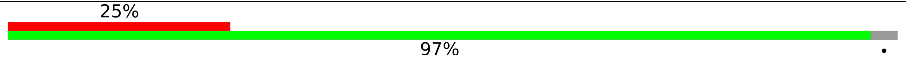
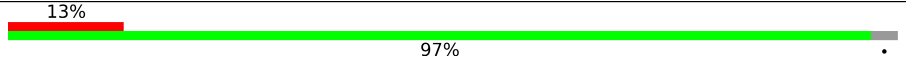
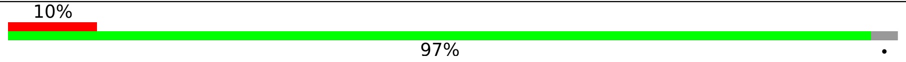
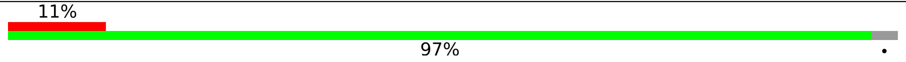
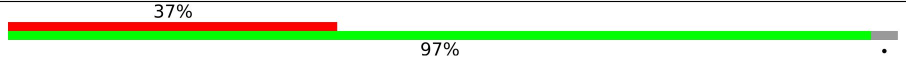
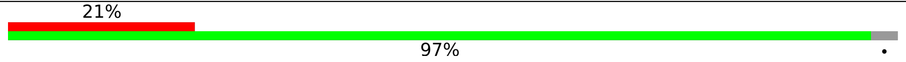
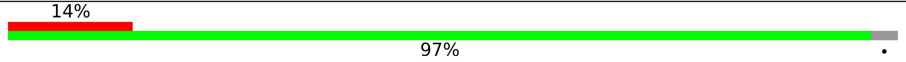
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	0I	976	
3	0J	976	
4	0K	528	
4	0L	528	
5	0M	758	
5	0N	758	
6	0O	201	
6	0P	201	
7	0Q	618	
7	0S	618	
8	0T	169	
9	0U	170	
10	0V	160	
11	0W	39	
12	0X	776	
12	0Y	776	
12	0Z	776	
12	1A	776	
13	1B	2257	
13	1C	2257	
14	1D	1074	
14	1E	1074	
14	1F	1074	
14	1G	1074	
15	1H	88	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	1L	174	
16	1M	174	
17	1a	443	
17	1c	443	
17	1e	443	
17	1g	443	
17	2a	443	
17	2c	443	
17	2e	443	
17	2g	443	
17	3a	443	
17	3c	443	
17	3e	443	
17	3g	443	
17	4a	443	
17	4c	443	
17	4e	443	
17	4g	443	
17	5a	443	
17	5c	443	
17	5e	443	
17	5g	443	
17	6a	443	
17	6c	443	
17	6e	443	

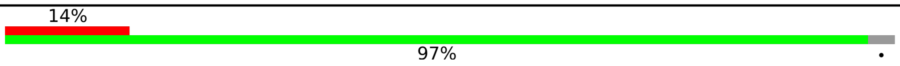
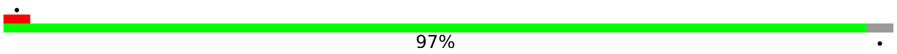
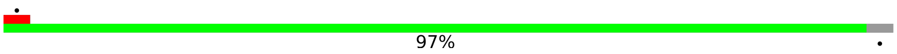
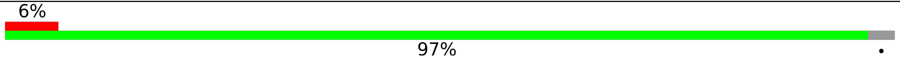
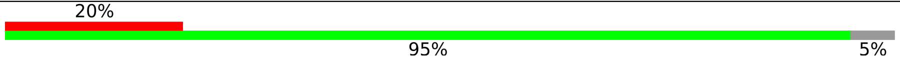
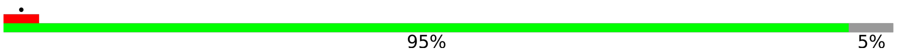
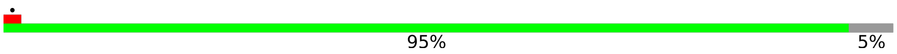
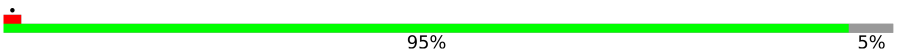
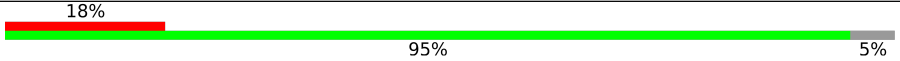
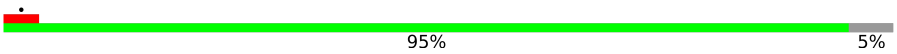
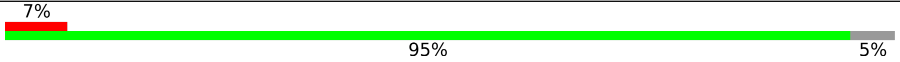
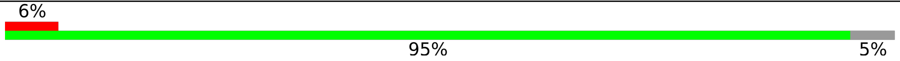
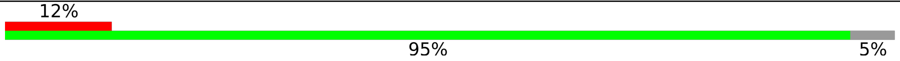
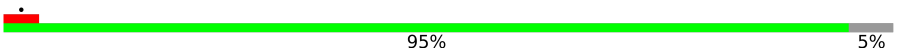
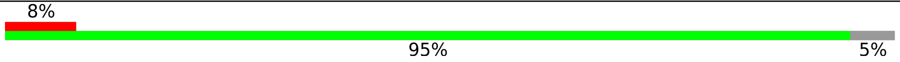
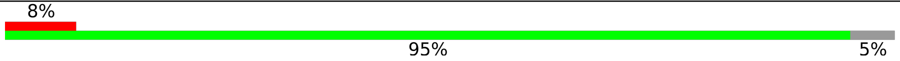
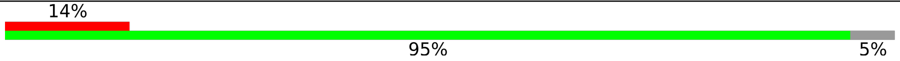
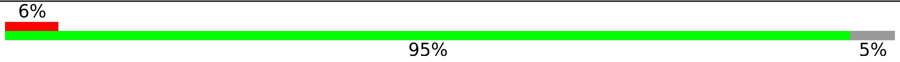
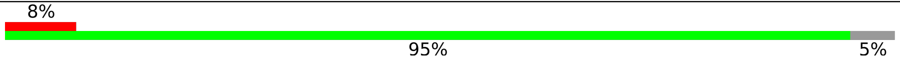
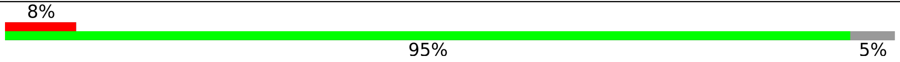
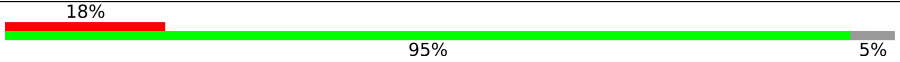
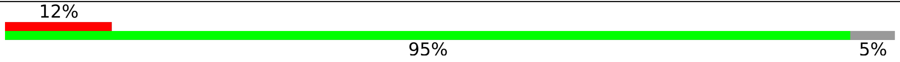
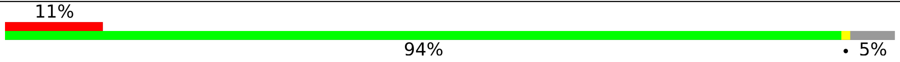
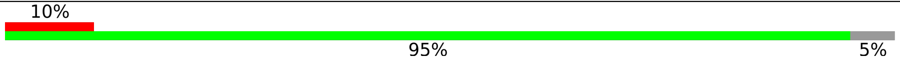
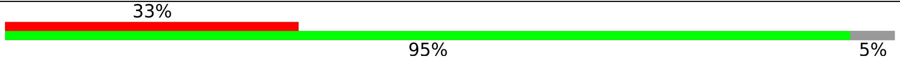
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
17	6g	443	19% 97% •
17	7a	443	17% 97% •
17	7c	443	6% 97% •
17	7e	443	6% 97% •
17	7g	443	6% 97% •
17	8a	443	15% 97% •
17	8c	443	• 97% •
17	8e	443	• 97% •
17	8g	443	• 97% •
17	9a	443	• 97% •
17	9c	443	• 97% •
17	9e	443	• 97% •
17	9g	443	• 97% •
17	Aa	443	11% 97% •
17	Ac	443	9% 97% •
17	Ae	443	5% 97% •
17	Ag	443	5% 97% •
17	Ba	443	17% 97% •
17	Bc	443	97% •
17	Be	443	• 97% •
17	Bg	443	• 97% •
17	Ca	443	15% 97% •
17	Cc	443	• 97% •
17	Ce	443	• 97% •
17	Cg	443	• 97% •

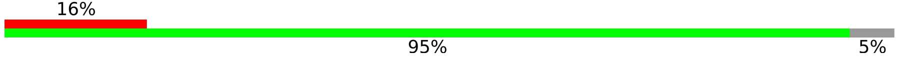
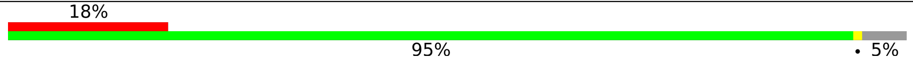
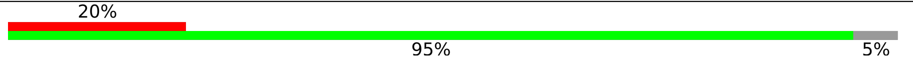
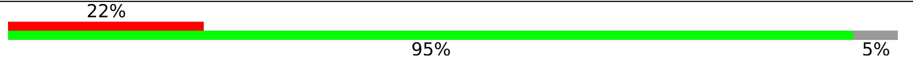
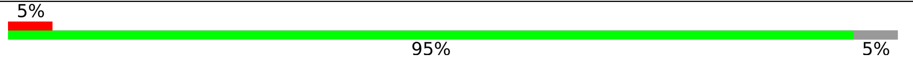
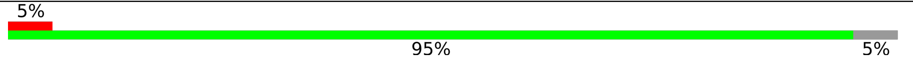
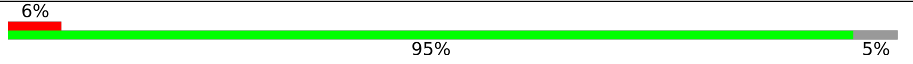
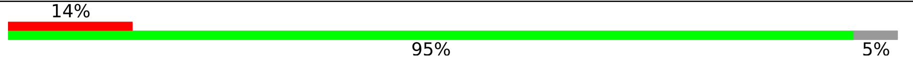
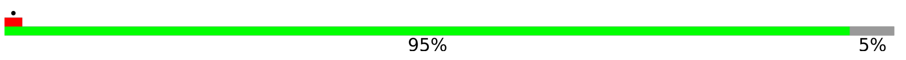
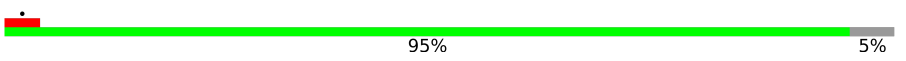
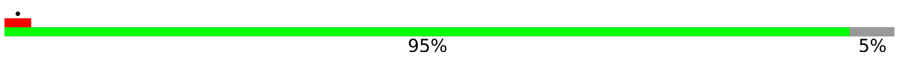
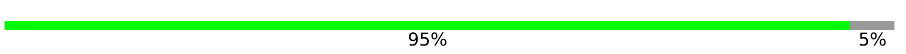
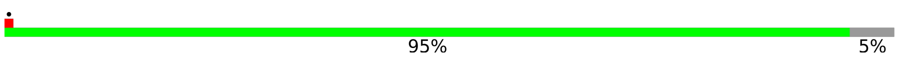
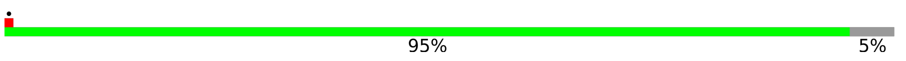
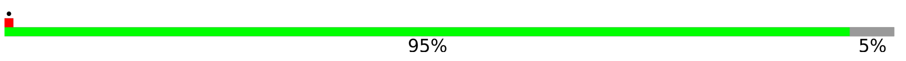
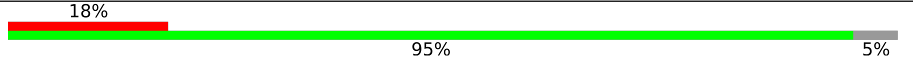
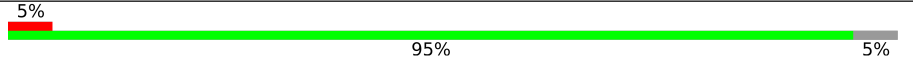
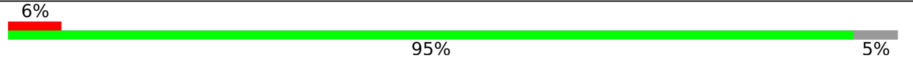
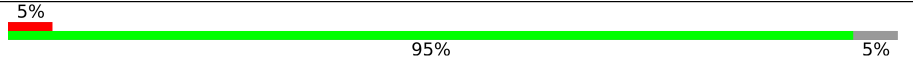
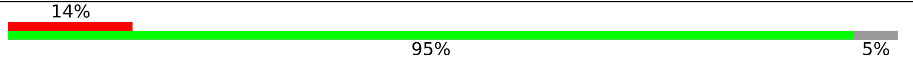
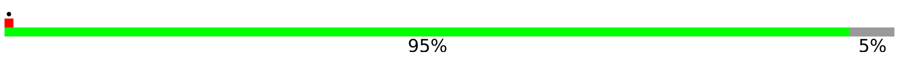
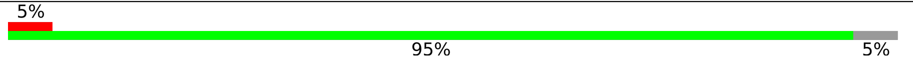
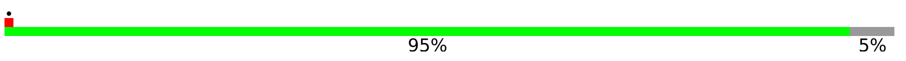
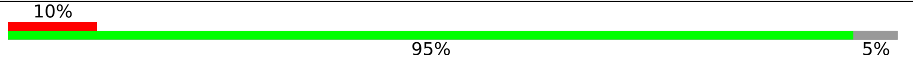
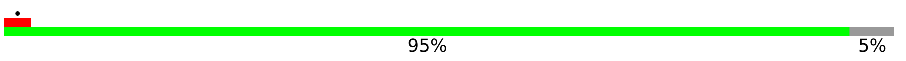
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
17	Da	443	
17	Dc	443	
17	De	443	
17	Dg	443	
18	1b	451	
18	1d	451	
18	1f	451	
18	1h	451	
18	2b	451	
18	2d	451	
18	2f	451	
18	2h	451	
18	3b	451	
18	3d	451	
18	3f	451	
18	3h	451	
18	4b	451	
18	4d	451	
18	4f	451	
18	4h	451	
18	5b	451	
18	5d	451	
18	5f	451	
18	5h	451	
18	6b	451	

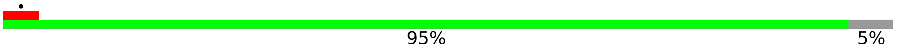
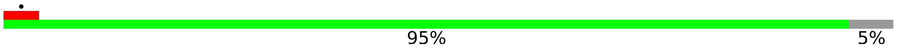
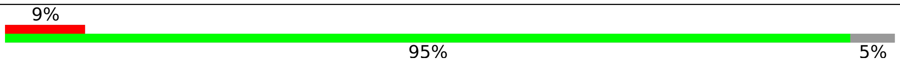
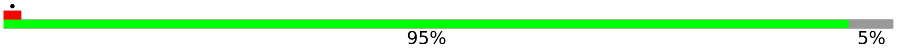
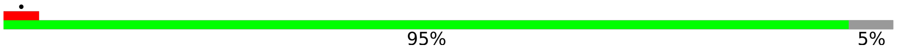
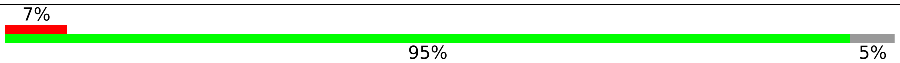
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
18	6d	451	
18	6f	451	
18	6h	451	
18	7b	451	
18	7d	451	
18	7f	451	
18	7h	451	
18	8b	451	
18	8d	451	
18	8f	451	
18	8h	451	
18	9b	451	
18	9d	451	
18	9f	451	
18	9h	451	
18	Ab	451	
18	Ad	451	
18	Af	451	
18	Ah	451	
18	Bb	451	
18	Bd	451	
18	Bf	451	
18	Bh	451	
18	Cb	451	
18	Cd	451	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
18	Cf	451	
18	Ch	451	
18	Db	451	
18	Dd	451	
18	Df	451	
18	Dh	451	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 443856 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Flagellar WD repeat-containing protein Pf20.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0A	467	Total 3656	C 2298	N 650	O 685	S 23	0	0
1	0B	467	Total 3656	C 2298	N 650	O 685	S 23	0	0
1	0C	476	Total 3726	C 2343	N 664	O 696	S 23	0	0
1	0D	476	Total 3726	C 2343	N 664	O 696	S 23	0	0

- Molecule 2 is a protein called FAP178.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0E	128	Total 1008	C 640	N 180	O 184	S 4	0	0
2	0F	128	Total 1008	C 640	N 180	O 184	S 4	0	0
2	0G	128	Total 1008	C 640	N 180	O 184	S 4	0	0
2	0H	128	Total 1008	C 640	N 180	O 184	S 4	0	0

- Molecule 3 is a protein called FAP147.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	0I	448	Total 3321	C 2062	N 633	O 616	S 10	0	0
3	0J	448	Total 3321	C 2062	N 633	O 616	S 10	0	0

- Molecule 4 is a protein called FAP239.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	0K	166	Total	C	N	O	S	0	0
			1216	747	229	239	1		
4	0L	166	Total	C	N	O	S	0	0
			1216	747	229	239	1		

- Molecule 5 is a protein called FAP225.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	0M	515	Total	C	N	O	S	0	0
			4037	2487	769	768	13		
5	0N	515	Total	C	N	O	S	0	0
			4037	2487	769	768	13		

- Molecule 6 is a protein called FAP213.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	0O	188	Total	C	N	O	S	0	0
			1481	897	294	287	3		
6	0P	188	Total	C	N	O	S	0	0
			1481	897	294	287	3		

- Molecule 7 is a protein called FAP196.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	0Q	617	Total	C	N	O	S	0	0
			4537	2823	824	857	33		
7	0S	617	Total	C	N	O	S	0	0
			4537	2823	824	857	33		

- Molecule 8 is a protein called Unassigned protein-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	0T	169	Total	C	N	O	0	0
			845	507	169	169		

- Molecule 9 is a protein called Unassigned protein-2.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	0U	170	Total	C	N	O	0	0
			850	510	170	170		

- Molecule 10 is a protein called Unassigned protein-3.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	0V	160	Total	C	N	O	0	0
			800	480	160	160		

- Molecule 11 is a protein called Unassigned protein-4.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	0W	39	Total	C	N	O	0	0
			195	117	39	39		

- Molecule 12 is a protein called Kinesin-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	0X	420	Total	C	N	O	S	0	0
			3098	1921	561	608	8		
12	0Y	404	Total	C	N	O	S	0	0
			2903	1800	527	569	7		
12	0Z	420	Total	C	N	O	S	0	0
			3098	1921	561	608	8		
12	1A	404	Total	C	N	O	S	0	0
			2903	1800	527	569	7		

- Molecule 13 is a protein called FAP65.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1B	630	Total	C	N	O	S	0	0
			4771	3018	865	874	14		
13	1C	630	Total	C	N	O	S	0	0
			4771	3018	865	874	14		

- Molecule 14 is a protein called FAP70.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1D	623	Total	C	N	O	S	0	0
			4079	2527	756	781	15		
14	1E	623	Total	C	N	O	S	0	0
			4079	2527	756	781	15		
14	1F	614	Total	C	N	O	S	0	0
			4370	2725	808	821	16		
14	1G	614	Total	C	N	O	S	0	0
			4370	2725	808	821	16		

- Molecule 15 is a protein called Unassigned protein-5.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	1H	88	Total	C	N	O	0	0
			440	264	88	88		

- Molecule 16 is a protein called Unassigned protein-6.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	1M	174	Total	C	N	O	0	0
			870	522	174	174		
16	1L	174	Total	C	N	O	0	0
			870	522	174	174		

- Molecule 17 is a protein called Tubulin beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1a	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
17	1c	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
17	1e	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
17	1g	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
17	2a	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
17	2c	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
17	2e	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
17	2g	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
17	3a	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
17	3c	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
17	3e	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
17	3g	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
17	4a	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
17	4c	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
17	4e	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf	Trace
17	4g	431	Total C N O S 3379 2121 579 649 30	0	0
17	5a	431	Total C N O S 3379 2121 579 649 30	0	0
17	5c	431	Total C N O S 3379 2121 579 649 30	0	0
17	5e	431	Total C N O S 3379 2121 579 649 30	0	0
17	5g	431	Total C N O S 3379 2121 579 649 30	0	0
17	6a	431	Total C N O S 3379 2121 579 649 30	0	0
17	6c	431	Total C N O S 3379 2121 579 649 30	0	0
17	6e	431	Total C N O S 3379 2121 579 649 30	0	0
17	6g	431	Total C N O S 3379 2121 579 649 30	0	0
17	7a	431	Total C N O S 3379 2121 579 649 30	0	0
17	7c	431	Total C N O S 3379 2121 579 649 30	0	0
17	7e	431	Total C N O S 3379 2121 579 649 30	0	0
17	7g	431	Total C N O S 3379 2121 579 649 30	0	0
17	8a	431	Total C N O S 3379 2121 579 649 30	0	0
17	8c	431	Total C N O S 3379 2121 579 649 30	0	0
17	8e	431	Total C N O S 3379 2121 579 649 30	0	0
17	8g	431	Total C N O S 3379 2121 579 649 30	0	0
17	9a	431	Total C N O S 3379 2121 579 649 30	0	0
17	9c	431	Total C N O S 3379 2121 579 649 30	0	0
17	9e	431	Total C N O S 3379 2121 579 649 30	0	0
17	9g	431	Total C N O S 3379 2121 579 649 30	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Aa	431	Total 3379	C 2121	N 579	O 649	S 30	0	0
17	Ac	431	Total 3379	C 2121	N 579	O 649	S 30	0	0
17	Ae	431	Total 3379	C 2121	N 579	O 649	S 30	0	0
17	Ag	431	Total 3379	C 2121	N 579	O 649	S 30	0	0
17	Ba	431	Total 3379	C 2121	N 579	O 649	S 30	0	0
17	Bc	431	Total 3379	C 2121	N 579	O 649	S 30	0	0
17	Be	431	Total 3379	C 2121	N 579	O 649	S 30	0	0
17	Bg	431	Total 3379	C 2121	N 579	O 649	S 30	0	0
17	Ca	431	Total 3379	C 2121	N 579	O 649	S 30	0	0
17	Cc	431	Total 3379	C 2121	N 579	O 649	S 30	0	0
17	Ce	431	Total 3379	C 2121	N 579	O 649	S 30	0	0
17	Cg	431	Total 3379	C 2121	N 579	O 649	S 30	0	0
17	Da	431	Total 3379	C 2121	N 579	O 649	S 30	0	0
17	Dc	431	Total 3379	C 2121	N 579	O 649	S 30	0	0
17	De	431	Total 3379	C 2121	N 579	O 649	S 30	0	0
17	Dg	431	Total 3379	C 2121	N 579	O 649	S 30	0	0

- Molecule 18 is a protein called Tubulin alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1b	430	Total 3339	C 2115	N 568	O 634	S 22	0	0
18	1d	430	Total 3339	C 2115	N 568	O 634	S 22	0	0
18	1f	430	Total 3339	C 2115	N 568	O 634	S 22	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf	Trace
18	1h	430	Total C N O S 3339 2115 568 634 22	0	0
18	2b	430	Total C N O S 3339 2115 568 634 22	0	0
18	2d	430	Total C N O S 3339 2115 568 634 22	0	0
18	2f	430	Total C N O S 3339 2115 568 634 22	0	0
18	2h	430	Total C N O S 3339 2115 568 634 22	0	0
18	3b	430	Total C N O S 3339 2115 568 634 22	0	0
18	3d	430	Total C N O S 3339 2115 568 634 22	0	0
18	3f	430	Total C N O S 3339 2115 568 634 22	0	0
18	3h	430	Total C N O S 3339 2115 568 634 22	0	0
18	4b	430	Total C N O S 3339 2115 568 634 22	0	0
18	4d	430	Total C N O S 3339 2115 568 634 22	0	0
18	4f	430	Total C N O S 3339 2115 568 634 22	0	0
18	4h	430	Total C N O S 3339 2115 568 634 22	0	0
18	5b	430	Total C N O S 3339 2115 568 634 22	0	0
18	5d	430	Total C N O S 3339 2115 568 634 22	0	0
18	5f	430	Total C N O S 3339 2115 568 634 22	0	0
18	5h	430	Total C N O S 3339 2115 568 634 22	0	0
18	6b	430	Total C N O S 3339 2115 568 634 22	0	0
18	6d	430	Total C N O S 3339 2115 568 634 22	0	0
18	6f	430	Total C N O S 3339 2115 568 634 22	0	0
18	6h	430	Total C N O S 3339 2115 568 634 22	0	0

Continued on next page...

Continued from previous page...

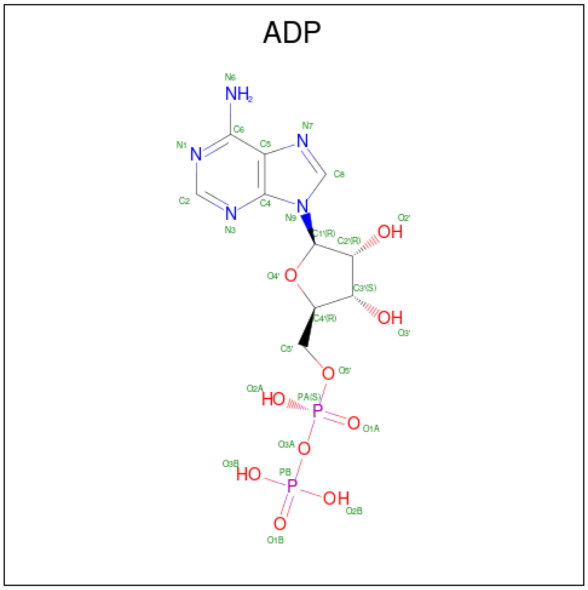
Mol	Chain	Residues	Atoms	AltConf	Trace
18	7b	430	Total C N O S 3339 2115 568 634 22	0	0
18	7d	430	Total C N O S 3339 2115 568 634 22	0	0
18	7f	430	Total C N O S 3339 2115 568 634 22	0	0
18	7h	430	Total C N O S 3339 2115 568 634 22	0	0
18	8b	430	Total C N O S 3339 2115 568 634 22	0	0
18	8d	430	Total C N O S 3339 2115 568 634 22	0	0
18	8f	430	Total C N O S 3339 2115 568 634 22	0	0
18	8h	430	Total C N O S 3339 2115 568 634 22	0	0
18	9b	430	Total C N O S 3339 2115 568 634 22	0	0
18	9d	430	Total C N O S 3339 2115 568 634 22	0	0
18	9f	430	Total C N O S 3339 2115 568 634 22	0	0
18	9h	430	Total C N O S 3339 2115 568 634 22	0	0
18	Ab	430	Total C N O S 3339 2115 568 634 22	0	0
18	Ad	430	Total C N O S 3339 2115 568 634 22	0	0
18	Af	430	Total C N O S 3339 2115 568 634 22	0	0
18	Ah	430	Total C N O S 3339 2115 568 634 22	0	0
18	Bb	430	Total C N O S 3339 2115 568 634 22	0	0
18	Bd	430	Total C N O S 3339 2115 568 634 22	0	0
18	Bf	430	Total C N O S 3339 2115 568 634 22	0	0
18	Bh	430	Total C N O S 3339 2115 568 634 22	0	0
18	Cb	430	Total C N O S 3339 2115 568 634 22	0	0

Continued on next page...

Continued from previous page...

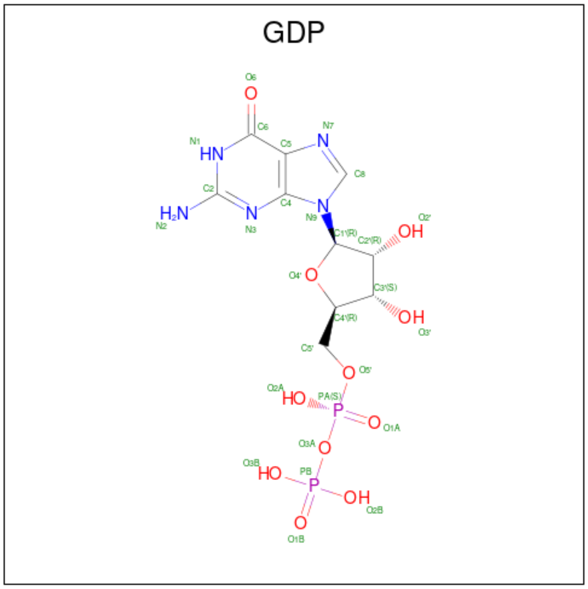
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Cd	430	3339	2115	568	634	22	0	0
18	Cf	430	3339	2115	568	634	22	0	0
18	Ch	430	3339	2115	568	634	22	0	0
18	Db	430	3339	2115	568	634	22	0	0
18	Dd	430	3339	2115	568	634	22	0	0
18	Df	430	3339	2115	568	634	22	0	0
18	Dh	430	3339	2115	568	634	22	0	0

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
19	0X	1	27	10	5	10	2	0
19	0Y	1	27	10	5	10	2	0
19	0Z	1	27	10	5	10	2	0
19	1A	1	27	10	5	10	2	0

- Molecule 20 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
20	1a	1	Total 28	C 10	N 5	O 11	P 2	0
20	1c	1	Total 28	C 10	N 5	O 11	P 2	0
20	1e	1	Total 28	C 10	N 5	O 11	P 2	0
20	1g	1	Total 28	C 10	N 5	O 11	P 2	0
20	2a	1	Total 28	C 10	N 5	O 11	P 2	0
20	2c	1	Total 28	C 10	N 5	O 11	P 2	0
20	2e	1	Total 28	C 10	N 5	O 11	P 2	0
20	2g	1	Total 28	C 10	N 5	O 11	P 2	0
20	3a	1	Total 28	C 10	N 5	O 11	P 2	0
20	3c	1	Total 28	C 10	N 5	O 11	P 2	0
20	3e	1	Total 28	C 10	N 5	O 11	P 2	0
20	3g	1	Total 28	C 10	N 5	O 11	P 2	0

Continued on next page...

Continued from previous page...

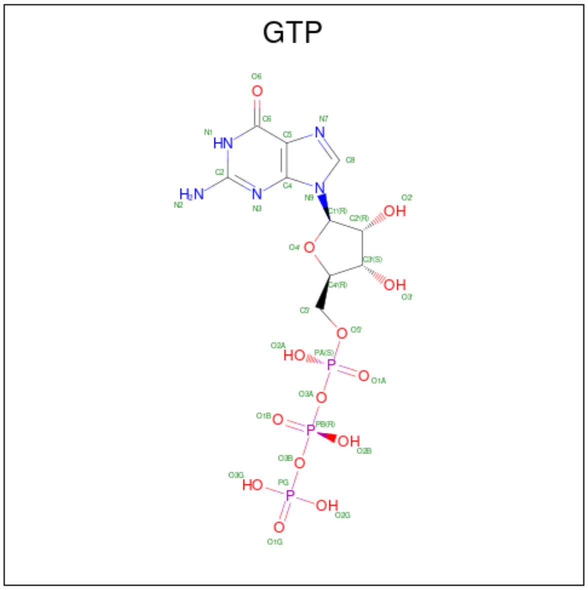
Mol	Chain	Residues	Atoms	AltConf
20	4a	1	Total C N O P 28 10 5 11 2	0
20	4c	1	Total C N O P 28 10 5 11 2	0
20	4e	1	Total C N O P 28 10 5 11 2	0
20	4g	1	Total C N O P 28 10 5 11 2	0
20	5a	1	Total C N O P 28 10 5 11 2	0
20	5c	1	Total C N O P 28 10 5 11 2	0
20	5e	1	Total C N O P 28 10 5 11 2	0
20	5g	1	Total C N O P 28 10 5 11 2	0
20	6a	1	Total C N O P 28 10 5 11 2	0
20	6c	1	Total C N O P 28 10 5 11 2	0
20	6e	1	Total C N O P 28 10 5 11 2	0
20	6g	1	Total C N O P 28 10 5 11 2	0
20	7a	1	Total C N O P 28 10 5 11 2	0
20	7c	1	Total C N O P 28 10 5 11 2	0
20	7e	1	Total C N O P 28 10 5 11 2	0
20	7g	1	Total C N O P 28 10 5 11 2	0
20	8a	1	Total C N O P 28 10 5 11 2	0
20	8c	1	Total C N O P 28 10 5 11 2	0
20	8e	1	Total C N O P 28 10 5 11 2	0
20	8g	1	Total C N O P 28 10 5 11 2	0
20	9a	1	Total C N O P 28 10 5 11 2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
20	9c	1	Total C N O P 28 10 5 11 2	0
20	9e	1	Total C N O P 28 10 5 11 2	0
20	9g	1	Total C N O P 28 10 5 11 2	0
20	Aa	1	Total C N O P 28 10 5 11 2	0
20	Ac	1	Total C N O P 28 10 5 11 2	0
20	Ae	1	Total C N O P 28 10 5 11 2	0
20	Ag	1	Total C N O P 28 10 5 11 2	0
20	Ba	1	Total C N O P 28 10 5 11 2	0
20	Bc	1	Total C N O P 28 10 5 11 2	0
20	Be	1	Total C N O P 28 10 5 11 2	0
20	Bg	1	Total C N O P 28 10 5 11 2	0
20	Ca	1	Total C N O P 28 10 5 11 2	0
20	Cc	1	Total C N O P 28 10 5 11 2	0
20	Ce	1	Total C N O P 28 10 5 11 2	0
20	Cg	1	Total C N O P 28 10 5 11 2	0
20	Da	1	Total C N O P 28 10 5 11 2	0
20	Dc	1	Total C N O P 28 10 5 11 2	0
20	De	1	Total C N O P 28 10 5 11 2	0
20	Dg	1	Total C N O P 28 10 5 11 2	0

- Molecule 21 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms	AltConf
21	1b	1	Total C N O P 32 10 5 14 3	0
21	1d	1	Total C N O P 32 10 5 14 3	0
21	1f	1	Total C N O P 32 10 5 14 3	0
21	1h	1	Total C N O P 32 10 5 14 3	0
21	2b	1	Total C N O P 32 10 5 14 3	0
21	2d	1	Total C N O P 32 10 5 14 3	0
21	2f	1	Total C N O P 32 10 5 14 3	0
21	2h	1	Total C N O P 32 10 5 14 3	0
21	3b	1	Total C N O P 32 10 5 14 3	0
21	3d	1	Total C N O P 32 10 5 14 3	0
21	3f	1	Total C N O P 32 10 5 14 3	0
21	3h	1	Total C N O P 32 10 5 14 3	0
21	4b	1	Total C N O P 32 10 5 14 3	0
21	4d	1	Total C N O P 32 10 5 14 3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
21	4f	1	Total C N O P 32 10 5 14 3	0
21	4h	1	Total C N O P 32 10 5 14 3	0
21	5b	1	Total C N O P 32 10 5 14 3	0
21	5d	1	Total C N O P 32 10 5 14 3	0
21	5f	1	Total C N O P 32 10 5 14 3	0
21	5h	1	Total C N O P 32 10 5 14 3	0
21	6b	1	Total C N O P 32 10 5 14 3	0
21	6d	1	Total C N O P 32 10 5 14 3	0
21	6f	1	Total C N O P 32 10 5 14 3	0
21	6h	1	Total C N O P 32 10 5 14 3	0
21	7b	1	Total C N O P 32 10 5 14 3	0
21	7d	1	Total C N O P 32 10 5 14 3	0
21	7f	1	Total C N O P 32 10 5 14 3	0
21	7h	1	Total C N O P 32 10 5 14 3	0
21	8b	1	Total C N O P 32 10 5 14 3	0
21	8d	1	Total C N O P 32 10 5 14 3	0
21	8f	1	Total C N O P 32 10 5 14 3	0
21	8h	1	Total C N O P 32 10 5 14 3	0
21	9b	1	Total C N O P 32 10 5 14 3	0
21	9d	1	Total C N O P 32 10 5 14 3	0
21	9f	1	Total C N O P 32 10 5 14 3	0

Continued on next page...

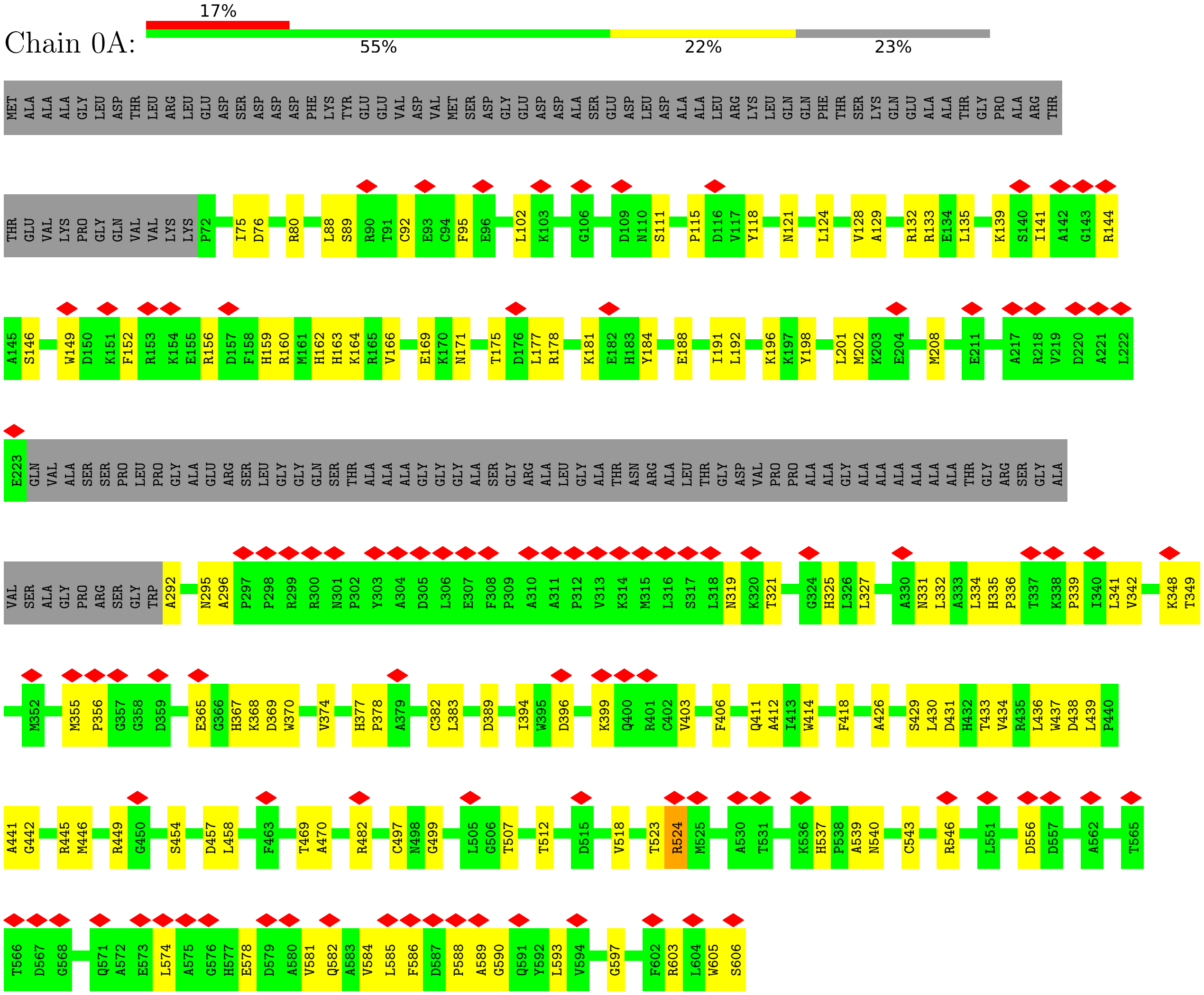
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
21	9h	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	Ab	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	Ad	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	Af	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	Ah	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	Bb	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	Bd	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	Bf	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	Bh	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	Cb	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	Cd	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	Cf	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	Ch	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	Db	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	Dd	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	Df	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	Dh	1	Total	C	N	O	P	0
			32	10	5	14	3	

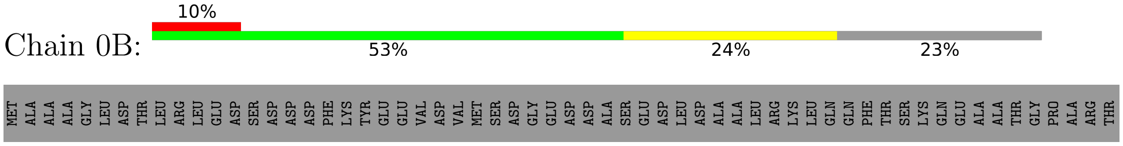
3 Residue-property plots ⓘ

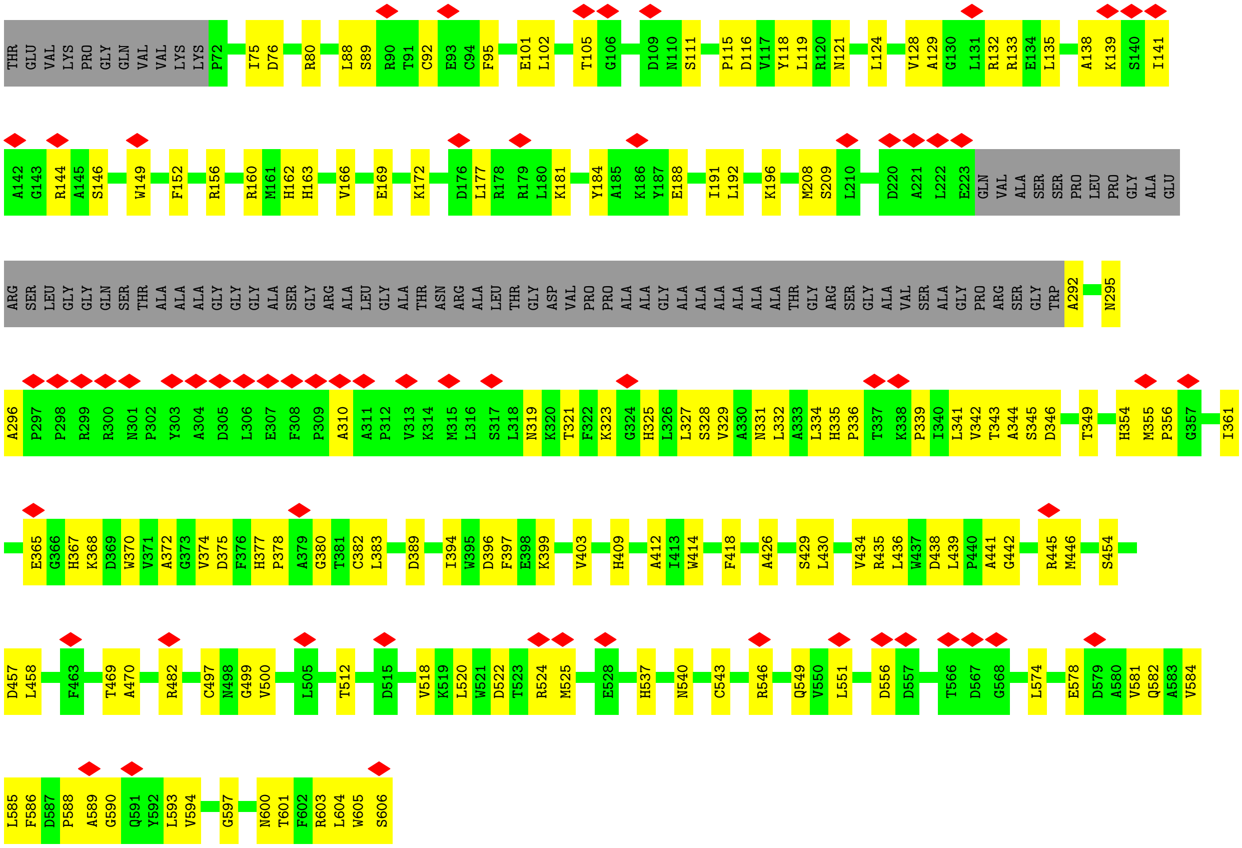
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Flagellar WD repeat-containing protein Pf20



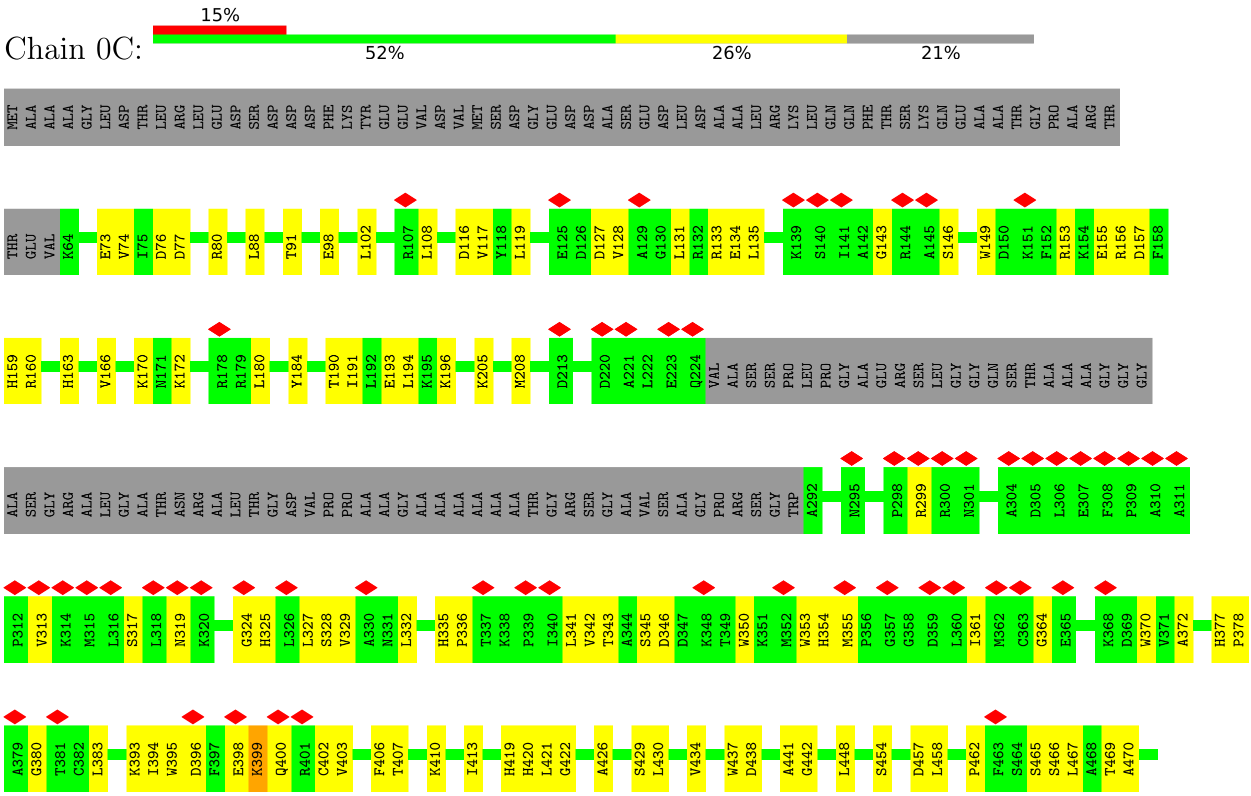
- Molecule 1: Flagellar WD repeat-containing protein Pf20

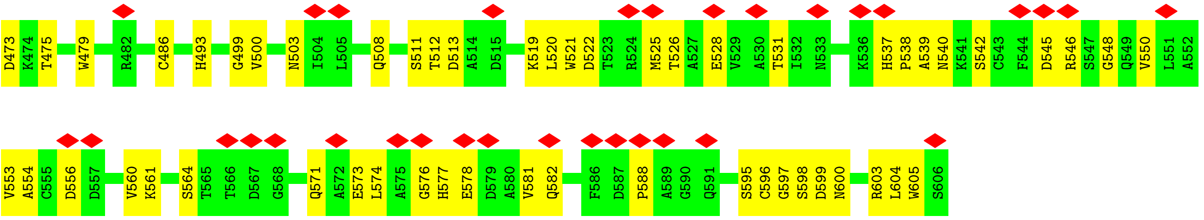




- Molecule 1: Flagellar WD repeat-containing protein Pf20

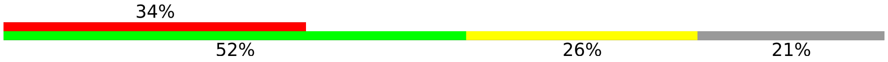
Chain 0C:

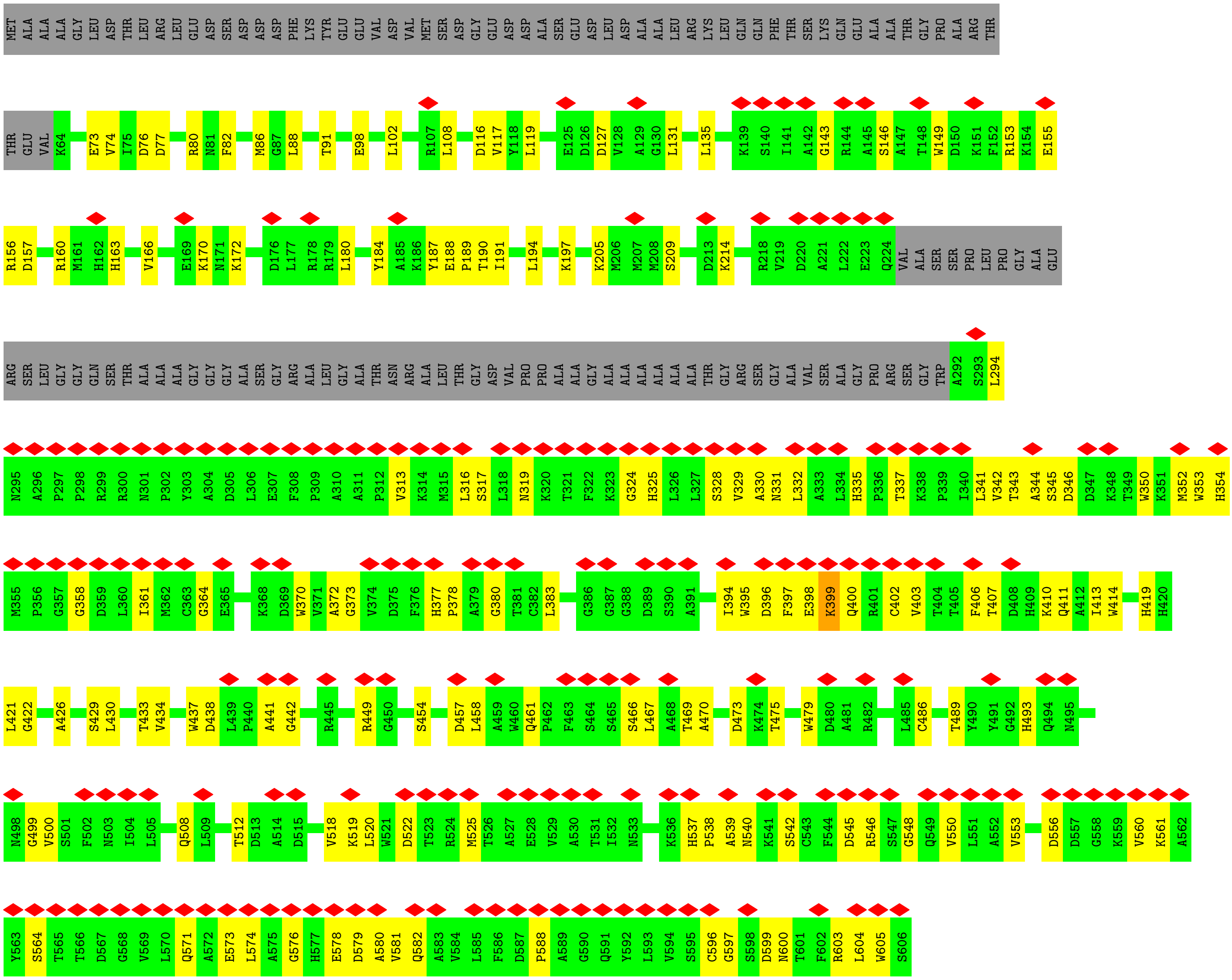




- Molecule 1: Flagellar WD repeat-containing protein Pf20

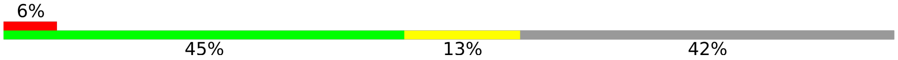
Chain 0D:

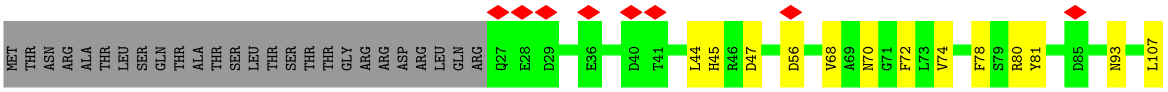


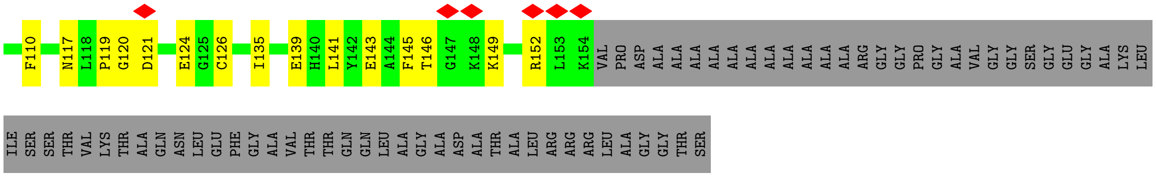


- Molecule 2: FAP178

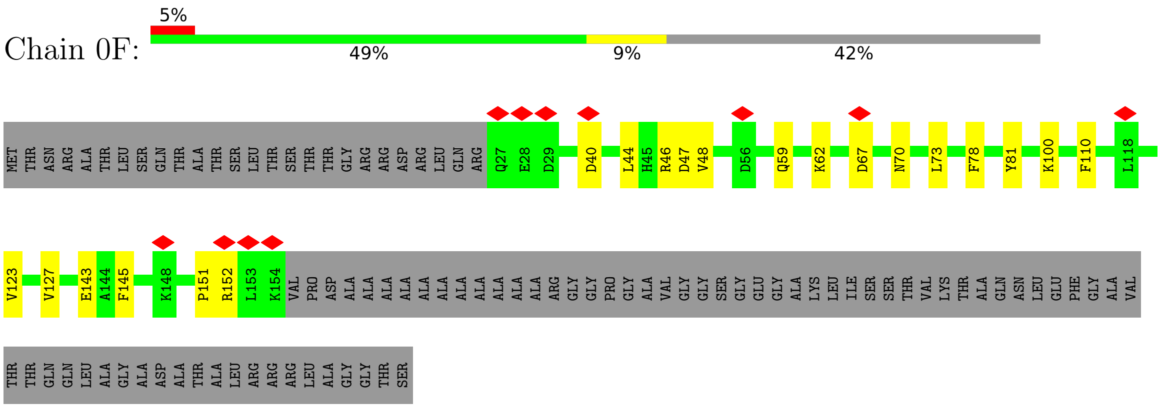
Chain 0E:



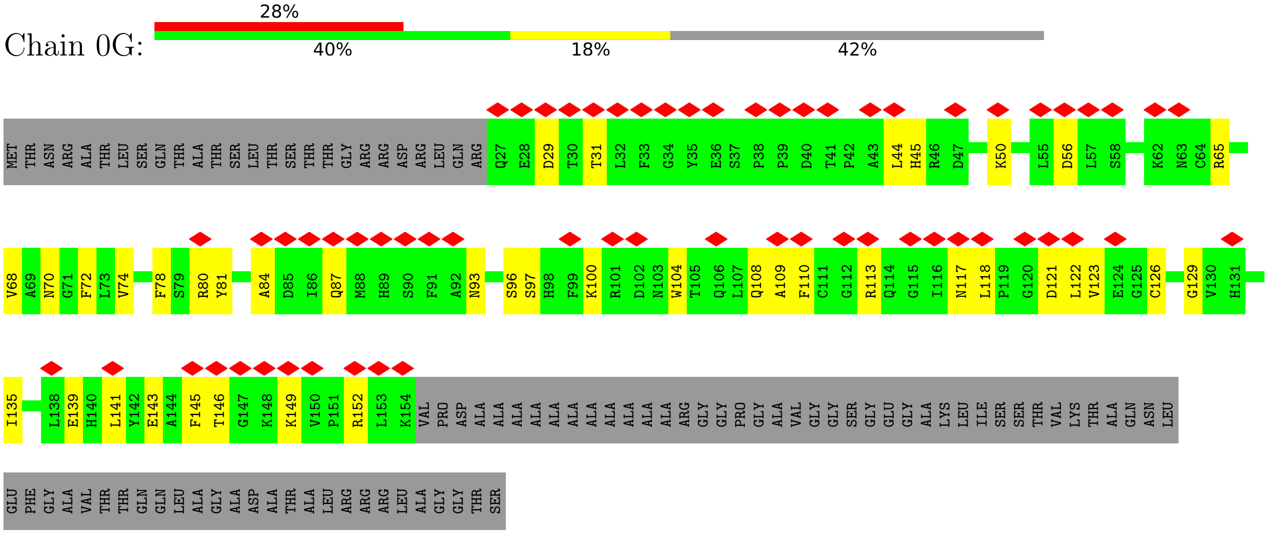




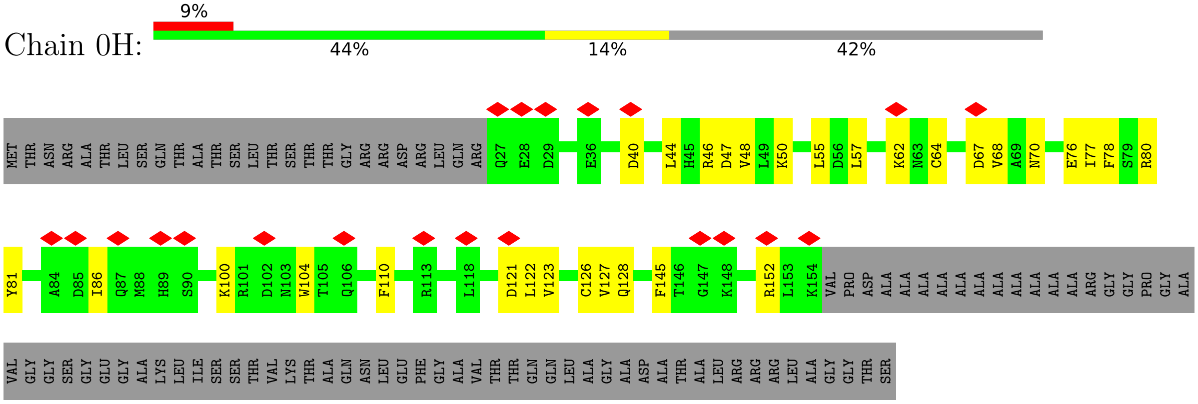
- Molecule 2: FAP178



- Molecule 2: FAP178

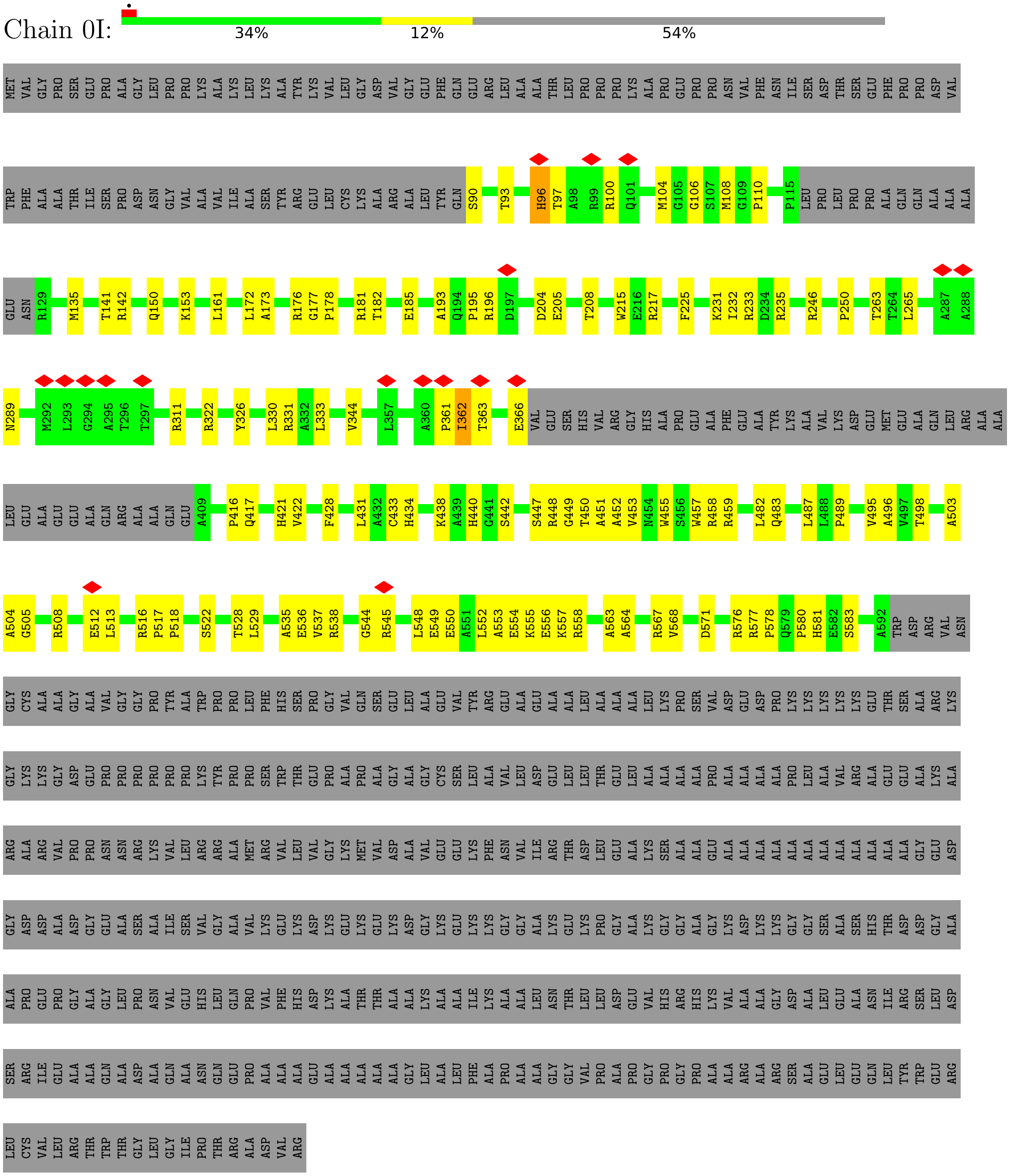


- Molecule 2: FAP178



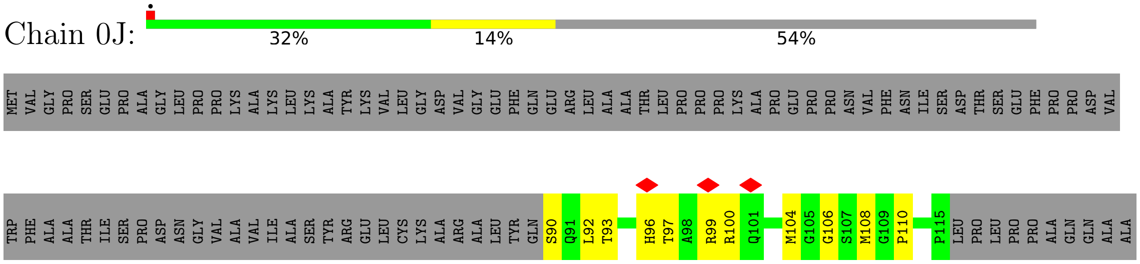
- Molecule 3: FAP147

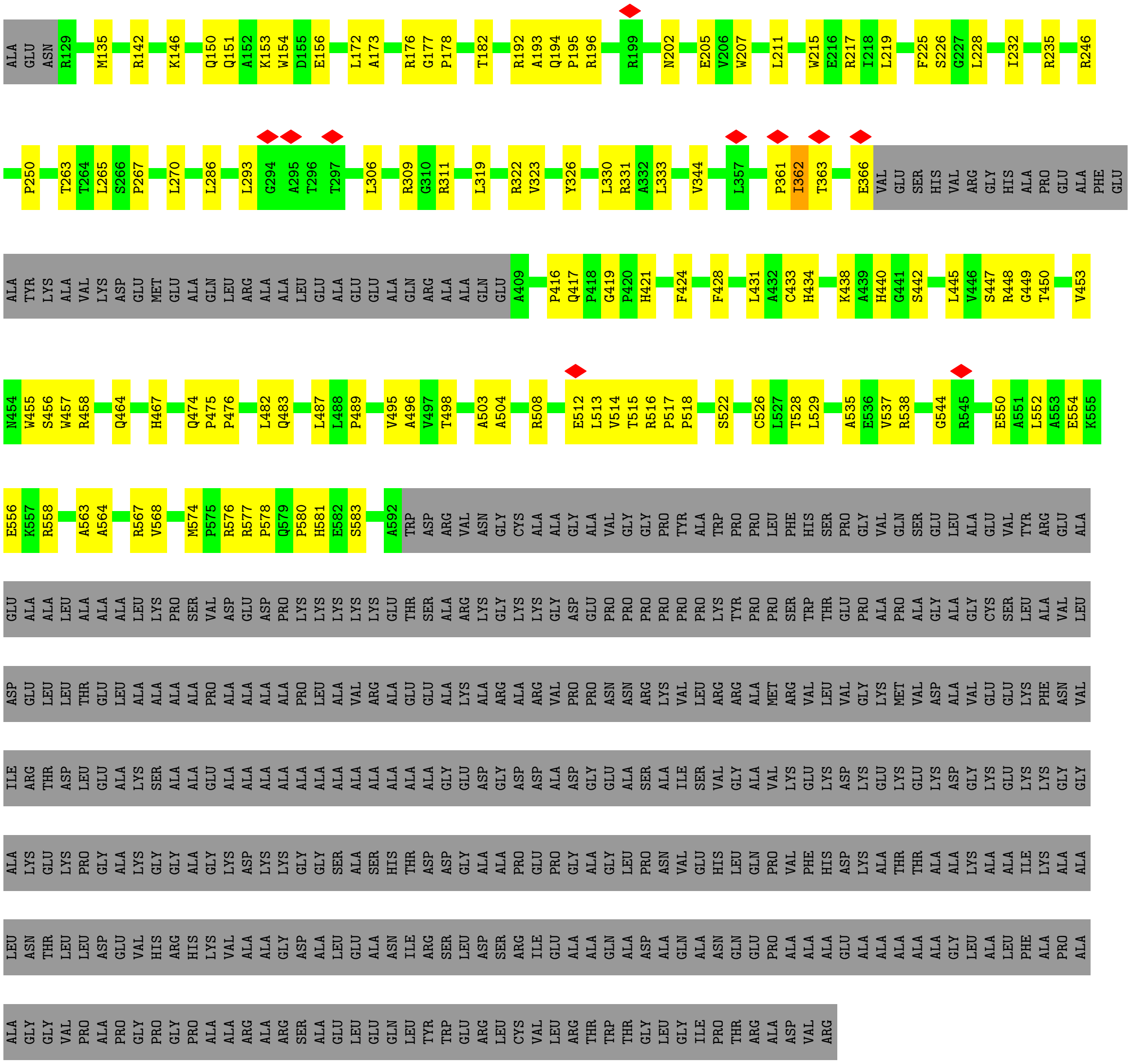
Chain 0I:



- Molecule 3: FAP147

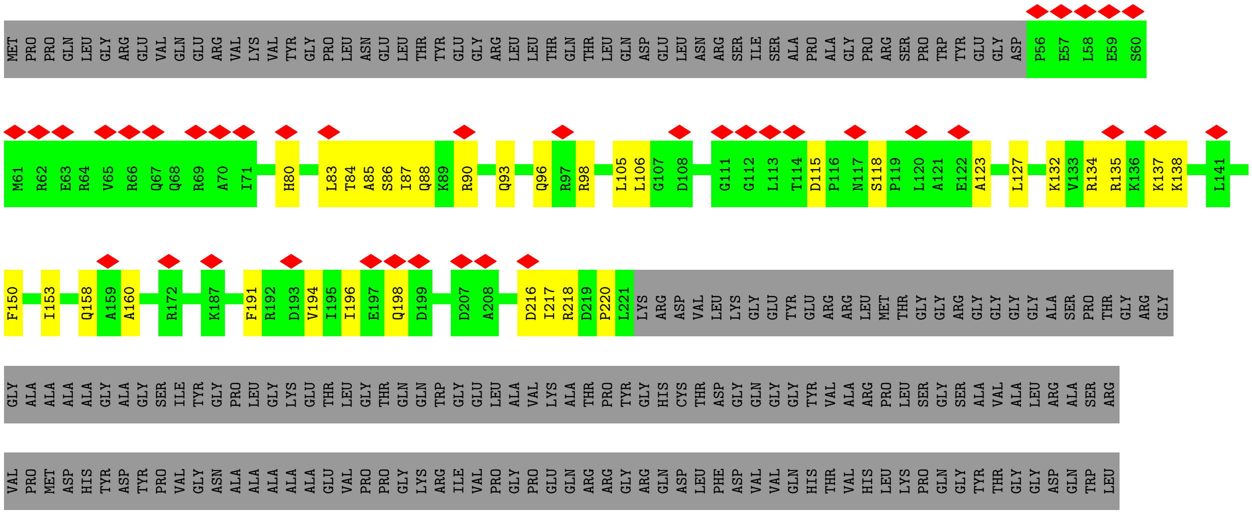
Chain 0J:

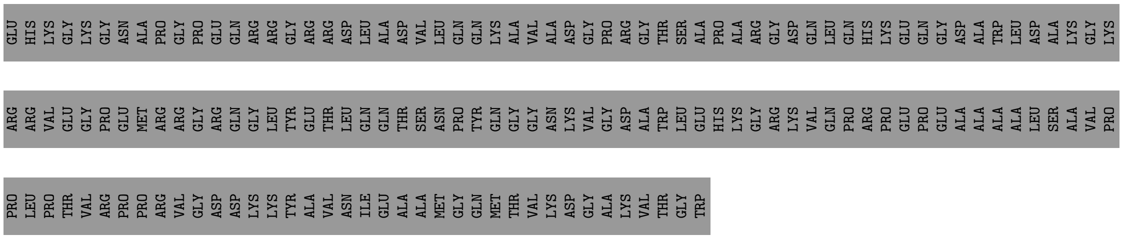




- Molecule 4: FAP239

Chain 0K:





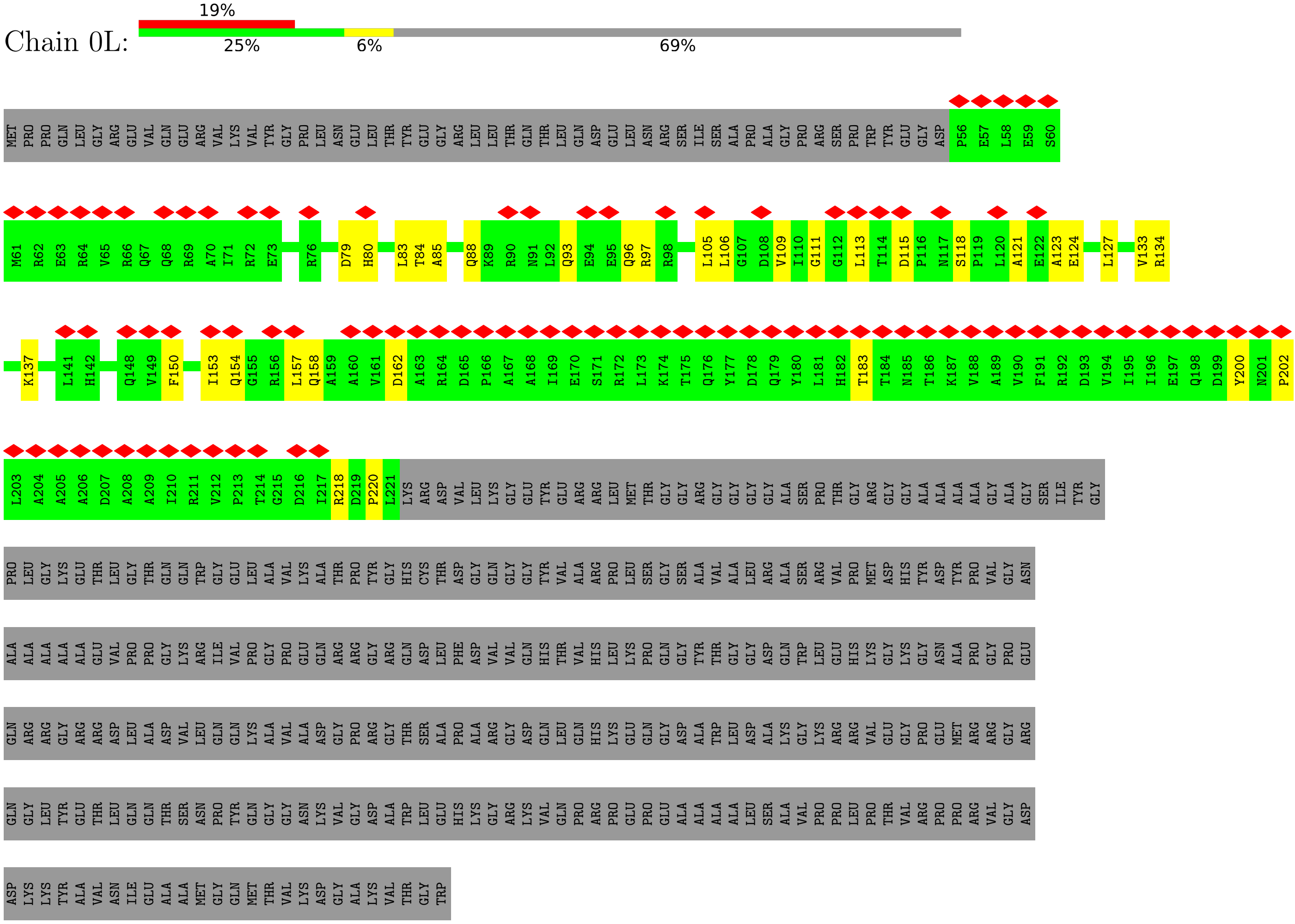
GLU HIS LYS GLY LYS GLY ASN ALA PRO GLY PRO GLU GLN ARG ARG GLY ARG ARG ASP LEU ALA ASP VAL LEU GLN GLN LYS ALA VAL ALA ASP GLY PRO ARG GLY THR SER ALA PRO ALA ARG GLY ASP GLN LEU GLN HIS LYS GLU GLN GLY ASP ALA TRP LEU ASP ALA LYS GLY LYS

ARG ARG VAL GLU GLY PRO GLU MET ARG ARG GLY ARG GLN GLY LEU TYR GLU THR LEU GLN GLN THR SER ASN PRO TYR GLN GLY GLY ASN LYS VAL GLY ASP ALA TRP LEU GLU HIS LYS GLY ARG LYS VAL GLN PRO ARG PRO GLU PRO GLU ALA ALA ALA ALA LEU SER ALA VAL PRO

PRO LEU PRO THR VAL ARG PRO PRO ARG VAL GLY ASP ASP LYS LYS TYR ALA VAL ASN ILE GLU ALA ALA MET GLY GLN MET THR VAL LYS ASP GLY ALA LYS VAL THR GLY TRP

- Molecule 4: FAP239

Chain 0L:



MET PRO PRO GLN LEU GLY ARG GLU VAL GLN GLU ARG VAL LYS VAL TYR GLY PRO LEU ASN GLU LEU THR TYR GLU GLY ARG LEU LEU THR GLN THR LEU GLN ASP GLU LEU ASN ARG SER ILE SER ALA PRO ALA GLY PRO ARG SER PRO TRP TYR GLU GLY ASP P56 E57 L58 E59 S60

M61 R62 E63 R64 V65 R66 Q67 Q68 R69 A70 I71 R72 E73 R76 D79 H80 L83 T84 A85 Q88 K89 R90 N91 L92 Q93 E94 E95 Q96 R97 R98 L105 L106 G107 D108 V109 I110 G111 G112 L113 T114 D115 P116 N117 S118 P119 L120 A121 E122 A123 E124 L127 V133 R134

K137 L141 H142 Q148 V149 F150 I153 Q154 G155 R156 L157 Q158 A159 A160 V161 D162 A163 R164 D165 P166 A167 A168 I169 E170 S171 R172 L173 K174 T175 Q176 Y177 D178 Q179 Y180 L181 H182 T183 T184 N185 T186 K187 V188 A189 V190 F191 R192 D193 V194 I195 I196 E197 Q198 D199 Y200 N201 P202

L203 A204 A205 A206 D207 A208 A209 I210 R211 V212 P213 T214 G215 D216 I217 R218 D219 P220 L221 LYS ARG ASP VAL LEU LYS GLY GLU TYR GLU ARG ARG LEU MET THR GLY GLY ARG GLY GLY GLY GLY ALA SER PRO THR GLY ARG GLY GLY ALA ALA ALA ALA GLY ALA GLY SER ILE TYR GLY

PRO LEU GLY LYS GLU THR LEU GLY THR GLN GLN TRP GLY GLU LEU ALA VAL LYS ALA THR PRO TYR GLY HIS CYS THR ASP GLY GLN GLY GLY TYR VAL ALA ARG PRO LEU SER GLY SER ALA VAL ALA LEU ARG ALA SER ARG VAL PRO MET ASP HIS TYR ASP TYR PRO VAL GLY ASN

ALA ALA ALA ALA ALA GLU VAL PRO PRO GLY LYS ARG ILE VAL PRO GLY PRO GLU GLN ARG ARG GLY ARG GLN ASP LEU PHE ASP VAL VAL GLN HIS THR VAL HIS LEU LYS PRO GLN GLY TYR THR GLY GLY ASP GLN TRP LEU GLU HIS LYS GLY LYS GLY ASN ALA PRO GLY PRO GLU

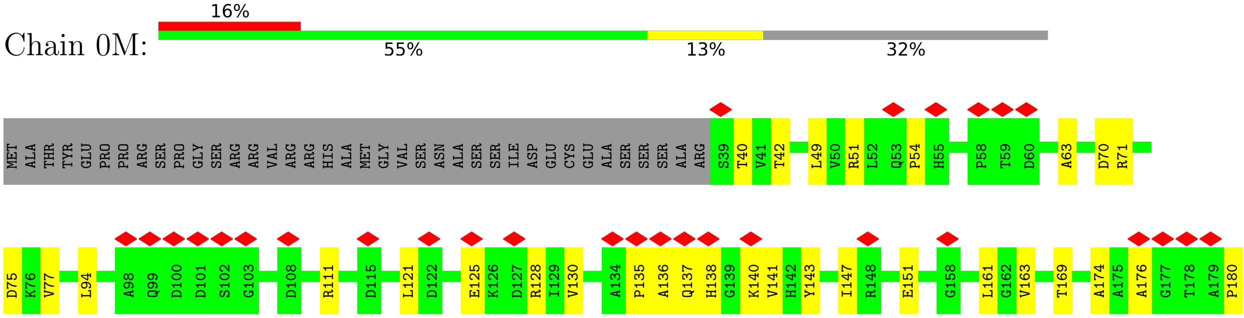
GLN ARG ARG GLY ARG ARG ASP LEU ALA ASP VAL LEU GLN GLN LYS ALA VAL ALA ASP GLY PRO ARG GLY THR SER ALA PRO ALA ARG GLY ASP GLN LEU GLN HIS LYS GLU GLN GLY ASP ALA TRP LEU ASP ALA LYS GLY LYS ARG ARG VAL GLU GLY PRO GLU MET ARG ARG GLY ARG

GLN GLY LEU TYR GLU THR LEU GLN GLN THR SER ASN PRO TYR GLN GLY GLY ASN LYS VAL GLY ASP ALA TRP LEU GLU HIS LYS GLY ARG LYS VAL GLN PRO ARG PRO GLU PRO GLU ALA ALA ALA ALA LEU SER ALA VAL PRO PRO LEU PRO THR VAL ARG PRO PRO ARG VAL GLY ASP

ASP LYS LYS TYR ALA VAL ASN ILE GLU ALA ALA MET GLY GLN MET THR VAL LYS ASP GLY ALA LYS VAL THR GLY TRP

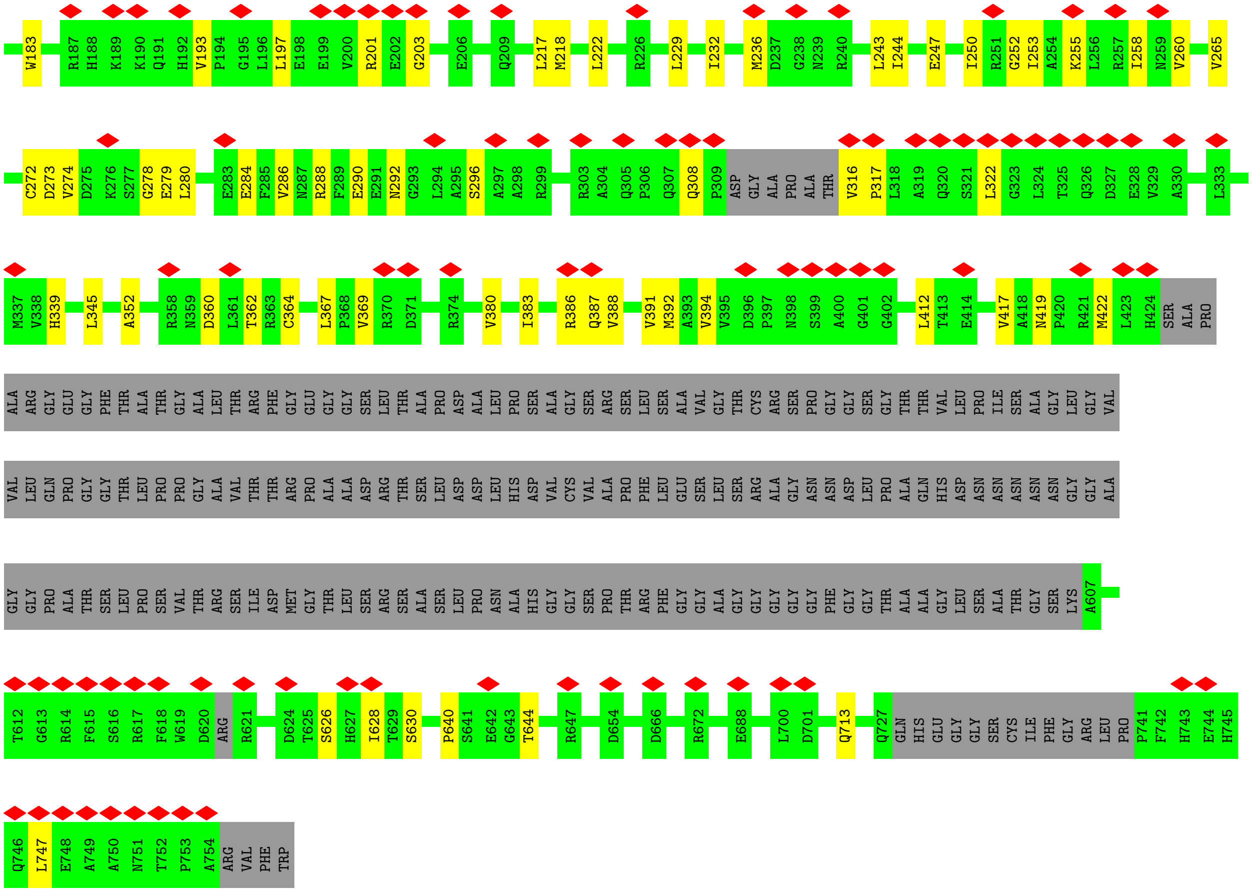
- Molecule 5: FAP225

Chain 0M:



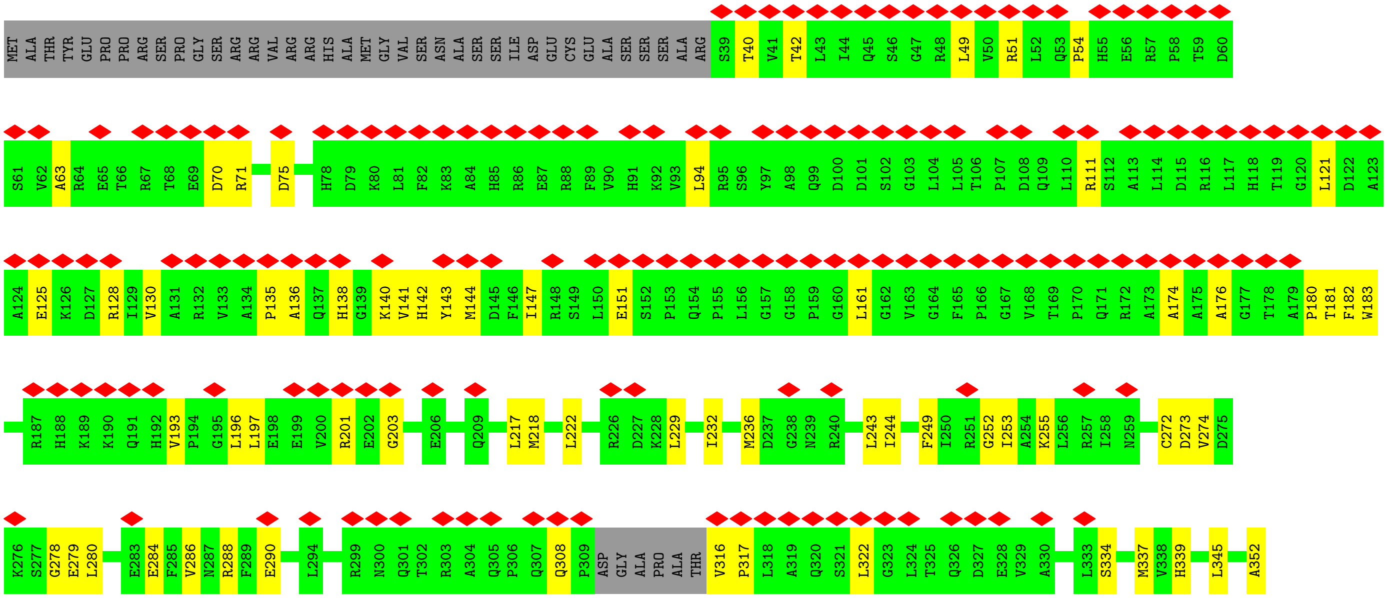
MET ALA THR TYR GLU PRO PRO ARG SER PRO GLY SER ARG ARG VAL ARG ARG HIS ALA MET GLY VAL SER ASN ALA SER SER ILE ASP GLU CYS GLU ALA SER SER SER ALA ARG S39 T40 V41 T42 L49 V50 R51 L52 Q53 P54 H55 P58 T59 D60 A63 D70 R71

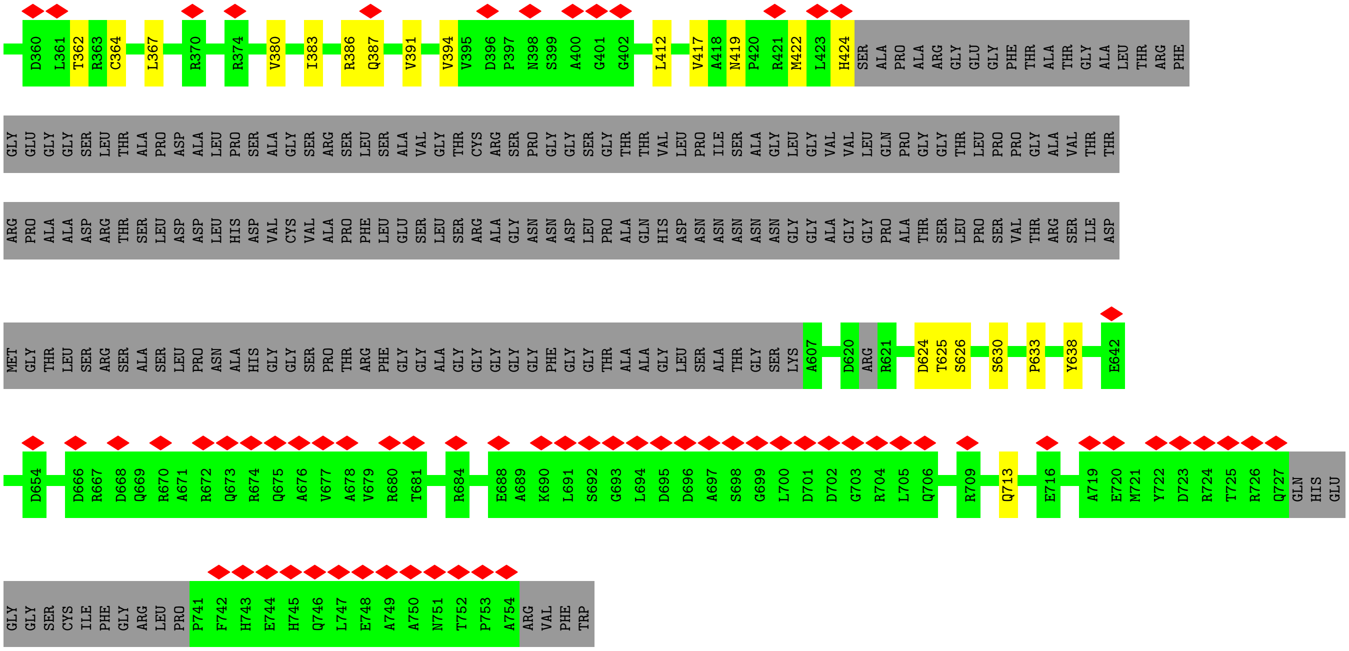
D75 K76 V77 L94 A98 Q99 D100 D101 S102 G103 D108 R111 D115 L121 D122 E125 K126 D127 R128 I129 V130 A134 P135 A136 Q137 H138 G139 K140 V141 H142 Y143 I147 R148 E151 G158 L161 G162 V163 T169 A174 A175 A176 G177 T178 A179 P180



- Molecule 5: FAP225

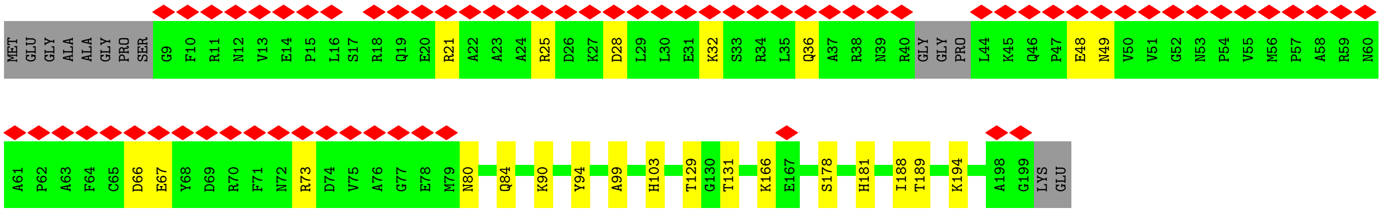
Chain 0N:





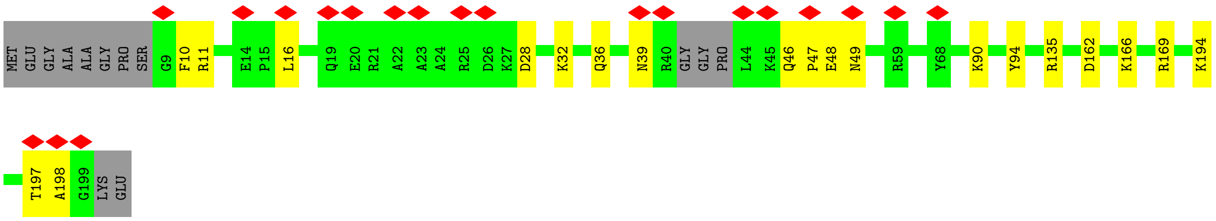
- Molecule 6: FAP213

Chain 0O:



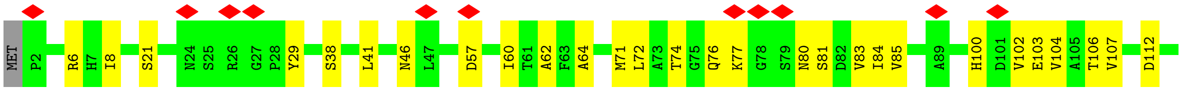
- Molecule 6: FAP213

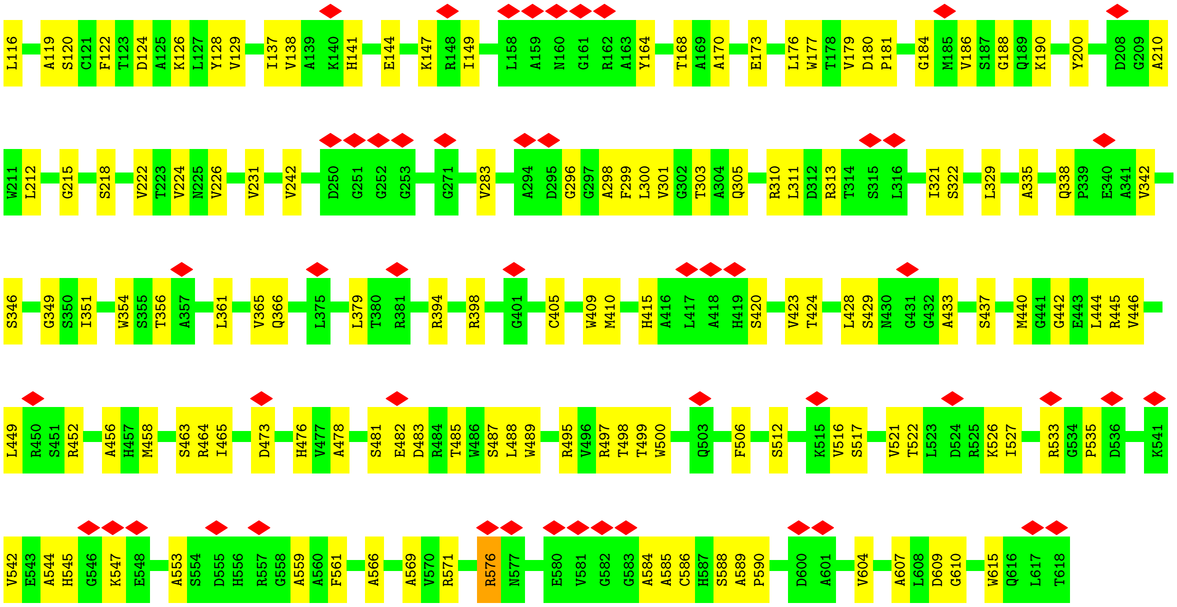
Chain 0P:



- Molecule 7: FAP196

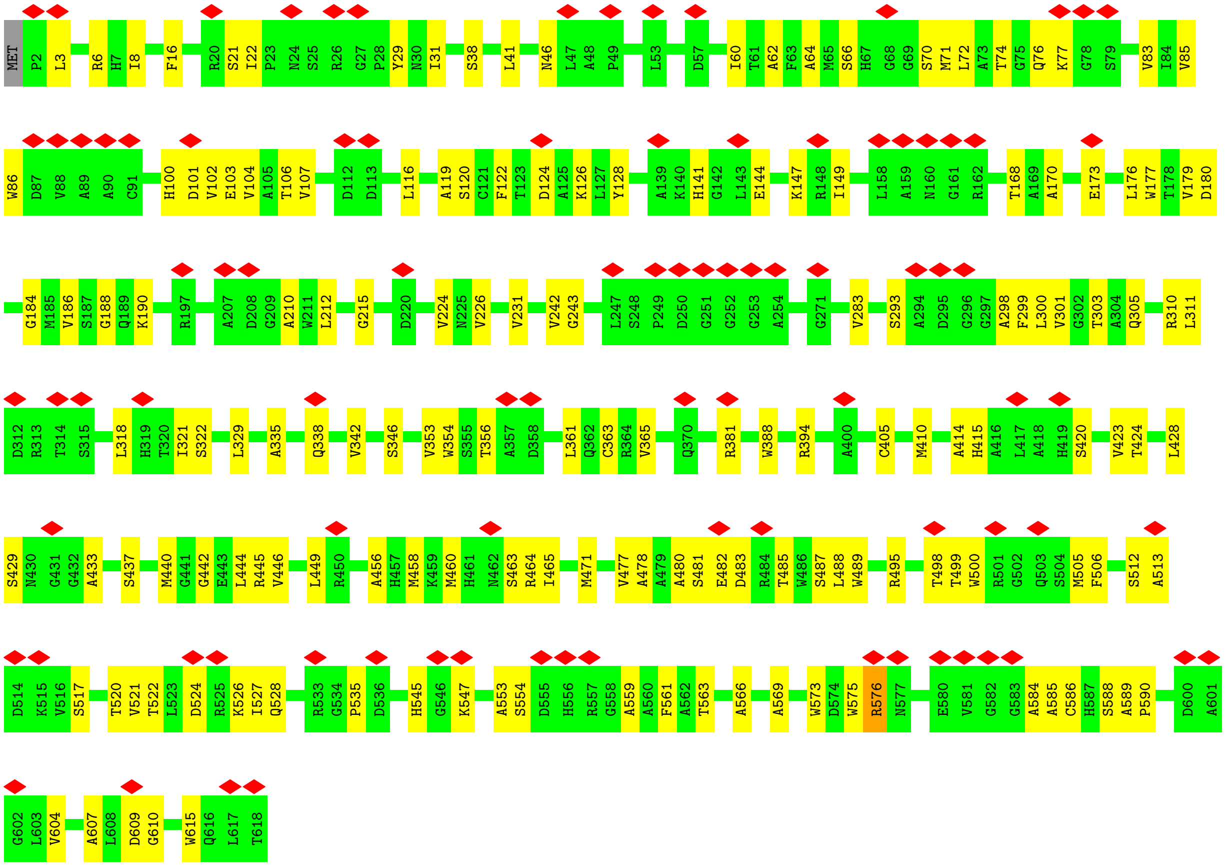
Chain 0Q:



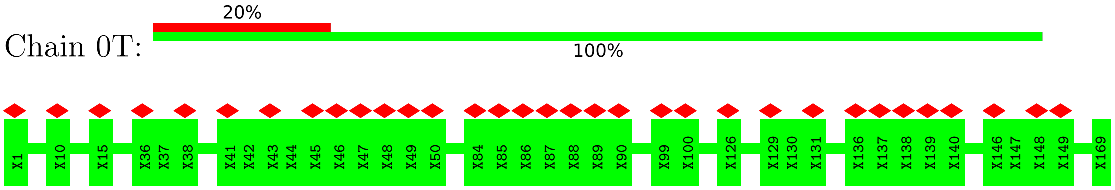


- Molecule 7: FAP196

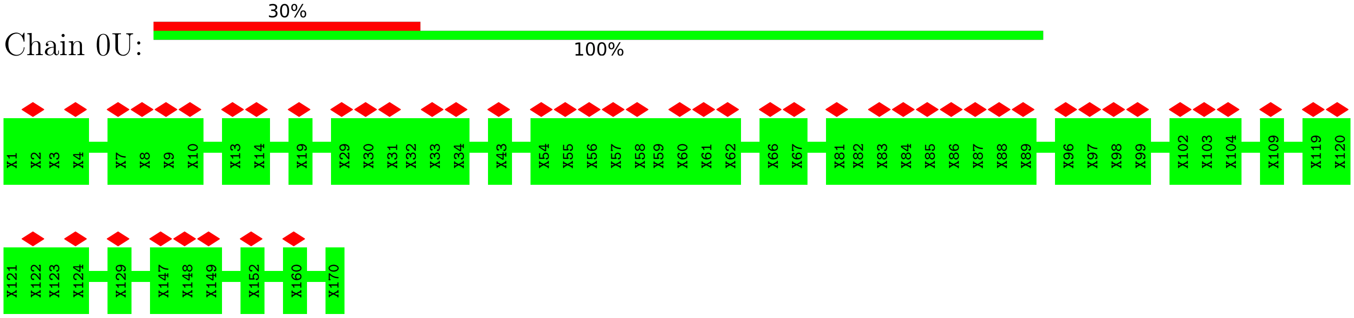
Chain 0S:



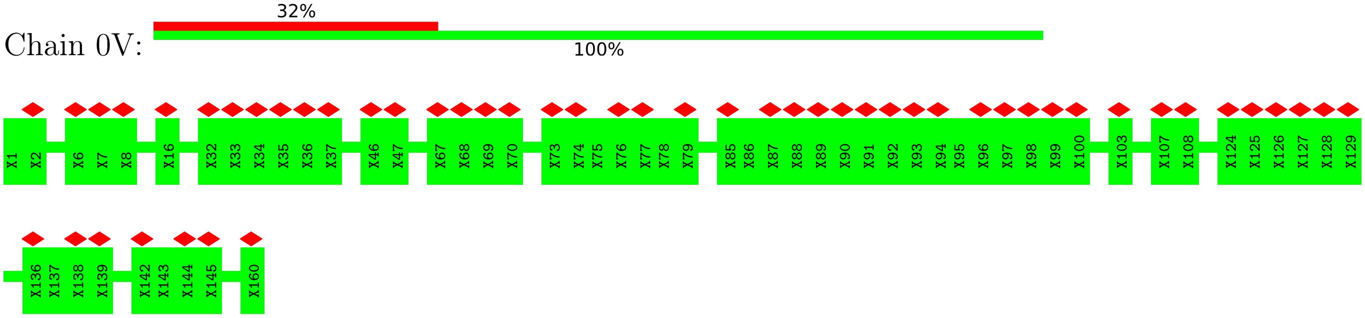
- Molecule 8: Unassigned protein-1



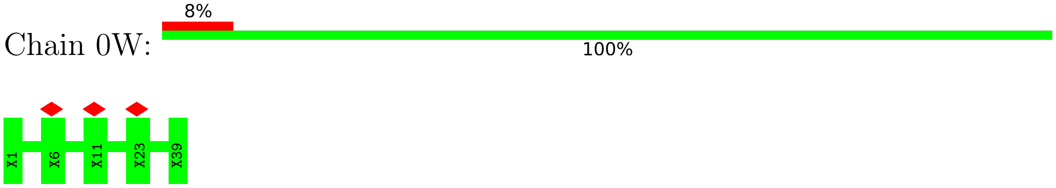
- Molecule 9: Unassigned protein-2



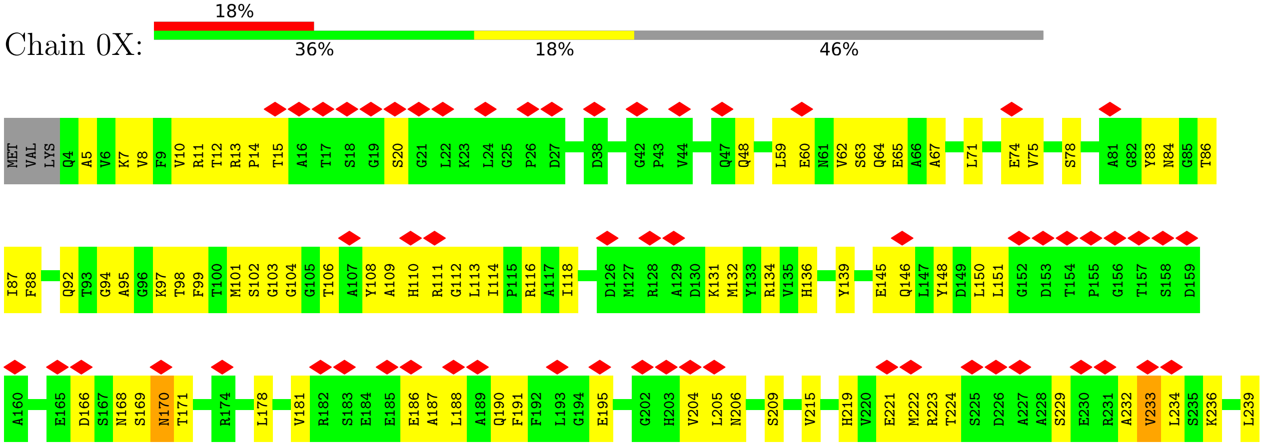
- Molecule 10: Unassigned protein-3

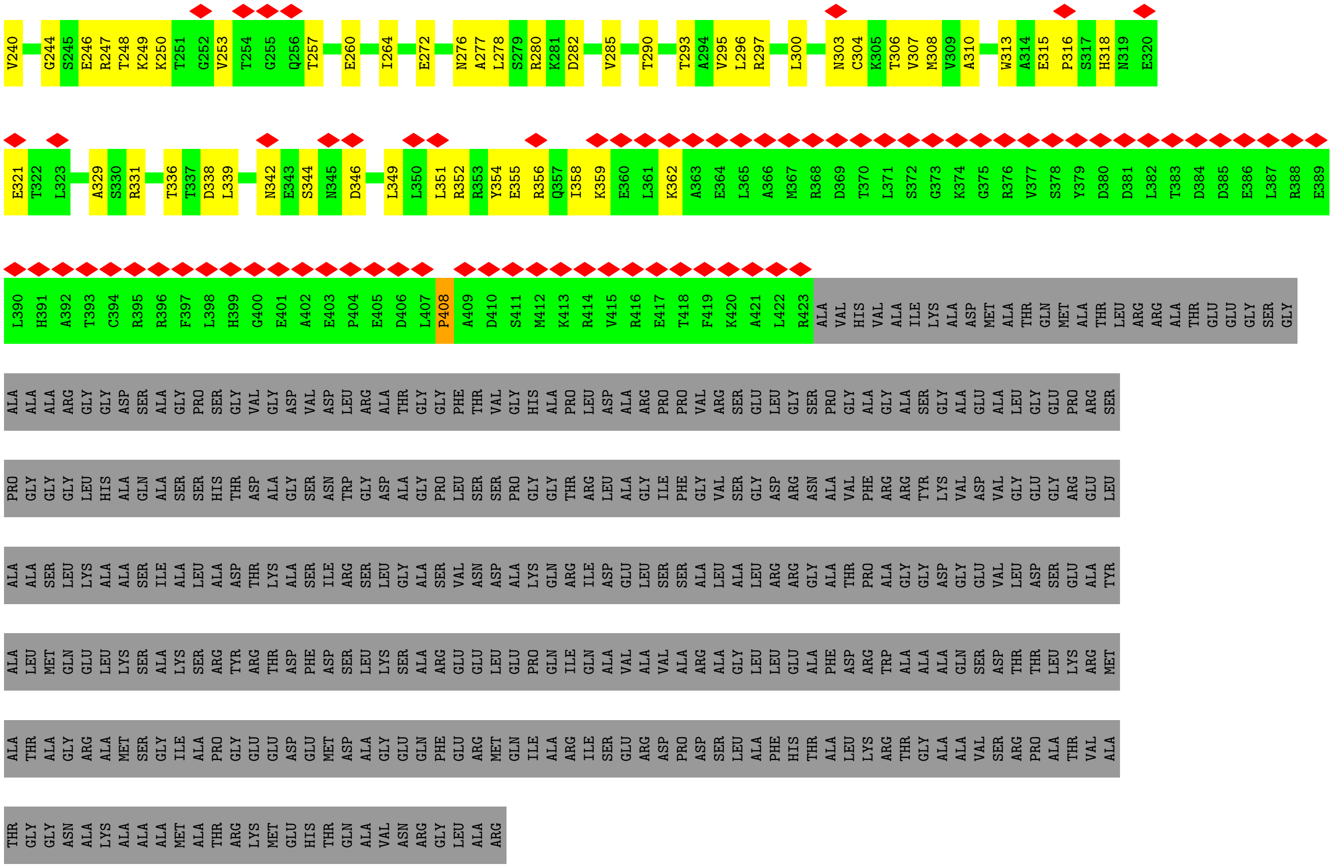


- Molecule 11: Unassigned protein-4

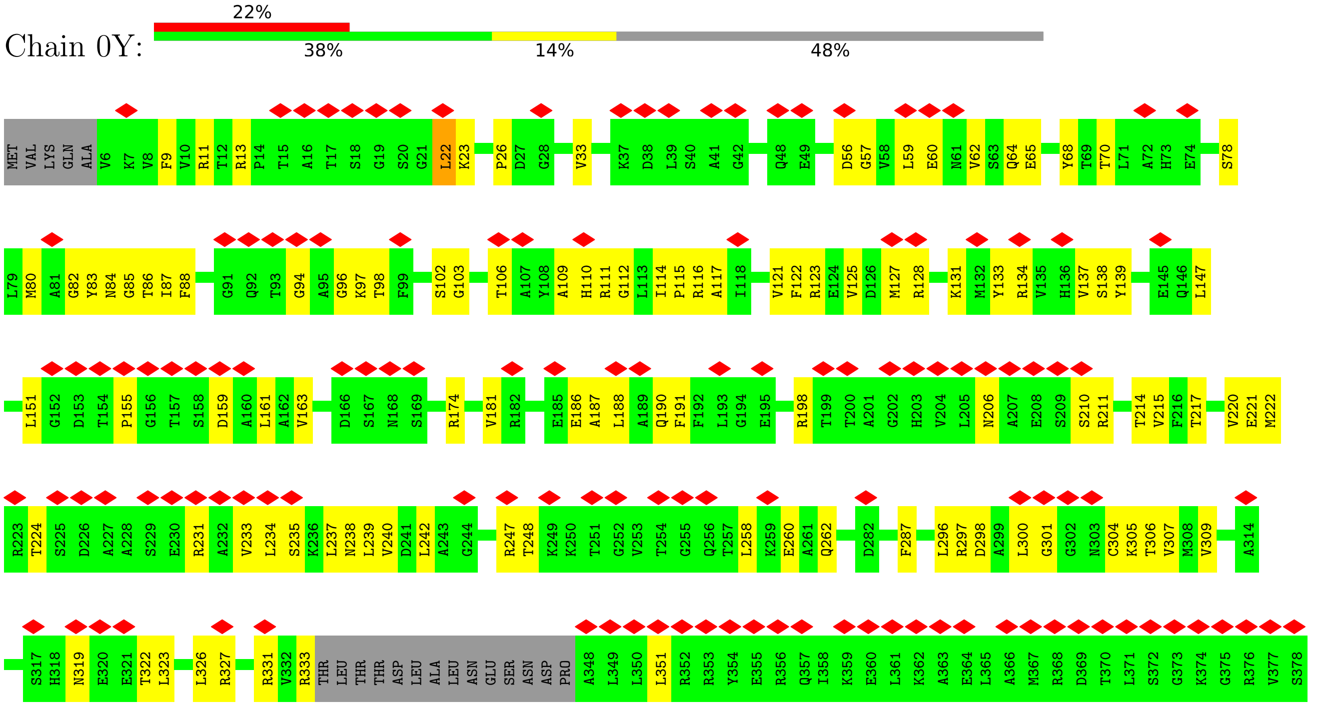


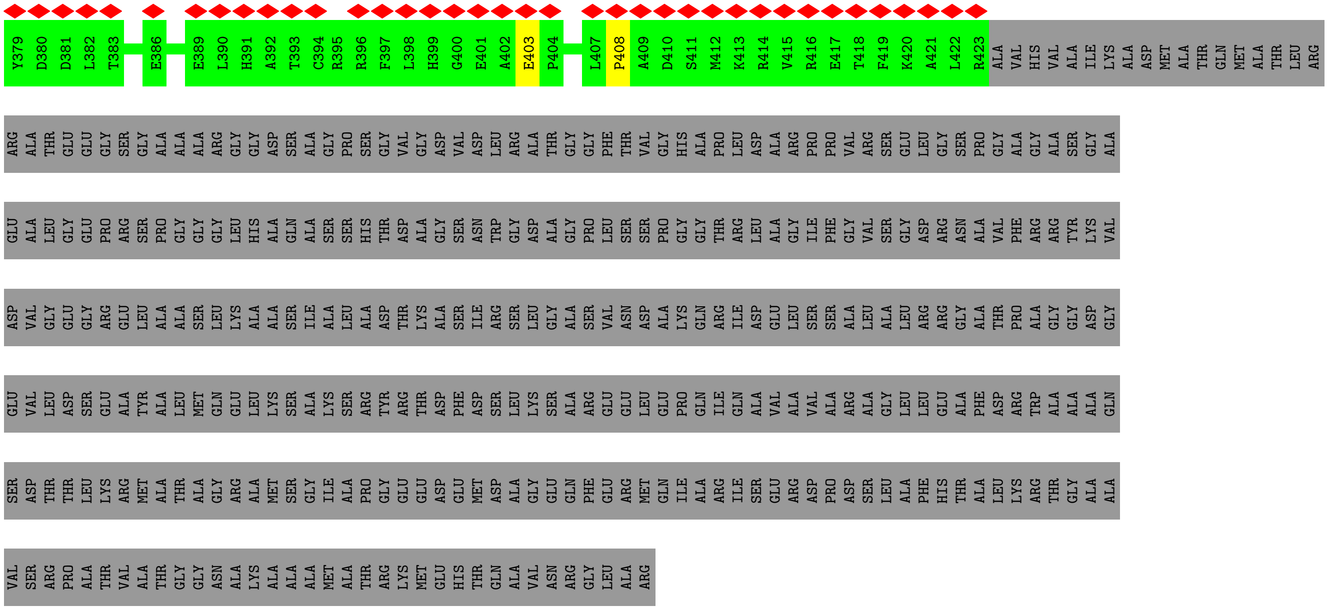
- Molecule 12: Kinesin-like protein





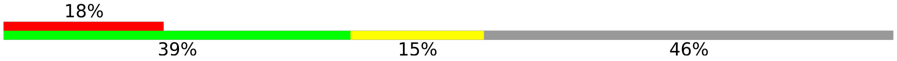
- Molecule 12: Kinesin-like protein

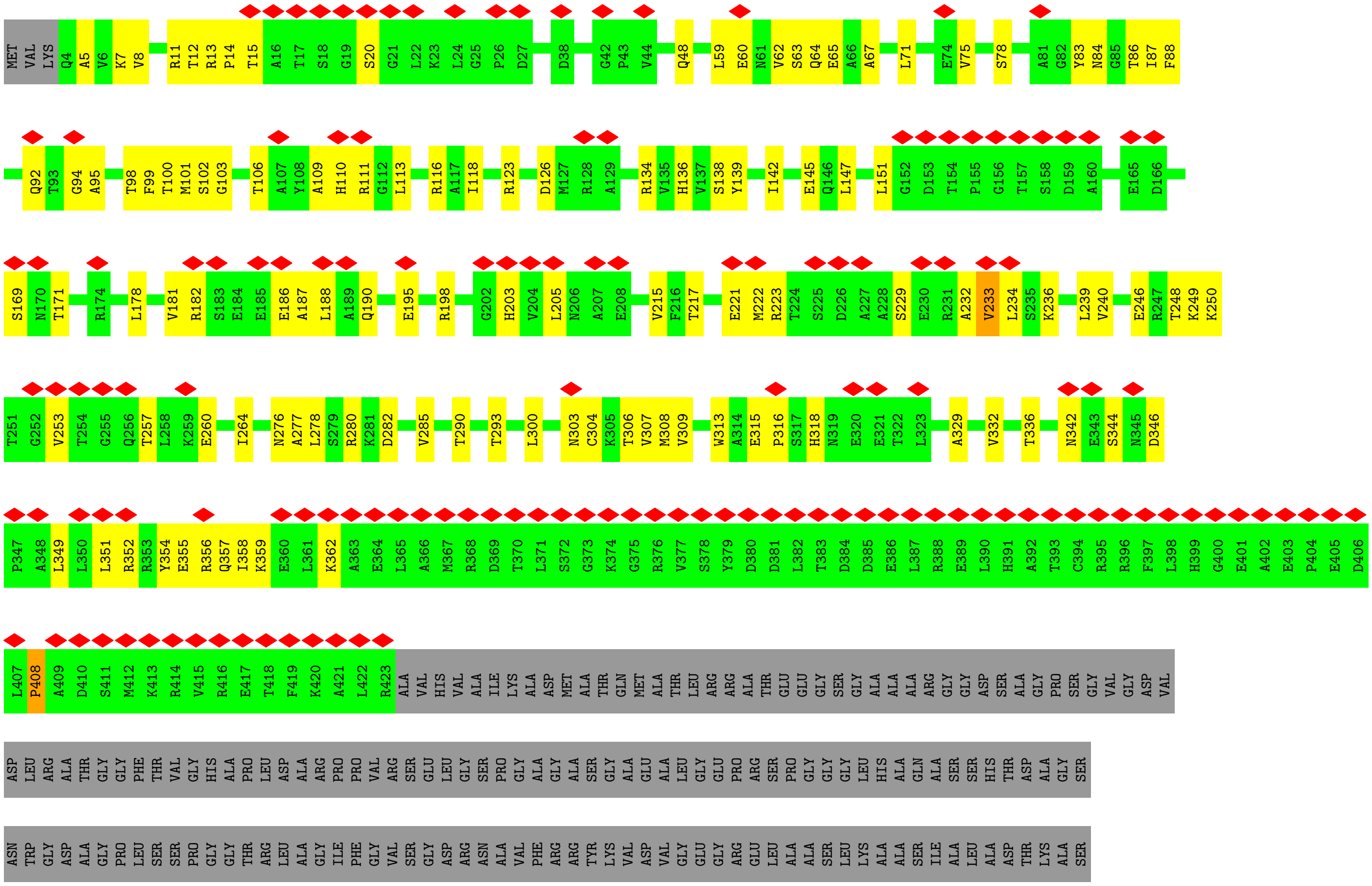


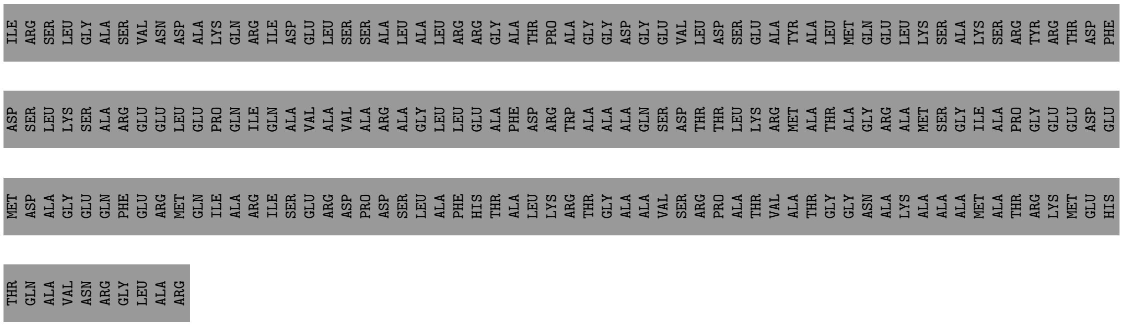


- Molecule 12: Kinesin-like protein

Chain 0Z:







ILE ARG SER LEU GLY ALA SER VAL ASN ASP ALA LYS GLN ARG ILE ASP GLU LEU SER SER ALA LEU ALA LEU ARG ARG GLY ALA THR PRO ALA GLY GLY ASP GLY GLU VAL LEU ASP SER GLU ALA TYR ALA LEU MET GLN GLU LEU LYS SER ALA LYS SER ARG TYR ARG THR ASP PHE

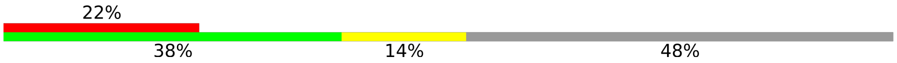
ASP SER LEU LYS SER ALA ARG GLU GLU LEU GLU PRO GLN ILE GLN ALA VAL ALA VAL ALA ARG ALA GLY LEU LEU GLU ALA PHE ASP ARG TRP ALA ALA ALA GLN SER ASP THR THR LEU LYS ARG MET ALA THR ALA GLY ARG ALA MET SER GLY ILE ALA PRO GLY GLU GLU ASP GLU

