Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 07:55 PM EDT

PDB ID	:	7MIZ
EMDB ID	:	EMD-23869
Title	:	Atomic structure of cortical microtubule from Toxoplasma gondii
Authors	:	Wang, X.; Brown, A.; Sibley, L.D.; Zhang, R.
Deposited on	:	2021-04-18
Resolution	:	3.40 Å(reported)
Based on initial models	:	6U42, 4FYU, 3JAS

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

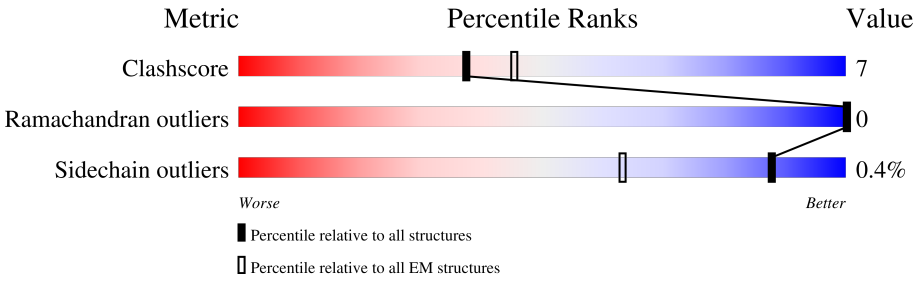
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	0	351	5% · 94%
1	1	351	5% · 94%
1	10	351	5% · 94%
1	11	351	6% 94%
1	12	351	5% · 94%
1	13	351	6% 94%
1	14	351	6% 94%
1	15	351	6% 94%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	16	351	6% 94%
1	17	351	6% 94%
1	18	351	6% 94%
1	19	351	6% 94%
1	2	351	6% 94%
1	20	351	6% 94%
1	21	351	6% 94%
1	22	351	5% 94%
1	23	351	5% 94%
1	3	351	6% 94%
1	4	351	6% 94%
1	5	351	6% 94%
1	6	351	6% 94%
1	7	351	5% 94%
1	8	351	6% 94%
1	9	351	5% 94%
2	A0	453	9% 76% 18% 6%
2	A2	453	8% 75% 19% 6%
2	A4	453	80% 14% 6%
2	A6	453	78% 17% 6%
2	A8	453	76% 18% 6%
2	B0	453	79% 15% 6%
2	B2	453	80% 15% 6%
2	B4	453	74% 20% 6%
2	B6	453	77% 17% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B8	453	74% 19% 6%
2	C0	453	74% 21% 6%
2	C2	453	74% 20% 6%
2	C4	453	68% 26% 6%
2	C6	453	70% 25% 6%
2	C8	453	80% 14% 6%
2	D0	453	82% 12% 6%
2	D2	453	81% 13% 6%
2	D4	453	80% 14% 6%
2	D6	453	79% 15% 6%
2	D8	453	82% 13% 6%
2	E0	453	82% 13% 6%
2	E2	453	80% 14% 6%
2	E4	453	77% 16% 6%
2	E6	453	78% 16% 6%
2	E8	453	72% 23% 6%
2	F0	453	75% 19% 6%
3	A1	449	74% 21% 5%
3	A3	449	76% 18% 5%
3	A5	449	76% 19% 5%
3	A7	449	80% 15% 5%
3	A9	449	74% 20% 5%
3	B1	449	78% 17% 5%
3	B3	449	77% 18% 5%
3	B5	449	78% 17% 5%

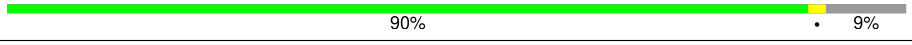
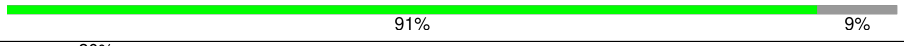
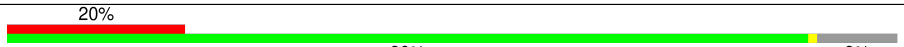
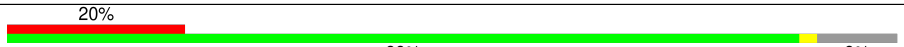
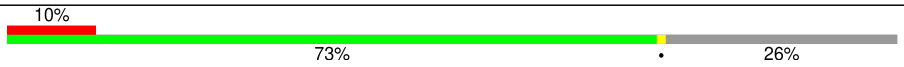
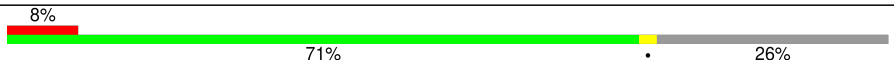
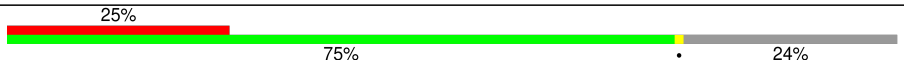
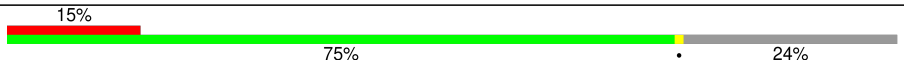
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	B7	449	78% 16% 5%
3	B9	449	77% 17% 5%
3	C1	449	72% 22% 5%
3	C3	449	72% 23% 5%
3	C5	449	72% 23% 5%
3	C7	449	71% 24% 5%
3	C9	449	77% 18% 5%
3	D1	449	78% 17% 5%
3	D3	449	78% 17% 5%
3	D5	449	73% 22% 5%
3	D7	449	75% 20% 5%
3	D9	449	77% 17% 5%
3	E1	449	82% 13% 5%
3	E3	449	79% 16% 5%
3	E5	449	73% 21% 5%
3	E7	449	78% 16% 5%
3	E9	449	73% 21% 5%
3	F1	449	71% 23% 5%
4	a	220	67% 32%
4	b	220	5% 68% 32%
4	c	220	91% 9%
4	d	220	91% 9%
4	e	220	90% 9%
4	f	220	90% 9%
4	g	220	90% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	h	220	
4	i	220	
4	j	220	
4	m	220	
4	n	220	
4	o	220	
4	p	220	
4	q	220	
4	r	220	
4	s	220	
4	t	220	
4	u	220	
4	v	220	
5	k	189	
5	l	189	
5	w	189	
5	x	189	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 214754 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 Microtubule associated protein SPM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	1	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	2	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	3	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	4	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	5	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	6	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	7	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	8	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	9	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	10	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	11	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	12	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	13	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	14	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	15	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	16	22	Total	C	N	O	S	0	0
			174	114	28	31	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	17	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	18	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	19	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	20	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	21	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	22	20	Total	C	N	O	S	0	0
			160	105	26	28	1		
1	23	20	Total	C	N	O	S	0	0
			160	105	26	28	1		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	93	ARG	PRO	conflict	UNP A0A7J6K285
1	93	ARG	PRO	conflict	UNP A0A7J6K285
2	93	ARG	PRO	conflict	UNP A0A7J6K285
3	93	ARG	PRO	conflict	UNP A0A7J6K285
4	93	ARG	PRO	conflict	UNP A0A7J6K285
5	93	ARG	PRO	conflict	UNP A0A7J6K285
6	93	ARG	PRO	conflict	UNP A0A7J6K285
7	93	ARG	PRO	conflict	UNP A0A7J6K285
8	93	ARG	PRO	conflict	UNP A0A7J6K285
9	93	ARG	PRO	conflict	UNP A0A7J6K285
10	93	ARG	PRO	conflict	UNP A0A7J6K285
11	93	ARG	PRO	conflict	UNP A0A7J6K285
12	93	ARG	PRO	conflict	UNP A0A7J6K285
13	93	ARG	PRO	conflict	UNP A0A7J6K285
14	93	ARG	PRO	conflict	UNP A0A7J6K285
15	93	ARG	PRO	conflict	UNP A0A7J6K285
16	93	ARG	PRO	conflict	UNP A0A7J6K285
17	93	ARG	PRO	conflict	UNP A0A7J6K285
18	93	ARG	PRO	conflict	UNP A0A7J6K285
19	93	ARG	PRO	conflict	UNP A0A7J6K285
20	93	ARG	PRO	conflict	UNP A0A7J6K285
21	93	ARG	PRO	conflict	UNP A0A7J6K285
22	93	ARG	PRO	conflict	UNP A0A7J6K285
23	93	ARG	PRO	conflict	UNP A0A7J6K285

- Molecule 2 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	A2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	A4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	A6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	A8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	B0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	B2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	B4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	B6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	B8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	C0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	C2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	C4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	C6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	C8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	D0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	D2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	D4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	D6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	D8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	E0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	E4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	E6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	E8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	F0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		

- Molecule 3 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A1	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	A3	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	A5	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	A7	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	A9	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	B1	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	B3	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	B5	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	B7	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	B9	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	C1	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	C3	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	C5	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	C7	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C9	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	D1	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	D3	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	D5	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	D7	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	D9	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	E1	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	E3	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	E5	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	E7	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	E9	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	F1	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		

- Molecule 4 is a protein called PDI family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	a	150	Total	C	N	O	S	0	0
			1198	763	213	217	5		
4	b	150	Total	C	N	O	S	0	0
			1198	763	213	217	5		
4	c	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	d	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	e	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	f	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	g	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	h	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	i	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	j	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	o	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	p	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	q	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	r	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	s	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	t	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	u	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	v	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	n	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	m	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		

- Molecule 5 is a protein called PDI family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	k	139	Total	C	N	O	S	0	0
			1140	738	203	195	4		
5	l	139	Total	C	N	O	S	0	0
			1140	738	203	195	4		
5	w	143	Total	C	N	O	S	0	0
			1172	755	207	205	5		
5	x	143	Total	C	N	O	S	0	0
			1172	755	207	205	5		

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	167	SER	-	insertion	UNP A0A7J6K232

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
k	168	ALA	-	insertion	UNP A0A7J6K232
k	169	GLN	-	insertion	UNP A0A7J6K232
k	170	ARG	-	insertion	UNP A0A7J6K232
k	171	LEU	-	insertion	UNP A0A7J6K232
k	172	ARG	-	insertion	UNP A0A7J6K232
k	173	THR	-	insertion	UNP A0A7J6K232
k	174	LEU	-	insertion	UNP A0A7J6K232
k	175	ASN	-	insertion	UNP A0A7J6K232
k	176	ASP	-	insertion	UNP A0A7J6K232
k	177	ALA	-	insertion	UNP A0A7J6K232
k	178	THR	-	insertion	UNP A0A7J6K232
k	179	ASP	-	insertion	UNP A0A7J6K232
k	180	PRO	-	insertion	UNP A0A7J6K232
k	181	TRP	-	insertion	UNP A0A7J6K232
k	182	LYS	-	insertion	UNP A0A7J6K232
k	183	LYS	-	insertion	UNP A0A7J6K232
k	184	ARG	-	insertion	UNP A0A7J6K232
k	185	LEU	-	insertion	UNP A0A7J6K232
k	186	PRO	-	insertion	UNP A0A7J6K232
k	187	GLN	-	insertion	UNP A0A7J6K232
k	188	ASN	-	insertion	UNP A0A7J6K232
k	189	VAL	-	insertion	UNP A0A7J6K232
l	167	SER	-	insertion	UNP A0A7J6K232
l	168	ALA	-	insertion	UNP A0A7J6K232
l	169	GLN	-	insertion	UNP A0A7J6K232
l	170	ARG	-	insertion	UNP A0A7J6K232
l	171	LEU	-	insertion	UNP A0A7J6K232
l	172	ARG	-	insertion	UNP A0A7J6K232
l	173	THR	-	insertion	UNP A0A7J6K232
l	174	LEU	-	insertion	UNP A0A7J6K232
l	175	ASN	-	insertion	UNP A0A7J6K232
l	176	ASP	-	insertion	UNP A0A7J6K232
l	177	ALA	-	insertion	UNP A0A7J6K232
l	178	THR	-	insertion	UNP A0A7J6K232
l	179	ASP	-	insertion	UNP A0A7J6K232
l	180	PRO	-	insertion	UNP A0A7J6K232
l	181	TRP	-	insertion	UNP A0A7J6K232
l	182	LYS	-	insertion	UNP A0A7J6K232
l	183	LYS	-	insertion	UNP A0A7J6K232
l	184	ARG	-	insertion	UNP A0A7J6K232
l	185	LEU	-	insertion	UNP A0A7J6K232
l	186	PRO	-	insertion	UNP A0A7J6K232

Continued on next page...

Continued from previous page...

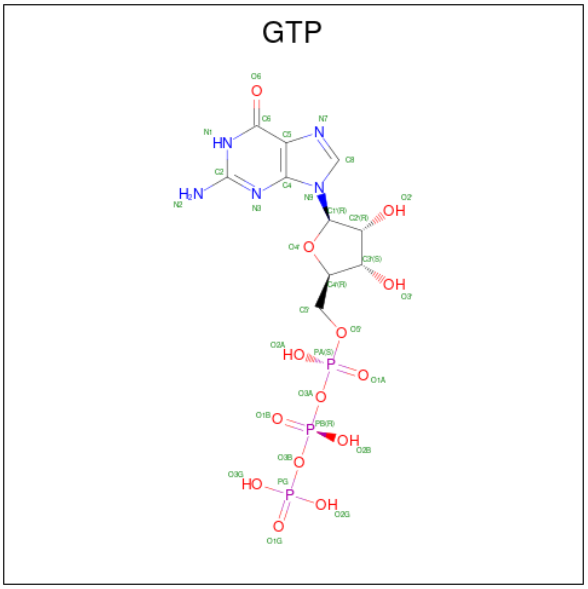
Chain	Residue	Modelled	Actual	Comment	Reference
l	187	GLN	-	insertion	UNP A0A7J6K232
l	188	ASN	-	insertion	UNP A0A7J6K232
l	189	VAL	-	insertion	UNP A0A7J6K232
w	167	SER	-	insertion	UNP A0A7J6K232
w	168	ALA	-	insertion	UNP A0A7J6K232
w	169	GLN	-	insertion	UNP A0A7J6K232
w	170	ARG	-	insertion	UNP A0A7J6K232
w	171	LEU	-	insertion	UNP A0A7J6K232
w	172	ARG	-	insertion	UNP A0A7J6K232
w	173	THR	-	insertion	UNP A0A7J6K232
w	174	LEU	-	insertion	UNP A0A7J6K232
w	175	ASN	-	insertion	UNP A0A7J6K232
w	176	ASP	-	insertion	UNP A0A7J6K232
w	177	ALA	-	insertion	UNP A0A7J6K232
w	178	THR	-	insertion	UNP A0A7J6K232
w	179	ASP	-	insertion	UNP A0A7J6K232
w	180	PRO	-	insertion	UNP A0A7J6K232
w	181	TRP	-	insertion	UNP A0A7J6K232
w	182	LYS	-	insertion	UNP A0A7J6K232
w	183	LYS	-	insertion	UNP A0A7J6K232
w	184	ARG	-	insertion	UNP A0A7J6K232
w	185	LEU	-	insertion	UNP A0A7J6K232
w	186	PRO	-	insertion	UNP A0A7J6K232
w	187	GLN	-	insertion	UNP A0A7J6K232
w	188	ASN	-	insertion	UNP A0A7J6K232
w	189	VAL	-	insertion	UNP A0A7J6K232
x	167	SER	-	insertion	UNP A0A7J6K232
x	168	ALA	-	insertion	UNP A0A7J6K232
x	169	GLN	-	insertion	UNP A0A7J6K232
x	170	ARG	-	insertion	UNP A0A7J6K232
x	171	LEU	-	insertion	UNP A0A7J6K232
x	172	ARG	-	insertion	UNP A0A7J6K232
x	173	THR	-	insertion	UNP A0A7J6K232
x	174	LEU	-	insertion	UNP A0A7J6K232
x	175	ASN	-	insertion	UNP A0A7J6K232
x	176	ASP	-	insertion	UNP A0A7J6K232
x	177	ALA	-	insertion	UNP A0A7J6K232
x	178	THR	-	insertion	UNP A0A7J6K232
x	179	ASP	-	insertion	UNP A0A7J6K232
x	180	PRO	-	insertion	UNP A0A7J6K232
x	181	TRP	-	insertion	UNP A0A7J6K232
x	182	LYS	-	insertion	UNP A0A7J6K232

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
x	183	LYS	-	insertion	UNP A0A7J6K232
x	184	ARG	-	insertion	UNP A0A7J6K232
x	185	LEU	-	insertion	UNP A0A7J6K232
x	186	PRO	-	insertion	UNP A0A7J6K232
x	187	GLN	-	insertion	UNP A0A7J6K232
x	188	ASN	-	insertion	UNP A0A7J6K232
x	189	VAL	-	insertion	UNP A0A7J6K232

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
6	A0	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	A2	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	A4	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	A6	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	A8	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	B0	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	B2	1	Total	C	N	O	P	0
			32	10	5	14	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
6	B4	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	B6	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	B8	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	C0	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	C2	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	C4	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	C6	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	C8	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	D0	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	D2	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	D4	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	D6	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	D8	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	E0	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	E2	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	E4	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	E6	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	E8	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	F0	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

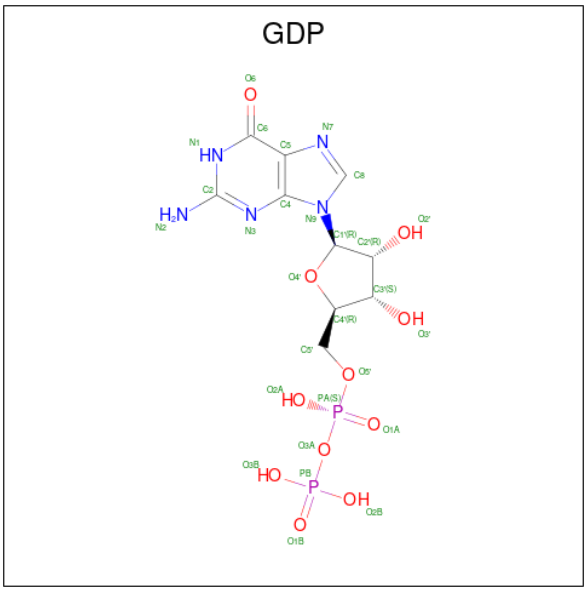
Mol	Chain	Residues	Atoms	AltConf
7	A0	1	Total Mg 1 1	0
7	A2	1	Total Mg 1 1	0
7	A4	1	Total Mg 1 1	0
7	A6	1	Total Mg 1 1	0
7	A8	1	Total Mg 1 1	0
7	B0	1	Total Mg 1 1	0
7	B2	1	Total Mg 1 1	0
7	B4	1	Total Mg 1 1	0
7	B6	1	Total Mg 1 1	0
7	B8	1	Total Mg 1 1	0
7	C0	1	Total Mg 1 1	0
7	C2	1	Total Mg 1 1	0
7	C4	1	Total Mg 1 1	0
7	C6	1	Total Mg 1 1	0
7	C8	1	Total Mg 1 1	0
7	D0	1	Total Mg 1 1	0
7	D2	1	Total Mg 1 1	0
7	D4	1	Total Mg 1 1	0
7	D6	1	Total Mg 1 1	0
7	D8	1	Total Mg 1 1	0
7	E0	1	Total Mg 1 1	0
7	E2	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
7	E4	1	Total Mg 1 1	0
7	E6	1	Total Mg 1 1	0
7	E8	1	Total Mg 1 1	0
7	F0	1	Total Mg 1 1	0

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms	AltConf
8	A1	1	Total C N O P 28 10 5 11 2	0
8	A3	1	Total C N O P 28 10 5 11 2	0
8	A5	1	Total C N O P 28 10 5 11 2	0
8	A7	1	Total C N O P 28 10 5 11 2	0
8	A9	1	Total C N O P 28 10 5 11 2	0
8	B1	1	Total C N O P 28 10 5 11 2	0
8	B3	1	Total C N O P 28 10 5 11 2	0

Continued on next page...

Continued from previous page...

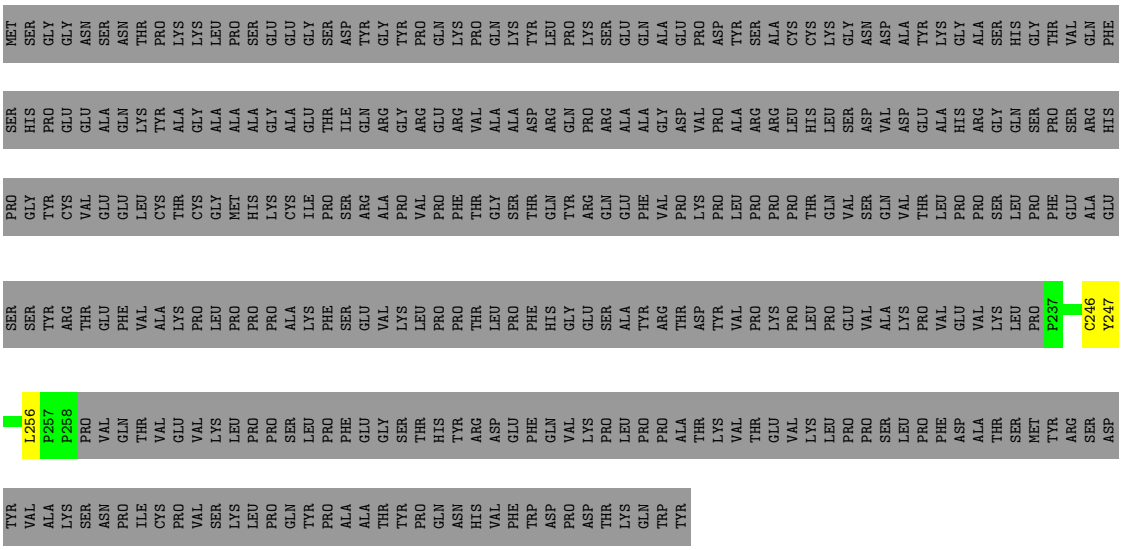
Mol	Chain	Residues	Atoms					AltConf
8	B5	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	B7	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	B9	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	C1	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	C3	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	C5	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	C7	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	C9	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	D1	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	D3	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	D5	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	D7	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	D9	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	E1	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	E3	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	E5	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	E7	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	E9	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	F1	1	Total	C	N	O	P	0
			28	10	5	11	2	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

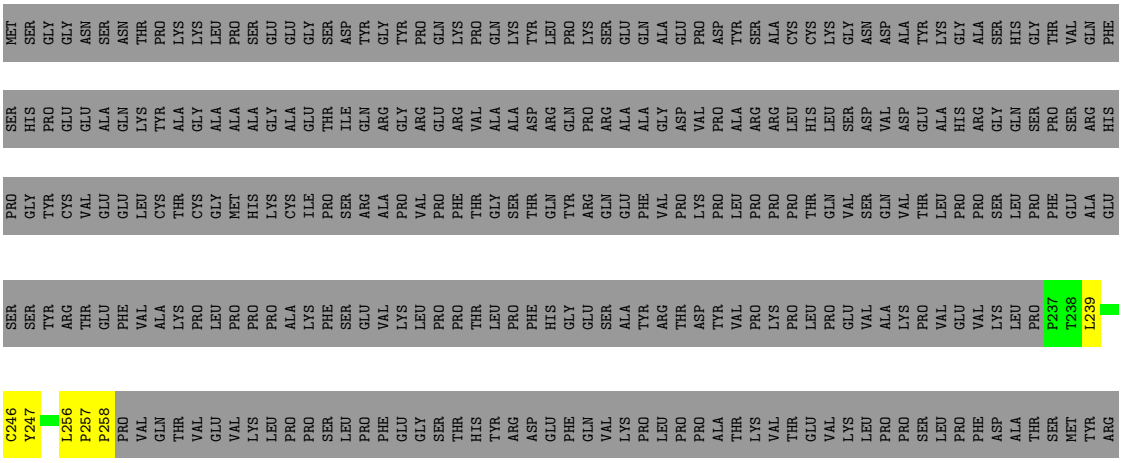
• Molecule 1: Microtubule associated protein SPM1

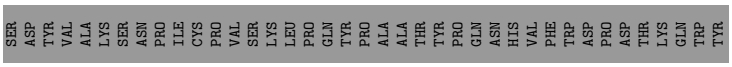
Chain 0:



• Molecule 1: Microtubule associated protein SPM1

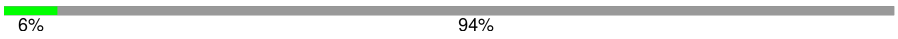
Chain 1:

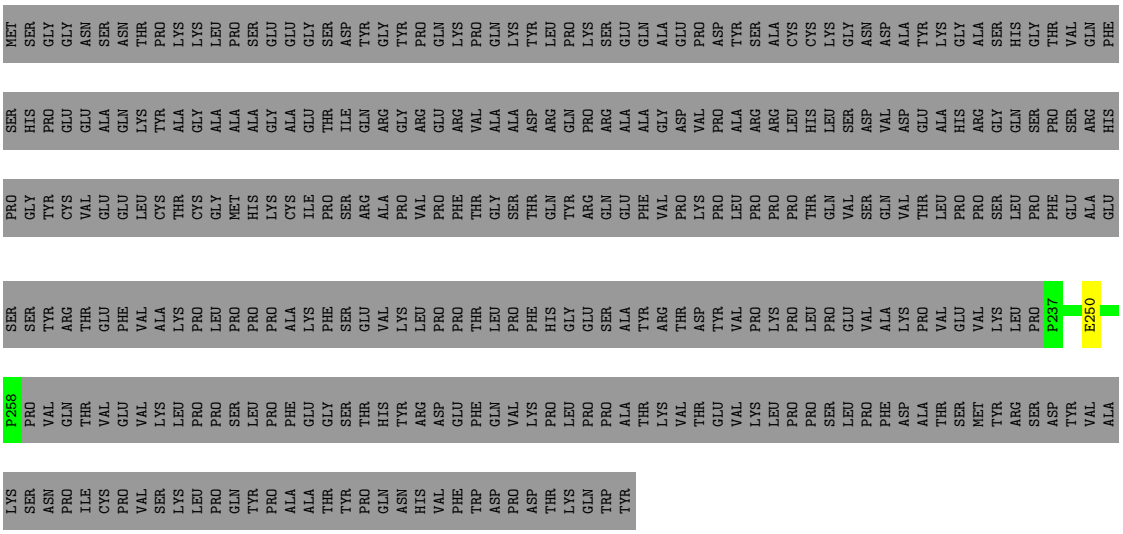




• Molecule 1: Microtubule associated protein SPM1

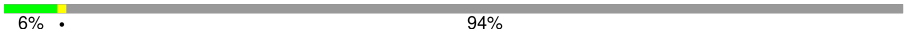
Chain 2:

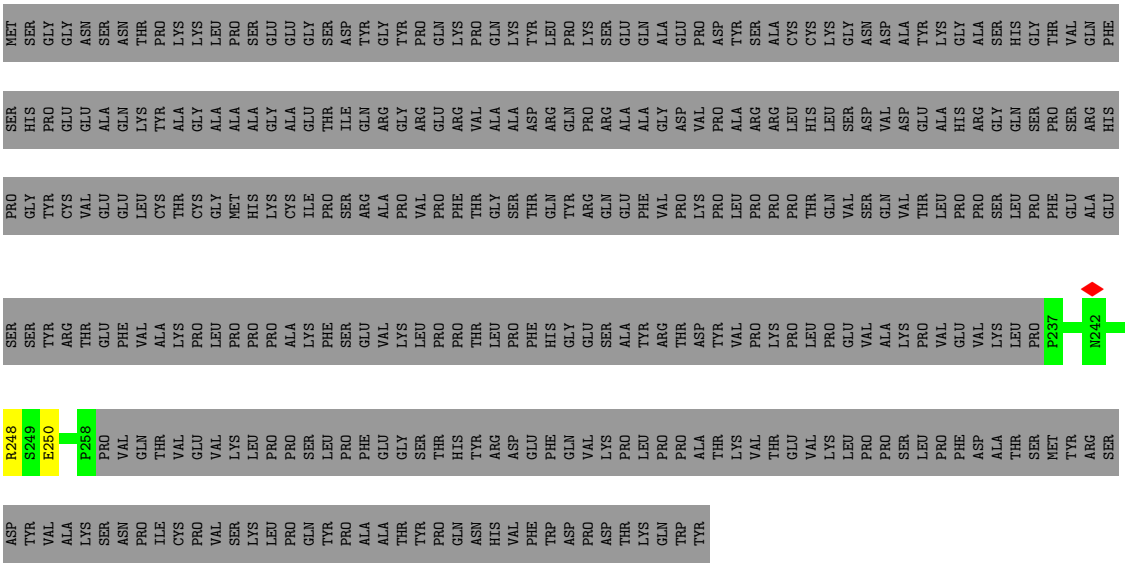




• Molecule 1: Microtubule associated protein SPM1

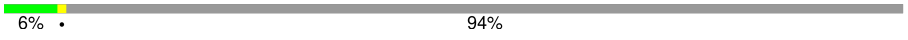
Chain 3:

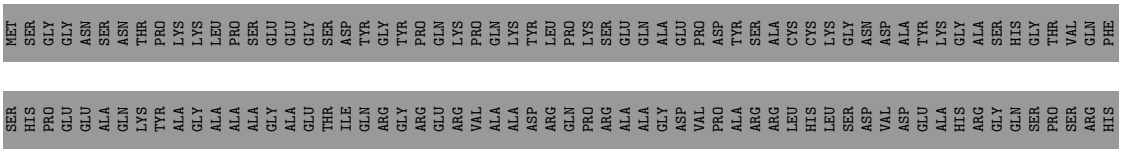


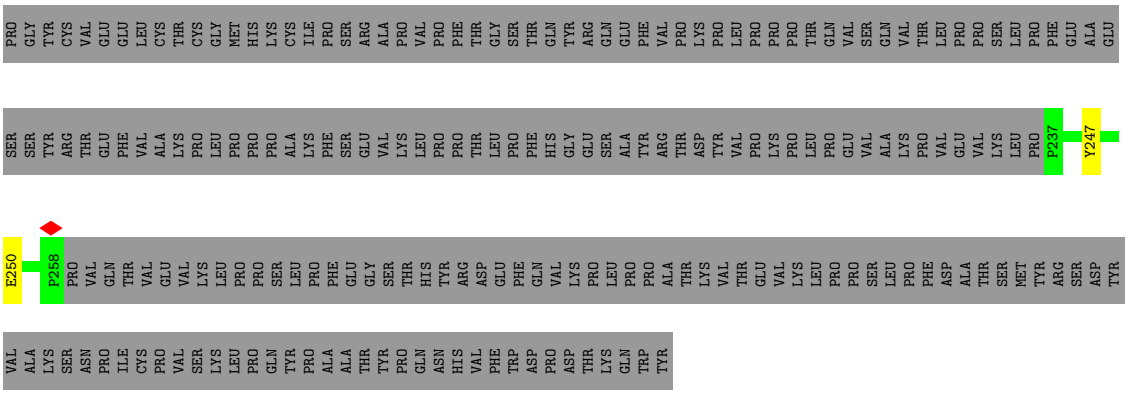


• Molecule 1: Microtubule associated protein SPM1

Chain 4:

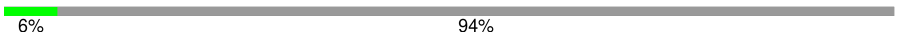






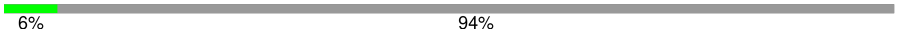
• Molecule 1: Microtubule associated protein SPM1

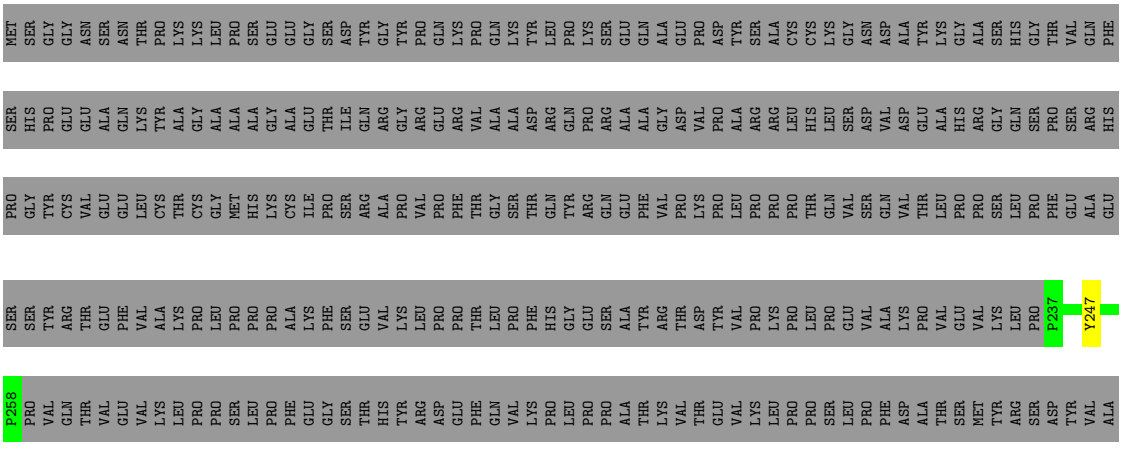
Chain 5:



• Molecule 1: Microtubule associated protein SPM1

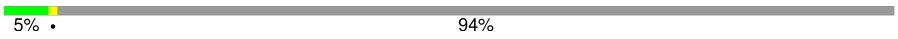
Chain 6:

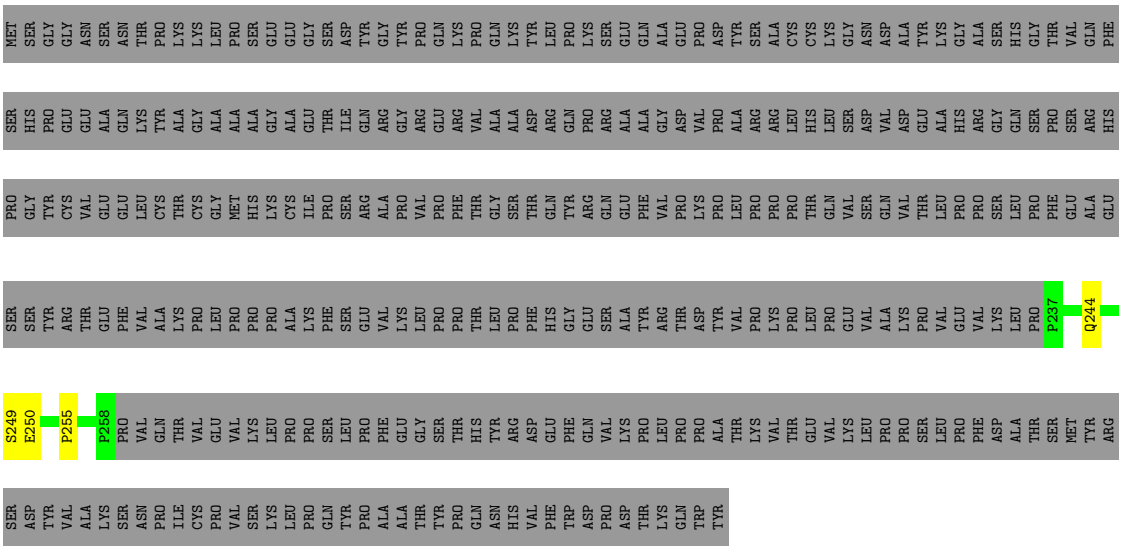




• Molecule 1: Microtubule associated protein SPM1

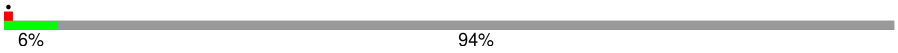
Chain 7:





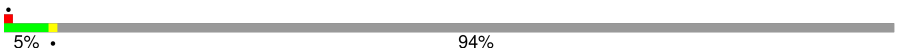
• Molecule 1: Microtubule associated protein SPM1

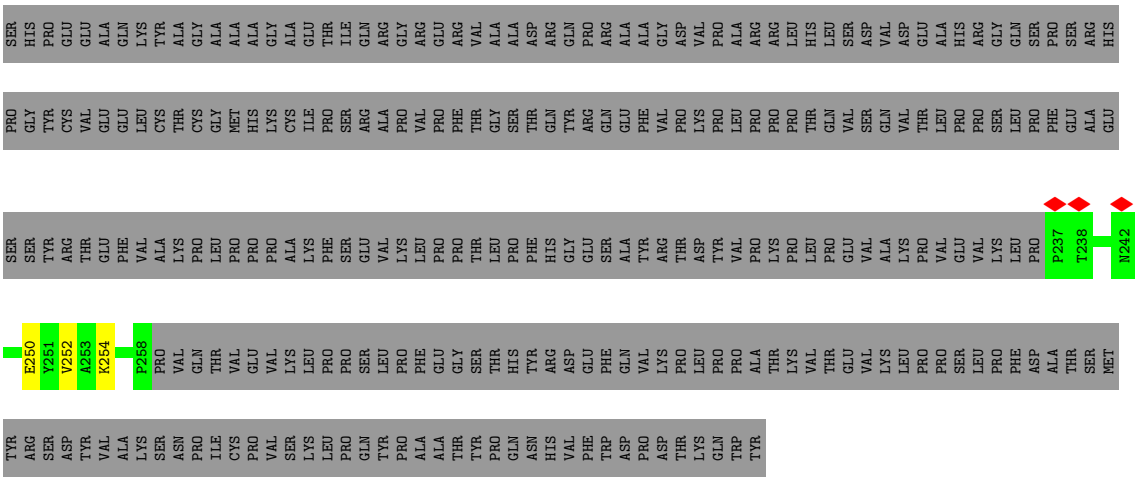
Chain 8:



• Molecule 1: Microtubule associated protein SPM1

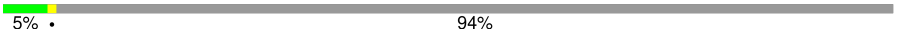
Chain 9:

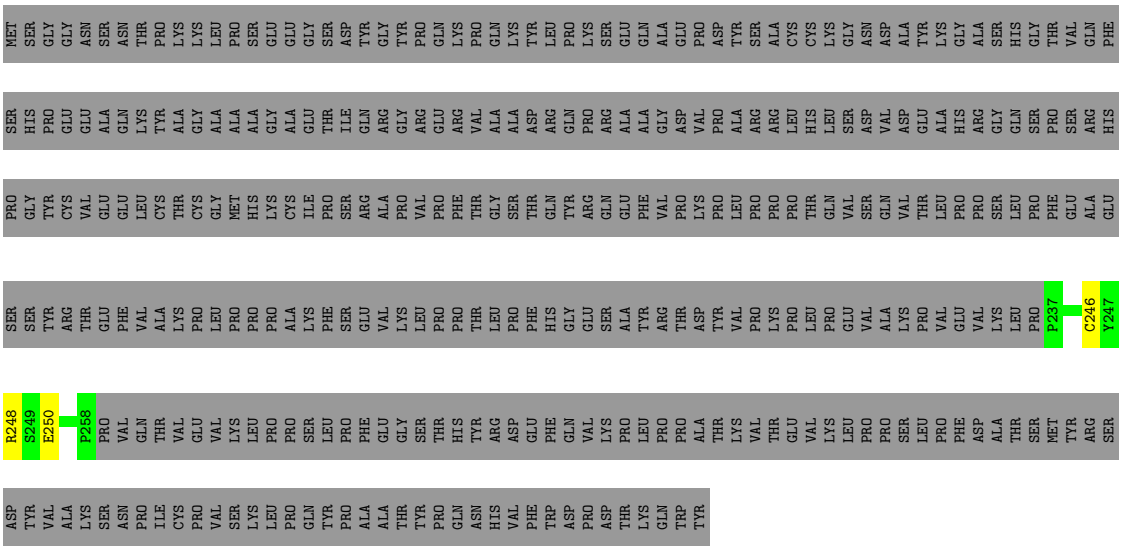




• Molecule 1: Microtubule associated protein SPM1

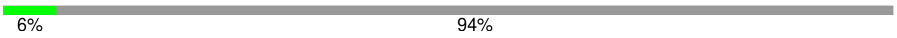
Chain 10:

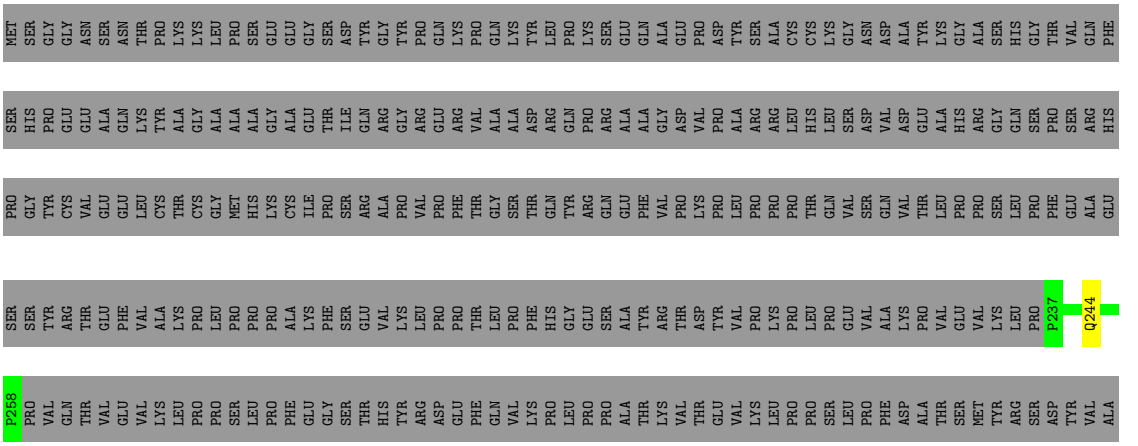




• Molecule 1: Microtubule associated protein SPM1

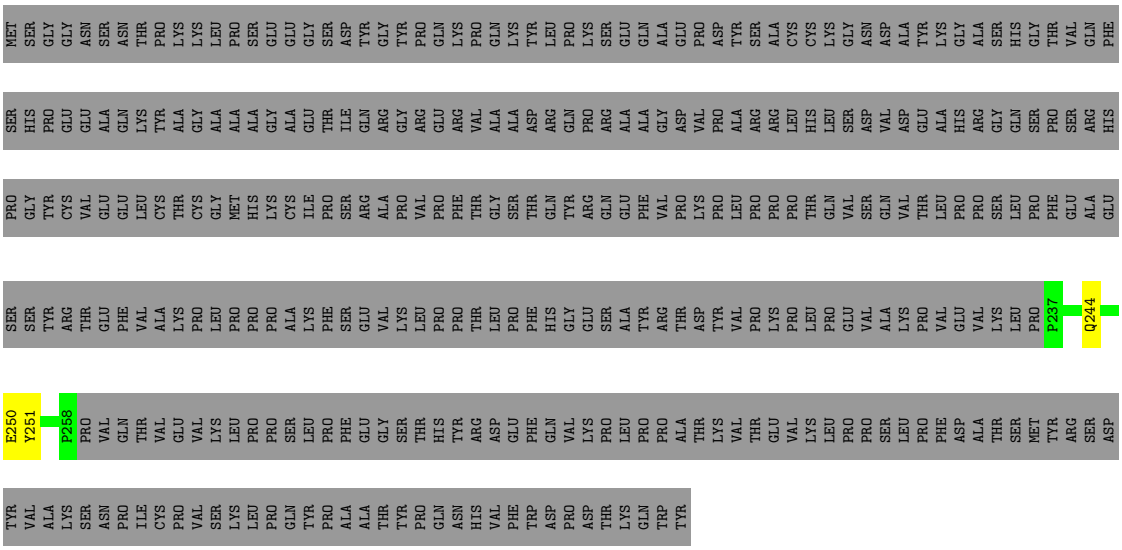
Chain 11:





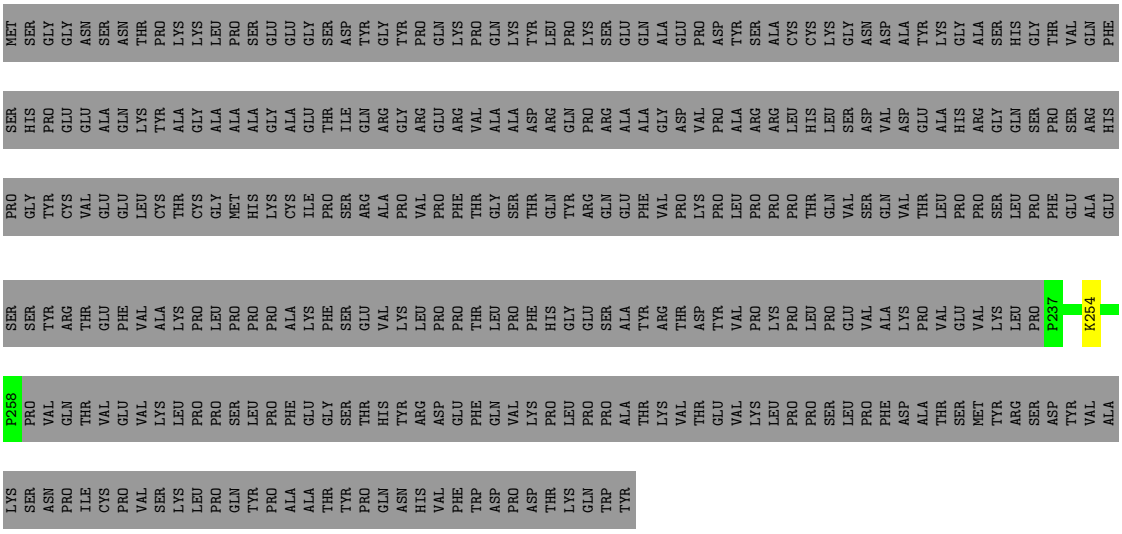
• Molecule 1: Microtubule associated protein SPM1

Chain 12: 5% 94%



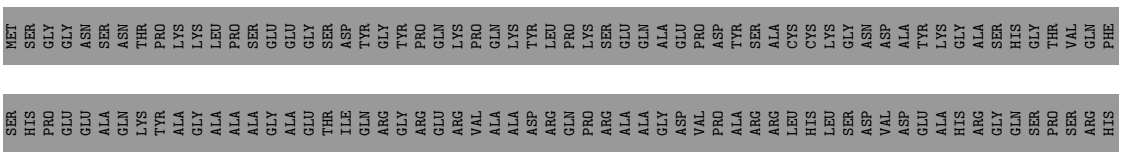
• Molecule 1: Microtubule associated protein SPM1

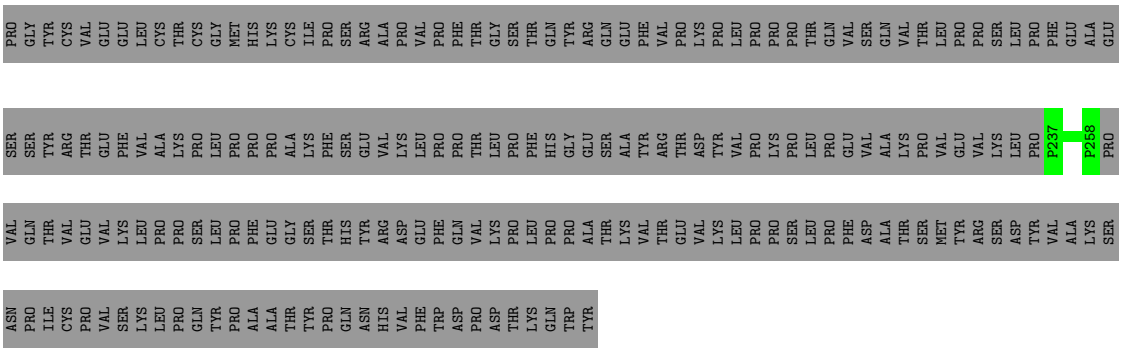
Chain 13: 6% 94%



• Molecule 1: Microtubule associated protein SPM1

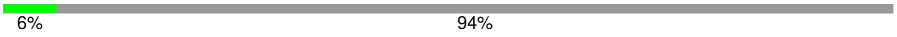
Chain 14: 6% 94%

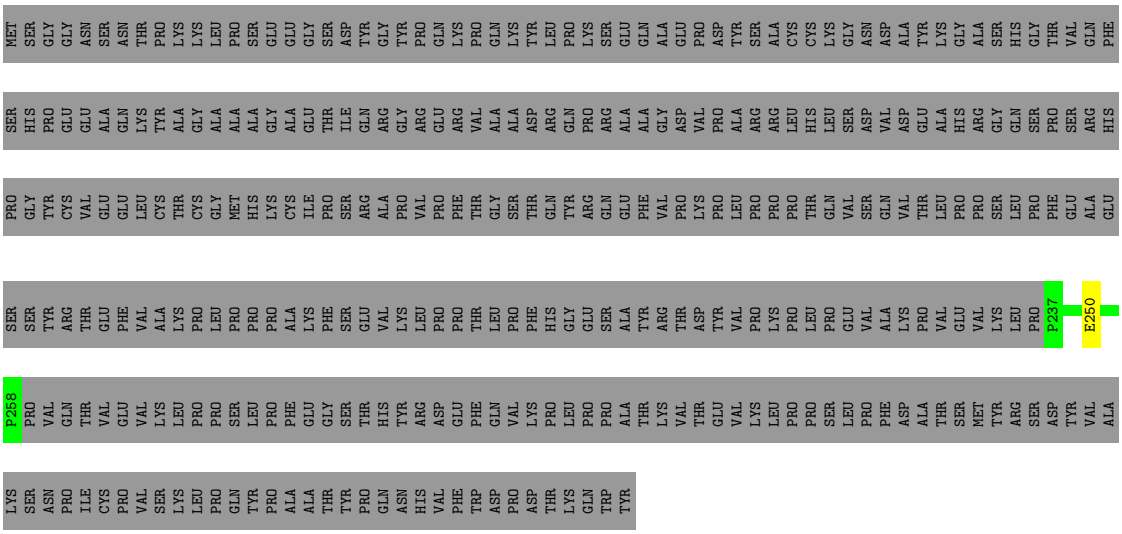




• Molecule 1: Microtubule associated protein SPM1

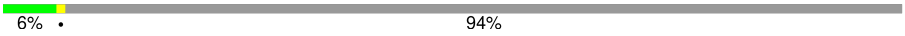
Chain 15:





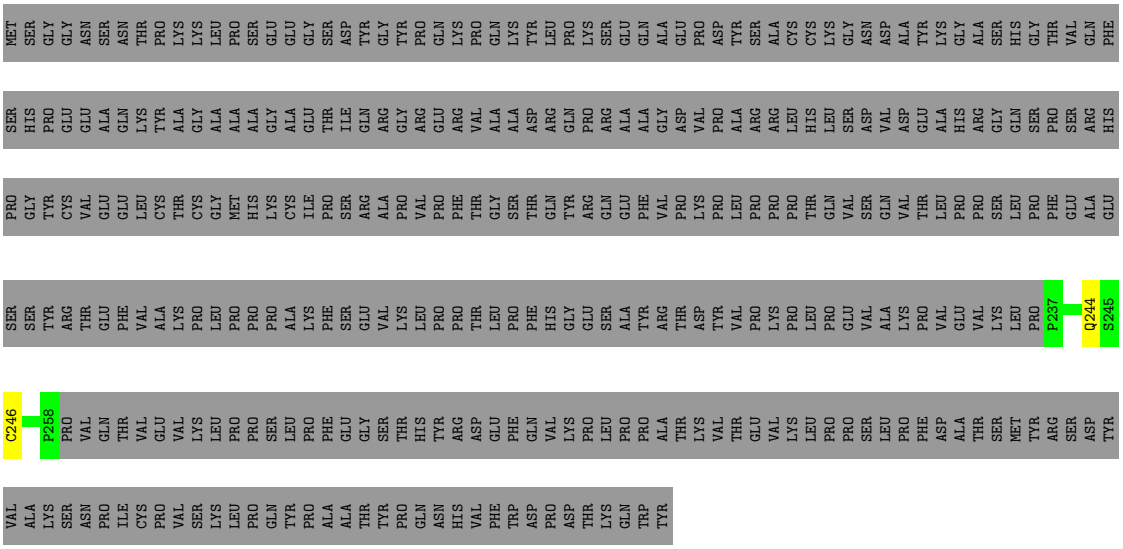
• Molecule 1: Microtubule associated protein SPM1

Chain 16:



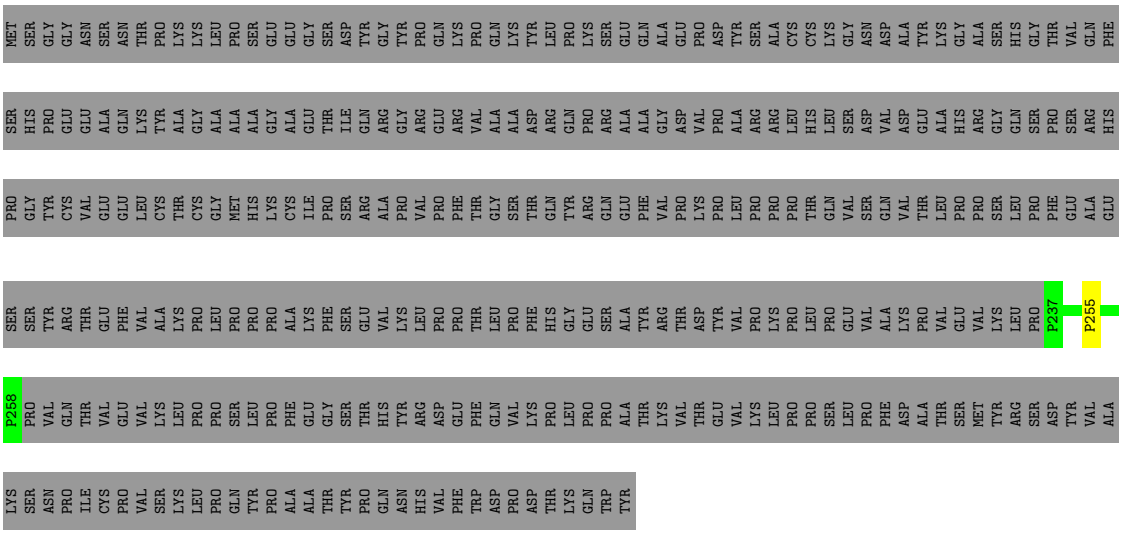
• Molecule 1: Microtubule associated protein SPM1

Chain 17:



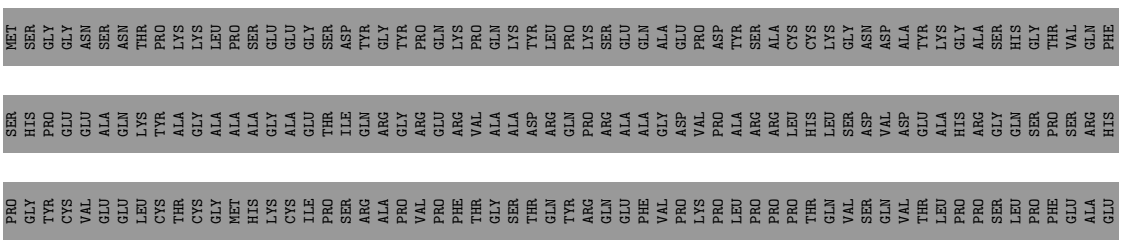
• Molecule 1: Microtubule associated protein SPM1

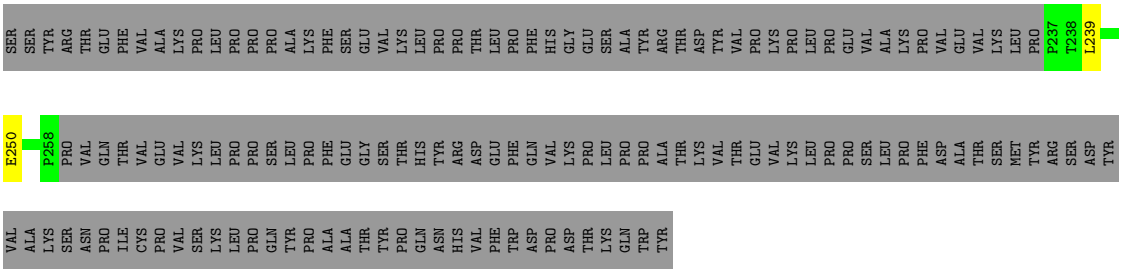
Chain 18:



• Molecule 1: Microtubule associated protein SPM1

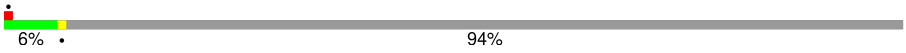
Chain 19:

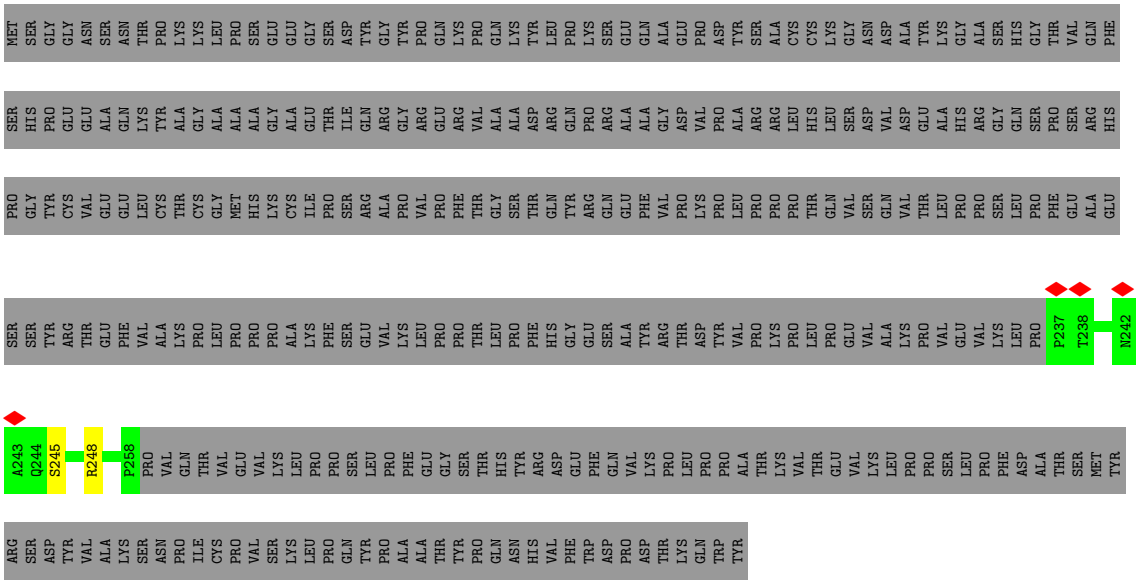




• Molecule 1: Microtubule associated protein SPM1

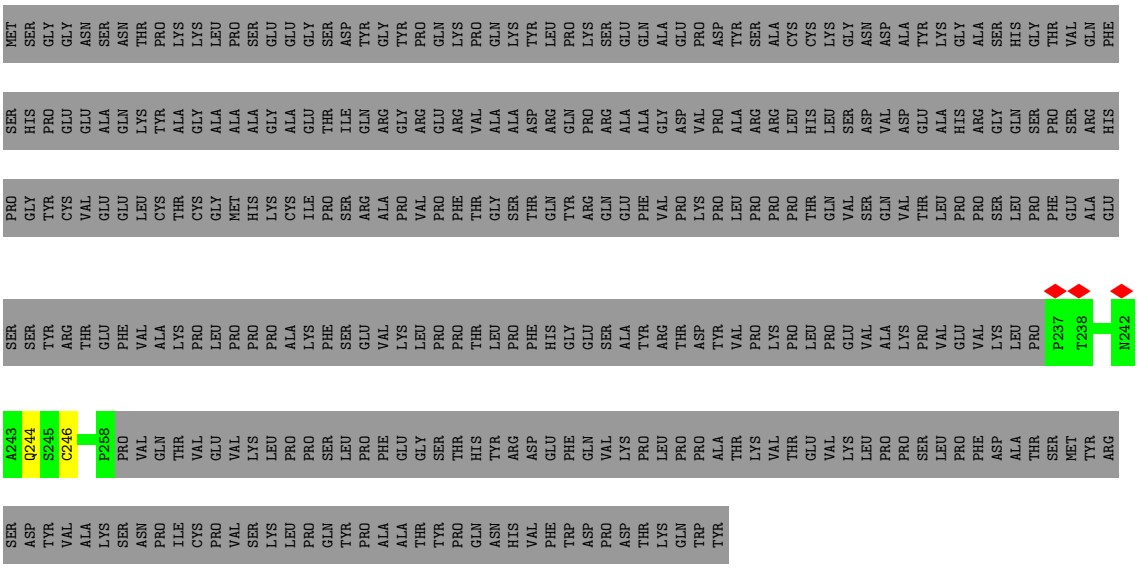
Chain 20:





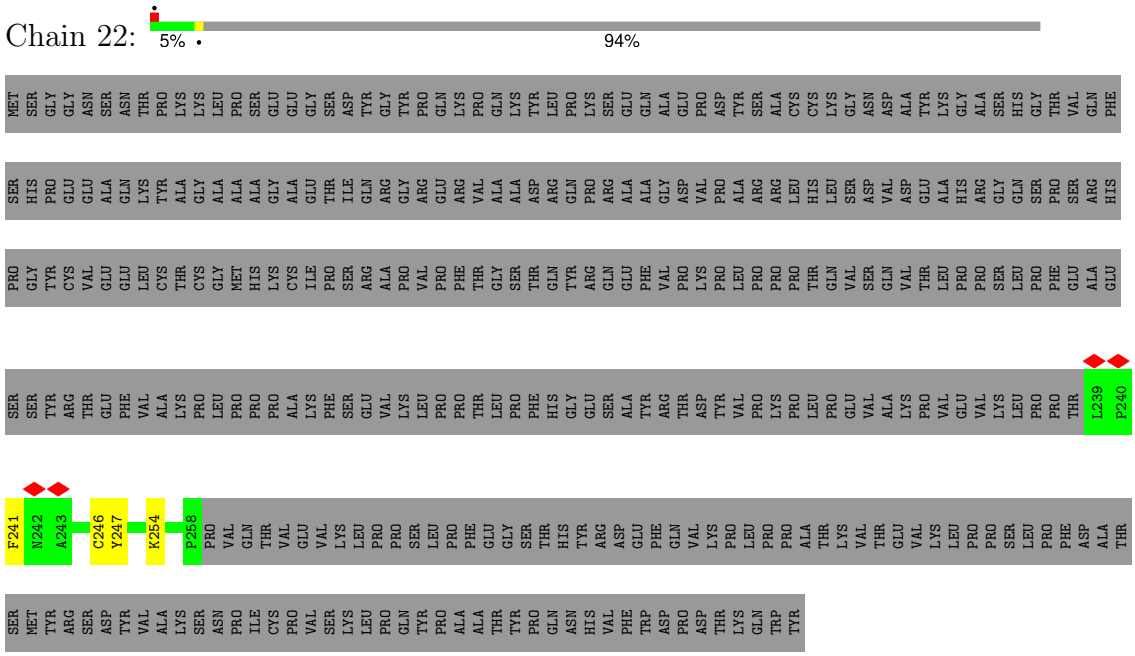
• Molecule 1: Microtubule associated protein SPM1

Chain 21:



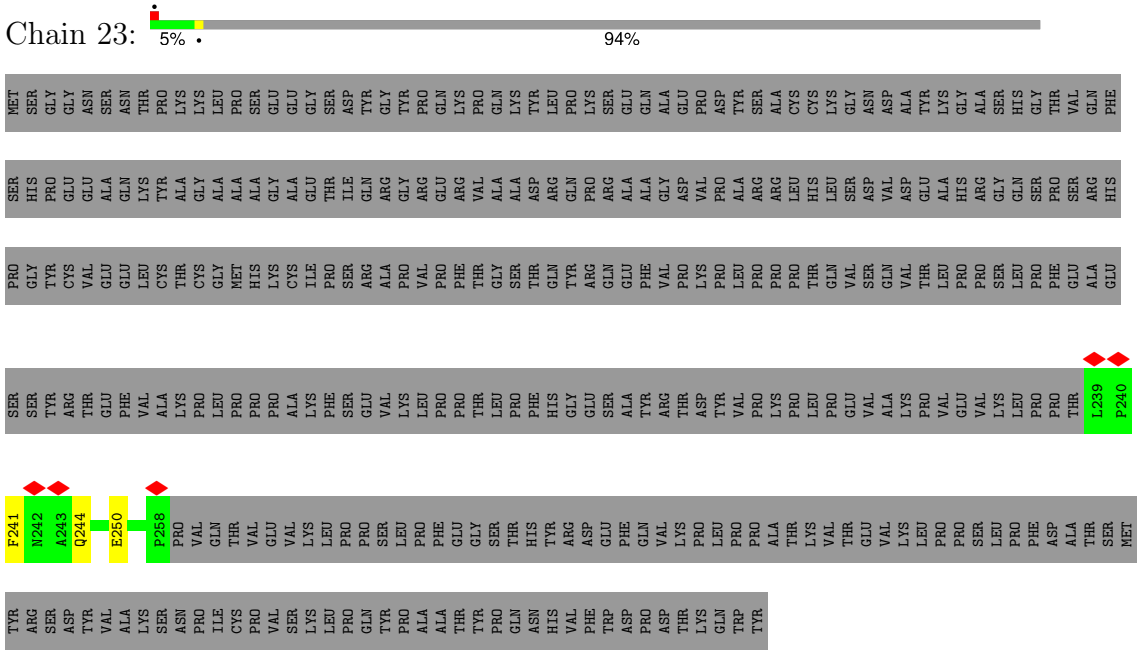
• Molecule 1: Microtubule associated protein SPM1

Chain 22:



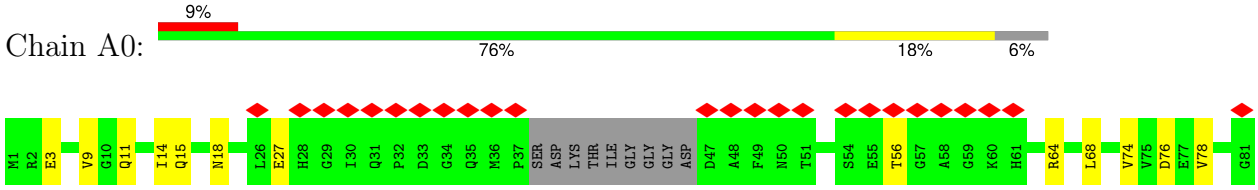
• Molecule 1: Microtubule associated protein SPM1

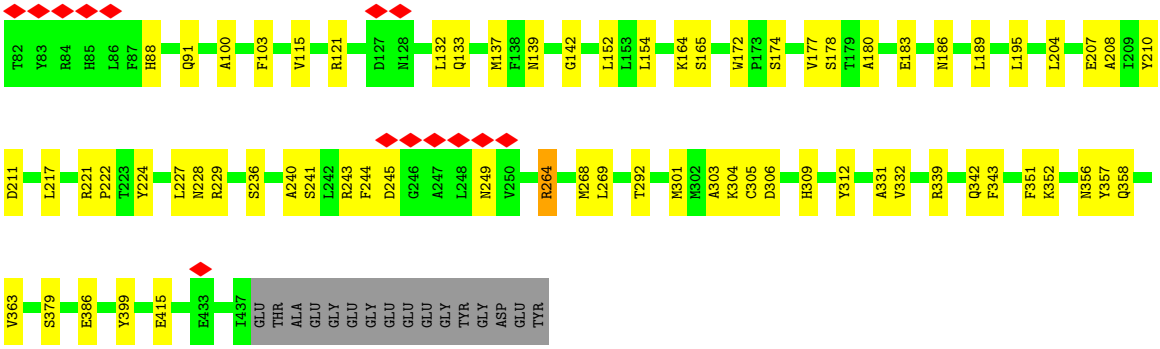
Chain 23:



• Molecule 2: Tubulin alpha chain

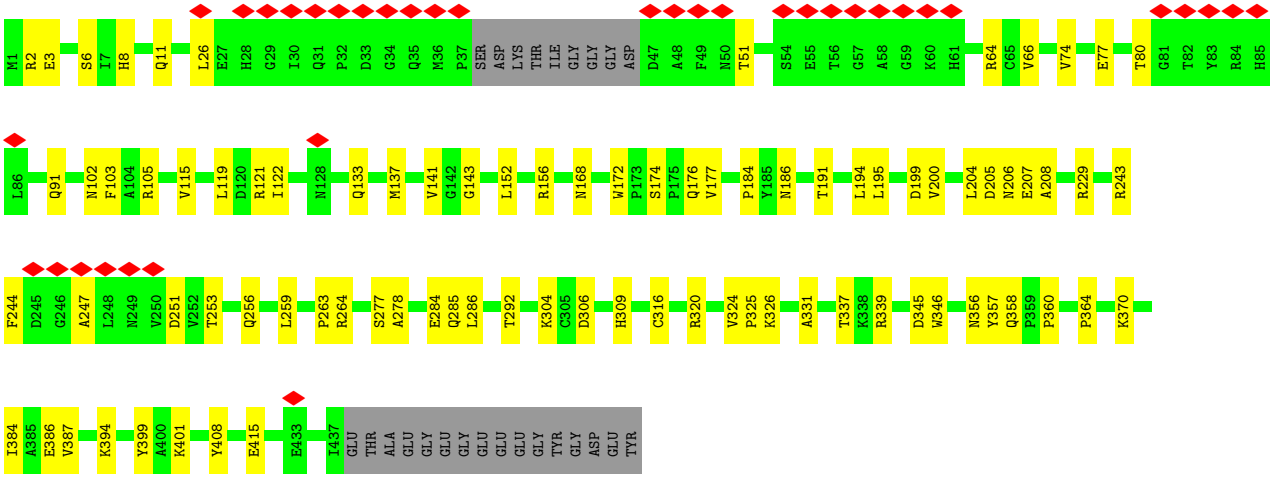
Chain A0:





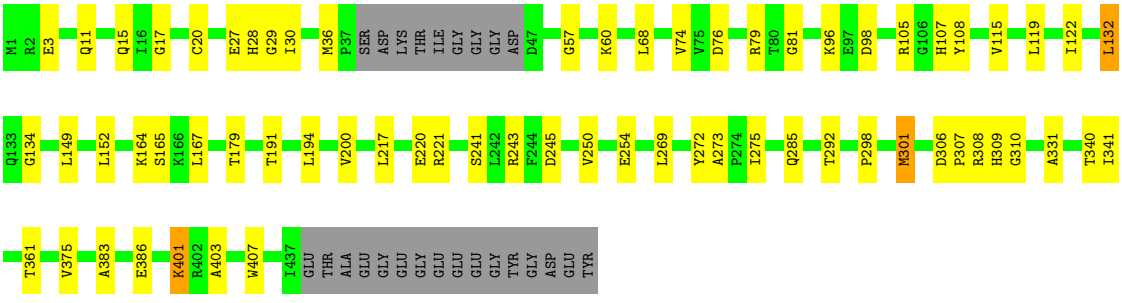
• Molecule 2: Tubulin alpha chain

Chain A2:



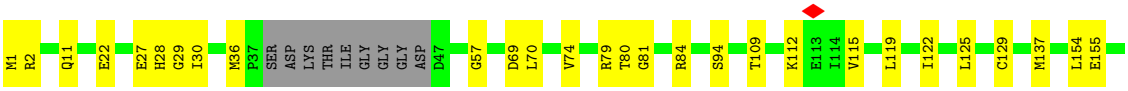
• Molecule 2: Tubulin alpha chain

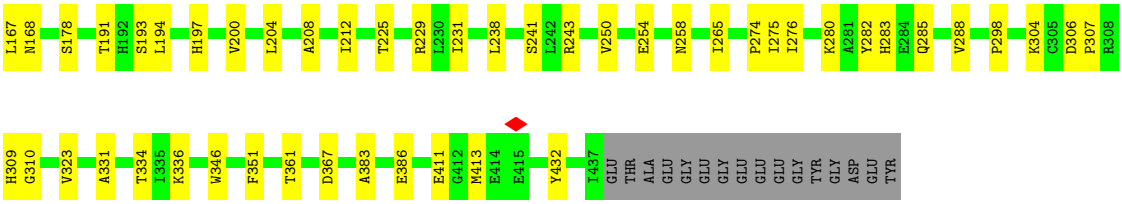
Chain A4:



• Molecule 2: Tubulin alpha chain

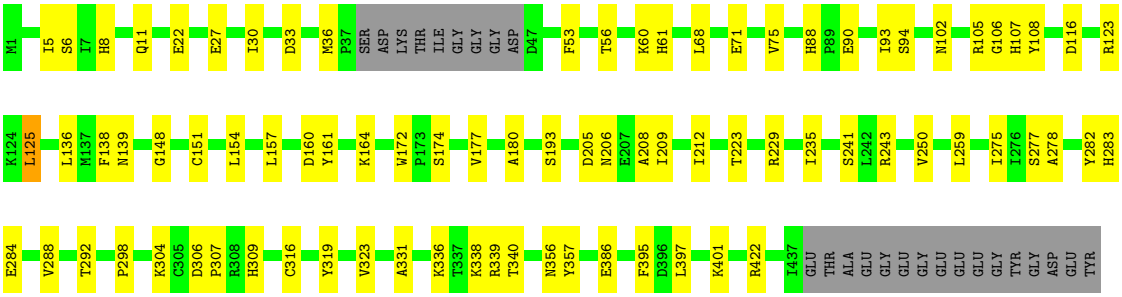
Chain A6:





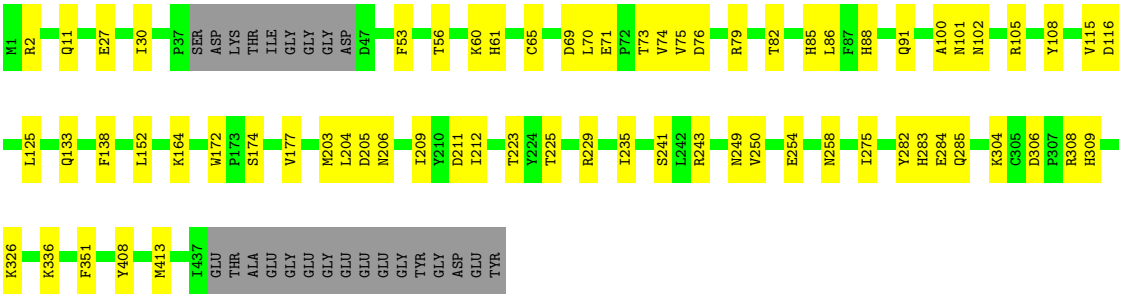
• Molecule 2: Tubulin alpha chain

Chain A8:



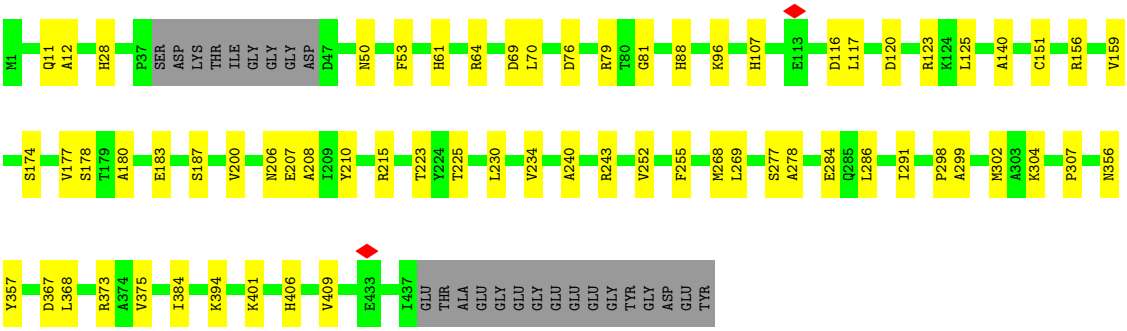
• Molecule 2: Tubulin alpha chain

Chain B0:



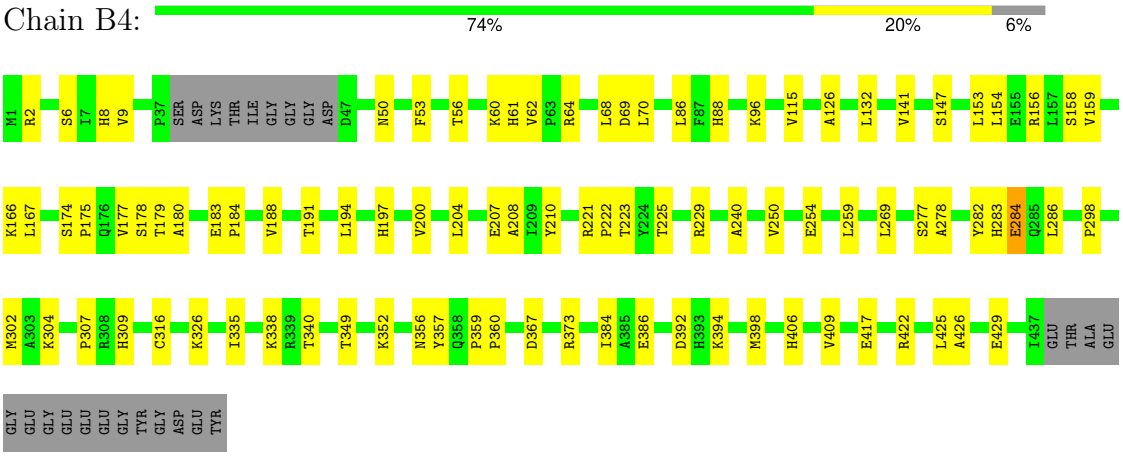
• Molecule 2: Tubulin alpha chain

Chain B2:



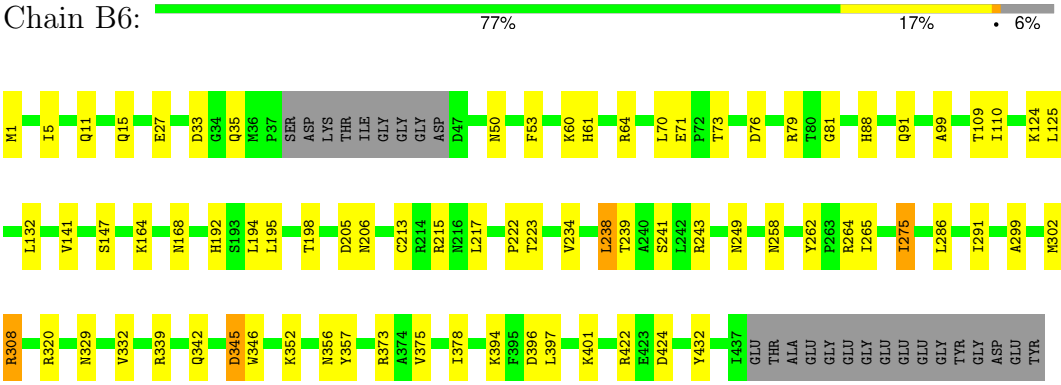
• Molecule 2: Tubulin alpha chain

Chain B4:



