



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:10 AM UTC

PDB ID : 9YA1 / pdb_00009ya1
EMDB ID : EMD-72717
Title : Cryo-EM structure of intraconoidal microtubule 2 (ICMT2) from *Toxoplasma gondii* (8-nm repeat)
Authors : Zeng, J.; Zhang, R.
Deposited on : 2025-09-15
Resolution : 3.52 Å(reported)

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

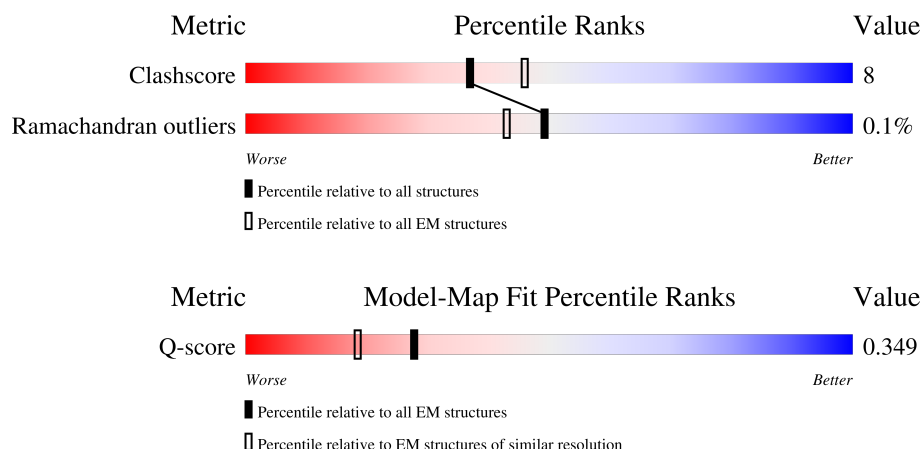
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

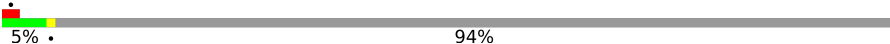
The reported resolution of this entry is 3.52 Å.

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.



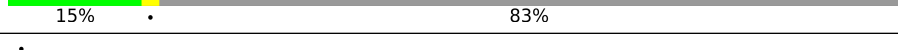
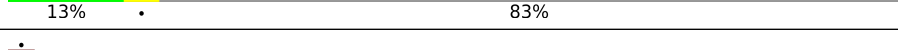
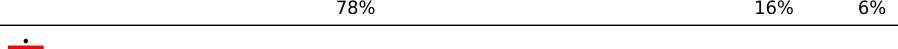
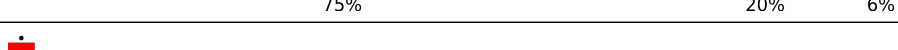
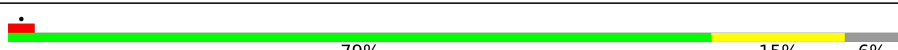
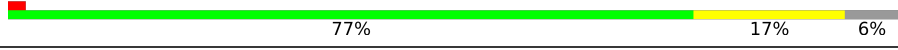
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	13017 (3.02 - 4.02)

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 $\leq 5\%$. 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	1	2041	 5% . 94%
1	2	2041	 5% . 94%
2	A	351	 15% . 83%
2	B	351	 15% . 83%
2	C	351	 15% . 83%