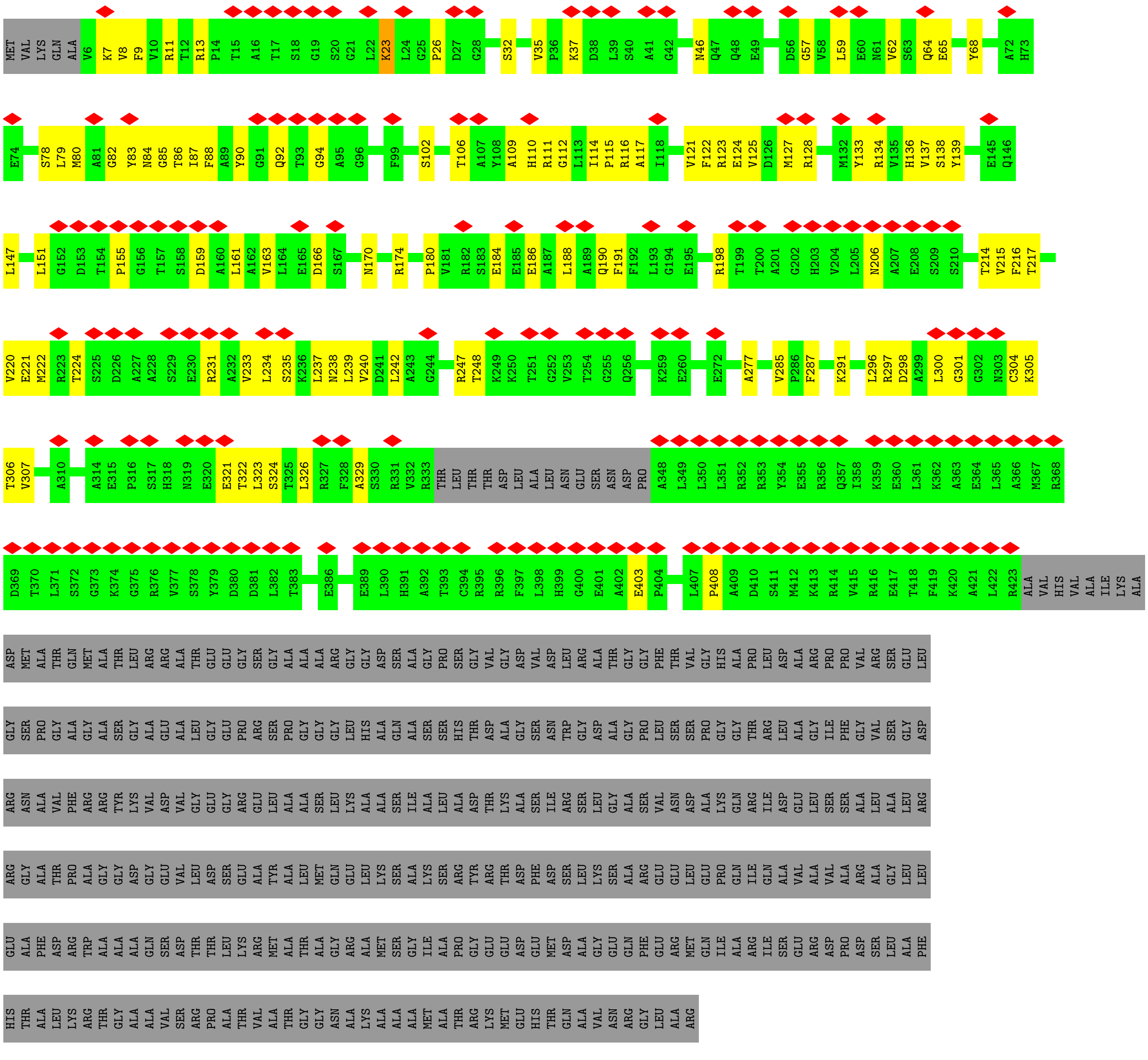
MET ASP ALA GLY GLU GLN PHE GLU ARG MET GLN ILE ALA ARG ILE SER GLU ARG ASP PRO ASP SER LEU ALA PHE HIS THR ALA LEU LYS ARG THR GLY ALA ALA VAL SER ARG PRO ALA THR VAL ALA THR GLY GLY ASN ALA LYS ALA ALA ALA MET ALA THR ARG LYS MET GLU HIS

THR GLN ALA VAL ASN ARG GLY LEU ALA ARG

- Molecule 12: Kinesin-like protein

Chain 1A:





MET VAL LYS GLN ALA V6 K7 V8 F9 V10 R11 T12 R13 P14 T15 A16 T17 S18 G19 S20 G21 L22 K23 L24 G25 P26 D27 G28 S32 V35 P36 K37 D38 L39 S40 A41 G42 N46 Q47 Q48 E49 D56 G57 V58 L59 E60 N61 V62 S63 Q64 E65 Y68 A72 H73

E74 S78 L79 M80 A81 G82 Y83 N84 G85 T86 I87 F88 A89 Y90 G91 Q92 T93 G94 A95 G96 F99 S102 T106 A107 Y108 A109 H110 R111 G112 L113 I114 P115 R116 A117 I118 V121 F122 R123 E124 V125 D126 M127 R128 M132 Y133 R134 V135 H136 V137 S138 Y139 E145 Q146

L147 L151 G152 D153 T154 P155 G156 T157 S158 D159 A160 L161 A162 V163 L164 E165 D166 S167 N170 R174 P180 V181 R182 S183 E184 E185 E186 A187 L188 A189 Q190 F191 F192 L193 G194 E195 R198 T199 T200 A201 G202 H203 V204 L205 N206 A207 E208 S209 S210 T214 V215 F216 T217

V220 E221 M222 R223 T224 S225 D226 A227 A228 S229 E230 R231 A232 V233 L234 S235 K236 L237 N238 L239 V240 D241 L242 A243 G244 R247 T248 K249 K250 T251 G252 V253 T254 G255 Q256 K259 E260 E272 A277 V285 P286 F287 K291 L296 R297 D298 A299 L300 G301 G302 N303 C304 K305

T306 V307 A310 A314 E315 P316 S317 H318 N319 E320 E321 T322 L323 S324 T325 L326 R327 F328 A329 S330 R331 V332 R333 THR LEU THR THR ASP LEU ALA LEU ASN GLU SER ASN ASP PRO A348 L349 L350 L351 R352 R353 Y354 E355 R356 Q357 I358 K359 E360 L361 K362 A363 E364 L365 A366 M367 R368

D369 T370 L371 S372 G373 K374 G375 R376 V377 S378 Y379 D380 D381 L382 T383 E386 E389 L390 H391 A392 T393 C394 R395 R396 F397 L398 H399 G400 E401 A402 E403 P404 L407 P408 A409 D410 S411 M412 K413 R414 V415 R416 E417 T418 F419 K420 A421 L422 R423 ALA VAL HIS VAL ALA ILE LYS ALA

ASP MET ALA THR GLN MET ALA THR LEU ARG ARG ALA THR GLU GLU GLY SER GLY ALA ALA ALA ARG GLY GLY ASP SER ALA GLY PRO SER GLY VAL GLY ASP VAL ASP LEU ARG ALA THR GLY PHE THR VAL GLY HIS ALA PRO LEU ASP ALA ARG PRO PRO VAL ARG SER GLU LEU

GLY SER PRO GLY ALA GLY ALA SER GLY ALA GLU ALA LEU GLY GLU PRO ARG SER PRO GLY GLY GLY LEU HIS ALA GLN ALA SER SER HIS THR ASP ALA GLY SER ASN TRP GLY ASP ALA GLY PRO LEU SER SER PRO GLY GLY THR ARG LEU ALA GLY ILE PHE GLY VAL SER GLY ASP

ARG ASN ALA VAL PHE ARG ARG TYR LYS VAL ASP VAL GLY GLU GLY ARG GLU LEU ALA ALA SER LEU LYS ALA ALA SER ILE ALA LEU ALA ASP THR LYS ALA SER ILE ARG SER LEU GLY ALA SER VAL ASN ASP ALA LYS GLN ARG ILE ASP GLU LEU SER SER ALA LEU ALA LEU ARG

ARG GLY ALA THR PRO ALA GLY GLY ASP GLY GLU VAL LEU ASP SER GLU ALA TYR ALA LEU MET GLN GLU LEU LYS SER ALA LYS SER ARG TYR ARG THR ASP PHE ASP SER LEU LYS SER ALA ARG GLU GLU LEU GLU PRO GLN ILE GLN ALA VAL ALA VAL ALA ARG ALA GLY LEU LEU

GLU ALA PHE ASP ARG TRP ALA ALA ALA GLN SER ASP THR THR LEU LYS ARG MET ALA THR ALA GLY ARG ALA MET SER GLY ILE ALA PRO GLY GLU GLU ASP GLU MET ASP ALA GLY GLU GLN PHE GLU ARG MET GLN ILE ALA ARG ILE SER GLU ARG ASP PRO ASP SER LEU ALA PHE

HIS THR ALA LEU LYS ARG THR GLY ALA ALA VAL SER ARG PRO ALA THR VAL ALA THR GLY GLY ASN ALA LYS ALA ALA ALA MET ALA THR ARG LYS MET GLU HIS THR GLN ALA VAL ASN ARG GLY LEU ALA ARG

- Molecule 13: FAP65

Chain 1B:

MET PRO ALA SER ASN GLY ALA ASP GLN GLY THR ALA PRO GLY GLY THR MET ALA TYR GLY VAL LEU SER ARG GLU GLN ARG LYS GLN MET PHE GLY LEU ASP CYS PRO GLU GLN LEU GLU TRP ARG HIS TRP ASN PRO GLY THR GLU TYR VAL LYS GLN LEU VAL LEU LYS ASN VAL SER

THR SER VAL LEU LYS ILE ARG PHE LYS GLN PRO THR SER LYS ALA PHE GLY MET ASP PHE PRO GLU PRO PHE LYS LEU ARG PRO GLY MET SER GLN PRO LEU LYS VAL VAL PHE ARG PRO LEU LYS GLN GLN HIS TYR SER ASP ASN VAL GLU LEU PHE VAL GLY ASN VAL SER CYS LEU

VAL PRO VAL HIS ALA TYR THR PRO VAL THR HIS ILE GLU VAL PRO PRO ALA LEU ASP PHE GLY PHE THR PRO THR LYS GLU THR VAL THR ALA GLN LEU PRO VAL ARG ASN THR GLY ASP VAL ARG VAL ASP VAL LEU TRP LYS LEU ASP ALA PRO PHE SER ILE SER PRO LEU PHE ALA

SER LEU ALA PRO GLY GLU VAL VAL ALA PHE THR ALA SER PHE THR PRO PRO GLU ALA CYS SER TYR THR ALA SER ALA ALA CYS GLN LEU GLU SER GLY ALA ALA ALA ILE CYS LYS ILE SER GLY ILE GLY LYS PHE PRO TYR LEU SER VAL GLU GLN ALA GLY VAL ASP PHE GLY ALA

VAL VAL VAL GLY GLN ARG VAL GLU ARG LEU VAL ARG PHE GLY ASN HIS SER VAL VAL PRO ALA HIS PHE ALA VAL THR HIS ASP GLU ALA GLY PRO ASP ASP GLY VAL PHE THR VAL GLY PRO ALA ARG GLY THR LEU GLY PRO GLU GLU TYR SER MET LEU LYS LEU SER TYR THR PRO

ARG ALA THR GLY THR PHE SER SER GLU THR PHE HIS ILE GLY THR ALA GLY GLY ASN ARG VAL ALA LEU ASN LEU ARG GLY THR ALA VAL ALA PRO LEU VAL THR LEU SER THR ARG ALA PHE ASN PHE GLY ASN VAL ALA ALA GLY ALA THR ALA SER ARG VAL LEU TYR ILE ARG ASN

HIS SER ALA VAL PRO VAL PRO TYR ASP PHE GLN VAL ASP PRO LEU ASP VAL PHE ALA ILE SER ARG THR ARG GLY VAL LEU ALA PRO ASP SER THR ALA HIS VAL THR ILE THR PHE ARG PRO MET ALA GLY LEU ALA ALA ASN LEU TRP ARG ARG VAL THR LEU LEU LEU LYS ASP ALA

GLU PRO GLN GLY VAL ASP LEU VAL ALA THR ALA TYR THR ASP LYS SER ARG PRO PRO PRO LEU SER GLN ARG HIS VAL GLU ARG TYR MET ALA ARG VAL LEU SER GLY GLY PRO ALA VAL GLU GLU SER GLN LEU ASP SER LYS PRO PRO SER ALA ALA THR GLY ALA GLY GLY LEU ASP

GLY ALA SER GLU GLY GLY ALA GLY PRO LEU LEU ALA GLY GLY GLY PHE GLY SER LEU LEU PRO PRO LEU GLY ASP ALA ALA GLU GLY GLY GLU GLY ALA ALA SER LYS LEU LEU GLY PRO ASP GLY TRP SER LEU LEU PHE GLY GLY GLN ASP PRO ALA ALA ALA LEU THR VAL ASP SER

ASP ALA LEU ASP PHE GLY SER CYS SER ARG LEU SER ALA SER GLU TYR ARG SER VAL THR VAL THR ASN HIS THR PRO ALA LYS LEU THR ALA PHE VAL LEU VAL PRO GLU TRP ALA ASP PRO GLY ALA ALA PRO GLY ASP ALA PRO GLN ARG VAL PHE GLN VAL PHE PRO GLU SER ALA

ASP MET ARG PRO TYR GLY GLN ALA THR PHE LYS VAL ALA PHE ARG PRO PRO ARG ASP ALA ALA PHE PHE SER GLN GLN LEU ALA LEU VAL ALA HIS THR LYS SER GLN ARG ASN PHE ARG LEU VAL ALA GLU HIS GLN VAL LEU PRO ALA TRP CYS VAL PRO LEU ARG ALA THR GLY ASN

THR PHE LEU HIS SER ASN PRO GLU PHE GLY PRO LYS VAL GLU LEU SER SER ARG ALA VAL ALA PHE PRO PRO CYS ARG PRO GLY GLU ARG VAL HIS GLN THR LEU LEU ILE ALA ASN SER GLY ASP THR PRO VAL ALA PHE SER PHE GLY ALA ALA GLY ALA ALA LEU GLY PRO LEU PHE

SER ALA LYS PRO ALA ALA GLY VAL VAL PRO PRO GLN GLY HIS VAL LEU VAL ALA LEU ARG PHE ALA PRO THR ASP THR ARG PRO ALA ALA ALA ASN ALA LEU VAL THR PHE ASN GLY VAL ALA SER ASN ALA VAL SER VAL SER LEU ARG GLY ALA ALA HIS THR PRO ARG LEU THR THR

ASP LEU PRO SER SER THR LEU TYR PHE ARG PRO THR CYS VAL GLY ALA SER SER GLN ARG ALA VAL THR LEU HIS ASN PRO SER ARG VAL PRO VAL ALA PHE ARG TRP ARG LEU PRO ALA ARG LEU GLN GLY LEU VAL THR VAL SER PRO ALA ALA GLY ALA LEU ARG GLY ASN GLU SER

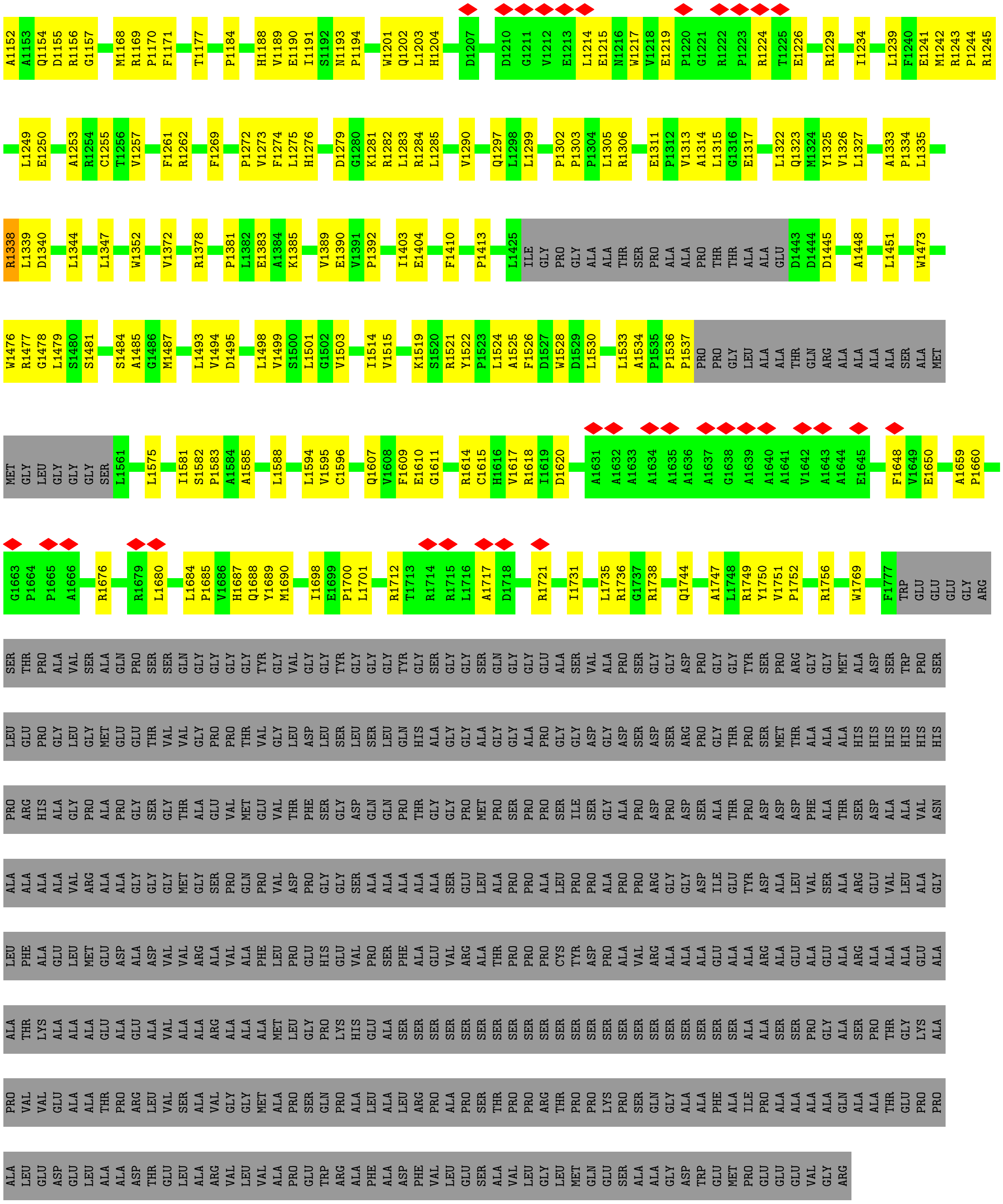
VAL GLN LEU GLN TRP SER PHE THR PRO ALA ALA GLN LYS LEU TYR GLU ALA ARG ALA ALA CYS LEU VAL MET SER PRO PRO GLU ALA ALA ASN GLY ASN ALA ALA GLY ALA THR ALA SER ALA ALA SER LEU PHE PRO GLY ALA GLY LEU ALA THR GLY ILE GLU TRP TYR GLU GLY ALA

GLY ALA THR ALA ALA LEU ALA GLY MET GLY GLU GLU GLU ALA ALA ASP ALA VAL LEU LEU SER LEU VAL GLY GLU GLY THR GLN GLY ALA VAL ALA LEU GLU PRO PRO SER LEU GLU LEU GLY ASP LEU ARG VAL GLY HIS PRO VAL ARG ARG PRO LEU LEU LEU GLN ASN CYS SER ASP

GLY VAL LEU ARG TYR SER LEU GLU VAL GLY PRO ALA GLU ASP ASP GLN PRO PRO ALA GLY ASP ALA THR LEU VAL ASP PHE THR ALA GLY LEU ASP SER ALA ALA GLU GLY GLY VAL GLY GLY GLY ALA GLY GLY ALA GLY GLY ALA ALA LEU GLU CYS TRP VAL ASP GLU PRO GLU GLY

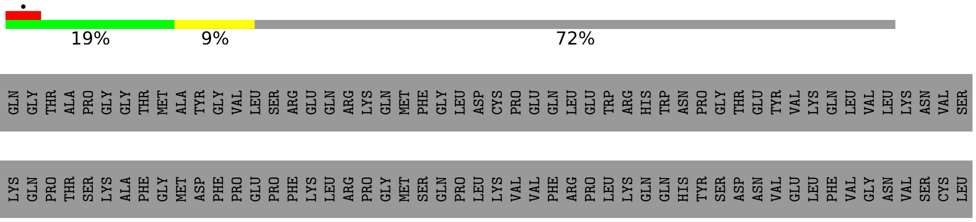
ALA LEU PRO ALA ARG ALA SER LYS THR VAL MET VAL THR LEU PHE PRO ARG TYR ARG LYS ARG TYR SER LEU GLN VAL ARG CYS ARG SER SER THR VAL ALA PRO LEU LEU THR GLY PRO ASN ARG PRO PRO SER GLY GLY ALA GLY PRO ARG PRO LEU ASP ALA GLY SER GLU ALA ALA

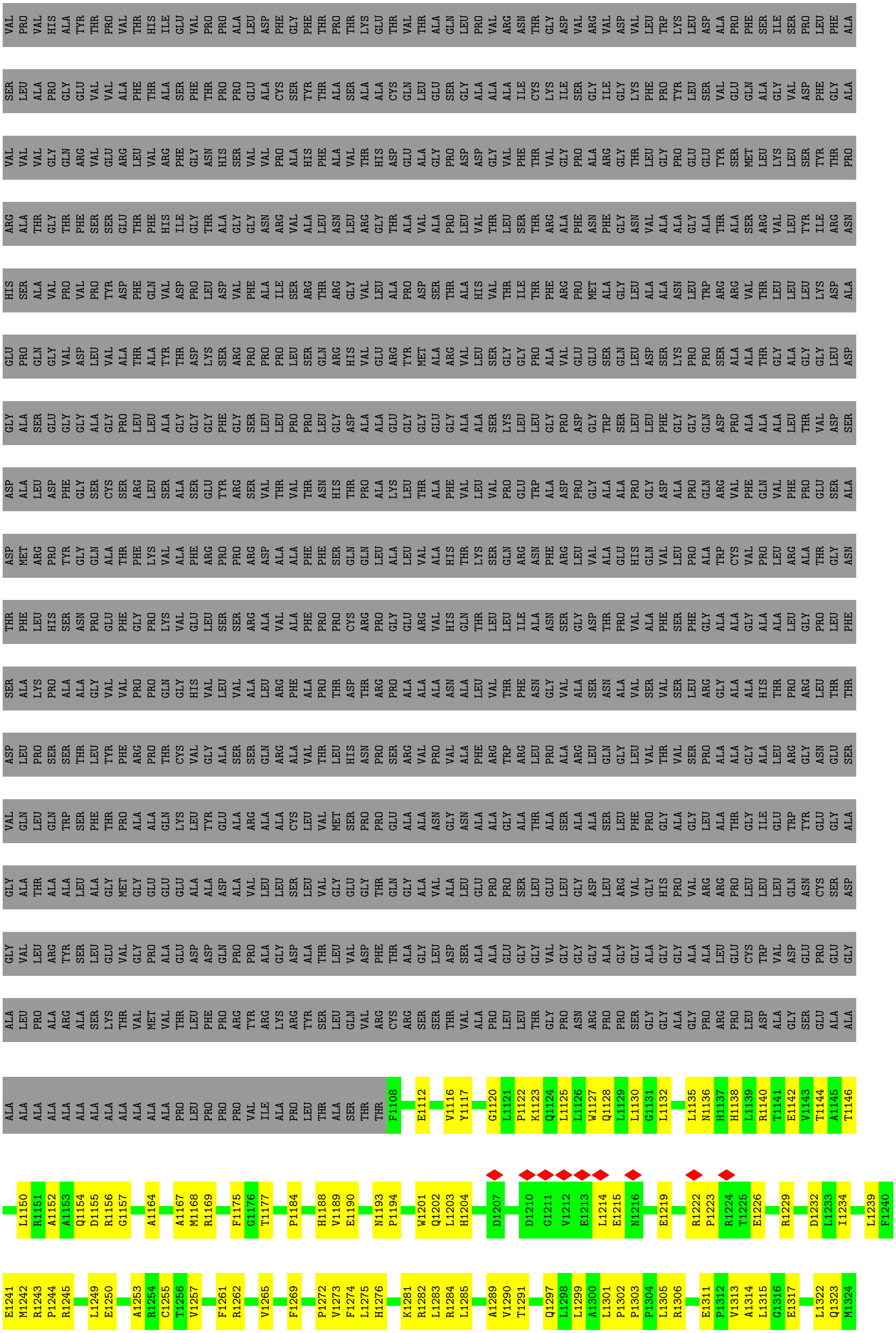
ALA ALA ALA ALA ALA ALA ALA ALA ALA ALA ALA ALA PRO LEU PRO PRO PRO VAL ILE ALA PRO LEU THR ALA SER THR THR 🟩 F1108 🟨 E1112 🟨 V1116 🟨 G1120 🟨 K1123 🟨 W1127 🟨 L1130 🟩 G1131 🟨 L1132 🟩 N1133 🟨 D1134 🟨 L1135 🟨 N1136 🟩 H1137 🟨 H1138 🟩 L1139 🟨 R1140 🟩 T1141 🟨 E1142 🟩 V1143 🟨 T1144 🟩 A1145 🟨 T1146 🟨 R1149 🟨 L1150 🟨 R1151

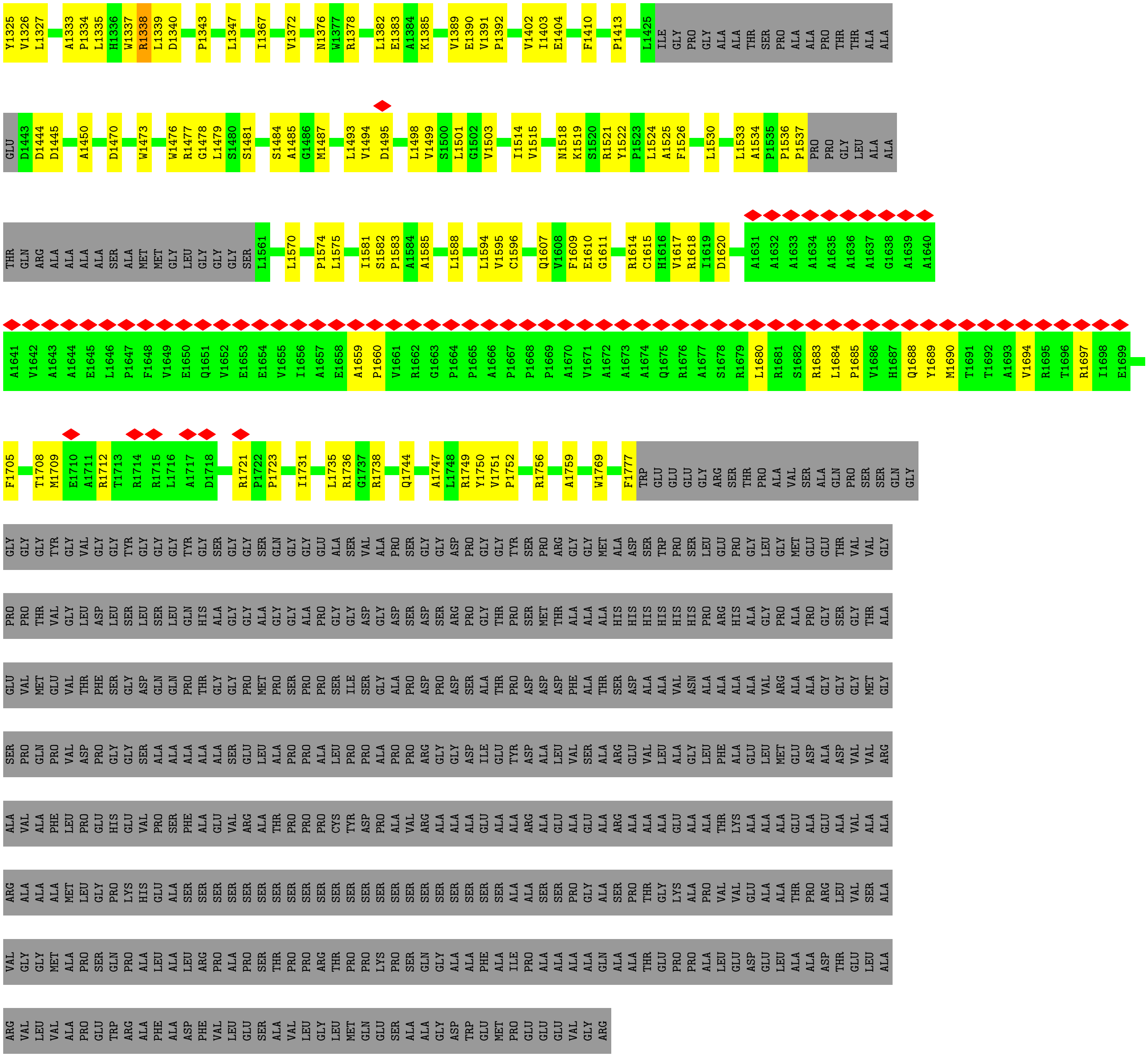


- Molecule 13: FAP65

Chain 1C:

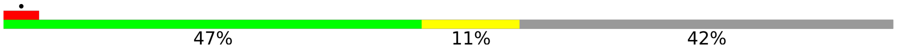


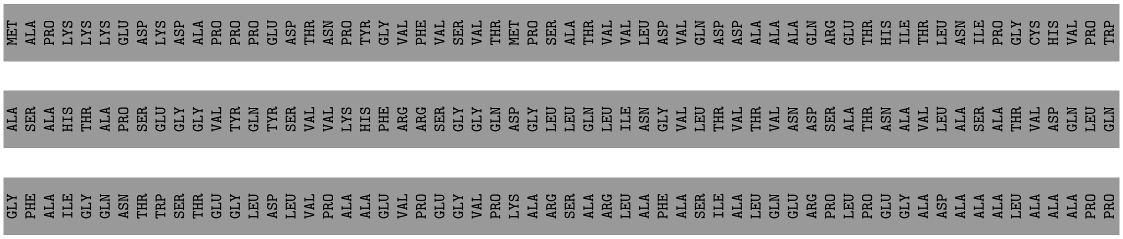

VAL PRO VAL HIS ALA TYR THR PRO VAL THR HIS ILE GLU VAL PRO PRO ALA LEU ASP PHE GLY PHE THR PRO THR LYS GLU THR VAL THR ALA GLN LEU PRO VAL ARG ASN THR GLY ASP VAL ARG VAL ASP VAL LEU TRP LYS LEU ASP ALA PRO PHE SER ILE SER PRO LEU PHE ALA
SER LEU ALA PRO GLY GLU VAL VAL ALA PHE THR ALA SER PHE THR PRO PRO GLU ALA CYS SER TYR THR ALA SER ALA ALA CYS GLN LEU GLU SER GLY ALA ALA ALA ILE CYS LYS ILE SER GLY ILE GLY LYS PHE PRO TYR LEU SER VAL GLU GLN ALA GLY VAL ASP PHE GLY ALA
VAL VAL VAL GLY GLN ARG VAL GLU ARG LEU VAL ARG PHE GLY ASN HIS SER VAL VAL PRO ALA HIS PHE ALA VAL THR HIS ASP GLU ALA GLY PRO ASP ASP GLY VAL PHE THR VAL GLY PRO ALA ARG GLY THR LEU GLY PRO GLU GLU TYR SER MET LEU LYS LEU SER TYR THR PRO
ARG ALA THR GLY THR PHE SER SER GLU THR PHE HIS ILE GLY THR ALA GLY GLY ASN ARG VAL ALA LEU ASN LEU ARG GLY THR ALA VAL ALA PRO LEU VAL THR LEU SER THR ARG ALA PHE ASN PHE GLY ASN VAL ALA ALA GLY ALA THR ALA SER ARG VAL LEU TYR ILE ARG ASN
HIS SER ALA VAL PRO VAL PRO TYR ASP PHE GLN VAL ASP PRO LEU ASP VAL PHE ALA ILE SER ARG THR ARG GLY VAL LEU ALA PRO ASP SER THR ALA HIS VAL THR ILE THR PHE ARG PRO MET ALA GLY LEU ALA ALA ASN LEU TRP ARG ARG VAL THR LEU LEU LEU LYS ASP ALA
GLU PRO GLN GLY VAL ASP LEU VAL ALA THR ALA TYR THR ASP LYS SER ARG PRO PRO PRO LEU SER GLN ARG HIS VAL GLU ARG TYR MET ALA ARG VAL LEU SER GLY GLY PRO ALA VAL GLU GLU SER GLN LEU ASP SER LYS PRO PRO SER ALA ALA THR GLY ALA GLY GLY LEU ASP
GLY ALA SER GLU GLY GLY ALA GLY PRO LEU LEU ALA GLY GLY GLY PHE GLY SER LEU LEU PRO PRO LEU GLY ASP ALA ALA GLU GLY GLY GLU GLY ALA ALA SER LYS LEU LEU GLY PRO ASP GLY TRP SER LEU LEU PHE GLY GLY GLN ASP PRO ALA ALA ALA LEU THR VAL ASP SER
ASP ALA LEU ASP PHE GLY SER CYS SER ARG LEU SER ALA SER GLU TYR ARG SER VAL THR VAL THR ASN HIS THR PRO ALA LYS LEU THR ALA PHE VAL LEU VAL PRO GLU TRP ALA ASP PRO GLY ALA ALA PRO GLY ASP ALA PRO GLN ARG VAL PHE GLN VAL PHE PRO GLU SER ALA
ASP MET ARG PRO TYR GLY GLN ALA THR PHE LYS VAL ALA PHE ARG PRO PRO ARG ASP ALA ALA PHE PHE SER GLN GLN LEU ALA LEU VAL ALA HIS THR LYS SER GLN ARG ASN PHE ARG LEU VAL ALA GLU HIS GLN VAL LEU PRO ALA TRP CYS VAL PRO LEU ARG ALA THR GLY ASN
THR PHE LEU HIS SER ASN PRO GLU PHE GLY PRO LYS VAL GLU LEU SER SER ARG ALA VAL ALA PHE PRO PRO CYS ARG PRO GLY GLU ARG VAL HIS GLN THR LEU LEU ILE ALA ASN SER GLY ASP THR PRO VAL ALA PHE SER PHE GLY ALA ALA GLY ALA ALA LEU GLY PRO LEU PHE
SER ALA LYS PRO ALA ALA GLY VAL VAL PRO PRO GLN GLY HIS VAL LEU VAL ALA LEU ARG PHE ALA PRO THR ASP THR ARG PRO ALA ALA ALA ASN ALA LEU VAL THR PHE ASN GLY VAL ALA SER ASN ALA VAL SER VAL SER LEU ARG GLY ALA ALA HIS THR PRO ARG LEU THR THR
ASP LEU PRO SER SER THR LEU TYR PHE ARG PRO THR CYS VAL GLY ALA SER SER GLN ARG ALA VAL THR LEU HIS ASN PRO SER ARG VAL PRO VAL ALA PHE ARG TRP ARG LEU PRO ALA ARG LEU GLN GLY LEU VAL THR VAL SER PRO ALA ALA GLY ALA LEU ARG GLY ASN GLU SER
VAL GLN LEU GLN TRP SER PHE THR PRO ALA ALA GLN LYS LEU TYR GLU ALA ARG ALA ALA CYS LEU VAL MET SER PRO PRO GLU ALA ALA ASN GLY ASN ALA ALA GLY ALA THR ALA SER ALA ALA SER LEU PHE PRO GLY ALA GLY LEU ALA THR GLY ILE GLU TRP TYR GLU GLY ALA
GLY ALA THR ALA ALA LEU ALA GLY MET GLY GLU GLU GLU ALA ALA ASP ALA VAL LEU LEU SER LEU VAL GLY GLU GLY THR GLN GLY ALA VAL ALA LEU GLU PRO PRO SER LEU GLU LEU GLY ASP LEU ARG VAL GLY HIS PRO VAL ARG ARG PRO LEU LEU LEU GLN ASN CYS SER ASP
GLY VAL LEU ARG TYR SER LEU GLU VAL GLY PRO ALA GLU ASP ASP GLN PRO PRO ALA GLY ASP ALA THR LEU VAL ASP PHE THR ALA GLY LEU ASP SER ALA ALA GLU GLY GLY VAL GLY GLY GLY ALA GLY GLY ALA GLY GLY ALA ALA LEU GLU CYS TRP VAL ASP GLU PRO GLU GLY
ALA LEU PRO ALA ARG ALA SER LYS THR VAL MET VAL THR LEU PHE PRO ARG TYR ARG LYS ARG TYR SER LEU GLN VAL ARG CYS ARG SER SER THR VAL ALA PRO LEU LEU THR GLY PRO ASN ARG PRO PRO SER GLY GLY ALA GLY PRO ARG PRO LEU ASP ALA GLY SER GLU ALA ALA
ALA ALA ALA ALA ALA ALA ALA ALA ALA ALA ALA ALA PRO LEU PRO PRO PRO VAL ILE ALA PRO LEU THR ALA SER THR THR F1108 E1112 V1116 Y1117 G1120 L1121 P1122 K1123 Q1124 L1125 L1126 W1127 Q1128 L1129 L1130 G1131 L1132 L1135 N1136 H1137 H1138 L1139 R1140 T1141 E1142 V1143 T1144 A1145 T1146
L1150 R1151 A1152 A1153 Q1154 D1155 R1156 G1157 A1164 A1167 M1168 R1169 F1175 G1176 T1177 P1184 H1188 V1189 E1190 N1193 P1194 W1201 Q1202 L1203 H1204 D1207 D1210 G1211 V1212 E1213 L1214 E1215 N1216 E1219 R1222 P1223 R1224 T1225 E1226 R1229 D1232 L1233 I1234 L1239 F1240
E1241 M1242 R1243 P1244 R1245 L1249 E1250 A1253 R1254 C1255 T1256 V1257 F1261 R1262 V1265 F1269 P1272 V1273 F1274 L1275 H1276 K1281 R1282 L1283 R1284 L1285 A1289 V1290 T1291 Q1297 L1298 L1299 A1300 L1301 P1302 P1303 P1304 L1305 R1306 E1311 P1312 V1313 A1314 L1315 G1316 E1317 L1322 Q1323 M1324

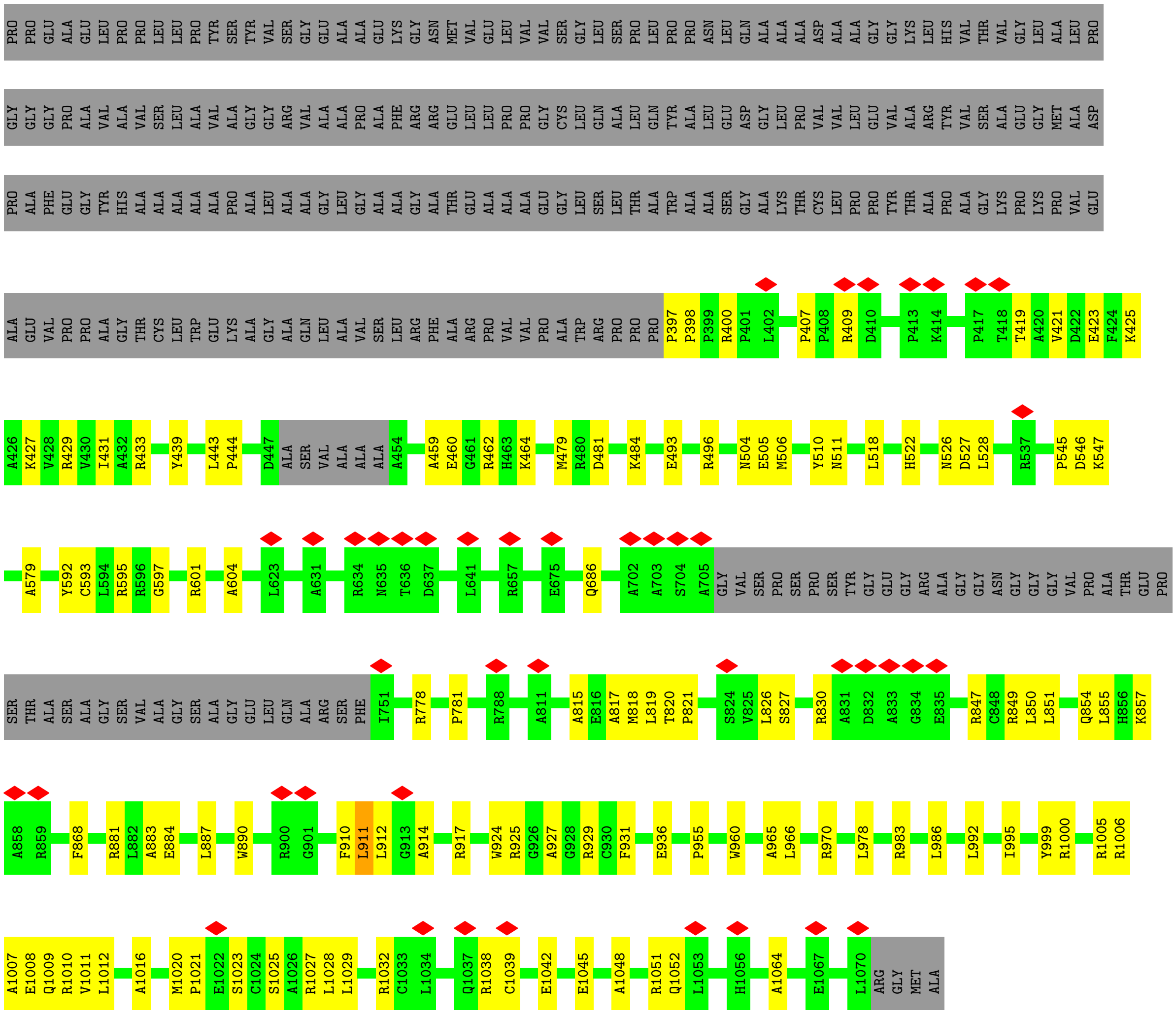


- Molecule 14: FAP70

Chain 1D:

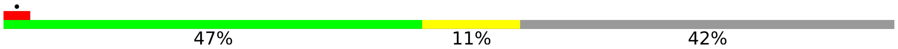


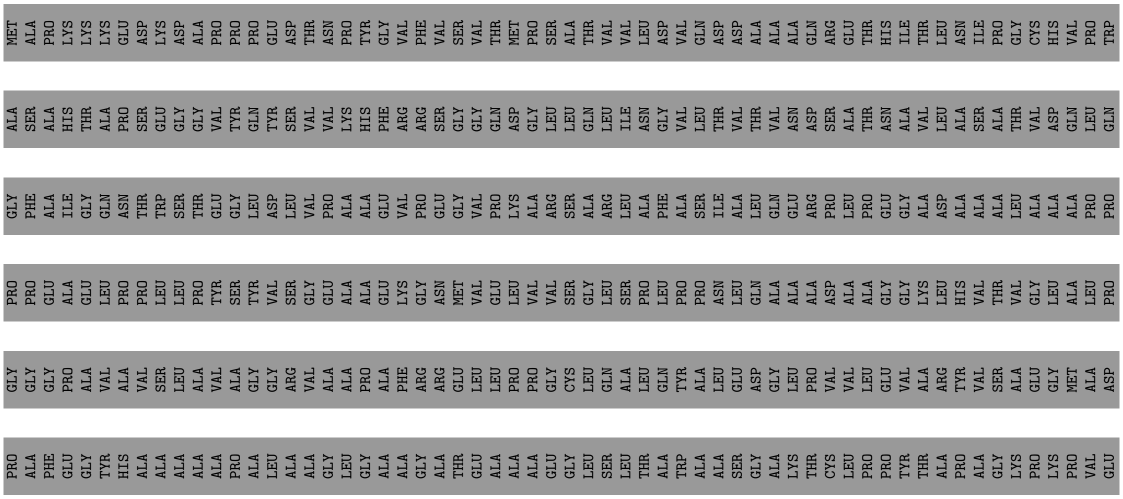


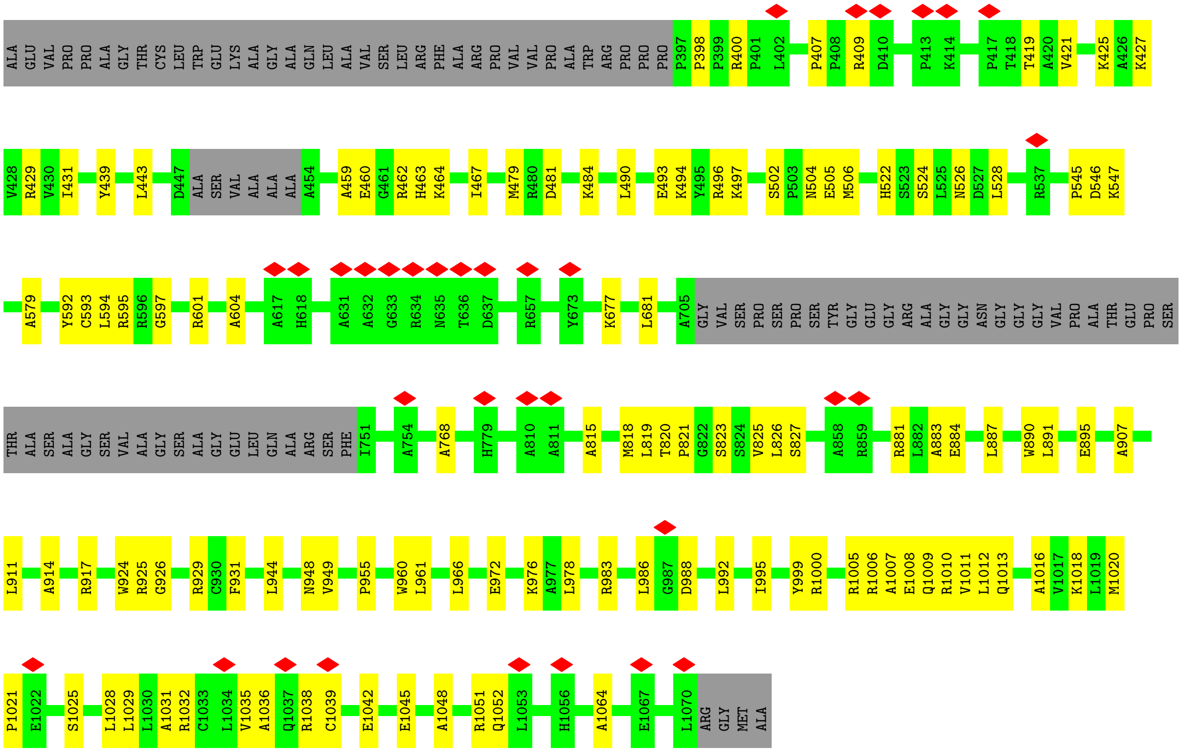


- Molecule 14: FAP70

Chain 1E:

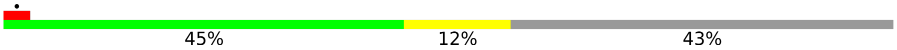


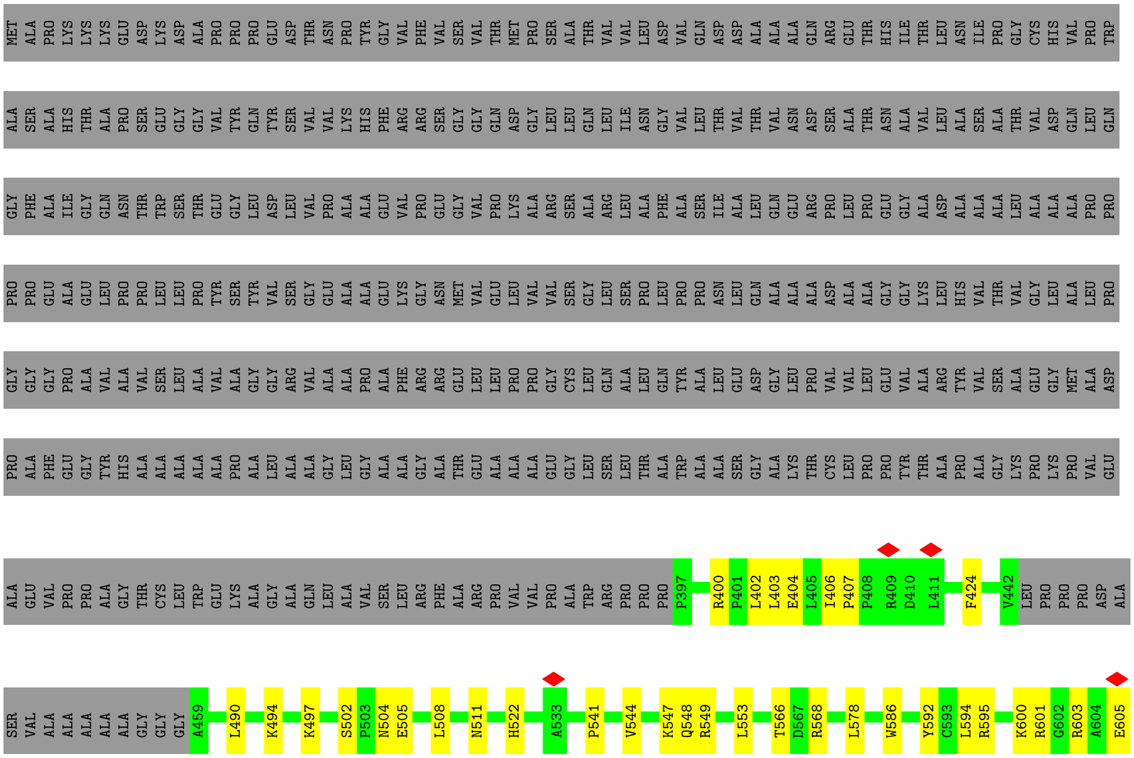


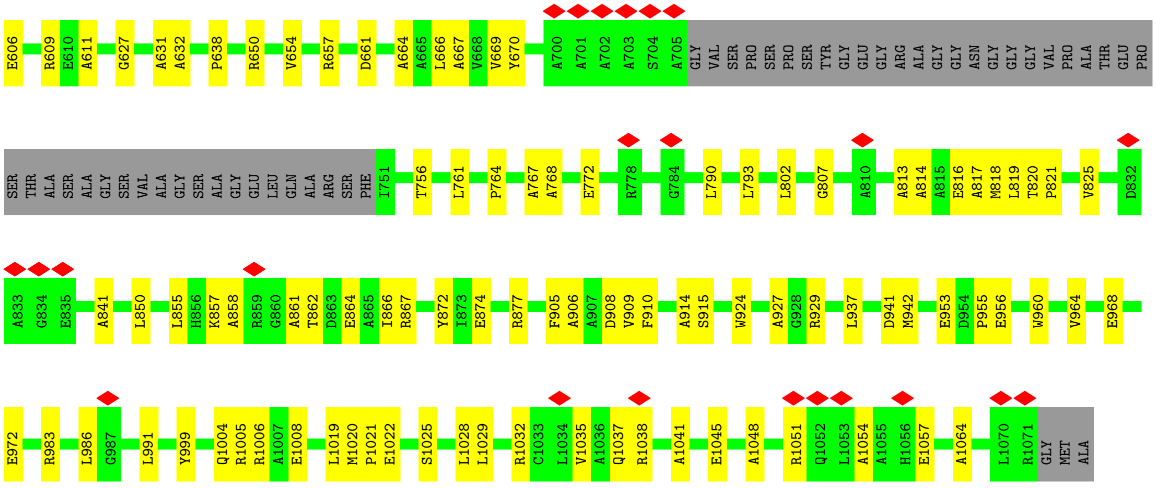


- Molecule 14: FAP70

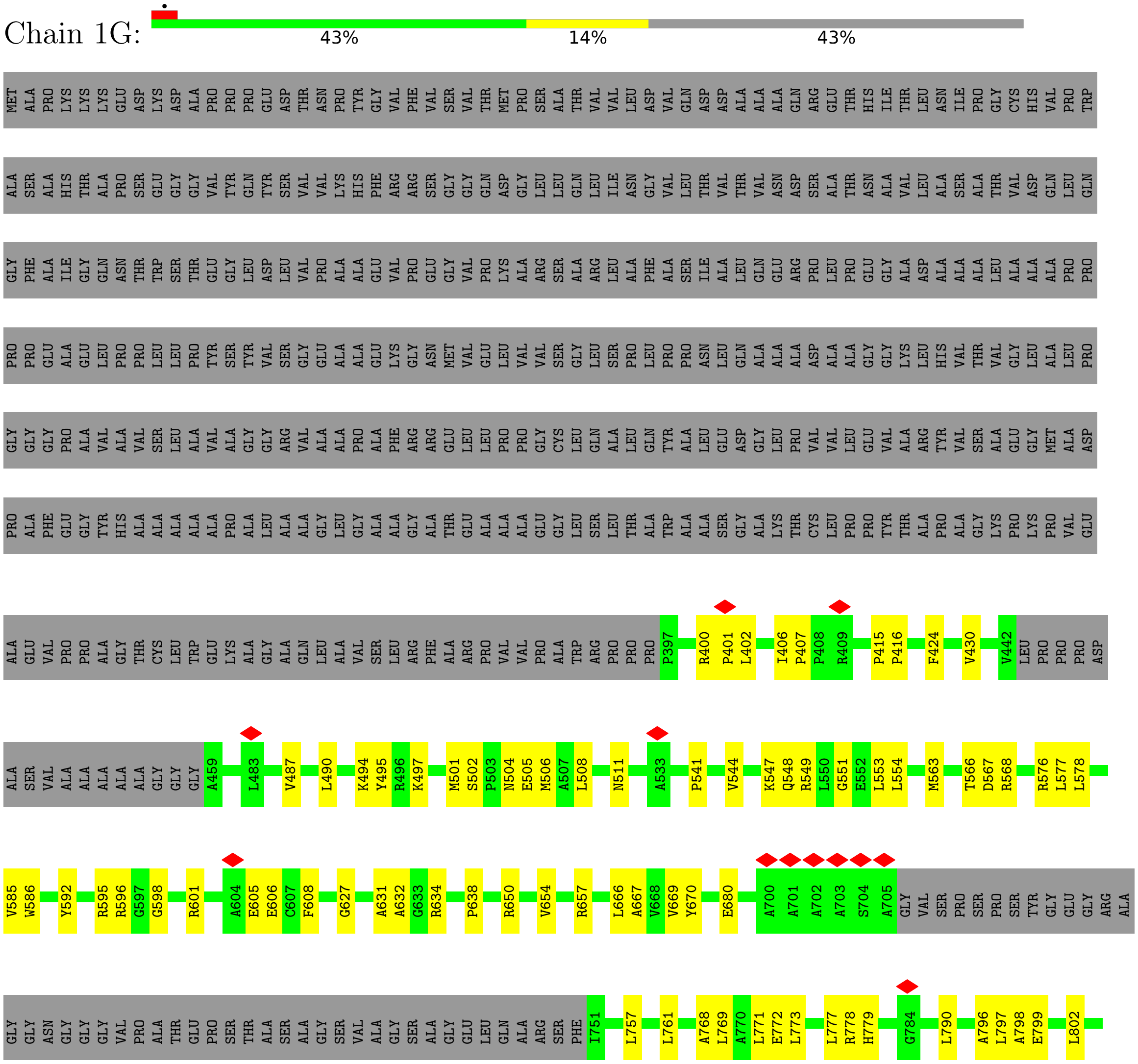
Chain 1F:

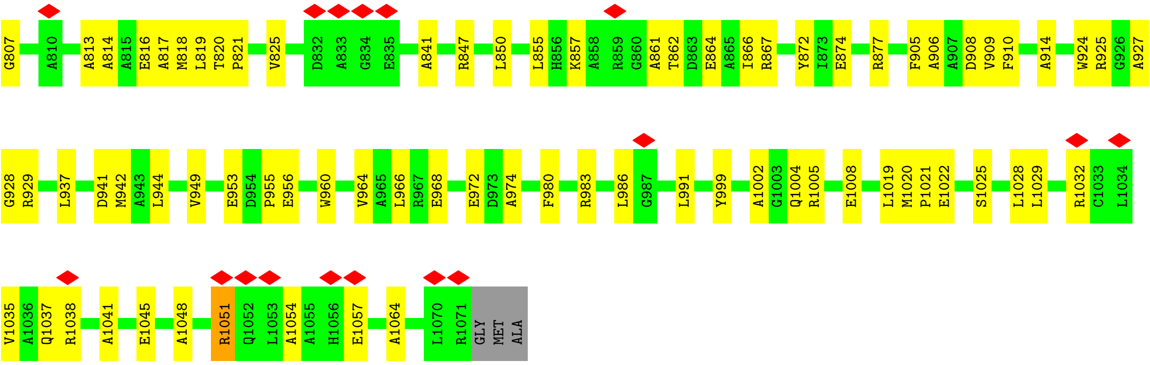






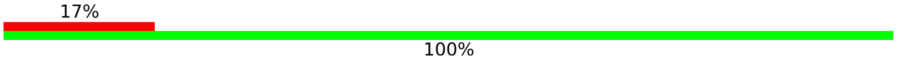
- Molecule 14: FAP70

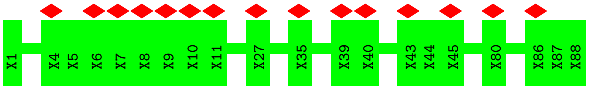




- Molecule 15: Unassigned protein-5

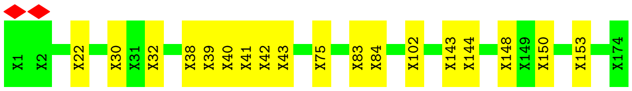
Chain 1H:





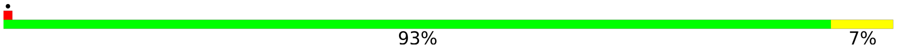
- Molecule 16: Unassigned protein-6

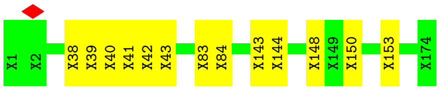
Chain 1M:



- Molecule 16: Unassigned protein-6

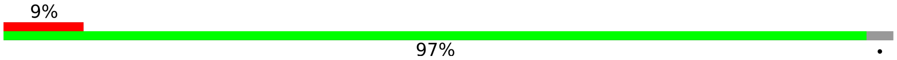
Chain 1L:

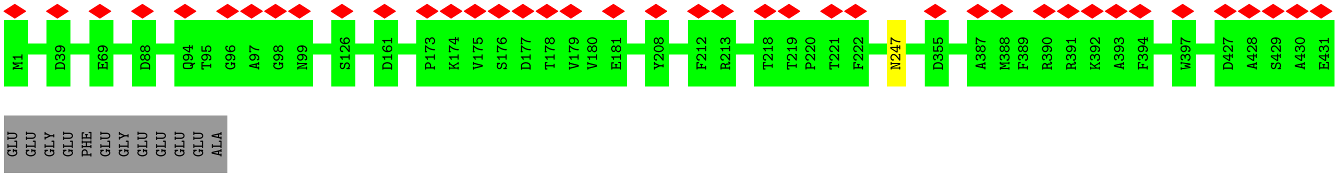




- Molecule 17: Tubulin beta

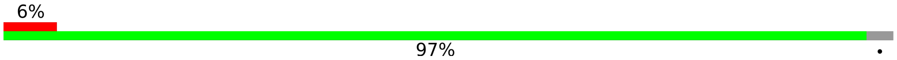
Chain 1a:

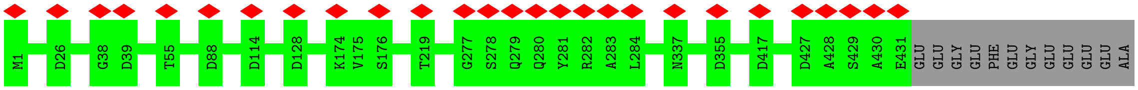




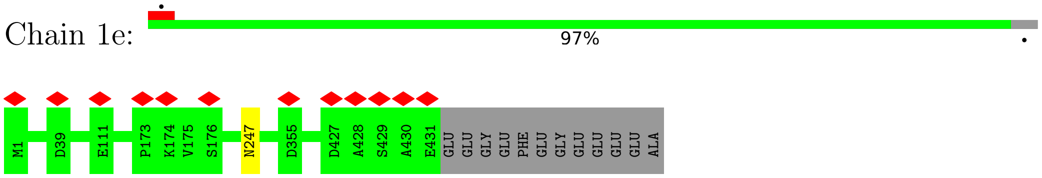
- Molecule 17: Tubulin beta

Chain 1c:

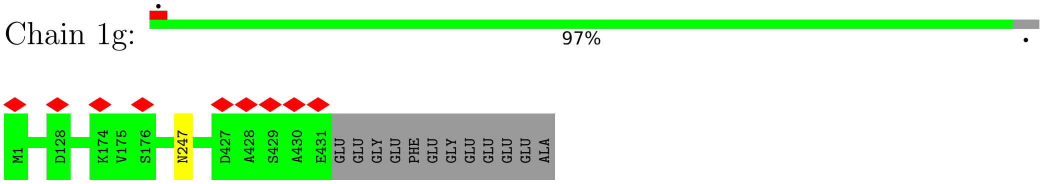




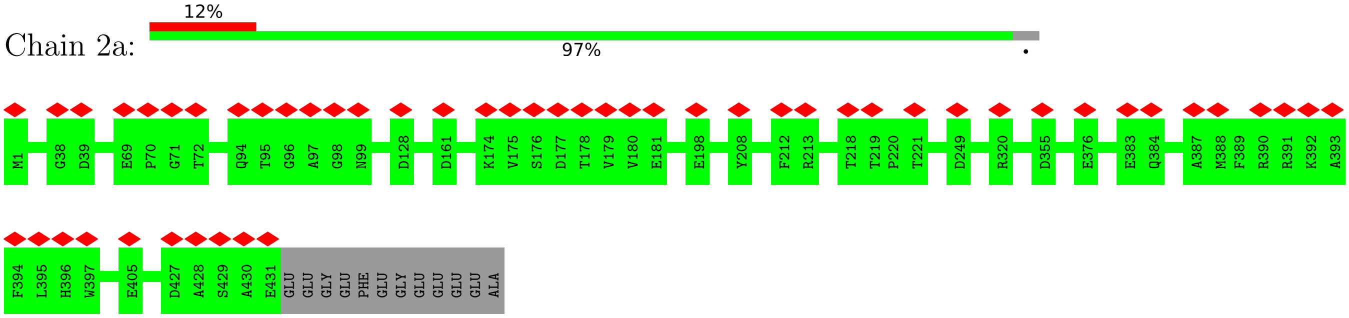
- Molecule 17: Tubulin beta



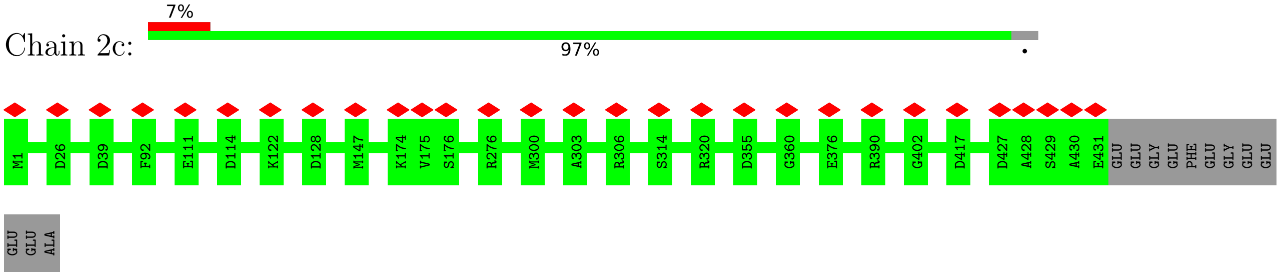
- Molecule 17: Tubulin beta



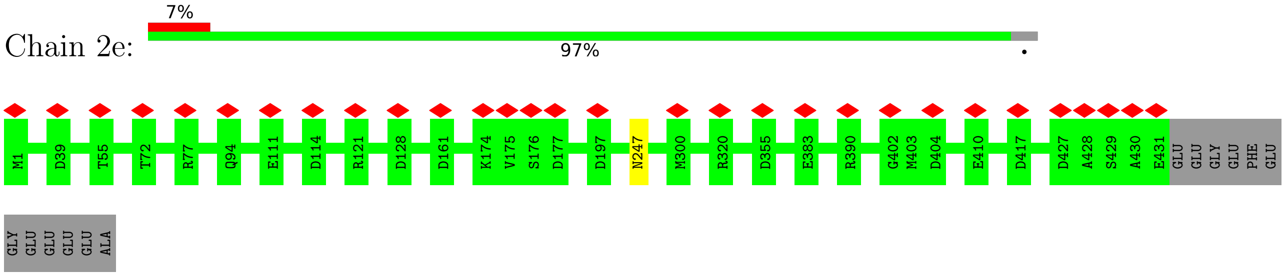
- Molecule 17: Tubulin beta



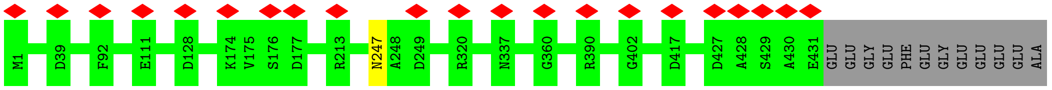
- Molecule 17: Tubulin beta



- Molecule 17: Tubulin beta

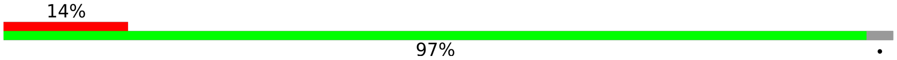


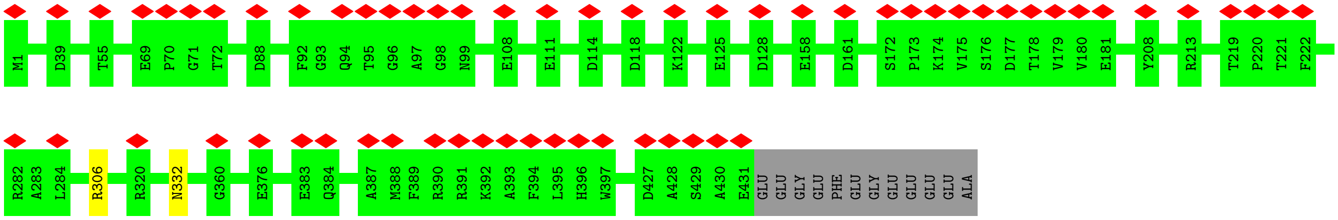
- Molecule 17: Tubulin beta



- Molecule 17: Tubulin beta

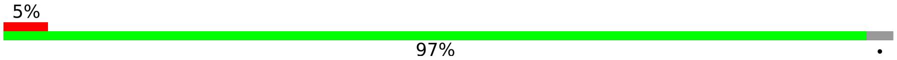
Chain 3a:

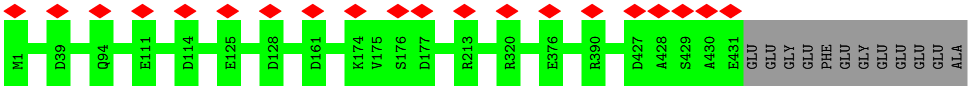




- Molecule 17: Tubulin beta

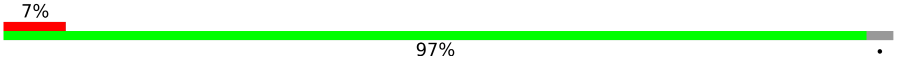
Chain 3c:

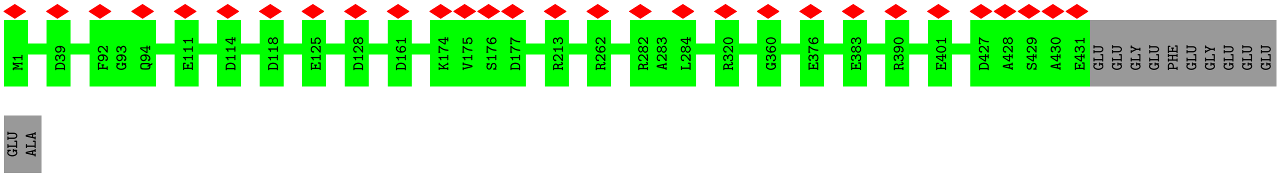




- Molecule 17: Tubulin beta

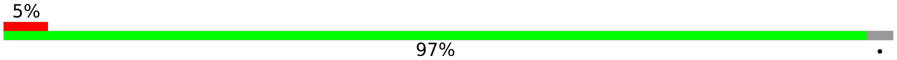
Chain 3e:

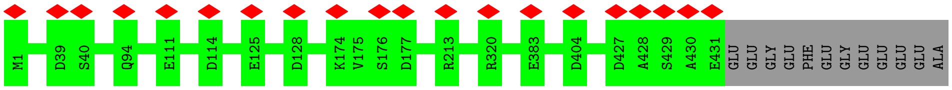




- Molecule 17: Tubulin beta

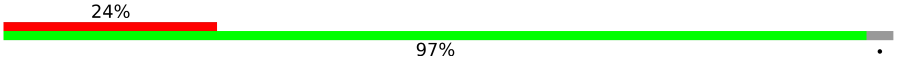
Chain 3g:

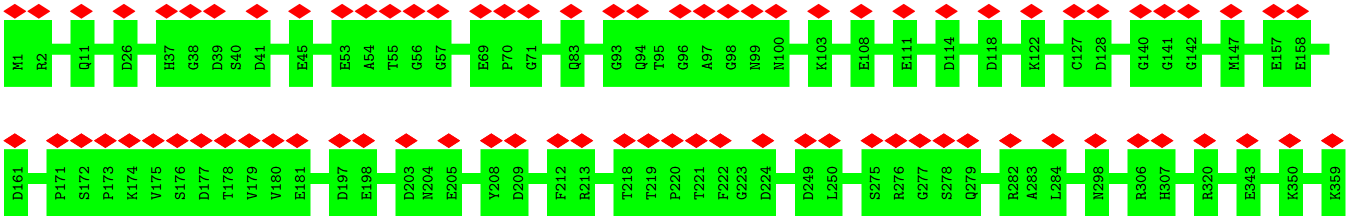


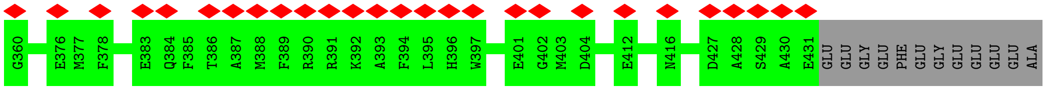


- Molecule 17: Tubulin beta

Chain 4a:

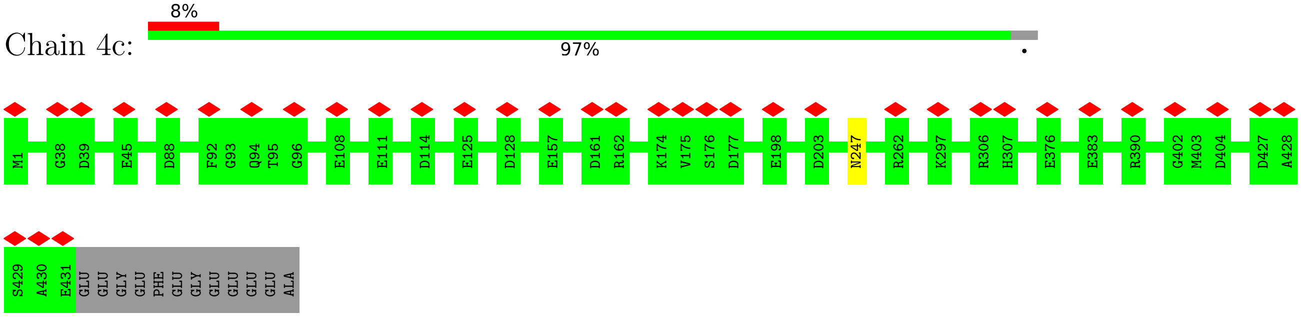






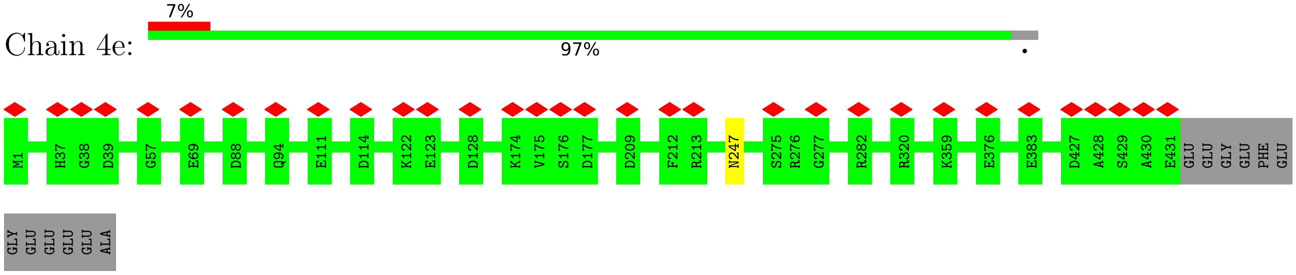
- Molecule 17: Tubulin beta

Chain 4c:



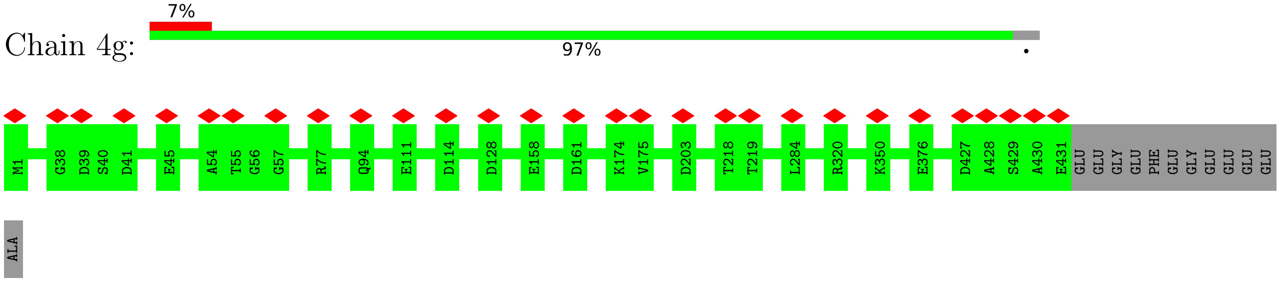
- Molecule 17: Tubulin beta

Chain 4e:



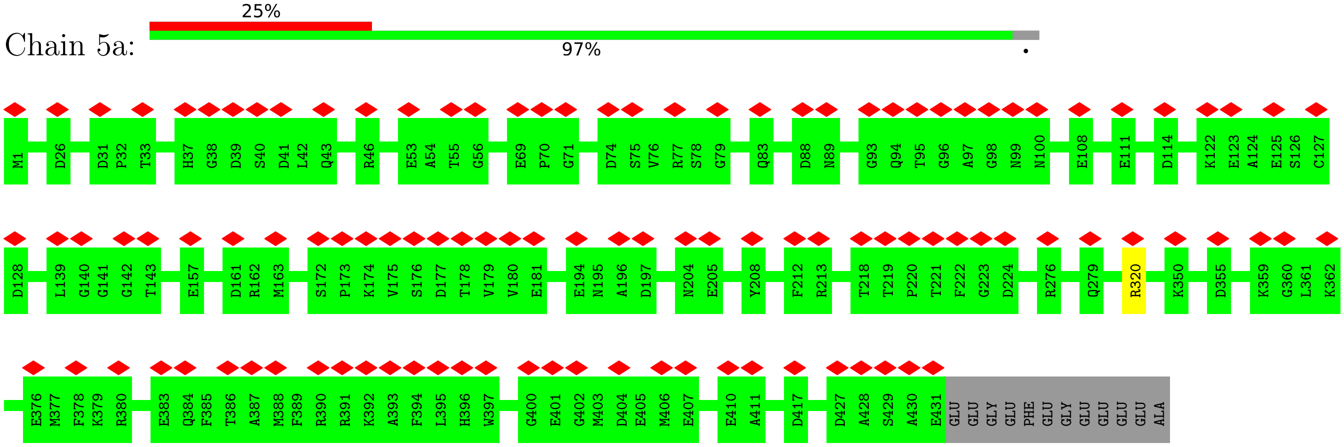
- Molecule 17: Tubulin beta

Chain 4g:



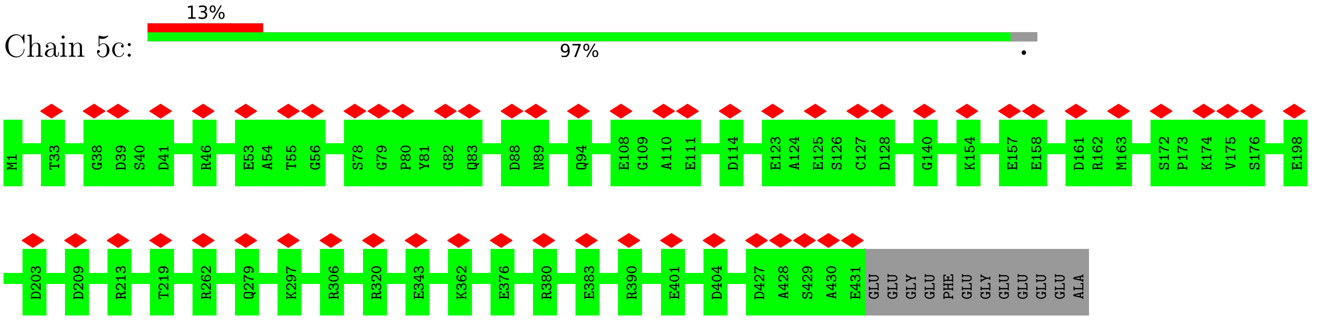
- Molecule 17: Tubulin beta

Chain 5a:



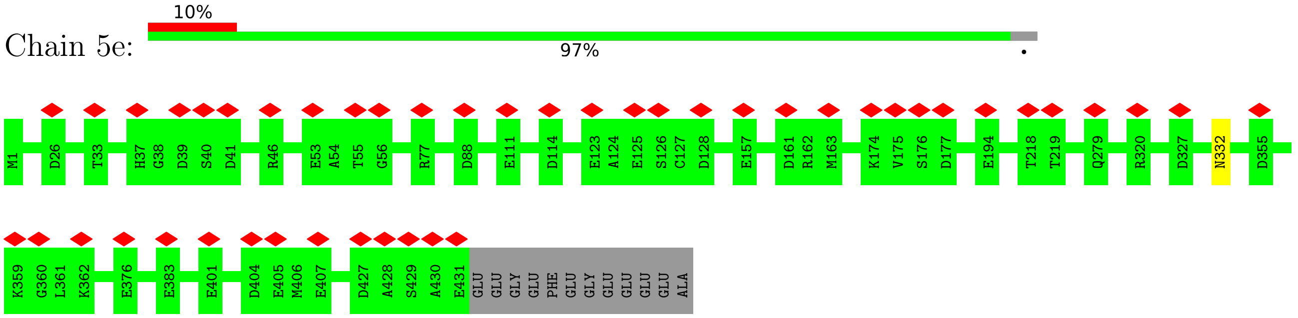
- Molecule 17: Tubulin beta

Chain 5c:



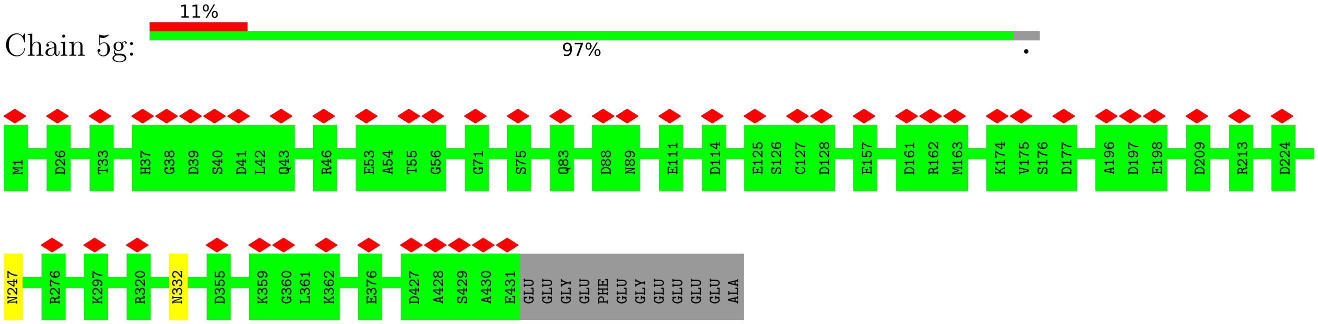
• Molecule 17: Tubulin beta

Chain 5e:



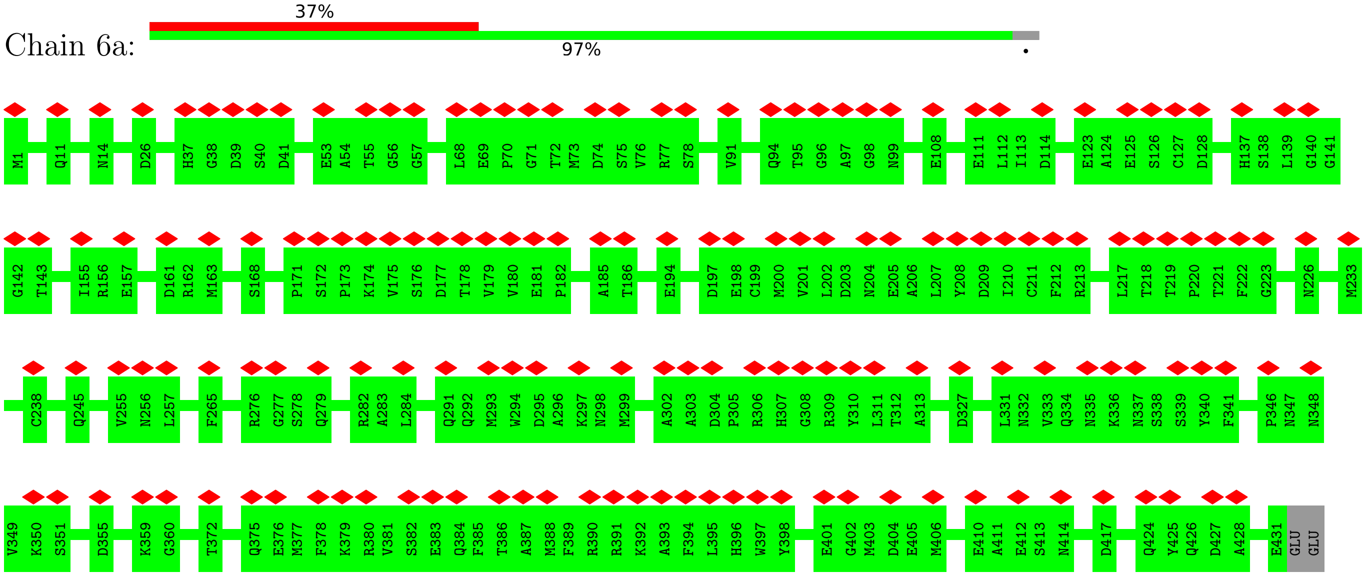
• Molecule 17: Tubulin beta

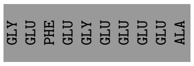
Chain 5g:



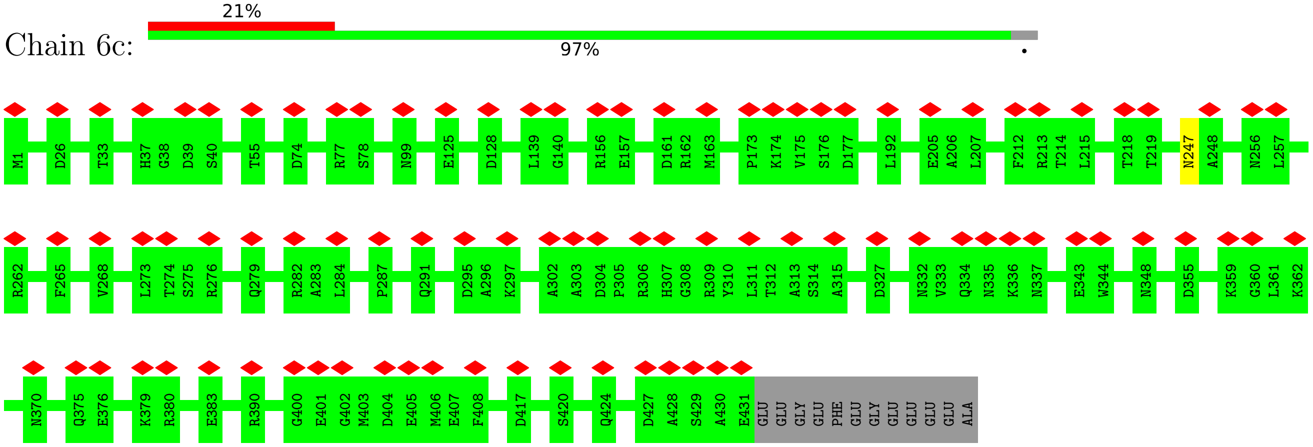
• Molecule 17: Tubulin beta

Chain 6a:

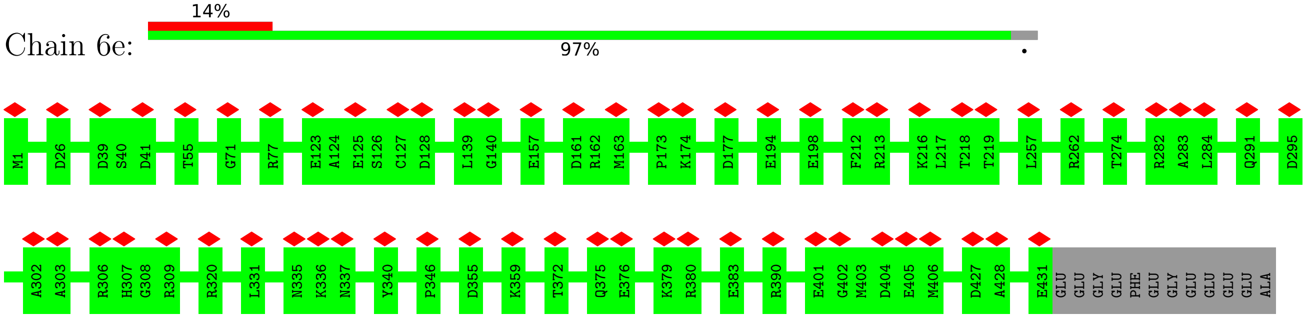




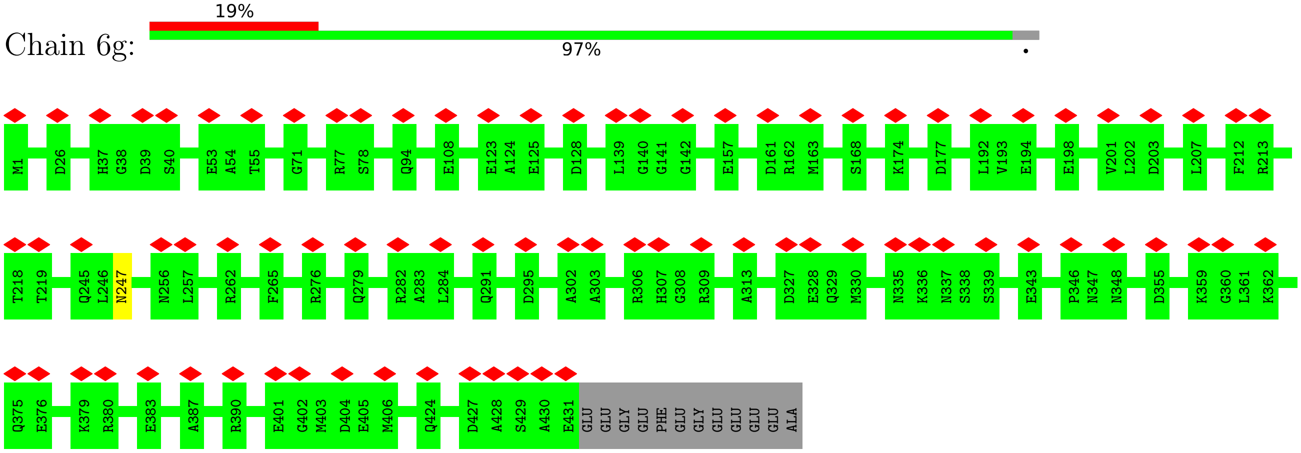
- Molecule 17: Tubulin beta



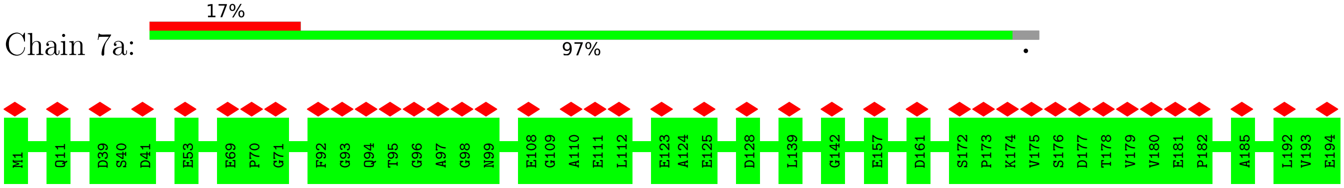
- Molecule 17: Tubulin beta

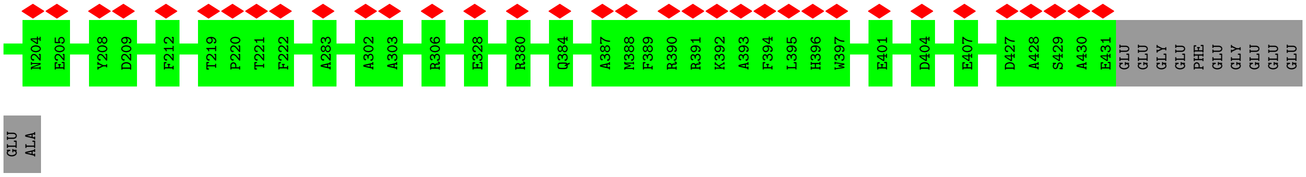


- Molecule 17: Tubulin beta



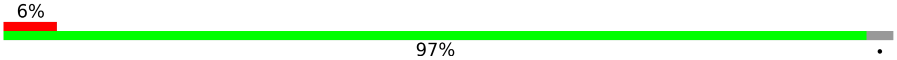
- Molecule 17: Tubulin beta

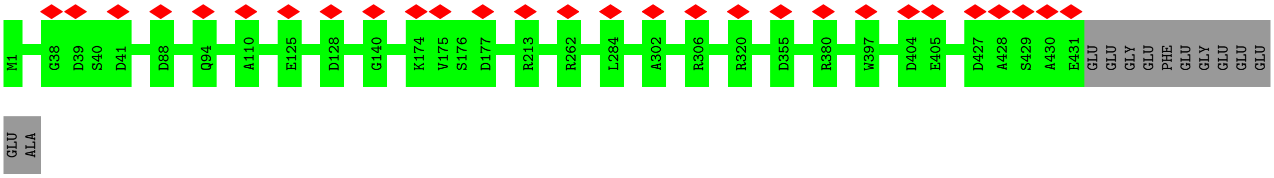




- Molecule 17: Tubulin beta

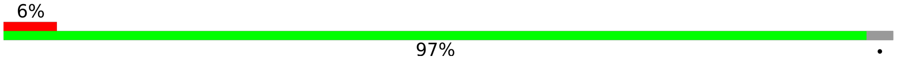
Chain 7c:

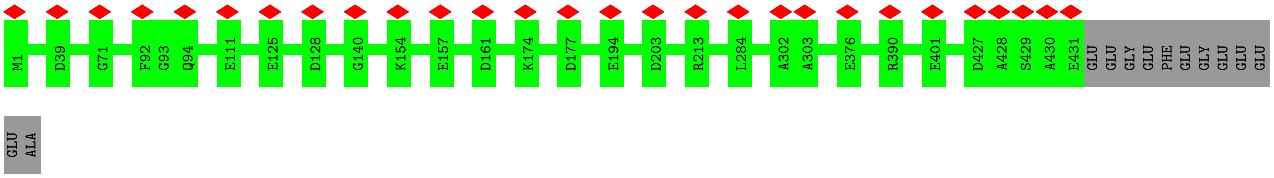




- Molecule 17: Tubulin beta

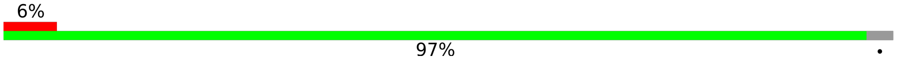
Chain 7e:

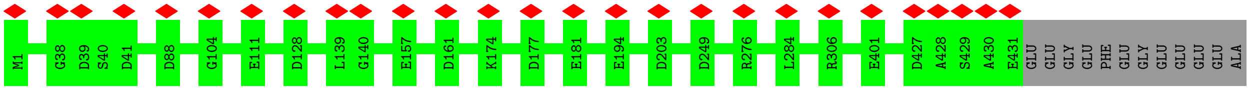




- Molecule 17: Tubulin beta

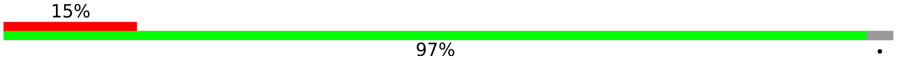
Chain 7g:

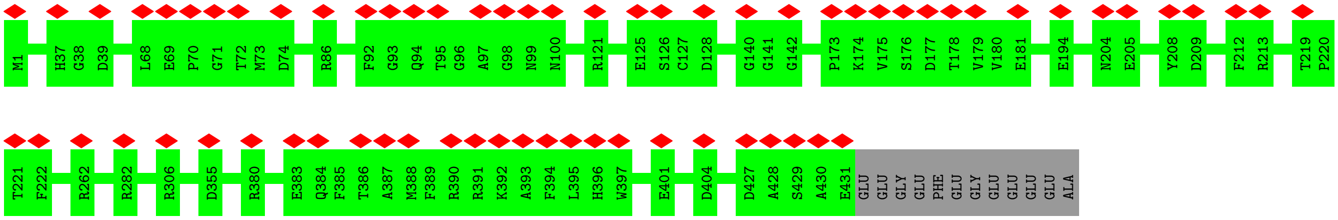




- Molecule 17: Tubulin beta

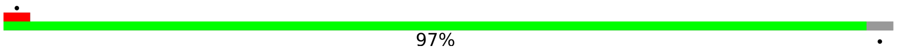
Chain 8a:

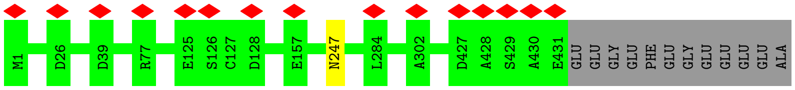




- Molecule 17: Tubulin beta

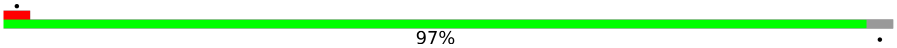
Chain 8c:

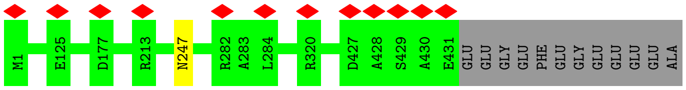




- Molecule 17: Tubulin beta

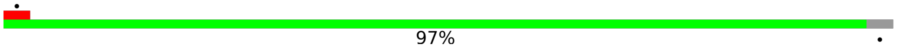
Chain 8e:

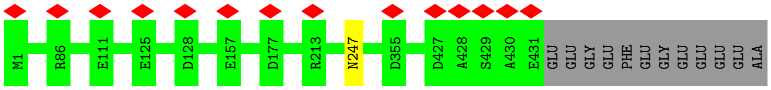




- Molecule 17: Tubulin beta

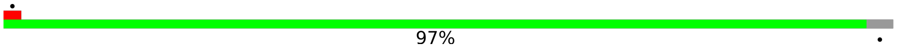
Chain 8g:

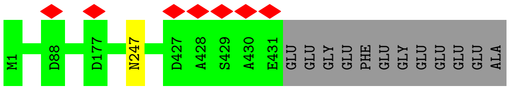




- Molecule 17: Tubulin beta

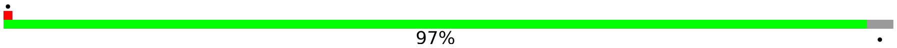
Chain 9a:

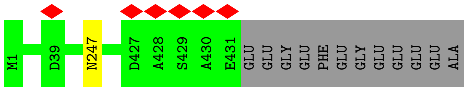




- Molecule 17: Tubulin beta

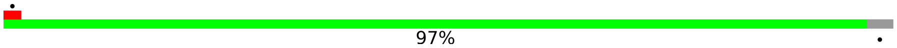
Chain 9c:

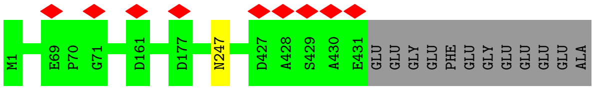




- Molecule 17: Tubulin beta

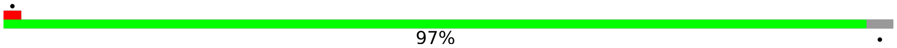
Chain 9e:

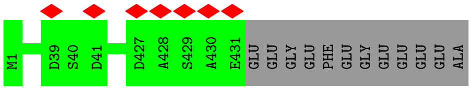




- Molecule 17: Tubulin beta

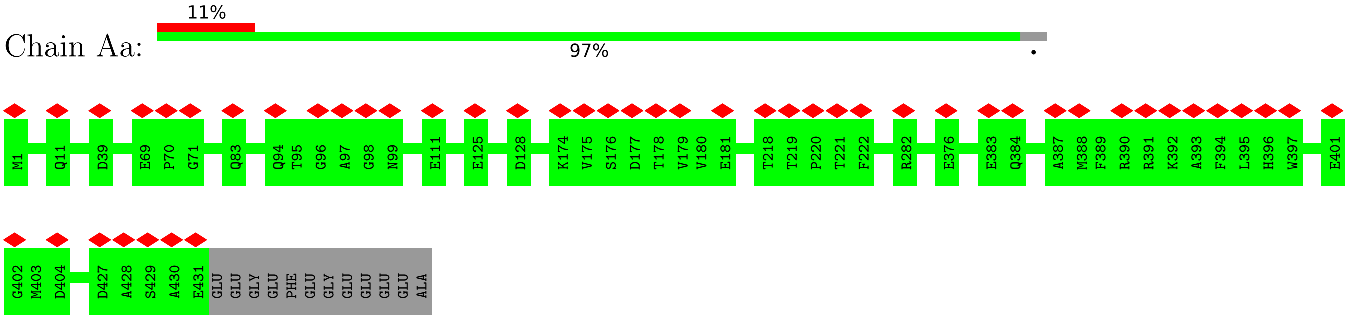
Chain 9g:





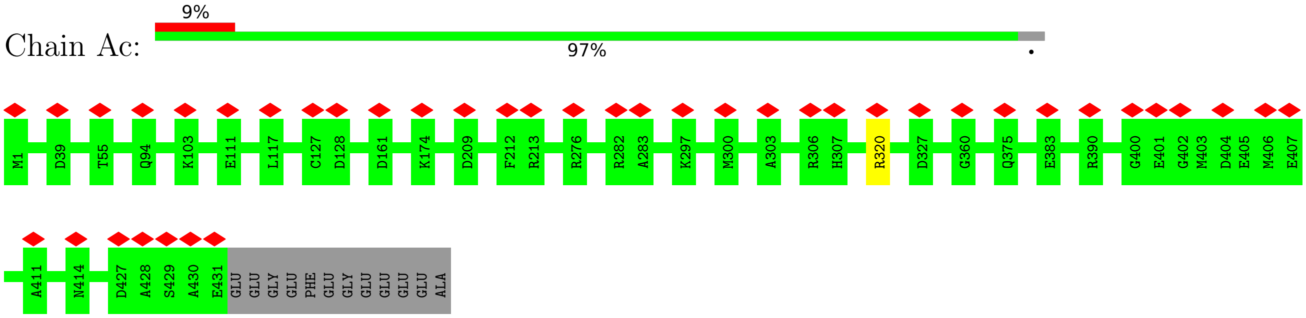
- Molecule 17: Tubulin beta

Chain Aa:



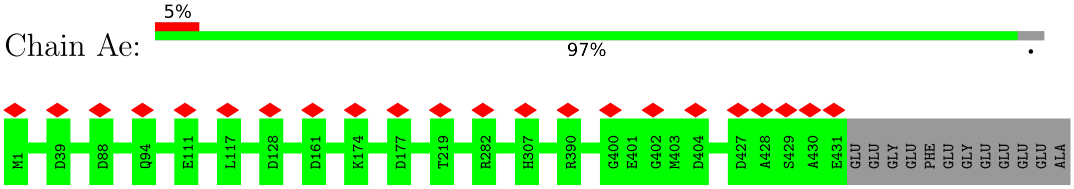
- Molecule 17: Tubulin beta

Chain Ac:



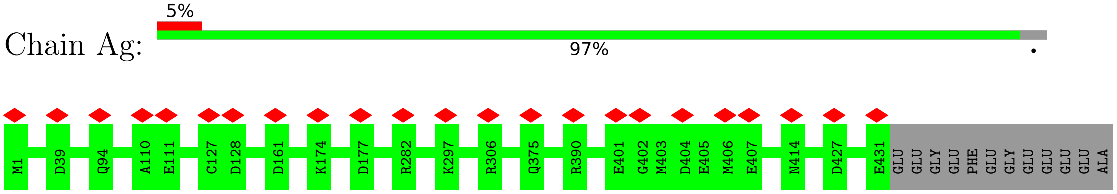
- Molecule 17: Tubulin beta

Chain Ae:



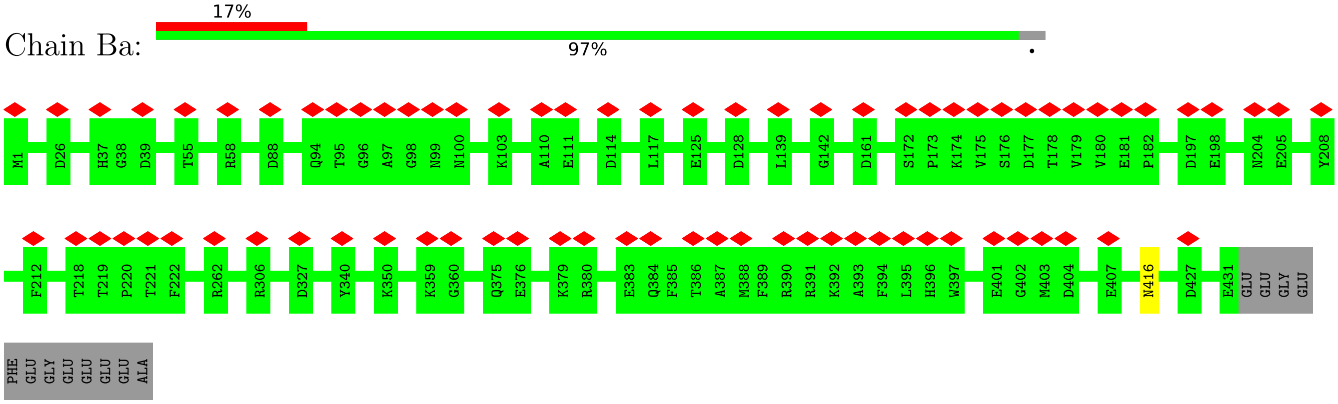
- Molecule 17: Tubulin beta

Chain Ag:

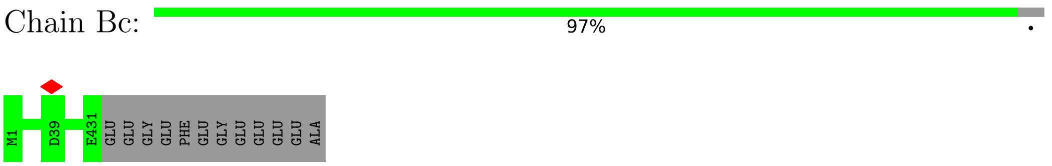


- Molecule 17: Tubulin beta

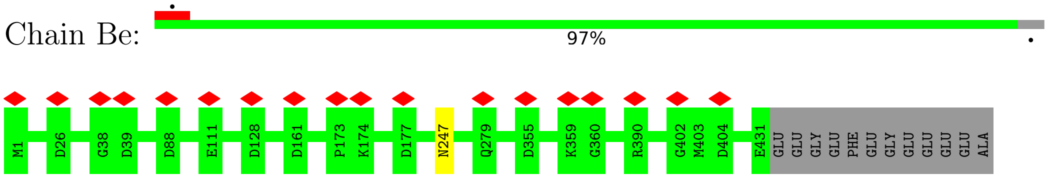
Chain Ba:



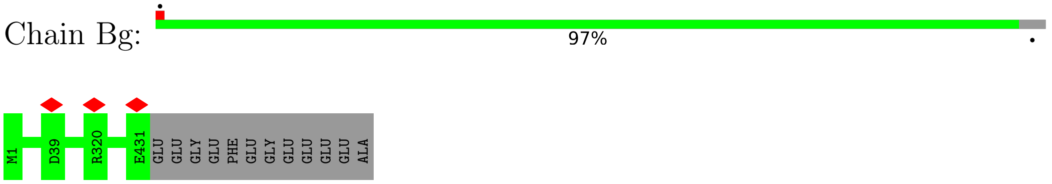
- Molecule 17: Tubulin beta



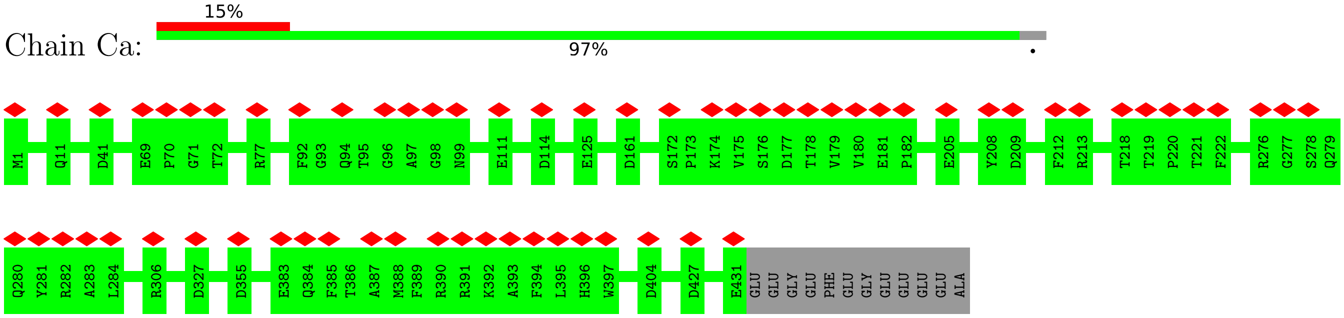
- Molecule 17: Tubulin beta



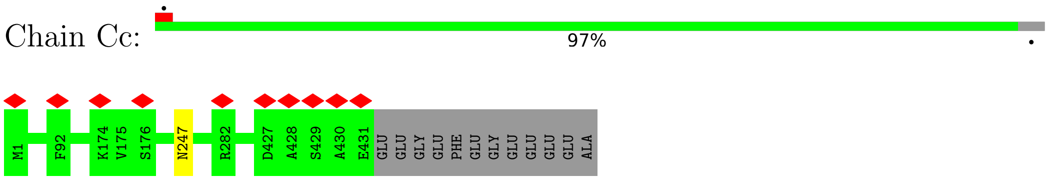
- Molecule 17: Tubulin beta



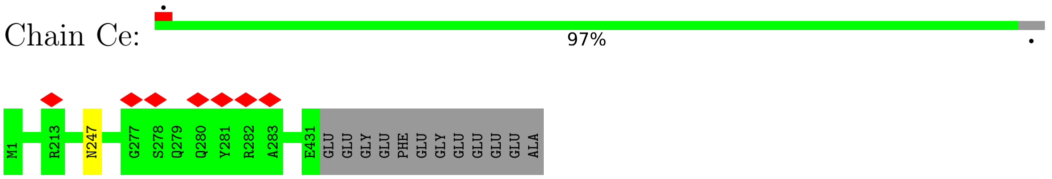
- Molecule 17: Tubulin beta



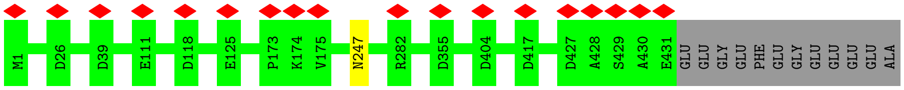
- Molecule 17: Tubulin beta



- Molecule 17: Tubulin beta

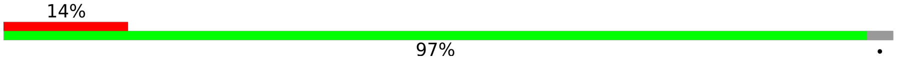


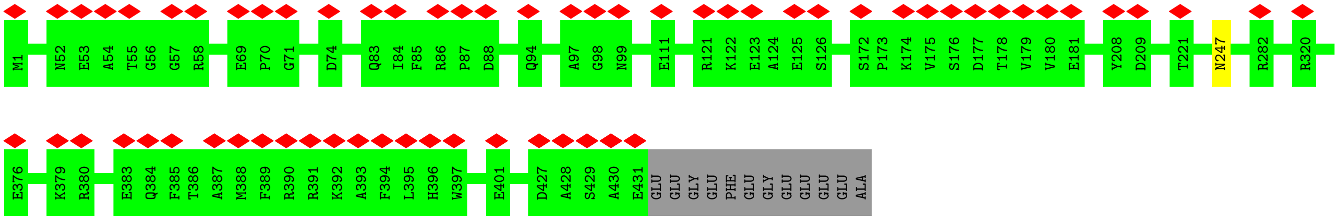
- Molecule 17: Tubulin beta



- Molecule 17: Tubulin beta

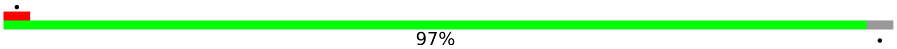
Chain Da:

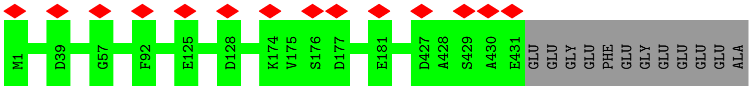




- Molecule 17: Tubulin beta

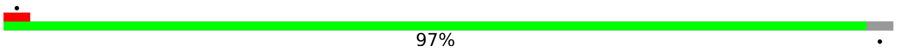
Chain Dc:

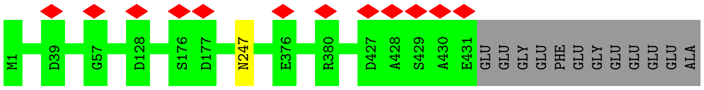




- Molecule 17: Tubulin beta

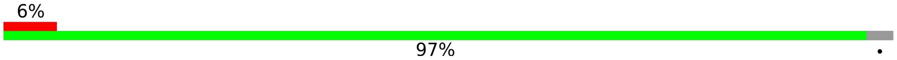
Chain De:

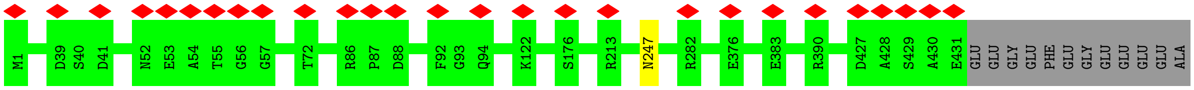




- Molecule 17: Tubulin beta

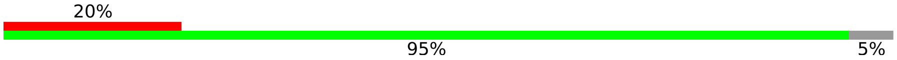
Chain Dg:

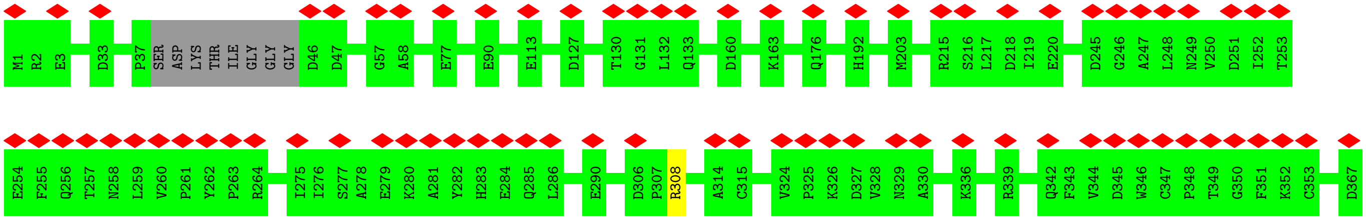


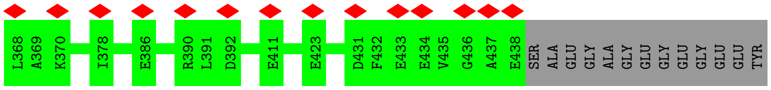


- Molecule 18: Tubulin alpha

Chain 1b:

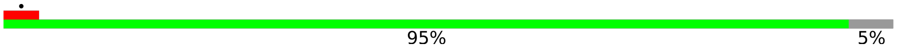


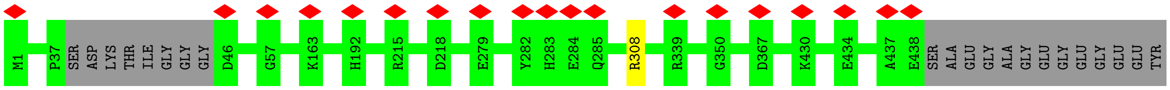




- Molecule 18: Tubulin alpha

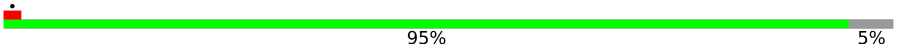
Chain 1d:

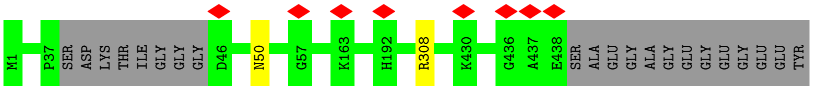




- Molecule 18: Tubulin alpha

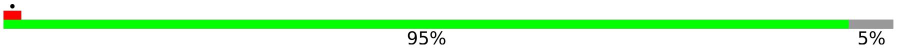
Chain 1f:

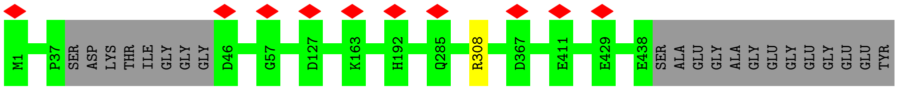




- Molecule 18: Tubulin alpha

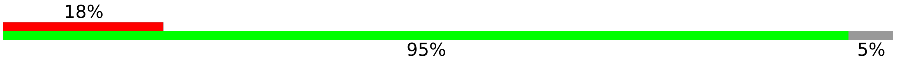
Chain 1h:

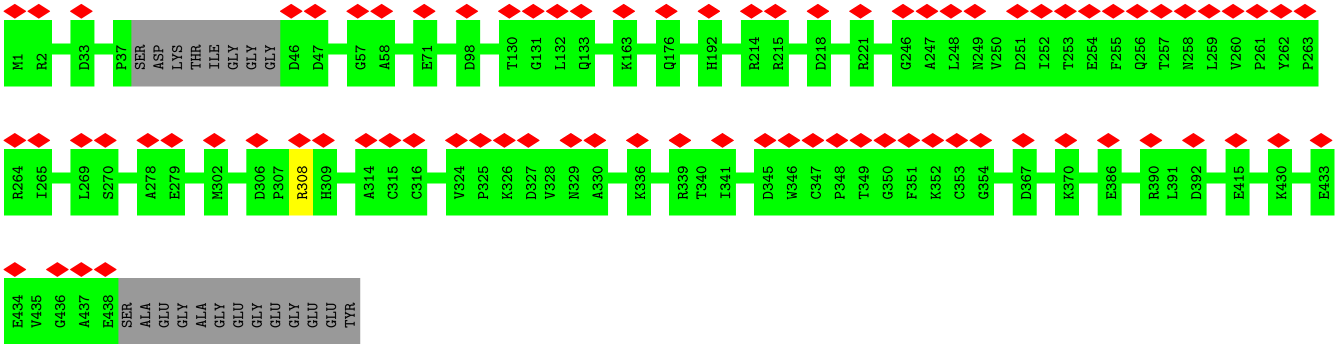




- Molecule 18: Tubulin alpha

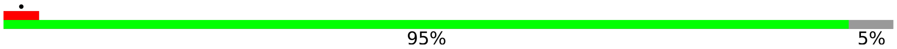
Chain 2b:

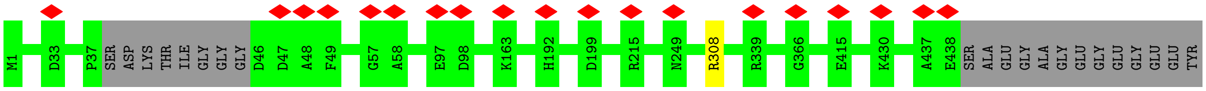




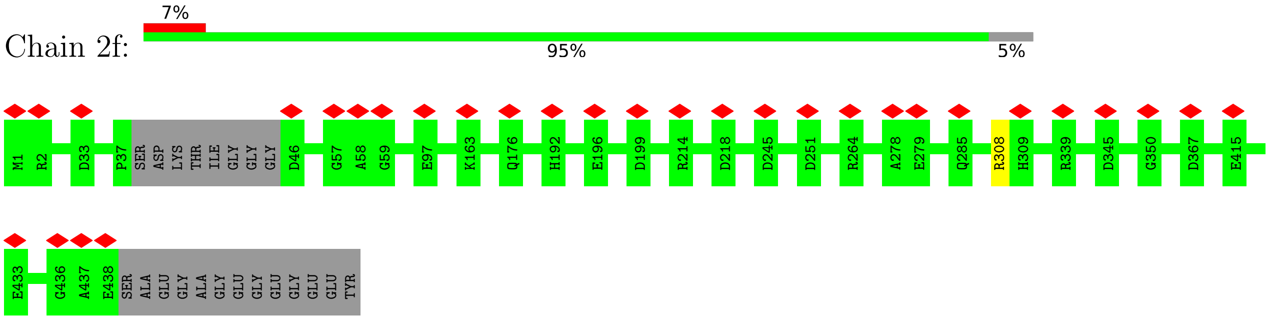
- Molecule 18: Tubulin alpha

Chain 2d:

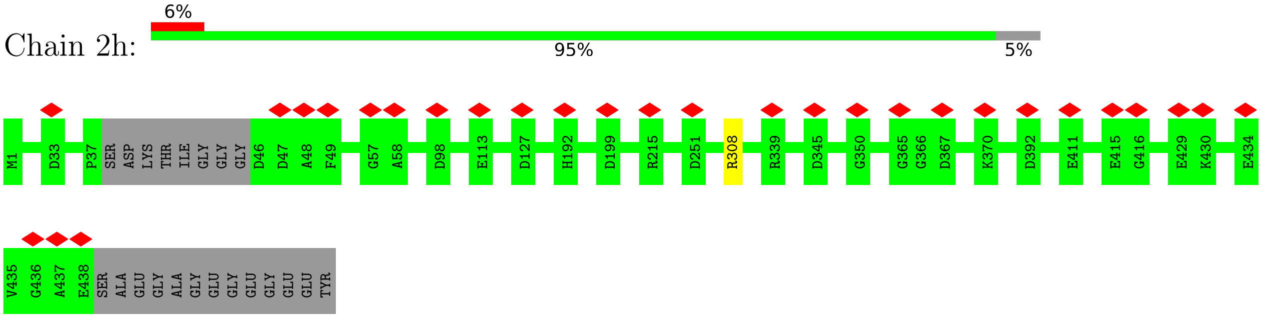




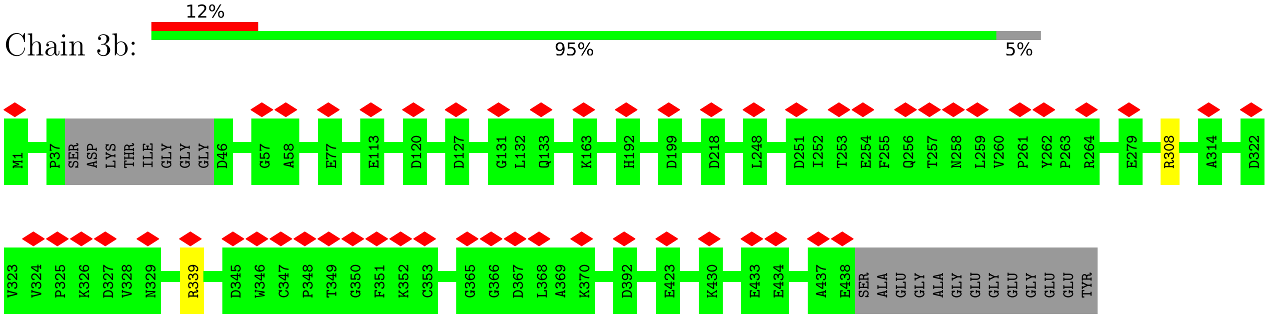
- Molecule 18: Tubulin alpha



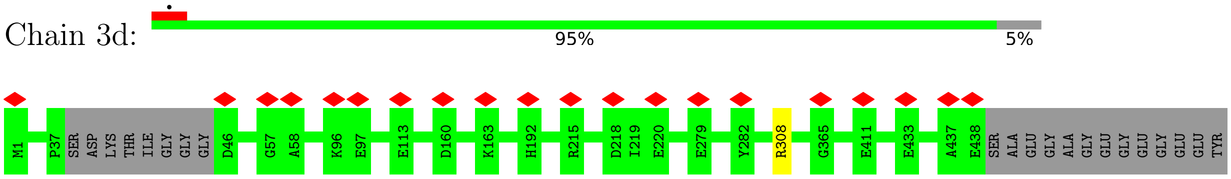
- Molecule 18: Tubulin alpha



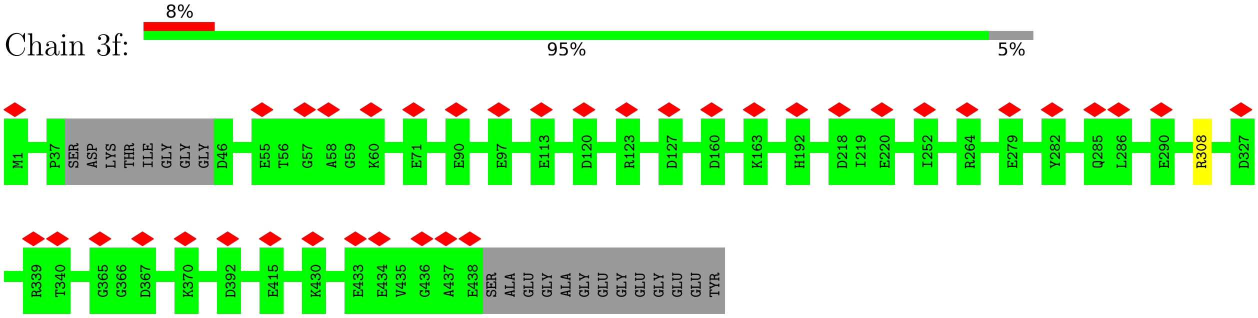
- Molecule 18: Tubulin alpha



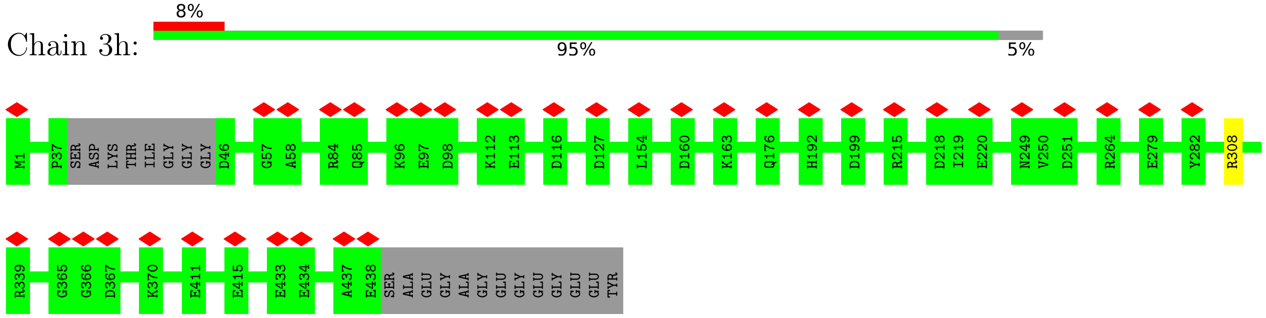
- Molecule 18: Tubulin alpha



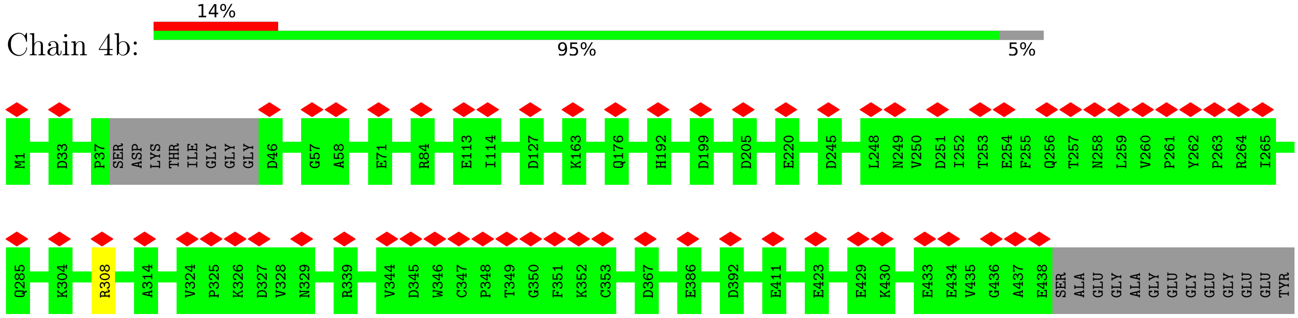
- Molecule 18: Tubulin alpha



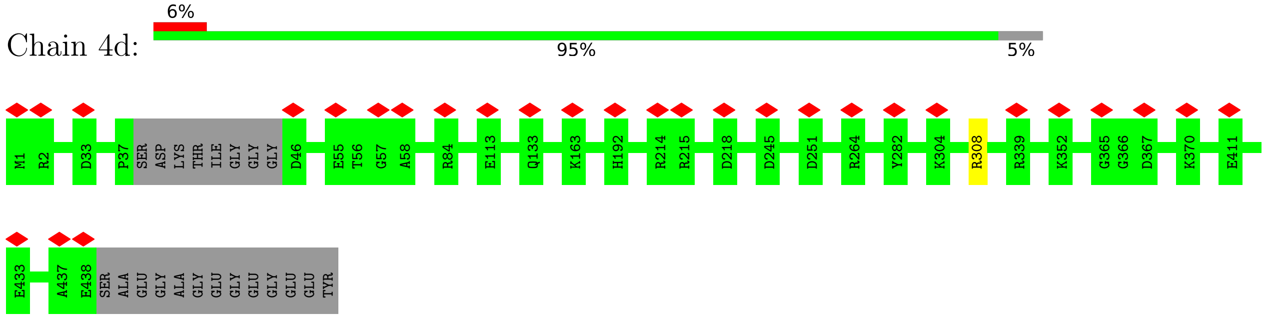
- Molecule 18: Tubulin alpha



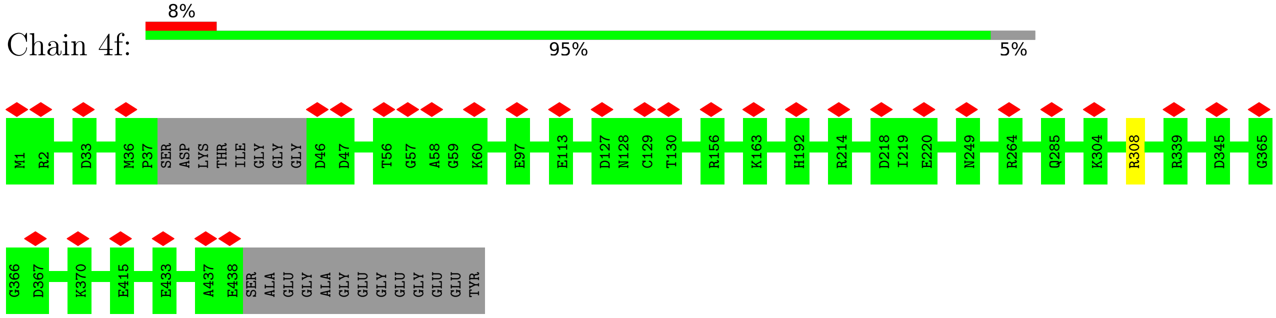
- Molecule 18: Tubulin alpha



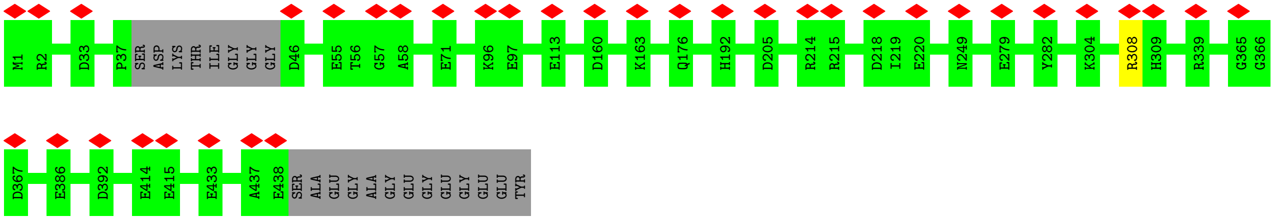
- Molecule 18: Tubulin alpha



- Molecule 18: Tubulin alpha

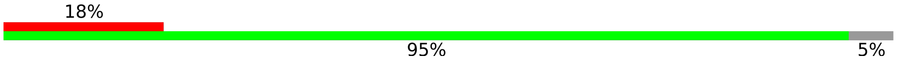


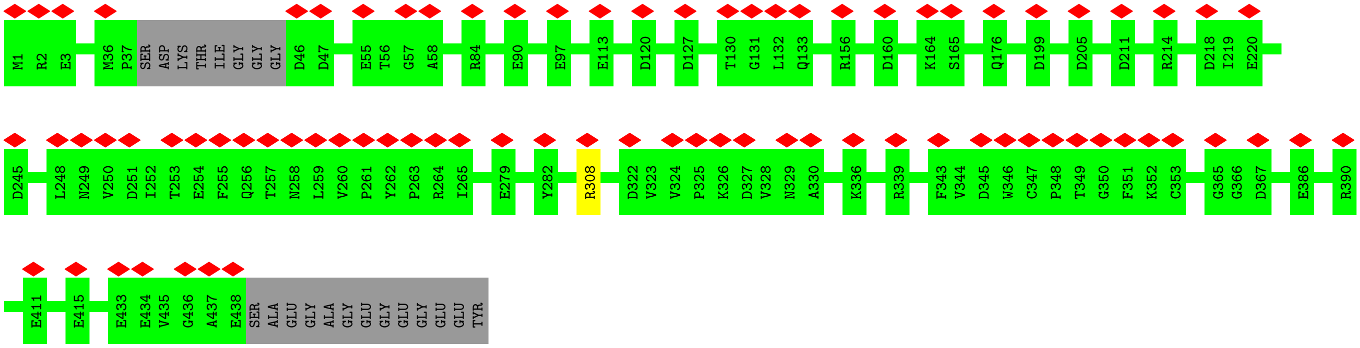
- Molecule 18: Tubulin alpha



- Molecule 18: Tubulin alpha

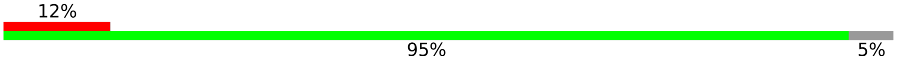
Chain 5b:

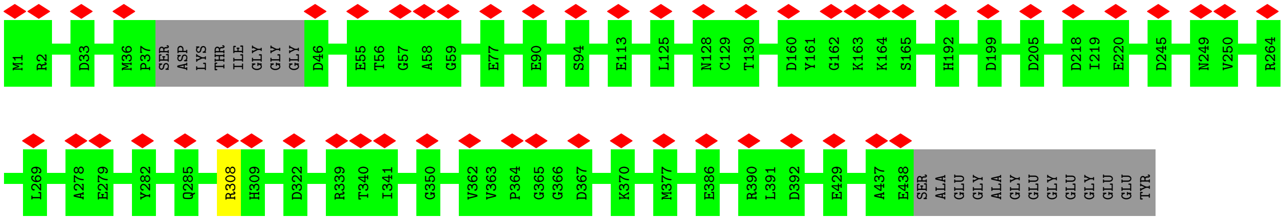




- Molecule 18: Tubulin alpha

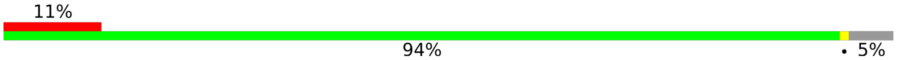
Chain 5d:

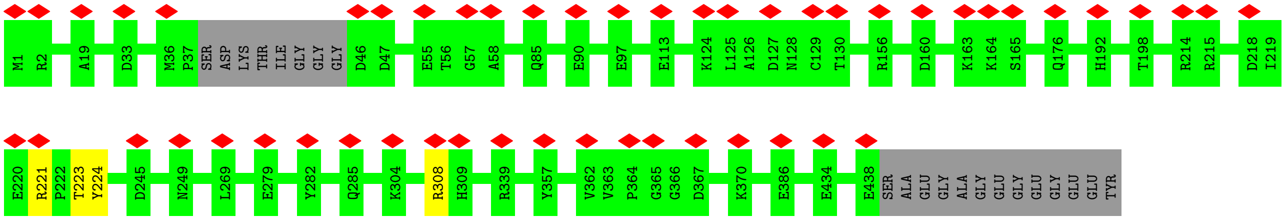




- Molecule 18: Tubulin alpha

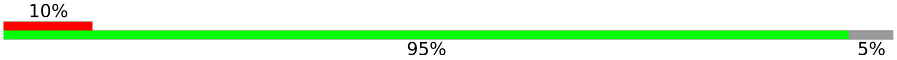
Chain 5f:

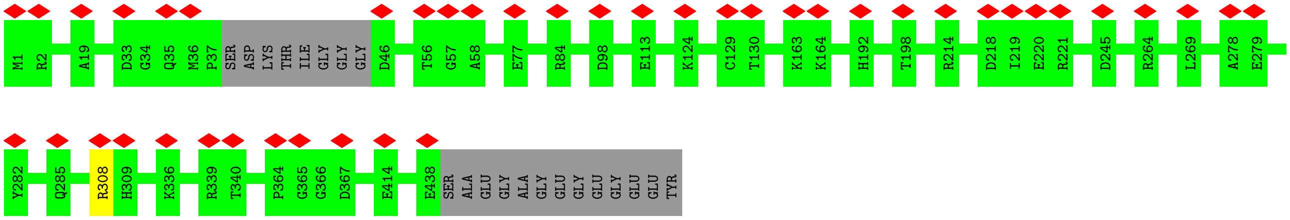




- Molecule 18: Tubulin alpha

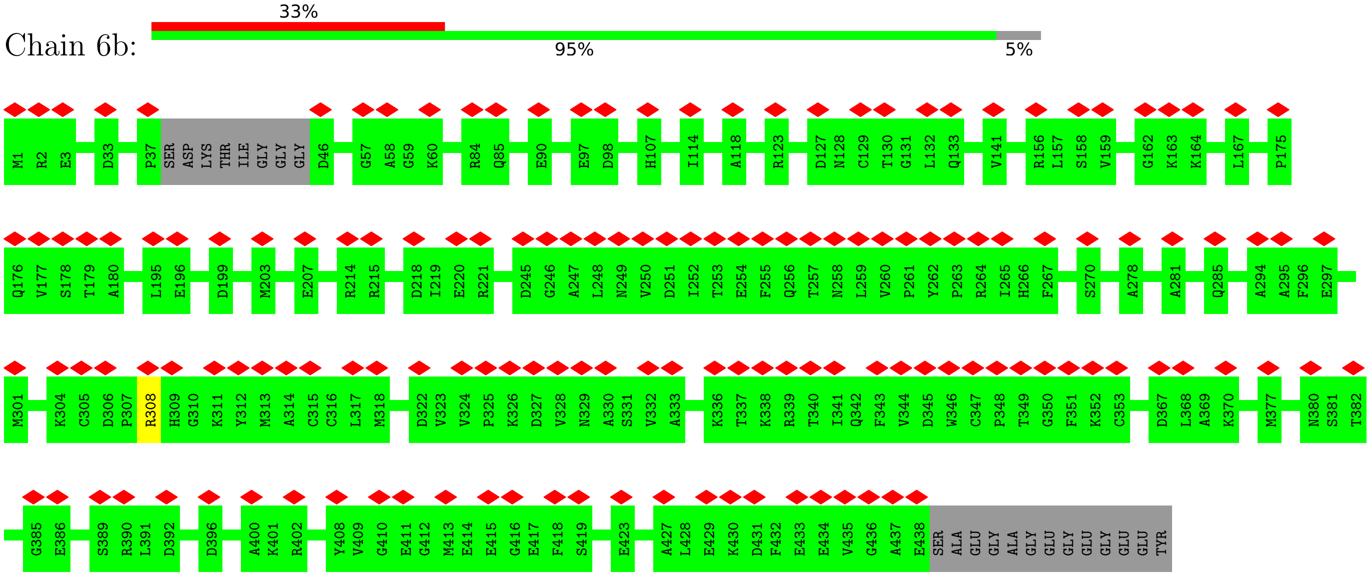
Chain 5h:





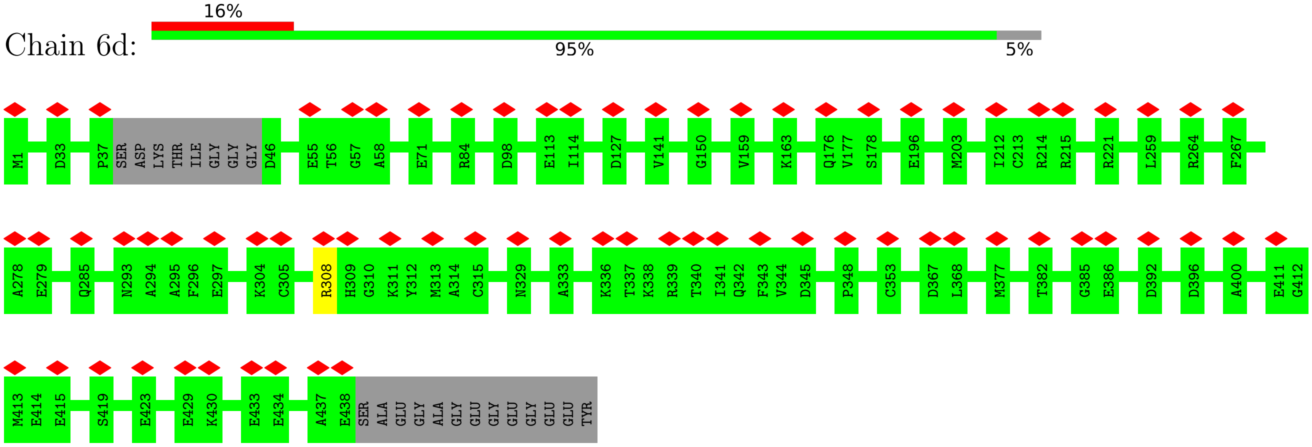
- Molecule 18: Tubulin alpha

Chain 6b:



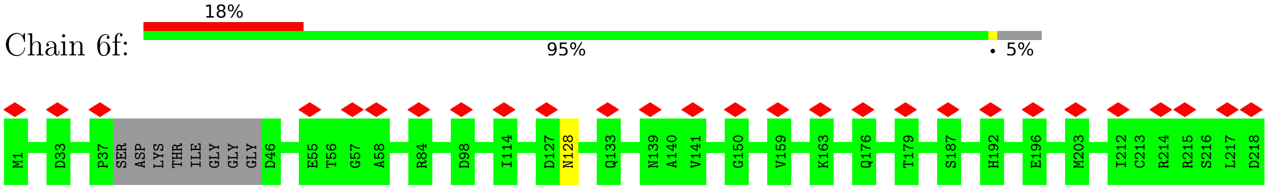
- Molecule 18: Tubulin alpha

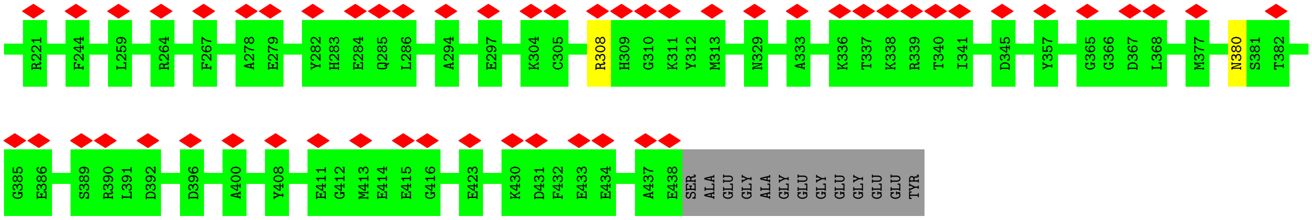
Chain 6d:



- Molecule 18: Tubulin alpha

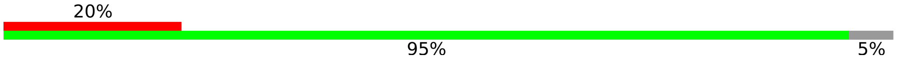
Chain 6f:

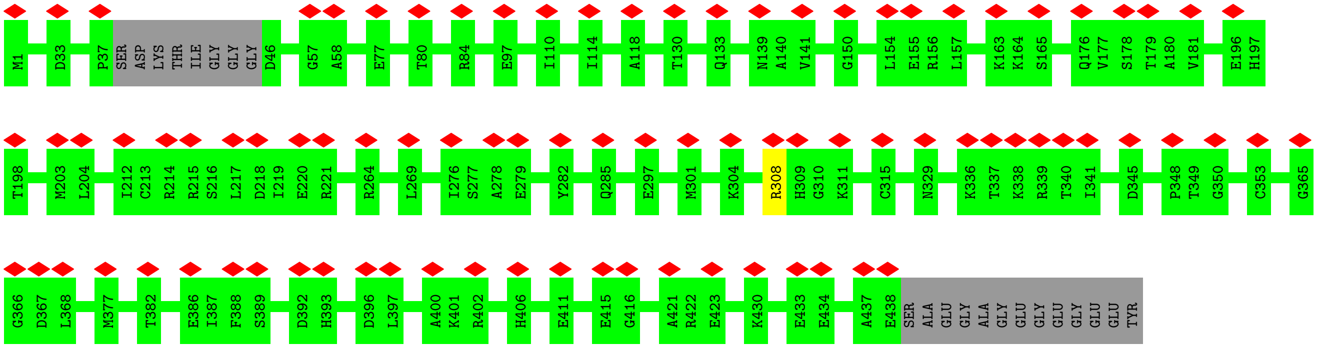




- Molecule 18: Tubulin alpha

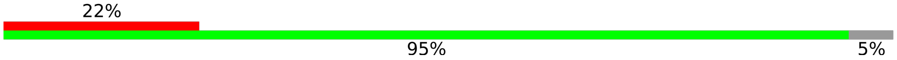
Chain 6h:

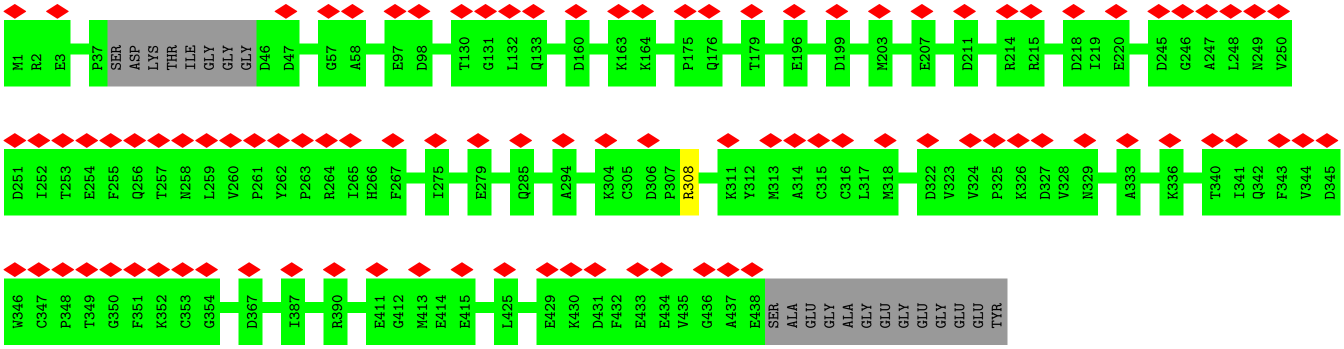




- Molecule 18: Tubulin alpha

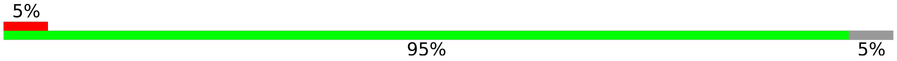
Chain 7b:

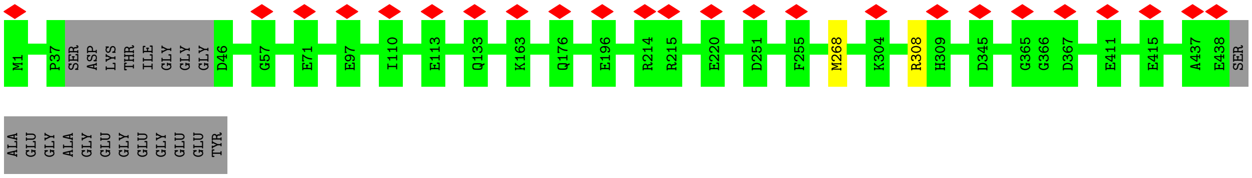




- Molecule 18: Tubulin alpha

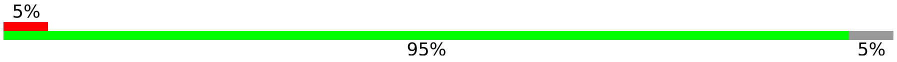
Chain 7d:

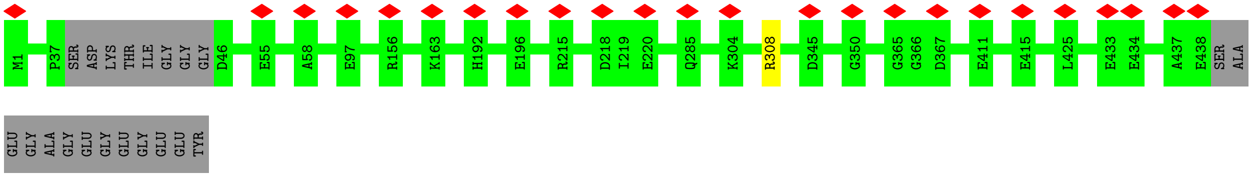




- Molecule 18: Tubulin alpha

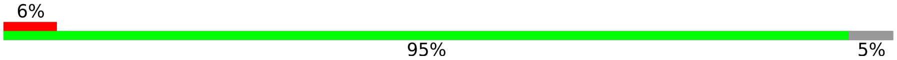
Chain 7f:

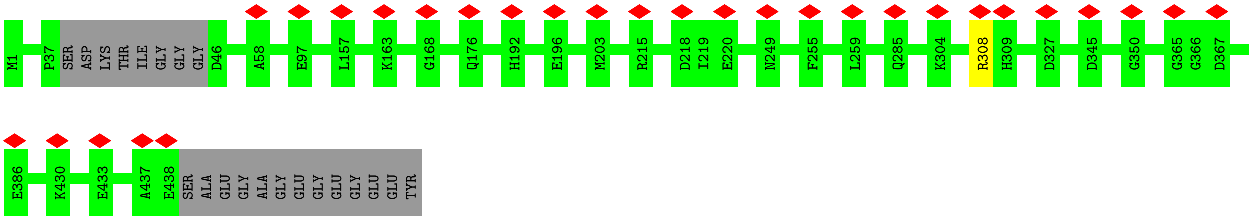




- Molecule 18: Tubulin alpha

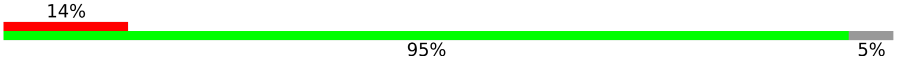
Chain 7h:

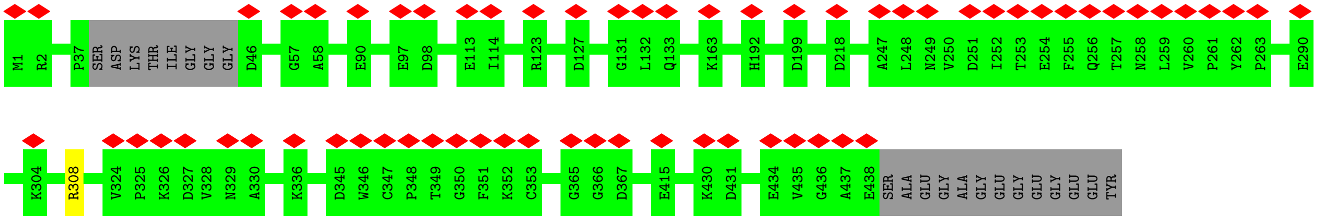




- Molecule 18: Tubulin alpha

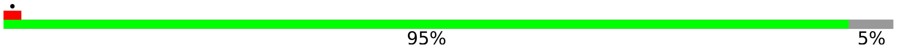
Chain 8b:

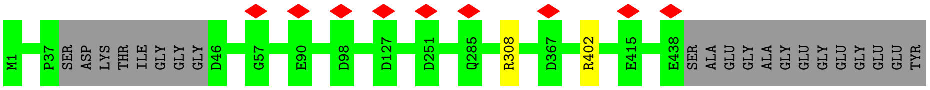




- Molecule 18: Tubulin alpha

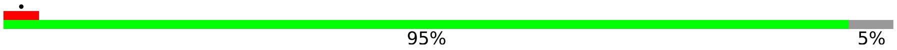
Chain 8d:

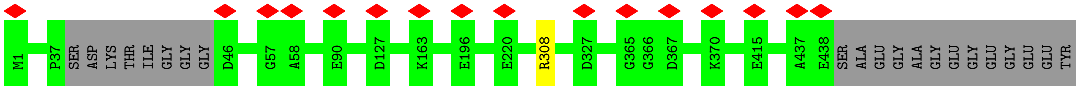




- Molecule 18: Tubulin alpha

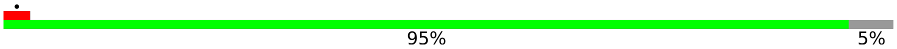
Chain 8f:

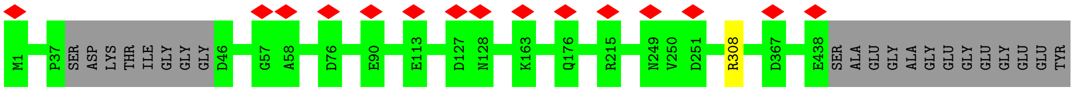




- Molecule 18: Tubulin alpha

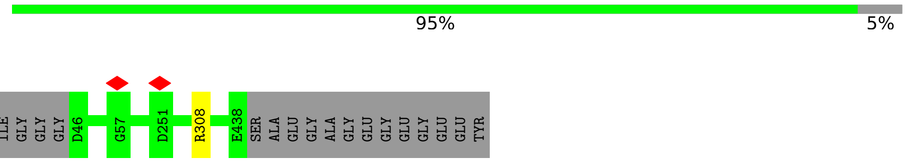
Chain 8h:





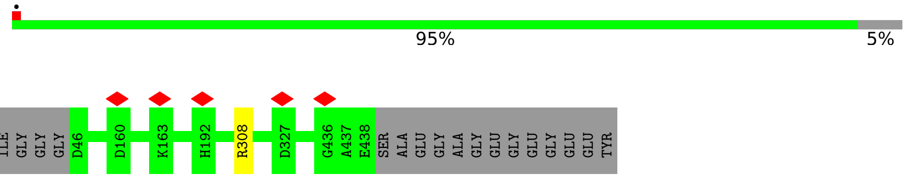
- Molecule 18: Tubulin alpha

Chain 9b:



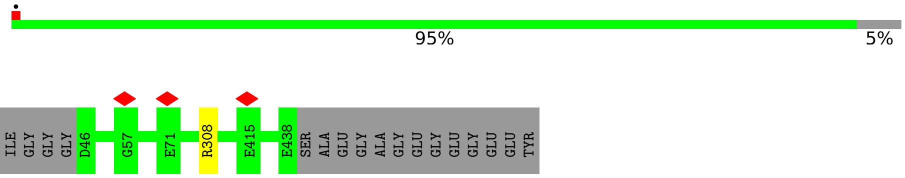
- Molecule 18: Tubulin alpha

Chain 9d:



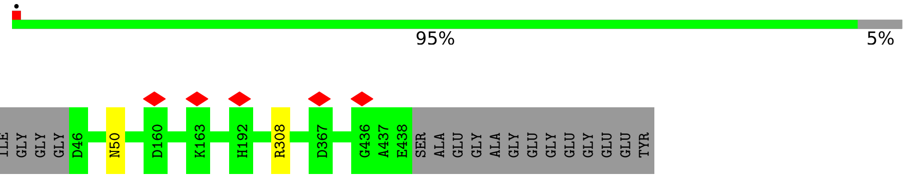
- Molecule 18: Tubulin alpha

Chain 9f:



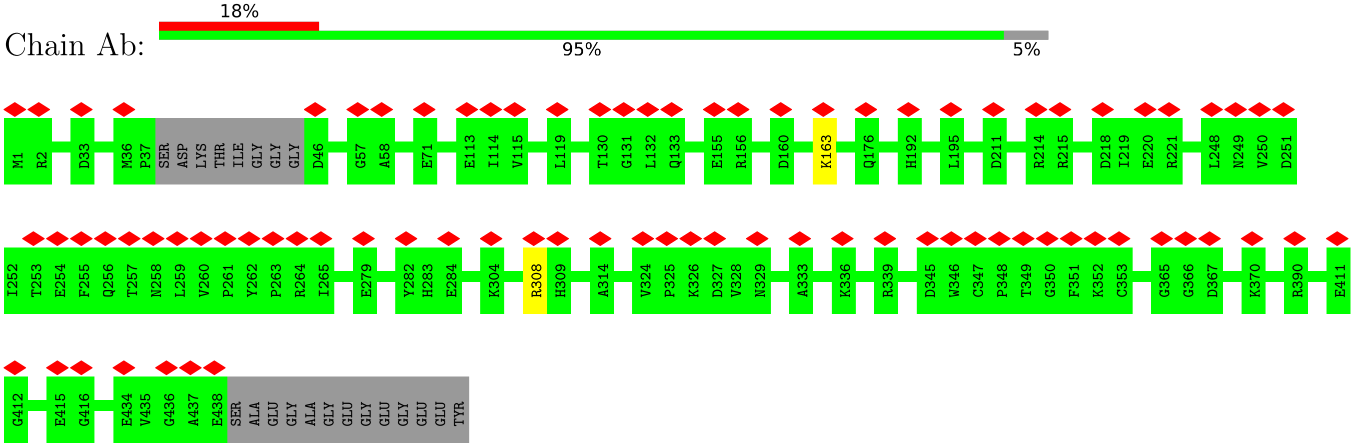
- Molecule 18: Tubulin alpha

Chain 9h:



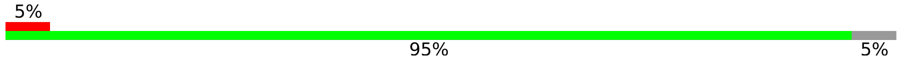
- Molecule 18: Tubulin alpha

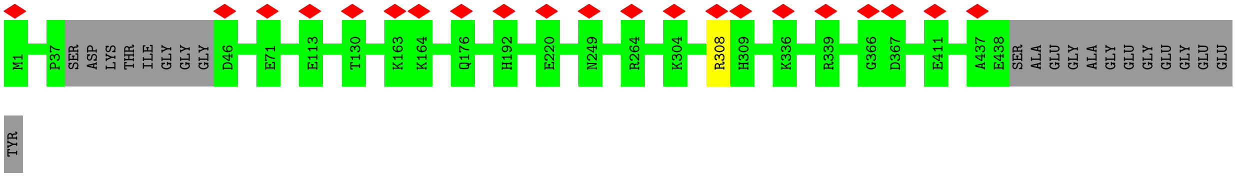
Chain Ab:



- Molecule 18: Tubulin alpha

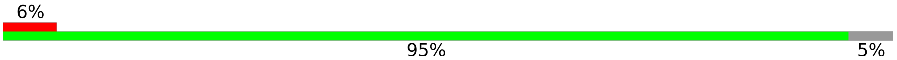
Chain Ad:

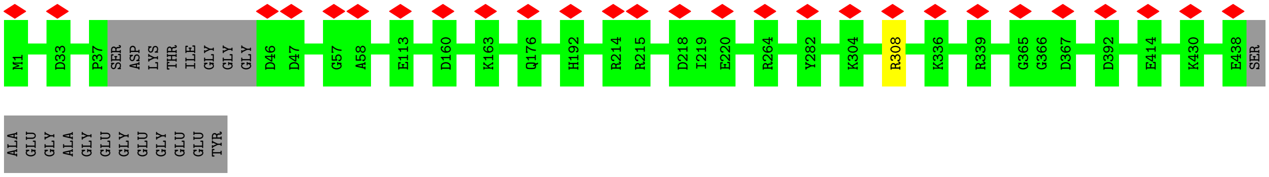




- Molecule 18: Tubulin alpha

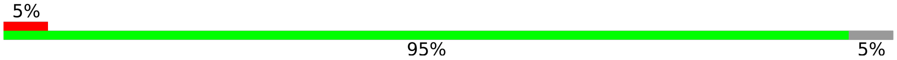
Chain Af:

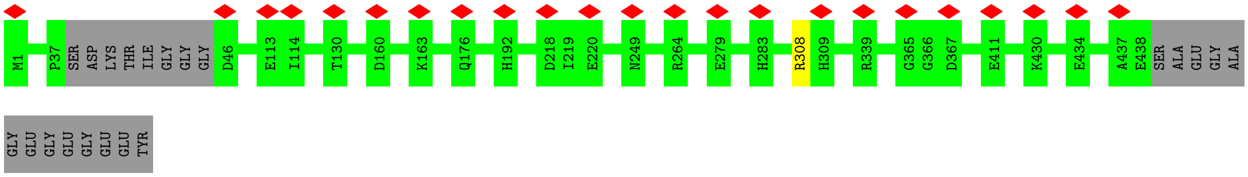




- Molecule 18: Tubulin alpha

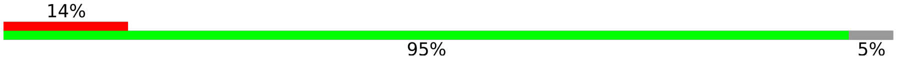
Chain Ah:

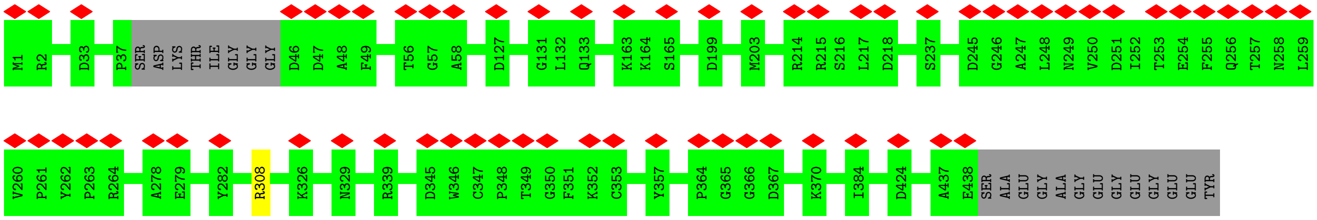




- Molecule 18: Tubulin alpha

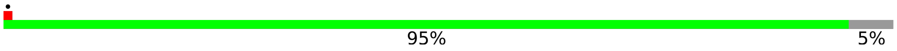
Chain Bb:

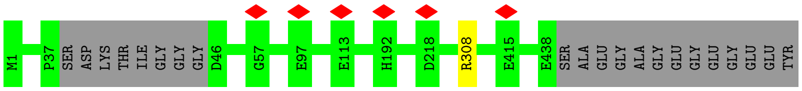




- Molecule 18: Tubulin alpha

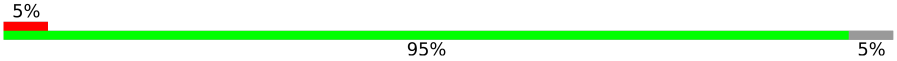
Chain Bd:

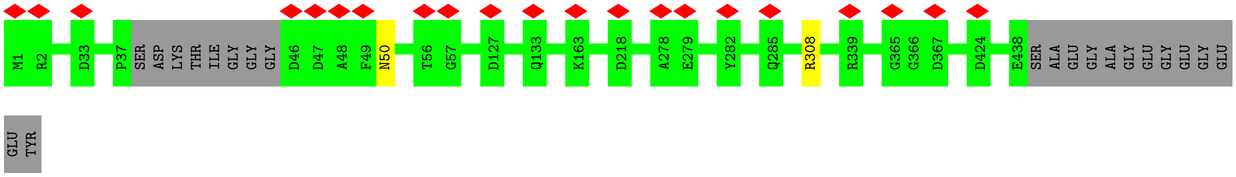




- Molecule 18: Tubulin alpha

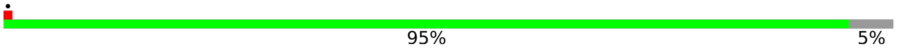
Chain Bf:

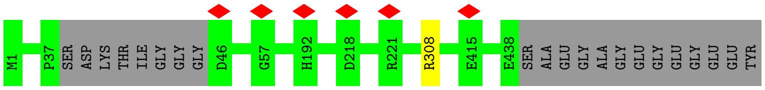




- Molecule 18: Tubulin alpha

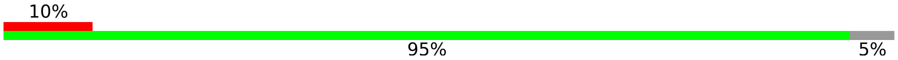
Chain Bh:

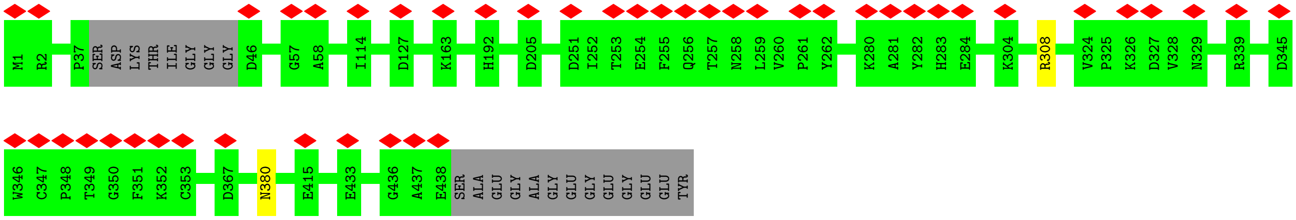




- Molecule 18: Tubulin alpha

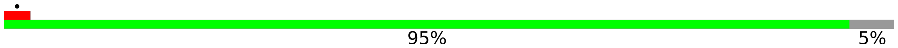
Chain Cb:

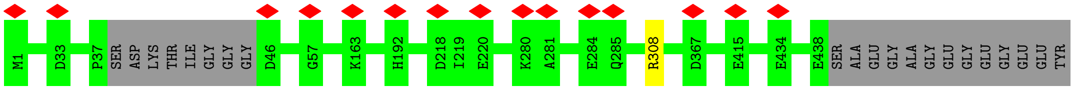




- Molecule 18: Tubulin alpha

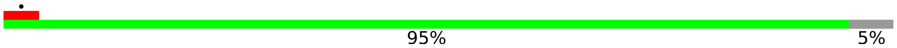
Chain Cd:

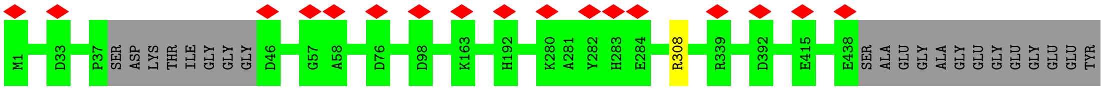




- Molecule 18: Tubulin alpha

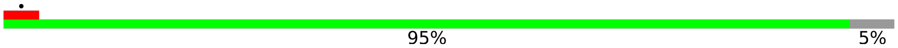
Chain Cf:

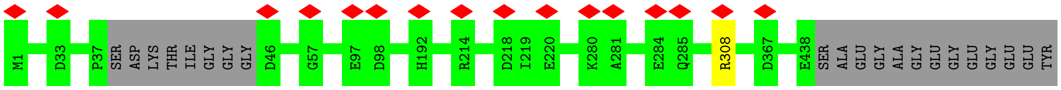




- Molecule 18: Tubulin alpha

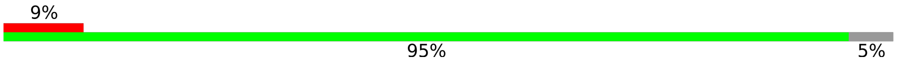
Chain Ch:





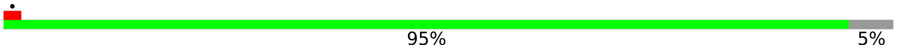
- Molecule 18: Tubulin alpha

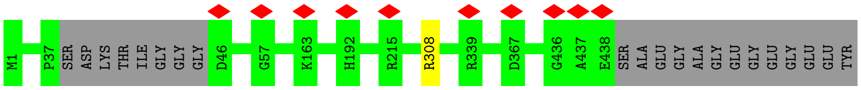
Chain Db:



- Molecule 18: Tubulin alpha

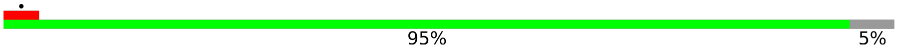
Chain Dd:

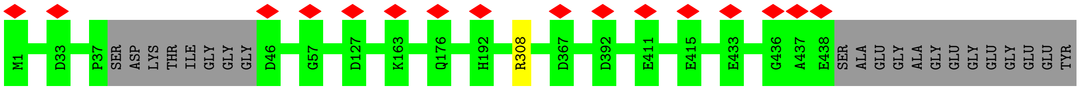




- Molecule 18: Tubulin alpha

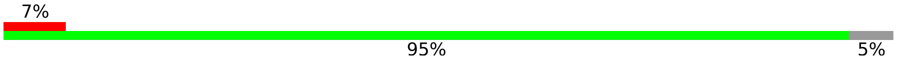
Chain Df:

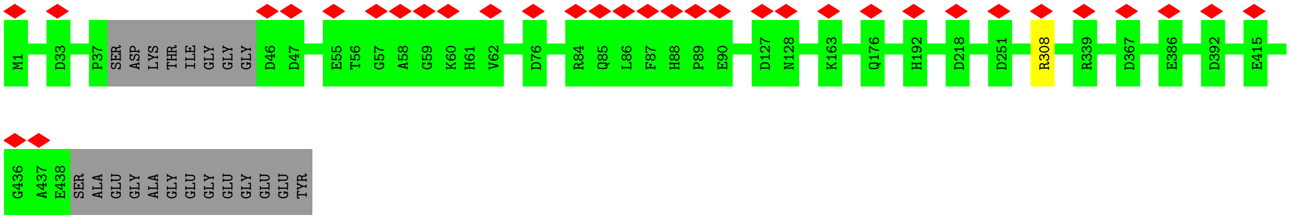




- Molecule 18: Tubulin alpha

Chain Dh:





4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	192253	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	38.6	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	9.616	Depositor
Minimum map value	0.000	Depositor
Average map value	0.046	Depositor
Map value standard deviation	0.138	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	805.9794, 699.57947, 699.57947	wwPDB
Map dimensions	606, 526, 526	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.329999, 1.329999, 1.329999	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, GDP, GTP

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	0A	0.29	0/3738	0.52	0/5058
1	0B	0.27	0/3738	0.53	0/5058
1	0C	0.26	0/3809	0.51	0/5153
1	0D	0.26	0/3809	0.51	0/5153
2	0E	0.27	0/1033	0.48	0/1399
2	0F	0.28	0/1033	0.50	0/1399
2	0G	0.27	0/1033	0.50	0/1399
2	0H	0.29	0/1033	0.49	0/1399
3	0I	0.29	0/3391	0.56	0/4613
3	0J	0.30	0/3391	0.57	0/4613
4	0K	0.26	0/1231	0.52	1/1674 (0.1%)
4	0L	0.24	0/1231	0.50	1/1674 (0.1%)
5	0M	0.26	0/4111	0.52	0/5556
5	0N	0.26	0/4111	0.52	0/5556
6	0O	0.26	0/1501	0.50	0/2016
6	0P	0.27	0/1501	0.51	0/2016
7	0Q	0.27	0/4634	0.53	0/6298
7	0S	0.26	0/4634	0.53	0/6298
12	0X	0.28	0/3143	0.56	1/4267 (0.0%)
12	0Y	0.30	0/2945	0.55	0/4003
12	0Z	0.28	0/3143	0.56	1/4267 (0.0%)
12	1A	0.29	0/2945	0.54	0/4003
13	1B	0.27	0/4891	0.53	0/6694
13	1C	0.28	0/4891	0.53	0/6694
14	1D	0.27	0/4141	0.50	0/5670
14	1E	0.26	0/4141	0.48	0/5670
14	1F	0.26	0/4441	0.51	0/6044
14	1G	0.27	0/4441	0.53	0/6044
17	1a	0.28	0/3453	0.48	0/4673
17	1c	0.28	0/3453	0.48	0/4673
17	1e	0.30	0/3453	0.49	0/4673
17	1g	0.29	0/3453	0.49	0/4673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	2a	0.29	0/3453	0.49	0/4673
17	2c	0.28	0/3453	0.49	0/4673
17	2e	0.28	0/3453	0.48	0/4673
17	2g	0.28	0/3453	0.48	0/4673
17	3a	0.27	0/3453	0.48	0/4673
17	3c	0.28	0/3453	0.48	0/4673
17	3e	0.28	0/3453	0.49	0/4673
17	3g	0.28	0/3453	0.49	0/4673
17	4a	0.27	0/3453	0.48	0/4673
17	4c	0.27	0/3453	0.48	0/4673
17	4e	0.27	0/3453	0.48	0/4673
17	4g	0.27	0/3453	0.48	0/4673
17	5a	0.26	0/3453	0.48	0/4673
17	5c	0.27	0/3453	0.48	0/4673
17	5e	0.27	0/3453	0.49	0/4673
17	5g	0.28	0/3453	0.48	0/4673
17	6a	0.26	0/3453	0.50	0/4673
17	6c	0.26	0/3453	0.49	0/4673
17	6e	0.27	0/3453	0.48	0/4673
17	6g	0.26	0/3453	0.48	0/4673
17	7a	0.26	0/3453	0.48	0/4673
17	7c	0.26	0/3453	0.48	0/4673
17	7e	0.26	0/3453	0.49	0/4673
17	7g	0.27	0/3453	0.49	0/4673
17	8a	0.27	0/3453	0.49	0/4673
17	8c	0.27	0/3453	0.49	0/4673
17	8e	0.27	0/3453	0.48	0/4673
17	8g	0.27	0/3453	0.49	0/4673
17	9a	0.33	0/3453	0.51	0/4673
17	9c	0.32	0/3453	0.50	0/4673
17	9e	0.32	0/3453	0.51	0/4673
17	9g	0.32	0/3453	0.51	0/4673
17	Aa	0.28	0/3453	0.50	0/4673
17	Ac	0.28	0/3453	0.49	0/4673
17	Ae	0.28	0/3453	0.48	0/4673
17	Ag	0.28	0/3453	0.49	0/4673
17	Ba	0.28	0/3453	0.51	0/4673
17	Bc	0.32	0/3453	0.52	0/4673
17	Be	0.29	0/3453	0.49	0/4673
17	Bg	0.32	0/3453	0.51	0/4673
17	Ca	0.27	0/3453	0.49	0/4673
17	Cc	0.30	0/3453	0.50	0/4673
17	Ce	0.30	0/3453	0.49	0/4673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	Cg	0.29	0/3453	0.49	0/4673
17	Da	0.28	0/3453	0.49	0/4673
17	Dc	0.29	0/3453	0.48	0/4673
17	De	0.29	0/3453	0.49	0/4673
17	Dg	0.29	0/3453	0.49	0/4673
18	1b	0.27	0/3410	0.49	0/4623
18	1d	0.29	0/3410	0.49	0/4623
18	1f	0.29	0/3410	0.49	0/4623
18	1h	0.28	0/3410	0.49	0/4623
18	2b	0.27	0/3410	0.48	0/4623
18	2d	0.28	0/3410	0.49	0/4623
18	2f	0.28	0/3410	0.49	0/4623
18	2h	0.28	0/3410	0.48	0/4623
18	3b	0.28	0/3410	0.48	0/4623
18	3d	0.29	0/3410	0.49	0/4623
18	3f	0.27	0/3410	0.49	0/4623
18	3h	0.28	0/3410	0.49	0/4623
18	4b	0.27	0/3410	0.49	0/4623
18	4d	0.27	0/3410	0.49	0/4623
18	4f	0.27	0/3410	0.49	0/4623
18	4h	0.27	0/3410	0.49	0/4623
18	5b	0.27	0/3410	0.48	0/4623
18	5d	0.27	0/3410	0.49	0/4623
18	5f	0.29	0/3410	0.49	0/4623
18	5h	0.27	0/3410	0.49	0/4623
18	6b	0.26	0/3410	0.48	0/4623
18	6d	0.29	0/3410	0.49	0/4623
18	6f	0.28	0/3410	0.49	0/4623
18	6h	0.28	0/3410	0.49	0/4623
18	7b	0.26	0/3410	0.48	0/4623
18	7d	0.28	0/3410	0.49	0/4623
18	7f	0.27	0/3410	0.48	0/4623
18	7h	0.27	0/3410	0.49	0/4623
18	8b	0.27	0/3410	0.49	0/4623
18	8d	0.29	0/3410	0.49	0/4623
18	8f	0.29	0/3410	0.50	0/4623
18	8h	0.27	0/3410	0.48	0/4623
18	9b	0.32	0/3410	0.50	0/4623
18	9d	0.33	0/3410	0.53	0/4623
18	9f	0.32	0/3410	0.50	0/4623
18	9h	0.33	0/3410	0.52	0/4623
18	Ab	0.27	0/3410	0.48	0/4623
18	Ad	0.28	0/3410	0.50	0/4623

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
18	Af	0.28	0/3410	0.49	0/4623
18	Ah	0.28	0/3410	0.49	0/4623
18	Bb	0.28	0/3410	0.48	0/4623
18	Bd	0.31	0/3410	0.51	0/4623
18	Bf	0.30	0/3410	0.50	0/4623
18	Bh	0.31	0/3410	0.51	0/4623
18	Cb	0.28	0/3410	0.49	0/4623
18	Cd	0.29	0/3410	0.49	0/4623
18	Cf	0.29	0/3410	0.49	0/4623
18	Ch	0.29	0/3410	0.49	0/4623
18	Db	0.28	0/3410	0.49	0/4623
18	Dd	0.29	0/3410	0.50	0/4623
18	Df	0.29	0/3410	0.49	0/4623
18	Dh	0.28	0/3410	0.49	0/4623
All	All	0.28	0/444960	0.50	4/603080 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	0X	408	PRO	N-CA-CB	6.46	111.06	103.30
12	0Z	408	PRO	N-CA-CB	6.45	111.04	103.30
4	0K	220	PRO	N-CA-CB	5.79	110.25	103.30
4	0L	220	PRO	N-CA-CB	5.77	110.22	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	0A	3656	0	3589	107	0
1	0B	3656	0	3589	116	0
1	0C	3726	0	3671	128	0
1	0D	3726	0	3671	130	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	0E	1008	0	980	25	0
2	0F	1008	0	980	17	0
2	0G	1008	0	980	27	0
2	0H	1008	0	980	19	0
3	0I	3321	0	3319	99	0
3	0J	3321	0	3319	108	0
4	0K	1216	0	1136	29	0
4	0L	1216	0	1136	28	0
5	0M	4037	0	3964	56	0
5	0N	4037	0	3964	56	0
6	0O	1481	0	1456	15	0
6	0P	1481	0	1456	17	0
7	0Q	4537	0	4426	110	0
7	0S	4537	0	4426	114	0
8	0T	845	0	185	0	0
9	0U	850	0	188	0	0
10	0V	800	0	171	0	0
11	0W	195	0	42	0	0
12	0X	3098	0	2933	101	0
12	0Y	2903	0	2675	75	0
12	0Z	3098	0	2933	84	0
12	1A	2903	0	2675	72	0
13	1B	4771	0	4774	152	0
13	1C	4771	0	4774	157	0
14	1D	4079	0	3607	95	0
14	1E	4079	0	3607	83	0
14	1F	4370	0	4195	93	0
14	1G	4370	0	4195	122	0
15	1H	440	0	97	0	0
16	1L	870	0	195	9	0
16	1M	870	0	195	19	0
17	1a	3379	0	3265	0	0
17	1c	3379	0	3265	0	0
17	1e	3379	0	3265	0	0
17	1g	3379	0	3265	0	0
17	2a	3379	0	3265	0	0
17	2c	3379	0	3265	0	0
17	2e	3379	0	3265	0	0
17	2g	3379	0	3265	0	0
17	3a	3379	0	3265	0	0
17	3c	3379	0	3265	0	0
17	3e	3379	0	3265	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	3g	3379	0	3265	0	0
17	4a	3379	0	3265	0	0
17	4c	3379	0	3265	0	0
17	4e	3379	0	3265	0	0
17	4g	3379	0	3265	0	0
17	5a	3379	0	3265	0	0
17	5c	3379	0	3265	0	0
17	5e	3379	0	3265	0	0
17	5g	3379	0	3265	0	0
17	6a	3379	0	3265	0	0
17	6c	3379	0	3265	0	0
17	6e	3379	0	3265	0	0
17	6g	3379	0	3265	0	0
17	7a	3379	0	3265	0	0
17	7c	3379	0	3265	0	0
17	7e	3379	0	3265	0	0
17	7g	3379	0	3265	0	0
17	8a	3379	0	3265	0	0
17	8c	3379	0	3265	0	0
17	8e	3379	0	3265	0	0
17	8g	3379	0	3265	0	0
17	9a	3379	0	3265	0	0
17	9c	3379	0	3265	0	0
17	9e	3379	0	3265	0	0
17	9g	3379	0	3265	0	0
17	Aa	3379	0	3265	0	0
17	Ac	3379	0	3265	0	0
17	Ae	3379	0	3265	0	0
17	Ag	3379	0	3265	0	0
17	Ba	3379	0	3265	0	0
17	Bc	3379	0	3265	0	0
17	Be	3379	0	3265	0	0
17	Bg	3379	0	3265	0	0
17	Ca	3379	0	3265	0	0
17	Cc	3379	0	3265	0	0
17	Ce	3379	0	3265	0	0
17	Cg	3379	0	3265	0	0
17	Da	3379	0	3265	0	0
17	Dc	3379	0	3265	0	0
17	De	3379	0	3265	0	0
17	Dg	3379	0	3265	0	0
18	1b	3339	0	3277	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	1d	3339	0	3277	0	0
18	1f	3339	0	3277	0	0
18	1h	3339	0	3277	0	0
18	2b	3339	0	3277	0	0
18	2d	3339	0	3277	0	0
18	2f	3339	0	3277	0	0
18	2h	3339	0	3277	0	0
18	3b	3339	0	3277	0	0
18	3d	3339	0	3277	0	0
18	3f	3339	0	3277	0	0
18	3h	3339	0	3277	0	0
18	4b	3339	0	3277	0	0
18	4d	3339	0	3277	0	0
18	4f	3339	0	3277	0	0
18	4h	3339	0	3277	0	0
18	5b	3339	0	3277	0	0
18	5d	3339	0	3277	0	0
18	5f	3339	0	3277	0	0
18	5h	3339	0	3277	0	0
18	6b	3339	0	3277	0	0
18	6d	3339	0	3277	0	0
18	6f	3339	0	3277	0	0
18	6h	3339	0	3277	0	0
18	7b	3339	0	3277	0	0
18	7d	3339	0	3277	0	0
18	7f	3339	0	3277	0	0
18	7h	3339	0	3277	0	0
18	8b	3339	0	3277	0	0
18	8d	3339	0	3277	0	0
18	8f	3339	0	3277	0	0
18	8h	3339	0	3277	0	0
18	9b	3339	0	3277	0	0
18	9d	3339	0	3277	0	0
18	9f	3339	0	3277	0	0
18	9h	3339	0	3277	0	0
18	Ab	3339	0	3277	0	0
18	Ad	3339	0	3277	0	0
18	Af	3339	0	3277	0	0
18	Ah	3339	0	3277	0	0
18	Bb	3339	0	3277	0	0
18	Bd	3339	0	3277	0	0
18	Bf	3339	0	3277	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	Bh	3339	0	3277	0	0
18	Cb	3339	0	3277	0	0
18	Cd	3339	0	3277	0	0
18	Cf	3339	0	3277	0	0
18	Ch	3339	0	3277	0	0
18	Db	3339	0	3277	0	0
18	Dd	3339	0	3277	0	0
18	Df	3339	0	3277	0	0
18	Dh	3339	0	3277	0	0
19	0X	27	0	12	2	0
19	0Y	27	0	12	4	0
19	0Z	27	0	12	2	0
19	1A	27	0	12	1	0
20	1a	28	0	12	0	0
20	1c	28	0	12	0	0
20	1e	28	0	12	0	0
20	1g	28	0	12	0	0
20	2a	28	0	12	0	0
20	2c	28	0	12	0	0
20	2e	28	0	12	0	0
20	2g	28	0	12	0	0
20	3a	28	0	12	0	0
20	3c	28	0	12	0	0
20	3e	28	0	12	0	0
20	3g	28	0	12	0	0
20	4a	28	0	12	0	0
20	4c	28	0	12	0	0
20	4e	28	0	12	0	0
20	4g	28	0	12	0	0
20	5a	28	0	12	0	0
20	5c	28	0	12	0	0
20	5e	28	0	12	0	0
20	5g	28	0	12	0	0
20	6a	28	0	12	0	0
20	6c	28	0	12	0	0
20	6e	28	0	12	0	0
20	6g	28	0	12	0	0
20	7a	28	0	12	0	0
20	7c	28	0	12	0	0
20	7e	28	0	12	0	0
20	7g	28	0	12	0	0
20	8a	28	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	8c	28	0	12	0	0
20	8e	28	0	12	0	0
20	8g	28	0	12	0	0
20	9a	28	0	12	0	0
20	9c	28	0	12	0	0
20	9e	28	0	12	0	0
20	9g	28	0	12	0	0
20	Aa	28	0	12	0	0
20	Ac	28	0	12	0	0
20	Ae	28	0	12	0	0
20	Ag	28	0	12	0	0
20	Ba	28	0	12	0	0
20	Bc	28	0	12	0	0
20	Be	28	0	12	0	0
20	Bg	28	0	12	0	0
20	Ca	28	0	12	0	0
20	Cc	28	0	12	0	0
20	Ce	28	0	12	0	0
20	Cg	28	0	12	0	0
20	Da	28	0	12	0	0
20	Dc	28	0	12	0	0
20	De	28	0	12	0	0
20	Dg	28	0	12	0	0
21	1b	32	0	12	0	0
21	1d	32	0	12	0	0
21	1f	32	0	12	0	0
21	1h	32	0	12	0	0
21	2b	32	0	12	0	0
21	2d	32	0	12	0	0
21	2f	32	0	12	0	0
21	2h	32	0	12	0	0
21	3b	32	0	12	0	0
21	3d	32	0	12	0	0
21	3f	32	0	12	0	0
21	3h	32	0	12	0	0
21	4b	32	0	12	0	0
21	4d	32	0	12	0	0
21	4f	32	0	12	0	0
21	4h	32	0	12	0	0
21	5b	32	0	12	0	0
21	5d	32	0	12	0	0
21	5f	32	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	5h	32	0	12	0	0
21	6b	32	0	12	0	0
21	6d	32	0	12	0	0
21	6f	32	0	12	0	0
21	6h	32	0	12	0	0
21	7b	32	0	12	0	0
21	7d	32	0	12	0	0
21	7f	32	0	12	0	0
21	7h	32	0	12	0	0
21	8b	32	0	12	0	0
21	8d	32	0	12	0	0
21	8f	32	0	12	0	0
21	8h	32	0	12	0	0
21	9b	32	0	12	0	0
21	9d	32	0	12	0	0
21	9f	32	0	12	0	0
21	9h	32	0	12	0	0
21	Ab	32	0	12	0	0
21	Ad	32	0	12	0	0
21	Af	32	0	12	0	0
21	Ah	32	0	12	0	0
21	Bb	32	0	12	0	0
21	Bd	32	0	12	0	0
21	Bf	32	0	12	0	0
21	Bh	32	0	12	0	0
21	Cb	32	0	12	0	0
21	Cd	32	0	12	0	0
21	Cf	32	0	12	0	0
21	Ch	32	0	12	0	0
21	Db	32	0	12	0	0
21	Dd	32	0	12	0	0
21	Df	32	0	12	0	0
21	Dh	32	0	12	0	0
All	All	443856	0	425963	2096	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 12.

All (2096) 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)
13:1B:1659:ALA:HB2	16:1M:22:UNK:CB	1.25	1.57
13:1B:1659:ALA:CB	16:1M:22:UNK:CB	2.19	1.20
13:1B:1650:GLU:OE1	16:1M:30:UNK:O	1.69	1.10
7:0Q:488:LEU:HB3	7:0Q:498:THR:HG21	1.53	0.91
7:0S:460:MET:HE2	7:0S:495:ARG:HH12	1.33	0.91
12:0Y:106:THR:H	12:0Y:111:ARG:HG2	1.36	0.88
12:1A:106:THR:H	12:1A:111:ARG:HG2	1.37	0.88
14:1G:551:GLY:H	14:1G:576:ARG:HH22	1.24	0.86
12:0Y:78:SER:O	12:0Y:82:GLY:HA3	1.77	0.85
12:1A:78:SER:O	12:1A:82:GLY:HA3	1.78	0.83
1:0B:430:LEU:O	2:0F:62:LYS:NZ	2.12	0.82
14:1F:632:ALA:H	14:1F:638:PRO:HB2	1.45	0.82
14:1G:772:GLU:HG2	14:1G:802:LEU:HD21	1.61	0.82
14:1G:632:ALA:H	14:1G:638:PRO:HB2	1.45	0.81
14:1G:1028:LEU:HB3	14:1G:1032:ARG:HH12	1.44	0.81
14:1G:769:LEU:HG	14:1G:771:LEU:H	1.48	0.79
7:0Q:329:LEU:HD13	7:0Q:610:GLY:HA2	1.65	0.79
14:1F:402:LEU:HB3	14:1F:406:ILE:HG21	1.63	0.79
14:1D:850:LEU:HG	14:1D:854:GLN:HE22	1.46	0.78
1:0D:508:GLN:HB3	1:0D:520:LEU:HD11	1.65	0.78
14:1G:400:ARG:HG3	14:1G:402:LEU:H	1.50	0.77
1:0C:508:GLN:HB3	1:0C:520:LEU:HD11	1.65	0.77
12:0X:99:PHE:HA	12:0X:103:GLY:HA3	1.65	0.77
12:0X:278:LEU:HG	12:0X:285:VAL:HG21	1.65	0.77
14:1F:1032:ARG:NH1	14:1F:1045:GLU:OE2	2.18	0.77
12:0Y:161:LEU:HA	12:0Y:174:ARG:O	1.85	0.77
7:0S:329:LEU:HD13	7:0S:610:GLY:HA2	1.66	0.76
1:0D:346:ASP:OD2	2:0G:152:ARG:NH2	2.18	0.76
7:0Q:487:SER:HG	7:0Q:489:TRP:HE1	1.32	0.76
14:1F:772:GLU:HG2	14:1F:802:LEU:HD21	1.66	0.76
14:1G:402:LEU:HB3	14:1G:406:ILE:HG21	1.67	0.76
3:0J:150:GLN:HG2	3:0J:153:LYS:HE3	1.67	0.76
14:1F:547:LYS:HG3	14:1F:548:GLN:HG2	1.67	0.76
12:0Z:300:LEU:H	12:0Z:306:THR:HG21	1.50	0.76
12:1A:161:LEU:HA	12:1A:174:ARG:O	1.86	0.76
13:1C:1487:MET:O	13:1C:1519:LYS:NZ	2.18	0.76
12:0Z:65:GLU:HG3	12:0Z:116:ARG:HH22	1.49	0.75
12:0X:65:GLU:HG3	12:0X:116:ARG:HH22	1.50	0.75
1:0B:177:LEU:HD11	1:0C:180:LEU:HD13	1.69	0.75
2:0F:70:ASN:HA	2:0F:100:LYS:HG2	1.69	0.75
7:0Q:46:ASN:ND2	7:0Q:321:ILE:O	2.20	0.74
13:1C:1581:ILE:HG12	13:1C:1583:PRO:HD2	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1C:1242:MET:SD	13:1C:1245:ARG:NH1	2.59	0.74
1:0A:537:HIS:HB3	1:0A:556:ASP:HB2	1.69	0.74
14:1E:1009:GLN:O	14:1E:1013:GLN:NE2	2.20	0.74
1:0D:328:SER:HA	1:0D:600:ASN:HA	1.69	0.74
2:0H:70:ASN:HA	2:0H:100:LYS:HG2	1.70	0.74
3:0J:151:GLN:HA	3:0J:154:TRP:HD1	1.52	0.74
3:0J:217:ARG:H	3:0J:232:ILE:HG12	1.52	0.74
12:0X:169:SER:OG	12:0X:342:ASN:ND2	2.21	0.74
12:0Z:13:ARG:NH1	12:0Z:94:GLY:O	2.21	0.74
14:1D:999:TYR:HB3	14:1D:1008:GLU:HG2	1.68	0.74
1:0A:177:LEU:HD11	1:0D:180:LEU:HD13	1.70	0.73
12:0Z:99:PHE:HA	12:0Z:103:GLY:HA3	1.69	0.73
13:1C:1493:LEU:HG	13:1C:1519:LYS:HE2	1.67	0.73
7:0S:495:ARG:NH1	7:0S:499:THR:OG1	2.21	0.73
7:0Q:72:LEU:HD21	7:0Q:83:VAL:HG13	1.69	0.72
12:0X:229:SER:HB3	12:0X:349:LEU:HA	1.70	0.72
1:0C:157:ASP:OD1	1:0C:160:ARG:NH2	2.22	0.72
13:1B:1242:MET:SD	13:1B:1245:ARG:NH1	2.62	0.72
12:0Z:278:LEU:HG	12:0Z:285:VAL:HG21	1.69	0.72
14:1D:849:ARG:CZ	14:1D:868:PHE:HA	2.19	0.72
4:0L:218:ARG:HH12	13:1C:1215:GLU:HG2	1.55	0.72
7:0Q:444:LEU:HD21	7:0Q:478:ALA:HB2	1.72	0.72
13:1C:1123:LYS:HB2	13:1C:1498:LEU:HD21	1.72	0.72
3:0J:455:TRP:HD1	3:0J:516:ARG:HH12	1.38	0.72
5:0N:244:ILE:HB	5:0N:280:LEU:HB2	1.71	0.72
13:1B:1648:PHE:HB3	16:1M:32:UNK:CB	2.19	0.72
1:0B:537:HIS:HB3	1:0B:556:ASP:HB2	1.70	0.72
6:0P:39:ASN:O	6:0P:46:GLN:NE2	2.21	0.72
12:0X:109:ALA:O	12:0X:110:HIS:ND1	2.23	0.72
12:1A:247:ARG:HH21	12:1A:324:SER:HB2	1.53	0.72
13:1C:1685:PRO:HG2	13:1C:1688:GLN:HB2	1.72	0.72
7:0S:46:ASN:ND2	7:0S:321:ILE:O	2.22	0.72
12:0Z:221:GLU:HG2	12:0Z:233:VAL:HG13	1.72	0.72
12:0Z:246:GLU:HG3	12:0Z:248:THR:H	1.55	0.71
1:0B:327:LEU:HD11	2:0F:152:ARG:HB3	1.72	0.71
12:0X:221:GLU:HG2	12:0X:233:VAL:HG13	1.73	0.71
12:0X:272:GLU:OE1	12:0X:331:ARG:NH2	2.24	0.71
3:0I:265:LEU:HD21	3:0I:330:LEU:HB3	1.70	0.71
13:1B:1123:LYS:HB2	13:1B:1498:LEU:HD21	1.72	0.71
14:1F:820:THR:HB	14:1F:825:VAL:HG21	1.73	0.71
12:0Z:229:SER:HB3	12:0Z:349:LEU:HA	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0I:225:PHE:HE1	6:0O:166:LYS:HG3	1.56	0.71
12:0X:59:LEU:HD23	12:0X:62:VAL:HG21	1.73	0.71
12:0Z:232:ALA:O	12:0Z:344:SER:N	2.23	0.71
14:1D:545:PRO:HD2	14:1D:579:ALA:HB1	1.72	0.71
14:1G:820:THR:HB	14:1G:825:VAL:HG21	1.71	0.71
12:0X:300:LEU:H	12:0X:306:THR:HG21	1.56	0.71
5:0M:244:ILE:HB	5:0M:280:LEU:HB2	1.73	0.70
1:0C:327:LEU:HD23	2:0E:152:ARG:HH11	1.55	0.70
3:0J:196:ARG:NH2	3:0J:205:GLU:O	2.25	0.70
13:1B:1581:ILE:HG12	13:1B:1583:PRO:HD2	1.72	0.70
13:1C:1588:LEU:HD21	13:1C:1594:LEU:HB2	1.72	0.70
12:0Z:169:SER:OG	12:0Z:342:ASN:ND2	2.24	0.70
13:1B:1297:GLN:HG2	13:1B:1335:LEU:HA	1.72	0.70
2:0G:70:ASN:HD21	2:0G:93:ASN:HA	1.57	0.70
3:0I:265:LEU:HD23	3:0I:331:ARG:HH21	1.55	0.70
14:1E:545:PRO:HD2	14:1E:579:ALA:HB1	1.72	0.70
12:0X:246:GLU:HG3	12:0X:248:THR:H	1.56	0.70
13:1C:1244:PRO:HG2	13:1C:1257:VAL:HA	1.73	0.70
1:0A:334:LEU:HD13	1:0A:585:LEU:HD23	1.75	0.69
3:0J:265:LEU:HD21	3:0J:330:LEU:HB3	1.74	0.69
13:1B:1347:LEU:HD22	13:1B:1389:VAL:HG21	1.75	0.69
7:0S:488:LEU:HB3	7:0S:498:THR:HG21	1.72	0.69
14:1F:544:VAL:HG13	14:1F:547:LYS:HG2	1.74	0.69
7:0S:500:TRP:HE1	7:0S:535:PRO:HA	1.58	0.69
13:1B:1272:PRO:HB2	13:1B:1284:ARG:HH11	1.56	0.69
1:0D:582:GLN:H	1:0D:597:GLY:HA2	1.56	0.69
4:0K:218:ARG:HH12	13:1B:1215:GLU:HG2	1.58	0.69
12:0X:181:VAL:HG11	12:0X:187:ALA:HB2	1.75	0.69
14:1E:425:LYS:HD2	14:1E:524:SER:HB3	1.74	0.69
5:0N:419:ASN:HB3	5:0N:422:MET:HG2	1.74	0.68
12:0X:232:ALA:O	12:0X:344:SER:N	2.23	0.68
1:0A:349:THR:HG22	1:0A:365:GLU:HB3	1.75	0.68
13:1C:1190:GLU:HG2	13:1C:1485:ALA:HB2	1.75	0.68
14:1G:1002:ALA:O	14:1G:1004:GLN:NE2	2.26	0.68
4:0K:137:LYS:NZ	13:1B:1217:TRP:O	2.24	0.68
1:0C:194:LEU:HD21	4:0K:106:LEU:HD11	1.75	0.68
2:0E:44:LEU:HD23	2:0E:135:ILE:HG23	1.74	0.68
3:0I:322:ARG:HE	3:0I:326:TYR:HE2	1.39	0.68
3:0J:92:LEU:O	3:0J:96:HIS:ND1	2.27	0.68
3:0J:135:MET:O	3:0J:142:ARG:NH2	2.26	0.68
12:0Z:59:LEU:HD23	12:0Z:62:VAL:HG21	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1E:1029:LEU:HD22	14:1E:1064:ALA:HB1	1.74	0.68
1:0C:146:SER:HA	1:0C:149:TRP:CD1	2.28	0.68
5:0M:161:LEU:HA	5:0M:174:ALA:HB3	1.76	0.67
14:1G:544:VAL:HG13	14:1G:547:LYS:HG2	1.75	0.67
3:0I:457:TRP:HE1	3:0I:483:GLN:HG2	1.59	0.67
13:1C:1250:GLU:HG3	13:1C:1253:ALA:HB2	1.76	0.67
1:0D:434:VAL:HG21	1:0D:469:THR:HG21	1.76	0.67
1:0C:332:LEU:HB3	1:0C:341:LEU:HD11	1.74	0.67
3:0I:217:ARG:H	3:0I:232:ILE:HG12	1.58	0.67
13:1C:1190:GLU:HG3	13:1C:1484:SER:HB3	1.77	0.67
13:1C:1481:SER:HA	13:1C:1498:LEU:HD12	1.76	0.67
3:0J:508:ARG:HH22	14:1F:942:MET:HA	1.60	0.67
12:0X:233:VAL:HG12	12:0X:234:LEU:H	1.59	0.67
13:1C:1347:LEU:HD22	13:1C:1389:VAL:HG21	1.76	0.67
1:0B:169:GLU:HA	1:0B:172:LYS:HD2	1.77	0.67
3:0J:424:PHE:HZ	3:0J:514:VAL:HG21	1.60	0.67
4:0L:218:ARG:NH2	13:1C:1214:LEU:O	2.28	0.67
6:0P:36:GLN:NE2	6:0P:49:ASN:O	2.27	0.67
1:0A:296:ALA:HB2	1:0A:482:ARG:HD3	1.75	0.67
13:1B:1390:GLU:HG3	13:1B:1404:GLU:HG2	1.75	0.67
1:0D:332:LEU:HD22	1:0D:341:LEU:HD21	1.76	0.66
1:0D:407:THR:O	1:0D:410:LYS:NZ	2.27	0.66
3:0J:265:LEU:HD23	3:0J:331:ARG:HH21	1.60	0.66
7:0Q:442:GLY:HA2	7:0Q:465:ILE:HG12	1.76	0.66
1:0D:157:ASP:OD1	1:0D:160:ARG:NH2	2.28	0.66
2:0E:70:ASN:HD21	2:0E:93:ASN:HA	1.61	0.66
7:0S:429:SER:HB3	7:0S:433:ALA:H	1.60	0.66
13:1B:1684:LEU:HD22	13:1B:1689:TYR:HB2	1.77	0.66
1:0B:88:LEU:HD22	1:0C:98:GLU:HG3	1.76	0.66
12:0X:106:THR:H	12:0X:111:ARG:HG2	1.60	0.66
14:1F:790:LEU:HD11	14:1F:841:ALA:HB2	1.77	0.66
13:1B:1250:GLU:HG3	13:1B:1253:ALA:HB2	1.78	0.66
13:1B:1659:ALA:HB2	16:1M:22:UNK:CA	2.20	0.66
12:0X:13:ARG:NH1	12:0X:94:GLY:O	2.29	0.66
12:0Z:233:VAL:HG12	12:0Z:234:LEU:H	1.60	0.66
1:0A:88:LEU:HD22	1:0D:98:GLU:HG3	1.77	0.66
1:0D:146:SER:HA	1:0D:149:TRP:CD1	2.30	0.66
13:1C:1313:VAL:HA	13:1C:1750:TYR:HE1	1.61	0.66
14:1E:883:ALA:O	14:1E:917:ARG:NH1	2.29	0.66
7:0S:589:ALA:HB3	7:0S:607:ALA:HB1	1.77	0.66
12:0X:249:LYS:HG3	12:0X:250:LYS:HD3	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1F:502:SER:OG	14:1F:505:GLU:OE1	2.12	0.66
1:0C:434:VAL:HG21	1:0C:469:THR:HG21	1.77	0.65
12:0Z:249:LYS:HG3	12:0Z:250:LYS:HD3	1.77	0.65
13:1B:1302:PRO:HD2	13:1B:1305:LEU:HB2	1.79	0.65
14:1E:522:HIS:O	14:1E:526:ASN:ND2	2.29	0.65
1:0A:76:ASP:OD1	1:0A:80:ARG:NH2	2.29	0.65
12:0X:20:SER:HB3	12:0X:316:PRO:HG3	1.77	0.65
14:1D:1007:ALA:HA	14:1D:1010:ARG:HD2	1.77	0.65
16:1L:83:UNK:O	16:1L:144:UNK:N	2.29	0.65
1:0C:194:LEU:HD11	4:0K:106:LEU:HD21	1.78	0.65
13:1B:1244:PRO:HG2	13:1B:1257:VAL:HA	1.76	0.65
14:1G:666:LEU:HG	14:1G:670:TYR:CE1	2.32	0.65
16:1M:83:UNK:O	16:1M:144:UNK:N	2.29	0.65
7:0Q:500:TRP:HE1	7:0Q:535:PRO:HA	1.61	0.65
7:0S:64:ALA:HB2	7:0S:107:VAL:HG13	1.78	0.65
7:0S:442:GLY:HA2	7:0S:465:ILE:HG12	1.79	0.65
13:1B:1190:GLU:HG2	13:1B:1485:ALA:HB2	1.79	0.65
13:1B:1313:VAL:HA	13:1B:1750:TYR:HE1	1.62	0.65
7:0S:460:MET:HE2	7:0S:495:ARG:NH1	2.09	0.65
14:1D:522:HIS:O	14:1D:526:ASN:ND2	2.29	0.65
12:0X:204:VAL:HG23	12:0X:205:LEU:HD12	1.78	0.65
12:0Y:94:GLY:HA2	12:0Y:206:ASN:HD22	1.62	0.65
14:1D:493:GLU:O	14:1D:496:ARG:NH1	2.30	0.65
5:0M:137:GLN:O	5:0M:138:HIS:ND1	2.29	0.65
6:0O:32:LYS:HE3	6:0O:48:GLU:HG3	1.77	0.65
3:0I:450:THR:HA	3:0I:489:PRO:HB3	1.79	0.64
7:0Q:46:ASN:HD21	7:0Q:322:SER:HB3	1.62	0.64
14:1E:929:ARG:HG2	14:1E:960:TRP:CE2	2.32	0.64
14:1G:551:GLY:H	14:1G:576:ARG:NH2	1.94	0.64
1:0B:116:ASP:HA	1:0B:119:LEU:HD12	1.79	0.64
3:0J:322:ARG:HE	3:0J:326:TYR:HE2	1.43	0.64
3:0J:482:LEU:HD23	3:0J:495:VAL:HG22	1.79	0.64
7:0Q:589:ALA:HB3	7:0Q:607:ALA:HB1	1.78	0.64
1:0B:146:SER:HA	1:0B:149:TRP:NE1	2.13	0.64
1:0C:582:GLN:H	1:0C:597:GLY:HA2	1.60	0.64
3:0I:496:ALA:O	14:1G:511:ASN:ND2	2.30	0.64
13:1B:1303:PRO:HA	13:1B:1306:ARG:HE	1.62	0.64
14:1D:883:ALA:O	14:1D:917:ARG:NH1	2.30	0.64
1:0B:578:GLU:OE1	1:0B:603:ARG:NH2	2.31	0.64
1:0D:332:LEU:HB3	1:0D:341:LEU:HD11	1.77	0.64
7:0Q:424:THR:OG1	7:0Q:465:ILE:O	2.16	0.64

Continued on next page...

Continued from previous page...

Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
13:1C:1297:GLN:HG2	13:1C:1335:LEU:HA	1.78	0.64
1:0D:346:ASP:HB2	2:0G:152:ARG:HH12	1.63	0.64
12:0Z:181:VAL:HG11	12:0Z:187:ALA:HB2	1.79	0.64
1:0D:458:LEU:HG	1:0D:467:LEU:HD11	1.79	0.64
6:0O:188:ILE:HG22	6:0O:189:THR:HG23	1.80	0.64
5:0M:138:HIS:H	5:0M:140:LYS:HG2	1.63	0.64
14:1F:400:ARG:HH12	14:1F:404:GLU:HA	1.63	0.64
1:0A:146:SER:HA	1:0A:149:TRP:NE1	2.13	0.64
12:0Z:221:GLU:HA	12:0Z:233:VAL:HA	1.78	0.64
13:1C:1526:PHE:O	13:1C:1585:ALA:HA	1.97	0.64
12:0Y:68:TYR:HB2	12:0Y:116:ARG:HE	1.62	0.63
13:1B:1659:ALA:CB	16:1M:22:UNK:C	2.76	0.63
7:0S:215:GLY:HA3	7:0S:242:VAL:HG11	1.80	0.63
13:1C:1501:LEU:HD12	13:1C:1609:PHE:HZ	1.64	0.63
1:0A:152:PHE:HD2	1:0D:149:TRP:HB2	1.64	0.63
7:0S:38:SER:H	7:0S:588:SER:HB2	1.63	0.63
12:0Y:88:PHE:HB3	12:0Y:240:VAL:HB	1.81	0.63
14:1D:1029:LEU:HD22	14:1D:1064:ALA:HB1	1.81	0.63
1:0C:325:HIS:NE2	1:0C:343:THR:OG1	2.30	0.63
1:0D:194:LEU:HD11	4:0L:106:LEU:HD21	1.80	0.63
7:0Q:429:SER:HB3	7:0Q:433:ALA:H	1.63	0.63
12:0Y:11:ARG:NH2	12:0Y:64:GLN:OE1	2.32	0.63
12:0Y:59:LEU:HD23	12:0Y:62:VAL:HG11	1.78	0.63
13:1B:1738:ARG:NH2	13:1B:1750:TYR:O	2.31	0.63
13:1C:1302:PRO:HD2	13:1C:1305:LEU:HB2	1.80	0.63
4:0K:137:LYS:HZ1	13:1B:1219:GLU:HG3	1.63	0.63
12:0X:221:GLU:HA	12:0X:233:VAL:HA	1.79	0.63
13:1B:1201:TRP:HZ2	13:1B:1255:CYS:HG	1.44	0.63
14:1D:911:LEU:HB2	14:1G:400:ARG:HH12	1.63	0.63
1:0A:198:TYR:O	1:0A:202:MET:HG2	1.99	0.63
13:1B:1481:SER:HA	13:1B:1498:LEU:HD12	1.81	0.63
1:0B:334:LEU:HD13	1:0B:585:LEU:HD23	1.79	0.63
14:1E:493:GLU:O	14:1E:496:ARG:NH1	2.32	0.63
14:1F:1005:ARG:NH1	14:1F:1008:GLU:OE2	2.32	0.63
1:0C:196:LYS:HB2	4:0K:98:ARG:NH2	2.12	0.63
12:0X:169:SER:HG	12:0X:342:ASN:ND2	1.96	0.63
12:0X:355:GLU:HA	12:0X:358:ILE:HG22	1.81	0.63
13:1B:1413:PRO:HD2	13:1B:1749:ARG:HH12	1.62	0.63
1:0D:419:HIS:HB3	1:0D:422:GLY:H	1.63	0.62
5:0M:193:VAL:HG11	5:0M:217:LEU:HD11	1.81	0.62
1:0C:419:HIS:HB3	1:0C:422:GLY:H	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:0Y:131:LYS:NZ	12:0Y:224:THR:OG1	2.30	0.62
13:1C:1390:GLU:HG3	13:1C:1404:GLU:HG2	1.79	0.62
14:1G:790:LEU:HD11	14:1G:841:ALA:HB2	1.81	0.62
7:0Q:21:SER:HB3	7:0Q:300:LEU:HD23	1.80	0.62
7:0Q:299:PHE:HD2	7:0Q:311:LEU:HD23	1.64	0.62
13:1B:1526:PHE:O	13:1B:1585:ALA:HA	1.98	0.62
14:1D:1039:CYS:HA	14:1D:1042:GLU:HB2	1.81	0.62
2:0G:108:GLN:NE2	2:0G:123:VAL:HG21	2.14	0.62
3:0I:482:LEU:HD23	3:0I:495:VAL:HG22	1.80	0.62
14:1E:999:TYR:HB3	14:1E:1008:GLU:HG2	1.81	0.62
1:0A:135:LEU:HB2	1:0D:135:LEU:HD13	1.81	0.62
1:0B:332:LEU:HD22	1:0B:341:LEU:HD21	1.81	0.62
7:0Q:149:ILE:HD13	7:0Q:170:ALA:HB2	1.82	0.62
14:1D:504:ASN:OD1	14:1D:505:GLU:N	2.32	0.62
1:0A:141:ILE:HD12	1:0A:144:ARG:HD2	1.82	0.62
1:0A:368:LYS:NZ	2:0H:40:ASP:OD2	2.32	0.62
1:0D:190:THR:HG22	4:0L:105:LEU:HB3	1.81	0.62
1:0C:458:LEU:HG	1:0C:467:LEU:HD11	1.81	0.62
12:0X:84:ASN:ND2	12:0X:303:ASN:O	2.32	0.62
1:0A:102:LEU:HD12	1:0D:88:LEU:HD23	1.82	0.62
1:0D:194:LEU:HD21	4:0L:106:LEU:HD11	1.82	0.62
14:1G:1005:ARG:NH1	14:1G:1008:GLU:OE2	2.33	0.62
3:0J:217:ARG:HH11	3:0J:219:LEU:HD21	1.64	0.62
5:0N:624:ASP:OD1	5:0N:625:THR:N	2.33	0.62
12:0Y:137:VAL:HG21	12:0Y:190:GLN:NE2	2.15	0.62
13:1B:1177:THR:HG22	13:1B:1290:VAL:HB	1.81	0.62
14:1F:1025:SER:HA	14:1F:1028:LEU:HD12	1.81	0.62
14:1G:1025:SER:HA	14:1G:1028:LEU:HD12	1.81	0.62
1:0C:335:HIS:HE2	1:0C:380:GLY:HA3	1.65	0.61
12:0X:171:THR:O	12:0X:236:LYS:NZ	2.31	0.61
13:1C:1120:GLY:HA2	13:1C:1614:ARG:HH22	1.65	0.61
13:1C:1272:PRO:HB2	13:1C:1284:ARG:HH11	1.65	0.61
13:1C:1738:ARG:NH2	13:1C:1750:TYR:O	2.33	0.61
14:1E:911:LEU:HG	14:1F:400:ARG:HD3	1.83	0.61
1:0A:149:TRP:HB3	1:0D:149:TRP:HB3	1.82	0.61
1:0B:102:LEU:HD12	1:0C:88:LEU:HD23	1.81	0.61
12:0Y:137:VAL:HG21	12:0Y:190:GLN:HE21	1.64	0.61
12:0Z:169:SER:HG	12:0Z:342:ASN:ND2	1.98	0.61
13:1B:1234:ILE:HD11	13:1B:1269:PHE:HB3	1.82	0.61
14:1F:666:LEU:HG	14:1F:670:TYR:CE1	2.35	0.61
14:1G:666:LEU:HD12	14:1G:669:VAL:HB	1.80	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0B:135:LEU:HB2	1:0C:135:LEU:HD13	1.81	0.61
5:0M:40:THR:HA	5:0M:54:PRO:HD3	1.82	0.61
12:1A:59:LEU:HD23	12:1A:62:VAL:HG11	1.81	0.61
14:1G:820:THR:OG1	14:1G:821:PRO:HD3	2.00	0.61
1:0C:299:ARG:HH21	1:0C:465:SER:HB3	1.66	0.61
7:0S:424:THR:OG1	7:0S:465:ILE:O	2.18	0.61
12:1A:68:TYR:HB2	12:1A:116:ARG:HE	1.65	0.61
13:1B:1120:GLY:HA2	13:1B:1614:ARG:HH22	1.65	0.61
14:1E:407:PRO:HB2	14:1E:409:ARG:HH12	1.64	0.61
1:0C:328:SER:OG	2:0E:152:ARG:NH2	2.34	0.61
1:0C:512:THR:HB	1:0C:539:ALA:HB3	1.82	0.61
7:0Q:72:LEU:HD22	7:0Q:107:VAL:HG21	1.83	0.61
1:0A:431:ASP:OD2	1:0A:433:THR:OG1	2.19	0.61
7:0S:446:VAL:HB	7:0S:456:ALA:HB3	1.82	0.61
13:1C:1610:GLU:HG3	13:1C:1736:ARG:HB2	1.81	0.61
14:1F:874:GLU:OE2	14:1F:877:ARG:NH2	2.33	0.61
12:0X:356:ARG:HA	12:0X:359:LYS:HE3	1.83	0.61
7:0S:149:ILE:HD13	7:0S:170:ALA:HB2	1.83	0.61
12:1A:13:ARG:NH1	12:1A:94:GLY:O	2.33	0.61
12:1A:123:ARG:O	12:1A:127:MET:HG2	2.01	0.61
13:1B:1533:LEU:HD21	13:1B:1611:GLY:HA3	1.81	0.61
13:1B:1688:GLN:OE1	13:1B:1712:ARG:NH2	2.34	0.61
14:1G:667:ALA:O	14:1G:778:ARG:NH1	2.34	0.61
5:0M:345:LEU:HD22	5:0M:352:ALA:HB1	1.82	0.61
7:0S:588:SER:OG	7:0S:609:ASP:OD2	2.18	0.61
12:0Z:106:THR:H	12:0Z:111:ARG:HG2	1.66	0.61
3:0I:508:ARG:HH22	14:1G:942:MET:HA	1.64	0.60
3:0J:554:GLU:HB2	3:0J:558:ARG:HH21	1.66	0.60
13:1B:1501:LEU:HD12	13:1B:1609:PHE:HZ	1.65	0.60
1:0B:296:ALA:HB2	1:0B:482:ARG:HD3	1.82	0.60
3:0J:496:ALA:O	14:1F:511:ASN:ND2	2.34	0.60
7:0Q:38:SER:H	7:0Q:588:SER:HB2	1.66	0.60
7:0S:423:VAL:HG21	7:0S:437:SER:HB2	1.83	0.60
12:0X:134:ARG:HB2	12:0X:221:GLU:HB2	1.83	0.60
13:1C:1688:GLN:OE1	13:1C:1712:ARG:NH2	2.34	0.60
1:0B:76:ASP:OD1	1:0B:80:ARG:NH2	2.34	0.60
1:0B:152:PHE:HD2	1:0C:149:TRP:HB2	1.66	0.60
3:0I:150:GLN:HA	3:0I:153:LYS:HG2	1.82	0.60
4:0K:115:ASP:HB2	4:0K:118:SER:HB3	1.82	0.60
14:1G:424:PHE:CG	14:1G:490:LEU:HD11	2.36	0.60
14:1G:501:MET:HA	14:1G:506:MET:HE3	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0B:436:LEU:HD12	1:0B:446:MET:HB2	1.84	0.60
1:0D:599:ASP:OD2	1:0D:603:ARG:NH2	2.34	0.60
12:1A:11:ARG:NH2	12:1A:64:GLN:OE1	2.34	0.60
13:1C:1530:LEU:HD12	13:1C:1534:ALA:HA	1.82	0.60
13:1C:1582:SER:OG	13:1C:1583:PRO:HD3	2.01	0.60
14:1F:424:PHE:CG	14:1F:490:LEU:HD11	2.36	0.60
13:1C:1226:GLU:HA	13:1C:1229:ARG:HG2	1.83	0.60
14:1G:490:LEU:O	14:1G:494:LYS:HG2	2.01	0.60
1:0C:342:VAL:HG11	1:0C:383:LEU:HD21	1.82	0.60
1:0B:349:THR:HG22	1:0B:365:GLU:HB3	1.83	0.60
1:0A:546:ARG:NH1	1:0A:588:PRO:O	2.35	0.60
5:0N:286:VAL:O	5:0N:290:GLU:HG3	2.02	0.60
3:0J:447:SER:HB3	3:0J:487:LEU:HD21	1.82	0.60
5:0M:42:THR:HA	5:0M:51:ARG:HA	1.83	0.60
6:0P:11:ARG:NH1	7:0Q:137:ILE:O	2.34	0.60
7:0Q:176:LEU:HD13	7:0Q:226:VAL:HG13	1.84	0.60
12:0Z:181:VAL:HG13	12:0Z:186:GLU:HG2	1.83	0.60
1:0B:141:ILE:HD12	1:0B:144:ARG:HD2	1.83	0.59
1:0C:346:ASP:HB2	2:0E:152:ARG:HH12	1.67	0.59
4:0K:218:ARG:NH2	13:1B:1214:LEU:O	2.35	0.59
4:0L:183:THR:HG21	4:0L:200:TYR:HB2	1.84	0.59
7:0Q:428:LEU:HD11	7:0Q:449:LEU:HD11	1.84	0.59
7:0S:444:LEU:HD21	7:0S:478:ALA:HB2	1.84	0.59
14:1E:460:GLU:O	14:1E:464:LYS:HG2	2.02	0.59
14:1E:1020:MET:SD	14:1E:1021:PRO:HD3	2.42	0.59
14:1G:807:GLY:HA2	14:1G:813:ALA:HB3	1.84	0.59
14:1G:1054:ALA:HB3	14:1G:1057:GLU:HB2	1.84	0.59
1:0B:169:GLU:OE1	1:0C:170:LYS:NZ	2.29	0.59
5:0N:626:SER:O	5:0N:630:SER:HB3	2.02	0.59
14:1F:490:LEU:O	14:1F:494:LYS:HG2	2.01	0.59
5:0N:94:LEU:HD13	5:0N:143:TYR:HB2	1.84	0.59
14:1D:1005:ARG:HA	14:1D:1008:GLU:HG3	1.85	0.59
1:0D:160:ARG:HH22	13:1C:1157:GLY:HA3	1.68	0.59
3:0I:512:GLU:HA	3:0I:529:LEU:H	1.67	0.59
7:0S:481:SER:HB2	7:0S:505:MET:HE1	1.84	0.59
13:1B:1154:GLN:HB2	13:1B:1282:ARG:HH12	1.68	0.59
13:1B:1493:LEU:HG	13:1B:1519:LYS:NZ	2.18	0.59
13:1B:1493:LEU:HG	13:1B:1519:LYS:HZ3	1.68	0.59
14:1E:1025:SER:OG	14:1E:1052:GLN:NE2	2.35	0.59
3:0I:196:ARG:NH2	3:0I:205:GLU:O	2.36	0.59
14:1G:400:ARG:HD3	14:1G:401:PRO:HD2	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0H:62:LYS:N	2:0H:67:ASP:OD2	2.36	0.59
3:0I:453:VAL:HG23	3:0I:516:ARG:HH11	1.66	0.59
5:0N:138:HIS:H	5:0N:140:LYS:HG2	1.67	0.59
7:0S:566:ALA:HA	7:0S:590:PRO:HB3	1.85	0.59
14:1E:504:ASN:OD1	14:1E:505:GLU:N	2.36	0.59
14:1F:820:THR:OG1	14:1F:821:PRO:HD3	2.02	0.59
14:1G:999:TYR:HB3	14:1G:1008:GLU:HG2	1.84	0.59
12:0Z:234:LEU:HD23	12:0Z:344:SER:HA	1.83	0.59
13:1B:1582:SER:OG	13:1B:1583:PRO:HD3	2.03	0.59
13:1C:1117:TYR:HA	13:1C:1123:LYS:NZ	2.17	0.59
14:1D:1020:MET:SD	14:1D:1021:PRO:HD3	2.43	0.59
1:0B:546:ARG:NH1	1:0B:588:PRO:O	2.36	0.59
1:0D:76:ASP:OD2	1:0D:80:ARG:NH2	2.36	0.59
3:0I:555:LYS:HG3	3:0I:558:ARG:HH21	1.68	0.59
5:0M:135:PRO:HA	5:0M:141:VAL:HG13	1.85	0.59
12:0Y:64:GLN:HB3	12:0Y:116:ARG:HH22	1.66	0.59
14:1E:497:LYS:NZ	14:1E:505:GLU:O	2.35	0.59
1:0A:434:VAL:HG21	1:0A:469:THR:HG21	1.83	0.58
1:0A:540:ASN:ND2	1:0A:581:VAL:O	2.34	0.58
1:0B:149:TRP:HB3	1:0C:149:TRP:HB3	1.85	0.58
5:0M:49:LEU:HD13	5:0M:51:ARG:HH21	1.68	0.58
12:1A:106:THR:N	12:1A:111:ARG:HG2	2.15	0.58
13:1C:1413:PRO:HD2	13:1C:1749:ARG:HH12	1.68	0.58
14:1F:999:TYR:HB3	14:1F:1008:GLU:HG2	1.85	0.58
7:0S:72:LEU:HD21	7:0S:83:VAL:HG13	1.84	0.58
12:0X:234:LEU:HD23	12:0X:344:SER:HA	1.85	0.58
12:0Z:134:ARG:HB2	12:0Z:221:GLU:HB2	1.85	0.58
1:0A:178:ARG:HH22	4:0L:134:ARG:HH12	1.51	0.58
1:0B:146:SER:HA	1:0B:149:TRP:CD1	2.39	0.58
12:0Z:84:ASN:ND2	12:0Z:303:ASN:O	2.36	0.58
1:0D:578:GLU:OE1	1:0D:603:ARG:NH2	2.35	0.58
13:1C:1338:ARG:NH1	13:1C:1339:LEU:O	2.37	0.58
14:1E:978:LEU:HD11	14:1E:995:ILE:HG21	1.85	0.58
1:0A:146:SER:HA	1:0A:149:TRP:CD1	2.39	0.58
7:0Q:495:ARG:NH1	7:0Q:497:ARG:O	2.35	0.58
1:0B:89:SER:HA	1:0B:92:CYS:HB2	1.85	0.58
3:0J:434:HIS:HB2	14:1E:1006:ARG:HH12	1.68	0.58
13:1B:1588:LEU:HD21	13:1B:1594:LEU:HB2	1.84	0.58
14:1E:1039:CYS:HA	14:1E:1042:GLU:HB2	1.85	0.58
14:1G:544:VAL:HG11	14:1G:548:GLN:HG3	1.85	0.58
1:0C:407:THR:O	1:0C:410:LYS:NZ	2.32	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0I:141:THR:HG22	16:1M:75:UNK:O	2.03	0.58
7:0Q:168:THR:HB	7:0Q:177:TRP:HE1	1.68	0.58
12:1A:64:GLN:HB3	12:1A:116:ARG:HH22	1.67	0.58
14:1D:978:LEU:HD11	14:1D:995:ILE:HG21	1.84	0.58
14:1G:1029:LEU:HD22	14:1G:1064:ALA:HB1	1.86	0.58
3:0J:438:LYS:HZ1	3:0J:498:THR:HB	1.69	0.58
13:1B:1525:ALA:HB3	13:1B:1618:ARG:HG3	1.86	0.58
2:0H:121:ASP:OD1	2:0H:122:LEU:N	2.36	0.58
3:0J:270:LEU:HD11	3:0J:323:VAL:HG11	1.86	0.58
7:0S:29:TYR:HB3	7:0S:41:LEU:HG	1.86	0.58
12:0Z:280:ARG:NH1	12:0Z:282:ASP:OD2	2.37	0.58
13:1C:1317:GLU:OE2	13:1C:1744:GLN:NE2	2.37	0.58
13:1C:1503:VAL:HG21	13:1C:1751:VAL:HG23	1.86	0.58
14:1E:443:LEU:HD21	14:1E:462:ARG:HE	1.69	0.58
1:0A:436:LEU:HD12	1:0A:446:MET:HB2	1.86	0.57
1:0C:578:GLU:OE1	1:0C:603:ARG:NH2	2.37	0.57
3:0I:193:ALA:HB2	3:0I:333:LEU:HD12	1.86	0.57
3:0I:536:GLU:HB2	14:1G:980:PHE:CE2	2.39	0.57
5:0M:232:ILE:O	5:0M:236:MET:HG2	2.04	0.57
7:0S:21:SER:HB3	7:0S:300:LEU:HD23	1.86	0.57
12:0Z:356:ARG:HA	12:0Z:359:LYS:HE3	1.87	0.57
12:1A:88:PHE:HB3	12:1A:240:VAL:HB	1.86	0.57
14:1F:1029:LEU:HD22	14:1F:1064:ALA:HB1	1.87	0.57
14:1F:960:TRP:CE2	14:1F:991:LEU:HD21	2.39	0.57
14:1G:595:ARG:HA	14:1G:768:ALA:HB2	1.86	0.57
1:0D:579:ASP:OD1	1:0D:580:ALA:N	2.37	0.57
12:0Y:151:LEU:HD21	12:0Y:190:GLN:HG3	1.85	0.57
14:1D:460:GLU:O	14:1D:464:LYS:HG2	2.03	0.57
3:0J:150:GLN:HA	3:0J:153:LYS:HG2	1.86	0.57
4:0K:191:PHE:HB2	4:0K:194:VAL:HB	1.86	0.57
12:0X:63:SER:OG	12:0X:65:GLU:OE1	2.19	0.57
12:0X:139:TYR:HB3	12:0X:151:LEU:HD13	1.87	0.57
13:1B:1338:ARG:NH1	13:1B:1339:LEU:O	2.38	0.57
13:1B:1530:LEU:HD12	13:1B:1534:ALA:HA	1.86	0.57
14:1G:821:PRO:HA	14:1G:825:VAL:HB	1.86	0.57
1:0C:346:ASP:OD2	2:0E:152:ARG:NH2	2.32	0.57
3:0I:538:ARG:HH22	14:1G:983:ARG:HB3	1.70	0.57
3:0J:450:THR:HA	3:0J:489:PRO:HB3	1.85	0.57
7:0Q:588:SER:OG	7:0Q:609:ASP:OD2	2.20	0.57
7:0S:342:VAL:HG11	7:0S:604:VAL:HG11	1.86	0.57
13:1B:1138:HIS:O	13:1B:1281:LYS:NZ	2.31	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1C:1184:PRO:HG2	13:1C:1262:ARG:HH11	1.67	0.57
3:0I:362:ILE:HA	3:0I:366:GLU:HB2	1.86	0.57
12:0X:277:ALA:HB3	12:0X:285:VAL:HG23	1.86	0.57
12:0Y:87:ILE:HG12	12:0Y:307:VAL:HB	1.86	0.57
12:0Z:63:SER:OG	12:0Z:65:GLU:OE1	2.19	0.57
1:0C:398:GLU:O	1:0C:400:GLN:NE2	2.37	0.57
13:1B:1299:LEU:HD21	13:1B:1327:LEU:HD13	1.86	0.57
14:1G:874:GLU:OE2	14:1G:877:ARG:NH2	2.38	0.57
1:0B:434:VAL:HG21	1:0B:469:THR:HG21	1.86	0.57
1:0B:540:ASN:ND2	1:0B:581:VAL:O	2.35	0.57
2:0G:56:ASP:O	2:0G:80:ARG:NE	2.36	0.57
7:0Q:487:SER:OG	7:0Q:489:TRP:NE1	2.26	0.57
7:0S:299:PHE:HD2	7:0S:311:LEU:HD23	1.69	0.57
13:1C:1751:VAL:HG21	13:1C:1759:ALA:HB2	1.85	0.57
14:1F:605:GLU:HG2	14:1F:627:GLY:HA3	1.86	0.57
3:0I:512:GLU:HA	3:0I:528:THR:HA	1.85	0.57
12:0X:351:LEU:O	12:0X:355:GLU:HG2	2.05	0.57
14:1F:406:ILE:HG13	14:1F:407:PRO:HD3	1.86	0.57
1:0D:512:THR:HB	1:0D:539:ALA:HB3	1.86	0.56
2:0F:81:TYR:CZ	2:0F:145:PHE:HB3	2.41	0.56
3:0J:512:GLU:HA	3:0J:528:THR:HA	1.87	0.56
5:0M:222:LEU:HD22	5:0M:232:ILE:HG13	1.86	0.56
12:1A:233:VAL:HG23	12:1A:234:LEU:H	1.69	0.56
14:1D:419:THR:HG22	14:1D:421:VAL:H	1.70	0.56
16:1M:38:UNK:O	16:1M:40:UNK:N	2.38	0.56
16:1L:38:UNK:O	16:1L:40:UNK:N	2.38	0.56
1:0A:184:TYR:CZ	1:0D:184:TYR:HB3	2.40	0.56
7:0Q:141:HIS:HE1	7:0Q:188:GLY:H	1.52	0.56
7:0Q:224:VAL:HG12	7:0Q:231:VAL:HA	1.87	0.56
14:1G:960:TRP:CE2	14:1G:991:LEU:HD21	2.40	0.56
1:0A:162:HIS:HB3	1:0D:163:HIS:CE1	2.40	0.56
1:0B:321:THR:HG22	1:0B:603:ARG:HG2	1.86	0.56
3:0J:504:ALA:HA	3:0J:535:ALA:HB3	1.87	0.56
5:0M:253:ILE:HD12	5:0M:265:VAL:HG13	1.87	0.56
5:0M:419:ASN:H	5:0M:422:MET:HE2	1.70	0.56
6:0O:90:LYS:HG2	6:0O:94:TYR:CE1	2.40	0.56
7:0Q:173:GLU:OE2	7:0Q:190:LYS:NZ	2.39	0.56
7:0Q:215:GLY:HA3	7:0Q:242:VAL:HG11	1.86	0.56
7:0S:559:ALA:HA	7:0S:576:ARG:HH22	1.69	0.56
12:0Z:171:THR:O	12:0Z:236:LYS:NZ	2.37	0.56
13:1B:1314:ALA:HB3	13:1B:1317:GLU:HB2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1B:1326:VAL:HG13	13:1B:1372:VAL:HG13	1.87	0.56
14:1E:1029:LEU:HB2	14:1E:1045:GLU:HB3	1.86	0.56
14:1G:666:LEU:HG	14:1G:670:TYR:HE1	1.69	0.56
3:0I:173:ALA:HA	3:0I:176:ARG:HE	1.70	0.56
3:0I:195:PRO:HD2	3:0I:326:TYR:HE1	1.71	0.56
12:0X:11:ARG:NH2	12:0X:64:GLN:OE1	2.38	0.56
12:1A:137:VAL:HG21	12:1A:190:GLN:NE2	2.19	0.56
14:1G:654:VAL:O	14:1G:657:ARG:C	2.44	0.56
5:0N:243:LEU:HB3	5:0N:279:GLU:HB3	1.86	0.56
7:0Q:559:ALA:HA	7:0Q:576:ARG:HH22	1.69	0.56
12:0X:315:GLU:HB2	12:0X:318:HIS:HB2	1.87	0.56
12:0Y:233:VAL:HG23	12:0Y:234:LEU:H	1.70	0.56
14:1E:820:THR:O	14:1E:823:SER:OG	2.19	0.56
1:0A:208:MET:HE3	1:0D:209:SER:N	2.21	0.56
1:0B:328:SER:HA	1:0B:600:ASN:HA	1.87	0.56
3:0I:452:ALA:HB2	3:0I:489:PRO:HD3	1.88	0.56
5:0M:70:ASP:OD2	5:0M:128:ARG:NH2	2.35	0.56
7:0Q:335:ALA:HB3	7:0Q:338:GLN:HB2	1.86	0.56
13:1B:1155:ASP:O	13:1B:1156:ARG:HG2	2.06	0.56
1:0A:95:PHE:HA	1:0D:91:THR:HG22	1.87	0.56
7:0Q:180:ASP:O	7:0Q:184:GLY:N	2.36	0.56
12:0Z:145:GLU:OE1	12:0Z:290:THR:OG1	2.23	0.56
12:1A:151:LEU:HD21	12:1A:190:GLN:HG3	1.87	0.56
1:0C:76:ASP:OD2	1:0C:80:ARG:NH2	2.39	0.56
1:0C:313:VAL:HG11	1:0C:550:VAL:HG11	1.88	0.56
12:0X:171:THR:HG21	12:0X:297:ARG:HB3	1.86	0.56
14:1D:965:ALA:HA	14:1D:970:ARG:HE	1.71	0.56
14:1E:820:THR:HB	14:1E:826:LEU:HD11	1.88	0.56
1:0C:561:LYS:HG2	1:0C:573:GLU:HG3	1.88	0.56
1:0D:370:TRP:HZ3	1:0D:372:ALA:HB2	1.71	0.56
7:0S:329:LEU:HA	7:0S:346:SER:HA	1.88	0.56
12:0Y:122:PHE:HA	12:0Y:125:VAL:HG22	1.86	0.56
5:0N:252:GLY:HA2	5:0N:255:LYS:HD2	1.88	0.56
7:0S:106:THR:HG22	7:0S:119:ALA:HB3	1.87	0.56
12:0X:170:ASN:O	12:0X:170:ASN:ND2	2.38	0.56
12:1A:155:PRO:HB3	12:1A:159:ASP:HB2	1.88	0.56
14:1D:929:ARG:HG2	14:1D:960:TRP:CE2	2.40	0.56
1:0C:457:ASP:HB3	1:0C:500:VAL:HG12	1.88	0.55
1:0D:394:ILE:O	1:0D:403:VAL:N	2.37	0.55
2:0G:70:ASN:ND2	2:0G:72:PHE:HB2	2.20	0.55
5:0M:274:VAL:HB	5:0M:278:GLY:H	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:0Q:210:ALA:HA	7:0Q:226:VAL:HB	1.87	0.55
12:0X:118:ILE:HD11	12:0X:188:LEU:HD23	1.87	0.55
12:0X:229:SER:HB2	12:0X:352:ARG:HD2	1.89	0.55
13:1C:1142:GLU:HG3	13:1C:1144:THR:H	1.70	0.55
13:1C:1326:VAL:HG13	13:1C:1372:VAL:HG13	1.88	0.55
14:1E:1007:ALA:HA	14:1E:1010:ARG:HD2	1.88	0.55
14:1F:1038:ARG:HG3	14:1F:1041:ALA:HB3	1.87	0.55
1:0D:457:ASP:HB3	1:0D:500:VAL:HG12	1.89	0.55
3:0J:150:GLN:O	3:0J:154:TRP:CD1	2.59	0.55
5:0M:180:PRO:O	5:0M:183:TRP:HD1	1.89	0.55
7:0Q:29:TYR:HB3	7:0Q:41:LEU:HG	1.86	0.55
7:0S:71:MET:HB2	7:0S:86:TRP:HB2	1.87	0.55
7:0S:176:LEU:HD13	7:0S:226:VAL:HG13	1.87	0.55
7:0S:414:ALA:O	7:0S:445:ARG:NH1	2.40	0.55
12:0Y:240:VAL:HG21	12:0Y:296:LEU:HD11	1.88	0.55
13:1C:1201:TRP:HZ2	13:1C:1255:CYS:HG	1.52	0.55
14:1D:820:THR:OG1	14:1D:821:PRO:HD3	2.06	0.55
14:1E:914:ALA:HB1	14:1E:924:TRP:CE2	2.41	0.55
14:1F:1054:ALA:HB3	14:1F:1057:GLU:HB2	1.88	0.55
7:0Q:409:TRP:CD2	7:0Q:452:ARG:HD3	2.40	0.55
13:1B:1317:GLU:OE2	13:1B:1744:GLN:NE2	2.38	0.55
13:1B:1525:ALA:N	13:1B:1620:ASP:OD1	2.39	0.55
16:1L:38:UNK:O	16:1L:39:UNK:C	2.53	0.55
1:0B:166:VAL:HG12	1:0C:166:VAL:HG12	1.88	0.55
1:0C:377:HIS:ND1	1:0C:378:PRO:O	2.40	0.55
6:0O:178:SER:HA	6:0O:181:HIS:CE1	2.41	0.55
7:0S:420:SER:HB2	7:0S:440:MET:HB3	1.88	0.55
13:1B:1314:ALA:HA	13:1B:1410:PHE:HB3	1.87	0.55
16:1M:38:UNK:O	16:1M:39:UNK:C	2.53	0.55
4:0L:137:LYS:HD3	13:1C:1219:GLU:HG3	1.89	0.55
12:0X:178:LEU:HD11	12:0X:219:HIS:HD2	1.72	0.55
12:0Y:155:PRO:HB3	12:0Y:159:ASP:HB2	1.88	0.55
12:0Z:11:ARG:NH2	12:0Z:64:GLN:OE1	2.39	0.55
13:1C:1314:ALA:HA	13:1C:1410:PHE:HB3	1.88	0.55
5:0N:161:LEU:HA	5:0N:174:ALA:HB3	1.88	0.55
12:0X:280:ARG:NH1	12:0X:282:ASP:OD2	2.40	0.55
13:1B:1152:ALA:O	13:1B:1156:ARG:NH1	2.38	0.55
13:1B:1494:VAL:HG13	13:1B:1514:ILE:HG23	1.88	0.55
13:1C:1204:HIS:HB3	13:1C:1274:PHE:CE2	2.42	0.55
14:1D:887:LEU:HA	14:1D:890:TRP:HD1	1.70	0.55
14:1G:406:ILE:HG13	14:1G:407:PRO:HD3	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0D:342:VAL:HG11	1:0D:383:LEU:HD21	1.89	0.55
3:0J:417:GLN:O	3:0J:449:GLY:HA2	2.06	0.55
12:0X:67:ALA:O	12:0X:71:LEU:HB2	2.07	0.55
12:1A:87:ILE:HG12	12:1A:307:VAL:HB	1.88	0.55
14:1E:439:TYR:CE1	14:1E:443:LEU:HD22	2.41	0.55
1:0B:325:HIS:NE2	1:0B:343:THR:OG1	2.35	0.55
1:0D:438:ASP:HB3	1:0D:441:ALA:HB3	1.88	0.55
1:0D:582:GLN:N	1:0D:596:CYS:O	2.40	0.55
13:1B:1204:HIS:HB3	13:1B:1274:PHE:CE2	2.41	0.55
1:0D:102:LEU:HD21	1:0D:108:LEU:HB2	1.89	0.55
3:0I:417:GLN:O	3:0I:449:GLY:HA2	2.06	0.55
7:0Q:423:VAL:HG21	7:0Q:437:SER:HB2	1.89	0.55
7:0S:141:HIS:HE1	7:0S:188:GLY:H	1.55	0.55
12:0Z:92:GLN:HB2	12:0Z:95:ALA:HB2	1.87	0.55
12:0Z:222:MET:SD	12:0Z:223:ARG:N	2.80	0.55
13:1C:1155:ASP:O	13:1C:1156:ARG:HG2	2.07	0.55
13:1C:1299:LEU:HD21	13:1C:1327:LEU:HD13	1.89	0.55
1:0C:370:TRP:HZ3	1:0C:372:ALA:HB2	1.72	0.55
3:0J:458:ARG:HH21	3:0J:513:LEU:HD22	1.72	0.55
7:0S:463:SER:OG	7:0S:483:ASP:OD1	2.25	0.55
14:1G:554:LEU:H	14:1G:576:ARG:HH21	1.54	0.55
5:0N:40:THR:HA	5:0N:54:PRO:HD3	1.89	0.54
6:0O:129:THR:HG23	6:0O:131:THR:H	1.70	0.54
7:0Q:303:THR:HG22	7:0Q:305:GLN:H	1.70	0.54
7:0Q:463:SER:OG	7:0Q:483:ASP:OD1	2.26	0.54
14:1G:1019:LEU:HB3	14:1G:1022:GLU:OE1	2.08	0.54
1:0A:89:SER:HA	1:0A:92:CYS:HB2	1.89	0.54
1:0D:342:VAL:HG22	1:0D:352:MET:HB2	1.87	0.54
7:0S:173:GLU:OE2	7:0S:190:LYS:NZ	2.41	0.54
7:0S:303:THR:HG22	7:0S:305:GLN:H	1.71	0.54
12:0X:92:GLN:HB2	12:0X:95:ALA:HB2	1.88	0.54
12:0Z:98:THR:N	19:0Z:801:ADP:O2A	2.40	0.54
13:1C:1525:ALA:HB3	13:1C:1618:ARG:HG3	1.89	0.54
2:0G:121:ASP:OD1	2:0G:122:LEU:N	2.41	0.54
5:0M:273:ASP:HB2	5:0M:284:GLU:HG2	1.88	0.54
12:0X:181:VAL:HG13	12:0X:186:GLU:HG2	1.88	0.54
12:0Z:139:TYR:HB3	12:0Z:151:LEU:HD13	1.90	0.54
12:1A:300:LEU:HA	12:1A:306:THR:HG21	1.90	0.54
13:1C:1383:GLU:HB2	13:1C:1385:LYS:HG2	1.89	0.54
14:1G:818:MET:HA	14:1G:855:LEU:HD21	1.90	0.54
1:0A:470:ALA:HB1	1:0A:497:CYS:HB2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0B:329:VAL:HA	1:0B:345:SER:HA	1.88	0.54
1:0C:160:ARG:NH2	13:1B:1156:ARG:O	2.41	0.54
3:0J:202:ASN:HB2	3:0J:205:GLU:HB3	1.90	0.54
14:1D:1009:GLN:HG2	14:1D:1032:ARG:HE	1.71	0.54
14:1E:820:THR:OG1	14:1E:821:PRO:HD3	2.07	0.54
14:1G:605:GLU:HG2	14:1G:627:GLY:HA3	1.89	0.54
5:0N:180:PRO:O	5:0N:183:TRP:HD1	1.90	0.54
5:0N:362:THR:HG1	5:0N:364:CYS:HG	1.56	0.54
6:0P:197:THR:OG1	6:0P:198:ALA:N	2.41	0.54
7:0Q:566:ALA:HA	7:0Q:590:PRO:HB3	1.89	0.54
14:1F:818:MET:HA	14:1F:855:LEU:HD21	1.89	0.54
14:1G:1028:LEU:HB3	14:1G:1032:ARG:NH1	2.19	0.54
1:0B:522:ASP:HB3	1:0B:525:MET:HB2	1.90	0.54
12:0Y:13:ARG:NH1	12:0Y:94:GLY:O	2.39	0.54
13:1B:1383:GLU:HB2	13:1B:1385:LYS:HG2	1.88	0.54
14:1D:443:LEU:HD21	14:1D:462:ARG:HE	1.71	0.54
7:0Q:545:HIS:NE2	7:0Q:569:ALA:O	2.34	0.54
12:0X:98:THR:N	19:0X:801:ADP:O2A	2.41	0.54
12:0Y:65:GLU:OE2	12:0Y:116:ARG:NH1	2.39	0.54
14:1F:1019:LEU:HD13	14:1F:1022:GLU:HG3	1.90	0.54
1:0B:115:PRO:HB2	1:0B:118:TYR:HD1	1.73	0.54
1:0C:394:ILE:O	1:0C:403:VAL:N	2.39	0.54
2:0G:44:LEU:HD23	2:0G:135:ILE:HG23	1.90	0.54
3:0J:577:ARG:HG3	3:0J:578:PRO:HD3	1.90	0.54
5:0M:136:ALA:HB3	5:0M:140:LYS:HB2	1.90	0.54
5:0N:135:PRO:HA	5:0N:141:VAL:HG13	1.90	0.54
7:0S:168:THR:HB	7:0S:177:TRP:HE1	1.71	0.54
1:0A:582:GLN:H	1:0A:597:GLY:HA2	1.71	0.54
1:0C:328:SER:HA	1:0C:600:ASN:HA	1.88	0.54
2:0G:81:TYR:CZ	2:0G:145:PHE:HB3	2.42	0.54
3:0J:442:SER:HA	3:0J:496:ALA:HA	1.89	0.54
4:0K:80:HIS:HA	4:0K:83:LEU:HD12	1.88	0.54
12:1A:137:VAL:HG21	12:1A:190:GLN:HE21	1.73	0.54
7:0S:545:HIS:NE2	7:0S:569:ALA:O	2.40	0.54
12:1A:94:GLY:N	19:1A:801:ADP:O3B	2.41	0.54
1:0A:335:HIS:CD2	1:0A:336:PRO:HD2	2.43	0.53
1:0A:396:ASP:HB3	1:0A:399:LYS:HG2	1.89	0.53
1:0B:95:PHE:HA	1:0C:91:THR:HG22	1.90	0.53
1:0C:599:ASP:OD2	1:0C:603:ARG:NH2	2.36	0.53
12:0Y:114:ILE:HG12	12:0Y:239:LEU:HD22	1.89	0.53
12:0Z:84:ASN:HB2	12:0Z:304:CYS:HA	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1D:597:GLY:O	14:1D:601:ARG:N	2.41	0.53
14:1G:563:MET:SD	14:1G:925:ARG:NH2	2.81	0.53
1:0C:540:ASN:ND2	1:0C:581:VAL:O	2.40	0.53
3:0I:453:VAL:HG21	3:0I:516:ARG:HD3	1.89	0.53
3:0J:225:PHE:CE2	6:0P:166:LYS:HG3	2.43	0.53
12:0X:222:MET:SD	12:0X:223:ARG:N	2.81	0.53
12:1A:240:VAL:HG21	12:1A:296:LEU:HD11	1.90	0.53
13:1C:1152:ALA:O	13:1C:1156:ARG:NH1	2.40	0.53
14:1F:666:LEU:HD12	14:1F:669:VAL:HB	1.90	0.53
1:0B:582:GLN:H	1:0B:597:GLY:HA2	1.72	0.53
1:0C:413:ILE:HD13	1:0C:429:SER:HB2	1.90	0.53
12:0Z:15:THR:HG22	12:0Z:313:TRP:HE1	1.73	0.53
13:1C:1525:ALA:N	13:1C:1620:ASP:OD1	2.40	0.53
14:1D:881:ARG:NH1	14:1D:884:GLU:OE1	2.36	0.53
14:1E:825:VAL:O	14:1E:827:SER:N	2.39	0.53
1:0A:578:GLU:OE1	1:0A:603:ARG:NH2	2.42	0.53
1:0B:341:LEU:HD22	1:0B:594:VAL:HG11	1.90	0.53
4:0L:200:TYR:CD1	4:0L:202:PRO:HD3	2.44	0.53
12:0Z:346:ASP:HB2	12:0Z:349:LEU:HB2	1.91	0.53
12:1A:122:PHE:HA	12:1A:125:VAL:HG22	1.90	0.53
14:1F:549:ARG:HG2	14:1F:553:LEU:HG	1.90	0.53
14:1G:567:ASP:OD1	14:1G:568:ARG:N	2.42	0.53
1:0A:377:HIS:ND1	1:0A:378:PRO:O	2.40	0.53
5:0N:222:LEU:HD22	5:0N:232:ILE:HG13	1.90	0.53
13:1B:1610:GLU:HG3	13:1B:1736:ARG:HB2	1.91	0.53
14:1E:597:GLY:O	14:1E:601:ARG:N	2.41	0.53
1:0A:132:ARG:HG3	1:0A:133:ARG:HG3	1.90	0.53
2:0E:70:ASN:ND2	2:0E:72:PHE:HB2	2.23	0.53
5:0N:232:ILE:O	5:0N:236:MET:HB2	2.09	0.53
5:0N:322:LEU:O	5:0N:386:ARG:NH2	2.42	0.53
12:0X:101:MET:HE1	12:0X:239:LEU:HB3	1.91	0.53
12:0X:233:VAL:HG12	12:0X:234:LEU:N	2.23	0.53
13:1B:1142:GLU:HG3	13:1B:1144:THR:H	1.73	0.53
5:0N:337:MET:HG3	5:0N:383:ILE:HG12	1.89	0.53
7:0S:365:VAL:HG22	7:0S:405:CYS:HB2	1.90	0.53
12:1A:184:GLU:O	12:1A:188:LEU:HG	2.09	0.53
13:1C:1112:GLU:HG3	13:1C:1194:PRO:HG3	1.90	0.53
13:1C:1518:ASN:HD21	13:1C:1588:LEU:HB3	1.72	0.53
13:1C:1533:LEU:HD21	13:1C:1611:GLY:HA3	1.90	0.53
14:1D:827:SER:O	14:1D:830:ARG:N	2.41	0.53
14:1G:937:LEU:HD13	14:1G:968:GLU:HG3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0C:457:ASP:HB2	1:0C:499:GLY:HA2	1.89	0.53
7:0Q:584:ALA:HB3	7:0Q:615:TRP:HZ3	1.73	0.53
13:1B:1184:PRO:HG2	13:1B:1262:ARG:HH11	1.72	0.53
1:0B:414:TRP:HZ3	2:0F:46:ARG:HG3	1.74	0.53
3:0J:362:ILE:HA	3:0J:366:GLU:HB2	1.91	0.53
5:0N:249:PHE:O	5:0N:253:ILE:HG12	2.08	0.53
6:0P:10:PHE:HD1	7:0Q:181:PRO:HB2	1.73	0.53
7:0Q:329:LEU:HA	7:0Q:346:SER:HA	1.91	0.53
7:0S:482:GLU:H	7:0S:505:MET:HB2	1.73	0.53
7:0S:512:SER:HB3	7:0S:517:SER:HB2	1.90	0.53
12:1A:80:MET:HG2	12:1A:124:GLU:HB3	1.91	0.53
13:1C:1249:LEU:HD11	13:1C:1255:CYS:HB2	1.89	0.53
13:1C:1314:ALA:HB3	13:1C:1317:GLU:HB2	1.91	0.53
1:0B:323:LYS:H	1:0B:601:THR:HG23	1.72	0.52
12:0X:145:GLU:OE1	12:0X:290:THR:OG1	2.27	0.52
14:1D:439:TYR:CE1	14:1D:443:LEU:HD22	2.44	0.52
14:1D:817:ALA:HB1	14:1D:855:LEU:HD13	1.91	0.52
1:0B:377:HIS:ND1	1:0B:378:PRO:O	2.41	0.52
1:0C:582:GLN:N	1:0C:596:CYS:O	2.42	0.52
7:0S:458:MET:HB3	7:0S:489:TRP:CZ3	2.44	0.52
12:0Z:118:ILE:HD11	12:0Z:188:LEU:HD12	1.90	0.52
14:1E:459:ALA:O	14:1E:462:ARG:HG2	2.10	0.52
14:1E:881:ARG:NH1	14:1E:884:GLU:OE1	2.37	0.52
1:0A:334:LEU:HD12	1:0A:341:LEU:HD13	1.91	0.52
1:0B:184:TYR:CZ	1:0C:184:TYR:HB3	2.44	0.52
3:0I:225:PHE:CE1	6:0O:166:LYS:HG3	2.40	0.52
4:0K:132:LYS:HG2	4:0K:135:ARG:HH21	1.75	0.52
5:0N:42:THR:HB	5:0N:49:LEU:HD22	1.90	0.52
12:0Z:106:THR:O	12:0Z:111:ARG:NH1	2.42	0.52
13:1C:1234:ILE:HD11	13:1C:1269:PHE:HB3	1.90	0.52
13:1C:1769:TRP:HB2	14:1D:522:HIS:NE2	2.25	0.52
1:0B:370:TRP:NE1	2:0F:44:LEU:O	2.42	0.52
1:0D:398:GLU:O	1:0D:400:GLN:NE2	2.42	0.52
3:0I:563:ALA:O	3:0I:567:ARG:HG3	2.07	0.52
3:0J:421:HIS:ND1	3:0J:522:SER:HB2	2.24	0.52
5:0N:193:VAL:HG11	5:0N:217:LEU:HD11	1.90	0.52
7:0Q:6:ARG:NH2	7:0Q:356:THR:O	2.43	0.52
12:0Y:9:PHE:CE2	12:0Y:57:GLY:HA3	2.45	0.52
12:0Z:233:VAL:HG12	12:0Z:234:LEU:N	2.24	0.52
13:1C:1738:ARG:NH1	13:1C:1752:PRO:HG3	2.24	0.52
14:1D:459:ALA:O	14:1D:462:ARG:HG2	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1E:419:THR:HG22	14:1E:421:VAL:H	1.74	0.52
14:1G:864:GLU:HA	14:1G:867:ARG:HD2	1.91	0.52
14:1G:1048:ALA:HA	14:1G:1051:ARG:NH1	2.24	0.52
1:0B:191:ILE:HD11	1:0C:191:ILE:HD11	1.90	0.52
5:0M:243:LEU:HB3	5:0M:279:GLU:HB3	1.91	0.52
12:0X:232:ALA:HB1	12:0X:233:VAL:HG23	1.92	0.52
12:0Z:276:ASN:HB3	12:0Z:280:ARG:HH21	1.75	0.52
13:1C:1234:ILE:HG12	13:1C:1239:LEU:HD12	1.92	0.52
13:1C:1299:LEU:HD11	13:1C:1327:LEU:HB3	1.90	0.52
14:1F:790:LEU:HD13	14:1F:793:LEU:HD12	1.91	0.52
1:0A:166:VAL:HG12	1:0D:166:VAL:HG12	1.91	0.52
3:0J:456:SER:HB2	3:0J:515:THR:HG23	1.91	0.52
5:0N:345:LEU:HD22	5:0N:352:ALA:HB1	1.91	0.52
7:0Q:283:VAL:HG11	7:0Q:301:VAL:HG11	1.92	0.52
7:0Q:342:VAL:HG11	7:0Q:604:VAL:HG11	1.89	0.52
13:1B:1116:VAL:HG22	13:1B:1189:VAL:HG22	1.92	0.52
5:0M:626:SER:O	5:0M:630:SER:HB3	2.09	0.52
7:0S:100:HIS:HD1	7:0S:120:SER:HB2	1.74	0.52
12:0X:215:VAL:HG13	12:0X:240:VAL:HG22	1.92	0.52
12:0Z:109:ALA:O	12:0Z:110:HIS:ND1	2.43	0.52
12:1A:94:GLY:HA2	12:1A:206:ASN:HD22	1.75	0.52
14:1E:1005:ARG:HA	14:1E:1008:GLU:HG3	1.90	0.52
3:0J:512:GLU:HA	3:0J:529:LEU:H	1.74	0.52
7:0S:8:ILE:HD11	7:0S:586:CYS:HB3	1.92	0.52
12:0Z:86:THR:HB	12:0Z:306:THR:HG22	1.92	0.52
13:1B:1769:TRP:HB2	14:1E:522:HIS:NE2	2.25	0.52
14:1D:820:THR:HB	14:1D:826:LEU:HD11	1.91	0.52
14:1D:1025:SER:OG	14:1D:1052:GLN:NE2	2.43	0.52
1:0B:335:HIS:CD2	1:0B:336:PRO:HD2	2.45	0.52
3:0I:450:THR:O	13:1C:1383:GLU:HG2	2.10	0.52
3:0J:512:GLU:HG2	3:0J:528:THR:HB	1.91	0.52
7:0Q:64:ALA:HB2	7:0Q:107:VAL:HG13	1.92	0.52
7:0S:465:ILE:HD12	7:0S:478:ALA:HB1	1.92	0.52
12:0Z:12:THR:OG1	12:0Z:60:GLU:O	2.28	0.52
13:1B:1305:LEU:HD22	13:1B:1325:TYR:HE1	1.75	0.52
13:1C:1127:TRP:HA	13:1C:1132:LEU:HD12	1.92	0.52
13:1C:1521:ARG:NH2	13:1C:1522:TYR:OH	2.42	0.52
14:1F:864:GLU:HA	14:1F:867:ARG:HD2	1.91	0.52
1:0A:367:HIS:ND1	1:0A:389:ASP:OD2	2.33	0.52
1:0D:180:LEU:HD11	4:0L:123:ALA:HB2	1.92	0.52
3:0I:433:CYS:O	3:0I:535:ALA:HA	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0I:453:VAL:HG12	3:0I:518:PRO:HG2	1.91	0.52
7:0Q:106:THR:HG22	7:0Q:119:ALA:HB3	1.90	0.52
7:0S:46:ASN:HD21	7:0S:322:SER:HB3	1.75	0.52
13:1B:1524:LEU:HB3	13:1B:1617:VAL:HG13	1.91	0.52
14:1D:999:TYR:CE2	14:1D:1007:ALA:HB1	2.45	0.52
14:1F:929:ARG:HG2	14:1F:960:TRP:CE2	2.45	0.52
5:0M:203:GLY:HA3	5:0M:308:GLN:HG2	1.92	0.51
5:0M:339:HIS:NE2	5:0M:417:VAL:O	2.40	0.51
7:0S:72:LEU:HD22	7:0S:107:VAL:HG21	1.92	0.51
13:1C:1116:VAL:HA	13:1C:1188:HIS:O	2.10	0.51
1:0A:191:ILE:HD11	1:0D:191:ILE:HD11	1.91	0.51
1:0C:180:LEU:HD11	4:0K:123:ALA:HB2	1.93	0.51
1:0D:316:LEU:HG	1:0D:317:SER:H	1.75	0.51
2:0E:56:ASP:O	2:0E:80:ARG:NE	2.43	0.51
3:0J:193:ALA:HB2	3:0J:333:LEU:HD12	1.93	0.51
5:0M:197:LEU:HD22	5:0M:201:ARG:HH21	1.75	0.51
5:0N:136:ALA:HB3	5:0N:140:LYS:HB2	1.92	0.51
14:1D:966:LEU:HD11	14:1D:999:TYR:CE1	2.45	0.51
1:0A:135:LEU:CB	1:0D:135:LEU:HB3	2.40	0.51
4:0K:196:ILE:HG13	4:0K:198:GLN:H	1.75	0.51
4:0L:80:HIS:O	4:0L:84:THR:HG23	2.11	0.51
12:0X:15:THR:HG22	12:0X:313:TRP:HE1	1.75	0.51
13:1C:1177:THR:HG22	13:1C:1290:VAL:HB	1.91	0.51
14:1F:594:LEU:HD23	14:1F:601:ARG:HG2	1.90	0.51
5:0N:203:GLY:HA3	5:0N:308:GLN:HG2	1.92	0.51
7:0S:298:ALA:HB1	7:0S:310:ARG:HG3	1.93	0.51
12:0Z:229:SER:HB2	12:0Z:352:ARG:HD2	1.93	0.51
13:1B:1325:TYR:HE2	13:1B:1403:ILE:HD13	1.75	0.51
14:1E:999:TYR:CE2	14:1E:1007:ALA:HB1	2.45	0.51
2:0H:81:TYR:CZ	2:0H:145:PHE:HB3	2.46	0.51
13:1C:1135:LEU:HD21	13:1C:1285:LEU:HD21	1.92	0.51
1:0B:132:ARG:HG3	1:0B:133:ARG:HG3	1.93	0.51
1:0C:564:SER:HB2	1:0C:571:GLN:HE21	1.75	0.51
3:0I:457:TRP:NE1	3:0I:483:GLN:HG2	2.25	0.51
5:0M:147:ILE:O	5:0M:151:GLU:HB2	2.10	0.51
5:0M:388:VAL:O	5:0M:392:MET:HG3	2.10	0.51
7:0S:428:LEU:HD11	7:0S:449:LEU:HD11	1.91	0.51
7:0S:584:ALA:HB3	7:0S:615:TRP:HZ3	1.76	0.51
13:1C:1313:VAL:HA	13:1C:1750:TYR:CE1	2.43	0.51
14:1D:493:GLU:HA	14:1D:496:ARG:HH22	1.75	0.51
14:1G:596:ARG:HA	14:1G:596:ARG:NH1	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0A:121:ASN:ND2	1:0D:117:VAL:HG23	2.25	0.51
1:0B:162:HIS:HB3	1:0C:163:HIS:CE1	2.45	0.51
7:0S:74:THR:HB	7:0S:104:VAL:HB	1.92	0.51
12:0Y:123:ARG:O	12:0Y:127:MET:HG2	2.11	0.51
12:0Z:67:ALA:O	12:0Z:71:LEU:HB2	2.11	0.51
12:0Z:215:VAL:HG13	12:0Z:240:VAL:HG22	1.92	0.51
12:1A:136:HIS:CE1	12:1A:180:PRO:HB3	2.46	0.51
1:0D:294:LEU:HD13	1:0D:421:LEU:HD12	1.93	0.51
5:0N:142:HIS:ND1	5:0N:144:MET:HB2	2.26	0.51
13:1B:1313:VAL:HA	13:1B:1750:TYR:CE1	2.43	0.51
1:0B:135:LEU:CB	1:0C:135:LEU:HB3	2.41	0.51
1:0C:537:HIS:HB3	1:0C:556:ASP:HB2	1.93	0.51
3:0I:577:ARG:HG3	3:0I:578:PRO:HD3	1.93	0.51
7:0Q:8:ILE:HD11	7:0Q:586:CYS:HB3	1.93	0.51
7:0Q:298:ALA:HB1	7:0Q:310:ARG:HG3	1.93	0.51
13:1B:1249:LEU:HD11	13:1B:1255:CYS:HB2	1.92	0.51
13:1C:1130:LEU:HB2	13:1C:1132:LEU:HG	1.93	0.51
13:1C:1747:ALA:HB3	13:1C:1749:ARG:HG2	1.91	0.51
3:0J:450:THR:O	13:1B:1383:GLU:HG2	2.11	0.51
5:0M:94:LEU:HD13	5:0M:143:TYR:HB2	1.92	0.51
12:1A:220:VAL:O	12:1A:235:SER:HB2	2.11	0.51
13:1B:1146:THR:HG22	13:1B:1150:LEU:HD13	1.93	0.51
14:1D:506:MET:HG3	14:1D:510:TYR:HE1	1.75	0.51
1:0C:329:VAL:HA	1:0C:345:SER:HA	1.93	0.50
1:0C:438:ASP:HB3	1:0C:441:ALA:HB3	1.93	0.50
4:0K:137:LYS:NZ	13:1B:1219:GLU:HG3	2.25	0.50
12:0Y:300:LEU:HA	12:0Y:306:THR:HG21	1.93	0.50
12:0Z:355:GLU:HA	12:0Z:358:ILE:HG22	1.93	0.50
12:1A:198:ARG:HH21	12:1A:214:THR:HG1	1.57	0.50
13:1B:1193:ASN:ND2	13:1B:1249:LEU:O	2.44	0.50
13:1B:1224:ARG:HD3	13:1B:1229:ARG:HH21	1.76	0.50
13:1C:1116:VAL:HG22	13:1C:1189:VAL:HG22	1.92	0.50
13:1C:1515:VAL:HG12	13:1C:1595:VAL:HA	1.93	0.50
14:1E:1025:SER:HA	14:1E:1028:LEU:HD12	1.92	0.50
4:0K:86:SER:O	4:0K:90:ARG:HG3	2.11	0.50
5:0N:111:ARG:HG3	5:0N:130:VAL:HG21	1.93	0.50
12:1A:65:GLU:OE2	12:1A:116:ARG:NH1	2.43	0.50
12:1A:85:GLY:HA2	12:1A:305:LYS:H	1.76	0.50
14:1D:992:LEU:HD12	14:1D:1011:VAL:HG13	1.93	0.50
14:1D:1006:ARG:HA	14:1D:1009:GLN:OE1	2.11	0.50
14:1G:549:ARG:HG2	14:1G:553:LEU:HG	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0B:368:LYS:NZ	2:0F:40:ASP:OD2	2.39	0.50
2:0G:65:ARG:NH2	2:0G:129:GLY:O	2.37	0.50
3:0J:90:SER:N	3:0J:93:THR:HG1	2.09	0.50
3:0J:196:ARG:HH22	3:0J:215:TRP:HZ3	1.58	0.50
3:0J:457:TRP:HE1	3:0J:483:GLN:HG2	1.76	0.50
7:0S:212:LEU:HB3	7:0S:224:VAL:HG22	1.94	0.50
14:1D:506:MET:HG3	14:1D:510:TYR:CE1	2.46	0.50
14:1G:598:GLY:HA2	14:1G:601:ARG:HG3	1.92	0.50
1:0A:321:THR:HG22	1:0A:603:ARG:HG2	1.92	0.50
1:0A:438:ASP:O	1:0A:442:GLY:N	2.41	0.50
1:0C:470:ALA:HB2	1:0C:500:VAL:HB	1.93	0.50
2:0F:78:PHE:HD1	2:0F:110:PHE:HE2	1.57	0.50
3:0I:545:ARG:HE	3:0I:548:LEU:HD12	1.76	0.50
12:0Z:351:LEU:O	12:0Z:355:GLU:HG2	2.11	0.50
13:1B:1487:MET:O	13:1B:1519:LYS:HE3	2.10	0.50
14:1G:680:GLU:O	14:1G:778:ARG:NH2	2.42	0.50
3:0I:447:SER:HB3	3:0I:487:LEU:HD21	1.93	0.50
3:0J:267:PRO:HG3	3:0J:323:VAL:HG13	1.94	0.50
12:0X:84:ASN:HB2	12:0X:304:CYS:HA	1.93	0.50
12:1A:287:PHE:CE1	12:1A:297:ARG:HA	2.47	0.50
13:1B:1521:ARG:NH2	13:1B:1522:TYR:OH	2.44	0.50
1:0A:115:PRO:HB2	1:0A:118:TYR:HD1	1.76	0.50
3:0I:442:SER:HA	3:0I:496:ALA:HA	1.93	0.50
7:0Q:465:ILE:HD12	7:0Q:478:ALA:HB1	1.93	0.50
12:0X:75:VAL:HG21	12:0X:87:ILE:HD11	1.93	0.50
12:0Z:75:VAL:HG21	12:0Z:87:ILE:HD11	1.94	0.50
14:1F:929:ARG:HE	14:1F:960:TRP:HE1	1.59	0.50
1:0D:329:VAL:HA	1:0D:345:SER:HA	1.93	0.50
3:0J:172:LEU:HD12	3:0J:173:ALA:H	1.77	0.50
3:0J:195:PRO:HD2	3:0J:326:TYR:HE1	1.76	0.50
6:0P:135:ARG:HG2	6:0P:135:ARG:HH11	1.76	0.50
13:1C:1311:GLU:HB2	13:1C:1323:GLN:HE22	1.75	0.50
13:1C:1524:LEU:HB3	13:1C:1617:VAL:HG13	1.94	0.50
14:1D:914:ALA:HB1	14:1D:924:TRP:CE2	2.47	0.50
14:1F:667:ALA:HA	14:1F:670:TYR:HD1	1.76	0.50
1:0D:354:HIS:HB2	1:0D:361:ILE:HD11	1.94	0.50
3:0J:563:ALA:O	3:0J:567:ARG:HG3	2.10	0.50
7:0S:415:HIS:NE2	7:0S:437:SER:OG	2.31	0.50
12:0Z:315:GLU:HB2	12:0Z:318:HIS:HB2	1.93	0.50
13:1C:1241:GLU:OE1	13:1C:1243:ARG:NH1	2.44	0.50
14:1D:397:PRO:HB3	14:1D:686:GLN:HA	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0D:582:GLN:HG2	1:0D:597:GLY:HA2	1.93	0.50
3:0J:564:ALA:O	3:0J:568:VAL:HG23	2.12	0.50
4:0K:80:HIS:O	4:0K:84:THR:HG23	2.12	0.50
4:0L:111:GLY:O	4:0L:115:ASP:HB2	2.11	0.50
5:0N:147:ILE:O	5:0N:151:GLU:HB2	2.12	0.50
12:1A:233:VAL:HG23	12:1A:234:LEU:N	2.26	0.50
14:1G:667:ALA:HB1	14:1G:778:ARG:CZ	2.41	0.50
5:0M:322:LEU:O	5:0M:386:ARG:NH2	2.45	0.49
12:0Y:85:GLY:HA2	12:0Y:305:LYS:H	1.76	0.49
12:0Y:233:VAL:HG23	12:0Y:234:LEU:N	2.27	0.49
13:1B:1146:THR:HG23	13:1B:1149:ARG:HD3	1.94	0.49
13:1B:1241:GLU:OE1	13:1B:1243:ARG:NH1	2.43	0.49
14:1F:807:GLY:HA2	14:1F:813:ALA:HB3	1.94	0.49
14:1G:554:LEU:N	14:1G:576:ARG:HH21	2.09	0.49
14:1G:816:GLU:HA	14:1G:819:LEU:HG	1.94	0.49
16:1L:41:UNK:O	16:1L:43:UNK:N	2.45	0.49
1:0B:367:HIS:ND1	1:0B:389:ASP:OD2	2.34	0.49
1:0C:574:LEU:HD13	1:0C:605:TRP:CD2	2.47	0.49
3:0I:580:PRO:O	3:0I:583:SER:OG	2.29	0.49
12:0Y:220:VAL:O	12:0Y:235:SER:HB2	2.12	0.49
12:0Z:101:MET:SD	12:0Z:113:LEU:HD23	2.51	0.49
12:0Z:136:HIS:HB3	12:0Z:178:LEU:HG	1.94	0.49
13:1B:1747:ALA:HB3	13:1B:1749:ARG:HG2	1.93	0.49
13:1C:1193:ASN:ND2	13:1C:1249:LEU:O	2.45	0.49
14:1D:592:TYR:HA	14:1D:595:ARG:HD2	1.94	0.49
14:1E:493:GLU:HA	14:1E:496:ARG:HH22	1.77	0.49
14:1E:1016:ALA:HB2	14:1E:1028:LEU:HD11	1.92	0.49
16:1M:41:UNK:O	16:1M:43:UNK:N	2.45	0.49
1:0A:319:ASN:HB2	1:0A:606:SER:H	1.78	0.49
1:0A:523:THR:HB	1:0A:524:ARG:HH11	1.77	0.49
1:0D:86:MET:SD	1:0D:86:MET:N	2.85	0.49
2:0G:139:GLU:O	2:0G:143:GLU:HG2	2.12	0.49
3:0I:135:MET:O	3:0I:142:ARG:NH2	2.45	0.49
5:0M:272:CYS:SG	5:0M:288:ARG:HD3	2.53	0.49
13:1B:1177:THR:HA	13:1B:1290:VAL:O	2.12	0.49
13:1B:1226:GLU:OE2	13:1B:1229:ARG:NH1	2.42	0.49
14:1F:606:GLU:HG2	14:1F:609:ARG:HD3	1.93	0.49
14:1G:929:ARG:HG2	14:1G:960:TRP:CE2	2.47	0.49
1:0A:438:ASP:HB3	1:0A:441:ALA:HB3	1.94	0.49
1:0D:335:HIS:HE2	1:0D:380:GLY:HA3	1.78	0.49
3:0J:433:CYS:O	3:0J:535:ALA:HA	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0J:517:PRO:HB2	3:0J:518:PRO:HD3	1.93	0.49
3:0J:574:MET:SD	3:0J:577:ARG:NH2	2.84	0.49
13:1B:1311:GLU:HB2	13:1B:1323:GLN:NE2	2.28	0.49
13:1B:1659:ALA:HB2	16:1M:22:UNK:C	2.39	0.49
1:0B:181:LYS:NZ	4:0K:127:LEU:HD12	2.27	0.49
5:0N:345:LEU:HD12	5:0N:412:LEU:HD23	1.95	0.49
7:0Q:420:SER:HB2	7:0Q:440:MET:HB3	1.94	0.49
12:0Y:94:GLY:N	19:0Y:801:ADP:O1B	2.45	0.49
13:1C:1305:LEU:HD22	13:1C:1325:TYR:HE1	1.77	0.49
14:1D:407:PRO:HB2	14:1D:409:ARG:HH12	1.77	0.49
14:1E:592:TYR:HA	14:1E:595:ARG:HD2	1.95	0.49
14:1G:502:SER:OG	14:1G:505:GLU:OE1	2.28	0.49
1:0A:163:HIS:HB2	1:0D:163:HIS:HB2	1.95	0.49
1:0A:430:LEU:HD12	1:0A:454:SER:HB2	1.93	0.49
1:0B:156:ARG:HG3	1:0C:155:GLU:HB3	1.95	0.49
1:0B:438:ASP:O	1:0B:442:GLY:N	2.42	0.49
2:0E:74:VAL:HG13	2:0E:141:LEU:HD11	1.94	0.49
4:0L:154:GLN:O	4:0L:157:LEU:N	2.45	0.49
5:0M:229:LEU:HD21	5:0M:286:VAL:HA	1.95	0.49
5:0M:252:GLY:HA2	5:0M:255:LYS:HD2	1.95	0.49
7:0Q:116:LEU:O	7:0Q:129:VAL:HA	2.13	0.49
13:1C:1275:LEU:HD12	13:1C:1283:LEU:HB2	1.95	0.49
14:1D:429:ARG:HG3	14:1D:528:LEU:HD11	1.93	0.49
14:1E:992:LEU:HD12	14:1E:1011:VAL:HG13	1.94	0.49
14:1F:654:VAL:O	14:1F:657:ARG:C	2.51	0.49
1:0B:470:ALA:HB2	1:0B:500:VAL:HG13	1.95	0.49
1:0C:332:LEU:HD22	1:0C:341:LEU:HD21	1.95	0.49
5:0N:273:ASP:HB2	5:0N:284:GLU:HG2	1.93	0.49
12:0X:88:PHE:CZ	12:0X:308:MET:HG3	2.47	0.49
12:1A:198:ARG:NH2	12:1A:214:THR:OG1	2.30	0.49
13:1C:1494:VAL:HG13	13:1C:1514:ILE:HG23	1.93	0.49
7:0S:283:VAL:HG11	7:0S:301:VAL:HG11	1.94	0.49
12:0Y:106:THR:N	12:0Y:111:ARG:HG2	2.15	0.49
12:0Z:232:ALA:HB1	12:0Z:233:VAL:HG23	1.95	0.49
13:1C:1146:THR:HG22	13:1C:1150:LEU:HD13	1.94	0.49
14:1D:818:MET:SD	14:1D:857:LYS:HA	2.52	0.49
1:0A:370:TRP:NE1	2:0H:44:LEU:O	2.45	0.49
1:0B:586:PHE:HE2	1:0B:590:GLY:HA2	1.77	0.49
4:0L:115:ASP:HB2	4:0L:118:SER:HB3	1.94	0.49
5:0M:121:LEU:HB3	5:0M:125:GLU:HB2	1.95	0.49
7:0S:463:SER:HB2	7:0S:482:GLU:HB2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:0D:574:LEU:HD13	1:0D:605:TRP:CD2	2.48	0.49
3:0J:215:TRP:CD1	3:0J:235:ARG:HD3	2.47	0.49
12:0X:48:GLN:HG2	12:0X:48:GLN:O	2.12	0.49
12:0X:170:ASN:HD22	12:0X:170:ASN:C	2.15	0.49
12:0Z:71:LEU:HD22	12:0Z:309:VAL:HG22	1.94	0.49
13:1B:1311:GLU:HB2	13:1B:1323:GLN:HE22	1.78	0.49
14:1E:677:LYS:O	14:1E:681:LEU:N	2.43	0.49
14:1E:948:ASN:OD1	14:1E:949:VAL:N	2.46	0.49
14:1G:568:ARG:NH2	14:1G:956:GLU:OE1	2.45	0.49
14:1G:960:TRP:CD2	14:1G:991:LEU:HD21	2.48	0.49
1:0A:75:ILE:HG22	1:0A:111:SER:HB3	1.95	0.48
1:0B:121:ASN:ND2	1:0C:117:VAL:HG23	2.28	0.48
1:0C:190:THR:HG22	4:0K:105:LEU:HB3	1.94	0.48
3:0I:106:GLY:O	3:0I:110:PRO:HD2	2.12	0.48
6:0P:90:LYS:HG2	6:0P:94:TYR:CE1	2.48	0.48
13:1C:1581:ILE:HD11	13:1C:1596:CYS:HB3	1.94	0.48
14:1D:481:ASP:O	14:1D:484:LYS:HG2	2.13	0.48
14:1D:1025:SER:HA	14:1D:1028:LEU:HB2	1.95	0.48
14:1F:650:ARG:CB	14:1F:666:LEU:HD13	2.43	0.48
1:0A:331:ASN:HD22	1:0A:374:VAL:H	1.61	0.48
1:0D:354:HIS:O	1:0D:358:GLY:N	2.45	0.48
2:0H:78:PHE:HD1	2:0H:110:PHE:HE2	1.61	0.48
3:0J:106:GLY:O	3:0J:110:PRO:HD2	2.12	0.48
3:0J:544:GLY:HA2	14:1F:578:LEU:HD11	1.95	0.48
6:0O:66:ASP:OD1	6:0O:67:GLU:N	2.44	0.48
7:0S:224:VAL:HG12	7:0S:231:VAL:HA	1.95	0.48
12:0X:136:HIS:HB3	12:0X:178:LEU:HG	1.95	0.48
13:1B:1135:LEU:HD21	13:1B:1285:LEU:HD21	1.94	0.48
13:1C:1322:LEU:HD23	13:1C:1378:ARG:HG2	1.96	0.48
13:1C:1473:TRP:NE1	13:1C:1498:LEU:HB3	2.29	0.48
1:0A:546:ARG:NH2	1:0A:589:ALA:O	2.46	0.48
1:0B:396:ASP:HB3	1:0B:399:LYS:HG2	1.94	0.48
1:0D:438:ASP:O	1:0D:442:GLY:N	2.42	0.48
3:0J:246:ARG:HH11	3:0J:263:THR:HG21	1.77	0.48
3:0J:306:LEU:HD23	3:0J:309:ARG:HH21	1.78	0.48
13:1C:1117:TYR:HA	13:1C:1123:LYS:HZ3	1.76	0.48
13:1C:1680:LEU:O	13:1C:1683:ARG:HB2	2.13	0.48
14:1D:847:ARG:HH11	14:1D:847:ARG:HA	1.78	0.48
14:1E:1025:SER:HA	14:1E:1028:LEU:HB2	1.95	0.48
14:1G:1038:ARG:HG3	14:1G:1041:ALA:HB3	1.94	0.48
1:0C:319:ASN:HB2	1:0C:604:LEU:HB3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
3:0I:440:HIS:CD2	14:1G:508:LEU:HD22	2.48	0.48
3:0J:580:PRO:O	3:0J:583:SER:OG	2.27	0.48
7:0Q:354:TRP:HD1	7:0Q:361:LEU:HA	1.78	0.48
13:1C:1444:ASP:O	13:1C:1450:ALA:HB2	2.14	0.48
14:1G:905:PHE:HA	14:1G:908:ASP:OD2	2.13	0.48
1:0B:292:ALA:HA	1:0B:295:ASN:HD22	1.77	0.48
1:0C:193:GLU:O	4:0K:98:ARG:NH2	2.47	0.48
1:0D:429:SER:OG	1:0D:430:LEU:N	2.47	0.48
1:0D:473:ASP:OD1	1:0D:475:THR:OG1	2.26	0.48
7:0Q:365:VAL:HG22	7:0Q:405:CYS:HB2	1.95	0.48
12:0X:10:VAL:HG22	12:0X:310:ALA:HB3	1.96	0.48
12:1A:138:SER:OG	12:1A:217:THR:OG1	2.19	0.48
12:1A:139:TYR:HB3	12:1A:151:LEU:HD13	1.96	0.48
13:1B:1495:ASP:HB2	13:1B:1515:VAL:HG23	1.94	0.48
14:1G:797:LEU:HD21	14:1G:847:ARG:HG2	1.95	0.48
1:0B:546:ARG:NH2	1:0B:589:ALA:O	2.46	0.48
3:0I:231:LYS:HE2	3:0I:233:ARG:HD3	1.94	0.48
5:0M:360:ASP:HA	5:0M:367:LEU:HD21	1.96	0.48
7:0Q:512:SER:HB3	7:0Q:517:SER:HB2	1.95	0.48
12:1A:114:ILE:HG12	12:1A:239:LEU:HD22	1.95	0.48
13:1B:1685:PRO:HG2	13:1B:1688:GLN:HB2	1.95	0.48
1:0D:537:HIS:HB3	1:0D:556:ASP:HB2	1.95	0.48
7:0S:354:TRP:HD1	7:0S:361:LEU:HA	1.79	0.48
12:0Y:287:PHE:CE1	12:0Y:297:ARG:HA	2.49	0.48
12:0Z:308:MET:HE2	12:0Z:332:VAL:HG11	1.96	0.48
14:1F:960:TRP:CD2	14:1F:991:LEU:HD21	2.49	0.48
14:1G:1020:MET:HB2	14:1G:1021:PRO:HD3	1.95	0.48
1:0C:116:ASP:HB2	1:0C:119:LEU:HB2	1.95	0.48
1:0C:522:ASP:HB3	1:0C:525:MET:HB3	1.94	0.48
1:0D:116:ASP:HB2	1:0D:119:LEU:HB2	1.94	0.48
12:0X:110:HIS:O	12:0X:116:ARG:NH2	2.43	0.48
12:0Y:64:GLN:HB3	12:0Y:116:ARG:NH2	2.27	0.48
12:0Z:48:GLN:O	12:0Z:48:GLN:HG2	2.13	0.48
14:1E:1000:ARG:HH21	14:1E:1012:LEU:HD21	1.78	0.48
1:0C:160:ARG:HH22	13:1B:1157:GLY:HA3	1.79	0.48
1:0C:577:HIS:NE2	1:0C:595:SER:OG	2.45	0.48
2:0H:68:VAL:HG12	2:0H:126:CYS:SG	2.54	0.48
3:0I:172:LEU:HD12	3:0I:173:ALA:H	1.79	0.48
3:0I:440:HIS:CD2	3:0I:498:THR:HG22	2.49	0.48
7:0Q:296:GLY:O	7:0Q:313:ARG:NH1	2.46	0.48
12:0X:86:THR:HB	12:0X:306:THR:HG22	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1C:1201:TRP:HZ3	13:1C:1203:LEU:HG	1.79	0.48
14:1F:850:LEU:HB2	14:1F:872:TYR:CE1	2.49	0.48
1:0A:411:GLN:HB3	1:0A:430:LEU:HB3	1.96	0.48
1:0C:406:PHE:HB3	1:0C:437:TRP:CH2	2.49	0.48
2:0G:104:TRP:O	2:0G:108:GLN:HG2	2.14	0.48
2:0H:44:LEU:HD11	2:0H:64:CYS:HB2	1.95	0.48
5:0M:49:LEU:HD13	5:0M:51:ARG:NH2	2.29	0.48
12:0X:168:ASN:O	12:0X:342:ASN:ND2	2.45	0.48
12:0Z:78:SER:HB2	12:0Z:83:TYR:HB2	1.96	0.48
13:1C:1311:GLU:HB2	13:1C:1323:GLN:NE2	2.29	0.48
1:0C:395:TRP:HA	1:0C:402:CYS:HA	1.95	0.47
2:0F:59:GLN:NE2	2:0F:73:LEU:HA	2.29	0.47
3:0I:196:ARG:HH22	3:0I:215:TRP:HZ3	1.62	0.47
3:0I:416:PRO:HB3	3:0I:448:ARG:HB2	1.96	0.47
5:0M:111:ARG:HG3	5:0M:130:VAL:HG21	1.95	0.47
12:0X:346:ASP:HB2	12:0X:349:LEU:HB2	1.94	0.47
12:1A:64:GLN:HB3	12:1A:116:ARG:NH2	2.28	0.47
13:1B:1201:TRP:HZ3	13:1B:1203:LEU:HG	1.79	0.47
13:1B:1340:ASP:HB2	13:1B:1392:PRO:HG2	1.96	0.47
14:1F:906:ALA:HA	14:1F:909:VAL:HG22	1.96	0.47
3:0J:458:ARG:HE	3:0J:513:LEU:HD13	1.79	0.47
3:0J:474:GLN:HG3	14:1F:522:HIS:CD2	2.49	0.47
5:0M:369:VAL:HA	5:0M:392:MET:HE1	1.95	0.47
5:0N:387:GLN:O	5:0N:391:VAL:HG23	2.14	0.47
12:0Y:147:LEU:HD11	12:0Y:163:VAL:HG13	1.97	0.47
13:1B:1501:LEU:HD12	13:1B:1609:PHE:CZ	2.48	0.47
14:1E:966:LEU:HD11	14:1E:999:TYR:CE1	2.49	0.47
1:0C:538:PRO:HD2	1:0C:556:ASP:HB2	1.95	0.47
1:0D:377:HIS:ND1	1:0D:378:PRO:O	2.47	0.47
2:0E:139:GLU:O	2:0E:143:GLU:HG2	2.14	0.47
5:0M:286:VAL:O	5:0M:290:GLU:HG3	2.14	0.47
5:0N:63:ALA:HB2	5:0N:128:ARG:HB3	1.97	0.47
5:0N:197:LEU:HD22	5:0N:201:ARG:HH21	1.79	0.47
6:0P:28:ASP:O	6:0P:32:LYS:HG2	2.15	0.47
12:0X:106:THR:O	12:0X:111:ARG:NH1	2.47	0.47
12:0Y:121:VAL:HG12	12:0Y:122:PHE:HD1	1.78	0.47
12:0Y:215:VAL:HG13	12:0Y:240:VAL:HG22	1.95	0.47
12:0Z:142:ILE:HG12	12:0Z:147:LEU:HD23	1.96	0.47
13:1B:1473:TRP:HA	13:1B:1476:TRP:CD2	2.49	0.47
1:0B:470:ALA:HB1	1:0B:497:CYS:HB3	1.96	0.47
2:0G:118:LEU:HD13	2:0G:141:LEU:HD21	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
3:0J:265:LEU:HB3	3:0J:331:ARG:NH2	2.30	0.47
7:0Q:473:ASP:OD1	7:0Q:473:ASP:N	2.47	0.47
7:0S:498:THR:OG1	7:0S:499:THR:N	2.46	0.47
12:0X:97:LYS:HZ3	12:0X:244:GLY:HA2	1.79	0.47
13:1B:1322:LEU:HB2	13:1B:1607:GLN:HG2	1.96	0.47
14:1F:857:LYS:H	14:1F:857:LYS:HD2	1.78	0.47
1:0C:193:GLU:HA	4:0K:98:ARG:HH22	1.80	0.47
3:0J:99:ARG:HG2	3:0J:362:ILE:HD11	1.95	0.47
5:0M:71:ARG:NH1	5:0M:75:ASP:OD2	2.47	0.47
7:0Q:74:THR:HB	7:0Q:104:VAL:HB	1.95	0.47
7:0Q:218:SER:O	7:0Q:218:SER:OG	2.31	0.47
7:0Q:394:ARG:HG2	7:0Q:410:MET:SD	2.54	0.47
12:0Y:301:GLY:N	12:0Y:304:CYS:SG	2.87	0.47
13:1B:1203:LEU:HD23	13:1B:1275:LEU:HA	1.96	0.47
13:1B:1322:LEU:HD23	13:1B:1378:ARG:HG2	1.97	0.47
14:1D:425:LYS:NZ	14:1D:527:ASP:OD2	2.45	0.47
14:1F:937:LEU:HD13	14:1F:968:GLU:HG3	1.97	0.47
5:0M:391:VAL:HA	5:0M:394:VAL:HG22	1.96	0.47
7:0Q:81:SER:OG	7:0Q:100:HIS:O	2.32	0.47
7:0Q:553:ALA:O	7:0Q:561:PHE:HB2	2.14	0.47
12:0X:131:LYS:HG3	12:0X:224:THR:HA	1.96	0.47
12:1A:9:PHE:CE2	12:1A:57:GLY:HA3	2.50	0.47
1:0A:160:ARG:HG2	1:0A:164:LYS:NZ	2.30	0.47
1:0A:208:MET:HE3	1:0D:209:SER:CA	2.44	0.47
1:0A:292:ALA:HA	1:0A:295:ASN:HD22	1.78	0.47
1:0B:75:ILE:HG22	1:0B:111:SER:HB3	1.95	0.47
1:0B:582:GLN:HG2	1:0B:597:GLY:HA2	1.97	0.47
1:0C:466:SER:HA	1:0C:479:TRP:O	2.15	0.47
1:0D:470:ALA:HB2	1:0D:500:VAL:HB	1.95	0.47
3:0I:361:PRO:O	3:0I:363:THR:HG23	2.14	0.47
3:0I:550:GLU:O	3:0I:554:GLU:OE1	2.33	0.47
5:0M:345:LEU:HD12	5:0M:412:LEU:HD23	1.97	0.47
7:0Q:138:VAL:HG21	7:0Q:186:VAL:HG23	1.96	0.47
7:0S:21:SER:HB2	7:0S:293:SER:HB2	1.96	0.47
7:0S:180:ASP:O	7:0S:184:GLY:N	2.46	0.47
13:1B:1116:VAL:HA	13:1B:1188:HIS:O	2.14	0.47
13:1B:1168:MET:SD	13:1B:1284:ARG:HB2	2.54	0.47
13:1B:1607:GLN:OE1	13:1B:1609:PHE:HB3	2.15	0.47
14:1D:912:LEU:HG	14:1G:400:ARG:HH21	1.80	0.47
14:1F:761:LEU:HD11	14:1F:802:LEU:HD11	1.97	0.47
14:1G:929:ARG:HE	14:1G:960:TRP:HE1	1.61	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1M:41:UNK:C	16:1M:43:UNK:N	2.78	0.47
16:1L:41:UNK:C	16:1L:43:UNK:N	2.78	0.47
1:0C:102:LEU:HD21	1:0C:108:LEU:HB2	1.97	0.47
1:0D:430:LEU:HD12	1:0D:454:SER:HB2	1.97	0.47
3:0I:250:PRO:HB2	3:0I:344:VAL:HG13	1.95	0.47
12:1A:291:LYS:HD3	12:1A:291:LYS:HA	1.74	0.47
13:1B:1239:LEU:O	13:1B:1261:PHE:HA	2.14	0.47
13:1C:1684:LEU:HD22	13:1C:1689:TYR:HD1	1.80	0.47
14:1E:481:ASP:O	14:1E:484:LYS:HG2	2.14	0.47
1:0A:543:CYS:SG	1:0A:585:LEU:HD12	2.54	0.47
7:0Q:506:PHE:HD1	7:0Q:522:THR:HG22	1.79	0.47
7:0S:335:ALA:HB3	7:0S:338:GLN:HB2	1.96	0.47
12:1A:37:LYS:HE2	12:1A:46:ASN:HB2	1.97	0.47
13:1C:1138:HIS:O	13:1C:1281:LYS:NZ	2.33	0.47
14:1F:631:ALA:HA	14:1F:638:PRO:HG2	1.97	0.47
14:1F:955:PRO:HB2	14:1F:986:LEU:H	1.79	0.47
14:1G:914:ALA:HB1	14:1G:924:TRP:CE2	2.50	0.47
1:0A:339:PRO:HB2	1:0A:356:PRO:HD3	1.97	0.47
13:1B:1138:HIS:HB3	13:1B:1283:LEU:HD11	1.97	0.47
14:1G:502:SER:O	14:1G:506:MET:HG2	2.15	0.47
1:0A:412:ALA:C	1:0A:429:SER:HG	2.18	0.46
1:0B:160:ARG:HG2	1:0C:159:HIS:NE2	2.30	0.46
2:0G:68:VAL:HG12	2:0G:126:CYS:SG	2.54	0.46
3:0I:311:ARG:HG2	3:0I:311:ARG:O	2.15	0.46
7:0Q:547:LYS:HB3	7:0Q:566:ALA:HB3	1.97	0.46
13:1C:1499:VAL:O	13:1C:1735:LEU:HA	2.15	0.46
1:0B:152:PHE:CD2	1:0C:149:TRP:HB2	2.49	0.46
3:0I:90:SER:N	3:0I:93:THR:HG1	2.13	0.46
12:0Y:210:SER:N	19:0Y:801:ADP:O3B	2.34	0.46
13:1B:1473:TRP:HA	13:1B:1476:TRP:CE2	2.50	0.46
13:1C:1325:TYR:HE2	13:1C:1403:ILE:HD13	1.80	0.46
14:1F:816:GLU:HA	14:1F:819:LEU:HG	1.96	0.46
14:1F:905:PHE:HA	14:1F:908:ASP:OD2	2.15	0.46
1:0A:169:GLU:OE1	1:0D:170:LYS:NZ	2.31	0.46
1:0C:479:TRP:CZ3	1:0C:486:CYS:HB2	2.49	0.46
1:0D:406:PHE:HB3	1:0D:437:TRP:CH2	2.50	0.46
3:0I:135:MET:SD	3:0I:142:ARG:NH1	2.81	0.46
7:0S:465:ILE:HD13	7:0S:480:ALA:HA	1.97	0.46
12:1A:68:TYR:CB	12:1A:116:ARG:HE	2.29	0.46
13:1B:1659:ALA:HB3	13:1B:1660:PRO:HD3	1.97	0.46
14:1D:966:LEU:HD23	14:1D:966:LEU:HA	1.77	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1G:544:VAL:HG21	14:1G:548:GLN:HE21	1.80	0.46
14:1G:631:ALA:HA	14:1G:638:PRO:HG2	1.96	0.46
14:1G:761:LEU:HD11	14:1G:802:LEU:HD11	1.96	0.46
16:1M:40:UNK:HA	16:1M:153:UNK:HA	1.97	0.46
2:0F:59:GLN:HE21	2:0F:73:LEU:HA	1.81	0.46
3:0I:421:HIS:ND1	3:0I:522:SER:HB2	2.30	0.46
3:0I:504:ALA:HA	3:0I:535:ALA:HB3	1.96	0.46
7:0Q:126:LYS:HE2	7:0Q:128:TYR:HE2	1.80	0.46
12:0X:104:GLY:HA2	12:0X:108:TYR:HE1	1.81	0.46
12:0Z:20:SER:HB3	12:0Z:316:PRO:HG3	1.97	0.46
12:1A:215:VAL:HG13	12:1A:240:VAL:HG22	1.96	0.46
12:1A:224:THR:HB	12:1A:231:ARG:NH2	2.31	0.46
13:1C:1479:LEU:HD21	13:1C:1498:LEU:HD13	1.97	0.46
14:1D:955:PRO:CB	14:1D:986:LEU:H	2.28	0.46
14:1D:999:TYR:CB	14:1D:1008:GLU:HG2	2.39	0.46
14:1D:1005:ARG:HA	14:1D:1008:GLU:CG	2.45	0.46
14:1G:504:ASN:O	14:1G:508:LEU:HG	2.15	0.46
16:1M:84:UNK:HA	16:1M:143:UNK:HA	1.97	0.46
1:0D:74:VAL:HG13	1:0D:77:ASP:H	1.80	0.46
1:0D:153:ARG:HA	1:0D:156:ARG:HG2	1.96	0.46
4:0L:150:PHE:HA	4:0L:153:ILE:HG22	1.98	0.46
5:0N:274:VAL:HB	5:0N:278:GLY:H	1.81	0.46
6:0O:99:ALA:O	6:0O:103:HIS:ND1	2.39	0.46
7:0S:547:LYS:HB3	7:0S:566:ALA:HB3	1.98	0.46
12:0Y:198:ARG:HH21	12:0Y:214:THR:HG1	1.61	0.46
12:0Z:182:ARG:HA	12:0Z:182:ARG:HD2	1.63	0.46
12:0Z:290:THR:HG23	12:0Z:293:THR:H	1.80	0.46
12:1A:301:GLY:N	12:1A:304:CYS:SG	2.89	0.46
13:1C:1136:ASN:ND2	13:1C:1478:GLY:HA3	2.31	0.46
14:1G:576:ARG:HH11	14:1G:585:VAL:HG12	1.79	0.46
14:1G:596:ARG:HA	14:1G:596:ARG:CZ	2.46	0.46
16:1L:40:UNK:HA	16:1L:153:UNK:HA	1.97	0.46
16:1L:84:UNK:HA	16:1L:143:UNK:HA	1.97	0.46
1:0A:406:PHE:HB3	1:0A:437:TRP:CH2	2.50	0.46
1:0B:163:HIS:HB2	1:0C:163:HIS:HB2	1.98	0.46
1:0C:430:LEU:HD12	1:0C:454:SER:HB2	1.97	0.46
1:0C:582:GLN:HG2	1:0C:597:GLY:HA2	1.97	0.46
7:0S:463:SER:OG	7:0S:481:SER:O	2.33	0.46
7:0S:512:SER:OG	7:0S:513:ALA:N	2.47	0.46
13:1C:1343:PRO:HG2	13:1C:1391:VAL:HG12	1.97	0.46
14:1G:906:ALA:HA	14:1G:909:VAL:HG22	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0D:316:LEU:HD12	1:0D:605:TRP:HZ3	1.80	0.46
5:0N:51:ARG:O	5:0N:51:ARG:HD2	2.16	0.46
5:0N:176:ALA:HB1	5:0N:713:GLN:NE2	2.31	0.46
12:0X:151:LEU:HD21	12:0X:190:GLN:HB3	1.97	0.46
12:0Y:22:LEU:HB3	12:0Y:33:VAL:HG13	1.97	0.46
12:0Y:134:ARG:HB3	12:0Y:221:GLU:CG	2.46	0.46
13:1B:1112:GLU:HG3	13:1B:1194:PRO:HG3	1.96	0.46
13:1C:1140:ARG:HD3	13:1C:1477:ARG:NH1	2.31	0.46
14:1E:926:GLY:HA2	14:1E:929:ARG:HD2	1.97	0.46
14:1G:910:PHE:HB3	14:1G:927:ALA:HB2	1.97	0.46
1:0B:139:LYS:HZ2	1:0C:135:LEU:HD23	1.80	0.46
1:0D:143:GLY:O	1:0D:146:SER:OG	2.23	0.46
2:0E:152:ARG:HD2	2:0E:152:ARG:O	2.16	0.46
2:0F:47:ASP:OD1	2:0F:48:VAL:N	2.49	0.46
3:0J:226:SER:HB3	3:0J:228:LEU:HD23	1.96	0.46
5:0N:236:MET:CE	5:0N:249:PHE:HA	2.46	0.46
12:0Z:151:LEU:HD21	12:0Z:190:GLN:HB3	1.97	0.46
12:0Z:253:VAL:HG23	12:0Z:257:THR:HB	1.98	0.46
13:1C:1519:LYS:HB2	13:1C:1519:LYS:HE3	1.60	0.46
1:0C:341:LEU:HB3	1:0C:355:MET:SD	2.56	0.46
2:0E:70:ASN:ND2	2:0E:93:ASN:OD1	2.48	0.46
3:0J:286:LEU:HD13	3:0J:293:LEU:HD21	1.97	0.46
12:0X:8:VAL:HG11	12:0X:329:ALA:HB1	1.98	0.46
12:0X:114:ILE:HG21	12:0X:191:PHE:CE1	2.51	0.46
13:1B:1276:HIS:HA	13:1B:1282:ARG:HG2	1.96	0.46
13:1C:1164:ALA:O	13:1C:1168:MET:HG3	2.15	0.46
13:1C:1322:LEU:HB2	13:1C:1607:GLN:HG2	1.98	0.46
14:1G:862:THR:O	14:1G:866:ILE:HG12	2.16	0.46
1:0A:160:ARG:HG2	1:0A:164:LYS:HZ3	1.81	0.46
1:0A:178:ARG:HG3	4:0L:127:LEU:HD22	1.98	0.46
1:0B:332:LEU:HB3	1:0B:341:LEU:HD11	1.98	0.46
1:0B:412:ALA:C	1:0B:429:SER:HG	2.19	0.46
1:0D:540:ASN:HD22	1:0D:582:GLN:HA	1.80	0.46
3:0I:458:ARG:HH21	3:0I:513:LEU:HD22	1.81	0.46
5:0N:121:LEU:HB3	5:0N:125:GLU:HB2	1.97	0.46
7:0Q:179:VAL:HG22	7:0Q:186:VAL:HG22	1.97	0.46
12:0X:101:MET:SD	12:0X:113:LEU:HD23	2.56	0.46
12:0X:290:THR:HG23	12:0X:293:THR:H	1.80	0.46
12:0Z:277:ALA:HB3	12:0Z:285:VAL:HG23	1.97	0.46
12:1A:86:THR:HG22	12:1A:238:ASN:HB2	1.98	0.46
13:1C:1154:GLN:HB2	13:1C:1282:ARG:HH12	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1E:1032:ARG:HD2	14:1E:1038:ARG:HD2	1.97	0.46
1:0A:584:VAL:HG23	1:0A:593:LEU:HD21	1.96	0.45
1:0B:543:CYS:SG	1:0B:585:LEU:HD12	2.56	0.45
1:0C:143:GLY:O	1:0C:146:SER:OG	2.23	0.45
1:0C:426:ALA:HB3	1:0C:458:LEU:HD21	1.98	0.45
1:0C:448:LEU:HD22	1:0C:479:TRP:CE3	2.51	0.45
2:0H:47:ASP:OD1	2:0H:48:VAL:N	2.49	0.45
3:0I:215:TRP:CD1	3:0I:235:ARG:HD3	2.50	0.45
3:0I:250:PRO:HD2	16:1M:102:UNK:HA	1.97	0.45
3:0I:550:GLU:O	3:0I:553:ALA:N	2.49	0.45
3:0I:564:ALA:O	3:0I:568:VAL:HG23	2.16	0.45
3:0J:416:PRO:HB3	3:0J:448:ARG:HB2	1.97	0.45
4:0K:85:ALA:O	4:0K:88:GLN:HG3	2.16	0.45
5:0N:236:MET:HE2	5:0N:249:PHE:HA	1.97	0.45
5:0N:316:VAL:HB	5:0N:317:PRO:HD3	1.98	0.45
7:0Q:349:GLY:O	7:0Q:366:GLN:NE2	2.50	0.45
7:0S:31:ILE:HG22	7:0S:300:LEU:HD21	1.98	0.45
12:0X:65:GLU:OE1	12:0X:65:GLU:N	2.38	0.45
12:0Y:9:PHE:CD2	12:0Y:57:GLY:HA3	2.51	0.45
12:1A:90:TYR:HB2	12:1A:242:LEU:HD12	1.98	0.45
13:1B:1581:ILE:HD11	13:1B:1596:CYS:HB3	1.98	0.45
13:1C:1164:ALA:O	13:1C:1167:ALA:N	2.49	0.45
14:1D:443:LEU:HB3	14:1D:444:PRO:HD3	1.98	0.45
14:1D:890:TRP:CZ3	14:1D:912:LEU:HB3	2.51	0.45
14:1E:429:ARG:HG3	14:1E:528:LEU:HD11	1.97	0.45
14:1E:490:LEU:HB3	14:1E:494:LYS:HE2	1.98	0.45
14:1F:910:PHE:HB3	14:1F:927:ALA:HB2	1.97	0.45
14:1G:650:ARG:CB	14:1G:666:LEU:HD13	2.46	0.45
1:0B:438:ASP:OD2	1:0B:445:ARG:NH2	2.49	0.45
1:0B:512:THR:HG22	1:0B:518:VAL:HG22	1.98	0.45
3:0I:246:ARG:HH11	3:0I:263:THR:HG21	1.81	0.45
3:0I:428:PHE:HE2	14:1G:972:GLU:HB3	1.81	0.45
4:0K:134:ARG:O	4:0K:138:LYS:HG2	2.17	0.45
4:0L:93:GLN:O	4:0L:96:GLN:HG3	2.17	0.45
6:0O:36:GLN:NE2	6:0O:49:ASN:O	2.49	0.45
12:0Y:128:ARG:HG3	12:0Y:133:TYR:HE2	1.82	0.45
13:1C:1301:LEU:HD21	13:1C:1306:ARG:HE	1.81	0.45
1:0A:166:VAL:HG13	1:0D:170:LYS:HZ1	1.81	0.45
3:0I:265:LEU:HB3	3:0I:331:ARG:NH2	2.31	0.45
3:0I:434:HIS:HB2	14:1D:1006:ARG:HH22	1.81	0.45
3:0J:225:PHE:CZ	6:0P:166:LYS:HE3	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
3:0J:440:HIS:CD2	14:1F:508:LEU:HD22	2.52	0.45
7:0Q:463:SER:OG	7:0Q:481:SER:O	2.32	0.45
7:0S:22:ILE:HD11	7:0S:41:LEU:HD11	1.98	0.45
7:0S:72:LEU:HD22	7:0S:107:VAL:HG11	1.98	0.45
12:0Y:138:SER:OG	12:0Y:217:THR:OG1	2.22	0.45
12:1A:7:LYS:HD2	12:1A:7:LYS:N	2.30	0.45
12:1A:134:ARG:HB3	12:1A:221:GLU:CG	2.47	0.45
13:1B:1201:TRP:CZ3	13:1B:1203:LEU:HG	2.52	0.45
13:1C:1615:CYS:SG	13:1C:1731:ILE:HB	2.56	0.45
14:1D:931:PHE:HD1	14:1D:936:GLU:HB2	1.80	0.45
14:1G:1032:ARG:NH1	14:1G:1045:GLU:OE2	2.50	0.45
1:0A:414:TRP:HZ3	2:0H:46:ARG:HG3	1.81	0.45
1:0B:188:GLU:HA	1:0B:191:ILE:HD13	1.98	0.45
1:0D:457:ASP:HB2	1:0D:499:GLY:HA2	1.97	0.45
2:0G:78:PHE:CD1	2:0G:110:PHE:HE2	2.34	0.45
3:0J:250:PRO:HB2	3:0J:344:VAL:HG13	1.97	0.45
4:0L:96:GLN:NE2	4:0L:97:ARG:HG3	2.31	0.45
7:0Q:521:VAL:HG12	7:0Q:527:ILE:HG12	1.98	0.45
13:1B:1130:LEU:HB2	13:1B:1132:LEU:HG	1.97	0.45
14:1E:1048:ALA:O	14:1E:1051:ARG:HG3	2.15	0.45
14:1F:914:ALA:HB1	14:1F:924:TRP:CE2	2.52	0.45
1:0C:396:ASP:HB2	1:0C:403:VAL:HG23	1.99	0.45
2:0E:44:LEU:HB3	2:0E:45:HIS:H	1.52	0.45
3:0I:552:LEU:O	3:0I:556:GLU:HG3	2.17	0.45
3:0J:513:LEU:HA	3:0J:526:CYS:SG	2.56	0.45
7:0S:477:VAL:HG23	7:0S:487:SER:O	2.17	0.45
7:0S:480:ALA:HB3	7:0S:485:THR:O	2.15	0.45
13:1B:1144:THR:CG2	13:1B:1281:LYS:HG2	2.46	0.45
14:1F:595:ARG:HA	14:1F:768:ALA:HB2	1.99	0.45
14:1F:818:MET:C	14:1F:821:PRO:HD2	2.37	0.45
1:0A:159:HIS:CG	1:0D:160:ARG:HG3	2.51	0.45
1:0D:160:ARG:NH2	13:1C:1156:ARG:O	2.50	0.45
3:0I:422:VAL:HG11	3:0I:516:ARG:NH2	2.32	0.45
3:0J:538:ARG:NH1	14:1F:983:ARG:HB3	2.32	0.45
12:0Y:112:GLY:C	12:0Y:115:PRO:HD2	2.37	0.45
12:0Z:65:GLU:OE1	12:0Z:65:GLU:N	2.39	0.45
13:1B:1528:TRP:CZ3	13:1B:1615:CYS:HB3	2.51	0.45
13:1B:1676:ARG:O	13:1B:1680:LEU:HG	2.17	0.45
13:1C:1144:THR:CG2	13:1C:1281:LYS:HG2	2.46	0.45
13:1C:1201:TRP:CZ3	13:1C:1203:LEU:HG	2.52	0.45
14:1D:815:ALA:O	14:1D:819:LEU:HG	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0B:586:PHE:CE2	1:0B:590:GLY:HA2	2.51	0.45
1:0C:156:ARG:HH22	13:1B:1156:ARG:HA	1.82	0.45
3:0J:207:TRP:O	3:0J:211:LEU:HG	2.17	0.45
5:0M:316:VAL:HB	5:0M:317:PRO:HD3	1.99	0.45
7:0S:64:ALA:HB3	7:0S:72:LEU:HB3	1.98	0.45
7:0S:124:ASP:HB3	7:0S:126:LYS:HZ2	1.82	0.45
12:0X:78:SER:HB2	12:0X:83:TYR:HB2	1.99	0.45
12:0X:222:MET:O	12:0X:232:ALA:HA	2.16	0.45
14:1D:1048:ALA:O	14:1D:1051:ARG:HG3	2.16	0.45
1:0C:346:ASP:CB	2:0E:152:ARG:HH12	2.30	0.45
1:0C:350:TRP:CE2	1:0C:364:GLY:HA3	2.51	0.45
1:0D:331:ASN:HD22	1:0D:373:GLY:HA2	1.82	0.45
3:0I:104:MET:O	3:0I:108:MET:HG2	2.17	0.45
3:0I:564:ALA:HA	3:0I:567:ARG:NE	2.32	0.45
3:0J:361:PRO:O	3:0J:363:THR:HG23	2.17	0.45
4:0K:83:LEU:O	4:0K:87:ILE:HG23	2.16	0.45
5:0M:77:VAL:HG22	5:0M:121:LEU:HD11	1.98	0.45
12:0X:253:VAL:HG23	12:0X:257:THR:HB	1.99	0.45
13:1B:1499:VAL:O	13:1B:1735:LEU:HA	2.15	0.45
13:1C:1177:THR:HA	13:1C:1290:VAL:O	2.16	0.45
13:1C:1705:PHE:O	13:1C:1709:MET:HG2	2.16	0.45
14:1E:966:LEU:HD21	14:1E:999:TYR:HE1	1.79	0.45
14:1E:1009:GLN:HB3	14:1E:1013:GLN:HE22	1.82	0.45
14:1F:661:ASP:HB3	14:1F:756:THR:HG23	1.98	0.45
14:1G:905:PHE:O	14:1G:909:VAL:HG13	2.17	0.45
1:0A:181:LYS:HZ1	4:0L:127:LEU:HD12	1.82	0.45
1:0A:411:GLN:HB3	1:0A:430:LEU:HD23	1.99	0.45
1:0B:141:ILE:HA	1:0B:144:ARG:HD2	1.98	0.45
1:0B:208:MET:HE1	1:0C:205:LYS:O	2.16	0.45
1:0B:520:LEU:HD11	1:0B:551:LEU:HD22	1.99	0.45
1:0C:493:HIS:ND1	1:0C:513:ASP:OD2	2.50	0.45
1:0D:350:TRP:CE2	1:0D:364:GLY:HA3	2.51	0.45
1:0D:395:TRP:HA	1:0D:402:CYS:HA	1.97	0.45
3:0I:204:ASP:HA	3:0I:208:THR:HG23	1.99	0.45
4:0L:85:ALA:O	4:0L:88:GLN:HG3	2.17	0.45
7:0Q:464:ARG:HB3	7:0Q:482:GLU:OE1	2.17	0.45
12:0X:146:GLN:HB2	12:0X:148:TYR:CE2	2.52	0.45
12:1A:35:VAL:HG11	12:1A:323:LEU:HD11	1.98	0.45
12:1A:92:GLN:NE2	12:1A:321:GLU:HG3	2.32	0.45
13:1C:1138:HIS:HB3	13:1C:1283:LEU:HD11	1.99	0.45
14:1G:400:ARG:HG3	14:1G:402:LEU:N	2.25	0.45

Continued on next page...

Continued from previous page...

Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:0B:135:LEU:HB3	1:0C:135:LEU:HB3	1.98	0.45
2:0E:81:TYR:CZ	2:0E:145:PHE:HB3	2.52	0.45
3:0I:93:THR:O	3:0I:97:THR:HG23	2.16	0.45
7:0Q:112:ASP:OD2	7:0Q:164:TYR:OH	2.28	0.45
13:1C:1607:GLN:OE1	13:1C:1609:PHE:HB3	2.16	0.45
14:1D:593:CYS:HB2	14:1D:604:ALA:HB2	1.98	0.45
14:1F:862:THR:O	14:1F:866:ILE:HG12	2.17	0.45
1:0A:135:LEU:HB3	1:0D:135:LEU:HB3	1.99	0.44
1:0A:139:LYS:HZ2	1:0D:135:LEU:HD23	1.82	0.44
1:0A:342:VAL:HG11	1:0A:383:LEU:HD21	1.98	0.44
1:0B:209:SER:HA	1:0C:208:MET:CE	2.48	0.44
1:0B:394:ILE:O	1:0B:403:VAL:N	2.46	0.44
1:0C:473:ASP:OD1	1:0C:475:THR:OG1	2.27	0.44
1:0D:330:ALA:N	1:0D:344:ALA:O	2.44	0.44
2:0E:119:PRO:HB2	2:0E:121:ASP:OD1	2.17	0.44
3:0J:503:ALA:HB2	14:1F:541:PRO:HA	1.98	0.44
13:1B:1317:GLU:OE1	13:1B:1750:TYR:OH	2.26	0.44
13:1B:1479:LEU:HD21	13:1B:1498:LEU:HD13	1.97	0.44
13:1C:1495:ASP:HB2	13:1C:1515:VAL:HG23	1.98	0.44
14:1D:1000:ARG:HH21	14:1D:1012:LEU:HD21	1.81	0.44
1:0A:181:LYS:NZ	4:0L:127:LEU:HD12	2.32	0.44
1:0A:394:ILE:O	1:0A:403:VAL:N	2.45	0.44
1:0B:335:HIS:HE2	1:0B:380:GLY:HA3	1.82	0.44
1:0B:346:ASP:CG	2:0F:46:ARG:HH12	2.19	0.44
1:0C:354:HIS:HB2	1:0C:361:ILE:HD11	1.98	0.44
3:0J:205:GLU:HB2	3:0J:217:ARG:HH21	1.83	0.44
3:0J:550:GLU:O	3:0J:554:GLU:HG3	2.17	0.44
7:0Q:124:ASP:HB3	7:0Q:126:LYS:HZ2	1.83	0.44
12:0Y:211:ARG:HB3	12:0Y:260:GLU:OE1	2.16	0.44
12:1A:112:GLY:C	12:1A:115:PRO:HD2	2.38	0.44
14:1D:546:ASP:OD1	14:1D:547:LYS:N	2.50	0.44
14:1D:983:ARG:HG2	14:1G:497:LYS:NZ	2.31	0.44
14:1D:1032:ARG:HH11	14:1D:1038:ARG:HD2	1.83	0.44
14:1E:955:PRO:CB	14:1E:986:LEU:H	2.31	0.44
14:1F:941:ASP:HB2	14:1F:964:VAL:HG11	1.99	0.44
14:1G:757:LEU:HD13	14:1G:779:HIS:HA	1.99	0.44
14:1G:941:ASP:HB2	14:1G:964:VAL:HG11	2.00	0.44
1:0B:319:ASN:HB2	1:0B:606:SER:H	1.82	0.44
1:0B:342:VAL:HG11	1:0B:383:LEU:HD21	2.00	0.44
1:0C:346:ASP:HB2	2:0E:152:ARG:NH1	2.32	0.44
1:0C:370:TRP:CZ3	1:0C:372:ALA:HB2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:0D:156:ARG:HH22	13:1C:1156:ARG:HA	1.82	0.44
1:0D:172:LYS:HE2	1:0D:172:LYS:HB3	1.77	0.44
1:0D:426:ALA:HB3	1:0D:458:LEU:HD21	1.99	0.44
12:0X:338:ASP:O	12:0X:339:LEU:HD23	2.17	0.44
12:0Y:22:LEU:HD12	12:0Y:22:LEU:HA	1.76	0.44
12:0Y:85:GLY:O	12:0Y:237:LEU:HD12	2.17	0.44
12:0Y:134:ARG:HB3	12:0Y:221:GLU:HG2	2.00	0.44
13:1B:1272:PRO:HB2	13:1B:1284:ARG:NH1	2.27	0.44
13:1B:1698:ILE:HD12	13:1B:1701:LEU:HD12	1.98	0.44
13:1B:1738:ARG:NH1	13:1B:1752:PRO:HG3	2.32	0.44
13:1C:1609:PHE:O	13:1C:1736:ARG:HA	2.18	0.44
14:1D:966:LEU:HD21	14:1D:999:TYR:HE1	1.81	0.44
14:1G:796:ALA:O	14:1G:799:GLU:HG3	2.17	0.44
1:0C:74:VAL:HG13	1:0C:77:ASP:H	1.82	0.44
1:0D:319:ASN:HB2	1:0D:604:LEU:HB3	1.99	0.44
3:0I:455:TRP:CH2	3:0I:495:VAL:HG21	2.52	0.44
6:0O:28:ASP:O	6:0O:32:LYS:HG2	2.16	0.44
12:0Y:97:LYS:NZ	12:0Y:242:LEU:O	2.50	0.44
13:1B:1615:CYS:SG	13:1B:1731:ILE:HB	2.57	0.44
13:1C:1533:LEU:HD12	13:1C:1575:LEU:HD22	1.99	0.44
14:1E:593:CYS:HB2	14:1E:604:ALA:HB2	1.98	0.44
14:1E:1032:ARG:HD3	14:1E:1032:ARG:HA	1.79	0.44
1:0A:121:ASN:HD21	1:0D:117:VAL:HG23	1.82	0.44
1:0A:198:TYR:O	1:0A:201:LEU:HG	2.16	0.44
1:0B:438:ASP:HB3	1:0B:441:ALA:HB3	1.99	0.44
1:0D:370:TRP:CZ3	1:0D:372:ALA:HB2	2.52	0.44
3:0I:512:GLU:HG2	3:0I:528:THR:HB	1.99	0.44
4:0L:133:VAL:O	4:0L:137:LYS:HG2	2.17	0.44
5:0M:163:VAL:O	5:0M:169:THR:OG1	2.20	0.44
7:0Q:200:TYR:HE1	7:0Q:222:VAL:HG21	1.83	0.44
7:0S:62:ALA:HB1	7:0S:107:VAL:HG12	2.00	0.44
12:1A:79:LEU:HD22	12:1A:237:LEU:HB2	2.00	0.44
13:1B:1533:LEU:HD12	13:1B:1575:LEU:HD22	2.00	0.44
13:1C:1273:VAL:HG12	13:1C:1274:PHE:N	2.33	0.44
14:1D:778:ARG:O	14:1D:781:PRO:HD2	2.18	0.44
14:1E:427:LYS:O	14:1E:431:ILE:HG12	2.16	0.44
14:1G:544:VAL:HG22	14:1G:547:LYS:NZ	2.32	0.44
14:1G:566:THR:O	14:1G:592:TYR:OH	2.36	0.44
14:1G:1004:GLN:O	14:1G:1008:GLU:HG3	2.18	0.44
1:0A:414:TRP:CZ3	2:0H:50:LYS:HE2	2.52	0.44
5:0M:218:MET:O	5:0M:222:LEU:HG	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:0Q:379:LEU:HD11	7:0Q:398:ARG:HH11	1.82	0.44
12:0Z:359:LYS:HA	12:0Z:362:LYS:HE2	2.00	0.44
13:1B:1297:GLN:HB3	13:1B:1335:LEU:HD12	1.99	0.44
14:1E:1031:ALA:O	14:1E:1035:VAL:HG23	2.17	0.44
14:1F:764:PRO:HA	14:1F:767:ALA:HB3	1.99	0.44
14:1G:955:PRO:HB2	14:1G:986:LEU:H	1.82	0.44
14:1G:1035:VAL:HG12	14:1G:1037:GLN:HG3	1.98	0.44
1:0A:348:LYS:HZ2	1:0A:369:ASP:HA	1.82	0.44
1:0D:313:VAL:HG11	1:0D:550:VAL:HG11	2.00	0.44
3:0I:161:LEU:HD23	3:0I:161:LEU:HA	1.82	0.44
3:0I:554:GLU:HG2	14:1G:606:GLU:CG	2.47	0.44
3:0J:362:ILE:HG22	3:0J:363:THR:N	2.33	0.44
12:0X:88:PHE:HA	12:0X:240:VAL:O	2.17	0.44
12:0X:102:SER:HA	12:0X:112:GLY:HA3	1.99	0.44
12:0Y:102:SER:HB2	12:0Y:191:PHE:HZ	1.81	0.44
12:0Z:110:HIS:O	12:0Z:116:ARG:NH2	2.42	0.44
12:1A:85:GLY:O	12:1A:237:LEU:HD12	2.17	0.44
13:1B:1144:THR:HG21	13:1B:1281:LYS:HG2	2.00	0.44
13:1B:1273:VAL:HG12	13:1B:1274:PHE:N	2.33	0.44
13:1B:1515:VAL:HA	13:1B:1594:LEU:O	2.17	0.44
13:1C:1659:ALA:HB3	13:1C:1660:PRO:HD3	2.00	0.44
14:1D:1005:ARG:HG3	14:1D:1008:GLU:OE2	2.18	0.44
14:1E:1036:ALA:HB1	14:1F:983:ARG:HG2	1.99	0.44
14:1F:544:VAL:HG11	14:1F:548:GLN:H	1.82	0.44
14:1G:577:LEU:HD11	14:1G:586:TRP:CD2	2.53	0.44
14:1G:857:LYS:H	14:1G:857:LYS:HD2	1.82	0.44
1:0C:438:ASP:O	1:0C:442:GLY:N	2.45	0.44
1:0D:461:GLN:OE1	1:0D:466:SER:OG	2.33	0.44
2:0E:146:THR:HG22	2:0E:149:LYS:HE3	2.00	0.44
2:0G:84:ALA:O	2:0G:87:GLN:NE2	2.51	0.44
2:0G:117:ASN:N	2:0G:117:ASN:OD1	2.51	0.44
3:0I:544:GLY:HA2	14:1G:578:LEU:HD11	2.00	0.44
5:0N:142:HIS:CE1	5:0N:144:MET:HB2	2.53	0.44
5:0N:236:MET:CE	5:0N:252:GLY:HA3	2.48	0.44
7:0Q:544:ALA:O	7:0Q:571:ARG:NH1	2.51	0.44
7:0S:500:TRP:NE1	7:0S:535:PRO:HA	2.31	0.44
12:0X:247:ARG:HH21	12:0X:321:GLU:HA	1.83	0.44
12:0Z:222:MET:O	12:0Z:232:ALA:HA	2.17	0.44
12:1A:186:GLU:O	12:1A:190:GLN:OE1	2.35	0.44
13:1C:1203:LEU:HD23	13:1C:1275:LEU:HA	1.99	0.44
14:1D:1032:ARG:NH1	14:1D:1038:ARG:HD2	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1E:925:ARG:O	14:1E:929:ARG:HG3	2.18	0.44
14:1E:961:LEU:HD23	14:1E:961:LEU:HA	1.86	0.44
14:1E:966:LEU:HD23	14:1E:966:LEU:HA	1.83	0.44
14:1F:814:ALA:HA	14:1F:817:ALA:HB3	2.00	0.44
1:0C:153:ARG:HA	1:0C:156:ARG:HG2	1.99	0.44
1:0C:191:ILE:H	1:0C:191:ILE:HD12	1.83	0.44
1:0C:546:ARG:NE	1:0C:588:PRO:HA	2.33	0.44
1:0D:396:ASP:HB3	1:0D:399:LYS:HG3	2.00	0.44
2:0G:70:ASN:ND2	2:0G:93:ASN:OD1	2.51	0.44
3:0I:250:PRO:CD	16:1M:102:UNK:HA	2.48	0.44
3:0I:538:ARG:HH22	14:1G:983:ARG:CB	2.30	0.44
3:0J:153:LYS:HA	3:0J:156:GLU:OE1	2.18	0.44
3:0J:537:VAL:HG21	14:1F:953:GLU:HG2	2.00	0.44
7:0Q:129:VAL:HB	7:0Q:138:VAL:HG12	1.99	0.44
7:0S:3:LEU:HD22	7:0S:615:TRP:HB3	2.00	0.44
7:0S:609:ASP:OD1	7:0S:610:GLY:N	2.51	0.44
12:0X:87:ILE:HB	12:0X:239:LEU:HD13	1.99	0.44
12:0Z:7:LYS:O	12:0Z:307:VAL:HG13	2.17	0.44
13:1B:1344:LEU:HD23	13:1B:1389:VAL:HG11	2.00	0.44
13:1B:1609:PHE:O	13:1B:1736:ARG:HA	2.18	0.44
14:1G:761:LEU:HD22	14:1G:798:ALA:HB1	1.99	0.44
1:0A:438:ASP:OD2	1:0A:445:ARG:NH2	2.50	0.43
1:0D:328:SER:HB2	1:0D:597:GLY:O	2.18	0.43
1:0D:383:LEU:HB2	1:0D:397:PHE:CZ	2.53	0.43
1:0D:546:ARG:NE	1:0D:588:PRO:HA	2.32	0.43
2:0G:29:ASP:OD2	2:0G:31:THR:OG1	2.20	0.43
3:0J:475:PRO:HA	3:0J:476:PRO:HD3	1.92	0.43
13:1C:1276:HIS:HA	13:1C:1282:ARG:HG2	2.00	0.43
14:1D:1032:ARG:HD3	14:1D:1032:ARG:HA	1.72	0.43
14:1E:978:LEU:HD23	14:1E:978:LEU:HA	1.88	0.43
14:1F:1004:GLN:O	14:1F:1008:GLU:HG3	2.18	0.43
1:0A:586:PHE:HE2	1:0A:590:GLY:HA2	1.82	0.43
1:0B:342:VAL:HG11	1:0B:374:VAL:HG11	1.99	0.43
1:0C:327:LEU:HD23	2:0E:152:ARG:NH1	2.28	0.43
7:0S:471:MET:HE1	7:0S:477:VAL:HG12	2.00	0.43
12:0X:232:ALA:HB3	12:0X:349:LEU:HD11	2.00	0.43
12:1A:122:PHE:O	12:1A:125:VAL:HG22	2.18	0.43
14:1E:887:LEU:HA	14:1E:890:TRP:HD1	1.82	0.43
14:1E:999:TYR:CB	14:1E:1008:GLU:HG2	2.47	0.43
14:1G:1048:ALA:HA	14:1G:1051:ARG:HH11	1.83	0.43
1:0A:95:PHE:HB2	1:0D:91:THR:HB	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0B:118:TYR:OH	1:0C:73:GLU:O	2.27	0.43
1:0B:310:ALA:HB2	1:0B:549:GLN:H	1.83	0.43
1:0C:335:HIS:CD2	1:0C:336:PRO:HD2	2.54	0.43
1:0D:191:ILE:H	1:0D:191:ILE:HD12	1.84	0.43
1:0D:411:GLN:HB3	1:0D:430:LEU:HB3	2.00	0.43
1:0D:564:SER:HB2	1:0D:571:GLN:HE21	1.84	0.43
3:0I:362:ILE:HG22	3:0I:363:THR:N	2.33	0.43
3:0J:207:TRP:CE2	3:0J:211:LEU:HD11	2.53	0.43
4:0K:93:GLN:O	4:0K:96:GLN:HG3	2.19	0.43
4:0L:105:LEU:HD23	4:0L:105:LEU:HA	1.83	0.43
5:0N:273:ASP:O	5:0N:284:GLU:HG2	2.18	0.43
7:0Q:212:LEU:HB3	7:0Q:224:VAL:CG2	2.49	0.43
7:0Q:415:HIS:NE2	7:0Q:437:SER:OG	2.38	0.43
7:0Q:526:LYS:HG2	7:0Q:542:VAL:HA	2.00	0.43
12:0Y:224:THR:HB	12:0Y:231:ARG:NH2	2.33	0.43
12:0Z:7:LYS:HB2	12:0Z:307:VAL:HG22	1.99	0.43
12:1A:322:THR:O	12:1A:326:LEU:HD23	2.18	0.43
13:1B:1299:LEU:HD11	13:1B:1327:LEU:HB3	2.01	0.43
13:1C:1242:MET:HG2	13:1C:1245:ARG:HD2	2.00	0.43
14:1G:577:LEU:HD21	14:1G:586:TRP:CZ3	2.52	0.43
14:1G:850:LEU:HB2	14:1G:872:TYR:CE1	2.53	0.43
1:0B:370:TRP:HZ3	1:0B:372:ALA:HB2	1.83	0.43
1:0C:493:HIS:CE1	1:0C:519:LYS:HB2	2.53	0.43
1:0C:576:GLY:O	1:0C:603:ARG:NH1	2.52	0.43
3:0I:549:GLU:HA	3:0I:552:LEU:HD13	2.00	0.43
3:0J:564:ALA:HA	3:0J:567:ARG:NE	2.33	0.43
3:0J:576:ARG:CZ	3:0J:577:ARG:HA	2.48	0.43
3:0J:578:PRO:HA	3:0J:581:HIS:ND1	2.34	0.43
5:0M:362:THR:OG1	5:0M:364:CYS:SG	2.66	0.43
5:0M:367:LEU:HD23	5:0M:367:LEU:HA	1.85	0.43
6:0O:73:ARG:HD3	6:0O:73:ARG:HA	1.77	0.43
7:0Q:60:ILE:HA	7:0Q:74:THR:O	2.18	0.43
7:0Q:446:VAL:HB	7:0Q:456:ALA:HB3	1.99	0.43
12:0Y:56:ASP:HB2	12:0Y:333:ARG:HH22	1.83	0.43
12:0Y:247:ARG:O	12:0Y:248:THR:OG1	2.36	0.43
12:0Z:65:GLU:HG3	12:0Z:116:ARG:NH2	2.27	0.43
12:1A:83:TYR:O	12:1A:235:SER:HA	2.19	0.43
12:1A:134:ARG:HB3	12:1A:221:GLU:HG2	2.00	0.43
13:1C:1272:PRO:HB2	13:1C:1284:ARG:NH1	2.32	0.43
14:1E:398:PRO:HG2	14:1E:400:ARG:NH2	2.33	0.43
14:1E:546:ASP:OD1	14:1E:547:LYS:N	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1F:400:ARG:HH22	14:1F:404:GLU:HB3	1.82	0.43
14:1G:773:LEU:O	14:1G:777:LEU:HG	2.18	0.43
7:0Q:458:MET:CE	7:0Q:489:TRP:HB3	2.48	0.43
7:0S:553:ALA:O	7:0S:561:PHE:HB2	2.17	0.43
12:0Y:139:TYR:HB3	12:0Y:151:LEU:HD13	2.00	0.43
12:0Z:8:VAL:HG11	12:0Z:329:ALA:HB1	2.01	0.43
12:1A:147:LEU:HD11	12:1A:163:VAL:HG13	2.01	0.43
13:1B:1151:ARG:HH22	13:1B:1279:ASP:HA	1.84	0.43
13:1C:1306:ARG:HB3	13:1C:1306:ARG:NH1	2.34	0.43
14:1F:818:MET:HG2	14:1F:858:ALA:HA	2.01	0.43
1:0A:574:LEU:HB3	1:0A:605:TRP:CZ3	2.53	0.43
1:0B:524:ARG:HG3	1:0B:525:MET:SD	2.59	0.43
1:0B:604:LEU:HD23	1:0B:605:TRP:N	2.33	0.43
1:0D:538:PRO:HD2	1:0D:556:ASP:HB2	1.99	0.43
1:0D:560:VAL:HG22	1:0D:581:VAL:HG11	2.01	0.43
2:0H:55:LEU:HD11	2:0H:80:ARG:HB3	2.01	0.43
3:0I:135:MET:HB3	3:0I:142:ARG:HH22	1.84	0.43
3:0J:453:VAL:HB	3:0J:516:ARG:CG	2.48	0.43
7:0S:141:HIS:CE1	7:0S:188:GLY:H	2.35	0.43
7:0S:212:LEU:HB3	7:0S:224:VAL:CG2	2.48	0.43
12:0Z:195:GLU:O	12:0Z:198:ARG:HG2	2.18	0.43
13:1C:1303:PRO:HA	13:1C:1306:ARG:HG3	1.99	0.43
14:1D:925:ARG:O	14:1D:929:ARG:HG3	2.19	0.43
14:1F:504:ASN:O	14:1F:508:LEU:HG	2.18	0.43
14:1G:592:TYR:HA	14:1G:595:ARG:HD2	2.00	0.43
14:1G:601:ARG:HH22	14:1G:634:ARG:CB	2.31	0.43
1:0A:377:HIS:HB3	1:0A:382:CYS:H	1.83	0.43
1:0B:139:LYS:NZ	1:0C:135:LEU:HD23	2.34	0.43
1:0D:542:SER:HB3	1:0D:553:VAL:HG12	2.00	0.43
7:0S:224:VAL:HG12	7:0S:231:VAL:HG22	1.99	0.43
7:0S:354:TRP:CD1	7:0S:361:LEU:HA	2.53	0.43
12:0Y:115:PRO:HB3	12:0Y:188:LEU:HD11	2.01	0.43
13:1B:1687:HIS:ND1	13:1B:1688:GLN:HG3	2.33	0.43
13:1C:1122:PRO:HD2	13:1C:1125:LEU:HD23	2.01	0.43
14:1D:910:PHE:HB3	14:1D:927:ALA:HB2	2.01	0.43
14:1F:566:THR:O	14:1F:592:TYR:OH	2.35	0.43
1:0B:426:ALA:HB3	1:0B:458:LEU:HD21	2.01	0.43
1:0B:574:LEU:HB3	1:0B:605:TRP:CZ3	2.54	0.43
1:0C:545:ASP:HB3	1:0C:548:GLY:HA3	2.01	0.43
1:0D:576:GLY:O	1:0D:603:ARG:NH1	2.52	0.43
3:0I:537:VAL:HG21	14:1G:953:GLU:HG2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:0Q:72:LEU:HG	7:0Q:84:ILE:O	2.18	0.43
7:0Q:354:TRP:CD1	7:0Q:361:LEU:HA	2.54	0.43
7:0S:506:PHE:HD1	7:0S:522:THR:HG22	1.83	0.43
7:0S:521:VAL:HG12	7:0S:527:ILE:HG12	2.00	0.43
12:0Z:87:ILE:HB	12:0Z:239:LEU:HD13	2.01	0.43
13:1B:1313:VAL:O	13:1B:1410:PHE:HB2	2.19	0.43
13:1C:1721:ARG:HH11	13:1C:1723:PRO:HA	1.83	0.43
14:1E:815:ALA:O	14:1E:819:LEU:HG	2.19	0.43
14:1E:891:LEU:O	14:1E:895:GLU:HG2	2.18	0.43
1:0B:191:ILE:H	1:0B:191:ILE:HD12	1.84	0.43
2:0E:45:HIS:HE1	2:0E:47:ASP:OD2	2.01	0.43
2:0E:74:VAL:HG12	2:0E:107:LEU:HD21	2.01	0.43
2:0H:104:TRP:CD1	2:0H:127:VAL:HG12	2.54	0.43
3:0J:100:ARG:O	3:0J:104:MET:HG2	2.19	0.43
3:0J:440:HIS:HD2	14:1F:508:LEU:HD22	1.83	0.43
5:0M:380:VAL:HB	5:0M:383:ILE:HD11	2.00	0.43
5:0N:272:CYS:SG	5:0N:288:ARG:HD3	2.58	0.43
5:0N:380:VAL:HB	5:0N:383:ILE:HD11	1.99	0.43
6:0O:21:ARG:HB3	6:0O:25:ARG:HH22	1.84	0.43
12:0Y:186:GLU:O	12:0Y:190:GLN:OE1	2.37	0.43
12:0Z:100:THR:O	12:0Z:113:LEU:HB2	2.19	0.43
12:0Z:123:ARG:NH1	12:0Z:126:ASP:OD2	2.50	0.43
12:0Z:354:TYR:HA	12:0Z:357:GLN:HB2	2.00	0.43
13:1B:1234:ILE:HG12	13:1B:1239:LEU:HD12	2.01	0.43
13:1B:1315:LEU:HD23	13:1B:1381:PRO:HG2	2.01	0.43
14:1E:907:ALA:HB1	14:1E:931:PHE:CE1	2.54	0.43
14:1F:1006:ARG:HD3	14:1F:1006:ARG:HA	1.85	0.43
16:1M:40:UNK:O	16:1M:42:UNK:N	2.52	0.43
1:0A:341:LEU:HB3	1:0A:355:MET:CE	2.48	0.43
1:0D:82:PHE:O	1:0D:86:MET:HG2	2.18	0.43
1:0D:188:GLU:HG2	1:0D:189:PRO:HD3	2.00	0.43
1:0D:324:GLY:HA3	1:0D:353:TRP:CH2	2.53	0.43
2:0E:68:VAL:HG12	2:0E:126:CYS:SG	2.59	0.43
3:0J:225:PHE:HZ	6:0P:162:ASP:HB3	1.84	0.43
5:0N:71:ARG:NH1	5:0N:75:ASP:OD2	2.52	0.43
7:0S:126:LYS:HE2	7:0S:128:TYR:HE2	1.83	0.43
7:0S:210:ALA:HA	7:0S:226:VAL:HB	1.99	0.43
12:1A:23:LYS:HA	12:1A:32:SER:O	2.18	0.43
13:1C:1445:ASP:OD1	13:1C:1445:ASP:N	2.51	0.43
14:1E:818:MET:O	14:1E:821:PRO:HD2	2.18	0.43
14:1G:966:LEU:HG	14:1G:974:ALA:HB1	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1G:1019:LEU:HB3	14:1G:1022:GLU:CD	2.38	0.43
16:1L:40:UNK:O	16:1L:42:UNK:N	2.52	0.43
1:0D:561:LYS:HG2	1:0D:573:GLU:HG3	2.01	0.42
2:0H:128:GLN:HA	2:0H:128:GLN:OE1	2.19	0.42
3:0J:453:VAL:HB	3:0J:516:ARG:HG2	2.00	0.42
7:0Q:516:VAL:HG21	7:0Q:533:ARG:HH21	1.84	0.42
12:1A:247:ARG:O	12:1A:248:THR:OG1	2.37	0.42
13:1B:1536:PRO:HA	13:1B:1537:PRO:HD3	1.90	0.42
14:1D:518:LEU:HD12	14:1D:522:HIS:HE1	1.83	0.42
1:0B:166:VAL:HG13	1:0C:170:LYS:HZ1	1.83	0.42
2:0G:97:SER:HA	2:0G:100:LYS:HE2	2.02	0.42
3:0J:424:PHE:HD1	3:0J:445:LEU:HB3	1.84	0.42
7:0Q:476:HIS:O	7:0Q:488:LEU:HD12	2.19	0.42
7:0S:102:VAL:HG11	7:0S:122:PHE:HB2	2.00	0.42
7:0S:520:THR:OG1	7:0S:528:GLN:HB2	2.19	0.42
12:0Y:13:ARG:NH2	19:0Y:801:ADP:H1'	2.34	0.42
12:0Y:86:THR:HG22	12:0Y:238:ASN:HB2	2.00	0.42
12:1A:102:SER:HB2	12:1A:191:PHE:HZ	1.83	0.42
13:1B:1473:TRP:NE1	13:1B:1498:LEU:HB3	2.34	0.42
13:1C:1223:PRO:HG3	13:1C:1232:ASP:OD2	2.19	0.42
14:1D:1029:LEU:HB2	14:1D:1045:GLU:HB3	2.01	0.42
1:0B:375:ASP:OD2	1:0B:418:PHE:N	2.44	0.42
1:0C:317:SER:HA	1:0C:605:TRP:HA	2.01	0.42
1:0D:127:ASP:O	1:0D:131:LEU:HB2	2.19	0.42
1:0D:414:TRP:CZ3	2:0G:50:LYS:HE3	2.54	0.42
1:0D:518:VAL:HG21	1:0D:553:VAL:HG11	2.02	0.42
1:0D:522:ASP:HB3	1:0D:525:MET:HB3	2.00	0.42
2:0G:109:ALA:O	2:0G:113:ARG:HG3	2.19	0.42
3:0I:178:PRO:O	3:0I:182:THR:HG23	2.20	0.42
3:0I:512:GLU:HA	3:0I:529:LEU:N	2.32	0.42
3:0I:578:PRO:HA	3:0I:581:HIS:ND1	2.35	0.42
5:0N:633:PRO:HA	5:0N:638:TYR:CG	2.54	0.42
7:0Q:144:GLU:HG3	7:0Q:147:LYS:HB2	2.01	0.42
7:0S:338:GLN:NE2	7:0S:381:ARG:HE	2.17	0.42
12:0Y:59:LEU:HD21	12:0Y:70:THR:HG21	2.01	0.42
12:0Y:68:TYR:OH	12:0Y:117:ALA:HA	2.19	0.42
12:0Z:5:ALA:HA	12:0Z:336:THR:HG23	2.02	0.42
13:1C:1473:TRP:CH2	13:1C:1736:ARG:HB3	2.54	0.42
14:1D:433:ARG:HA	14:1D:433:ARG:HD2	1.89	0.42
1:0A:191:ILE:H	1:0A:191:ILE:HD12	1.84	0.42
1:0B:584:VAL:HG23	1:0B:593:LEU:HD21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0I:553:ALA:HA	3:0I:556:GLU:CD	2.40	0.42
5:0N:70:ASP:OD2	5:0N:128:ARG:NH2	2.39	0.42
5:0N:391:VAL:HA	5:0N:394:VAL:HG22	2.00	0.42
7:0Q:62:ALA:HB1	7:0Q:107:VAL:HG12	2.00	0.42
7:0Q:445:ARG:HA	7:0Q:456:ALA:O	2.20	0.42
13:1B:1120:GLY:HA2	13:1B:1614:ARG:NH2	2.33	0.42
13:1B:1445:ASP:OD1	13:1B:1445:ASP:N	2.51	0.42
14:1D:427:LYS:O	14:1D:431:ILE:HG12	2.19	0.42
14:1G:818:MET:HE3	14:1G:821:PRO:HB2	2.01	0.42
1:0B:355:MET:SD	1:0B:604:LEU:HD12	2.59	0.42
1:0C:127:ASP:O	1:0C:131:LEU:HB2	2.19	0.42
1:0C:393:LYS:HB3	1:0C:402:CYS:SG	2.60	0.42
2:0G:44:LEU:HB3	2:0G:45:HIS:H	1.56	0.42
3:0I:517:PRO:HB2	3:0I:518:PRO:HD3	1.99	0.42
3:0I:568:VAL:O	3:0I:571:ASP:HB2	2.19	0.42
3:0J:104:MET:O	3:0J:108:MET:HG2	2.20	0.42
6:0P:16:LEU:HD23	6:0P:16:LEU:H	1.84	0.42
7:0Q:57:ASP:OD2	7:0Q:80:ASN:ND2	2.53	0.42
7:0S:22:ILE:HD12	7:0S:29:TYR:O	2.20	0.42
12:0Z:14:PRO:HD2	19:0Z:801:ADP:C6	2.55	0.42
13:1C:1265:VAL:O	13:1C:1291:THR:OG1	2.29	0.42
13:1C:1297:GLN:HB3	13:1C:1335:LEU:HD12	2.01	0.42
14:1E:594:LEU:HB3	14:1E:768:ALA:HB3	2.00	0.42
2:0H:123:VAL:O	2:0H:127:VAL:HG13	2.20	0.42
3:0I:503:ALA:HB2	14:1G:541:PRO:HA	2.00	0.42
3:0I:576:ARG:CZ	3:0I:577:ARG:HA	2.50	0.42
12:0X:5:ALA:HA	12:0X:336:THR:HG23	2.02	0.42
12:0X:14:PRO:HD2	19:0X:801:ADP:C6	2.55	0.42
12:0X:139:TYR:HD1	12:0X:150:LEU:HD13	1.84	0.42
12:0Y:98:THR:O	12:0Y:103:GLY:HA2	2.19	0.42
13:1B:1202:GLN:O	13:1B:1276:HIS:HB3	2.20	0.42
13:1C:1175:PHE:HB2	13:1C:1289:ALA:HB2	2.00	0.42
13:1C:1244:PRO:HD2	13:1C:1257:VAL:HG13	2.01	0.42
14:1E:983:ARG:HG2	14:1F:497:LYS:NZ	2.34	0.42
14:1E:988:ASP:O	14:1E:1018:LYS:NZ	2.52	0.42
1:0A:327:LEU:HD12	1:0A:327:LEU:HA	1.78	0.42
1:0B:129:ALA:HA	1:0B:132:ARG:HG2	2.02	0.42
1:0D:329:VAL:HB	1:0D:596:CYS:HB2	2.01	0.42
2:0H:55:LEU:HD23	2:0H:77:ILE:HG12	2.02	0.42
3:0J:419:GLY:HA2	13:1B:1352:TRP:NE1	2.35	0.42
5:0M:63:ALA:HB2	5:0M:128:ARG:HB3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:0S:353:VAL:HB	7:0S:363:CYS:SG	2.60	0.42
12:0X:260:GLU:O	12:0X:264:ILE:HG12	2.20	0.42
12:0X:276:ASN:HB3	12:0X:280:ARG:HH21	1.84	0.42
13:1B:1448:ALA:HA	13:1B:1451:LEU:HD13	2.01	0.42
13:1B:1751:VAL:HG13	13:1B:1756:ARG:HG2	2.01	0.42
14:1D:1023:SER:C	14:1D:1027:ARG:HH21	2.23	0.42
14:1F:1035:VAL:HG12	14:1F:1037:GLN:HG3	2.01	0.42
14:1F:1048:ALA:HA	14:1F:1051:ARG:NH1	2.34	0.42
1:0A:507:THR:HG23	1:0A:524:ARG:HH22	1.84	0.42
1:0B:377:HIS:HB3	1:0B:382:CYS:H	1.85	0.42
1:0D:493:HIS:CE1	1:0D:519:LYS:HB2	2.55	0.42
2:0F:62:LYS:N	2:0F:67:ASP:OD2	2.53	0.42
3:0J:270:LEU:HD13	3:0J:319:LEU:HG	2.01	0.42
4:0L:109:VAL:O	4:0L:113:LEU:HG	2.20	0.42
4:0L:121:ALA:O	4:0L:124:GLU:HG3	2.19	0.42
5:0M:640:PRO:O	5:0M:644:THR:HG23	2.19	0.42
5:0N:193:VAL:HB	5:0N:196:LEU:HD12	2.02	0.42
6:0O:194:LYS:HA	6:0O:194:LYS:HD3	1.86	0.42
7:0Q:100:HIS:ND1	7:0Q:120:SER:HB2	2.34	0.42
7:0Q:102:VAL:HG11	7:0Q:122:PHE:HD2	1.84	0.42
7:0Q:506:PHE:CD1	7:0Q:522:THR:HG22	2.55	0.42
12:0X:12:THR:OG1	12:0X:60:GLU:O	2.37	0.42
12:0Z:88:PHE:HA	12:0Z:240:VAL:O	2.19	0.42
12:1A:68:TYR:OH	12:1A:117:ALA:HA	2.20	0.42
13:1B:1140:ARG:HD3	13:1B:1477:ARG:NH1	2.35	0.42
13:1B:1515:VAL:HG12	13:1B:1595:VAL:HG22	2.02	0.42
13:1B:1701:LEU:HD23	13:1B:1701:LEU:HA	1.88	0.42
14:1D:849:ARG:NE	14:1D:868:PHE:HA	2.35	0.42
14:1F:761:LEU:O	14:1F:764:PRO:HD2	2.20	0.42
14:1G:814:ALA:HA	14:1G:817:ALA:HB3	2.02	0.42
1:0B:129:ALA:HB1	1:0B:133:ARG:CZ	2.49	0.42
1:0C:133:ARG:HG3	1:0C:134:GLU:N	2.35	0.42
1:0C:396:ASP:HB2	1:0C:403:VAL:CG2	2.49	0.42
1:0D:205:LYS:HE2	1:0D:205:LYS:HB3	1.91	0.42
2:0G:146:THR:HG22	2:0G:149:LYS:HE3	2.02	0.42
3:0J:467:HIS:CD2	14:1F:915:SER:HB2	2.54	0.42
4:0K:84:THR:HA	4:0K:87:ILE:HG12	2.01	0.42
4:0L:79:ASP:O	4:0L:83:LEU:HG	2.20	0.42
7:0Q:224:VAL:HG12	7:0Q:231:VAL:HG22	2.01	0.42
7:0Q:609:ASP:OD1	7:0Q:610:GLY:N	2.52	0.42
7:0S:283:VAL:HG12	7:0S:318:LEU:HD11	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:0Z:138:SER:OG	12:0Z:217:THR:OG1	2.36	0.42
12:1A:8:VAL:HG11	12:1A:329:ALA:HB1	2.00	0.42
13:1C:1390:GLU:HG2	13:1C:1402:VAL:HG22	2.01	0.42
13:1C:1690:MET:HE2	13:1C:1705:PHE:HB2	2.02	0.42
14:1D:965:ALA:HB1	14:1D:970:ARG:HG3	2.02	0.42
14:1F:1020:MET:HB2	14:1F:1021:PRO:HD3	2.02	0.42
1:0A:332:LEU:HB3	1:0A:341:LEU:HD11	2.02	0.42
1:0D:582:GLN:N	1:0D:597:GLY:HA2	2.28	0.42
3:0I:451:ALA:HA	13:1C:1382:LEU:O	2.19	0.42
5:0M:628:ILE:HD12	5:0M:628:ILE:H	1.85	0.42
5:0N:412:LEU:HD12	5:0N:412:LEU:HA	1.89	0.42
6:0P:194:LYS:HA	6:0P:194:LYS:HD3	1.88	0.42
12:0X:7:LYS:HB2	12:0X:307:VAL:HG22	2.02	0.42
12:0Z:221:GLU:HB3	12:0Z:233:VAL:HG22	2.00	0.42
12:1A:139:TYR:HD1	12:1A:216:PHE:CD1	2.38	0.42
13:1B:1170:PRO:HG3	13:1B:1284:ARG:HD2	2.01	0.42
13:1C:1202:GLN:O	13:1C:1276:HIS:HB3	2.20	0.42
13:1C:1769:TRP:HB2	14:1D:522:HIS:CD2	2.54	0.42
14:1D:851:LEU:HA	14:1D:854:GLN:OE1	2.20	0.42
14:1D:966:LEU:HD12	14:1D:995:ILE:HD13	2.02	0.42
14:1D:1016:ALA:HB2	14:1D:1028:LEU:HD11	2.01	0.42
14:1E:972:GLU:HB3	14:1E:976:LYS:NZ	2.35	0.42
14:1F:400:ARG:NH1	14:1F:403:LEU:O	2.53	0.42
14:1G:1022:GLU:OE1	14:1G:1022:GLU:N	2.53	0.42
1:0A:418:PHE:HE1	1:0A:439:LEU:HD11	1.85	0.41
1:0A:433:THR:HG21	1:0A:449:ARG:HH11	1.85	0.41
1:0A:582:GLN:HG2	1:0A:597:GLY:HA2	2.02	0.41
1:0B:344:ALA:HB2	1:0B:374:VAL:HG23	2.02	0.41
1:0C:324:GLY:HA3	1:0C:353:TRP:CH2	2.55	0.41
1:0D:214:LYS:HD3	1:0D:214:LYS:HA	1.89	0.41
2:0G:74:VAL:HG13	2:0G:141:LEU:HD11	2.01	0.41
3:0I:453:VAL:CG2	3:0I:516:ARG:HD3	2.49	0.41
3:0J:93:THR:O	3:0J:97:THR:HG23	2.20	0.41
3:0J:192:ARG:HA	3:0J:192:ARG:HD3	1.83	0.41
5:0N:218:MET:O	5:0N:222:LEU:HG	2.20	0.41
6:0P:135:ARG:HG2	6:0P:135:ARG:NH1	2.35	0.41
7:0S:464:ARG:HB3	7:0S:482:GLU:OE1	2.20	0.41
12:0Y:322:THR:O	12:0Y:326:LEU:HD23	2.19	0.41
13:1C:1239:LEU:O	13:1C:1261:PHE:HA	2.20	0.41
1:0B:101:GLU:O	1:0B:105:THR:HG23	2.20	0.41
1:0D:396:ASP:HB2	1:0D:403:VAL:CG2	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0J:265:LEU:HD21	3:0J:330:LEU:HD22	2.03	0.41
3:0J:311:ARG:O	3:0J:311:ARG:HG2	2.20	0.41
3:0J:552:LEU:O	3:0J:556:GLU:HG3	2.20	0.41
4:0K:150:PHE:HA	4:0K:153:ILE:HG22	2.02	0.41
5:0M:176:ALA:HB1	5:0M:713:GLN:NE2	2.35	0.41
5:0M:292:ASN:HA	5:0M:296:SER:HB3	2.02	0.41
5:0N:334:SER:HA	5:0N:424:HIS:HD1	1.84	0.41
6:0P:32:LYS:HE3	6:0P:48:GLU:HG3	2.02	0.41
7:0S:60:ILE:HA	7:0S:74:THR:O	2.20	0.41
7:0S:72:LEU:HD13	7:0S:116:LEU:HD11	2.01	0.41
7:0S:524:ASP:HB3	7:0S:526:LYS:HE2	2.02	0.41
12:0Y:258:LEU:O	12:0Y:262:GLN:HG2	2.20	0.41
12:0Y:319:ASN:O	12:0Y:323:LEU:HD23	2.19	0.41
13:1B:1136:ASN:ND2	13:1B:1478:GLY:HA3	2.35	0.41
14:1D:1009:GLN:O	14:1D:1010:ARG:C	2.57	0.41
14:1G:544:VAL:HG22	14:1G:547:LYS:HZ3	1.85	0.41
1:0A:586:PHE:CE2	1:0A:590:GLY:HA2	2.55	0.41
1:0B:339:PRO:HB2	1:0B:356:PRO:HD3	2.03	0.41
1:0C:396:ASP:HB3	1:0C:399:LYS:HG3	2.03	0.41
1:0D:352:MET:HG2	1:0D:361:ILE:HB	2.02	0.41
1:0D:413:ILE:HD13	1:0D:429:SER:HB2	2.01	0.41
2:0F:78:PHE:CD1	2:0F:110:PHE:HE2	2.38	0.41
3:0I:177:GLY:N	3:0I:178:PRO:HD2	2.35	0.41
3:0I:181:ARG:NE	3:0I:185:GLU:OE2	2.53	0.41
5:0N:229:LEU:HD21	5:0N:286:VAL:HA	2.02	0.41
7:0Q:72:LEU:HD12	7:0Q:85:VAL:HG22	2.02	0.41
7:0Q:584:ALA:HB3	7:0Q:615:TRP:CZ3	2.54	0.41
7:0S:72:LEU:HD12	7:0S:85:VAL:HG22	2.02	0.41
13:1B:1698:ILE:HG22	13:1B:1700:PRO:HD2	2.01	0.41
13:1C:1313:VAL:O	13:1C:1410:PHE:HB2	2.20	0.41
13:1C:1536:PRO:HA	13:1C:1537:PRO:HD3	1.92	0.41
14:1E:502:SER:O	14:1E:506:MET:HG2	2.19	0.41
14:1G:605:GLU:O	14:1G:608:PHE:HB2	2.20	0.41
14:1G:654:VAL:O	14:1G:657:ARG:N	2.52	0.41
14:1G:861:ALA:O	14:1G:864:GLU:HG3	2.21	0.41
1:0B:457:ASP:CB	1:0B:499:GLY:HA2	2.49	0.41
1:0C:542:SER:HB3	1:0C:553:VAL:HG12	2.03	0.41
1:0D:396:ASP:HB2	1:0D:403:VAL:HG23	2.02	0.41
2:0F:143:GLU:OE2	2:0F:151:PRO:HD3	2.20	0.41
2:0G:70:ASN:ND2	2:0G:93:ASN:HA	2.31	0.41
3:0J:226:SER:HA	6:0P:169:ARG:HH12	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1G:415:PRO:HA	14:1G:416:PRO:HD3	1.89	0.41
1:0A:156:ARG:HG3	1:0D:155:GLU:HB3	2.02	0.41
1:0B:409:HIS:CE1	1:0B:435:ARG:HG3	2.55	0.41
1:0B:418:PHE:HE1	1:0B:439:LEU:HD11	1.85	0.41
1:0C:328:SER:HB2	1:0C:598:SER:HA	2.02	0.41
2:0E:117:ASN:OD1	2:0E:117:ASN:N	2.51	0.41
3:0I:434:HIS:HB2	14:1D:1006:ARG:HH12	1.86	0.41
3:0J:428:PHE:HE2	14:1F:972:GLU:HB3	1.84	0.41
3:0J:431:LEU:HD23	3:0J:431:LEU:HA	1.86	0.41
5:0M:747:LEU:HD23	5:0M:747:LEU:HA	1.92	0.41
7:0S:76:GLN:HG2	7:0S:103:GLU:HB3	2.03	0.41
12:0X:7:LYS:O	12:0X:307:VAL:HG13	2.20	0.41
12:0X:88:PHE:CE1	12:0X:308:MET:HG3	2.55	0.41
12:0X:354:TYR:OH	12:0Y:351:LEU:O	2.39	0.41
12:0Y:327:ARG:HB3	12:0Y:331:ARG:NH2	2.35	0.41
13:1B:1690:MET:SD	13:1B:1701:LEU:HD13	2.60	0.41
13:1C:1694:VAL:HG22	13:1C:1697:ARG:HH21	1.86	0.41
14:1D:518:LEU:HD12	14:1D:522:HIS:CE1	2.56	0.41
14:1F:600:LYS:HE3	14:1F:603:ARG:HD2	2.02	0.41
1:0A:192:LEU:O	1:0A:196:LYS:HG3	2.20	0.41
1:0D:187:TYR:HD1	4:0L:109:VAL:HG22	1.86	0.41
3:0I:452:ALA:HB3	13:1C:1315:LEU:HB3	2.02	0.41
7:0S:569:ALA:HA	7:0S:585:ALA:HA	2.02	0.41
12:0X:74:GLU:OE2	12:0X:74:GLU:N	2.49	0.41
12:1A:128:ARG:HG3	12:1A:133:TYR:HE2	1.86	0.41
13:1C:1128:GLN:NE2	13:1C:1470:ASP:O	2.54	0.41
1:0A:512:THR:HG22	1:0A:518:VAL:HG22	2.03	0.41
1:0B:124:LEU:O	1:0B:128:VAL:HG23	2.21	0.41
1:0B:429:SER:OG	1:0B:430:LEU:N	2.52	0.41
1:0C:420:HIS:CE1	1:0C:421:LEU:HG	2.56	0.41
1:0C:511:SER:OG	1:0C:521:TRP:HZ3	2.04	0.41
1:0D:486:CYS:SG	1:0D:489:THR:OG1	2.79	0.41
6:0O:80:ASN:O	6:0O:84:GLN:HG2	2.21	0.41
6:0P:46:GLN:OE1	6:0P:47:PRO:HD2	2.20	0.41
7:0Q:495:ARG:NH1	7:0Q:499:THR:OG1	2.54	0.41
7:0S:179:VAL:HG22	7:0S:186:VAL:HG22	2.03	0.41
12:0Y:68:TYR:CB	12:0Y:116:ARG:HE	2.29	0.41
13:1B:1191:ILE:HD12	13:1B:1257:VAL:HG21	2.02	0.41
13:1C:1120:GLY:HA2	13:1C:1614:ARG:NH2	2.34	0.41
13:1C:1515:VAL:HA	13:1C:1594:LEU:O	2.21	0.41
13:1C:1777:PHE:HB2	14:1G:430:VAL:HG12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1D:419:THR:HG22	14:1D:421:VAL:N	2.35	0.41
1:0A:171:ASN:O	1:0A:175:THR:HG23	2.19	0.41
1:0B:192:LEU:O	1:0B:196:LYS:HG3	2.21	0.41
1:0B:383:LEU:HB2	1:0B:397:PHE:CZ	2.56	0.41
3:0J:207:TRP:NE1	3:0J:211:LEU:HD21	2.36	0.41
3:0J:554:GLU:HB3	14:1F:606:GLU:OE1	2.20	0.41
5:0M:247:GLU:HA	5:0M:250:ILE:HG22	2.03	0.41
7:0Q:102:VAL:HG12	7:0Q:103:GLU:N	2.36	0.41
12:1A:84:ASN:ND2	12:1A:298:ASP:OD1	2.53	0.41
12:1A:147:LEU:HD21	12:1A:291:LYS:HB3	2.03	0.41
12:1A:166:ASP:HA	12:1A:170:ASN:O	2.21	0.41
13:1B:1127:TRP:HA	13:1B:1132:LEU:HD12	2.03	0.41
13:1C:1340:ASP:HB2	13:1C:1392:PRO:HG2	2.03	0.41
14:1E:431:ILE:HG23	14:1E:479:MET:SD	2.60	0.41
14:1E:1005:ARG:HG3	14:1E:1008:GLU:OE2	2.21	0.41
1:0A:457:ASP:CB	1:0A:499:GLY:HA2	2.50	0.41
1:0B:409:HIS:CE1	1:0B:429:SER:HB3	2.56	0.41
1:0C:462:PRO:HG2	1:0C:503:ASN:O	2.20	0.41
1:0D:335:HIS:CE1	1:0D:337:THR:HB	2.56	0.41
1:0D:545:ASP:HB3	1:0D:548:GLY:HA3	2.03	0.41
2:0G:96:SER:O	2:0G:100:LYS:HG3	2.21	0.41
3:0I:505:GLY:HA3	14:1G:949:VAL:HG22	2.02	0.41
3:0J:177:GLY:N	3:0J:178:PRO:HD2	2.36	0.41
3:0J:554:GLU:O	3:0J:558:ARG:HG3	2.21	0.41
4:0K:216:ASP:OD1	4:0K:217:ILE:N	2.51	0.41
4:0L:158:GLN:HB3	4:0L:162:ASP:OD2	2.20	0.41
5:0M:387:GLN:O	5:0M:391:VAL:HG23	2.21	0.41
5:0N:367:LEU:HD23	5:0N:367:LEU:HA	1.86	0.41
7:0S:66:SER:OG	7:0S:70:SER:HB2	2.21	0.41
7:0S:101:ASP:OD1	7:0S:101:ASP:N	2.53	0.41
7:0S:394:ARG:HG2	7:0S:410:MET:HG3	2.02	0.41
12:0X:101:MET:O	12:0X:102:SER:OG	2.38	0.41
12:0X:132:MET:CE	12:0X:223:ARG:HD2	2.51	0.41
12:0X:178:LEU:HD11	12:0X:219:HIS:CD2	2.53	0.41
12:0Y:83:TYR:O	12:0Y:235:SER:HA	2.21	0.41
12:0Y:181:VAL:HG21	12:0Y:187:ALA:HB2	2.02	0.41
12:0Z:102:SER:H	12:0Z:113:LEU:H	1.68	0.41
12:0Z:260:GLU:O	12:0Z:264:ILE:HG12	2.21	0.41
12:1A:109:ALA:O	12:1A:110:HIS:CG	2.74	0.41
13:1B:1243:ARG:HB2	13:1B:1244:PRO:HD3	2.02	0.41
13:1C:1317:GLU:OE1	13:1C:1750:TYR:OH	2.27	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1C:1337:TRP:CD1	13:1C:1367:ILE:HG13	2.56	0.41
13:1C:1473:TRP:HA	13:1C:1476:TRP:CD2	2.56	0.41
13:1C:1708:THR:HB	13:1C:1712:ARG:NH1	2.35	0.41
13:1C:1751:VAL:HG13	13:1C:1756:ARG:HG2	2.03	0.41
14:1D:423:GLU:O	14:1D:427:LYS:HG2	2.21	0.41
14:1D:504:ASN:OD1	14:1D:505:GLU:HG3	2.20	0.41
14:1E:463:HIS:O	14:1E:467:ILE:HG13	2.20	0.41
14:1F:821:PRO:HA	14:1F:825:VAL:HB	2.02	0.41
1:0A:129:ALA:HA	1:0A:132:ARG:HG2	2.03	0.41
1:0A:129:ALA:HB1	1:0A:133:ARG:CZ	2.50	0.41
1:0A:457:ASP:HB2	1:0A:499:GLY:HA2	2.03	0.41
1:0B:128:VAL:HG22	1:0C:128:VAL:HG23	2.02	0.41
1:0B:331:ASN:HD22	1:0B:374:VAL:H	1.67	0.41
1:0C:522:ASP:O	1:0C:526:THR:N	2.53	0.41
1:0C:554:ALA:HB1	1:0C:581:VAL:HB	2.03	0.41
2:0E:120:GLY:O	2:0E:124:GLU:HG2	2.21	0.41
3:0I:96:HIS:CG	3:0I:100:ARG:HH21	2.39	0.41
3:0I:431:LEU:HD23	3:0I:431:LEU:HA	1.87	0.41
3:0J:173:ALA:HA	3:0J:176:ARG:HH21	1.85	0.41
7:0Q:498:THR:OG1	7:0Q:499:THR:N	2.52	0.41
7:0S:563:THR:HB	7:0S:573:TRP:HE1	1.86	0.41
12:0Y:109:ALA:O	12:0Y:110:HIS:CG	2.74	0.41
12:0Y:187:ALA:HA	12:0Y:190:GLN:NE2	2.35	0.41
12:0Z:203:HIS:CD2	12:0Z:205:LEU:HB2	2.56	0.41
13:1B:1333:ALA:HB1	13:1B:1334:PRO:HD2	2.03	0.41
13:1C:1184:PRO:HB3	13:1C:1262:ARG:HD3	2.03	0.41
13:1C:1376:ASN:HD21	13:1C:1574:PRO:HA	1.85	0.41
14:1D:911:LEU:H	14:1D:911:LEU:HG	1.76	0.41
14:1D:911:LEU:HD12	14:1G:400:ARG:NH2	2.36	0.41
14:1E:504:ASN:OD1	14:1E:505:GLU:HG3	2.21	0.41
14:1E:955:PRO:HB2	14:1E:986:LEU:H	1.86	0.41
1:0A:88:LEU:HD21	1:0D:102:LEU:HD12	2.03	0.40
1:0A:188:GLU:HA	1:0A:191:ILE:HD13	2.03	0.40
1:0A:426:ALA:HB3	1:0A:458:LEU:HD21	2.03	0.40
1:0B:430:LEU:HD12	1:0B:454:SER:HB2	2.03	0.40
1:0C:172:LYS:HE2	1:0C:172:LYS:HB3	1.76	0.40
1:0C:560:VAL:HG22	1:0C:581:VAL:HG11	2.03	0.40
1:0D:466:SER:HA	1:0D:479:TRP:O	2.21	0.40
3:0J:194:GLN:HG2	3:0J:326:TYR:CE1	2.56	0.40
7:0Q:71:MET:N	7:0Q:71:MET:SD	2.94	0.40
7:0Q:77:LYS:NZ	7:0Q:102:VAL:HG13	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:0Q:500:TRP:NE1	7:0Q:535:PRO:HA	2.33	0.40
7:0Q:569:ALA:HA	7:0Q:585:ALA:HA	2.04	0.40
7:0S:144:GLU:HG3	7:0S:147:LYS:HB2	2.03	0.40
12:0X:206:ASN:HB3	12:0X:209:SER:OG	2.20	0.40
12:0Y:9:PHE:O	12:0Y:309:VAL:HA	2.21	0.40
13:1B:1190:GLU:HG3	13:1B:1484:SER:HB3	2.02	0.40
14:1E:944:LEU:HB3	14:1E:961:LEU:HG	2.03	0.40
14:1G:928:GLY:HA3	14:1G:944:LEU:HG	2.02	0.40
16:1M:148:UNK:O	16:1M:150:UNK:N	2.54	0.40
1:0C:528:GLU:OE2	1:0C:531:THR:HB	2.22	0.40
3:0I:457:TRP:HZ3	3:0I:459:ARG:HB2	1.87	0.40
3:0J:178:PRO:O	3:0J:182:THR:HG23	2.22	0.40
3:0J:306:LEU:HD23	3:0J:309:ARG:NH2	2.35	0.40
5:0M:258:ILE:HG22	5:0M:260:VAL:HG23	2.02	0.40
7:0Q:409:TRP:CG	7:0Q:452:ARG:HD3	2.56	0.40
12:0X:295:VAL:HG12	12:0X:296:LEU:HD12	2.03	0.40
12:1A:277:ALA:HB1	12:1A:285:VAL:HG12	2.04	0.40
13:1B:1503:VAL:HG13	13:1B:1738:ARG:HB2	2.04	0.40
13:1B:1717:ALA:O	13:1B:1721:ARG:HG3	2.21	0.40
13:1C:1570:LEU:HD23	13:1C:1570:LEU:HA	1.96	0.40
14:1D:1006:ARG:HG3	14:1D:1010:ARG:NE	2.36	0.40
14:1E:1005:ARG:HB3	14:1E:1035:VAL:HG22	2.03	0.40
14:1F:818:MET:O	14:1F:821:PRO:HD2	2.20	0.40
14:1F:861:ALA:O	14:1F:864:GLU:HG3	2.22	0.40
14:1F:905:PHE:O	14:1F:909:VAL:HG13	2.22	0.40
14:1G:494:LYS:HG3	14:1G:495:TYR:CD2	2.56	0.40
16:1L:148:UNK:O	16:1L:150:UNK:N	2.54	0.40
1:0A:512:THR:HB	1:0A:539:ALA:HB3	2.02	0.40
1:0B:457:ASP:HB2	1:0B:499:GLY:HA2	2.03	0.40
1:0D:197:LYS:HB2	1:0D:197:LYS:HE2	1.75	0.40
2:0F:123:VAL:O	2:0F:127:VAL:HG13	2.22	0.40
2:0H:57:LEU:HD22	2:0H:76:GLU:HB3	2.02	0.40
3:0I:557:LYS:HA	3:0I:557:LYS:HD2	1.84	0.40
3:0J:146:LYS:HE2	3:0J:150:GLN:NE2	2.36	0.40
5:0N:181:THR:O	5:0N:182:PHE:HB2	2.22	0.40
7:0Q:463:SER:HB2	7:0Q:482:GLU:HB2	2.02	0.40
7:0Q:483:ASP:OD2	7:0Q:485:THR:HG22	2.20	0.40
7:0S:6:ARG:NH2	7:0S:356:THR:O	2.54	0.40
7:0S:77:LYS:NZ	7:0S:102:VAL:HG13	2.37	0.40
12:0X:166:ASP:HA	12:0X:170:ASN:O	2.20	0.40
12:0X:195:GLU:HA	12:0X:195:GLU:OE2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
12:0X:359:LYS:O	12:0X:362:LYS:HG2	2.21	0.40
12:0Y:96:GLY:HA2	19:0Y:801:ADP:H5’2	2.03	0.40
12:0Y:215:VAL:HG22	12:0Y:240:VAL:HG13	2.03	0.40
12:1A:121:VAL:O	12:1A:125:VAL:HG13	2.20	0.40
13:1B:1134:ASP:HB3	13:1B:1171:PHE:HE2	1.87	0.40
13:1C:1333:ALA:HB1	13:1C:1334:PRO:HD2	2.03	0.40
13:1C:1518:ASN:HD21	13:1C:1588:LEU:CB	2.34	0.40
14:1F:586:TRP:HB3	14:1F:611:ALA:HB2	2.02	0.40
14:1F:664:ALA:HB3	14:1F:756:THR:HG21	2.02	0.40
14:1G:487:VAL:HA	14:1G:490:LEU:HD12	2.02	0.40
1:0A:124:LEU:O	1:0A:128:VAL:HG23	2.22	0.40
1:0B:354:HIS:HB2	1:0B:361:ILE:HD11	2.02	0.40
1:0C:429:SER:OG	1:0C:430:LEU:N	2.54	0.40
1:0D:325:HIS:NE2	1:0D:343:THR:OG1	2.44	0.40
1:0D:433:THR:HG22	1:0D:449:ARG:HG2	2.02	0.40
2:0H:78:PHE:HB3	2:0H:86:ILE:HG13	2.04	0.40
3:0I:265:LEU:HD11	3:0I:330:LEU:HD13	2.04	0.40
4:0K:105:LEU:HD23	4:0K:105:LEU:HA	1.84	0.40
4:0K:158:GLN:C	4:0K:160:ALA:H	2.23	0.40
5:0N:339:HIS:NE2	5:0N:417:VAL:O	2.53	0.40
7:0S:124:ASP:HB3	7:0S:126:LYS:NZ	2.36	0.40
7:0S:388:TRP:NE1	7:0S:394:ARG:HD2	2.36	0.40
7:0S:554:SER:HB3	7:0S:575:TRP:HZ2	1.86	0.40
12:0X:102:SER:HB3	12:0X:114:ILE:HB	2.03	0.40
12:0Z:109:ALA:C	12:0Z:110:HIS:ND1	2.75	0.40
13:1B:1473:TRP:CH2	13:1B:1736:ARG:HB3	2.56	0.40
13:1C:1222:ARG:HD2	13:1C:1222:ARG:HA	1.98	0.40
14:1D:398:PRO:HG2	14:1D:400:ARG:NH2	2.37	0.40
14:1D:431:ILE:HG23	14:1D:479:MET:SD	2.62	0.40
14:1F:568:ARG:NH2	14:1F:956:GLU:OE1	2.54	0.40
1:0A:118:TYR:OH	1:0D:73:GLU:O	2.29	0.40
1:0A:332:LEU:HD22	1:0A:341:LEU:HD21	2.03	0.40
1:0B:138:ALA:HA	1:0B:141:ILE:HG22	2.03	0.40
2:0E:78:PHE:CD1	2:0E:110:PHE:HE2	2.40	0.40
2:0F:62:LYS:HA	2:0F:62:LYS:HE2	2.03	0.40
3:0J:464:GLN:HA	14:1F:942:MET:CE	2.51	0.40
7:0Q:76:GLN:HG2	7:0Q:103:GLU:HB3	2.02	0.40
7:0Q:351:ILE:HB	7:0Q:365:VAL:HB	2.03	0.40
7:0S:16:PHE:HE1	7:0S:243:GLY:HA2	1.87	0.40
7:0S:62:ALA:N	7:0S:74:THR:OG1	2.54	0.40
7:0S:584:ALA:HB3	7:0S:615:TRP:CZ3	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:0Y:80:MET:HA	12:0Y:80:MET:HE3	2.02	0.40
12:0Y:84:ASN:ND2	12:0Y:298:ASP:OD1	2.54	0.40
13:1C:1144:THR:HG22	13:1C:1281:LYS:HG2	2.03	0.40
13:1C:1499:VAL:HG13	14:1D:511:ASN:HD21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	0A	463/606 (76%)	447 (96%)	16 (4%)	0	100	100
1	0B	463/606 (76%)	449 (97%)	14 (3%)	0	100	100
1	0C	472/606 (78%)	454 (96%)	18 (4%)	0	100	100
1	0D	472/606 (78%)	458 (97%)	14 (3%)	0	100	100
2	0E	126/222 (57%)	122 (97%)	4 (3%)	0	100	100
2	0F	126/222 (57%)	121 (96%)	5 (4%)	0	100	100
2	0G	126/222 (57%)	122 (97%)	4 (3%)	0	100	100
2	0H	126/222 (57%)	121 (96%)	5 (4%)	0	100	100
3	0I	442/976 (45%)	424 (96%)	17 (4%)	1 (0%)	47	81
3	0J	442/976 (45%)	426 (96%)	15 (3%)	1 (0%)	47	81
4	0K	164/528 (31%)	162 (99%)	2 (1%)	0	100	100
4	0L	164/528 (31%)	161 (98%)	3 (2%)	0	100	100
5	0M	507/758 (67%)	488 (96%)	19 (4%)	0	100	100
5	0N	507/758 (67%)	491 (97%)	16 (3%)	0	100	100
6	0O	184/201 (92%)	180 (98%)	4 (2%)	0	100	100
6	0P	184/201 (92%)	180 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	0Q	615/618 (100%)	564 (92%)	51 (8%)	0	100	100
7	0S	615/618 (100%)	566 (92%)	49 (8%)	0	100	100
12	0X	418/776 (54%)	390 (93%)	26 (6%)	2 (0%)	29	68
12	0Y	400/776 (52%)	371 (93%)	25 (6%)	4 (1%)	15	54
12	0Z	418/776 (54%)	390 (93%)	26 (6%)	2 (0%)	29	68
12	1A	400/776 (52%)	373 (93%)	24 (6%)	3 (1%)	19	58
13	1B	624/2257 (28%)	595 (95%)	29 (5%)	0	100	100
13	1C	624/2257 (28%)	595 (95%)	29 (5%)	0	100	100
14	1D	617/1074 (57%)	584 (95%)	33 (5%)	0	100	100
14	1E	617/1074 (57%)	584 (95%)	33 (5%)	0	100	100
14	1F	608/1074 (57%)	576 (95%)	32 (5%)	0	100	100
14	1G	608/1074 (57%)	573 (94%)	35 (6%)	0	100	100
17	1a	429/443 (97%)	420 (98%)	9 (2%)	0	100	100
17	1c	429/443 (97%)	420 (98%)	9 (2%)	0	100	100
17	1e	429/443 (97%)	421 (98%)	8 (2%)	0	100	100
17	1g	429/443 (97%)	419 (98%)	10 (2%)	0	100	100
17	2a	429/443 (97%)	418 (97%)	11 (3%)	0	100	100
17	2c	429/443 (97%)	420 (98%)	9 (2%)	0	100	100
17	2e	429/443 (97%)	418 (97%)	11 (3%)	0	100	100
17	2g	429/443 (97%)	420 (98%)	9 (2%)	0	100	100
17	3a	429/443 (97%)	422 (98%)	7 (2%)	0	100	100
17	3c	429/443 (97%)	420 (98%)	9 (2%)	0	100	100
17	3e	429/443 (97%)	421 (98%)	8 (2%)	0	100	100
17	3g	429/443 (97%)	422 (98%)	7 (2%)	0	100	100
17	4a	429/443 (97%)	419 (98%)	10 (2%)	0	100	100
17	4c	429/443 (97%)	420 (98%)	9 (2%)	0	100	100
17	4e	429/443 (97%)	420 (98%)	9 (2%)	0	100	100
17	4g	429/443 (97%)	418 (97%)	11 (3%)	0	100	100
17	5a	429/443 (97%)	419 (98%)	10 (2%)	0	100	100
17	5c	429/443 (97%)	421 (98%)	8 (2%)	0	100	100
17	5e	429/443 (97%)	418 (97%)	11 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	5g	429/443 (97%)	420 (98%)	9 (2%)	0	100	100
17	6a	429/443 (97%)	421 (98%)	8 (2%)	0	100	100
17	6c	429/443 (97%)	419 (98%)	10 (2%)	0	100	100
17	6e	429/443 (97%)	421 (98%)	8 (2%)	0	100	100
17	6g	429/443 (97%)	419 (98%)	10 (2%)	0	100	100
17	7a	429/443 (97%)	418 (97%)	11 (3%)	0	100	100
17	7c	429/443 (97%)	421 (98%)	8 (2%)	0	100	100
17	7e	429/443 (97%)	420 (98%)	9 (2%)	0	100	100
17	7g	429/443 (97%)	419 (98%)	10 (2%)	0	100	100
17	8a	429/443 (97%)	418 (97%)	11 (3%)	0	100	100
17	8c	429/443 (97%)	421 (98%)	8 (2%)	0	100	100
17	8e	429/443 (97%)	420 (98%)	9 (2%)	0	100	100
17	8g	429/443 (97%)	419 (98%)	10 (2%)	0	100	100
17	9a	429/443 (97%)	418 (97%)	11 (3%)	0	100	100
17	9c	429/443 (97%)	419 (98%)	10 (2%)	0	100	100
17	9e	429/443 (97%)	420 (98%)	9 (2%)	0	100	100
17	9g	429/443 (97%)	417 (97%)	12 (3%)	0	100	100
17	Aa	429/443 (97%)	419 (98%)	10 (2%)	0	100	100
17	Ac	429/443 (97%)	422 (98%)	7 (2%)	0	100	100
17	Ae	429/443 (97%)	422 (98%)	7 (2%)	0	100	100
17	Ag	429/443 (97%)	422 (98%)	7 (2%)	0	100	100
17	Ba	429/443 (97%)	419 (98%)	10 (2%)	0	100	100
17	Bc	429/443 (97%)	421 (98%)	8 (2%)	0	100	100
17	Be	429/443 (97%)	421 (98%)	8 (2%)	0	100	100
17	Bg	429/443 (97%)	420 (98%)	9 (2%)	0	100	100
17	Ca	429/443 (97%)	422 (98%)	7 (2%)	0	100	100
17	Cc	429/443 (97%)	418 (97%)	11 (3%)	0	100	100
17	Ce	429/443 (97%)	421 (98%)	8 (2%)	0	100	100
17	Cg	429/443 (97%)	414 (96%)	15 (4%)	0	100	100
17	Da	429/443 (97%)	421 (98%)	8 (2%)	0	100	100
17	Dc	429/443 (97%)	420 (98%)	9 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	De	429/443 (97%)	419 (98%)	10 (2%)	0	100	100
17	Dg	429/443 (97%)	418 (97%)	11 (3%)	0	100	100
18	1b	426/451 (94%)	414 (97%)	12 (3%)	0	100	100
18	1d	426/451 (94%)	416 (98%)	10 (2%)	0	100	100
18	1f	426/451 (94%)	414 (97%)	12 (3%)	0	100	100
18	1h	426/451 (94%)	415 (97%)	11 (3%)	0	100	100
18	2b	426/451 (94%)	414 (97%)	12 (3%)	0	100	100
18	2d	426/451 (94%)	415 (97%)	11 (3%)	0	100	100
18	2f	426/451 (94%)	411 (96%)	15 (4%)	0	100	100
18	2h	426/451 (94%)	416 (98%)	10 (2%)	0	100	100
18	3b	426/451 (94%)	415 (97%)	11 (3%)	0	100	100
18	3d	426/451 (94%)	413 (97%)	13 (3%)	0	100	100
18	3f	426/451 (94%)	417 (98%)	9 (2%)	0	100	100
18	3h	426/451 (94%)	415 (97%)	11 (3%)	0	100	100
18	4b	426/451 (94%)	414 (97%)	12 (3%)	0	100	100
18	4d	426/451 (94%)	414 (97%)	12 (3%)	0	100	100
18	4f	426/451 (94%)	416 (98%)	10 (2%)	0	100	100
18	4h	426/451 (94%)	411 (96%)	15 (4%)	0	100	100
18	5b	426/451 (94%)	416 (98%)	10 (2%)	0	100	100
18	5d	426/451 (94%)	416 (98%)	10 (2%)	0	100	100
18	5f	426/451 (94%)	420 (99%)	6 (1%)	0	100	100
18	5h	426/451 (94%)	411 (96%)	15 (4%)	0	100	100
18	6b	426/451 (94%)	417 (98%)	9 (2%)	0	100	100
18	6d	426/451 (94%)	413 (97%)	13 (3%)	0	100	100
18	6f	426/451 (94%)	416 (98%)	10 (2%)	0	100	100
18	6h	426/451 (94%)	416 (98%)	10 (2%)	0	100	100
18	7b	426/451 (94%)	417 (98%)	9 (2%)	0	100	100
18	7d	426/451 (94%)	417 (98%)	9 (2%)	0	100	100
18	7f	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
18	7h	426/451 (94%)	415 (97%)	11 (3%)	0	100	100
18	8b	426/451 (94%)	416 (98%)	10 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	8d	426/451 (94%)	416 (98%)	10 (2%)	0	100	100
18	8f	426/451 (94%)	414 (97%)	12 (3%)	0	100	100
18	8h	426/451 (94%)	417 (98%)	9 (2%)	0	100	100
18	9b	426/451 (94%)	415 (97%)	11 (3%)	0	100	100
18	9d	426/451 (94%)	413 (97%)	13 (3%)	0	100	100
18	9f	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
18	9h	426/451 (94%)	411 (96%)	15 (4%)	0	100	100
18	Ab	426/451 (94%)	417 (98%)	9 (2%)	0	100	100
18	Ad	426/451 (94%)	415 (97%)	11 (3%)	0	100	100
18	Af	426/451 (94%)	414 (97%)	12 (3%)	0	100	100
18	Ah	426/451 (94%)	415 (97%)	11 (3%)	0	100	100
18	Bb	426/451 (94%)	419 (98%)	7 (2%)	0	100	100
18	Bd	426/451 (94%)	414 (97%)	12 (3%)	0	100	100
18	Bf	426/451 (94%)	415 (97%)	11 (3%)	0	100	100
18	Bh	426/451 (94%)	414 (97%)	12 (3%)	0	100	100
18	Cb	426/451 (94%)	414 (97%)	12 (3%)	0	100	100
18	Cd	426/451 (94%)	418 (98%)	8 (2%)	0	100	100
18	Cf	426/451 (94%)	418 (98%)	8 (2%)	0	100	100
18	Ch	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
18	Db	426/451 (94%)	419 (98%)	7 (2%)	0	100	100
18	Dd	426/451 (94%)	414 (97%)	12 (3%)	0	100	100
18	Df	426/451 (94%)	416 (98%)	10 (2%)	0	100	100
18	Dh	426/451 (94%)	415 (97%)	11 (3%)	0	100	100
All	All	55992/67876 (82%)	54371 (97%)	1608 (3%)	13 (0%)	100	100