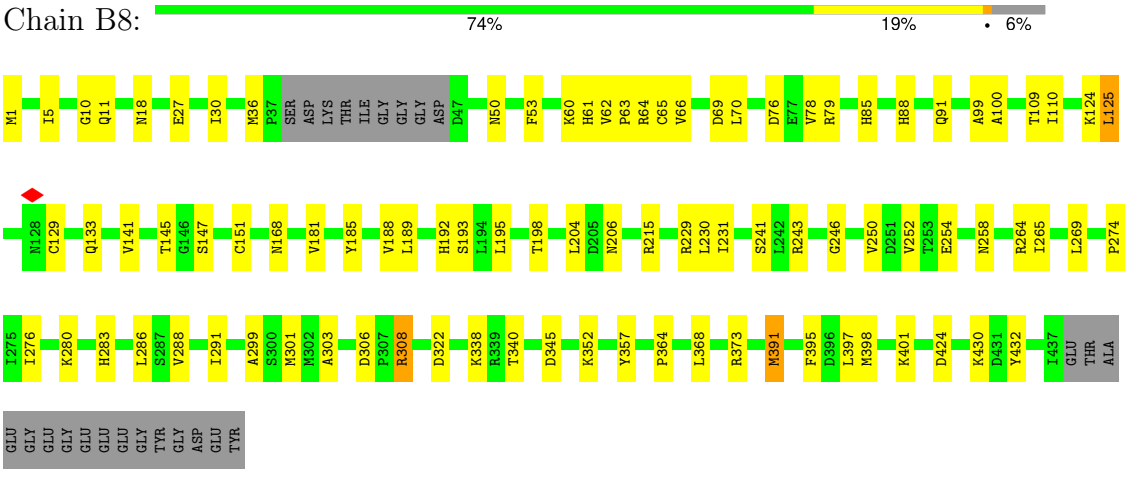
• Molecule 2: Tubulin alpha chain

Chain B6:



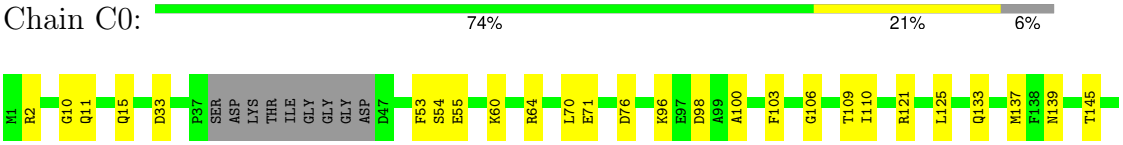
• Molecule 2: Tubulin alpha chain

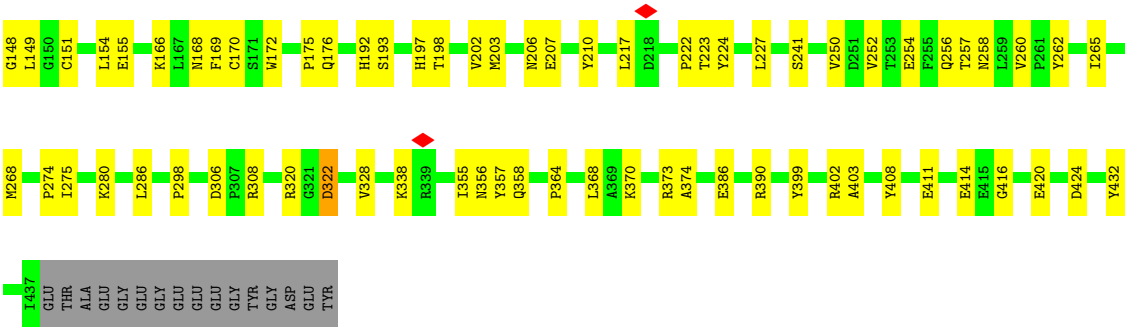
Chain B8:



• Molecule 2: Tubulin alpha chain

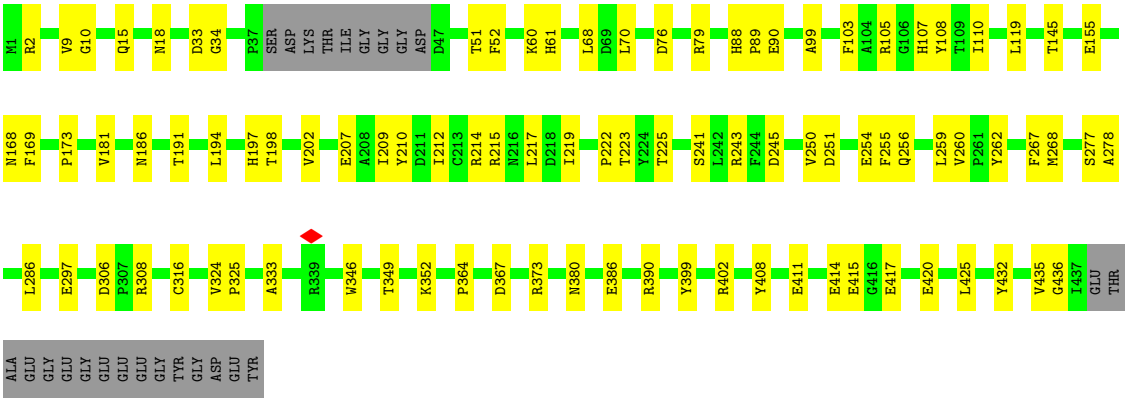
Chain C0:





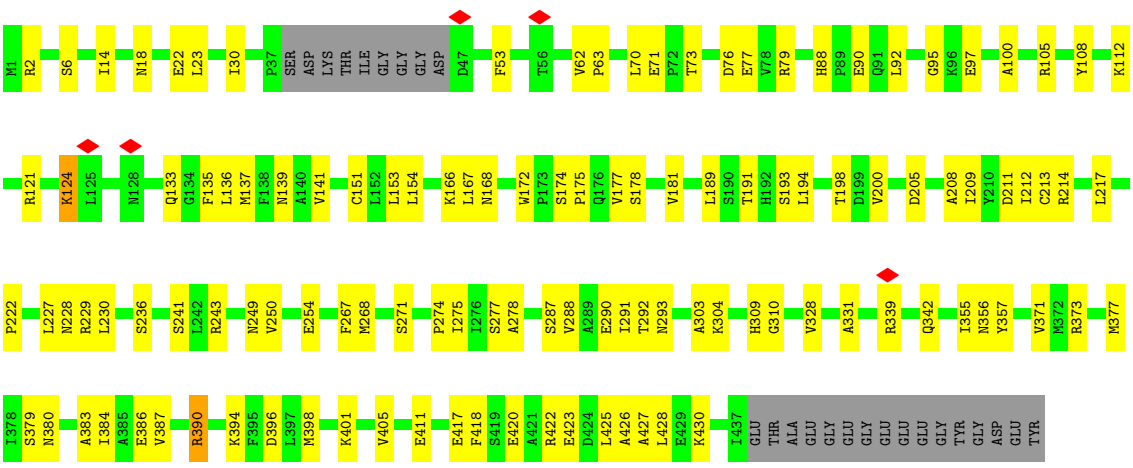
• Molecule 2: Tubulin alpha chain

Chain C2:



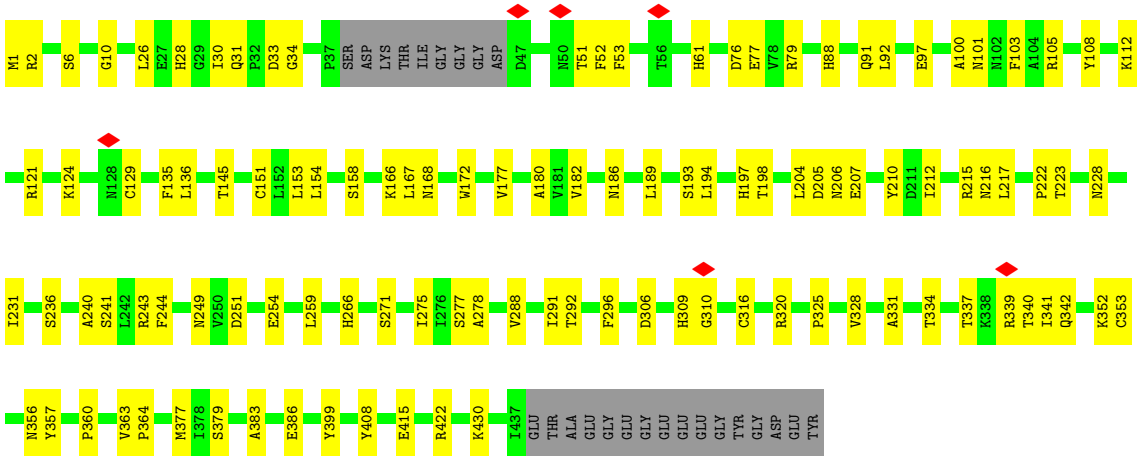
• Molecule 2: Tubulin alpha chain

Chain C4:



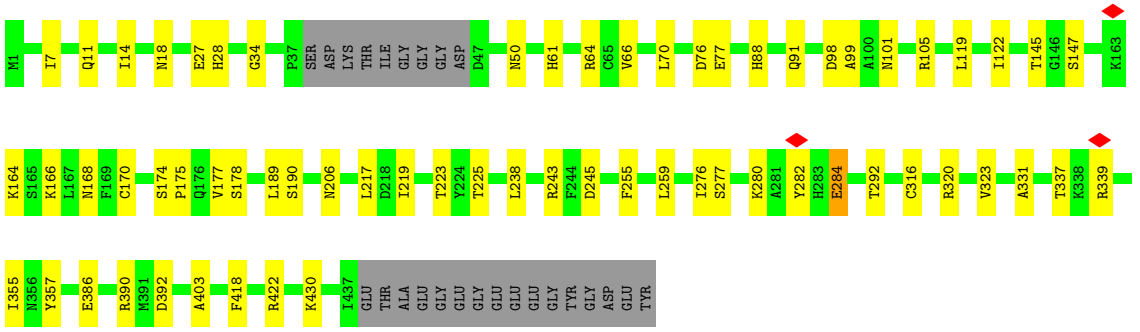
• Molecule 2: Tubulin alpha chain

Chain C6:



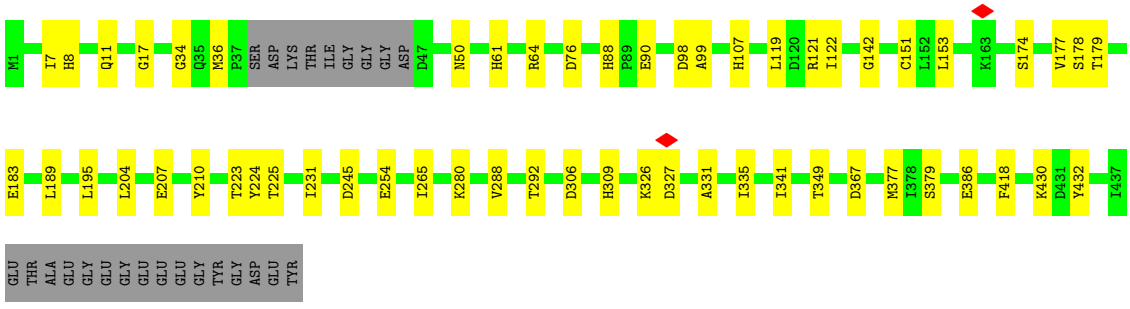
• Molecule 2: Tubulin alpha chain

Chain C8:



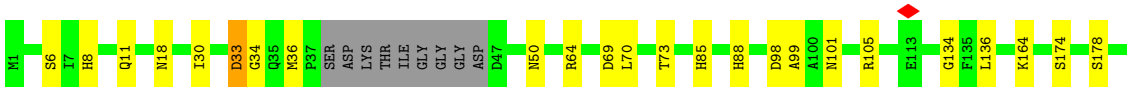
• Molecule 2: Tubulin alpha chain

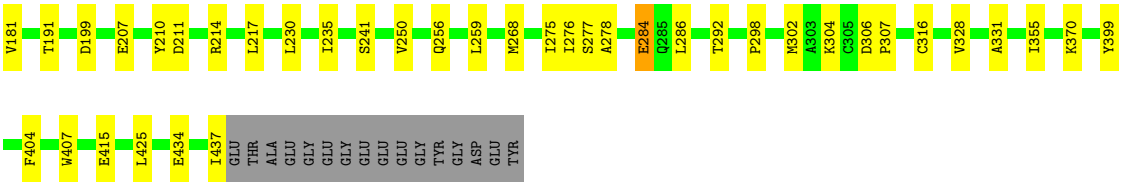
Chain D0:



• Molecule 2: Tubulin alpha chain

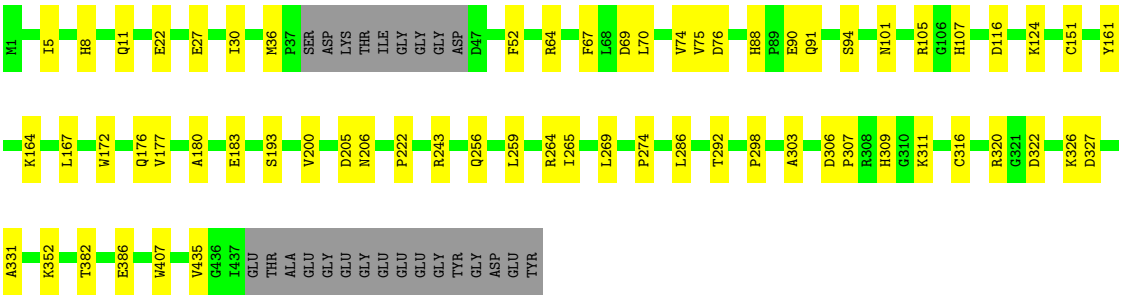
Chain D2:





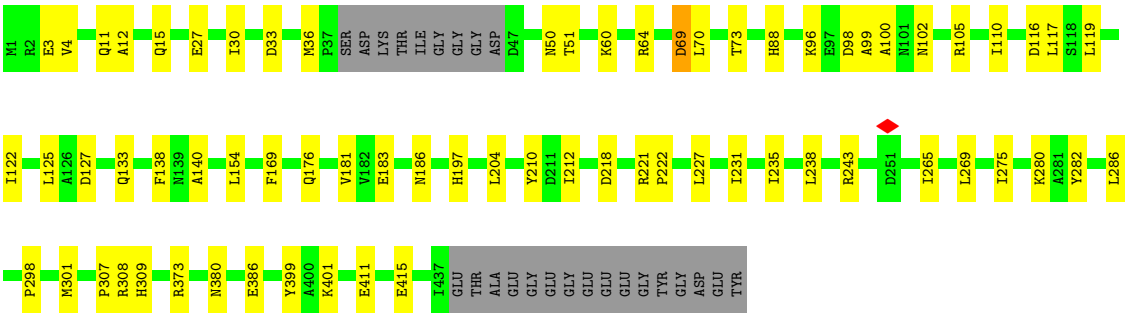
• Molecule 2: Tubulin alpha chain

Chain D4:



• Molecule 2: Tubulin alpha chain

Chain D6:



• Molecule 2: Tubulin alpha chain

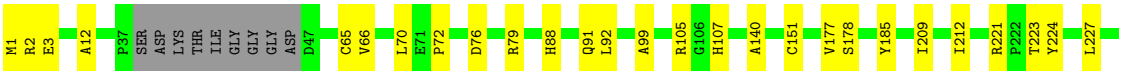
Chain D8:

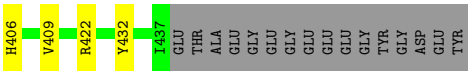
• Molecule 2: Tubulin alpha chain

Chain E0:

• Molecule 2: Tubulin alpha chain

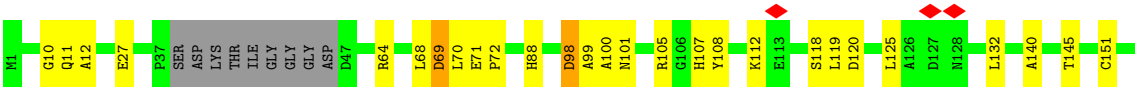
Chain E2:

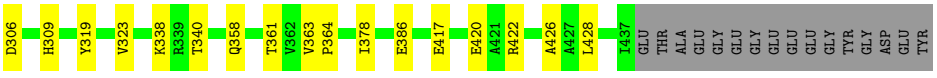




• Molecule 2: Tubulin alpha chain

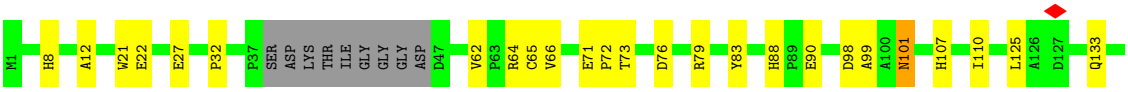
Chain E4:

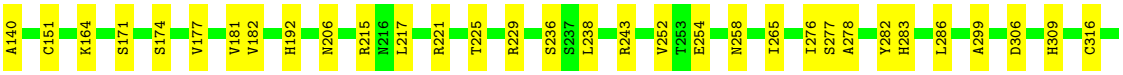




• Molecule 2: Tubulin alpha chain

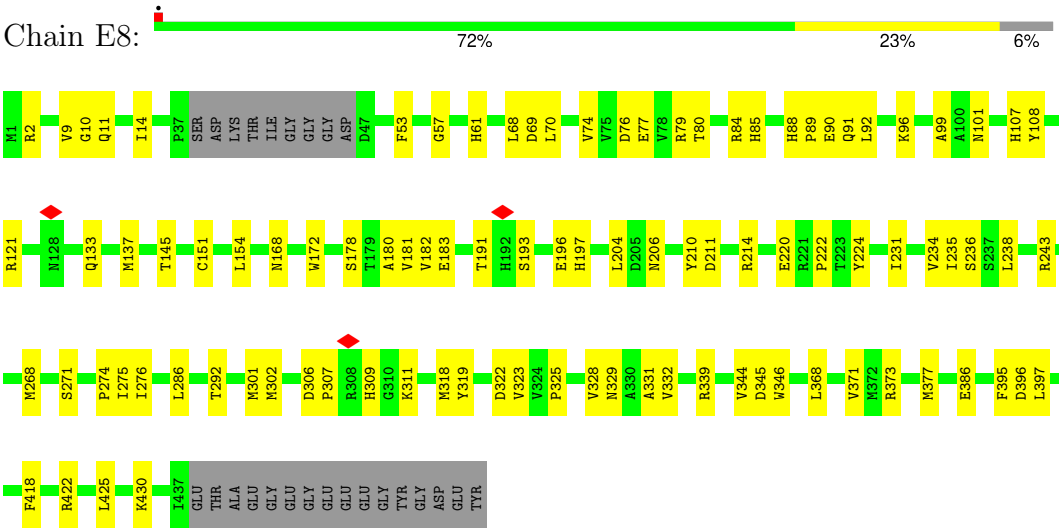
Chain E6:





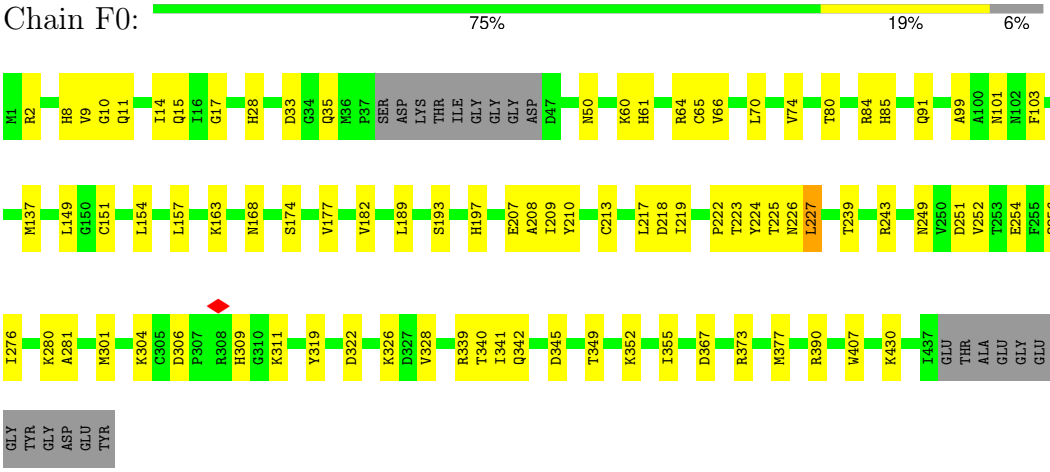
• Molecule 2: Tubulin alpha chain

Chain E8:



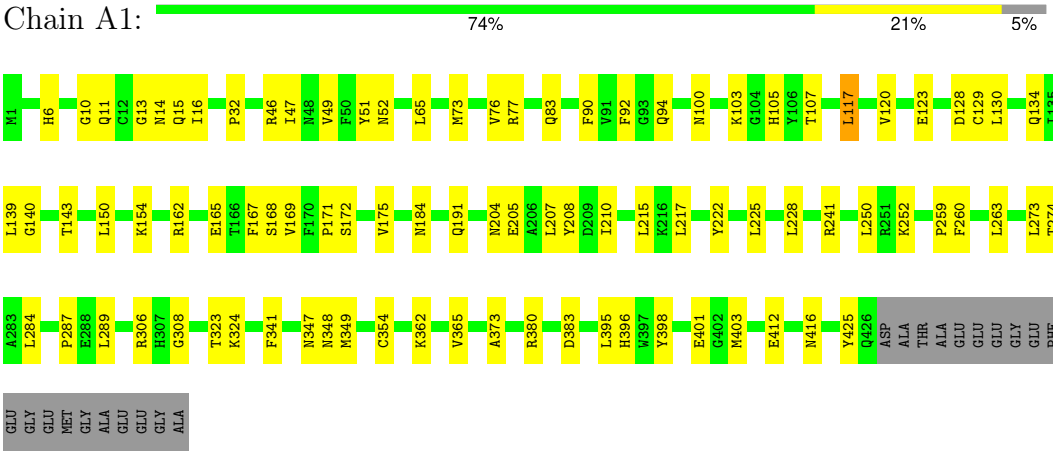
• Molecule 2: Tubulin alpha chain

Chain F0:



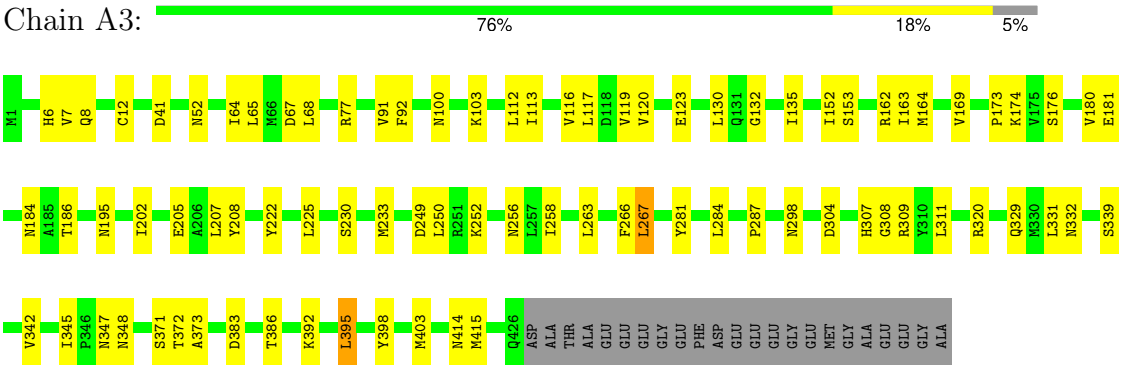
• Molecule 3: Tubulin beta chain

Chain A1:



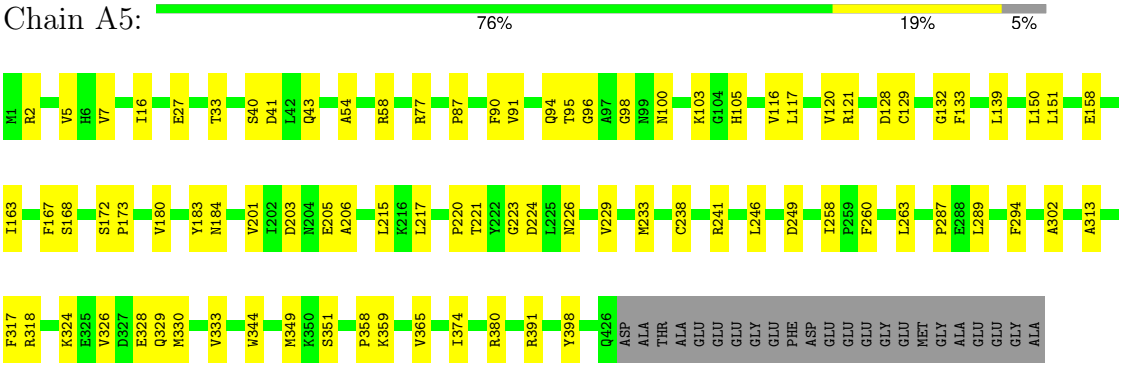
• Molecule 3: Tubulin beta chain

Chain A3:



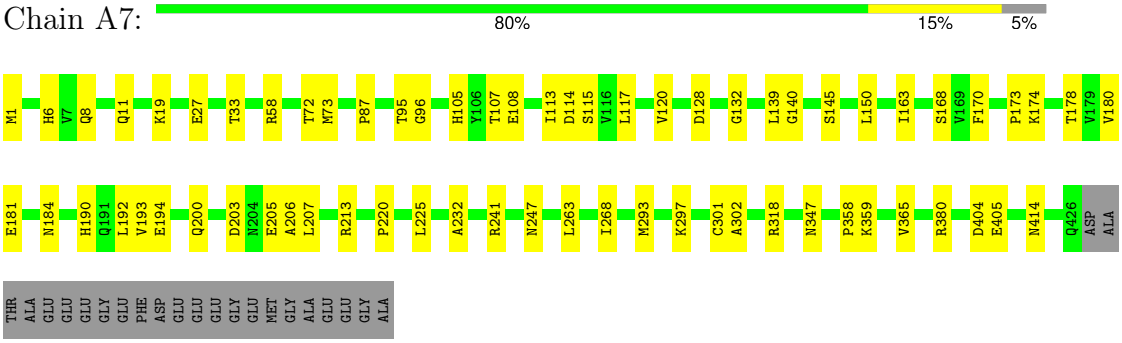
• Molecule 3: Tubulin beta chain

Chain A5:



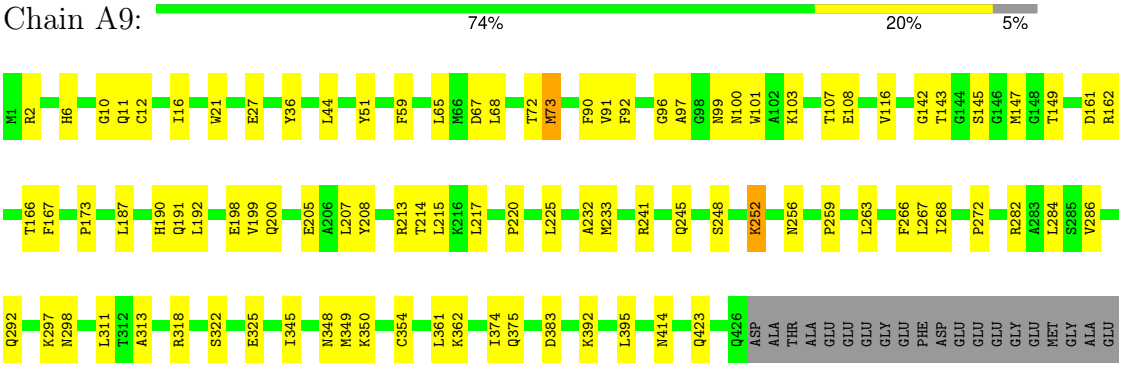
• Molecule 3: Tubulin beta chain

Chain A7:



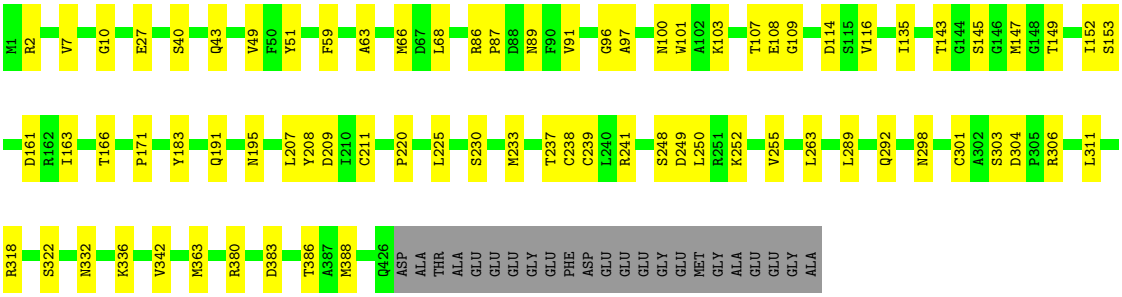
• Molecule 3: Tubulin beta chain

Chain A9:



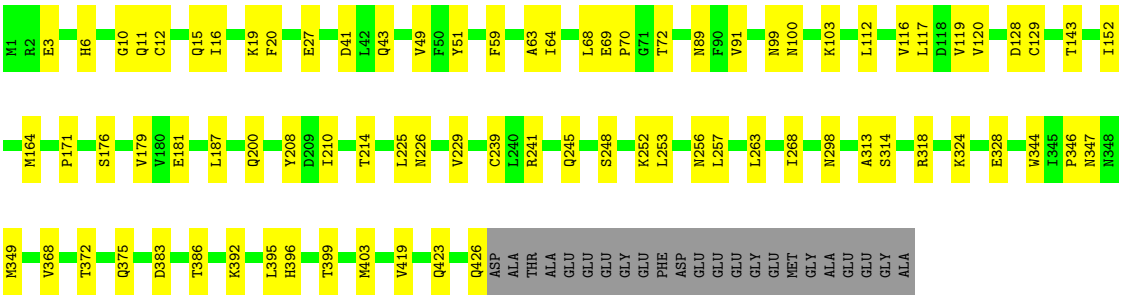
• Molecule 3: Tubulin beta chain

Chain B1:



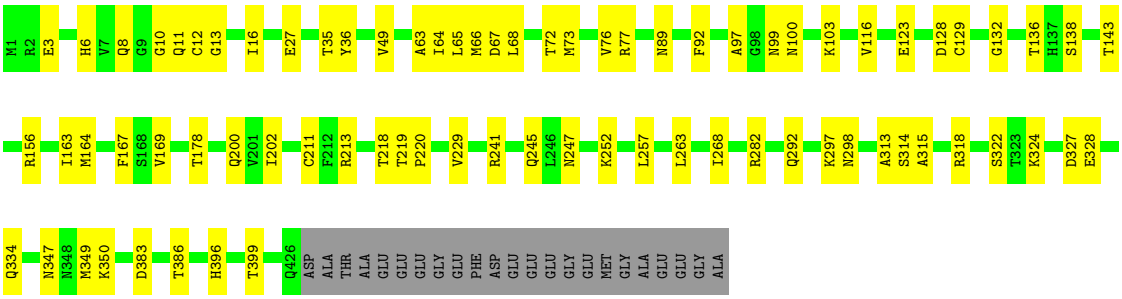
• Molecule 3: Tubulin beta chain

Chain B3:



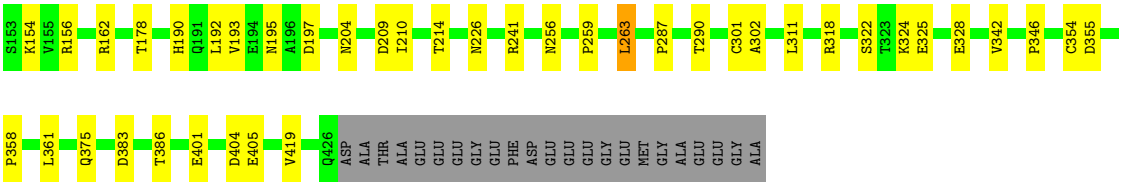
• Molecule 3: Tubulin beta chain

Chain B5:



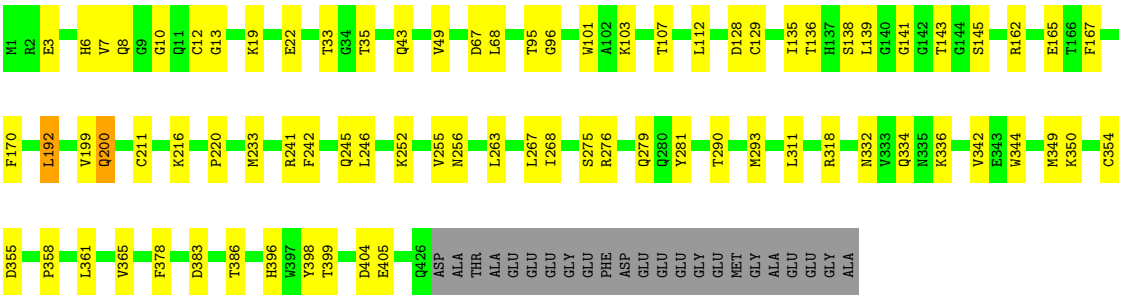
• Molecule 3: Tubulin beta chain

Chain B7:



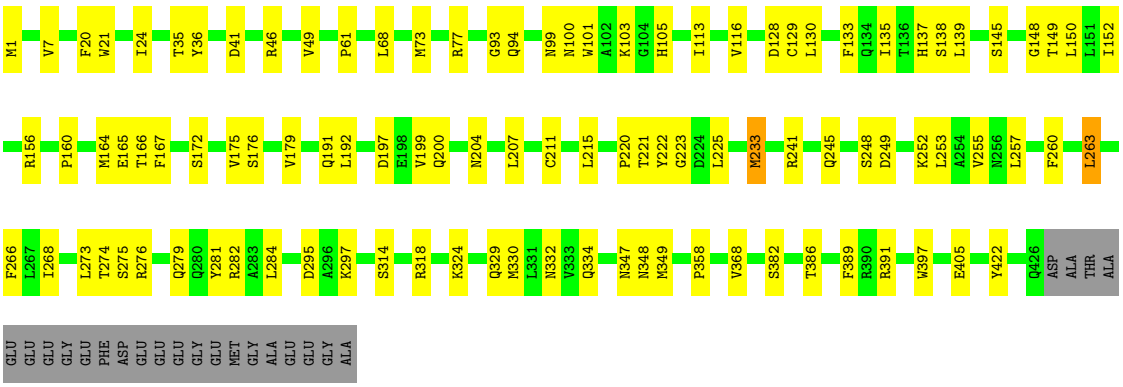
• Molecule 3: Tubulin beta chain

Chain B9:



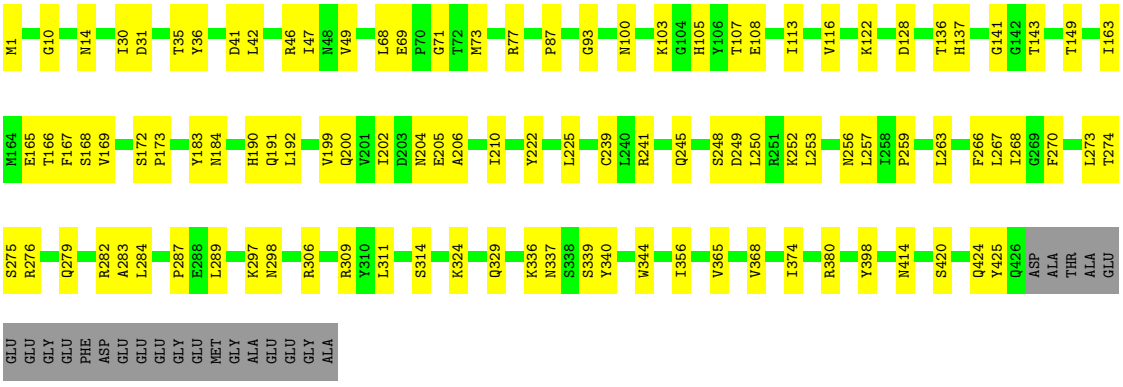
• Molecule 3: Tubulin beta chain

Chain C1:



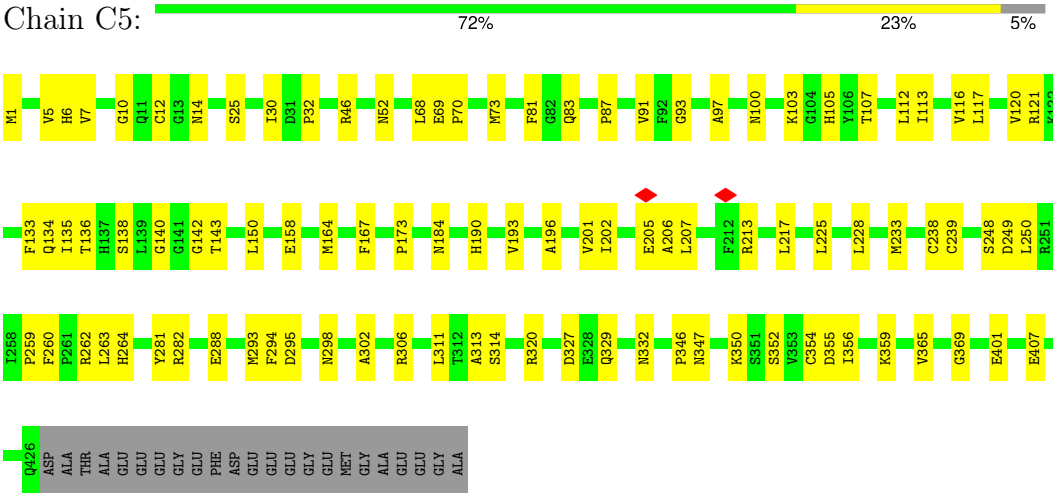
• Molecule 3: Tubulin beta chain

Chain C3:



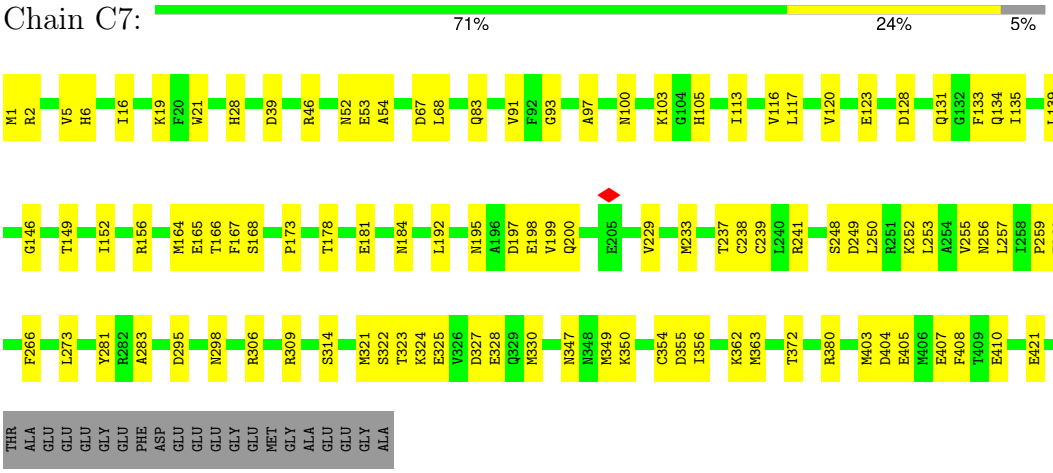
• Molecule 3: Tubulin beta chain

Chain C5:



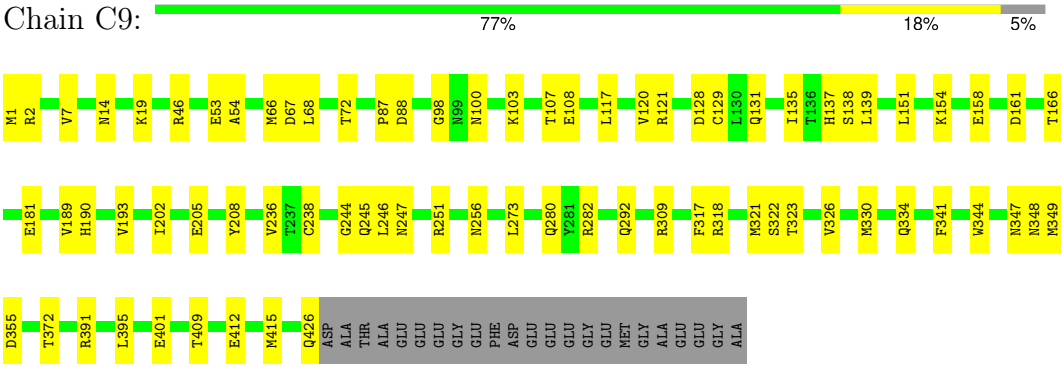
• Molecule 3: Tubulin beta chain

Chain C7:



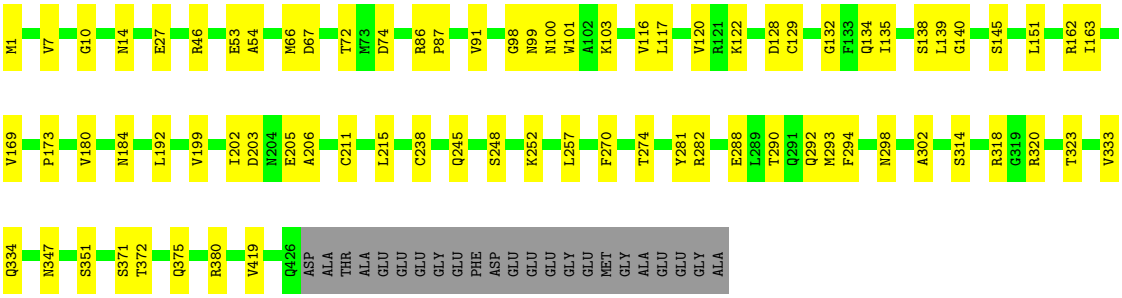
• Molecule 3: Tubulin beta chain

Chain C9:



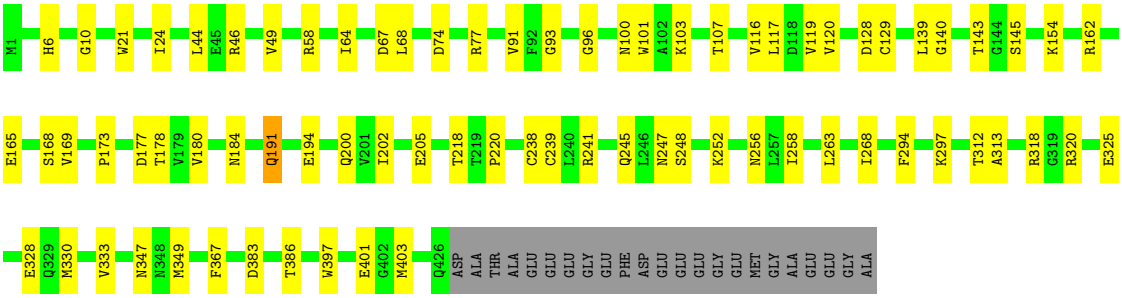
• Molecule 3: Tubulin beta chain

Chain D1:



• Molecule 3: Tubulin beta chain

Chain D3:

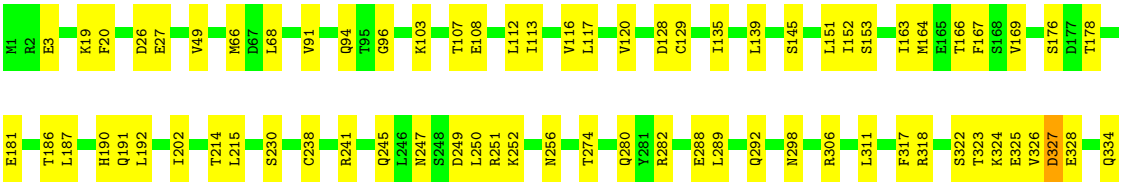


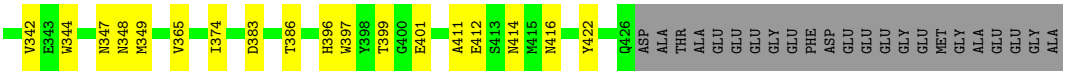
• Molecule 3: Tubulin beta chain

Chain D5:

• Molecule 3: Tubulin beta chain

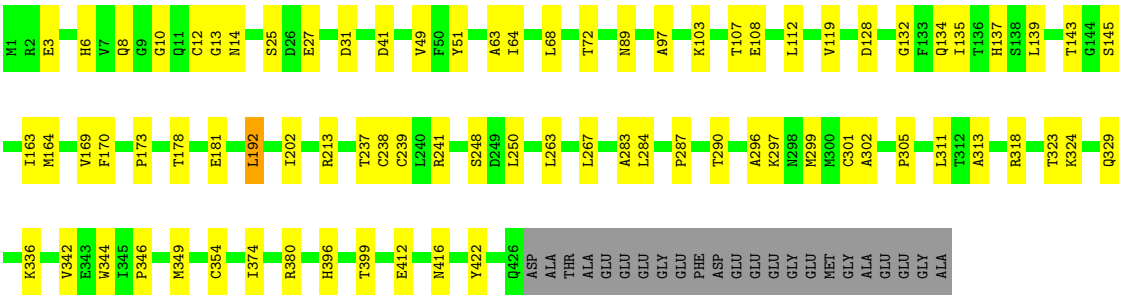
Chain D7:





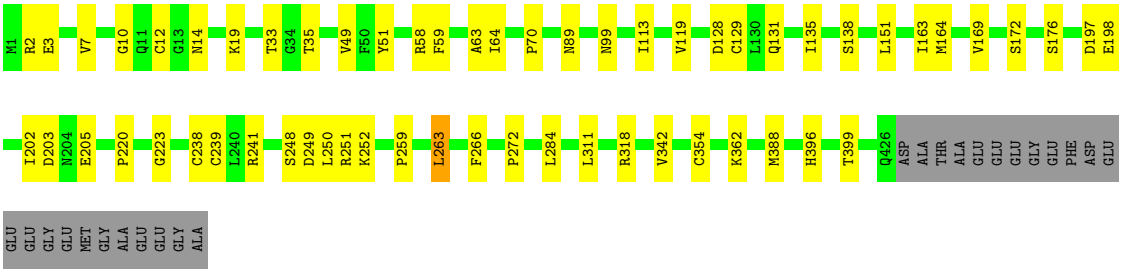
• Molecule 3: Tubulin beta chain

Chain D9:



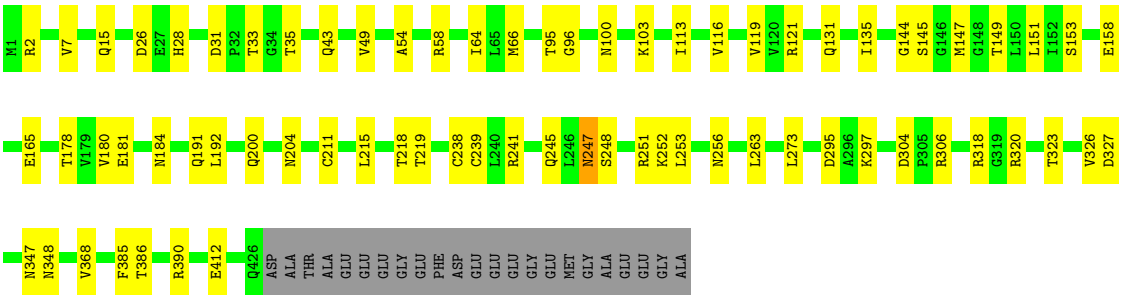
• Molecule 3: Tubulin beta chain

Chain E1:



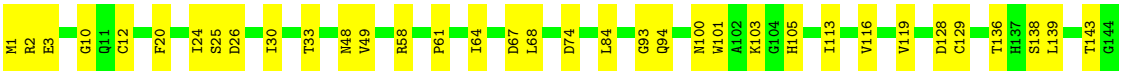
• Molecule 3: Tubulin beta chain

Chain E3:



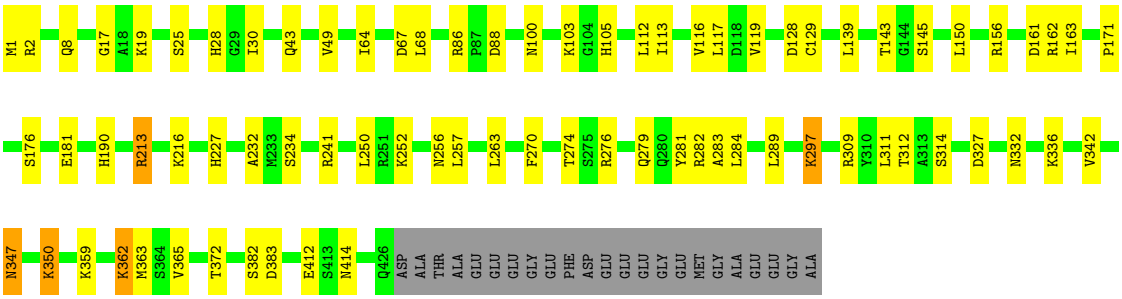
• Molecule 3: Tubulin beta chain

Chain E5:



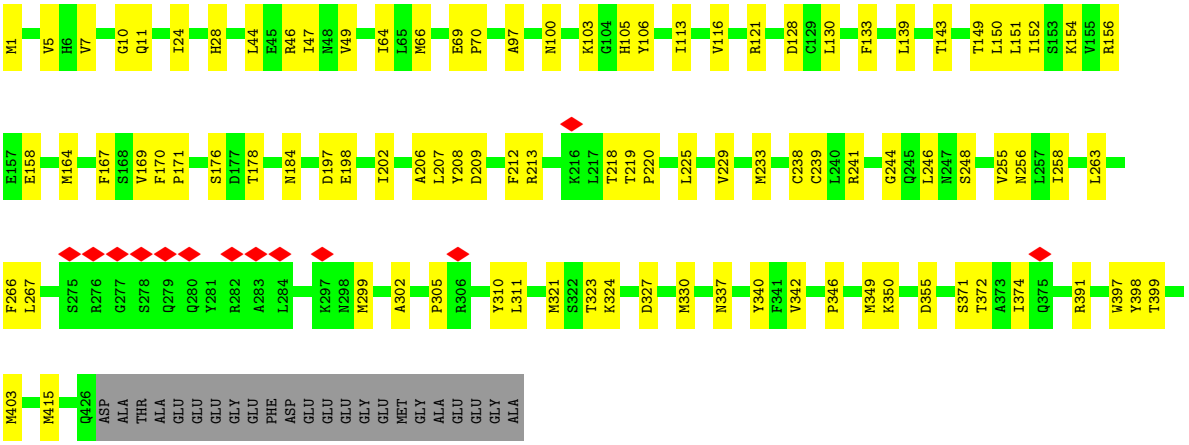
• Molecule 3: Tubulin beta chain

Chain E7:



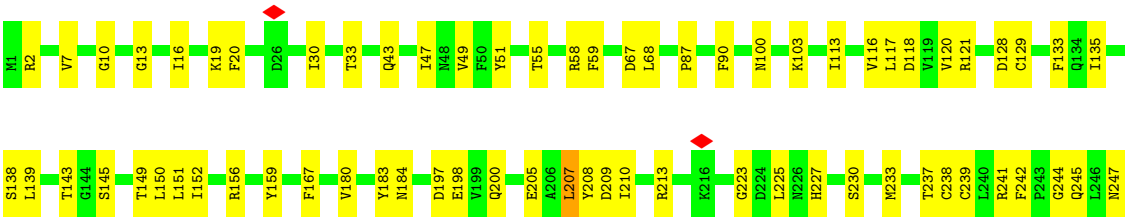
• Molecule 3: Tubulin beta chain

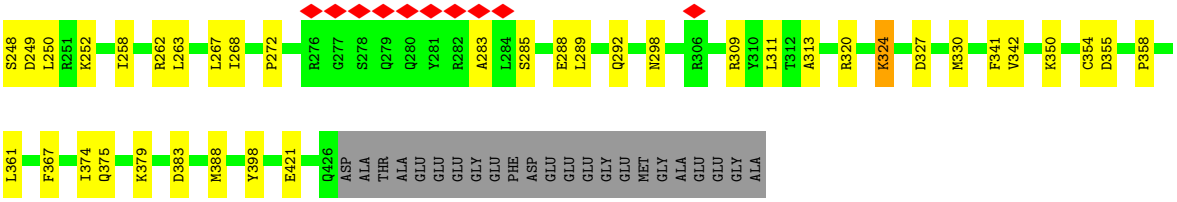
Chain E9:



• Molecule 3: Tubulin beta chain

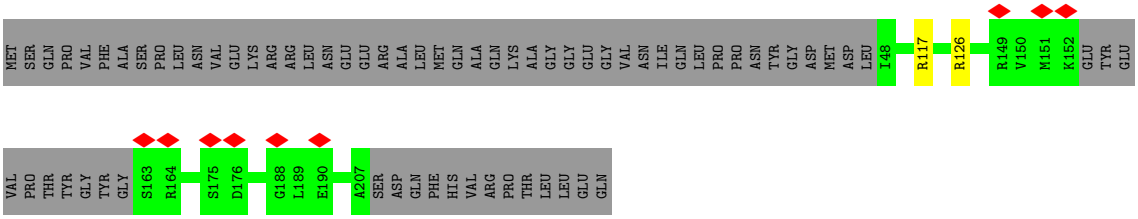
Chain F1:





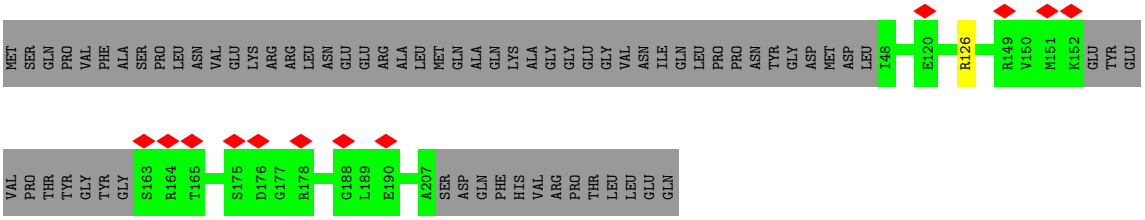
• Molecule 4: PDI family protein

Chain a:



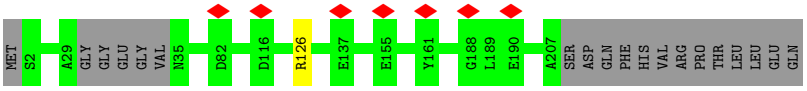
• Molecule 4: PDI family protein

Chain b:



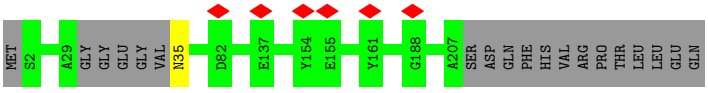
• Molecule 4: PDI family protein

Chain c:



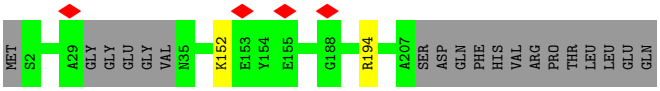
• Molecule 4: PDI family protein

Chain d:



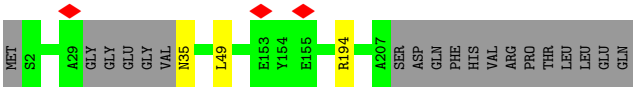
• Molecule 4: PDI family protein

Chain e:



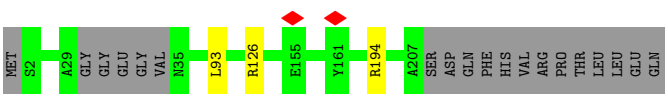
• Molecule 4: PDI family protein

Chain f:



• Molecule 4: PDI family protein

Chain g:

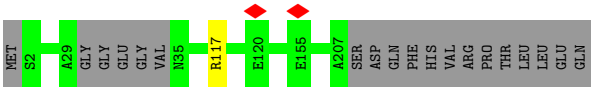


• Molecule 4: PDI family protein

Chain h:

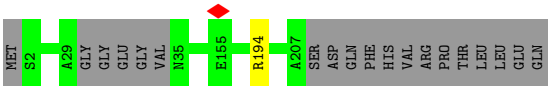
• Molecule 4: PDI family protein

Chain i:



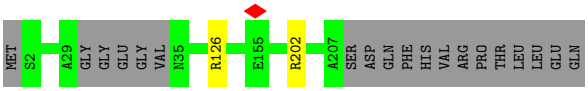
• Molecule 4: PDI family protein

Chain j:



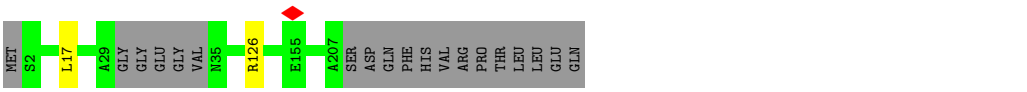
• Molecule 4: PDI family protein

Chain o:



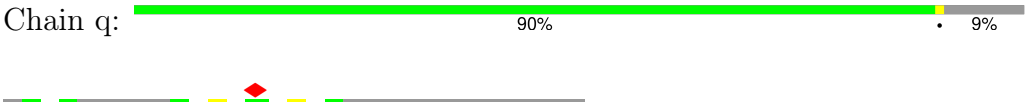
• Molecule 4: PDI family protein

Chain p:



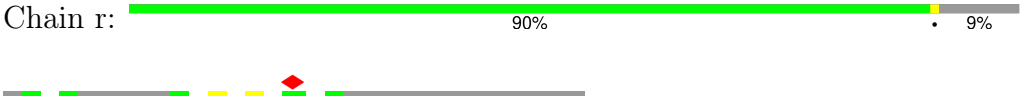
• Molecule 4: PDI family protein

Chain q:



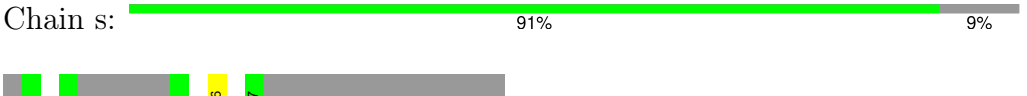
• Molecule 4: PDI family protein

Chain r:



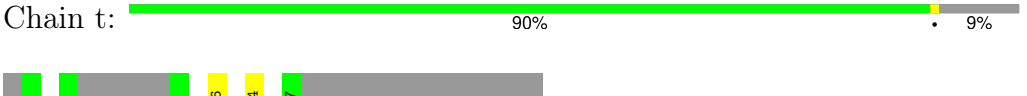
• Molecule 4: PDI family protein

Chain s:



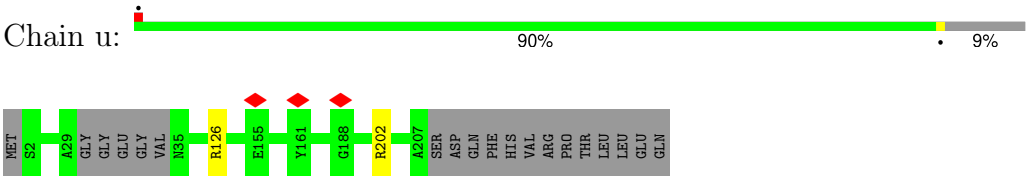
• Molecule 4: PDI family protein

Chain t:



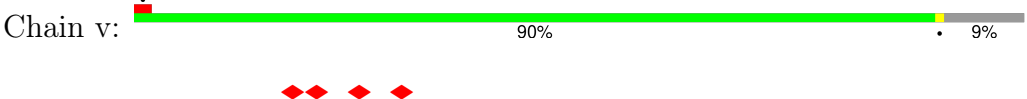
• Molecule 4: PDI family protein

Chain u:



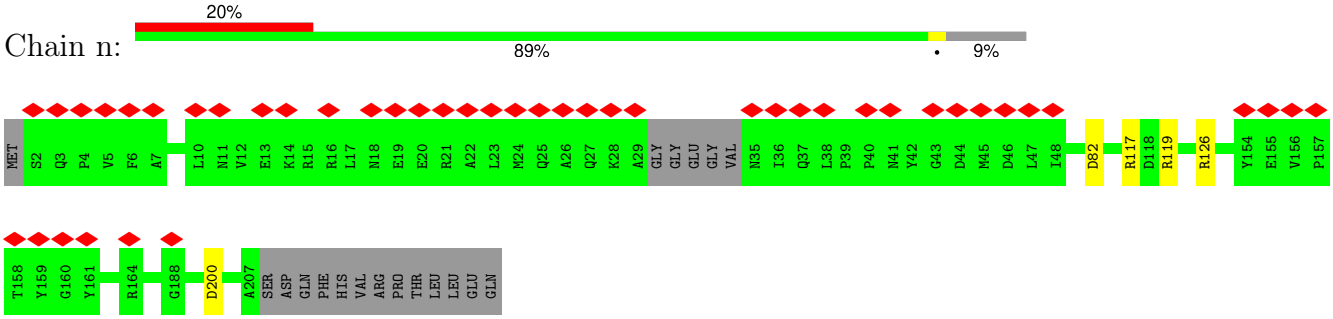
• Molecule 4: PDI family protein

Chain v:



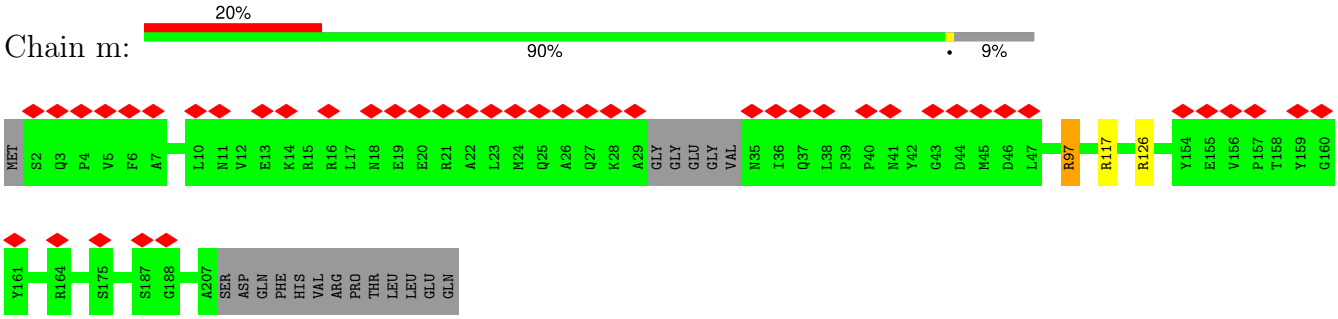
• Molecule 4: PDI family protein

Chain n:



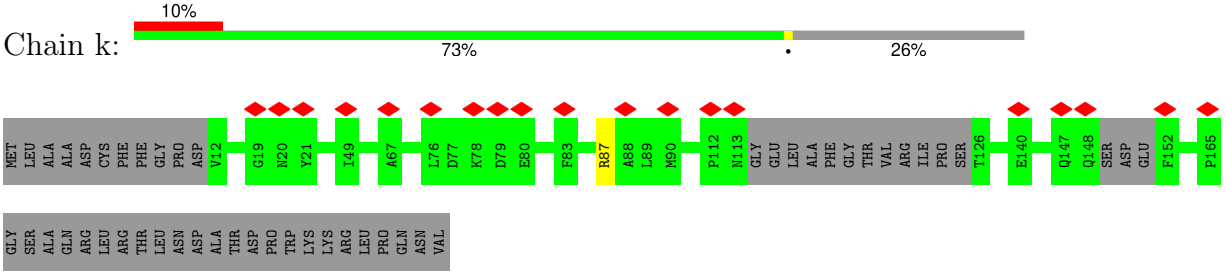
• Molecule 4: PDI family protein

Chain m:



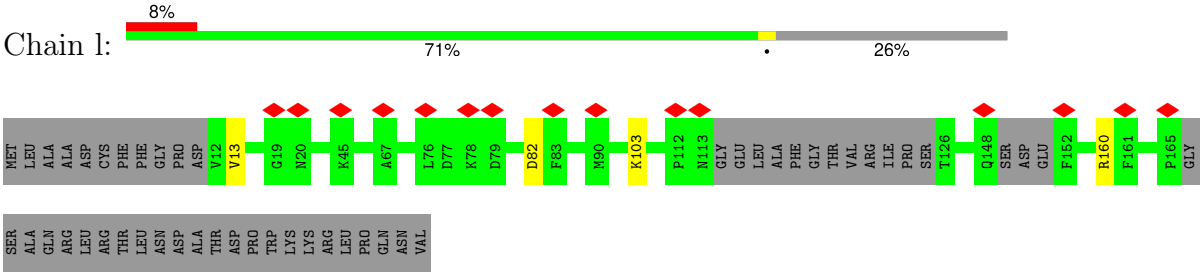
• Molecule 5: PDI family protein

Chain k:



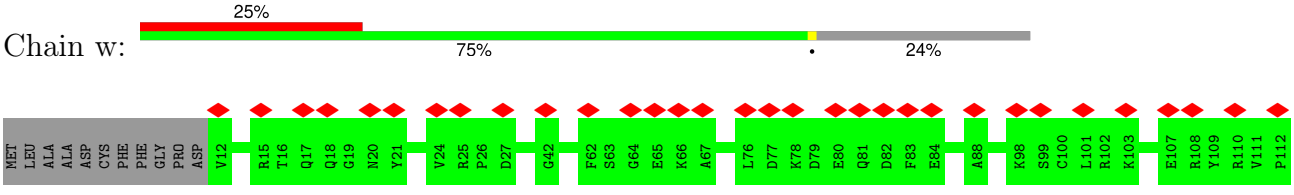
• Molecule 5: PDI family protein

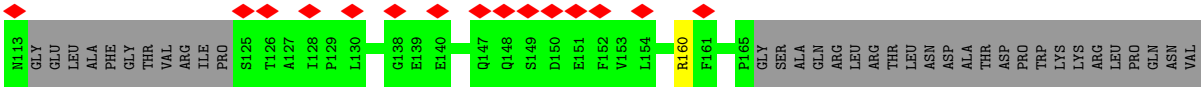
Chain l:



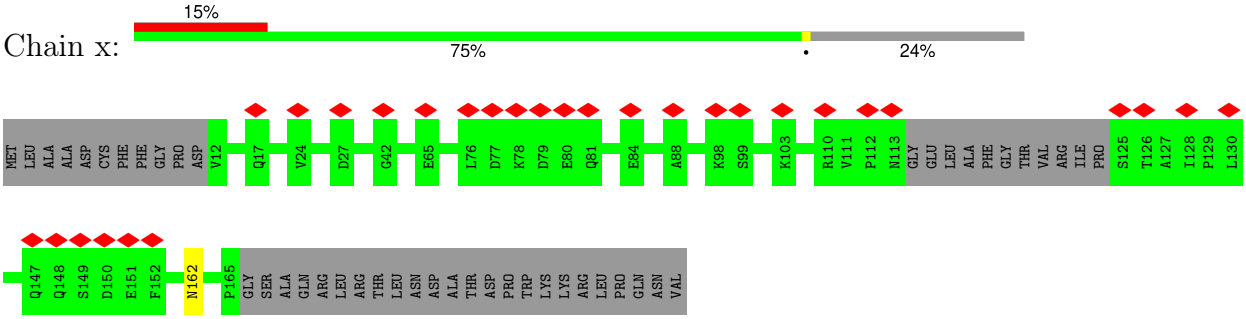
• Molecule 5: PDI family protein

Chain w:





• Molecule 5: PDI family protein



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	220139	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF amplitude correction was performed as part of the 3D reconstruction.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	63.7	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.228	Depositor
Minimum map value	0.000	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	438.4, 438.4, 438.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.096, 1.096, 1.096	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0	0.47	0/181	0.55	0/248
1	1	0.42	0/181	0.58	0/248
1	10	0.49	0/181	0.61	0/248
1	11	0.53	0/181	0.60	0/248
1	12	0.47	0/181	0.51	0/248
1	13	0.50	0/181	0.50	0/248
1	14	0.47	0/181	0.48	0/248
1	15	0.53	0/181	0.42	0/248
1	16	0.40	0/181	0.49	0/248
1	17	0.47	0/181	0.51	0/248
1	18	0.44	0/181	0.48	0/248
1	19	0.57	0/181	0.53	0/248
1	2	0.54	0/181	0.59	0/248
1	20	0.39	0/181	0.59	0/248
1	21	0.43	0/181	0.52	0/248
1	22	0.42	0/166	0.48	0/227
1	23	0.46	0/166	0.47	0/227
1	3	0.53	0/181	0.49	0/248
1	4	0.51	0/181	0.50	0/248
1	5	0.55	0/181	0.52	0/248
1	6	0.49	0/181	0.46	0/248
1	7	0.48	0/181	0.48	0/248
1	8	0.47	0/181	0.65	0/248
1	9	0.45	0/181	0.63	0/248
2	A0	0.42	0/3398	0.61	2/4606 (0.0%)
2	A2	0.39	0/3398	0.61	1/4606 (0.0%)
2	A4	0.53	0/3398	0.63	2/4606 (0.0%)
2	A6	0.48	0/3398	0.62	0/4606
2	A8	0.50	0/3398	0.60	2/4606 (0.0%)
2	B0	0.50	0/3398	0.62	4/4606 (0.1%)
2	B2	0.53	0/3398	0.62	1/4606 (0.0%)
2	B4	0.52	0/3398	0.63	2/4606 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	B6	0.53	0/3398	0.63	6/4606 (0.1%)
2	B8	0.55	0/3398	0.66	6/4606 (0.1%)
2	C0	0.44	0/3398	0.61	1/4606 (0.0%)
2	C2	0.45	0/3398	0.65	0/4606
2	C4	0.43	0/3398	0.65	4/4606 (0.1%)
2	C6	0.44	0/3398	0.68	3/4606 (0.1%)
2	C8	0.45	0/3398	0.60	1/4606 (0.0%)
2	D0	0.50	0/3398	0.61	0/4606
2	D2	0.45	0/3398	0.62	5/4606 (0.1%)
2	D4	0.52	0/3398	0.62	2/4606 (0.0%)
2	D6	0.42	0/3398	0.61	3/4606 (0.1%)
2	D8	0.52	0/3398	0.62	1/4606 (0.0%)
2	E0	0.37	0/3398	0.56	1/4606 (0.0%)
2	E2	0.44	0/3398	0.59	0/4606
2	E4	0.38	0/3398	0.65	6/4606 (0.1%)
2	E6	0.45	0/3398	0.58	0/4606
2	E8	0.39	0/3398	0.59	0/4606
2	F0	0.45	0/3398	0.60	2/4606 (0.0%)
3	A1	0.47	0/3404	0.66	6/4606 (0.1%)
3	A3	0.40	0/3404	0.62	3/4606 (0.1%)
3	A5	0.50	0/3404	0.65	2/4606 (0.0%)
3	A7	0.45	0/3404	0.61	3/4606 (0.1%)
3	A9	0.52	0/3404	0.68	6/4606 (0.1%)
3	B1	0.46	0/3404	0.65	3/4606 (0.1%)
3	B3	0.54	0/3404	0.62	2/4606 (0.0%)
3	B5	0.48	0/3404	0.61	1/4606 (0.0%)
3	B7	0.54	0/3404	0.63	3/4606 (0.1%)
3	B9	0.50	0/3404	0.63	3/4606 (0.1%)
3	C1	0.46	0/3404	0.66	3/4606 (0.1%)
3	C3	0.44	0/3404	0.68	3/4606 (0.1%)
3	C5	0.44	0/3404	0.65	1/4606 (0.0%)
3	C7	0.44	0/3404	0.63	2/4606 (0.0%)
3	C9	0.52	0/3404	0.64	2/4606 (0.0%)
3	D1	0.49	0/3404	0.64	1/4606 (0.0%)
3	D3	0.50	0/3404	0.63	2/4606 (0.0%)
3	D5	0.50	0/3404	0.66	6/4606 (0.1%)
3	D7	0.51	0/3404	0.65	4/4606 (0.1%)
3	D9	0.51	0/3404	0.64	4/4606 (0.1%)
3	E1	0.41	0/3404	0.58	2/4606 (0.0%)
3	E3	0.45	0/3404	0.62	5/4606 (0.1%)
3	E5	0.41	0/3404	0.64	3/4606 (0.1%)
3	E7	0.45	0/3404	0.61	3/4606 (0.1%)
3	E9	0.41	0/3404	0.64	4/4606 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	F1	0.45	0/3404	0.69	7/4606 (0.2%)
4	a	0.46	0/1225	0.62	0/1654
4	b	0.39	0/1225	0.55	0/1654
4	c	0.50	0/1645	0.64	0/2225
4	d	0.44	0/1645	0.65	0/2225
4	e	0.50	0/1645	0.63	0/2225
4	f	0.47	0/1645	0.61	1/2225 (0.0%)
4	g	0.50	0/1645	0.65	1/2225 (0.0%)
4	h	0.48	0/1645	0.58	0/2225
4	i	0.48	0/1645	0.66	0/2225
4	j	0.47	0/1645	0.67	1/2225 (0.0%)
4	m	0.41	0/1645	0.62	1/2225 (0.0%)
4	n	0.41	0/1645	0.66	3/2225 (0.1%)
4	o	0.49	0/1645	0.65	1/2225 (0.0%)
4	p	0.47	0/1645	0.64	1/2225 (0.0%)
4	q	0.45	0/1645	0.60	0/2225
4	r	0.49	0/1645	0.60	1/2225 (0.0%)
4	s	0.41	0/1645	0.61	0/2225
4	t	0.48	0/1645	0.62	0/2225
4	u	0.36	0/1645	0.57	1/2225 (0.0%)
4	v	0.45	0/1645	0.63	0/2225
5	k	0.37	0/1168	0.59	0/1578
5	l	0.37	0/1168	0.69	2/1578 (0.1%)
5	w	0.35	0/1201	0.55	0/1623
5	x	0.37	0/1201	0.54	0/1623
All	All	0.47	0/217964	0.63	152/295182 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A2	0	1
2	A4	0	2
2	A8	0	1
2	B4	0	1
2	B6	0	1
2	C8	0	1
2	D2	0	1
3	A1	0	1
3	B3	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
3	B9	0	1
3	E5	0	2
5	l	0	1
All	All	0	14

There are no bond length outliers.