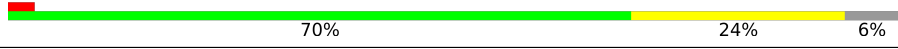
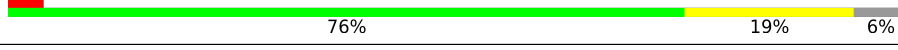
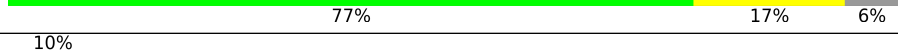
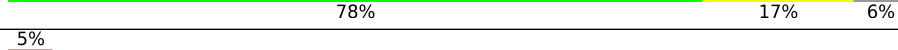
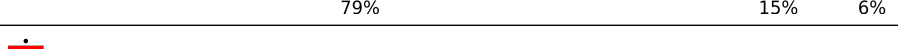
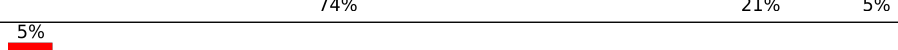
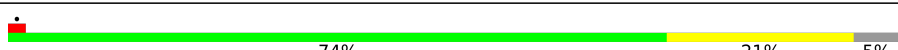
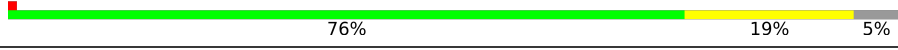
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Mol	Chain	Length	Quality of chain
2	D	351	
2	E	351	
2	F	351	
2	G	351	
2	H	351	
2	I	351	
2	J	351	
2	K	351	
3	A0	453	
3	A2	453	
3	A4	453	
3	A6	453	
3	A8	453	
3	B0	453	
3	B2	453	
3	B4	453	
3	B6	453	
3	B8	453	
3	C0	453	
3	C2	453	
3	C4	453	
3	C6	453	
3	C8	453	
3	D0	453	
3	D2	453	

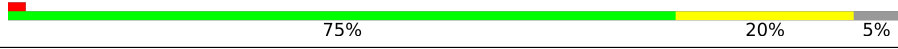
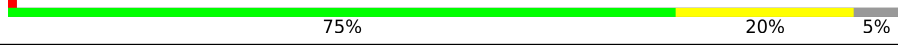
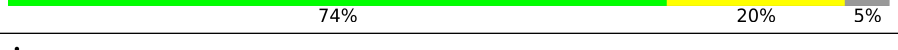
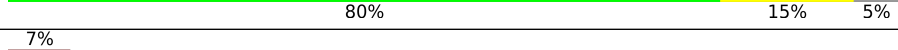
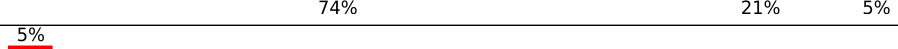
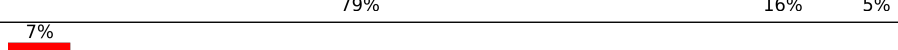
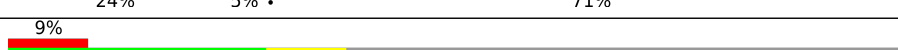
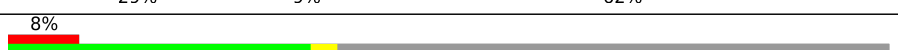
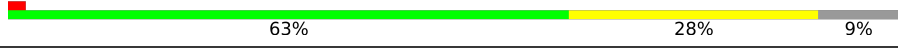
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Mol	Chain	Length	Quality of chain
3	D4	453	
3	D6	453	
3	D8	453	
3	E0	453	
3	E2	453	
3	E4	453	
3	E6	453	
3	E8	453	
3	F0	453	
4	A1	449	
4	A3	449	
4	A5	449	
4	A7	449	
4	A9	449	
4	B1	449	
4	B3	449	
4	B5	449	
4	B7	449	
4	B9	449	
4	C1	449	
4	C3	449	
4	C5	449	
4	C7	449	
4	C9	449	
4	D1	449	