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	0X	233	VAL
12	0X	408	PRO
12	0Y	408	PRO
12	0Z	233	VAL
12	0Z	408	PRO
12	1A	408	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	0Y	60	GLU
12	0Y	403	GLU
12	1A	403	GLU
12	0Y	26	PRO
3	0I	362	ILE
3	0J	362	ILE
12	1A	26	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	0A	389/482 (81%)	387 (100%)	2 (0%)	88	94
1	0B	389/482 (81%)	389 (100%)	0	100	100
1	0C	397/482 (82%)	396 (100%)	1 (0%)	92	97
1	0D	397/482 (82%)	396 (100%)	1 (0%)	92	97
2	0E	106/166 (64%)	106 (100%)	0	100	100
2	0F	106/166 (64%)	106 (100%)	0	100	100
2	0G	106/166 (64%)	106 (100%)	0	100	100
2	0H	106/166 (64%)	105 (99%)	1 (1%)	78	90
3	0I	325/697 (47%)	322 (99%)	3 (1%)	78	90
3	0J	325/697 (47%)	325 (100%)	0	100	100
4	0K	113/410 (28%)	113 (100%)	0	100	100
4	0L	113/410 (28%)	113 (100%)	0	100	100
5	0M	426/598 (71%)	426 (100%)	0	100	100
5	0N	426/598 (71%)	426 (100%)	0	100	100
6	0O	152/159 (96%)	152 (100%)	0	100	100
6	0P	152/159 (96%)	152 (100%)	0	100	100
7	0Q	461/462 (100%)	460 (100%)	1 (0%)	93	98
7	0S	461/462 (100%)	460 (100%)	1 (0%)	93	98

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	0X	306/600 (51%)	305 (100%)	1 (0%)	92	97
12	0Y	274/600 (46%)	271 (99%)	3 (1%)	73	88
12	0Z	306/600 (51%)	306 (100%)	0	100	100
12	1A	274/600 (46%)	272 (99%)	2 (1%)	84	93
13	1B	487/1666 (29%)	485 (100%)	2 (0%)	91	96
13	1C	487/1666 (29%)	485 (100%)	2 (0%)	91	96
14	1D	291/753 (39%)	290 (100%)	1 (0%)	92	97
14	1E	291/753 (39%)	291 (100%)	0	100	100
14	1F	373/753 (50%)	373 (100%)	0	100	100
14	1G	373/753 (50%)	372 (100%)	1 (0%)	92	97
17	1a	370/379 (98%)	369 (100%)	1 (0%)	92	97
17	1c	370/379 (98%)	370 (100%)	0	100	100
17	1e	370/379 (98%)	369 (100%)	1 (0%)	92	97
17	1g	370/379 (98%)	369 (100%)	1 (0%)	92	97
17	2a	370/379 (98%)	370 (100%)	0	100	100
17	2c	370/379 (98%)	370 (100%)	0	100	100
17	2e	370/379 (98%)	369 (100%)	1 (0%)	92	97
17	2g	370/379 (98%)	369 (100%)	1 (0%)	92	97
17	3a	370/379 (98%)	368 (100%)	2 (0%)	88	94
17	3c	370/379 (98%)	370 (100%)	0	100	100
17	3e	370/379 (98%)	370 (100%)	0	100	100
17	3g	370/379 (98%)	370 (100%)	0	100	100
17	4a	370/379 (98%)	370 (100%)	0	100	100
17	4c	370/379 (98%)	369 (100%)	1 (0%)	92	97
17	4e	370/379 (98%)	369 (100%)	1 (0%)	92	97
17	4g	370/379 (98%)	370 (100%)	0	100	100
17	5a	370/379 (98%)	369 (100%)	1 (0%)	92	97
17	5c	370/379 (98%)	370 (100%)	0	100	100
17	5e	370/379 (98%)	369 (100%)	1 (0%)	92	97
17	5g	370/379 (98%)	368 (100%)	2 (0%)	88	94
17	6a	370/379 (98%)	370 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	6c	370/379 (98%)	369 (100%)	1 (0%)	92	97
17	6e	370/379 (98%)	370 (100%)	0	100	100
17	6g	370/379 (98%)	369 (100%)	1 (0%)	92	97
17	7a	370/379 (98%)	370 (100%)	0	100	100
17	7c	370/379 (98%)	370 (100%)	0	100	100
17	7e	370/379 (98%)	370 (100%)	0	100	100
17	7g	370/379 (98%)	370 (100%)	0	100	100
17	8a	370/379 (98%)	370 (100%)	0	100	100
17	8c	370/379 (98%)	369 (100%)	1 (0%)	92	97
17	8e	370/379 (98%)	369 (100%)	1 (0%)	92	97
17	8g	370/379 (98%)	369 (100%)	1 (0%)	92	97
17	9a	370/379 (98%)	369 (100%)	1 (0%)	92	97
17	9c	370/379 (98%)	369 (100%)	1 (0%)	92	97
17	9e	370/379 (98%)	369 (100%)	1 (0%)	92	97
17	9g	370/379 (98%)	370 (100%)	0	100	100
17	Aa	370/379 (98%)	370 (100%)	0	100	100
17	Ac	370/379 (98%)	369 (100%)	1 (0%)	92	97
17	Ae	370/379 (98%)	370 (100%)	0	100	100
17	Ag	370/379 (98%)	370 (100%)	0	100	100
17	Ba	370/379 (98%)	369 (100%)	1 (0%)	92	97
17	Bc	370/379 (98%)	370 (100%)	0	100	100
17	Be	370/379 (98%)	369 (100%)	1 (0%)	92	97
17	Bg	370/379 (98%)	370 (100%)	0	100	100
17	Ca	370/379 (98%)	370 (100%)	0	100	100
17	Cc	370/379 (98%)	369 (100%)	1 (0%)	92	97
17	Ce	370/379 (98%)	369 (100%)	1 (0%)	92	97
17	Cg	370/379 (98%)	369 (100%)	1 (0%)	92	97
17	Da	370/379 (98%)	369 (100%)	1 (0%)	92	97
17	Dc	370/379 (98%)	370 (100%)	0	100	100
17	De	370/379 (98%)	369 (100%)	1 (0%)	92	97
17	Dg	370/379 (98%)	369 (100%)	1 (0%)	92	97

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	1b	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	1d	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	1f	361/374 (96%)	359 (99%)	2 (1%)	86	94
18	1h	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	2b	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	2d	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	2f	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	2h	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	3b	361/374 (96%)	359 (99%)	2 (1%)	86	94
18	3d	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	3f	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	3h	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	4b	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	4d	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	4f	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	4h	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	5b	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	5d	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	5f	361/374 (96%)	357 (99%)	4 (1%)	73	88
18	5h	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	6b	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	6d	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	6f	361/374 (96%)	358 (99%)	3 (1%)	81	91
18	6h	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	7b	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	7d	361/374 (96%)	359 (99%)	2 (1%)	86	94
18	7f	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	7h	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	8b	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	8d	361/374 (96%)	359 (99%)	2 (1%)	86	94
18	8f	361/374 (96%)	360 (100%)	1 (0%)	92	97

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	8h	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	9b	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	9d	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	9f	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	9h	361/374 (96%)	359 (99%)	2 (1%)	86	94
18	Ab	361/374 (96%)	359 (99%)	2 (1%)	86	94
18	Ad	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	Af	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	Ah	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	Bb	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	Bd	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	Bf	361/374 (96%)	359 (99%)	2 (1%)	86	94
18	Bh	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	Cb	361/374 (96%)	359 (99%)	2 (1%)	86	94
18	Cd	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	Cf	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	Ch	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	Db	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	Dd	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	Df	361/374 (96%)	360 (100%)	1 (0%)	92	97
18	Dh	361/374 (96%)	360 (100%)	1 (0%)	92	97
All	All	46424/55144 (84%)	46307 (100%)	117 (0%)	92	97

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0A	325	HIS
1	0A	524	ARG
1	0C	399	LYS
1	0D	399	LYS
2	0H	152	ARG
3	0I	96	HIS
3	0I	289	ASN
3	0I	438	LYS
7	0Q	576	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	0S	576	ARG
12	0X	170	ASN
12	0Y	22	LEU
12	0Y	23	LYS
12	0Y	222	MET
12	1A	23	LYS
12	1A	222	MET
13	1B	1169	ARG
13	1B	1338	ARG
13	1C	1169	ARG
13	1C	1338	ARG
14	1D	911	LEU
14	1G	1051	ARG
17	1a	247	ASN
18	1b	308	ARG
18	1d	308	ARG
17	1e	247	ASN
18	1f	50	ASN
18	1f	308	ARG
17	1g	247	ASN
18	1h	308	ARG
18	2b	308	ARG
18	2d	308	ARG
17	2e	247	ASN
18	2f	308	ARG
17	2g	247	ASN
18	2h	308	ARG
17	3a	306	ARG
17	3a	332	ASN
18	3b	308	ARG
18	3b	339	ARG
18	3d	308	ARG
18	3f	308	ARG
18	3h	308	ARG
18	4b	308	ARG
17	4c	247	ASN
18	4d	308	ARG
17	4e	247	ASN
18	4f	308	ARG
18	4h	308	ARG
17	5a	320	ARG
18	5b	308	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	5d	308	ARG
17	5e	332	ASN
18	5f	221	ARG
18	5f	223	THR
18	5f	224	TYR
18	5f	308	ARG
17	5g	247	ASN
17	5g	332	ASN
18	5h	308	ARG
18	6b	308	ARG
17	6c	247	ASN
18	6d	308	ARG
18	6f	128	ASN
18	6f	308	ARG
18	6f	380	ASN
17	6g	247	ASN
18	6h	308	ARG
18	7b	308	ARG
18	7d	268	MET
18	7d	308	ARG
18	7f	308	ARG
18	7h	308	ARG
18	8b	308	ARG
17	8c	247	ASN
18	8d	308	ARG
18	8d	402	ARG
17	8e	247	ASN
18	8f	308	ARG
17	8g	247	ASN
18	8h	308	ARG
17	9a	247	ASN
18	9b	308	ARG
17	9c	247	ASN
18	9d	308	ARG
17	9e	247	ASN
18	9f	308	ARG
18	9h	50	ASN
18	9h	308	ARG
18	Ab	163	LYS
18	Ab	308	ARG
17	Ac	320	ARG
18	Ad	308	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	Af	308	ARG
18	Ah	308	ARG
17	Ba	416	ASN
18	Bb	308	ARG
18	Bd	308	ARG
17	Be	247	ASN
18	Bf	50	ASN
18	Bf	308	ARG
18	Bh	308	ARG
18	Cb	308	ARG
18	Cb	380	ASN
17	Cc	247	ASN
18	Cd	308	ARG
17	Ce	247	ASN
18	Cf	308	ARG
17	Cg	247	ASN
18	Ch	308	ARG
17	Da	247	ASN
18	Db	308	ARG
18	Dd	308	ARG
17	De	247	ASN
18	Df	308	ARG
17	Dg	247	ASN
18	Dh	308	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (184) such sidechains are listed below:

Mol	Chain	Res	Type
1	0A	121	ASN
1	0A	295	ASN
1	0A	331	ASN
1	0A	432	HIS
1	0B	295	ASN
1	0C	432	HIS
1	0D	159	HIS
2	0E	45	HIS
2	0E	70	ASN
2	0E	93	ASN
2	0G	70	ASN
2	0G	93	ASN
2	0G	108	GLN
3	0I	520	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	0P	143	ASN
7	0Q	46	ASN
7	0S	46	ASN
12	0X	92	GLN
12	0X	289	GLN
12	0Y	120	HIS
12	0Z	289	GLN
12	1A	47	GLN
13	1B	1154	GLN
13	1C	1154	GLN
13	1C	1518	ASN
14	1D	1052	GLN
14	1E	1013	GLN
14	1E	1052	GLN
14	1F	526	ASN
14	1G	526	ASN
14	1G	548	GLN
17	1a	256	ASN
18	1b	101	ASN
17	1c	256	ASN
18	1f	28	HIS
18	1f	101	ASN
17	1g	256	ASN
18	1h	101	ASN
17	2a	11	GLN
17	2a	204	ASN
17	2a	256	ASN
18	2b	101	ASN
18	2b	283	HIS
17	2c	134	GLN
17	2c	256	ASN
18	2d	15	GLN
18	2d	101	ASN
17	2e	247	ASN
17	2e	256	ASN
18	2f	61	HIS
18	2f	101	ASN
17	2g	134	GLN
17	2g	256	ASN
18	2h	101	ASN
17	3a	256	ASN
18	3b	101	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	3c	134	GLN
17	3c	247	ASN
17	3c	256	ASN
18	3d	101	ASN
17	3e	134	GLN
17	3e	256	ASN
18	3f	101	ASN
17	3g	134	GLN
17	3g	245	GLN
17	3g	256	ASN
18	3h	101	ASN
18	3h	283	HIS
18	4b	101	ASN
17	4c	256	ASN
18	4d	61	HIS
18	4d	101	ASN
17	4e	256	ASN
18	4f	101	ASN
18	4f	283	HIS
17	4g	256	ASN
18	4h	61	HIS
17	5a	256	ASN
17	5c	245	GLN
17	5c	332	ASN
18	5f	101	ASN
17	5g	256	ASN
18	5h	101	ASN
18	6b	101	ASN
17	6c	245	GLN
17	6c	256	ASN
18	6d	101	ASN
17	6e	245	GLN
17	6e	256	ASN
18	6f	101	ASN
17	6g	256	ASN
18	6h	266	HIS
17	7a	256	ASN
18	7b	101	ASN
18	7b	283	HIS
17	7c	256	ASN
18	7d	101	ASN
18	7d	266	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	7e	256	ASN
18	7f	283	HIS
18	7h	101	ASN
17	8a	134	GLN
17	8a	256	ASN
18	8b	101	ASN
17	8c	256	ASN
17	8e	245	GLN
17	8e	247	ASN
18	8f	88	HIS
18	8f	101	ASN
18	8f	283	HIS
17	8g	99	ASN
17	8g	134	GLN
17	8g	247	ASN
17	8g	256	ASN
17	8g	375	GLN
18	8h	88	HIS
18	8h	101	ASN
17	9a	256	ASN
17	9a	334	GLN
17	9a	347	ASN
18	9b	101	ASN
17	9c	256	ASN
18	9d	61	HIS
18	9d	101	ASN
18	9d	197	HIS
17	9e	256	ASN
17	9e	334	GLN
18	9f	101	ASN
18	9f	256	GLN
18	9f	283	HIS
18	9f	329	ASN
17	9g	256	ASN
18	9h	61	HIS
18	9h	101	ASN
18	9h	197	HIS
17	Aa	134	GLN
17	Aa	256	ASN
18	Ab	61	HIS
18	Ab	101	ASN
17	Ac	99	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	Ac	256	ASN
18	Ad	101	ASN
17	Ae	256	ASN
18	Ah	101	ASN
17	Ba	256	ASN
17	Ba	396	HIS
18	Bb	15	GLN
18	Bb	101	ASN
17	Bc	247	ASN
17	Bc	256	ASN
17	Bc	348	ASN
18	Bd	101	ASN
17	Be	134	GLN
17	Be	256	ASN
18	Bf	15	GLN
18	Bf	101	ASN
18	Bf	393	HIS
17	Bg	94	GLN
17	Bg	247	ASN
17	Bg	256	ASN
17	Bg	348	ASN
17	Bg	396	HIS
18	Bh	101	ASN
17	Ca	256	ASN
18	Cb	101	ASN
17	Cc	256	ASN
18	Cd	101	ASN
17	Ce	256	ASN
18	Cf	101	ASN
17	Cg	94	GLN
17	Cg	256	ASN
18	Ch	101	ASN
18	Ch	393	HIS
17	Da	134	GLN
17	Da	256	ASN
17	Da	332	ASN
18	Db	101	ASN
17	Dc	256	ASN
18	Dd	28	HIS
18	Dd	101	ASN
17	De	256	ASN
18	Dh	28	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	Dh	61	HIS
18	Dh	101	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

108 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	GTP	3f	501	-	26,34,34	1.18	2 (7%)	32,54,54	1.63	7 (21%)
20	GDP	Da	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
21	GTP	Bf	501	-	26,34,34	1.21	2 (7%)	32,54,54	1.61	7 (21%)
20	GDP	1a	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.37	4 (13%)
20	GDP	De	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.36	4 (13%)
21	GTP	3h	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.63	7 (21%)
20	GDP	7a	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
21	GTP	2b	501	-	26,34,34	1.19	2 (7%)	32,54,54	1.61	7 (21%)
21	GTP	1d	501	-	26,34,34	1.20	2 (7%)	32,54,54	1.61	7 (21%)

Continued on next page...

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
20	GDP	9e	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.43	5 (16%)
21	GTP	9f	501	-	26,34,34	1.22	2 (7%)	32,54,54	1.65	7 (21%)
20	GDP	7g	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
21	GTP	Ab	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.60	7 (21%)
21	GTP	6b	501	-	26,34,34	1.15	2 (7%)	32,54,54	1.59	7 (21%)
20	GDP	3a	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.38	4 (13%)
20	GDP	2a	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.38	4 (13%)
20	GDP	Dc	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.38	4 (13%)
20	GDP	5g	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.38	4 (13%)
21	GTP	4h	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.60	7 (21%)
20	GDP	Bg	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.39	4 (13%)
20	GDP	5a	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.36	4 (13%)
20	GDP	8c	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.39	4 (13%)
21	GTP	Df	501	-	26,34,34	1.18	2 (7%)	32,54,54	1.64	7 (21%)
21	GTP	Dh	501	-	26,34,34	1.18	2 (7%)	32,54,54	1.64	7 (21%)
19	ADP	1A	801	-	24,29,29	0.94	1 (4%)	29,45,45	1.34	4 (13%)
20	GDP	Ca	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.37	4 (13%)
20	GDP	9a	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.41	4 (13%)
21	GTP	1f	501	-	26,34,34	1.18	2 (7%)	32,54,54	1.60	7 (21%)
19	ADP	0Z	801	-	24,29,29	0.94	1 (4%)	29,45,45	1.40	4 (13%)
20	GDP	9c	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.41	4 (13%)
20	GDP	Cc	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.40	4 (13%)
21	GTP	9d	501	-	26,34,34	1.20	2 (7%)	32,54,54	1.63	7 (21%)
20	GDP	4c	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
20	GDP	Ac	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.31	4 (13%)
21	GTP	8b	501	-	26,34,34	1.14	2 (7%)	32,54,54	1.63	6 (18%)
20	GDP	7e	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.37	4 (13%)
20	GDP	2c	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
20	GDP	1g	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.35	4 (13%)
21	GTP	9b	501	-	26,34,34	1.22	2 (7%)	32,54,54	1.66	7 (21%)
20	GDP	1c	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.40	4 (13%)
21	GTP	Ad	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.60	7 (21%)
21	GTP	7f	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.61	7 (21%)
20	GDP	4g	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
21	GTP	9h	501	-	26,34,34	1.21	2 (7%)	32,54,54	1.62	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
21	GTP	1b	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.60	7 (21%)
20	GDP	6e	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.33	4 (13%)
21	GTP	Bb	501	-	26,34,34	1.19	2 (7%)	32,54,54	1.64	7 (21%)
21	GTP	8d	501	-	26,34,34	1.15	2 (7%)	32,54,54	1.63	7 (21%)
21	GTP	Cb	501	-	26,34,34	1.19	2 (7%)	32,54,54	1.61	7 (21%)
20	GDP	5e	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.32	4 (13%)
19	ADP	0X	801	-	24,29,29	0.94	1 (4%)	29,45,45	1.41	4 (13%)
21	GTP	Bd	501	-	26,34,34	1.21	2 (7%)	32,54,54	1.61	7 (21%)
21	GTP	Dd	501	-	26,34,34	1.18	2 (7%)	32,54,54	1.61	7 (21%)
20	GDP	Ba	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.31	4 (13%)
20	GDP	3e	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.37	4 (13%)
21	GTP	2f	501	-	26,34,34	1.19	2 (7%)	32,54,54	1.61	7 (21%)
21	GTP	7d	501	-	26,34,34	1.18	2 (7%)	32,54,54	1.60	7 (21%)
21	GTP	8h	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.61	7 (21%)
21	GTP	Ch	501	-	26,34,34	1.18	2 (7%)	32,54,54	1.64	7 (21%)
20	GDP	Dg	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.38	4 (13%)
21	GTP	4b	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.61	7 (21%)
21	GTP	7h	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.60	7 (21%)
21	GTP	2h	501	-	26,34,34	1.19	2 (7%)	32,54,54	1.60	7 (21%)
20	GDP	7c	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
19	ADP	0Y	801	-	24,29,29	0.94	1 (4%)	29,45,45	1.32	4 (13%)
21	GTP	1h	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.58	6 (18%)
21	GTP	4d	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.63	7 (21%)
21	GTP	4f	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.62	7 (21%)
20	GDP	6g	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.36	4 (13%)
21	GTP	5b	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.60	7 (21%)
21	GTP	Af	501	-	26,34,34	1.19	2 (7%)	32,54,54	1.63	7 (21%)
21	GTP	2d	501	-	26,34,34	1.18	2 (7%)	32,54,54	1.63	7 (21%)
21	GTP	Cf	501	-	26,34,34	1.18	2 (7%)	32,54,54	1.62	7 (21%)
20	GDP	4a	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.33	4 (13%)
20	GDP	Ae	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.33	4 (13%)
21	GTP	5f	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.60	7 (21%)
20	GDP	4e	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.37	4 (13%)
20	GDP	9g	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.42	4 (13%)
21	GTP	7b	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.59	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	GDP	3g	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.35	4 (13%)
20	GDP	6a	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.37	4 (13%)
20	GDP	8g	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.35	4 (13%)
21	GTP	6h	501	-	26,34,34	1.14	2 (7%)	32,54,54	1.59	6 (18%)
21	GTP	Bh	501	-	26,34,34	1.20	2 (7%)	32,54,54	1.64	7 (21%)
21	GTP	8f	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.59	7 (21%)
21	GTP	6f	501	-	26,34,34	1.14	2 (7%)	32,54,54	1.58	6 (18%)
20	GDP	2e	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.35	4 (13%)
20	GDP	8e	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.37	4 (13%)
21	GTP	Ah	501	-	26,34,34	1.18	2 (7%)	32,54,54	1.61	7 (21%)
20	GDP	Aa	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.38	4 (13%)
20	GDP	Bc	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.41	4 (13%)
20	GDP	5c	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
21	GTP	Db	501	-	26,34,34	1.18	2 (7%)	32,54,54	1.62	7 (21%)
20	GDP	Be	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
21	GTP	5h	501	-	26,34,34	1.15	2 (7%)	32,54,54	1.59	7 (21%)
20	GDP	6c	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.36	4 (13%)
20	GDP	1e	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.40	4 (13%)
20	GDP	3c	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.39	4 (13%)
21	GTP	Cd	501	-	26,34,34	1.18	2 (7%)	32,54,54	1.62	7 (21%)
20	GDP	2g	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.37	4 (13%)
20	GDP	Ce	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.38	4 (13%)
21	GTP	3d	501	-	26,34,34	1.18	2 (7%)	32,54,54	1.63	7 (21%)
20	GDP	Ag	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
21	GTP	3b	501	-	26,34,34	1.20	2 (7%)	32,54,54	1.64	7 (21%)
21	GTP	6d	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.58	7 (21%)
21	GTP	5d	501	-	26,34,34	1.15	2 (7%)	32,54,54	1.58	7 (21%)
20	GDP	Cg	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.40	4 (13%)
20	GDP	8a	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)

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
21	GTP	3f	501	-	-	3/18/38/38	0/3/3/3
20	GDP	Da	501	-	-	3/12/32/32	0/3/3/3
21	GTP	Bf	501	-	-	3/18/38/38	0/3/3/3
20	GDP	1a	501	-	-	3/12/32/32	0/3/3/3
20	GDP	De	501	-	-	3/12/32/32	0/3/3/3
21	GTP	3h	501	-	-	3/18/38/38	0/3/3/3
20	GDP	7a	501	-	-	3/12/32/32	0/3/3/3
21	GTP	2b	501	-	-	2/18/38/38	0/3/3/3
21	GTP	1d	501	-	-	2/18/38/38	0/3/3/3
20	GDP	9e	501	-	-	3/12/32/32	0/3/3/3
21	GTP	9f	501	-	-	3/18/38/38	0/3/3/3
20	GDP	7g	501	-	-	3/12/32/32	0/3/3/3
21	GTP	Ab	501	-	-	3/18/38/38	0/3/3/3
21	GTP	6b	501	-	-	3/18/38/38	0/3/3/3
20	GDP	3a	501	-	-	3/12/32/32	0/3/3/3
20	GDP	2a	501	-	-	3/12/32/32	0/3/3/3
20	GDP	Dc	501	-	-	3/12/32/32	0/3/3/3
20	GDP	5g	501	-	-	3/12/32/32	0/3/3/3
21	GTP	4h	501	-	-	2/18/38/38	0/3/3/3
20	GDP	Bg	501	-	-	3/12/32/32	0/3/3/3
20	GDP	5a	501	-	-	3/12/32/32	0/3/3/3
20	GDP	8c	501	-	-	3/12/32/32	0/3/3/3
21	GTP	Df	501	-	-	3/18/38/38	0/3/3/3
21	GTP	Dh	501	-	-	2/18/38/38	0/3/3/3
19	ADP	1A	801	-	-	4/12/32/32	0/3/3/3
20	GDP	Ca	501	-	-	3/12/32/32	0/3/3/3
20	GDP	9a	501	-	-	3/12/32/32	0/3/3/3
21	GTP	1f	501	-	-	2/18/38/38	0/3/3/3
19	ADP	0Z	801	-	-	4/12/32/32	0/3/3/3
20	GDP	9c	501	-	-	3/12/32/32	0/3/3/3
20	GDP	Cc	501	-	-	3/12/32/32	0/3/3/3
21	GTP	9d	501	-	-	3/18/38/38	0/3/3/3
20	GDP	4c	501	-	-	3/12/32/32	0/3/3/3
20	GDP	Ac	501	-	-	3/12/32/32	0/3/3/3
21	GTP	8b	501	-	-	3/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	GDP	7e	501	-	-	3/12/32/32	0/3/3/3
20	GDP	2c	501	-	-	3/12/32/32	0/3/3/3
20	GDP	1g	501	-	-	3/12/32/32	0/3/3/3
21	GTP	9b	501	-	-	3/18/38/38	0/3/3/3
20	GDP	1c	501	-	-	3/12/32/32	0/3/3/3
21	GTP	Ad	501	-	-	3/18/38/38	0/3/3/3
21	GTP	7f	501	-	-	2/18/38/38	0/3/3/3
20	GDP	4g	501	-	-	3/12/32/32	0/3/3/3
21	GTP	9h	501	-	-	3/18/38/38	0/3/3/3
21	GTP	1b	501	-	-	3/18/38/38	0/3/3/3
20	GDP	6e	501	-	-	3/12/32/32	0/3/3/3
21	GTP	Bb	501	-	-	3/18/38/38	0/3/3/3
21	GTP	8d	501	-	-	3/18/38/38	0/3/3/3
21	GTP	Cb	501	-	-	3/18/38/38	0/3/3/3
20	GDP	5e	501	-	-	3/12/32/32	0/3/3/3
19	ADP	0X	801	-	-	3/12/32/32	0/3/3/3
21	GTP	Bd	501	-	-	2/18/38/38	0/3/3/3
21	GTP	Dd	501	-	-	2/18/38/38	0/3/3/3
20	GDP	Ba	501	-	-	3/12/32/32	0/3/3/3
20	GDP	3e	501	-	-	3/12/32/32	0/3/3/3
21	GTP	2f	501	-	-	3/18/38/38	0/3/3/3
21	GTP	7d	501	-	-	3/18/38/38	0/3/3/3
21	GTP	8h	501	-	-	3/18/38/38	0/3/3/3
21	GTP	Ch	501	-	-	3/18/38/38	0/3/3/3
20	GDP	Dg	501	-	-	3/12/32/32	0/3/3/3
21	GTP	4b	501	-	-	3/18/38/38	0/3/3/3
21	GTP	7h	501	-	-	3/18/38/38	0/3/3/3
21	GTP	2h	501	-	-	2/18/38/38	0/3/3/3
20	GDP	7c	501	-	-	3/12/32/32	0/3/3/3
19	ADP	0Y	801	-	-	5/12/32/32	0/3/3/3
21	GTP	1h	501	-	-	2/18/38/38	0/3/3/3
21	GTP	4d	501	-	-	3/18/38/38	0/3/3/3
21	GTP	4f	501	-	-	3/18/38/38	0/3/3/3
20	GDP	6g	501	-	-	3/12/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	GTP	5b	501	-	-	3/18/38/38	0/3/3/3
21	GTP	Af	501	-	-	3/18/38/38	0/3/3/3
21	GTP	2d	501	-	-	3/18/38/38	0/3/3/3
21	GTP	Cf	501	-	-	3/18/38/38	0/3/3/3
20	GDP	4a	501	-	-	3/12/32/32	0/3/3/3
20	GDP	Ae	501	-	-	3/12/32/32	0/3/3/3
21	GTP	5f	501	-	-	3/18/38/38	0/3/3/3
20	GDP	4e	501	-	-	3/12/32/32	0/3/3/3
20	GDP	9g	501	-	-	3/12/32/32	0/3/3/3
21	GTP	7b	501	-	-	3/18/38/38	0/3/3/3
20	GDP	3g	501	-	-	3/12/32/32	0/3/3/3
20	GDP	6a	501	-	-	3/12/32/32	0/3/3/3
20	GDP	8g	501	-	-	3/12/32/32	0/3/3/3
21	GTP	6h	501	-	-	3/18/38/38	0/3/3/3
21	GTP	Bh	501	-	-	3/18/38/38	0/3/3/3
21	GTP	8f	501	-	-	3/18/38/38	0/3/3/3
21	GTP	6f	501	-	-	3/18/38/38	0/3/3/3
20	GDP	2e	501	-	-	3/12/32/32	0/3/3/3
20	GDP	8e	501	-	-	3/12/32/32	0/3/3/3
21	GTP	Ah	501	-	-	2/18/38/38	0/3/3/3
20	GDP	Aa	501	-	-	3/12/32/32	0/3/3/3
20	GDP	Bc	501	-	-	3/12/32/32	0/3/3/3
20	GDP	5c	501	-	-	3/12/32/32	0/3/3/3
21	GTP	Db	501	-	-	3/18/38/38	0/3/3/3
20	GDP	Be	501	-	-	3/12/32/32	0/3/3/3
21	GTP	5h	501	-	-	3/18/38/38	0/3/3/3
20	GDP	6c	501	-	-	3/12/32/32	0/3/3/3
20	GDP	1e	501	-	-	3/12/32/32	0/3/3/3
20	GDP	3c	501	-	-	3/12/32/32	0/3/3/3
21	GTP	Cd	501	-	-	2/18/38/38	0/3/3/3
20	GDP	2g	501	-	-	3/12/32/32	0/3/3/3
20	GDP	Ce	501	-	-	3/12/32/32	0/3/3/3
21	GTP	3d	501	-	-	3/18/38/38	0/3/3/3
20	GDP	Ag	501	-	-	3/12/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	GTP	3b	501	-	-	2/18/38/38	0/3/3/3
21	GTP	6d	501	-	-	3/18/38/38	0/3/3/3
21	GTP	5d	501	-	-	3/18/38/38	0/3/3/3
20	GDP	Cg	501	-	-	3/12/32/32	0/3/3/3
20	GDP	8a	501	-	-	3/12/32/32	0/3/3/3

All (160) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	9b	501	GTP	C5-C6	-4.33	1.38	1.47
21	9f	501	GTP	C5-C6	-4.29	1.38	1.47
21	Af	501	GTP	C5-C6	-4.28	1.38	1.47
21	9h	501	GTP	C5-C6	-4.27	1.38	1.47
21	Bf	501	GTP	C5-C6	-4.27	1.38	1.47
21	1d	501	GTP	C5-C6	-4.26	1.38	1.47
21	Bd	501	GTP	C5-C6	-4.25	1.38	1.47
21	Bh	501	GTP	C5-C6	-4.22	1.38	1.47
21	9d	501	GTP	C5-C6	-4.22	1.38	1.47
21	2b	501	GTP	C5-C6	-4.21	1.38	1.47
21	3f	501	GTP	C5-C6	-4.21	1.38	1.47
21	3b	501	GTP	C5-C6	-4.20	1.38	1.47
21	Ab	501	GTP	C5-C6	-4.20	1.38	1.47
21	2f	501	GTP	C5-C6	-4.20	1.38	1.47
21	Ah	501	GTP	C5-C6	-4.20	1.38	1.47
21	2h	501	GTP	C5-C6	-4.19	1.38	1.47
21	Ch	501	GTP	C5-C6	-4.19	1.38	1.47
21	Dh	501	GTP	C5-C6	-4.19	1.38	1.47
21	1f	501	GTP	C5-C6	-4.19	1.38	1.47
21	Bb	501	GTP	C5-C6	-4.18	1.38	1.47
21	2d	501	GTP	C5-C6	-4.18	1.38	1.47
21	4f	501	GTP	C5-C6	-4.18	1.38	1.47
21	3d	501	GTP	C5-C6	-4.17	1.38	1.47
21	3h	501	GTP	C5-C6	-4.17	1.38	1.47
21	5f	501	GTP	C5-C6	-4.17	1.39	1.47
21	5b	501	GTP	C5-C6	-4.16	1.39	1.47
21	7d	501	GTP	C5-C6	-4.16	1.39	1.47
21	Cb	501	GTP	C5-C6	-4.15	1.39	1.47
21	Df	501	GTP	C5-C6	-4.15	1.39	1.47
21	4b	501	GTP	C5-C6	-4.15	1.39	1.47
21	7b	501	GTP	C5-C6	-4.15	1.39	1.47
21	8h	501	GTP	C5-C6	-4.15	1.39	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Cf	501	GTP	C5-C6	-4.14	1.39	1.47
21	7h	501	GTP	C5-C6	-4.14	1.39	1.47
21	Dd	501	GTP	C5-C6	-4.14	1.39	1.47
21	4d	501	GTP	C5-C6	-4.14	1.39	1.47
21	1b	501	GTP	C5-C6	-4.13	1.39	1.47
21	Cd	501	GTP	C5-C6	-4.13	1.39	1.47
21	Db	501	GTP	C5-C6	-4.13	1.39	1.47
21	Ad	501	GTP	C5-C6	-4.13	1.39	1.47
21	1h	501	GTP	C5-C6	-4.12	1.39	1.47
21	8f	501	GTP	C5-C6	-4.10	1.39	1.47
21	4h	501	GTP	C5-C6	-4.10	1.39	1.47
21	7f	501	GTP	C5-C6	-4.09	1.39	1.47
21	5d	501	GTP	C5-C6	-4.08	1.39	1.47
21	8d	501	GTP	C5-C6	-4.08	1.39	1.47
21	6b	501	GTP	C5-C6	-4.06	1.39	1.47
21	6d	501	GTP	C5-C6	-4.05	1.39	1.47
21	8b	501	GTP	C5-C6	-4.00	1.39	1.47
21	5h	501	GTP	C5-C6	-3.97	1.39	1.47
21	6f	501	GTP	C5-C6	-3.97	1.39	1.47
21	6h	501	GTP	C5-C6	-3.92	1.39	1.47
20	Bg	501	GDP	C6-N1	-2.63	1.33	1.37
20	De	501	GDP	C6-N1	-2.62	1.34	1.37
20	9a	501	GDP	C6-N1	-2.61	1.34	1.37
20	9e	501	GDP	C6-N1	-2.61	1.34	1.37
20	Be	501	GDP	C6-N1	-2.61	1.34	1.37
20	9c	501	GDP	C6-N1	-2.60	1.34	1.37
20	Ce	501	GDP	C6-N1	-2.60	1.34	1.37
20	Da	501	GDP	C6-N1	-2.60	1.34	1.37
20	9g	501	GDP	C6-N1	-2.58	1.34	1.37
20	5a	501	GDP	C6-N1	-2.58	1.34	1.37
20	Cc	501	GDP	C6-N1	-2.58	1.34	1.37
20	Bc	501	GDP	C6-N1	-2.57	1.34	1.37
20	Cg	501	GDP	C6-N1	-2.56	1.34	1.37
20	Ag	501	GDP	C6-N1	-2.55	1.34	1.37
20	1e	501	GDP	C6-N1	-2.55	1.34	1.37
20	1a	501	GDP	C6-N1	-2.55	1.34	1.37
20	1c	501	GDP	C6-N1	-2.53	1.34	1.37
20	Ba	501	GDP	C6-N1	-2.53	1.34	1.37
20	Dg	501	GDP	C6-N1	-2.53	1.34	1.37
20	5c	501	GDP	C6-N1	-2.53	1.34	1.37
20	2g	501	GDP	C6-N1	-2.53	1.34	1.37
20	2a	501	GDP	C6-N1	-2.52	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Dc	501	GDP	C6-N1	-2.52	1.34	1.37
20	5e	501	GDP	C6-N1	-2.52	1.34	1.37
20	2e	501	GDP	C6-N1	-2.51	1.34	1.37
20	8a	501	GDP	C6-N1	-2.51	1.34	1.37
20	3e	501	GDP	C6-N1	-2.51	1.34	1.37
20	4a	501	GDP	C6-N1	-2.51	1.34	1.37
20	4c	501	GDP	C6-N1	-2.50	1.34	1.37
20	6g	501	GDP	C6-N1	-2.50	1.34	1.37
20	Ae	501	GDP	C6-N1	-2.49	1.34	1.37
20	4g	501	GDP	C6-N1	-2.49	1.34	1.37
20	7c	501	GDP	C6-N1	-2.48	1.34	1.37
20	Aa	501	GDP	C6-N1	-2.48	1.34	1.37
20	3g	501	GDP	C6-N1	-2.47	1.34	1.37
20	Ac	501	GDP	C6-N1	-2.47	1.34	1.37
20	3a	501	GDP	C6-N1	-2.47	1.34	1.37
19	1A	801	ADP	C5-C4	2.46	1.47	1.40
20	1g	501	GDP	C6-N1	-2.46	1.34	1.37
20	6a	501	GDP	C6-N1	-2.46	1.34	1.37
20	4e	501	GDP	C6-N1	-2.45	1.34	1.37
20	Ca	501	GDP	C6-N1	-2.45	1.34	1.37
19	0Y	801	ADP	C5-C4	2.45	1.47	1.40
20	3c	501	GDP	C6-N1	-2.45	1.34	1.37
20	2c	501	GDP	C6-N1	-2.44	1.34	1.37
20	7g	501	GDP	C6-N1	-2.43	1.34	1.37
19	0Z	801	ADP	C5-C4	2.43	1.47	1.40
20	5g	501	GDP	C6-N1	-2.42	1.34	1.37
19	0X	801	ADP	C5-C4	2.42	1.47	1.40
20	8c	501	GDP	C6-N1	-2.41	1.34	1.37
20	8g	501	GDP	C6-N1	-2.40	1.34	1.37
20	6e	501	GDP	C6-N1	-2.39	1.34	1.37
20	7e	501	GDP	C6-N1	-2.39	1.34	1.37
20	8e	501	GDP	C6-N1	-2.39	1.34	1.37
20	7a	501	GDP	C6-N1	-2.39	1.34	1.37
20	6c	501	GDP	C6-N1	-2.34	1.34	1.37
21	6d	501	GTP	C2-N3	2.26	1.38	1.33
21	5h	501	GTP	C2-N3	2.25	1.38	1.33
21	5d	501	GTP	C2-N3	2.23	1.38	1.33
21	Ad	501	GTP	C2-N3	2.22	1.38	1.33
21	6h	501	GTP	C2-N3	2.22	1.38	1.33
21	3b	501	GTP	C2-N3	2.21	1.38	1.33
21	Af	501	GTP	C2-N3	2.21	1.38	1.33
21	5b	501	GTP	C2-N3	2.20	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Ab	501	GTP	C2-N3	2.19	1.38	1.33
21	4d	501	GTP	C2-N3	2.19	1.38	1.33
21	6f	501	GTP	C2-N3	2.19	1.38	1.33
21	4h	501	GTP	C2-N3	2.18	1.38	1.33
21	Ch	501	GTP	C2-N3	2.18	1.38	1.33
21	7d	501	GTP	C2-N3	2.18	1.38	1.33
21	5f	501	GTP	C2-N3	2.18	1.38	1.33
21	7h	501	GTP	C2-N3	2.18	1.38	1.33
21	Ah	501	GTP	C2-N3	2.17	1.38	1.33
21	6b	501	GTP	C2-N3	2.17	1.38	1.33
21	3f	501	GTP	C2-N3	2.16	1.38	1.33
21	Cd	501	GTP	C2-N3	2.16	1.38	1.33
21	Dh	501	GTP	C2-N3	2.15	1.38	1.33
21	7b	501	GTP	C2-N3	2.15	1.38	1.33
21	4b	501	GTP	C2-N3	2.13	1.38	1.33
21	9d	501	GTP	C2-N3	2.13	1.38	1.33
21	3d	501	GTP	C2-N3	2.13	1.38	1.33
21	1b	501	GTP	C2-N3	2.13	1.38	1.33
21	9h	501	GTP	C2-N3	2.13	1.38	1.33
21	1d	501	GTP	C2-N3	2.12	1.38	1.33
21	4f	501	GTP	C2-N3	2.12	1.38	1.33
21	2f	501	GTP	C2-N3	2.12	1.38	1.33
21	1f	501	GTP	C2-N3	2.12	1.38	1.33
21	2b	501	GTP	C2-N3	2.11	1.38	1.33
21	Bf	501	GTP	C2-N3	2.10	1.38	1.33
21	7f	501	GTP	C2-N3	2.10	1.38	1.33
21	2d	501	GTP	C2-N3	2.09	1.38	1.33
21	Cb	501	GTP	C2-N3	2.09	1.38	1.33
21	3h	501	GTP	C2-N3	2.09	1.38	1.33
21	Bh	501	GTP	C2-N3	2.09	1.38	1.33
21	Dd	501	GTP	C2-N3	2.09	1.38	1.33
21	Df	501	GTP	C2-N3	2.08	1.38	1.33
21	8b	501	GTP	C2-N3	2.08	1.38	1.33
21	9f	501	GTP	C2-N3	2.08	1.38	1.33
21	Db	501	GTP	C2-N3	2.08	1.38	1.33
21	Bd	501	GTP	C2-N3	2.08	1.38	1.33
21	9b	501	GTP	C2-N3	2.07	1.38	1.33
21	2h	501	GTP	C2-N3	2.07	1.38	1.33
21	Bb	501	GTP	C2-N3	2.07	1.38	1.33
21	8h	501	GTP	C2-N3	2.07	1.38	1.33
21	8d	501	GTP	C2-N3	2.06	1.38	1.33
21	8f	501	GTP	C2-N3	2.05	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1h	501	GTP	C2-N3	2.02	1.38	1.33
21	Cf	501	GTP	C2-N3	2.01	1.38	1.33

All (585) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	9a	501	GDP	PA-O3A-PB	-4.71	116.66	132.83
20	9g	501	GDP	PA-O3A-PB	-4.70	116.69	132.83
20	9c	501	GDP	PA-O3A-PB	-4.63	116.95	132.83
20	9e	501	GDP	PA-O3A-PB	-4.60	117.05	132.83
20	Cc	501	GDP	PA-O3A-PB	-4.58	117.10	132.83
20	1c	501	GDP	PA-O3A-PB	-4.50	117.40	132.83
20	8c	501	GDP	PA-O3A-PB	-4.48	117.45	132.83
20	Cg	501	GDP	PA-O3A-PB	-4.48	117.45	132.83
20	Bc	501	GDP	PA-O3A-PB	-4.42	117.65	132.83
20	1e	501	GDP	PA-O3A-PB	-4.42	117.66	132.83
20	4e	501	GDP	PA-O3A-PB	-4.42	117.67	132.83
20	7g	501	GDP	PA-O3A-PB	-4.39	117.75	132.83
20	Bg	501	GDP	PA-O3A-PB	-4.39	117.76	132.83
20	2g	501	GDP	PA-O3A-PB	-4.35	117.92	132.83
20	Dg	501	GDP	PA-O3A-PB	-4.35	117.92	132.83
20	Ca	501	GDP	PA-O3A-PB	-4.33	117.96	132.83
20	7e	501	GDP	PA-O3A-PB	-4.33	117.96	132.83
20	Dc	501	GDP	PA-O3A-PB	-4.32	118.00	132.83
20	3c	501	GDP	PA-O3A-PB	-4.31	118.04	132.83
20	1a	501	GDP	PA-O3A-PB	-4.30	118.05	132.83
20	Aa	501	GDP	PA-O3A-PB	-4.29	118.09	132.83
20	2a	501	GDP	PA-O3A-PB	-4.28	118.13	132.83
20	3a	501	GDP	PA-O3A-PB	-4.27	118.16	132.83
20	Ce	501	GDP	PA-O3A-PB	-4.27	118.16	132.83
20	3e	501	GDP	PA-O3A-PB	-4.27	118.17	132.83
20	6g	501	GDP	PA-O3A-PB	-4.25	118.24	132.83
20	6c	501	GDP	PA-O3A-PB	-4.25	118.25	132.83
20	8e	501	GDP	PA-O3A-PB	-4.24	118.27	132.83
20	5g	501	GDP	PA-O3A-PB	-4.23	118.32	132.83
20	4c	501	GDP	PA-O3A-PB	-4.19	118.44	132.83
20	7c	501	GDP	PA-O3A-PB	-4.19	118.46	132.83
20	2e	501	GDP	PA-O3A-PB	-4.18	118.48	132.83
20	6a	501	GDP	PA-O3A-PB	-4.18	118.49	132.83
20	Da	501	GDP	PA-O3A-PB	-4.17	118.50	132.83
20	7a	501	GDP	PA-O3A-PB	-4.17	118.53	132.83
20	3g	501	GDP	PA-O3A-PB	-4.16	118.53	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	5a	501	GDP	PA-O3A-PB	-4.16	118.54	132.83
20	4g	501	GDP	PA-O3A-PB	-4.16	118.55	132.83
20	Ag	501	GDP	PA-O3A-PB	-4.15	118.59	132.83
20	1g	501	GDP	PA-O3A-PB	-4.12	118.68	132.83
20	Be	501	GDP	PA-O3A-PB	-4.11	118.71	132.83
20	4a	501	GDP	PA-O3A-PB	-4.09	118.78	132.83
20	Ae	501	GDP	PA-O3A-PB	-4.08	118.83	132.83
20	8g	501	GDP	PA-O3A-PB	-4.07	118.87	132.83
20	6e	501	GDP	PA-O3A-PB	-4.06	118.88	132.83
20	8a	501	GDP	PA-O3A-PB	-4.06	118.88	132.83
21	Dh	501	GTP	PA-O3A-PB	-4.06	118.90	132.83
21	7f	501	GTP	PA-O3A-PB	-4.03	118.99	132.83
21	3d	501	GTP	PA-O3A-PB	-4.03	119.00	132.83
20	2c	501	GDP	PA-O3A-PB	-4.03	119.01	132.83
20	De	501	GDP	PA-O3A-PB	-4.02	119.03	132.83
21	Cf	501	GTP	PA-O3A-PB	-4.01	119.06	132.83
21	7d	501	GTP	PA-O3A-PB	-4.00	119.11	132.83
20	5c	501	GDP	PA-O3A-PB	-4.00	119.12	132.83
21	3h	501	GTP	PA-O3A-PB	-3.99	119.13	132.83
21	9f	501	GTP	PB-O3B-PG	-3.99	119.15	132.83
21	9b	501	GTP	PB-O3B-PG	-3.98	119.15	132.83
21	Bh	501	GTP	PA-O3A-PB	-3.97	119.21	132.83
20	5e	501	GDP	PA-O3A-PB	-3.96	119.25	132.83
21	2d	501	GTP	PA-O3A-PB	-3.93	119.34	132.83
21	4b	501	GTP	PA-O3A-PB	-3.92	119.37	132.83
21	Dd	501	GTP	PA-O3A-PB	-3.90	119.43	132.83
21	4f	501	GTP	PA-O3A-PB	-3.89	119.47	132.83
21	1f	501	GTP	PA-O3A-PB	-3.88	119.52	132.83
21	8b	501	GTP	PA-O3A-PB	-3.88	119.53	132.83
21	Bb	501	GTP	PB-O3B-PG	-3.87	119.53	132.83
21	Bb	501	GTP	PA-O3A-PB	-3.87	119.53	132.83
20	Ac	501	GDP	PA-O3A-PB	-3.86	119.57	132.83
21	4d	501	GTP	PA-O3A-PB	-3.86	119.57	132.83
21	4h	501	GTP	PA-O3A-PB	-3.86	119.57	132.83
21	Df	501	GTP	PB-O3B-PG	-3.86	119.59	132.83
21	8h	501	GTP	PA-O3A-PB	-3.85	119.61	132.83
21	5f	501	GTP	PA-O3A-PB	-3.85	119.63	132.83
21	Ah	501	GTP	PA-O3A-PB	-3.84	119.64	132.83
21	6h	501	GTP	PA-O3A-PB	-3.84	119.65	132.83
21	6b	501	GTP	PA-O3A-PB	-3.84	119.66	132.83
21	Df	501	GTP	PA-O3A-PB	-3.84	119.66	132.83
21	2b	501	GTP	PA-O3A-PB	-3.84	119.66	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1d	501	GTP	PA-O3A-PB	-3.83	119.67	132.83
21	8f	501	GTP	PA-O3A-PB	-3.83	119.68	132.83
21	3f	501	GTP	PA-O3A-PB	-3.83	119.70	132.83
21	Af	501	GTP	PA-O3A-PB	-3.82	119.73	132.83
21	Cb	501	GTP	PA-O3A-PB	-3.81	119.76	132.83
21	9h	501	GTP	PA-O3A-PB	-3.80	119.78	132.83
21	Ch	501	GTP	PA-O3A-PB	-3.80	119.79	132.83
21	5d	501	GTP	PA-O3A-PB	-3.80	119.80	132.83
20	Ba	501	GDP	PA-O3A-PB	-3.79	119.81	132.83
21	5b	501	GTP	PA-O3A-PB	-3.79	119.81	132.83
21	7b	501	GTP	PA-O3A-PB	-3.79	119.81	132.83
21	7h	501	GTP	PA-O3A-PB	-3.79	119.82	132.83
21	Ab	501	GTP	PA-O3A-PB	-3.79	119.82	132.83
21	Db	501	GTP	PB-O3B-PG	-3.77	119.88	132.83
21	1b	501	GTP	PA-O3A-PB	-3.77	119.89	132.83
21	4f	501	GTP	PB-O3B-PG	-3.77	119.89	132.83
21	6f	501	GTP	PA-O3A-PB	-3.77	119.89	132.83
21	9d	501	GTP	PA-O3A-PB	-3.76	119.93	132.83
21	Bf	501	GTP	PB-O3B-PG	-3.76	119.94	132.83
21	3b	501	GTP	PA-O3A-PB	-3.76	119.94	132.83
21	2f	501	GTP	PA-O3A-PB	-3.75	119.97	132.83
21	2h	501	GTP	PA-O3A-PB	-3.75	119.97	132.83
21	8b	501	GTP	PB-O3B-PG	-3.74	119.98	132.83
21	Cd	501	GTP	PA-O3A-PB	-3.73	120.01	132.83
21	8d	501	GTP	PA-O3A-PB	-3.73	120.02	132.83
19	0X	801	ADP	PA-O3A-PB	-3.73	120.03	132.83
21	4d	501	GTP	PB-O3B-PG	-3.71	120.09	132.83
19	0Z	801	ADP	PA-O3A-PB	-3.71	120.10	132.83
21	8d	501	GTP	PB-O3B-PG	-3.69	120.16	132.83
21	Db	501	GTP	PA-O3A-PB	-3.69	120.16	132.83
21	5h	501	GTP	PA-O3A-PB	-3.69	120.17	132.83
21	Bd	501	GTP	PA-O3A-PB	-3.69	120.17	132.83
21	3h	501	GTP	PB-O3B-PG	-3.69	120.17	132.83
21	Ah	501	GTP	PB-O3B-PG	-3.69	120.18	132.83
21	2d	501	GTP	PB-O3B-PG	-3.68	120.19	132.83
21	3f	501	GTP	PB-O3B-PG	-3.66	120.28	132.83
21	Ad	501	GTP	PA-O3A-PB	-3.66	120.28	132.83
21	3b	501	GTP	PB-O3B-PG	-3.65	120.29	132.83
21	Ch	501	GTP	PB-O3B-PG	-3.65	120.31	132.83
21	Bf	501	GTP	PA-O3A-PB	-3.65	120.31	132.83
21	Af	501	GTP	PB-O3B-PG	-3.64	120.33	132.83
21	9b	501	GTP	PA-O3A-PB	-3.64	120.34	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1h	501	GTP	PA-O3A-PB	-3.62	120.41	132.83
21	3d	501	GTP	PB-O3B-PG	-3.62	120.42	132.83
21	9f	501	GTP	PA-O3A-PB	-3.60	120.47	132.83
21	6d	501	GTP	PA-O3A-PB	-3.59	120.50	132.83
21	Bd	501	GTP	PB-O3B-PG	-3.57	120.58	132.83
21	Cb	501	GTP	PB-O3B-PG	-3.55	120.64	132.83
21	2h	501	GTP	PB-O3B-PG	-3.55	120.66	132.83
21	2f	501	GTP	PB-O3B-PG	-3.53	120.71	132.83
21	Bh	501	GTP	PB-O3B-PG	-3.52	120.74	132.83
21	Ab	501	GTP	PB-O3B-PG	-3.52	120.75	132.83
19	1A	801	ADP	PA-O3A-PB	-3.52	120.75	132.83
21	4h	501	GTP	PB-O3B-PG	-3.51	120.79	132.83
21	9d	501	GTP	PB-O3B-PG	-3.48	120.87	132.83
21	7f	501	GTP	PB-O3B-PG	-3.48	120.89	132.83
21	7b	501	GTP	PB-O3B-PG	-3.47	120.91	132.83
21	1d	501	GTP	PB-O3B-PG	-3.47	120.91	132.83
21	6h	501	GTP	PB-O3B-PG	-3.47	120.92	132.83
21	Cf	501	GTP	PB-O3B-PG	-3.47	120.93	132.83
21	8f	501	GTP	PB-O3B-PG	-3.46	120.96	132.83
21	Dd	501	GTP	PB-O3B-PG	-3.46	120.97	132.83
21	8h	501	GTP	PB-O3B-PG	-3.45	120.98	132.83
21	1b	501	GTP	PB-O3B-PG	-3.45	121.00	132.83
21	Ad	501	GTP	PB-O3B-PG	-3.44	121.00	132.83
21	7h	501	GTP	PB-O3B-PG	-3.44	121.03	132.83
21	Bh	501	GTP	C5-C6-N1	3.43	120.01	113.95
21	6f	501	GTP	PB-O3B-PG	-3.43	121.07	132.83
20	Aa	501	GDP	C3'-C2'-C1'	3.42	106.13	100.98
21	4b	501	GTP	PB-O3B-PG	-3.42	121.08	132.83
21	Cd	501	GTP	PB-O3B-PG	-3.42	121.08	132.83
21	5h	501	GTP	C5-C6-N1	3.42	119.98	113.95
21	9d	501	GTP	C5-C6-N1	3.41	119.97	113.95
21	7d	501	GTP	PB-O3B-PG	-3.40	121.14	132.83
21	Bd	501	GTP	C5-C6-N1	3.39	119.94	113.95
21	9h	501	GTP	C5-C6-N1	3.39	119.94	113.95
21	2b	501	GTP	C5-C6-N1	3.39	119.93	113.95
21	Bb	501	GTP	C5-C6-N1	3.39	119.93	113.95
21	4d	501	GTP	C5-C6-N1	3.39	119.93	113.95
21	3b	501	GTP	C5-C6-N1	3.39	119.93	113.95
21	1h	501	GTP	PB-O3B-PG	-3.38	121.22	132.83
21	5f	501	GTP	C5-C6-N1	3.38	119.92	113.95
21	9h	501	GTP	PB-O3B-PG	-3.37	121.25	132.83
21	Af	501	GTP	C5-C6-N1	3.36	119.88	113.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5h	501	GTP	PB-O3B-PG	-3.36	121.31	132.83
21	6d	501	GTP	C5-C6-N1	3.36	119.88	113.95
21	2f	501	GTP	C5-C6-N1	3.35	119.87	113.95
21	6d	501	GTP	PB-O3B-PG	-3.35	121.33	132.83
21	2b	501	GTP	PB-O3B-PG	-3.35	121.33	132.83
21	5b	501	GTP	C5-C6-N1	3.35	119.86	113.95
21	Cd	501	GTP	C5-C6-N1	3.35	119.86	113.95
21	3f	501	GTP	C5-C6-N1	3.35	119.86	113.95
21	Ab	501	GTP	C5-C6-N1	3.35	119.86	113.95
20	Cg	501	GDP	C3'-C2'-C1'	3.35	106.02	100.98
21	4b	501	GTP	C5-C6-N1	3.34	119.85	113.95
21	6b	501	GTP	C5-C6-N1	3.34	119.85	113.95
21	Cb	501	GTP	C5-C6-N1	3.34	119.84	113.95
21	9f	501	GTP	C5-C6-N1	3.33	119.84	113.95
21	7d	501	GTP	C5-C6-N1	3.33	119.83	113.95
21	5b	501	GTP	PB-O3B-PG	-3.33	121.39	132.83
21	8b	501	GTP	C5-C6-N1	3.33	119.83	113.95
21	4h	501	GTP	C5-C6-N1	3.33	119.83	113.95
21	Dh	501	GTP	PB-O3B-PG	-3.33	121.41	132.83
21	1d	501	GTP	C5-C6-N1	3.33	119.83	113.95
21	Ah	501	GTP	C5-C6-N1	3.33	119.83	113.95
21	1f	501	GTP	C5-C6-N1	3.32	119.82	113.95
21	3d	501	GTP	C5-C6-N1	3.32	119.82	113.95
21	5d	501	GTP	PB-O3B-PG	-3.32	121.43	132.83
21	Bf	501	GTP	C5-C6-N1	3.32	119.81	113.95
21	5f	501	GTP	PB-O3B-PG	-3.32	121.44	132.83
21	Db	501	GTP	C5-C6-N1	3.31	119.79	113.95
20	3a	501	GDP	C3'-C2'-C1'	3.31	105.95	100.98
21	5d	501	GTP	C5-C6-N1	3.30	119.78	113.95
21	Cf	501	GTP	C5-C6-N1	3.30	119.78	113.95
21	Dh	501	GTP	C5-C6-N1	3.30	119.78	113.95
21	6b	501	GTP	PB-O3B-PG	-3.30	121.50	132.83
21	8d	501	GTP	C5-C6-N1	3.30	119.77	113.95
21	4f	501	GTP	C5-C6-N1	3.29	119.77	113.95
21	6f	501	GTP	C5-C6-N1	3.29	119.77	113.95
21	Df	501	GTP	C5-C6-N1	3.29	119.76	113.95
21	6h	501	GTP	C5-C6-N1	3.29	119.76	113.95
20	1e	501	GDP	C3'-C2'-C1'	3.29	105.93	100.98
21	Dd	501	GTP	C5-C6-N1	3.28	119.75	113.95
21	Ch	501	GTP	C5-C6-N1	3.28	119.75	113.95
20	Bc	501	GDP	C3'-C2'-C1'	3.28	105.92	100.98
21	9b	501	GTP	C5-C6-N1	3.28	119.74	113.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	7h	501	GTP	C5-C6-N1	3.28	119.74	113.95
21	8h	501	GTP	C5-C6-N1	3.28	119.73	113.95
19	0Y	801	ADP	PA-O3A-PB	-3.27	121.59	132.83
20	De	501	GDP	C3'-C2'-C1'	3.27	105.91	100.98
21	3h	501	GTP	C5-C6-N1	3.27	119.73	113.95
20	4g	501	GDP	C3'-C2'-C1'	3.27	105.90	100.98
21	Ad	501	GTP	C5-C6-N1	3.27	119.73	113.95
21	1h	501	GTP	C5-C6-N1	3.27	119.72	113.95
21	1b	501	GTP	C5-C6-N1	3.26	119.72	113.95
21	2d	501	GTP	C5-C6-N1	3.26	119.70	113.95
21	7b	501	GTP	C5-C6-N1	3.25	119.70	113.95
21	2h	501	GTP	C5-C6-N1	3.25	119.68	113.95
21	8f	501	GTP	C5-C6-N1	3.24	119.67	113.95
20	Bg	501	GDP	C3'-C2'-C1'	3.23	105.85	100.98
21	7f	501	GTP	C5-C6-N1	3.23	119.65	113.95
20	Ca	501	GDP	C3'-C2'-C1'	3.23	105.83	100.98
20	3e	501	GDP	C3'-C2'-C1'	3.21	105.82	100.98
21	1f	501	GTP	PB-O3B-PG	-3.21	121.80	132.83
20	Da	501	GDP	C3'-C2'-C1'	3.21	105.81	100.98
20	6a	501	GDP	C3'-C2'-C1'	3.20	105.80	100.98
20	2a	501	GDP	C3'-C2'-C1'	3.19	105.78	100.98
20	3c	501	GDP	C3'-C2'-C1'	3.19	105.78	100.98
20	5a	501	GDP	C3'-C2'-C1'	3.18	105.77	100.98
20	Be	501	GDP	C3'-C2'-C1'	3.16	105.74	100.98
20	8a	501	GDP	C3'-C2'-C1'	3.15	105.73	100.98
20	3g	501	GDP	C3'-C2'-C1'	3.14	105.70	100.98
19	0X	801	ADP	N3-C2-N1	-3.14	123.77	128.68
20	7a	501	GDP	C3'-C2'-C1'	3.13	105.69	100.98
20	Ce	501	GDP	C3'-C2'-C1'	3.13	105.69	100.98
20	8g	501	GDP	C3'-C2'-C1'	3.12	105.67	100.98
20	4a	501	GDP	C3'-C2'-C1'	3.12	105.67	100.98
19	0Z	801	ADP	N3-C2-N1	-3.11	123.81	128.68
20	4e	501	GDP	C3'-C2'-C1'	3.11	105.66	100.98
20	8e	501	GDP	C3'-C2'-C1'	3.11	105.65	100.98
20	5c	501	GDP	C3'-C2'-C1'	3.10	105.64	100.98
20	Ag	501	GDP	C3'-C2'-C1'	3.08	105.62	100.98
20	8c	501	GDP	C3'-C2'-C1'	3.08	105.62	100.98
20	5e	501	GDP	C3'-C2'-C1'	3.08	105.61	100.98
21	Ch	501	GTP	C8-N7-C5	3.08	108.85	102.99
21	6f	501	GTP	C8-N7-C5	3.07	108.85	102.99
20	Ba	501	GDP	C3'-C2'-C1'	3.07	105.61	100.98
20	6c	501	GDP	C3'-C2'-C1'	3.07	105.60	100.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Bf	501	GTP	C8-N7-C5	3.07	108.84	102.99
21	6h	501	GTP	C8-N7-C5	3.07	108.83	102.99
20	2c	501	GDP	C3'-C2'-C1'	3.06	105.59	100.98
20	4c	501	GDP	C3'-C2'-C1'	3.06	105.59	100.98
21	Dh	501	GTP	C2-N1-C6	-3.06	119.46	125.10
20	1a	501	GDP	C3'-C2'-C1'	3.06	105.59	100.98
21	Ad	501	GTP	C8-N7-C5	3.06	108.82	102.99
21	1h	501	GTP	C8-N7-C5	3.05	108.81	102.99
21	8b	501	GTP	C8-N7-C5	3.05	108.80	102.99
21	5h	501	GTP	C8-N7-C5	3.05	108.80	102.99
21	Bd	501	GTP	C2-N1-C6	-3.05	119.48	125.10
21	Cd	501	GTP	C2-N1-C6	-3.04	119.49	125.10
21	Bb	501	GTP	C8-N7-C5	3.04	108.78	102.99
19	1A	801	ADP	N3-C2-N1	-3.04	123.93	128.68
21	Bh	501	GTP	C8-N7-C5	3.04	108.78	102.99
21	4d	501	GTP	C8-N7-C5	3.04	108.78	102.99
20	5g	501	GDP	C3'-C2'-C1'	3.03	105.54	100.98
21	Db	501	GTP	C8-N7-C5	3.03	108.77	102.99
21	Dd	501	GTP	C8-N7-C5	3.03	108.77	102.99
21	5d	501	GTP	C8-N7-C5	3.03	108.76	102.99
21	2d	501	GTP	C8-N7-C5	3.03	108.76	102.99
21	8f	501	GTP	C8-N7-C5	3.03	108.76	102.99
21	7b	501	GTP	C8-N7-C5	3.03	108.76	102.99
21	5h	501	GTP	C2-N1-C6	-3.03	119.53	125.10
21	5b	501	GTP	C3'-C2'-C1'	3.02	105.53	100.98
21	Bd	501	GTP	C8-N7-C5	3.02	108.75	102.99
21	8d	501	GTP	C8-N7-C5	3.02	108.75	102.99
21	Cd	501	GTP	C8-N7-C5	3.02	108.75	102.99
20	6e	501	GDP	C3'-C2'-C1'	3.02	105.53	100.98
20	Dg	501	GDP	C3'-C2'-C1'	3.02	105.53	100.98
21	3b	501	GTP	C8-N7-C5	3.02	108.74	102.99
21	6d	501	GTP	C8-N7-C5	3.02	108.74	102.99
21	6b	501	GTP	C8-N7-C5	3.02	108.74	102.99
21	9b	501	GTP	C8-N7-C5	3.02	108.74	102.99
21	1f	501	GTP	C2-N1-C6	-3.02	119.55	125.10
21	Ch	501	GTP	C3'-C2'-C1'	3.01	105.52	100.98
21	Cb	501	GTP	C8-N7-C5	3.01	108.73	102.99
20	6g	501	GDP	C3'-C2'-C1'	3.01	105.52	100.98
20	1c	501	GDP	C3'-C2'-C1'	3.01	105.51	100.98
21	4b	501	GTP	C8-N7-C5	3.01	108.72	102.99
21	8h	501	GTP	C8-N7-C5	3.01	108.72	102.99
21	9d	501	GTP	C8-N7-C5	3.01	108.72	102.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3b	501	GTP	C2-N1-C6	-3.01	119.56	125.10
21	7f	501	GTP	C8-N7-C5	3.01	108.72	102.99
21	Cd	501	GTP	C3'-C2'-C1'	3.00	105.50	100.98
21	9d	501	GTP	C2-N1-C6	-3.00	119.57	125.10
21	3d	501	GTP	C2-N1-C6	-3.00	119.57	125.10
21	1f	501	GTP	C8-N7-C5	3.00	108.71	102.99
20	2e	501	GDP	C3'-C2'-C1'	3.00	105.49	100.98
21	5b	501	GTP	C8-N7-C5	3.00	108.70	102.99
20	Ae	501	GDP	C3'-C2'-C1'	3.00	105.49	100.98
19	0Y	801	ADP	N3-C2-N1	-3.00	124.00	128.68
21	2f	501	GTP	C8-N7-C5	3.00	108.70	102.99
21	4d	501	GTP	C2-N1-C6	-2.99	119.58	125.10
21	7h	501	GTP	C8-N7-C5	2.99	108.69	102.99
20	1g	501	GDP	C3'-C2'-C1'	2.99	105.48	100.98
21	6b	501	GTP	C2-N1-C6	-2.99	119.59	125.10
21	Dh	501	GTP	C8-N7-C5	2.99	108.68	102.99
21	4f	501	GTP	C8-N7-C5	2.99	108.68	102.99
21	4h	501	GTP	C8-N7-C5	2.99	108.68	102.99
21	Ch	501	GTP	C2-N1-C6	-2.99	119.60	125.10
21	9h	501	GTP	C8-N7-C5	2.99	108.68	102.99
21	2f	501	GTP	C2-N1-C6	-2.99	119.60	125.10
21	1b	501	GTP	C8-N7-C5	2.98	108.67	102.99
21	Bh	501	GTP	C2-N1-C6	-2.98	119.61	125.10
21	2b	501	GTP	C8-N7-C5	2.98	108.67	102.99
21	Cb	501	GTP	C2-N1-C6	-2.98	119.61	125.10
21	Af	501	GTP	C8-N7-C5	2.98	108.67	102.99
21	Ab	501	GTP	C2-N1-C6	-2.98	119.61	125.10
21	Cf	501	GTP	C2-N1-C6	-2.98	119.61	125.10
21	9f	501	GTP	C8-N7-C5	2.97	108.66	102.99
21	Cf	501	GTP	C8-N7-C5	2.97	108.66	102.99
21	3f	501	GTP	C2-N1-C6	-2.97	119.63	125.10
21	5f	501	GTP	C8-N7-C5	2.97	108.64	102.99
21	9f	501	GTP	C2-N1-C6	-2.97	119.63	125.10
21	Df	501	GTP	C2-N1-C6	-2.97	119.63	125.10
21	3d	501	GTP	C8-N7-C5	2.97	108.64	102.99
21	5b	501	GTP	C2-N1-C6	-2.97	119.63	125.10
21	8d	501	GTP	C3'-C2'-C1'	2.97	105.44	100.98
21	3h	501	GTP	C8-N7-C5	2.97	108.64	102.99
21	2b	501	GTP	C2-N1-C6	-2.97	119.64	125.10
21	6d	501	GTP	C2-N1-C6	-2.97	119.64	125.10
21	4h	501	GTP	C2-N1-C6	-2.97	119.64	125.10
21	1d	501	GTP	C2-N1-C6	-2.96	119.64	125.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2g	501	GDP	C3'-C2'-C1'	2.96	105.44	100.98
21	5d	501	GTP	C2-N1-C6	-2.96	119.64	125.10
21	9b	501	GTP	C2-N1-C6	-2.96	119.64	125.10
21	2h	501	GTP	C8-N7-C5	2.96	108.63	102.99
21	7d	501	GTP	C8-N7-C5	2.96	108.62	102.99
21	Bb	501	GTP	C2-N1-C6	-2.96	119.65	125.10
21	Ah	501	GTP	C2-N1-C6	-2.95	119.66	125.10
21	Af	501	GTP	C2-N1-C6	-2.95	119.66	125.10
21	3f	501	GTP	C8-N7-C5	2.95	108.61	102.99
21	8h	501	GTP	C3'-C2'-C1'	2.95	105.42	100.98
21	5f	501	GTP	C2-N1-C6	-2.95	119.67	125.10
20	Ac	501	GDP	C3'-C2'-C1'	2.95	105.42	100.98
21	7h	501	GTP	C3'-C2'-C1'	2.95	105.42	100.98
21	Ab	501	GTP	C8-N7-C5	2.95	108.61	102.99
21	6f	501	GTP	C2-N1-C6	-2.95	119.67	125.10
21	3h	501	GTP	C2-N1-C6	-2.94	119.68	125.10
21	4b	501	GTP	C2-N1-C6	-2.94	119.68	125.10
21	Df	501	GTP	C8-N7-C5	2.94	108.60	102.99
21	5d	501	GTP	C3'-C2'-C1'	2.94	105.41	100.98
21	1d	501	GTP	C8-N7-C5	2.94	108.59	102.99
21	7b	501	GTP	C3'-C2'-C1'	2.94	105.40	100.98
21	Dd	501	GTP	C2-N1-C6	-2.94	119.69	125.10
21	9h	501	GTP	C2-N1-C6	-2.94	119.69	125.10
21	Ad	501	GTP	C2-N1-C6	-2.93	119.70	125.10
21	7d	501	GTP	C2-N1-C6	-2.93	119.70	125.10
21	8d	501	GTP	C2-N1-C6	-2.93	119.70	125.10
21	2d	501	GTP	C2-N1-C6	-2.93	119.71	125.10
21	Bf	501	GTP	C2-N1-C6	-2.93	119.71	125.10
21	1b	501	GTP	C3'-C2'-C1'	2.93	105.38	100.98
21	3f	501	GTP	C3'-C2'-C1'	2.92	105.38	100.98
21	8b	501	GTP	C3'-C2'-C1'	2.92	105.37	100.98
20	9a	501	GDP	C3'-C2'-C1'	2.92	105.37	100.98
21	3b	501	GTP	C3'-C2'-C1'	2.92	105.37	100.98
20	7g	501	GDP	C3'-C2'-C1'	2.92	105.37	100.98
21	5f	501	GTP	C3'-C2'-C1'	2.91	105.37	100.98
21	Db	501	GTP	C3'-C2'-C1'	2.91	105.37	100.98
21	7h	501	GTP	C2-N1-C6	-2.91	119.74	125.10
20	Cc	501	GDP	C3'-C2'-C1'	2.91	105.36	100.98
21	4f	501	GTP	C2-N1-C6	-2.91	119.74	125.10
21	6d	501	GTP	C3'-C2'-C1'	2.91	105.36	100.98
21	1b	501	GTP	C2-N1-C6	-2.91	119.75	125.10
21	Db	501	GTP	C2-N1-C6	-2.91	119.75	125.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	8b	501	GTP	C2-N1-C6	-2.91	119.75	125.10
21	3h	501	GTP	C3'-C2'-C1'	2.91	105.35	100.98
21	Ah	501	GTP	C8-N7-C5	2.90	108.51	102.99
20	7c	501	GDP	C3'-C2'-C1'	2.90	105.34	100.98
21	7b	501	GTP	C2-N1-C6	-2.90	119.77	125.10
20	Dc	501	GDP	C3'-C2'-C1'	2.90	105.34	100.98
21	3d	501	GTP	C3'-C2'-C1'	2.90	105.34	100.98
21	4h	501	GTP	C3'-C2'-C1'	2.89	105.34	100.98
21	8h	501	GTP	C2-N1-C6	-2.89	119.77	125.10
20	9g	501	GDP	C3'-C2'-C1'	2.89	105.33	100.98
21	2f	501	GTP	C3'-C2'-C1'	2.89	105.33	100.98
21	Cf	501	GTP	C3'-C2'-C1'	2.89	105.33	100.98
21	7f	501	GTP	C2-N1-C6	-2.89	119.78	125.10
21	Df	501	GTP	C3'-C2'-C1'	2.88	105.32	100.98
21	5h	501	GTP	C3'-C2'-C1'	2.88	105.31	100.98
21	6h	501	GTP	C2-N1-C6	-2.88	119.80	125.10
21	1h	501	GTP	C2-N1-C6	-2.88	119.80	125.10
21	1f	501	GTP	C3'-C2'-C1'	2.87	105.30	100.98
21	2h	501	GTP	C2-N1-C6	-2.86	119.82	125.10
21	Dh	501	GTP	C3'-C2'-C1'	2.86	105.29	100.98
21	Ad	501	GTP	C3'-C2'-C1'	2.86	105.29	100.98
21	Af	501	GTP	C3'-C2'-C1'	2.86	105.28	100.98
21	8f	501	GTP	C2-N1-C6	-2.85	119.84	125.10
21	1d	501	GTP	C3'-C2'-C1'	2.85	105.27	100.98
21	Bd	501	GTP	C3'-C2'-C1'	2.85	105.27	100.98
20	9c	501	GDP	C3'-C2'-C1'	2.85	105.27	100.98
21	Cb	501	GTP	C3'-C2'-C1'	2.85	105.26	100.98
21	6b	501	GTP	C3'-C2'-C1'	2.84	105.26	100.98
21	9f	501	GTP	C3'-C2'-C1'	2.84	105.25	100.98
21	Ab	501	GTP	C3'-C2'-C1'	2.84	105.25	100.98
21	4b	501	GTP	C3'-C2'-C1'	2.84	105.25	100.98
21	4d	501	GTP	C3'-C2'-C1'	2.83	105.24	100.98
21	7d	501	GTP	C3'-C2'-C1'	2.83	105.24	100.98
21	Ah	501	GTP	C3'-C2'-C1'	2.83	105.24	100.98
21	1h	501	GTP	C3'-C2'-C1'	2.83	105.24	100.98
21	9b	501	GTP	C3'-C2'-C1'	2.83	105.23	100.98
20	7e	501	GDP	C3'-C2'-C1'	2.82	105.22	100.98
21	2b	501	GTP	C3'-C2'-C1'	2.82	105.22	100.98
21	Dd	501	GTP	C3'-C2'-C1'	2.81	105.22	100.98
20	9e	501	GDP	C3'-C2'-C1'	2.81	105.20	100.98
21	2d	501	GTP	C3'-C2'-C1'	2.80	105.19	100.98
21	4f	501	GTP	C3'-C2'-C1'	2.80	105.19	100.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6f	501	GTP	C3’-C2’-C1’	2.79	105.17	100.98
21	Bh	501	GTP	C3’-C2’-C1’	2.78	105.16	100.98
21	7f	501	GTP	C3’-C2’-C1’	2.78	105.16	100.98
21	2h	501	GTP	C3’-C2’-C1’	2.77	105.15	100.98
19	0X	801	ADP	C3’-C2’-C1’	2.76	105.13	100.98
19	0Y	801	ADP	C4-C5-N7	-2.75	106.53	109.40
21	Bf	501	GTP	C3’-C2’-C1’	2.75	105.11	100.98
21	6h	501	GTP	C3’-C2’-C1’	2.75	105.11	100.98
19	0Z	801	ADP	C3’-C2’-C1’	2.74	105.11	100.98
21	9d	501	GTP	C3’-C2’-C1’	2.74	105.11	100.98
21	Bb	501	GTP	C3’-C2’-C1’	2.73	105.09	100.98
21	8f	501	GTP	C3’-C2’-C1’	2.73	105.09	100.98
19	1A	801	ADP	C4-C5-N7	-2.72	106.57	109.40
21	9h	501	GTP	C3’-C2’-C1’	2.71	105.06	100.98
19	0X	801	ADP	C4-C5-N7	-2.51	106.78	109.40
19	0Z	801	ADP	C4-C5-N7	-2.48	106.81	109.40
20	9e	501	GDP	C5-C6-N1	2.47	118.32	113.95
20	9c	501	GDP	C8-N7-C5	2.45	107.65	102.99
20	Cc	501	GDP	C8-N7-C5	2.44	107.63	102.99
20	6g	501	GDP	C8-N7-C5	2.43	107.62	102.99
20	6e	501	GDP	C8-N7-C5	2.43	107.61	102.99
20	5a	501	GDP	C8-N7-C5	2.42	107.61	102.99
20	6a	501	GDP	C8-N7-C5	2.41	107.58	102.99
20	9g	501	GDP	C8-N7-C5	2.40	107.55	102.99
20	5g	501	GDP	C8-N7-C5	2.39	107.55	102.99
20	3c	501	GDP	C5-C6-N1	2.39	118.17	113.95
20	1e	501	GDP	C8-N7-C5	2.38	107.53	102.99
20	3c	501	GDP	C8-N7-C5	2.38	107.52	102.99
20	8e	501	GDP	C8-N7-C5	2.38	107.52	102.99
20	Da	501	GDP	C8-N7-C5	2.38	107.52	102.99
20	Ca	501	GDP	C8-N7-C5	2.37	107.51	102.99
20	7a	501	GDP	C8-N7-C5	2.37	107.51	102.99
20	Ba	501	GDP	C5-C6-N1	2.37	118.14	113.95
20	8c	501	GDP	C8-N7-C5	2.37	107.50	102.99
20	6c	501	GDP	C8-N7-C5	2.37	107.50	102.99
20	Bc	501	GDP	C8-N7-C5	2.37	107.50	102.99
20	Bc	501	GDP	C5-C6-N1	2.37	118.13	113.95
20	Cc	501	GDP	C5-C6-N1	2.37	118.13	113.95
20	5g	501	GDP	C5-C6-N1	2.37	118.13	113.95
20	5c	501	GDP	C5-C6-N1	2.36	118.13	113.95
20	Ag	501	GDP	C8-N7-C5	2.36	107.49	102.99
20	Bg	501	GDP	C8-N7-C5	2.36	107.49	102.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	6a	501	GDP	C5-C6-N1	2.36	118.12	113.95
20	7c	501	GDP	C8-N7-C5	2.36	107.48	102.99
20	1c	501	GDP	C5-C6-N1	2.36	118.11	113.95
20	2e	501	GDP	C8-N7-C5	2.35	107.47	102.99
20	Ae	501	GDP	C8-N7-C5	2.35	107.47	102.99
20	5e	501	GDP	C8-N7-C5	2.35	107.47	102.99
20	Ac	501	GDP	C8-N7-C5	2.35	107.47	102.99
20	8g	501	GDP	C8-N7-C5	2.35	107.47	102.99
20	Ba	501	GDP	C8-N7-C5	2.35	107.47	102.99
21	Af	501	GTP	O6-C6-C5	-2.35	119.78	124.37
20	4c	501	GDP	C8-N7-C5	2.35	107.47	102.99
20	7e	501	GDP	C8-N7-C5	2.35	107.46	102.99
20	9a	501	GDP	C8-N7-C5	2.35	107.46	102.99
20	1a	501	GDP	C8-N7-C5	2.35	107.46	102.99
20	8a	501	GDP	C8-N7-C5	2.34	107.45	102.99
20	Be	501	GDP	C8-N7-C5	2.34	107.45	102.99
20	6g	501	GDP	C5-C6-N1	2.34	118.09	113.95
21	9b	501	GTP	O6-C6-C5	-2.34	119.80	124.37
20	Bg	501	GDP	C5-C6-N1	2.34	118.08	113.95
20	3e	501	GDP	C8-N7-C5	2.34	107.44	102.99
20	Dg	501	GDP	C8-N7-C5	2.34	107.44	102.99
19	1A	801	ADP	C3'-C2'-C1'	2.34	104.50	100.98
20	5e	501	GDP	C5-C6-N1	2.34	118.08	113.95
20	2c	501	GDP	C5-C6-N1	2.33	118.08	113.95
20	De	501	GDP	C5-C6-N1	2.33	118.08	113.95
20	Ag	501	GDP	C5-C6-N1	2.33	118.07	113.95
20	4a	501	GDP	C8-N7-C5	2.33	107.44	102.99
20	5c	501	GDP	C8-N7-C5	2.33	107.44	102.99
20	2g	501	GDP	C5-C6-N1	2.33	118.07	113.95
20	Dc	501	GDP	C8-N7-C5	2.33	107.43	102.99
19	0Y	801	ADP	C3'-C2'-C1'	2.33	104.49	100.98
20	3a	501	GDP	C8-N7-C5	2.33	107.43	102.99
20	1e	501	GDP	C5-C6-N1	2.33	118.07	113.95
20	4c	501	GDP	C5-C6-N1	2.33	118.06	113.95
20	2c	501	GDP	C8-N7-C5	2.33	107.42	102.99
20	7g	501	GDP	C8-N7-C5	2.33	107.42	102.99
20	4g	501	GDP	C8-N7-C5	2.32	107.42	102.99
20	7e	501	GDP	C5-C6-N1	2.32	118.05	113.95
20	Ce	501	GDP	C8-N7-C5	2.32	107.41	102.99
20	1c	501	GDP	C8-N7-C5	2.32	107.41	102.99
20	2g	501	GDP	C8-N7-C5	2.32	107.41	102.99
20	9g	501	GDP	C5-C6-N1	2.32	118.04	113.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	De	501	GDP	C8-N7-C5	2.32	107.40	102.99
20	Aa	501	GDP	C8-N7-C5	2.32	107.40	102.99
20	9a	501	GDP	C5-C6-N1	2.32	118.04	113.95
20	Cg	501	GDP	C5-C6-N1	2.31	118.04	113.95
20	Dg	501	GDP	C5-C6-N1	2.31	118.04	113.95
21	9d	501	GTP	O6-C6-C5	-2.31	119.85	124.37
20	Ac	501	GDP	C5-C6-N1	2.31	118.04	113.95
20	9c	501	GDP	C5-C6-N1	2.31	118.03	113.95
20	8a	501	GDP	C5-C6-N1	2.31	118.03	113.95
20	Be	501	GDP	C5-C6-N1	2.31	118.02	113.95
20	6c	501	GDP	C5-C6-N1	2.30	118.02	113.95
20	1g	501	GDP	C8-N7-C5	2.30	107.38	102.99
20	4a	501	GDP	C5-C6-N1	2.30	118.02	113.95
21	3d	501	GTP	O6-C6-C5	-2.30	119.88	124.37
20	4e	501	GDP	C5-C6-N1	2.30	118.01	113.95
21	9h	501	GTP	O6-C6-C5	-2.30	119.88	124.37
20	4g	501	GDP	C5-C6-N1	2.30	118.01	113.95
20	Dc	501	GDP	C5-C6-N1	2.30	118.01	113.95
20	9e	501	GDP	C8-N7-C5	2.30	107.37	102.99
20	6e	501	GDP	C5-C6-N1	2.30	118.01	113.95
20	Ce	501	GDP	C5-C6-N1	2.30	118.01	113.95
20	Ca	501	GDP	C5-C6-N1	2.30	118.01	113.95
20	7a	501	GDP	C5-C6-N1	2.29	118.00	113.95
20	4e	501	GDP	C8-N7-C5	2.29	107.36	102.99
20	2a	501	GDP	C5-C6-N1	2.29	118.00	113.95
20	8g	501	GDP	C5-C6-N1	2.29	117.99	113.95
20	Da	501	GDP	C5-C6-N1	2.29	117.99	113.95
21	9f	501	GTP	O6-C6-C5	-2.29	119.90	124.37
21	2b	501	GTP	O6-C6-C5	-2.29	119.91	124.37
20	3a	501	GDP	C5-C6-N1	2.28	117.98	113.95
20	7c	501	GDP	C5-C6-N1	2.28	117.98	113.95
21	3b	501	GTP	O6-C6-C5	-2.28	119.92	124.37
20	5a	501	GDP	C5-C6-N1	2.28	117.98	113.95
20	3g	501	GDP	C5-C6-N1	2.28	117.98	113.95
21	Ab	501	GTP	O6-C6-C5	-2.28	119.92	124.37
20	Ae	501	GDP	C5-C6-N1	2.28	117.97	113.95
20	3g	501	GDP	C8-N7-C5	2.28	107.33	102.99
20	3e	501	GDP	C5-C6-N1	2.28	117.97	113.95
20	2e	501	GDP	C5-C6-N1	2.28	117.97	113.95
21	3h	501	GTP	O6-C6-C5	-2.27	119.93	124.37
20	Aa	501	GDP	C5-C6-N1	2.27	117.96	113.95
21	Ah	501	GTP	O6-C6-C5	-2.27	119.94	124.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1f	501	GTP	O6-C6-C5	-2.27	119.95	124.37
20	Cg	501	GDP	C8-N7-C5	2.26	107.30	102.99
20	8c	501	GDP	C5-C6-N1	2.26	117.94	113.95
20	1a	501	GDP	C5-C6-N1	2.26	117.94	113.95
21	1b	501	GTP	O6-C6-C5	-2.25	119.97	124.37
20	8e	501	GDP	C5-C6-N1	2.24	117.91	113.95
21	3f	501	GTP	O6-C6-C5	-2.24	120.00	124.37
20	2a	501	GDP	C8-N7-C5	2.23	107.24	102.99
20	7g	501	GDP	C5-C6-N1	2.23	117.89	113.95
20	1g	501	GDP	C5-C6-N1	2.22	117.88	113.95
21	Ad	501	GTP	O6-C6-C5	-2.22	120.03	124.37
21	1d	501	GTP	O6-C6-C5	-2.22	120.03	124.37
21	Ch	501	GTP	O6-C6-C5	-2.21	120.06	124.37
21	2h	501	GTP	O6-C6-C5	-2.21	120.06	124.37
21	4h	501	GTP	O6-C6-C5	-2.20	120.08	124.37
21	8h	501	GTP	O6-C6-C5	-2.19	120.10	124.37
21	2f	501	GTP	O6-C6-C5	-2.19	120.10	124.37
21	Dh	501	GTP	O6-C6-C5	-2.18	120.11	124.37
21	2d	501	GTP	O6-C6-C5	-2.18	120.11	124.37
21	Df	501	GTP	O6-C6-C5	-2.18	120.12	124.37
21	4f	501	GTP	O6-C6-C5	-2.17	120.14	124.37
21	Cd	501	GTP	O6-C6-C5	-2.16	120.16	124.37
21	Bf	501	GTP	O6-C6-C5	-2.15	120.17	124.37
21	4d	501	GTP	O6-C6-C5	-2.15	120.17	124.37
21	5f	501	GTP	O6-C6-C5	-2.15	120.17	124.37
21	7h	501	GTP	O6-C6-C5	-2.14	120.19	124.37
21	5h	501	GTP	O6-C6-C5	-2.14	120.19	124.37
21	Bh	501	GTP	O6-C6-C5	-2.13	120.22	124.37
21	5d	501	GTP	O6-C6-C5	-2.13	120.22	124.37
21	4b	501	GTP	O6-C6-C5	-2.12	120.23	124.37
21	7d	501	GTP	O6-C6-C5	-2.11	120.24	124.37
21	8d	501	GTP	O6-C6-C5	-2.11	120.25	124.37
21	Dd	501	GTP	O6-C6-C5	-2.11	120.25	124.37
21	8f	501	GTP	O6-C6-C5	-2.10	120.26	124.37
21	7b	501	GTP	O6-C6-C5	-2.10	120.28	124.37
21	5b	501	GTP	O6-C6-C5	-2.09	120.29	124.37
21	7f	501	GTP	O6-C6-C5	-2.09	120.30	124.37
21	Db	501	GTP	O6-C6-C5	-2.09	120.30	124.37
21	Bd	501	GTP	O6-C6-C5	-2.08	120.30	124.37
20	9e	501	GDP	O6-C6-C5	-2.08	120.31	124.37
21	Cb	501	GTP	O6-C6-C5	-2.08	120.31	124.37
21	Cf	501	GTP	O6-C6-C5	-2.08	120.31	124.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6b	501	GTP	O6-C6-C5	-2.08	120.31	124.37
21	6d	501	GTP	O6-C6-C5	-2.07	120.33	124.37
21	Bb	501	GTP	O6-C6-C5	-2.06	120.35	124.37

There are no chirality outliers.

All (315) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	0X	801	ADP	C3'-C4'-C5'-O5'
19	0Y	801	ADP	PA-O3A-PB-O2B
19	0Y	801	ADP	PA-O3A-PB-O3B
19	1A	801	ADP	PA-O3A-PB-O2B
20	1a	501	GDP	C5'-O5'-PA-O1A
20	1a	501	GDP	C5'-O5'-PA-O2A
20	1c	501	GDP	C5'-O5'-PA-O1A
20	1c	501	GDP	C5'-O5'-PA-O2A
20	1e	501	GDP	C5'-O5'-PA-O1A
20	1e	501	GDP	C5'-O5'-PA-O2A
20	1g	501	GDP	C5'-O5'-PA-O1A
20	1g	501	GDP	C5'-O5'-PA-O2A
20	2a	501	GDP	C5'-O5'-PA-O1A
20	2a	501	GDP	C5'-O5'-PA-O2A
20	2c	501	GDP	C5'-O5'-PA-O1A
20	2c	501	GDP	C5'-O5'-PA-O2A
20	2e	501	GDP	C5'-O5'-PA-O1A
20	2e	501	GDP	C5'-O5'-PA-O2A
20	2g	501	GDP	C5'-O5'-PA-O1A
20	2g	501	GDP	C5'-O5'-PA-O2A
20	3a	501	GDP	C5'-O5'-PA-O1A
20	3a	501	GDP	C5'-O5'-PA-O2A
20	3c	501	GDP	C5'-O5'-PA-O1A
20	3c	501	GDP	C5'-O5'-PA-O2A
20	3e	501	GDP	C5'-O5'-PA-O1A
20	3e	501	GDP	C5'-O5'-PA-O2A
20	3g	501	GDP	C5'-O5'-PA-O1A
20	3g	501	GDP	C5'-O5'-PA-O2A
20	4a	501	GDP	C5'-O5'-PA-O2A
20	4c	501	GDP	C5'-O5'-PA-O2A
20	4e	501	GDP	C5'-O5'-PA-O1A
20	4e	501	GDP	C5'-O5'-PA-O2A
20	4g	501	GDP	C5'-O5'-PA-O1A
20	4g	501	GDP	C5'-O5'-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	5a	501	GDP	C5'-O5'-PA-O2A
20	5c	501	GDP	C5'-O5'-PA-O3A
20	5c	501	GDP	C5'-O5'-PA-O2A
20	5e	501	GDP	C5'-O5'-PA-O3A
20	5e	501	GDP	C5'-O5'-PA-O2A
20	5g	501	GDP	C5'-O5'-PA-O3A
20	6a	501	GDP	C5'-O5'-PA-O3A
20	6a	501	GDP	C5'-O5'-PA-O2A
20	6c	501	GDP	C5'-O5'-PA-O1A
20	6c	501	GDP	C5'-O5'-PA-O2A
20	6e	501	GDP	C5'-O5'-PA-O2A
20	6g	501	GDP	C5'-O5'-PA-O2A
20	7a	501	GDP	C5'-O5'-PA-O3A
20	7a	501	GDP	C5'-O5'-PA-O2A
20	7c	501	GDP	C5'-O5'-PA-O1A
20	7c	501	GDP	C5'-O5'-PA-O2A
20	7e	501	GDP	C5'-O5'-PA-O2A
20	7g	501	GDP	C5'-O5'-PA-O1A
20	7g	501	GDP	C5'-O5'-PA-O2A
20	8a	501	GDP	C5'-O5'-PA-O1A
20	8a	501	GDP	C5'-O5'-PA-O2A
20	8c	501	GDP	C5'-O5'-PA-O1A
20	8c	501	GDP	C5'-O5'-PA-O2A
20	8e	501	GDP	C5'-O5'-PA-O1A
20	8e	501	GDP	C5'-O5'-PA-O2A
20	8g	501	GDP	C5'-O5'-PA-O1A
20	8g	501	GDP	C5'-O5'-PA-O2A
20	9a	501	GDP	C5'-O5'-PA-O3A
20	9c	501	GDP	C5'-O5'-PA-O1A
20	9c	501	GDP	C5'-O5'-PA-O2A
20	9e	501	GDP	C5'-O5'-PA-O3A
20	9e	501	GDP	C5'-O5'-PA-O2A
20	9g	501	GDP	C5'-O5'-PA-O1A
20	9g	501	GDP	C5'-O5'-PA-O2A
20	Aa	501	GDP	C5'-O5'-PA-O1A
20	Aa	501	GDP	C5'-O5'-PA-O2A
20	Ac	501	GDP	C5'-O5'-PA-O3A
20	Ac	501	GDP	C5'-O5'-PA-O2A
20	Ae	501	GDP	C5'-O5'-PA-O2A
20	Ag	501	GDP	C5'-O5'-PA-O1A
20	Ag	501	GDP	C5'-O5'-PA-O2A
20	Ba	501	GDP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	Ba	501	GDP	C5'-O5'-PA-O2A
20	Bc	501	GDP	C5'-O5'-PA-O1A
20	Bc	501	GDP	C5'-O5'-PA-O2A
20	Be	501	GDP	C5'-O5'-PA-O3A
20	Be	501	GDP	C5'-O5'-PA-O1A
20	Be	501	GDP	C5'-O5'-PA-O2A
20	Bg	501	GDP	C5'-O5'-PA-O1A
20	Bg	501	GDP	C5'-O5'-PA-O2A
20	Ca	501	GDP	C5'-O5'-PA-O3A
20	Ca	501	GDP	C5'-O5'-PA-O1A
20	Ca	501	GDP	C5'-O5'-PA-O2A
20	Cc	501	GDP	C5'-O5'-PA-O3A
20	Cc	501	GDP	C5'-O5'-PA-O1A
20	Cc	501	GDP	C5'-O5'-PA-O2A
20	Ce	501	GDP	C5'-O5'-PA-O1A
20	Ce	501	GDP	C5'-O5'-PA-O2A
20	Cg	501	GDP	C5'-O5'-PA-O1A
20	Cg	501	GDP	C5'-O5'-PA-O2A
20	Da	501	GDP	C5'-O5'-PA-O1A
20	Da	501	GDP	C5'-O5'-PA-O2A
20	Dc	501	GDP	C5'-O5'-PA-O1A
20	Dc	501	GDP	C5'-O5'-PA-O2A
20	De	501	GDP	C5'-O5'-PA-O1A
20	De	501	GDP	C5'-O5'-PA-O2A
20	Dg	501	GDP	C5'-O5'-PA-O1A
20	Dg	501	GDP	C5'-O5'-PA-O2A
21	1b	501	GTP	PB-O3B-PG-O2G
21	1b	501	GTP	O4'-C4'-C5'-O5'
21	1b	501	GTP	C3'-C4'-C5'-O5'
21	1d	501	GTP	O4'-C4'-C5'-O5'
21	1d	501	GTP	C3'-C4'-C5'-O5'
21	1f	501	GTP	O4'-C4'-C5'-O5'
21	1f	501	GTP	C3'-C4'-C5'-O5'
21	2b	501	GTP	O4'-C4'-C5'-O5'
21	2b	501	GTP	C3'-C4'-C5'-O5'
21	2d	501	GTP	O4'-C4'-C5'-O5'
21	2d	501	GTP	C3'-C4'-C5'-O5'
21	2f	501	GTP	O4'-C4'-C5'-O5'
21	2f	501	GTP	C3'-C4'-C5'-O5'
21	2h	501	GTP	O4'-C4'-C5'-O5'
21	2h	501	GTP	C3'-C4'-C5'-O5'
21	3b	501	GTP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	3b	501	GTP	C3'-C4'-C5'-O5'
21	3d	501	GTP	O4'-C4'-C5'-O5'
21	3d	501	GTP	C3'-C4'-C5'-O5'
21	3f	501	GTP	O4'-C4'-C5'-O5'
21	3f	501	GTP	C3'-C4'-C5'-O5'
21	3h	501	GTP	PB-O3B-PG-O2G
21	3h	501	GTP	O4'-C4'-C5'-O5'
21	3h	501	GTP	C3'-C4'-C5'-O5'
21	4b	501	GTP	O4'-C4'-C5'-O5'
21	4b	501	GTP	C3'-C4'-C5'-O5'
21	4d	501	GTP	O4'-C4'-C5'-O5'
21	4d	501	GTP	C3'-C4'-C5'-O5'
21	4f	501	GTP	O4'-C4'-C5'-O5'
21	4f	501	GTP	C3'-C4'-C5'-O5'
21	4h	501	GTP	O4'-C4'-C5'-O5'
21	4h	501	GTP	C3'-C4'-C5'-O5'
21	5b	501	GTP	PB-O3B-PG-O2G
21	5b	501	GTP	O4'-C4'-C5'-O5'
21	5b	501	GTP	C3'-C4'-C5'-O5'
21	5d	501	GTP	PB-O3B-PG-O2G
21	5d	501	GTP	O4'-C4'-C5'-O5'
21	5d	501	GTP	C3'-C4'-C5'-O5'
21	5f	501	GTP	PB-O3B-PG-O2G
21	5f	501	GTP	O4'-C4'-C5'-O5'
21	5f	501	GTP	C3'-C4'-C5'-O5'
21	5h	501	GTP	PB-O3B-PG-O2G
21	5h	501	GTP	O4'-C4'-C5'-O5'
21	5h	501	GTP	C3'-C4'-C5'-O5'
21	6b	501	GTP	O4'-C4'-C5'-O5'
21	6b	501	GTP	C3'-C4'-C5'-O5'
21	6d	501	GTP	PB-O3B-PG-O2G
21	6d	501	GTP	O4'-C4'-C5'-O5'
21	6d	501	GTP	C3'-C4'-C5'-O5'
21	6f	501	GTP	PB-O3B-PG-O2G
21	6f	501	GTP	O4'-C4'-C5'-O5'
21	6f	501	GTP	C3'-C4'-C5'-O5'
21	6h	501	GTP	PB-O3B-PG-O2G
21	6h	501	GTP	O4'-C4'-C5'-O5'
21	6h	501	GTP	C3'-C4'-C5'-O5'
21	7b	501	GTP	O4'-C4'-C5'-O5'
21	7b	501	GTP	C3'-C4'-C5'-O5'
21	7d	501	GTP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	7d	501	GTP	C3'-C4'-C5'-O5'
21	7f	501	GTP	O4'-C4'-C5'-O5'
21	7f	501	GTP	C3'-C4'-C5'-O5'
21	7h	501	GTP	C3'-C4'-C5'-O5'
21	8b	501	GTP	PB-O3B-PG-O2G
21	8b	501	GTP	O4'-C4'-C5'-O5'
21	8b	501	GTP	C3'-C4'-C5'-O5'
21	8d	501	GTP	PB-O3B-PG-O2G
21	8d	501	GTP	O4'-C4'-C5'-O5'
21	8d	501	GTP	C3'-C4'-C5'-O5'
21	8f	501	GTP	PB-O3B-PG-O2G
21	8f	501	GTP	O4'-C4'-C5'-O5'
21	8f	501	GTP	C3'-C4'-C5'-O5'
21	8h	501	GTP	O4'-C4'-C5'-O5'
21	8h	501	GTP	C3'-C4'-C5'-O5'
21	9b	501	GTP	O4'-C4'-C5'-O5'
21	9b	501	GTP	C3'-C4'-C5'-O5'
21	9d	501	GTP	O4'-C4'-C5'-O5'
21	9d	501	GTP	C3'-C4'-C5'-O5'
21	9f	501	GTP	O4'-C4'-C5'-O5'
21	9f	501	GTP	C3'-C4'-C5'-O5'
21	9h	501	GTP	C3'-C4'-C5'-O5'
21	Ab	501	GTP	O4'-C4'-C5'-O5'
21	Ab	501	GTP	C3'-C4'-C5'-O5'
21	Ad	501	GTP	O4'-C4'-C5'-O5'
21	Ad	501	GTP	C3'-C4'-C5'-O5'
21	Af	501	GTP	O4'-C4'-C5'-O5'
21	Af	501	GTP	C3'-C4'-C5'-O5'
21	Ah	501	GTP	O4'-C4'-C5'-O5'
21	Ah	501	GTP	C3'-C4'-C5'-O5'
21	Bb	501	GTP	O4'-C4'-C5'-O5'
21	Bb	501	GTP	C3'-C4'-C5'-O5'
21	Bd	501	GTP	O4'-C4'-C5'-O5'
21	Bd	501	GTP	C3'-C4'-C5'-O5'
21	Bf	501	GTP	PB-O3B-PG-O2G
21	Bf	501	GTP	O4'-C4'-C5'-O5'
21	Bf	501	GTP	C3'-C4'-C5'-O5'
21	Bh	501	GTP	O4'-C4'-C5'-O5'
21	Bh	501	GTP	C3'-C4'-C5'-O5'
21	Cb	501	GTP	O4'-C4'-C5'-O5'
21	Cb	501	GTP	C3'-C4'-C5'-O5'
21	Cd	501	GTP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	Cd	501	GTP	C3'-C4'-C5'-O5'
21	Cf	501	GTP	C3'-C4'-C5'-O5'
21	Ch	501	GTP	PB-O3B-PG-O2G
21	Ch	501	GTP	O4'-C4'-C5'-O5'
21	Ch	501	GTP	C3'-C4'-C5'-O5'
21	Db	501	GTP	PB-O3B-PG-O2G
21	Db	501	GTP	O4'-C4'-C5'-O5'
21	Db	501	GTP	C3'-C4'-C5'-O5'
21	Dd	501	GTP	O4'-C4'-C5'-O5'
21	Dd	501	GTP	C3'-C4'-C5'-O5'
21	Df	501	GTP	O4'-C4'-C5'-O5'
21	Df	501	GTP	C3'-C4'-C5'-O5'
21	Dh	501	GTP	C3'-C4'-C5'-O5'
19	0Y	801	ADP	O4'-C4'-C5'-O5'
19	0Y	801	ADP	C3'-C4'-C5'-O5'
19	0Z	801	ADP	C3'-C4'-C5'-O5'
19	1A	801	ADP	O4'-C4'-C5'-O5'
19	1A	801	ADP	C3'-C4'-C5'-O5'
21	1h	501	GTP	O4'-C4'-C5'-O5'
21	1h	501	GTP	C3'-C4'-C5'-O5'
21	7h	501	GTP	O4'-C4'-C5'-O5'
21	9h	501	GTP	O4'-C4'-C5'-O5'
21	Cf	501	GTP	O4'-C4'-C5'-O5'
21	Dh	501	GTP	O4'-C4'-C5'-O5'
19	0X	801	ADP	O4'-C4'-C5'-O5'
19	0Z	801	ADP	O4'-C4'-C5'-O5'
19	1A	801	ADP	PA-O3A-PB-O1B
21	2f	501	GTP	PB-O3B-PG-O2G
21	4d	501	GTP	PB-O3B-PG-O2G
21	6b	501	GTP	PB-O3B-PG-O2G
21	9d	501	GTP	PB-O3B-PG-O2G
21	9f	501	GTP	PB-O3B-PG-O2G
21	9h	501	GTP	PB-O3B-PG-O2G
21	Ab	501	GTP	PB-O3B-PG-O2G
21	Df	501	GTP	PB-O3B-PG-O2G
20	1a	501	GDP	C5'-O5'-PA-O3A
20	1c	501	GDP	C5'-O5'-PA-O3A
20	4a	501	GDP	C5'-O5'-PA-O3A
20	4c	501	GDP	C5'-O5'-PA-O3A
20	5a	501	GDP	C5'-O5'-PA-O3A
20	6e	501	GDP	C5'-O5'-PA-O3A
20	6g	501	GDP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	7e	501	GDP	C5'-O5'-PA-O3A
20	Ae	501	GDP	C5'-O5'-PA-O3A
20	Ba	501	GDP	C5'-O5'-PA-O3A
20	4a	501	GDP	C5'-O5'-PA-O1A
20	4c	501	GDP	C5'-O5'-PA-O1A
20	5a	501	GDP	C5'-O5'-PA-O1A
20	5c	501	GDP	C5'-O5'-PA-O1A
20	5e	501	GDP	C5'-O5'-PA-O1A
20	5g	501	GDP	C5'-O5'-PA-O1A
20	6a	501	GDP	C5'-O5'-PA-O1A
20	6e	501	GDP	C5'-O5'-PA-O1A
20	6g	501	GDP	C5'-O5'-PA-O1A
20	7a	501	GDP	C5'-O5'-PA-O1A
20	7e	501	GDP	C5'-O5'-PA-O1A
20	9a	501	GDP	C5'-O5'-PA-O1A
20	9a	501	GDP	C5'-O5'-PA-O2A
20	9e	501	GDP	C5'-O5'-PA-O1A
20	Ac	501	GDP	C5'-O5'-PA-O1A
20	Ae	501	GDP	C5'-O5'-PA-O1A
21	2d	501	GTP	PB-O3B-PG-O2G
21	3d	501	GTP	PB-O3B-PG-O2G
21	3f	501	GTP	PB-O3B-PG-O2G
21	4b	501	GTP	PB-O3B-PG-O2G
21	4f	501	GTP	PB-O3B-PG-O2G
21	7b	501	GTP	PB-O3B-PG-O2G
21	7d	501	GTP	PB-O3B-PG-O2G
21	7h	501	GTP	PB-O3B-PG-O2G
21	8h	501	GTP	PB-O3B-PG-O2G
21	9b	501	GTP	PB-O3B-PG-O2G
21	Ad	501	GTP	PB-O3B-PG-O2G
21	Af	501	GTP	PB-O3B-PG-O2G
21	Bb	501	GTP	PB-O3B-PG-O2G
21	Bh	501	GTP	PB-O3B-PG-O2G
21	Cb	501	GTP	PB-O3B-PG-O2G
21	Cf	501	GTP	PB-O3B-PG-O2G
19	0X	801	ADP	C5'-O5'-PA-O3A
19	0Z	801	ADP	C5'-O5'-PA-O3A
20	1e	501	GDP	C5'-O5'-PA-O3A
20	1g	501	GDP	C5'-O5'-PA-O3A
20	2a	501	GDP	C5'-O5'-PA-O3A
20	2c	501	GDP	C5'-O5'-PA-O3A
20	2e	501	GDP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	2g	501	GDP	C5’-O5’-PA-O3A
20	3a	501	GDP	C5’-O5’-PA-O3A
20	3c	501	GDP	C5’-O5’-PA-O3A
20	3e	501	GDP	C5’-O5’-PA-O3A
20	3g	501	GDP	C5’-O5’-PA-O3A
20	4e	501	GDP	C5’-O5’-PA-O3A
20	4g	501	GDP	C5’-O5’-PA-O3A
20	6c	501	GDP	C5’-O5’-PA-O3A
20	7c	501	GDP	C5’-O5’-PA-O3A
20	7g	501	GDP	C5’-O5’-PA-O3A
20	8a	501	GDP	C5’-O5’-PA-O3A
20	8c	501	GDP	C5’-O5’-PA-O3A
20	8e	501	GDP	C5’-O5’-PA-O3A
20	8g	501	GDP	C5’-O5’-PA-O3A
20	9c	501	GDP	C5’-O5’-PA-O3A
20	9g	501	GDP	C5’-O5’-PA-O3A
20	Aa	501	GDP	C5’-O5’-PA-O3A
20	Ag	501	GDP	C5’-O5’-PA-O3A
20	Bc	501	GDP	C5’-O5’-PA-O3A
20	Bg	501	GDP	C5’-O5’-PA-O3A
20	Ce	501	GDP	C5’-O5’-PA-O3A
20	Cg	501	GDP	C5’-O5’-PA-O3A
20	Da	501	GDP	C5’-O5’-PA-O3A
20	Dc	501	GDP	C5’-O5’-PA-O3A
20	De	501	GDP	C5’-O5’-PA-O3A
20	Dg	501	GDP	C5’-O5’-PA-O3A
19	0Y	801	ADP	C5’-O5’-PA-O1A
19	0Z	801	ADP	C5’-O5’-PA-O2A
20	5g	501	GDP	C5’-O5’-PA-O2A

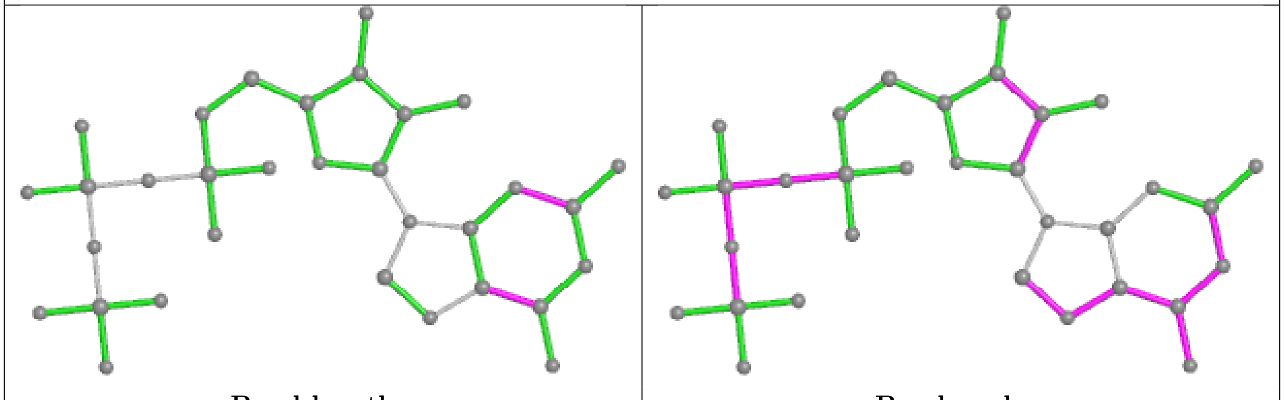
There are no ring outliers.