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C6	30	ILE	C-N-CA	10.74	148.56	121.70
3	A9	383	ASP	CB-CG-OD1	8.05	125.55	118.30
3	E9	130	LEU	CA-CB-CG	7.97	133.64	115.30
3	A9	73	MET	CG-SD-CE	-7.75	87.80	100.20
3	D5	41	ASP	CB-CG-OD1	7.71	125.24	118.30
3	B7	209	ASP	CB-CG-OD1	7.68	125.21	118.30
2	D2	33	ASP	CB-CG-OD1	7.61	125.14	118.30
2	E4	120	ASP	CB-CG-OD1	7.47	125.03	118.30
2	B6	345	ASP	CB-CG-OD1	7.47	125.03	118.30
2	B4	60	LYS	CD-CE-NZ	-7.37	94.74	111.70
3	E3	263	LEU	CA-CB-CG	7.31	132.12	115.30
3	C3	41	ASP	CB-CG-OD1	7.18	124.76	118.30
3	B3	41	ASP	CB-CG-OD1	7.14	124.73	118.30
3	B7	263	LEU	CA-CB-CG	7.08	131.57	115.30
3	E5	26	ASP	CB-CG-OD1	7.04	124.64	118.30
3	C5	263	LEU	CA-CB-CG	7.04	131.48	115.30
3	C3	31	ASP	CB-CG-OD1	6.92	124.53	118.30
3	B1	161	ASP	CB-CG-OD1	6.90	124.51	118.30
3	C3	263	LEU	CA-CB-CG	6.88	131.13	115.30
2	D6	218	ASP	CB-CG-OD1	6.84	124.46	118.30
2	A4	301	MET	CG-SD-CE	-6.79	89.34	100.20
3	D9	41	ASP	CB-CG-OD1	6.77	124.39	118.30
3	E3	26	ASP	CB-CG-OD1	6.76	124.39	118.30
3	E1	263	LEU	CA-CB-CG	6.62	130.53	115.30
3	A1	383	ASP	CB-CG-OD1	6.56	124.20	118.30
3	A5	41	ASP	CB-CG-OD1	6.55	124.20	118.30
4	n	82	ASP	CB-CG-OD1	6.54	124.19	118.30
2	E4	98	ASP	CB-CG-OD1	6.53	124.18	118.30
3	C9	88	ASP	CB-CG-OD1	6.53	124.18	118.30
3	D5	209	ASP	CB-CG-OD1	6.49	124.14	118.30
3	C1	263	LEU	CA-CB-CG	6.48	130.20	115.30
4	o	202	ARG	NE-CZ-NH1	6.48	123.54	120.30
3	D9	192	LEU	CA-CB-CG	6.46	130.15	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D8	211	ASP	CB-CG-OD1	6.39	124.05	118.30
3	D9	263	LEU	CA-CB-CG	6.38	129.96	115.30
2	B8	322	ASP	CB-CG-OD1	6.32	123.99	118.30
3	A3	395	LEU	CA-CB-CG	6.25	129.69	115.30
2	D2	214	ARG	NE-CZ-NH1	6.23	123.42	120.30
3	B9	267	LEU	CA-CB-CG	6.20	129.56	115.30
2	C6	306	ASP	CB-CG-OD1	6.18	123.86	118.30
2	B8	345	ASP	CB-CG-OD1	6.18	123.86	118.30
2	C0	322	ASP	CB-CG-OD1	6.14	123.82	118.30
3	D7	327	ASP	CB-CG-OD1	6.12	123.81	118.30
3	E3	348	ASN	CA-C-N	6.12	130.65	117.20
3	D9	31	ASP	CB-CG-OD1	6.11	123.80	118.30
3	D5	263	LEU	CA-CB-CG	6.10	129.34	115.30
2	E0	98	ASP	CB-CG-OD1	6.09	123.78	118.30
2	C4	194	LEU	CA-CB-CG	6.08	129.28	115.30
5	l	82	ASP	CB-CG-OD1	6.08	123.77	118.30
4	g	93	LEU	CA-CB-CG	6.03	129.17	115.30
4	r	97	ARG	NE-CZ-NH1	-6.02	117.29	120.30
3	D1	74	ASP	CB-CG-OD1	5.99	123.69	118.30
3	C1	41	ASP	CB-CG-OD1	5.97	123.67	118.30
3	A9	252	LYS	CA-CB-CG	5.94	126.48	113.40
2	E4	69	ASP	CB-CG-OD1	5.92	123.63	118.30
2	C4	217	LEU	CA-CB-CG	5.92	128.91	115.30
3	E5	263	LEU	CA-CB-CG	5.90	128.86	115.30
3	D3	263	LEU	CA-CB-CG	5.87	128.79	115.30
2	D6	127	ASP	CB-CG-OD1	5.85	123.56	118.30
2	C6	217	LEU	CA-CB-CG	5.84	128.72	115.30
2	B8	125	LEU	CA-CB-CG	5.82	128.69	115.30
2	A8	125	LEU	CA-CB-CG	5.80	128.64	115.30
3	E7	263	LEU	CA-CB-CG	5.78	128.59	115.30
3	F1	207	LEU	CA-CB-CG	5.75	128.53	115.30
2	B6	125	LEU	CA-CB-CG	5.74	128.51	115.30
2	B6	205	ASP	CB-CG-OD1	5.71	123.44	118.30
3	C7	263	LEU	CA-CB-CG	5.68	128.35	115.30
3	C1	233	MET	CG-SD-CE	5.65	109.25	100.20
3	E9	171	PRO	C-N-CA	5.63	135.76	121.70
3	E1	203	ASP	CB-CG-OD1	5.62	123.36	118.30
2	D2	211	ASP	CB-CG-OD1	5.58	123.32	118.30
2	D2	306	ASP	CB-CG-OD1	5.58	123.32	118.30
2	F0	227	LEU	CA-CB-CG	5.57	128.12	115.30
3	E9	263	LEU	CA-CB-CG	5.56	128.08	115.30
2	D2	302	MET	CA-CB-CG	5.55	122.74	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D5	192	LEU	CA-CB-CG	5.55	128.06	115.30
3	C9	395	LEU	CA-CB-CG	5.54	128.05	115.30
3	E7	350	LYS	CD-CE-NZ	-5.53	98.99	111.70
2	E4	217	LEU	CB-CG-CD2	-5.52	101.61	111.00
3	A3	263	LEU	CA-CB-CG	5.52	127.99	115.30
2	F0	33	ASP	CB-CG-OD1	5.51	123.26	118.30
3	F1	354	CYS	CA-CB-SG	5.50	123.91	114.00
3	F1	263	LEU	CA-CB-CG	5.50	127.95	115.30
3	D5	320	ARG	NE-CZ-NH1	5.48	123.04	120.30
2	B2	125	LEU	CA-CB-CG	5.46	127.86	115.30
4	n	200	ASP	CB-CG-OD1	5.46	123.22	118.30
2	B4	86	LEU	CA-CB-CG	5.45	127.84	115.30
3	E7	383	ASP	CB-CG-OD1	5.45	123.20	118.30
2	C8	357	TYR	C-N-CA	-5.44	108.10	121.70
3	A1	354	CYS	CA-CB-SG	5.43	123.78	114.00
2	C4	23	LEU	CA-CB-CG	5.43	127.78	115.30
2	E4	221	ARG	CG-CD-NE	5.42	123.18	111.80
3	F1	383	ASP	CB-CG-OD1	5.41	123.17	118.30
3	B9	263	LEU	CA-CB-CG	5.40	127.72	115.30
4	n	119	ARG	NE-CZ-NH1	5.39	122.99	120.30
3	A7	192	LEU	CA-CB-CG	5.38	127.67	115.30
2	B0	125	LEU	CA-CB-CG	5.38	127.67	115.30
4	m	97	ARG	CA-CB-CG	5.37	125.21	113.40
3	A1	263	LEU	CA-CB-CG	5.37	127.65	115.30
4	p	17	LEU	CA-CB-CG	5.34	127.59	115.30
3	F1	324	LYS	CD-CE-NZ	-5.34	99.41	111.70
2	B8	391	MET	CB-CG-SD	-5.32	96.43	112.40
3	A9	192	LEU	CA-CB-CG	5.32	127.53	115.30
3	A1	395	LEU	CA-CB-CG	5.31	127.52	115.30
2	C4	230	LEU	CA-CB-CG	5.31	127.52	115.30
3	A7	263	LEU	CA-CB-CG	5.30	127.50	115.30
3	D7	192	LEU	CA-CB-CG	5.30	127.49	115.30
3	D7	348	ASN	CA-C-N	5.29	128.85	117.20
3	B1	209	ASP	CB-CG-OD1	5.29	123.06	118.30
3	B7	192	LEU	CA-CB-CG	5.29	127.47	115.30
3	E9	415	MET	CA-CB-CG	5.29	122.30	113.30
3	A1	117	LEU	CA-CB-CG	-5.28	103.16	115.30
2	A4	132	LEU	CA-CB-CG	5.28	127.44	115.30
3	D3	44	LEU	CA-CB-CG	5.28	127.44	115.30
5	l	160	ARG	CG-CD-NE	-5.28	100.71	111.80
2	B0	86	LEU	CA-CB-CG	5.28	127.44	115.30
2	D4	322	ASP	CB-CG-OD1	5.28	123.05	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E3	192	LEU	CA-CB-CG	5.26	127.41	115.30
2	D4	264	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	B8	60	LYS	CD-CE-NZ	-5.26	99.61	111.70
3	A1	287	PRO	CA-N-CD	-5.25	104.14	111.50
3	E5	74	ASP	CB-CG-OD1	5.25	123.02	118.30
2	B6	238	LEU	CB-CG-CD1	-5.24	102.09	111.00
2	A0	217	LEU	CA-CB-CG	5.23	127.32	115.30
2	D6	69	ASP	CB-CG-OD1	5.22	123.00	118.30
3	B5	263	LEU	CA-CB-CG	5.21	127.28	115.30
3	A9	263	LEU	CA-CB-CG	5.19	127.24	115.30
2	A2	229	ARG	NE-CZ-NH1	5.18	122.89	120.30
3	B1	263	LEU	CA-CB-CG	5.17	127.18	115.30
3	F1	207	LEU	CB-CG-CD2	-5.16	102.22	111.00
3	F1	118	ASP	CB-CG-OD1	5.16	122.94	118.30
2	B6	275	ILE	CG1-CB-CG2	-5.15	100.08	111.40
3	A5	263	LEU	CA-CB-CG	5.14	127.13	115.30
3	B3	263	LEU	CA-CB-CG	5.14	127.13	115.30
3	D7	26	ASP	CB-CG-OD1	5.14	122.92	118.30
2	A8	397	LEU	CA-CB-CG	5.13	127.10	115.30
4	j	194	ARG	NE-CZ-NH1	5.12	122.86	120.30
2	E4	217	LEU	CA-CB-CG	5.12	127.08	115.30
2	B0	282	TYR	CA-CB-CG	5.12	123.13	113.40
3	C7	39	ASP	CB-CG-OD1	5.12	122.90	118.30
3	E3	31	ASP	CB-CG-OD1	5.09	122.88	118.30
3	D5	252	LYS	CA-CB-CG	5.08	124.57	113.40
2	A0	264	ARG	NE-CZ-NH1	5.07	122.83	120.30
3	A3	267	LEU	CB-CG-CD1	5.06	119.60	111.00
3	A9	161	ASP	CB-CG-OD1	5.05	122.84	118.30
2	B0	203	MET	CB-CG-SD	5.05	127.54	112.40
3	B9	192	LEU	CA-CB-CG	5.05	126.91	115.30
4	u	202	ARG	CA-CB-CG	5.05	124.50	113.40
3	A7	73	MET	CG-SD-CE	-5.03	92.15	100.20
4	f	49	LEU	CB-CG-CD2	5.03	119.55	111.00
2	B8	397	LEU	CA-CB-CG	5.03	126.86	115.30
2	B6	194	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A1	191	GLN	Peptide
2	A2	401	LYS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	A4	254	GLU	Peptide
2	A4	401	LYS	Peptide
2	A8	401	LYS	Peptide
3	B3	43	GLN	Peptide
2	B4	284	GLU	Peptide
2	B6	401	LYS	Peptide
3	B9	200	GLN	Peptide
2	C8	284	GLU	Peptide
2	D2	284	GLU	Peptide
3	E5	321	MET	Peptide
3	E5	322	SER	Peptide
5	l	13	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	174	0	171	3	0
1	1	174	0	171	5	0
1	10	174	0	171	3	0
1	11	174	0	171	1	0
1	12	174	0	171	3	0
1	13	174	0	171	1	0
1	14	174	0	171	0	0
1	15	174	0	171	1	0
1	16	174	0	171	2	0
1	17	174	0	171	2	0
1	18	174	0	171	1	0
1	19	174	0	171	2	0
1	2	174	0	171	1	0
1	20	174	0	171	2	0
1	21	174	0	171	3	0
1	22	160	0	156	3	0
1	23	160	0	156	3	0
1	3	174	0	171	2	0
1	4	174	0	171	2	0
1	5	174	0	171	2	0
1	6	174	0	171	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	7	174	0	171	3	0
1	8	174	0	171	1	0
1	9	174	0	171	2	0
2	A0	3325	0	3251	54	0
2	A2	3325	0	3252	54	0
2	A4	3325	0	3252	43	0
2	A6	3325	0	3252	48	0
2	A8	3325	0	3252	54	0
2	B0	3325	0	3252	47	0
2	B2	3325	0	3252	44	0
2	B4	3325	0	3252	62	0
2	B6	3325	0	3252	47	0
2	B8	3325	0	3252	61	0
2	C0	3325	0	3252	65	0
2	C2	3325	0	3252	69	0
2	C4	3325	0	3252	74	0
2	C6	3325	0	3251	69	0
2	C8	3325	0	3252	45	0
2	D0	3325	0	3252	38	0
2	D2	3325	0	3252	39	0
2	D4	3325	0	3252	41	0
2	D6	3325	0	3252	43	0
2	D8	3325	0	3252	38	0
2	E0	3325	0	3252	35	0
2	E2	3325	0	3252	45	0
2	E4	3325	0	3252	55	0
2	E6	3325	0	3252	50	0
2	E8	3325	0	3252	71	0
2	F0	3325	0	3252	67	0
3	A1	3331	0	3207	58	0
3	A3	3331	0	3209	52	0
3	A5	3331	0	3207	53	0
3	A7	3331	0	3207	41	0
3	A9	3331	0	3207	58	0
3	B1	3331	0	3209	47	0
3	B3	3331	0	3207	50	0
3	B5	3331	0	3207	48	0
3	B7	3331	0	3209	47	0
3	B9	3331	0	3209	44	0
3	C1	3331	0	3209	72	0
3	C3	3331	0	3209	62	0
3	C5	3331	0	3209	65	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C7	3331	0	3209	66	0
3	C9	3331	0	3209	59	0
3	D1	3331	0	3209	50	0
3	D3	3331	0	3207	56	0
3	D5	3331	0	3207	61	0
3	D7	3331	0	3207	63	0
3	D9	3331	0	3207	49	0
3	E1	3331	0	3207	39	0
3	E3	3331	0	3209	44	0
3	E5	3331	0	3207	60	0
3	E7	3331	0	3207	50	0
3	E9	3331	0	3206	68	0
3	F1	3331	0	3207	72	0
4	a	1198	0	1194	0	0
4	b	1198	0	1194	0	0
4	c	1608	0	1590	0	0
4	d	1608	0	1590	0	0
4	e	1608	0	1590	0	0
4	f	1608	0	1590	0	0
4	g	1608	0	1590	0	0
4	h	1608	0	1590	0	0
4	i	1608	0	1590	0	0
4	j	1608	0	1590	0	0
4	m	1608	0	1590	0	0
4	n	1608	0	1590	0	0
4	o	1608	0	1590	0	0
4	p	1608	0	1590	0	0
4	q	1608	0	1590	0	0
4	r	1608	0	1590	0	0
4	s	1608	0	1590	0	0
4	t	1608	0	1590	0	0
4	u	1608	0	1590	0	0
4	v	1608	0	1590	0	0
5	k	1140	0	1143	0	0
5	l	1140	0	1143	0	0
5	w	1172	0	1171	0	0
5	x	1172	0	1171	0	0
6	A0	32	0	12	2	0
6	A2	32	0	12	0	0
6	A4	32	0	12	0	0
6	A6	32	0	12	0	0
6	A8	32	0	12	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B0	32	0	12	1	0
6	B2	32	0	12	1	0
6	B4	32	0	12	0	0
6	B6	32	0	12	2	0
6	B8	32	0	12	1	0
6	C0	32	0	12	2	0
6	C2	32	0	12	0	0
6	C4	32	0	12	1	0
6	C6	32	0	12	3	0
6	C8	32	0	12	1	0
6	D0	32	0	12	0	0
6	D2	32	0	12	0	0
6	D4	32	0	12	1	0
6	D6	32	0	12	0	0
6	D8	32	0	12	1	0
6	E0	32	0	12	0	0
6	E2	32	0	12	1	0
6	E4	32	0	12	0	0
6	E6	32	0	12	3	0
6	E8	32	0	12	2	0
6	F0	32	0	12	1	0
7	A0	1	0	0	0	0
7	A2	1	0	0	0	0
7	A4	1	0	0	0	0
7	A6	1	0	0	0	0
7	A8	1	0	0	0	0
7	B0	1	0	0	0	0
7	B2	1	0	0	0	0
7	B4	1	0	0	0	0
7	B6	1	0	0	0	0
7	B8	1	0	0	0	0
7	C0	1	0	0	0	0
7	C2	1	0	0	0	0
7	C4	1	0	0	0	0
7	C6	1	0	0	0	0
7	C8	1	0	0	0	0
7	D0	1	0	0	0	0
7	D2	1	0	0	0	0
7	D4	1	0	0	0	0
7	D6	1	0	0	0	0
7	D8	1	0	0	0	0
7	E0	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E2	1	0	0	0	0
7	E4	1	0	0	0	0
7	E6	1	0	0	0	0
7	E8	1	0	0	0	0
7	F0	1	0	0	0	0
8	A1	28	0	12	2	0
8	A3	28	0	12	2	0
8	A5	28	0	12	0	0
8	A7	28	0	12	0	0
8	A9	28	0	12	1	0
8	B1	28	0	12	0	0
8	B3	28	0	12	1	0
8	B5	28	0	12	0	0
8	B7	28	0	12	1	0
8	B9	28	0	12	0	0
8	C1	28	0	12	1	0
8	C3	28	0	12	2	0
8	C5	28	0	12	1	0
8	C7	28	0	12	0	0
8	C9	28	0	12	0	0
8	D1	28	0	12	0	0
8	D3	28	0	12	0	0
8	D5	28	0	12	1	0
8	D7	28	0	12	0	0
8	D9	28	0	12	0	0
8	E1	28	0	12	0	0
8	E3	28	0	12	3	0
8	E5	28	0	12	0	0
8	E7	28	0	12	0	0
8	E9	28	0	12	0	0
8	F1	28	0	12	1	0
All	All	214754	0	208287	2539	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 7.