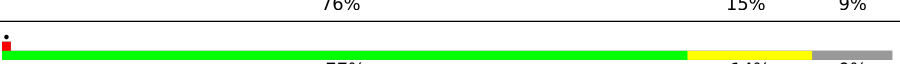
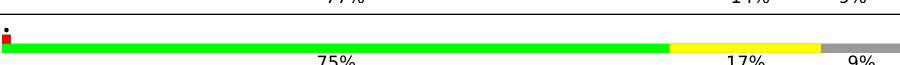
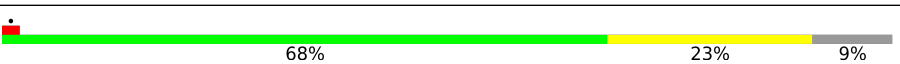
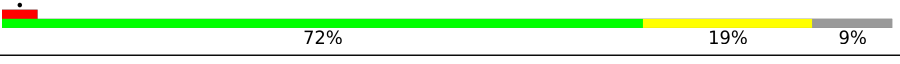
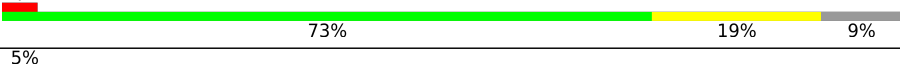
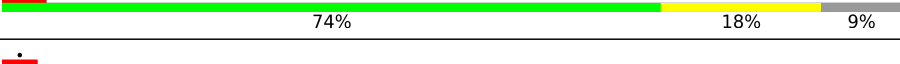
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Mol	Chain	Length	Quality of chain
4	D3	449	
4	D5	449	
4	D7	449	
4	D9	449	
4	E1	449	
4	E3	449	
4	E5	449	
4	E7	449	
4	E9	449	
4	F1	449	
5	O	583	
5	P	583	
5	R	583	
6	U	336	
6	V	336	
6	W	336	
6	X	336	
7	a	220	
7	b	220	
7	c	220	
7	d	220	
7	e	220	
7	f	220	
7	g	220	
7	h	220	

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

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 226608 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 ICMAP4, TGME49_225340.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	130	Total	C	N	O	S	0	0
			1054	670	185	197	2		
1	2	130	Total	C	N	O	S	0	0
			1054	670	185	197	2		

- Molecule 2 is a protein called Microtubule associated protein SPM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	59	Total	C	N	O	S	0	0
			464	306	74	83	1		
2	B	60	Total	C	N	O	S	0	0
			471	311	75	84	1		
2	C	59	Total	C	N	O	S	0	0
			464	306	74	83	1		
2	D	59	Total	C	N	O	S	0	0
			464	306	74	83	1		
2	E	60	Total	C	N	O	S	0	0
			471	311	75	84	1		
2	F	56	Total	C	N	O	S	0	0
			441	292	70	78	1		
2	G	60	Total	C	N	O	S	0	0
			471	311	75	84	1		
2	H	56	Total	C	N	O	S	0	0
			441	292	70	78	1		
2	I	60	Total	C	N	O	S	0	0
			471	311	75	84	1		
2	J	60	Total	C	N	O	S	0	0
			471	311	75	84	1		
2	K	60	Total	C	N	O	S	0	0
			471	311	75	84	1		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	93	ARG	PRO	conflict	UNP A0A7J6K285
B	93	ARG	PRO	conflict	UNP A0A7J6K285
C	93	ARG	PRO	conflict	UNP A0A7J6K285
D	93	ARG	PRO	conflict	UNP A0A7J6K285
E	93	ARG	PRO	conflict	UNP A0A7J6K285
F	93	ARG	PRO	conflict	UNP A0A7J6K285
G	93	ARG	PRO	conflict	UNP A0A7J6K285
H	93	ARG	PRO	conflict	UNP A0A7J6K285
I	93	ARG	PRO	conflict	UNP A0A7J6K285
J	93	ARG	PRO	conflict	UNP A0A7J6K285
K	93	ARG	PRO	conflict	UNP A0A7J6K285

- Molecule 3 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	A2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	A4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	A6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	A8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	B0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	B2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	B4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	B6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	B8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	C0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	C2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	C4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	C6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	C8	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	D0	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	D2	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	D4	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	D6	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	D8	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	E0	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	E2	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	E4	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	E6	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	E8	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	F0	428	Total 3325	C 2105	N 569	O 625	S 26	0	0

- Molecule 4 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A1	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	A3	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	A5	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	A7	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	A9	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	B1	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	B3	426	Total 3331	C 2094	N 569	O 641	S 27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	B5	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	B7	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	B9	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	C1	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	C3	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	C5	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	C7	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	C9	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	D1	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	D3	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	D5	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	D7	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	D9	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	E1	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	E3	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	E5	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	E7	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	E9	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	F1	426	Total 3331	C 2094	N 569	O 641	S 27	0	0

- Molecule 5 is a protein called TLAP3 (apical cap protein AC5), TGME49_235380.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	O	171	Total	C	N	O	S	0	0
			1360	844	255	259	2		
5	P	220	Total	C	N	O	S	0	0
			1744	1084	329	329	2		
5	R	220	Total	C	N	O	S	0	0
			1744	1084	329	329	2		