4 monomers are involved in 9 short contacts:

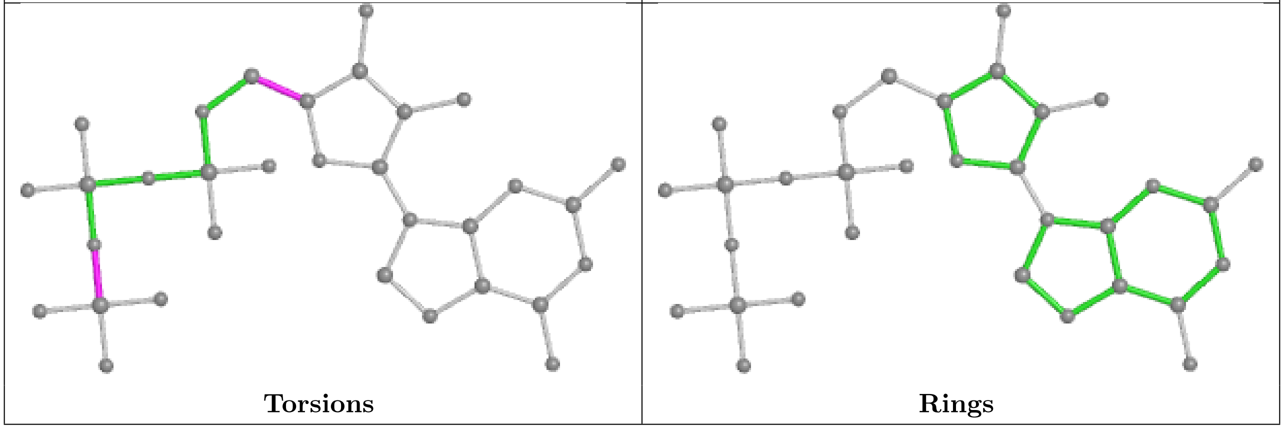
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	1A	801	ADP	1	0
19	0Z	801	ADP	2	0
19	0X	801	ADP	2	0
19	0Y	801	ADP	4	0

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 then 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.

Ligand GTP 3f 501

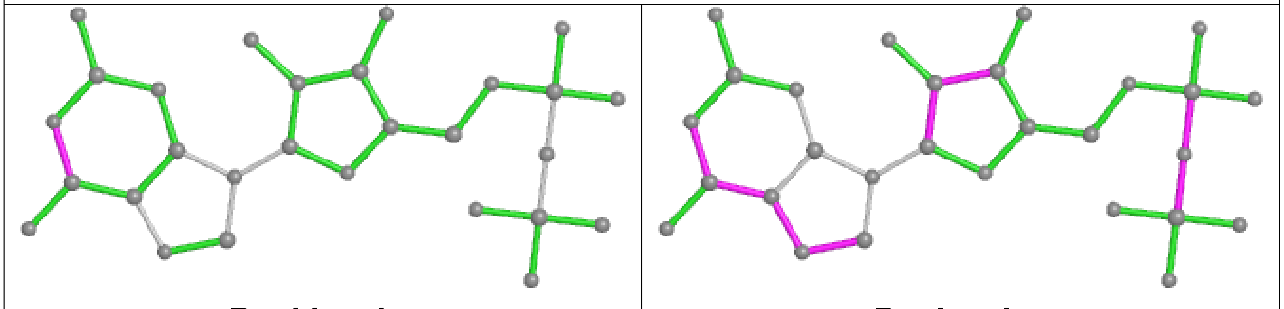


Bond lengths **Bond angles**

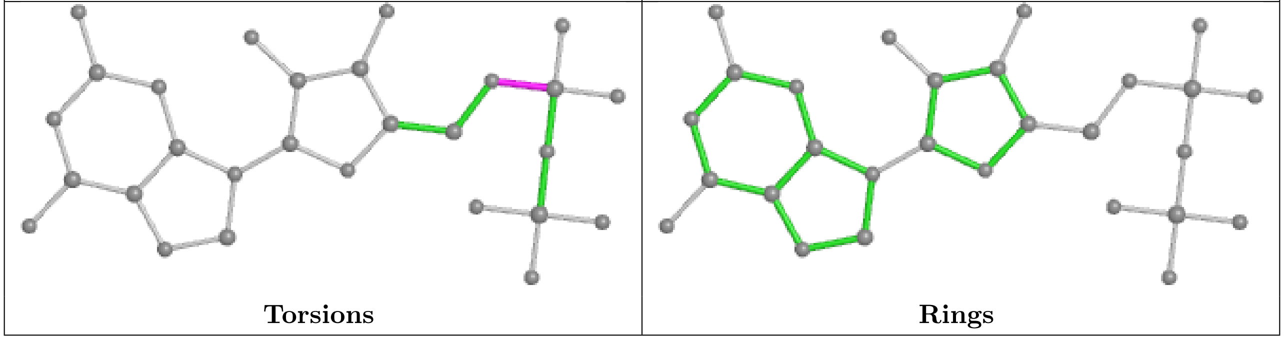


Torsions **Rings**

Ligand GDP Da 501

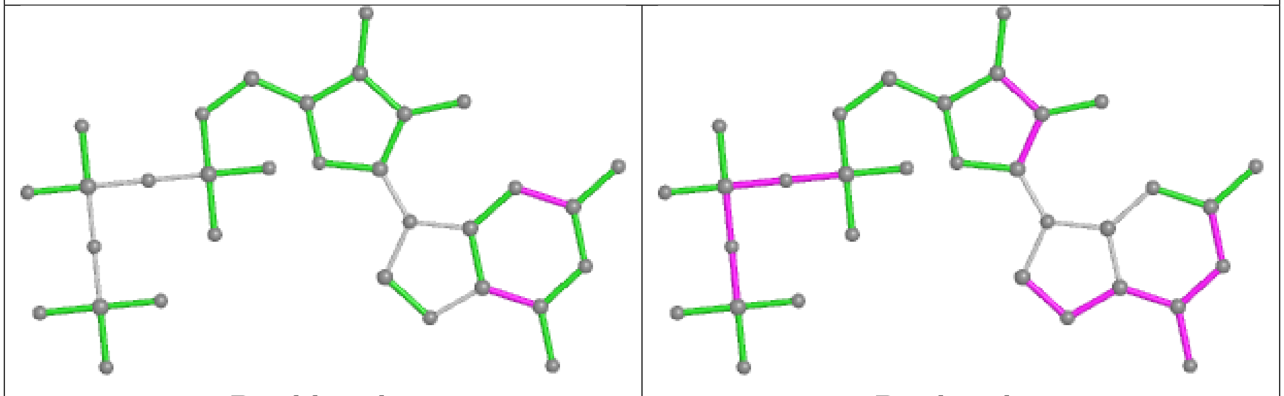


Bond lengths Bond angles

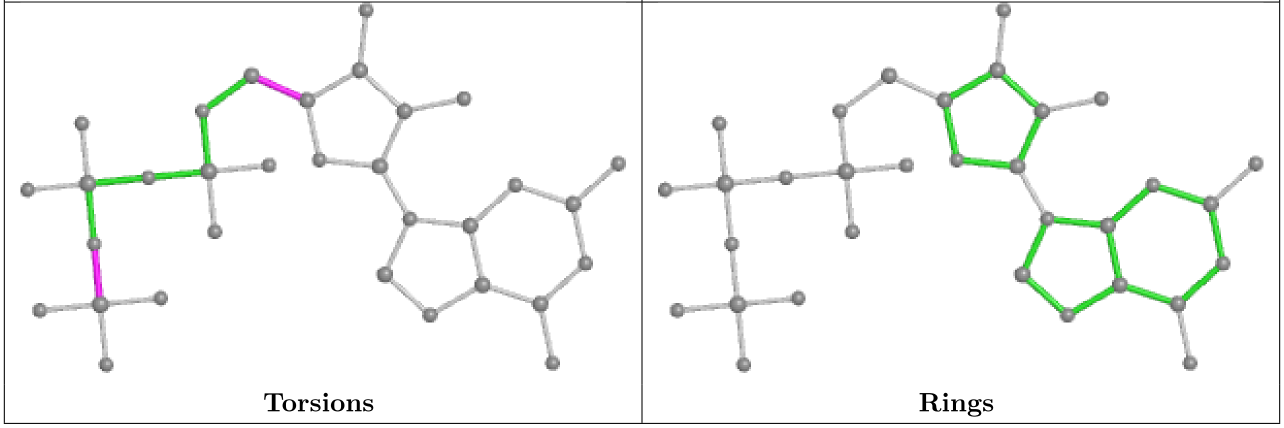


Torsions Rings

Ligand GTP Bf 501

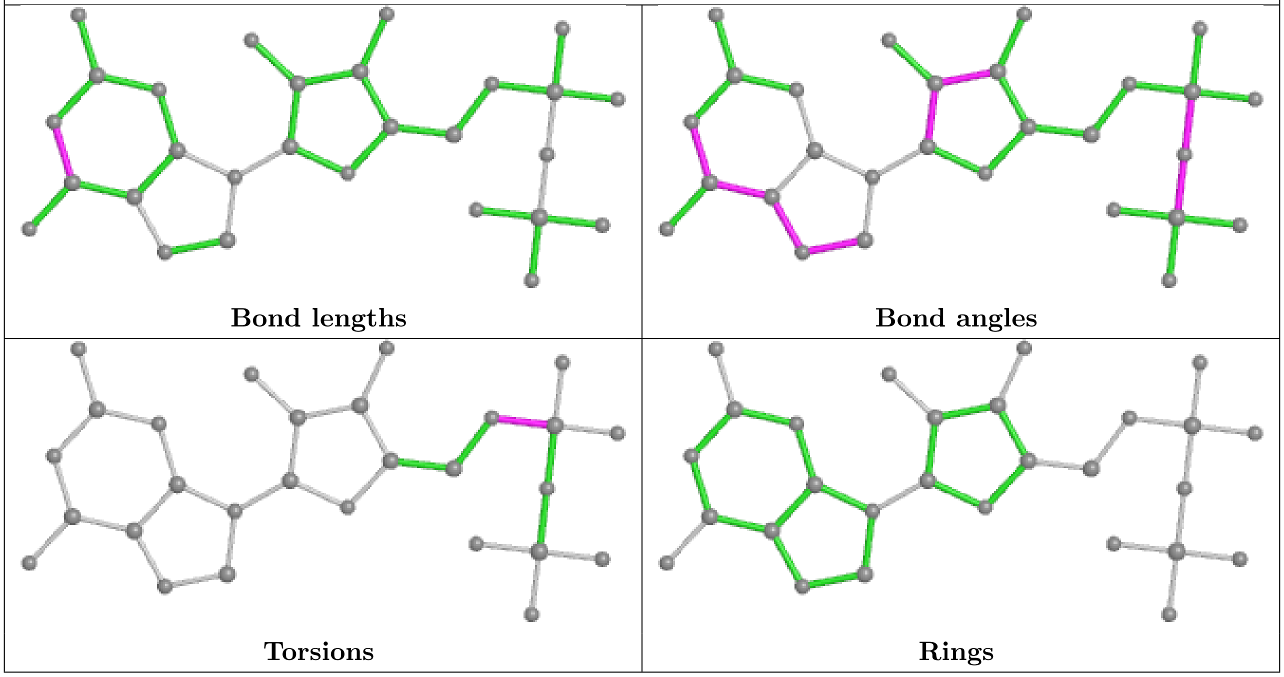


Bond lengths Bond angles

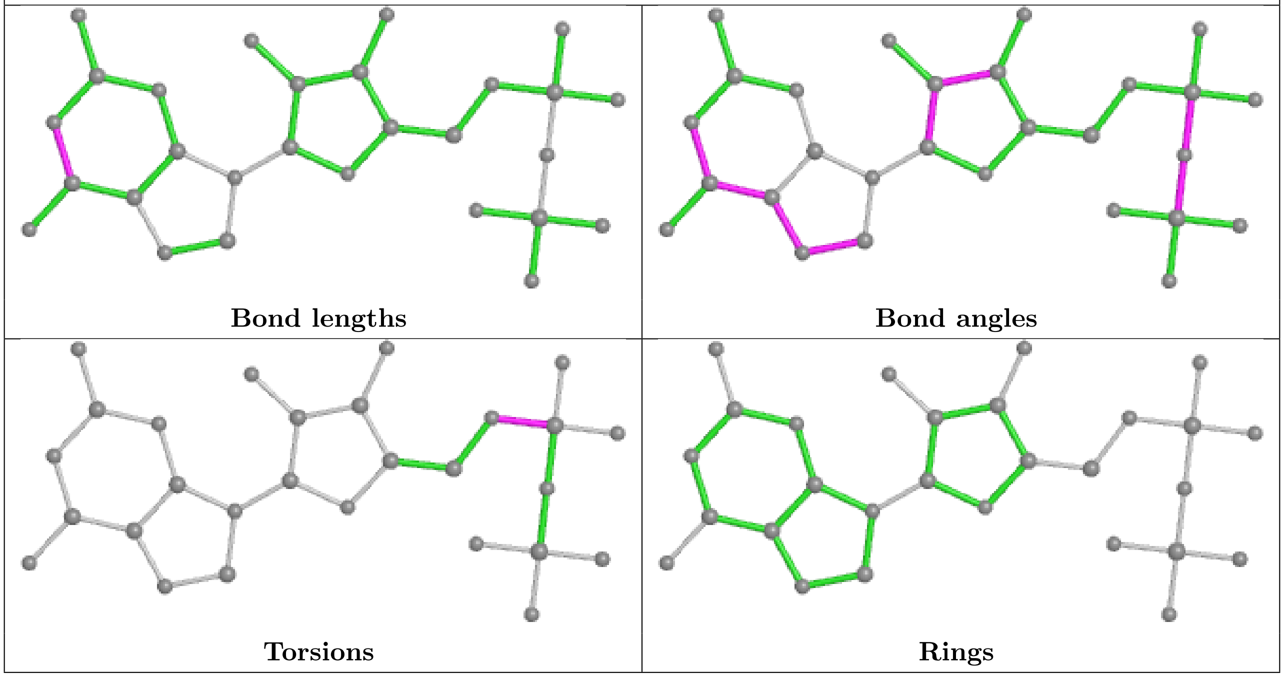


Torsions Rings

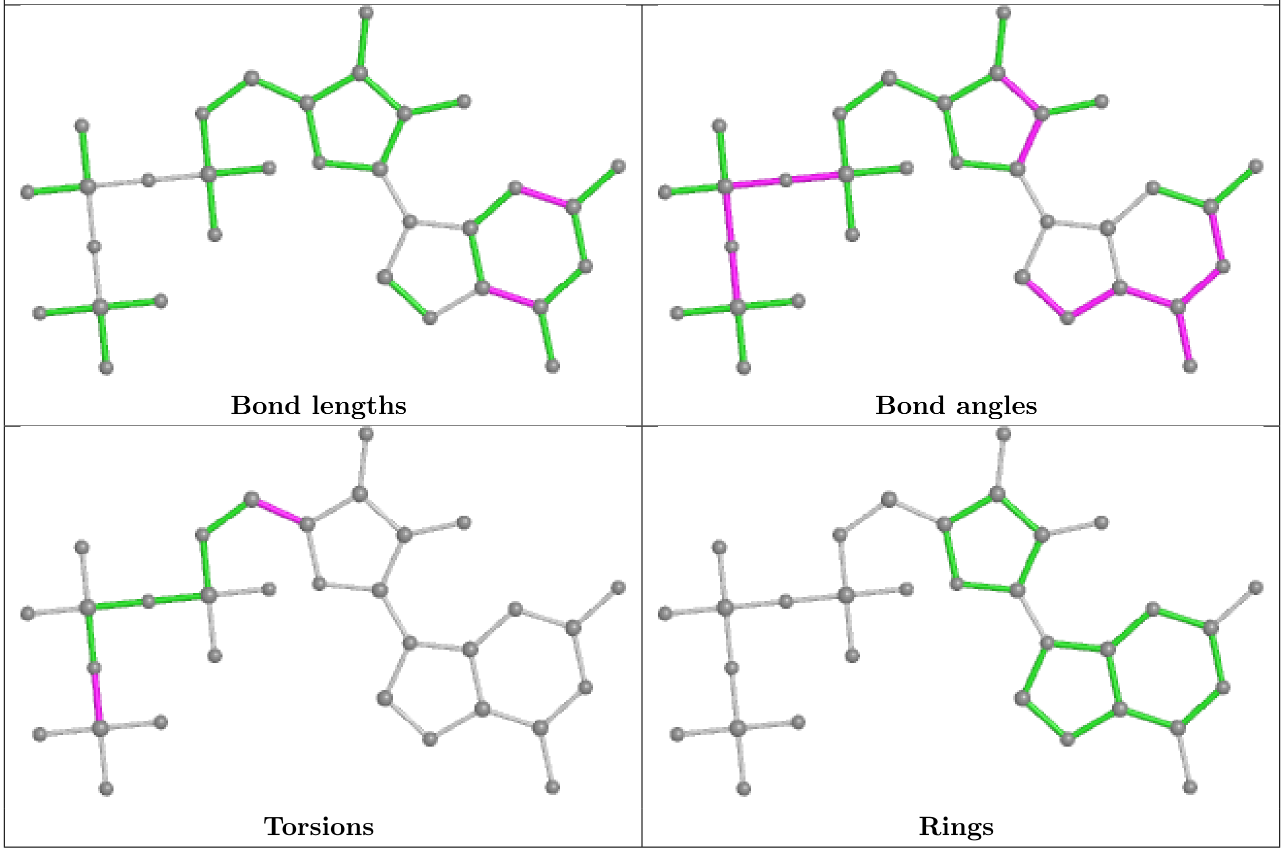
Ligand GDP 1a 501



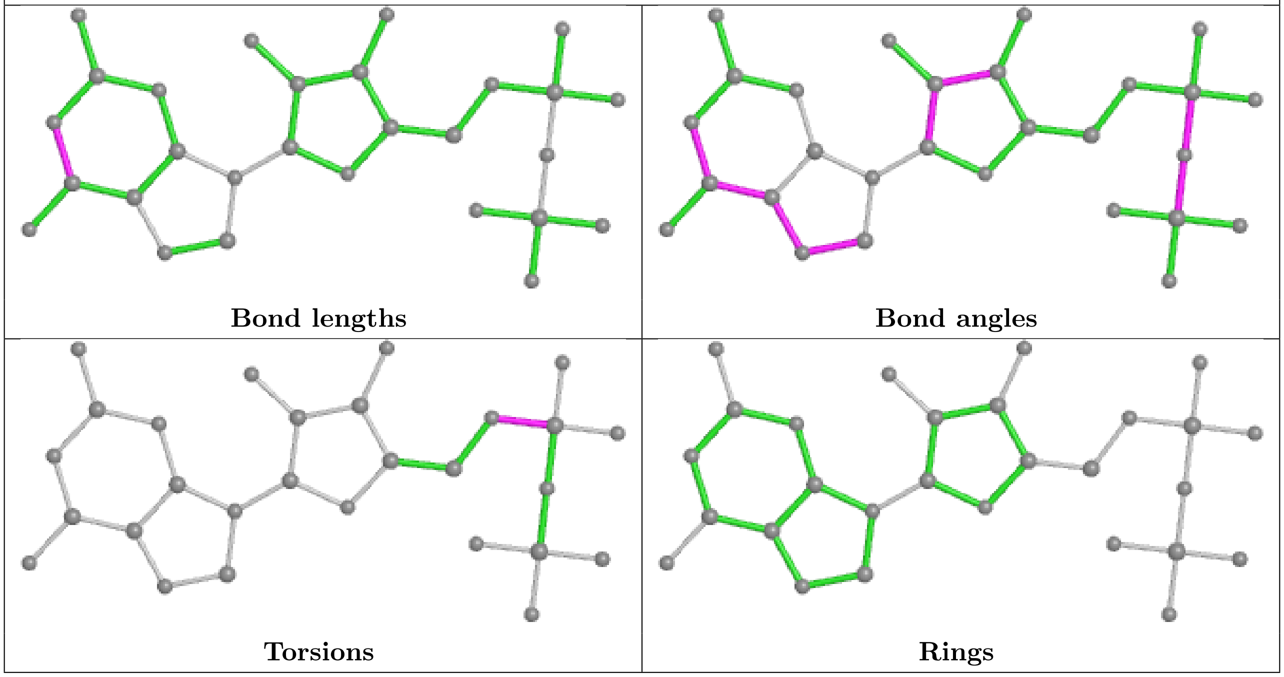
Ligand GDP De 501



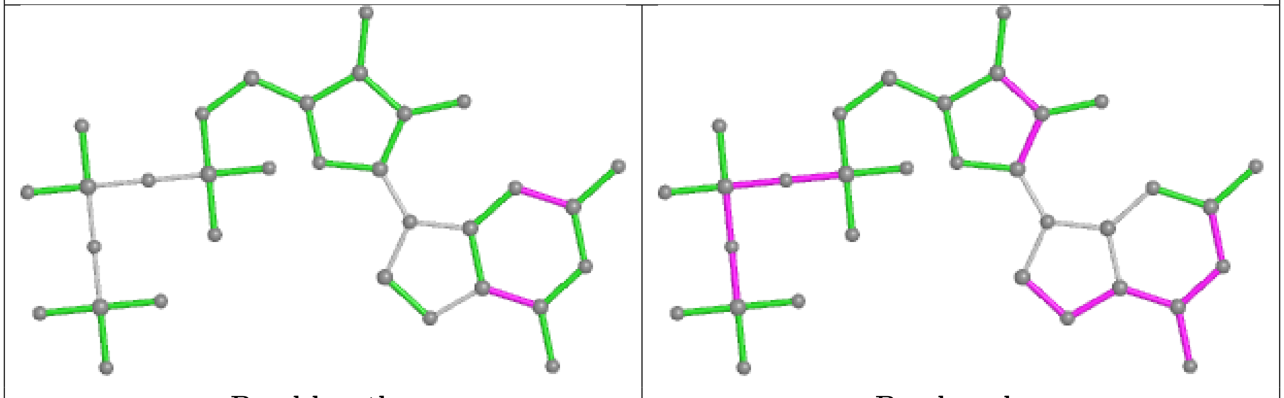
Ligand GTP 3h 501



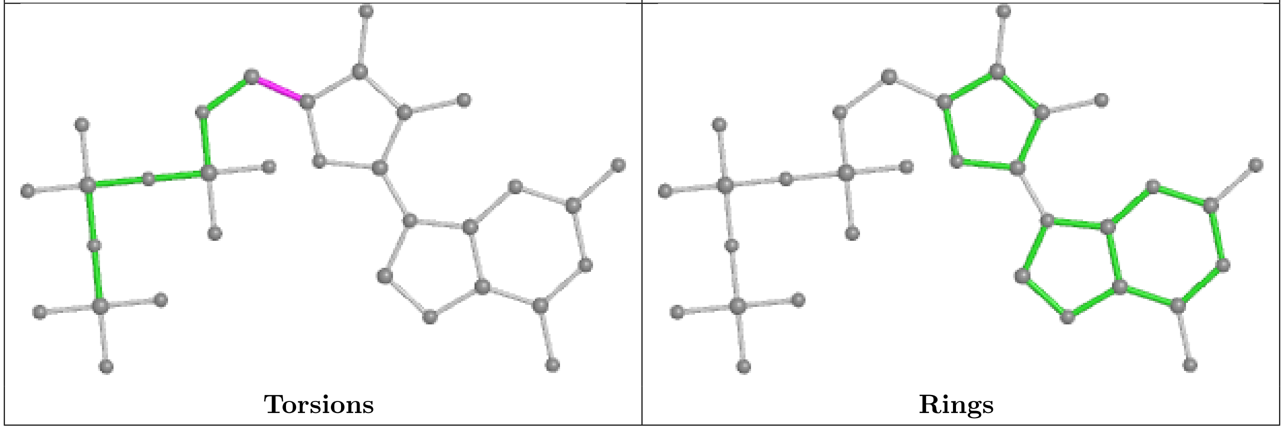
Ligand GDP 7a 501



Ligand GTP 2b 501

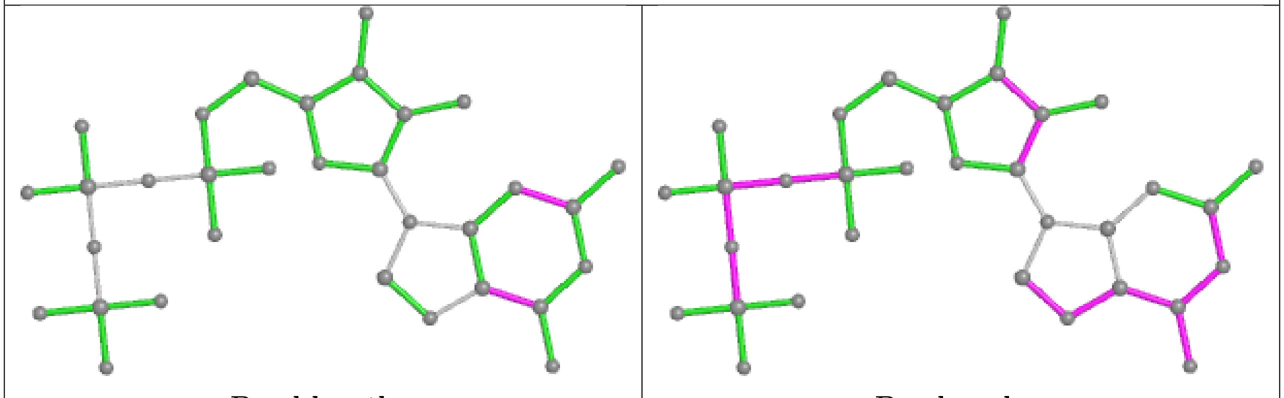


Bond lengths Bond angles

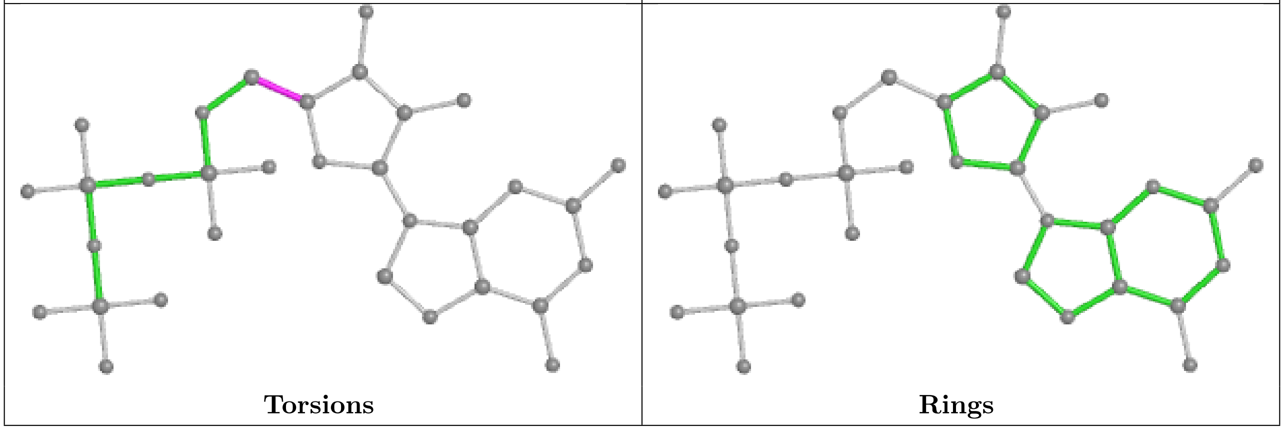


Torsions Rings

Ligand GTP 1d 501

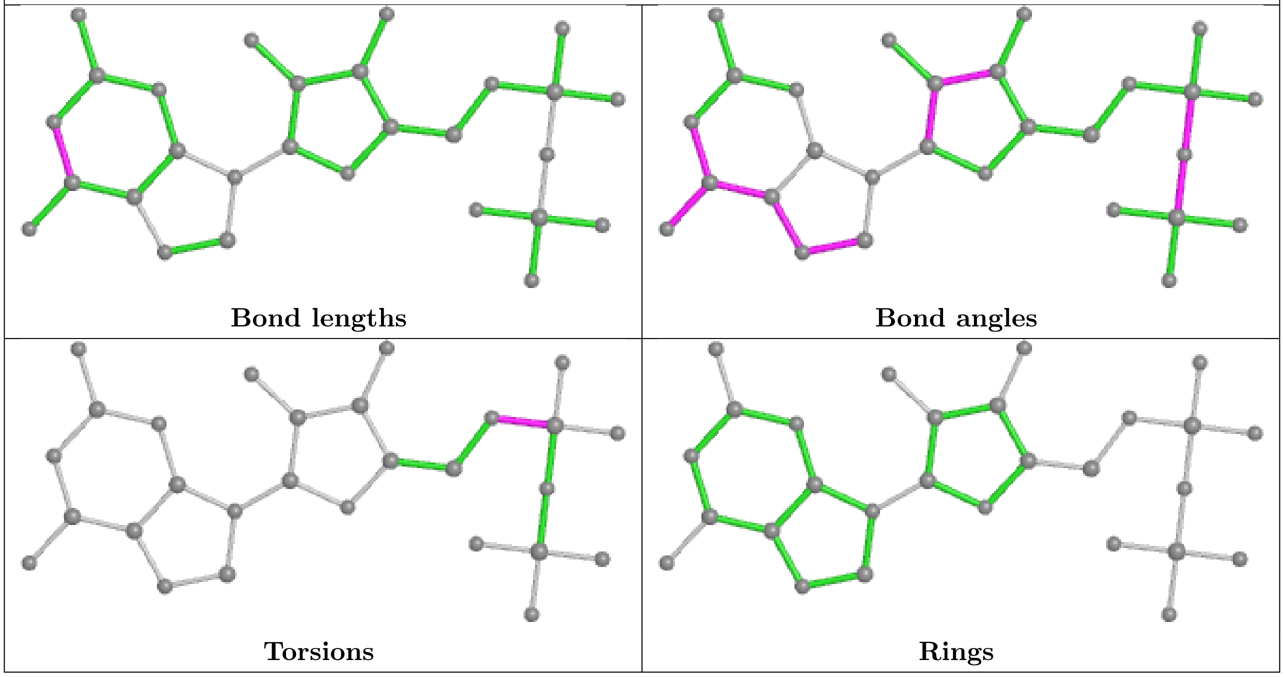


Bond lengths Bond angles

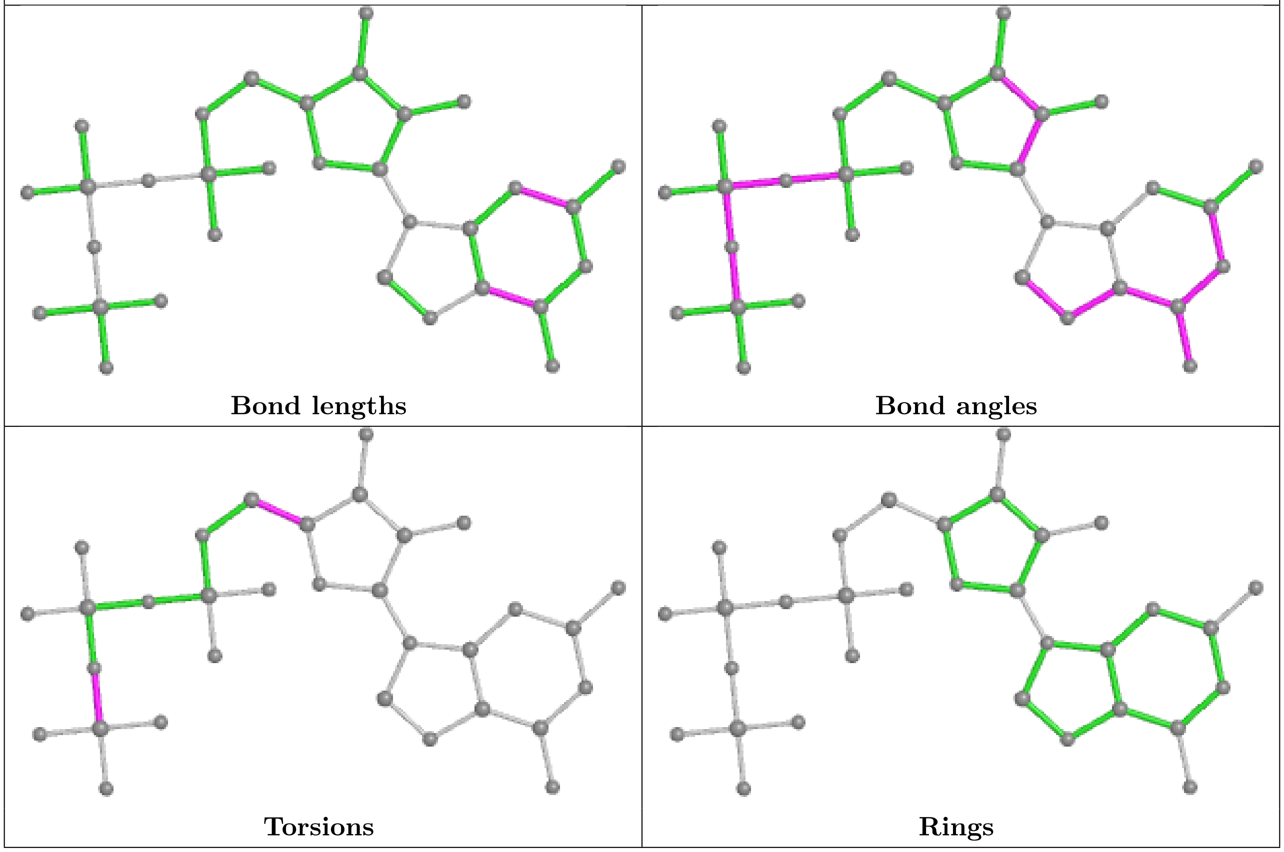


Torsions Rings

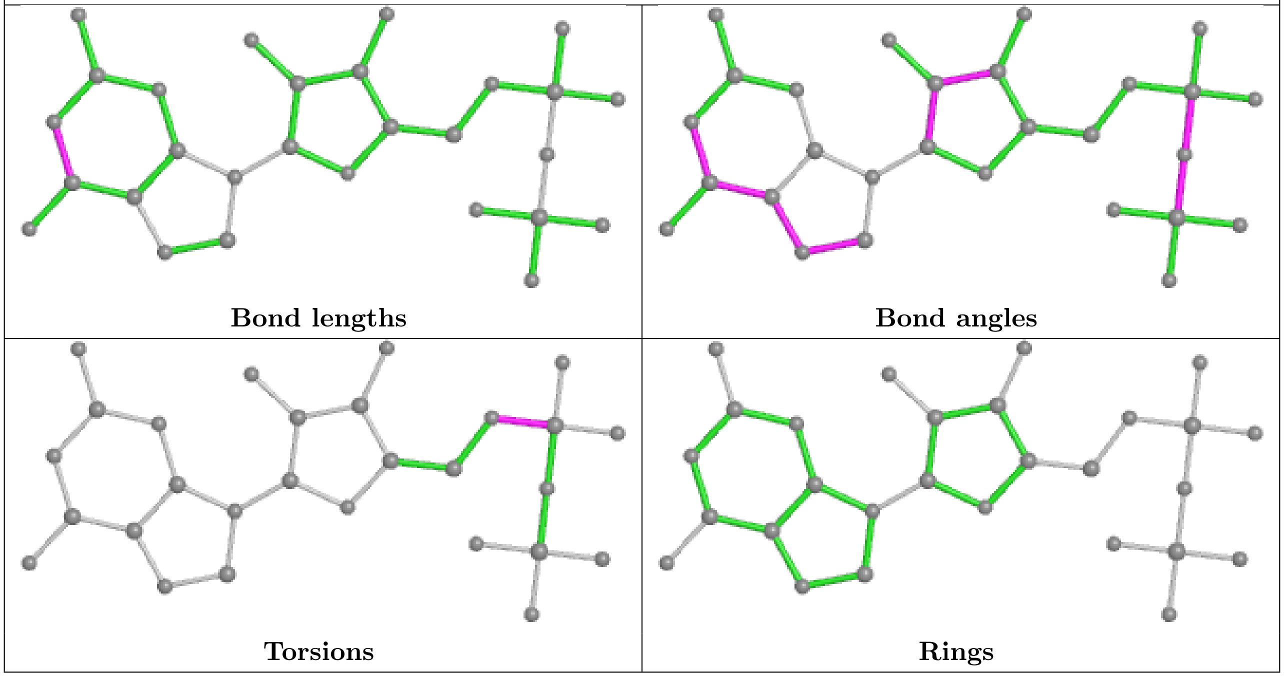
Ligand GDP 9e 501



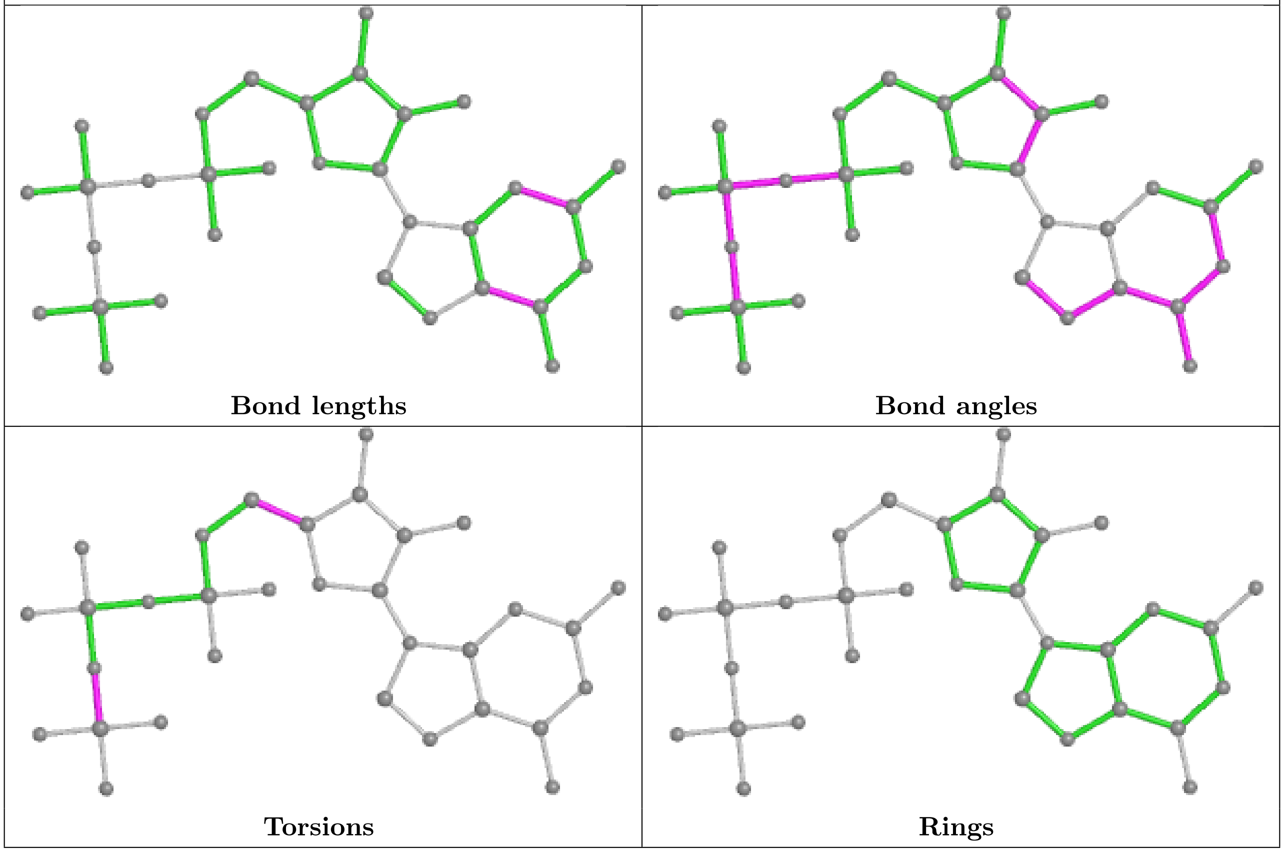
Ligand GTP 9f 501



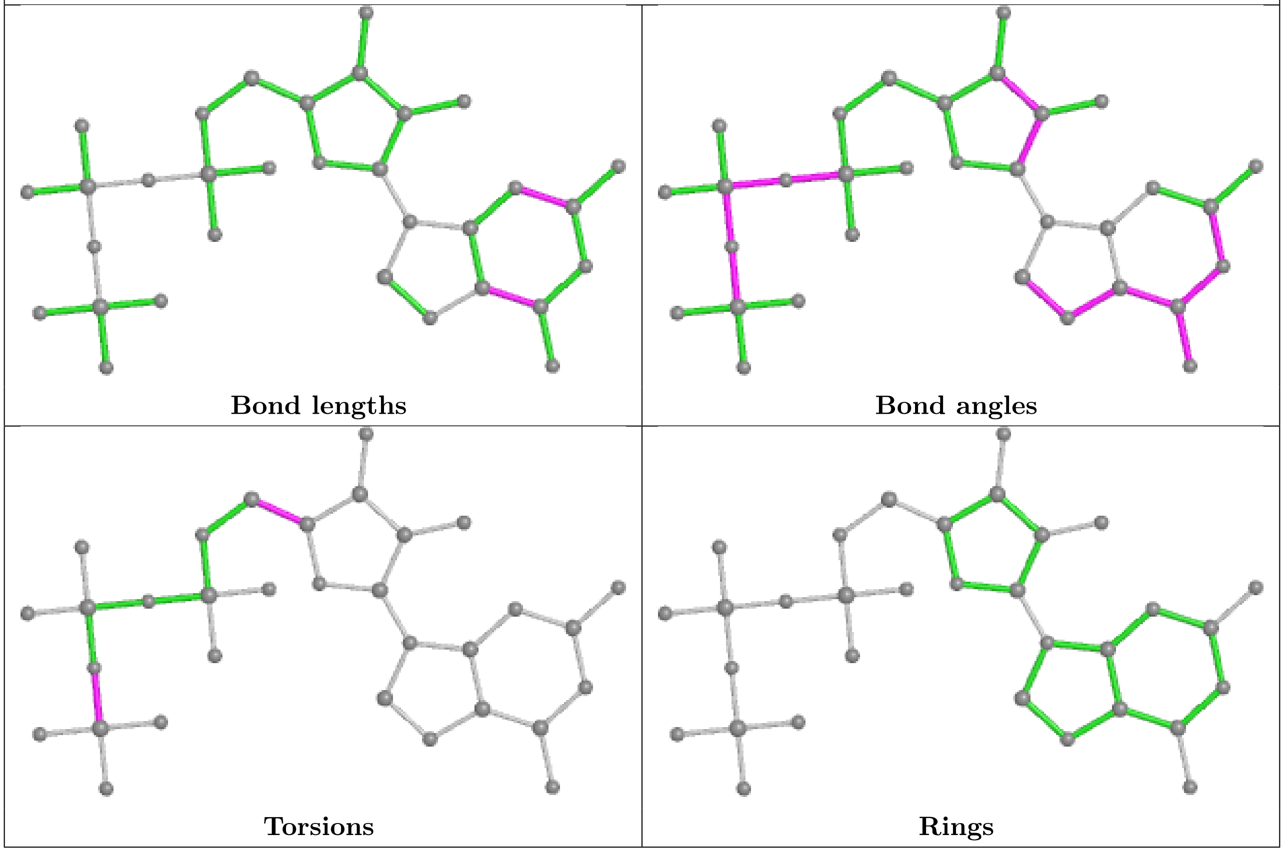
Ligand GDP 7g 501



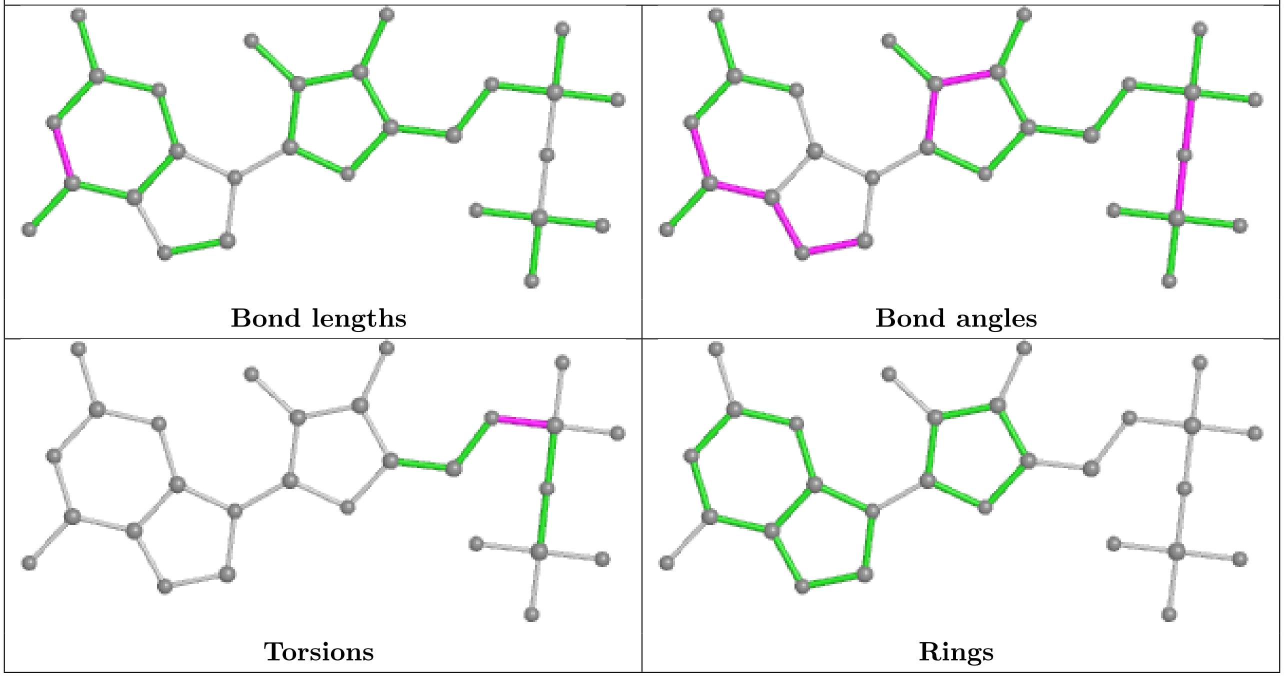
Ligand GTP Ab 501



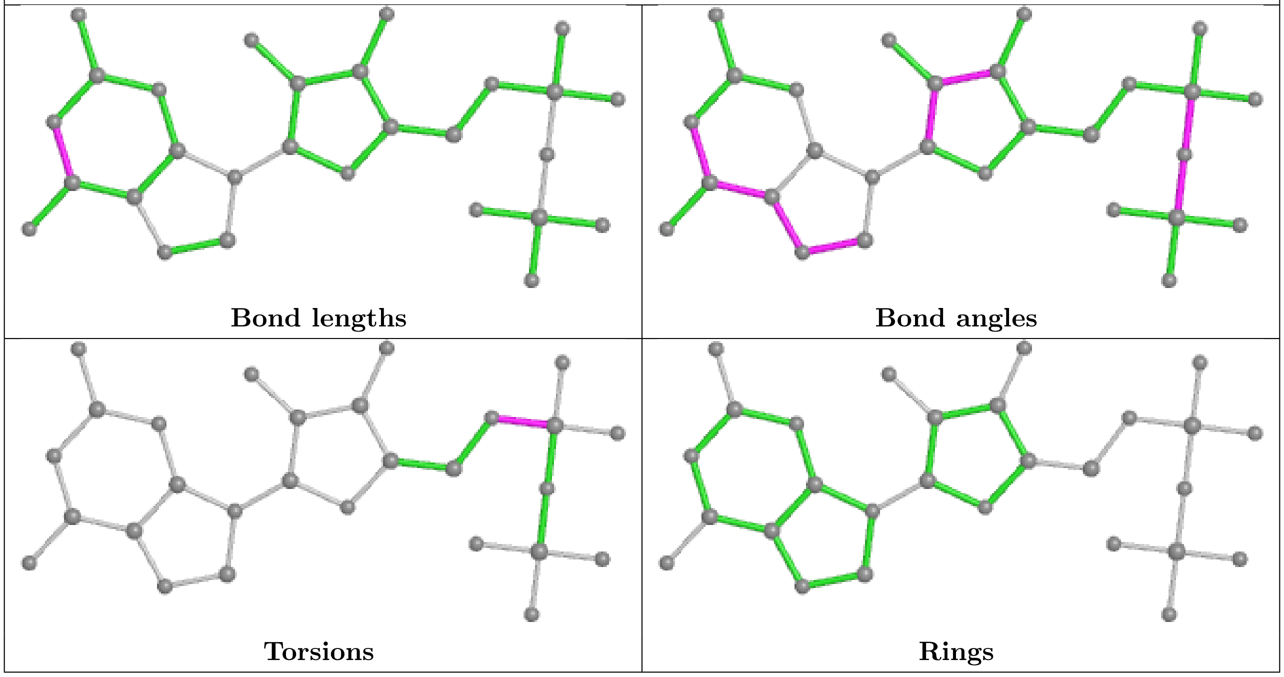
Ligand GTP 6b 501



Ligand GDP 3a 501



Ligand GDP 2a 501



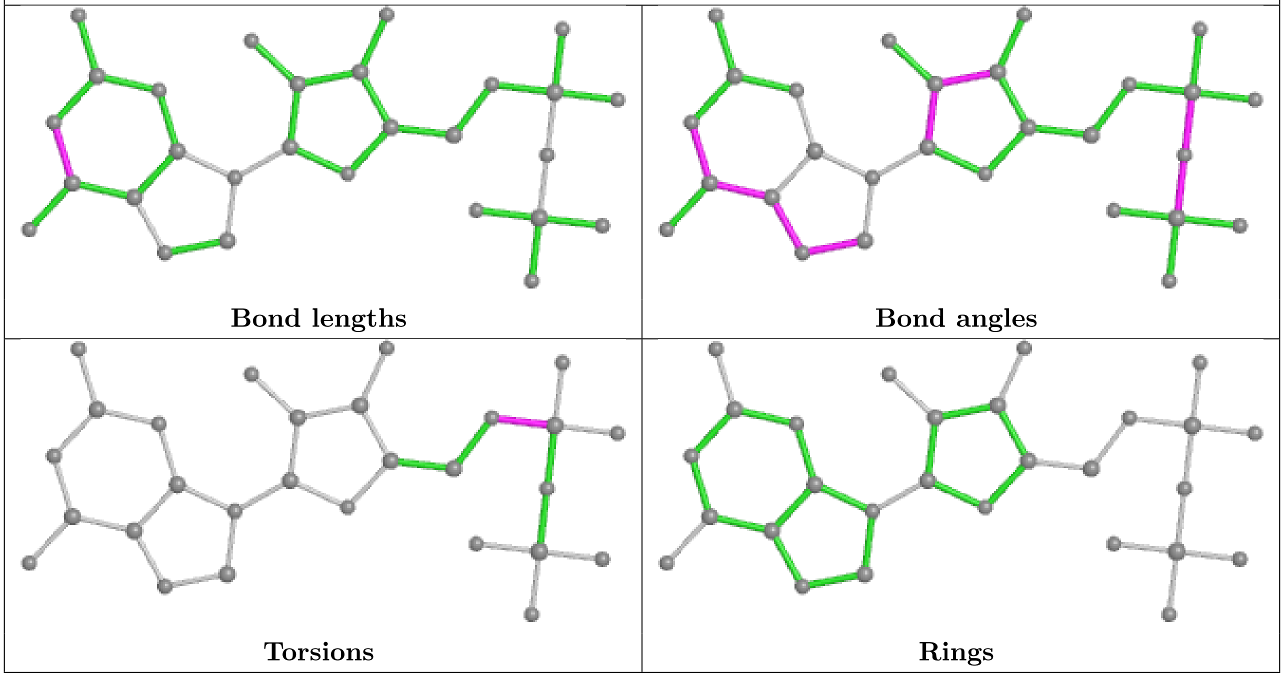
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP Dc 501



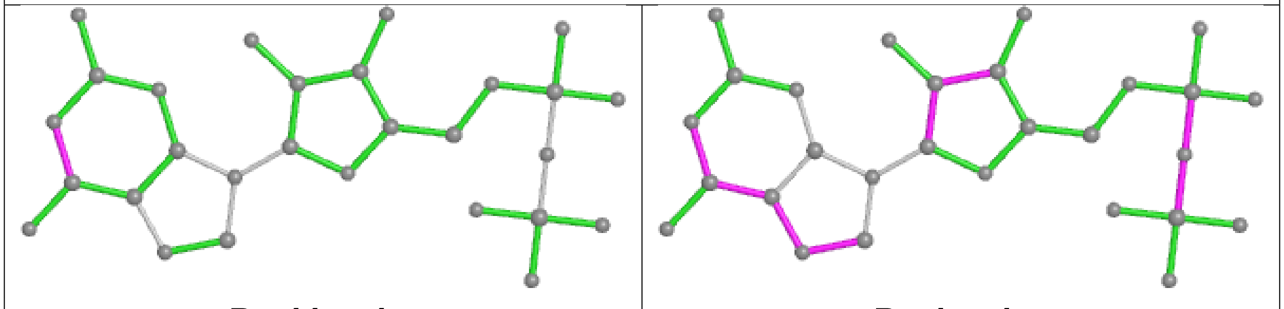
Bond lengths

Bond angles

Torsions

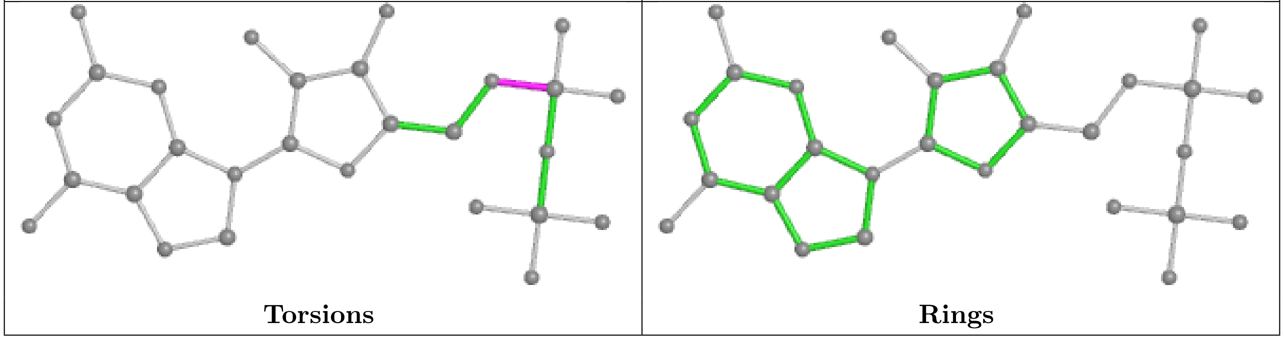
Rings

Ligand GDP 5g 501



Bond lengths

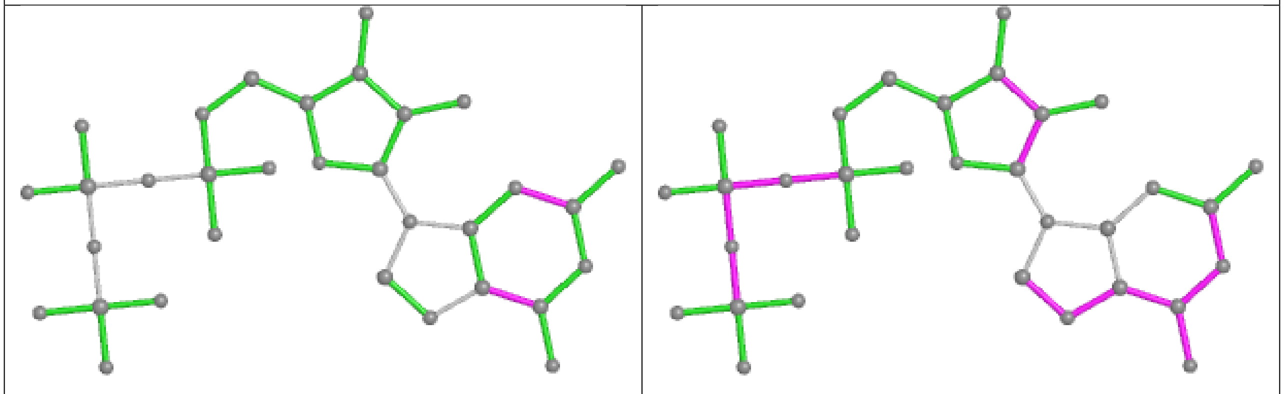
Bond angles



Torsions

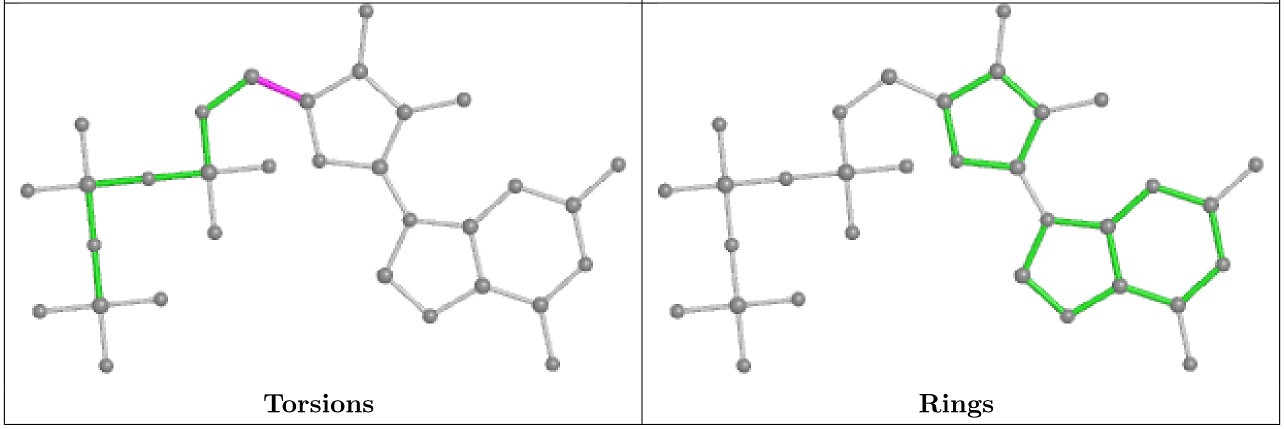
Rings

Ligand GTP 4h 501



Bond lengths

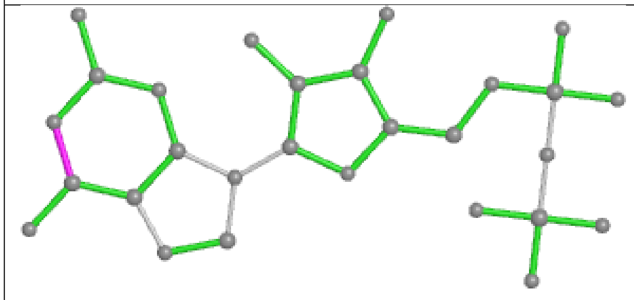
Bond angles



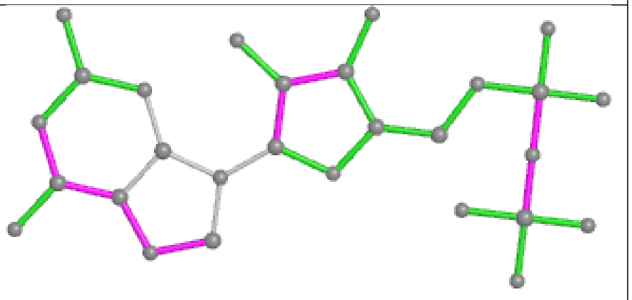
Torsions

Rings

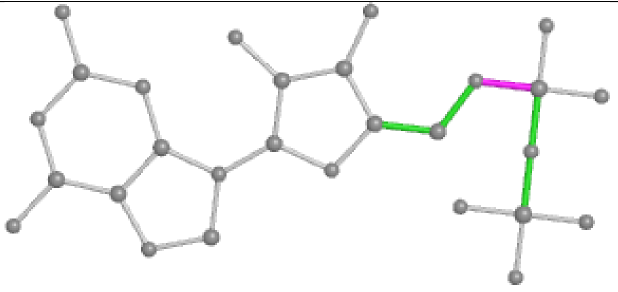
Ligand GDP Bg 501



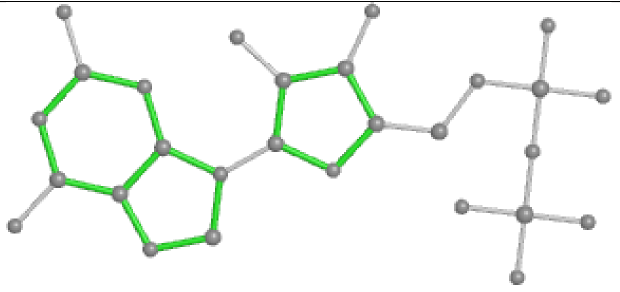
Bond lengths



Bond angles

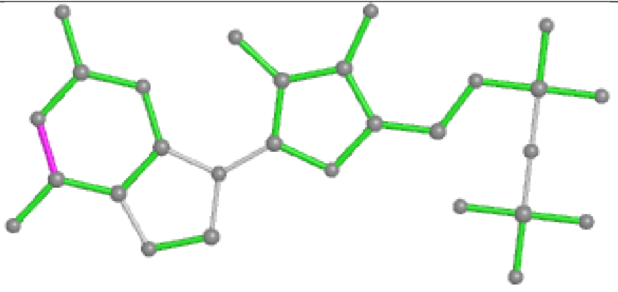


Torsions

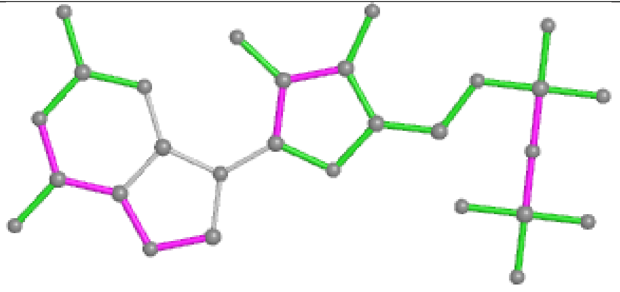


Rings

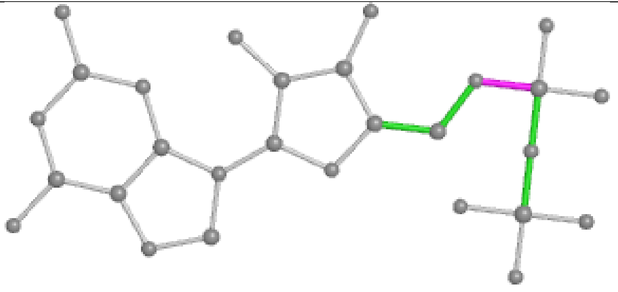
Ligand GDP 5a 501



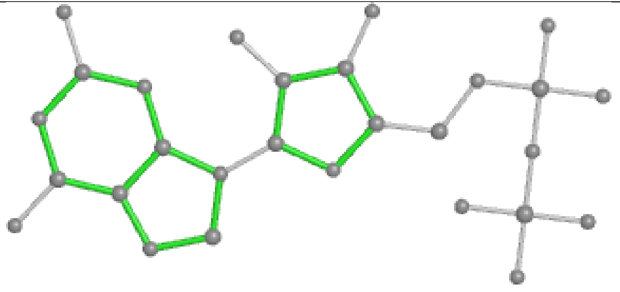
Bond lengths



Bond angles

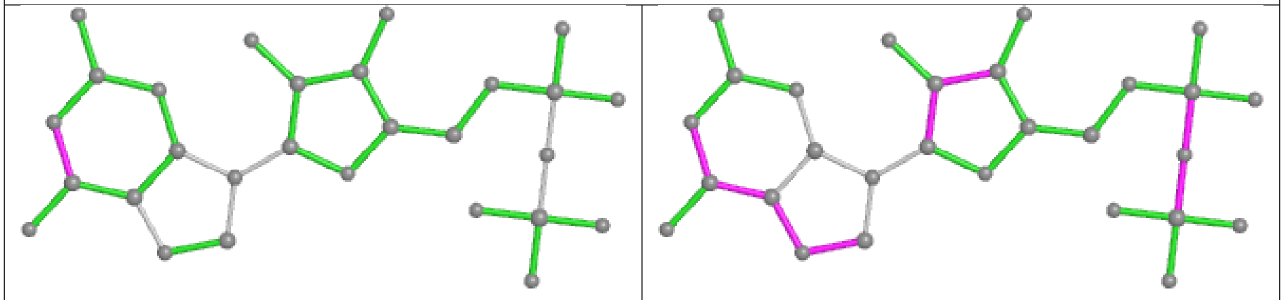


Torsions



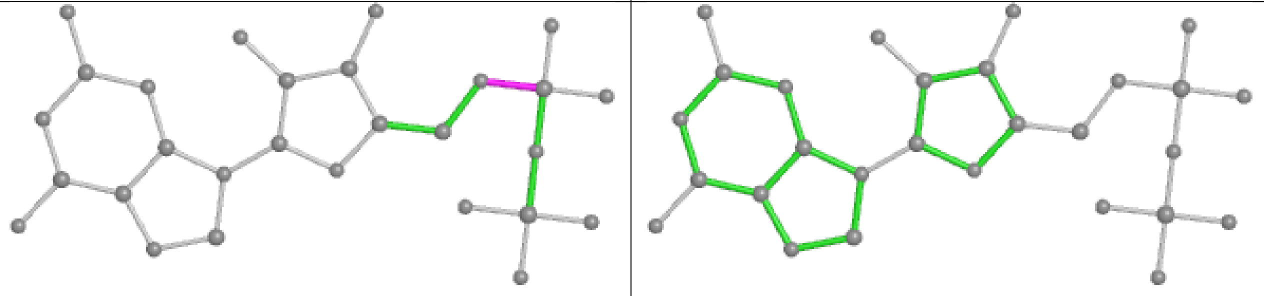
Rings

Ligand GDP 8c 501



Bond lengths

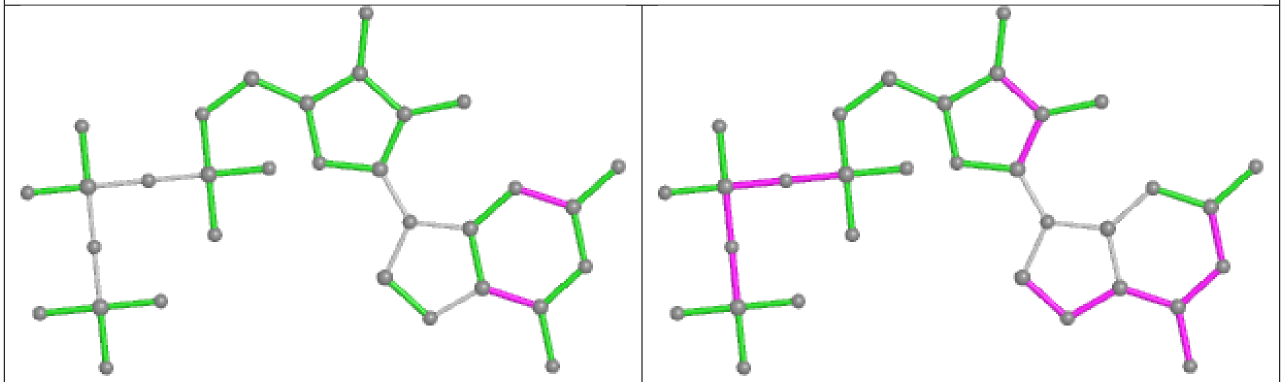
Bond angles



Torsions

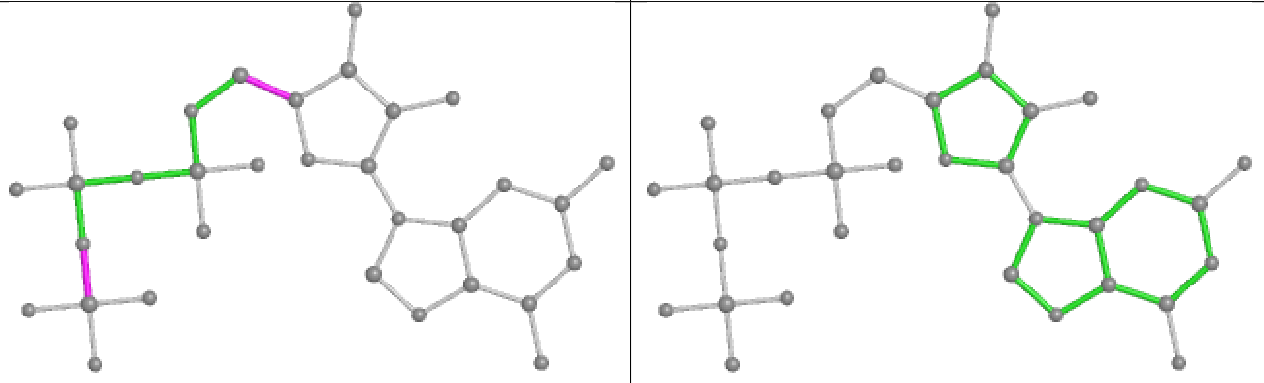
Rings

Ligand GTP Df 501



Bond lengths

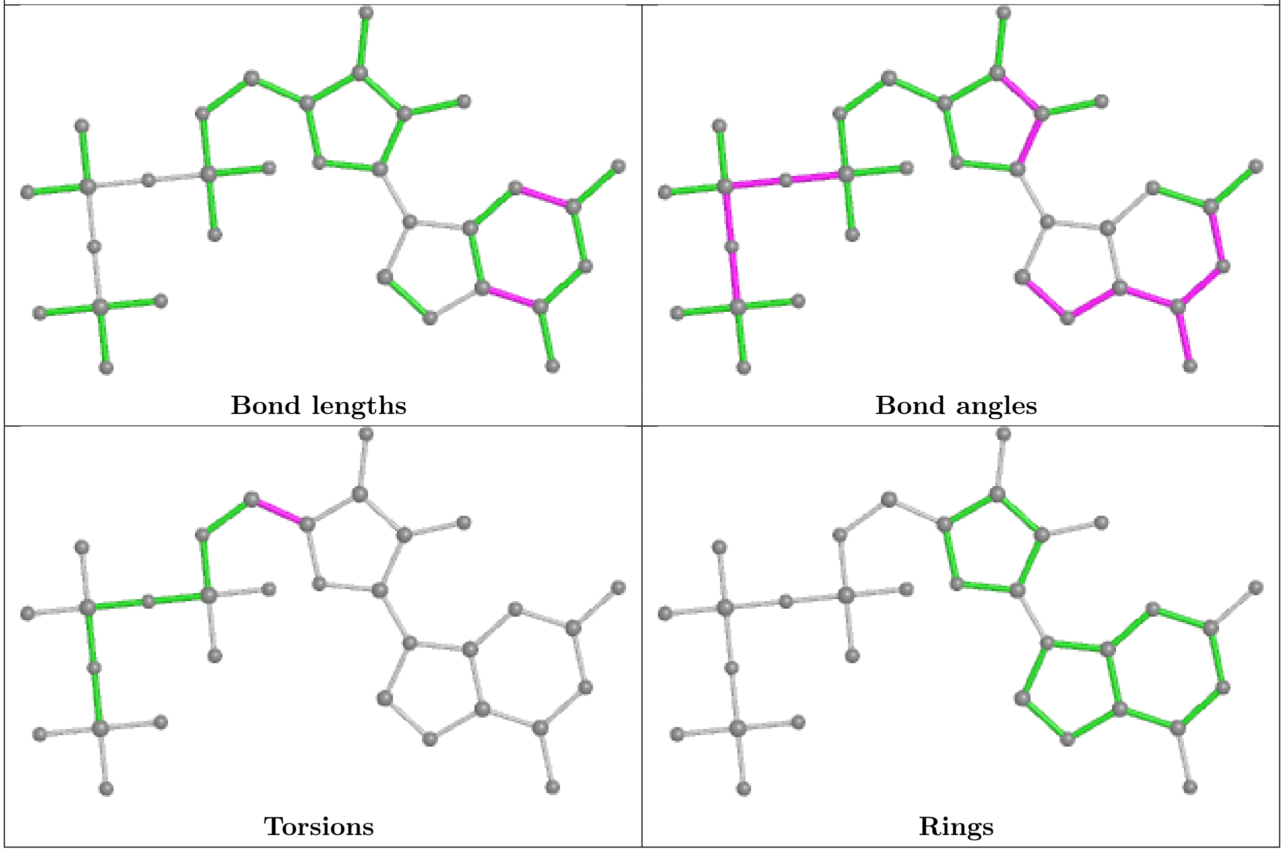
Bond angles



Torsions

Rings

Ligand GTP Dh 501



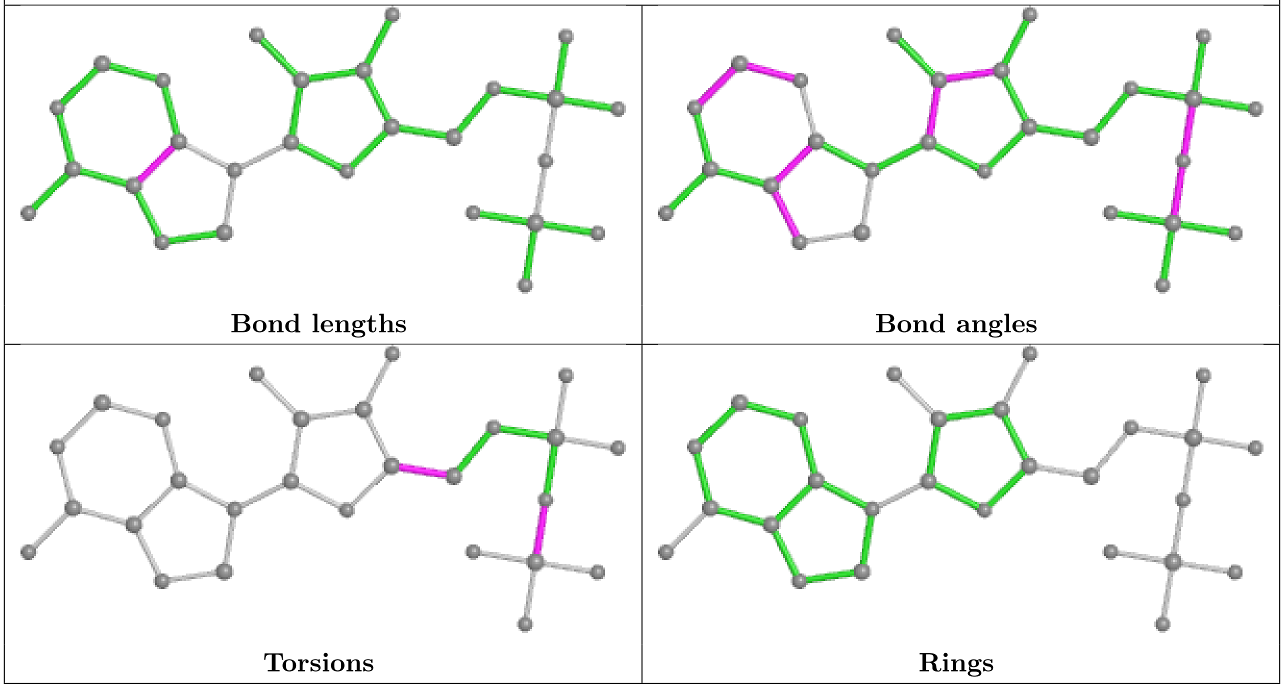
Bond lengths

Bond angles

Torsions

Rings

Ligand ADP 1A 801



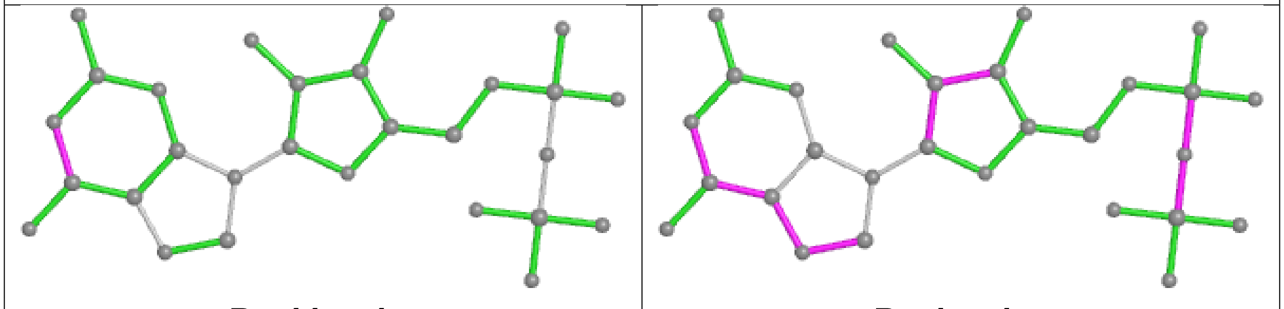
Bond lengths

Bond angles

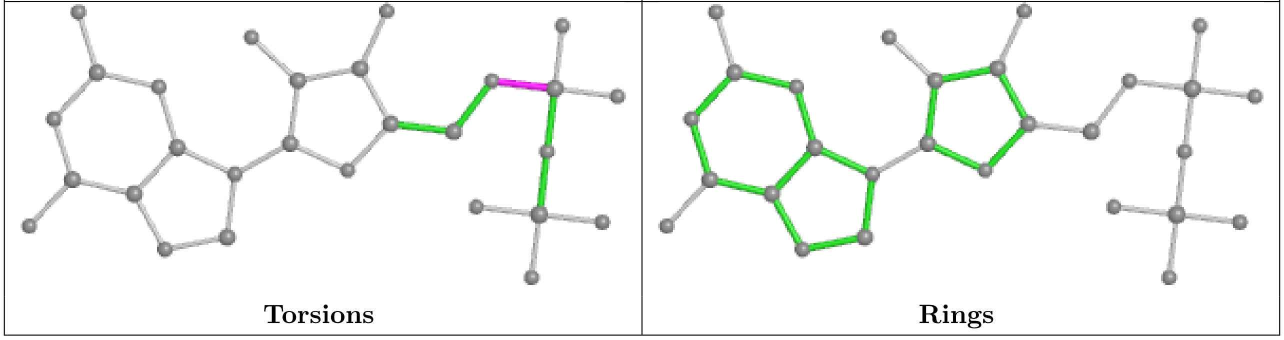
Torsions

Rings

Ligand GDP Ca 501

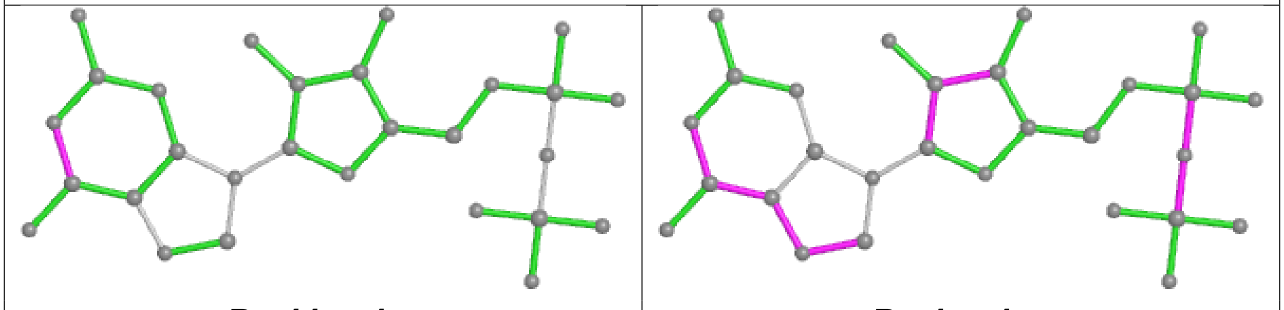


Bond lengths Bond angles

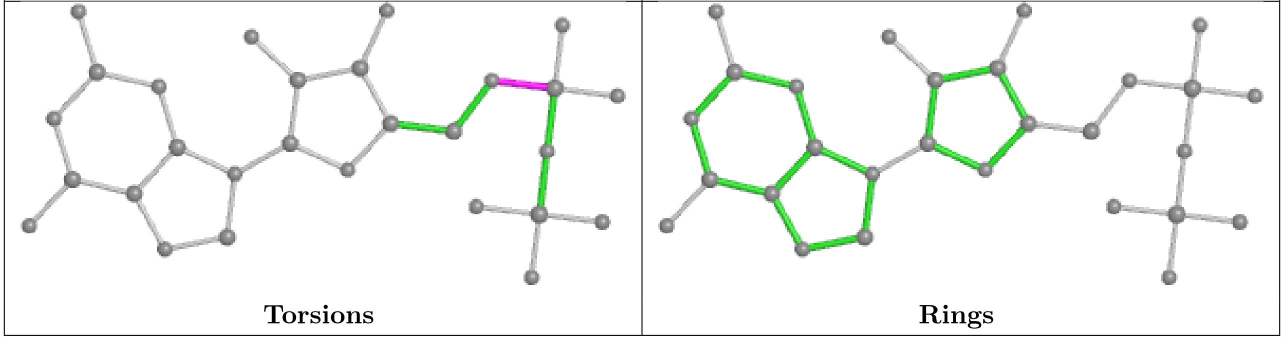


Torsions Rings

Ligand GDP 9a 501

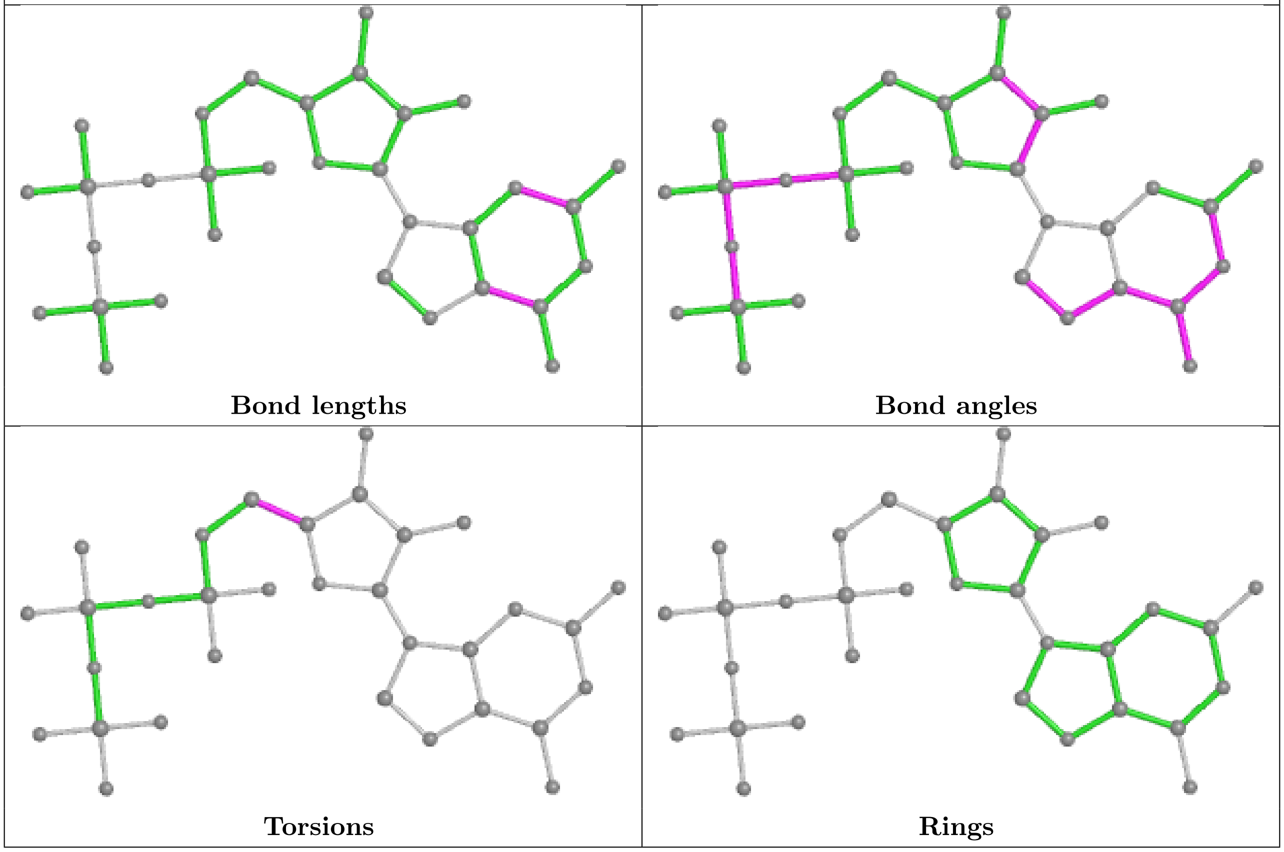


Bond lengths Bond angles

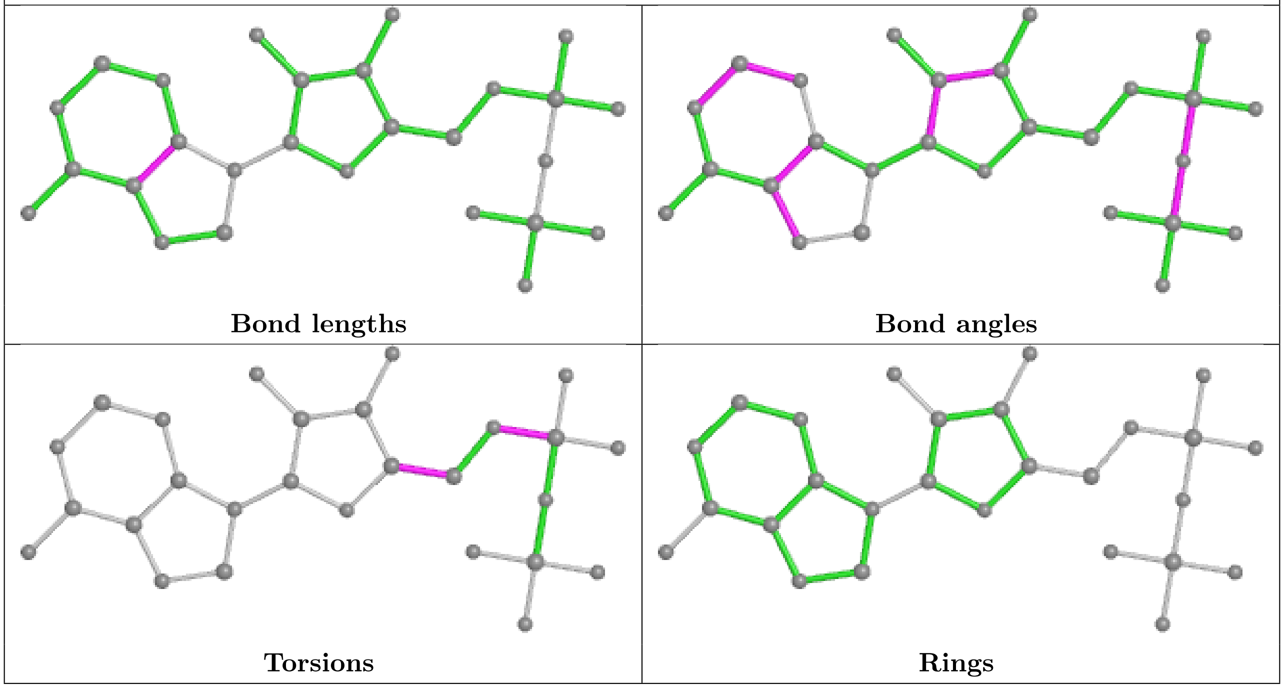


Torsions Rings

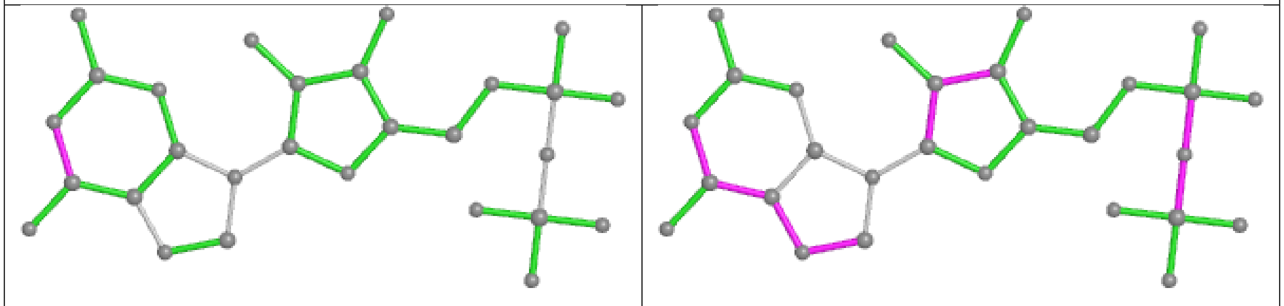
Ligand GTP 1f 501



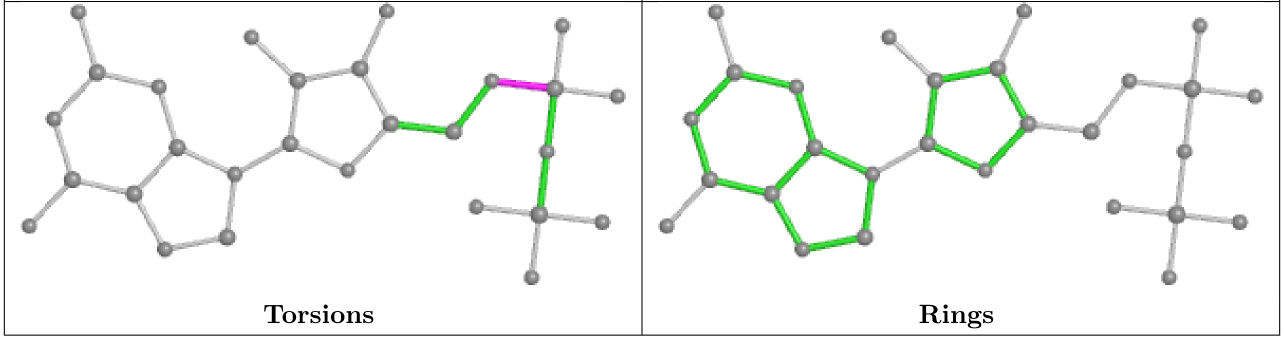
Ligand ADP 0Z 801



Ligand GDP 9c 501

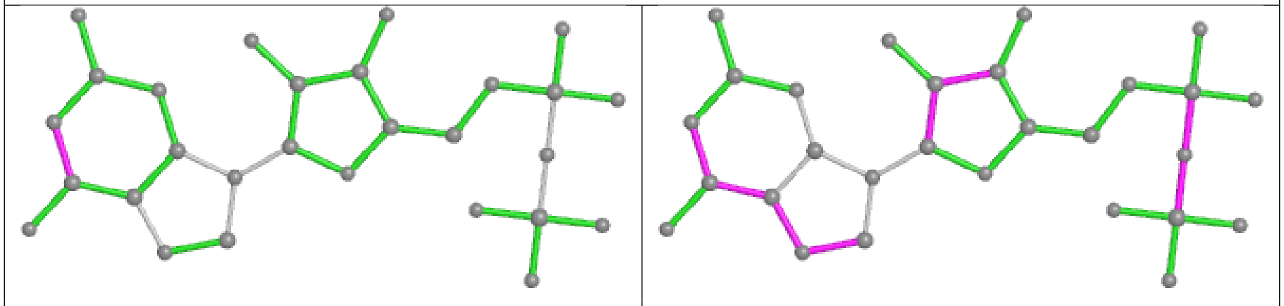


Bond lengths **Bond angles**

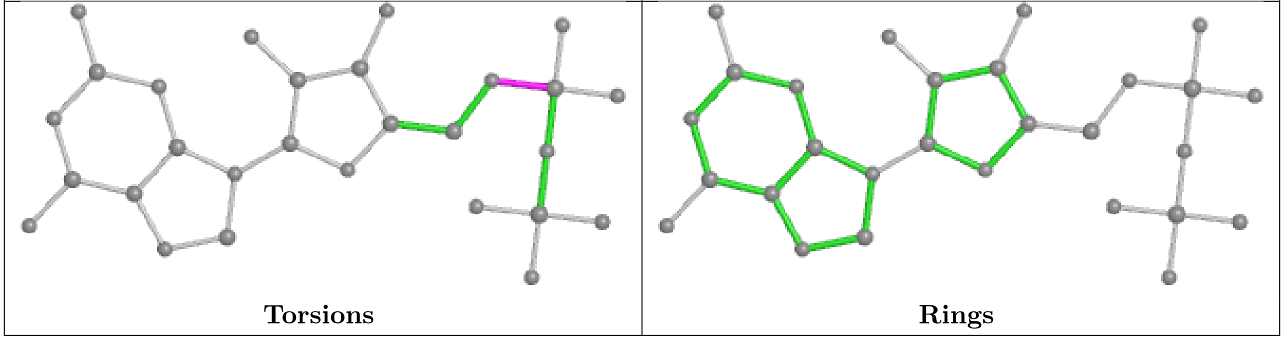


Torsions **Rings**

Ligand GDP Cc 501

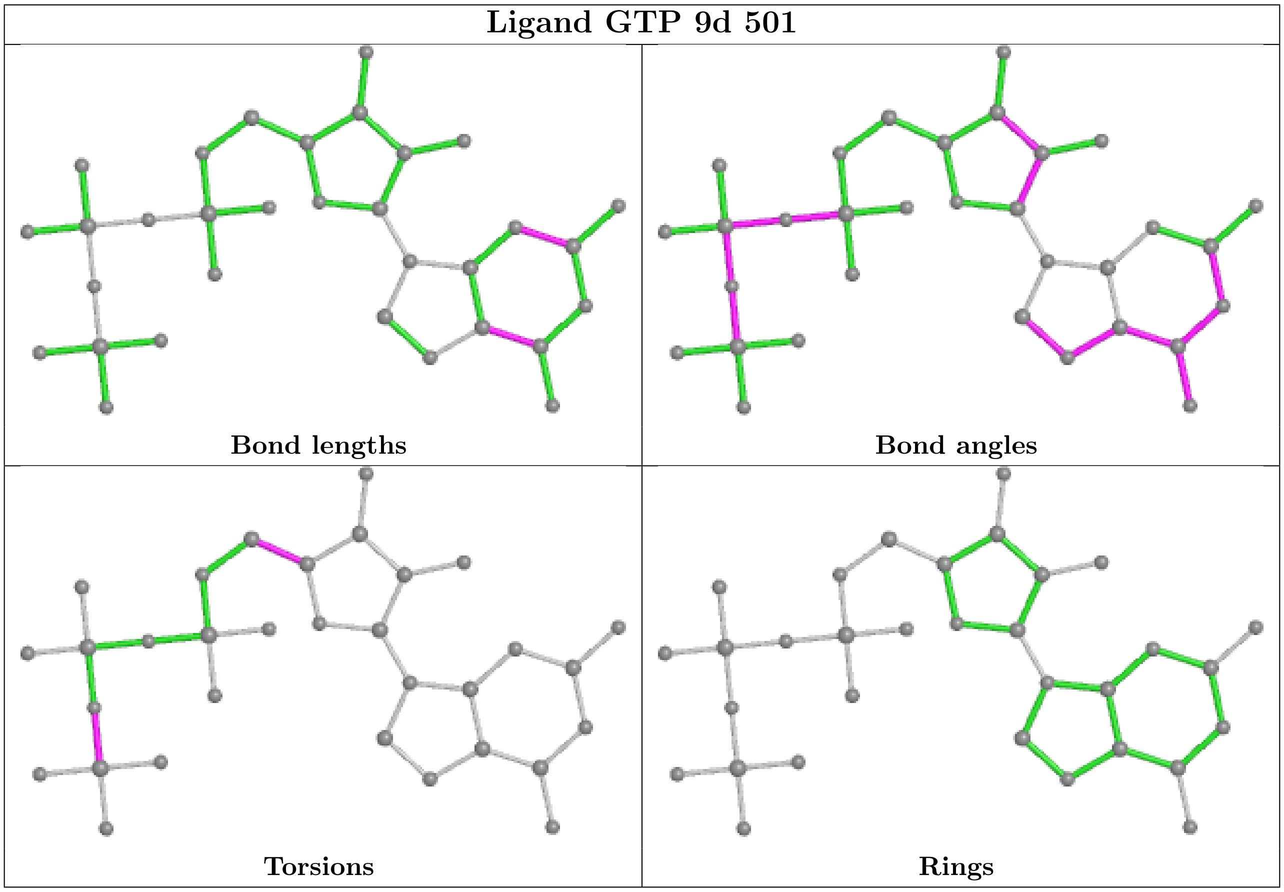


Bond lengths **Bond angles**

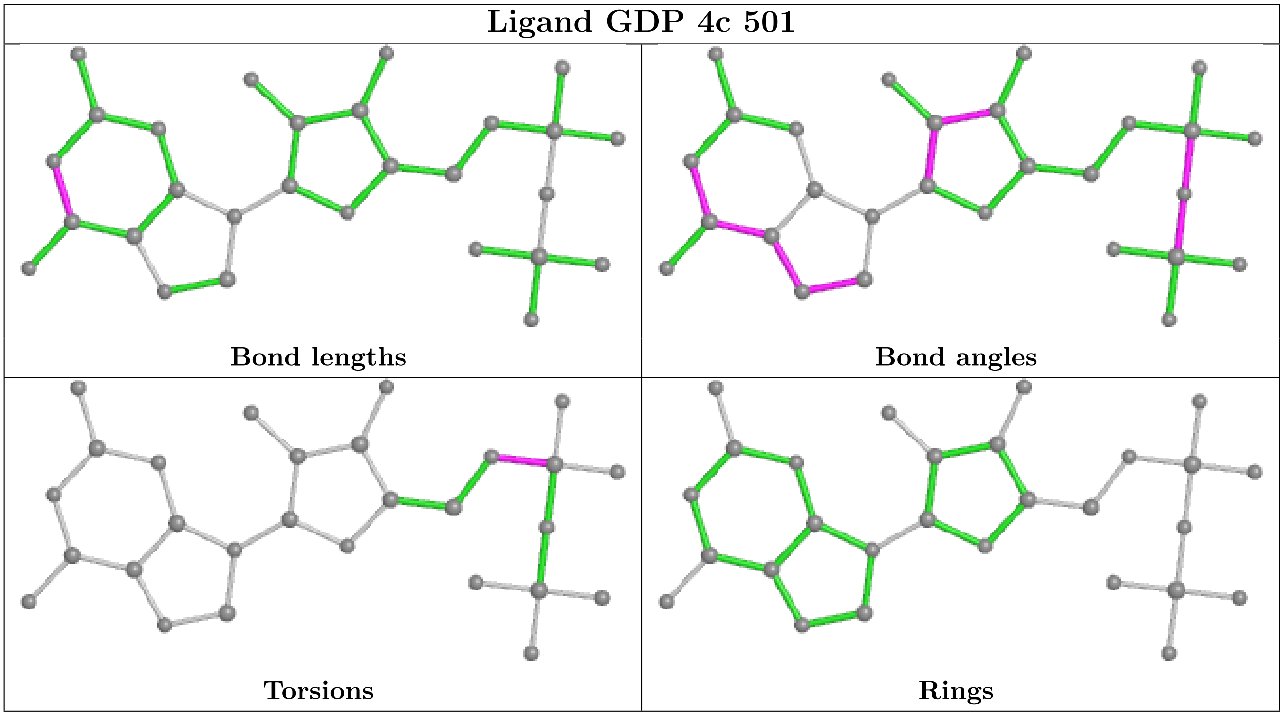


Torsions **Rings**

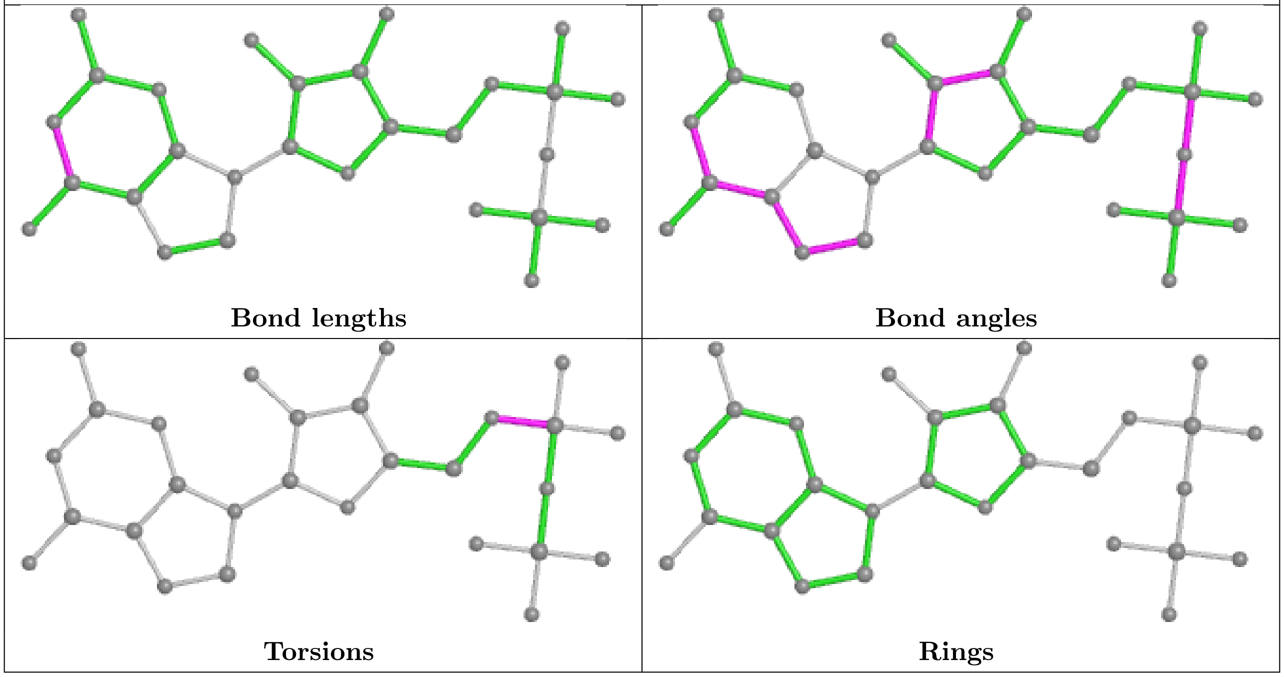
Ligand GTP 9d 501



Ligand GDP 4c 501



Ligand GDP Ac 501



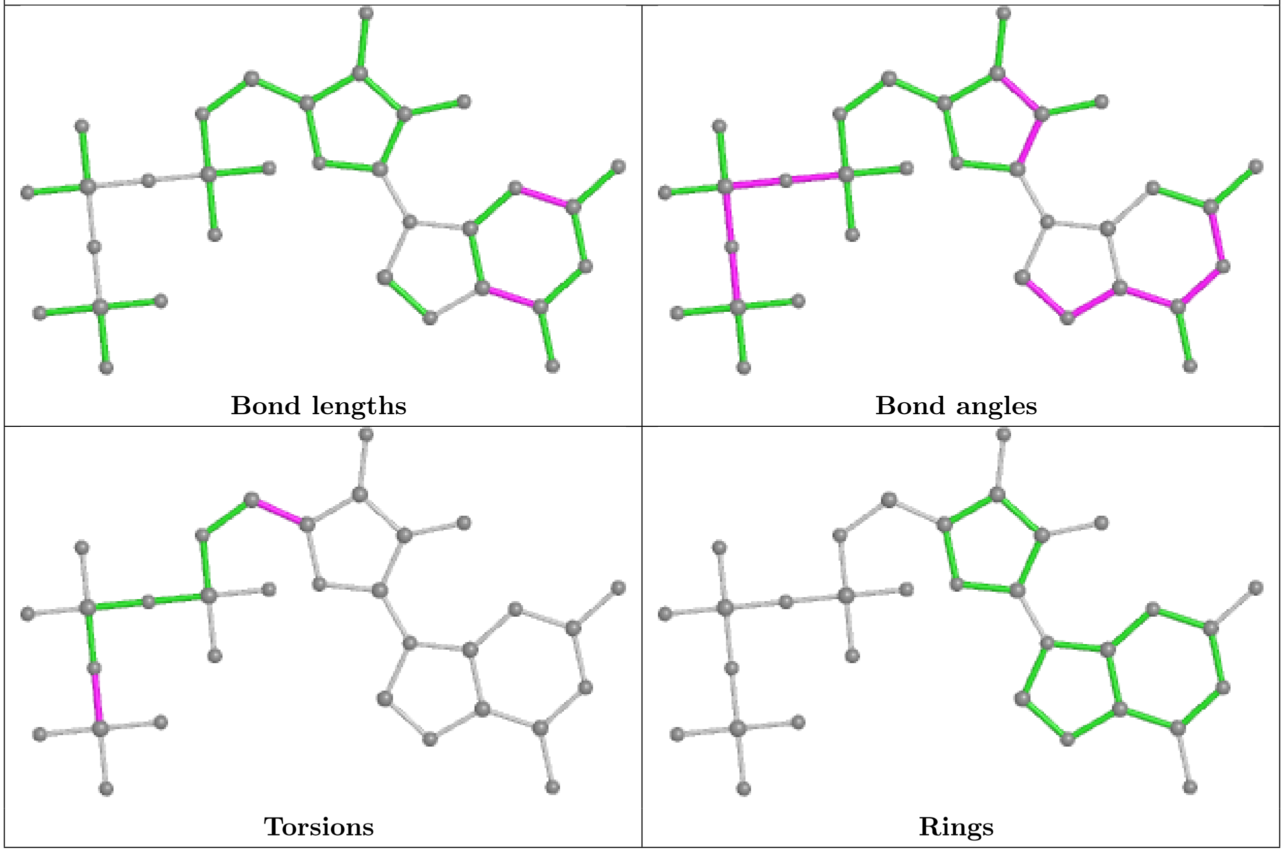
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP 8b 501



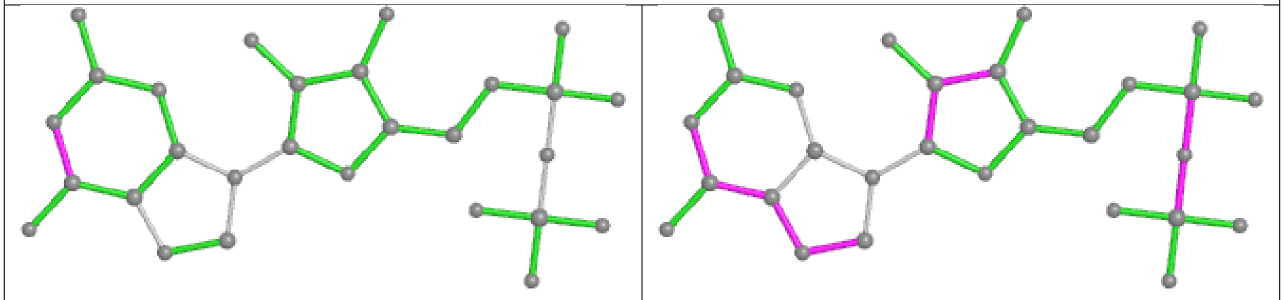
Bond lengths

Bond angles

Torsions

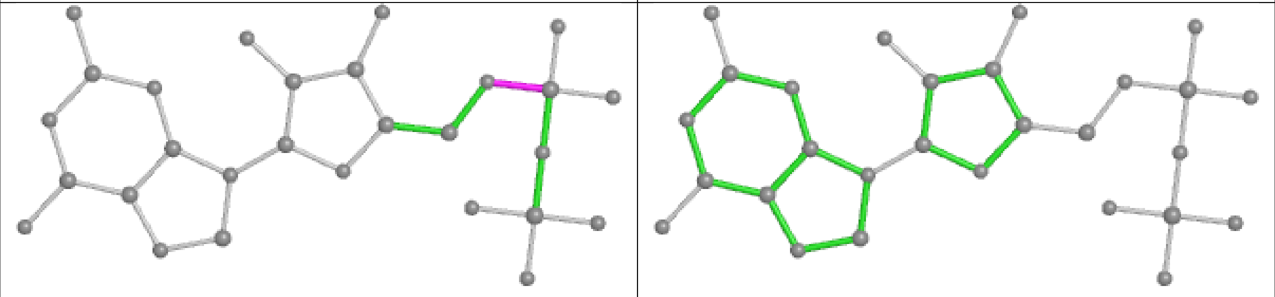
Rings

Ligand GDP 7e 501



Bond lengths

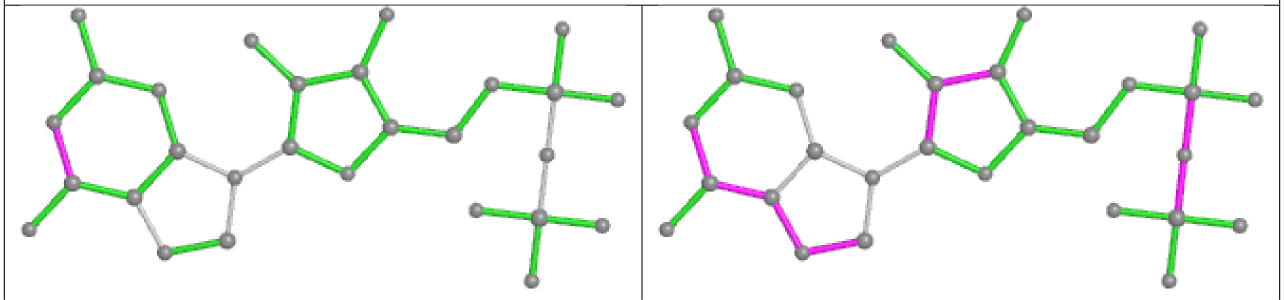
Bond angles



Torsions

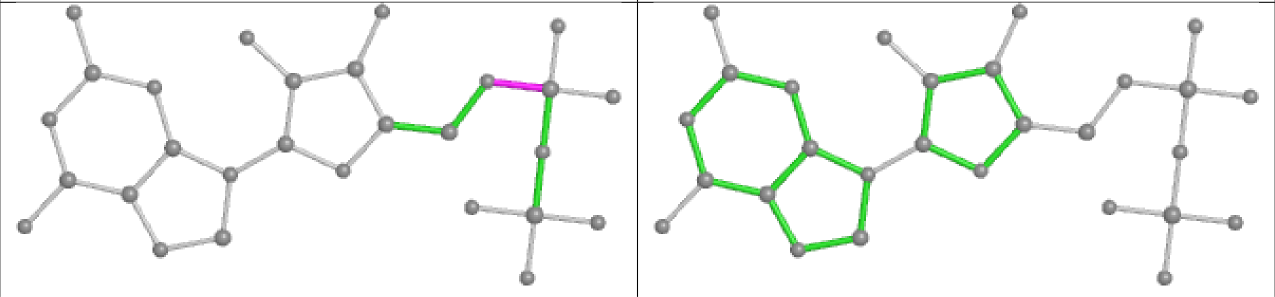
Rings

Ligand GDP 2c 501



Bond lengths

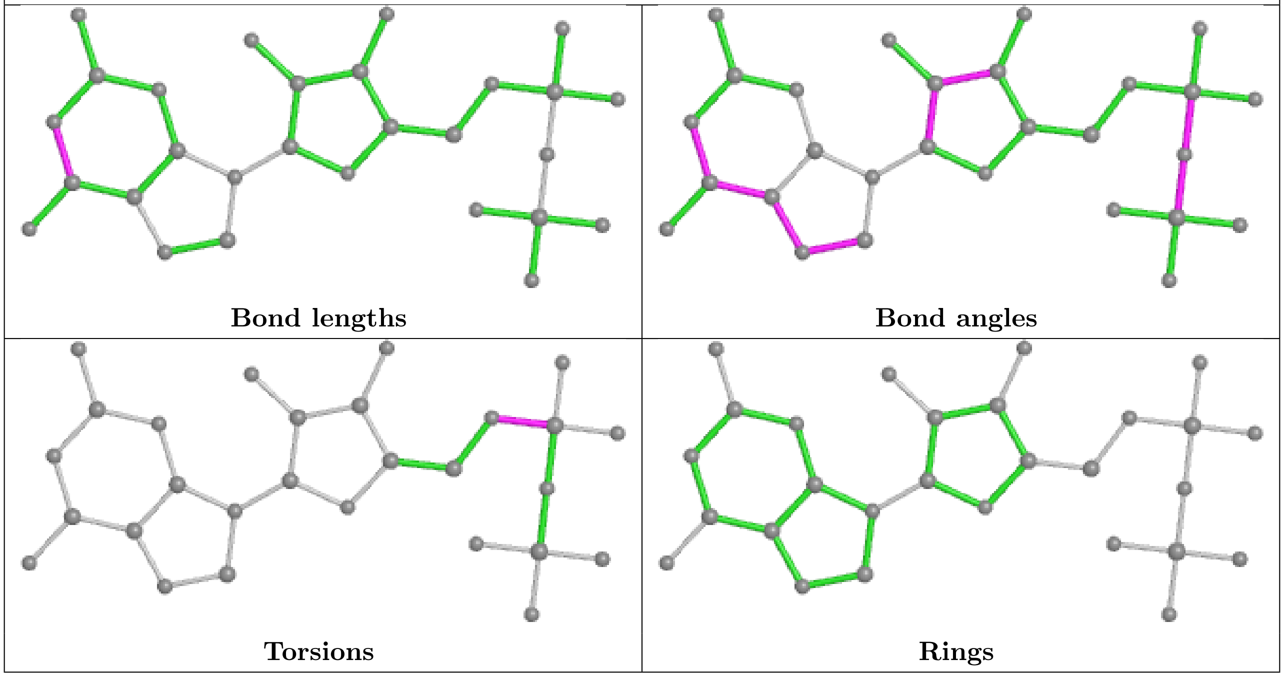
Bond angles



Torsions

Rings

Ligand GDP 1g 501



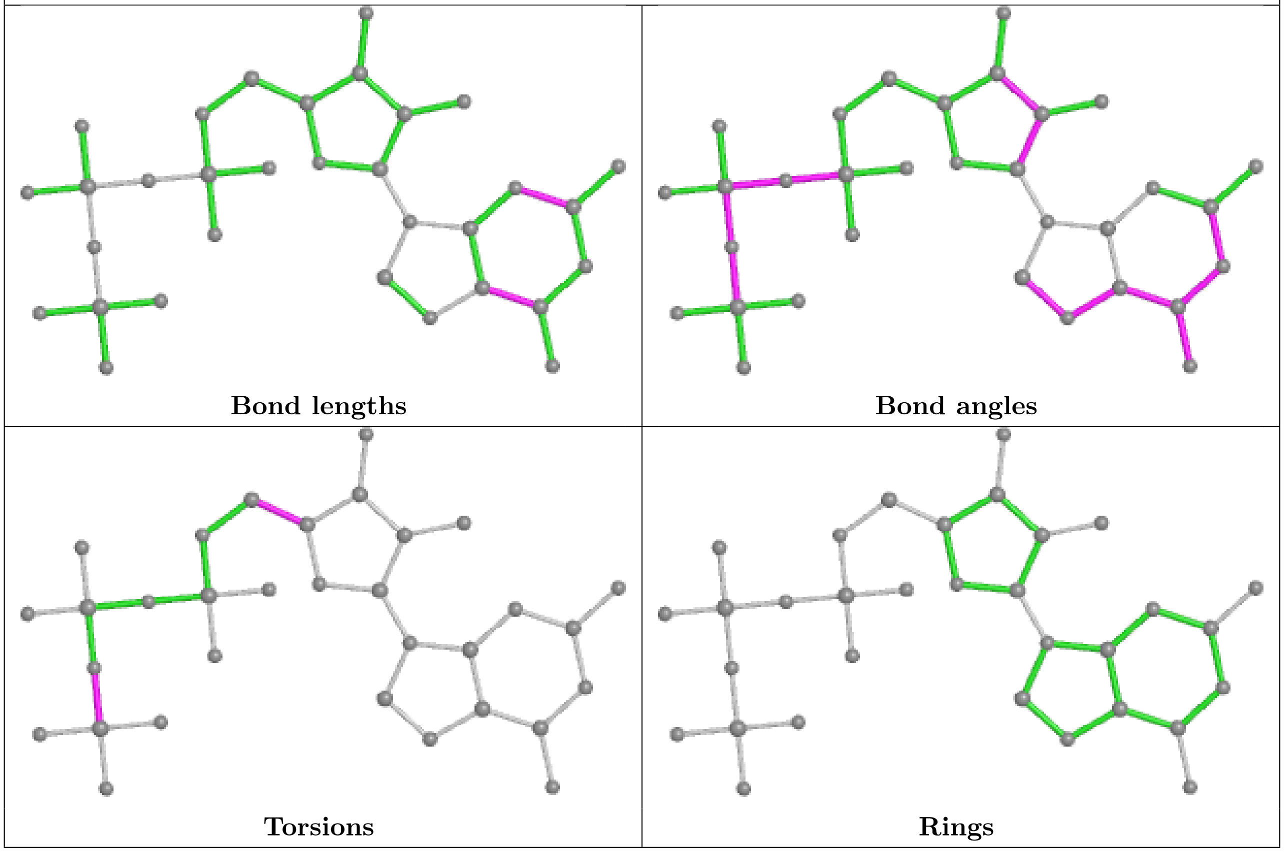
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP 9b 501