All (2539) 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)
2:D4:151:CYS:HG	2:D4:193:SER:HG	1.23	0.83
3:A9:248:SER:HA	3:A9:252:LYS:HG2	1.67	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E2:88:HIS:HB3	2:E2:91:GLN:HG2	1.65	0.77
2:C6:6:SER:HA	2:C6:136:LEU:HB2	1.67	0.76
2:D0:142:GLY:HA3	2:D0:183:GLU:HG2	1.66	0.76
3:A9:100:ASN:HB2	3:A9:103:LYS:HG2	1.67	0.76
3:B1:49:VAL:HG21	3:B1:241:ARG:HG2	1.67	0.76
3:E7:213:ARG:HH22	3:E7:297:LYS:HB2	1.50	0.76
3:B5:12:CYS:HG	3:B5:138:SER:HG	1.32	0.76
2:F0:222:PRO:O	3:F1:324:LYS:NZ	2.19	0.76
2:B4:178:SER:OG	3:B5:347:ASN:ND2	2.19	0.75
2:C4:151:CYS:SG	2:C4:193:SER:OG	2.44	0.75
2:B4:284:GLU:OE2	2:B8:88:HIS:NE2	2.20	0.74
2:C6:168:ASN:HD21	2:C6:194:LEU:HD11	1.50	0.74
3:C9:208:TYR:HB3	2:D0:326:LYS:HE2	1.70	0.74
3:B5:324:LYS:HA	3:B5:327:ASP:HB2	1.70	0.73
3:A9:256:ASN:HB2	3:A9:350:LYS:HE3	1.69	0.73
2:C2:222:PRO:O	3:C3:324:LYS:NZ	2.22	0.73
2:D4:292:THR:HG21	2:D4:331:ALA:HB1	1.70	0.73
2:C0:176:GLN:O	3:C1:347:ASN:ND2	2.22	0.72
2:A8:212:ILE:HG12	2:A8:275:ILE:HD11	1.71	0.72
3:F1:207:LEU:HD21	3:F1:225:LEU:HB3	1.72	0.72
2:B2:96:LYS:NZ	3:B3:129:CYS:SG	2.62	0.71
3:C9:354:CYS:SG	3:C9:355:ASP:N	2.64	0.71
2:B2:234:VAL:HG21	2:B2:302:MET:HE1	1.71	0.71
2:D6:222:PRO:O	3:D7:324:LYS:NZ	2.23	0.71
2:A8:151:CYS:SG	2:A8:193:SER:OG	2.48	0.71
2:A8:151:CYS:HG	2:A8:193:SER:HG	1.37	0.71
2:E4:107:HIS:NE2	2:E4:151:CYS:SG	2.64	0.71
3:D9:169:VAL:HG12	3:D9:202:ILE:HB	1.74	0.70
2:E0:292:THR:HG21	2:E0:331:ALA:HB1	1.73	0.70
2:A8:284:GLU:OE2	2:B2:88:HIS:NE2	2.24	0.70
3:B7:99:ASN:ND2	2:B8:254:GLU:OE1	2.24	0.70
2:E8:80:THR:HA	2:E8:84:ARG:HE	1.56	0.70
2:B0:212:ILE:HG12	2:B0:275:ILE:HD11	1.72	0.70
3:D3:248:SER:HA	3:D3:252:LYS:HD3	1.72	0.70
3:C3:190:HIS:HB2	3:C3:414:ASN:HD21	1.56	0.69
2:E2:259:LEU:HD21	2:E2:316:CYS:HB2	1.73	0.69
2:B6:238:LEU:HD11	2:B6:378:ILE:HD11	1.73	0.69
3:C5:354:CYS:SG	3:C5:355:ASP:N	2.65	0.69
3:D1:274:THR:HG21	3:D1:282:ARG:HD2	1.73	0.69
3:A5:313:ALA:HB3	3:A5:349:MET:HG2	1.73	0.69
3:D9:12:CYS:SG	3:D9:13:GLY:N	2.65	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D2:181:VAL:HG22	3:D3:256:ASN:HD22	1.57	0.69
2:A0:132:LEU:HG	2:A0:164:LYS:HE2	1.74	0.69
3:D5:129:CYS:SG	3:D5:162:ARG:NH2	2.65	0.69
3:F1:267:LEU:HD21	3:F1:374:ILE:HD11	1.75	0.69
3:D7:169:VAL:HG12	3:D7:202:ILE:HB	1.74	0.69
3:D1:98:GLY:H	3:D1:103:LYS:HD3	1.59	0.68
3:A1:15:GLN:NE2	8:A1:501:GDP:O6	2.27	0.68
2:D0:292:THR:HG21	2:D0:331:ALA:HB1	1.74	0.68
2:B8:280:LYS:NZ	2:C2:90:GLU:OE1	2.26	0.68
3:E1:220:PRO:HD2	2:E2:326:LYS:HD2	1.74	0.68
2:C4:398:MET:HE1	3:C5:346:PRO:HD2	1.75	0.68
2:A6:137:MET:HB3	2:A6:168:ASN:HA	1.77	0.67
3:C3:306:ARG:HA	3:C3:340:TYR:HE1	1.59	0.67
3:C3:204:ASN:HD21	8:C3:501:GDP:HN22	1.40	0.67
2:B4:96:LYS:NZ	3:B5:129:CYS:SG	2.61	0.67
3:C3:166:THR:HB	3:C3:199:VAL:HG22	1.76	0.67
3:E9:256:ASN:HD21	3:E9:350:LYS:HG2	1.58	0.67
2:B0:174:SER:OG	2:B0:177:VAL:O	2.12	0.67
2:C6:108:TYR:O	2:C6:112:LYS:NZ	2.27	0.67
3:C9:100:ASN:HB3	3:C9:103:LYS:HG2	1.75	0.67
3:D3:49:VAL:HG21	3:D3:241:ARG:HG2	1.76	0.67
2:A0:142:GLY:O	2:A0:186:ASN:ND2	2.28	0.67
3:A7:207:LEU:HB3	3:A7:225:LEU:HD12	1.76	0.67
2:B2:53:PHE:HB3	2:B2:61:HIS:HB3	1.76	0.67
3:C1:166:THR:HB	3:C1:199:VAL:HG12	1.77	0.67
2:C6:151:CYS:SG	2:C6:193:SER:OG	2.52	0.67
2:D2:292:THR:HG21	2:D2:331:ALA:HB1	1.77	0.67
3:B1:207:LEU:HB3	3:B1:225:LEU:HD22	1.76	0.66
3:A1:10:GLY:HA2	3:A1:143:THR:HG23	1.77	0.66
3:D3:202:ILE:HD11	3:D3:268:ILE:HD12	1.78	0.66
3:D3:220:PRO:HD2	2:D4:326:LYS:HD3	1.77	0.66
2:A0:229:ARG:HD3	2:A0:363:VAL:HG21	1.77	0.66
3:A5:33:THR:O	3:A5:58:ARG:NH2	2.28	0.66
2:F0:70:LEU:HD12	2:F0:99:ALA:HB2	1.77	0.66
2:D4:105:ARG:HH12	3:D5:251:ARG:HD3	1.60	0.66
2:E0:284:GLU:OE2	2:E4:88:HIS:NE2	2.25	0.66
3:A5:221:THR:HG23	3:A5:223:GLY:H	1.61	0.66
3:C7:135:ILE:HB	3:C7:166:THR:HG22	1.76	0.66
3:D3:129:CYS:SG	3:D3:162:ARG:NH2	2.69	0.66
2:B4:269:LEU:HD21	2:B4:384:ILE:HD11	1.77	0.66
3:A3:6:HIS:NE2	3:A3:8:GLN:OE1	2.29	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A8:22:GLU:OE2	2:A8:229:ARG:NH1	2.28	0.66
3:D9:311:LEU:HD12	3:D9:342:VAL:HG11	1.78	0.66
3:B3:91:VAL:HG21	3:B3:116:VAL:HG22	1.78	0.66
3:C7:1:MET:N	3:C7:128:ASP:OD2	2.28	0.66
2:E2:76:ASP:HA	2:E2:79:ARG:HD2	1.78	0.66
3:E7:284:LEU:HB3	3:E7:362:LYS:HE3	1.78	0.66
2:E8:180:ALA:HB3	2:E8:183:GLU:HG2	1.78	0.66
3:C5:257:LEU:HD11	3:C5:314:SER:HB3	1.78	0.65
1:8:254:LYS:NZ	2:C0:364:PRO:O	2.25	0.65
2:B0:284:GLU:OE2	2:B4:88:HIS:NE2	2.29	0.65
3:C7:2:ARG:NH1	3:C7:249:ASP:OD2	2.29	0.65
2:E0:298:PRO:HG3	2:E0:308:ARG:HH22	1.61	0.65
2:E4:274:PRO:HD3	2:E4:291:ILE:HD11	1.78	0.65
2:A2:195:LEU:HD21	2:A2:264:ARG:HE	1.60	0.65
3:C1:164:MET:HB2	3:C1:197:ASP:H	1.60	0.65
2:D2:98:ASP:O	2:D2:105:ARG:NH2	2.27	0.65
2:A0:115:VAL:HG21	2:A0:152:LEU:HD22	1.78	0.65
2:C0:399:TYR:O	2:C0:402:ARG:NH2	2.30	0.65
3:D7:49:VAL:HG21	3:D7:241:ARG:HG2	1.79	0.65
2:D2:284:GLU:OE2	2:D6:88:HIS:NE2	2.30	0.65
3:E1:248:SER:HA	3:E1:252:LYS:HG3	1.78	0.65
2:B4:254:GLU:OE1	2:B4:352:LYS:NZ	2.30	0.65
2:C6:121:ARG:HH12	2:C6:124:LYS:HE3	1.61	0.65
2:D6:221:ARG:HA	3:D7:324:LYS:HE3	1.77	0.65
3:A1:281:TYR:HD2	3:A5:87:PRO:HD3	1.62	0.65
3:A7:33:THR:O	3:A7:58:ARG:NH2	2.30	0.65
2:D0:174:SER:OG	2:D0:177:VAL:O	2.13	0.65
2:C8:76:ASP:OD2	3:C9:46:ARG:NH2	2.28	0.65
2:A0:309:HIS:NE2	2:A0:386:GLU:OE2	2.30	0.65
3:C1:221:THR:HG22	3:C1:223:GLY:H	1.62	0.65
2:C6:31:GLN:NE2	2:C6:33:ASP:OD2	2.30	0.65
3:F1:210:ILE:HD11	3:F1:298:ASN:HA	1.79	0.65
2:D6:27:GLU:OE1	2:D6:243:ARG:NH1	2.30	0.64
2:B6:50:ASN:O	2:B6:64:ARG:NH2	2.31	0.64
2:D2:30:ILE:HG22	2:D2:36:MET:HB3	1.79	0.64
2:C0:298:PRO:HG3	2:C0:308:ARG:HH12	1.63	0.64
2:D8:210:TYR:HH	3:D9:323:THR:HG1	1.44	0.64
3:A1:412:GLU:OE2	3:A1:416:ASN:ND2	2.31	0.64
3:B3:208:TYR:HB3	2:B4:326:LYS:HE3	1.79	0.64
3:D7:68:LEU:HB3	3:D7:96:GLY:HA2	1.78	0.64
3:D7:334:GLN:HE21	3:D7:349:MET:HG2	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E7:163:ILE:HD13	3:E7:250:LEU:HB3	1.80	0.64
2:A6:212:ILE:HG12	2:A6:275:ILE:HD11	1.79	0.64
2:B2:174:SER:OG	2:B2:177:VAL:O	2.15	0.64
2:B8:195:LEU:HD21	2:B8:264:ARG:HE	1.62	0.64
2:C6:76:ASP:OD2	3:C7:46:ARG:NH1	2.30	0.64
2:C2:202:VAL:HG22	2:C2:268:MET:HG3	1.79	0.64
3:E9:139:LEU:HD12	3:E9:170:PHE:HE1	1.62	0.64
3:A7:27:GLU:OE2	3:A7:241:ARG:NH2	2.31	0.64
3:B1:171:PRO:O	3:B1:380:ARG:NH1	2.30	0.64
2:B6:132:LEU:HB3	2:B6:164:LYS:HE2	1.79	0.64
2:C2:399:TYR:O	2:C2:402:ARG:NH2	2.31	0.64
3:C3:165:GLU:OE2	3:C3:200:GLN:NE2	2.31	0.64
2:D6:30:ILE:HG22	2:D6:36:MET:HB3	1.80	0.64
3:F1:10:GLY:HA2	3:F1:143:THR:HG23	1.80	0.64
2:A6:155:GLU:OE1	2:A6:197:HIS:NE2	2.27	0.63
2:F0:219:ILE:HG13	2:F0:222:PRO:HD3	1.80	0.63
6:A0:501:GTP:O3G	3:A1:252:LYS:NZ	2.28	0.63
2:D0:76:ASP:OD2	3:D1:46:ARG:NH1	2.31	0.63
3:E9:113:ILE:HA	3:E9:116:VAL:HG12	1.80	0.63
2:C0:207:GLU:HA	2:C0:210:TYR:HB2	1.80	0.63
2:D0:309:HIS:NE2	2:D0:386:GLU:OE1	2.27	0.63
2:E0:259:LEU:HD21	2:E0:316:CYS:HB2	1.79	0.63
2:E4:151:CYS:SG	2:E4:193:SER:OG	2.52	0.63
3:E5:267:LEU:HD12	3:E5:301:CYS:HB3	1.80	0.63
2:A0:245:ASP:O	2:A0:358:GLN:NE2	2.28	0.63
3:B7:325:GLU:HA	3:B7:328:GLU:HG3	1.80	0.63
3:D7:153:SER:HB2	3:D7:191:GLN:HE22	1.63	0.63
2:C2:76:ASP:OD2	3:C3:46:ARG:NH1	2.32	0.63
2:B0:2:ARG:HB2	2:B0:133:GLN:HE22	1.63	0.63
2:C4:6:SER:HA	2:C4:136:LEU:HB2	1.81	0.63
2:C4:387:VAL:HA	2:C4:390:ARG:HH21	1.64	0.63
3:C9:244:GLY:HA2	3:C9:355:ASP:HB2	1.81	0.63
2:C6:339:ARG:O	2:C6:342:GLN:NE2	2.32	0.63
3:B7:7:VAL:HB	3:B7:135:ILE:HG12	1.81	0.63
2:D6:11:GLN:NE2	2:D6:15:GLN:OE1	2.31	0.63
3:E7:100:ASN:HB3	3:E7:103:LYS:HG2	1.79	0.63
3:E7:49:VAL:HG11	3:E7:241:ARG:HG2	1.81	0.62
3:F1:2:ARG:NH2	3:F1:249:ASP:OD2	2.32	0.62
2:B6:258:ASN:HB3	2:B6:352:LYS:HG3	1.81	0.62
2:C8:284:GLU:OE2	2:D2:88:HIS:NE2	2.33	0.62
3:A1:107:THR:HG21	3:A1:401:GLU:HG2	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A5:287:PRO:HA	3:A5:329:GLN:HE22	1.64	0.62
3:A7:1:MET:N	3:A7:128:ASP:OD2	2.28	0.62
2:C6:97:GLU:OE2	2:C6:105:ARG:NH2	2.27	0.62
2:A8:136:LEU:HD13	2:A8:235:ILE:HD11	1.81	0.62
3:C7:178:THR:OG1	3:C7:181:GLU:OE2	2.18	0.62
2:D8:259:LEU:HD11	2:D8:316:CYS:HB2	1.79	0.62
3:B3:49:VAL:HG21	3:B3:241:ARG:HG2	1.80	0.62
2:B6:234:VAL:HG21	2:B6:302:MET:HE1	1.80	0.62
2:C0:222:PRO:HD2	3:C1:324:LYS:HG2	1.81	0.62
2:D4:407:TRP:HH2	3:D5:258:ILE:HB	1.65	0.62
3:C5:1:MET:N	3:C5:128:ASP:OD2	2.33	0.62
2:E6:76:ASP:OD1	2:E6:79:ARG:NH2	2.32	0.62
3:E7:332:ASN:OD1	3:E7:336:LYS:NZ	2.32	0.62
2:E8:292:THR:HG21	2:E8:331:ALA:HB1	1.80	0.62
3:E9:150:LEU:HD21	3:E9:154:LYS:HZ2	1.65	0.62
3:A3:7:VAL:HB	3:A3:135:ILE:HG22	1.81	0.62
3:B1:135:ILE:HB	3:B1:166:THR:HG22	1.81	0.62
3:B1:238:CYS:SG	3:B1:241:ARG:NH2	2.72	0.62
3:B3:375:GLN:NE2	3:B3:423:GLN:OE1	2.32	0.62
2:C2:202:VAL:HA	2:C2:268:MET:HB2	1.81	0.62
3:C5:68:LEU:HD12	3:C5:97:ALA:HB2	1.81	0.62
3:C7:165:GLU:OE2	3:C7:200:GLN:NE2	2.33	0.62
3:D3:91:VAL:HG21	3:D3:116:VAL:HG22	1.82	0.62
2:B0:53:PHE:HB3	2:B0:61:HIS:HB3	1.80	0.62
2:E4:221:ARG:NH2	3:E5:322:SER:O	2.33	0.62
2:B2:120:ASP:OD1	2:B2:123:ARG:NH2	2.33	0.61
3:D7:280:GLN:HE22	3:E1:58:ARG:HH11	1.44	0.61
2:F0:66:VAL:HG12	2:F0:91:GLN:HB2	1.82	0.61
2:A0:3:GLU:OE2	2:A0:64:ARG:NH1	2.33	0.61
3:A5:27:GLU:OE1	3:A5:241:ARG:NH2	2.33	0.61
3:B9:318:ARG:HD2	3:B9:358:PRO:HD3	1.81	0.61
3:C1:249:ASP:H	3:C1:252:LYS:HB2	1.65	0.61
3:E1:99:ASN:HD21	2:E2:258:ASN:HD21	1.45	0.61
2:D4:11:GLN:HG3	2:D4:74:VAL:HG21	1.81	0.61
3:E5:1:MET:N	3:E5:128:ASP:OD2	2.31	0.61
3:A1:52:ASN:ND2	3:A1:123:GLU:OE2	2.33	0.61
2:A4:191:THR:HA	2:A4:194:LEU:HG	1.83	0.61
2:C4:2:ARG:HB3	2:C4:133:GLN:HE21	1.65	0.61
3:A1:140:GLY:O	3:A1:184:ASN:ND2	2.34	0.61
2:A2:91:GLN:HA	2:A2:121:ARG:HH12	1.65	0.61
3:A5:132:GLY:HA3	3:A5:163:ILE:HG22	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C0:202:VAL:HA	2:C0:268:MET:HB2	1.83	0.61
2:D6:176:GLN:O	3:D7:347:ASN:ND2	2.34	0.61
2:A2:356:ASN:OD1	2:A2:358:GLN:NE2	2.34	0.61
2:B0:101:ASN:OD1	3:B1:252:LYS:NZ	2.29	0.61
3:B1:248:SER:HA	3:B1:252:LYS:HG2	1.83	0.61
2:C0:10:GLY:HA2	2:C0:145:THR:HG23	1.81	0.61
3:C1:49:VAL:HG11	3:C1:241:ARG:HG2	1.83	0.61
2:C6:236:SER:O	2:C6:243:ARG:NH2	2.34	0.61
3:E9:218:THR:O	2:F0:326:LYS:NZ	2.34	0.61
3:B3:248:SER:HA	3:B3:252:LYS:HE2	1.83	0.61
2:B4:174:SER:OG	2:B4:177:VAL:O	2.18	0.61
3:C7:354:CYS:SG	3:C7:355:ASP:N	2.73	0.61
3:A7:107:THR:OG1	3:A7:108:GLU:OE1	2.18	0.61
3:B5:132:GLY:HA3	3:B5:163:ILE:HG22	1.81	0.61
3:B5:156:ARG:HD3	3:B5:164:MET:HG2	1.82	0.61
2:E8:311:LYS:HE2	2:E8:344:VAL:HA	1.82	0.61
2:A6:119:LEU:HD13	2:A6:122:ILE:HD11	1.82	0.61
2:A6:241:SER:OG	2:A6:250:VAL:O	2.18	0.61
3:D5:135:ILE:HG13	3:D5:152:ILE:HD11	1.81	0.61
2:E6:339:ARG:NH2	2:E6:342:GLN:OE1	2.34	0.61
3:C3:200:GLN:HG3	3:C3:268:ILE:HD11	1.83	0.60
3:A3:329:GLN:HA	3:A3:332:ASN:HB2	1.83	0.60
3:A7:132:GLY:HA3	3:A7:163:ILE:HG22	1.83	0.60
2:A8:292:THR:HG21	2:A8:331:ALA:HB1	1.82	0.60
2:A4:119:LEU:HD13	2:A4:122:ILE:HD11	1.82	0.60
3:B5:218:THR:HG23	3:B5:219:THR:HG23	1.84	0.60
2:A4:30:ILE:HG22	2:A4:36:MET:HB3	1.83	0.60
3:A5:180:VAL:O	3:A5:184:ASN:ND2	2.34	0.60
3:C3:267:LEU:HD11	3:C3:374:ILE:HD13	1.83	0.60
3:D5:49:VAL:HG21	3:D5:241:ARG:HG2	1.84	0.60
3:E3:248:SER:HA	3:E3:252:LYS:HG2	1.82	0.60
3:F1:100:ASN:HB3	3:F1:103:LYS:HG2	1.83	0.60
2:B6:33:ASP:OD2	2:B6:35:GLN:NE2	2.35	0.60
2:C4:241:SER:HB2	2:C4:249:ASN:HB2	1.84	0.60
2:D0:280:LYS:NZ	2:D4:90:GLU:OE2	2.33	0.60
2:B0:223:THR:HG22	3:B1:322:SER:HA	1.83	0.60
2:C0:151:CYS:SG	2:C0:193:SER:OG	2.56	0.60
2:C4:310:GLY:HA3	2:C4:383:ALA:HB2	1.83	0.60
3:E5:100:ASN:HB3	3:E5:103:LYS:HG2	1.81	0.60
2:A0:292:THR:HG21	2:A0:331:ALA:HB1	1.84	0.60
3:A5:27:GLU:HA	3:A5:359:LYS:HD2	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A6:254:GLU:O	2:A6:258:ASN:ND2	2.35	0.60
2:A8:259:LEU:HD11	2:A8:316:CYS:HB2	1.84	0.60
2:B0:138:PHE:HZ	2:B0:235:ILE:HD12	1.66	0.60
3:B9:332:ASN:OD1	3:B9:336:LYS:NZ	2.34	0.60
2:C0:403:ALA:HA	3:C1:260:PHE:HE1	1.65	0.60
3:E9:209:ASP:OD1	3:E9:213:ARG:NH1	2.35	0.60
2:B8:27:GLU:OE2	2:B8:243:ARG:NH1	2.35	0.60
3:E1:172:SER:HB3	3:E1:205:GLU:HG2	1.84	0.60
3:E5:105:HIS:HD2	3:E5:150:LEU:HD22	1.66	0.60
3:E5:172:SER:HB2	3:E5:205:GLU:HG2	1.84	0.60
3:A9:27:GLU:OE2	3:A9:241:ARG:NH1	2.32	0.60
2:B6:396:ASP:OD2	2:B6:422:ARG:NH2	2.35	0.60
3:C3:100:ASN:HB3	3:C3:103:LYS:HG2	1.82	0.60
2:B0:115:VAL:HG21	2:B0:152:LEU:HD22	1.83	0.60
3:C1:165:GLU:OE2	3:C1:200:GLN:NE2	2.34	0.60
2:C6:151:CYS:HG	2:C6:193:SER:HG	1.49	0.60
2:D4:88:HIS:HB3	2:D4:91:GLN:HG2	1.83	0.60
3:D9:25:SER:HG	3:D9:51:TYR:HH	1.48	0.60
2:C2:215:ARG:NH2	2:C2:297:GLU:OE2	2.35	0.59
3:C3:249:ASP:H	3:C3:252:LYS:HB2	1.66	0.59
2:C6:244:PHE:HB2	2:C6:356:ASN:HD21	1.66	0.59
2:C8:292:THR:HG21	2:C8:331:ALA:HB1	1.83	0.59
2:D2:199:ASP:OD2	2:D2:256:GLN:NE2	2.35	0.59
2:D8:123:ARG:NH1	2:D8:160:ASP:OD2	2.31	0.59
2:E4:277:SER:OG	2:E4:278:ALA:N	2.35	0.59
3:E9:10:GLY:HA2	3:E9:143:THR:HG23	1.82	0.59
3:F1:285:SER:N	3:F1:288:GLU:OE2	2.35	0.59
3:C3:163:ILE:HD13	3:C3:250:LEU:HB3	1.85	0.59
3:C3:337:ASN:HB3	3:C3:340:TYR:HB2	1.81	0.59
3:A7:180:VAL:O	3:A7:184:ASN:ND2	2.35	0.59
2:C8:101:ASN:HD22	3:C9:256:ASN:HD21	1.50	0.59
2:C6:309:HIS:NE2	2:C6:386:GLU:OE1	2.36	0.59
3:B5:16:ILE:HD11	3:B5:229:VAL:HG11	1.85	0.59
2:B8:241:SER:OG	2:B8:250:VAL:O	2.17	0.59
2:C0:223:THR:OG1	3:C1:245:GLN:OE1	2.20	0.59
2:C6:180:ALA:O	3:C7:347:ASN:ND2	2.36	0.59
3:E9:239:CYS:SG	3:E9:248:SER:N	2.73	0.59
2:C2:255:PHE:HB3	2:C2:259:LEU:HD12	1.85	0.59
3:C5:100:ASN:HB3	3:C5:103:LYS:HG2	1.84	0.59
2:E2:76:ASP:OD1	2:E2:79:ARG:NH2	2.33	0.59
3:E9:398:TYR:HB3	3:E9:403:MET:HG3	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D5:127:CYS:SG	3:D5:128:ASP:N	2.73	0.59
1:20:248:ARG:NH1	2:E8:77:GLU:OE2	2.36	0.59
2:A8:106:GLY:HA3	2:A8:148:GLY:HA3	1.84	0.59
2:B8:76:ASP:HA	2:B8:79:ARG:HD2	1.85	0.59
3:C9:67:ASP:OD2	3:C9:72:THR:OG1	2.20	0.59
3:D5:64:ILE:HD11	3:D5:123:GLU:HG3	1.85	0.59
1:10:246:CYS:N	3:C9:355:ASP:OD2	2.35	0.59
2:B4:180:ALA:O	3:B5:347:ASN:ND2	2.33	0.59
3:C7:262:ARG:NH1	3:C7:421:GLU:OE2	2.35	0.59
2:D4:298:PRO:HB3	2:D4:307:PRO:HD2	1.84	0.59
2:E6:107:HIS:NE2	2:E6:151:CYS:SG	2.69	0.59
3:F1:113:ILE:HA	3:F1:116:VAL:HG12	1.84	0.59
2:D4:101:ASN:OD1	3:D5:252:LYS:NZ	2.35	0.59
2:A0:268:MET:N	2:A0:268:MET:SD	2.76	0.58
3:E5:169:VAL:HG12	3:E5:202:ILE:HB	1.85	0.58
2:E6:283:HIS:NE2	2:F0:85:HIS:O	2.34	0.58
2:B2:284:GLU:OE2	2:B6:88:HIS:NE2	2.36	0.58
2:B6:286:LEU:O	2:B6:373:ARG:NH1	2.28	0.58
3:C1:1:MET:N	3:C1:128:ASP:OD2	2.36	0.58
3:C3:30:ILE:HD11	3:C3:47:ILE:HD11	1.84	0.58
3:C5:350:LYS:NZ	3:C5:352:SER:OG	2.36	0.58
2:E4:280:LYS:HZ1	2:E8:90:GLU:HB2	1.67	0.58
1:1:239:LEU:HD22	3:A7:359:LYS:HB3	1.85	0.58
1:4:247:TYR:HE1	2:B2:81:GLY:HA3	1.67	0.58
3:B3:152:ILE:HG23	3:B3:164:MET:HE1	1.84	0.58
3:D1:67:ASP:OD2	3:D1:72:THR:OG1	2.21	0.58
2:D6:286:LEU:O	2:D6:373:ARG:NH1	2.31	0.58
3:F1:244:GLY:HA2	3:F1:355:ASP:HB2	1.85	0.58
2:B6:195:LEU:HD21	2:B6:264:ARG:HE	1.68	0.58
2:C4:405:VAL:HG13	2:C4:418:PHE:HE2	1.69	0.58
2:C6:26:LEU:HD21	2:C6:363:VAL:HG12	1.86	0.58
3:D1:66:MET:HE1	3:D1:151:LEU:HD22	1.84	0.58
2:D6:33:ASP:O	2:D6:60:LYS:NZ	2.37	0.58
1:21:244:GLN:O	3:F1:320:ARG:NH2	2.32	0.58
2:A4:164:LYS:NZ	2:A4:165:SER:O	2.36	0.58
3:A9:68:LEU:HB3	3:A9:96:GLY:HA2	1.85	0.58
3:A9:107:THR:OG1	3:A9:108:GLU:OE1	2.18	0.58
3:A9:292:GLN:O	3:A9:298:ASN:ND2	2.37	0.58
2:C0:306:ASP:N	2:C0:386:GLU:OE2	2.36	0.58
2:C2:51:THR:HG23	2:C2:52:PHE:HD1	1.69	0.58
2:C2:259:LEU:HD21	2:C2:316:CYS:HB2	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D7:249:ASP:OD1	3:D7:250:LEU:N	2.36	0.58
2:E4:338:LYS:HZ3	2:E4:340:THR:HG22	1.68	0.58
2:A2:102:ASN:HB2	2:A2:105:ARG:HB2	1.86	0.58
3:A7:117:LEU:HA	3:A7:120:VAL:HG12	1.85	0.58
2:C4:121:ARG:HH22	2:C4:124:LYS:HE3	1.67	0.58
2:C4:287:SER:HA	2:C4:373:ARG:HH21	1.68	0.58
2:C4:309:HIS:NE2	2:C4:386:GLU:OE1	2.36	0.58
2:A8:102:ASN:HB2	2:A8:105:ARG:HB2	1.85	0.58
2:B2:107:HIS:NE2	2:B2:151:CYS:SG	2.76	0.58
2:B6:73:THR:HG22	3:B7:46:ARG:HE	1.66	0.58
2:C4:70:LEU:HD13	2:C4:95:GLY:HA3	1.85	0.58
3:E9:105:HIS:HD2	3:E9:150:LEU:HD12	1.68	0.58
1:13:254:LYS:NZ	2:D4:22:GLU:OE2	2.37	0.58
3:C3:282:ARG:NH2	3:C3:284:LEU:HD13	2.18	0.58
2:E6:181:VAL:HG13	3:E7:350:LYS:NZ	2.19	0.58
3:A1:130:LEU:O	3:A1:162:ARG:NH1	2.37	0.58
3:A9:149:THR:OG1	3:A9:191:GLN:OE1	2.21	0.58
3:B1:292:GLN:NE2	3:B1:298:ASN:OD1	2.37	0.58
2:C2:10:GLY:HA2	2:C2:145:THR:HG23	1.85	0.58
3:D5:248:SER:HA	3:D5:252:LYS:HG2	1.85	0.58
3:E3:15:GLN:NE2	8:E3:501:GDP:N7	2.51	0.58
2:E8:252:VAL:HA	2:E8:255:PHE:HD2	1.67	0.58
2:F0:322:ASP:O	2:F0:373:ARG:NH2	2.36	0.58
3:F1:180:VAL:O	3:F1:184:ASN:ND2	2.37	0.58
3:B1:237:THR:HG22	3:B1:250:LEU:HD11	1.86	0.58
3:B7:318:ARG:HD3	3:B7:358:PRO:HD3	1.84	0.58
2:C4:181:VAL:HG12	3:C5:256:ASN:HB2	1.85	0.58
3:C5:294:PHE:O	3:C5:306:ARG:NH2	2.33	0.58
3:C7:407:GLU:HA	3:C7:410:GLU:HB3	1.86	0.58
2:D6:298:PRO:HB3	2:D6:307:PRO:HD2	1.86	0.58
2:E8:151:CYS:SG	2:E8:193:SER:OG	2.51	0.58
2:C8:223:THR:HG22	3:C9:322:SER:HA	1.85	0.57
2:E6:217:LEU:HD21	2:E6:367:ASP:HB3	1.85	0.57
3:A5:318:ARG:HD3	3:A5:358:PRO:HD3	1.85	0.57
2:A6:30:ILE:HG22	2:A6:36:MET:HB3	1.86	0.57
2:C4:236:SER:O	2:C4:243:ARG:NH2	2.37	0.57
2:C8:50:ASN:O	2:C8:64:ARG:NH2	2.35	0.57
3:D7:117:LEU:HA	3:D7:120:VAL:HG12	1.85	0.57
3:E9:219:THR:HA	2:F0:326:LYS:HZ1	1.69	0.57
2:A0:210:TYR:HE1	2:A0:227:LEU:HD21	1.69	0.57
2:B6:1:MET:N	2:B6:129:CYS:SG	2.77	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C9:7:VAL:HB	3:C9:135:ILE:HG12	1.86	0.57
3:D9:313:ALA:HB3	3:D9:349:MET:HG2	1.86	0.57
2:E4:238:LEU:HD11	2:E4:378:ILE:HG13	1.86	0.57
2:E6:206:ASN:ND2	6:E6:501:GTP:O2'	2.37	0.57
3:A1:205:GLU:HA	3:A1:208:TYR:HD2	1.70	0.57
2:A2:259:LEU:HD21	2:A2:316:CYS:HB2	1.87	0.57
2:A6:11:GLN:HG3	2:A6:74:VAL:HG21	1.86	0.57
2:C4:229:ARG:NH2	1:23:250:GLU:OE2	2.37	0.57
3:D3:100:ASN:HB3	3:D3:103:LYS:HB2	1.86	0.57
2:D4:151:CYS:SG	2:D4:193:SER:OG	2.47	0.57
2:F0:11:GLN:HG3	2:F0:74:VAL:HG21	1.86	0.57
2:A0:180:ALA:HB3	2:A0:183:GLU:HG2	1.86	0.57
3:A9:345:ILE:O	3:A9:348:ASN:ND2	2.37	0.57
2:B0:283:HIS:HB2	2:B4:88:HIS:HD2	1.70	0.57
2:B2:286:LEU:O	2:B2:373:ARG:NH1	2.33	0.57
3:B3:10:GLY:HA2	3:B3:143:THR:HG23	1.85	0.57
3:B3:16:ILE:HD11	3:B3:229:VAL:HG11	1.86	0.57
2:C0:2:ARG:NH2	2:C0:133:GLN:OE1	2.36	0.57
2:C2:286:LEU:O	2:C2:373:ARG:NH1	2.36	0.57
3:C3:49:VAL:HG11	3:C3:241:ARG:HG2	1.87	0.57
3:C7:91:VAL:HG21	3:C7:116:VAL:HG12	1.87	0.57
2:C8:11:GLN:NE2	3:C9:245:GLN:O	2.37	0.57
2:E8:178:SER:HB3	2:E8:183:GLU:HG3	1.85	0.57
3:B3:3:GLU:HA	3:B3:49:VAL:HA	1.87	0.57
3:B5:257:LEU:HD21	3:B5:314:SER:HB2	1.87	0.57
3:C1:204:ASN:OD1	8:C1:501:GDP:N2	2.36	0.57
3:C9:323:THR:HA	3:C9:326:VAL:HG12	1.87	0.57
2:E2:242:LEU:HD11	2:E2:252:VAL:HG23	1.87	0.57
2:E4:215:ARG:NH1	2:E4:216:ASN:OD1	2.37	0.57
3:E5:207:LEU:HB3	3:E5:225:LEU:HD22	1.86	0.57
3:E7:1:MET:N	3:E7:128:ASP:OD2	2.36	0.57
2:B6:53:PHE:HB3	2:B6:61:HIS:HB3	1.87	0.57
2:C6:352:LYS:NZ	2:C6:353:CYS:O	2.38	0.57
3:D5:95:THR:OG1	3:D5:108:GLU:OE2	2.23	0.57
2:E4:229:ARG:HD2	2:E4:363:VAL:HG21	1.86	0.57
1:11:244:GLN:O	3:D1:320:ARG:NH2	2.36	0.57
3:D7:274:THR:HG21	3:D7:282:ARG:HD2	1.86	0.57
3:A3:12:CYS:SG	8:A3:501:GDP:N2	2.75	0.57
2:E6:174:SER:OG	2:E6:177:VAL:O	2.17	0.57
3:E7:176:SER:OG	3:E7:181:GLU:OE1	2.23	0.57
3:A3:174:LYS:NZ	3:A3:205:GLU:OE1	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C0:15:GLN:NE2	6:C0:501:GTP:O6	2.38	0.56
2:C0:96:LYS:NZ	3:C1:129:CYS:SG	2.71	0.56
3:E3:100:ASN:HB3	3:E3:103:LYS:HG2	1.87	0.56
3:E5:172:SER:OG	3:E5:175:VAL:O	2.22	0.56
2:E8:274:PRO:HB2	2:E8:276:ILE:HG12	1.86	0.56
3:F1:49:VAL:HG11	3:F1:241:ARG:HG2	1.86	0.56
2:A0:339:ARG:O	2:A0:342:GLN:NE2	2.38	0.56
2:B0:65:CYS:O	2:B0:91:GLN:NE2	2.38	0.56
3:C1:94:GLN:O	2:C2:2:ARG:NH2	2.37	0.56
2:D6:138:PHE:HZ	2:D6:235:ILE:HD12	1.70	0.56
3:D7:135:ILE:HB	3:D7:166:THR:HG22	1.86	0.56
2:E4:285:GLN:OE1	2:E8:57:GLY:N	2.38	0.56
3:A1:210:ILE:HD11	3:A1:228:LEU:HD21	1.86	0.56
2:A8:27:GLU:OE2	2:A8:243:ARG:NH2	2.38	0.56
3:A9:10:GLY:HA2	3:A9:143:THR:HG23	1.86	0.56
2:B2:180:ALA:O	3:B3:347:ASN:ND2	2.38	0.56
2:C0:356:ASN:OD1	2:C0:357:TYR:N	2.39	0.56
2:C2:306:ASP:OD1	2:C2:308:ARG:NH1	2.38	0.56
2:C4:71:GLU:HG2	2:C4:73:THR:HG22	1.86	0.56
2:D0:107:HIS:NE2	2:D0:151:CYS:SG	2.69	0.56
2:D2:328:VAL:HG21	2:D2:355:ILE:HD11	1.87	0.56
3:D3:101:TRP:NE1	3:D3:145:SER:O	2.37	0.56
3:D5:100:ASN:ND2	3:D5:397:TRP:O	2.37	0.56
2:E0:244:PHE:HB2	2:E0:356:ASN:HD21	1.70	0.56
2:E2:311:LYS:NZ	2:E2:342:GLN:OE1	2.38	0.56
3:F1:183:TYR:OH	3:F1:388:MET:O	2.20	0.56
3:F1:248:SER:OG	3:F1:350:LYS:NZ	2.38	0.56
3:A1:32:PRO:O	3:A1:83:GLN:NE2	2.38	0.56
3:A9:207:LEU:HB3	3:A9:225:LEU:HD22	1.87	0.56
3:B3:200:GLN:HB3	3:B3:268:ILE:HD11	1.88	0.56
3:C7:156:ARG:HG2	3:C7:195:ASN:HB2	1.88	0.56
2:C8:168:ASN:ND2	2:C8:170:CYS:SG	2.79	0.56
3:D7:322:SER:OG	3:D7:325:GLU:OE2	2.23	0.56
2:D8:69:ASP:OD1	2:D8:70:LEU:N	2.38	0.56
2:E4:221:ARG:NH1	3:E5:325:GLU:H	2.04	0.56
1:0:247:TYR:HE2	2:A4:81:GLY:HA3	1.70	0.56
3:B3:372:THR:HG21	3:B3:426:GLN:HB3	1.88	0.56
2:C0:76:ASP:OD2	3:C1:46:ARG:NH1	2.39	0.56
2:C4:271:SER:HB3	2:C4:377:MET:HB3	1.88	0.56
3:C9:245:GLN:HB2	3:C9:353:VAL:HG13	1.88	0.56
3:D9:412:GLU:O	3:D9:416:ASN:ND2	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B8:50:ASN:O	2:B8:64:ARG:NH2	2.38	0.56
3:C1:200:GLN:HG3	3:C1:268:ILE:HD11	1.88	0.56
2:C4:108:TYR:O	2:C4:112:LYS:NZ	2.39	0.56
2:D8:5:ILE:HD12	2:D8:125:LEU:HG	1.87	0.56
3:D9:238:CYS:SG	3:D9:318:ARG:NE	2.78	0.56
2:E4:221:ARG:HH12	3:E5:324:LYS:H	1.54	0.56
2:E4:241:SER:HB2	2:E4:249:ASN:HB2	1.88	0.56
2:E6:22:GLU:OE1	2:E6:229:ARG:NH1	2.38	0.56
2:E8:396:ASP:OD1	2:E8:422:ARG:NH1	2.39	0.56
2:A8:223:THR:HG22	3:A9:322:SER:HA	1.87	0.56
3:B1:2:ARG:NH1	3:B1:249:ASP:OD2	2.38	0.56
3:C7:100:ASN:HB3	3:C7:103:LYS:HG2	1.88	0.56
2:D4:309:HIS:NE2	2:D4:386:GLU:OE1	2.39	0.56
3:D7:139:LEU:HA	3:D7:145:SER:HB2	1.87	0.56
3:D7:396:HIS:HA	3:D7:399:THR:HG22	1.87	0.56
3:E1:49:VAL:HG21	3:E1:241:ARG:HG2	1.88	0.56
6:E6:501:GTP:O3G	3:E7:252:LYS:NZ	2.35	0.56
3:E7:156:ARG:NH1	3:E7:162:ARG:O	2.38	0.56
3:A1:11:GLN:NE2	2:A2:247:ALA:O	2.39	0.56
2:A8:33:ASP:O	2:A8:60:LYS:NZ	2.39	0.56
2:D0:11:GLN:NE2	3:D1:245:GLN:O	2.38	0.56
2:E4:272:TYR:HB3	2:E4:275:ILE:HD11	1.88	0.56
3:E9:69:GLU:OE1	2:F0:2:ARG:NH1	2.39	0.56
2:F0:60:LYS:O	2:F0:61:HIS:ND1	2.39	0.56
3:A3:91:VAL:HG21	3:A3:116:VAL:HG12	1.88	0.56
2:C2:168:ASN:HD22	2:C2:198:THR:HG21	1.70	0.56
2:C6:198:THR:O	2:C6:266:HIS:NE2	2.39	0.56
3:D3:107:THR:HG21	3:D3:401:GLU:HB2	1.87	0.56
3:D7:282:ARG:NH1	3:D7:288:GLU:OE2	2.39	0.56
3:E3:180:VAL:O	3:E3:184:ASN:ND2	2.38	0.56
3:E5:113:ILE:HA	3:E5:116:VAL:HG12	1.88	0.56
2:E8:101:ASN:HB3	2:E8:182:VAL:HG21	1.86	0.56
3:A3:52:ASN:ND2	3:A3:123:GLU:OE2	2.39	0.56
2:E4:71:GLU:HB3	2:E4:98:ASP:HB2	1.87	0.56
3:E9:169:VAL:HG12	3:E9:202:ILE:HB	1.86	0.56
2:A4:292:THR:HG21	2:A4:331:ALA:HB1	1.89	0.55
2:A8:11:GLN:NE2	3:A9:245:GLN:O	2.39	0.55
2:A8:123:ARG:NH2	2:A8:160:ASP:OD2	2.38	0.55
3:B5:334:GLN:HE21	3:B5:349:MET:HG2	1.71	0.55
2:B6:88:HIS:HB3	2:B6:91:GLN:HG3	1.88	0.55
2:C4:339:ARG:O	2:C4:342:GLN:NE2	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C6:240:ALA:HB1	2:C6:356:ASN:HD22	1.71	0.55
3:D5:324:LYS:HA	3:D5:327:ASP:HB2	1.88	0.55
3:E1:12:CYS:HB3	3:E1:138:SER:HB2	1.89	0.55
2:E6:64:ARG:HB3	2:E6:125:LEU:HD21	1.88	0.55
2:A2:253:THR:O	2:A2:256:GLN:NE2	2.39	0.55
2:B4:286:LEU:O	2:B4:373:ARG:NH1	2.35	0.55
2:D0:204:LEU:HD13	2:D0:231:ILE:HD12	1.88	0.55
3:D1:282:ARG:NH1	3:D1:292:GLN:OE1	2.40	0.55
2:A0:356:ASN:OD1	2:A0:358:GLN:NE2	2.38	0.55
3:A3:383:ASP:HA	3:A3:386:THR:HG22	1.89	0.55
2:B6:11:GLN:NE2	6:B6:501:GTP:O1A	2.37	0.55
3:B9:252:LYS:HG3	3:B9:350:LYS:HE3	1.87	0.55
3:C3:73:MET:HB3	3:C3:77:ARG:HH22	1.71	0.55
2:C4:287:SER:OG	2:C4:290:GLU:OE1	2.22	0.55
3:C9:66:MET:HE3	3:C9:151:LEU:HD22	1.88	0.55
2:D2:69:ASP:OD1	2:D2:70:LEU:N	2.39	0.55
2:D4:222:PRO:O	3:D5:322:SER:OG	2.21	0.55
3:F1:358:PRO:HG2	3:F1:361:LEU:HB3	1.88	0.55
2:A2:26:LEU:HD22	2:A2:364:PRO:HD3	1.89	0.55
3:A9:208:TYR:CD1	2:B0:326:LYS:HE3	2.42	0.55
3:C3:35:THR:OG1	3:C3:36:TYR:N	2.40	0.55
3:C5:97:ALA:HB3	3:C5:143:THR:HB	1.88	0.55
2:D0:50:ASN:O	2:D0:64:ARG:NH2	2.36	0.55
3:D1:91:VAL:HG11	3:D1:116:VAL:HG22	1.87	0.55
3:D9:6:HIS:HD2	3:D9:134:GLN:HE21	1.53	0.55
3:D9:97:ALA:HA	3:D9:103:LYS:HE2	1.89	0.55
3:E9:178:THR:HA	2:F0:352:LYS:HE3	1.87	0.55
1:12:244:GLN:O	3:D3:320:ARG:NH2	2.40	0.55
3:A3:207:LEU:HB3	3:A3:225:LEU:HD22	1.88	0.55
3:B5:97:ALA:HA	3:B5:103:LYS:HE2	1.88	0.55
3:B9:354:CYS:SG	3:B9:355:ASP:N	2.80	0.55
2:D2:134:GLY:HA2	2:D2:164:LYS:HE2	1.88	0.55
2:A4:285:GLN:HB2	2:A8:56:THR:HA	1.88	0.55
2:A4:401:LYS:HE3	3:A5:344:TRP:CD2	2.42	0.55
3:B1:97:ALA:HA	3:B1:103:LYS:HE3	1.87	0.55
3:C7:140:GLY:O	3:C7:184:ASN:ND2	2.39	0.55
3:D3:238:CYS:SG	3:D3:318:ARG:NE	2.80	0.55
6:E2:501:GTP:O3G	3:E3:252:LYS:NZ	2.37	0.55
2:E6:277:SER:OG	2:E6:278:ALA:N	2.39	0.55
2:E8:206:ASN:ND2	6:E8:501:GTP:O2'	2.40	0.55
3:A3:186:THR:HG23	3:A3:415:MET:HG3	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A4:76:ASP:HA	2:A4:79:ARG:HG2	1.88	0.55
3:B1:149:THR:OG1	3:B1:191:GLN:OE1	2.19	0.55
2:C4:290:GLU:HA	2:C4:293:ASN:HB2	1.88	0.55
2:C4:417:GLU:HA	2:C4:420:GLU:HG3	1.89	0.55
3:C7:257:LEU:HD21	3:C7:314:SER:HB2	1.89	0.55
3:D5:192:LEU:HD21	3:D5:199:VAL:HG11	1.88	0.55
2:E4:319:TYR:HB3	2:E4:323:VAL:HG21	1.89	0.55
2:A0:91:GLN:HA	2:A0:121:ARG:HH12	1.72	0.55
3:B1:163:ILE:HD13	3:B1:250:LEU:HB3	1.88	0.55
2:B8:206:ASN:OD1	6:B8:501:GTP:N2	2.39	0.55
2:C0:217:LEU:HD21	2:C0:275:ILE:HG13	1.89	0.55
3:C7:68:LEU:HD13	3:C7:93:GLY:HA3	1.88	0.55
2:D6:73:THR:OG1	3:D7:247:ASN:ND2	2.40	0.55
2:D8:30:ILE:HG22	2:D8:36:MET:HB3	1.89	0.55
3:E5:68:LEU:HA	3:E5:93:GLY:HA3	1.89	0.55
2:E6:177:VAL:HG11	3:E7:327:ASP:HB3	1.89	0.55
3:F1:7:VAL:HB	3:F1:135:ILE:HG12	1.89	0.55
3:C1:334:GLN:OE1	3:C1:348:ASN:N	2.39	0.55
3:C3:105:HIS:HE1	3:C3:191:GLN:HE22	1.54	0.55
3:D9:27:GLU:OE2	3:D9:241:ARG:NH1	2.36	0.55
3:F1:238:CYS:SG	3:F1:239:CYS:N	2.80	0.55
2:A8:88:HIS:NE2	2:A8:90:GLU:OE1	2.41	0.54
2:B8:53:PHE:HB3	2:B8:61:HIS:HB3	1.88	0.54
3:D7:152:ILE:HA	3:D7:164:MET:HE1	1.88	0.54
2:E6:101:ASN:HB3	2:E6:182:VAL:HG11	1.88	0.54
2:F0:208:ALA:HB2	2:F0:304:LYS:HB2	1.89	0.54
3:A1:94:GLN:O	2:A2:2:ARG:NH1	2.31	0.54
2:A2:292:THR:HG21	2:A2:331:ALA:HB1	1.89	0.54
3:A5:183:TYR:HB3	3:A5:398:TYR:HE2	1.72	0.54
3:B9:49:VAL:HG11	3:B9:241:ARG:HG2	1.88	0.54
2:C6:10:GLY:HA2	2:C6:145:THR:HG23	1.88	0.54
3:D5:202:ILE:HD11	3:D5:268:ILE:HD12	1.90	0.54
2:D6:269:LEU:HD23	2:D6:301:MET:HG2	1.89	0.54
3:E5:334:GLN:OE1	3:E5:348:ASN:ND2	2.39	0.54
2:E6:181:VAL:HG13	3:E7:350:LYS:HZ1	1.71	0.54
3:A1:207:LEU:HB3	3:A1:225:LEU:HD22	1.90	0.54
3:A5:40:SER:HB3	3:A5:43:GLN:HG3	1.90	0.54
2:B0:206:ASN:OD1	6:B0:501:GTP:N2	2.40	0.54
2:B8:1:MET:N	2:B8:129:CYS:SG	2.81	0.54
3:B9:12:CYS:HB3	3:B9:138:SER:HB2	1.89	0.54
3:C1:35:THR:OG1	3:C1:36:TYR:N	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C9:280:GLN:HE22	3:D3:58:ARG:HH11	1.54	0.54
3:D1:180:VAL:O	3:D1:184:ASN:ND2	2.40	0.54
2:D6:69:ASP:OD1	2:D6:70:LEU:N	2.40	0.54
2:F0:151:CYS:SG	2:F0:193:SER:OG	2.52	0.54
2:A8:138:PHE:HZ	2:A8:235:ILE:HD12	1.72	0.54
2:B0:102:ASN:HB3	2:B0:105:ARG:H	1.71	0.54
2:B8:306:ASP:OD2	2:B8:308:ARG:NH2	2.38	0.54
2:C8:178:SER:HB2	3:C9:347:ASN:ND2	2.22	0.54
3:D5:200:GLN:HB3	3:D5:268:ILE:HD11	1.90	0.54
3:D5:274:THR:OG1	3:D5:279:GLN:OE1	2.25	0.54
3:E5:284:LEU:HD23	3:E5:362:LYS:HG2	1.89	0.54
2:F0:65:CYS:SG	2:F0:66:VAL:N	2.81	0.54
3:A1:130:LEU:H	3:A1:162:ARG:HH12	1.55	0.54
3:A5:238:CYS:SG	3:A5:318:ARG:NE	2.78	0.54
2:A8:309:HIS:NE2	2:A8:386:GLU:OE1	2.36	0.54
3:D9:68:LEU:HD23	3:D9:112:LEU:HD13	1.89	0.54
3:E5:248:SER:HA	3:E5:252:LYS:HG2	1.87	0.54
2:A0:332:VAL:HG13	2:A0:351:PHE:HD2	1.72	0.54
3:A5:289:LEU:HD13	3:A5:365:VAL:HG23	1.90	0.54
2:A6:109:THR:HG21	2:A6:411:GLU:HB2	1.88	0.54
2:A6:208:ALA:HB2	2:A6:304:LYS:HG2	1.89	0.54
2:B4:259:LEU:HD11	2:B4:316:CYS:HB2	1.88	0.54
2:B6:262:TYR:HB2	2:B6:265:ILE:HD12	1.88	0.54
2:C6:204:LEU:HD13	2:C6:231:ILE:HD12	1.88	0.54
2:E0:192:HIS:NE2	2:E0:420:GLU:OE2	2.40	0.54
3:E1:10:GLY:O	3:E1:14:ASN:ND2	2.40	0.54
2:E2:178:SER:OG	3:E3:347:ASN:ND2	2.41	0.54
2:A2:337:THR:O	2:A2:339:ARG:NH1	2.40	0.54
3:A5:172:SER:HB3	3:A5:205:GLU:HG2	1.90	0.54
3:A7:203:ASP:HB2	3:A7:301:CYS:HA	1.89	0.54
3:B5:66:MET:HG3	3:B5:116:VAL:HG21	1.90	0.54
3:B7:404:ASP:OD1	3:B7:405:GLU:N	2.40	0.54
2:C8:386:GLU:OE1	2:C8:390:ARG:NH1	2.41	0.54
2:D4:326:LYS:NZ	2:D4:327:ASP:OD1	2.36	0.54
3:E5:304:ASP:OD2	3:E5:306:ARG:NH1	2.41	0.54
2:E8:137:MET:HE3	2:E8:154:LEU:HD12	1.88	0.54
2:A0:18:ASN:HD21	2:A0:78:VAL:HG22	1.71	0.54
3:B5:27:GLU:OE1	3:B5:318:ARG:NH2	2.36	0.54
3:D7:292:GLN:O	3:D7:298:ASN:ND2	2.41	0.54
2:E0:76:ASP:HA	2:E0:79:ARG:HD2	1.89	0.54
3:E9:66:MET:HG3	3:E9:116:VAL:HG21	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E9:184:ASN:OD1	3:E9:398:TYR:OH	2.25	0.54
2:A4:179:THR:HG1	3:A5:351:SER:HG	1.56	0.54
2:B4:188:VAL:HG23	2:B4:425:LEU:HD22	1.90	0.54
2:B4:338:LYS:HG2	2:B4:340:THR:HG22	1.90	0.54
2:B6:306:ASP:OD2	2:B6:308:ARG:NH2	2.39	0.54
2:B8:274:PRO:HB2	2:B8:276:ILE:HG12	1.90	0.54
3:B9:358:PRO:HG2	3:B9:361:LEU:HD12	1.89	0.54
3:C1:248:SER:HA	3:C1:252:LYS:HG3	1.89	0.54
3:C5:140:GLY:O	3:C5:184:ASN:ND2	2.38	0.54
2:D2:207:GLU:HA	2:D2:210:TYR:HB2	1.90	0.54
2:D8:222:PRO:HD2	3:D9:324:LYS:HD3	1.90	0.54
3:D9:107:THR:OG1	3:D9:108:GLU:OE1	2.25	0.54
2:F0:80:THR:HA	2:F0:84:ARG:HE	1.73	0.54
3:A5:117:LEU:HA	3:A5:120:VAL:HG12	1.89	0.54
2:A6:283:HIS:NE2	2:B0:85:HIS:O	2.39	0.54
3:B1:91:VAL:HG21	3:B1:116:VAL:HG12	1.89	0.54
3:B7:15:GLN:O	3:B7:226:ASN:ND2	2.41	0.54
3:C1:175:VAL:HG21	2:C2:333:ALA:HA	1.90	0.54
2:F0:11:GLN:NE2	3:F1:245:GLN:O	2.41	0.54
3:A3:117:LEU:HA	3:A3:120:VAL:HG12	1.89	0.53
3:A3:135:ILE:HG21	3:A3:152:ILE:HD11	1.89	0.53
3:B3:117:LEU:HA	3:B3:120:VAL:HG12	1.90	0.53
3:B9:10:GLY:HA2	3:B9:143:THR:HG23	1.90	0.53
2:C2:168:ASN:OD1	2:C2:169:PHE:N	2.41	0.53
3:C5:167:PHE:CD2	3:C5:233:MET:HG2	2.43	0.53
2:E4:239:THR:OG1	2:E4:243:ARG:NH1	2.41	0.53
3:A1:171:PRO:O	3:A1:380:ARG:NH1	2.30	0.53
2:A2:176:GLN:HB3	3:A3:331:LEU:HD22	1.90	0.53
3:A3:311:LEU:HD12	3:A3:342:VAL:HG11	1.88	0.53
3:B1:100:ASN:HB3	3:B1:103:LYS:HG2	1.90	0.53
3:B5:3:GLU:HA	3:B5:49:VAL:HA	1.89	0.53
2:C6:79:ARG:NH1	2:C6:92:LEU:O	2.41	0.53
3:D1:14:ASN:ND2	3:D1:67:ASP:OD1	2.41	0.53
3:D7:311:LEU:HD12	3:D7:342:VAL:HG11	1.90	0.53
2:B4:282:TYR:HD2	2:B4:283:HIS:CE1	2.26	0.53
3:C3:68:LEU:HD12	3:C3:143:THR:HG22	1.91	0.53
2:C6:277:SER:OG	2:C6:278:ALA:N	2.40	0.53
3:D1:238:CYS:SG	3:D1:318:ARG:NE	2.81	0.53
2:D4:30:ILE:HG22	2:D4:36:MET:HB3	1.89	0.53
3:E5:10:GLY:HA2	3:E5:143:THR:HG23	1.89	0.53
3:E7:68:LEU:HD12	3:E7:143:THR:HG22	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F0:137:MET:O	2:F0:168:ASN:ND2	2.38	0.53
2:A2:115:VAL:HG21	2:A2:152:LEU:HG	1.90	0.53
2:B8:181:VAL:HG22	3:B9:256:ASN:OD1	2.08	0.53
3:C3:172:SER:OG	3:C3:205:GLU:OE2	2.26	0.53
2:E8:268:MET:N	2:E8:268:MET:SD	2.81	0.53
3:A3:8:GLN:HG3	3:A3:65:LEU:HD13	1.89	0.53
3:B5:64:ILE:HD11	3:B5:123:GLU:HG3	1.89	0.53
2:B6:33:ASP:O	2:B6:60:LYS:NZ	2.41	0.53
3:C5:91:VAL:HB	3:C5:112:LEU:HD11	1.90	0.53
2:C6:186:ASN:OD1	2:C6:408:TYR:OH	2.25	0.53
3:D3:128:ASP:N	3:D3:128:ASP:OD1	2.41	0.53
3:D3:165:GLU:OE2	3:D3:200:GLN:NE2	2.42	0.53
3:D5:128:ASP:OD1	3:D5:129:CYS:N	2.41	0.53
2:D6:116:ASP:OD1	2:D6:117:LEU:N	2.42	0.53
3:D7:66:MET:HE2	3:D7:116:VAL:HG21	1.91	0.53
2:F0:328:VAL:HG21	2:F0:355:ILE:HD11	1.90	0.53
1:17:244:GLN:HG2	3:E3:320:ARG:HH21	1.73	0.53
3:A3:130:LEU:H	3:A3:162:ARG:HH21	1.56	0.53
2:A6:22:GLU:OE2	2:A6:229:ARG:NH1	2.42	0.53
2:A8:71:GLU:HG3	3:A9:2:ARG:HH22	1.72	0.53
3:B1:107:THR:OG1	3:B1:108:GLU:OE1	2.26	0.53
3:B1:230:SER:HA	3:B1:233:MET:HG2	1.90	0.53
3:B7:49:VAL:HG11	3:B7:241:ARG:HG2	1.90	0.53
3:C1:7:VAL:HB	3:C1:135:ILE:HD13	1.89	0.53
3:C1:113:ILE:HA	3:C1:116:VAL:HG12	1.91	0.53
3:C5:6:HIS:CD2	3:C5:134:GLN:HG3	2.43	0.53
2:F0:122:ILE:HG21	2:F0:157:LEU:HD21	1.89	0.53
3:A1:128:ASP:OD1	3:A1:129:CYS:N	2.40	0.53
3:C3:10:GLY:O	3:C3:14:ASN:ND2	2.42	0.53
2:C6:158:SER:OG	2:C6:166:LYS:NZ	2.42	0.53
3:D5:77:ARG:HH22	3:D5:92:PHE:HZ	1.55	0.53
3:D7:324:LYS:O	3:D7:327:ASP:N	2.40	0.53
3:D9:173:PRO:HB3	3:D9:380:ARG:CZ	2.39	0.53
3:E3:385:PHE:HE2	3:E3:412:GLU:HB3	1.73	0.53
2:B8:280:LYS:HZ3	2:C2:89:PRO:HB2	1.74	0.53
2:C2:186:ASN:OD1	2:C2:408:TYR:OH	2.26	0.53
2:C4:135:PHE:HB2	2:C4:166:LYS:HA	1.91	0.53
3:C5:52:ASN:ND2	3:C5:123:GLU:OE2	2.29	0.53
3:C5:356:ILE:HD12	1:23:241:PHE:HZ	1.74	0.53
2:B8:269:LEU:HD12	2:B8:303:ALA:HB3	1.90	0.53
2:C6:399:TYR:OH	2:C6:415:GLU:OE2	2.26	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D5:107:THR:OG1	3:D5:108:GLU:N	2.40	0.53
3:D5:238:CYS:SG	3:D5:318:ARG:NE	2.82	0.53
2:E0:102:ASN:HB3	2:E0:105:ARG:HB3	1.91	0.53
2:E0:311:LYS:NZ	2:E0:342:GLN:OE1	2.40	0.53
2:E2:209:ILE:HB	2:E2:227:LEU:HD22	1.91	0.53
2:F0:101:ASN:HB3	2:F0:182:VAL:HG21	1.91	0.53
1:5:250:GLU:OE2	2:B4:229:ARG:NH2	2.42	0.53
3:A1:117:LEU:HD13	3:A1:154:LYS:NZ	2.24	0.53
2:C2:250:VAL:HG23	2:C2:352:LYS:HZ3	1.74	0.53
2:C4:268:MET:SD	2:C4:380:ASN:ND2	2.82	0.53
3:D5:209:ASP:OD1	3:D5:213:ARG:NH1	2.42	0.53
3:E1:164:MET:HB3	3:E1:197:ASP:H	1.72	0.53
2:E2:65:CYS:SG	2:E2:66:VAL:N	2.80	0.53
1:7:255:PRO:HD2	2:B8:364:PRO:HG2	1.90	0.52
2:A4:57:GLY:HA3	2:A4:60:LYS:HD3	1.90	0.52
2:C0:11:GLN:NE2	2:C0:15:GLN:OE1	2.41	0.52
2:C0:286:LEU:O	2:C0:373:ARG:NH1	2.42	0.52
3:C1:391:ARG:HD2	2:C2:346:TRP:CG	2.44	0.52
2:C4:97:GLU:OE2	2:C4:105:ARG:NH2	2.29	0.52
3:C7:149:THR:HG23	3:C7:152:ILE:HD12	1.91	0.52
3:C9:2:ARG:HB3	3:C9:131:GLN:HB2	1.89	0.52
3:D3:68:LEU:HB3	3:D3:96:GLY:HA2	1.91	0.52
2:E4:256:GLN:HE21	2:E4:256:GLN:H	1.56	0.52
2:A6:79:ARG:NH1	2:A6:94:SER:OG	2.42	0.52
2:B4:6:SER:OG	2:B4:8:HIS:NE2	2.43	0.52
2:B6:206:ASN:OD1	6:B6:501:GTP:N2	2.42	0.52
2:C4:288:VAL:HA	2:C4:291:ILE:HG12	1.91	0.52
3:C9:139:LEU:HD13	3:C9:168:SER:HB2	1.92	0.52
2:D2:11:GLN:NE2	3:D3:245:GLN:O	2.42	0.52
3:E7:311:LEU:HD12	3:E7:342:VAL:HG11	1.91	0.52
2:E8:191:THR:HG23	2:E8:425:LEU:HD21	1.91	0.52
3:B9:200:GLN:HB2	3:B9:268:ILE:HD11	1.92	0.52
3:E3:215:LEU:HD21	3:E3:273:LEU:HD22	1.90	0.52
2:A2:244:PHE:HD2	2:A2:358:GLN:HG2	1.75	0.52
2:A6:306:ASP:HB3	2:A6:309:HIS:CE1	2.44	0.52
2:C2:254:GLU:HG2	2:C2:352:LYS:HZ3	1.74	0.52
2:C4:79:ARG:NH1	2:C4:92:LEU:O	2.43	0.52
3:C5:196:ALA:O	3:C5:264:HIS:NE2	2.42	0.52
3:D3:139:LEU:HG	3:D3:168:SER:HB2	1.91	0.52
3:A1:77:ARG:HH22	3:A1:92:PHE:HZ	1.56	0.52
3:A3:249:ASP:H	3:A3:252:LYS:HB2	1.73	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A4:306:ASP:HB3	2:A4:309:HIS:CE1	2.45	0.52
3:B5:73:MET:HA	3:B5:76:VAL:HG12	1.92	0.52
3:C1:253:LEU:HD11	3:C1:368:VAL:HG21	1.91	0.52
3:C3:149:THR:O	3:C3:191:GLN:NE2	2.42	0.52
3:C7:164:MET:N	3:C7:197:ASP:OD2	2.40	0.52
2:D0:335:ILE:HG23	2:D0:341:ILE:HD13	1.90	0.52
3:A9:68:LEU:HG	3:A9:147:MET:HE1	1.90	0.52
2:C2:267:PHE:O	2:C2:380:ASN:ND2	2.43	0.52
2:C4:76:ASP:OD2	3:C5:46:ARG:NH2	2.42	0.52
2:C4:191:THR:HB	2:C4:425:LEU:HD21	1.92	0.52
2:D8:241:SER:OG	2:D8:250:VAL:O	2.22	0.52
3:D9:128:ASP:OD1	3:D9:128:ASP:N	2.42	0.52
3:E1:2:ARG:HB2	3:E1:131:GLN:HB2	1.91	0.52
3:E1:3:GLU:HA	3:E1:49:VAL:HA	1.91	0.52
2:A0:208:ALA:HB2	2:A0:304:LYS:HB2	1.91	0.52
3:A1:10:GLY:O	3:A1:14:ASN:ND2	2.34	0.52
2:A4:217:LEU:HD11	2:A4:275:ILE:HG22	1.90	0.52
3:A7:200:GLN:HG2	3:A7:268:ILE:HD11	1.92	0.52
3:B3:239:CYS:SG	3:B3:248:SER:N	2.75	0.52
3:B3:324:LYS:O	3:B3:328:GLU:N	2.42	0.52
3:C5:282:ARG:NH1	3:C5:288:GLU:OE2	2.43	0.52
3:C9:347:ASN:OD1	3:C9:349:MET:HB3	2.09	0.52
2:D0:90:GLU:HG3	2:D0:121:ARG:HD3	1.92	0.52
2:D2:98:ASP:OD1	2:D2:99:ALA:N	2.42	0.52
3:D3:397:TRP:NE1	2:D4:256:GLN:OE1	2.42	0.52
3:D7:324:LYS:O	3:D7:328:GLU:N	2.30	0.52
2:D8:206:ASN:ND2	6:D8:501:GTP:O2'	2.43	0.52
3:E3:239:CYS:SG	3:E3:248:SER:N	2.80	0.52
2:A2:191:THR:HA	2:A2:194:LEU:HB3	1.92	0.52
2:A4:96:LYS:NZ	3:A5:129:CYS:SG	2.82	0.52
3:A7:11:GLN:HA	3:A7:72:THR:HG21	1.92	0.52
3:A9:313:ALA:HB3	3:A9:349:MET:HG2	1.92	0.52
2:B4:392:ASP:OD1	2:B4:422:ARG:NE	2.43	0.52
2:B8:109:THR:HG22	2:B8:110:ILE:HG23	1.91	0.52
2:C2:51:THR:HG21	2:C2:243:ARG:HG2	1.92	0.52
2:C4:175:PRO:HG3	2:C4:304:LYS:HG2	1.91	0.52
3:D1:282:ARG:NH1	3:D1:288:GLU:OE2	2.42	0.52
3:D3:191:GLN:HA	3:D3:194:GLU:HG2	1.92	0.52
2:E2:105:ARG:HH12	3:E3:251:ARG:HD3	1.74	0.52
3:E7:234:SER:O	3:E7:241:ARG:NH2	2.43	0.52
3:E7:257:LEU:HD21	3:E7:314:SER:HB3	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A1:341:PHE:HB3	3:A1:348:ASN:HD22	1.75	0.52
3:A3:308:GLY:HA3	3:A3:373:ALA:HB2	1.90	0.52
2:B4:183:GLU:HG2	2:B4:184:PRO:HD3	1.92	0.52
3:C3:200:GLN:HB3	3:C3:266:PHE:HB2	1.92	0.52
2:C4:274:PRO:HG2	2:C4:371:VAL:HG11	1.92	0.52
2:D2:298:PRO:HB3	2:D2:307:PRO:HD2	1.92	0.52
2:D2:407:TRP:HZ2	3:D3:258:ILE:HD11	1.74	0.52
2:D6:309:HIS:NE2	2:D6:386:GLU:OE1	2.43	0.52
2:A8:36:MET:SD	2:A8:61:HIS:NE2	2.74	0.52
3:B5:247:ASN:O	3:B5:252:LYS:NZ	2.39	0.52
2:C4:427:ALA:HA	2:C4:430:LYS:HE3	1.91	0.52
2:D2:136:LEU:HD23	2:D2:235:ILE:HD11	1.92	0.52
2:F0:8:HIS:CD2	2:F0:17:GLY:HA3	2.43	0.52
2:F0:239:THR:OG1	2:F0:243:ARG:NH1	2.43	0.52
3:A1:208:TYR:HD1	2:A2:326:LYS:HG2	1.74	0.51
3:B9:276:ARG:NH2	3:B9:279:GLN:OE1	2.43	0.51
2:C2:277:SER:OG	2:C2:278:ALA:N	2.43	0.51
3:C7:139:LEU:HD13	3:C7:168:SER:HB2	1.92	0.51
2:C8:392:ASP:OD1	2:C8:422:ARG:NE	2.38	0.51
3:D5:114:ASP:OD1	3:D5:114:ASP:N	2.42	0.51
2:A0:174:SER:OG	2:A0:177:VAL:O	2.27	0.51
2:B0:71:GLU:HG2	2:B0:73:THR:HG22	1.92	0.51
2:B2:206:ASN:ND2	6:B2:501:GTP:O2'	2.43	0.51
2:B6:73:THR:HA	3:B7:46:ARG:HH11	1.76	0.51
3:B9:167:PHE:CZ	3:B9:233:MET:HG2	2.45	0.51
2:C2:207:GLU:HA	2:C2:210:TYR:HB2	1.93	0.51
2:C6:101:ASN:HB3	2:C6:182:VAL:HG21	1.93	0.51
3:C7:403:MET:HB3	3:C7:408:PHE:HE1	1.75	0.51
2:C8:245:ASP:N	2:C8:245:ASP:OD1	2.44	0.51
3:D5:334:GLN:HE22	3:D5:347:ASN:HA	1.75	0.51
3:E7:190:HIS:HB2	3:E7:414:ASN:HD22	1.75	0.51
3:F1:117:LEU:HB3	3:F1:121:ARG:HH22	1.75	0.51
2:A0:137:MET:HG3	2:A0:154:LEU:HD12	1.93	0.51
3:B1:311:LEU:HD12	3:B1:342:VAL:HG11	1.92	0.51
2:C4:277:SER:OG	2:C4:278:ALA:N	2.42	0.51
3:C9:137:HIS:HE1	3:C9:166:THR:HB	1.74	0.51
3:E5:113:ILE:HD11	3:E5:147:MET:HG3	1.92	0.51
2:A2:324:VAL:HG12	2:A2:326:LYS:H	1.76	0.51
3:A3:67:ASP:OD1	3:A3:68:LEU:N	2.43	0.51
3:A3:222:TYR:OH	8:A3:501:GDP:N2	2.44	0.51
2:A6:27:GLU:HG3	2:A6:361:THR:HG21	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A9:91:VAL:HG21	3:A9:116:VAL:HG22	1.91	0.51
2:B2:183:GLU:OE2	2:B2:187:SER:OG	2.28	0.51
2:B2:394:LYS:HG2	3:B3:346:PRO:HG3	1.92	0.51
3:B3:15:GLN:O	3:B3:226:ASN:ND2	2.43	0.51
3:B7:383:ASP:HA	3:B7:386:THR:HG22	1.92	0.51
2:C0:53:PHE:O	2:C0:64:ARG:NH2	2.43	0.51
3:C5:327:ASP:OD1	3:C5:327:ASP:N	2.40	0.51
2:D0:224:TYR:CZ	3:D1:323:THR:HG21	2.46	0.51
2:D8:298:PRO:HB3	2:D8:307:PRO:HD2	1.91	0.51
2:E0:306:ASP:OD1	2:E0:308:ARG:NH1	2.44	0.51
3:E5:128:ASP:OD1	3:E5:129:CYS:N	2.41	0.51
2:A2:3:GLU:OE1	2:A2:64:ARG:NH1	2.44	0.51
3:B9:7:VAL:HB	3:B9:135:ILE:HG13	1.93	0.51
3:C1:397:TRP:HH2	2:C2:260:VAL:HG23	1.75	0.51
3:C3:68:LEU:HA	3:C3:93:GLY:HA3	1.93	0.51
3:D3:173:PRO:HD2	3:D3:205:GLU:HG3	1.93	0.51
3:A7:318:ARG:HD3	3:A7:358:PRO:HD3	1.92	0.51
2:A8:338:LYS:HG2	2:A8:340:THR:HG22	1.93	0.51
3:A9:11:GLN:HB2	3:A9:72:THR:HG21	1.93	0.51
3:C5:107:THR:OG1	3:C5:401:GLU:OE2	2.27	0.51
2:D4:206:ASN:OD1	6:D4:501:GTP:N2	2.43	0.51
3:D5:392:LYS:HG2	3:D5:395:LEU:HD22	1.92	0.51
3:D9:301:CYS:SG	3:D9:302:ALA:N	2.84	0.51
3:E9:207:LEU:HB3	3:E9:225:LEU:HD22	1.93	0.51
3:F1:19:LYS:NZ	3:F1:223:GLY:O	2.44	0.51
2:B0:241:SER:OG	2:B0:250:VAL:O	2.24	0.51
2:B8:250:VAL:HG23	2:B8:254:GLU:HG2	1.91	0.51
3:C5:262:ARG:O	3:C5:264:HIS:ND1	2.44	0.51
2:C6:136:LEU:HD22	2:C6:167:LEU:HD23	1.93	0.51
3:D1:173:PRO:HD3	3:D1:380:ARG:CZ	2.40	0.51
2:D8:50:ASN:O	2:D8:64:ARG:NH2	2.44	0.51
3:E1:163:ILE:HD12	3:E1:250:LEU:HB2	1.92	0.51
3:F1:249:ASP:OD1	3:F1:250:LEU:N	2.43	0.51
2:A6:168:ASN:HD22	2:A6:194:LEU:HD11	1.76	0.51
2:A6:178:SER:OG	3:A7:347:ASN:ND2	2.35	0.51
2:A8:336:LYS:O	2:A8:339:ARG:NH2	2.43	0.51
3:B5:169:VAL:HG12	3:B5:202:ILE:HB	1.91	0.51
2:B6:76:ASP:HA	2:B6:79:ARG:HD2	1.93	0.51
3:C5:238:CYS:SG	3:C5:239:CYS:N	2.84	0.51
2:C6:207:GLU:HA	2:C6:210:TYR:HB2	1.93	0.51
3:C9:117:LEU:HA	3:C9:120:VAL:HG12	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D4:259:LEU:HD21	2:D4:316:CYS:HB2	1.93	0.51
2:D6:265:ILE:HG22	2:D6:380:ASN:HD21	1.75	0.51
2:E2:292:THR:HG21	2:E2:331:ALA:HB1	1.93	0.51
3:E5:309:ARG:NH1	3:E5:341:PHE:O	2.42	0.51
3:E9:121:ARG:NH2	3:E9:158:GLU:OE2	2.44	0.51
3:A3:398:TYR:HB3	3:A3:403:MET:HG3	1.93	0.51
3:A5:203:ASP:OD2	3:A5:302:ALA:N	2.35	0.51
2:A6:204:LEU:HD13	2:A6:231:ILE:HD12	1.93	0.51
2:A8:180:ALA:HA	3:A9:350:LYS:HB3	1.92	0.51
3:A9:187:LEU:HA	3:A9:190:HIS:CE1	2.45	0.51
3:C3:113:ILE:HA	3:C3:116:VAL:HG12	1.93	0.51
3:E7:139:LEU:HA	3:E7:145:SER:HB2	1.93	0.51
3:A3:135:ILE:HD13	3:A3:152:ILE:HD11	1.93	0.51
2:C4:14:ILE:O	2:C4:18:ASN:N	2.44	0.51
3:C7:237:THR:HG22	3:C7:250:LEU:HD11	1.93	0.51
3:C9:317:PHE:HB3	3:C9:321:MET:HE1	1.92	0.51
2:D2:33:ASP:OD1	2:D2:34:GLY:N	2.44	0.51
3:D5:307:HIS:ND1	3:D5:376:GLU:OE2	2.40	0.51
3:E7:128:ASP:OD1	3:E7:129:CYS:N	2.41	0.51
2:F0:50:ASN:O	2:F0:64:ARG:NH2	2.41	0.51
3:A1:208:TYR:CD1	2:A2:326:LYS:HG2	2.46	0.50
2:B4:367:ASP:OD1	2:B4:367:ASP:N	2.44	0.50
3:B9:290:THR:HA	3:B9:293:MET:HE3	1.93	0.50
3:C5:329:GLN:HA	3:C5:332:ASN:HB3	1.93	0.50
2:C6:271:SER:HB3	2:C6:377:MET:HB3	1.91	0.50
3:C9:121:ARG:NH2	3:C9:158:GLU:OE2	2.43	0.50
2:D0:377:MET:HE2	2:D0:379:SER:HB3	1.93	0.50
3:D7:91:VAL:HG11	3:D7:116:VAL:HB	1.93	0.50
3:E7:382:SER:OG	3:E7:412:GLU:OE1	2.28	0.50
2:F0:367:ASP:OD1	2:F0:367:ASP:N	2.44	0.50
3:F1:43:GLN:HA	3:F1:242:PHE:HE1	1.76	0.50
3:A3:230:SER:HA	3:A3:233:MET:HB3	1.93	0.50
2:A6:80:THR:HA	2:A6:84:ARG:HH21	1.76	0.50
2:B2:174:SER:HB2	2:B2:207:GLU:HG2	1.93	0.50
3:B7:139:LEU:HA	3:B7:145:SER:HB3	1.93	0.50
2:C2:9:VAL:HG22	2:C2:68:LEU:HB2	1.92	0.50
3:C3:69:GLU:HG2	3:C3:71:GLY:H	1.76	0.50
3:C9:208:TYR:CB	2:D0:326:LYS:HE2	2.38	0.50
3:E3:238:CYS:SG	3:E3:318:ARG:NE	2.85	0.50
3:E7:25:SER:HB3	3:E7:30:ILE:HB	1.94	0.50
2:A0:88:HIS:HB3	2:A0:91:GLN:HB2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A0:133:GLN:O	2:A0:165:SER:OG	2.30	0.50
3:A5:128:ASP:OD1	3:A5:129:CYS:N	2.42	0.50
3:A9:167:PHE:CE2	3:A9:233:MET:HG2	2.46	0.50
2:B0:27:GLU:OE1	2:B0:243:ARG:NH2	2.45	0.50
2:B6:329:ASN:HA	2:B6:332:VAL:HG12	1.94	0.50
2:B8:188:VAL:HG23	2:B8:189:LEU:HD12	1.93	0.50
3:B9:128:ASP:OD1	3:B9:129:CYS:N	2.38	0.50
3:C1:100:ASN:HD22	3:C1:103:LYS:HE3	1.76	0.50
3:C1:275:SER:OG	3:C1:276:ARG:N	2.43	0.50
2:C2:306:ASP:N	2:C2:386:GLU:OE2	2.45	0.50
3:C3:287:PRO:HB3	3:C3:329:GLN:HE21	1.75	0.50
3:C9:309:ARG:H	3:C9:372:THR:HG22	1.76	0.50
3:D1:117:LEU:HA	3:D1:120:VAL:HG12	1.92	0.50
2:E0:65:CYS:SG	2:E0:66:VAL:N	2.84	0.50
3:E1:238:CYS:SG	3:E1:239:CYS:N	2.85	0.50
3:E5:179:VAL:H	2:E6:352:LYS:NZ	2.10	0.50
2:E8:2:ARG:HE	2:E8:133:GLN:HE21	1.60	0.50
3:F1:309:ARG:NH1	3:F1:341:PHE:O	2.43	0.50
3:A5:105:HIS:CD2	3:A5:150:LEU:HB2	2.46	0.50
3:B9:311:LEU:HD12	3:B9:342:VAL:HG11	1.94	0.50
3:C1:139:LEU:HA	3:C1:145:SER:HB2	1.93	0.50
3:C1:281:TYR:OH	3:C5:83:GLN:O	2.29	0.50
2:C4:209:ILE:HG23	2:C4:227:LEU:HD22	1.93	0.50
2:C6:251:ASP:N	2:C6:254:GLU:OE2	2.41	0.50
3:C7:295:ASP:HB3	3:C7:298:ASN:HB2	1.92	0.50
2:C8:98:ASP:O	2:C8:105:ARG:NH2	2.44	0.50
2:D2:101:ASN:ND2	3:D3:256:ASN:OD1	2.43	0.50
2:E0:98:ASP:OD1	2:E0:99:ALA:N	2.44	0.50
2:E2:72:PRO:HD2	3:E3:2:ARG:HH21	1.77	0.50
2:E2:107:HIS:NE2	2:E2:151:CYS:SG	2.84	0.50
3:B5:324:LYS:O	3:B5:328:GLU:N	2.39	0.50
3:B7:150:LEU:HD21	3:B7:154:LYS:HZ2	1.77	0.50
2:B8:5:ILE:HD12	2:B8:125:LEU:HD23	1.94	0.50
2:C2:245:ASP:OD1	2:C2:245:ASP:N	2.42	0.50
3:C5:7:VAL:HB	3:C5:135:ILE:HG22	1.94	0.50
2:C6:51:THR:HG23	2:C6:52:PHE:HD1	1.77	0.50
2:C8:259:LEU:HD21	2:C8:316:CYS:HB2	1.92	0.50
2:D6:50:ASN:O	2:D6:64:ARG:NH2	2.43	0.50
2:D8:205:ASP:OD1	2:D8:206:ASN:N	2.44	0.50
3:D9:10:GLY:HA2	3:D9:143:THR:HG23	1.94	0.50
2:E2:79:ARG:NH1	2:E2:92:LEU:O	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F0:209:ILE:HB	2:F0:227:LEU:HD13	1.92	0.50
2:A2:6:SER:OG	2:A2:8:HIS:NE2	2.44	0.50
3:B3:171:PRO:HB3	3:B3:181:GLU:OE1	2.12	0.50
3:B9:383:ASP:HA	3:B9:386:THR:HG22	1.92	0.50
3:C3:136:THR:HG23	3:C3:167:PHE:HB2	1.93	0.50
3:E3:64:ILE:HD12	3:E3:119:VAL:HG12	1.94	0.50
2:E4:11:GLN:NE2	3:E5:245:GLN:O	2.44	0.50
2:E8:395:PHE:HZ	2:E8:418:PHE:HB3	1.77	0.50
3:F1:113:ILE:HG13	3:F1:150:LEU:HD22	1.94	0.50
3:A3:163:ILE:HG12	3:A3:250:LEU:HB3	1.94	0.50
3:A3:281:TYR:HD2	3:A7:87:PRO:HD3	1.76	0.50
3:A5:94:GLN:O	2:A6:2:ARG:NH2	2.45	0.50
3:A7:139:LEU:HA	3:A7:145:SER:HB2	1.93	0.50
3:B9:334:GLN:HE21	3:B9:349:MET:HG2	1.77	0.50
3:C1:382:SER:O	3:C1:386:THR:N	2.40	0.50
2:C2:103:PHE:H	2:C2:408:TYR:HE1	1.60	0.50
3:D9:283:ALA:HB2	3:E3:54:ALA:HA	1.92	0.50
3:D9:296:ALA:HB2	3:D9:305:PRO:HD2	1.93	0.50
3:E7:289:LEU:HD12	3:E7:365:VAL:HG12	1.94	0.50
1:7:250:GLU:HG3	2:B8:229:ARG:HH22	1.77	0.50
3:C1:274:THR:OG1	3:C1:282:ARG:NE	2.41	0.50
2:D2:174:SER:HB3	2:D2:207:GLU:HG2	1.94	0.50
3:D5:8:GLN:HE21	3:D5:65:LEU:HG	1.77	0.50
3:E3:144:GLY:N	8:E3:501:GDP:O3B	2.43	0.50
3:E7:256:ASN:HB3	3:E7:350:LYS:HE2	1.92	0.50
3:F1:139:LEU:HA	3:F1:145:SER:HB2	1.92	0.50
3:A3:173:PRO:HD2	3:A3:205:GLU:HG2	1.94	0.50
3:A3:267:LEU:HD21	3:A3:371:SER:HB3	1.93	0.50
3:B5:12:CYS:SG	3:B5:138:SER:OG	2.55	0.50
2:B8:88:HIS:HB3	2:B8:91:GLN:HG3	1.93	0.50
3:C3:141:GLY:O	3:C3:184:ASN:ND2	2.42	0.50
3:C5:142:GLY:N	8:C5:501:GDP:O3B	2.44	0.50
2:C8:282:TYR:CE2	2:D2:85:HIS:HB3	2.47	0.50
2:D6:119:LEU:HA	2:D6:122:ILE:HG22	1.93	0.50
3:D7:163:ILE:HD11	3:D7:251:ARG:HG3	1.94	0.50
2:E4:224:TYR:HA	2:E4:227:LEU:HD23	1.94	0.50
1:19:239:LEU:O	3:E7:359:LYS:NZ	2.36	0.49
2:A6:282:TYR:O	2:B0:60:LYS:NZ	2.43	0.49
3:B5:10:GLY:HA2	3:B5:143:THR:HG23	1.94	0.49
2:C2:155:GLU:HG2	2:C2:197:HIS:CD2	2.47	0.49
3:C7:356:ILE:HD12	1:22:241:PHE:HZ	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D1:10:GLY:O	3:D1:14:ASN:ND2	2.40	0.49
2:D6:64:ARG:HG2	2:D6:125:LEU:HD11	1.94	0.49
3:E9:11:GLN:NE2	2:F0:249:ASN:OD1	2.45	0.49
2:A4:241:SER:OG	2:A4:250:VAL:O	2.21	0.49
3:A7:140:GLY:O	3:A7:184:ASN:ND2	2.44	0.49
2:B8:30:ILE:HG22	2:B8:36:MET:HB3	1.94	0.49
3:D3:67:ASP:OD1	3:D3:68:LEU:N	2.45	0.49
3:D9:139:LEU:HD12	3:D9:170:PHE:HE1	1.77	0.49
2:E2:185:TYR:HE2	2:E2:404:PHE:HB2	1.78	0.49
3:E7:309:ARG:H	3:E7:372:THR:HG22	1.76	0.49
3:E9:267:LEU:HB3	3:E9:299:MET:SD	2.53	0.49
3:A1:105:HIS:CD2	3:A1:150:LEU:HB2	2.47	0.49
2:A2:277:SER:OG	2:A2:278:ALA:N	2.44	0.49
2:A4:107:HIS:HB3	2:A4:108:TYR:HD1	1.77	0.49
2:B6:27:GLU:OE2	2:B6:320:ARG:NH2	2.45	0.49
3:C9:330:MET:HE2	3:C9:349:MET:HG3	1.95	0.49
2:D0:36:MET:SD	2:D0:61:HIS:NE2	2.75	0.49
3:D3:169:VAL:HG12	3:D3:202:ILE:HB	1.95	0.49
3:D5:239:CYS:SG	3:D5:247:ASN:HB3	2.52	0.49
3:D9:163:ILE:HD13	3:D9:250:LEU:HB3	1.93	0.49
2:E0:195:LEU:HD13	2:E0:264:ARG:HH21	1.77	0.49
2:E6:72:PRO:HD2	3:E7:2:ARG:HH22	1.75	0.49
2:A8:30:ILE:HG22	2:A8:36:MET:HB3	1.94	0.49
3:B5:213:ARG:HE	3:B5:297:LYS:HD3	1.77	0.49
2:B8:168:ASN:HD22	2:B8:198:THR:HG21	1.77	0.49
3:D1:192:LEU:HD21	3:D1:199:VAL:HG11	1.94	0.49
2:D8:53:PHE:O	2:D8:64:ARG:NH2	2.46	0.49
3:D9:6:HIS:HE1	3:D9:8:GLN:HE21	1.60	0.49
2:E0:97:GLU:OE2	3:E1:251:ARG:NH1	2.44	0.49
3:E1:176:SER:HB3	2:E2:351:PHE:HB2	1.95	0.49
2:E4:236:SER:OG	2:E4:243:ARG:NH2	2.45	0.49
3:F1:128:ASP:OD1	3:F1:129:CYS:N	2.44	0.49
3:F1:184:ASN:OD1	3:F1:398:TYR:OH	2.26	0.49
2:A4:269:LEU:HB3	2:A4:301:MET:HE1	1.94	0.49
2:B6:241:SER:HB2	2:B6:249:ASN:HB2	1.93	0.49
2:C2:223:THR:OG1	3:C3:245:GLN:OE1	2.30	0.49
3:C5:239:CYS:SG	3:C5:248:SER:N	2.77	0.49
2:C8:98:ASP:OD1	2:C8:99:ALA:N	2.46	0.49
3:C9:1:MET:N	3:C9:128:ASP:OD2	2.38	0.49
2:D0:8:HIS:CD2	2:D0:17:GLY:HA3	2.47	0.49
3:D3:178:THR:HA	2:D4:352:LYS:HD2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D4:274:PRO:HG3	2:D4:286:LEU:HD23	1.93	0.49
3:D5:226:ASN:OD1	8:D5:501:GDP:N1	2.41	0.49
3:D7:27:GLU:OE1	3:D7:318:ARG:NH2	2.42	0.49
3:E1:311:LEU:HD12	3:E1:342:VAL:HG11	1.94	0.49
2:E4:309:HIS:NE2	2:E4:386:GLU:OE1	2.34	0.49
2:E4:422:ARG:HH12	2:E4:426:ALA:HB2	1.77	0.49
3:E9:267:LEU:HD21	3:E9:374:ILE:HD11	1.93	0.49
2:F0:222:PRO:HG2	3:F1:324:LYS:HZ1	1.77	0.49
2:A2:199:ASP:OD1	2:A2:200:VAL:N	2.46	0.49
3:A9:208:TYR:HD1	2:B0:326:LYS:HE3	1.77	0.49
3:B1:153:SER:HA	3:B1:195:ASN:HD22	1.78	0.49
2:C0:320:ARG:NH2	2:C0:358:GLN:OE1	2.46	0.49
2:C2:399:TYR:OH	2:C2:415:GLU:OE2	2.31	0.49
3:D1:140:GLY:O	3:D1:184:ASN:ND2	2.44	0.49
3:E1:33:THR:HG23	3:E1:35:THR:HG23	1.94	0.49
2:E6:133:GLN:HG3	2:E6:252:VAL:HG22	1.95	0.49
2:E6:417:GLU:HA	2:E6:420:GLU:HG3	1.95	0.49
3:F1:200:GLN:HG3	3:F1:268:ILE:HD11	1.95	0.49
2:A4:310:GLY:HA3	2:A4:383:ALA:HB2	1.95	0.49
2:B0:204:LEU:HD12	2:B0:209:ILE:HD11	1.94	0.49
3:B1:135:ILE:HG13	3:B1:152:ILE:HG12	1.94	0.49
2:B4:298:PRO:HB3	2:B4:307:PRO:HD2	1.93	0.49
3:C7:97:ALA:HB3	3:C7:143:THR:HG22	1.95	0.49
3:C7:404:ASP:OD1	3:C7:405:GLU:N	2.45	0.49
2:D0:223:THR:HG23	2:D0:225:THR:HG22	1.95	0.49
3:E5:219:THR:O	3:E5:219:THR:OG1	2.30	0.49
2:F0:218:ASP:OD2	2:F0:280:LYS:NZ	2.39	0.49
3:A1:100:ASN:HB3	3:A1:103:LYS:HB2	1.94	0.49
3:A3:309:ARG:NE	3:A3:339:SER:O	2.45	0.49
3:C9:282:ARG:NH1	3:C9:292:GLN:OE1	2.46	0.49
3:D3:117:LEU:HA	3:D3:120:VAL:HG12	1.94	0.49
3:D3:177:ASP:HB3	3:D3:178:THR:HG23	1.94	0.49
2:E2:223:THR:OG1	3:E3:245:GLN:OE1	2.31	0.49
3:E3:153:SER:HB2	3:E3:191:GLN:NE2	2.27	0.49
3:E5:318:ARG:HG2	3:E5:354:CYS:HB3	1.94	0.49
2:E6:65:CYS:SG	2:E6:66:VAL:N	2.85	0.49
3:E7:67:ASP:OD1	3:E7:68:LEU:N	2.44	0.49
3:A1:222:TYR:HB2	2:A2:325:PRO:HG2	1.95	0.49
2:A2:77:GLU:HA	2:A2:80:THR:HG22	1.95	0.49
2:A4:27:GLU:HG3	2:A4:361:THR:HG21	1.95	0.49
2:A4:309:HIS:NE2	2:A4:386:GLU:OE1	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A5:226:ASN:HA	3:A5:229:VAL:HG12	1.95	0.49
2:B0:209:ILE:HA	2:B0:212:ILE:HG22	1.94	0.49
3:B5:67:ASP:OD1	3:B5:68:LEU:N	2.45	0.49
3:C1:329:GLN:OE1	3:C1:332:ASN:ND2	2.46	0.49
2:E4:68:LEU:HD11	2:E4:118:SER:HB2	1.95	0.49
3:E5:49:VAL:HG11	3:E5:241:ARG:HG2	1.95	0.49
2:A0:103:PHE:HD2	2:A0:189:LEU:HD23	1.76	0.49
2:A6:1:MET:N	2:A6:129:CYS:SG	2.74	0.49
3:A9:220:PRO:HB2	2:B0:326:LYS:NZ	2.27	0.49
2:B4:50:ASN:O	2:B4:64:ARG:NH2	2.46	0.49
2:B6:71:GLU:OE2	3:B7:2:ARG:NH2	2.45	0.49
3:C3:1:MET:N	3:C3:128:ASP:OD2	2.31	0.49
2:D0:245:ASP:OD1	2:D0:245:ASP:N	2.44	0.49
2:D6:154:LEU:HB3	2:D6:197:HIS:HB3	1.95	0.49
3:E1:7:VAL:HB	3:E1:135:ILE:HG13	1.95	0.49
3:E3:204:ASN:ND2	8:E3:501:GDP:O2'	2.46	0.49
2:E4:64:ARG:HB3	2:E4:125:LEU:HD21	1.95	0.49
3:E5:175:VAL:HG11	2:E6:332:VAL:HG13	1.95	0.49
3:E7:113:ILE:HA	3:E7:116:VAL:HG12	1.95	0.49
3:E9:49:VAL:HG21	3:E9:241:ARG:HG2	1.95	0.49
3:F1:375:GLN:HE21	3:F1:379:LYS:HD3	1.78	0.49
2:A0:56:THR:HA	3:F1:283:ALA:HB2	1.95	0.48
3:A3:252:LYS:O	3:A3:256:ASN:ND2	2.46	0.48
3:A7:293:MET:SD	3:A7:365:VAL:HG11	2.53	0.48
3:B5:63:ALA:O	3:B5:89:ASN:ND2	2.46	0.48
3:B7:178:THR:HA	2:B8:258:ASN:HD21	1.78	0.48
3:C5:68:LEU:HA	3:C5:93:GLY:HA3	1.95	0.48
2:C8:175:PRO:HB3	2:C8:390:ARG:HD3	1.96	0.48
2:D2:191:THR:HG21	2:D2:425:LEU:HD13	1.95	0.48
2:D6:96:LYS:HE2	3:D7:129:CYS:HB2	1.95	0.48
3:D9:139:LEU:HA	3:D9:145:SER:HB2	1.95	0.48
3:E1:318:ARG:HG2	3:E1:354:CYS:HB3	1.95	0.48
3:E1:396:HIS:HA	3:E1:399:THR:HG22	1.95	0.48
2:E8:301:MET:HE3	2:E8:307:PRO:HG3	1.95	0.48
3:A1:204:ASN:OD1	8:A1:501:GDP:O2'	2.31	0.48
3:A3:77:ARG:HH22	3:A3:92:PHE:HZ	1.61	0.48
3:A3:132:GLY:HA3	3:A3:163:ILE:HG22	1.95	0.48
3:A7:27:GLU:HA	3:A7:359:LYS:HD2	1.94	0.48
2:C2:223:THR:HG23	2:C2:225:THR:HG22	1.95	0.48
3:C5:133:PHE:HB2	3:C5:164:MET:HB3	1.95	0.48
3:D5:107:THR:HG21	3:D5:401:GLU:HB2	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D8:2:ARG:HD2	2:D8:133:GLN:HE21	1.77	0.48
3:E3:49:VAL:HG21	3:E3:241:ARG:HG2	1.95	0.48
2:E4:69:ASP:OD1	2:E4:70:LEU:N	2.46	0.48
3:F1:311:LEU:HD12	3:F1:342:VAL:HG21	1.94	0.48
2:A2:184:PRO:HG3	2:A2:394:LYS:HD3	1.95	0.48
3:A3:392:LYS:HE2	3:A3:395:LEU:HD13	1.94	0.48
3:A9:392:LYS:HD3	3:A9:395:LEU:HG	1.95	0.48
2:B8:276:ILE:HG23	2:B8:280:LYS:HG3	1.96	0.48
3:C1:101:TRP:NE1	3:C1:145:SER:O	2.40	0.48
2:C2:217:LEU:HB3	2:C2:219:ILE:HG13	1.95	0.48
3:C7:330:MET:HB3	3:C7:349:MET:HG3	1.96	0.48
3:D1:248:SER:HA	3:D1:252:LYS:HG3	1.94	0.48
3:E5:213:ARG:HH12	3:E5:297:LYS:HB3	1.77	0.48
3:E7:281:TYR:CD2	3:F1:87:PRO:HD3	2.49	0.48
2:E8:181:VAL:HG11	2:E8:404:PHE:CE1	2.48	0.48
3:A3:205:GLU:HA	3:A3:208:TYR:HD2	1.78	0.48
2:A8:53:PHE:HB3	2:A8:61:HIS:HB3	1.95	0.48
3:B1:68:LEU:HB3	3:B1:96:GLY:HA2	1.95	0.48
3:B5:13:GLY:HA2	3:B5:16:ILE:HG22	1.94	0.48
3:B5:383:ASP:HA	3:B5:386:THR:HG22	1.95	0.48
2:B8:254:GLU:HG2	2:B8:352:LYS:HE2	1.96	0.48
2:C0:103:PHE:H	2:C0:408:TYR:HE1	1.62	0.48
2:C2:251:ASP:OD1	2:C2:254:GLU:N	2.47	0.48
3:D9:139:LEU:HD12	3:D9:170:PHE:CE1	2.49	0.48
2:A0:15:GLN:NE2	6:A0:501:GTP:O6	2.47	0.48
2:A0:172:TRP:N	2:A0:204:LEU:O	2.42	0.48
2:A8:306:ASP:HB3	2:A8:309:HIS:CE1	2.48	0.48
3:A9:67:ASP:OD1	3:A9:68:LEU:N	2.47	0.48
3:B1:239:CYS:SG	3:B1:248:SER:N	2.86	0.48
3:D7:238:CYS:SG	3:D7:318:ARG:NE	2.86	0.48
3:D9:135:ILE:HG22	3:D9:137:HIS:HD2	1.79	0.48
3:D9:239:CYS:SG	3:D9:248:SER:N	2.79	0.48
2:E4:12:ALA:HB3	2:E4:140:ALA:HB2	1.95	0.48
3:E7:274:THR:HG21	3:E7:282:ARG:HD2	1.95	0.48
3:F1:87:PRO:HA	3:F1:90:PHE:HD1	1.78	0.48
2:A2:345:ASP:OD1	2:A2:346:TRP:N	2.47	0.48
2:B0:211:ASP:OD2	2:B0:304:LYS:NZ	2.31	0.48
3:B1:301:CYS:SG	3:B1:303:SER:OG	2.56	0.48
2:B6:223:THR:HG22	3:B7:322:SER:HA	1.95	0.48
2:B8:151:CYS:SG	2:B8:193:SER:OG	2.58	0.48
2:C0:54:SER:OG	2:C0:55:GLU:N	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C6:135:PHE:HB2	2:C6:166:LYS:HG2	1.95	0.48
2:C6:212:ILE:HD13	2:C6:215:ARG:HH22	1.79	0.48
2:D4:75:VAL:HG11	2:D4:94:SER:HB3	1.95	0.48
2:E2:392:ASP:OD1	2:E2:422:ARG:NH1	2.46	0.48
3:E5:257:LEU:HD21	3:E5:314:SER:HB2	1.96	0.48
3:E9:149:THR:HA	3:E9:152:ILE:HD12	1.95	0.48
2:F0:339:ARG:O	2:F0:342:GLN:NE2	2.47	0.48
2:A4:272:TYR:HB3	2:A4:275:ILE:HD11	1.96	0.48
3:A5:98:GLY:H	3:A5:103:LYS:HD3	1.79	0.48
2:A8:209:ILE:HA	2:A8:212:ILE:HG22	1.94	0.48
2:B2:252:VAL:HA	2:B2:255:PHE:HD2	1.78	0.48
3:B3:70:PRO:HD2	2:B4:2:ARG:HH21	1.79	0.48
3:C5:69:GLU:HG2	2:C6:2:ARG:HH22	1.78	0.48
3:C5:173:PRO:HD2	3:C5:205:GLU:HG2	1.95	0.48
2:C8:337:THR:O	2:C8:339:ARG:NH1	2.47	0.48
2:D0:189:LEU:HD11	2:D0:418:PHE:CD1	2.49	0.48
3:D1:375:GLN:HG3	3:D1:419:VAL:HG13	1.94	0.48
3:D7:178:THR:HG22	2:D8:352:LYS:HZ3	1.77	0.48
2:E8:306:ASP:HB3	2:E8:309:HIS:CE1	2.48	0.48
3:F1:33:THR:O	3:F1:58:ARG:NH2	2.47	0.48
1:12:250:GLU:HG3	1:12:251:TYR:CD1	2.48	0.48
2:A2:309:HIS:NE2	2:A2:386:GLU:OE1	2.43	0.48
3:A5:95:THR:OG1	3:A5:96:GLY:N	2.47	0.48
2:B0:172:TRP:HB3	2:B0:205:ASP:OD1	2.13	0.48
3:B5:314:SER:OG	3:B5:315:ALA:N	2.46	0.48
2:C4:390:ARG:O	2:C4:394:LYS:N	2.47	0.48
2:C6:206:ASN:ND2	6:C6:501:GTP:O2'	2.47	0.48
2:C8:217:LEU:HB3	2:C8:219:ILE:HG13	1.95	0.48
2:D4:265:ILE:HD11	2:D4:435:VAL:HG21	1.96	0.48
3:E1:113:ILE:HD11	3:E1:151:LEU:HD13	1.96	0.48
2:E8:79:ARG:NH1	2:E8:92:LEU:O	2.47	0.48
2:E8:274:PRO:HG3	2:E8:286:LEU:HD13	1.95	0.48
3:F1:138:SER:OG	8:F1:501:GDP:O2A	2.31	0.48
2:A4:269:LEU:HD23	2:A4:301:MET:HE2	1.96	0.48
3:A7:113:ILE:HG13	3:A7:117:LEU:HD23	1.95	0.48
2:B4:9:VAL:HG12	2:B4:68:LEU:HB2	1.95	0.48
2:C0:370:LYS:HE2	2:C0:370:LYS:HB2	1.70	0.48
3:C1:391:ARG:O	2:C2:262:TYR:OH	2.32	0.48
2:D6:98:ASP:OD1	2:D6:99:ALA:N	2.46	0.48
3:E5:308:GLY:HA2	3:E5:426:GLN:HE21	1.78	0.48
2:E6:192:HIS:ND1	2:E6:424:ASP:OD2	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F0:340:THR:HG23	2:F0:341:ILE:HG13	1.95	0.48
2:A0:139:ASN:OD1	2:A0:139:ASN:N	2.46	0.48
2:A6:288:VAL:HG21	2:A6:323:VAL:HG23	1.96	0.48
2:B2:240:ALA:HB1	2:B2:356:ASN:HD22	1.79	0.48
2:B8:280:LYS:NZ	2:C2:89:PRO:HB2	2.29	0.48
2:C2:417:GLU:HA	2:C2:420:GLU:HG3	1.94	0.48
2:D4:306:ASP:HB3	2:D4:309:HIS:CE1	2.49	0.48
2:D8:324:VAL:HG23	2:D8:327:ASP:H	1.78	0.48
2:E4:174:SER:OG	2:E4:177:VAL:O	2.27	0.48
2:F0:15:GLN:NE2	6:F0:501:GTP:O6	2.47	0.48
1:1:256:LEU:HD12	2:A6:29:GLY:HA2	1.96	0.47
3:A3:281:TYR:CD2	3:A7:87:PRO:HD3	2.49	0.47
3:B3:12:CYS:HB2	8:B3:501:GDP:C8	2.49	0.47
3:B9:68:LEU:HD23	3:B9:112:LEU:HD13	1.95	0.47
2:C0:109:THR:OG1	2:C0:110:ILE:N	2.46	0.47
3:D9:6:HIS:CE1	3:D9:8:GLN:HE21	2.32	0.47
2:E0:406:HIS:HA	2:E0:409:VAL:HG12	1.95	0.47
2:E2:277:SER:OG	2:E2:278:ALA:N	2.47	0.47
2:E6:12:ALA:HB3	2:E6:140:ALA:HB2	1.96	0.47
3:E9:244:GLY:HA2	3:E9:355:ASP:HB2	1.96	0.47
3:F1:149:THR:HA	3:F1:152:ILE:HD12	1.95	0.47
1:6:247:TYR:HE2	2:B6:81:GLY:HA3	1.78	0.47
2:A8:282:TYR:HD2	2:A8:283:HIS:CE1	2.32	0.47
3:A9:232:ALA:HB1	3:A9:268:ILE:HG21	1.96	0.47
2:B0:108:TYR:HE2	2:B0:413:MET:HB3	1.79	0.47
3:B1:332:ASN:OD1	3:B1:336:LYS:NZ	2.43	0.47
2:C6:222:PRO:HD2	3:C7:324:LYS:HG2	1.95	0.47
3:C9:53:GLU:OE2	3:C9:54:ALA:N	2.47	0.47
3:D1:128:ASP:OD1	3:D1:129:CYS:N	2.40	0.47
2:D2:101:ASN:OD1	3:D3:252:LYS:NZ	2.48	0.47
3:E3:247:ASN:C	3:E3:247:ASN:HD22	2.15	0.47
2:E8:69:ASP:OD1	2:E8:70:LEU:N	2.47	0.47
2:E8:407:TRP:HE1	3:E9:258:ILE:HG13	1.79	0.47
2:A2:51:THR:HG21	2:A2:243:ARG:HA	1.95	0.47
3:A5:206:ALA:HB2	3:A5:302:ALA:HB2	1.96	0.47
2:A6:191:THR:HA	2:A6:194:LEU:HB3	1.96	0.47
2:A6:276:ILE:HB	2:A6:280:LYS:HB2	1.96	0.47
3:A7:139:LEU:HG	3:A7:168:SER:HB3	1.96	0.47
2:D4:180:ALA:HB3	2:D4:183:GLU:HG3	1.96	0.47
2:D8:132:LEU:HG	2:D8:164:LYS:HD3	1.96	0.47
2:E6:27:GLU:OE2	2:E6:320:ARG:NH2	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:250:GLU:OE2	2:B0:229:ARG:NH2	2.47	0.47
1:10:248:ARG:HH22	2:C8:77:GLU:HG2	1.78	0.47
2:A0:211:ASP:OD2	2:A0:304:LYS:NZ	2.48	0.47
2:A2:384:ILE:HA	2:A2:387:VAL:HG12	1.96	0.47
3:B7:128:ASP:OD1	3:B7:129:CYS:N	2.39	0.47
2:C2:191:THR:HG21	2:C2:425:LEU:HD21	1.96	0.47
2:C8:238:LEU:HD11	2:C8:255:PHE:HE2	1.79	0.47
3:C9:334:GLN:HE22	3:C9:348:ASN:H	1.62	0.47
2:D2:277:SER:OG	2:D2:278:ALA:N	2.48	0.47
2:E8:9:VAL:HG22	2:E8:68:LEU:HB3	1.96	0.47
2:E8:107:HIS:NE2	2:E8:151:CYS:SG	2.80	0.47
2:A2:320:ARG:NH1	2:A2:360:PRO:HA	2.30	0.47
3:A5:167:PHE:CE2	3:A5:233:MET:HG2	2.49	0.47
3:B1:114:ASP:N	3:B1:114:ASP:OD1	2.47	0.47
2:C2:76:ASP:HA	2:C2:79:ARG:HD2	1.96	0.47
2:C8:105:ARG:HH12	3:C9:251:ARG:HG2	1.79	0.47
2:C8:174:SER:OG	2:C8:177:VAL:O	2.23	0.47
3:D5:25:SER:OG	3:D5:51:TYR:OH	2.33	0.47
2:F0:223:THR:HG23	2:F0:225:THR:HG22	1.95	0.47
3:F1:198:GLU:OE2	3:F1:200:GLN:NE2	2.43	0.47
2:A0:27:GLU:OE2	2:A0:236:SER:OG	2.33	0.47
3:A7:139:LEU:HD12	3:A7:170:PHE:HE1	1.79	0.47
3:B7:259:PRO:HD2	3:B7:263:LEU:HD11	1.95	0.47
2:B8:133:GLN:HG3	2:B8:252:VAL:HB	1.97	0.47
2:C0:100:ALA:HA	3:C1:252:LYS:HE2	1.97	0.47
3:C3:42:LEU:HD21	3:C3:356:ILE:HG13	1.96	0.47
2:C4:30:ILE:HD13	2:C4:53:PHE:CE2	2.50	0.47
2:C8:7:ILE:HG23	2:C8:66:VAL:HG23	1.96	0.47
3:D3:180:VAL:O	3:D3:184:ASN:ND2	2.48	0.47
3:E3:145:SER:O	3:E3:149:THR:OG1	2.27	0.47
1:19:250:GLU:HG3	2:E6:225:THR:HG21	1.96	0.47
2:A0:269:LEU:HD23	2:A0:303:ALA:HB3	1.96	0.47
2:A0:301:MET:HE1	2:A0:305:CYS:H	1.78	0.47
3:A1:341:PHE:HB3	3:A1:348:ASN:ND2	2.30	0.47
3:A1:398:TYR:HB3	3:A1:403:MET:HG3	1.96	0.47
3:A5:91:VAL:HG21	3:A5:116:VAL:HG22	1.97	0.47
2:B2:28:HIS:CE1	2:B2:243:ARG:HD2	2.50	0.47
2:B2:76:ASP:HA	2:B2:79:ARG:HG2	1.96	0.47
2:B2:277:SER:OG	2:B2:278:ALA:N	2.46	0.47
3:B3:208:TYR:CE1	3:B3:225:LEU:HD11	2.50	0.47
3:B3:257:LEU:HD21	3:B3:314:SER:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B4:184:PRO:HG2	2:B4:398:MET:HE3	1.95	0.47
2:B4:240:ALA:O	2:B4:356:ASN:ND2	2.47	0.47
3:B5:211:CYS:SG	3:B5:220:PRO:HB3	2.54	0.47
2:B8:185:TYR:HE1	2:B8:398:MET:HG2	1.80	0.47
2:B8:192:HIS:ND1	2:B8:424:ASP:OD2	2.44	0.47
3:C1:130:LEU:HD11	3:C1:133:PHE:HE1	1.80	0.47
3:C1:149:THR:O	3:C1:191:GLN:NE2	2.48	0.47
2:C2:105:ARG:HG2	2:C2:411:GLU:HG2	1.95	0.47
2:C4:205:ASP:HB2	2:C4:303:ALA:HA	1.96	0.47
2:C6:1:MET:HA	2:C6:129:CYS:HB3	1.97	0.47
2:D0:98:ASP:OD1	2:D0:99:ALA:N	2.48	0.47
3:D3:21:TRP:HA	3:D3:24:ILE:HG22	1.96	0.47
3:D3:294:PHE:CD2	3:D3:333:VAL:HG21	2.50	0.47
3:D5:323:THR:O	3:D5:327:ASP:N	2.46	0.47
3:D5:404:ASP:OD1	3:D5:405:GLU:N	2.47	0.47
2:E4:132:LEU:HG	2:E4:164:LYS:NZ	2.29	0.47
3:E5:379:LYS:O	3:E5:383:ASP:N	2.45	0.47
2:E6:8:HIS:HE1	2:E6:21:TRP:HE1	1.61	0.47
2:E6:238:LEU:HD11	2:E6:378:ILE:HG13	1.96	0.47
3:E7:64:ILE:HD13	3:E7:119:VAL:HG13	1.96	0.47
2:E8:236:SER:O	2:E8:243:ARG:NH2	2.40	0.47
2:E8:271:SER:HB3	2:E8:377:MET:HB3	1.97	0.47
2:F0:390:ARG:NH2	2:F0:390:ARG:HB3	2.29	0.47
3:A1:13:GLY:HA2	3:A1:16:ILE:HG22	1.96	0.47
3:A1:136:THR:HG22	3:A1:167:PHE:HD2	1.80	0.47
2:A4:28:HIS:CE1	2:A4:243:ARG:HD2	2.50	0.47
2:A4:269:LEU:HB3	2:A4:301:MET:CE	2.45	0.47
3:B3:179:VAL:HA	2:B4:349:THR:HG22	1.96	0.47
2:B4:115:VAL:HG23	2:B4:153:LEU:HD12	1.97	0.47
3:B5:100:ASN:HB3	3:B5:103:LYS:HG2	1.97	0.47
3:B7:100:ASN:HB3	3:B7:103:LYS:HD3	1.97	0.47
3:C9:334:GLN:HE22	3:C9:348:ASN:N	2.12	0.47
3:D1:203:ASP:OD2	3:D1:302:ALA:N	2.40	0.47
3:D9:63:ALA:O	3:D9:89:ASN:ND2	2.47	0.47
3:D9:64:ILE:HD12	3:D9:119:VAL:HG12	1.96	0.47
2:E0:212:ILE:HD11	2:E0:300:SER:HA	1.96	0.47
3:E1:64:ILE:HD12	3:E1:119:VAL:HG12	1.97	0.47
2:E8:11:GLN:HG3	2:E8:74:VAL:HG21	1.96	0.47
2:E8:70:LEU:HD12	2:E8:99:ALA:HB2	1.96	0.47
2:E8:319:TYR:HB3	2:E8:323:VAL:HG11	1.96	0.47
3:F1:292:GLN:O	3:F1:298:ASN:ND2	2.35	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B0:76:ASP:HA	2:B0:79:ARG:HG2	1.97	0.47
3:B1:63:ALA:O	3:B1:89:ASN:ND2	2.48	0.47
3:C1:192:LEU:HD11	3:C1:199:VAL:HG11	1.96	0.47
2:C8:147:SER:HB2	2:C8:190:SER:HB3	1.96	0.47
3:D1:270:PHE:O	3:D1:298:ASN:ND2	2.47	0.47
2:D8:265:ILE:HG22	2:D8:380:ASN:HD21	1.80	0.47
2:E6:236:SER:OG	2:E6:243:ARG:NH2	2.48	0.47
2:A0:241:SER:HB3	2:A0:249:ASN:HB3	1.97	0.47
3:A3:41:ASP:N	3:A3:41:ASP:OD1	2.48	0.47
3:A7:404:ASP:OD1	3:A7:405:GLU:N	2.48	0.47
2:B8:301:MET:HE2	2:B8:301:MET:HA	1.97	0.47
2:B8:391:MET:O	2:B8:395:PHE:N	2.47	0.47
2:C0:275:ILE:HD12	2:C0:368:LEU:HD11	1.96	0.47
3:C1:156:ARG:HD3	3:C1:160:PRO:HA	1.97	0.47
2:C6:135:PHE:HD2	2:C6:166:LYS:HG2	1.81	0.47
2:C6:210:TYR:HH	3:C7:323:THR:HG1	1.62	0.47
2:D0:34:GLY:O	2:D0:61:HIS:N	2.41	0.47
3:D3:6:HIS:HD1	3:D3:21:TRP:HE1	1.63	0.47
2:D8:392:ASP:OD1	2:D8:422:ARG:NH2	2.43	0.47
3:E3:33:THR:O	3:E3:58:ARG:NH2	2.48	0.47
2:E8:211:ASP:N	2:E8:211:ASP:OD1	2.48	0.47
2:E8:325:PRO:HA	2:E8:328:VAL:HG12	1.97	0.47
3:F1:117:LEU:HA	3:F1:120:VAL:HG12	1.97	0.47
2:A2:208:ALA:HB2	2:A2:304:LYS:HB2	1.97	0.46
3:A7:95:THR:OG1	3:A7:96:GLY:N	2.48	0.46
3:B1:383:ASP:HA	3:B1:386:THR:HG22	1.95	0.46
2:B4:178:SER:OG	2:B4:179:THR:N	2.47	0.46
3:C1:68:LEU:HA	3:C1:93:GLY:HA3	1.96	0.46
3:C1:105:HIS:O	3:C1:105:HIS:ND1	2.47	0.46
3:C1:263:LEU:HB2	3:C1:422:TYR:CZ	2.49	0.46
3:C3:183:TYR:HB3	3:C3:398:TYR:HE2	1.80	0.46
2:D2:217:LEU:HD11	2:D2:275:ILE:HG22	1.96	0.46
2:D2:241:SER:OG	2:D2:250:VAL:O	2.25	0.46
3:D3:100:ASN:ND2	3:D3:401:GLU:OE2	2.47	0.46
3:D7:94:GLN:O	2:D8:2:ARG:NH2	2.48	0.46
2:D8:1:MET:N	2:D8:3:GLU:OE2	2.38	0.46
3:E7:105:HIS:CD2	3:E7:150:LEU:HB2	2.50	0.46
2:E8:306:ASP:N	2:E8:386:GLU:OE2	2.48	0.46
2:E8:397:LEU:HD23	3:E9:346:PRO:HD3	1.97	0.46
3:E9:5:VAL:HB	3:E9:133:PHE:HD1	1.79	0.46
2:A8:116:ASP:N	2:A8:116:ASP:OD1	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B0:254:GLU:O	2:B0:258:ASN:ND2	2.45	0.46
3:B7:375:GLN:HE22	3:B7:419:VAL:HA	1.81	0.46
2:B8:70:LEU:HD12	2:B8:99:ALA:HB2	1.96	0.46
3:C3:184:ASN:OD1	3:C3:398:TYR:OH	2.30	0.46
3:C3:309:ARG:NH1	3:C3:339:SER:O	2.48	0.46
2:C6:34:GLY:O	2:C6:61:HIS:N	2.37	0.46
2:C8:88:HIS:HB3	2:C8:91:GLN:HB2	1.97	0.46
3:D7:190:HIS:HB2	3:D7:414:ASN:ND2	2.30	0.46
2:E4:72:PRO:HD2	3:E5:2:ARG:HH22	1.80	0.46
3:E7:19:LYS:HE3	3:E7:227:HIS:HB2	1.96	0.46
2:E8:10:GLY:HA2	2:E8:145:THR:HG23	1.96	0.46
1:1:246:CYS:SG	1:1:247:TYR:N	2.88	0.46
2:A4:115:VAL:HG21	2:A4:152:LEU:HG	1.97	0.46
2:A6:331:ALA:O	2:A6:334:THR:OG1	2.28	0.46
2:B6:222:PRO:O	3:B7:322:SER:OG	2.26	0.46
2:C0:172:TRP:HB2	2:C0:203:MET:HB3	1.96	0.46
3:C9:205:GLU:HA	3:C9:208:TYR:HD2	1.81	0.46
3:D1:7:VAL:HB	3:D1:135:ILE:HG12	1.97	0.46
3:D5:96:GLY:N	3:D5:108:GLU:OE2	2.49	0.46
2:D8:398:MET:HE2	3:D9:346:PRO:HD2	1.97	0.46
2:E6:423:GLU:O	2:E6:427:ALA:N	2.42	0.46
2:F0:207:GLU:HA	2:F0:210:TYR:HB2	1.96	0.46
1:3:248:ARG:NH2	2:B0:82:THR:H	2.13	0.46
3:A3:113:ILE:HA	3:A3:116:VAL:HG22	1.96	0.46
2:A8:277:SER:OG	2:A8:278:ALA:N	2.48	0.46
3:B7:66:MET:HE3	3:B7:116:VAL:HG21	1.96	0.46
2:C6:340:THR:HG23	2:C6:341:ILE:HG13	1.97	0.46
3:D7:19:LYS:HA	3:D7:19:LYS:HD2	1.74	0.46
3:D9:290:THR:HG21	3:D9:329:GLN:HB3	1.98	0.46
3:E5:101:TRP:HD1	3:E5:145:SER:HG	1.63	0.46
3:E5:274:THR:HG21	3:E5:282:ARG:HD2	1.98	0.46
2:E6:206:ASN:OD1	6:E6:501:GTP:N2	2.49	0.46
2:E8:329:ASN:HA	2:E8:332:VAL:HG12	1.98	0.46
2:A0:356:ASN:OD1	2:A0:357:TYR:N	2.48	0.46
3:A5:139:LEU:HG	3:A5:168:SER:HB3	1.98	0.46
3:A9:6:HIS:HD1	3:A9:21:TRP:HE1	1.64	0.46
3:B9:13:GLY:HA2	3:B9:136:THR:HG22	1.98	0.46
2:C0:322:ASP:OD1	2:C0:373:ARG:NH2	2.49	0.46
2:C6:228:ASN:ND2	6:C6:501:GTP:O6	2.43	0.46
3:E1:198:GLU:HB2	3:E1:266:PHE:HE2	1.81	0.46
3:E5:261:PRO:O	3:E5:264:HIS:ND1	2.47	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E7:232:ALA:HB2	3:E7:270:PHE:HB2	1.97	0.46
2:E8:210:TYR:HB3	3:E9:324:LYS:HD3	1.98	0.46
3:E9:105:HIS:HB3	3:E9:106:TYR:CD1	2.51	0.46
2:F0:271:SER:HB2	2:F0:377:MET:HB3	1.97	0.46
2:A0:224:TYR:CZ	3:A1:323:THR:HG21	2.51	0.46
2:A4:98:ASP:O	2:A4:105:ARG:NH1	2.47	0.46
3:A9:272:PRO:HG3	3:A9:284:LEU:HD11	1.97	0.46
3:B3:27:GLU:OE2	3:B3:318:ARG:NH2	2.33	0.46
2:B8:11:GLN:NE2	3:B9:245:GLN:O	2.49	0.46
2:C6:100:ALA:HA	3:C7:252:LYS:HB3	1.96	0.46
2:D0:306:ASP:HB3	2:D0:309:HIS:CE1	2.50	0.46
3:E5:94:GLN:OE1	3:E5:94:GLN:N	2.49	0.46
3:A3:176:SER:HB2	3:A3:181:GLU:HG3	1.98	0.46
2:A6:193:SER:O	2:A6:197:HIS:ND1	2.49	0.46
3:B5:77:ARG:HH22	3:B5:92:PHE:HZ	1.64	0.46
3:C3:259:PRO:HG2	3:C3:311:LEU:HD21	1.97	0.46
2:C4:105:ARG:HG2	2:C4:411:GLU:HG2	1.97	0.46
2:C6:364:PRO:HG2	1:22:254:LYS:HB3	1.97	0.46
2:C8:206:ASN:OD1	6:C8:501:GTP:O2'	2.32	0.46
2:D2:73:THR:HA	3:D3:46:ARG:HH11	1.81	0.46
3:D7:383:ASP:HA	3:D7:386:THR:HG22	1.98	0.46
3:E1:70:PRO:HD2	2:E2:2:ARG:NH2	2.31	0.46
2:E6:8:HIS:HD1	2:E6:65:CYS:HG	1.64	0.46
2:E8:172:TRP:N	2:E8:204:LEU:O	2.40	0.46
3:E9:69:GLU:HG2	2:F0:2:ARG:HH12	1.80	0.46
2:F0:9:VAL:HG13	2:F0:149:LEU:HD23	1.97	0.46
2:F0:60:LYS:HE3	2:F0:60:LYS:HB3	1.82	0.46
1:7:244:GLN:HE22	1:7:249:SER:N	2.14	0.46
2:A4:245:ASP:N	2:A4:245:ASP:OD1	2.49	0.46
3:A9:213:ARG:HH21	3:A9:297:LYS:HD3	1.80	0.46
3:B3:210:ILE:O	3:B3:214:THR:OG1	2.27	0.46
3:C1:105:HIS:CE1	3:C1:150:LEU:HD13	2.51	0.46
2:C2:241:SER:OG	2:C2:250:VAL:O	2.24	0.46
3:C3:275:SER:OG	3:C3:276:ARG:N	2.48	0.46
2:D4:8:HIS:HD2	2:D4:67:PHE:CE1	2.33	0.46
3:D5:213:ARG:HH12	3:D5:297:LYS:HB2	1.81	0.46
2:D6:298:PRO:HG2	2:D6:308:ARG:NH1	2.31	0.46
3:E5:3:GLU:HA	3:E5:49:VAL:HA	1.98	0.46
2:E6:71:GLU:HG2	2:E6:73:THR:HG22	1.98	0.46
2:E6:282:TYR:OH	2:F0:35:GLN:NE2	2.49	0.46
2:F0:103:PHE:CD2	2:F0:189:LEU:HB3	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F0:223:THR:OG1	2:F0:224:TYR:N	2.49	0.46
2:F0:306:ASP:HB3	2:F0:309:HIS:CE1	2.50	0.46
2:A0:9:VAL:HG22	2:A0:68:LEU:HD22	1.98	0.46
3:A5:7:VAL:HG11	3:A5:151:LEU:HD21	1.98	0.46
2:A8:6:SER:OG	2:A8:8:HIS:NE2	2.43	0.46
3:B1:40:SER:OG	3:B1:43:GLN:OE1	2.30	0.46
2:B2:356:ASN:OD1	2:B2:357:TYR:N	2.49	0.46
3:B3:176:SER:HB2	2:B4:349:THR:HG23	1.97	0.46
3:B7:358:PRO:HG2	3:B7:361:LEU:HD12	1.97	0.46
2:C2:70:LEU:HD12	2:C2:99:ALA:HB2	1.97	0.46
2:C4:141:VAL:HG11	2:C4:172:TRP:CE3	2.51	0.46
2:D0:178:SER:HB3	2:D0:183:GLU:OE2	2.16	0.46
2:D8:2:ARG:HG3	2:D8:51:THR:HG22	1.98	0.46
2:E2:283:HIS:HB3	2:E6:62:VAL:HG11	1.98	0.46
3:E5:64:ILE:HD12	3:E5:119:VAL:HG12	1.98	0.46
3:E9:28:HIS:CE1	3:E9:241:ARG:HE	2.33	0.46
3:A1:117:LEU:HA	3:A1:120:VAL:HG12	1.98	0.46
2:B0:11:GLN:HG3	2:B0:74:VAL:HG21	1.98	0.46
2:C0:121:ARG:HD2	2:C0:121:ARG:HA	1.64	0.46
2:C4:396:ASP:N	2:C4:396:ASP:OD1	2.46	0.46
3:C7:192:LEU:HG	3:C7:199:VAL:HG21	1.98	0.46
3:C7:362:LYS:HD2	3:C7:363:MET:HG3	1.97	0.46
2:D6:401:LYS:HD2	3:D7:344:TRP:CD2	2.51	0.46
3:D7:374:ILE:HD11	3:D7:422:TYR:CZ	2.51	0.46
2:E0:100:ALA:HA	3:E1:252:LYS:HD2	1.98	0.46
2:E4:241:SER:OG	2:E4:250:VAL:O	2.28	0.46
3:E9:7:VAL:HG22	3:E9:64:ILE:HB	1.98	0.46
3:F1:133:PHE:HZ	3:F1:159:TYR:HD2	1.63	0.46
1:21:246:CYS:SG	3:F1:245:GLN:NE2	2.88	0.45
3:A9:318:ARG:HG2	3:A9:354:CYS:HB3	1.99	0.45
2:B4:223:THR:OG1	3:B5:245:GLN:OE1	2.33	0.45
2:B4:356:ASN:OD1	2:B4:357:TYR:N	2.49	0.45
3:B9:404:ASP:OD1	3:B9:405:GLU:N	2.46	0.45
2:C0:155:GLU:HA	2:C0:197:HIS:CE1	2.51	0.45
2:C0:241:SER:OG	2:C0:250:VAL:O	2.22	0.45
3:C1:99:ASN:HD22	2:C2:254:GLU:CD	2.20	0.45
3:C1:137:HIS:ND1	3:C1:138:SER:O	2.36	0.45
3:C1:222:TYR:HD1	3:C1:225:LEU:HD12	1.81	0.45
2:C4:76:ASP:OD1	2:C4:77:GLU:N	2.49	0.45
1:2:250:GLU:OE2	2:A8:229:ARG:NH2	2.49	0.45
2:A0:195:LEU:HD21	2:A0:264:ARG:HE	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B1:208:TYR:CE1	3:B1:225:LEU:HD11	2.51	0.45
3:B3:396:HIS:HA	3:B3:399:THR:HG22	1.98	0.45
2:B4:406:HIS:HA	2:B4:409:VAL:HG12	1.97	0.45
2:B8:215:ARG:NH2	2:B8:299:ALA:O	2.49	0.45
2:B8:401:LYS:HE2	3:B9:344:TRP:CD2	2.50	0.45
2:C0:71:GLU:HB3	2:C0:98:ASP:HB3	1.98	0.45
3:C1:330:MET:HB3	3:C1:349:MET:HG2	1.97	0.45
3:C5:6:HIS:HE2	3:C5:136:THR:HG23	1.81	0.45
3:C7:165:GLU:HG3	3:C7:198:GLU:HG3	1.98	0.45
3:D1:371:SER:OG	3:D1:372:THR:N	2.48	0.45
2:D2:399:TYR:OH	2:D2:415:GLU:OE2	2.25	0.45
3:D5:318:ARG:HD3	3:D5:358:PRO:HD3	1.99	0.45
2:E4:306:ASP:HB3	2:E4:309:HIS:CE1	2.52	0.45
3:E9:198:GLU:HG3	3:E9:266:PHE:CE2	2.51	0.45
2:F0:407:TRP:HE1	3:F1:258:ILE:HG13	1.81	0.45
2:A0:11:GLN:HG3	2:A0:74:VAL:HG11	1.98	0.45
2:A2:356:ASN:OD1	2:A2:357:TYR:N	2.49	0.45
2:A8:107:HIS:HB2	2:A8:108:TYR:CD1	2.51	0.45
2:A8:157:LEU:HD23	2:A8:157:LEU:HA	1.86	0.45
2:A8:356:ASN:OD1	2:A8:357:TYR:N	2.50	0.45
3:B3:6:HIS:CE1	3:B3:20:PHE:CD2	3.05	0.45
3:B5:313:ALA:HB3	3:B5:349:MET:SD	2.56	0.45
3:B9:67:ASP:OD1	3:B9:68:LEU:N	2.49	0.45
2:C0:106:GLY:HA3	2:C0:148:GLY:HA3	1.98	0.45
2:C0:133:GLN:HG3	2:C0:252:VAL:HG22	1.97	0.45
2:C0:137:MET:SD	2:C0:139:ASN:ND2	2.89	0.45
3:C3:283:ALA:HB2	3:C7:54:ALA:HA	1.97	0.45
3:C7:5:VAL:HB	3:C7:133:PHE:CD1	2.51	0.45
3:C7:252:LYS:HA	3:C7:255:VAL:HG22	1.97	0.45
2:D8:395:PHE:HD2	2:D8:422:ARG:HD3	1.81	0.45
2:E2:177:VAL:HG13	3:E3:327:ASP:HB3	1.99	0.45
2:E4:221:ARG:CZ	3:E5:325:GLU:H	2.29	0.45
2:E8:96:LYS:NZ	3:E9:1:MET:O	2.33	0.45
2:B4:282:TYR:HE2	2:B8:85:HIS:HB3	1.80	0.45
3:C3:107:THR:OG1	3:C3:108:GLU:N	2.50	0.45
2:C4:18:ASN:O	2:C4:22:GLU:HG2	2.17	0.45
3:C5:248:SER:HA	3:C5:252:LYS:HE3	1.98	0.45
2:C6:296:PHE:HE1	2:C6:377:MET:HG3	1.81	0.45
2:C8:34:GLY:O	2:C8:61:HIS:N	2.42	0.45
2:D6:12:ALA:HB3	2:D6:140:ALA:HB2	1.99	0.45
2:D6:280:LYS:HG2	2:E0:89:PRO:HG2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D9:178:THR:O	3:D9:181:GLU:HG2	2.16	0.45
2:E8:214:ARG:HH22	2:E8:220:GLU:HG2	1.81	0.45
3:F1:327:ASP:HA	3:F1:330:MET:HE1	1.98	0.45
3:A1:47:ILE:HG12	3:A1:51:TYR:HB2	1.98	0.45
3:B1:27:GLU:OE1	3:B1:318:ARG:NH2	2.50	0.45
3:B1:249:ASP:H	3:B1:252:LYS:HB2	1.82	0.45
2:B4:207:GLU:HA	2:B4:210:TYR:HB2	1.98	0.45
2:C0:224:TYR:HD2	6:C0:501:GTP:C6	2.35	0.45
3:C1:211:CYS:HA	3:C1:215:LEU:HB2	1.97	0.45
2:D8:388:PHE:HB2	2:D8:429:GLU:OE2	2.17	0.45
2:E2:2:ARG:HD3	2:E2:2:ARG:HA	1.86	0.45
3:E3:178:THR:HG23	3:E3:181:GLU:HG3	1.99	0.45
1:20:245:SER:HB3	1:20:248:ARG:HD3	1.98	0.45
2:B0:223:THR:OG1	2:B0:225:THR:HG22	2.17	0.45
3:B1:27:GLU:OE2	3:B1:241:ARG:NH1	2.35	0.45
2:B2:156:ARG:HA	2:B2:159:VAL:HG12	1.99	0.45
2:C2:33:ASP:O	2:C2:60:LYS:NZ	2.33	0.45
2:C2:181:VAL:HG22	3:C3:256:ASN:OD1	2.17	0.45
3:C5:320:ARG:NH2	1:23:244:GLN:O	2.50	0.45
2:C6:103:PHE:HB3	2:C6:189:LEU:HD23	1.99	0.45
3:D1:53:GLU:OE2	3:D1:54:ALA:N	2.49	0.45
2:D4:69:ASP:OD1	2:D4:70:LEU:N	2.50	0.45
3:D5:13:GLY:HA2	3:D5:16:ILE:HG22	1.98	0.45
2:D6:212:ILE:HG12	2:D6:275:ILE:HD11	1.99	0.45
3:D7:66:MET:HE1	3:D7:151:LEU:HD22	1.99	0.45
2:D8:422:ARG:HA	2:D8:422:ARG:HD2	1.65	0.45
2:E4:195:LEU:HD11	2:E4:428:LEU:HD22	1.98	0.45
3:E9:327:ASP:HA	3:E9:330:MET:HB3	1.98	0.45
2:A6:69:ASP:OD1	2:A6:70:LEU:N	2.50	0.45
3:B9:216:LYS:HE2	3:B9:275:SER:HB3	1.99	0.45
2:C0:254:GLU:HA	2:C0:257:THR:HG22	1.99	0.45
3:C1:167:PHE:CE2	3:C1:233:MET:HB2	2.52	0.45
3:C3:169:VAL:HG12	3:C3:202:ILE:HB	1.98	0.45
2:C4:154:LEU:HD21	2:C4:198:THR:HB	1.99	0.45
2:D0:119:LEU:HA	2:D0:122:ILE:HG22	1.98	0.45
2:D2:259:LEU:HD21	2:D2:316:CYS:HB2	1.98	0.45
2:D4:107:HIS:NE2	2:D4:151:CYS:SG	2.80	0.45
3:D9:3:GLU:HA	3:D9:49:VAL:HA	1.99	0.45
3:D9:6:HIS:CE1	3:D9:8:GLN:HG2	2.52	0.45
3:E7:276:ARG:NH2	3:E7:279:GLN:OE1	2.38	0.45
3:E9:238:CYS:SG	3:E9:239:CYS:N	2.89	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A8:288:VAL:HG13	2:A8:319:TYR:HE2	1.82	0.45
3:B3:63:ALA:O	3:B3:89:ASN:ND2	2.50	0.45
3:B7:311:LEU:HD12	3:B7:342:VAL:HG11	1.99	0.45
3:B9:192:LEU:HD21	3:B9:199:VAL:HG11	1.98	0.45
2:C4:356:ASN:OD1	2:C4:357:TYR:N	2.50	0.45
2:C6:53:PHE:HB3	2:C6:61:HIS:HB3	1.98	0.45
3:D1:294:PHE:CD2	3:D1:333:VAL:HG21	2.52	0.45
3:D3:313:ALA:HB1	3:D3:367:PHE:HE1	1.81	0.45
3:E1:284:LEU:HD23	3:E1:362:LYS:HG2	1.98	0.45
2:E8:2:ARG:NE	2:E8:133:GLN:HE21	2.15	0.45
3:F1:239:CYS:SG	3:F1:248:SER:N	2.73	0.45
2:A2:205:ASP:OD1	2:A2:206:ASN:N	2.50	0.45
2:A2:247:ALA:HB2	2:A2:357:TYR:CZ	2.52	0.45
2:A2:284:GLU:HG2	2:A2:286:LEU:HD22	1.97	0.45
3:A5:2:ARG:NH2	3:A5:249:ASP:OD2	2.50	0.45
2:B8:286:LEU:O	2:B8:373:ARG:NH1	2.41	0.45
3:C3:253:LEU:HD11	3:C3:368:VAL:HG21	1.98	0.45
3:C3:289:LEU:HD12	3:C3:365:VAL:HG12	1.98	0.45
2:D4:76:ASP:OD2	3:D5:46:ARG:NH1	2.41	0.45
3:D9:6:HIS:HD2	3:D9:134:GLN:NE2	2.14	0.45
3:D9:139:LEU:HD11	3:D9:192:LEU:HD13	1.97	0.45
3:F1:7:VAL:HG11	3:F1:151:LEU:HD23	1.97	0.45
2:A2:174:SER:HB3	2:A2:177:VAL:O	2.17	0.45
2:B2:230:LEU:HD21	2:B2:368:LEU:HD11	1.98	0.45
2:B4:141:VAL:O	2:B4:147:SER:OG	2.34	0.45
2:B8:265:ILE:HG23	2:B8:432:TYR:HE1	1.82	0.45
2:C0:338:LYS:HA	2:C0:338:LYS:HD2	1.84	0.45
3:C1:179:VAL:HG23	2:C2:349:THR:HG23	1.98	0.45
2:C2:105:ARG:HE	2:C2:105:ARG:HB3	1.66	0.45
2:C2:346:TRP:HZ2	2:C2:435:VAL:HG13	1.81	0.45
3:C3:204:ASN:HD21	8:C3:501:GDP:N2	2.11	0.45
2:C4:417:GLU:OE2	2:C4:417:GLU:N	2.48	0.45
2:E2:262:TYR:HD2	2:E2:265:ILE:HD12	1.82	0.45
3:A1:289:LEU:HD21	3:A1:365:VAL:HG11	1.99	0.44
3:A5:5:VAL:HB	3:A5:133:PHE:CD1	2.52	0.44
3:A5:220:PRO:HB2	3:A5:224:ASP:HB2	1.98	0.44
3:A7:174:LYS:HE3	3:A7:205:GLU:HG3	1.97	0.44
2:B2:178:SER:HB2	3:B3:347:ASN:ND2	2.32	0.44
3:B7:204:ASN:ND2	8:B7:501:GDP:O2'	2.50	0.44
2:B8:141:VAL:HA	2:B8:147:SER:HB2	1.99	0.44
2:C0:222:PRO:HG2	3:C1:324:LYS:NZ	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C3:173:PRO:HA	3:C3:380:ARG:HH21	1.82	0.44
2:C4:137:MET:HB3	2:C4:168:ASN:HA	1.99	0.44
3:C5:259:PRO:HB2	3:C5:260:PHE:CD1	2.52	0.44
2:C8:28:HIS:CE1	2:C8:243:ARG:HH11	2.35	0.44
3:D9:132:GLY:HA3	3:D9:163:ILE:HG22	1.98	0.44
3:E5:173:PRO:HB3	3:E5:380:ARG:CZ	2.47	0.44
2:E6:71:GLU:HB2	2:E6:98:ASP:HB3	1.97	0.44
2:E8:88:HIS:HA	2:E8:89:PRO:HD3	1.89	0.44
3:E9:70:PRO:HD2	2:F0:2:ARG:HH11	1.81	0.44
2:A0:91:GLN:HA	2:A0:121:ARG:NH1	2.32	0.44
3:A5:16:ILE:HG22	3:A5:226:ASN:CG	2.37	0.44
3:A5:100:ASN:HB3	3:A5:103:LYS:HG2	1.99	0.44
3:A7:232:ALA:HB1	3:A7:268:ILE:HG21	1.99	0.44
3:A9:142:GLY:N	8:A9:501:GDP:O1B	2.48	0.44
3:A9:214:THR:OG1	3:A9:215:LEU:N	2.50	0.44
3:A9:286:VAL:HB	3:A9:325:GLU:HG2	1.99	0.44
2:B0:88:HIS:HB3	2:B0:91:GLN:HG2	1.98	0.44
2:B2:215:ARG:HH11	2:B2:299:ALA:HB1	1.83	0.44
2:B4:156:ARG:HA	2:B4:159:VAL:HG12	1.99	0.44
2:B8:69:ASP:OD1	2:B8:70:LEU:N	2.49	0.44
2:B8:283:HIS:HB2	2:C2:88:HIS:CD2	2.52	0.44
3:B9:170:PHE:HE2	3:B9:378:PHE:HE1	1.65	0.44
2:C6:154:LEU:HG	2:C6:197:HIS:HB3	1.98	0.44
3:C7:2:ARG:HG3	3:C7:131:GLN:HB2	1.99	0.44
3:C9:161:ASP:OD1	3:C9:161:ASP:N	2.47	0.44
3:C9:205:GLU:HA	3:C9:208:TYR:CD2	2.52	0.44
3:C9:409:THR:HA	3:C9:412:GLU:HG3	2.00	0.44
2:D6:181:VAL:H	3:D7:256:ASN:ND2	2.15	0.44
2:E2:319:TYR:HB3	2:E2:323:VAL:HG21	1.99	0.44
3:E3:218:THR:HG23	3:E3:219:THR:HG23	1.99	0.44
2:E6:316:CYS:HA	2:E6:352:LYS:HB2	1.99	0.44
3:F1:13:GLY:HA2	3:F1:16:ILE:HG22	1.97	0.44
3:A1:139:LEU:HD13	3:A1:168:SER:HB2	1.99	0.44
2:A2:103:PHE:H	2:A2:408:TYR:HE1	1.66	0.44
2:A4:340:THR:HG23	2:A4:341:ILE:HG13	1.99	0.44
2:A8:241:SER:OG	2:A8:250:VAL:O	2.23	0.44
3:B3:51:TYR:HB3	3:B3:59:PHE:HB3	2.00	0.44
3:B5:11:GLN:HA	3:B5:72:THR:HG21	2.00	0.44
2:B6:168:ASN:HD22	2:B6:198:THR:HG21	1.83	0.44
2:C2:219:ILE:HG22	2:C2:222:PRO:HD3	1.99	0.44
3:C5:10:GLY:O	3:C5:14:ASN:ND2	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E1:249:ASP:OD1	3:E1:252:LYS:HG2	2.16	0.44
2:E8:53:PHE:HB3	2:E8:61:HIS:HB3	1.99	0.44
2:E8:80:THR:HG22	2:E8:84:ARG:HH21	1.83	0.44
3:A1:215:LEU:HD11	3:A1:273:LEU:HD22	1.99	0.44
3:A1:396:HIS:CD2	2:A2:263:PRO:HD3	2.53	0.44
3:A3:287:PRO:HB3	3:A3:329:GLN:HE22	1.82	0.44
3:A7:114:ASP:OD1	3:A7:115:SER:N	2.51	0.44
3:A7:128:ASP:OD1	3:A7:128:ASP:N	2.49	0.44
2:A8:208:ALA:HB2	2:A8:304:LYS:HB2	2.00	0.44
2:B2:269:LEU:HD11	2:B2:384:ILE:HD11	2.00	0.44
2:B4:426:ALA:HA	2:B4:429:GLU:HG2	1.99	0.44
3:B5:136:THR:HG22	3:B5:167:PHE:HB2	1.98	0.44
2:B6:265:ILE:HG23	2:B6:432:TYR:CZ	2.53	0.44
2:C0:411:GLU:OE1	2:C0:411:GLU:N	2.51	0.44
3:C7:324:LYS:HB2	3:C7:324:LYS:HE3	1.69	0.44
3:C9:181:GLU:HB2	2:D0:349:THR:HG21	1.99	0.44
3:D1:100:ASN:HB3	3:D1:103:LYS:HG2	1.99	0.44
2:D6:282:TYR:CE2	2:E0:60:LYS:HD2	2.52	0.44
2:D8:175:PRO:O	2:D8:394:LYS:NZ	2.38	0.44
2:E4:108:TYR:O	2:E4:112:LYS:NZ	2.34	0.44
3:E5:67:ASP:OD1	3:E5:68:LEU:N	2.51	0.44
3:E9:220:PRO:HD2	2:F0:326:LYS:NZ	2.32	0.44
2:A8:139:ASN:N	2:A8:139:ASN:OD1	2.51	0.44
3:A9:272:PRO:HB2	3:A9:282:ARG:HH12	1.83	0.44
3:A9:361:LEU:HD23	3:A9:361:LEU:HA	1.84	0.44
2:B2:11:GLN:NE2	3:B3:245:GLN:O	2.50	0.44
3:B7:210:ILE:O	3:B7:214:THR:OG1	2.27	0.44
3:B9:103:LYS:HA	3:B9:107:THR:HG22	1.99	0.44
2:C0:224:TYR:HA	2:C0:227:LEU:HD12	1.99	0.44
2:C2:105:ARG:HH21	2:C2:110:ILE:HG21	1.83	0.44
2:C4:166:LYS:HE3	2:C4:166:LYS:HB2	1.88	0.44
3:C7:256:ASN:HD21	3:C7:350:LYS:HD3	1.82	0.44
2:D0:367:ASP:OD1	2:D0:367:ASP:N	2.50	0.44
2:D4:116:ASP:OD1	2:D4:116:ASP:N	2.48	0.44
3:D5:141:GLY:O	3:D5:145:SER:OG	2.26	0.44
2:E2:316:CYS:HA	2:E2:352:LYS:HB2	2.00	0.44
3:E5:20:PHE:HA	3:E5:230:SER:OG	2.18	0.44
3:E5:33:THR:O	3:E5:58:ARG:NH2	2.50	0.44
2:A2:137:MET:HB3	2:A2:168:ASN:HA	1.99	0.44
2:A6:367:ASP:OD1	2:A6:367:ASP:N	2.45	0.44
2:B0:75:VAL:HG13	2:B0:79:ARG:HH11	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C0:137:MET:HE2	2:C0:154:LEU:HD21	1.99	0.44
2:C0:206:ASN:O	2:C0:210:TYR:N	2.50	0.44
3:D1:86:ARG:HH22	3:D1:122:LYS:HZ2	1.65	0.44
3:D1:334:GLN:HE22	3:D1:347:ASN:HA	1.83	0.44
3:D3:140:GLY:O	3:D3:184:ASN:ND2	2.44	0.44
2:D8:223:THR:HG23	2:D8:225:THR:H	1.83	0.44
3:E7:139:LEU:HB2	3:E7:171:PRO:HD3	1.99	0.44
2:E8:345:ASP:OD1	2:E8:346:TRP:N	2.51	0.44
3:E9:246:LEU:HD12	3:E9:246:LEU:HA	1.88	0.44
1:12:251:TYR:CE2	2:D2:18:ASN:HB3	2.53	0.44
3:A5:246:LEU:HD12	3:A5:246:LEU:HA	1.86	0.44
2:A8:288:VAL:HG21	2:A8:323:VAL:HG13	1.99	0.44
3:B3:383:ASP:HA	3:B3:386:THR:HG22	2.00	0.44
2:B4:222:PRO:HD2	3:B5:324:LYS:HG2	1.99	0.44
2:C0:256:GLN:O	2:C0:260:VAL:HG22	2.17	0.44
2:C4:213:CYS:SG	2:C4:222:PRO:HG3	2.57	0.44
3:C5:206:ALA:HB2	3:C5:302:ALA:HA	1.99	0.44
2:C6:223:THR:HG22	3:C7:322:SER:HA	1.99	0.44
2:D6:100:ALA:HA	3:D7:252:LYS:HG3	2.00	0.44
2:E2:251:ASP:OD1	2:E2:254:GLU:HG2	2.17	0.44
2:E4:101:ASN:N	3:E5:252:LYS:HZ3	2.16	0.44
3:E7:161:ASP:OD1	3:E7:162:ARG:NH1	2.47	0.44
2:A0:332:VAL:HG13	2:A0:351:PHE:CD2	2.52	0.44
3:A3:180:VAL:O	3:A3:184:ASN:ND2	2.51	0.44
3:A5:54:ALA:HB3	3:A5:58:ARG:HG2	1.99	0.44
2:A6:112:LYS:HA	2:A6:115:VAL:HG12	1.99	0.44
3:A9:51:TYR:HB3	3:A9:59:PHE:HB3	1.99	0.44
3:A9:259:PRO:HG2	3:A9:311:LEU:HD21	1.99	0.44
3:B3:100:ASN:HB3	3:B3:103:LYS:HG2	2.00	0.44
3:B7:156:ARG:NH1	3:B7:197:ASP:OD1	2.50	0.44
3:C1:281:TYR:CE2	3:C5:87:PRO:HD3	2.53	0.44
3:C5:295:ASP:HB3	3:C5:298:ASN:HB2	2.00	0.44
2:C8:70:LEU:HD12	2:C8:145:THR:HG22	1.99	0.44
2:D0:178:SER:HB2	3:D1:347:ASN:ND2	2.33	0.44
3:D1:173:PRO:HD2	3:D1:205:GLU:OE2	2.17	0.44
3:D5:259:PRO:HG2	3:D5:311:LEU:HD13	2.00	0.44
2:D8:12:ALA:HB3	2:D8:140:ALA:HB2	1.99	0.44
2:E0:352:LYS:HA	2:E0:352:LYS:HD3	1.73	0.44
3:E1:128:ASP:OD1	3:E1:129:CYS:N	2.45	0.44
3:E3:386:THR:O	3:E3:390:ARG:HG3	2.17	0.44
3:F1:19:LYS:HZ1	3:F1:227:HIS:HB2	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A0:164:LYS:HD2	2:A0:164:LYS:HA	1.72	0.44
3:A1:49:VAL:HG11	3:A1:241:ARG:HG2	2.00	0.44
2:A4:403:ALA:HB2	3:A5:344:TRP:HZ3	1.82	0.44
2:A6:336:LYS:HD3	2:A6:351:PHE:HE2	1.83	0.44
2:B2:50:ASN:O	2:B2:64:ARG:NH2	2.51	0.44
2:B6:70:LEU:HD12	2:B6:99:ALA:HB2	1.99	0.44
2:B8:288:VAL:HA	2:B8:291:ILE:HG12	2.00	0.44
3:B9:293:MET:HE2	3:B9:365:VAL:HG11	2.00	0.44
2:C0:274:PRO:HG3	2:C0:286:LEU:HD13	1.99	0.44
3:C1:103:LYS:HB3	3:C1:103:LYS:HE2	1.81	0.44
3:C1:172:SER:HB3	3:C1:176:SER:HB3	2.00	0.44
2:C2:119:LEU:HD23	2:C2:119:LEU:HA	1.81	0.44
3:C5:281:TYR:CD2	3:C9:87:PRO:HD3	2.53	0.44
2:C6:320:ARG:HH22	2:C6:360:PRO:HA	1.82	0.44
3:C7:113:ILE:HA	3:C7:116:VAL:HG22	2.00	0.44
3:C7:238:CYS:SG	3:C7:239:CYS:N	2.91	0.44
2:D2:207:GLU:HG3	2:D2:304:LYS:HG3	1.99	0.44
3:D7:186:THR:HG22	3:D7:411:ALA:HB1	2.00	0.44
2:E2:1:MET:N	2:E2:3:GLU:OE2	2.43	0.44
3:E3:113:ILE:HA	3:E3:116:VAL:HG12	1.98	0.44
2:E4:132:LEU:O	2:E4:164:LYS:NZ	2.51	0.44
3:E5:136:THR:HG22	3:E5:167:PHE:HB2	2.00	0.44
2:E6:345:ASP:OD1	2:E6:346:TRP:N	2.51	0.44
3:A1:138:SER:HA	3:A1:169:VAL:HG22	2.00	0.43
2:A2:306:ASP:HB3	2:A2:309:HIS:CE1	2.53	0.43
2:A8:75:VAL:HG11	2:A8:94:SER:HB3	2.00	0.43
3:A9:284:LEU:HD12	3:A9:284:LEU:HA	1.82	0.43
3:A9:362:LYS:HA	3:A9:362:LYS:HD2	1.86	0.43
2:B4:417:GLU:N	2:B4:417:GLU:OE2	2.50	0.43
2:C0:155:GLU:HG2	2:C0:197:HIS:CE1	2.53	0.43
2:C4:377:MET:SD	2:C4:379:SER:HB3	2.58	0.43
2:C6:177:VAL:HB	2:C6:207:GLU:HB3	1.99	0.43
2:C8:323:VAL:HG13	2:C8:355:ILE:HG23	2.00	0.43
2:D4:52:PHE:HD2	2:D4:243:ARG:HD3	1.83	0.43
2:E8:275:ILE:HG23	2:E8:368:LEU:HD21	2.00	0.43
2:F0:210:TYR:CD1	3:F1:324:LYS:HD3	2.53	0.43
2:A0:352:LYS:HD3	2:A0:352:LYS:HA	1.79	0.43
2:A0:399:TYR:OH	2:A0:415:GLU:OE2	2.36	0.43
2:A4:68:LEU:HD21	2:A4:149:LEU:HD21	1.99	0.43
3:A9:190:HIS:HB2	3:A9:414:ASN:HB3	1.99	0.43
2:B6:192:HIS:ND1	2:B6:424:ASP:OD2	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C8:28:HIS:NE2	2:C8:243:ARG:HD2	2.32	0.43
3:C9:128:ASP:OD1	3:C9:129:CYS:N	2.43	0.43
2:D2:276:ILE:HD11	2:D2:286:LEU:HD11	2.00	0.43
3:D3:64:ILE:HD12	3:D3:119:VAL:HG22	2.00	0.43
3:D3:239:CYS:SG	3:D3:248:SER:N	2.88	0.43
3:D5:32:PRO:HD3	3:D5:81:PHE:CZ	2.53	0.43
2:D6:4:VAL:HG12	2:D6:133:GLN:HB3	2.00	0.43
3:D7:397:TRP:NE1	2:D8:256:GLN:O	2.51	0.43
2:E2:300:SER:O	2:E2:300:SER:OG	2.29	0.43
2:E6:286:LEU:O	2:E6:373:ARG:NH1	2.48	0.43
3:E9:399:THR:HA	3:E9:403:MET:HB2	1.99	0.43
3:F1:156:ARG:NH2	3:F1:197:ASP:OD1	2.51	0.43
1:10:250:GLU:OE1	2:C8:225:THR:HG21	2.18	0.43
3:A1:103:LYS:HB2	3:A1:103:LYS:HE2	1.78	0.43
2:A4:134:GLY:CA	2:A4:164:LYS:HZ1	2.32	0.43
3:B5:6:HIS:HE2	3:B5:8:GLN:HB3	1.83	0.43
3:B5:49:VAL:HG21	3:B5:241:ARG:HG2	1.99	0.43
2:B6:109:THR:OG1	2:B6:110:ILE:N	2.51	0.43
3:C1:295:ASP:HB3	3:C1:297:LYS:HG2	1.99	0.43
2:C2:417:GLU:OE2	2:C2:417:GLU:N	2.50	0.43
2:C4:153:LEU:HA	2:C4:153:LEU:HD12	1.73	0.43
2:C4:241:SER:OG	2:C4:250:VAL:O	2.26	0.43
3:C5:12:CYS:HB3	3:C5:138:SER:HB3	1.99	0.43
3:C5:207:LEU:HG	3:C5:228:LEU:HD11	2.00	0.43
2:C6:28:HIS:HE1	2:C6:243:ARG:HD2	1.82	0.43
3:C9:167:PHE:HZ	3:C9:236:VAL:HG11	1.84	0.43
2:E0:214:ARG:NH1	2:E0:220:GLU:OE2	2.50	0.43
3:E5:25:SER:HB3	3:E5:30:ILE:HB	1.99	0.43
3:E7:86:ARG:HG2	3:E7:88:ASP:H	1.83	0.43
1:4:250:GLU:HG3	2:B2:225:THR:HG21	2.00	0.43
2:A0:244:PHE:CD2	2:A0:358:GLN:HG2	2.53	0.43
3:A7:220:PRO:HB2	3:A7:225:LEU:HD21	1.99	0.43
2:B4:53:PHE:HB3	2:B4:61:HIS:HB3	2.00	0.43
2:C0:33:ASP:O	2:C0:60:LYS:NZ	2.32	0.43
2:C0:416:GLY:O	2:C0:420:GLU:N	2.43	0.43
2:C4:287:SER:N	2:C4:290:GLU:OE2	2.45	0.43
3:C5:121:ARG:NH1	3:C5:158:GLU:OE1	2.51	0.43
3:C5:190:HIS:HA	3:C5:193:VAL:HG22	2.00	0.43
2:C6:377:MET:SD	2:C6:379:SER:HB3	2.58	0.43
3:C9:238:CYS:SG	3:C9:318:ARG:NE	2.87	0.43
3:D3:117:LEU:HD11	3:D3:154:LYS:HD3	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D8:36:MET:HG2	2:D8:61:HIS:NE2	2.33	0.43
2:E6:8:HIS:ND1	2:E6:65:CYS:SG	2.90	0.43
3:E9:7:VAL:HG11	3:E9:151:LEU:HD23	1.99	0.43
1:0:256:LEU:HD12	2:A4:29:GLY:HA2	2.00	0.43
1:21:246:CYS:N	3:F1:355:ASP:OD2	2.48	0.43
3:A5:317:PHE:CD1	3:A5:365:VAL:HG22	2.54	0.43
3:A9:99:ASN:ND2	2:B0:254:GLU:OE1	2.52	0.43
2:B0:306:ASP:HB3	2:B0:309:HIS:CE1	2.53	0.43
2:B2:208:ALA:HB2	2:B2:304:LYS:HB2	1.99	0.43
2:B4:221:ARG:HB3	3:B5:322:SER:HB2	2.01	0.43
3:B5:8:GLN:HE21	3:B5:65:LEU:HD11	1.84	0.43
3:C9:246:LEU:HD12	3:C9:246:LEU:HA	1.88	0.43
2:D0:88:HIS:CD2	2:D0:90:GLU:HB3	2.53	0.43
3:D7:289:LEU:HD22	3:D7:365:VAL:HG12	2.00	0.43
3:E3:323:THR:HA	3:E3:326:VAL:HG12	1.99	0.43
3:E5:180:VAL:HB	3:E5:183:TYR:HB2	2.00	0.43
2:E8:196:GLU:OE2	2:E8:197:HIS:NE2	2.52	0.43
2:E8:407:TRP:CG	3:E9:255:VAL:HG23	2.54	0.43
2:F0:107:HIS:NE2	2:F0:151:CYS:SG	2.84	0.43
3:F1:313:ALA:HB1	3:F1:367:PHE:CE1	2.54	0.43
1:16:256:LEU:HD12	2:E0:29:GLY:HA2	2.00	0.43
3:A5:391:ARG:HD2	2:A6:346:TRP:CD1	2.53	0.43
3:A9:73:MET:HG2	3:A9:92:PHE:CE1	2.53	0.43
2:B0:164:LYS:HA	2:B0:164:LYS:HD3	1.73	0.43
3:B1:10:GLY:HA2	3:B1:143:THR:HG23	1.99	0.43
2:B2:200:VAL:HG13	2:B2:268:MET:SD	2.58	0.43
3:B7:10:GLY:HA2	3:B7:143:THR:HG23	2.00	0.43
3:B7:107:THR:HG21	3:B7:401:GLU:OE2	2.19	0.43
3:B9:33:THR:HG23	3:B9:35:THR:HG23	2.00	0.43
2:C2:367:ASP:N	2:C2:367:ASP:OD1	2.48	0.43
3:C7:19:LYS:HA	3:C7:19:LYS:HD3	1.78	0.43
3:C7:28:HIS:NE2	3:C7:241:ARG:HD2	2.34	0.43
2:C8:178:SER:HB2	3:C9:347:ASN:HD21	1.84	0.43
3:D7:187:LEU:HD23	3:D7:190:HIS:HE1	1.84	0.43
2:E2:244:PHE:HB2	2:E2:356:ASN:HD21	1.82	0.43
2:E6:306:ASP:HB3	2:E6:309:HIS:CE1	2.54	0.43
2:F0:28:HIS:NE2	2:F0:243:ARG:HD2	2.34	0.43
3:F1:67:ASP:OD1	3:F1:68:LEU:N	2.51	0.43
3:A1:165:GLU:HG2	3:A1:250:LEU:HD13	2.01	0.43
2:A2:141:VAL:HG11	2:A2:172:TRP:CE3	2.54	0.43
3:A3:64:ILE:HD12	3:A3:119:VAL:HG12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A4:11:GLN:HG3	2:A4:74:VAL:HG21	2.00	0.43
3:A7:206:ALA:HB2	3:A7:302:ALA:HB2	2.01	0.43
2:B0:100:ALA:O	3:B1:255:VAL:HG11	2.18	0.43
2:B4:175:PRO:O	2:B4:394:LYS:NZ	2.52	0.43
2:B8:65:CYS:SG	2:B8:66:VAL:N	2.92	0.43
2:C2:173:PRO:O	2:C2:390:ARG:NH1	2.48	0.43
2:C2:432:TYR:O	2:C2:436:GLY:N	2.49	0.43
3:C5:293:MET:HE1	3:C5:365:VAL:HG21	2.01	0.43
3:C7:67:ASP:OD1	3:C7:68:LEU:N	2.48	0.43
3:D1:169:VAL:HA	3:D1:202:ILE:HB	2.00	0.43
3:D3:100:ASN:ND2	3:D3:397:TRP:O	2.51	0.43
2:D4:176:GLN:HG3	2:D4:177:VAL:HG23	2.01	0.43
2:D6:3:GLU:HA	2:D6:51:THR:HA	2.00	0.43
3:D7:214:THR:OG1	3:D7:215:LEU:N	2.52	0.43
3:E3:113:ILE:HD11	3:E3:151:LEU:HB2	2.00	0.43
2:E4:283:HIS:NE2	2:E8:85:HIS:O	2.49	0.43
2:E6:276:ILE:HD12	2:E6:276:ILE:HA	1.94	0.43
2:E8:137:MET:HB3	2:E8:168:ASN:HA	2.01	0.43
2:A0:222:PRO:HD2	3:A1:324:LYS:HG2	2.01	0.43
3:A1:308:GLY:HA3	3:A1:373:ALA:HB2	2.01	0.43
3:A5:326:VAL:O	3:A5:330:MET:HG2	2.18	0.43
2:A8:206:ASN:OD1	6:A8:501:GTP:N2	2.51	0.43
2:A8:283:HIS:HB2	2:B2:88:HIS:HD2	1.84	0.43
3:A9:198:GLU:HG2	3:A9:266:PHE:HE2	1.84	0.43
3:B3:392:LYS:HD3	3:B3:395:LEU:HD22	2.01	0.43
3:C1:215:LEU:HD21	3:C1:273:LEU:HD22	2.01	0.43
3:C3:192:LEU:HD21	3:C3:199:VAL:HG11	2.00	0.43
3:C3:284:LEU:HD12	3:C3:284:LEU:HA	1.81	0.43
3:C5:70:PRO:HA	3:C5:73:MET:HE2	2.01	0.43
3:C5:249:ASP:OD1	3:C5:250:LEU:N	2.51	0.43
2:C8:403:ALA:HB2	3:C9:344:TRP:HZ3	1.84	0.43
3:D5:61:PRO:HD3	3:D5:84:LEU:HG	2.00	0.43
3:D7:324:LYS:HZ3	3:D7:324:LYS:HG3	1.68	0.43
2:E4:221:ARG:HH11	2:E4:221:ARG:HD2	1.60	0.43
2:E6:254:GLU:O	2:E6:258:ASN:ND2	2.50	0.43
3:E7:281:TYR:HD2	3:F1:87:PRO:HD3	1.83	0.43
2:F0:213:CYS:HA	2:F0:217:LEU:HB2	2.00	0.43
3:F1:151:LEU:HA	3:F1:151:LEU:HD12	1.77	0.43
3:F1:237:THR:O	3:F1:241:ARG:NH1	2.51	0.43
1:0:246:CYS:SG	1:0:247:TYR:N	2.92	0.43
2:A2:119:LEU:HD11	2:A2:156:ARG:HB3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:306:ASP:HB3	2:A2:309:HIS:HE1	1.82	0.43
2:A6:28:HIS:CE1	2:A6:243:ARG:HD2	2.54	0.43
2:A6:383:ALA:O	2:A6:386:GLU:HG2	2.18	0.43
3:B7:3:GLU:HA	3:B7:49:VAL:HA	2.01	0.43
2:B8:36:MET:SD	2:B8:61:HIS:NE2	2.90	0.43
3:B9:141:GLY:O	3:B9:145:SER:OG	2.27	0.43
3:C1:257:LEU:HB3	3:C1:266:PHE:CE1	2.54	0.43
2:C2:34:GLY:O	2:C2:61:HIS:N	2.44	0.43
3:C7:321:MET:N	3:C7:321:MET:SD	2.92	0.43
3:C9:68:LEU:HD22	3:C9:108:GLU:HG3	2.00	0.43
3:D3:68:LEU:HA	3:D3:93:GLY:HA3	2.01	0.43
2:D6:105:ARG:HG2	2:D6:110:ILE:HG12	2.00	0.43
2:E2:406:HIS:HA	2:E2:409:VAL:HG12	1.99	0.43
2:E4:119:LEU:HD22	2:E4:157:LEU:HD21	2.00	0.43
2:E4:221:ARG:HH12	3:E5:325:GLU:H	1.66	0.43
3:F1:30:ILE:HD12	3:F1:51:TYR:HE2	1.84	0.43
2:B0:30:ILE:HG21	2:B0:61:HIS:HD2	1.83	0.43
3:B5:35:THR:OG1	3:B5:36:TYR:N	2.52	0.43
3:B5:252:LYS:HG3	3:B5:350:LYS:HE3	2.01	0.43
3:B7:63:ALA:O	3:B7:89:ASN:ND2	2.51	0.43
3:B7:152:ILE:HG22	3:B7:195:ASN:HB3	2.01	0.43
3:B7:190:HIS:HA	3:B7:193:VAL:HG12	2.00	0.43
2:C2:209:ILE:HA	2:C2:212:ILE:HG22	2.01	0.43
3:C7:6:HIS:HD1	3:C7:21:TRP:HE1	1.67	0.43
2:D4:5:ILE:HD13	2:D4:64:ARG:HB3	2.00	0.43
3:D9:237:THR:HG23	3:D9:241:ARG:HH21	1.83	0.43
2:E4:98:ASP:OD1	2:E4:100:ALA:N	2.40	0.43
2:E4:417:GLU:HA	2:E4:420:GLU:HG3	2.01	0.43
3:E5:48:ASN:N	3:E5:48:ASN:OD1	2.50	0.43
2:E6:215:ARG:HH12	2:E6:299:ALA:HB1	1.83	0.43
3:E7:362:LYS:HD2	3:E7:363:MET:HB2	2.01	0.43
2:A2:143:GLY:O	2:A2:186:ASN:ND2	2.52	0.42
3:A5:121:ARG:NH1	3:A5:158:GLU:OE2	2.51	0.42
2:A8:164:LYS:HD3	2:A8:164:LYS:HA	1.83	0.42
2:B4:158:SER:OG	2:B4:166:LYS:NZ	2.51	0.42
2:B4:250:VAL:HG23	2:B4:254:GLU:HG3	2.00	0.42
2:B4:277:SER:OG	2:B4:278:ALA:N	2.52	0.42
2:B6:356:ASN:OD1	2:B6:357:TYR:N	2.52	0.42
2:C0:168:ASN:HD22	2:C0:198:THR:HG21	1.84	0.42
2:C0:265:ILE:HG13	2:C0:432:TYR:CZ	2.53	0.42
2:C4:139:ASN:OD1	2:C4:139:ASN:N	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C4:254:GLU:N	2:C4:254:GLU:OE2	2.52	0.42
2:C8:27:GLU:OE1	2:C8:320:ARG:NH2	2.37	0.42
3:D1:132:GLY:HA3	3:D1:163:ILE:HG22	2.01	0.42
3:D3:10:GLY:HA2	3:D3:143:THR:HG23	2.01	0.42
3:D5:139:LEU:HD12	3:D5:170:PHE:HE1	1.84	0.42
3:E1:19:LYS:NZ	3:E1:223:GLY:O	2.52	0.42
2:E2:224:TYR:HD1	2:E2:227:LEU:HD12	1.84	0.42
3:E9:156:ARG:HH21	3:E9:164:MET:HG3	1.84	0.42
3:F1:205:GLU:HA	3:F1:208:TYR:HB2	2.01	0.42
3:A3:112:LEU:HD12	3:A3:112:LEU:HA	1.89	0.42
3:A5:324:LYS:HD3	3:A5:328:GLU:HB2	2.01	0.42
3:A7:19:LYS:HD2	3:A7:19:LYS:HA	1.67	0.42
3:A7:178:THR:O	3:A7:181:GLU:HG2	2.18	0.42
2:B4:154:LEU:HB3	2:B4:197:HIS:HB3	2.00	0.42
2:B6:397:LEU:HD23	2:B6:397:LEU:HA	1.91	0.42
2:B8:11:GLN:HE22	3:B9:246:LEU:HA	1.84	0.42
2:C0:280:LYS:NZ	2:C4:90:GLU:HG2	2.34	0.42
3:C1:148:GLY:O	3:C1:152:ILE:HG13	2.19	0.42
2:C2:259:LEU:HD23	2:C2:259:LEU:HA	1.85	0.42
2:C4:328:VAL:HG21	2:C4:355:ILE:HD11	2.02	0.42
3:C5:117:LEU:HA	3:C5:120:VAL:HG12	2.00	0.42
3:C7:52:ASN:ND2	3:C7:123:GLU:OE2	2.53	0.42
3:C7:309:ARG:H	3:C7:372:THR:HG22	1.84	0.42
3:C7:325:GLU:HA	3:C7:328:GLU:HG2	2.00	0.42
2:C8:119:LEU:HA	2:C8:122:ILE:HG22	2.01	0.42
3:D3:313:ALA:HB1	3:D3:367:PHE:CE1	2.54	0.42
3:D5:105:HIS:CE1	3:D5:150:LEU:HB2	2.53	0.42
3:E3:304:ASP:OD2	3:E3:306:ARG:NH2	2.52	0.42
3:E5:209:ASP:CG	3:E5:213:ARG:HH21	2.22	0.42
2:E6:404:PHE:HZ	3:E7:312:THR:HG21	1.84	0.42
3:E7:28:HIS:HA	3:E7:43:GLN:HG2	2.01	0.42
2:E8:91:GLN:OE1	2:E8:91:GLN:N	2.51	0.42
3:E9:100:ASN:HB3	3:E9:103:LYS:HG2	2.01	0.42
3:E9:128:ASP:OD1	3:E9:128:ASP:N	2.51	0.42
3:A1:65:LEU:HD22	3:A1:90:PHE:HE1	1.85	0.42
2:A4:167:LEU:HD23	2:A4:200:VAL:HB	2.01	0.42
2:A6:265:ILE:HG23	2:A6:432:TYR:CZ	2.54	0.42
2:B2:223:THR:HG23	2:B2:225:THR:HG22	2.01	0.42
2:B6:345:ASP:OD1	2:B6:346:TRP:N	2.52	0.42
2:C2:414:GLU:HG2	2:C2:417:GLU:OE2	2.19	0.42
2:C6:88:HIS:HB3	2:C6:91:GLN:HE22	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C7:117:LEU:HA	3:C7:120:VAL:HG12	2.01	0.42
3:D1:138:SER:HA	3:D1:169:VAL:HG22	2.01	0.42
3:D1:211:CYS:HA	3:D1:215:LEU:HB2	2.00	0.42
3:D5:375:GLN:HB2	3:D5:419:VAL:HG13	2.01	0.42
3:D7:412:GLU:O	3:D7:416:ASN:N	2.45	0.42
2:D8:207:GLU:HA	2:D8:210:TYR:HB2	2.01	0.42
3:D9:396:HIS:HA	3:D9:399:THR:HG22	2.02	0.42
3:E5:337:ASN:HB3	3:E5:340:TYR:HB2	2.01	0.42
2:E8:76:ASP:OD2	3:E9:46:ARG:NH1	2.52	0.42
3:F1:262:ARG:NH2	3:F1:421:GLU:OE1	2.53	0.42
2:A0:312:TYR:HE1	2:A0:379:SER:HB3	1.84	0.42
2:A6:125:LEU:HD23	2:A6:125:LEU:HA	1.87	0.42
3:A7:190:HIS:HB2	3:A7:414:ASN:HD22	1.84	0.42
2:A8:309:HIS:HE2	2:A8:386:GLU:CD	2.23	0.42
3:A9:65:LEU:HD22	3:A9:90:PHE:HE1	1.83	0.42
3:A9:173:PRO:HG2	3:A9:205:GLU:OE2	2.20	0.42
2:B0:102:ASN:HA	2:B0:408:TYR:HE1	1.84	0.42
2:B2:367:ASP:OD1	2:B2:367:ASP:N	2.41	0.42
3:B5:396:HIS:HA	3:B5:399:THR:HG22	2.01	0.42
3:B7:287:PRO:HA	3:B7:290:THR:HG22	2.01	0.42
3:B7:301:CYS:SG	3:B7:302:ALA:N	2.92	0.42
3:B9:3:GLU:HA	3:B9:49:VAL:HA	2.00	0.42
3:C3:273:LEU:HD23	3:C3:273:LEU:HA	1.89	0.42
3:C3:344:TRP:HZ2	3:C3:425:TYR:HB3	1.84	0.42
2:C4:212:ILE:HG23	2:C4:275:ILE:HD12	2.01	0.42
3:C5:164:MET:SD	3:C5:196:ALA:HA	2.59	0.42
3:C5:262:ARG:NH1	3:C5:421:GLU:OE2	2.53	0.42
2:C6:172:TRP:HB3	2:C6:205:ASP:OD1	2.19	0.42
2:C6:288:VAL:HA	2:C6:291:ILE:HG12	2.00	0.42
3:C7:273:LEU:HD23	3:C7:273:LEU:HA	1.76	0.42
3:D1:281:TYR:CD2	3:D5:87:PRO:HD3	2.54	0.42
2:D6:183:GLU:HA	2:D6:186:ASN:HD22	1.83	0.42
3:D7:103:LYS:HB3	3:D7:401:GLU:HG2	2.00	0.42
3:D9:213:ARG:NH1	3:D9:297:LYS:HD3	2.35	0.42
2:E4:27:GLU:HB3	2:E4:361:THR:HG21	2.02	0.42
2:E4:98:ASP:O	2:E4:105:ARG:NH1	2.50	0.42
3:E5:211:CYS:SG	3:E5:220:PRO:HB3	2.59	0.42
2:E6:32:PRO:HG3	2:E6:83:TYR:HE1	1.84	0.42
3:E9:167:PHE:CE1	3:E9:233:MET:HG2	2.54	0.42
3:F1:167:PHE:CZ	3:F1:233:MET:HG3	2.55	0.42
3:F1:272:PRO:HD2	3:F1:361:LEU:HD21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A0:224:TYR:O	2:A0:228:ASN:ND2	2.53	0.42
2:A2:207:GLU:HG3	2:A2:304:LYS:HE3	2.01	0.42
3:A3:113:ILE:HG23	3:A3:117:LEU:HD23	2.02	0.42
2:A4:28:HIS:NE2	2:A4:243:ARG:HD2	2.34	0.42
2:A8:5:ILE:HD12	2:A8:125:LEU:HG	2.01	0.42
2:B0:285:GLN:HB3	2:B4:56:THR:HA	2.01	0.42
2:B2:12:ALA:HB3	2:B2:140:ALA:HB2	2.01	0.42
2:B8:338:LYS:NZ	2:B8:340:THR:OG1	2.42	0.42
2:C2:191:THR:HA	2:C2:194:LEU:HG	2.00	0.42
2:C6:177:VAL:HG13	3:C7:327:ASP:HB3	2.02	0.42
2:C6:310:GLY:HA3	2:C6:383:ALA:HB2	2.02	0.42
2:C8:11:GLN:OE1	3:C9:247:ASN:ND2	2.52	0.42
3:C9:138:SER:HA	3:C9:169:VAL:HG22	2.01	0.42
3:D1:290:THR:HA	3:D1:293:MET:HE2	2.02	0.42
2:D6:169:PHE:HZ	2:D6:238:LEU:HD13	1.85	0.42
3:D7:113:ILE:HA	3:D7:116:VAL:HG12	2.02	0.42
3:D7:167:PHE:HD2	3:D7:202:ILE:HD11	1.85	0.42
3:D9:374:ILE:HD11	3:D9:422:TYR:CZ	2.55	0.42
2:E0:282:TYR:HB2	2:E0:283:HIS:CD2	2.54	0.42
2:E2:318:MET:SD	2:E2:318:MET:N	2.93	0.42
2:E8:318:MET:N	2:E8:318:MET:SD	2.93	0.42
2:A0:14:ILE:HD13	2:A0:14:ILE:HA	1.88	0.42
3:A1:73:MET:HA	3:A1:76:VAL:HG12	2.01	0.42
2:A4:298:PRO:HB3	2:A4:307:PRO:HD2	2.02	0.42
3:A7:193:VAL:HG13	3:A7:194:GLU:HG2	2.02	0.42
2:A8:154:LEU:HD23	2:A8:154:LEU:HA	1.85	0.42
2:A8:160:ASP:OD1	2:A8:161:TYR:N	2.52	0.42
3:A9:162:ARG:HA	3:A9:162:ARG:HD3	1.88	0.42
3:A9:167:PHE:CD1	3:A9:200:GLN:HB2	2.55	0.42
3:A9:267:LEU:HD21	3:A9:374:ILE:HG22	2.02	0.42
2:B4:191:THR:HA	2:B4:194:LEU:HG	2.02	0.42
2:B8:246:GLY:HA2	2:B8:357:TYR:HD1	1.83	0.42
3:C1:207:LEU:HB3	3:C1:225:LEU:HD22	2.00	0.42
2:C2:107:HIS:HB3	2:C2:108:TYR:CD2	2.55	0.42
3:C3:73:MET:HB3	3:C3:77:ARG:NH2	2.34	0.42
2:C4:189:LEU:HD11	2:C4:418:PHE:CD1	2.54	0.42
2:C6:356:ASN:OD1	2:C6:357:TYR:N	2.52	0.42
3:D3:239:CYS:SG	3:D3:247:ASN:HB3	2.60	0.42
3:D5:113:ILE:HD11	3:D5:151:LEU:HD13	2.00	0.42
2:D6:210:TYR:HE1	2:D6:227:LEU:HD11	1.84	0.42
2:D8:276:ILE:HD12	2:D8:281:ALA:HA	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E1:169:VAL:HG12	3:E1:202:ILE:HB	2.02	0.42
2:E4:98:ASP:OD1	2:E4:99:ALA:N	2.52	0.42
3:A1:259:PRO:HB2	3:A1:260:PHE:CD2	2.54	0.42
3:A3:304:ASP:CG	3:A3:307:HIS:HD1	2.23	0.42
3:A3:345:ILE:O	3:A3:348:ASN:ND2	2.53	0.42
2:A6:225:THR:O	2:A6:229:ARG:HG2	2.20	0.42
2:A8:172:TRP:HB3	2:A8:205:ASP:OD1	2.19	0.42
2:B0:283:HIS:HB3	2:B4:62:VAL:HG11	2.02	0.42
2:B0:336:LYS:HZ3	2:B0:351:PHE:HE2	1.68	0.42
2:B2:401:LYS:HD2	3:B3:344:TRP:CD2	2.54	0.42
3:B5:282:ARG:NH2	3:B5:292:GLN:OE1	2.52	0.42
2:B6:124:LYS:HE2	2:B6:124:LYS:HB2	1.71	0.42
2:B6:339:ARG:NH1	2:B6:342:GLN:OE1	2.52	0.42
2:C4:100:ALA:HA	3:C5:252:LYS:HD3	2.02	0.42
2:C4:167:LEU:HA	2:C4:200:VAL:HG13	2.01	0.42
3:C5:32:PRO:HD3	3:C5:81:PHE:CZ	2.55	0.42
3:D3:297:LYS:HE2	3:D3:297:LYS:HB2	1.69	0.42
3:D5:189:VAL:O	3:D5:193:VAL:N	2.52	0.42
2:D6:11:GLN:NE2	3:D7:245:GLN:O	2.50	0.42
3:D7:112:LEU:HD12	3:D7:112:LEU:HA	1.78	0.42
3:D7:128:ASP:OD1	3:D7:129:CYS:N	2.44	0.42
2:E4:223:THR:HG23	2:E4:225:THR:HG22	2.01	0.42
3:F1:247:ASN:O	3:F1:252:LYS:NZ	2.53	0.42
1:16:250:GLU:HG3	2:E0:225:THR:HG21	2.01	0.42
2:A0:100:ALA:HA	3:A1:252:LYS:HZ2	1.84	0.42
3:A1:284:LEU:HD12	3:A1:284:LEU:HA	1.86	0.42
2:A4:28:HIS:HE2	2:A4:243:ARG:HD2	1.84	0.42
3:A5:105:HIS:CE1	3:A5:150:LEU:HD12	2.54	0.42
2:A6:238:LEU:HD12	2:A6:238:LEU:HA	1.84	0.42
3:B1:109:GLY:HA2	3:B1:147:MET:HE2	2.01	0.42
2:B2:96:LYS:HZ1	3:B3:129:CYS:H	1.66	0.42
2:B2:207:GLU:HA	2:B2:210:TYR:HB2	2.02	0.42
3:B3:19:LYS:HD3	3:B3:19:LYS:HA	1.83	0.42
2:B8:258:ASN:ND2	2:B8:352:LYS:HD2	2.35	0.42
3:B9:43:GLN:HA	3:B9:242:PHE:HE1	1.85	0.42
3:B9:396:HIS:HA	3:B9:399:THR:HG22	2.01	0.42
2:C0:100:ALA:O	3:C1:255:VAL:HG11	2.20	0.42
3:C1:284:LEU:HD12	3:C1:284:LEU:HA	1.87	0.42
3:C3:274:THR:OG1	3:C3:279:GLN:OE1	2.30	0.42
2:D4:311:LYS:H	2:D4:382:THR:HG1	1.68	0.42
3:D7:3:GLU:HA	3:D7:49:VAL:HA	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E1:51:TYR:HB3	3:E1:59:PHE:HB3	2.01	0.42
2:E8:322:ASP:O	2:E8:373:ARG:NE	2.53	0.42
3:E9:97:ALA:HA	3:E9:103:LYS:HD2	2.02	0.42
1:1:257:PRO:HA	1:1:258:PRO:HD3	1.91	0.42
3:A1:349:MET:HE3	3:A1:349:MET:HB2	1.96	0.42
2:A2:172:TRP:N	2:A2:204:LEU:O	2.48	0.42
2:B0:249:ASN:OD1	2:B0:249:ASN:N	2.51	0.42
3:B3:181:GLU:HG3	2:B4:349:THR:HG21	2.00	0.42
2:B4:208:ALA:HB2	2:B4:304:LYS:HB2	2.01	0.42
2:C0:328:VAL:HG11	2:C0:355:ILE:HD11	2.02	0.42
3:C1:20:PHE:CE1	3:C1:24:ILE:HG13	2.55	0.42
2:D2:434:GLU:HA	2:D2:437:ILE:HD12	2.02	0.42
2:D6:102:ASN:ND2	2:D6:411:GLU:OE1	2.53	0.42
3:E3:253:LEU:HD11	3:E3:368:VAL:HG21	2.00	0.42
3:E7:216:LYS:HD3	3:E7:216:LYS:HA	1.87	0.42
3:F1:209:ASP:OD1	3:F1:213:ARG:NH1	2.53	0.42
1:5:250:GLU:HG3	2:B4:225:THR:HG21	2.01	0.42
3:B1:289:LEU:HD22	3:B1:363:MET:HG2	2.01	0.42
2:B6:141:VAL:HA	2:B6:147:SER:HB3	2.01	0.42
3:B7:322:SER:HB3	3:B7:325:GLU:OE2	2.20	0.42
3:C3:239:CYS:SG	3:C3:248:SER:N	2.88	0.42
2:C4:62:VAL:HA	2:C4:63:PRO:HD3	1.92	0.42
2:C4:211:ASP:HA	2:C4:214:ARG:HG2	2.02	0.42
3:C5:407:GLU:O	3:C5:411:ALA:N	2.47	0.42
3:C7:16:ILE:HD11	3:C7:229:VAL:HG11	2.01	0.42
3:C7:248:SER:HA	3:C7:252:LYS:HD3	2.01	0.42
2:D0:207:GLU:HA	2:D0:210:TYR:HB2	2.01	0.42
2:D0:288:VAL:HB	2:D0:327:ASP:HB3	2.01	0.42
2:D2:230:LEU:HD23	2:D2:230:LEU:HA	1.85	0.42
2:D2:259:LEU:HD13	2:D2:268:MET:HE2	2.02	0.42
3:D3:330:MET:HE3	3:D3:349:MET:HB3	2.01	0.42
2:D6:399:TYR:OH	2:D6:415:GLU:OE2	2.24	0.42
3:D7:282:ARG:HH12	3:D7:292:GLN:HG3	1.84	0.42
2:D8:174:SER:HB2	2:D8:177:VAL:O	2.20	0.42
2:E0:166:LYS:N	2:E0:199:ASP:OD2	2.51	0.42
3:E1:272:PRO:HG3	3:E1:284:LEU:HD11	2.02	0.42
2:E2:212:ILE:HD11	2:E2:300:SER:HA	2.01	0.42
2:E2:230:LEU:HD21	2:E2:368:LEU:HD21	2.00	0.42
3:E5:139:LEU:HA	3:E5:145:SER:HB2	2.01	0.42
2:E6:171:SER:O	2:E6:171:SER:OG	2.35	0.42
3:E9:208:TYR:CE1	3:E9:225:LEU:HD11	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E9:229:VAL:HG12	3:E9:233:MET:HE2	2.01	0.42
3:F1:51:TYR:HB3	3:F1:59:PHE:HB3	2.02	0.42
1:22:246:CYS:SG	1:22:247:TYR:N	2.93	0.42
3:A5:16:ILE:HD13	3:A5:16:ILE:HG21	1.87	0.41
2:B2:69:ASP:OD1	2:B2:70:LEU:N	2.53	0.41
2:B2:406:HIS:HA	2:B2:409:VAL:HG12	2.00	0.41
3:C1:73:MET:HB3	3:C1:77:ARG:HH22	1.84	0.41
3:C1:274:THR:O	3:C1:279:GLN:NE2	2.50	0.41
2:C4:208:ALA:O	2:C4:212:ILE:HG12	2.19	0.41
3:D5:172:SER:HB3	3:D5:205:GLU:HG2	2.02	0.41
3:D5:310:TYR:CD1	3:D5:371:SER:HB2	2.55	0.41
3:D7:176:SER:HB3	3:D7:181:GLU:OE1	2.20	0.41
3:D7:323:THR:HA	3:D7:326:VAL:HG12	2.01	0.41
2:E0:105:ARG:HH12	3:E1:251:ARG:HD3	1.84	0.41
3:E7:283:ALA:HA	3:F1:55:THR:HG23	2.02	0.41
2:E8:91:GLN:HB3	2:E8:121:ARG:HG2	2.00	0.41
3:E9:206:ALA:HB2	3:E9:302:ALA:HB2	2.02	0.41
1:9:250:GLU:O	1:9:252:VAL:N	2.54	0.41
1:17:246:CYS:HA	3:E3:320:ARG:HH12	1.85	0.41
3:A3:100:ASN:HB3	3:A3:103:LYS:HB3	2.02	0.41
3:A5:294:PHE:CD2	3:A5:333:VAL:HG21	2.56	0.41
3:A9:97:ALA:HA	3:A9:103:LYS:HD2	2.02	0.41
2:B0:116:ASP:N	2:B0:116:ASP:OD1	2.51	0.41
3:B3:11:GLN:HA	3:B3:72:THR:HG21	2.01	0.41
2:B4:126:ALA:HB1	2:B4:132:LEU:HD22	2.02	0.41
2:B6:394:LYS:HG2	3:B7:346:PRO:HG3	2.02	0.41
3:C7:83:GLN:OE1	3:C7:83:GLN:N	2.53	0.41
2:D6:210:TYR:CE1	2:D6:227:LEU:HD11	2.55	0.41
3:D9:318:ARG:HG2	3:D9:354:CYS:HB3	2.02	0.41
2:E0:189:LEU:HD11	2:E0:418:PHE:HE1	1.84	0.41
3:E7:213:ARG:NH2	3:E7:297:LYS:HB2	2.27	0.41
2:E8:116:ASP:OD1	2:E8:117:LEU:N	2.53	0.41
2:E8:222:PRO:HD2	3:E9:324:LYS:HB3	2.03	0.41
2:E8:224:TYR:HD1	3:E9:323:THR:HG1	1.68	0.41
3:E9:208:TYR:CD1	2:F0:326:LYS:HB3	2.55	0.41
3:E9:397:TRP:NE1	2:F0:256:GLN:O	2.53	0.41
2:F0:222:PRO:HB3	2:F0:226:ASN:HD22	1.85	0.41
2:F0:311:LYS:HD2	2:F0:311:LYS:HA	1.84	0.41
3:A1:217:LEU:HD12	3:A1:217:LEU:HA	1.92	0.41
3:A3:284:LEU:HD12	3:A3:284:LEU:HA	1.81	0.41
2:A6:285:GLN:HB2	2:B0:56:THR:HA	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A7:105:HIS:CE1	3:A7:150:LEU:HB2	2.55	0.41
3:A9:101:TRP:NE1	3:A9:145:SER:O	2.49	0.41
3:A9:166:THR:HG23	3:A9:199:VAL:HG13	2.02	0.41
2:C0:192:HIS:ND1	2:C0:424:ASP:OD2	2.40	0.41
3:C5:201:VAL:O	3:C5:202:ILE:HD13	2.20	0.41
2:C6:292:THR:HG21	2:C6:331:ALA:HB1	2.03	0.41
3:C7:6:HIS:CD2	3:C7:134:GLN:HG3	2.55	0.41
3:D1:257:LEU:HD21	3:D1:314:SER:HB3	2.02	0.41
2:D2:404:PHE:HZ	3:D3:312:THR:HG21	1.85	0.41
3:D3:74:ASP:OD1	3:D3:77:ARG:NH2	2.53	0.41
2:D4:161:TYR:HB3	2:D4:164:LYS:HG3	2.02	0.41
3:D5:349:MET:HB3	3:D5:349:MET:HE3	1.88	0.41
2:D6:221:ARG:HA	3:D7:324:LYS:CE	2.49	0.41
2:E0:178:SER:HB3	2:E0:183:GLU:HG2	2.01	0.41
2:E2:284:GLU:OE2	2:E6:88:HIS:NE2	2.53	0.41
3:E3:66:MET:HG2	3:E3:147:MET:HE1	2.01	0.41
2:E4:256:GLN:HE21	2:E4:256:GLN:N	2.17	0.41
2:E8:238:LEU:HA	2:E8:238:LEU:HD12	1.73	0.41
2:E8:339:ARG:HA	2:E8:339:ARG:HD2	1.80	0.41
1:1:247:TYR:HE2	2:A6:81:GLY:HA3	1.85	0.41
1:15:250:GLU:OE2	2:D8:225:THR:OG1	2.38	0.41
2:A0:178:SER:HB2	3:A1:347:ASN:HD22	1.84	0.41
3:A1:172:SER:OG	3:A1:175:VAL:O	2.36	0.41
2:A2:370:LYS:HE3	2:A2:370:LYS:HB3	1.85	0.41
3:A7:139:LEU:HD12	3:A7:170:PHE:CE1	2.56	0.41
2:B6:11:GLN:O	2:B6:15:GLN:HG3	2.20	0.41
3:B7:178:THR:HG22	2:B8:352:LYS:HZ3	1.85	0.41
3:B9:139:LEU:HA	3:B9:145:SER:HB3	2.02	0.41
2:C0:168:ASN:OD1	2:C0:169:PHE:N	2.54	0.41
3:C1:73:MET:HB3	3:C1:77:ARG:NH2	2.35	0.41
3:C1:100:ASN:HB3	3:C1:103:LYS:HG2	2.02	0.41
2:C2:15:GLN:HA	2:C2:18:ASN:HB2	2.01	0.41
3:C3:222:TYR:HA	3:C3:225:LEU:HB2	2.01	0.41
3:C3:270:PHE:O	3:C3:298:ASN:ND2	2.38	0.41
2:C6:259:LEU:HD11	2:C6:316:CYS:HB2	2.02	0.41
3:D1:101:TRP:HD1	3:D1:145:SER:HG	1.65	0.41
3:D3:313:ALA:HB3	3:D3:349:MET:SD	2.61	0.41
3:D5:377:MET:HA	3:D5:380:ARG:HG2	2.03	0.41
3:D7:20:PHE:HA	3:D7:230:SER:HB2	2.02	0.41
3:D9:164:MET:HE2	3:D9:164:MET:HB2	1.84	0.41
2:F0:174:SER:HB3	2:F0:177:VAL:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F0:254:GLU:OE1	2:F0:352:LYS:NZ	2.40	0.41
2:A0:76:ASP:OD2	3:A1:46:ARG:NH1	2.53	0.41
2:A2:133:GLN:NE2	2:A2:251:ASP:HB3	2.35	0.41
3:A5:77:ARG:HG3	3:A5:90:PHE:HE2	1.86	0.41
2:A8:298:PRO:HB3	2:A8:307:PRO:HD2	2.02	0.41
2:B4:174:SER:HB2	2:B4:207:GLU:HG2	2.02	0.41
2:B4:204:LEU:HD22	2:B4:302:MET:HE3	2.01	0.41
3:B9:95:THR:OG1	3:B9:96:GLY:N	2.53	0.41
3:B9:165:GLU:OE2	3:B9:200:GLN:NE2	2.52	0.41
2:C0:262:TYR:HB2	2:C0:265:ILE:HG22	2.01	0.41
2:C2:324:VAL:HA	2:C2:325:PRO:HD3	1.94	0.41
3:C3:336:LYS:HE2	3:C3:336:LYS:HB2	1.94	0.41
2:C4:178:SER:HB3	3:C5:347:ASN:ND2	2.35	0.41
3:C5:25:SER:OG	3:C5:30:ILE:O	2.36	0.41
2:C6:241:SER:HB2	2:C6:249:ASN:HB2	2.01	0.41
3:C7:200:GLN:HB3	3:C7:266:PHE:HB2	2.01	0.41
3:C7:259:PRO:HB2	3:C7:260:PHE:CD2	2.55	0.41
3:D3:403:MET:HB2	3:D3:403:MET:HE3	1.90	0.41
3:D5:68:LEU:HB3	3:D5:96:GLY:HA2	2.03	0.41
3:D5:237:THR:HG22	3:D5:250:LEU:HD21	2.03	0.41
2:D8:401:LYS:HD2	3:D9:344:TRP:CD2	2.55	0.41
3:E3:95:THR:OG1	3:E3:96:GLY:N	2.52	0.41
3:E3:211:CYS:HA	3:E3:215:LEU:HB2	2.01	0.41
2:E4:221:ARG:HD2	2:E4:221:ARG:HA	1.73	0.41
2:E8:193:SER:O	2:E8:197:HIS:ND1	2.48	0.41
1:18:255:PRO:HD2	2:E4:364:PRO:HG2	2.02	0.41
3:A1:6:HIS:CD2	3:A1:134:GLN:HG3	2.55	0.41
3:A1:274:THR:HG21	3:A1:282:ARG:HD2	2.03	0.41
2:A8:174:SER:HB2	2:A8:177:VAL:O	2.20	0.41
3:A9:213:ARG:HE	3:A9:297:LYS:HG3	1.85	0.41
3:B3:69:GLU:HG3	2:B4:2:ARG:HH21	1.85	0.41
3:B3:253:LEU:HD21	3:B3:368:VAL:HG11	2.02	0.41
3:B7:354:CYS:SG	3:B7:355:ASP:N	2.94	0.41
2:B8:100:ALA:O	3:B9:255:VAL:HG11	2.21	0.41
3:B9:281:TYR:CE2	3:C3:87:PRO:HD3	2.56	0.41
2:C6:334:THR:O	2:C6:337:THR:OG1	2.34	0.41
2:C8:430:LYS:HA	2:C8:430:LYS:HD3	1.90	0.41
3:C9:169:VAL:HA	3:C9:202:ILE:HB	2.01	0.41
2:D0:179:THR:OG1	3:D1:351:SER:OG	2.35	0.41
3:D1:27:GLU:OE1	3:D1:318:ARG:NH2	2.43	0.41
3:D1:206:ALA:HB2	3:D1:302:ALA:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D5:156:ARG:NH2	3:D5:197:ASP:HB2	2.36	0.41
3:D7:280:GLN:NE2	3:E1:58:ARG:HH11	2.16	0.41
2:E0:304:LYS:HA	2:E0:304:LYS:HD3	1.91	0.41
3:E3:7:VAL:HB	3:E3:135:ILE:HG13	2.02	0.41
3:E7:68:LEU:HD23	3:E7:112:LEU:HD13	2.02	0.41
2:E8:181:VAL:HG22	3:E9:350:LYS:HZ3	1.85	0.41
2:F0:251:ASP:OD1	2:F0:252:VAL:N	2.53	0.41
3:F1:20:PHE:HA	3:F1:230:SER:HB2	2.01	0.41
2:A2:285:GLN:OE1	2:A6:57:GLY:N	2.28	0.41
2:A8:395:PHE:HD2	2:A8:422:ARG:HD3	1.86	0.41
3:B3:128:ASP:OD1	3:B3:128:ASP:N	2.52	0.41
3:B5:128:ASP:OD1	3:B5:128:ASP:N	2.53	0.41
2:B6:239:THR:OG1	2:B6:243:ARG:NH1	2.53	0.41
3:B7:13:GLY:HA2	3:B7:136:THR:HG22	2.02	0.41
2:B8:124:LYS:HB2	2:B8:124:LYS:HE2	1.69	0.41
3:B9:101:TRP:H	3:B9:398:TYR:HE1	1.67	0.41
2:C4:174:SER:HB3	2:C4:177:VAL:O	2.20	0.41
2:C6:206:ASN:OD1	6:C6:501:GTP:N2	2.53	0.41
3:C7:192:LEU:HD12	3:C7:192:LEU:HA	1.91	0.41
3:C9:309:ARG:NH1	3:C9:341:PHE:O	2.54	0.41
3:D7:317:PHE:CD1	3:D7:326:VAL:HG23	2.56	0.41
2:E0:392:ASP:OD1	2:E0:422:ARG:NE	2.53	0.41
3:E1:259:PRO:HD2	3:E1:263:LEU:HD11	2.03	0.41
3:E3:33:THR:HG23	3:E3:35:THR:HG23	2.01	0.41
3:E7:117:LEU:HD23	3:E7:117:LEU:HA	1.89	0.41
3:F1:47:ILE:HD12	3:F1:47:ILE:HA	1.94	0.41
3:F1:139:LEU:HA	3:F1:139:LEU:HD23	1.89	0.41
2:A0:240:ALA:HA	2:A0:243:ARG:HE	1.85	0.41
3:A3:153:SER:HA	3:A3:195:ASN:HD22	1.86	0.41
2:A4:403:ALA:HA	3:A5:260:PHE:HE1	1.85	0.41
2:B2:298:PRO:HB3	2:B2:307:PRO:HD2	2.02	0.41
3:B3:68:LEU:HD23	3:B3:112:LEU:HD22	2.02	0.41
3:B3:375:GLN:HG3	3:B3:419:VAL:HG13	2.03	0.41
3:B5:99:ASN:ND2	3:B5:178:THR:HG23	2.35	0.41
2:B6:291:ILE:HD12	2:B6:375:VAL:HG23	2.02	0.41
2:B8:18:ASN:HD21	2:B8:78:VAL:HG22	1.85	0.41
2:B8:430:LYS:HB3	2:B8:430:LYS:HE3	1.86	0.41
2:C0:175:PRO:HA	2:C0:390:ARG:HH11	1.86	0.41
2:C0:414:GLU:N	2:C0:414:GLU:OE2	2.54	0.41
3:C1:149:THR:HG22	3:C1:191:GLN:NE2	2.35	0.41
2:C4:423:GLU:HA	2:C4:426:ALA:HB3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C6:153:LEU:HD12	2:C6:153:LEU:HA	1.84	0.41
3:C7:173:PRO:HA	3:C7:380:ARG:HD3	2.01	0.41
3:C7:283:ALA:HB2	3:D1:54:ALA:HA	2.03	0.41
3:C9:19:LYS:HD3	3:C9:19:LYS:HA	1.86	0.41
3:C9:107:THR:OG1	3:C9:401:GLU:OE2	2.29	0.41
2:D0:195:LEU:HD23	2:D0:195:LEU:HA	1.88	0.41
2:D2:425:LEU:HD12	2:D2:425:LEU:HA	1.89	0.41
3:D5:105:HIS:CD2	3:D5:150:LEU:HD12	2.55	0.41
3:D9:267:LEU:HB3	3:D9:299:MET:HE2	2.03	0.41
3:D9:284:LEU:HD12	3:D9:284:LEU:HA	1.92	0.41
3:E1:63:ALA:O	3:E1:89:ASN:ND2	2.53	0.41
2:E8:206:ASN:OD1	6:E8:501:GTP:N2	2.49	0.41
2:E8:231:ILE:O	2:E8:235:ILE:HG12	2.20	0.41
2:E8:234:VAL:HG21	2:E8:302:MET:HE1	2.02	0.41
2:F0:154:LEU:HG	2:F0:197:HIS:HB3	2.02	0.41
3:F1:30:ILE:HD12	3:F1:51:TYR:CE2	2.56	0.41
2:A0:207:GLU:HA	2:A0:210:TYR:HB2	2.03	0.41
2:A0:306:ASP:HB3	2:A0:309:HIS:CE1	2.56	0.41
2:A2:11:GLN:HB3	2:A2:74:VAL:HG11	2.03	0.41
2:A2:66:VAL:HG21	2:A2:122:ILE:HD11	2.02	0.41
3:A3:152:ILE:HD12	3:A3:164:MET:HE1	2.03	0.41
2:A6:310:GLY:HA3	2:A6:383:ALA:HB2	2.03	0.41
3:B1:101:TRP:NE1	3:B1:145:SER:O	2.51	0.41
3:B1:135:ILE:HG21	3:B1:152:ILE:HD11	2.01	0.41
3:B1:211:CYS:SG	3:B1:220:PRO:HB3	2.61	0.41
2:B2:291:ILE:HD12	2:B2:375:VAL:HG23	2.03	0.41
3:B3:64:ILE:HD12	3:B3:119:VAL:HG13	2.02	0.41
3:B3:99:ASN:HD22	3:B3:99:ASN:HA	1.61	0.41
3:B3:187:LEU:HD21	3:B3:403:MET:HE1	2.02	0.41
2:B4:167:LEU:HD22	2:B4:200:VAL:HB	2.03	0.41
2:B4:309:HIS:NE2	2:B4:386:GLU:HG2	2.36	0.41
2:B6:5:ILE:HG12	2:B6:132:LEU:HD11	2.01	0.41
2:B6:213:CYS:HA	2:B6:217:LEU:HD13	2.02	0.41
3:B7:2:ARG:H	3:B7:2:ARG:HG2	1.80	0.41
3:B7:33:THR:HG23	3:B7:35:THR:HG23	2.02	0.41
3:C1:318:ARG:HD3	3:C1:358:PRO:HD3	2.03	0.41
3:C3:137:HIS:CE1	3:C3:168:SER:HB3	2.56	0.41
2:C4:88:HIS:O	2:C4:90:GLU:N	2.54	0.41
2:C4:383:ALA:O	2:C4:386:GLU:HG2	2.20	0.41
3:C5:113:ILE:HA	3:C5:116:VAL:HG12	2.01	0.41
3:C5:313:ALA:HA	3:C5:369:GLY:HA2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C6:216:ASN:HB3	2:C6:275:ILE:O	2.21	0.41
3:C7:53:GLU:OE2	3:C7:54:ALA:N	2.51	0.41
2:C8:14:ILE:O	2:C8:18:ASN:N	2.49	0.41
2:C8:276:ILE:HG23	2:C8:280:LYS:HB2	2.03	0.41
3:C9:190:HIS:HA	3:C9:193:VAL:HG12	2.02	0.41
3:C9:273:LEU:HD23	3:C9:273:LEU:HA	1.92	0.41
3:C9:391:ARG:HA	3:C9:391:ARG:HD2	1.85	0.41
2:D0:430:LYS:HA	2:D0:430:LYS:HD3	1.84	0.41
2:D2:6:SER:OG	2:D2:8:HIS:NE2	2.54	0.41
3:D3:218:THR:O	2:D4:326:LYS:HE2	2.20	0.41
2:D4:27:GLU:OE2	2:D4:320:ARG:NH2	2.53	0.41
2:D4:407:TRP:CH2	3:D5:258:ILE:HB	2.50	0.41
3:D5:239:CYS:SG	3:D5:248:SER:N	2.87	0.41
2:D6:204:LEU:HD13	2:D6:231:ILE:HD12	2.03	0.41
3:D7:280:GLN:HE22	3:E1:58:ARG:HD2	1.86	0.41
3:D9:14:ASN:HD22	3:D9:72:THR:HG23	1.86	0.41
2:E0:64:ARG:HB3	2:E0:125:LEU:HD21	2.02	0.41
2:E2:12:ALA:HB3	2:E2:140:ALA:HB2	2.02	0.41
2:E2:324:VAL:HG13	2:E2:327:ASP:H	1.86	0.41
3:E3:295:ASP:OD2	3:E3:297:LYS:HG2	2.21	0.41
2:E4:422:ARG:NH1	2:E4:426:ALA:HB2	2.35	0.41
3:E5:238:CYS:SG	3:E5:239:CYS:N	2.94	0.41
3:E5:286:VAL:HG23	3:E5:287:PRO:HD3	2.03	0.41
3:E7:8:GLN:OE1	3:E7:17:GLY:HA3	2.21	0.41
3:E9:24:ILE:HD13	3:E9:24:ILE:HA	1.92	0.41
3:E9:44:LEU:HB2	3:E9:47:ILE:HB	2.02	0.41
2:F0:301:MET:HB3	2:F0:301:MET:HE2	1.93	0.41
3:F1:19:LYS:NZ	3:F1:227:HIS:HB2	2.36	0.41
3:F1:289:LEU:HD23	3:F1:289:LEU:HA	1.90	0.41
2:A2:399:TYR:OH	2:A2:415:GLU:OE1	2.39	0.41
3:A3:258:ILE:HG12	3:A3:266:PHE:HZ	1.86	0.41
2:A4:220:GLU:HG2	2:A4:221:ARG:HG3	2.03	0.41
3:A5:173:PRO:HB3	3:A5:380:ARG:CZ	2.51	0.41
3:A5:215:LEU:HB3	3:A5:217:LEU:HD13	2.02	0.41
2:A6:298:PRO:HB3	2:A6:307:PRO:HD2	2.03	0.41
3:A9:36:TYR:CD2	3:A9:44:LEU:HD12	2.56	0.41
2:B0:69:ASP:OD1	2:B0:70:LEU:N	2.54	0.41
3:B1:7:VAL:HB	3:B1:135:ILE:HD13	2.02	0.41
3:B1:51:TYR:HB3	3:B1:59:PHE:HB3	2.03	0.41
3:B1:66:MET:HA	3:B1:91:VAL:HG23	2.03	0.41
2:B4:69:ASP:OD1	2:B4:70:LEU:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B4:359:PRO:HA	2:B4:360:PRO:HD3	1.95	0.41
3:B5:77:ARG:HE	3:B5:77:ARG:HB2	1.70	0.41
3:C3:206:ALA:O	3:C3:210:ILE:HG12	2.21	0.41
2:C4:191:THR:HG21	2:C4:425:LEU:HD11	2.02	0.41
2:C4:384:ILE:H	2:C4:384:ILE:HG12	1.73	0.41
2:D0:7:ILE:HD13	2:D0:153:LEU:HD21	2.02	0.41
2:E2:223:THR:OG1	2:E2:224:TYR:N	2.54	0.41
3:E3:165:GLU:OE1	3:E3:200:GLN:NE2	2.54	0.41
3:E5:61:PRO:HD3	3:E5:84:LEU:HG	2.02	0.41
2:E6:99:ALA:HA	2:E6:110:ILE:HD11	2.03	0.41
2:F0:276:ILE:HD12	2:F0:281:ALA:HA	2.03	0.41
2:A2:156:ARG:HD3	2:A2:156:ARG:HA	1.86	0.40
2:A4:17:GLY:HA2	2:A4:20:CYS:HB2	2.03	0.40
3:B1:2:ARG:H	3:B1:2:ARG:HG2	1.72	0.40
3:B7:105:HIS:CD2	3:B7:150:LEU:HD12	2.56	0.40
2:B8:62:VAL:HA	2:B8:63:PRO:HD3	1.94	0.40
2:B8:204:LEU:HD13	2:B8:231:ILE:HD12	2.03	0.40
3:C3:257:LEU:HD21	3:C3:314:SER:HB2	2.03	0.40
3:C5:5:VAL:HB	3:C5:133:PHE:CD1	2.56	0.40
3:C5:217:LEU:HD23	3:C5:217:LEU:HA	1.85	0.40
3:C5:311:LEU:HD23	3:C5:311:LEU:HA	1.95	0.40
3:C7:167:PHE:CD2	3:C7:233:MET:HG2	2.56	0.40
3:C9:14:ASN:ND2	3:C9:67:ASP:OD2	2.54	0.40
2:D0:265:ILE:HG23	2:D0:432:TYR:CZ	2.56	0.40
3:D3:294:PHE:HE2	3:D3:333:VAL:HG11	1.85	0.40
2:D4:269:LEU:HD23	2:D4:303:ALA:HB3	2.03	0.40
2:E0:96:LYS:NZ	3:E1:129:CYS:HB2	2.35	0.40
2:E2:70:LEU:HD12	2:E2:99:ALA:HB2	2.02	0.40
3:E3:28:HIS:ND1	3:E3:43:GLN:O	2.52	0.40
2:E8:14:ILE:HD13	2:E8:14:ILE:HA	1.93	0.40
2:E8:274:PRO:HG2	2:E8:371:VAL:HG11	2.03	0.40
3:E9:212:PHE:CE1	2:F0:326:LYS:HD2	2.56	0.40
3:E9:321:MET:N	3:E9:321:MET:SD	2.95	0.40
3:E9:371:SER:OG	3:E9:372:THR:N	2.54	0.40
2:A0:210:TYR:CE1	2:A0:227:LEU:HD21	2.53	0.40
2:A2:304:LYS:HD3	2:A2:304:LYS:HA	1.94	0.40
3:A3:8:GLN:HB2	3:A3:65:LEU:HA	2.02	0.40
3:A3:169:VAL:HG12	3:A3:202:ILE:HB	2.03	0.40
2:A4:407:TRP:CH2	3:A5:258:ILE:HB	2.56	0.40
3:A5:201:VAL:HG11	3:A5:374:ILE:HD11	2.03	0.40
2:A6:154:LEU:HD23	2:A6:154:LEU:HA	1.88	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A6:413:MET:HE2	2:A6:413:MET:HB3	1.99	0.40
3:A7:173:PRO:HB3	3:A7:380:ARG:HD2	2.04	0.40
3:A7:213:ARG:HD2	3:A7:297:LYS:HD3	2.02	0.40
3:A9:12:CYS:O	3:A9:16:ILE:HG12	2.22	0.40
3:B1:304:ASP:OD2	3:B1:306:ARG:NH1	2.55	0.40
3:B7:2:ARG:HB2	3:B7:131:GLN:HB2	2.03	0.40
3:B9:6:HIS:CD2	3:B9:8:GLN:HG3	2.57	0.40
2:C0:168:ASN:ND2	2:C0:170:CYS:SG	2.94	0.40
2:C2:214:ARG:O	2:C2:214:ARG:NH1	2.55	0.40
2:C4:228:ASN:OD1	6:C4:501:GTP:N1	2.40	0.40
3:C5:105:HIS:ND1	3:C5:150:LEU:HB2	2.36	0.40
2:C8:28:HIS:HE1	2:C8:243:ARG:HH11	1.68	0.40
3:C9:98:GLY:HA3	2:D0:254:GLU:HB3	2.02	0.40
3:D1:1:MET:N	3:D1:128:ASP:OD2	2.38	0.40
3:D1:162:ARG:HA	3:D1:162:ARG:HD3	1.86	0.40
3:D3:325:GLU:HA	3:D3:328:GLU:HG2	2.03	0.40
2:D4:167:LEU:HD13	2:D4:200:VAL:HB	2.03	0.40
3:D9:287:PRO:HA	3:D9:290:THR:HG22	2.03	0.40
3:E3:256:ASN:HD22	3:E3:256:ASN:HA	1.74	0.40
3:E5:12:CYS:HB3	3:E5:138:SER:HB2	2.03	0.40
3:E5:344:TRP:CE3	3:E5:345:ILE:HG13	2.56	0.40
2:E6:164:LYS:HA	2:E6:164:LYS:HD3	1.84	0.40
2:E6:265:ILE:HG23	2:E6:432:TYR:CZ	2.56	0.40
3:E9:337:ASN:HB3	3:E9:340:TYR:HB2	2.03	0.40
2:A4:273:ALA:O	2:A4:375:VAL:N	2.42	0.40
3:A7:318:ARG:HH11	3:A7:358:PRO:HD3	1.86	0.40
3:B1:183:TYR:OH	3:B1:388:MET:O	2.36	0.40
2:B2:116:ASP:OD1	2:B2:117:LEU:N	2.55	0.40
3:B5:200:GLN:HB3	3:B5:268:ILE:HD11	2.02	0.40
3:B7:28:HIS:ND1	3:B7:43:GLN:O	2.53	0.40
3:B7:50:PHE:CD2	3:B7:241:ARG:HD3	2.57	0.40
2:B8:230:LEU:HD21	2:B8:368:LEU:HD11	2.04	0.40
2:C0:125:LEU:HD12	2:C0:125:LEU:HA	1.94	0.40
3:C1:211:CYS:SG	3:C1:220:PRO:HB3	2.60	0.40
3:C1:389:PHE:HZ	3:C1:405:GLU:HG2	1.86	0.40
3:C3:200:GLN:CB	3:C3:266:PHE:HB2	2.51	0.40
2:C4:267:PHE:HE2	2:C4:428:LEU:HD21	1.86	0.40
2:C6:76:ASP:OD1	2:C6:77:GLU:N	2.55	0.40
2:C6:325:PRO:HA	2:C6:328:VAL:HB	2.03	0.40
3:C7:105:HIS:ND1	3:C7:146:GLY:O	2.51	0.40
2:C8:164:LYS:O	2:C8:166:LYS:NZ	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C8:189:LEU:HD11	2:C8:418:PHE:CD1	2.56	0.40
2:C8:217:LEU:HD13	2:C8:277:SER:HB3	2.03	0.40
3:C9:151:LEU:HD12	3:C9:151:LEU:HA	1.97	0.40
3:C9:154:LYS:HA	3:C9:154:LYS:HD3	1.71	0.40
3:D1:151:LEU:HD12	3:D1:151:LEU:HA	1.77	0.40
3:D5:309:ARG:H	3:D5:372:THR:HG22	1.86	0.40
2:E0:399:TYR:OH	2:E0:415:GLU:OE1	2.38	0.40
3:E1:388:MET:HG2	2:E2:346:TRP:O	2.21	0.40
2:E2:280:LYS:NZ	2:E6:90:GLU:OE2	2.54	0.40
3:E3:121:ARG:NE	3:E3:158:GLU:OE2	2.55	0.40
2:E4:10:GLY:HA2	2:E4:145:THR:HG23	2.03	0.40
2:E8:107:HIS:HB3	2:E8:108:TYR:HD1	1.86	0.40
3:E9:176:SER:OG	2:F0:349:THR:OG1	2.24	0.40
3:E9:220:PRO:HD2	2:F0:326:LYS:HZ1	1.87	0.40
3:E9:311:LEU:HD12	3:E9:342:VAL:HG11	2.03	0.40
3:E9:349:MET:C	3:E9:350:LYS:HD2	2.41	0.40
2:F0:10:GLY:O	2:F0:14:ILE:HG12	2.21	0.40
2:F0:163:LYS:HD2	2:F0:163:LYS:HA	1.80	0.40
2:F0:345:ASP:N	2:F0:345:ASP:OD1	2.53	0.40
2:A0:343:PHE:HZ	2:A0:351:PHE:CE1	2.39	0.40
3:A1:260:PHE:CE2	3:A1:425:TYR:HE2	2.39	0.40
2:A6:274:PRO:HB2	2:A6:276:ILE:HG23	2.04	0.40
3:B1:86:ARG:HG2	3:B1:87:PRO:HD2	2.03	0.40
2:B2:28:HIS:HE1	2:B2:243:ARG:HD2	1.86	0.40
3:B3:313:ALA:HB3	3:B3:349:MET:SD	2.62	0.40
2:B4:335:ILE:HD13	2:B4:335:ILE:HA	1.93	0.40
2:B6:215:ARG:NH2	2:B6:299:ALA:O	2.52	0.40
3:B7:8:GLN:HG2	3:B7:14:ASN:HA	2.04	0.40
3:B7:324:LYS:HE3	3:B7:324:LYS:HB2	1.86	0.40
2:B8:10:GLY:HA2	2:B8:145:THR:HG23	2.04	0.40
3:B9:19:LYS:HA	3:B9:22:GLU:HG2	2.04	0.40
3:B9:211:CYS:SG	3:B9:220:PRO:HB3	2.61	0.40
2:C0:70:LEU:HD21	2:C0:149:LEU:HD22	2.02	0.40
2:C0:166:LYS:HE3	2:C0:166:LYS:HB2	1.77	0.40
2:C0:274:PRO:HD2	2:C0:374:ALA:HA	2.03	0.40
3:C3:420:SER:O	3:C3:424:GLN:N	2.55	0.40
3:C5:207:LEU:HB3	3:C5:225:LEU:HD12	2.04	0.40
3:C7:253:LEU:HD12	3:C7:253:LEU:HA	1.89	0.40
3:C7:281:TYR:CD2	3:D1:87:PRO:HD3	2.56	0.40
3:D1:139:LEU:HD23	3:D1:139:LEU:HA	1.91	0.40
3:D3:383:ASP:HA	3:D3:386:THR:HG22	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D4:172:TRP:HB3	2:D4:205:ASP:OD1	2.21	0.40
3:D5:117:LEU:O	3:D5:121:ARG:HG2	2.22	0.40
2:D8:322:ASP:OD1	2:D8:373:ARG:NE	2.52	0.40
2:D8:338:LYS:HE2	2:D8:338:LYS:HB2	1.93	0.40
2:E0:216:ASN:HB3	2:E0:275:ILE:O	2.22	0.40
2:E2:265:ILE:HG23	2:E2:432:TYR:CE1	2.57	0.40
3:E3:2:ARG:HB2	3:E3:131:GLN:HB2	2.04	0.40
3:E7:347:ASN:C	3:E7:347:ASN:HD22	2.24	0.40
3:E9:305:PRO:HB2	3:E9:310:TYR:HE1	1.87	0.40
2:F0:319:TYR:HB2	2:F0:355:ILE:HG12	2.02	0.40
1:9:254:LYS:HE2	2:C2:364:PRO:HB2	2.02	0.40
3:A3:309:ARG:H	3:A3:372:THR:HG22	1.87	0.40
2:A4:3:GLU:OE1	2:A4:132:LEU:HD13	2.22	0.40
2:A6:167:LEU:HG	2:A6:200:VAL:HB	2.04	0.40
3:A7:6:HIS:CD2	3:A7:8:GLN:HG3	2.57	0.40
2:A8:68:LEU:HD23	2:A8:93:ILE:HB	2.02	0.40
3:A9:65:LEU:HD22	3:A9:90:PHE:CE1	2.57	0.40
3:A9:217:LEU:HD23	3:A9:217:LEU:HA	1.86	0.40
3:A9:375:GLN:NE2	3:A9:423:GLN:OE1	2.53	0.40
2:B6:217:LEU:HD11	2:B6:275:ILE:HG22	2.04	0.40
3:C1:21:TRP:CH2	3:C1:61:PRO:HB3	2.57	0.40
3:C1:257:LEU:HD21	3:C1:314:SER:HB2	2.04	0.40
2:C4:292:THR:HG21	2:C4:331:ALA:HB1	2.02	0.40
3:C5:10:GLY:HA2	3:C5:143:THR:HG23	2.03	0.40
2:C6:135:PHE:HB2	2:C6:166:LYS:HA	2.03	0.40
3:C9:189:VAL:HG11	3:C9:415:MET:SD	2.62	0.40
2:D2:50:ASN:O	2:D2:64:ARG:NH2	2.50	0.40
2:D2:178:SER:OG	3:D3:347:ASN:ND2	2.44	0.40
3:D5:215:LEU:HD11	3:D5:273:LEU:HD22	2.04	0.40
3:D7:27:GLU:OE2	3:D7:241:ARG:NH1	2.50	0.40
3:D7:107:THR:OG1	3:D7:108:GLU:N	2.54	0.40
2:E0:155:GLU:HG3	2:E0:197:HIS:NE2	2.36	0.40
2:E4:269:LEU:HD23	2:E4:303:ALA:HB3	2.04	0.40
3:E5:24:ILE:HD13	3:E5:24:ILE:HA	1.96	0.40
3:E5:309:ARG:H	3:E5:372:THR:HG22	1.86	0.40
3:E9:156:ARG:HH22	3:E9:197:ASP:HB2	1.87	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	0	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	1	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	10	20/351 (6%)	16 (80%)	4 (20%)	0	100	100
1	11	20/351 (6%)	17 (85%)	3 (15%)	0	100	100
1	12	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	13	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	14	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	15	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	16	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	17	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	18	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	19	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	2	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	20	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	21	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	22	18/351 (5%)	16 (89%)	2 (11%)	0	100	100
1	23	18/351 (5%)	16 (89%)	2 (11%)	0	100	100
1	3	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	4	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	5	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	6	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	7	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	8	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	9	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
2	A0	424/453 (94%)	402 (95%)	22 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A2	424/453 (94%)	397 (94%)	27 (6%)	0	100	100
2	A4	424/453 (94%)	398 (94%)	26 (6%)	0	100	100
2	A6	424/453 (94%)	397 (94%)	27 (6%)	0	100	100
2	A8	424/453 (94%)	407 (96%)	17 (4%)	0	100	100
2	B0	424/453 (94%)	406 (96%)	18 (4%)	0	100	100
2	B2	424/453 (94%)	405 (96%)	19 (4%)	0	100	100
2	B4	424/453 (94%)	409 (96%)	15 (4%)	0	100	100
2	B6	424/453 (94%)	409 (96%)	15 (4%)	0	100	100
2	B8	424/453 (94%)	401 (95%)	23 (5%)	0	100	100
2	C0	424/453 (94%)	404 (95%)	20 (5%)	0	100	100
2	C2	424/453 (94%)	400 (94%)	24 (6%)	0	100	100
2	C4	424/453 (94%)	385 (91%)	39 (9%)	0	100	100
2	C6	424/453 (94%)	396 (93%)	28 (7%)	0	100	100
2	C8	424/453 (94%)	404 (95%)	20 (5%)	0	100	100
2	D0	424/453 (94%)	402 (95%)	22 (5%)	0	100	100
2	D2	424/453 (94%)	409 (96%)	15 (4%)	0	100	100
2	D4	424/453 (94%)	407 (96%)	17 (4%)	0	100	100
2	D6	424/453 (94%)	410 (97%)	14 (3%)	0	100	100
2	D8	424/453 (94%)	408 (96%)	16 (4%)	0	100	100
2	E0	424/453 (94%)	403 (95%)	21 (5%)	0	100	100
2	E2	424/453 (94%)	404 (95%)	20 (5%)	0	100	100
2	E4	424/453 (94%)	401 (95%)	23 (5%)	0	100	100
2	E6	424/453 (94%)	403 (95%)	21 (5%)	0	100	100
2	E8	424/453 (94%)	403 (95%)	21 (5%)	0	100	100
2	F0	424/453 (94%)	403 (95%)	21 (5%)	0	100	100
3	A1	424/449 (94%)	391 (92%)	33 (8%)	0	100	100
3	A3	424/449 (94%)	403 (95%)	21 (5%)	0	100	100
3	A5	424/449 (94%)	388 (92%)	36 (8%)	0	100	100
3	A7	424/449 (94%)	402 (95%)	22 (5%)	0	100	100
3	A9	424/449 (94%)	398 (94%)	26 (6%)	0	100	100
3	B1	424/449 (94%)	400 (94%)	24 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B3	424/449 (94%)	401 (95%)	23 (5%)	0	100	100
3	B5	424/449 (94%)	400 (94%)	24 (6%)	0	100	100
3	B7	424/449 (94%)	401 (95%)	23 (5%)	0	100	100
3	B9	424/449 (94%)	405 (96%)	19 (4%)	0	100	100
3	C1	424/449 (94%)	402 (95%)	22 (5%)	0	100	100
3	C3	424/449 (94%)	396 (93%)	28 (7%)	0	100	100
3	C5	424/449 (94%)	401 (95%)	23 (5%)	0	100	100
3	C7	424/449 (94%)	394 (93%)	30 (7%)	0	100	100
3	C9	424/449 (94%)	398 (94%)	26 (6%)	0	100	100
3	D1	424/449 (94%)	401 (95%)	23 (5%)	0	100	100
3	D3	424/449 (94%)	395 (93%)	29 (7%)	0	100	100
3	D5	424/449 (94%)	399 (94%)	25 (6%)	0	100	100
3	D7	424/449 (94%)	401 (95%)	23 (5%)	0	100	100
3	D9	424/449 (94%)	401 (95%)	23 (5%)	0	100	100
3	E1	424/449 (94%)	403 (95%)	21 (5%)	0	100	100
3	E3	424/449 (94%)	399 (94%)	25 (6%)	0	100	100
3	E5	424/449 (94%)	399 (94%)	25 (6%)	0	100	100
3	E7	424/449 (94%)	402 (95%)	22 (5%)	0	100	100
3	E9	424/449 (94%)	395 (93%)	29 (7%)	0	100	100
3	F1	424/449 (94%)	388 (92%)	36 (8%)	0	100	100
4	a	146/220 (66%)	136 (93%)	10 (7%)	0	100	100
4	b	146/220 (66%)	135 (92%)	11 (8%)	0	100	100
4	c	197/220 (90%)	187 (95%)	10 (5%)	0	100	100
4	d	197/220 (90%)	183 (93%)	14 (7%)	0	100	100
4	e	197/220 (90%)	186 (94%)	11 (6%)	0	100	100
4	f	197/220 (90%)	187 (95%)	10 (5%)	0	100	100
4	g	197/220 (90%)	184 (93%)	13 (7%)	0	100	100
4	h	197/220 (90%)	185 (94%)	12 (6%)	0	100	100
4	i	197/220 (90%)	185 (94%)	12 (6%)	0	100	100
4	j	197/220 (90%)	184 (93%)	13 (7%)	0	100	100
4	m	197/220 (90%)	184 (93%)	13 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	n	197/220 (90%)	187 (95%)	10 (5%)	0	100	100
4	o	197/220 (90%)	181 (92%)	16 (8%)	0	100	100
4	p	197/220 (90%)	186 (94%)	11 (6%)	0	100	100
4	q	197/220 (90%)	185 (94%)	12 (6%)	0	100	100
4	r	197/220 (90%)	186 (94%)	11 (6%)	0	100	100
4	s	197/220 (90%)	184 (93%)	13 (7%)	0	100	100
4	t	197/220 (90%)	186 (94%)	11 (6%)	0	100	100
4	u	197/220 (90%)	188 (95%)	9 (5%)	0	100	100
4	v	197/220 (90%)	181 (92%)	16 (8%)	0	100	100
5	k	133/189 (70%)	128 (96%)	5 (4%)	0	100	100
5	l	133/189 (70%)	128 (96%)	5 (4%)	0	100	100
5	w	139/189 (74%)	134 (96%)	5 (4%)	0	100	100
5	x	139/189 (74%)	129 (93%)	10 (7%)	0	100	100
All	All	26906/37032 (73%)	25394 (94%)	1512 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	0	20/305 (7%)	20 (100%)	0	100	100
1	1	20/305 (7%)	20 (100%)	0	100	100
1	10	20/305 (7%)	20 (100%)	0	100	100
1	11	20/305 (7%)	20 (100%)	0	100	100
1	12	20/305 (7%)	20 (100%)	0	100	100
1	13	20/305 (7%)	20 (100%)	0	100	100
1	14	20/305 (7%)	20 (100%)	0	100	100
1	15	20/305 (7%)	20 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	16	20/305 (7%)	20 (100%)	0	100	100
1	17	20/305 (7%)	20 (100%)	0	100	100
1	18	20/305 (7%)	20 (100%)	0	100	100
1	19	20/305 (7%)	20 (100%)	0	100	100
1	2	20/305 (7%)	20 (100%)	0	100	100
1	20	20/305 (7%)	20 (100%)	0	100	100
1	21	20/305 (7%)	20 (100%)	0	100	100
1	22	18/305 (6%)	18 (100%)	0	100	100
1	23	18/305 (6%)	18 (100%)	0	100	100
1	3	20/305 (7%)	20 (100%)	0	100	100
1	4	20/305 (7%)	20 (100%)	0	100	100
1	5	20/305 (7%)	20 (100%)	0	100	100
1	6	20/305 (7%)	20 (100%)	0	100	100
1	7	20/305 (7%)	20 (100%)	0	100	100
1	8	20/305 (7%)	20 (100%)	0	100	100
1	9	20/305 (7%)	20 (100%)	0	100	100
2	A0	359/379 (95%)	358 (100%)	1 (0%)	91	95
2	A2	359/379 (95%)	359 (100%)	0	100	100
2	A4	359/379 (95%)	357 (99%)	2 (1%)	84	90
2	A6	359/379 (95%)	359 (100%)	0	100	100
2	A8	359/379 (95%)	359 (100%)	0	100	100
2	B0	359/379 (95%)	358 (100%)	1 (0%)	91	95
2	B2	359/379 (95%)	359 (100%)	0	100	100
2	B4	359/379 (95%)	359 (100%)	0	100	100
2	B6	359/379 (95%)	358 (100%)	1 (0%)	91	95
2	B8	359/379 (95%)	358 (100%)	1 (0%)	91	95
2	C0	359/379 (95%)	358 (100%)	1 (0%)	91	95
2	C2	359/379 (95%)	358 (100%)	1 (0%)	91	95
2	C4	359/379 (95%)	355 (99%)	4 (1%)	70	81
2	C6	359/379 (95%)	357 (99%)	2 (1%)	84	90
2	C8	359/379 (95%)	359 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D0	359/379 (95%)	359 (100%)	0	100 100
2	D2	359/379 (95%)	358 (100%)	1 (0%)	91 95
2	D4	359/379 (95%)	358 (100%)	1 (0%)	91 95
2	D6	359/379 (95%)	359 (100%)	0	100 100
2	D8	359/379 (95%)	359 (100%)	0	100 100
2	E0	359/379 (95%)	358 (100%)	1 (0%)	91 95
2	E2	359/379 (95%)	358 (100%)	1 (0%)	91 95
2	E4	359/379 (95%)	357 (99%)	2 (1%)	84 90
2	E6	359/379 (95%)	357 (99%)	2 (1%)	84 90
2	E8	359/379 (95%)	358 (100%)	1 (0%)	91 95
2	F0	359/379 (95%)	358 (100%)	1 (0%)	91 95
3	A1	364/381 (96%)	362 (100%)	2 (0%)	86 91
3	A3	364/381 (96%)	360 (99%)	4 (1%)	70 81
3	A5	364/381 (96%)	364 (100%)	0	100 100
3	A7	364/381 (96%)	363 (100%)	1 (0%)	91 95
3	A9	364/381 (96%)	364 (100%)	0	100 100
3	B1	364/381 (96%)	364 (100%)	0	100 100
3	B3	364/381 (96%)	362 (100%)	2 (0%)	86 91
3	B5	364/381 (96%)	363 (100%)	1 (0%)	91 95
3	B7	364/381 (96%)	362 (100%)	2 (0%)	86 91
3	B9	364/381 (96%)	363 (100%)	1 (0%)	91 95
3	C1	364/381 (96%)	364 (100%)	0	100 100
3	C3	364/381 (96%)	362 (100%)	2 (0%)	86 91
3	C5	364/381 (96%)	362 (100%)	2 (0%)	86 91
3	C7	364/381 (96%)	363 (100%)	1 (0%)	91 95
3	C9	364/381 (96%)	363 (100%)	1 (0%)	91 95
3	D1	364/381 (96%)	362 (100%)	2 (0%)	86 91
3	D3	364/381 (96%)	363 (100%)	1 (0%)	91 95
3	D5	364/381 (96%)	363 (100%)	1 (0%)	91 95
3	D7	364/381 (96%)	363 (100%)	1 (0%)	91 95
3	D9	364/381 (96%)	363 (100%)	1 (0%)	91 95