- Molecule 6 is a protein called TLAP4 (thioredoxin-like associated protein), TGME49_201760.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	U	22	Total	C	N	O	S	0	0
			182	112	38	31	1		
6	V	113	Total	C	N	O	S	0	0
			954	592	182	179	1		
6	W	113	Total	C	N	O	S	0	0
			954	592	182	179	1		
6	X	91	Total	C	N	O		0	0
			772	480	144	148			

- Molecule 7 is a protein called TRXL1, TGME49_232410.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	161	Total	C	N	O	S	0	0
			1289	824	224	236	5		
7	b	161	Total	C	N	O	S	0	0
			1289	824	224	236	5		
7	c	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	d	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	e	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	f	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	g	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	h	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	i	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	j	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	m	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	n	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	o	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	p	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	q	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	r	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	s	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	t	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	u	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	v	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	w	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	x	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		

- Molecule 8 is a protein called TRXL2, TGME49_225790.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	k	141	Total	C	N	O	S	0	0
			1155	747	205	199	4		
8	l	141	Total	C	N	O	S	0	0
			1155	747	205	199	4		

There are 46 discrepancies between the modelled and reference sequences:

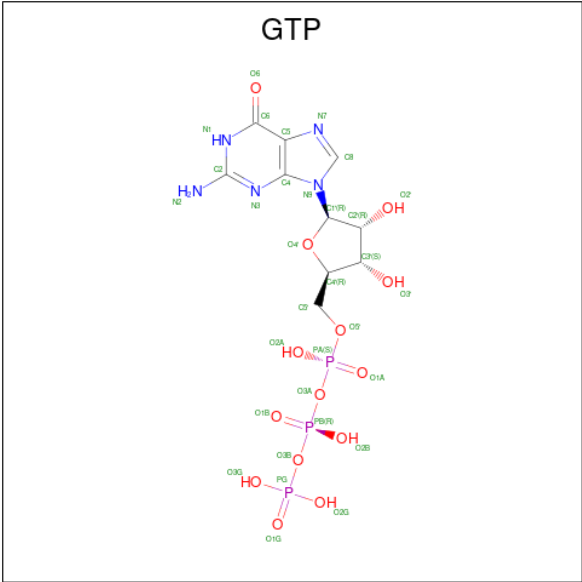
Chain	Residue	Modelled	Actual	Comment	Reference
k	167	SER	-	expression tag	UNP A0A7J6K232
k	168	ALA	-	expression tag	UNP A0A7J6K232
k	169	GLN	-	expression tag	UNP A0A7J6K232
k	170	ARG	-	expression tag	UNP A0A7J6K232
k	171	LEU	-	expression tag	UNP A0A7J6K232
k	172	ARG	-	expression tag	UNP A0A7J6K232
k	173	THR	-	expression tag	UNP A0A7J6K232
k	174	LEU	-	expression tag	UNP A0A7J6K232

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

- Molecule 9 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	A0	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	A2	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	A4	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	A6	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	A8	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	B0	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	B2	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	B4	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	B6	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	B8	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	C0	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	C2	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	C4	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	C6	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
9	C8	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	D0	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	D2	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	D4	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	D6	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	D8	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	E0	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	E2	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	E4	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	E7	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	E8	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	F0	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