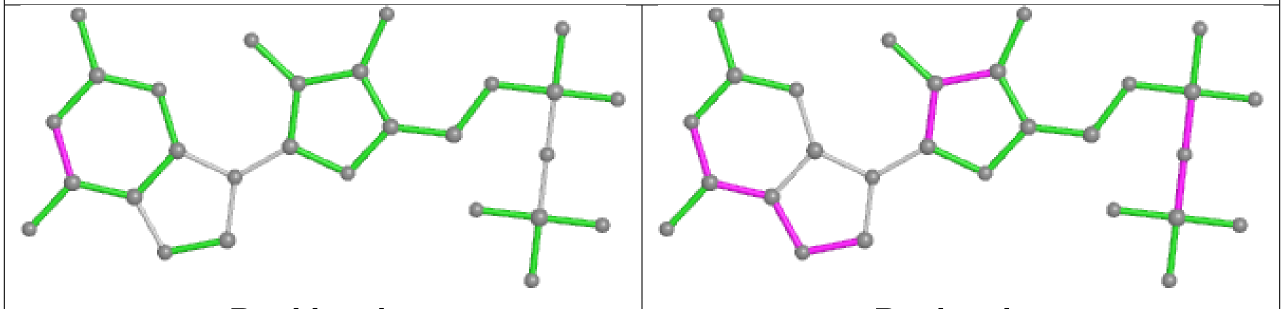
Bond lengths

Bond angles

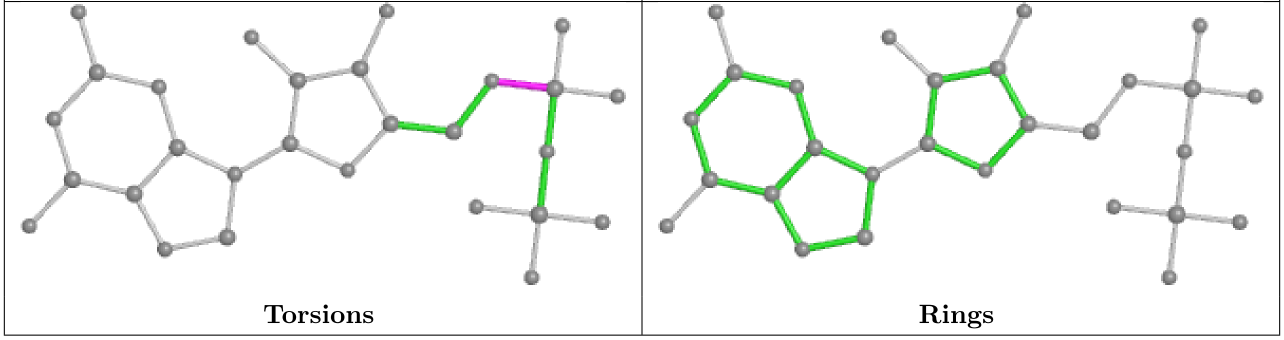
Torsions

Rings

Ligand GDP 1c 501

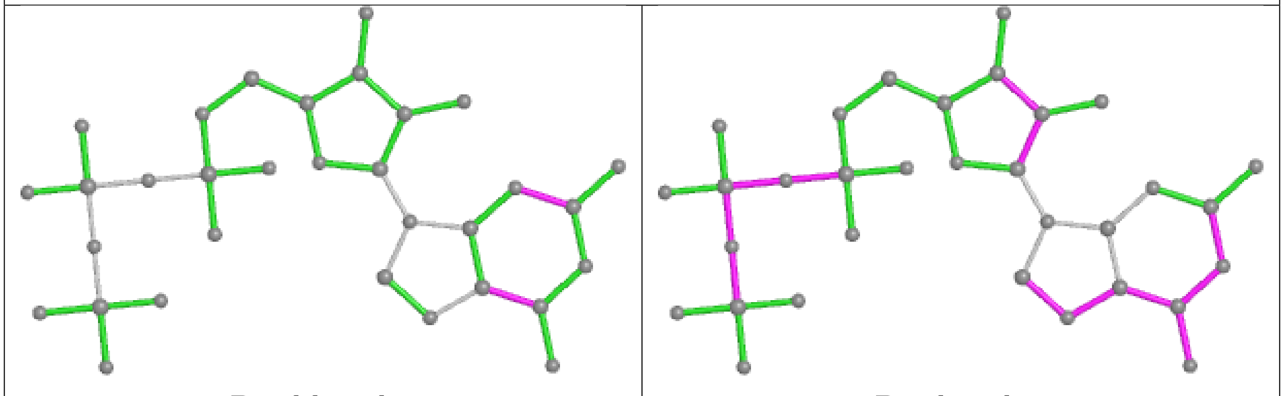


Bond lengths **Bond angles**

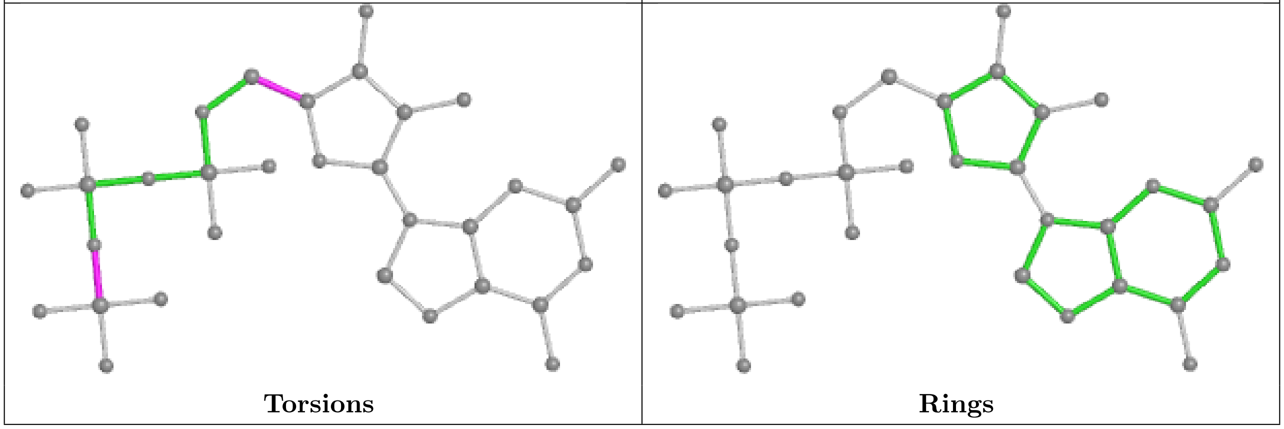


Torsions **Rings**

Ligand GTP Ad 501

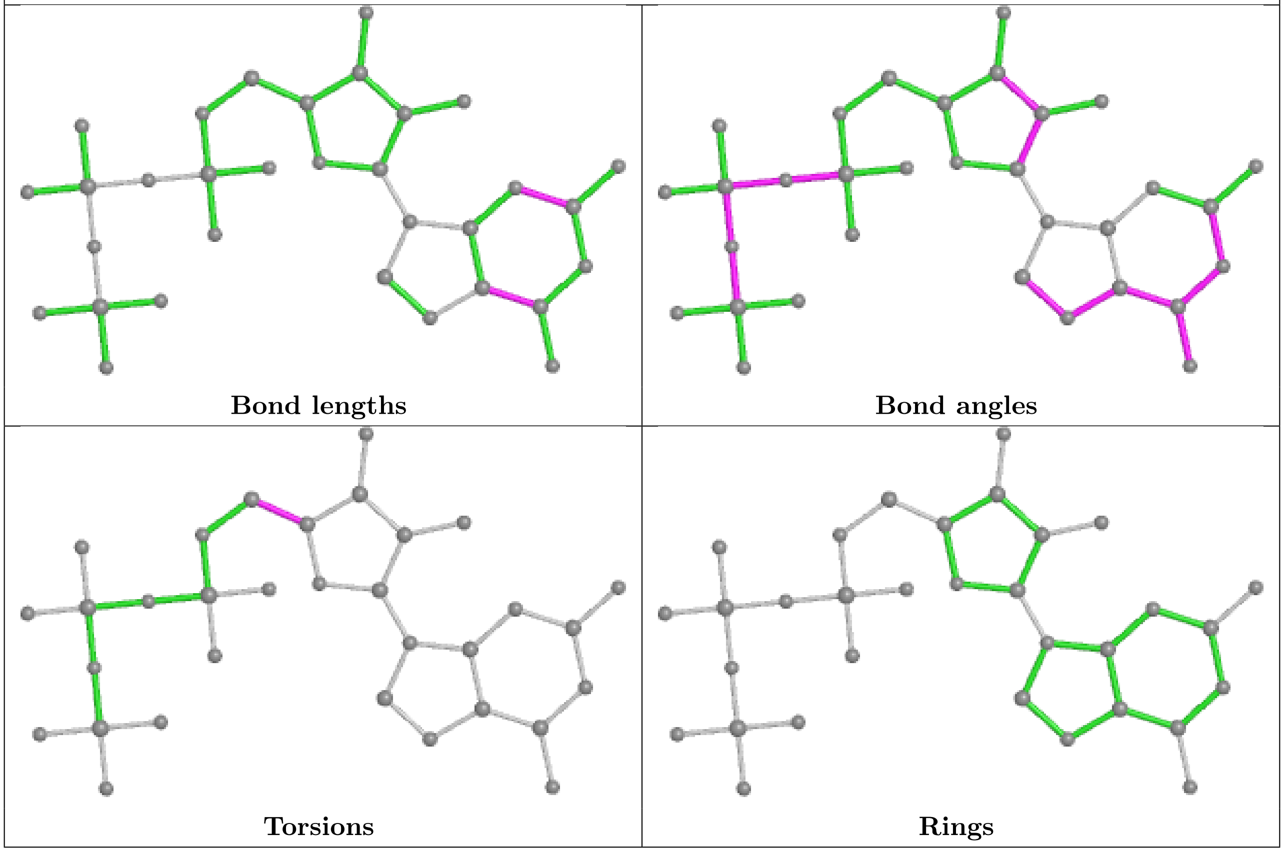


Bond lengths **Bond angles**



Torsions **Rings**

Ligand GTP 7f 501



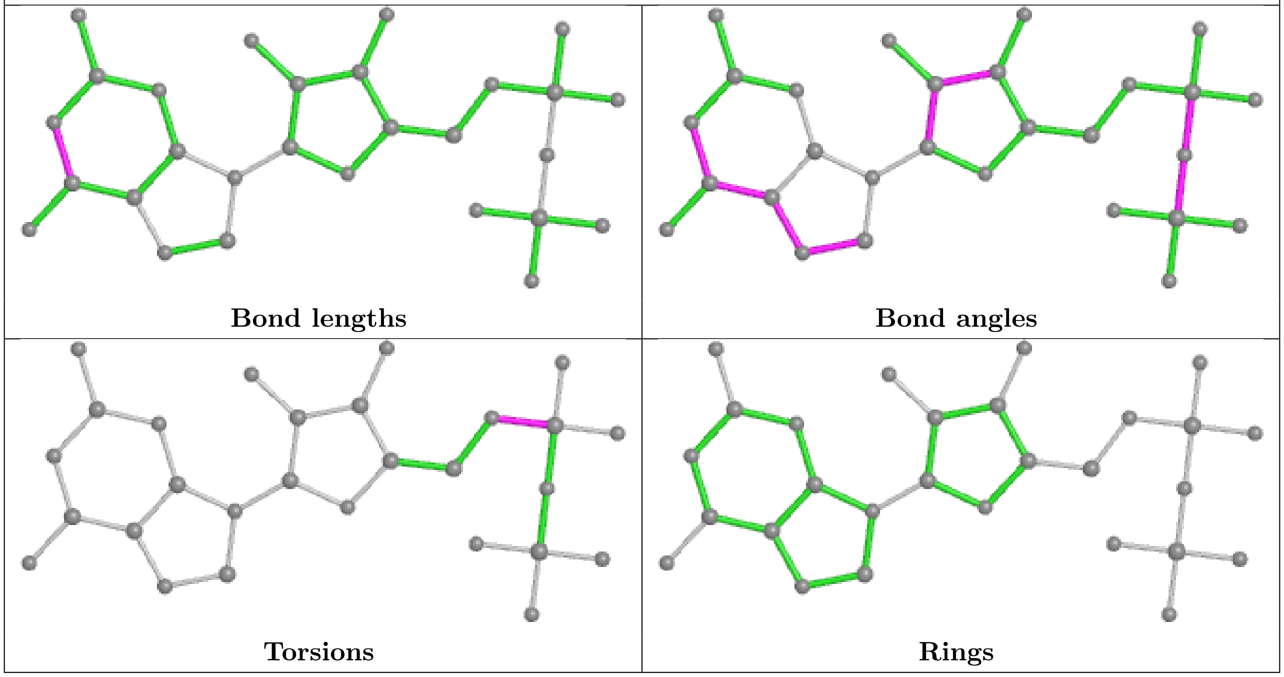
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP 4g 501



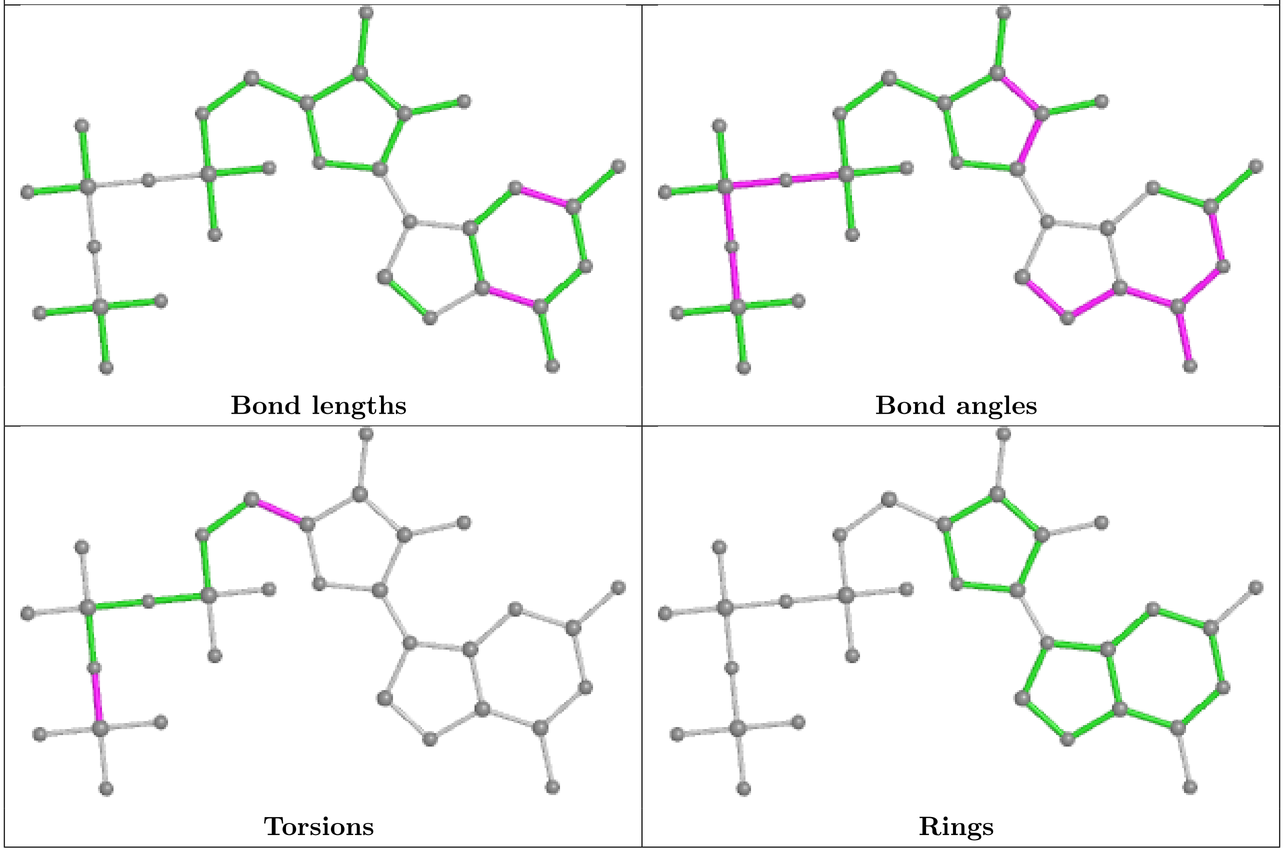
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP 9h 501



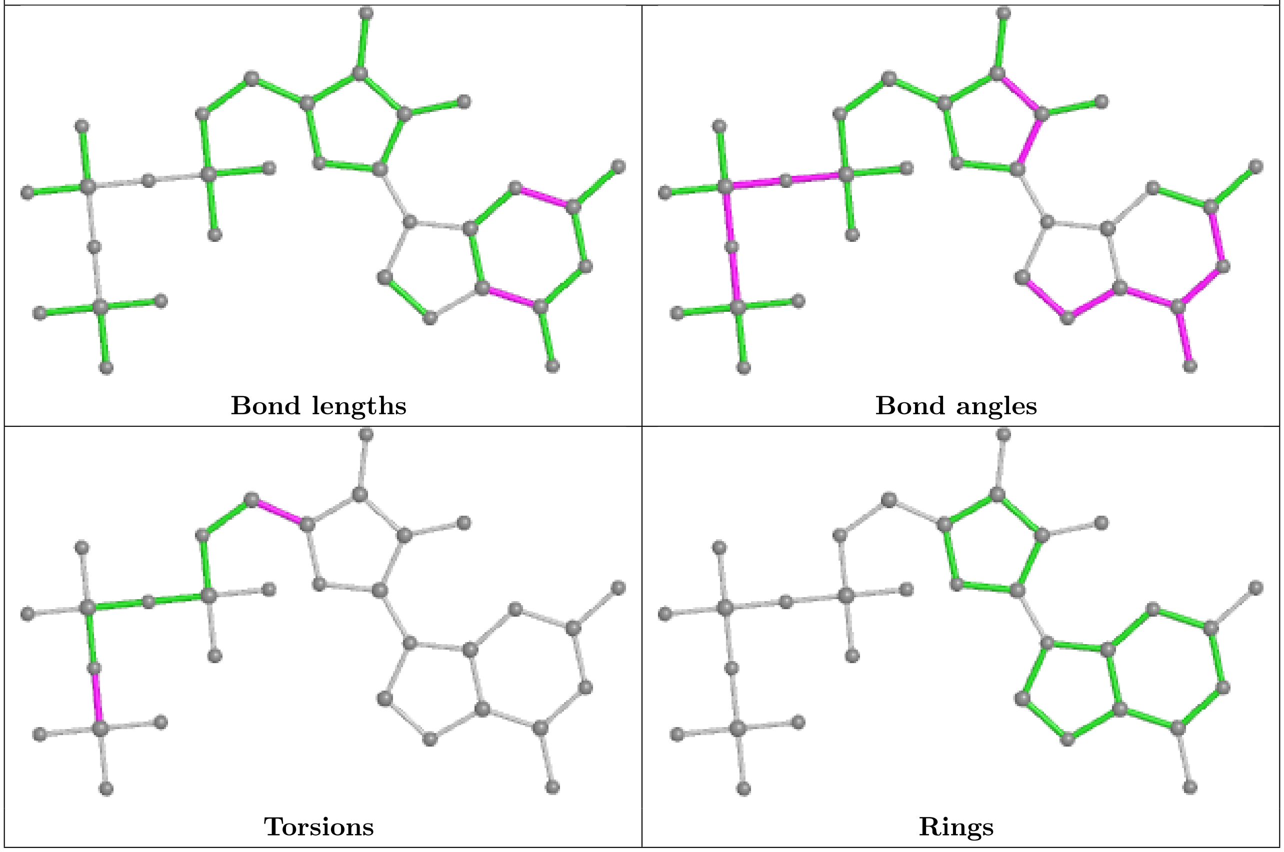
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP 1b 501



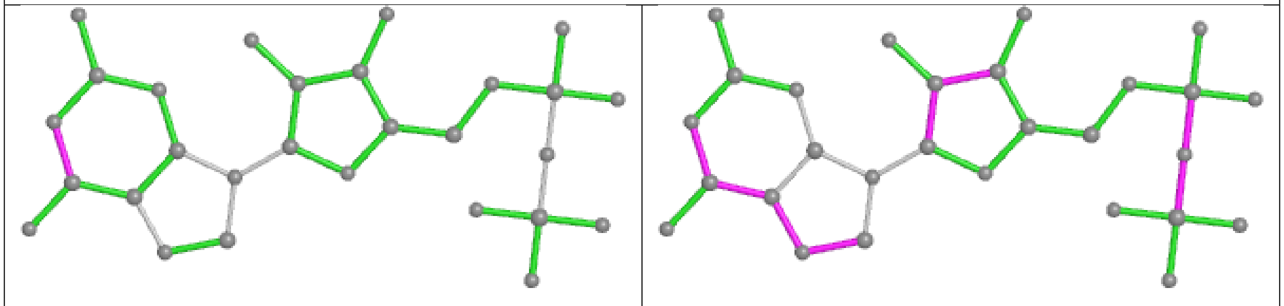
Bond lengths

Bond angles

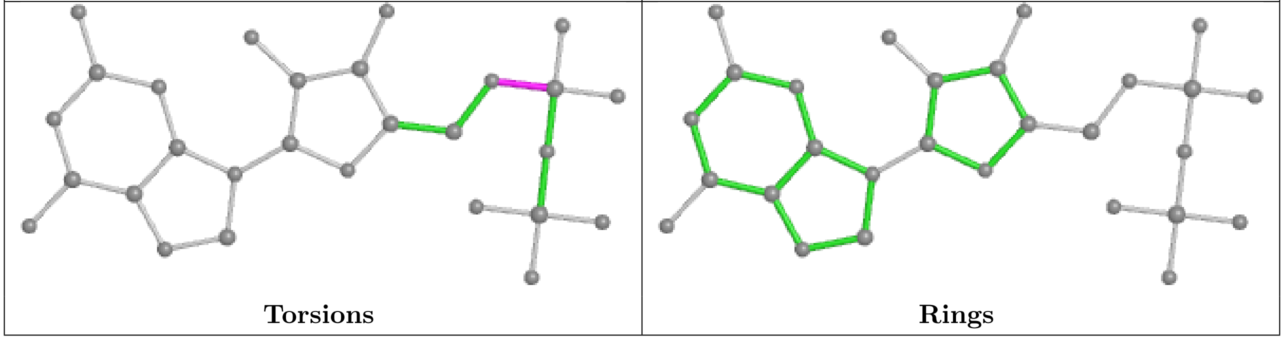
Torsions

Rings

Ligand GDP 6e 501

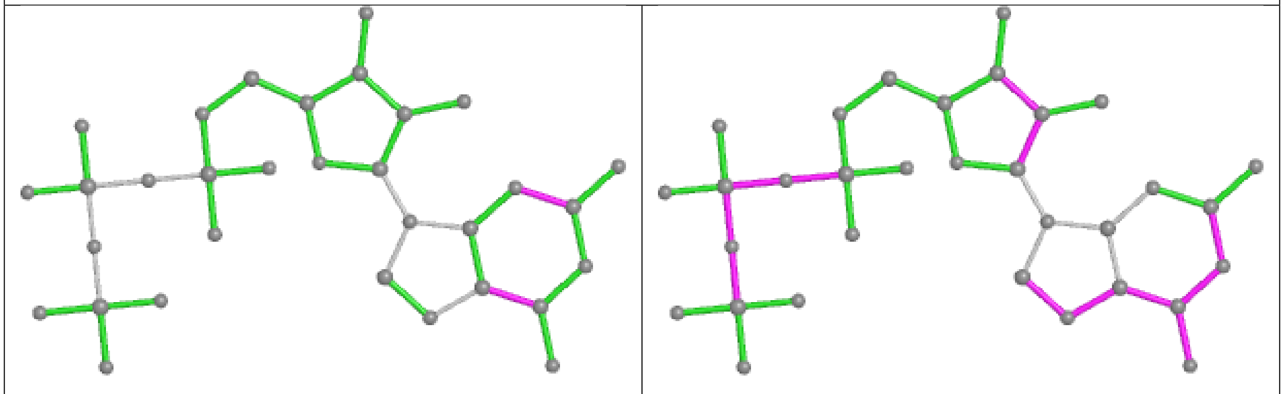


Bond lengths Bond angles

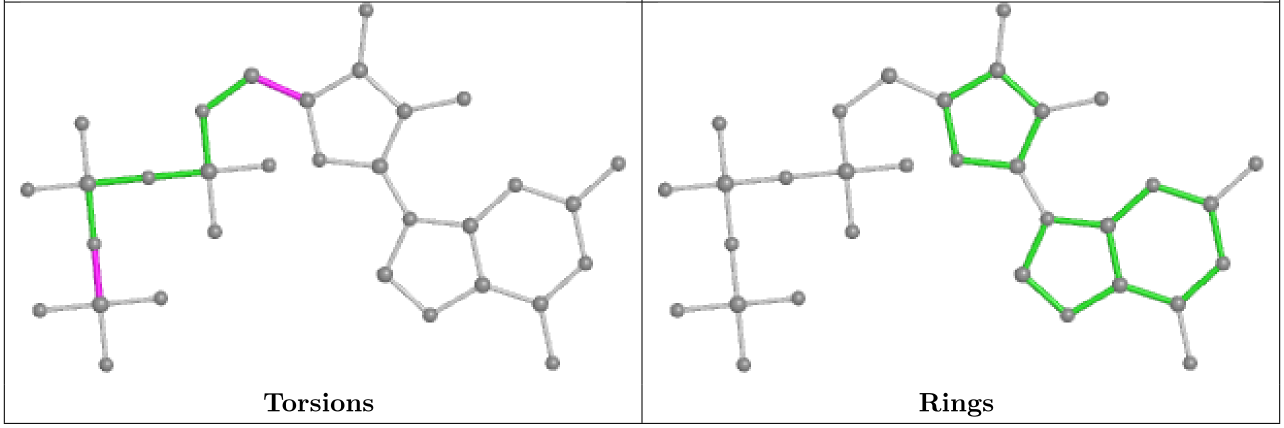


Torsions Rings

Ligand GTP Bb 501

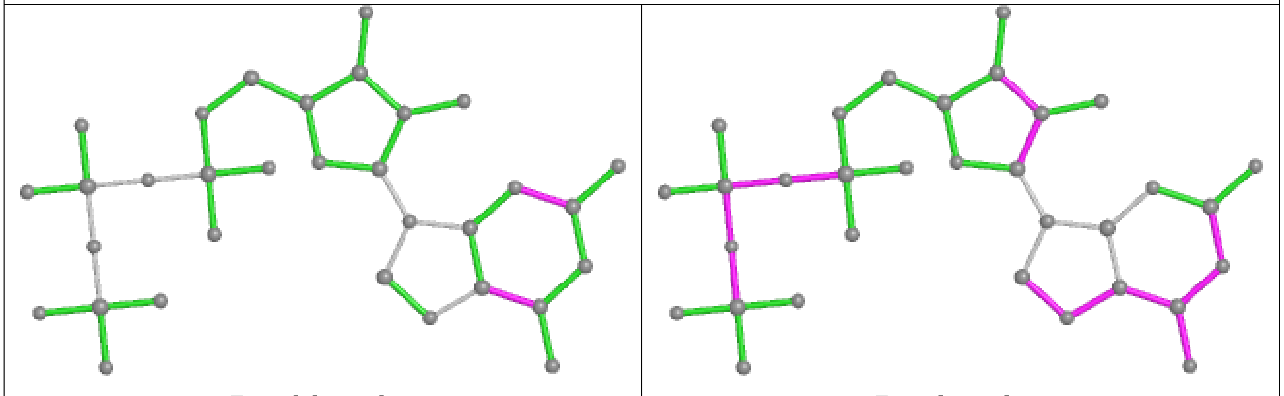


Bond lengths Bond angles



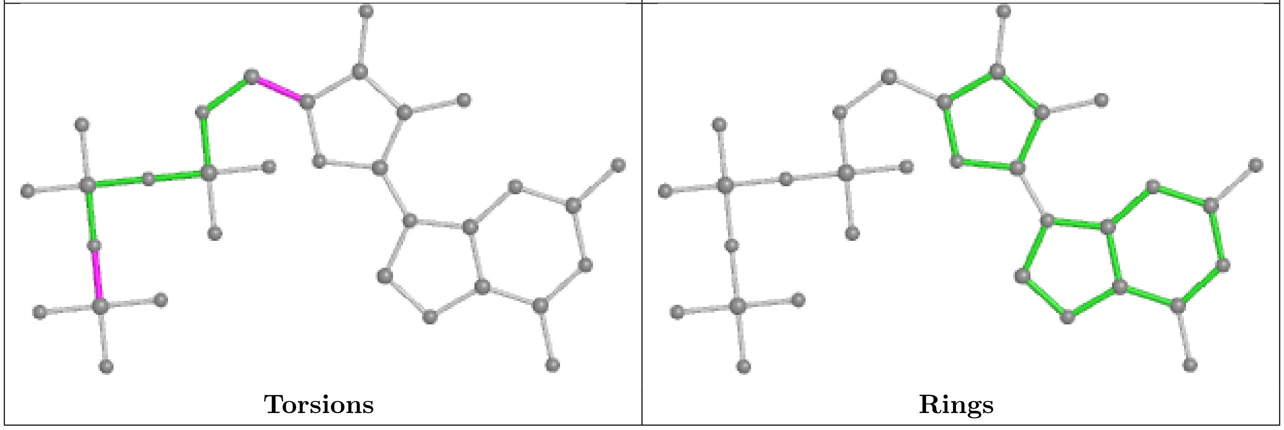
Torsions Rings

Ligand GTP 8d 501



Bond lengths

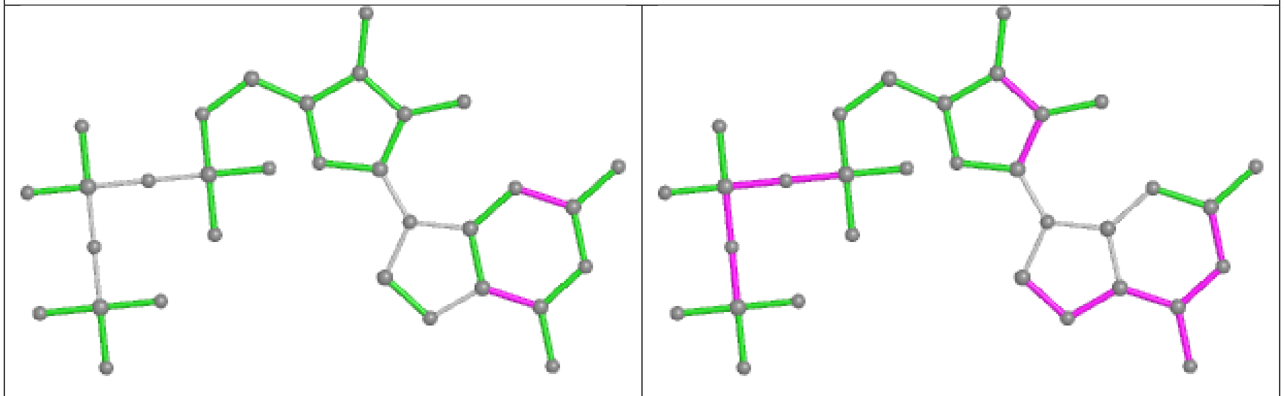
Bond angles



Torsions

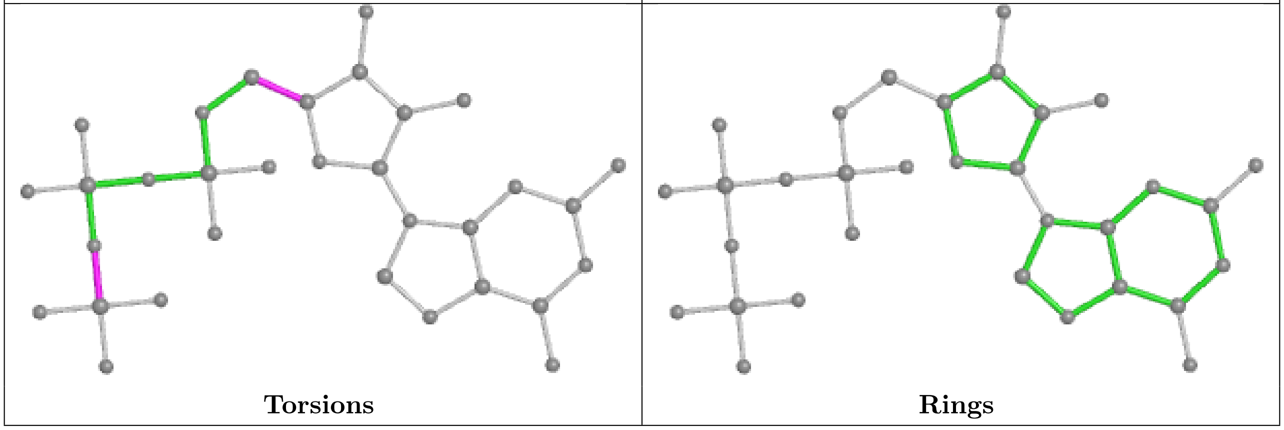
Rings

Ligand GTP Cb 501



Bond lengths

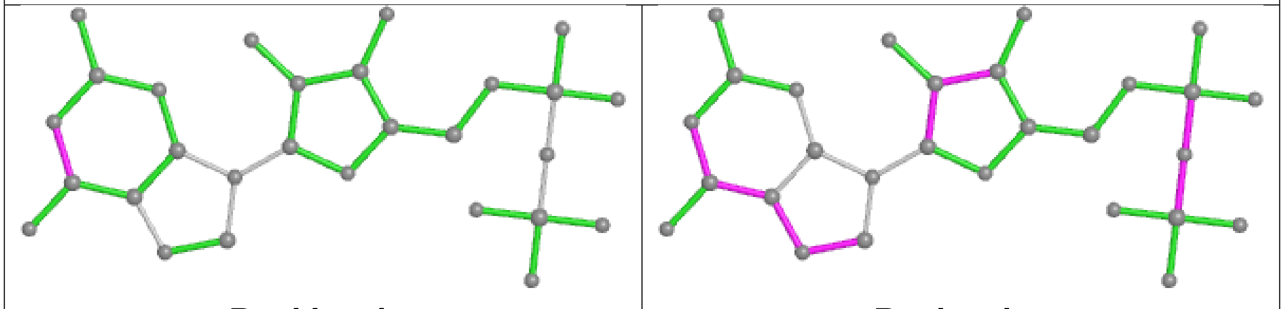
Bond angles



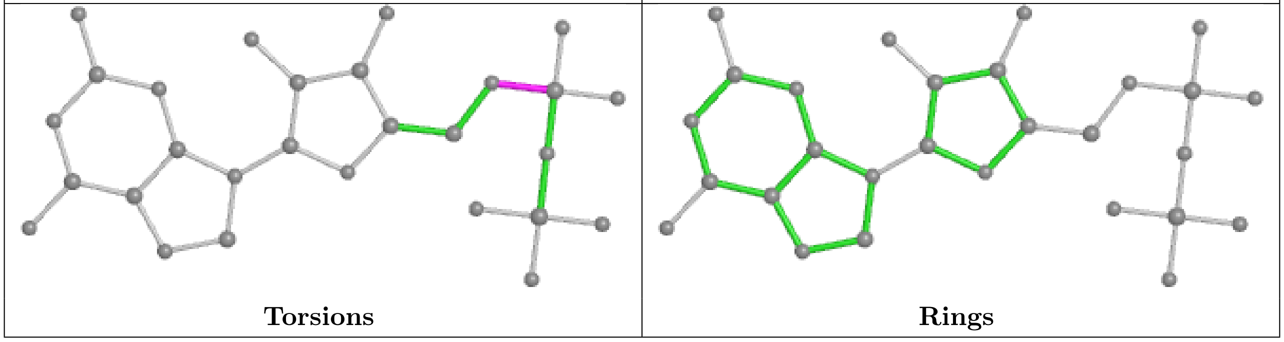
Torsions

Rings

Ligand GDP 5e 501

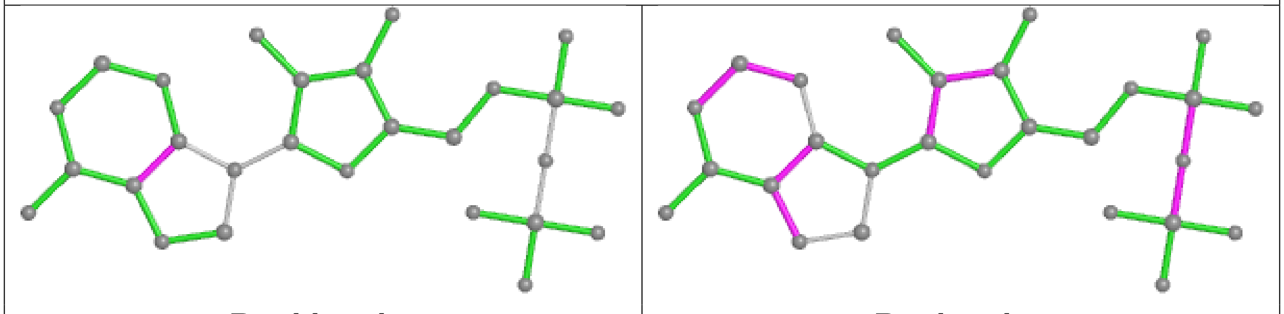


Bond lengths Bond angles

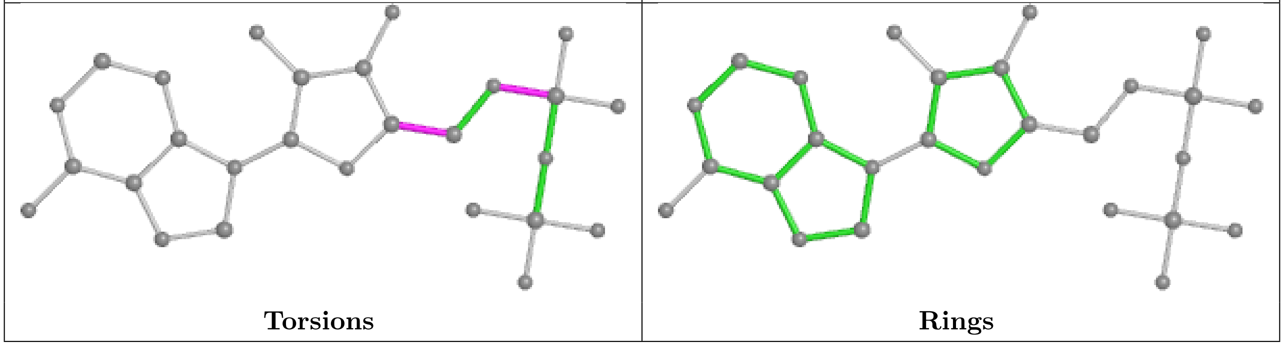


Torsions Rings

Ligand ADP 0X 801

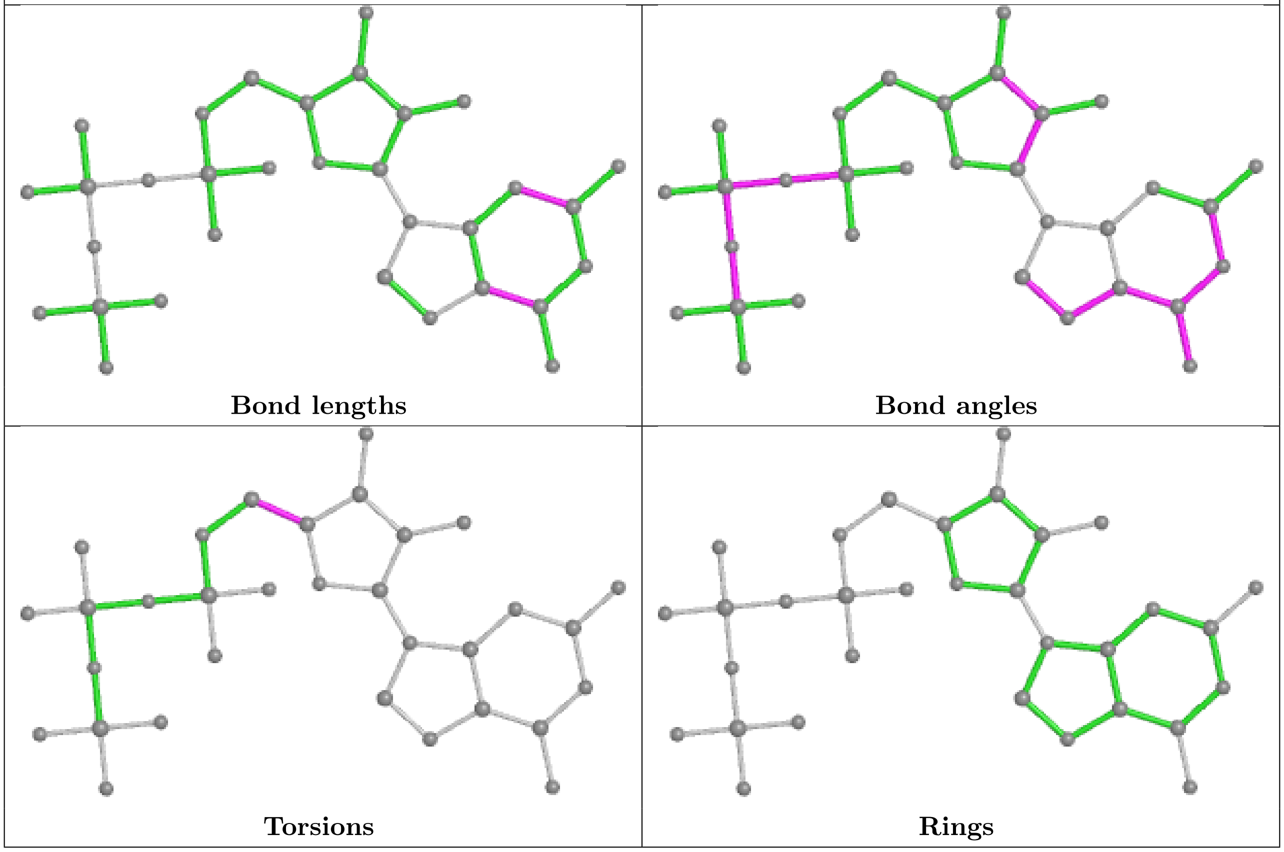


Bond lengths Bond angles

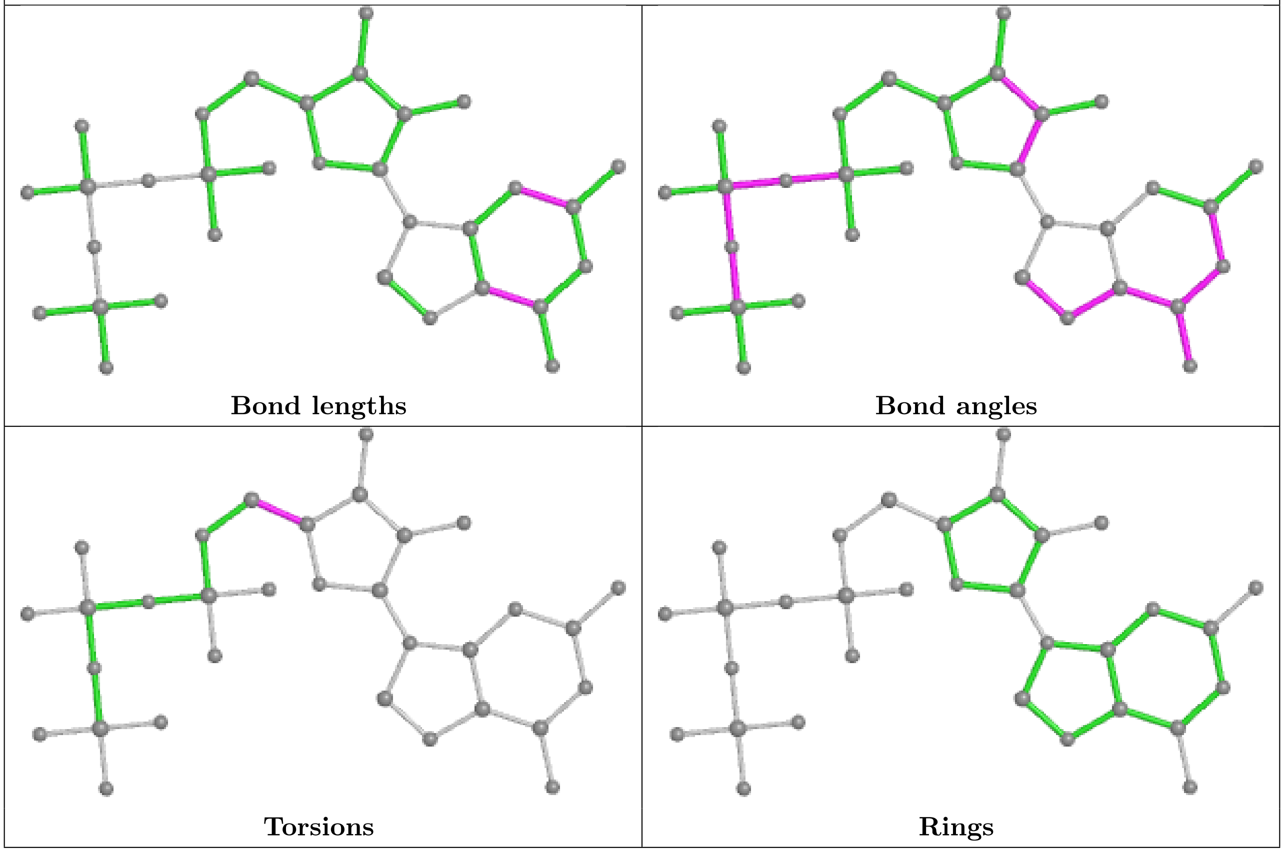


Torsions Rings

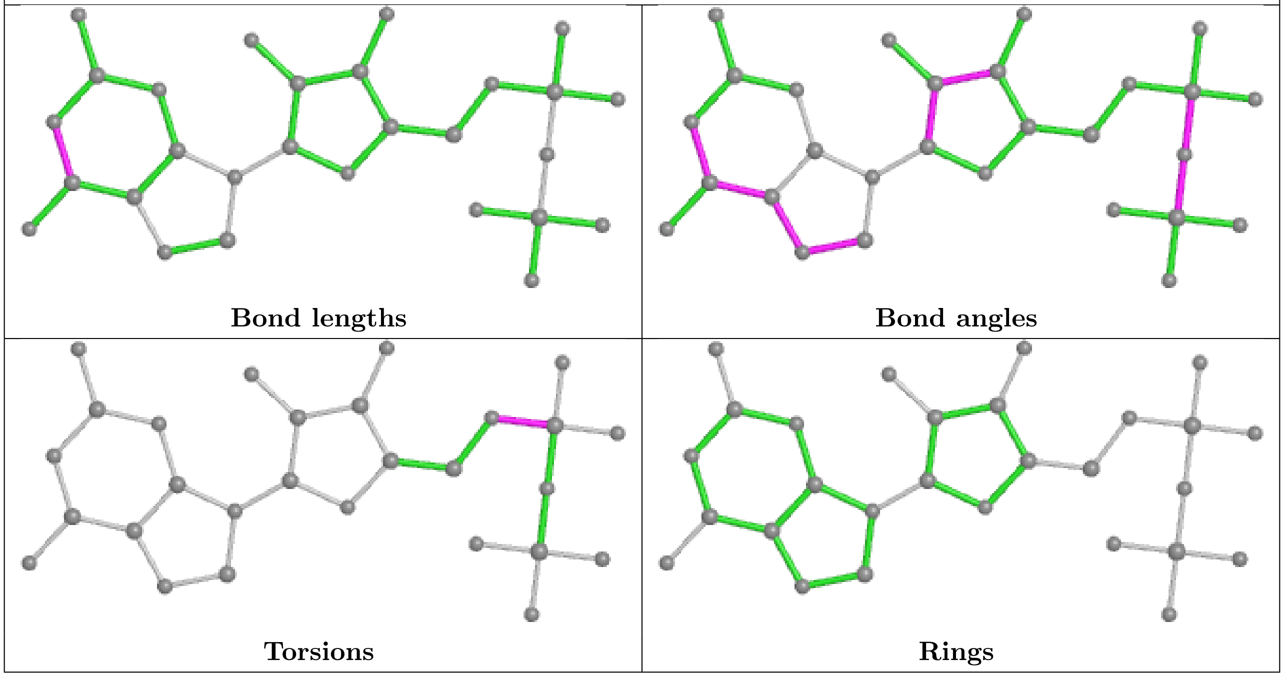
Ligand GTP Bd 501


Bond lengths
Bond angles
Torsions
Rings

Ligand GTP Dd 501


Bond lengths
Bond angles
Torsions
Rings

Ligand GDP Ba 501



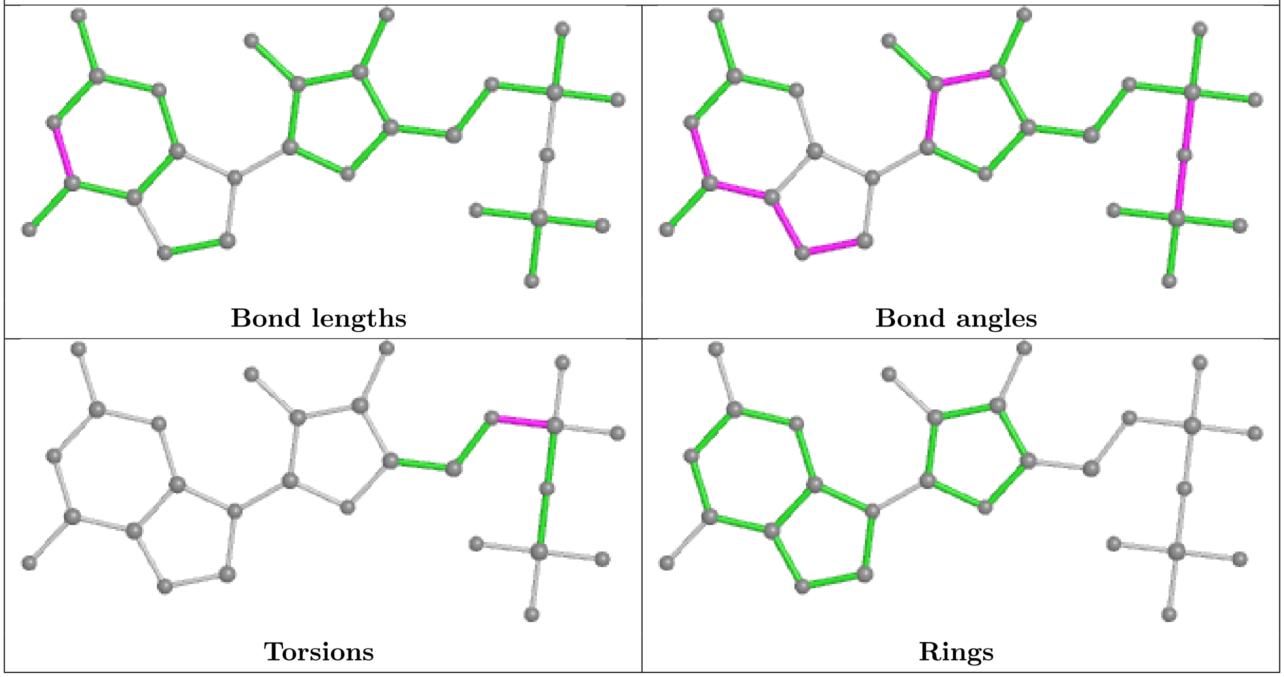
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP 3e 501



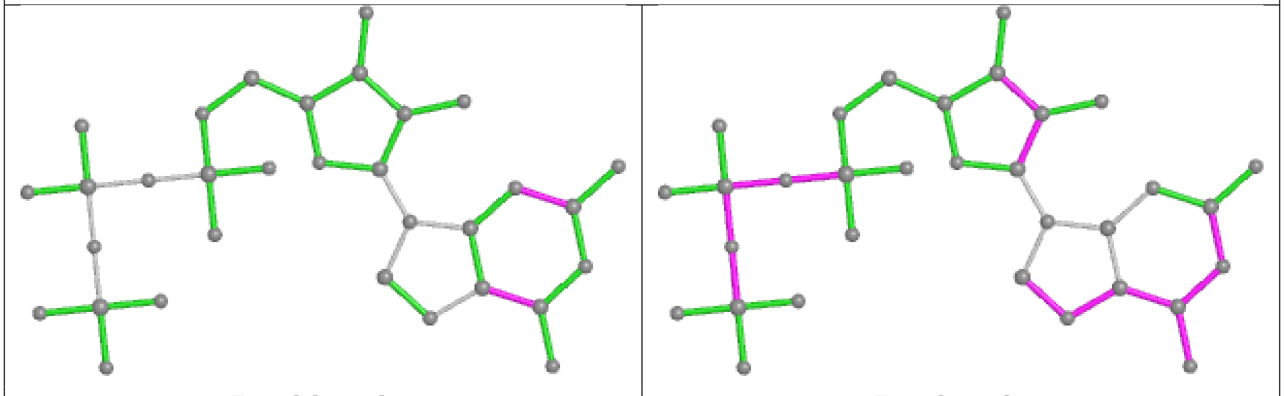
Bond lengths

Bond angles

Torsions

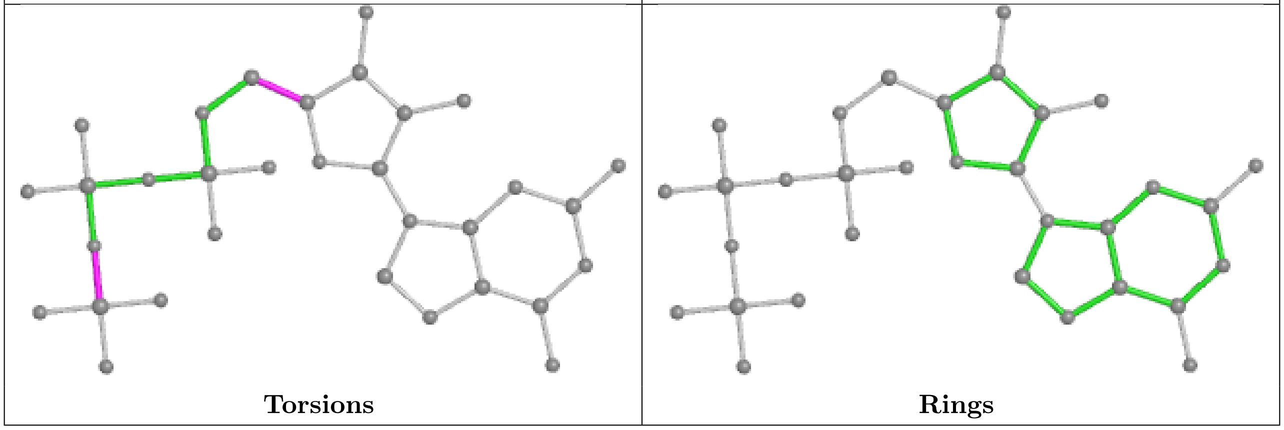
Rings

Ligand GTP 2f 501



Bond lengths

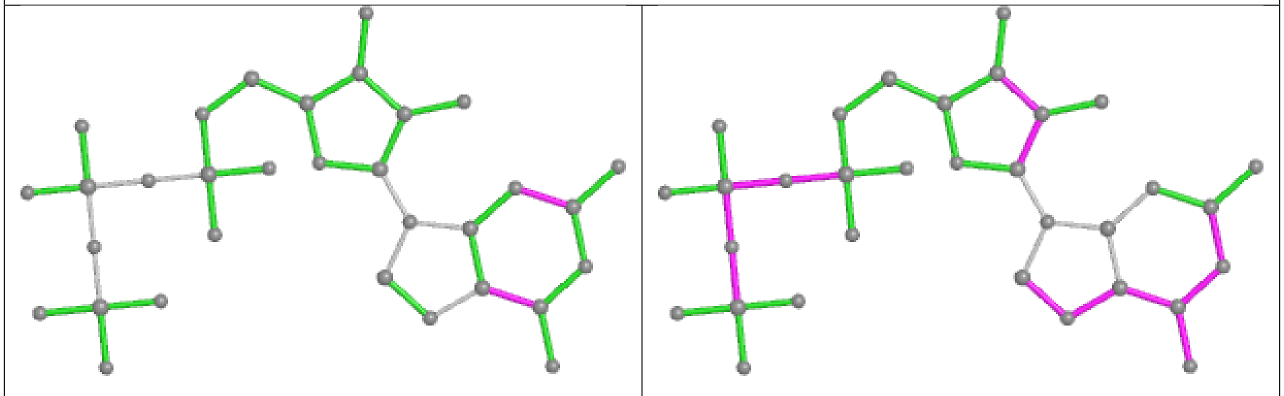
Bond angles



Torsions

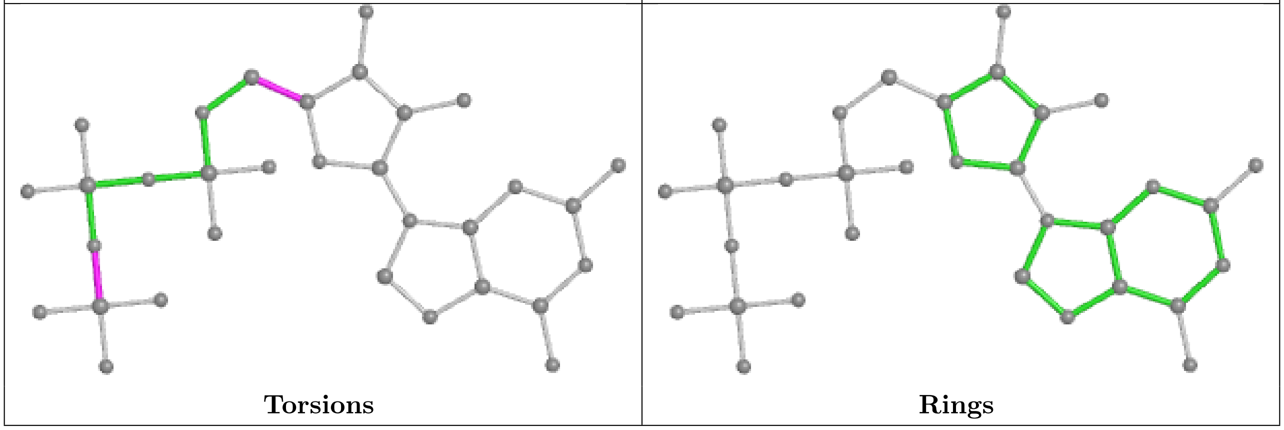
Rings

Ligand GTP 7d 501



Bond lengths

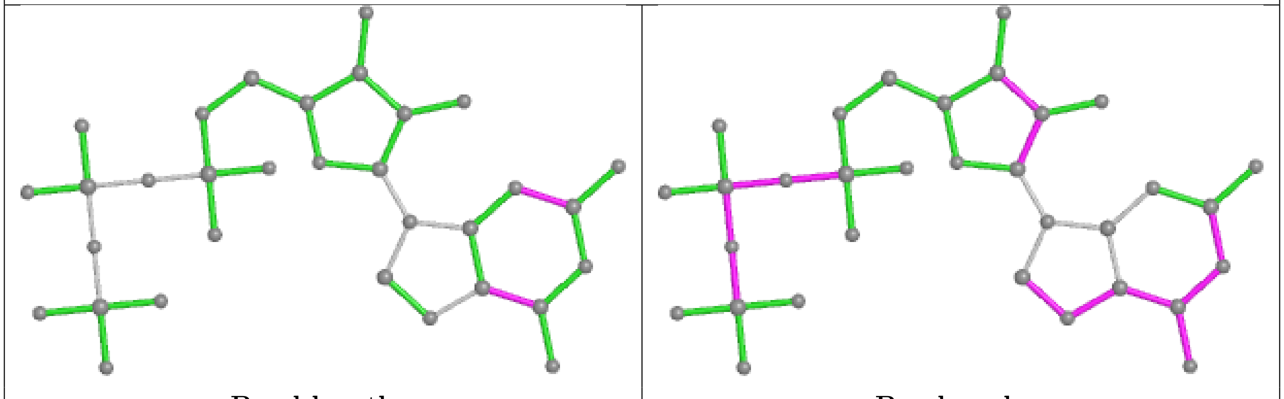
Bond angles



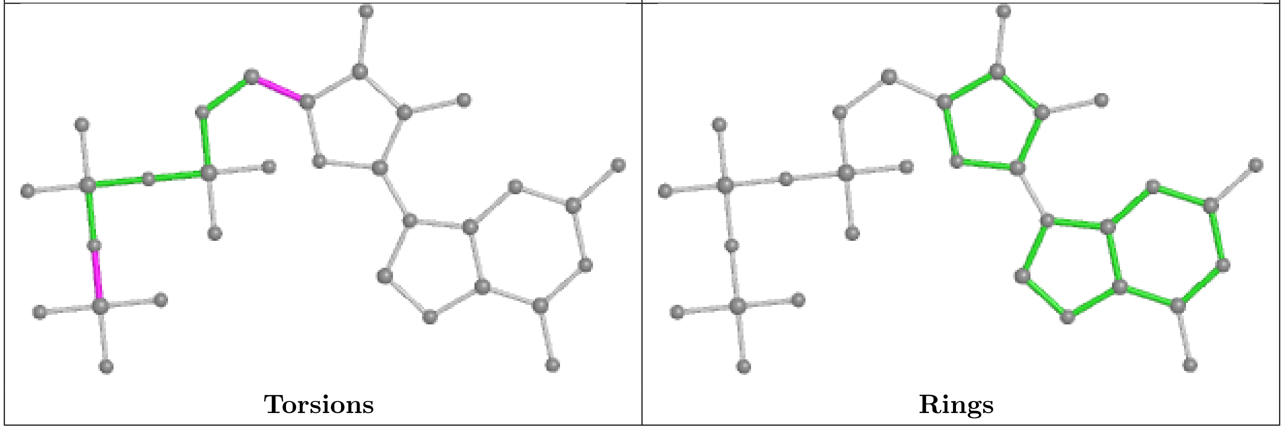
Torsions

Rings

Ligand GTP 8h 501

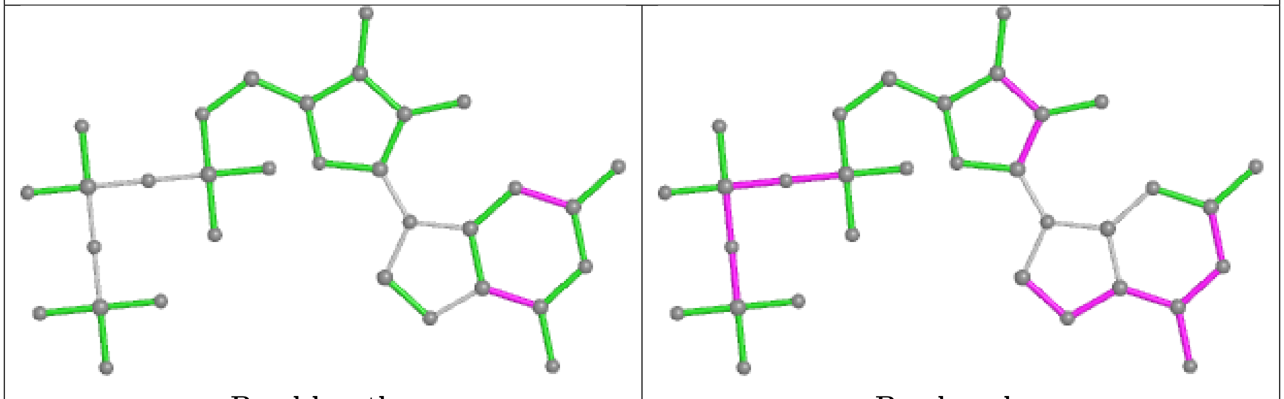


Bond lengths Bond angles

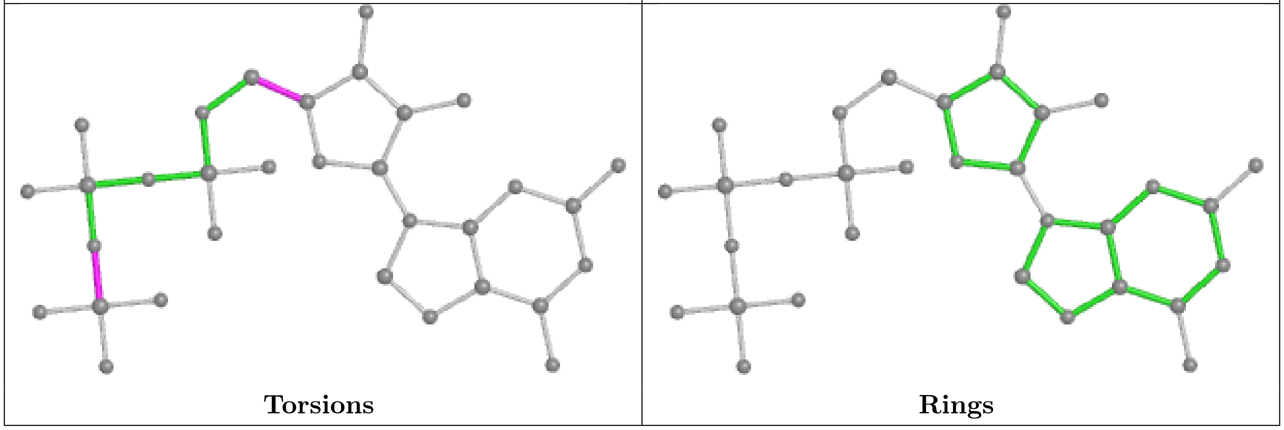


Torsions Rings

Ligand GTP Ch 501

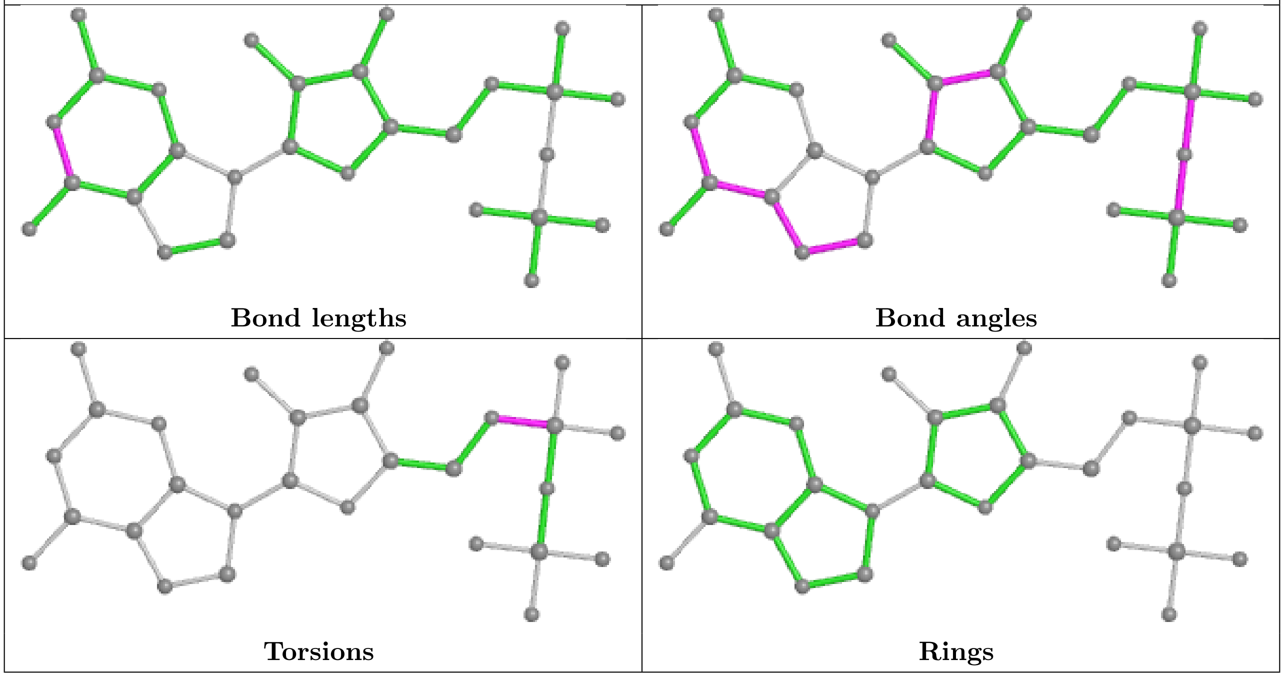


Bond lengths Bond angles

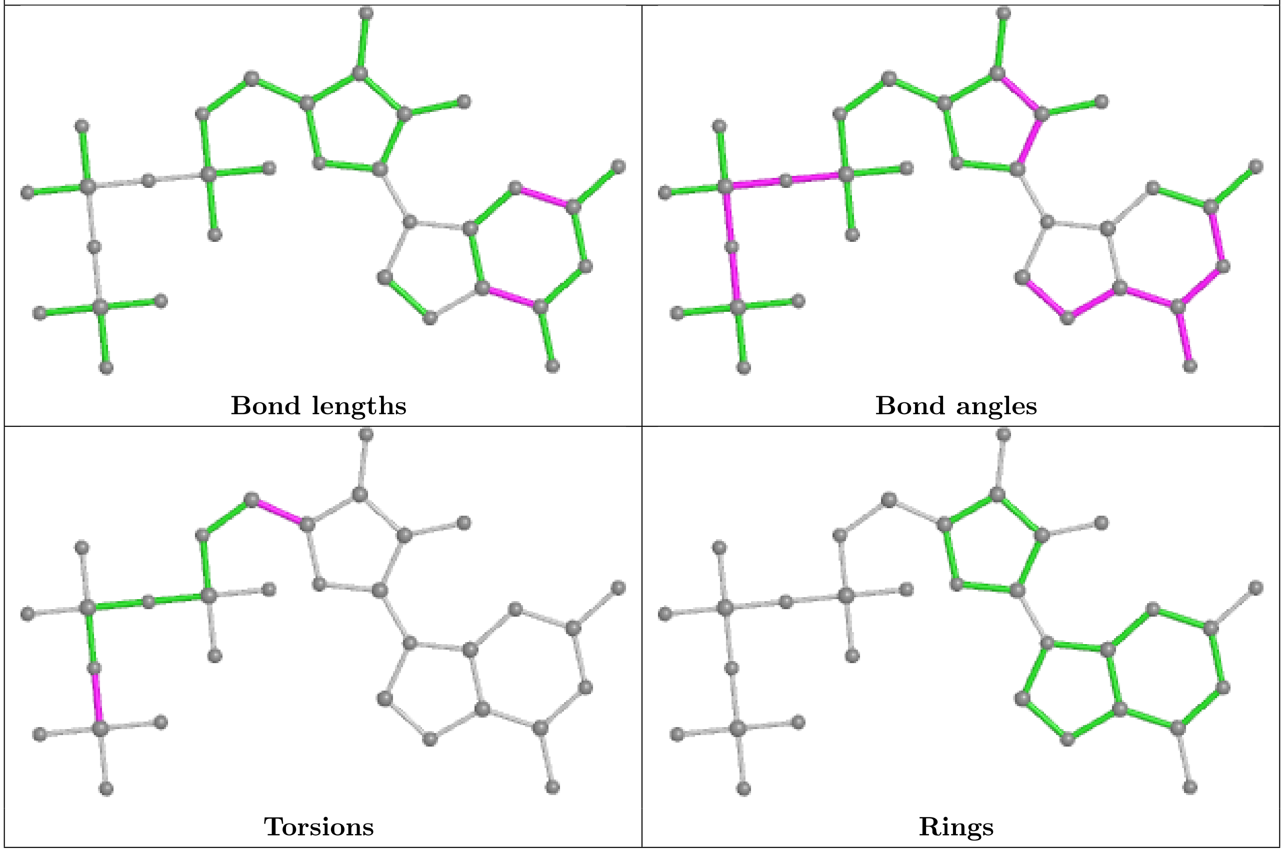


Torsions Rings

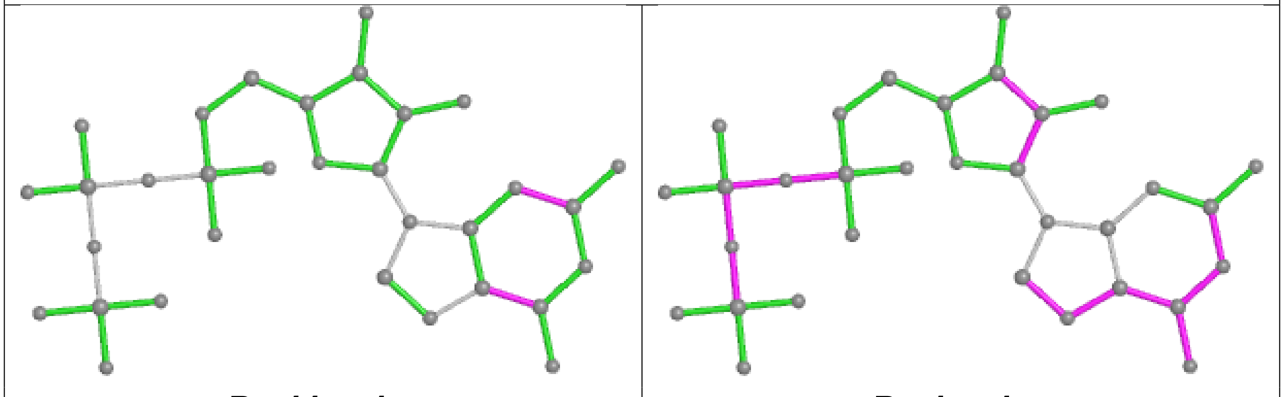
Ligand GDP Dg 501



Ligand GTP 4b 501

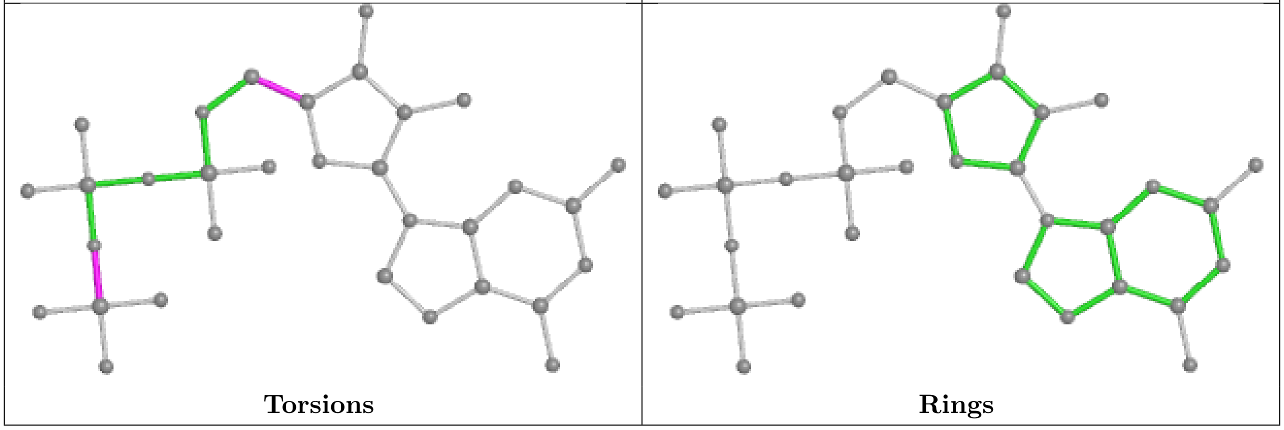


Ligand GTP 7h 501



Bond lengths

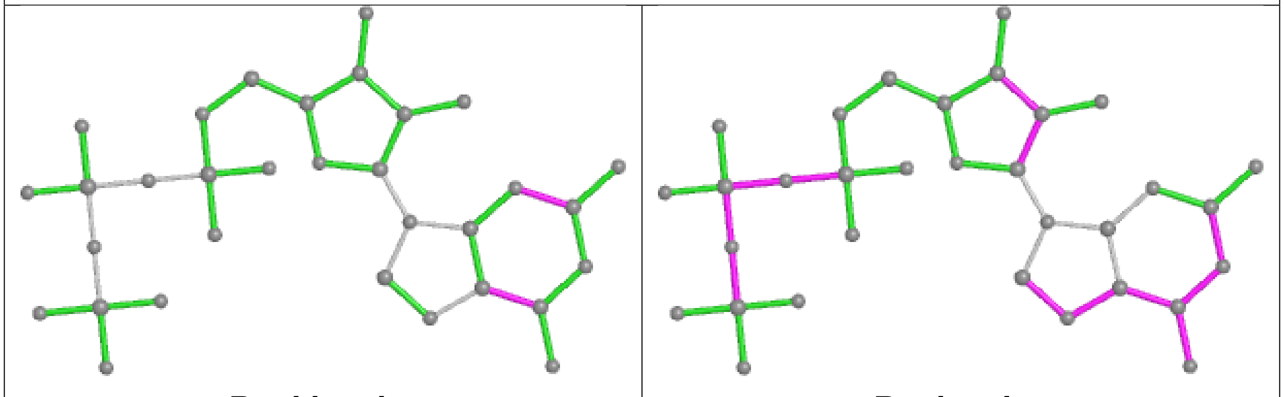
Bond angles



Torsions

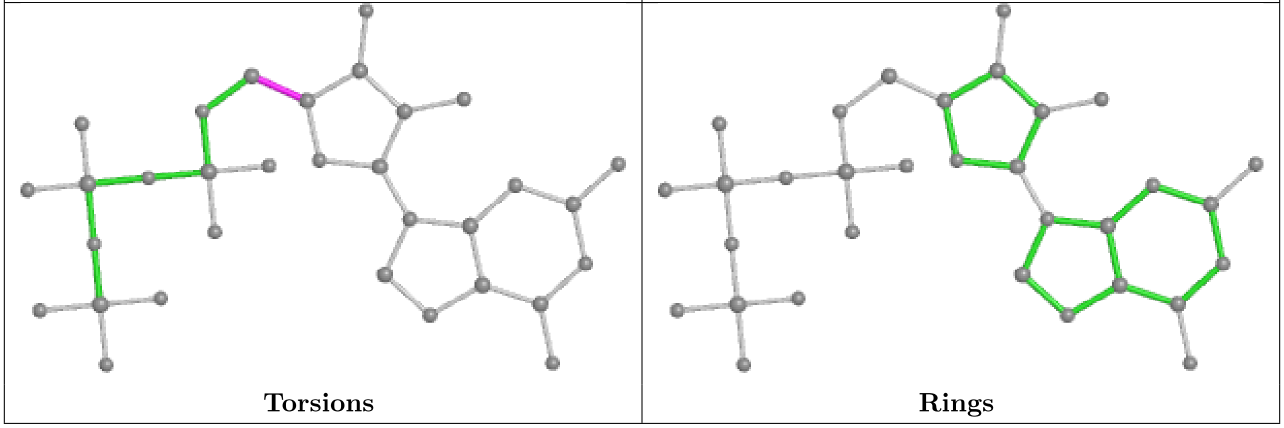
Rings

Ligand GTP 2h 501



Bond lengths

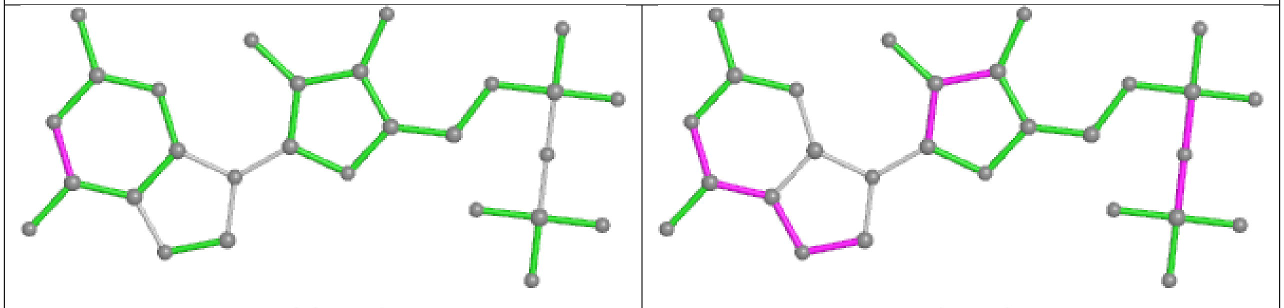
Bond angles



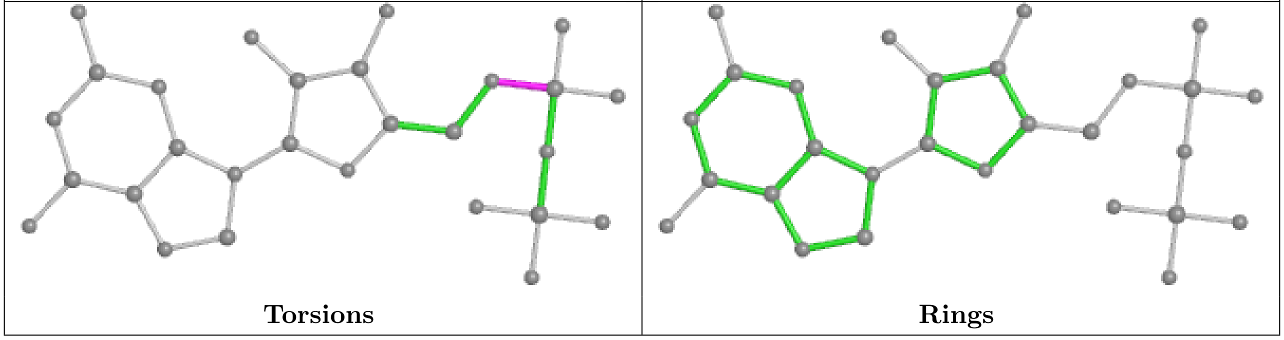
Torsions

Rings

Ligand GDP 7c 501

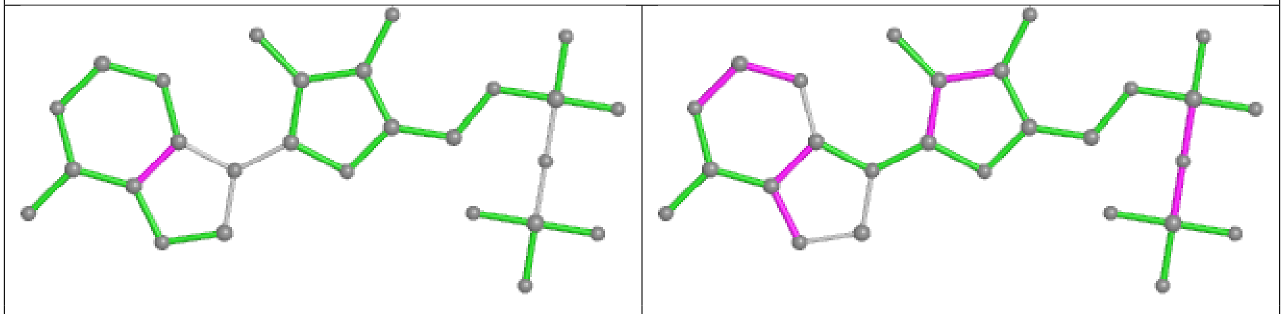


Bond lengths Bond angles

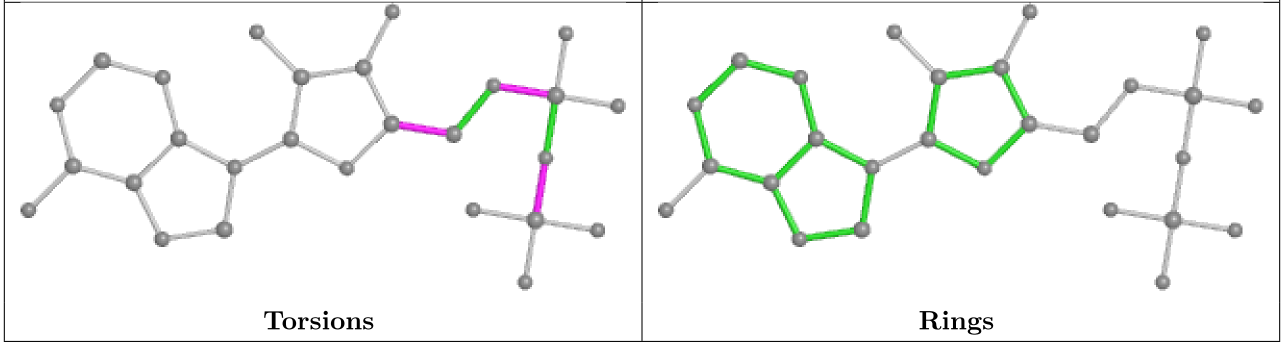


Torsions Rings

Ligand ADP 0Y 801

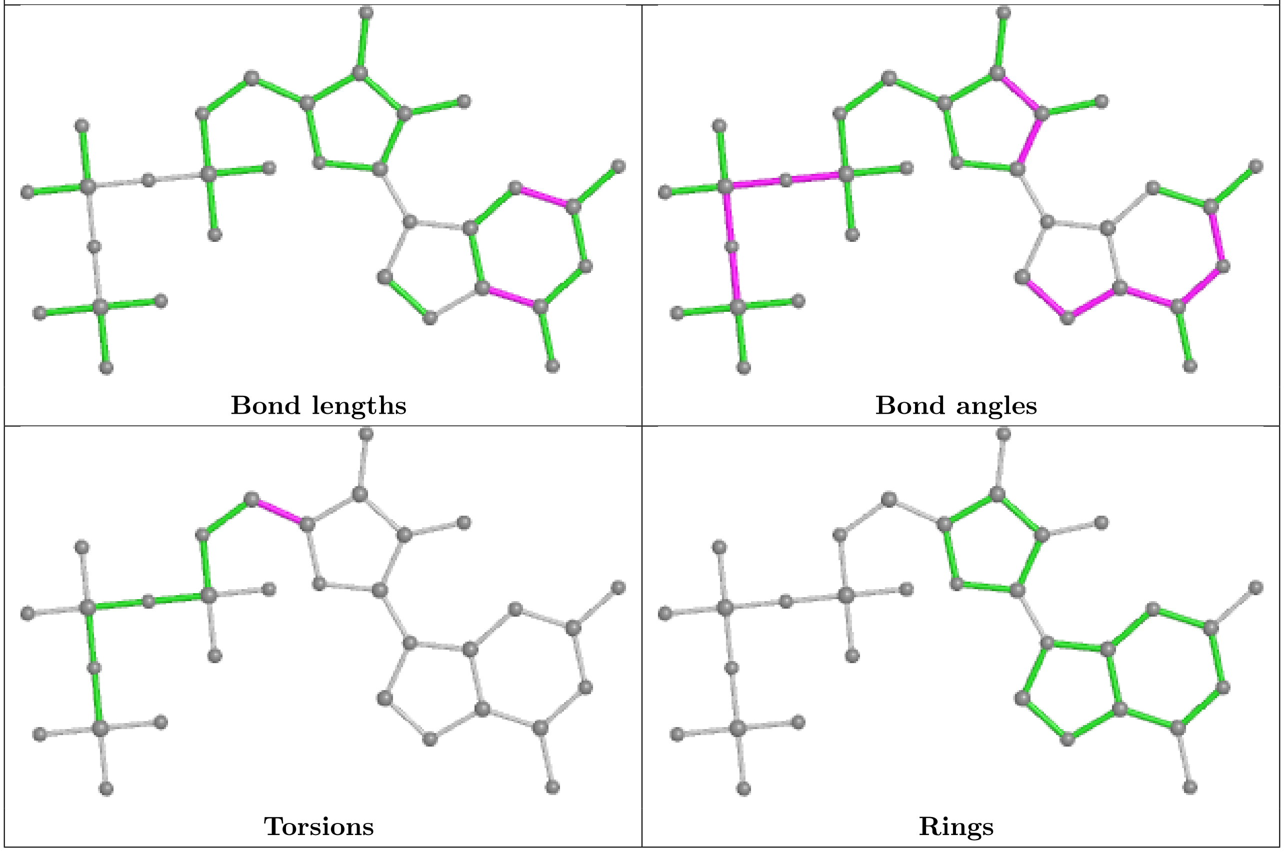


Bond lengths Bond angles

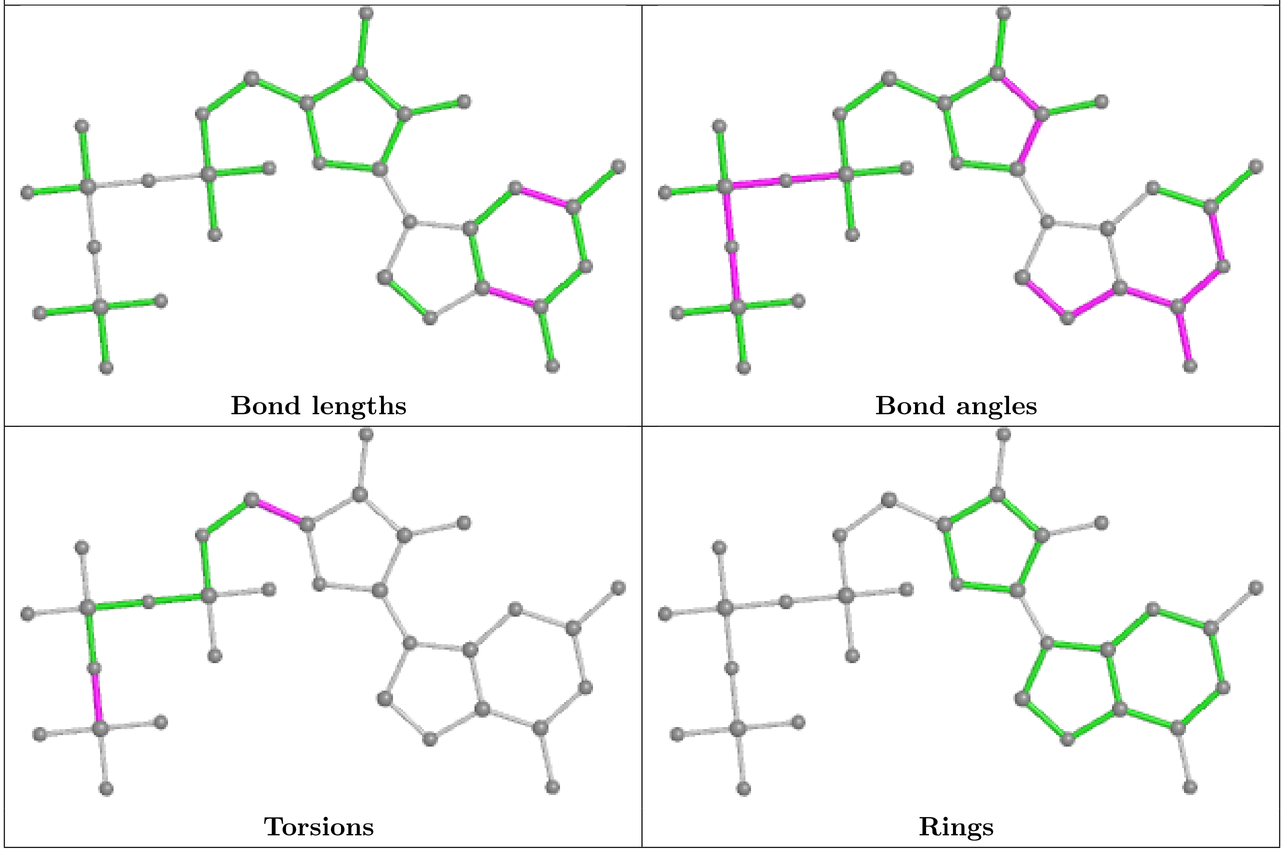


Torsions Rings

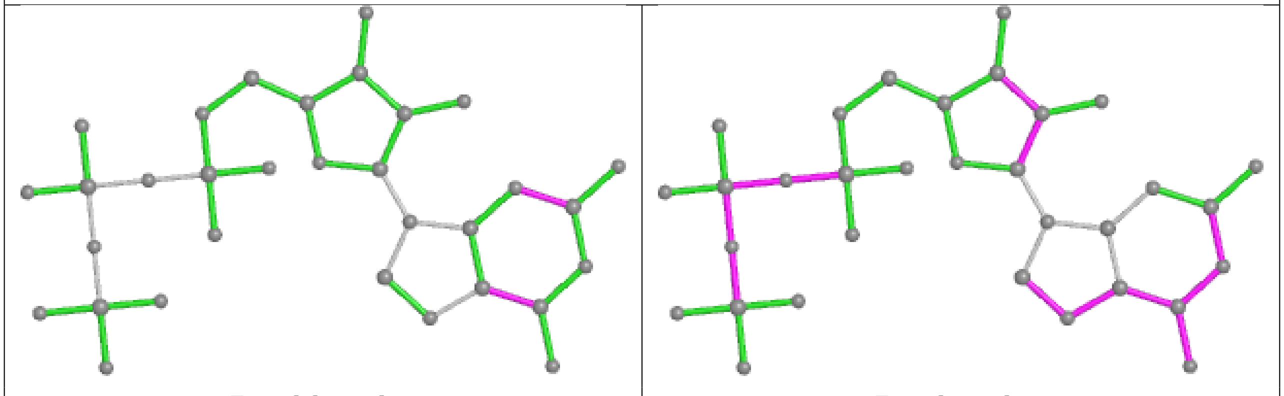
Ligand GTP 1h 501



Ligand GTP 4d 501

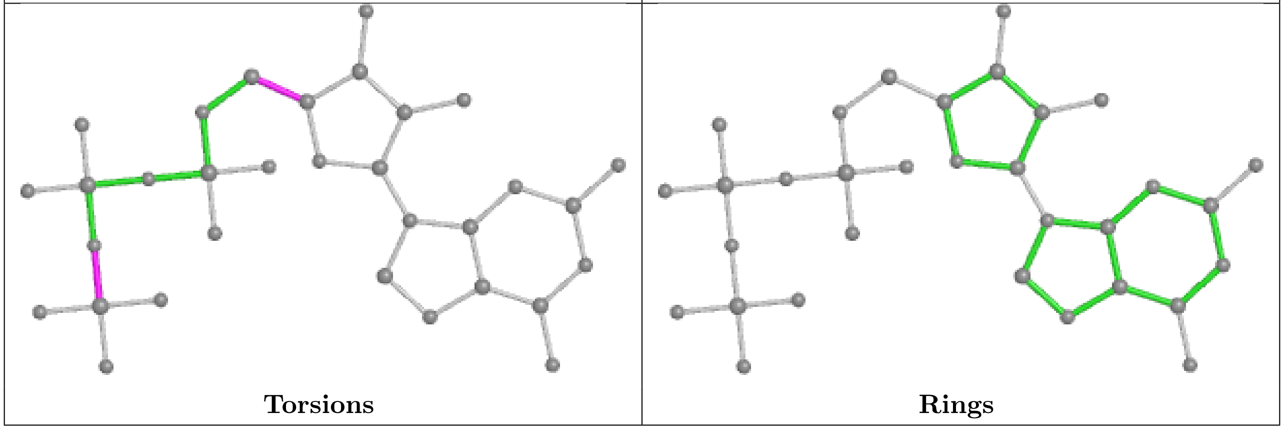


Ligand GTP 4f 501



Bond lengths

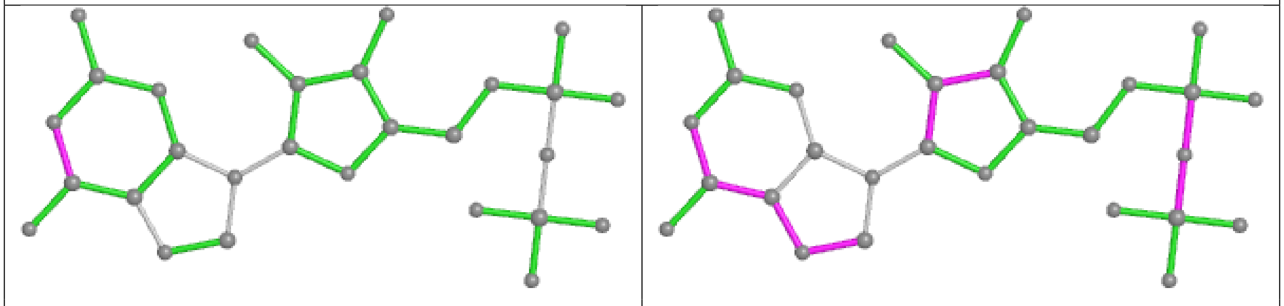
Bond angles



Torsions

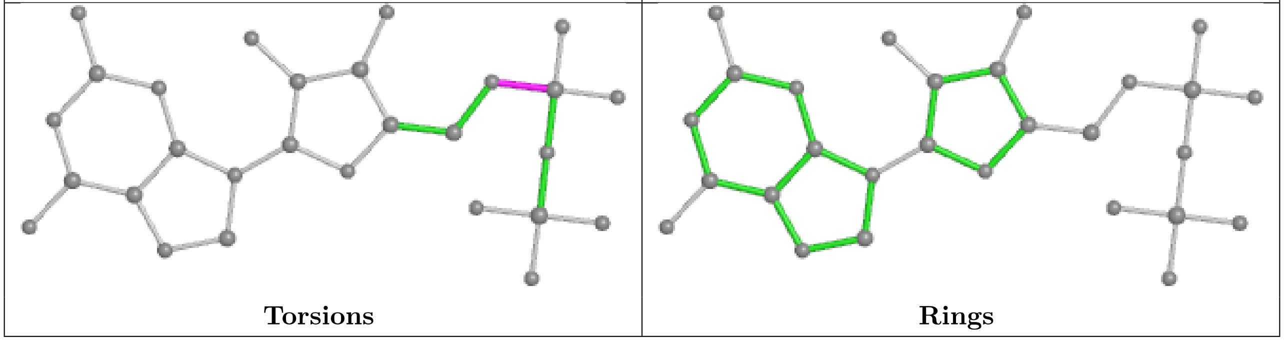
Rings

Ligand GDP 6g 501



Bond lengths

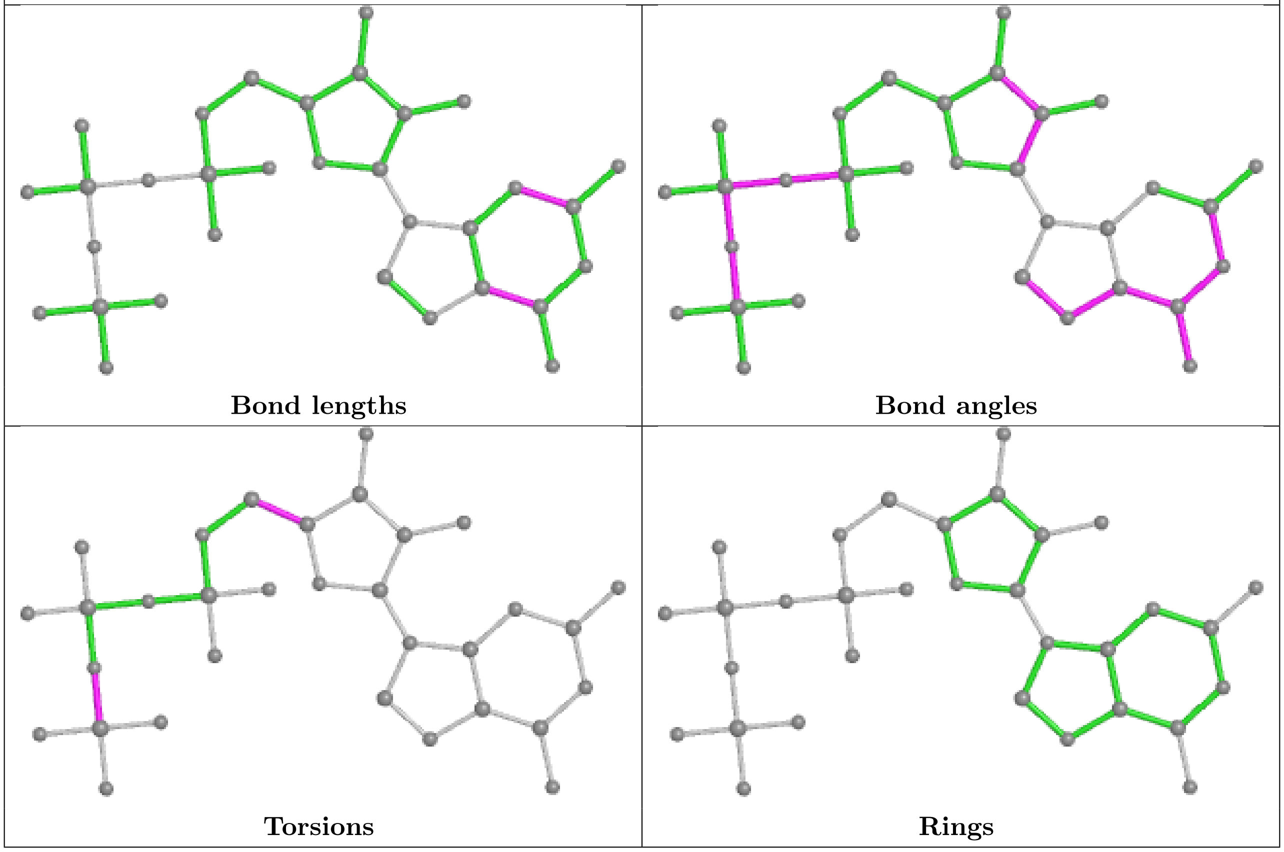
Bond angles



Torsions

Rings

Ligand GTP 5b 501



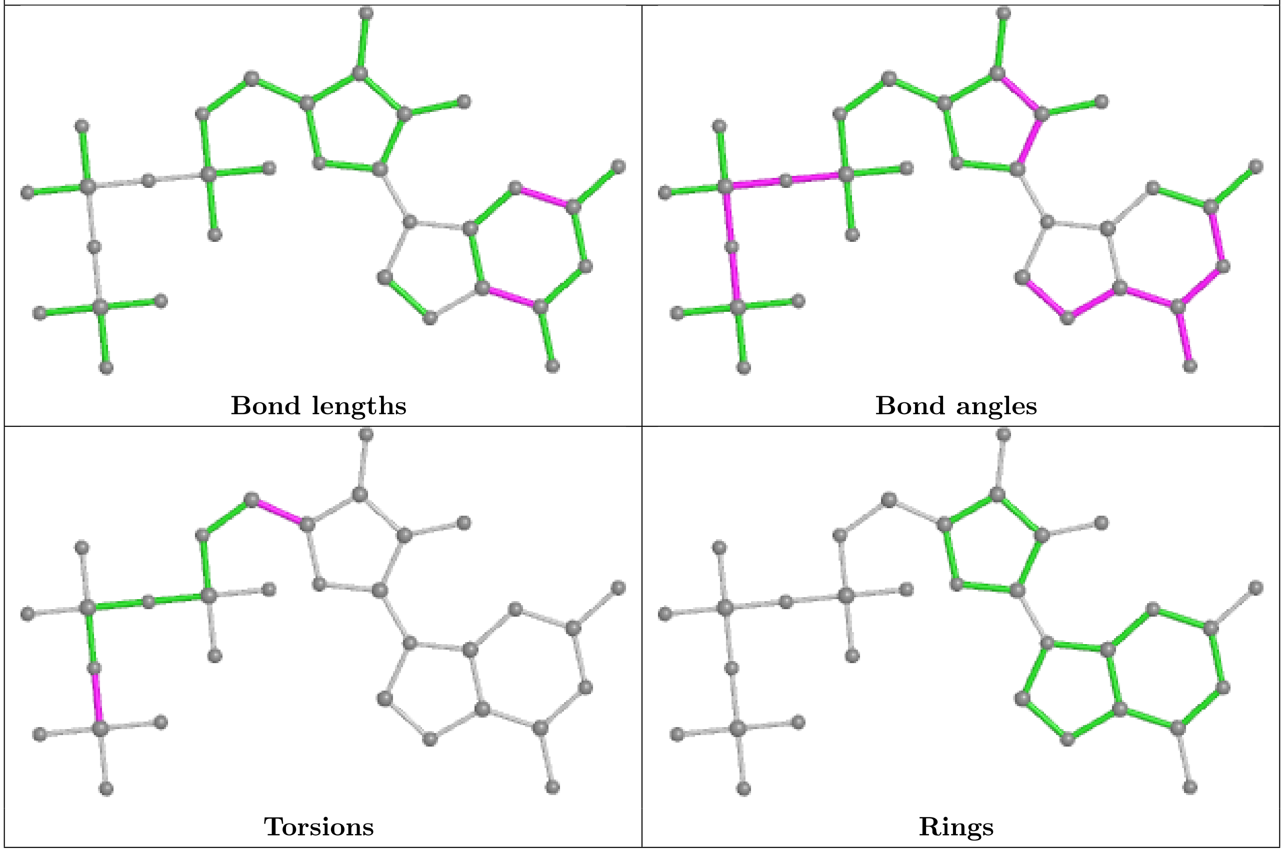
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP Af 501



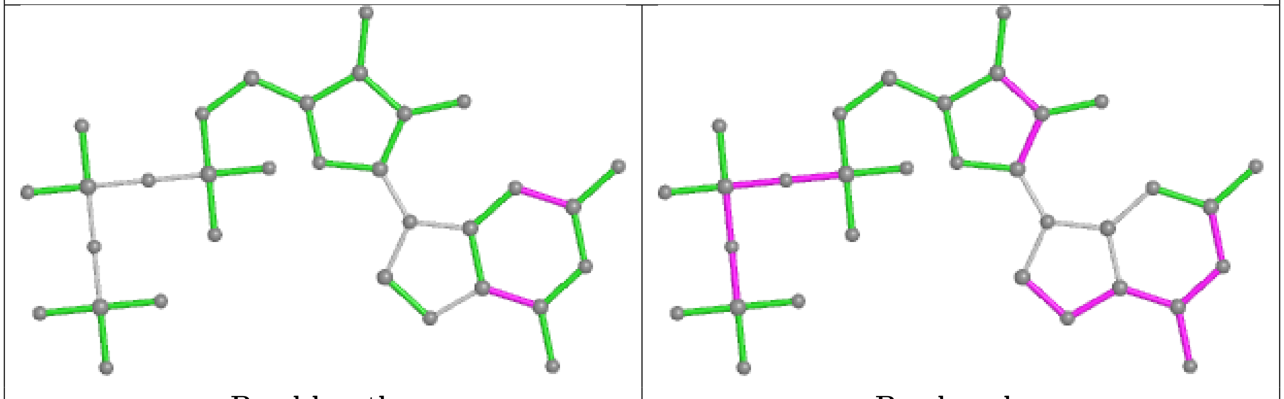
Bond lengths

Bond angles

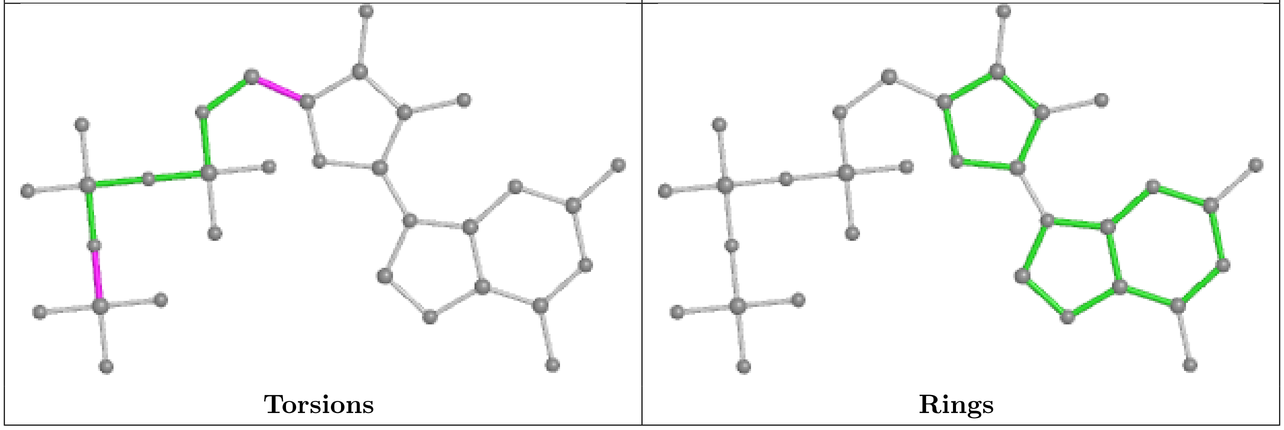
Torsions

Rings

Ligand GTP 2d 501

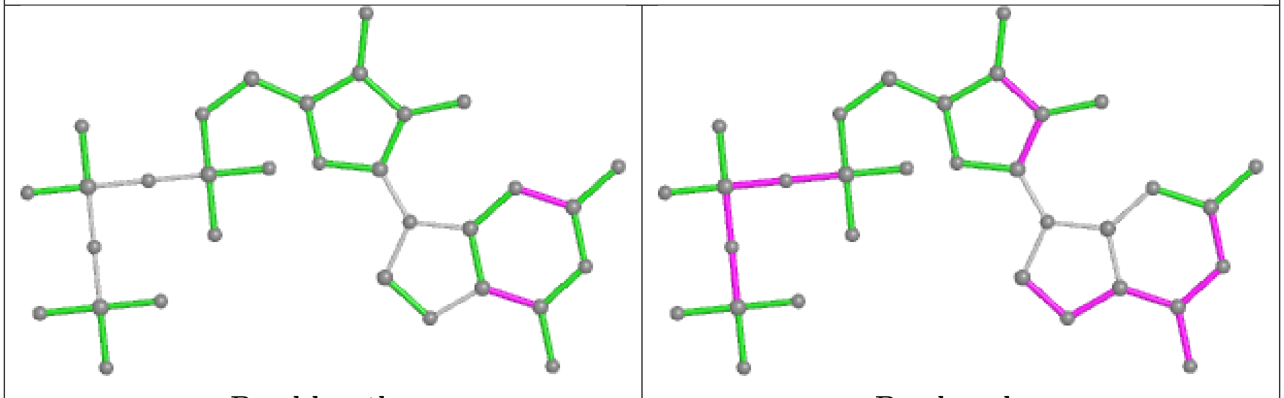


Bond lengths Bond angles

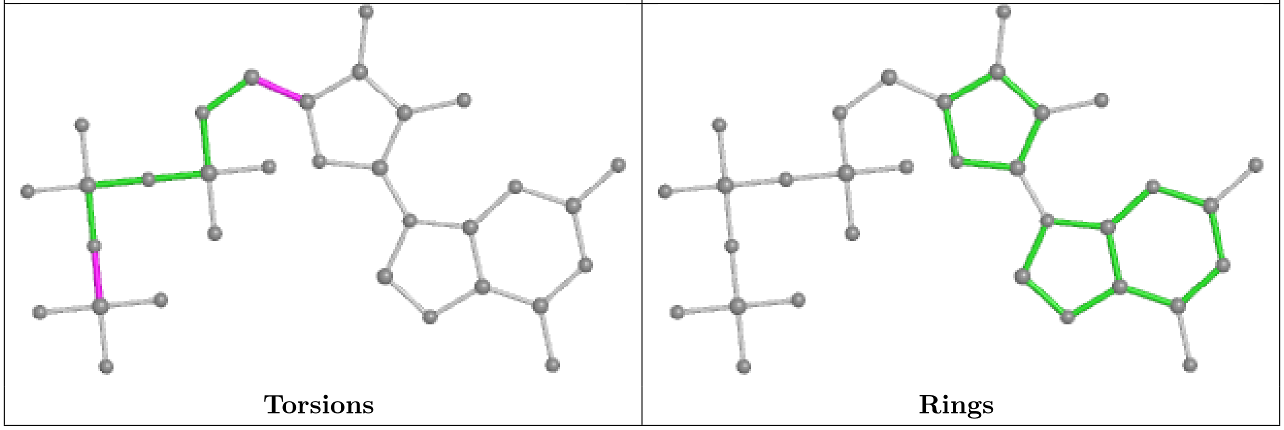


Torsions Rings

Ligand GTP Cf 501

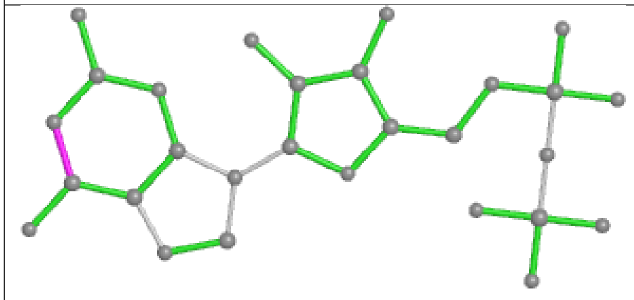


Bond lengths Bond angles

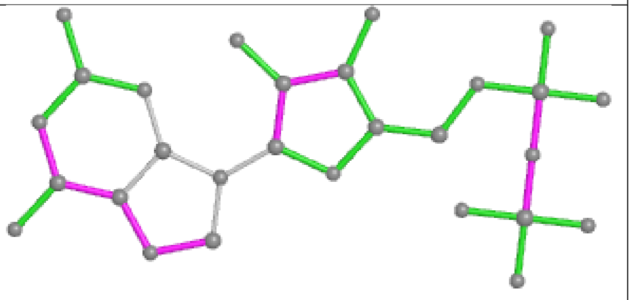


Torsions Rings

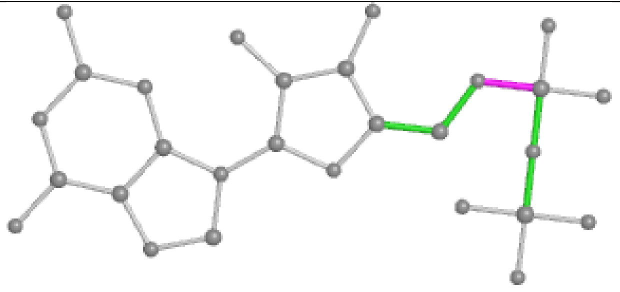
Ligand GDP 4a 501



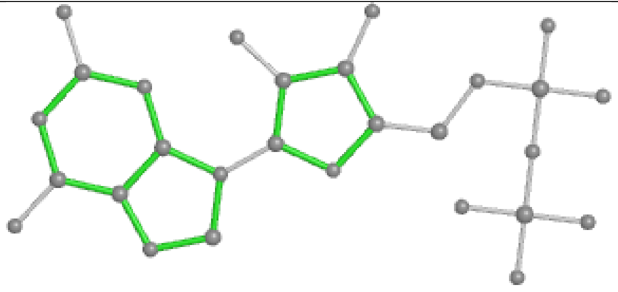
Bond lengths



Bond angles

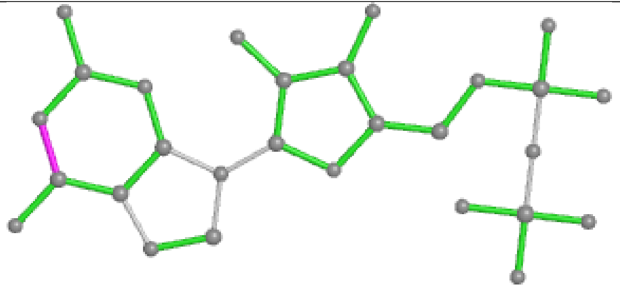


Torsions

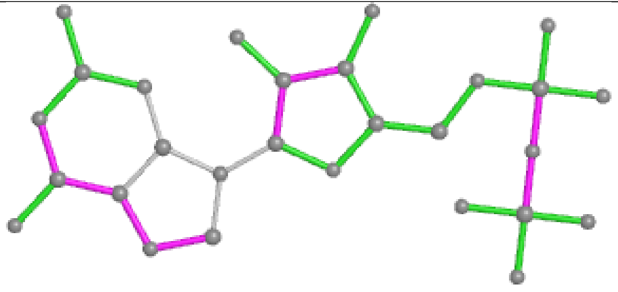


Rings

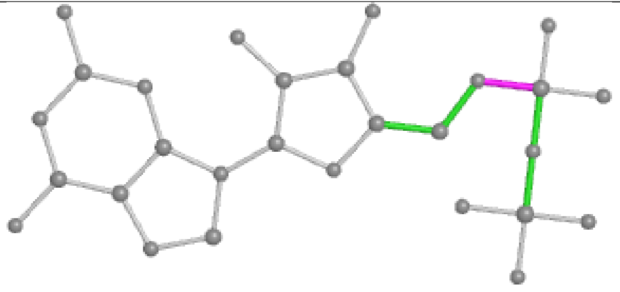
Ligand GDP Ae 501



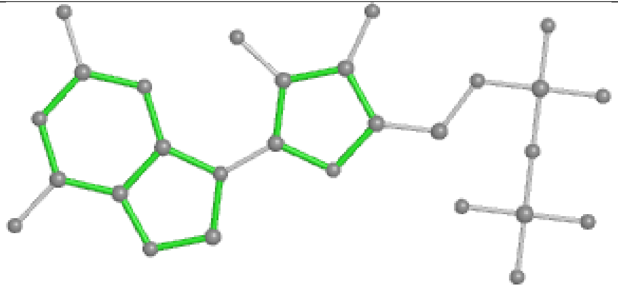
Bond lengths



Bond angles

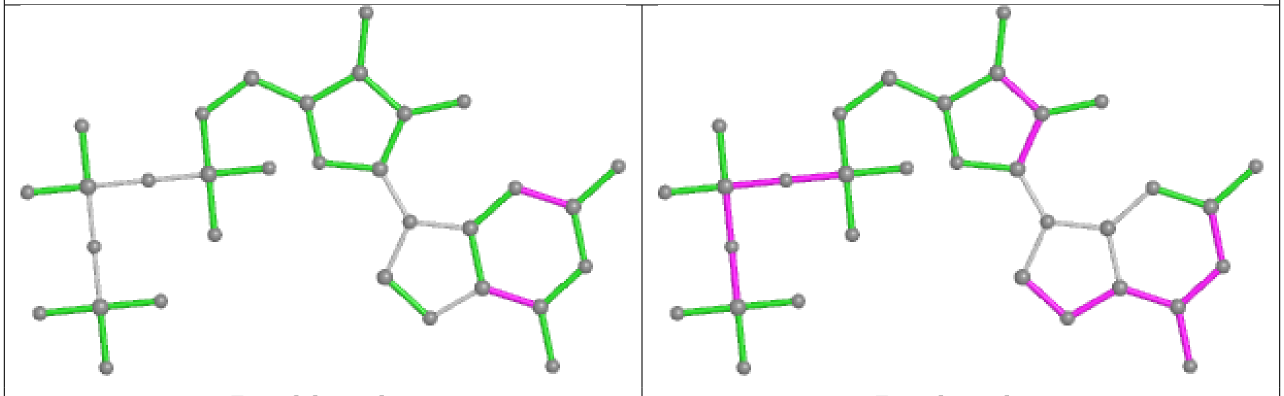


Torsions

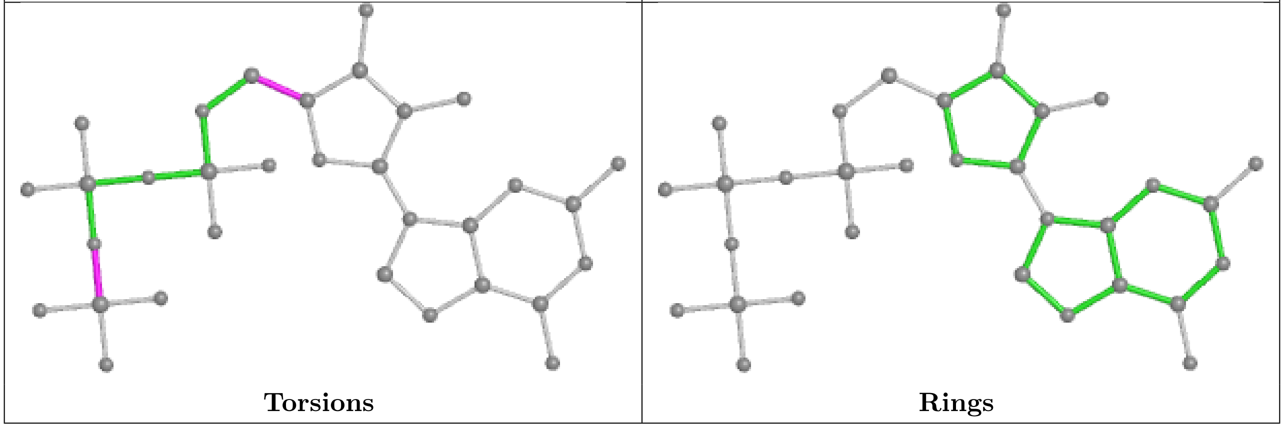


Rings

Ligand GTP 5f 501

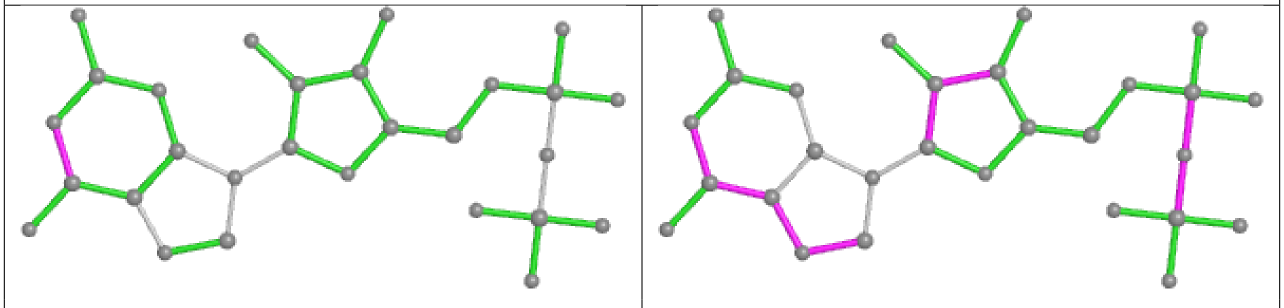


Bond lengths **Bond angles**

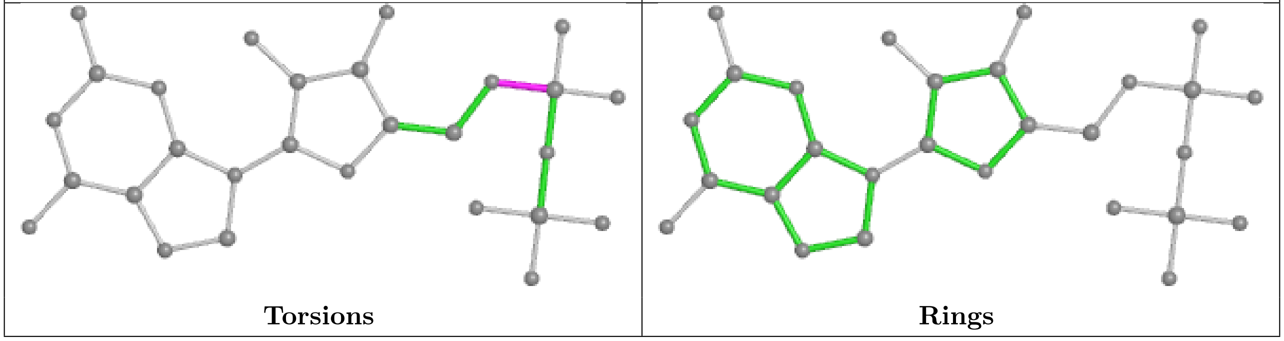


Torsions **Rings**

Ligand GDP 4e 501

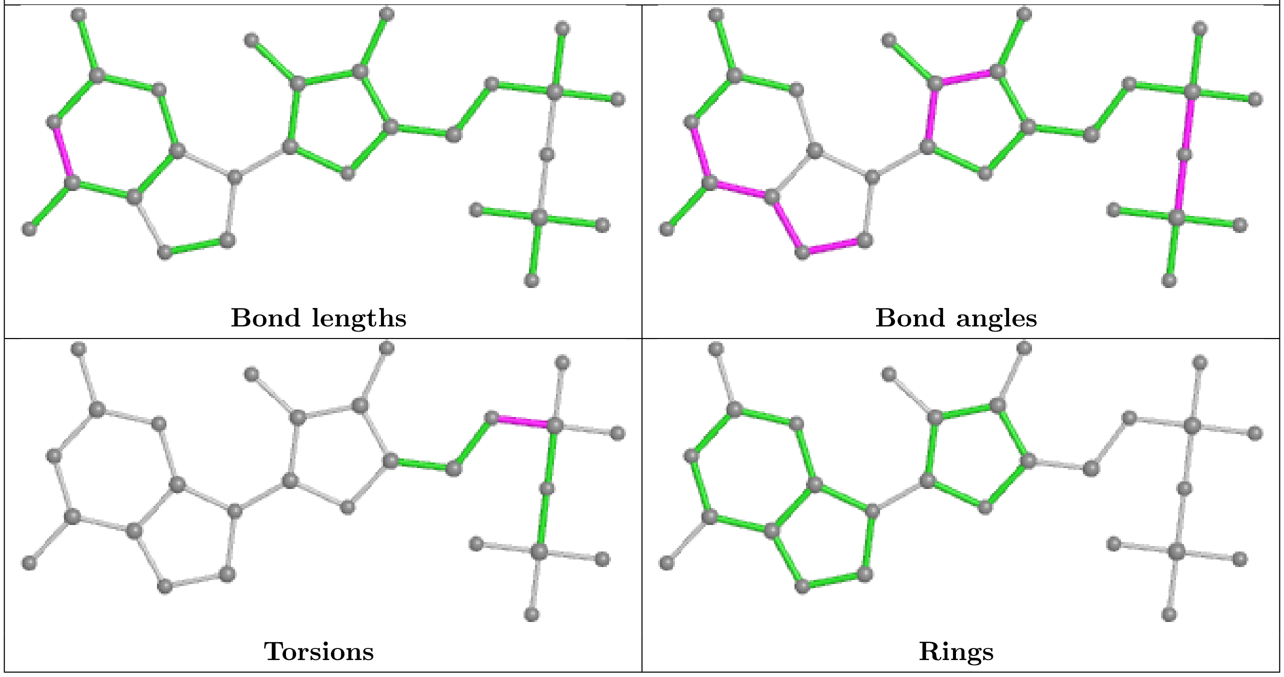


Bond lengths **Bond angles**



Torsions **Rings**

Ligand GDP 9g 501



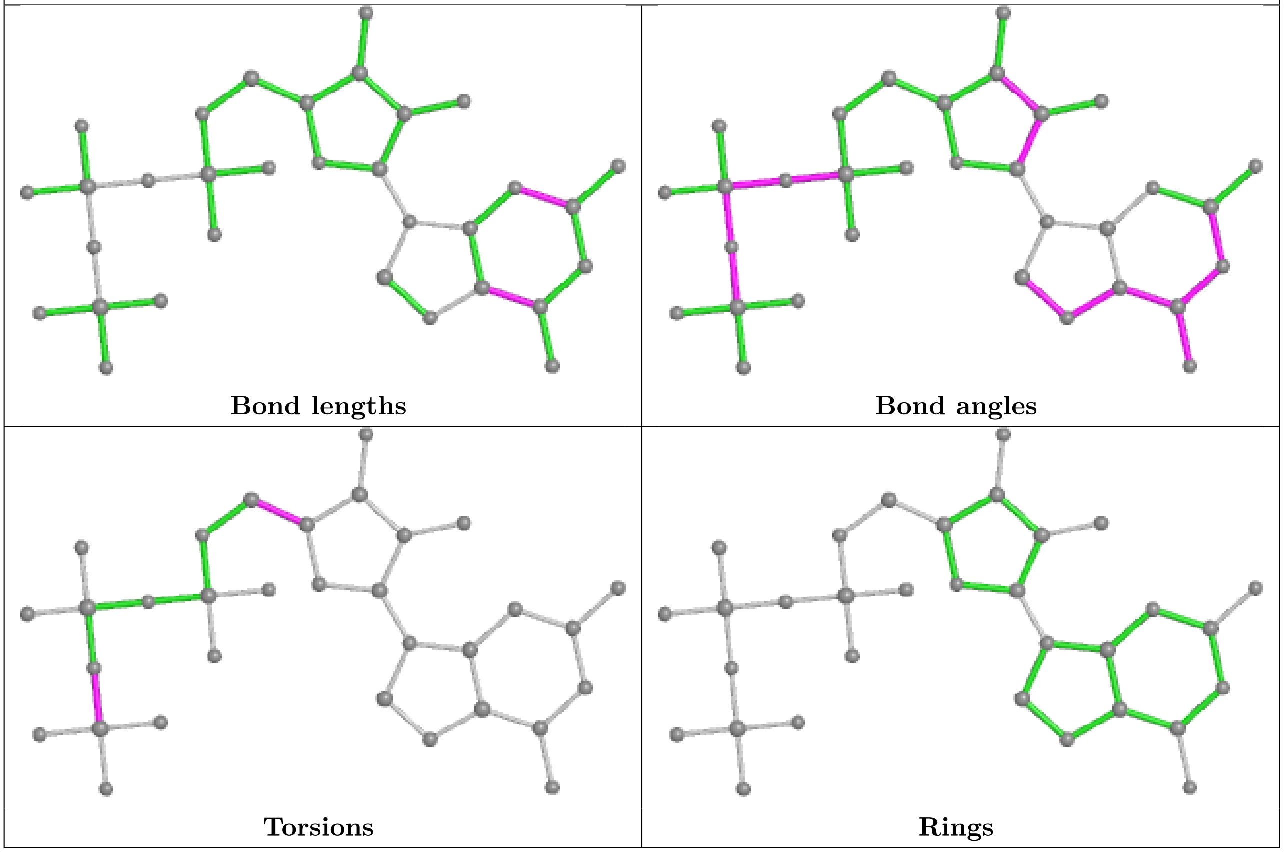
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP 7b 501