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E1	364/381 (96%)	364 (100%)	0	100	100
3	E3	364/381 (96%)	363 (100%)	1 (0%)	91	95
3	E5	364/381 (96%)	363 (100%)	1 (0%)	91	95
3	E7	364/381 (96%)	360 (99%)	4 (1%)	70	81
3	E9	364/381 (96%)	363 (100%)	1 (0%)	91	95
3	F1	364/381 (96%)	364 (100%)	0	100	100
4	a	130/190 (68%)	128 (98%)	2 (2%)	60	76
4	b	130/190 (68%)	129 (99%)	1 (1%)	79	87
4	c	174/190 (92%)	173 (99%)	1 (1%)	84	90
4	d	174/190 (92%)	173 (99%)	1 (1%)	84	90
4	e	174/190 (92%)	172 (99%)	2 (1%)	70	81
4	f	174/190 (92%)	172 (99%)	2 (1%)	70	81
4	g	174/190 (92%)	172 (99%)	2 (1%)	70	81
4	h	174/190 (92%)	170 (98%)	4 (2%)	45	67
4	i	174/190 (92%)	173 (99%)	1 (1%)	84	90
4	j	174/190 (92%)	174 (100%)	0	100	100
4	m	174/190 (92%)	171 (98%)	3 (2%)	56	74
4	n	174/190 (92%)	172 (99%)	2 (1%)	70	81
4	o	174/190 (92%)	173 (99%)	1 (1%)	84	90
4	p	174/190 (92%)	173 (99%)	1 (1%)	84	90
4	q	174/190 (92%)	172 (99%)	2 (1%)	70	81
4	r	174/190 (92%)	173 (99%)	1 (1%)	84	90
4	s	174/190 (92%)	173 (99%)	1 (1%)	84	90
4	t	174/190 (92%)	172 (99%)	2 (1%)	70	81
4	u	174/190 (92%)	173 (99%)	1 (1%)	84	90
4	v	174/190 (92%)	171 (98%)	3 (2%)	56	74
5	k	122/164 (74%)	121 (99%)	1 (1%)	79	87
5	l	122/164 (74%)	121 (99%)	1 (1%)	79	87
5	w	127/164 (77%)	126 (99%)	1 (1%)	79	87
5	x	127/164 (77%)	126 (99%)	1 (1%)	79	87
All	All	23164/31536 (74%)	23071 (100%)	93 (0%)	88	93