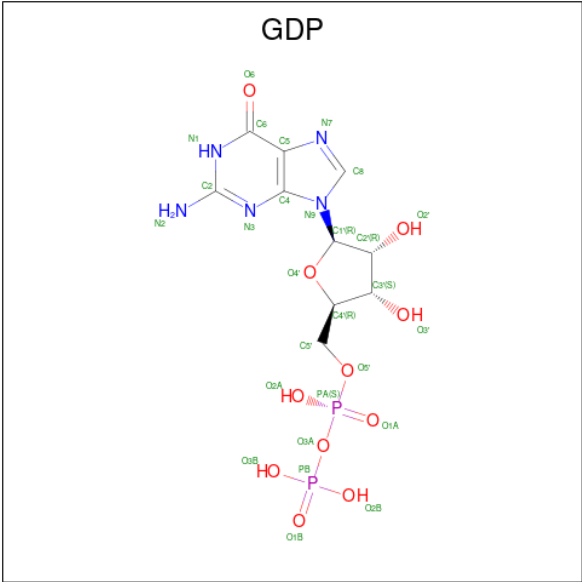
Mol	Chain	Residues	Atoms		AltConf
10	A0	1	Total	Mg	0
			1	1	
10	A2	1	Total	Mg	0
			1	1	
10	A4	1	Total	Mg	0
			1	1	
10	A6	1	Total	Mg	0
			1	1	
10	A8	1	Total	Mg	0
			1	1	
10	B0	1	Total	Mg	0
			1	1	
10	B2	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
10	B4	1	Total 1	Mg 1	0
10	B6	1	Total 1	Mg 1	0
10	B8	1	Total 1	Mg 1	0
10	C0	1	Total 1	Mg 1	0
10	C2	1	Total 1	Mg 1	0
10	C4	1	Total 1	Mg 1	0
10	C6	1	Total 1	Mg 1	0
10	C9	1	Total 1	Mg 1	0
10	D1	1	Total 1	Mg 1	0
10	D3	1	Total 1	Mg 1	0
10	D4	1	Total 1	Mg 1	0
10	D6	1	Total 1	Mg 1	0
10	D8	1	Total 1	Mg 1	0
10	E0	1	Total 1	Mg 1	0
10	E2	1	Total 1	Mg 1	0
10	E4	1	Total 1	Mg 1	0
10	E6	1	Total 1	Mg 1	0
10	E8	1	Total 1	Mg 1	0
10	F0	1	Total 1	Mg 1	0

- Molecule 11 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
11	A1	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	A3	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	A5	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	A7	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	B3	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	B5	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	B7	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	B9	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	C1	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	C3	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	C5	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	C7	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	C9	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	D1	1	Total	C	N	O	P	0
			28	10	5	11	2	

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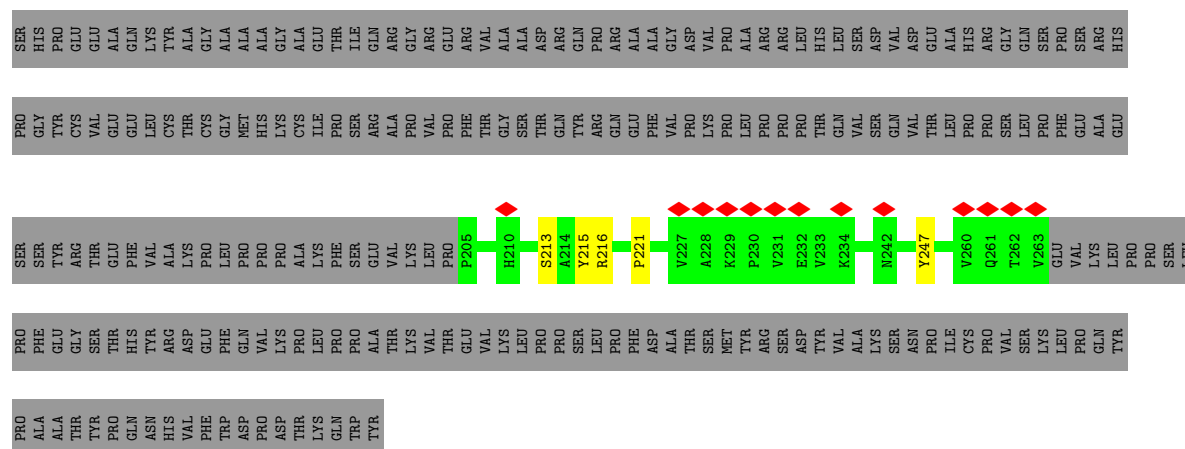
Mol	Chain	Residues	Atoms					AltConf
11	D3	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	D5	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	D7	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	D9	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	E1	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	E3	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	E5	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	E7	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	E9	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	F1	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	O	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	P	1	Total	C	N	O	P	0
			28	10	5	11	2	