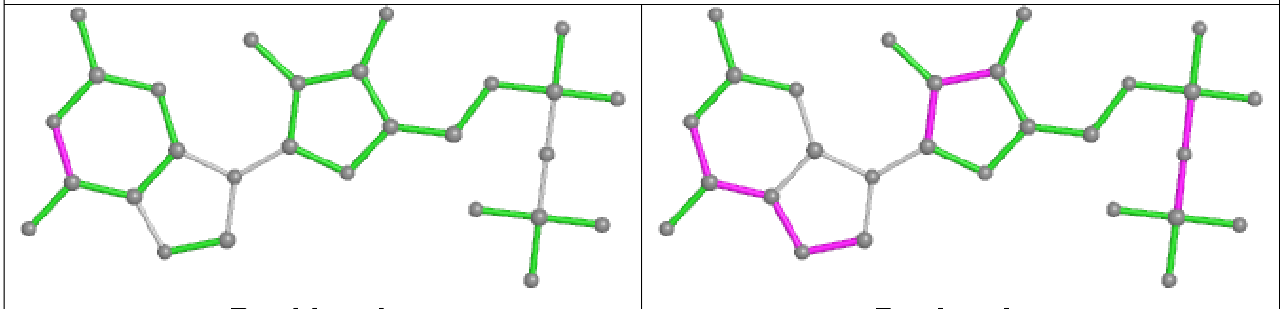
Bond lengths

Bond angles

Torsions

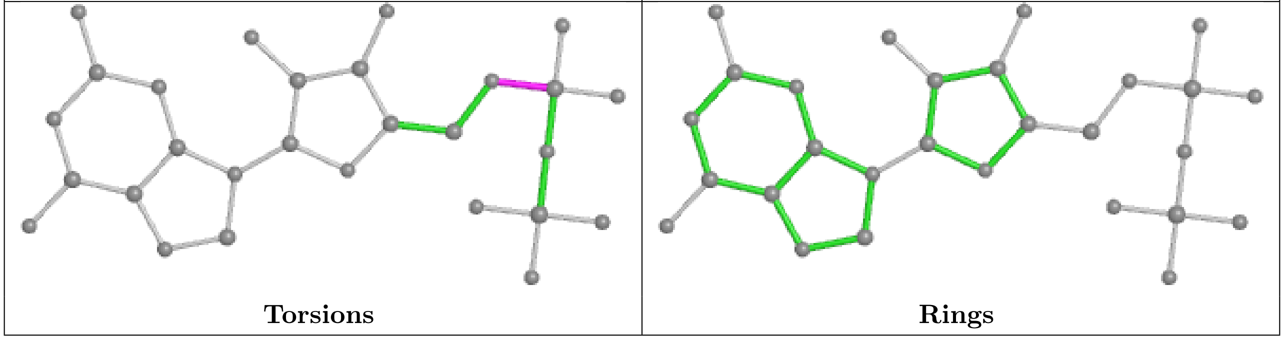
Rings

Ligand GDP 3g 501



Bond lengths

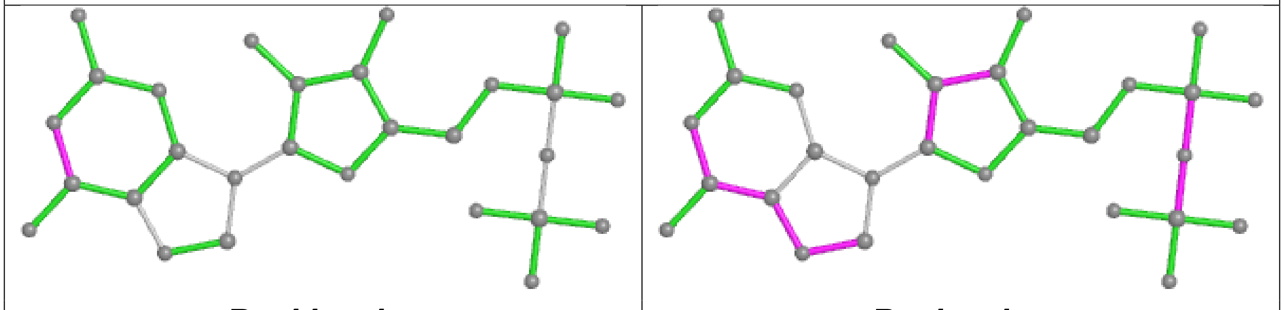
Bond angles



Torsions

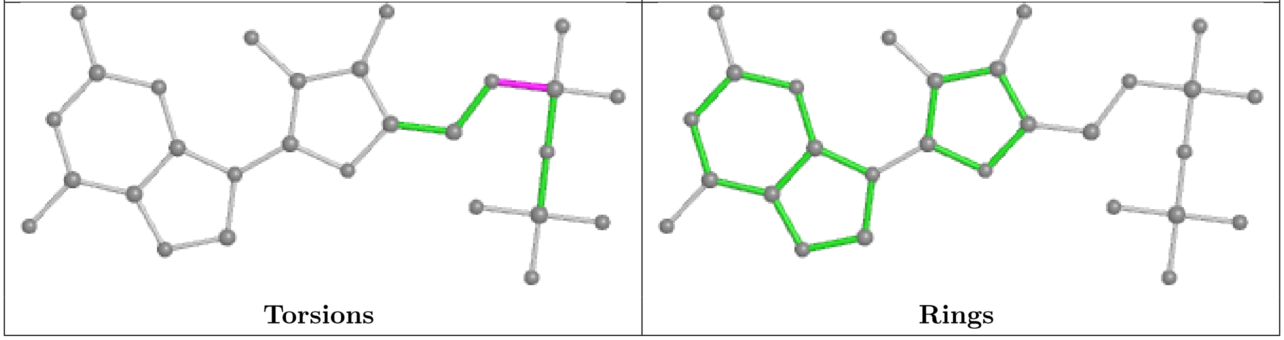
Rings

Ligand GDP 6a 501



Bond lengths

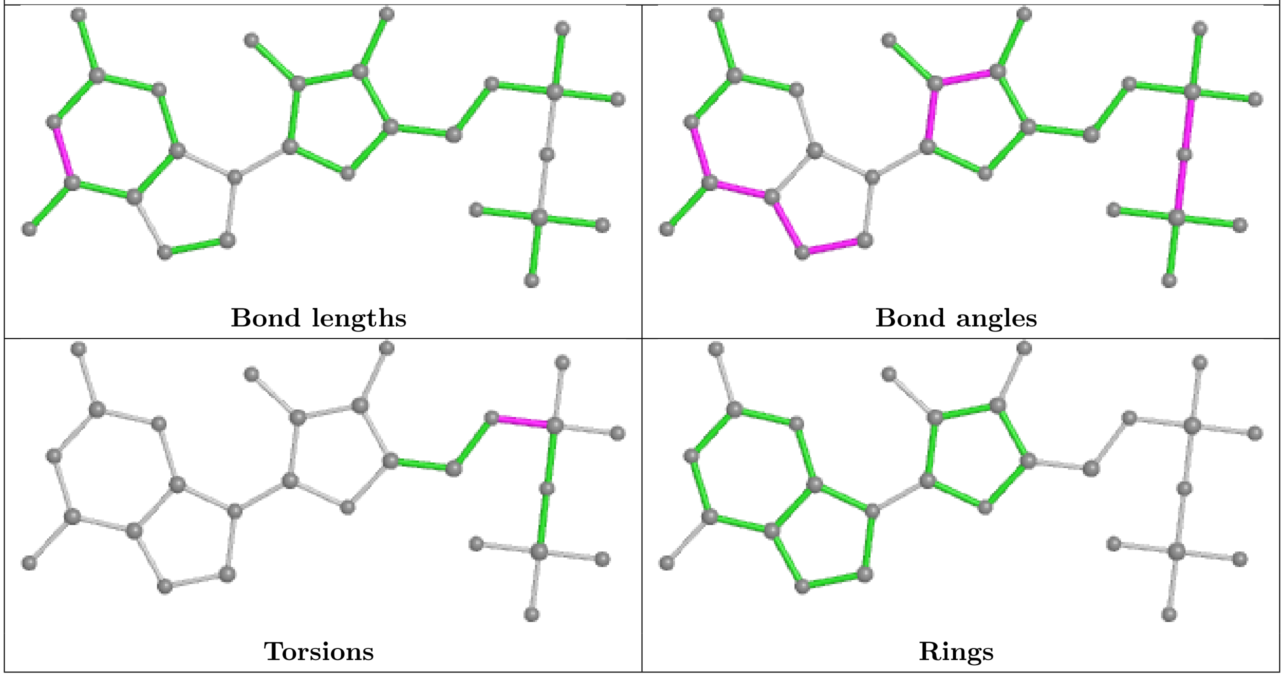
Bond angles



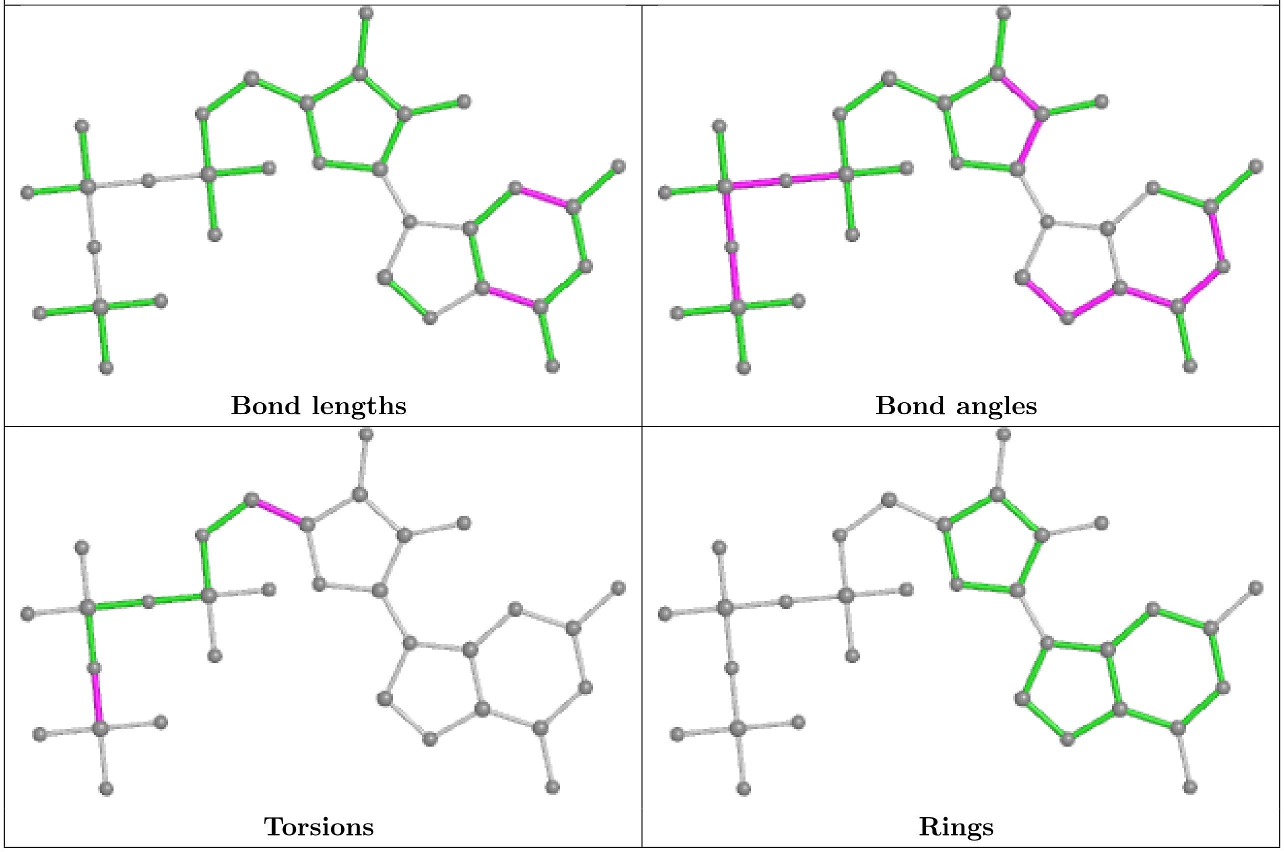
Torsions

Rings

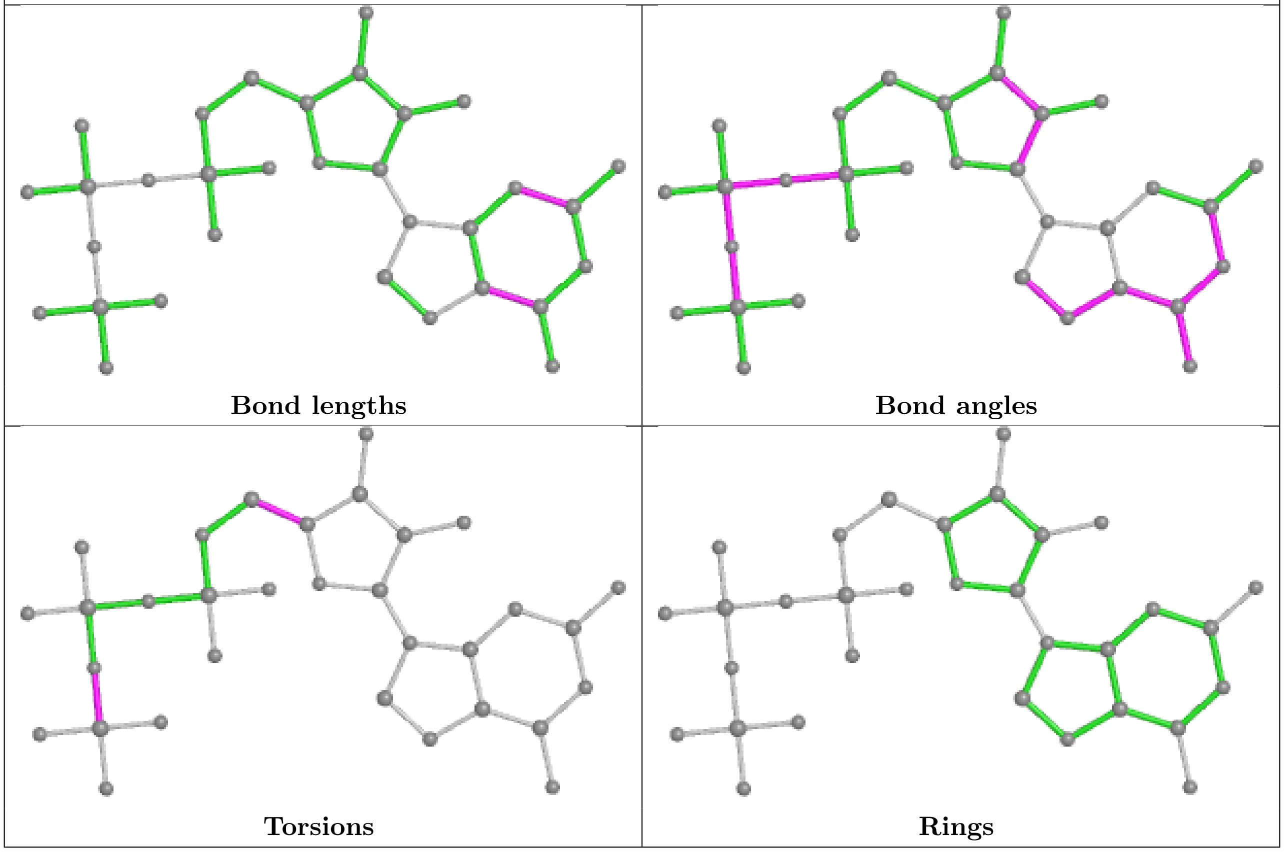
Ligand GDP 8g 501



Ligand GTP 6h 501



Ligand GTP Bh 501



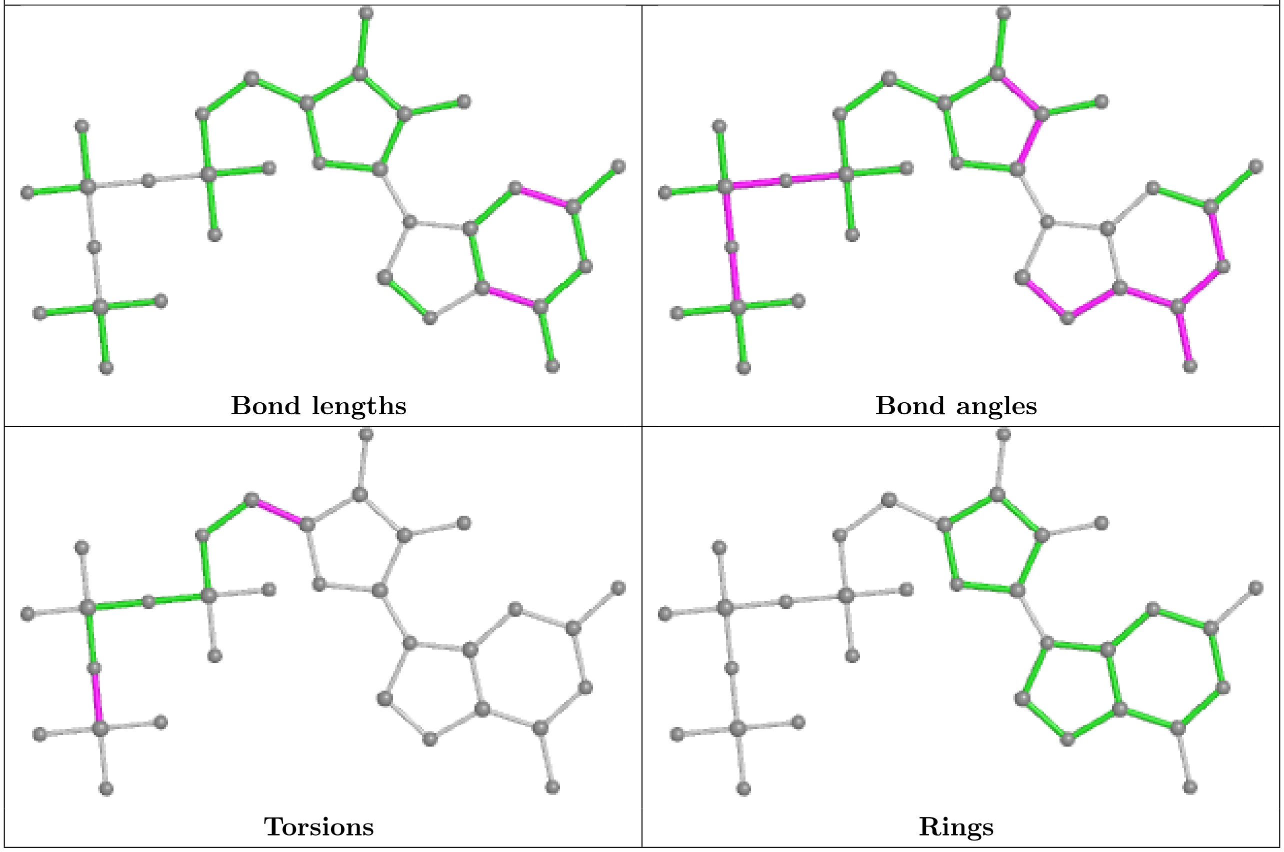
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP 8f 501



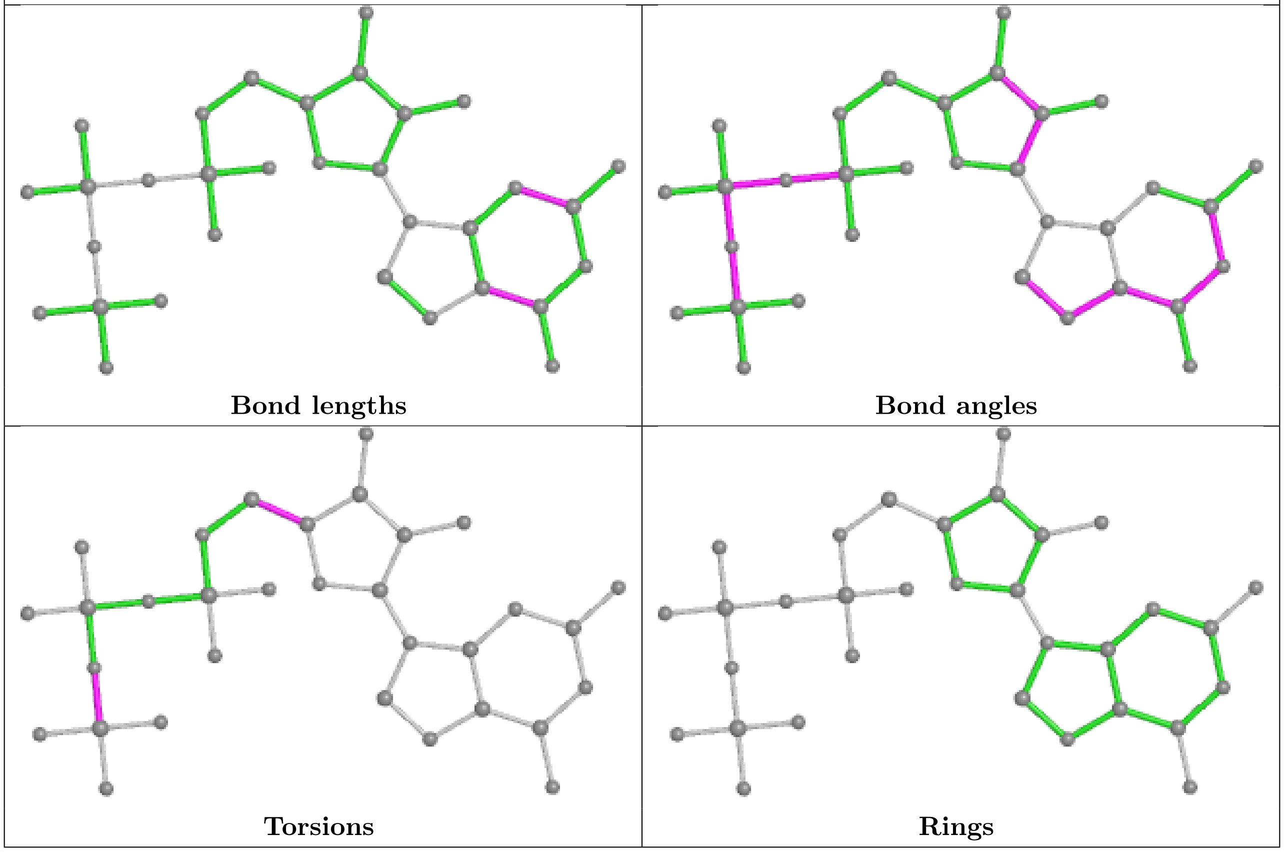
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP 6f 501



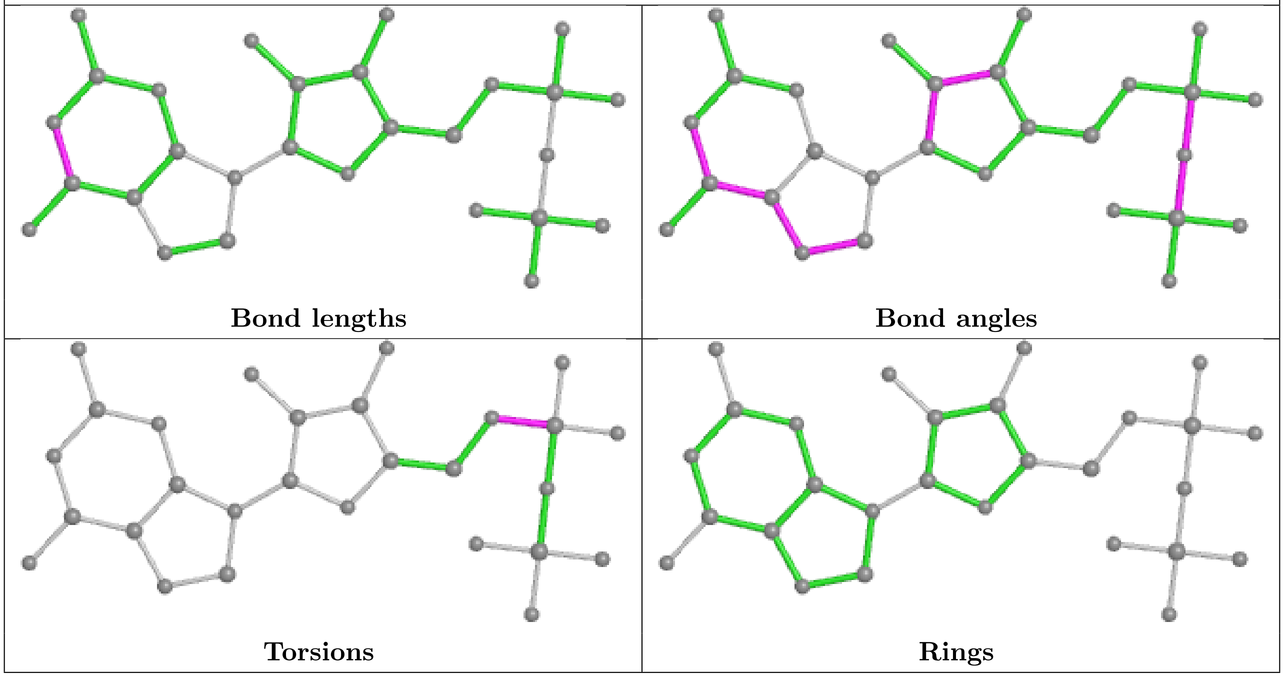
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP 2e 501



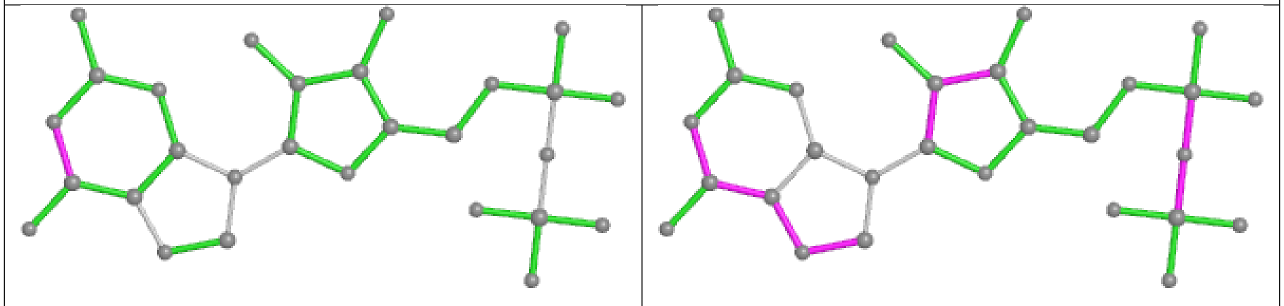
Bond lengths

Bond angles

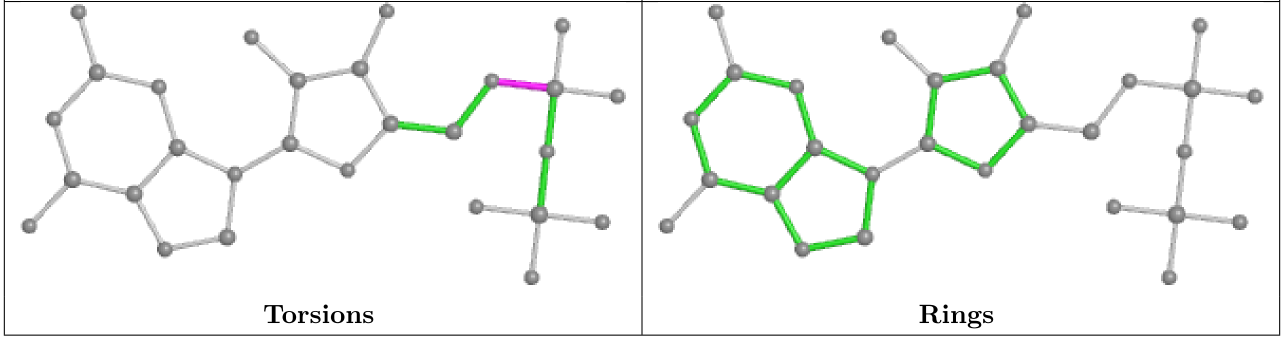
Torsions

Rings

Ligand GDP 8e 501

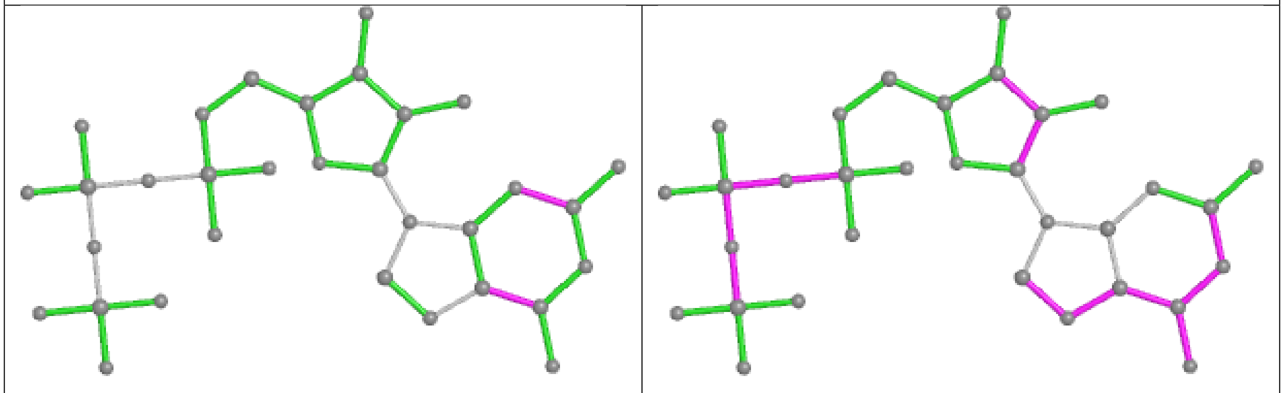


Bond lengths **Bond angles**

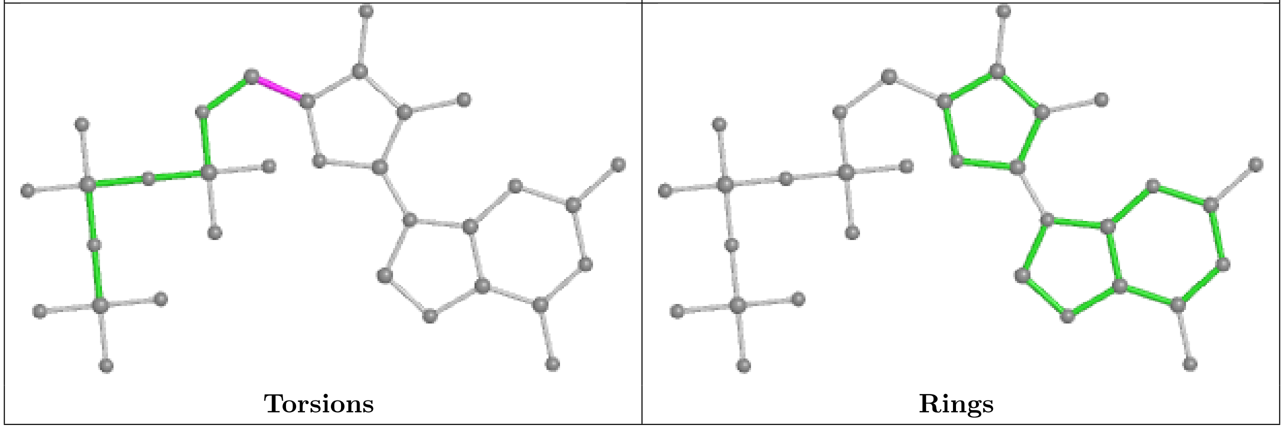


Torsions **Rings**

Ligand GTP Ah 501

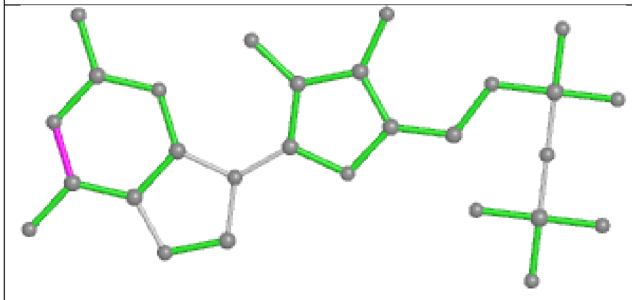


Bond lengths **Bond angles**

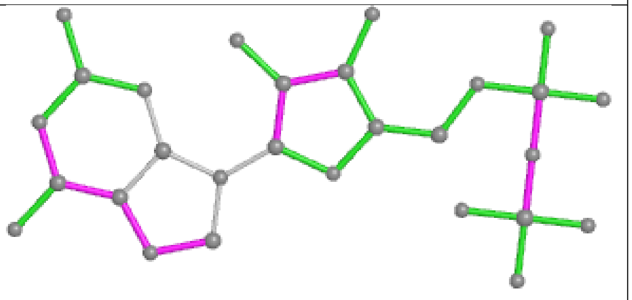


Torsions **Rings**

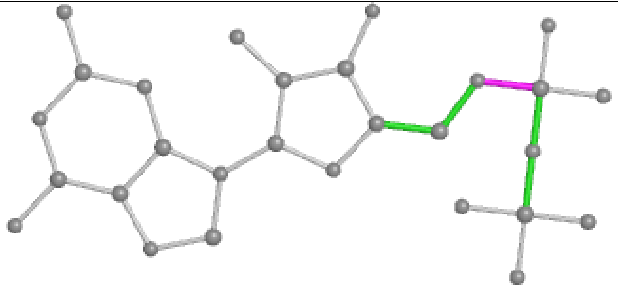
Ligand GDP Aa 501



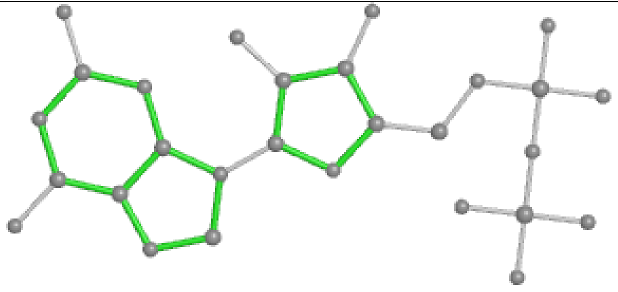
Bond lengths



Bond angles

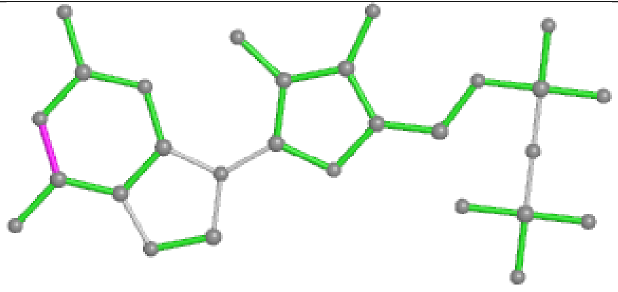


Torsions

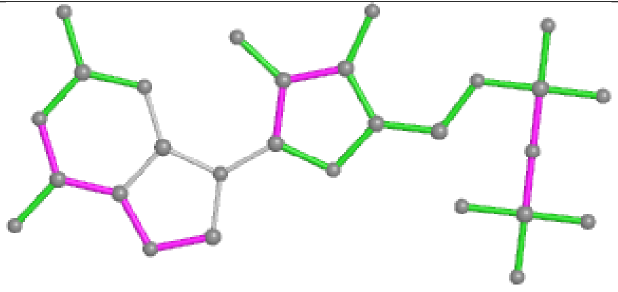


Rings

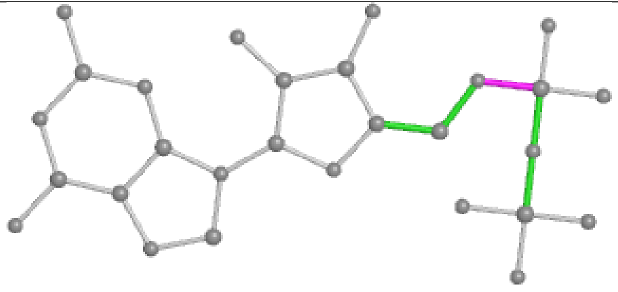
Ligand GDP Bc 501



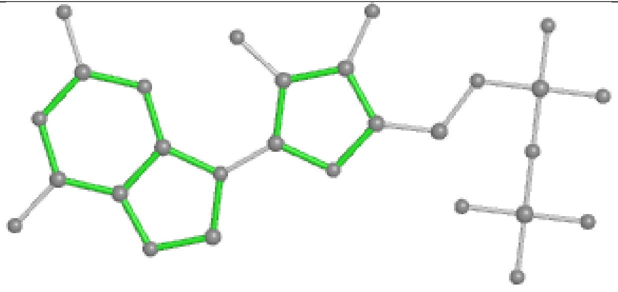
Bond lengths



Bond angles

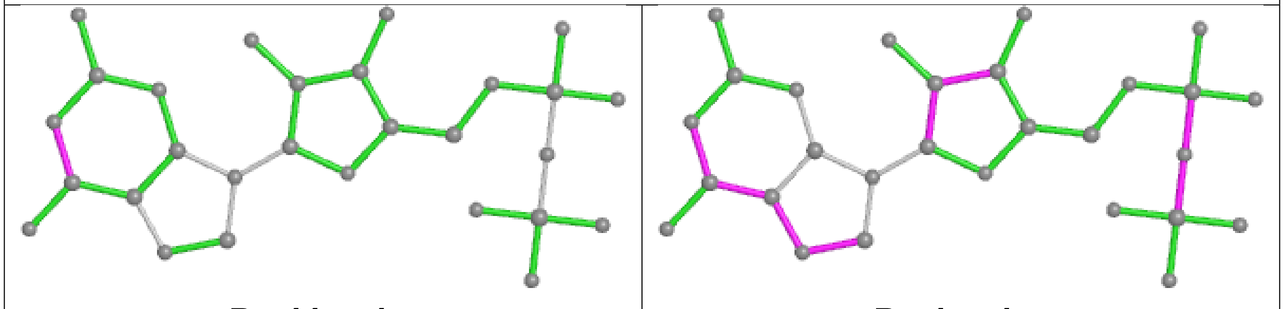


Torsions

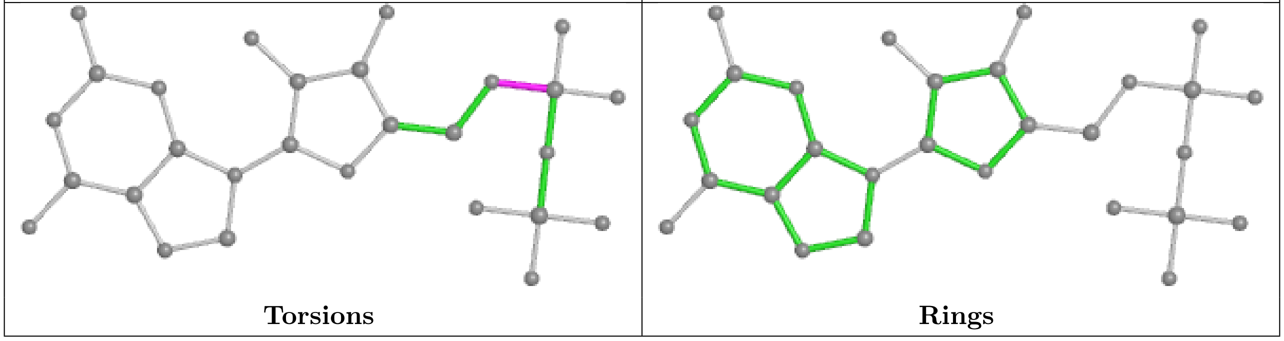


Rings

Ligand GDP 5c 501

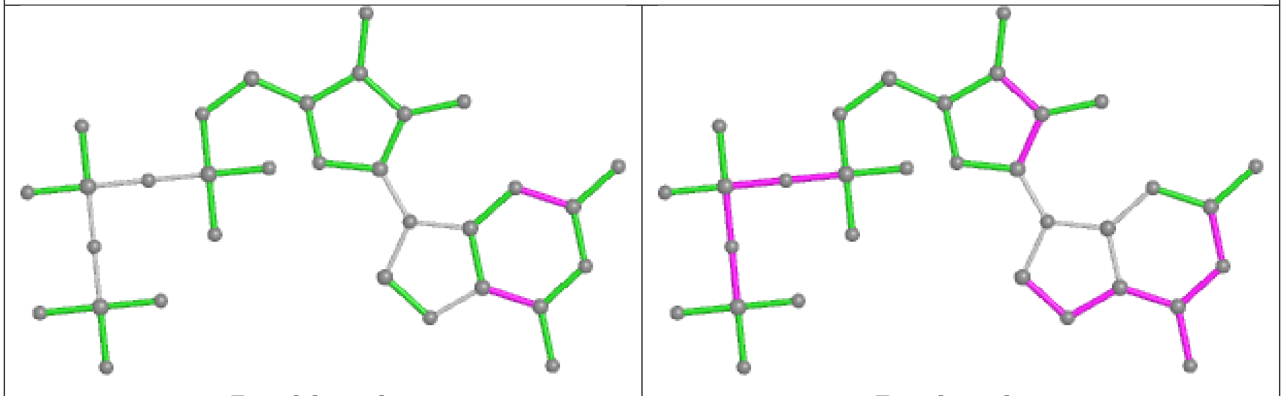


Bond lengths **Bond angles**

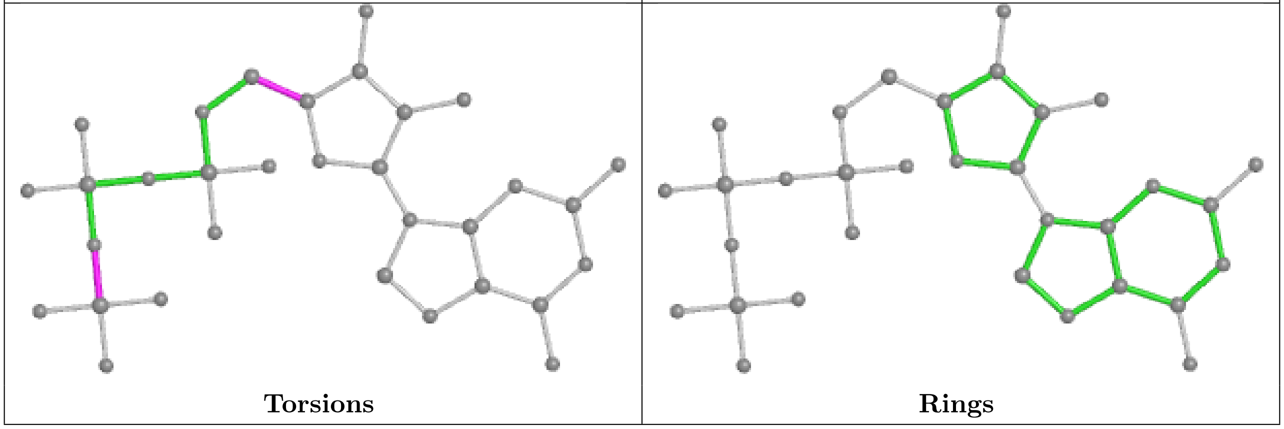


Torsions **Rings**

Ligand GTP Db 501

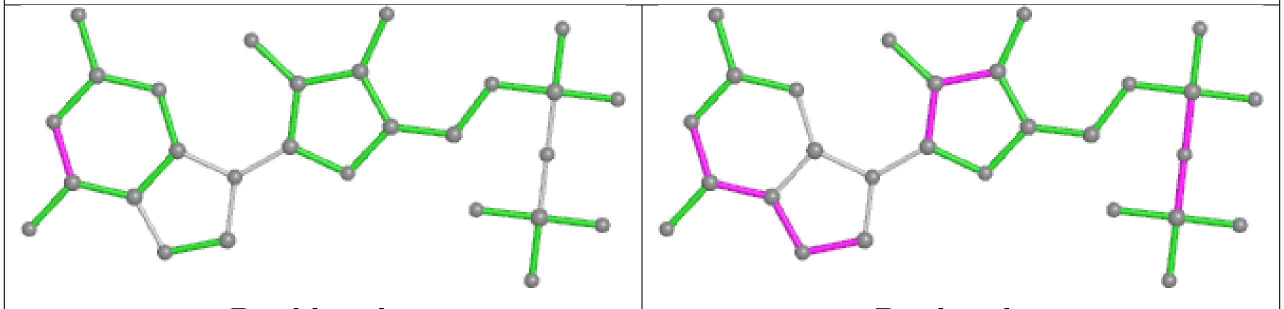


Bond lengths **Bond angles**

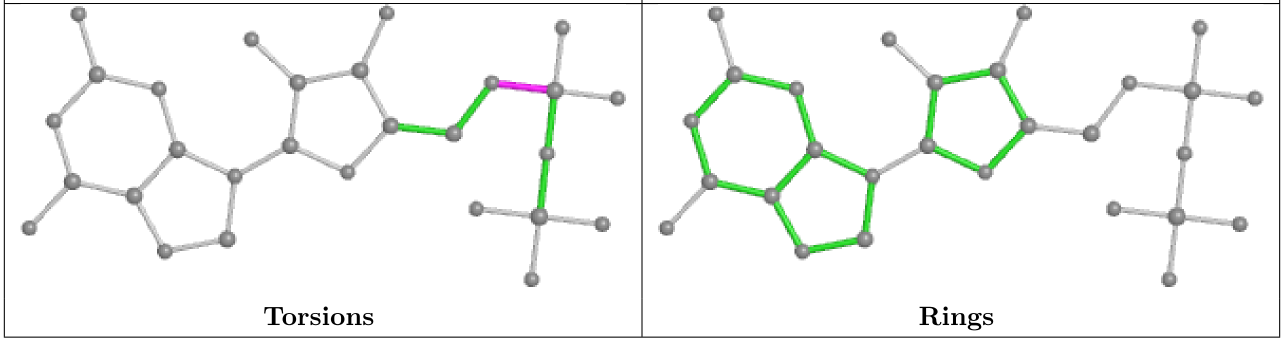


Torsions **Rings**

Ligand GDP Be 501

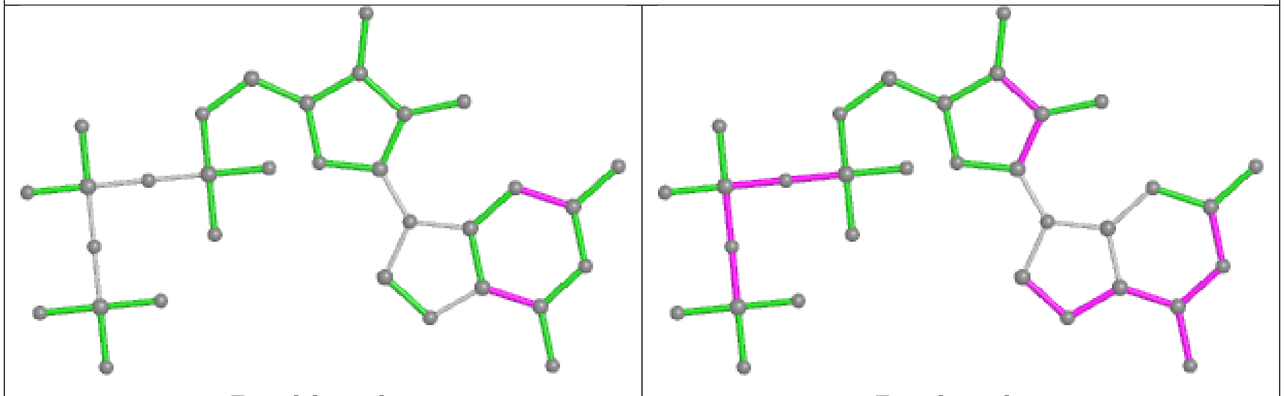


Bond lengths **Bond angles**

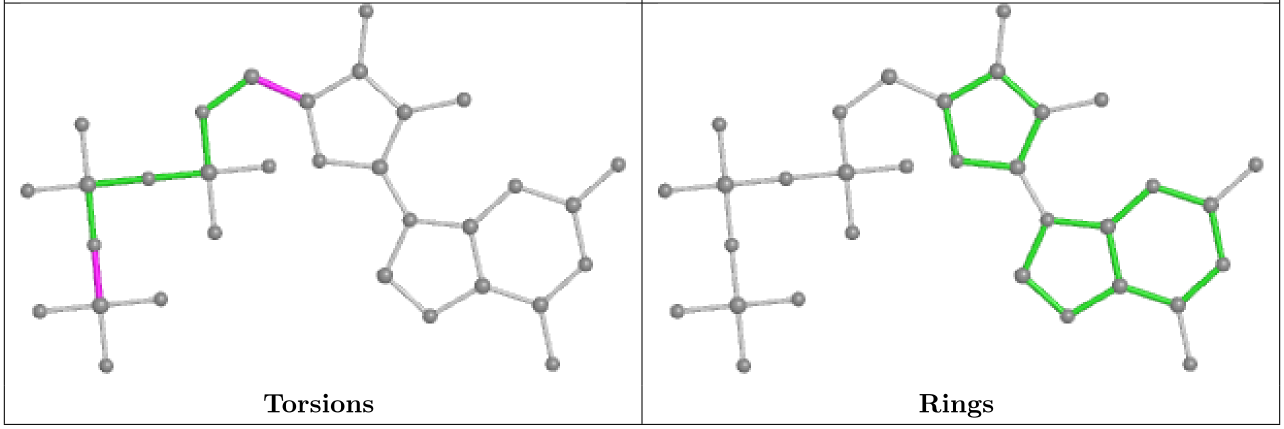


Torsions **Rings**

Ligand GTP 5h 501

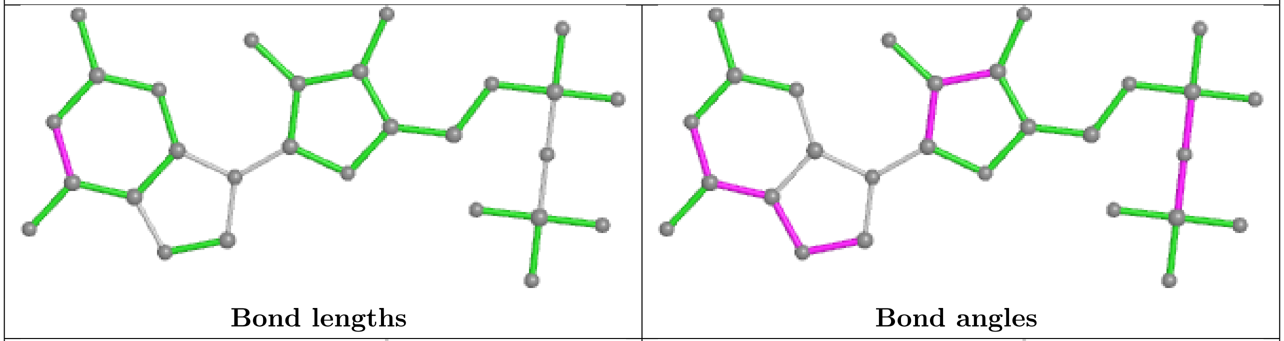


Bond lengths **Bond angles**



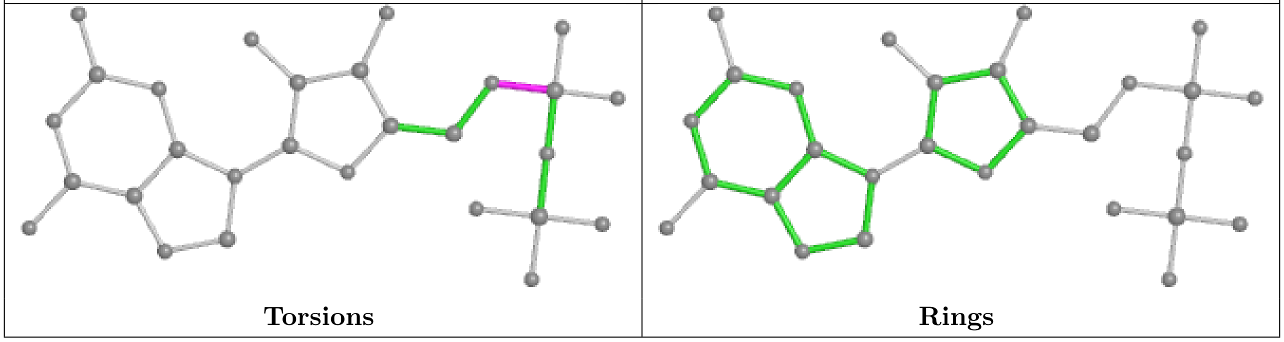
Torsions **Rings**

Ligand GDP 6c 501



Bond lengths

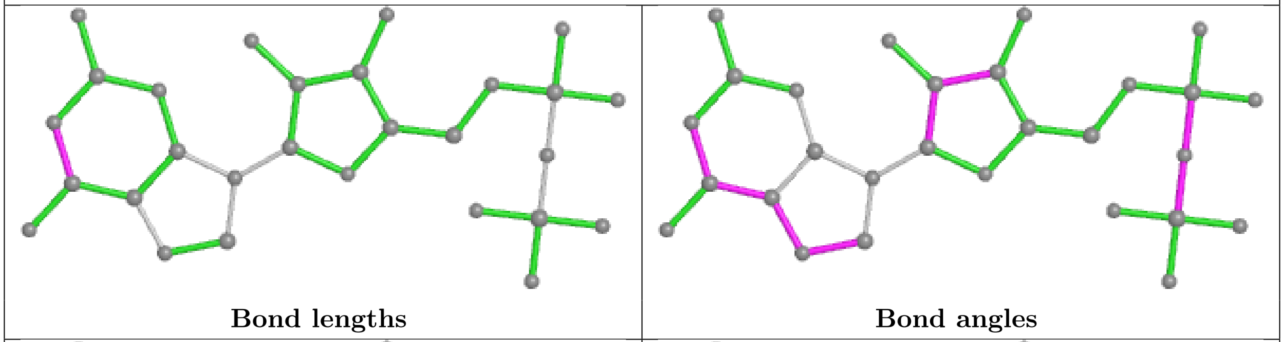
Bond angles



Torsions

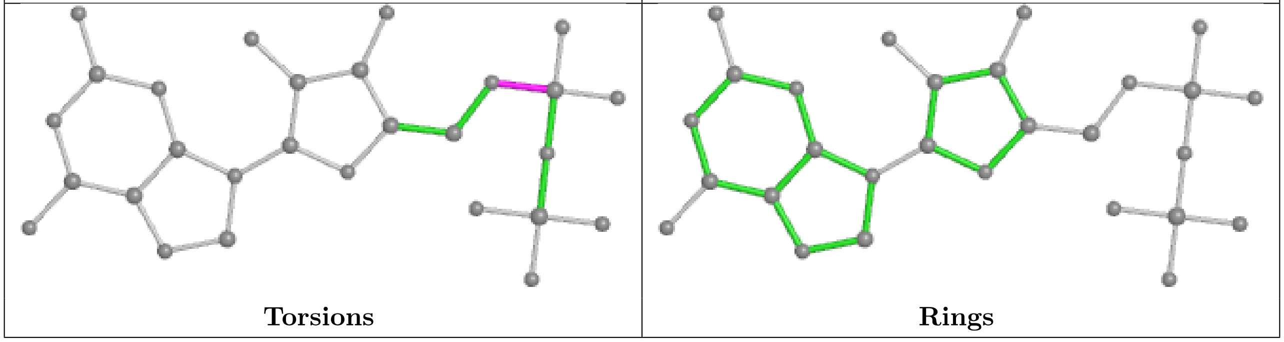
Rings

Ligand GDP 1e 501



Bond lengths

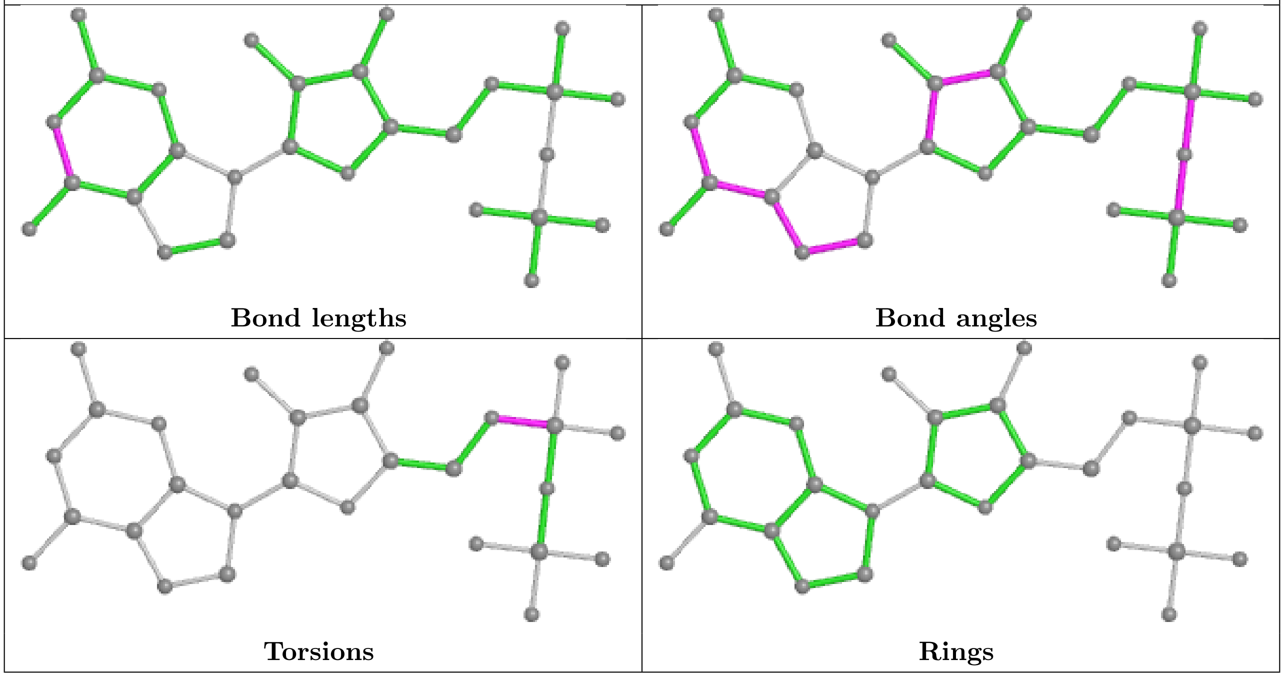
Bond angles



Torsions

Rings

Ligand GDP 3c 501



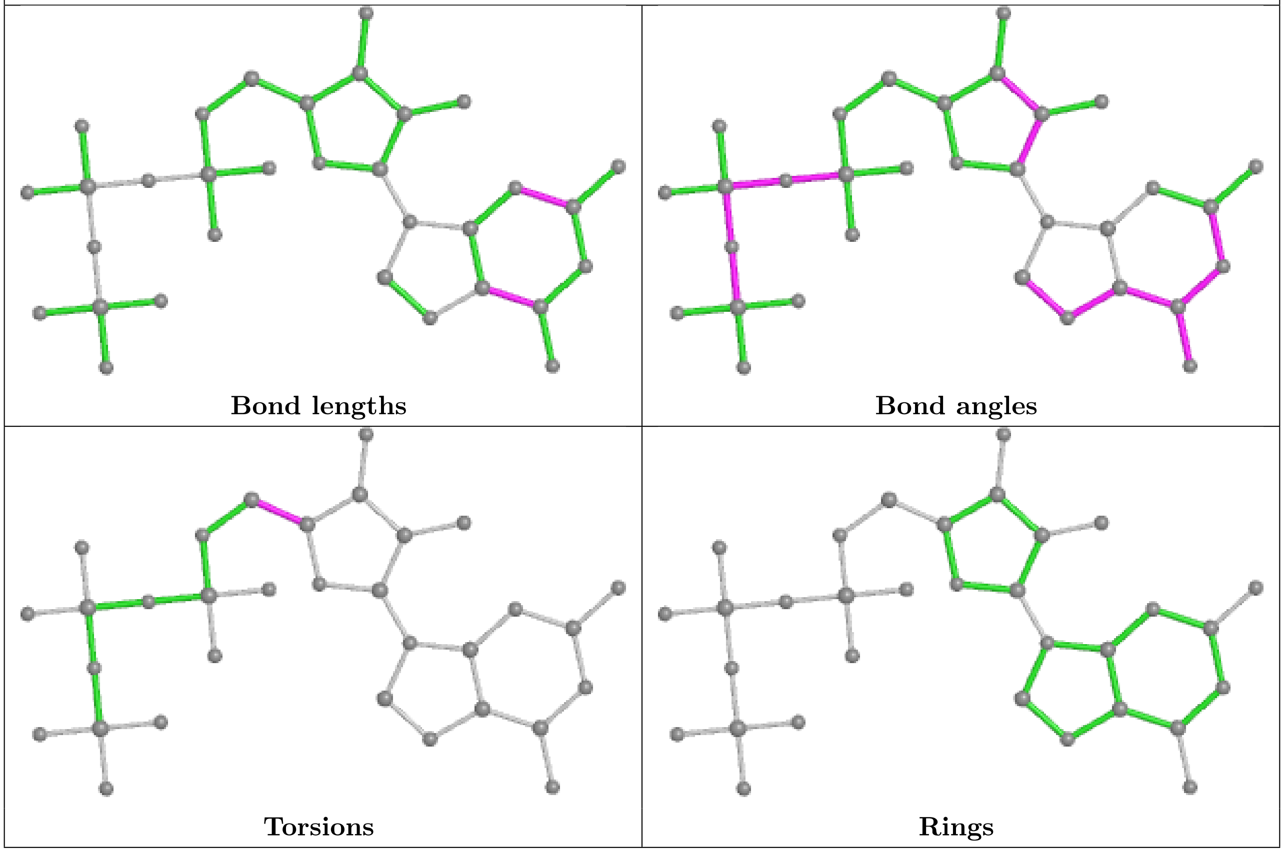
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP Cd 501



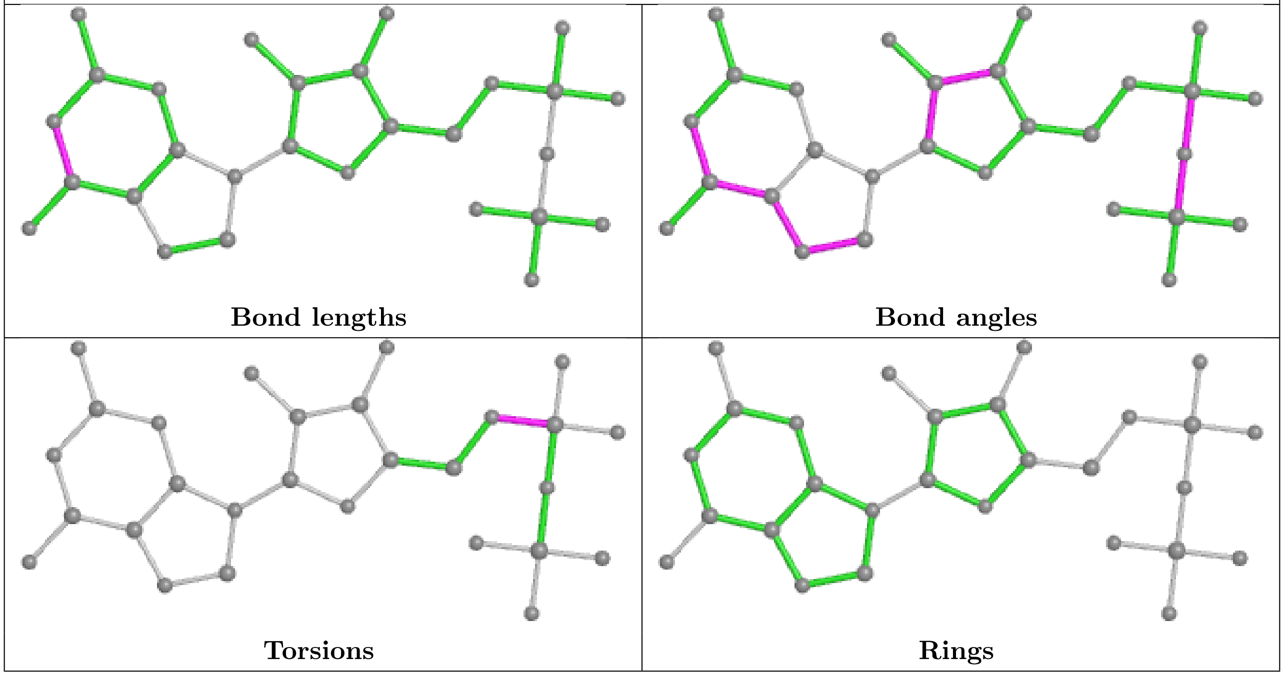
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP 2g 501



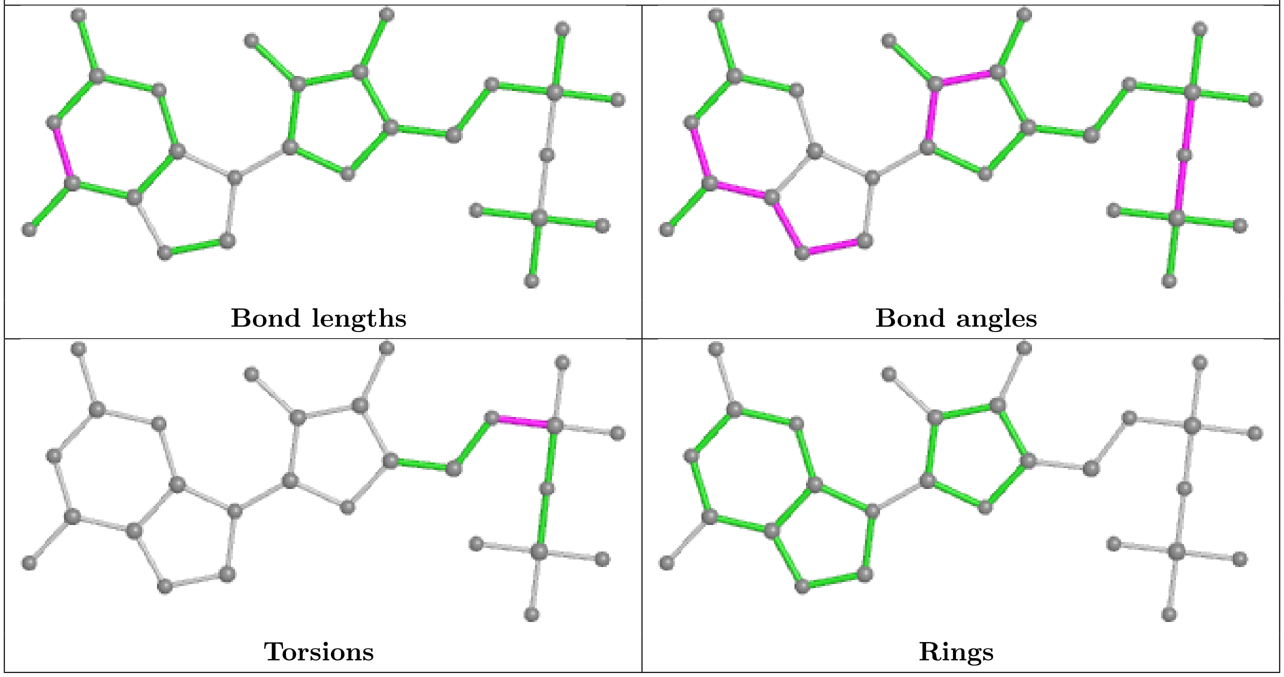
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP Ce 501



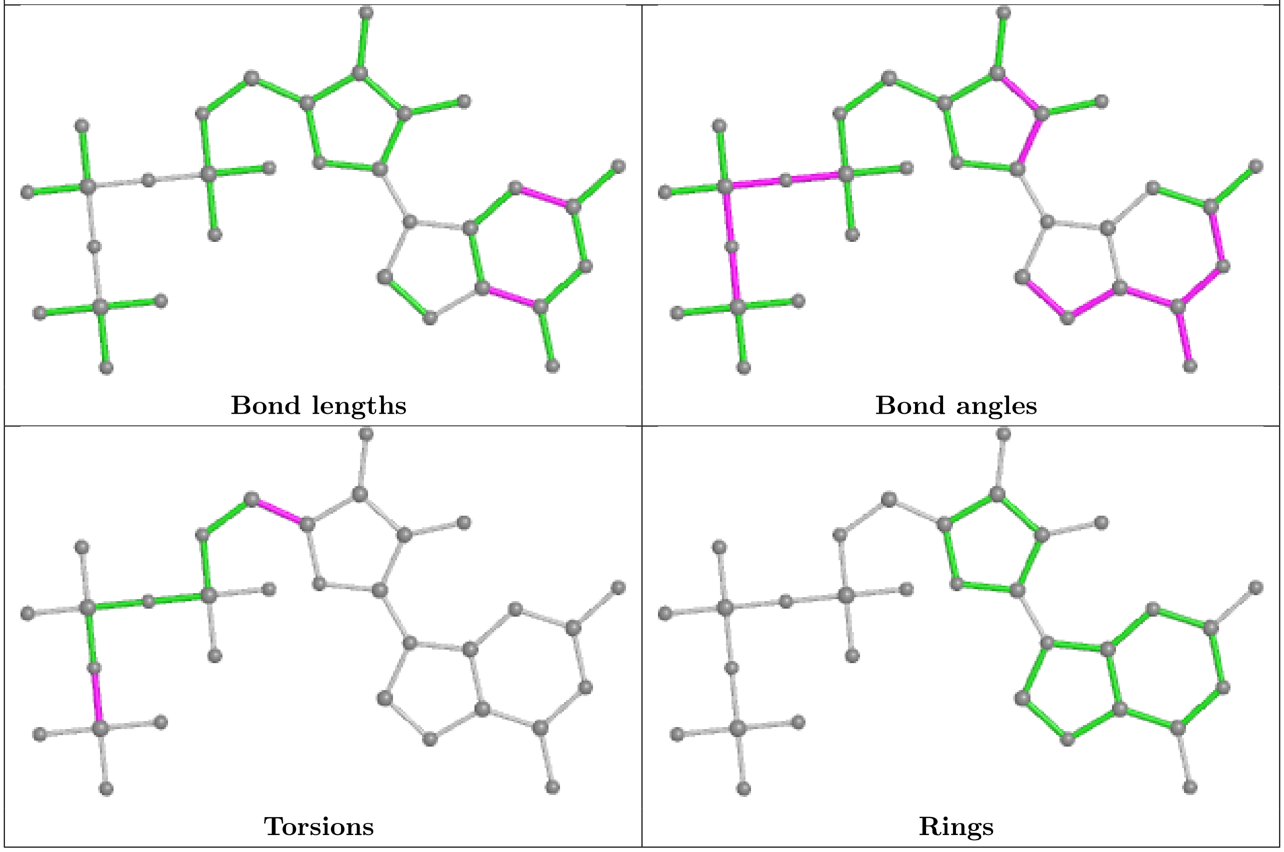
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP 3d 501



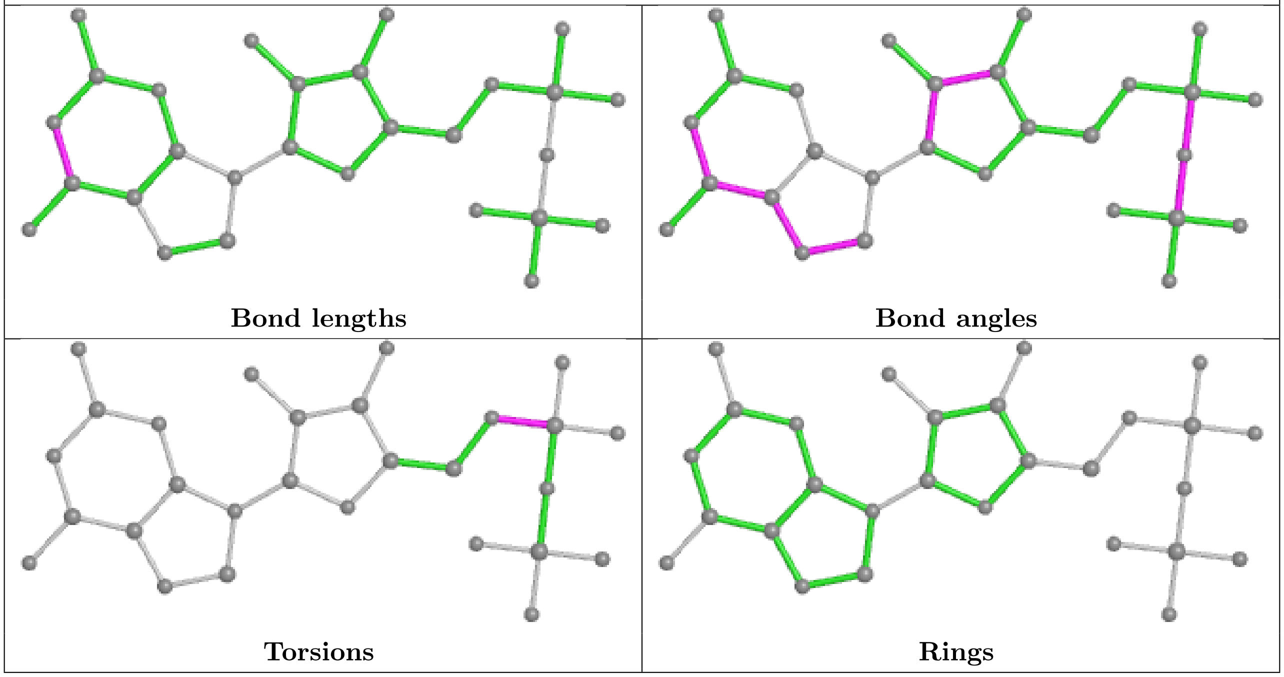
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP Ag 501



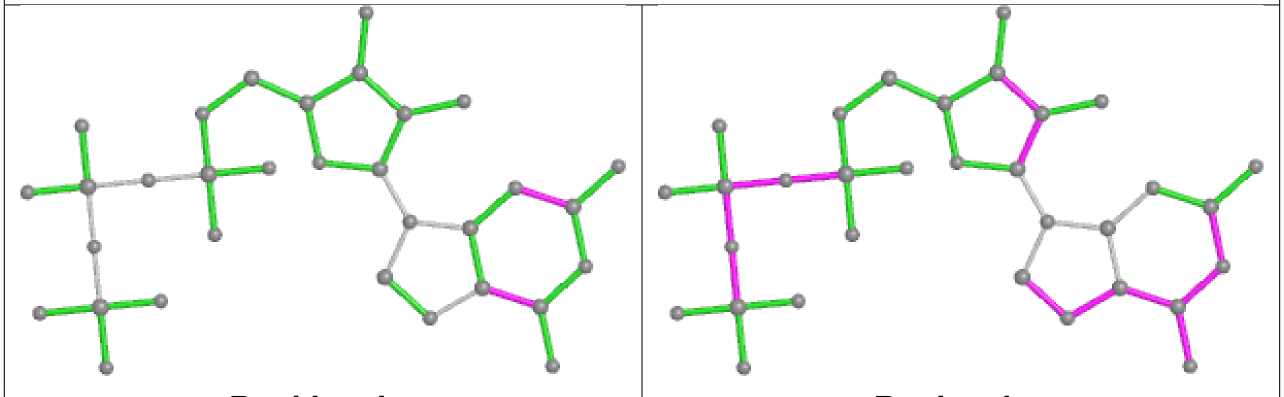
Bond lengths

Bond angles

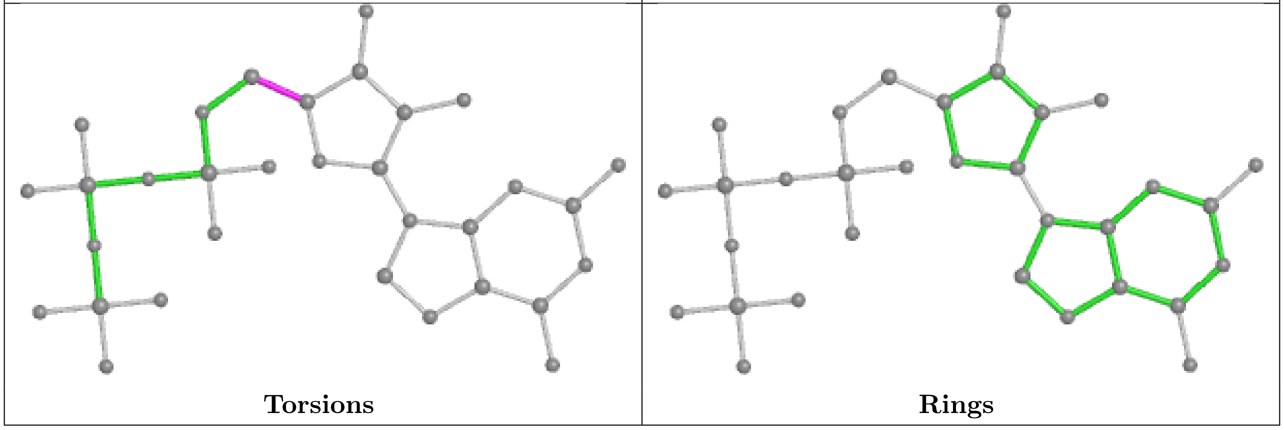
Torsions

Rings

Ligand GTP 3b 501

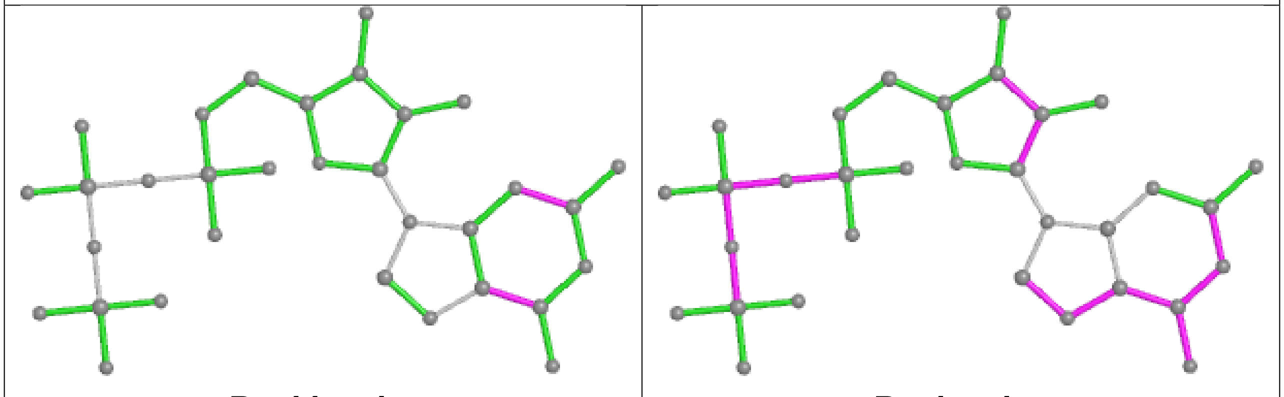


Bond lengths Bond angles

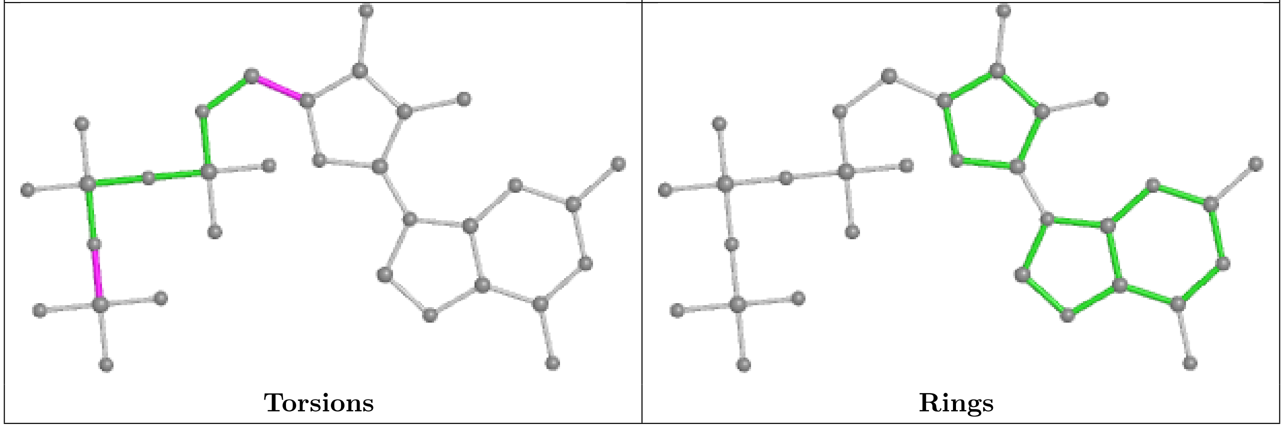


Torsions Rings

Ligand GTP 6d 501

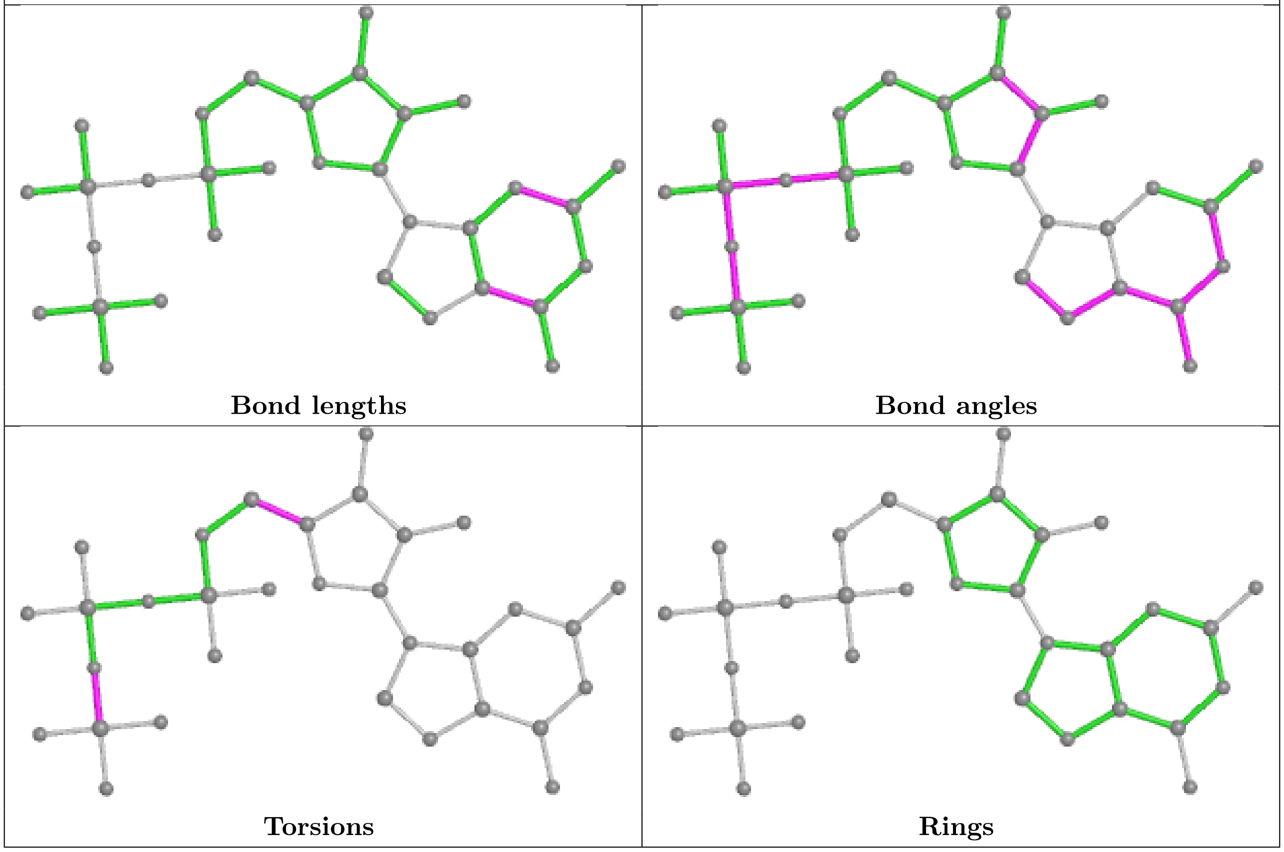


Bond lengths Bond angles



Torsions Rings

Ligand GTP 5d 501



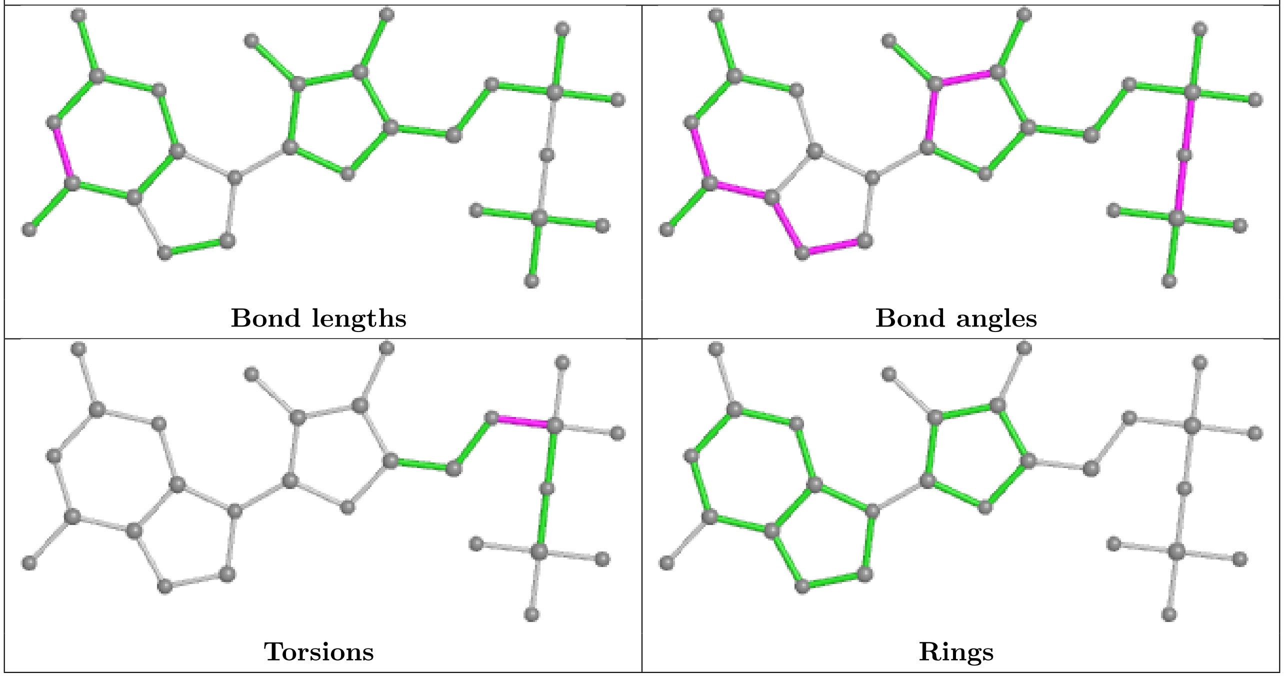
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP Cg 501



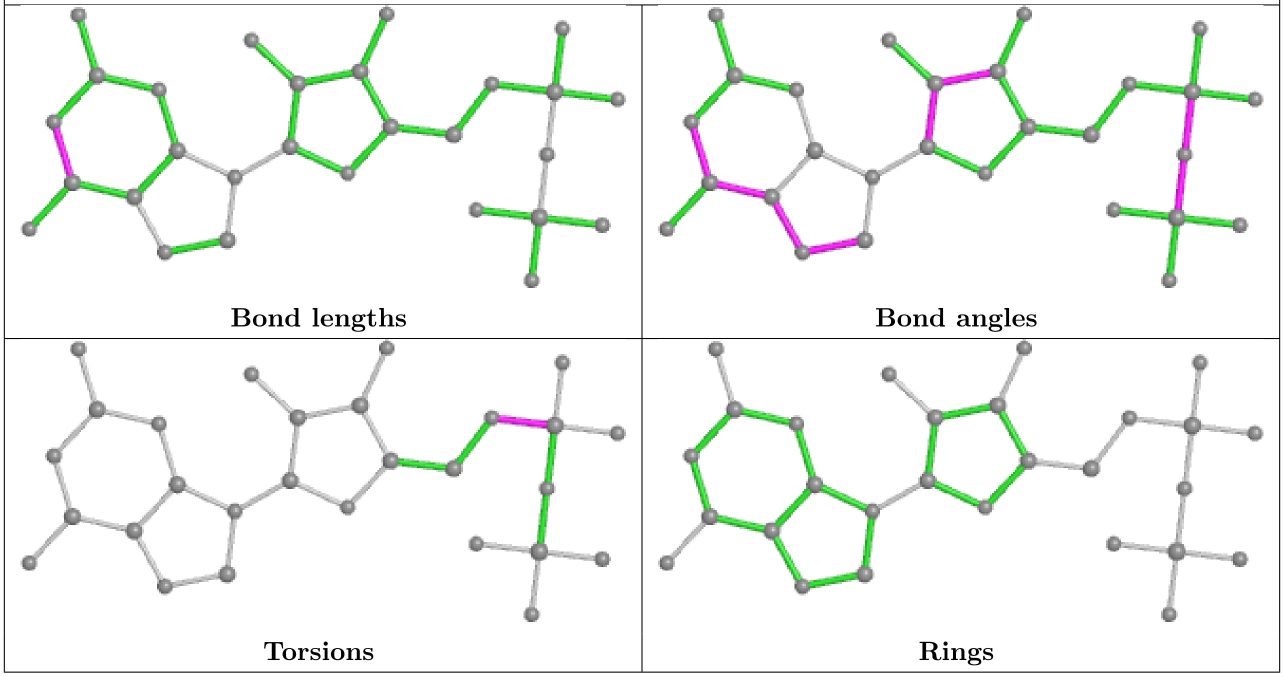
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP 8a 501



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-24191. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

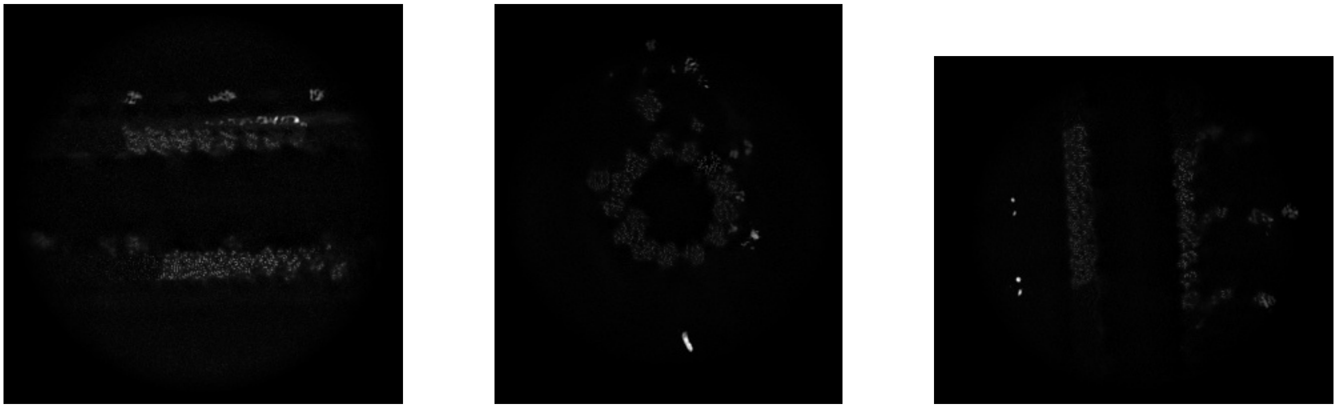
6.1.1 Primary map


X Y Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

6.2.1 Primary map


X Index: 303 Y Index: 263 Z Index: 263

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

6.3.1 Primary map


X Index: 147 Y Index: 294 Z Index: 288

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

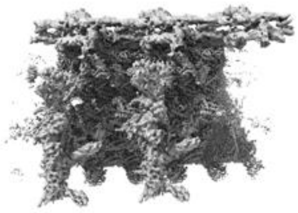
6.4.1 Primary map


X Y Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

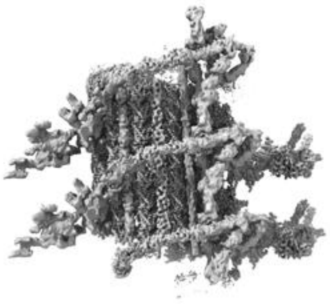
6.5 Orthogonal surface views

6.5.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

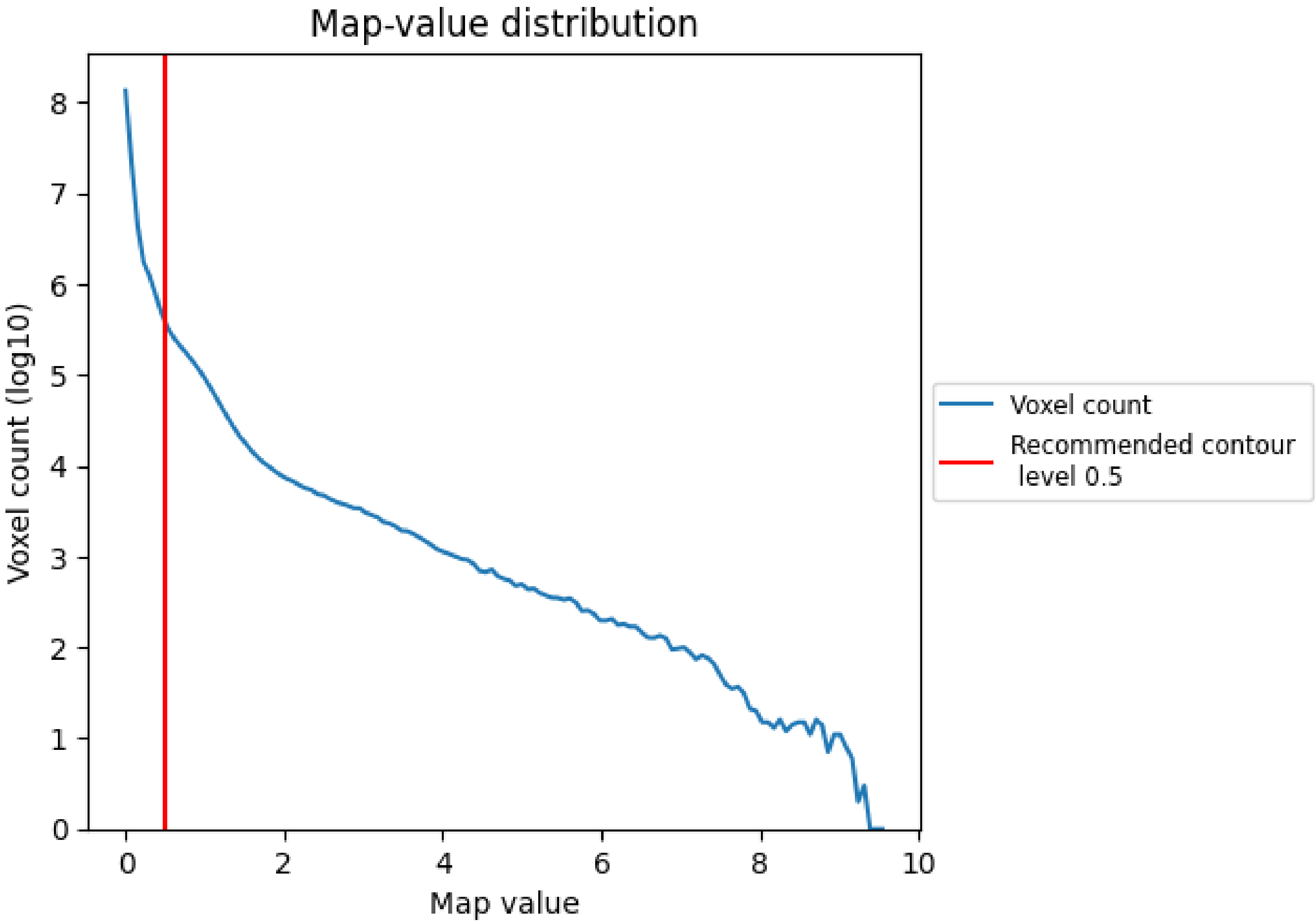
6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

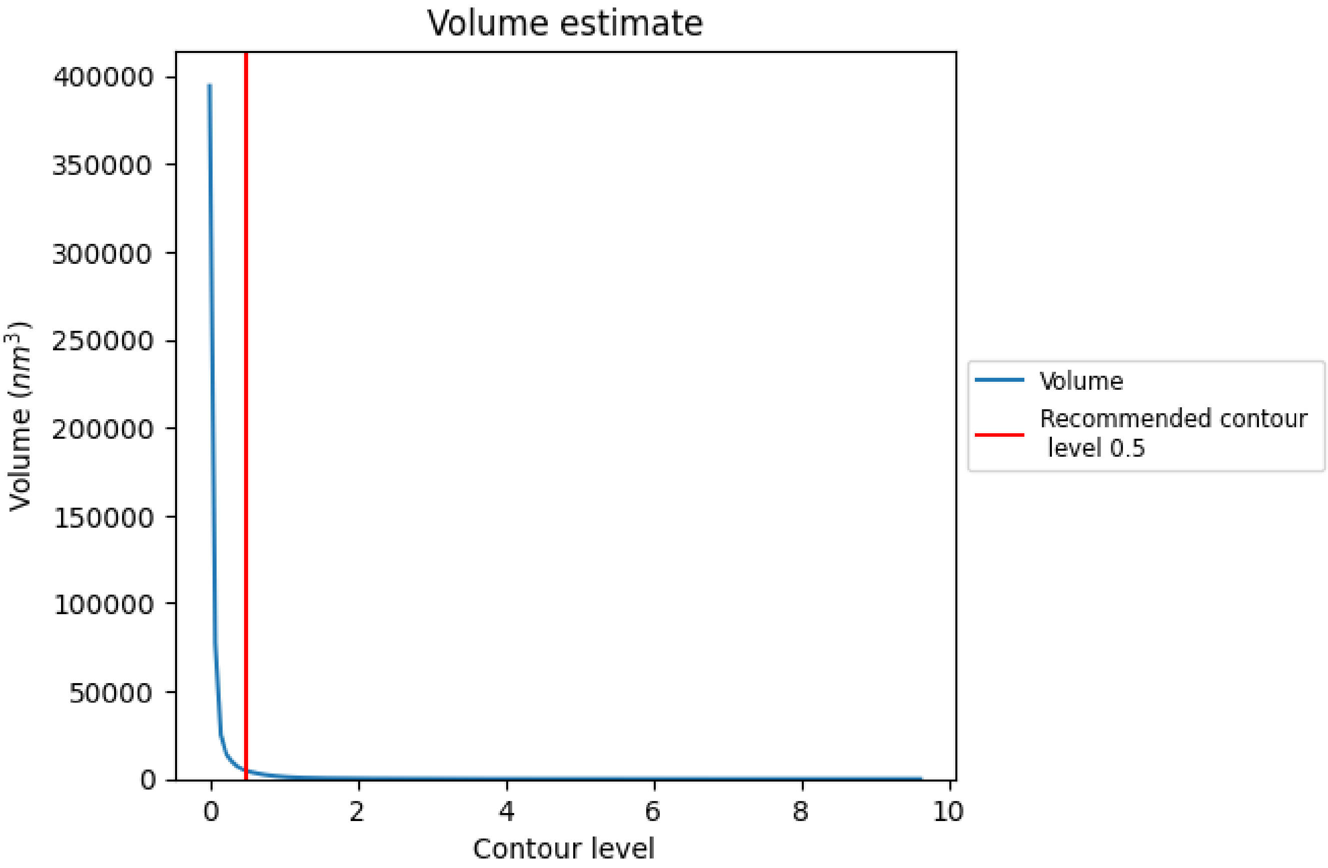
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ



The volume at the recommended contour level is 4655 nm^3; this corresponds to an approximate mass of 4205 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-24191 and PDB model 7N61. Per-residue inclusion information can be found in section 3 on page 24.

9.1 Map-model overlay ⓘ

X Y Z

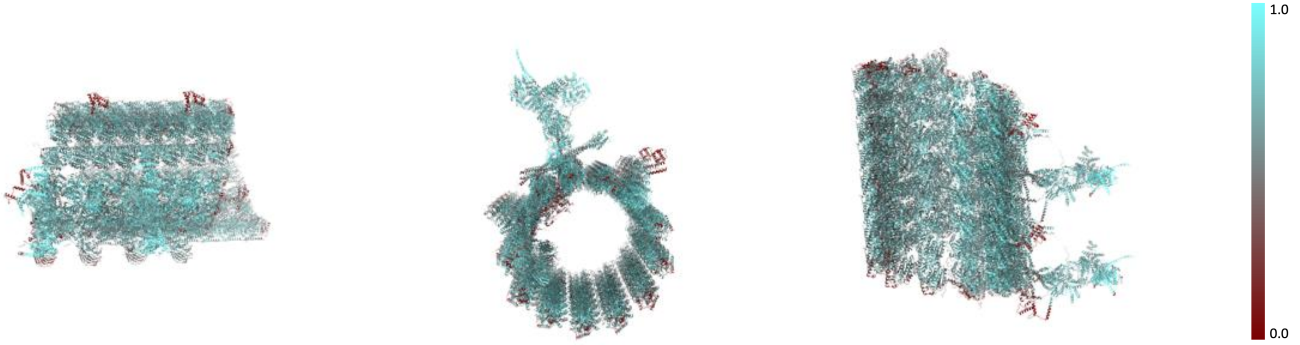
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ

X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

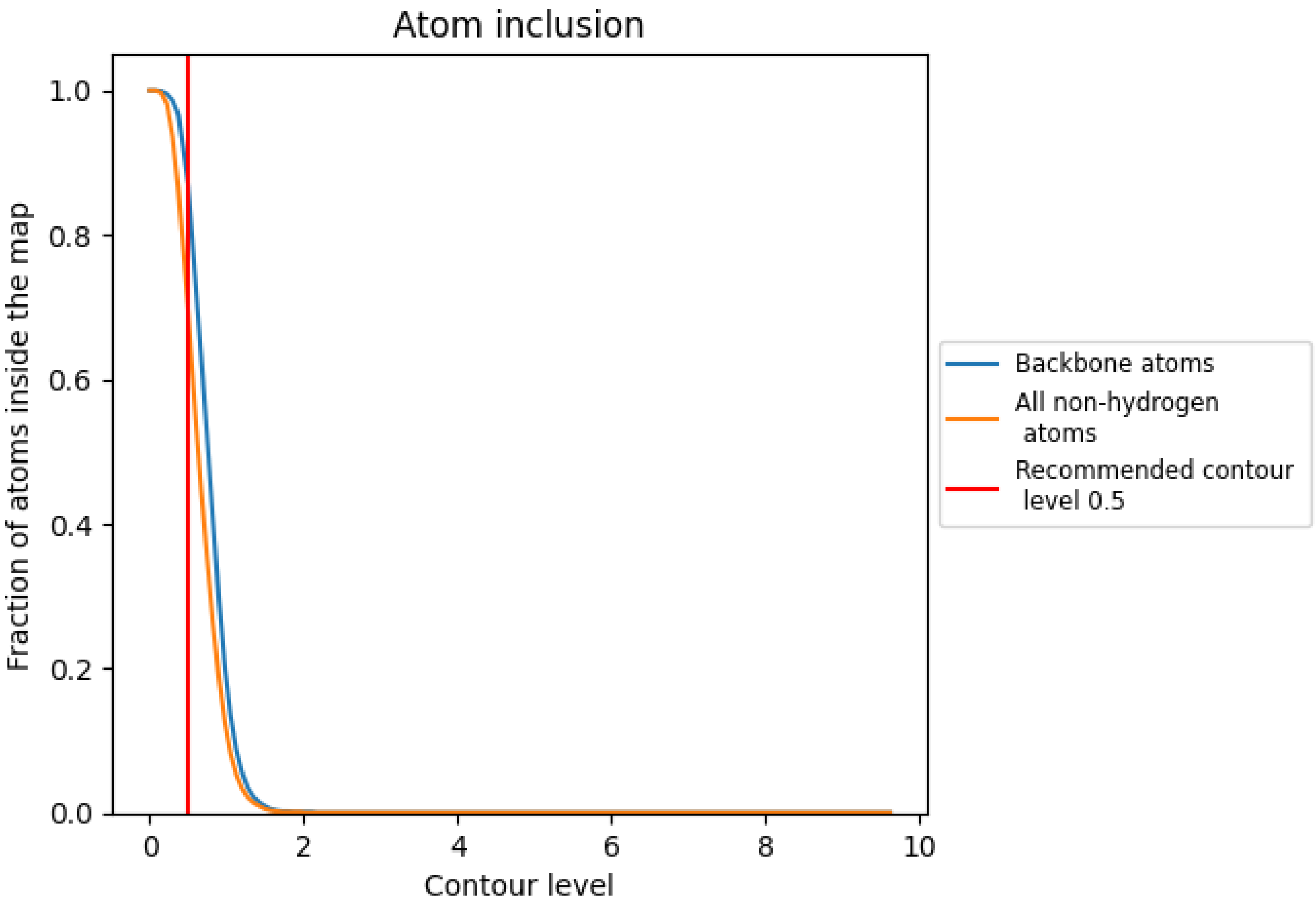
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion ⓘ



At the recommended contour level, 87% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6950	0.4050
0A	0.5700	0.3440
0B	0.6230	0.3750
0C	0.5950	0.3680
0D	0.4350	0.3010
0E	0.6710	0.4680
0F	0.7080	0.4710
0G	0.4120	0.3520
0H	0.6160	0.4340
0I	0.7720	0.3700
0J	0.7870	0.3700
0K	0.5770	0.3620
0L	0.3180	0.2630
0M	0.5730	0.4280
0N	0.4340	0.3900
0O	0.4650	0.3740
0P	0.6640	0.4190
0Q	0.6920	0.4490
0S	0.6390	0.4290
0T	0.6710	0.4930
0U	0.5750	0.4690
0V	0.6030	0.4890
0W	0.8360	0.4680
0X	0.5370	0.4480
0Y	0.4750	0.4020
0Z	0.5290	0.4490
1A	0.4610	0.4040
1B	0.7520	0.3620
1C	0.6740	0.3370
1D	0.7460	0.2730
1E	0.7550	0.2830
1F	0.7520	0.2980
1G	0.7550	0.3060
1H	0.7430	0.4800
1L	0.9580	0.4980

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
1M	0.9600	0.4900
1a	0.7160	0.4460
1b	0.5890	0.3780
1c	0.7430	0.4320
1d	0.7750	0.4650
1e	0.8190	0.4800
1f	0.8030	0.4700
1g	0.8120	0.4690
1h	0.7790	0.4610
2a	0.6370	0.4260
2b	0.5930	0.3910
2c	0.7010	0.4230
2d	0.7290	0.4460
2e	0.7050	0.4370
2f	0.6960	0.4390
2g	0.7460	0.4500
2h	0.6950	0.4330
3a	0.6250	0.4080
3b	0.6710	0.4280
3c	0.7430	0.4390
3d	0.7500	0.4490
3e	0.7170	0.4340
3f	0.6620	0.4190
3g	0.7230	0.4290
3h	0.6850	0.4220
4a	0.5430	0.3810
4b	0.6330	0.4040
4c	0.6700	0.4010
4d	0.6920	0.4170
4e	0.6960	0.4160
4f	0.6750	0.4090
4g	0.7270	0.4230
4h	0.6780	0.4000
5a	0.5660	0.3480
5b	0.5980	0.3720
5c	0.6590	0.3680
5d	0.6490	0.3590
5e	0.6920	0.3760
5f	0.6580	0.3600
5g	0.6980	0.3820
5h	0.6850	0.3680
6a	0.4780	0.2610

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
6b	0.5190	0.3180
6c	0.5830	0.3060
6d	0.6120	0.3220
6e	0.6390	0.3150
6f	0.5940	0.3040
6g	0.6100	0.3000
6h	0.5990	0.2920
7a	0.6030	0.3430
7b	0.5940	0.3630
7c	0.7040	0.3780
7d	0.7040	0.3810
7e	0.7070	0.3680
7f	0.7060	0.3670
7g	0.7080	0.3580
7h	0.6850	0.3530
8a	0.6170	0.3630
8b	0.6490	0.3800
8c	0.7590	0.3980
8d	0.7880	0.4150
8e	0.7750	0.4090
8f	0.7590	0.3890
8g	0.7790	0.3900
8h	0.7380	0.3870
9a	0.7940	0.4710
9b	0.8250	0.5090
9c	0.8380	0.5110
9d	0.8180	0.4800
9e	0.7850	0.4580
9f	0.8260	0.5090
9g	0.8310	0.5060
9h	0.8120	0.4790
Aa	0.6880	0.4040
Ab	0.6060	0.3800
Ac	0.6910	0.3760
Ad	0.7370	0.4000
Ae	0.7450	0.3950
Af	0.7370	0.4100
Ag	0.7500	0.4030
Ah	0.7380	0.4120
Ba	0.5970	0.3670
Bb	0.6530	0.3960
Bc	0.8280	0.4370

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Bd	0.8070	0.4330
Be	0.7300	0.4110
Bf	0.7520	0.4220
Bg	0.8240	0.4410
Bh	0.7980	0.4220
Ca	0.6550	0.4240
Cb	0.6950	0.4330
Cc	0.7850	0.4510
Cd	0.7930	0.4650
Ce	0.8140	0.4710
Cf	0.7770	0.4600
Cg	0.7700	0.4540
Ch	0.7640	0.4510
Da	0.6700	0.4300
Db	0.7180	0.4480
Dc	0.7890	0.4780
Dd	0.8060	0.4770
De	0.8170	0.4830
Df	0.7750	0.4630
Dg	0.7590	0.4680
Dh	0.7190	0.4500