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A0	221	ARG
3	A1	306	ARG
3	A1	362	LYS
3	A3	298	ASN
3	A3	320	ARG
3	A3	347	ASN
3	A3	414	ASN
2	A4	15	GLN
2	A4	308	ARG
3	A7	247	ASN
2	B0	308	ARG
3	B3	256	ASN
3	B3	298	ASN
3	B5	298	ASN
2	B6	308	ARG
3	B7	162	ARG
3	B7	256	ASN
2	B8	308	ARG
3	B9	162	ARG
2	C0	258	ASN
2	C2	256	GLN
3	C3	122	LYS
3	C3	297	LYS
2	C4	124	LYS
2	C4	390	ARG
2	C4	401	LYS
2	C4	422	ARG
3	C5	213	ARG
3	C5	359	LYS
2	C6	422	ARG
2	C6	430	LYS
3	C7	306	ARG
3	C9	426	GLN
3	D1	99	ASN
3	D1	134	GLN
2	D2	370	LYS
3	D3	191	GLN
2	D4	124	LYS
3	D5	298	ASN
3	D7	306	ARG
3	D9	336	LYS
2	E0	221	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E2	221	ARG
3	E3	247	ASN
2	E4	256	GLN
2	E4	358	GLN
3	E5	306	ARG
2	E6	101	ASN
2	E6	221	ARG
3	E7	213	ARG
3	E7	297	LYS
3	E7	347	ASN
3	E7	362	LYS
2	E8	430	LYS
3	E9	391	ARG
2	F0	430	LYS
4	a	117	ARG
4	a	126	ARG
4	b	126	ARG
4	c	126	ARG
4	d	35	ASN
4	e	152	LYS
4	e	194	ARG
4	f	35	ASN
4	f	194	ARG
4	g	126	ARG
4	g	194	ARG
4	h	15	ARG
4	h	18	ASN
4	h	126	ARG
4	h	194	ARG
4	i	117	ARG
5	k	87	ARG
5	l	103	LYS
4	o	126	ARG
4	p	126	ARG
4	q	126	ARG
4	q	164	ARG
4	r	126	ARG
4	s	126	ARG
4	t	126	ARG
4	t	194	ARG
4	u	126	ARG
4	v	94	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	v	126	ARG
4	v	202	ARG
5	w	160	ARG
5	x	162	ASN
4	n	117	ARG
4	n	126	ARG
4	m	97	ARG
4	m	117	ARG
4	m	126	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
3	A1	83	GLN
3	A1	396	HIS
2	A2	358	GLN
3	A3	348	ASN
3	A5	191	GLN
3	A5	329	GLN
2	A6	11	GLN
2	B0	91	GLN
2	B2	206	ASN
3	B3	6	HIS
3	B3	99	ASN
3	B3	134	GLN
3	B5	14	ASN
3	B5	334	GLN
3	B5	347	ASN
2	B6	31	GLN
2	C0	197	HIS
2	C2	380	ASN
3	C3	14	ASN
3	C3	105	HIS
2	C4	18	ASN
2	C6	168	ASN
3	C7	8	GLN
3	C7	134	GLN
3	C7	347	ASN
2	C8	11	GLN
2	C8	28	HIS
2	C8	168	ASN
3	C9	247	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C9	334	GLN
3	C9	423	GLN
2	D0	139	ASN
2	D2	11	GLN
3	D3	247	ASN
2	D4	11	GLN
3	D5	6	HIS
3	D5	298	ASN
3	D5	347	ASN
3	D7	14	ASN
3	D7	99	ASN
3	D9	6	HIS
3	D9	134	GLN
3	E1	14	ASN
3	E1	99	ASN
3	E3	204	ASN
3	E3	347	ASN
2	E4	256	GLN
3	E5	426	GLN
2	E8	88	HIS
2	E8	133	GLN
3	E9	99	ASN
3	F1	105	HIS
4	h	37	GLN
4	p	18	ASN
4	q	37	GLN
4	q	181	GLN
4	s	37	GLN
4	t	11	ASN
4	t	37	GLN
4	t	181	GLN
4	u	181	GLN
4	n	105	ASN
4	m	11	ASN
4	m	147	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 78 ligands modelled in this entry, 26 are monoatomic - leaving 52 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	GTP	E4	501	7	29,34,34	1.24	1 (3%)	35,54,54	1.30	4 (11%)
6	GTP	D0	501	7	29,34,34	1.34	3 (10%)	35,54,54	1.36	4 (11%)
6	GTP	B6	501	7	29,34,34	1.36	3 (10%)	35,54,54	1.38	4 (11%)
6	GTP	B0	501	7	29,34,34	1.27	2 (6%)	35,54,54	1.36	4 (11%)
6	GTP	E6	501	7	29,34,34	1.27	3 (10%)	35,54,54	1.31	4 (11%)
6	GTP	A6	501	7	29,34,34	1.32	3 (10%)	35,54,54	1.33	4 (11%)
8	GDP	A5	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.08	2 (6%)
8	GDP	E7	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.21	3 (10%)
8	GDP	E9	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
8	GDP	A1	501	-	25,30,30	1.03	1 (4%)	30,47,47	1.22	2 (6%)
6	GTP	E2	501	7	29,34,34	1.33	3 (10%)	35,54,54	1.34	4 (11%)
8	GDP	C9	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.20	3 (10%)
8	GDP	B7	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.07	2 (6%)
6	GTP	A4	501	7	29,34,34	1.37	3 (10%)	35,54,54	1.34	4 (11%)
6	GTP	A8	501	7	29,34,34	1.30	2 (6%)	35,54,54	1.40	4 (11%)
8	GDP	C7	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.16	2 (6%)
6	GTP	A2	501	7	29,34,34	1.26	2 (6%)	35,54,54	1.30	4 (11%)
6	GTP	B2	501	7	29,34,34	1.35	3 (10%)	35,54,54	1.39	5 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	GDP	A9	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.19	5 (16%)
8	GDP	B3	501	-	25,30,30	1.03	1 (4%)	30,47,47	1.17	2 (6%)
8	GDP	B5	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.07	2 (6%)
6	GTP	C0	501	7	29,34,34	1.30	3 (10%)	35,54,54	1.33	4 (11%)
8	GDP	D5	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
8	GDP	E3	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.14	2 (6%)
6	GTP	D8	501	7	29,34,34	1.30	2 (6%)	35,54,54	1.33	4 (11%)
6	GTP	D2	501	7	29,34,34	1.30	2 (6%)	35,54,54	1.36	4 (11%)
6	GTP	C2	501	7	29,34,34	1.28	2 (6%)	35,54,54	1.31	3 (8%)
8	GDP	E1	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.17	2 (6%)
8	GDP	C3	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.23	3 (10%)
8	GDP	D1	501	-	25,30,30	1.02	1 (4%)	30,47,47	1.14	3 (10%)
8	GDP	F1	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.10	3 (10%)
8	GDP	C5	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.30	5 (16%)
8	GDP	D7	501	-	25,30,30	1.03	1 (4%)	30,47,47	1.08	2 (6%)
8	GDP	E5	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.16	4 (13%)
6	GTP	B4	501	7	29,34,34	1.38	3 (10%)	35,54,54	1.33	5 (14%)
6	GTP	F0	501	7	29,34,34	1.28	3 (10%)	35,54,54	1.31	4 (11%)
6	GTP	C6	501	7	29,34,34	1.30	2 (6%)	35,54,54	1.38	5 (14%)
6	GTP	E8	501	7	29,34,34	1.25	3 (10%)	35,54,54	1.36	4 (11%)
8	GDP	A3	501	-	25,30,30	1.02	1 (4%)	30,47,47	1.18	2 (6%)
8	GDP	B1	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	2 (6%)
6	GTP	C4	501	7	29,34,34	1.33	2 (6%)	35,54,54	1.32	5 (14%)
6	GTP	B8	501	7	29,34,34	1.35	3 (10%)	35,54,54	1.36	4 (11%)
6	GTP	D4	501	7	29,34,34	1.36	2 (6%)	35,54,54	1.45	5 (14%)
6	GTP	E0	501	7	29,34,34	1.26	2 (6%)	35,54,54	1.33	4 (11%)
6	GTP	A0	501	7	29,34,34	1.29	3 (10%)	35,54,54	1.33	4 (11%)
6	GTP	D6	501	7	29,34,34	1.21	2 (6%)	35,54,54	1.39	4 (11%)
8	GDP	A7	501	-	25,30,30	1.01	1 (4%)	30,47,47	1.15	3 (10%)
8	GDP	D3	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.17	2 (6%)
8	GDP	B9	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.07	2 (6%)
8	GDP	D9	501	-	25,30,30	1.01	1 (4%)	30,47,47	1.15	2 (6%)
8	GDP	C1	501	-	25,30,30	1.03	1 (4%)	30,47,47	1.15	2 (6%)
6	GTP	C8	501	7	29,34,34	1.33	3 (10%)	35,54,54	1.33	4 (11%)

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
6	GTP	E4	501	7	-	6/18/38/38	0/3/3/3
6	GTP	D0	501	7	-	3/18/38/38	0/3/3/3
6	GTP	B6	501	7	-	6/18/38/38	0/3/3/3
6	GTP	B0	501	7	-	7/18/38/38	0/3/3/3
6	GTP	E6	501	7	-	5/18/38/38	0/3/3/3
6	GTP	A6	501	7	-	6/18/38/38	0/3/3/3
8	GDP	A5	501	-	-	3/12/32/32	0/3/3/3
8	GDP	E7	501	-	-	3/12/32/32	0/3/3/3
8	GDP	E9	501	-	-	4/12/32/32	0/3/3/3
8	GDP	A1	501	-	-	6/12/32/32	0/3/3/3
6	GTP	E2	501	7	-	4/18/38/38	0/3/3/3
8	GDP	C9	501	-	-	3/12/32/32	0/3/3/3
8	GDP	B7	501	-	-	3/12/32/32	0/3/3/3
6	GTP	A4	501	7	-	4/18/38/38	0/3/3/3
6	GTP	A8	501	7	-	4/18/38/38	0/3/3/3
8	GDP	C7	501	-	-	1/12/32/32	0/3/3/3
6	GTP	A2	501	7	-	7/18/38/38	0/3/3/3
6	GTP	B2	501	7	-	6/18/38/38	0/3/3/3
8	GDP	A9	501	-	-	5/12/32/32	0/3/3/3
8	GDP	B3	501	-	-	4/12/32/32	0/3/3/3
8	GDP	B5	501	-	-	2/12/32/32	0/3/3/3
6	GTP	C0	501	7	-	8/18/38/38	0/3/3/3
8	GDP	D5	501	-	-	6/12/32/32	0/3/3/3
8	GDP	E3	501	-	-	0/12/32/32	0/3/3/3
6	GTP	D8	501	7	-	5/18/38/38	0/3/3/3
6	GTP	D2	501	7	-	7/18/38/38	0/3/3/3
6	GTP	C2	501	7	-	3/18/38/38	0/3/3/3
8	GDP	E1	501	-	-	2/12/32/32	0/3/3/3
8	GDP	C3	501	-	-	4/12/32/32	0/3/3/3
8	GDP	D1	501	-	-	3/12/32/32	0/3/3/3
8	GDP	F1	501	-	-	4/12/32/32	0/3/3/3
8	GDP	C5	501	-	-	6/12/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GDP	D7	501	-	-	4/12/32/32	0/3/3/3
8	GDP	E5	501	-	-	3/12/32/32	0/3/3/3
6	GTP	B4	501	7	-	4/18/38/38	0/3/3/3
6	GTP	F0	501	7	-	7/18/38/38	0/3/3/3
6	GTP	C6	501	7	-	4/18/38/38	0/3/3/3
6	GTP	E8	501	7	-	6/18/38/38	0/3/3/3
8	GDP	A3	501	-	-	2/12/32/32	0/3/3/3
8	GDP	B1	501	-	-	5/12/32/32	0/3/3/3
6	GTP	C4	501	7	-	5/18/38/38	0/3/3/3
6	GTP	B8	501	7	-	6/18/38/38	0/3/3/3
6	GTP	D4	501	7	-	4/18/38/38	0/3/3/3
6	GTP	E0	501	7	-	2/18/38/38	0/3/3/3
6	GTP	A0	501	7	-	8/18/38/38	0/3/3/3
6	GTP	D6	501	7	-	7/18/38/38	0/3/3/3
8	GDP	A7	501	-	-	4/12/32/32	0/3/3/3
8	GDP	D3	501	-	-	4/12/32/32	0/3/3/3
8	GDP	B9	501	-	-	3/12/32/32	0/3/3/3
8	GDP	D9	501	-	-	5/12/32/32	0/3/3/3
8	GDP	C1	501	-	-	5/12/32/32	0/3/3/3
6	GTP	C8	501	7	-	3/18/38/38	0/3/3/3

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A4	501	GTP	C5-C6	-5.28	1.37	1.47
6	D4	501	GTP	C5-C6	-5.21	1.37	1.47
6	B4	501	GTP	C5-C6	-5.08	1.37	1.47
6	A6	501	GTP	C5-C6	-5.07	1.37	1.47
6	C8	501	GTP	C5-C6	-5.07	1.37	1.47
6	D0	501	GTP	C5-C6	-5.04	1.37	1.47
6	D2	501	GTP	C5-C6	-5.00	1.37	1.47
6	B2	501	GTP	C5-C6	-4.99	1.37	1.47
6	B8	501	GTP	C5-C6	-4.96	1.37	1.47
6	E2	501	GTP	C5-C6	-4.94	1.37	1.47
6	B6	501	GTP	C5-C6	-4.91	1.37	1.47
6	F0	501	GTP	C5-C6	-4.90	1.37	1.47
6	A8	501	GTP	C5-C6	-4.88	1.37	1.47
6	C0	501	GTP	C5-C6	-4.83	1.37	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C4	501	GTP	C5-C6	-4.82	1.37	1.47
6	C2	501	GTP	C5-C6	-4.82	1.37	1.47
6	D8	501	GTP	C5-C6	-4.82	1.37	1.47
6	A0	501	GTP	C5-C6	-4.81	1.37	1.47
6	E0	501	GTP	C5-C6	-4.76	1.38	1.47
6	B0	501	GTP	C5-C6	-4.75	1.38	1.47
6	C6	501	GTP	C5-C6	-4.72	1.38	1.47
6	E8	501	GTP	C5-C6	-4.72	1.38	1.47
6	A2	501	GTP	C5-C6	-4.63	1.38	1.47
6	E4	501	GTP	C5-C6	-4.61	1.38	1.47
6	E6	501	GTP	C5-C6	-4.61	1.38	1.47
6	D6	501	GTP	C5-C6	-4.61	1.38	1.47
8	D1	501	GDP	C6-N1	-3.28	1.32	1.37
8	D7	501	GDP	C6-N1	-3.21	1.32	1.37
8	B5	501	GDP	C6-N1	-3.16	1.33	1.37
8	A1	501	GDP	C6-N1	-3.15	1.33	1.37
8	C9	501	GDP	C6-N1	-3.11	1.33	1.37
8	C1	501	GDP	C6-N1	-3.11	1.33	1.37
8	A3	501	GDP	C6-N1	-3.10	1.33	1.37
8	B3	501	GDP	C6-N1	-3.07	1.33	1.37
8	C7	501	GDP	C6-N1	-3.05	1.33	1.37
8	F1	501	GDP	C6-N1	-3.05	1.33	1.37
8	A9	501	GDP	C6-N1	-3.04	1.33	1.37
8	D9	501	GDP	C6-N1	-3.01	1.33	1.37
8	A7	501	GDP	C6-N1	-3.00	1.33	1.37
8	E3	501	GDP	C6-N1	-2.99	1.33	1.37
8	B7	501	GDP	C6-N1	-2.97	1.33	1.37
8	A5	501	GDP	C6-N1	-2.96	1.33	1.37
8	E5	501	GDP	C6-N1	-2.96	1.33	1.37
8	D3	501	GDP	C6-N1	-2.95	1.33	1.37
8	B1	501	GDP	C6-N1	-2.94	1.33	1.37
8	B9	501	GDP	C6-N1	-2.92	1.33	1.37
8	C5	501	GDP	C6-N1	-2.92	1.33	1.37
8	D5	501	GDP	C6-N1	-2.89	1.33	1.37
8	C3	501	GDP	C6-N1	-2.85	1.33	1.37
8	E1	501	GDP	C6-N1	-2.85	1.33	1.37
8	E9	501	GDP	C6-N1	-2.81	1.33	1.37
8	E7	501	GDP	C6-N1	-2.81	1.33	1.37
6	E2	501	GTP	C5-C4	-2.56	1.36	1.43
6	B6	501	GTP	C5-C4	-2.51	1.36	1.43
6	D4	501	GTP	C5-C4	-2.50	1.36	1.43
6	A4	501	GTP	C5-C4	-2.49	1.36	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B8	501	GTP	C5-C4	-2.48	1.37	1.43
6	B6	501	GTP	O4'-C4'	-2.46	1.39	1.45
6	B4	501	GTP	C5-C4	-2.44	1.37	1.43
6	C0	501	GTP	C5-C4	-2.42	1.37	1.43
6	D8	501	GTP	C5-C4	-2.41	1.37	1.43
6	B2	501	GTP	C5-C4	-2.40	1.37	1.43
6	C6	501	GTP	C5-C4	-2.38	1.37	1.43
6	A6	501	GTP	C5-C4	-2.36	1.37	1.43
6	D0	501	GTP	C5-C4	-2.36	1.37	1.43
6	A8	501	GTP	C5-C4	-2.33	1.37	1.43
6	F0	501	GTP	C5-C4	-2.32	1.37	1.43
6	B4	501	GTP	O4'-C4'	-2.31	1.39	1.45
6	B8	501	GTP	O4'-C4'	-2.29	1.39	1.45
6	C4	501	GTP	C5-C4	-2.28	1.37	1.43
6	C2	501	GTP	C5-C4	-2.27	1.37	1.43
6	A0	501	GTP	C5-C4	-2.26	1.37	1.43
6	B2	501	GTP	O4'-C4'	-2.26	1.40	1.45
6	D2	501	GTP	C5-C4	-2.25	1.37	1.43
6	E8	501	GTP	C5-C4	-2.24	1.37	1.43
6	E0	501	GTP	C5-C4	-2.24	1.37	1.43
6	B0	501	GTP	C5-C4	-2.20	1.37	1.43
6	E6	501	GTP	C5-C4	-2.20	1.37	1.43
6	D6	501	GTP	C5-C4	-2.18	1.37	1.43
6	C8	501	GTP	C5-C4	-2.16	1.37	1.43
6	A2	501	GTP	C5-C4	-2.14	1.37	1.43
6	E2	501	GTP	O4'-C4'	-2.13	1.40	1.45
6	E6	501	GTP	O4'-C4'	-2.13	1.40	1.45
6	C0	501	GTP	O4'-C4'	-2.11	1.40	1.45
6	C8	501	GTP	O4'-C4'	-2.09	1.40	1.45
6	A4	501	GTP	O4'-C4'	-2.06	1.40	1.45
6	A6	501	GTP	O4'-C4'	-2.04	1.40	1.45
6	D0	501	GTP	O4'-C4'	-2.04	1.40	1.45
6	A0	501	GTP	O4'-C4'	-2.02	1.40	1.45
6	E8	501	GTP	C2-N3	2.02	1.38	1.33
6	F0	501	GTP	C2-N3	2.01	1.38	1.33

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E8	501	GTP	C8-N7-C5	3.81	109.04	102.55
6	C2	501	GTP	C8-N7-C5	3.76	108.96	102.55
6	D8	501	GTP	C8-N7-C5	3.76	108.96	102.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A0	501	GTP	C8-N7-C5	3.75	108.93	102.55
6	B6	501	GTP	C8-N7-C5	3.74	108.91	102.55
6	F0	501	GTP	C8-N7-C5	3.73	108.89	102.55
6	D6	501	GTP	C8-N7-C5	3.72	108.89	102.55
6	B8	501	GTP	C8-N7-C5	3.72	108.88	102.55
6	B0	501	GTP	C8-N7-C5	3.70	108.85	102.55
6	A2	501	GTP	C8-N7-C5	3.70	108.85	102.55
6	C0	501	GTP	C8-N7-C5	3.70	108.85	102.55
6	B2	501	GTP	C8-N7-C5	3.67	108.80	102.55
6	A8	501	GTP	C8-N7-C5	3.67	108.79	102.55
6	E0	501	GTP	C8-N7-C5	3.64	108.74	102.55
6	D4	501	GTP	C8-N7-C5	3.63	108.72	102.55
6	C4	501	GTP	C8-N7-C5	3.62	108.72	102.55
6	E4	501	GTP	C8-N7-C5	3.62	108.72	102.55
6	B4	501	GTP	C8-N7-C5	3.61	108.69	102.55
6	E2	501	GTP	C8-N7-C5	3.60	108.68	102.55
6	C6	501	GTP	C8-N7-C5	3.60	108.68	102.55
6	B8	501	GTP	C2-N1-C6	-3.58	118.56	125.11
6	D0	501	GTP	C8-N7-C5	3.57	108.63	102.55
6	E6	501	GTP	C8-N7-C5	3.55	108.60	102.55
6	B6	501	GTP	C2-N1-C6	-3.54	118.63	125.11
6	D2	501	GTP	C8-N7-C5	3.53	108.56	102.55
6	C8	501	GTP	C8-N7-C5	3.51	108.53	102.55
6	A6	501	GTP	C8-N7-C5	3.51	108.52	102.55
6	A4	501	GTP	C8-N7-C5	3.46	108.44	102.55
6	B6	501	GTP	C5-C6-N1	3.43	120.61	114.07
6	B8	501	GTP	C5-C6-N1	3.42	120.59	114.07
6	B4	501	GTP	C2-N1-C6	-3.40	118.89	125.11
6	B2	501	GTP	C2-N1-C6	-3.35	118.98	125.11
6	C6	501	GTP	C5-C6-N1	3.34	120.43	114.07
6	C0	501	GTP	C5-C6-N1	3.32	120.41	114.07
6	F0	501	GTP	C2-N1-C6	-3.32	119.04	125.11
6	E8	501	GTP	C5-C6-N1	3.29	120.35	114.07
6	C6	501	GTP	C2-N1-C6	-3.29	119.09	125.11
6	A8	501	GTP	C5-C6-N1	3.27	120.32	114.07
6	D4	501	GTP	C4'-O4'-C1'	-3.27	106.93	109.92
6	E2	501	GTP	C5-C6-N1	3.27	120.31	114.07
6	C0	501	GTP	C2-N1-C6	-3.26	119.14	125.11
6	E8	501	GTP	C2-N1-C6	-3.25	119.16	125.11
6	C4	501	GTP	C5-C6-N1	3.25	120.27	114.07
6	E2	501	GTP	C2-N1-C6	-3.24	119.17	125.11
6	F0	501	GTP	C5-C6-N1	3.23	120.24	114.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C2	501	GTP	C5-C6-N1	3.22	120.22	114.07
6	A8	501	GTP	C2-N1-C6	-3.22	119.22	125.11
6	D4	501	GTP	C2-N1-C6	-3.20	119.25	125.11
6	C4	501	GTP	C2-N1-C6	-3.18	119.28	125.11
6	E0	501	GTP	C2-N1-C6	-3.17	119.30	125.11
6	D0	501	GTP	C2-N1-C6	-3.16	119.33	125.11
6	A4	501	GTP	C5-C6-N1	3.16	120.09	114.07
6	E0	501	GTP	C5-C6-N1	3.15	120.08	114.07
6	B0	501	GTP	C5-C6-N1	3.14	120.06	114.07
8	C3	501	GDP	C4'-O4'-C1'	-3.13	107.06	109.92
6	B0	501	GTP	C2-N1-C6	-3.13	119.39	125.11
8	C9	501	GDP	C8-N7-C5	3.12	107.87	102.55
6	D2	501	GTP	C5-C6-N1	3.12	120.02	114.07
6	B4	501	GTP	C5-C6-N1	3.12	120.02	114.07
6	E6	501	GTP	C2-N1-C6	-3.11	119.42	125.11
6	D2	501	GTP	C2-N1-C6	-3.10	119.43	125.11
8	C5	501	GDP	C8-N7-C5	3.10	107.83	102.55
6	D6	501	GTP	C5-C6-N1	3.10	119.99	114.07
8	C7	501	GDP	C8-N7-C5	3.09	107.81	102.55
6	E6	501	GTP	C5-C6-N1	3.08	119.95	114.07
6	A6	501	GTP	C5-C6-N1	3.08	119.94	114.07
6	C2	501	GTP	C2-N1-C6	-3.07	119.48	125.11
6	D6	501	GTP	C2-N1-C6	-3.06	119.51	125.11
6	A6	501	GTP	C2-N1-C6	-3.06	119.51	125.11
6	B2	501	GTP	C5-C6-N1	3.06	119.90	114.07
6	A0	501	GTP	C2-N1-C6	-3.05	119.53	125.11
6	E4	501	GTP	C5-C6-N1	3.05	119.88	114.07
6	D0	501	GTP	C5-C6-N1	3.03	119.86	114.07
6	A2	501	GTP	C2-N1-C6	-3.03	119.56	125.11
6	C8	501	GTP	C5-C6-N1	3.03	119.85	114.07
6	E4	501	GTP	C2-N1-C6	-3.03	119.56	125.11
8	E3	501	GDP	C8-N7-C5	3.02	107.70	102.55
6	D4	501	GTP	C5-C6-N1	3.01	119.82	114.07
6	C8	501	GTP	C2-N1-C6	-3.00	119.62	125.11
8	A5	501	GDP	C8-N7-C5	3.00	107.65	102.55
8	D1	501	GDP	C8-N7-C5	2.99	107.64	102.55
8	C3	501	GDP	C8-N7-C5	2.99	107.64	102.55
6	D8	501	GTP	C5-C6-N1	2.99	119.77	114.07
6	D8	501	GTP	C2-N1-C6	-2.97	119.67	125.11
8	E9	501	GDP	C8-N7-C5	2.96	107.59	102.55
8	D3	501	GDP	C8-N7-C5	2.94	107.55	102.55
8	F1	501	GDP	C8-N7-C5	2.93	107.53	102.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C1	501	GDP	C8-N7-C5	2.92	107.52	102.55
8	D9	501	GDP	C8-N7-C5	2.92	107.52	102.55
8	E5	501	GDP	C8-N7-C5	2.91	107.50	102.55
8	E1	501	GDP	C8-N7-C5	2.90	107.49	102.55
8	B1	501	GDP	C8-N7-C5	2.90	107.49	102.55
6	A4	501	GTP	C2-N1-C6	-2.89	119.82	125.11
6	A2	501	GTP	C5-C6-N1	2.88	119.56	114.07
8	E7	501	GDP	C8-N7-C5	2.87	107.44	102.55
8	B3	501	GDP	C8-N7-C5	2.87	107.43	102.55
6	A0	501	GTP	C5-C6-N1	2.85	119.52	114.07
6	B2	501	GTP	C4'-O4'-C1'	-2.83	107.33	109.92
8	A9	501	GDP	C8-N7-C5	2.82	107.35	102.55
8	B9	501	GDP	C8-N7-C5	2.81	107.33	102.55
8	A7	501	GDP	C8-N7-C5	2.79	107.31	102.55
8	B5	501	GDP	C8-N7-C5	2.79	107.30	102.55
8	C5	501	GDP	C4'-O4'-C1'	-2.77	107.39	109.92
8	D7	501	GDP	C8-N7-C5	2.77	107.26	102.55
8	B7	501	GDP	C8-N7-C5	2.76	107.25	102.55
8	A3	501	GDP	O4'-C1'-N9	-2.76	105.09	108.75
8	D5	501	GDP	C8-N7-C5	2.75	107.23	102.55
8	A3	501	GDP	C8-N7-C5	2.67	107.09	102.55
6	D0	501	GTP	O6-C6-C5	-2.66	119.04	124.32
8	A1	501	GDP	C8-N7-C5	2.58	106.94	102.55
8	C5	501	GDP	O2B-PB-O3A	2.56	113.21	104.64
6	C8	501	GTP	O6-C6-C5	-2.54	119.29	124.32
6	A6	501	GTP	O6-C6-C5	-2.51	119.34	124.32
8	C5	501	GDP	O2A-PA-O3A	2.49	113.99	107.27
8	D1	501	GDP	C5-C6-N1	2.48	118.79	114.07
6	D4	501	GTP	O6-C6-C5	-2.47	119.42	124.32
6	A8	501	GTP	O6-C6-C5	-2.47	119.42	124.32
6	A4	501	GTP	O6-C6-C5	-2.46	119.45	124.32
6	A0	501	GTP	O2B-PB-O3B	2.46	113.91	107.27
6	D2	501	GTP	O6-C6-C5	-2.45	119.45	124.32
8	C9	501	GDP	C5-C6-N1	2.42	118.69	114.07
8	F1	501	GDP	C5-C6-N1	2.41	118.67	114.07
6	F0	501	GTP	O6-C6-C5	-2.40	119.56	124.32
8	D3	501	GDP	C5-C6-N1	2.39	118.62	114.07
6	B0	501	GTP	O6-C6-C5	-2.38	119.60	124.32
6	B4	501	GTP	C4'-O4'-C1'	-2.37	107.76	109.92
8	A1	501	GDP	C5-C6-N1	2.33	118.52	114.07
6	B4	501	GTP	O6-C6-C5	-2.30	119.75	124.32
6	E0	501	GTP	O6-C6-C5	-2.30	119.76	124.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D5	501	GDP	C5-C6-N1	2.30	118.46	114.07
8	C1	501	GDP	C5-C6-N1	2.29	118.44	114.07
6	C6	501	GTP	O2B-PB-O3B	2.28	113.44	107.27
8	A5	501	GDP	C5-C6-N1	2.28	118.42	114.07
6	B6	501	GTP	O6-C6-C5	-2.28	119.81	124.32
8	E7	501	GDP	C5-C6-N1	2.25	118.36	114.07
6	E8	501	GTP	O6-C6-C5	-2.25	119.86	124.32
6	E6	501	GTP	O6-C6-C5	-2.24	119.87	124.32
6	E4	501	GTP	O6-C6-C5	-2.24	119.87	124.32
8	E1	501	GDP	C5-C6-N1	2.24	118.34	114.07
8	E5	501	GDP	C5-C6-N1	2.23	118.33	114.07
8	B1	501	GDP	C5-C6-N1	2.23	118.33	114.07
6	B8	501	GTP	O6-C6-C5	-2.21	119.93	124.32
8	B7	501	GDP	C5-C6-N1	2.21	118.29	114.07
8	C3	501	GDP	C5-C6-N1	2.21	118.28	114.07
6	C4	501	GTP	O2B-PB-O3B	2.20	113.23	107.27
8	E3	501	GDP	C5-C6-N1	2.20	118.27	114.07
8	C7	501	GDP	C5-C6-N1	2.20	118.26	114.07
8	D7	501	GDP	C5-C6-N1	2.19	118.25	114.07
8	E9	501	GDP	C5-C6-N1	2.18	118.23	114.07
6	B2	501	GTP	O6-C6-C5	-2.18	120.00	124.32
6	D6	501	GTP	O6-C6-C5	-2.17	120.03	124.32
6	C0	501	GTP	O6-C6-C5	-2.16	120.03	124.32
8	A7	501	GDP	C5-C6-N1	2.15	118.18	114.07
6	E2	501	GTP	O6-C6-C5	-2.15	120.05	124.32
8	B5	501	GDP	C5-C6-N1	2.15	118.16	114.07
6	D8	501	GTP	O6-C6-C5	-2.14	120.07	124.32
8	E7	501	GDP	O2A-PA-O3A	2.14	113.06	107.27
6	A2	501	GTP	O6-C6-C5	-2.14	120.07	124.32
8	A9	501	GDP	C5-C6-N1	2.13	118.13	114.07
8	B9	501	GDP	C5-C6-N1	2.12	118.11	114.07
8	C9	501	GDP	C2-N1-C6	-2.10	121.26	125.11
8	A7	501	GDP	C4'-O4'-C1'	2.10	111.85	109.92
6	C4	501	GTP	O6-C6-C5	-2.10	120.16	124.32
8	D9	501	GDP	C5-C6-N1	2.10	118.07	114.07
8	E5	501	GDP	O2A-PA-O3A	2.09	112.94	107.27
8	C5	501	GDP	C5-C6-N1	2.09	118.06	114.07
8	E5	501	GDP	O2B-PB-O3A	2.09	111.63	104.64
8	A9	501	GDP	O2A-PA-O3A	2.08	112.89	107.27
8	A9	501	GDP	C4'-O4'-C1'	-2.05	108.04	109.92
6	C6	501	GTP	O6-C6-C5	-2.05	120.26	124.32
8	B3	501	GDP	C5-C6-N1	2.04	117.97	114.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D1	501	GDP	C2-N1-C6	-2.02	121.41	125.11
8	A9	501	GDP	O3B-PB-O3A	2.02	111.40	104.64
8	F1	501	GDP	C2-N1-C6	-2.00	121.44	125.11

There are no chirality outliers.

All (231) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A0	501	GTP	PB-O3A-PA-O5'
6	A0	501	GTP	C5'-O5'-PA-O3A
6	A0	501	GTP	C5'-O5'-PA-O1A
6	A0	501	GTP	C5'-O5'-PA-O2A
6	A2	501	GTP	C5'-O5'-PA-O3A
6	A2	501	GTP	C5'-O5'-PA-O1A
6	A2	501	GTP	C5'-O5'-PA-O2A
6	A4	501	GTP	C5'-O5'-PA-O3A
6	A4	501	GTP	C5'-O5'-PA-O1A
6	A4	501	GTP	C5'-O5'-PA-O2A
6	A6	501	GTP	C5'-O5'-PA-O3A
6	A6	501	GTP	C5'-O5'-PA-O1A
6	A6	501	GTP	C5'-O5'-PA-O2A
6	A8	501	GTP	C5'-O5'-PA-O3A
6	A8	501	GTP	C5'-O5'-PA-O1A
6	A8	501	GTP	C5'-O5'-PA-O2A
6	B0	501	GTP	C5'-O5'-PA-O3A
6	B0	501	GTP	C5'-O5'-PA-O1A
6	B0	501	GTP	C5'-O5'-PA-O2A
6	B2	501	GTP	C5'-O5'-PA-O3A
6	B2	501	GTP	C5'-O5'-PA-O1A
6	B4	501	GTP	C5'-O5'-PA-O3A
6	B4	501	GTP	C5'-O5'-PA-O1A
6	B6	501	GTP	C5'-O5'-PA-O3A
6	B6	501	GTP	C5'-O5'-PA-O1A
6	B8	501	GTP	C5'-O5'-PA-O1A
6	B8	501	GTP	O4'-C4'-C5'-O5'
6	C0	501	GTP	PB-O3B-PG-O2G
6	C0	501	GTP	C5'-O5'-PA-O3A
6	C0	501	GTP	C5'-O5'-PA-O1A
6	C0	501	GTP	C5'-O5'-PA-O2A
6	C2	501	GTP	C5'-O5'-PA-O3A
6	C2	501	GTP	C5'-O5'-PA-O2A
6	C4	501	GTP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	C4	501	GTP	C5'-O5'-PA-O1A
6	C4	501	GTP	C5'-O5'-PA-O2A
6	C6	501	GTP	C5'-O5'-PA-O3A
6	C6	501	GTP	C5'-O5'-PA-O1A
6	C6	501	GTP	C5'-O5'-PA-O2A
6	C8	501	GTP	C5'-O5'-PA-O3A
6	C8	501	GTP	C5'-O5'-PA-O2A
6	D0	501	GTP	C5'-O5'-PA-O3A
6	D0	501	GTP	C5'-O5'-PA-O2A
6	D2	501	GTP	C5'-O5'-PA-O3A
6	D2	501	GTP	C5'-O5'-PA-O1A
6	D2	501	GTP	C5'-O5'-PA-O2A
6	D6	501	GTP	C5'-O5'-PA-O3A
6	D6	501	GTP	C5'-O5'-PA-O1A
6	D6	501	GTP	C5'-O5'-PA-O2A
6	D8	501	GTP	C5'-O5'-PA-O3A
6	D8	501	GTP	C5'-O5'-PA-O1A
6	D8	501	GTP	C5'-O5'-PA-O2A
6	E0	501	GTP	C5'-O5'-PA-O3A
6	E2	501	GTP	C5'-O5'-PA-O3A
6	E2	501	GTP	C5'-O5'-PA-O2A
6	E4	501	GTP	C5'-O5'-PA-O3A
6	E4	501	GTP	C5'-O5'-PA-O1A
6	E4	501	GTP	C5'-O5'-PA-O2A
6	E6	501	GTP	C5'-O5'-PA-O3A
6	E6	501	GTP	C5'-O5'-PA-O2A
6	E8	501	GTP	C5'-O5'-PA-O3A
6	E8	501	GTP	C5'-O5'-PA-O1A
6	E8	501	GTP	C5'-O5'-PA-O2A
6	F0	501	GTP	C5'-O5'-PA-O3A
6	F0	501	GTP	C5'-O5'-PA-O1A
6	F0	501	GTP	C5'-O5'-PA-O2A
8	A1	501	GDP	C5'-O5'-PA-O3A
8	A1	501	GDP	C5'-O5'-PA-O1A
8	A5	501	GDP	C5'-O5'-PA-O3A
8	A5	501	GDP	C5'-O5'-PA-O1A
8	A5	501	GDP	C5'-O5'-PA-O2A
8	A7	501	GDP	C5'-O5'-PA-O3A
8	A7	501	GDP	C5'-O5'-PA-O1A
8	A7	501	GDP	C5'-O5'-PA-O2A
8	A9	501	GDP	C5'-O5'-PA-O3A
8	A9	501	GDP	C5'-O5'-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	B1	501	GDP	C5'-O5'-PA-O3A
8	B1	501	GDP	C5'-O5'-PA-O2A
8	B3	501	GDP	C5'-O5'-PA-O3A
8	B3	501	GDP	C5'-O5'-PA-O1A
8	B3	501	GDP	C5'-O5'-PA-O2A
8	B7	501	GDP	C5'-O5'-PA-O3A
8	B7	501	GDP	C5'-O5'-PA-O1A
8	B7	501	GDP	C5'-O5'-PA-O2A
8	B9	501	GDP	C5'-O5'-PA-O3A
8	B9	501	GDP	C5'-O5'-PA-O1A
8	B9	501	GDP	C5'-O5'-PA-O2A
8	C1	501	GDP	C5'-O5'-PA-O3A
8	C1	501	GDP	C5'-O5'-PA-O1A
8	C3	501	GDP	C5'-O5'-PA-O3A
8	C3	501	GDP	C5'-O5'-PA-O1A
8	C3	501	GDP	C5'-O5'-PA-O2A
8	C5	501	GDP	C5'-O5'-PA-O3A
8	C5	501	GDP	C5'-O5'-PA-O1A
8	C5	501	GDP	C5'-O5'-PA-O2A
8	C9	501	GDP	C5'-O5'-PA-O3A
8	C9	501	GDP	C5'-O5'-PA-O1A
8	C9	501	GDP	C5'-O5'-PA-O2A
8	D1	501	GDP	C5'-O5'-PA-O3A
8	D1	501	GDP	C5'-O5'-PA-O1A
8	D1	501	GDP	C5'-O5'-PA-O2A
8	D3	501	GDP	C5'-O5'-PA-O3A
8	D3	501	GDP	C5'-O5'-PA-O2A
8	D5	501	GDP	C5'-O5'-PA-O3A
8	D5	501	GDP	C5'-O5'-PA-O1A
8	D5	501	GDP	C5'-O5'-PA-O2A
8	D7	501	GDP	C5'-O5'-PA-O3A
8	D7	501	GDP	C5'-O5'-PA-O1A
8	D7	501	GDP	C5'-O5'-PA-O2A
8	D9	501	GDP	C5'-O5'-PA-O3A
8	D9	501	GDP	C5'-O5'-PA-O1A
8	D9	501	GDP	C5'-O5'-PA-O2A
8	E1	501	GDP	C5'-O5'-PA-O3A
8	E1	501	GDP	C5'-O5'-PA-O2A
8	E7	501	GDP	C5'-O5'-PA-O3A
8	E7	501	GDP	C5'-O5'-PA-O2A
8	E9	501	GDP	C5'-O5'-PA-O3A
8	E9	501	GDP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	F1	501	GDP	C5'-O5'-PA-O3A
8	F1	501	GDP	C5'-O5'-PA-O1A
6	B6	501	GTP	O4'-C4'-C5'-O5'
6	B6	501	GTP	C3'-C4'-C5'-O5'
6	B8	501	GTP	C3'-C4'-C5'-O5'
6	A2	501	GTP	C3'-C4'-C5'-O5'
6	D4	501	GTP	O4'-C4'-C5'-O5'
6	D4	501	GTP	C3'-C4'-C5'-O5'
8	D5	501	GDP	C3'-C4'-C5'-O5'
6	E8	501	GTP	C3'-C4'-C5'-O5'
6	A2	501	GTP	O4'-C4'-C5'-O5'
6	F0	501	GTP	C3'-C4'-C5'-O5'
6	A6	501	GTP	C3'-C4'-C5'-O5'
6	E8	501	GTP	O4'-C4'-C5'-O5'
8	D5	501	GDP	O4'-C4'-C5'-O5'
8	D5	501	GDP	PA-O3A-PB-O1B
6	D6	501	GTP	PB-O3A-PA-O1A
6	C8	501	GTP	C4'-C5'-O5'-PA
6	E0	501	GTP	C4'-C5'-O5'-PA
6	C6	501	GTP	C4'-C5'-O5'-PA
6	D4	501	GTP	PB-O3A-PA-O5'
6	B0	501	GTP	PB-O3B-PG-O2G
6	F0	501	GTP	PB-O3B-PG-O2G
6	C0	501	GTP	C3'-C4'-C5'-O5'
6	B6	501	GTP	C4'-C5'-O5'-PA
8	A9	501	GDP	PB-O3A-PA-O2A
8	C7	501	GDP	PB-O3A-PA-O2A
6	E4	501	GTP	C3'-C4'-C5'-O5'
8	B5	501	GDP	C3'-C4'-C5'-O5'
6	A0	501	GTP	C4'-C5'-O5'-PA
6	A2	501	GTP	C4'-C5'-O5'-PA
6	A6	501	GTP	C4'-C5'-O5'-PA
6	A8	501	GTP	C4'-C5'-O5'-PA
6	C4	501	GTP	C4'-C5'-O5'-PA
6	D0	501	GTP	C4'-C5'-O5'-PA
6	D6	501	GTP	C4'-C5'-O5'-PA
6	D8	501	GTP	C4'-C5'-O5'-PA
6	E6	501	GTP	C4'-C5'-O5'-PA
8	E9	501	GDP	C4'-C5'-O5'-PA
6	A6	501	GTP	O4'-C4'-C5'-O5'
6	F0	501	GTP	O4'-C4'-C5'-O5'
6	B2	501	GTP	C5'-O5'-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	B4	501	GTP	C5'-O5'-PA-O2A
6	B6	501	GTP	C5'-O5'-PA-O2A
6	B8	501	GTP	C5'-O5'-PA-O3A
6	B8	501	GTP	C5'-O5'-PA-O2A
8	A1	501	GDP	C5'-O5'-PA-O2A
8	B5	501	GDP	C5'-O5'-PA-O3A
8	C1	501	GDP	C5'-O5'-PA-O2A
8	E9	501	GDP	C5'-O5'-PA-O2A
8	F1	501	GDP	C5'-O5'-PA-O2A
6	A4	501	GTP	C4'-C5'-O5'-PA
6	B0	501	GTP	C4'-C5'-O5'-PA
6	C2	501	GTP	C4'-C5'-O5'-PA
6	D2	501	GTP	C4'-C5'-O5'-PA
6	E2	501	GTP	C4'-C5'-O5'-PA
6	E4	501	GTP	C4'-C5'-O5'-PA
6	E8	501	GTP	C4'-C5'-O5'-PA
6	F0	501	GTP	C4'-C5'-O5'-PA
8	A9	501	GDP	C4'-C5'-O5'-PA
8	F1	501	GDP	C4'-C5'-O5'-PA
8	C1	501	GDP	PA-O3A-PB-O1B
6	D2	501	GTP	C3'-C4'-C5'-O5'
6	B8	501	GTP	C4'-C5'-O5'-PA
6	A0	501	GTP	PA-O3A-PB-O2B
6	B2	501	GTP	PB-O3A-PA-O2A
6	D2	501	GTP	PA-O3A-PB-O2B
6	D8	501	GTP	PB-O3A-PA-O1A
6	E2	501	GTP	PB-O3A-PA-O2A
8	A1	501	GDP	PB-O3A-PA-O2A
8	B1	501	GDP	PB-O3A-PA-O2A
8	B3	501	GDP	PB-O3A-PA-O2A
8	C5	501	GDP	PB-O3A-PA-O2A
6	B4	501	GTP	C4'-C5'-O5'-PA
6	D4	501	GTP	C4'-C5'-O5'-PA
8	C1	501	GDP	C4'-C5'-O5'-PA
8	C3	501	GDP	C4'-C5'-O5'-PA
6	B2	501	GTP	PB-O3A-PA-O1A
6	C0	501	GTP	PB-O3A-PA-O1A
6	E6	501	GTP	PB-O3A-PA-O2A
8	A1	501	GDP	PB-O3A-PA-O1A
6	B2	501	GTP	C4'-C5'-O5'-PA
6	C0	501	GTP	C4'-C5'-O5'-PA
8	E5	501	GDP	C4'-C5'-O5'-PA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	A7	501	GDP	C3'-C4'-C5'-O5'
8	B1	501	GDP	C4'-C5'-O5'-PA
8	C5	501	GDP	C4'-C5'-O5'-PA
6	C4	501	GTP	PB-O3B-PG-O2G
8	A1	501	GDP	C4'-C5'-O5'-PA
6	E4	501	GTP	O4'-C4'-C5'-O5'
8	D3	501	GDP	C3'-C4'-C5'-O5'
8	D9	501	GDP	C4'-C5'-O5'-PA
6	A2	501	GTP	PA-O3A-PB-O2B
6	B0	501	GTP	PA-O3A-PB-O2B
6	C0	501	GTP	PB-O3A-PA-O2A
6	D6	501	GTP	PB-O3A-PA-O2A
6	E6	501	GTP	PB-O3A-PA-O1A
8	A3	501	GDP	PB-O3A-PA-O2A
8	A9	501	GDP	PB-O3A-PA-O1A
8	B1	501	GDP	PB-O3A-PA-O1A
8	E5	501	GDP	PB-O3A-PA-O2A
6	D6	501	GTP	C3'-C4'-C5'-O5'
8	D7	501	GDP	C4'-C5'-O5'-PA
8	D9	501	GDP	PA-O3A-PB-O1B
6	A0	501	GTP	C3'-C4'-C5'-O5'
6	A0	501	GTP	PA-O3A-PB-O1B
6	B0	501	GTP	PA-O3A-PB-O1B
6	D2	501	GTP	PA-O3A-PB-O1B
8	A3	501	GDP	PB-O3A-PA-O1A
8	C5	501	GDP	PB-O3A-PA-O1A
8	D3	501	GDP	PB-O3A-PA-O1A
8	E5	501	GDP	PB-O3A-PA-O1A
8	E7	501	GDP	C3'-C4'-C5'-O5'

There are no ring outliers.

27 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B6	501	GTP	2	0
6	B0	501	GTP	1	0
6	E6	501	GTP	3	0
8	A1	501	GDP	2	0
6	E2	501	GTP	1	0
8	B7	501	GDP	1	0
6	A8	501	GTP	1	0
6	B2	501	GTP	1	0

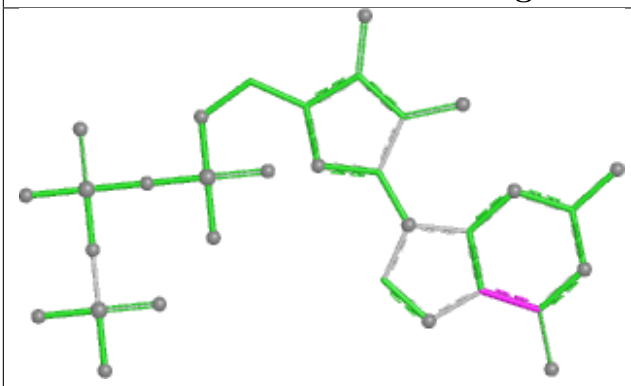
Continued on next page...

Continued from previous page...

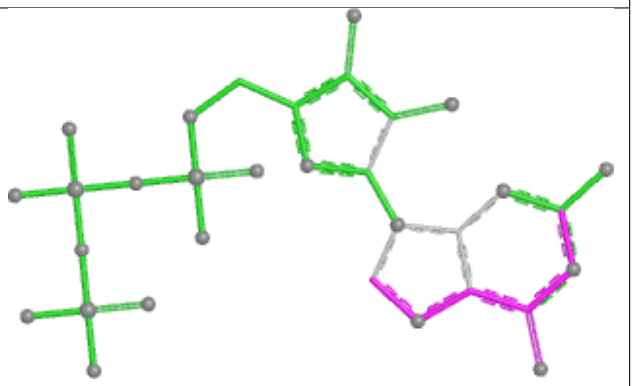
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A9	501	GDP	1	0
8	B3	501	GDP	1	0
6	C0	501	GTP	2	0
8	D5	501	GDP	1	0
8	E3	501	GDP	3	0
6	D8	501	GTP	1	0
8	C3	501	GDP	2	0
8	F1	501	GDP	1	0
8	C5	501	GDP	1	0
6	F0	501	GTP	1	0
6	C6	501	GTP	3	0
6	E8	501	GTP	2	0
8	A3	501	GDP	2	0
6	C4	501	GTP	1	0
6	B8	501	GTP	1	0
6	D4	501	GTP	1	0
6	A0	501	GTP	2	0
8	C1	501	GDP	1	0
6	C8	501	GTP	1	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.

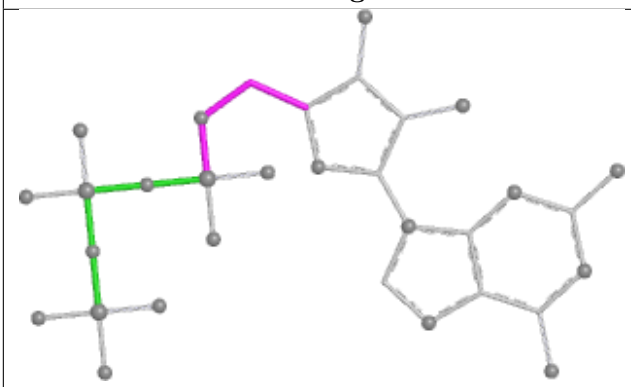
Ligand GTP E4 501



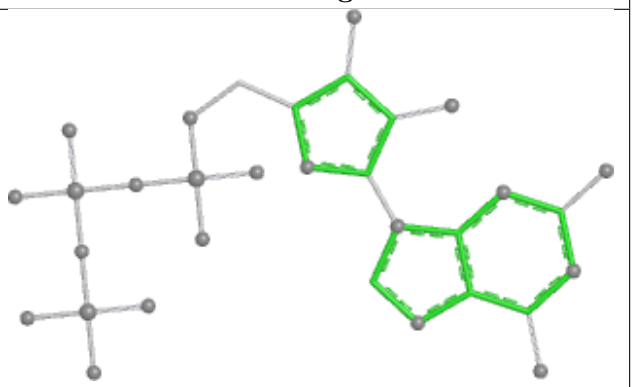
Bond lengths



Bond angles

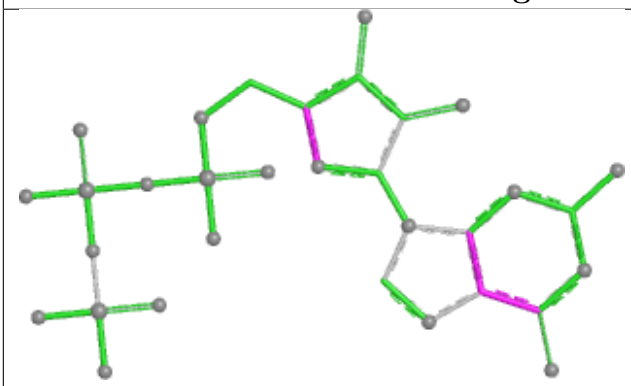


Torsions

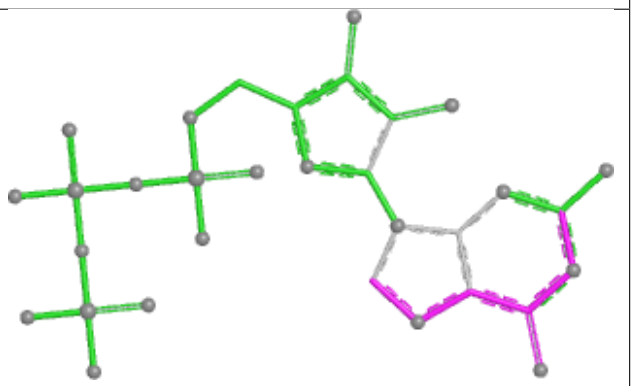


Rings

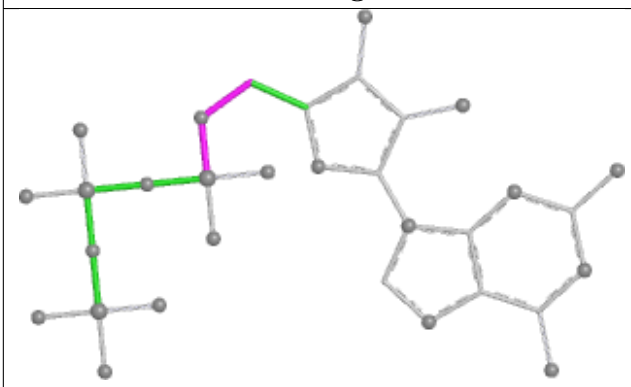
Ligand GTP D0 501



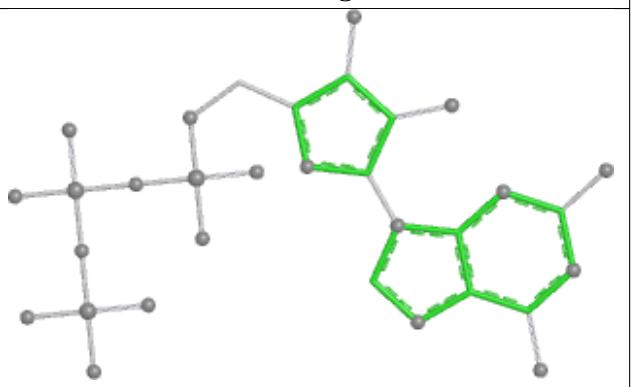
Bond lengths



Bond angles

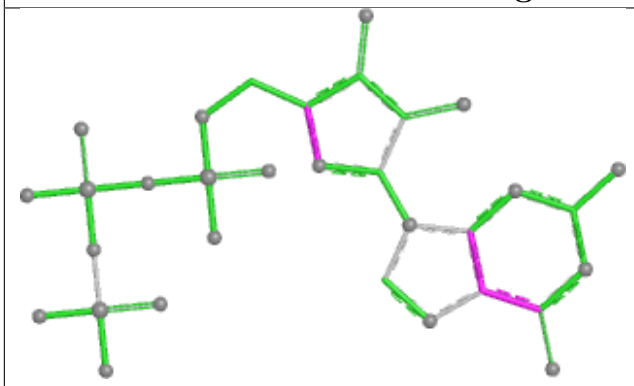


Torsions

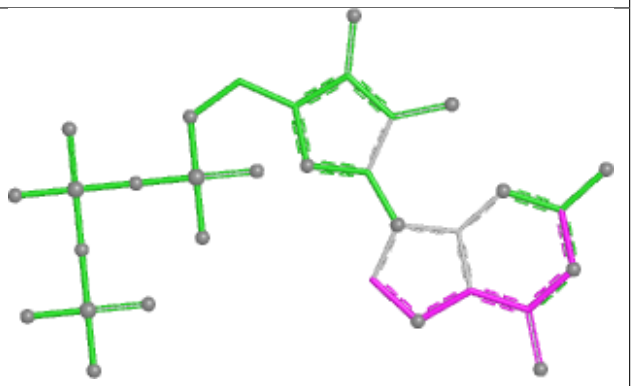


Rings

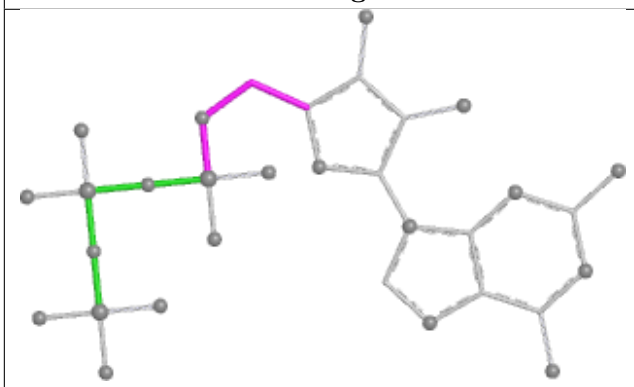
Ligand GTP B6 501



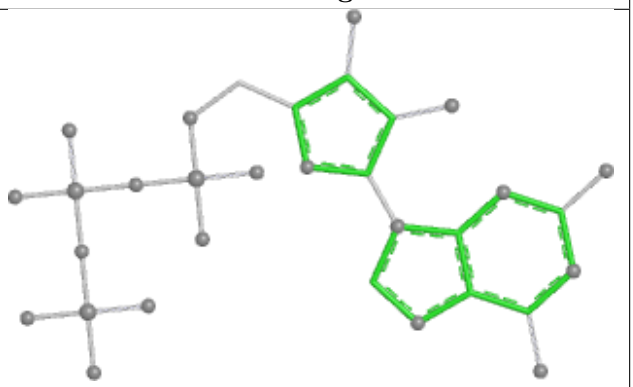
Bond lengths



Bond angles

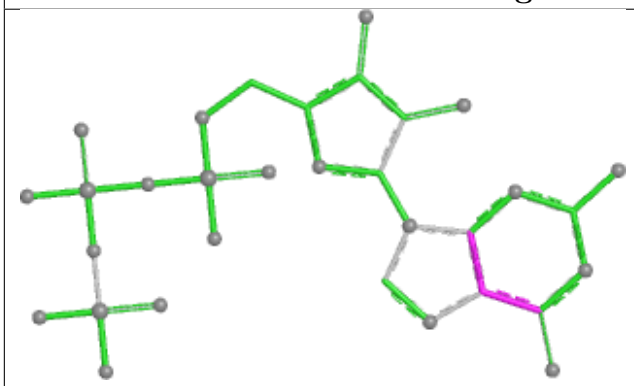


Torsions

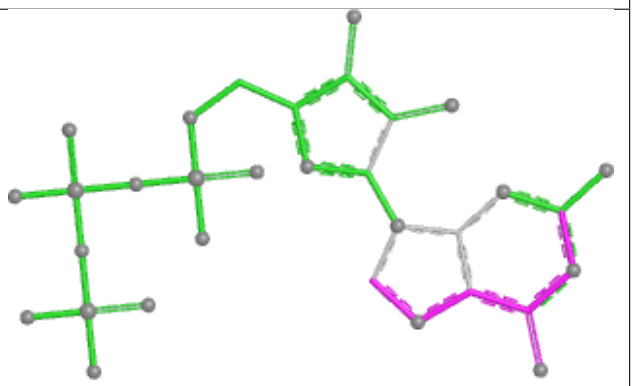


Rings

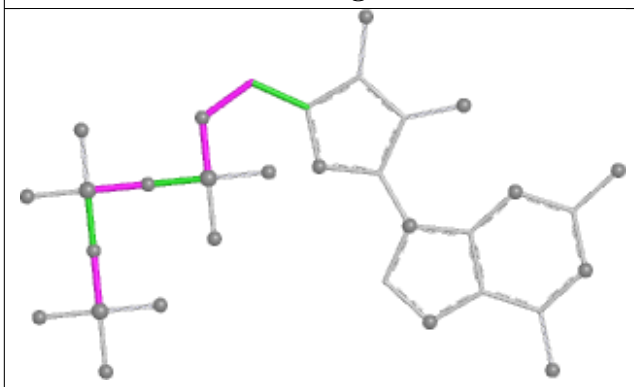
Ligand GTP B0 501



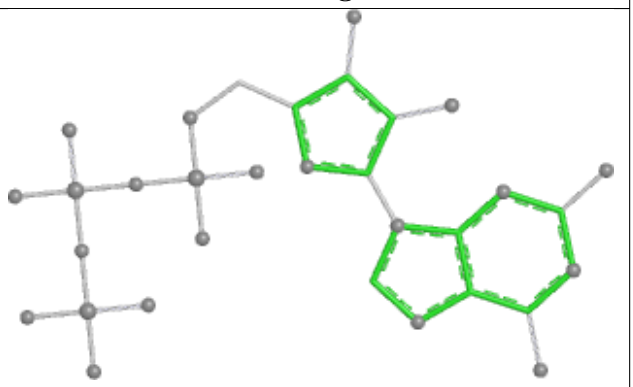
Bond lengths



Bond angles

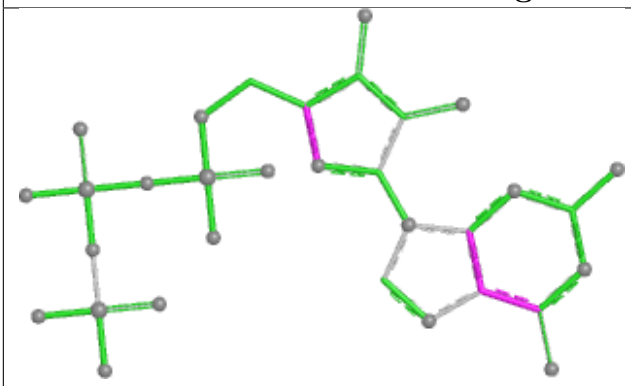


Torsions

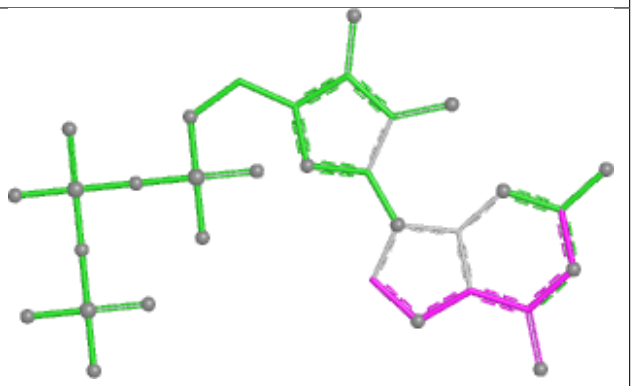


Rings

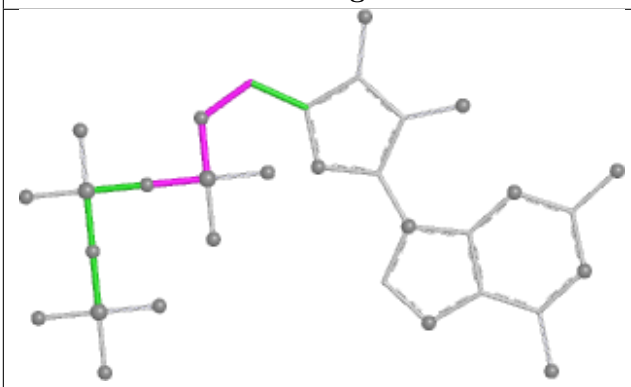
Ligand GTP E6 501



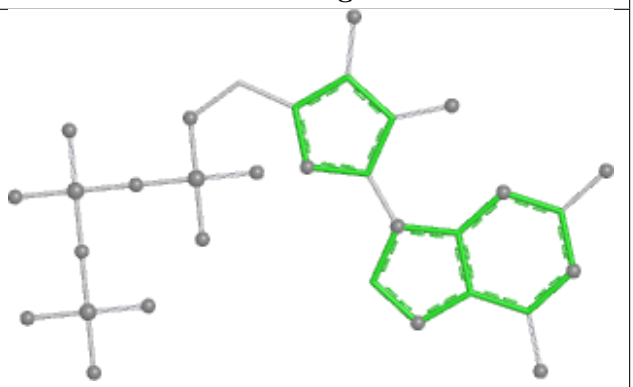
Bond lengths



Bond angles

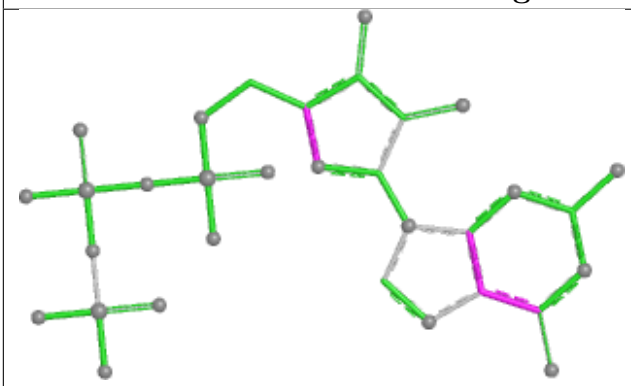


Torsions

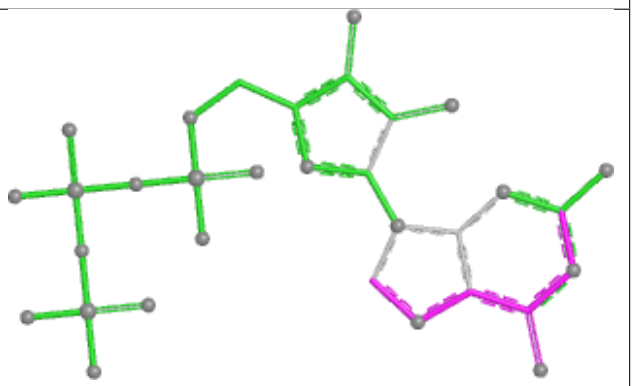


Rings

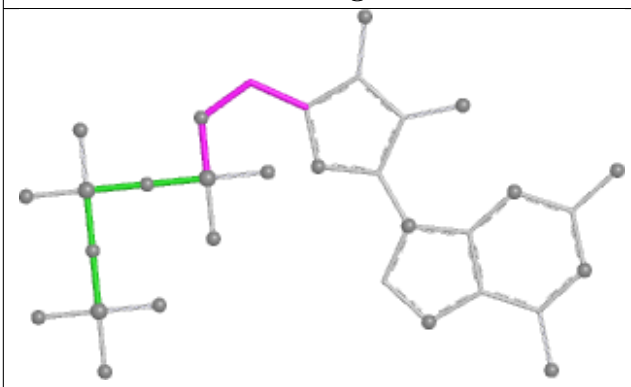
Ligand GTP A6 501



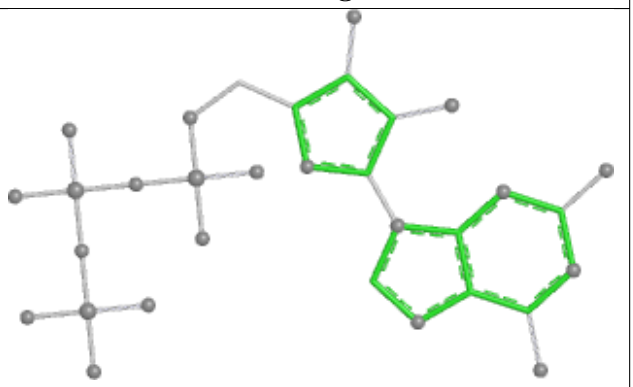
Bond lengths



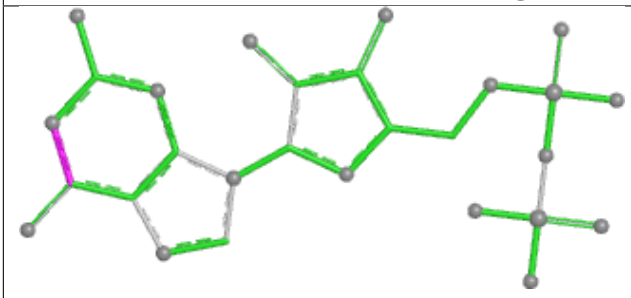
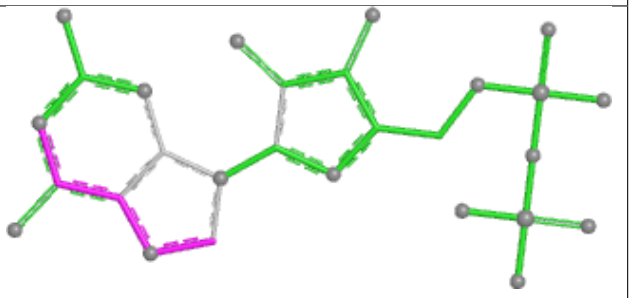
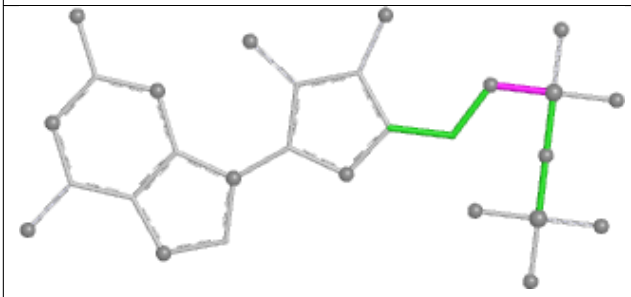
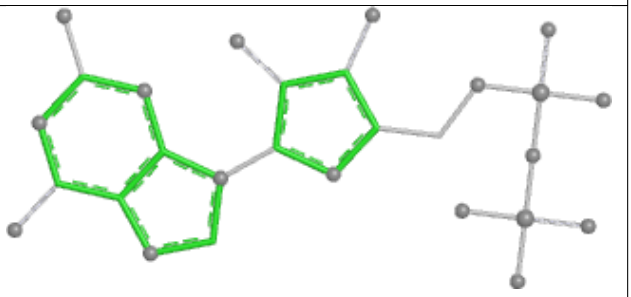
Bond angles