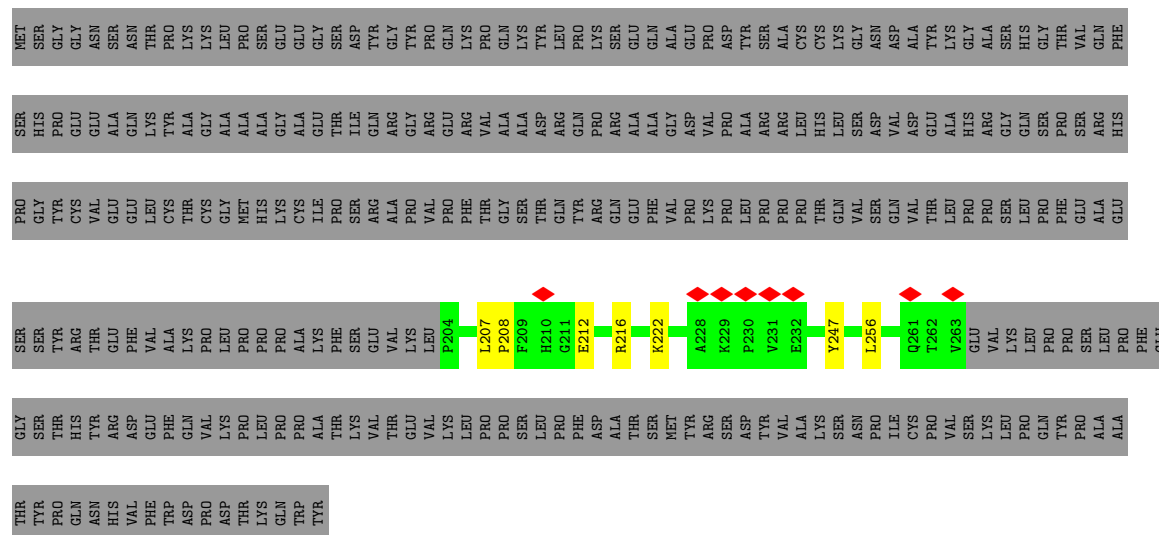
- Molecule 2: Microtubule associated protein SPM1



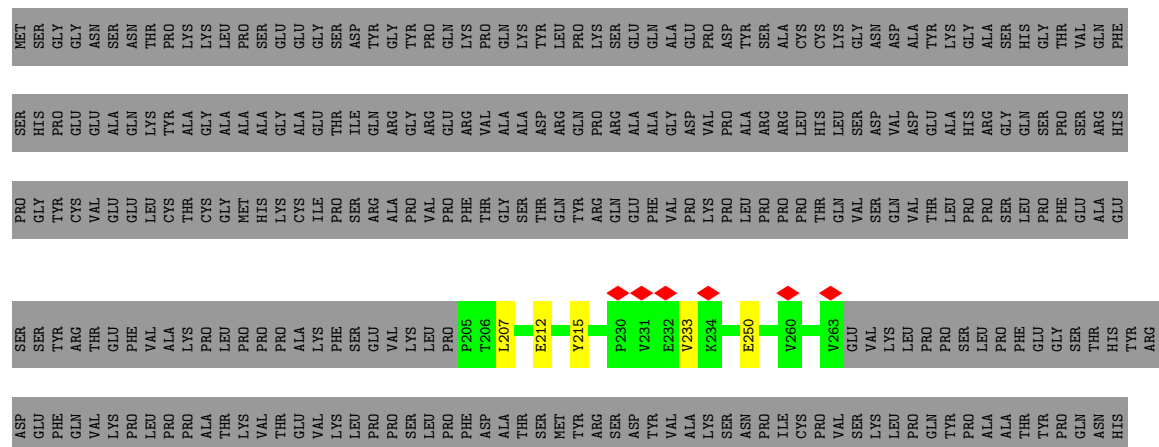
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-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