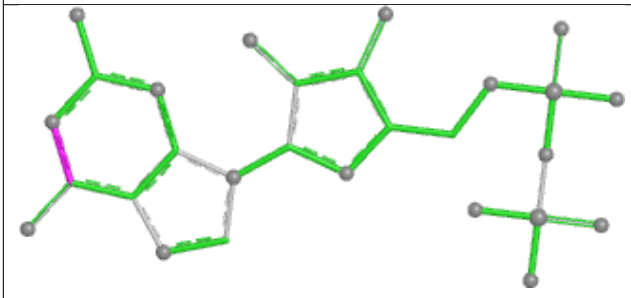
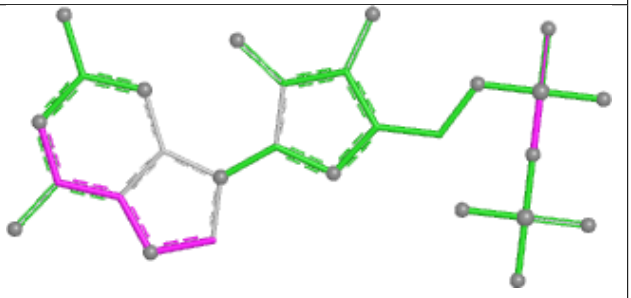
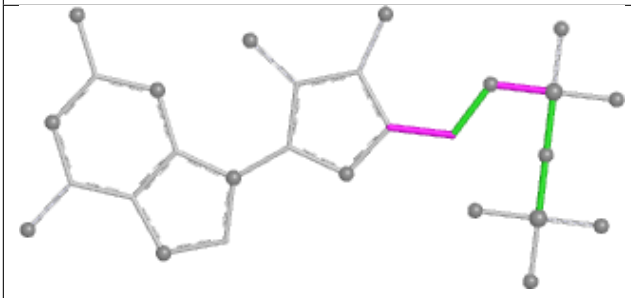
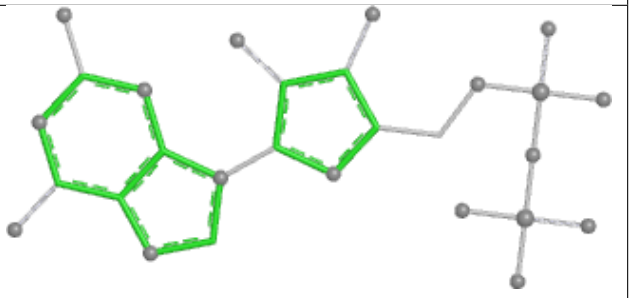


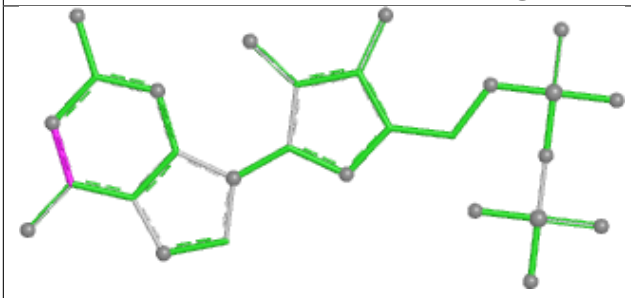
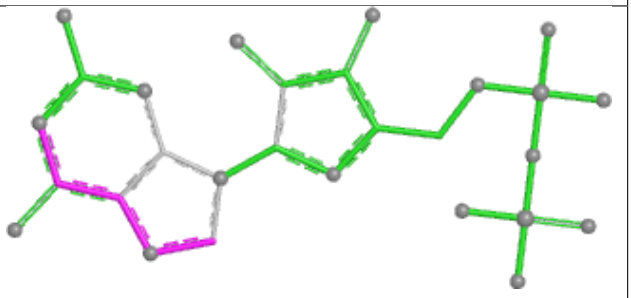
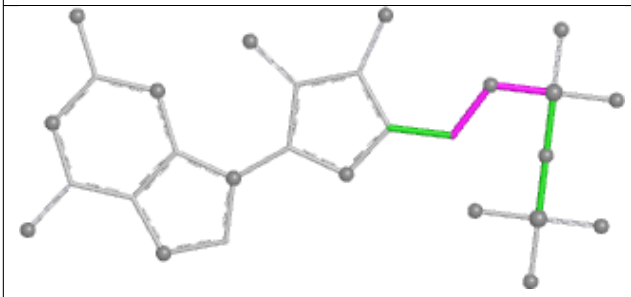
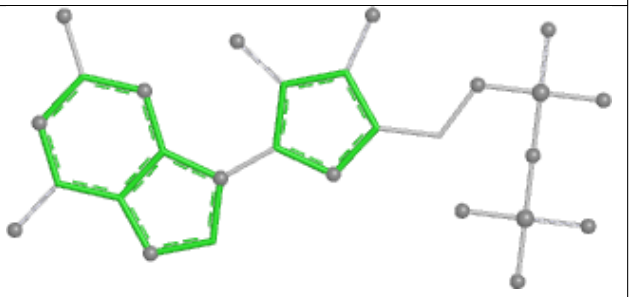
Torsions

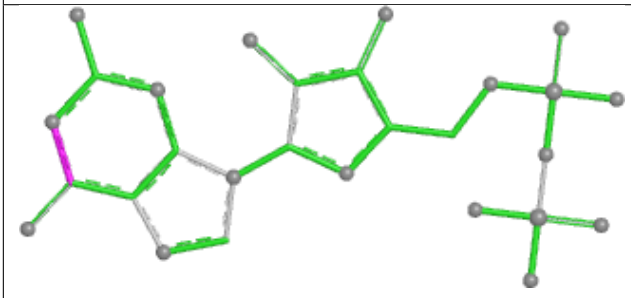
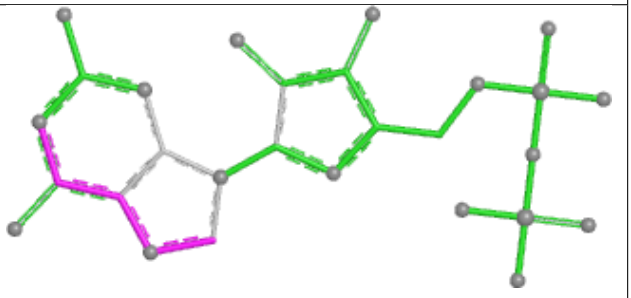
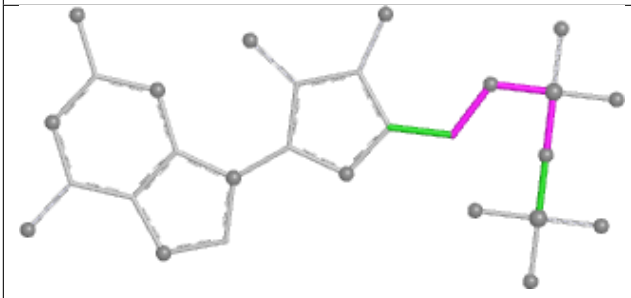
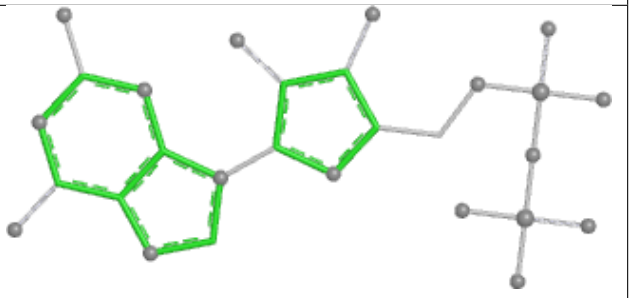


Rings

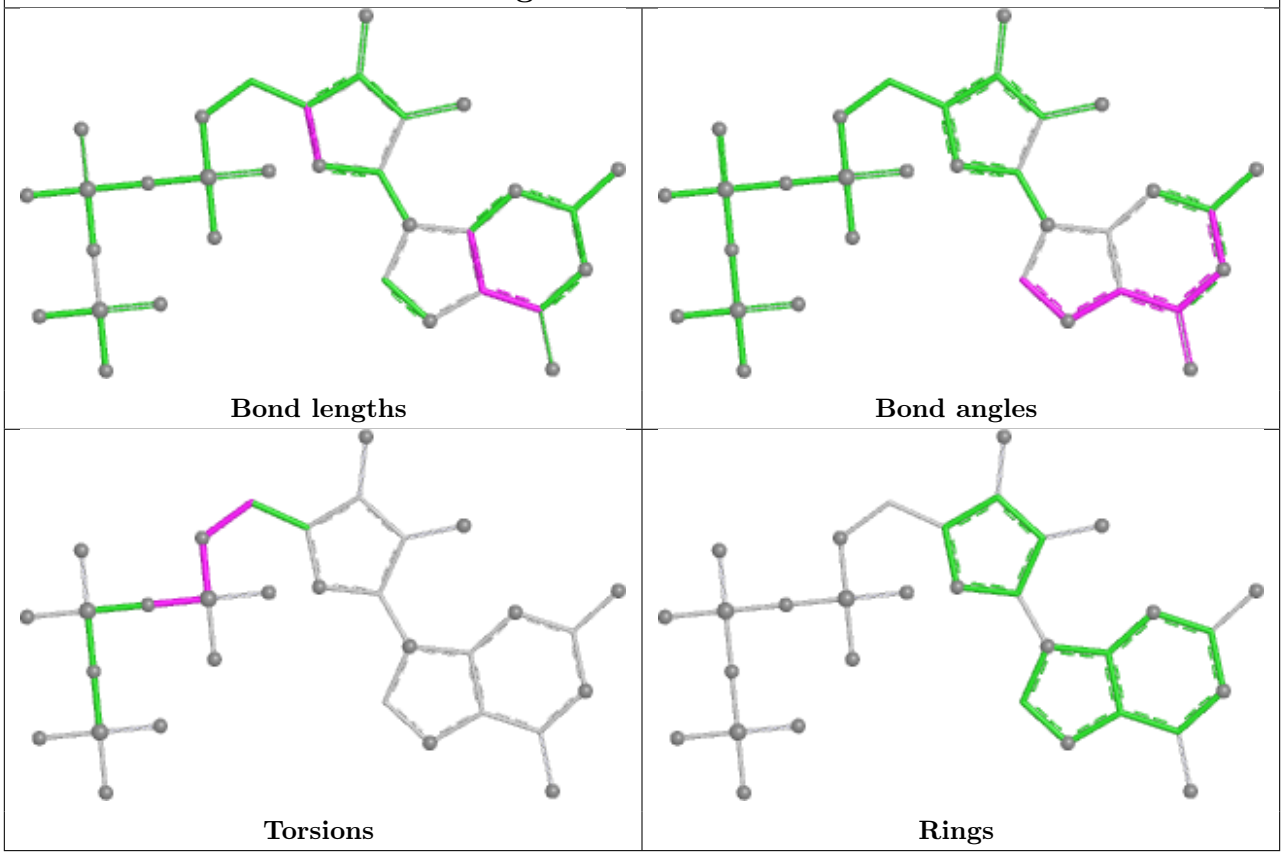
Ligand GDP A5 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP E7 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

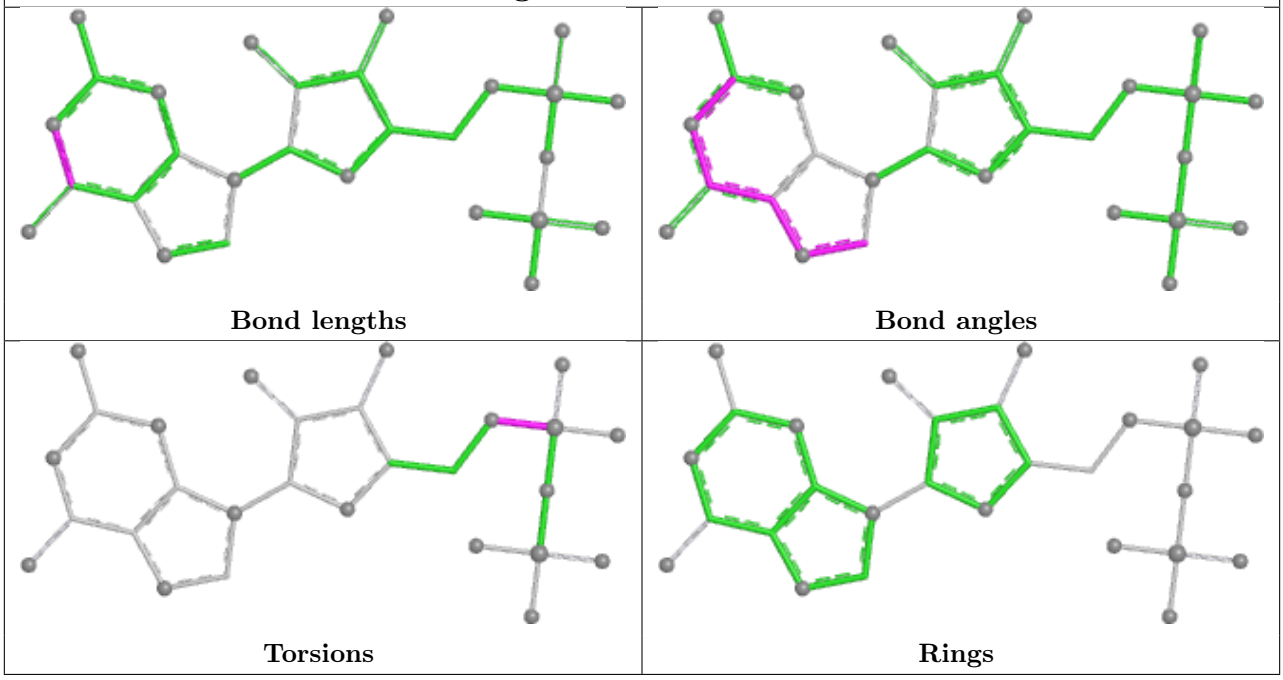
Ligand GDP E9 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

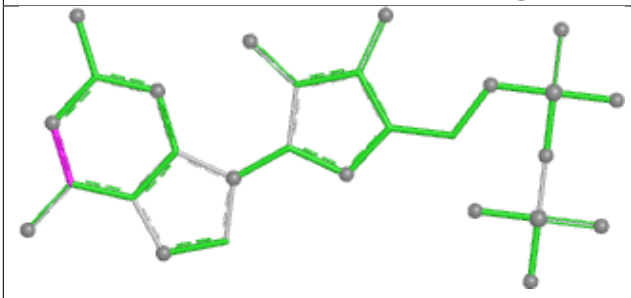
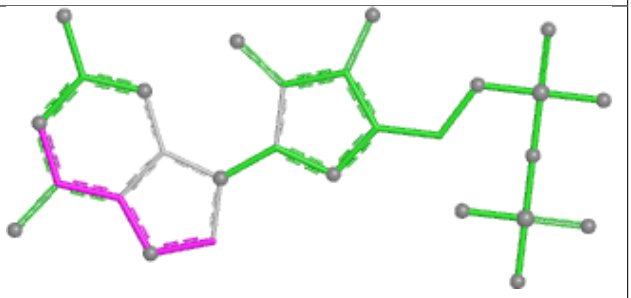
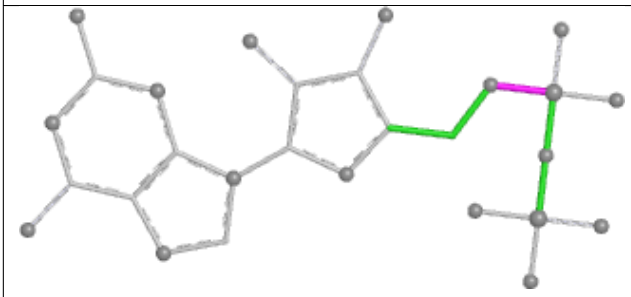
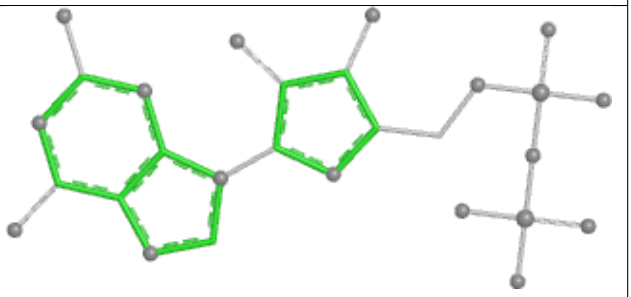
Ligand GDP A1 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

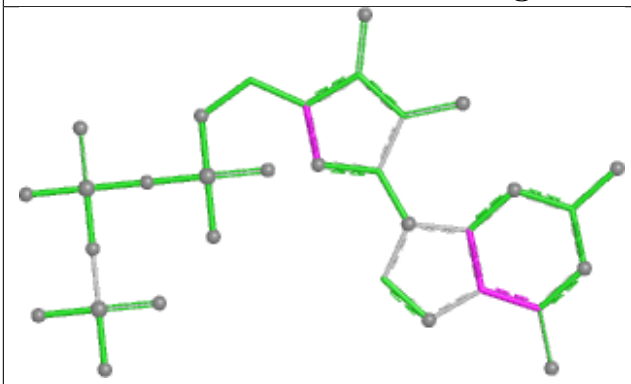
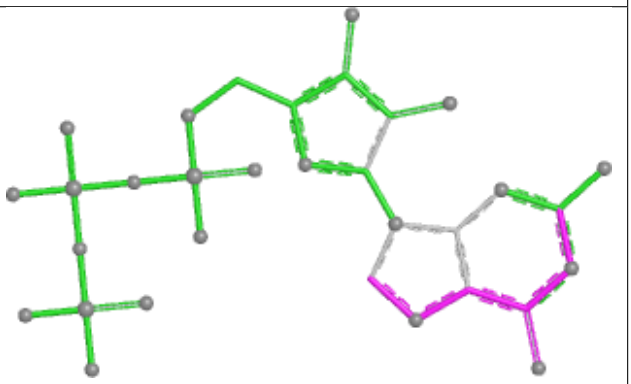
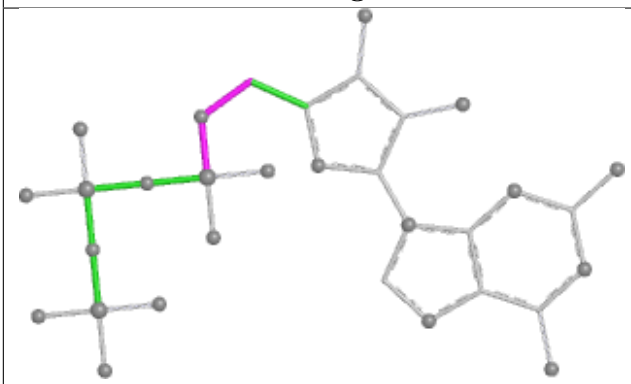
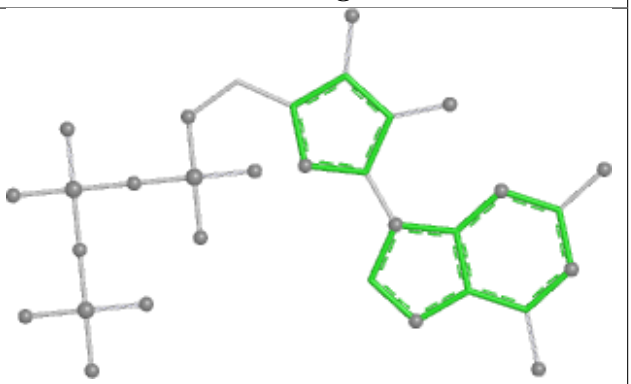
Ligand GTP E2 501



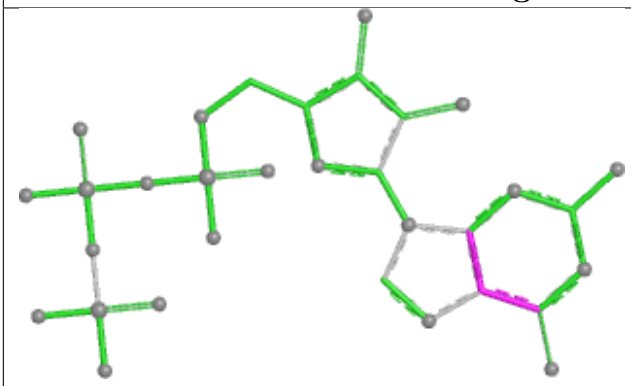
Ligand GDP C9 501



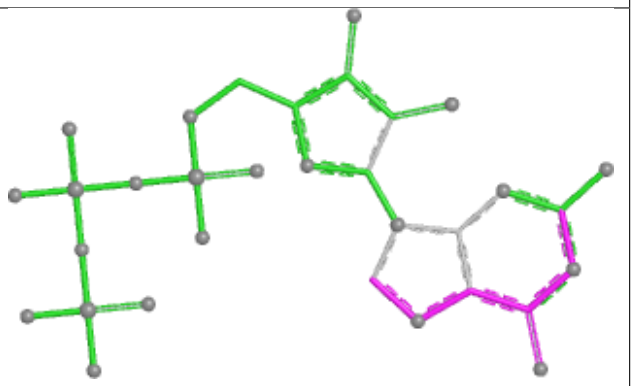
Ligand GDP B7 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GTP A4 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

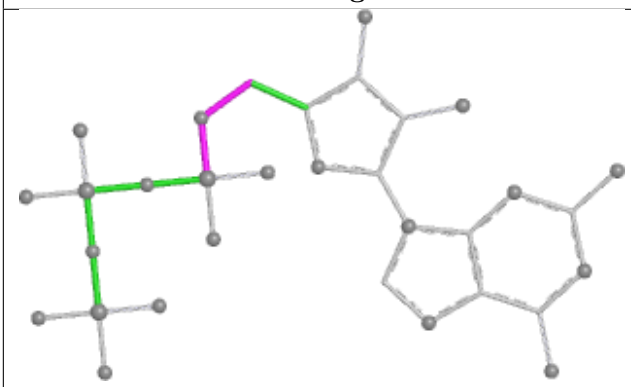
Ligand GTP A8 501



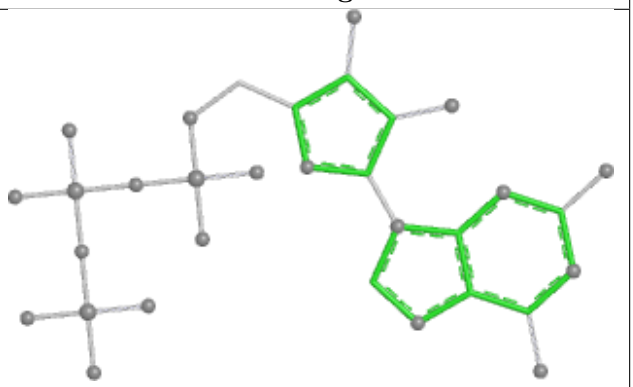
Bond lengths



Bond angles

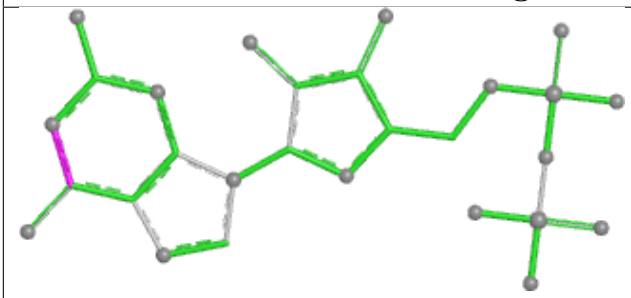


Torsions

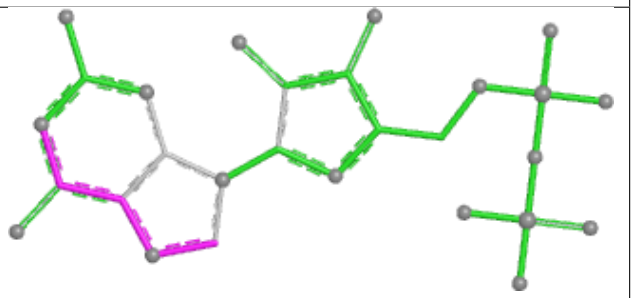


Rings

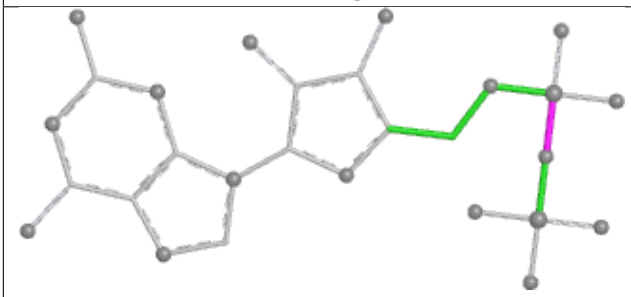
Ligand GDP C7 501



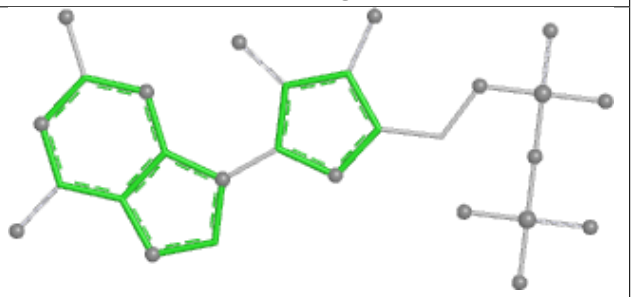
Bond lengths



Bond angles

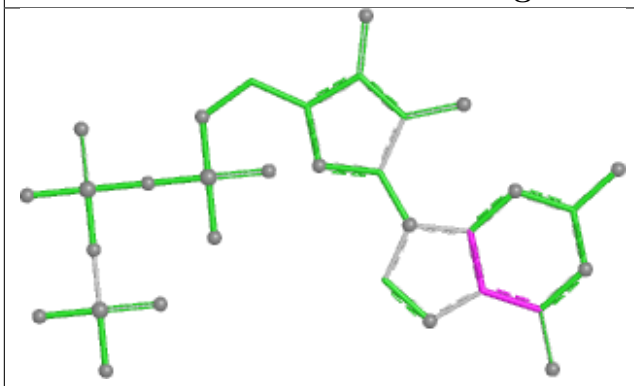


Torsions

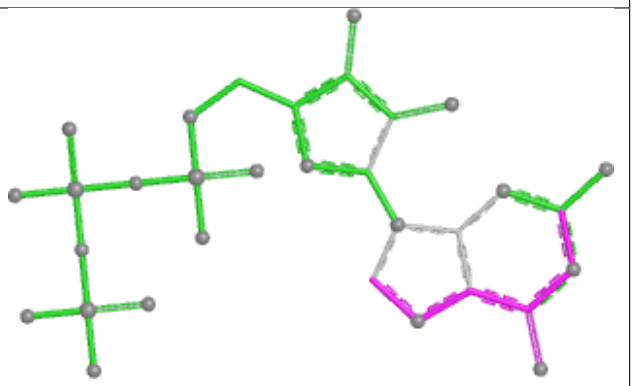


Rings

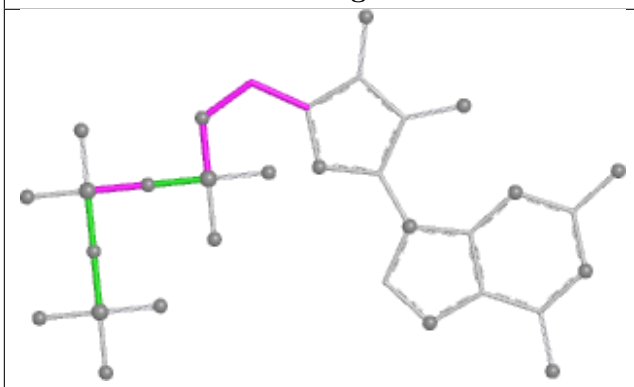
Ligand GTP A2 501



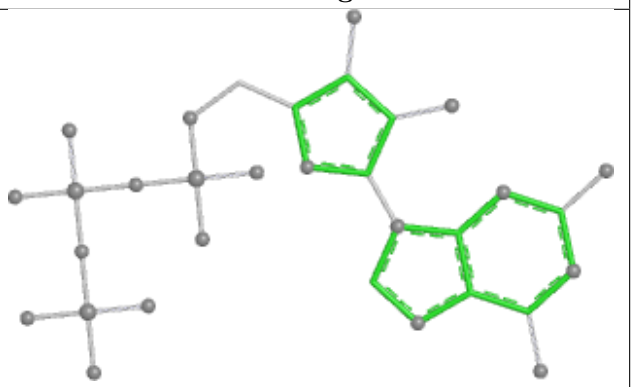
Bond lengths



Bond angles

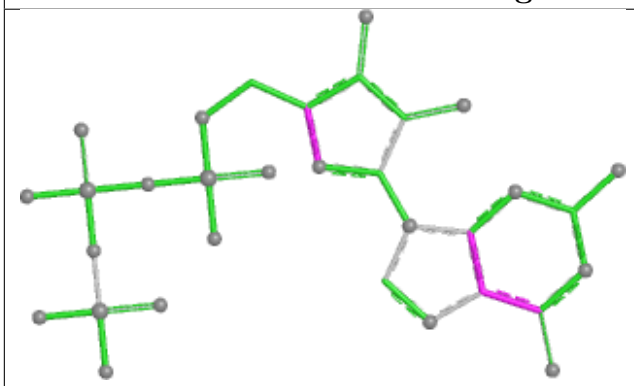


Torsions

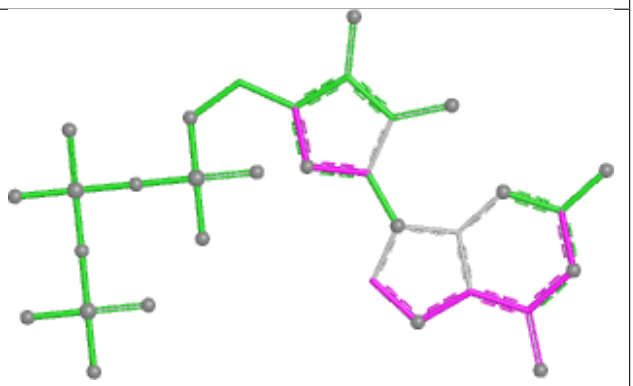


Rings

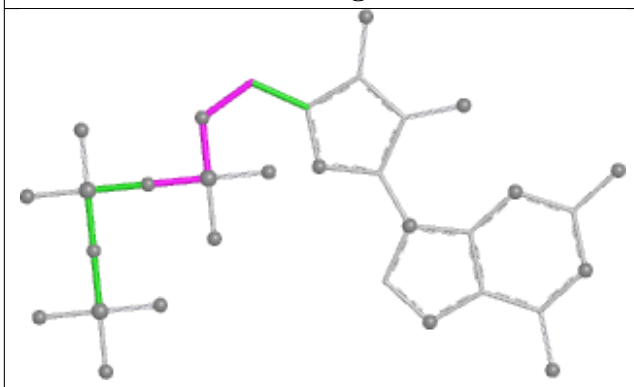
Ligand GTP B2 501



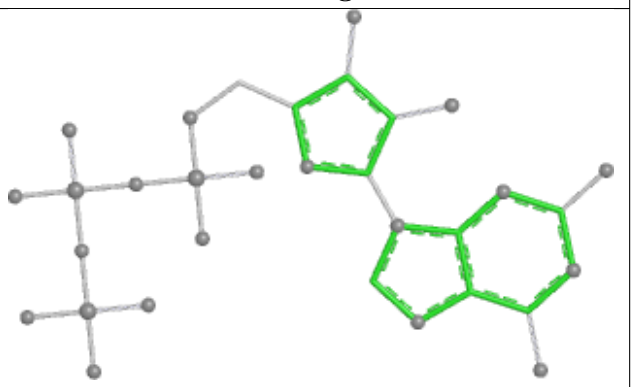
Bond lengths



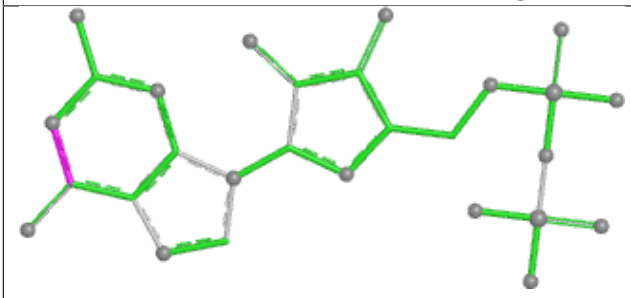
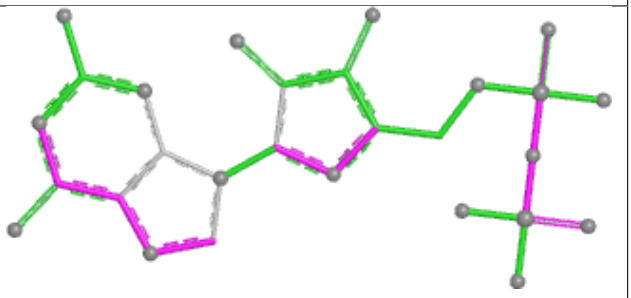
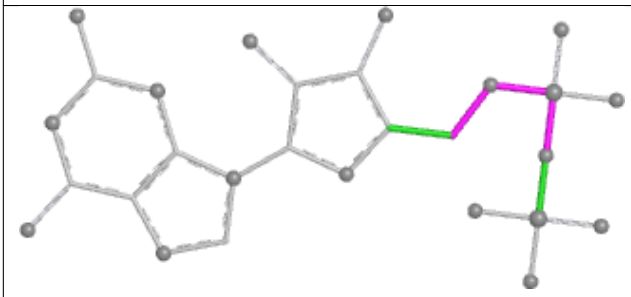
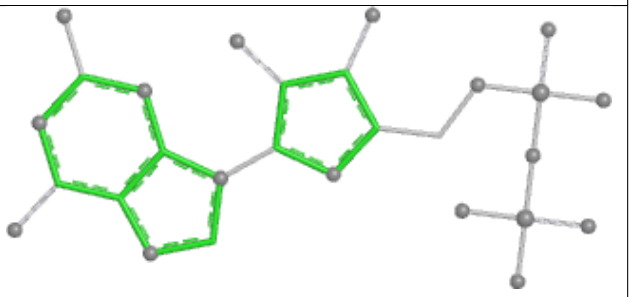
Bond angles

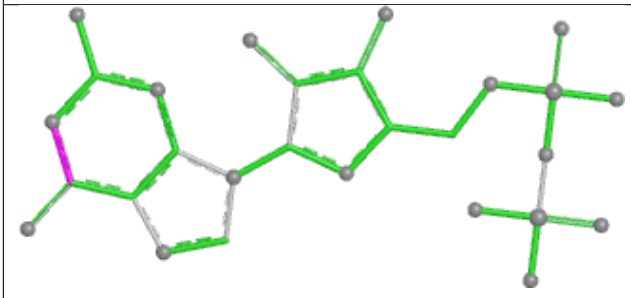
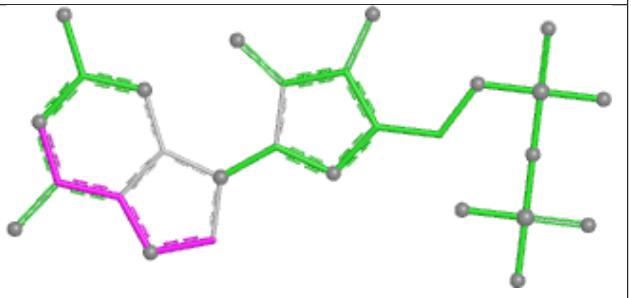
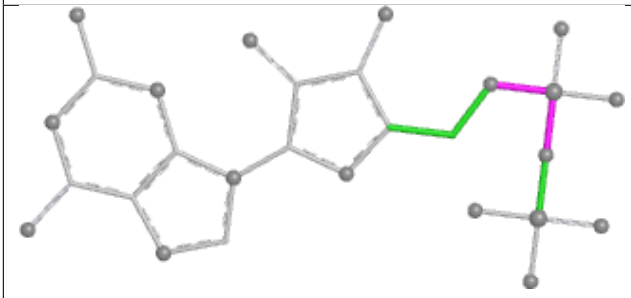
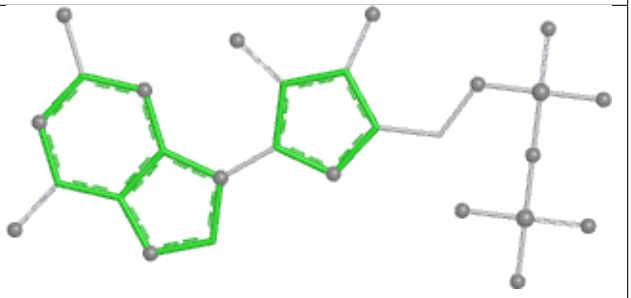


Torsions

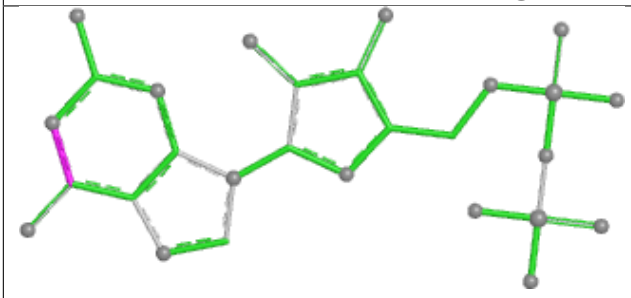


Rings

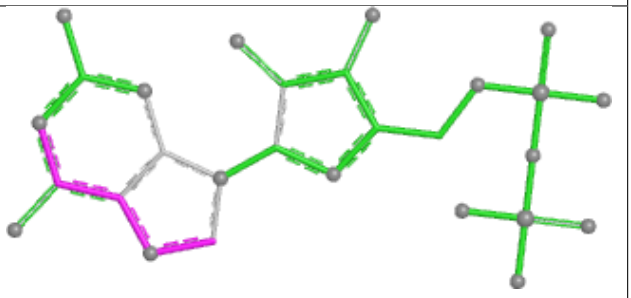
Ligand GDP A9 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP B3 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

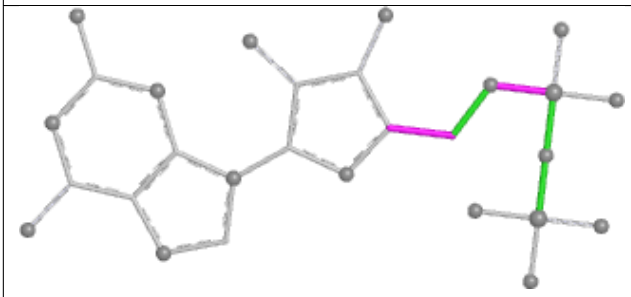
Ligand GDP B5 501



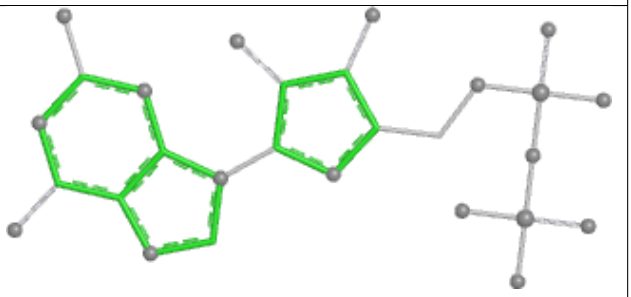
Bond lengths



Bond angles

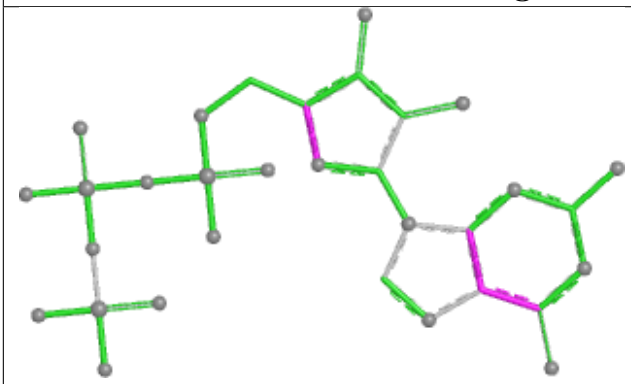


Torsions

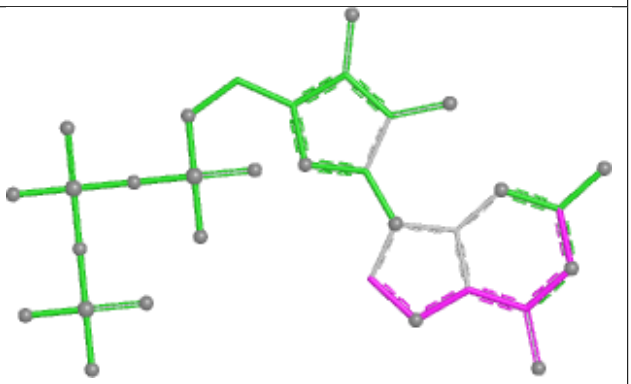


Rings

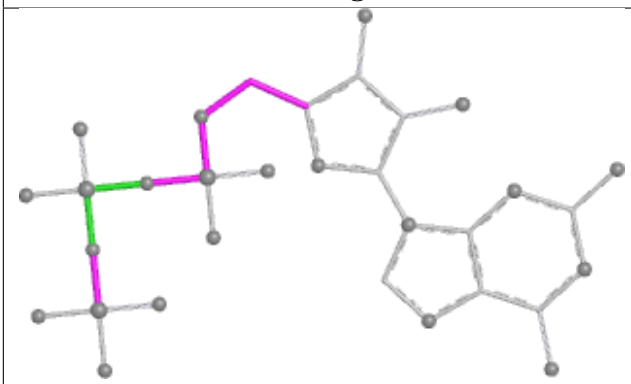
Ligand GTP C0 501



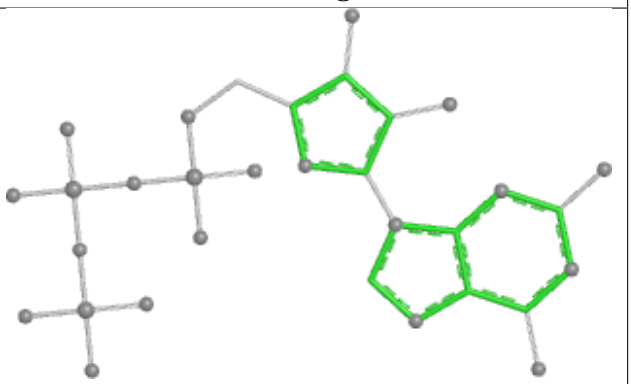
Bond lengths



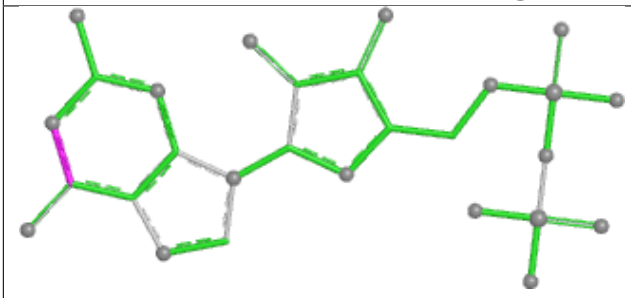
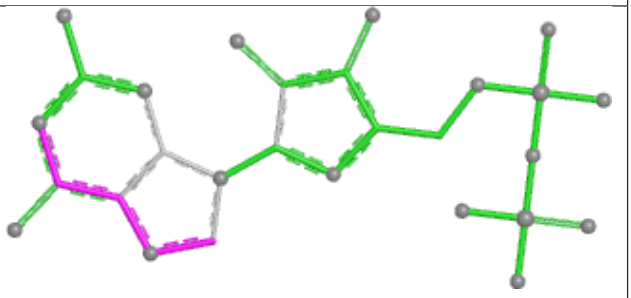
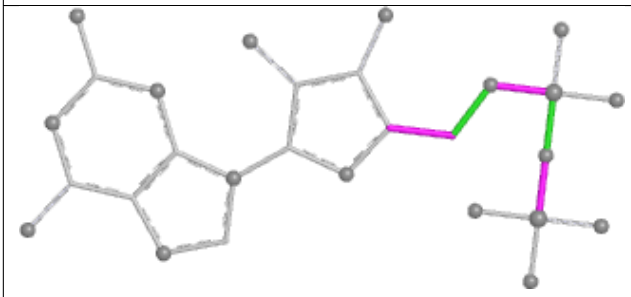
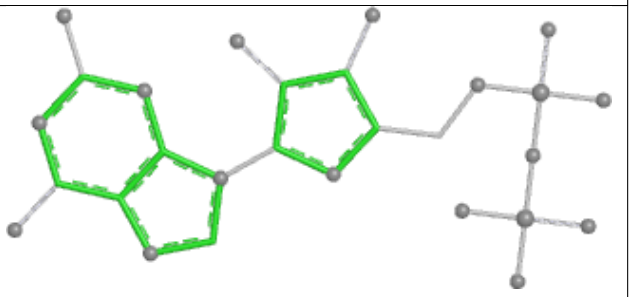
Bond angles

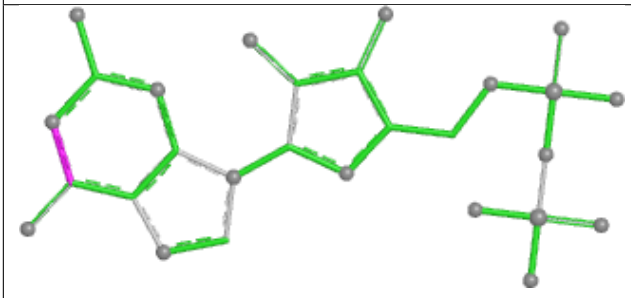
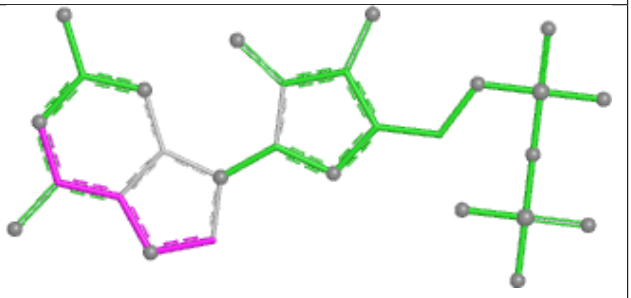
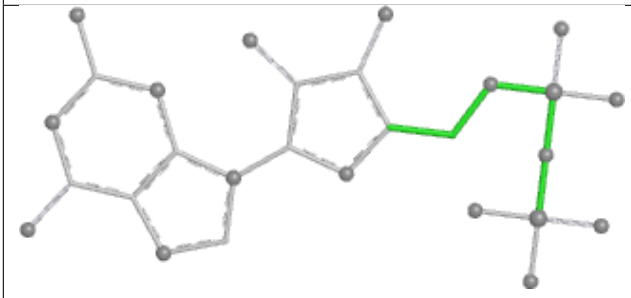
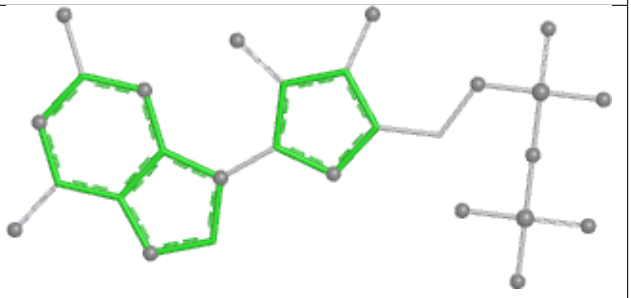


Torsions

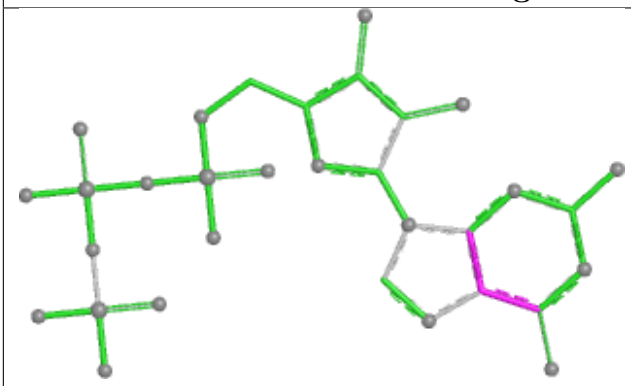


Rings

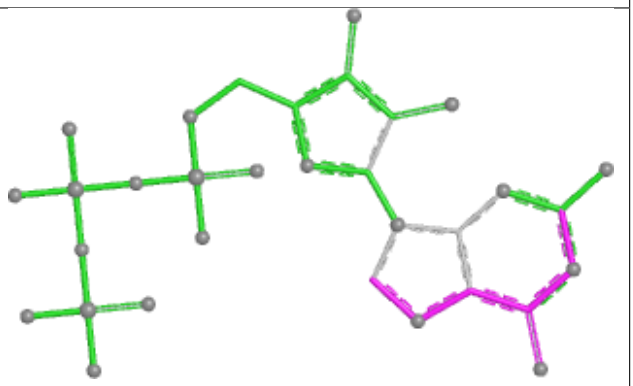
Ligand GDP D5 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP E3 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

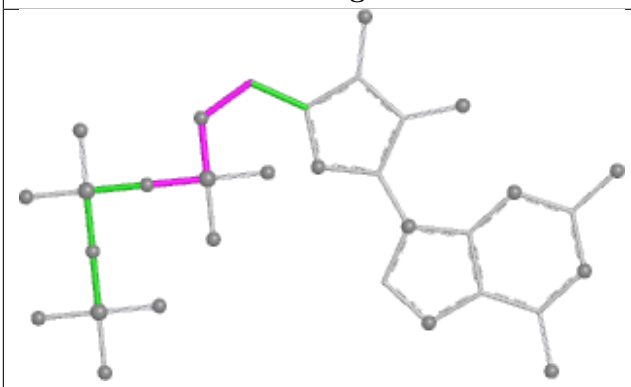
Ligand GTP D8 501



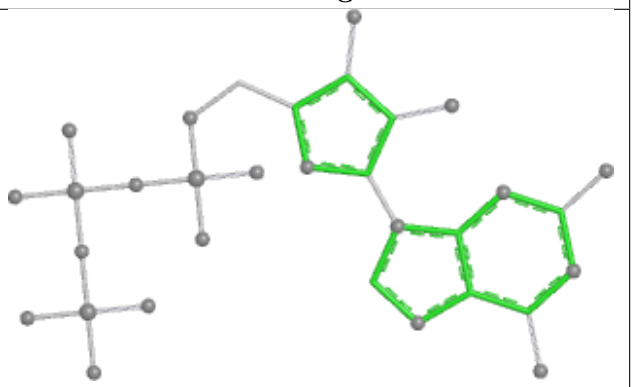
Bond lengths



Bond angles

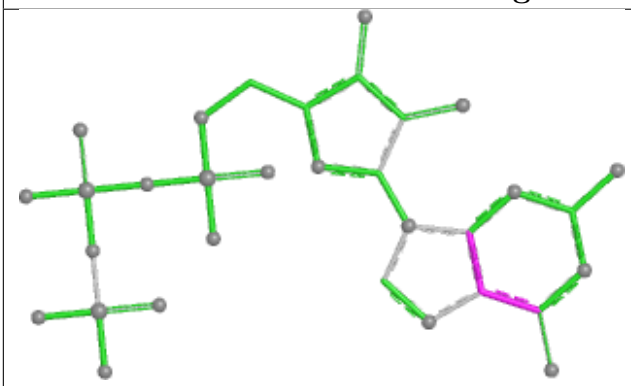


Torsions

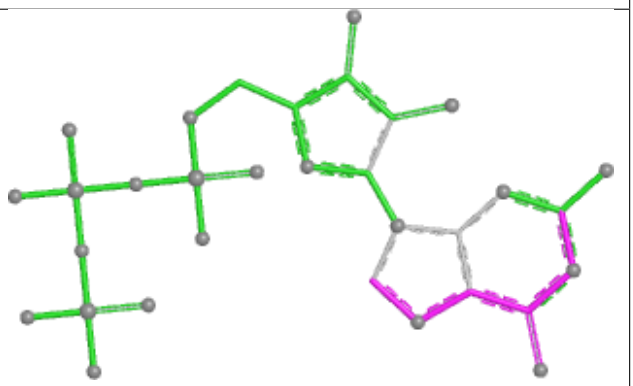


Rings

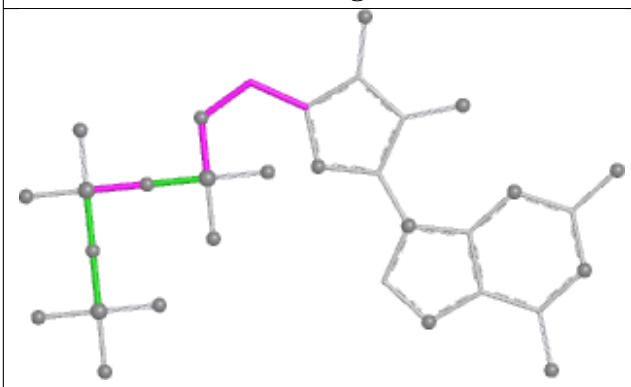
Ligand GTP D2 501



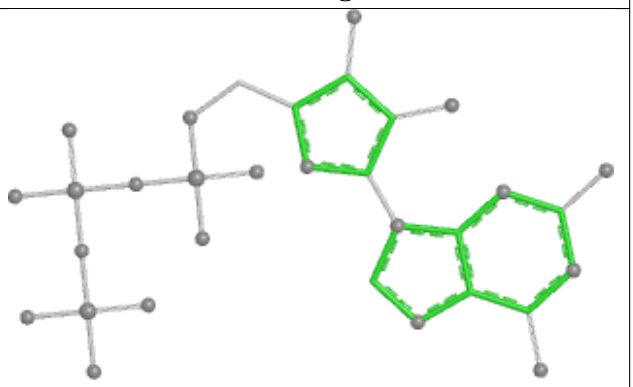
Bond lengths



Bond angles

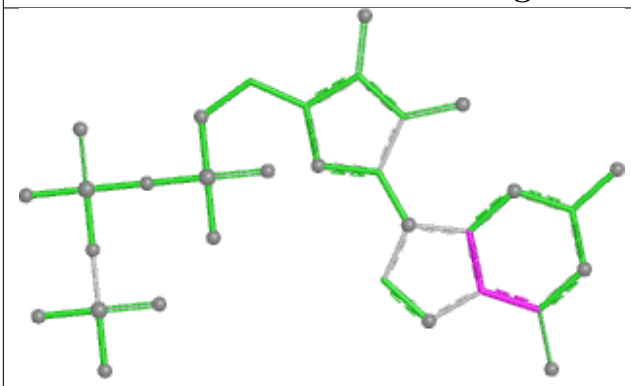


Torsions

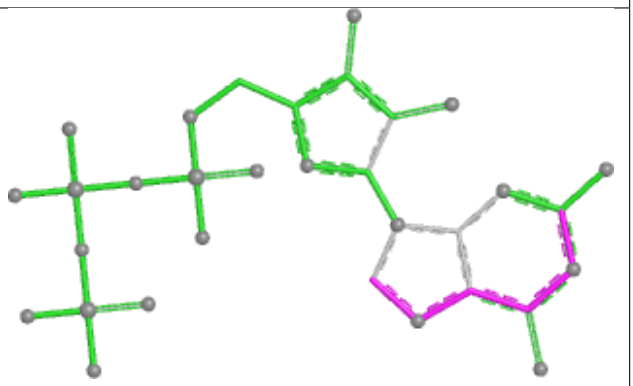


Rings

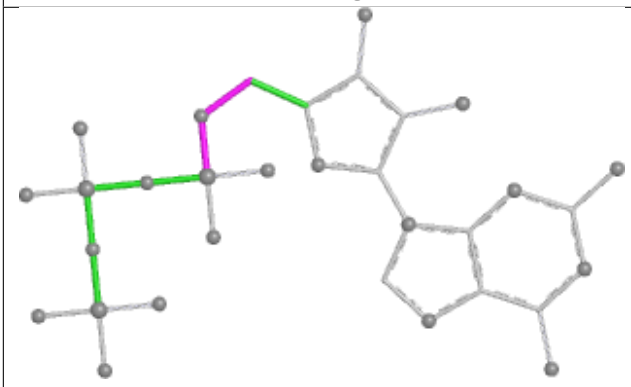
Ligand GTP C2 501



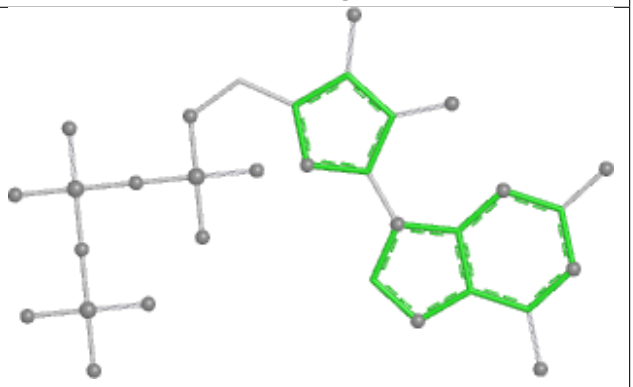
Bond lengths



Bond angles

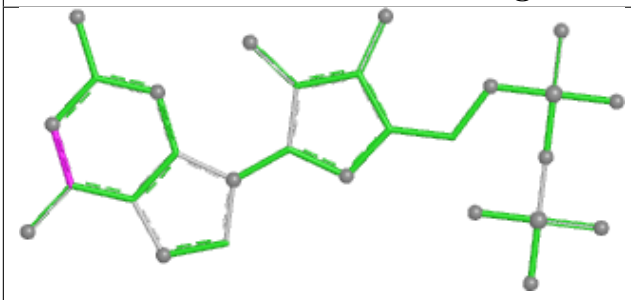


Torsions

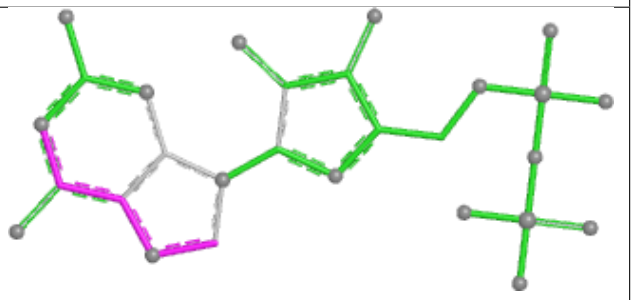


Rings

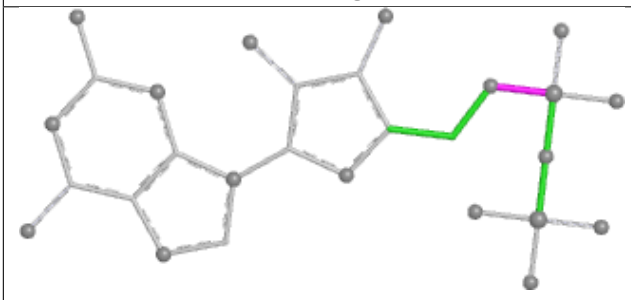
Ligand GDP E1 501



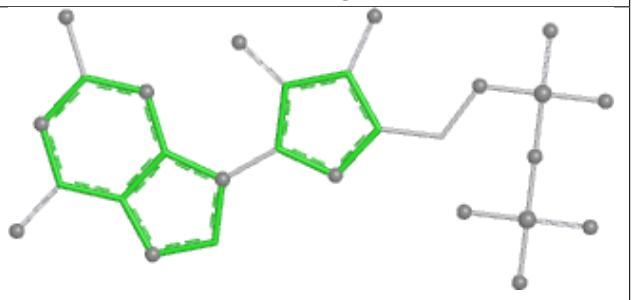
Bond lengths



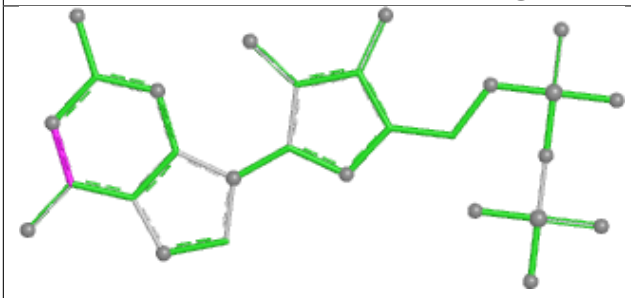
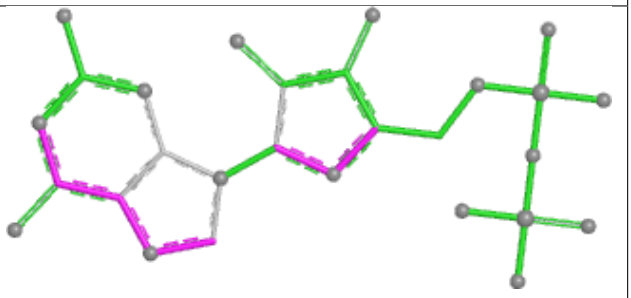
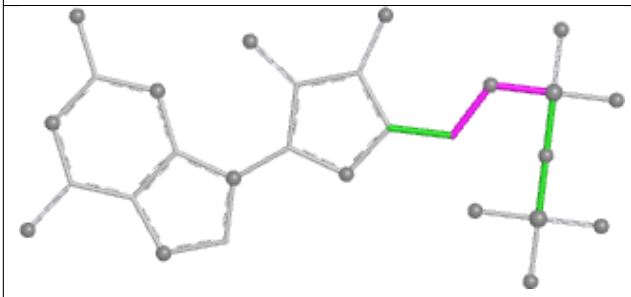
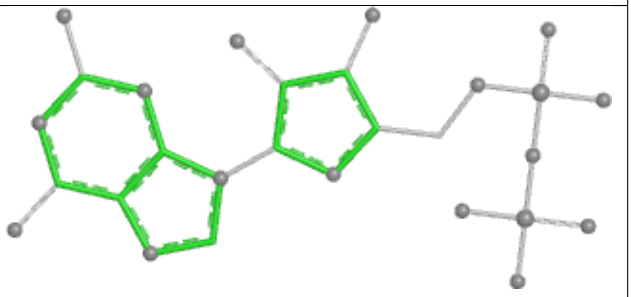
Bond angles

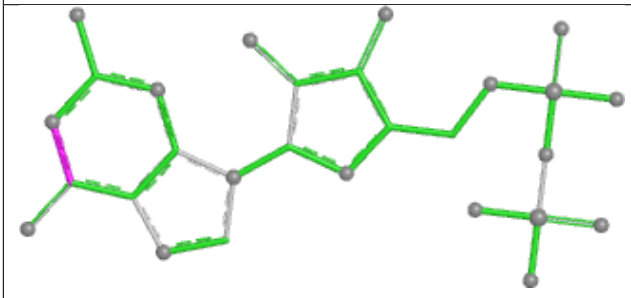
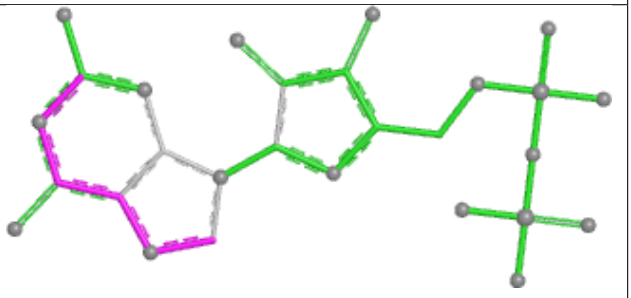
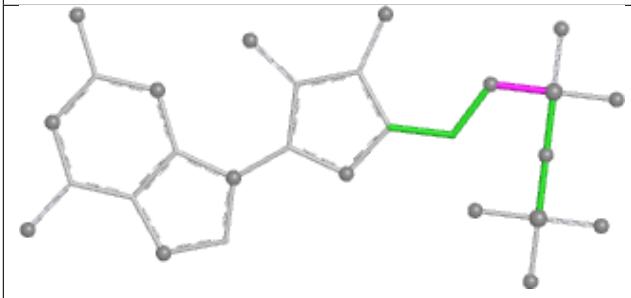
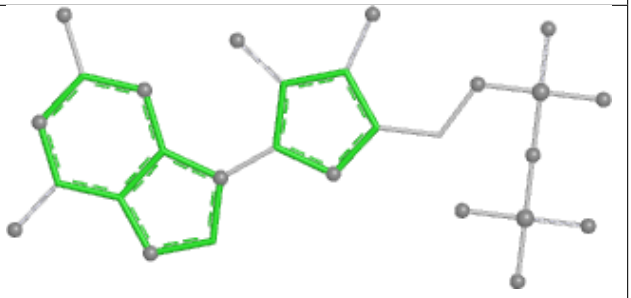


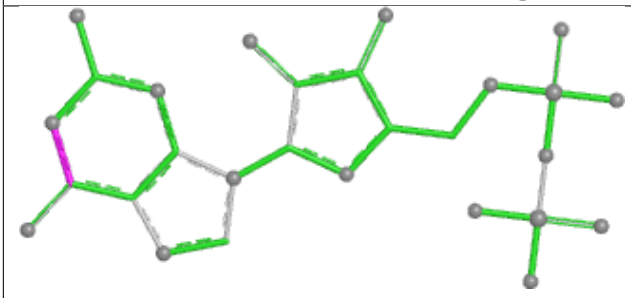
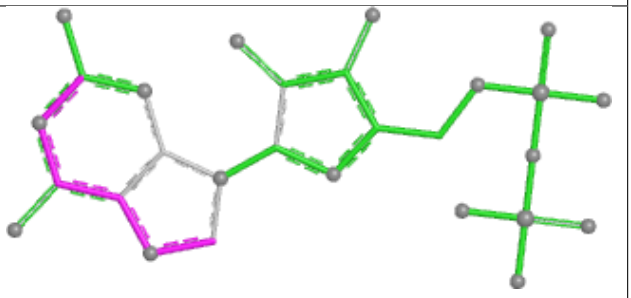
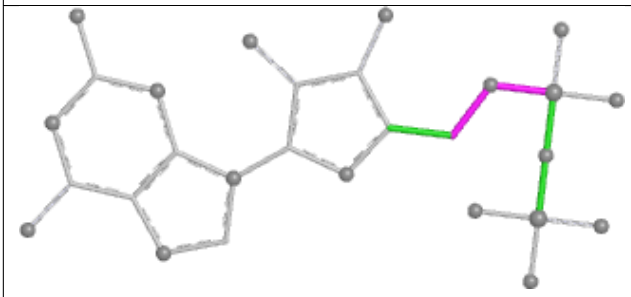
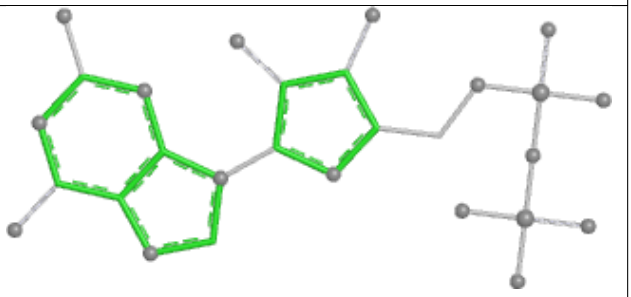
Torsions

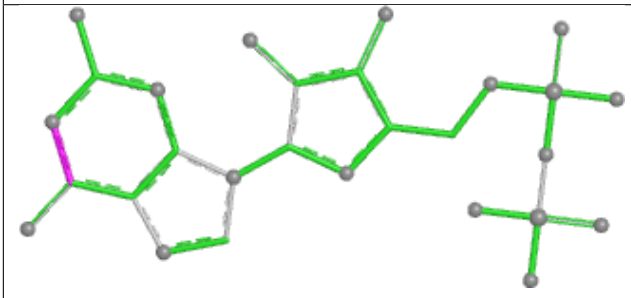
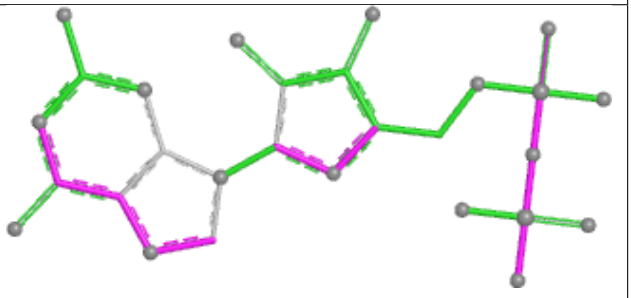
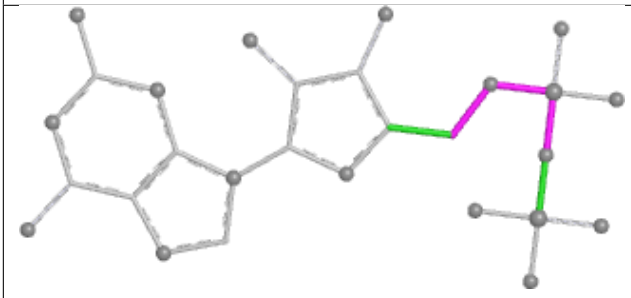
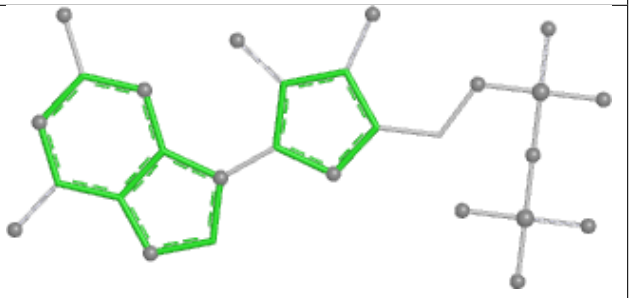


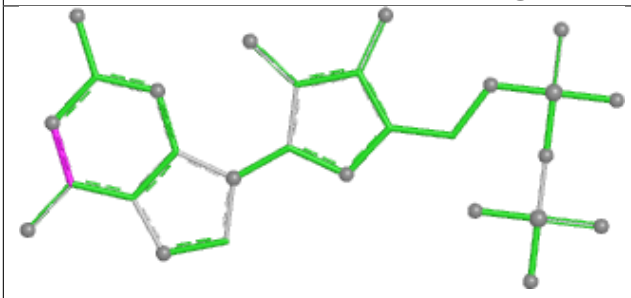
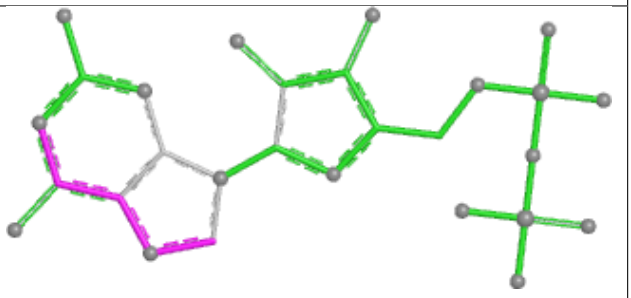
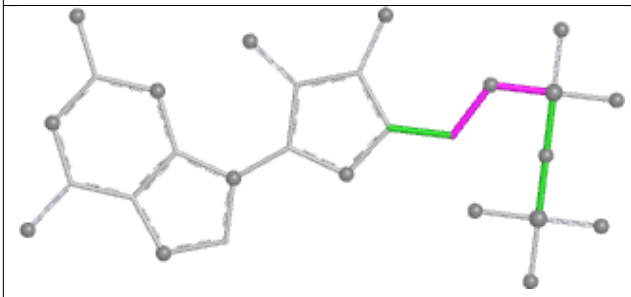
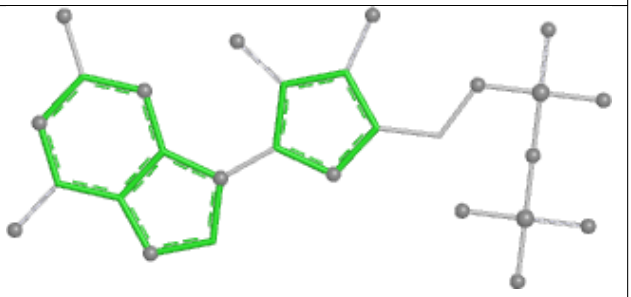
Rings

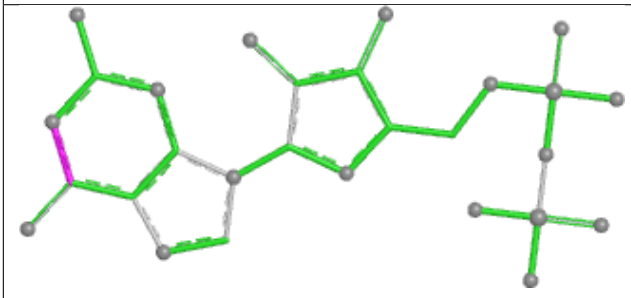
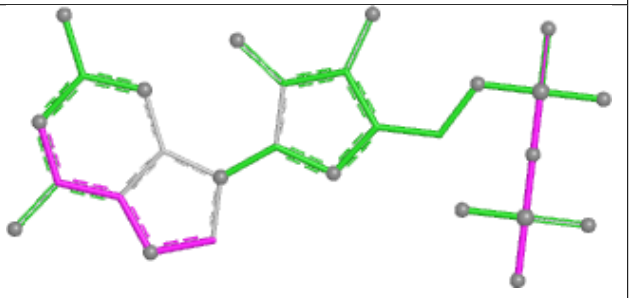
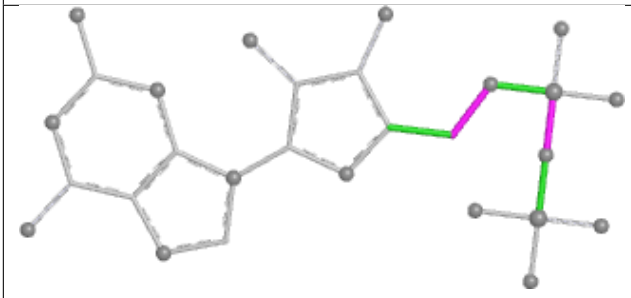
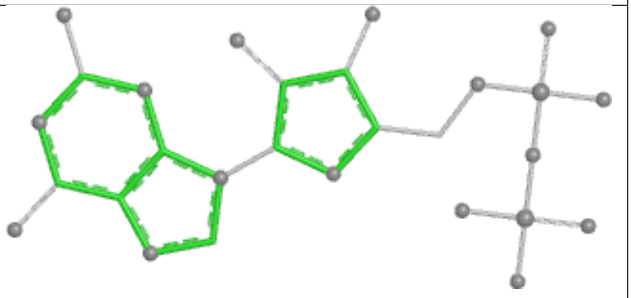
Ligand GDP C3 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand GDP D1 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

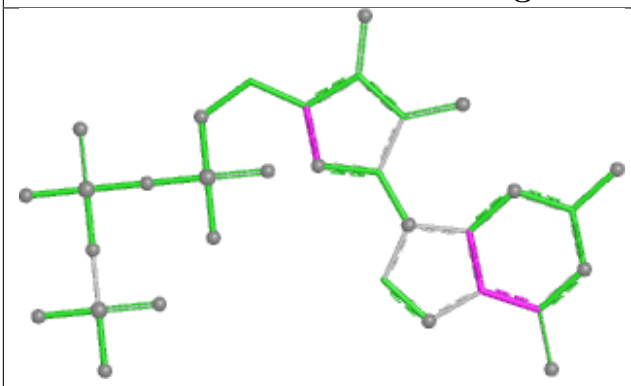
Ligand GDP F1 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP C5 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

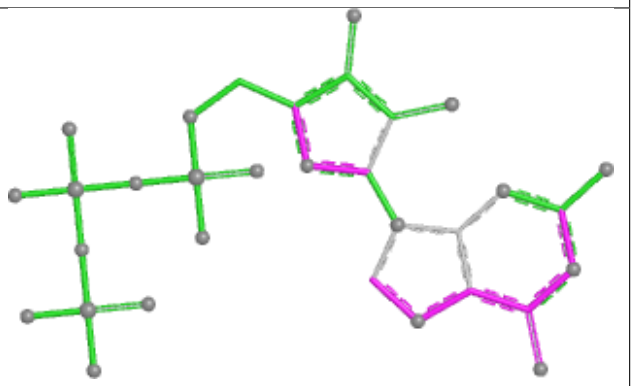
Ligand GDP D7 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand GDP E5 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