- Molecule 2: Microtubule associated protein SPM1



- Molecule 2: Microtubule associated protein SPM1



VAL
PHE
TRP
ASP
PRO
ASP
THR
GLN
TRP
TYR

• Molecule 2: Microtubule associated protein SPM1

Chain D: 14% 83%

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

SER HIS PRO GLU GLY ALA GLN LYS TYR ALA GLY ALA PRO MET HIS HIS CYS ILE GLY THR SER ARG GLN ARG VAL ARG GLN

PRO GLY TYR CYS VAL GLU GLY LEU CYS THR CYS GLY MET HIS HIS CYS ILE GLY THR SER ARG GLN ARG VAL ARG GLN

SER SER TYR ARG THR GLU PHE VAL LYS PRO PRO PRO PRO LYS PHE LEU P204 K214 D218 P221 P227 A228 K229 P230 V231 E232 V233 K234 Y247 Y251 V252 A253 K254 P255 L256 P257 V260 Q261 T262 VAL GLU VAL LYS LEU PRO

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

GLN TYR PRO ALA ALA THR TYR PRO GLN ASN HIS ASP PHE TRP ASP PRO TYR

• Molecule 2: Microtubule associated protein SPM1

Chain E: 14% 83%

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

SER HIS PRO GLU GLY ALA GLN LYS TYR ALA GLY ALA PRO MET HIS HIS CYS ILE GLY THR SER ARG GLN ARG VAL ARG GLN

PRO GLY TYR CYS VAL GLU GLY LEU CYS THR CYS GLY MET HIS HIS CYS ILE GLY THR SER ARG GLN ARG VAL ARG GLN

SER SER TYR THR GLU PHE VAL LYS PRO PRO PRO PRO LYS PHE LEU P204 T217 P221 K222 P223 L224 P225 E226 V227 A228 K229 P230 V231 E232 V233 K234 L235 F241 N242 A243 Q244 S249 E250 Y251 K254 V260 Q261 T262 V263 GLU VAL

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

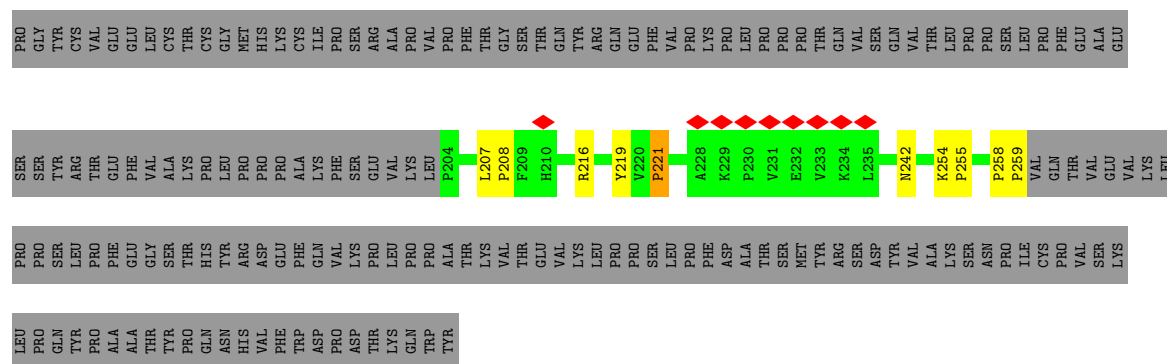
SER LYS LEU PRO PRO GLN TYR PRO ALA ALA TYR PRO GLN ASN HIS VAL ASP THR ASP PRO PRO TYR THR LYS TRP TYR