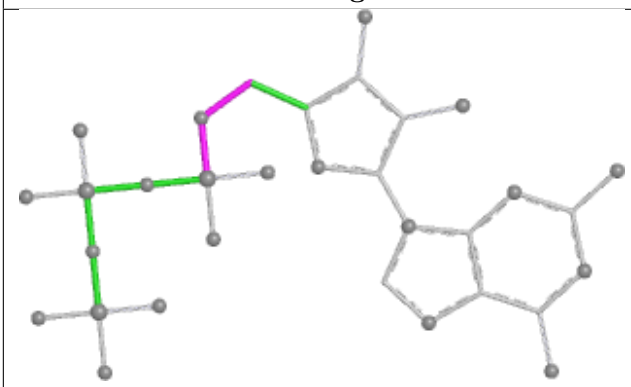
Ligand GTP B4 501



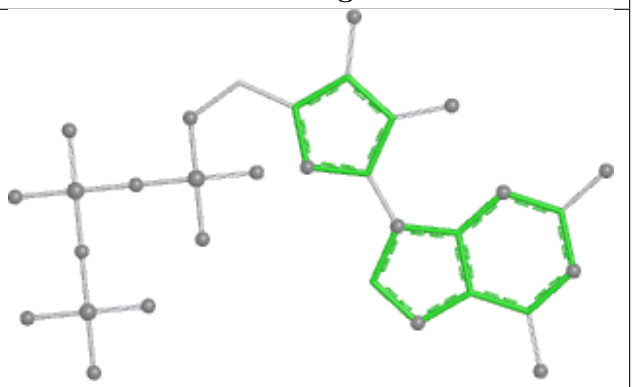
Bond lengths



Bond angles

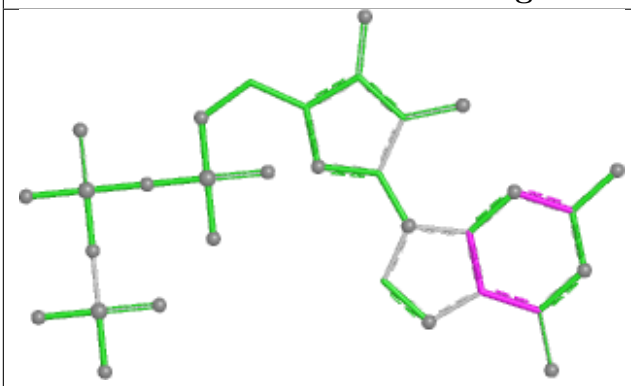


Torsions

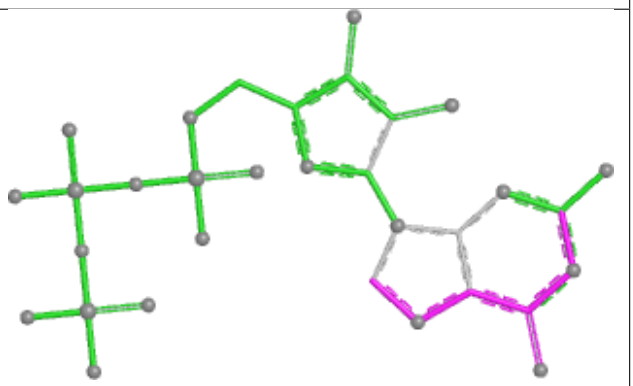


Rings

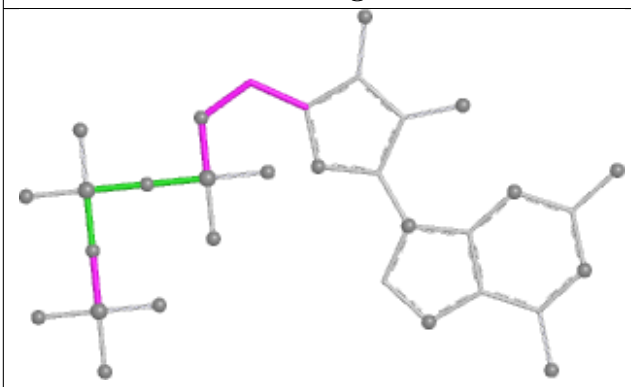
Ligand GTP F0 501



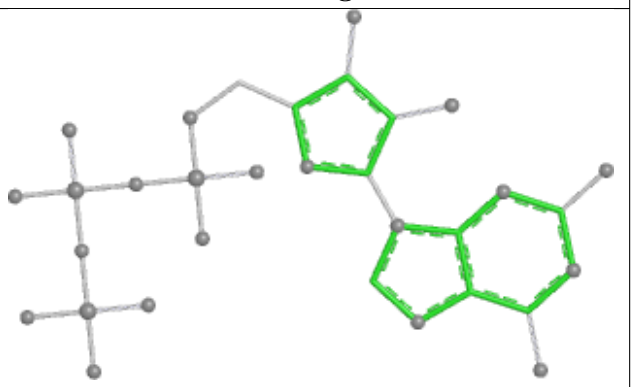
Bond lengths



Bond angles

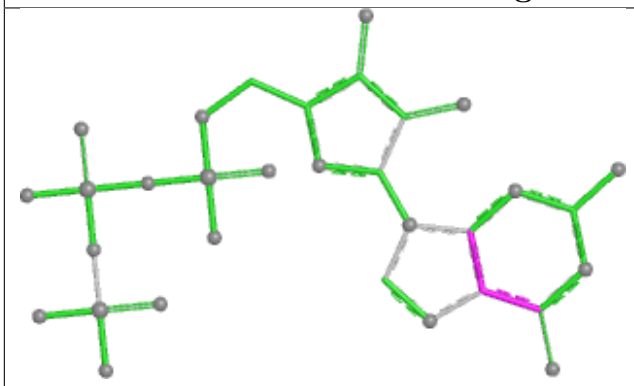


Torsions

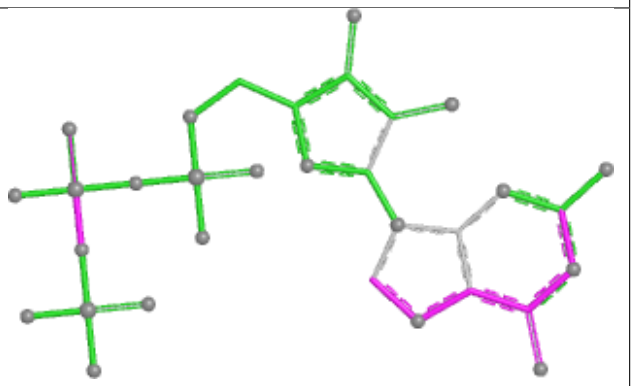


Rings

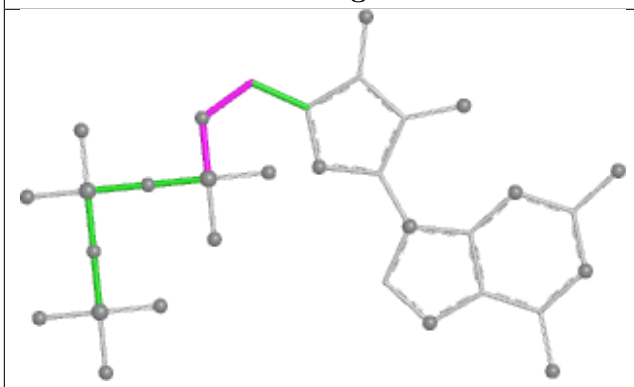
Ligand GTP C6 501



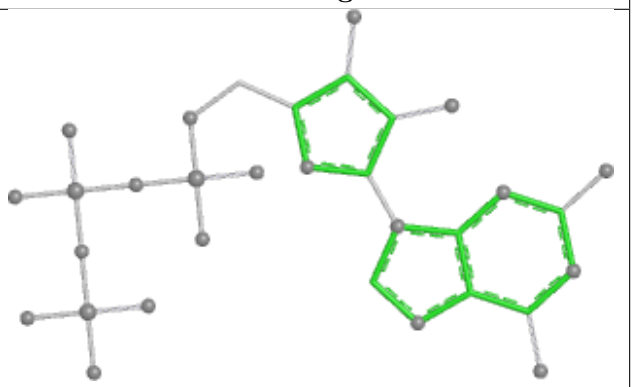
Bond lengths



Bond angles

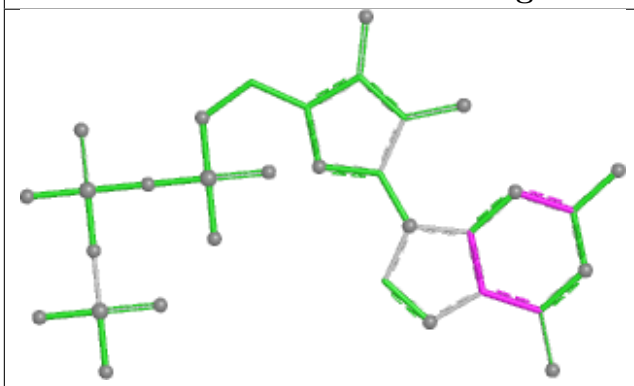


Torsions

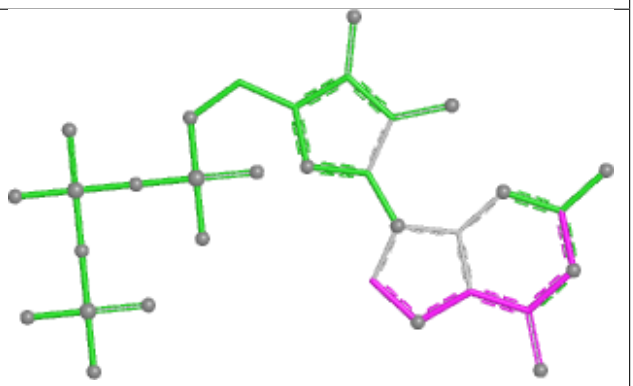


Rings

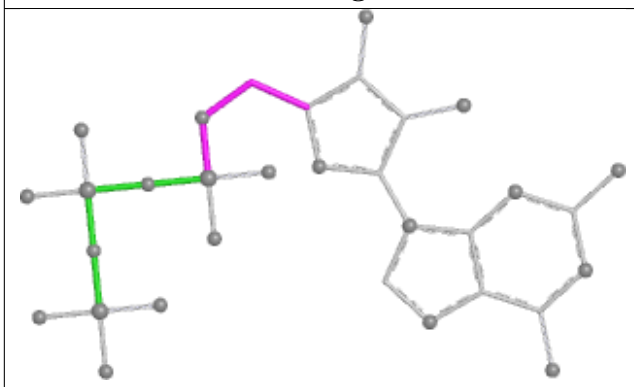
Ligand GTP E8 501



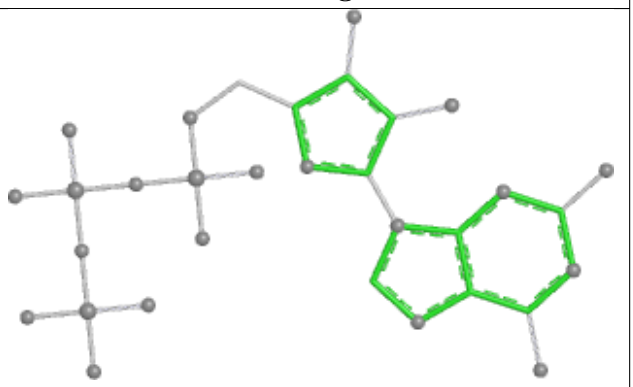
Bond lengths



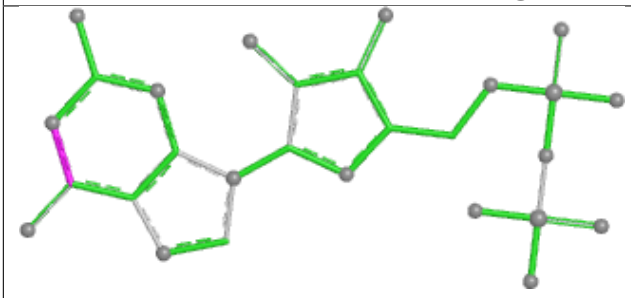
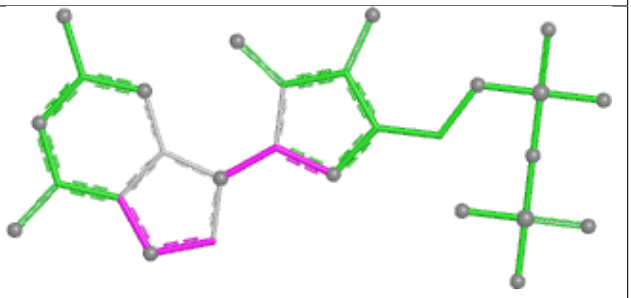
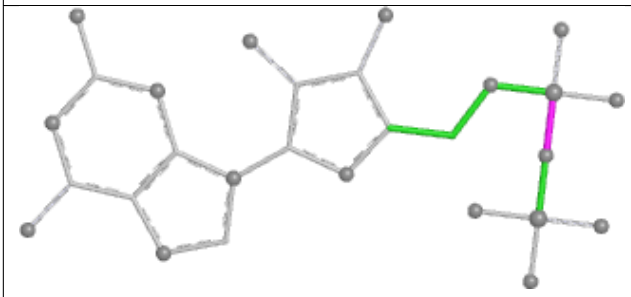
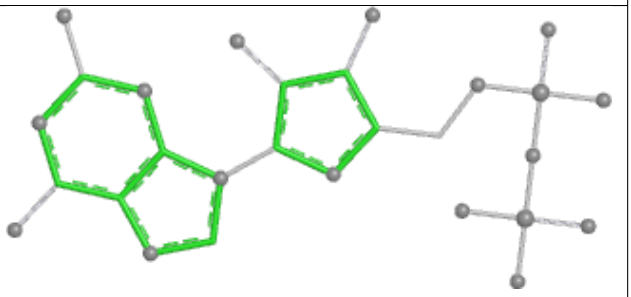
Bond angles

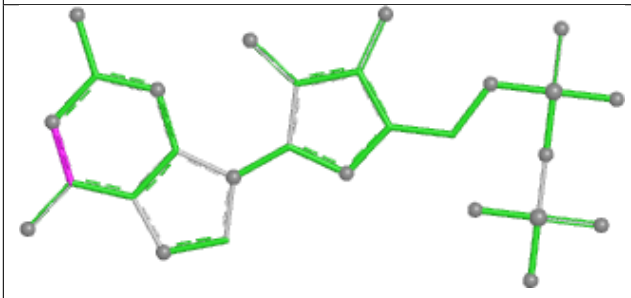
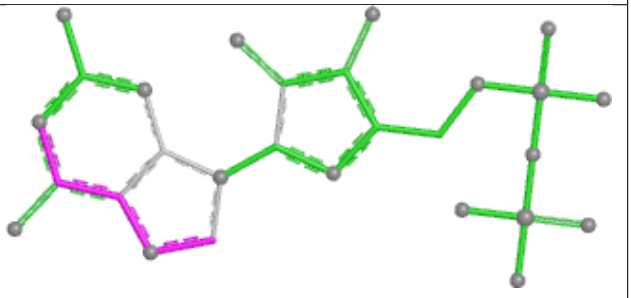
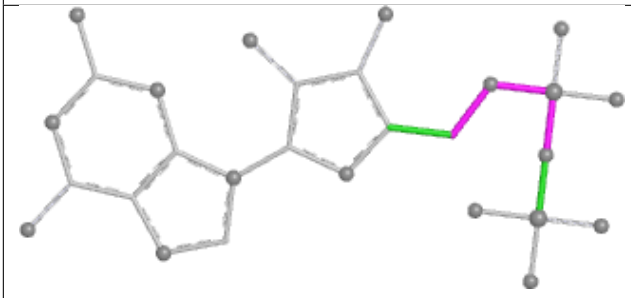
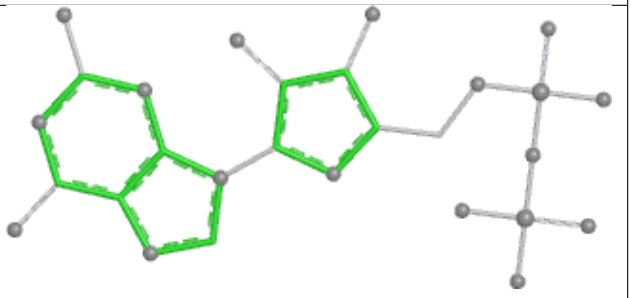


Torsions

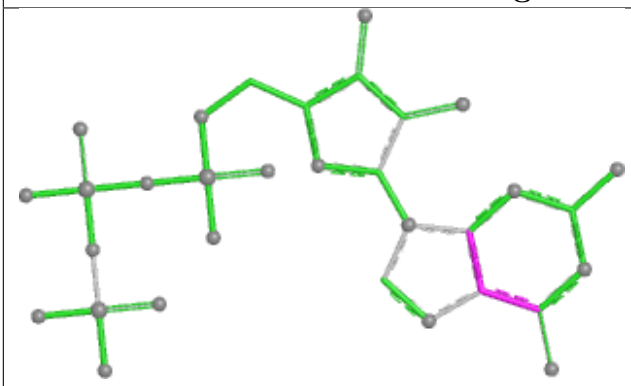


Rings

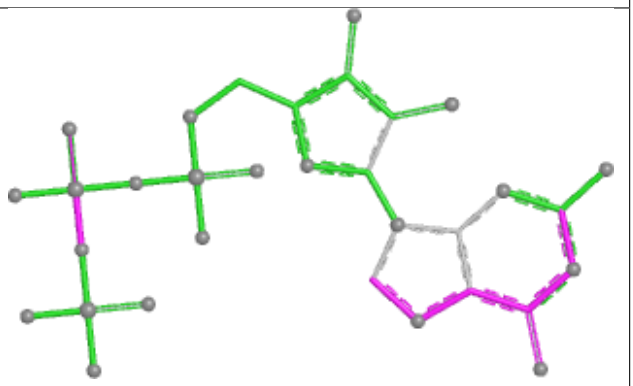
Ligand GDP A3 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP B1 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

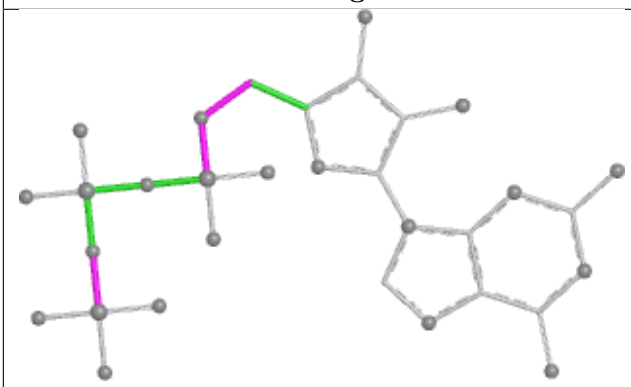
Ligand GTP C4 501



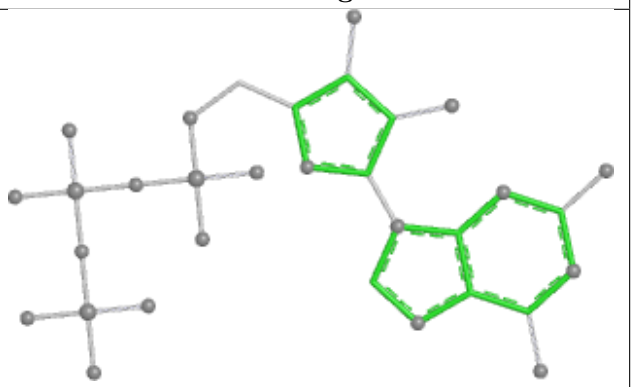
Bond lengths



Bond angles

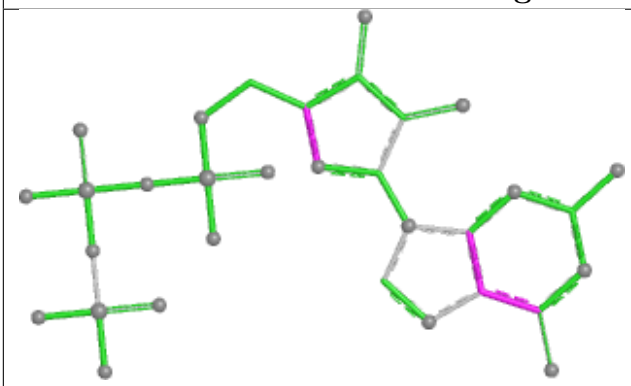


Torsions

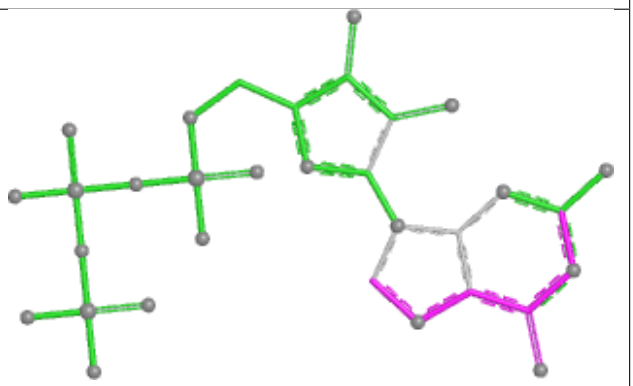


Rings

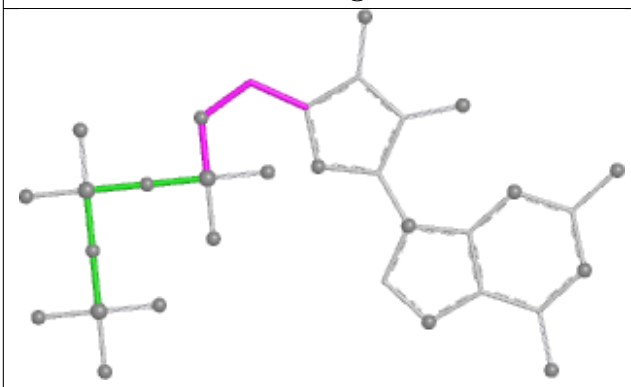
Ligand GTP B8 501



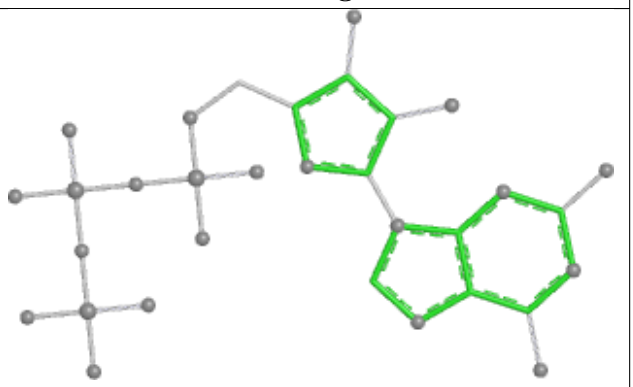
Bond lengths



Bond angles

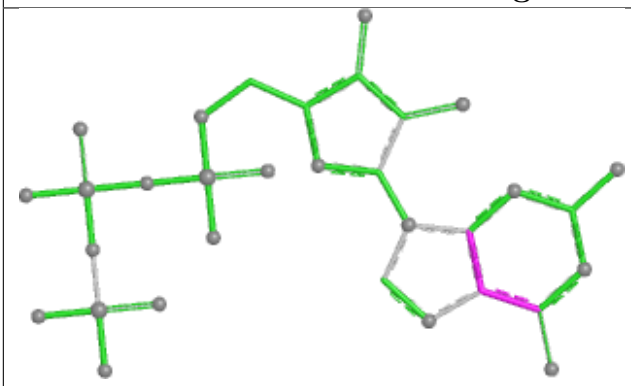


Torsions

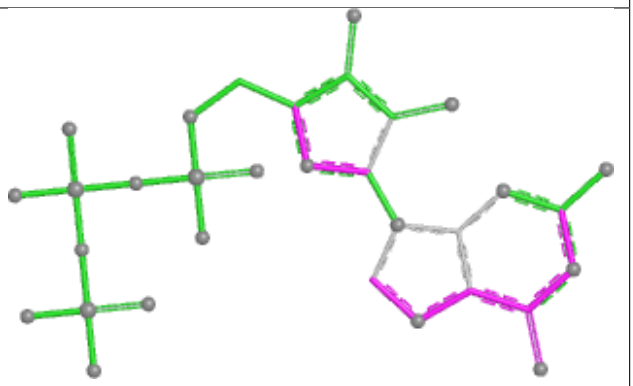


Rings

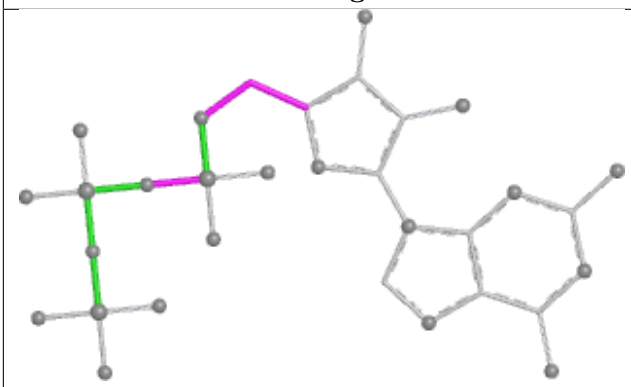
Ligand GTP D4 501



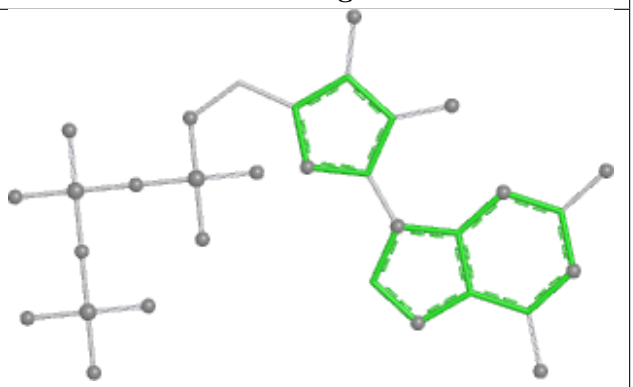
Bond lengths



Bond angles

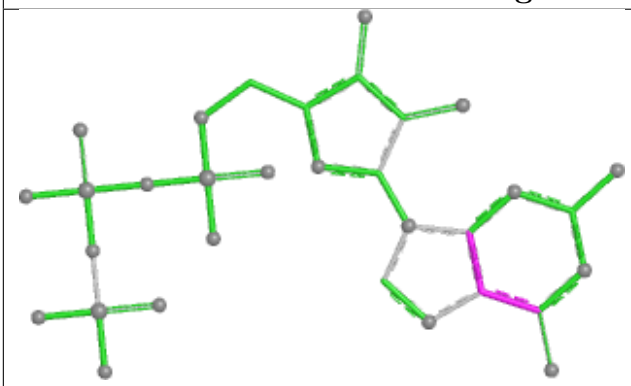


Torsions

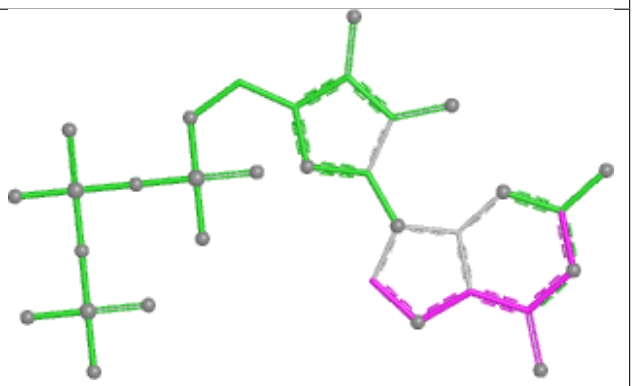


Rings

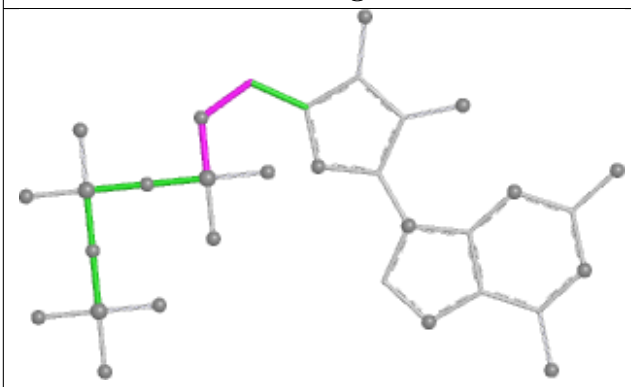
Ligand GTP E0 501



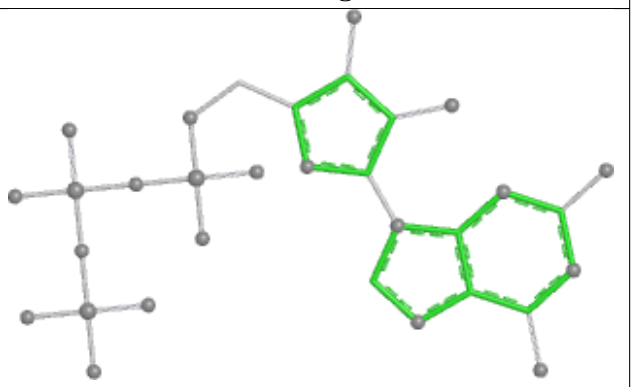
Bond lengths



Bond angles

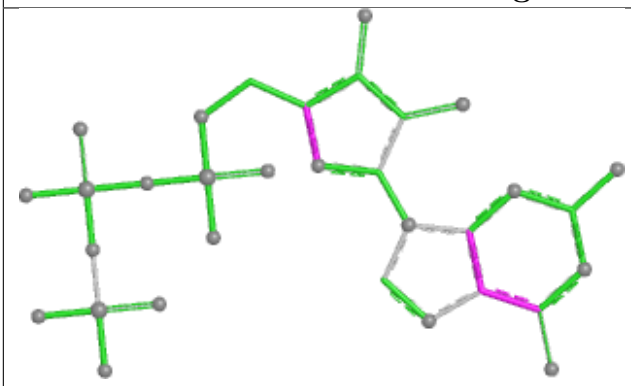


Torsions

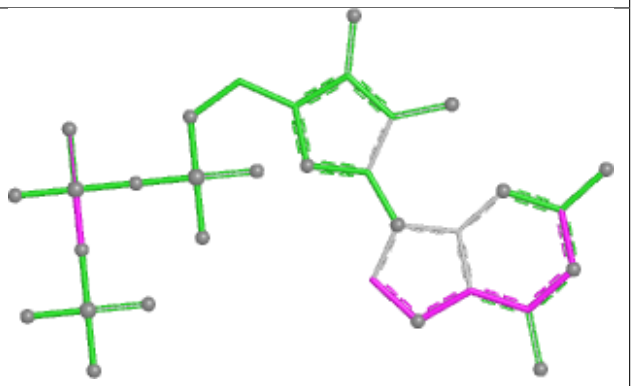


Rings

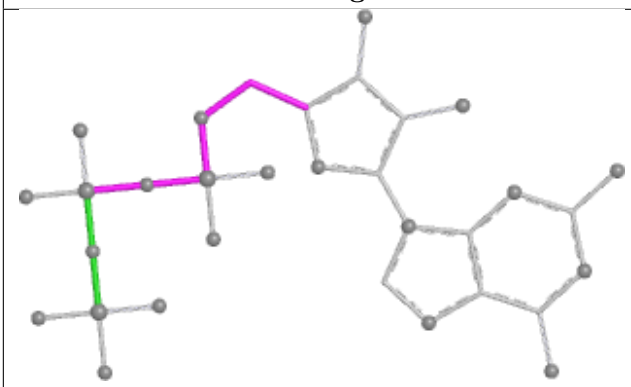
Ligand GTP A0 501



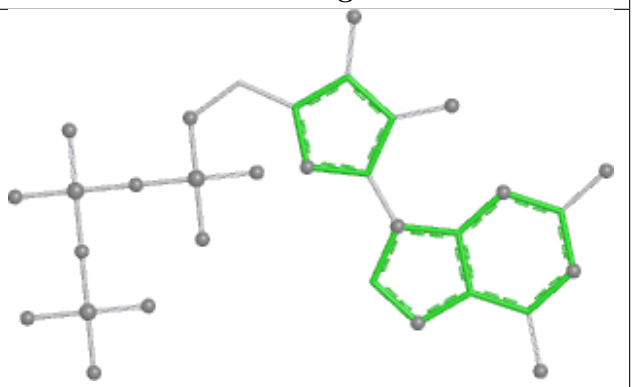
Bond lengths



Bond angles

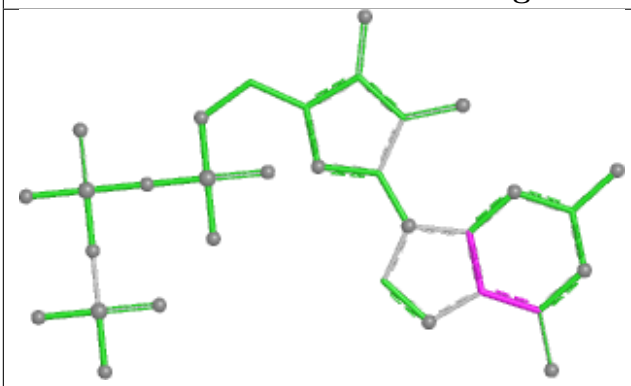


Torsions

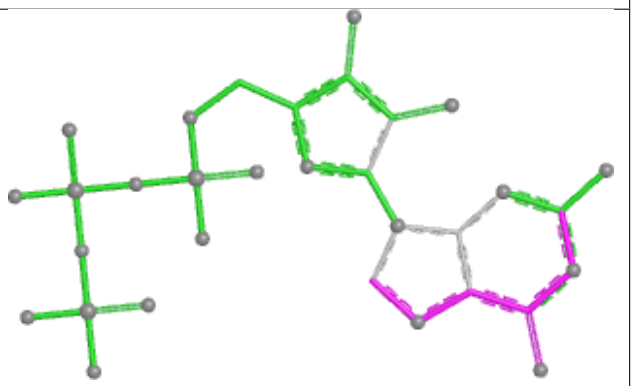


Rings

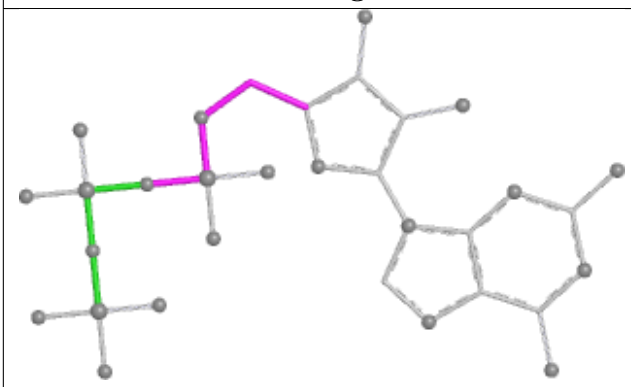
Ligand GTP D6 501



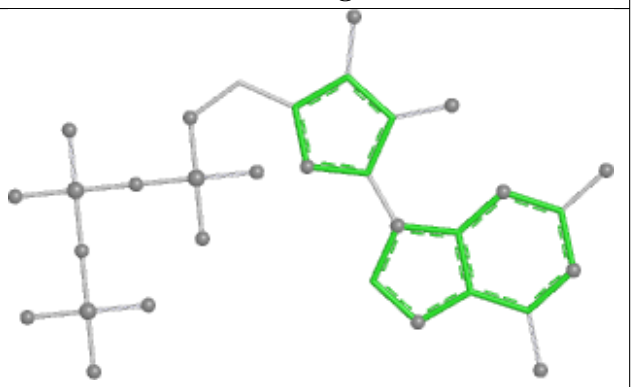
Bond lengths



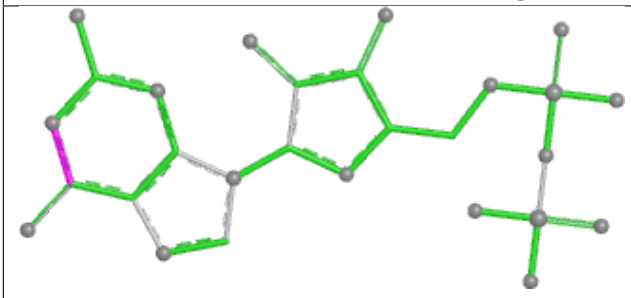
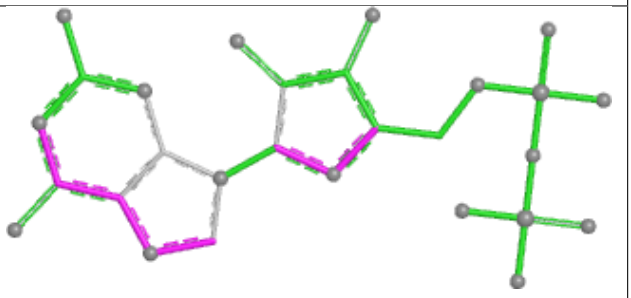
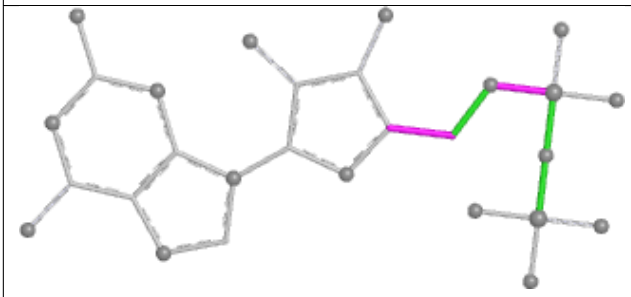
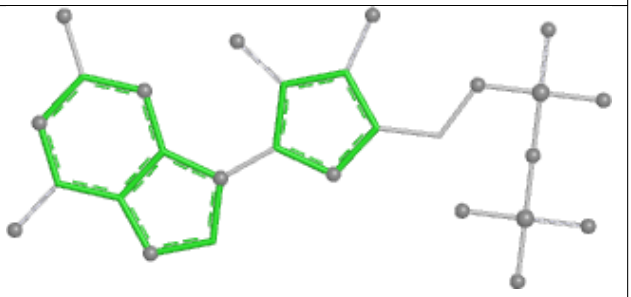
Bond angles

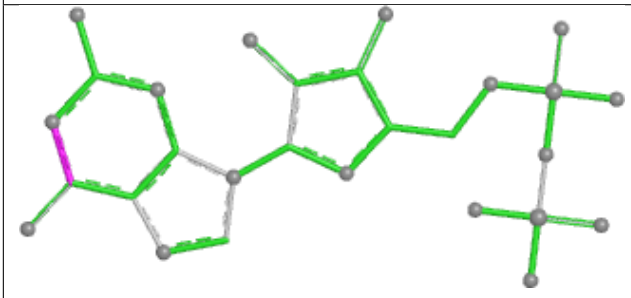
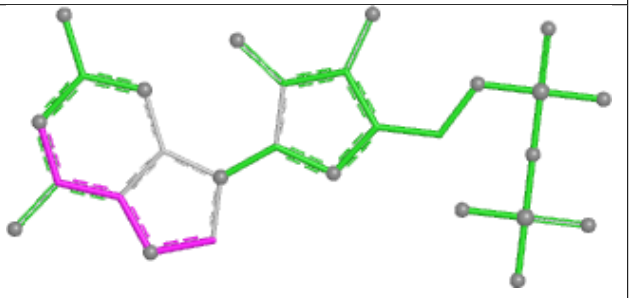
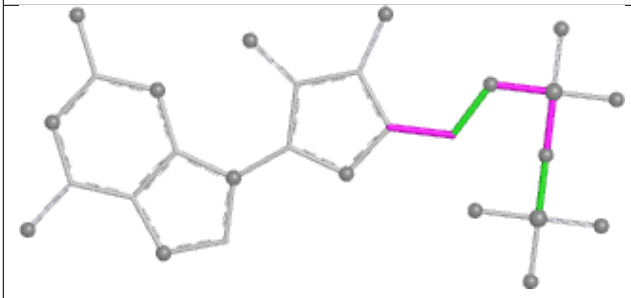
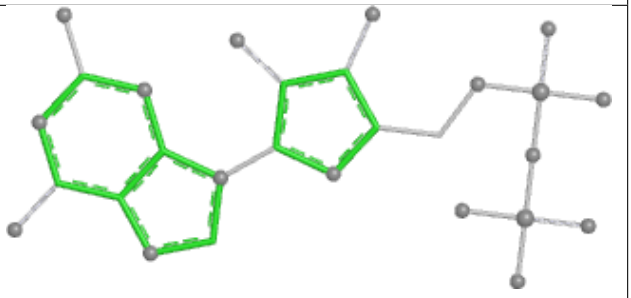


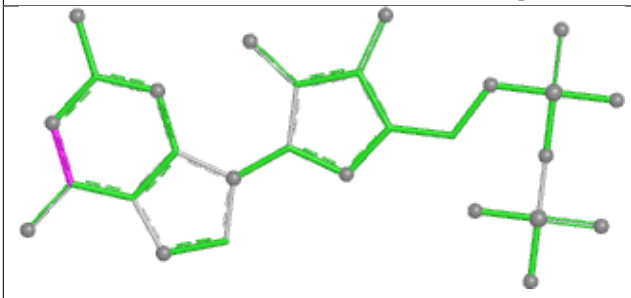
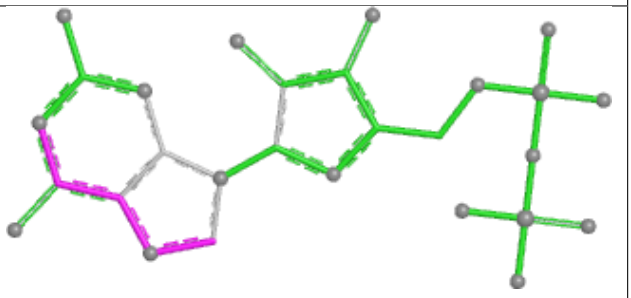
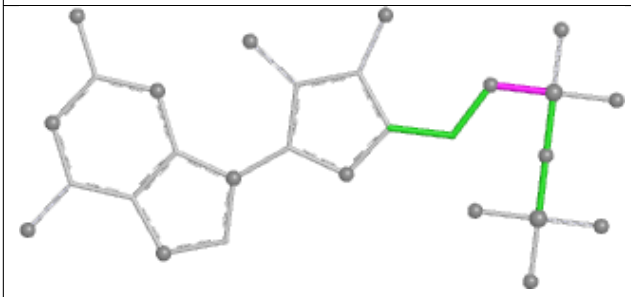
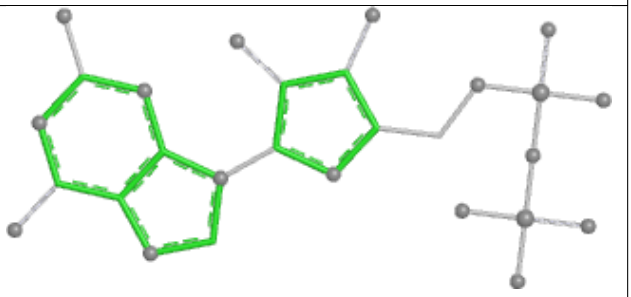
Torsions

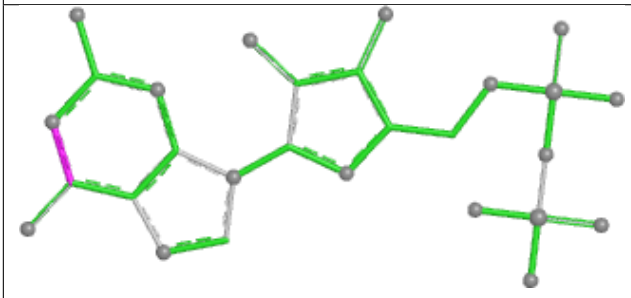
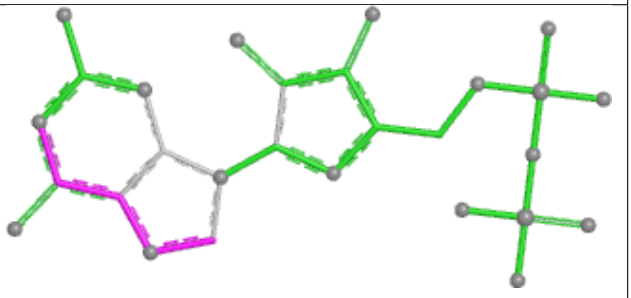
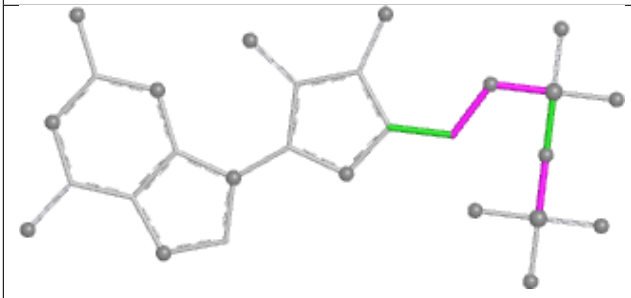
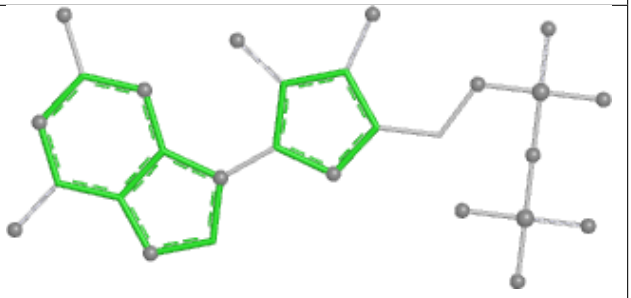


Rings

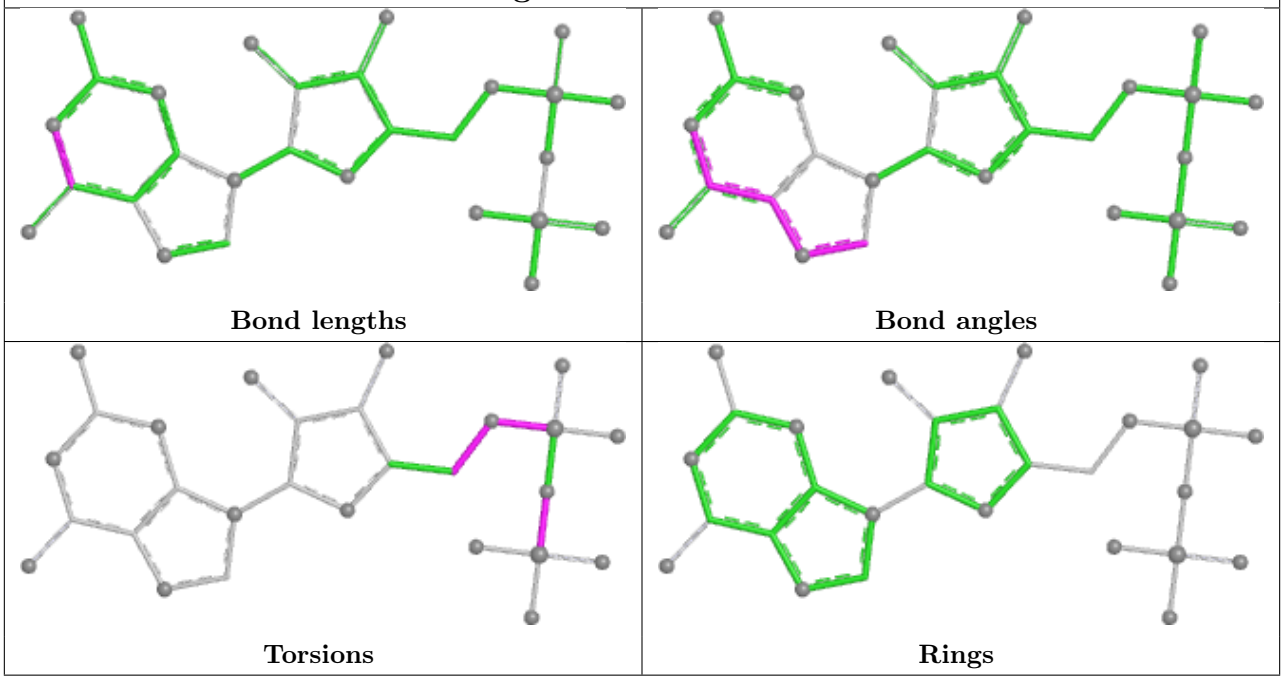
Ligand GDP A7 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP D3 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

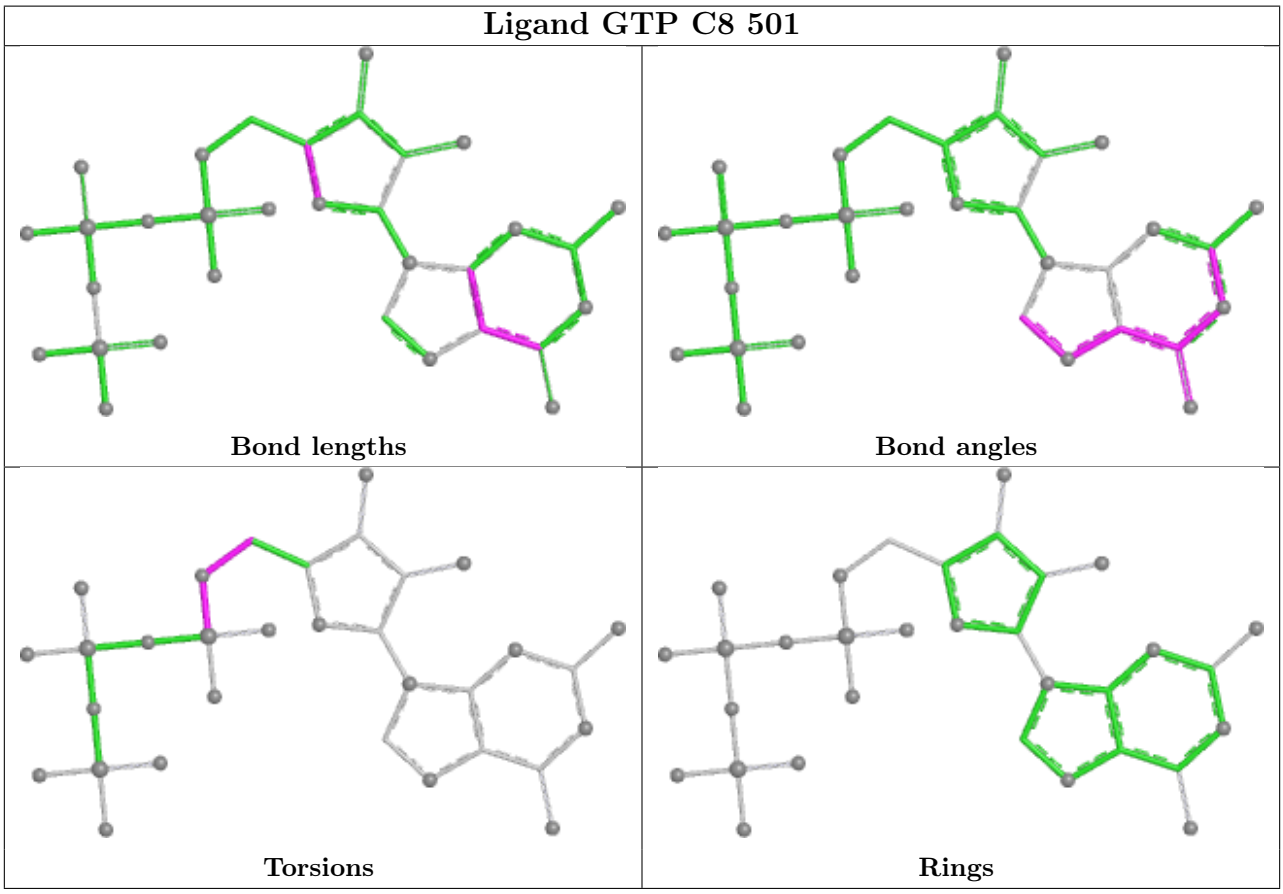
Ligand GDP B9 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP D9 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP C1 501



Ligand GTP C8 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

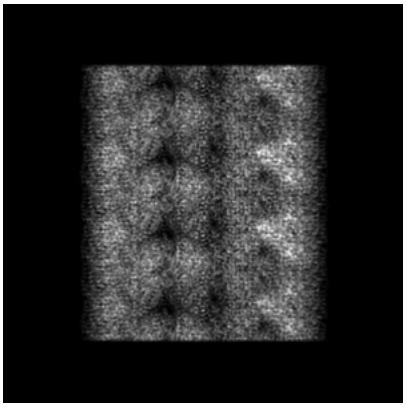
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23869. These allow visual inspection of the internal detail of the map and identification of artifacts.

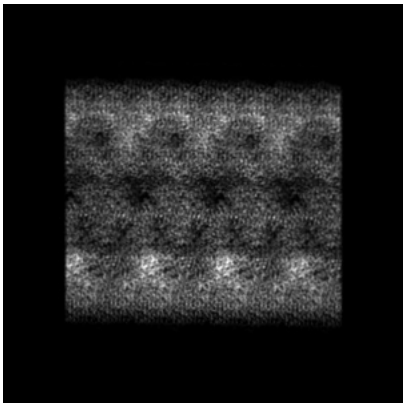
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

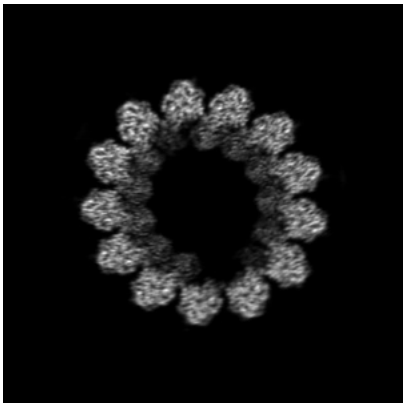
6.1.1 Primary map



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: 200

Y Index: 200

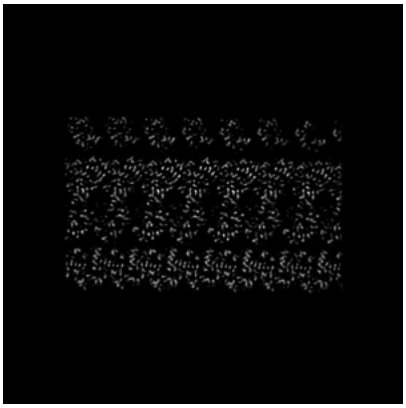
Z Index: 200

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

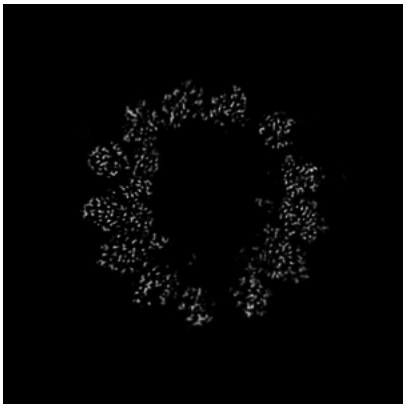
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 121



Y Index: 287

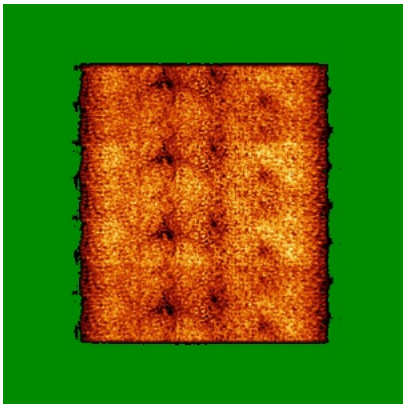


Z Index: 146

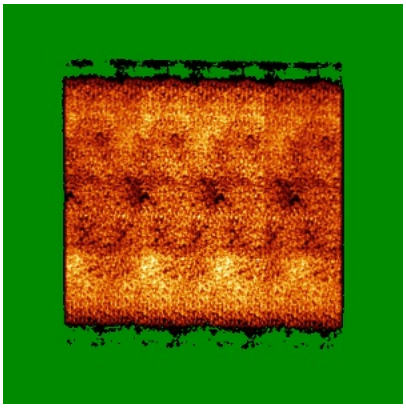
The images above show the largest variance slices of the map in three orthogonal directions.

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

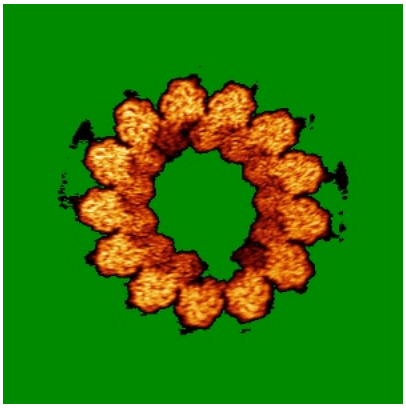
6.4.1 Primary map



X



Y

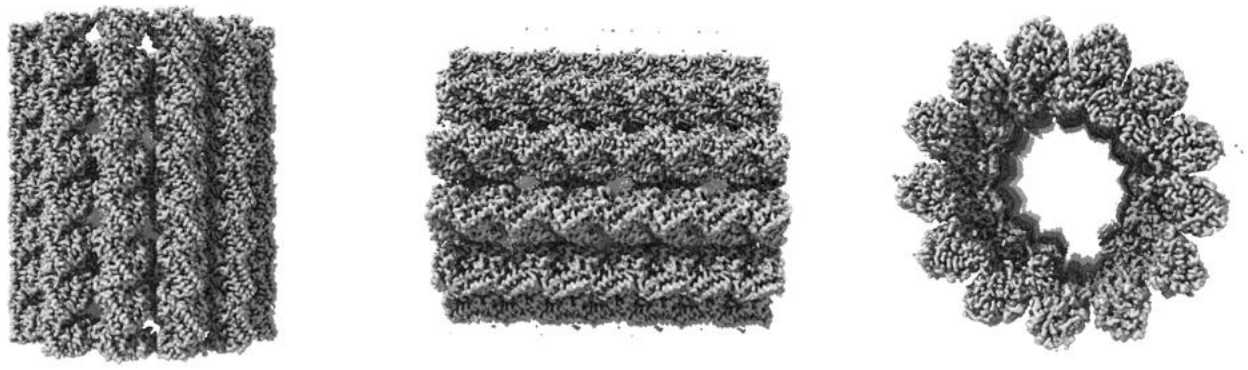


Z

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 (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

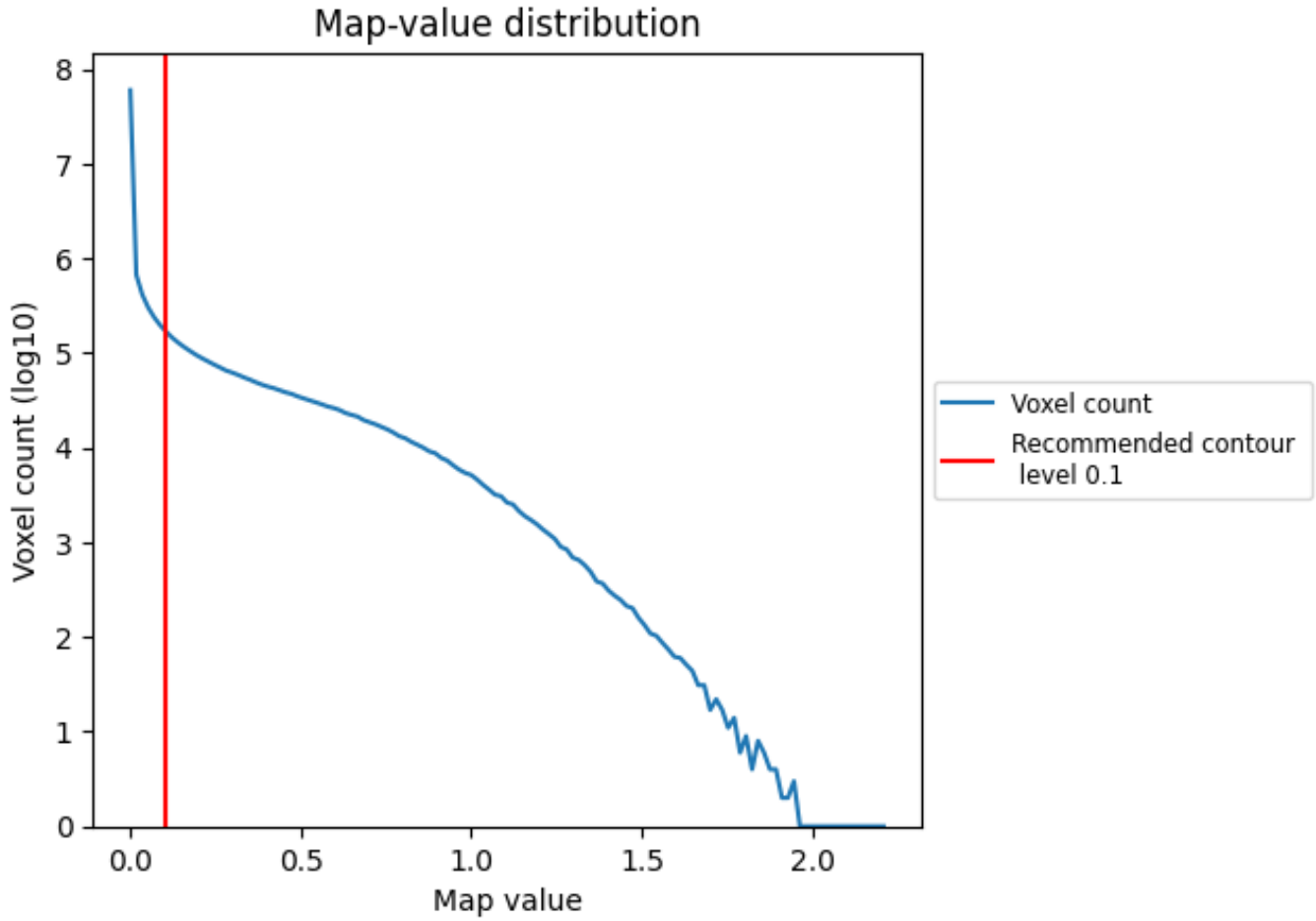
6.6 Mask visualisation (i)

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

7 Map analysis

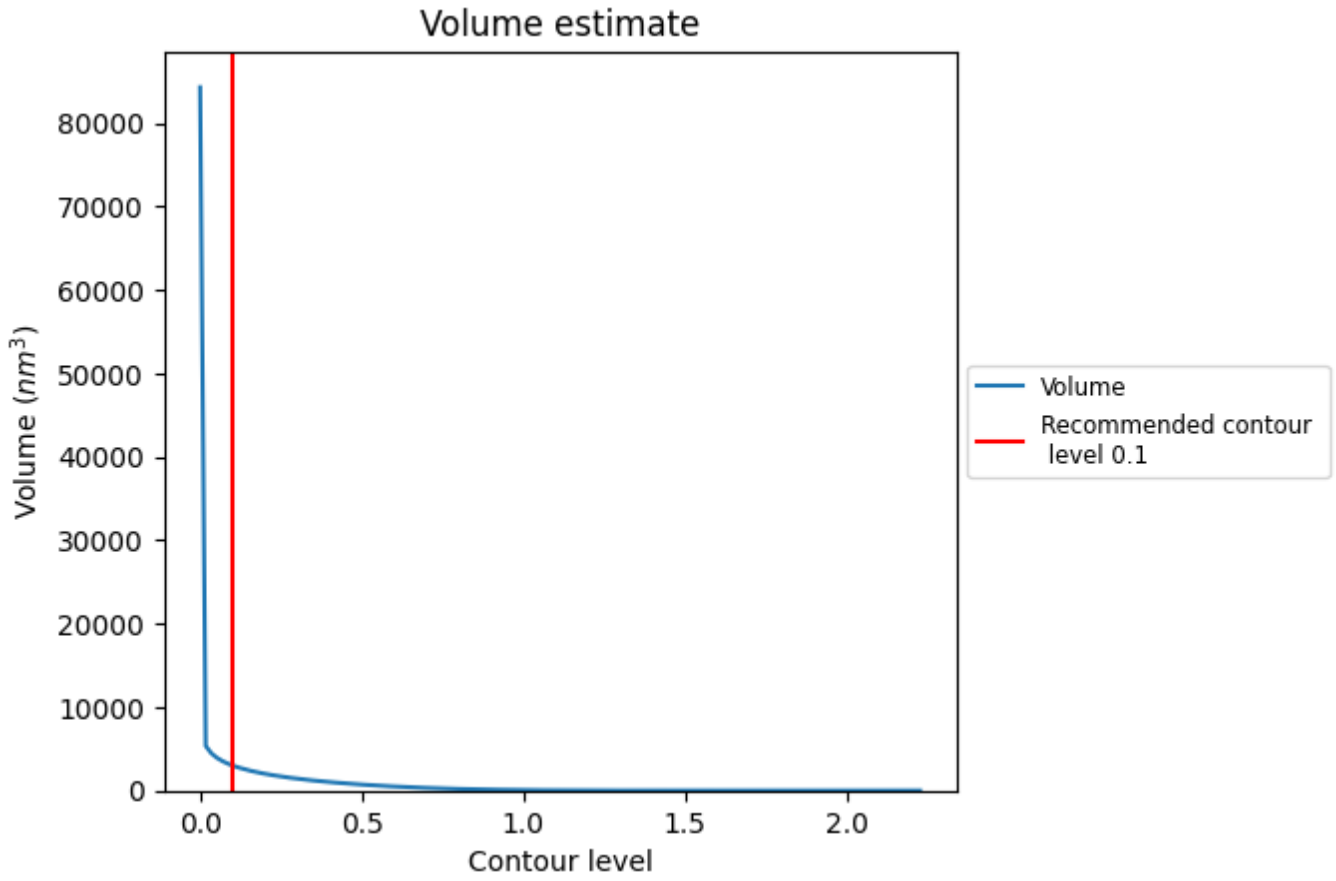
This section contains the results of statistical analysis of the map.

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.

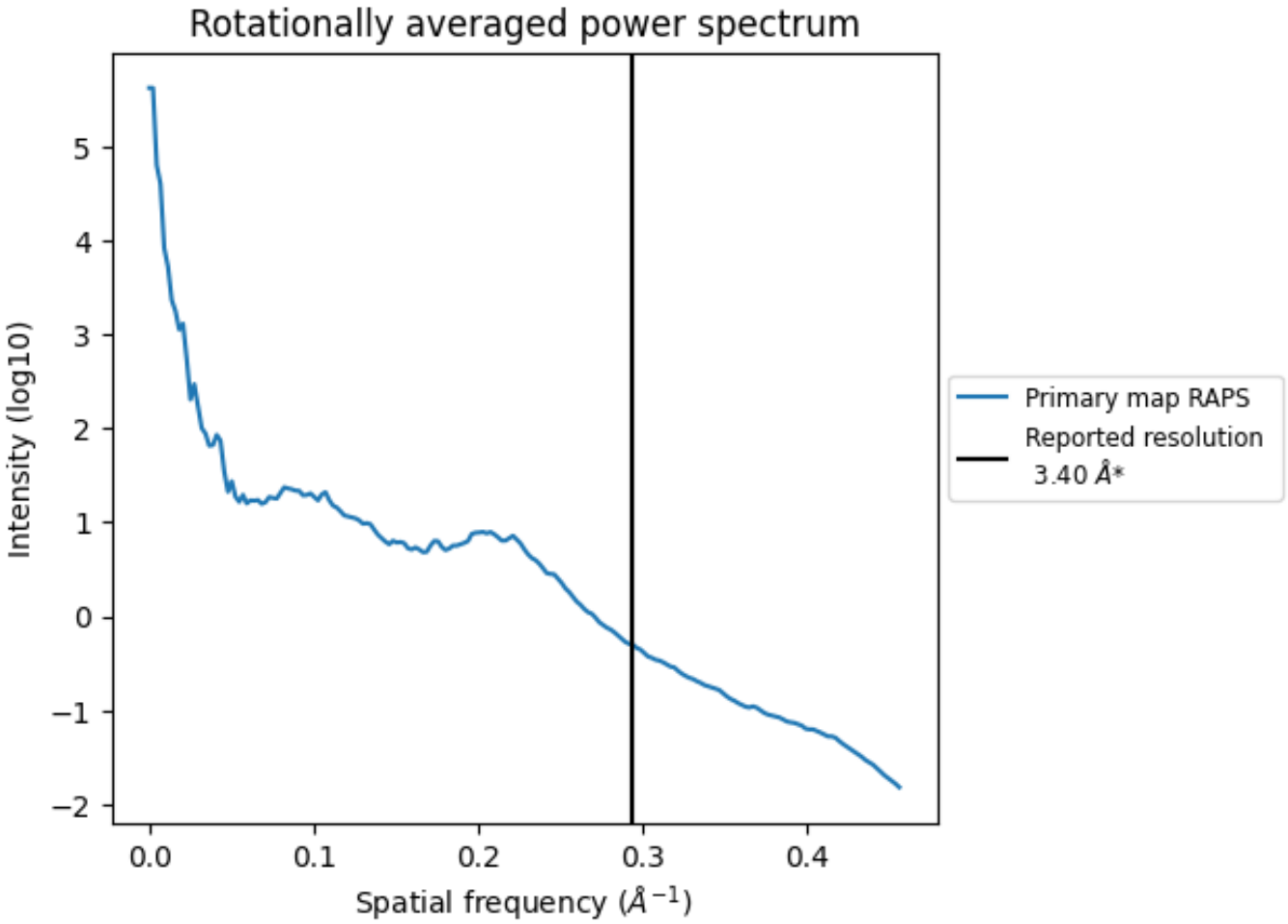
7.2 Volume estimate



The volume at the recommended contour level is 3014 nm^3; this corresponds to an approximate mass of 2723 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 (i)



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

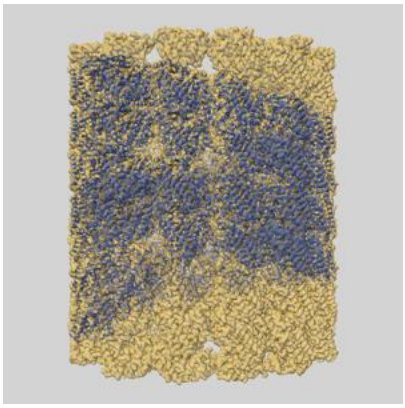
8 Fourier-Shell correlation (i)

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

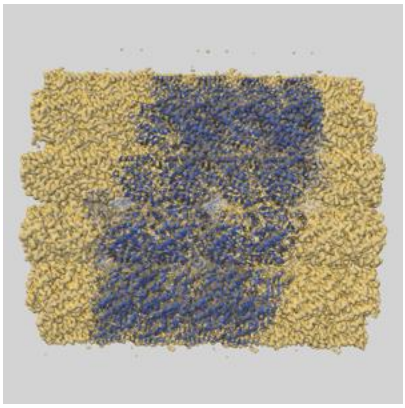
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23869 and PDB model 7MIZ. Per-residue inclusion information can be found in section 3 on page 20.

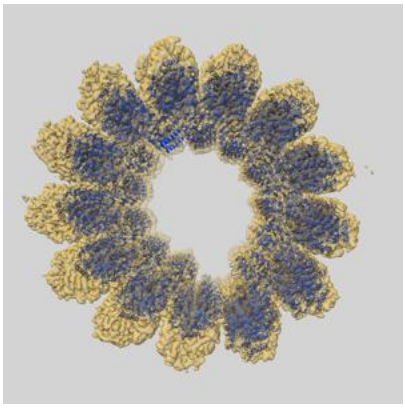
9.1 Map-model overlay



X



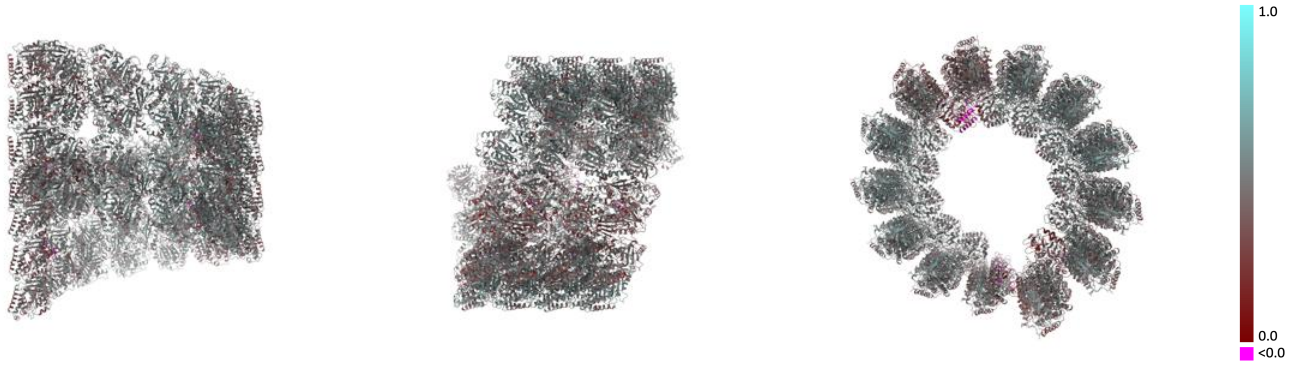
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

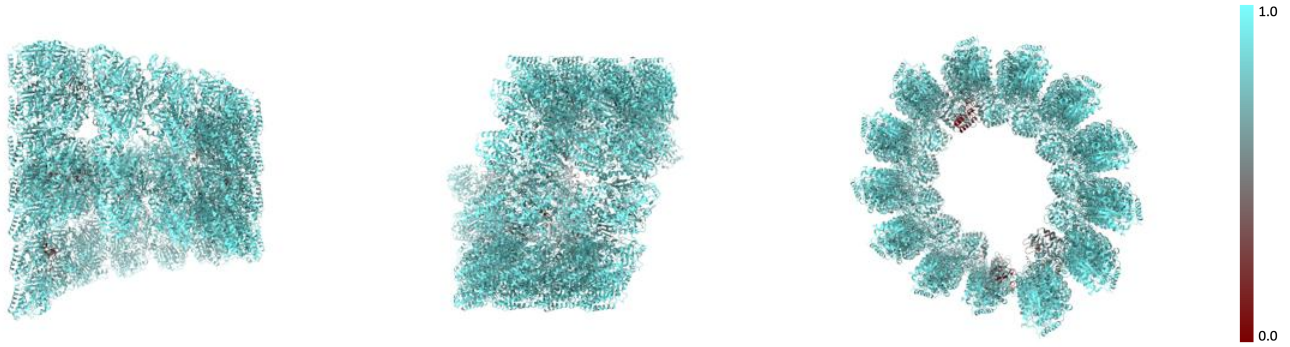
9.2 Q-score mapped to coordinate model



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.

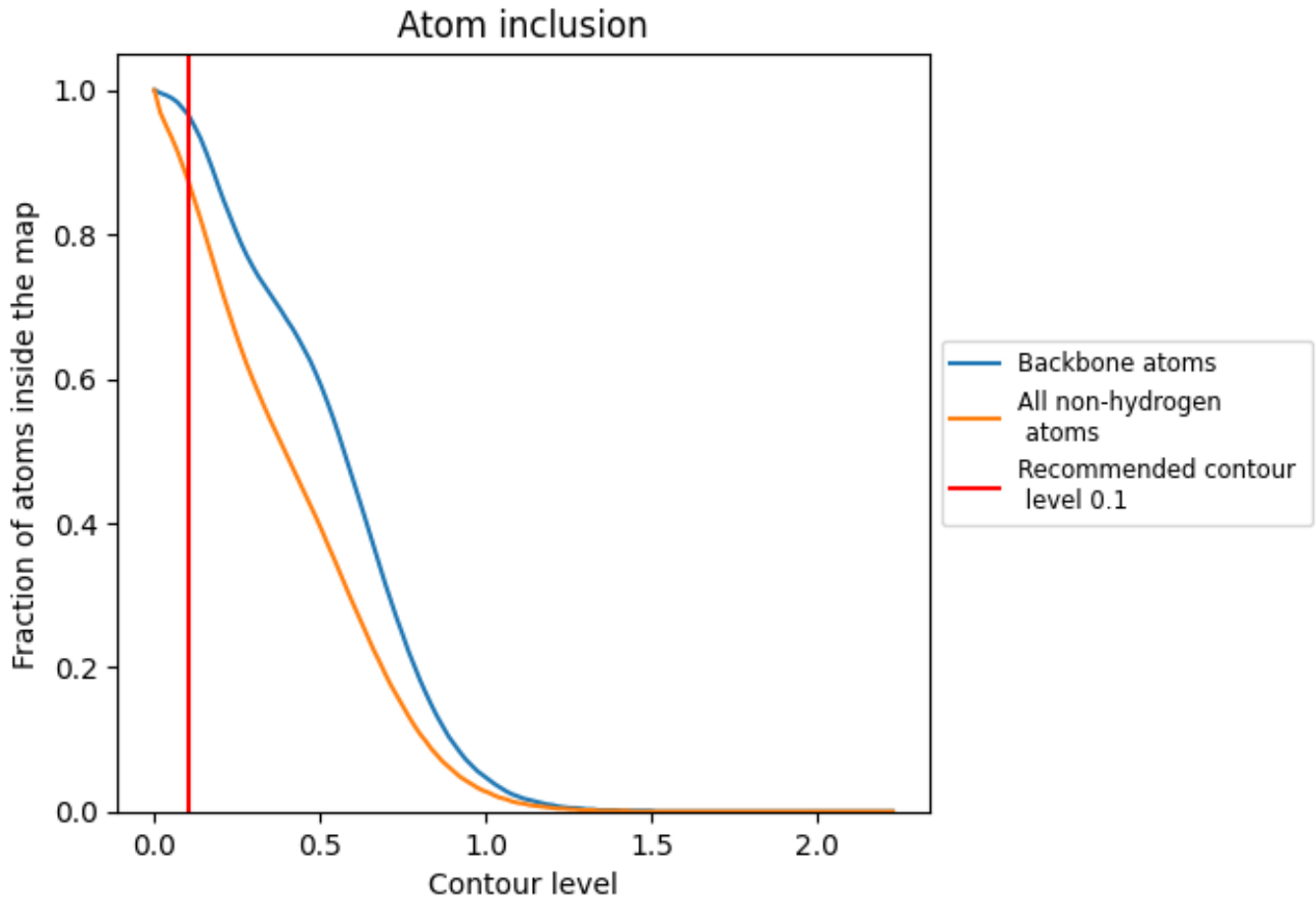
9.3 Atom inclusion mapped to coordinate model



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 88% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8770	0.4600
0	0.8650	0.4810
1	0.8350	0.4680
10	0.9060	0.4870
11	0.9060	0.4880
12	0.8820	0.4790
13	0.8760	0.4810
14	0.8710	0.4930
15	0.8530	0.4860
16	0.8650	0.4610
17	0.8820	0.4620
18	0.9350	0.4860
19	0.9410	0.4850
2	0.8350	0.4640
20	0.6940	0.4110
21	0.7350	0.4290
22	0.5900	0.3640
23	0.6150	0.3760
3	0.8410	0.4650
4	0.8240	0.4800
5	0.8410	0.4860
6	0.8590	0.4920
7	0.8590	0.4880
8	0.8240	0.4230
9	0.8290	0.4280
A0	0.7810	0.3990
A1	0.8960	0.4390
A2	0.7860	0.3920
A3	0.8560	0.4180
A4	0.8830	0.4680
A5	0.9020	0.4770
A6	0.8920	0.4680
A7	0.8820	0.4700
A8	0.9040	0.4900
A9	0.8970	0.4830

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
B0	0.8950	0.4860
B1	0.8860	0.4820
B2	0.9100	0.5040
B3	0.8940	0.5030
B4	0.9090	0.5030
B5	0.8870	0.4990
B6	0.9100	0.4990
B7	0.8980	0.5050
B8	0.9170	0.5000
B9	0.9050	0.4990
C0	0.8770	0.4160
C1	0.8490	0.4190
C2	0.8820	0.4190
C3	0.8550	0.4150
C4	0.8620	0.4020
C5	0.8630	0.4040
C6	0.8560	0.4050
C7	0.8680	0.4040
C8	0.8970	0.4740
C9	0.9070	0.4830
D0	0.8860	0.4810
D1	0.9190	0.4890
D2	0.8970	0.4870
D3	0.9200	0.5010
D4	0.8800	0.4960
D5	0.9220	0.5020
D6	0.9080	0.4910
D7	0.9230	0.4990
D8	0.8990	0.5050
D9	0.9200	0.5020
E0	0.8960	0.4680
E1	0.9110	0.4820
E2	0.9100	0.4810
E3	0.9150	0.4910
E4	0.9000	0.4530
E5	0.9080	0.4680
E6	0.9180	0.4730
E7	0.9060	0.4790
E8	0.8710	0.4230
E9	0.8510	0.4190
F0	0.8990	0.4420
F1	0.8530	0.4330

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
a	0.7830	0.4260
b	0.7790	0.4120
c	0.8410	0.4650
d	0.8490	0.4550
e	0.8780	0.4830
f	0.8900	0.4800
g	0.8840	0.4870
h	0.8810	0.4840
i	0.8820	0.4470
j	0.8820	0.4450
k	0.6920	0.2870
l	0.6830	0.2870
m	0.6830	0.3280
n	0.6800	0.3290
o	0.8890	0.4830
p	0.8850	0.4830
q	0.8950	0.4800
r	0.8940	0.4950
s	0.8990	0.4730
t	0.8970	0.4920
u	0.8750	0.4490
v	0.8770	0.4640
w	0.5560	0.2960
x	0.6150	0.3200