• Molecule 2: Microtubule associated protein SPM1

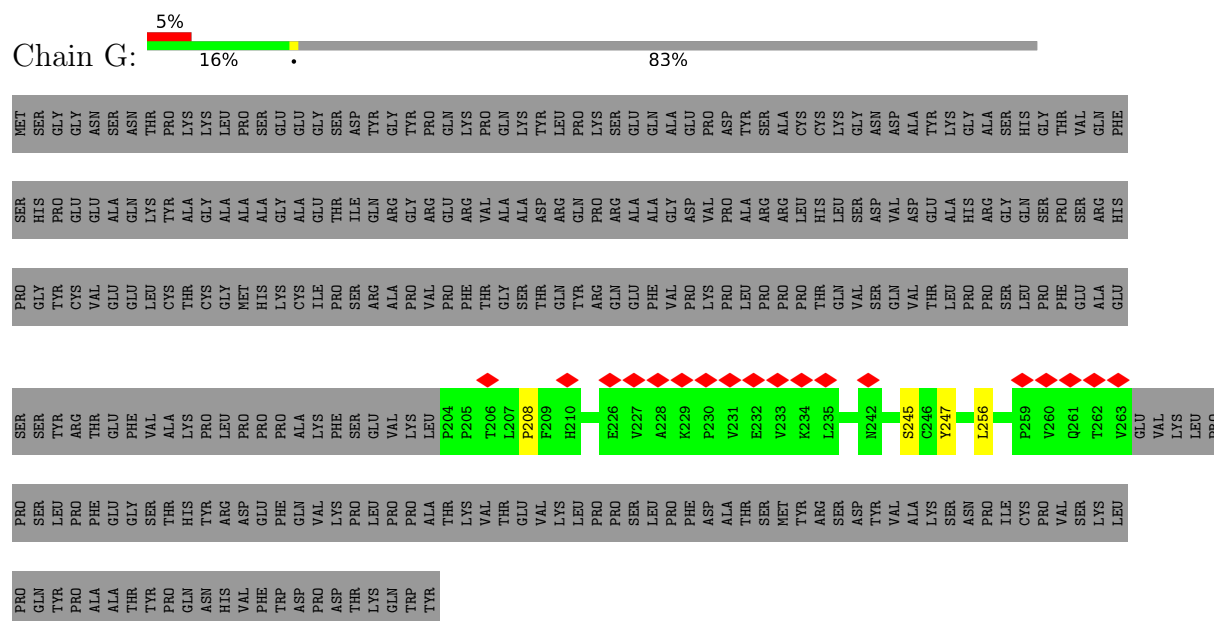
Chain F: 13% 84%

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

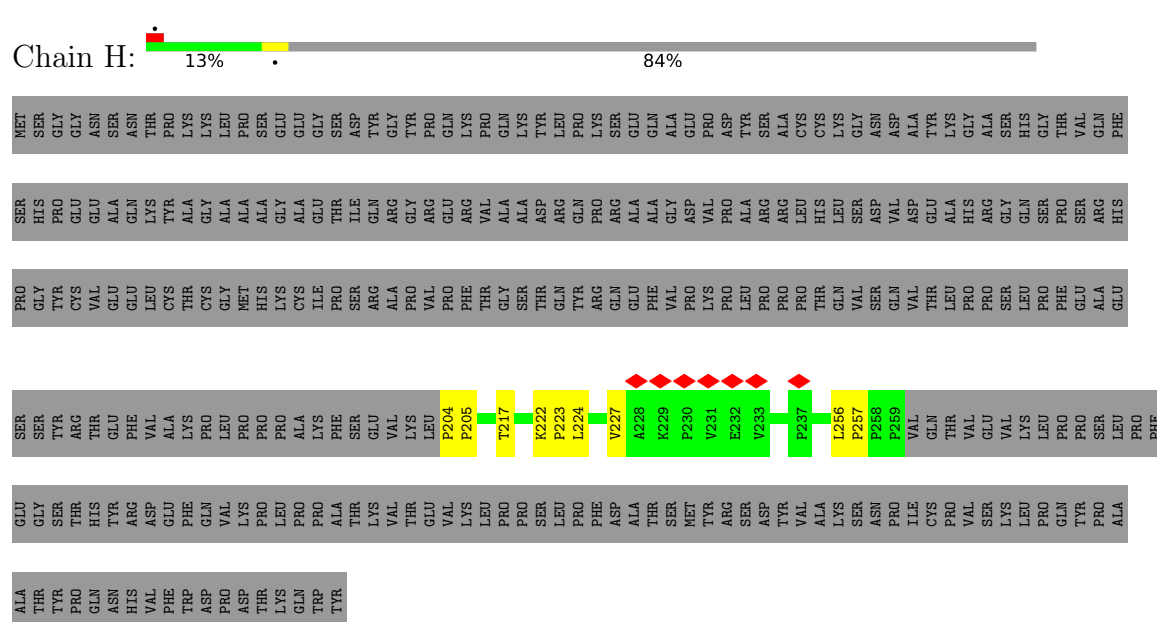
SER HIS PRO GLU GLY ALA GLN LYS TYR ALA GLY ALA PRO MET HIS HIS CYS ILE GLY THR SER ARG GLN ARG VAL ARG GLN



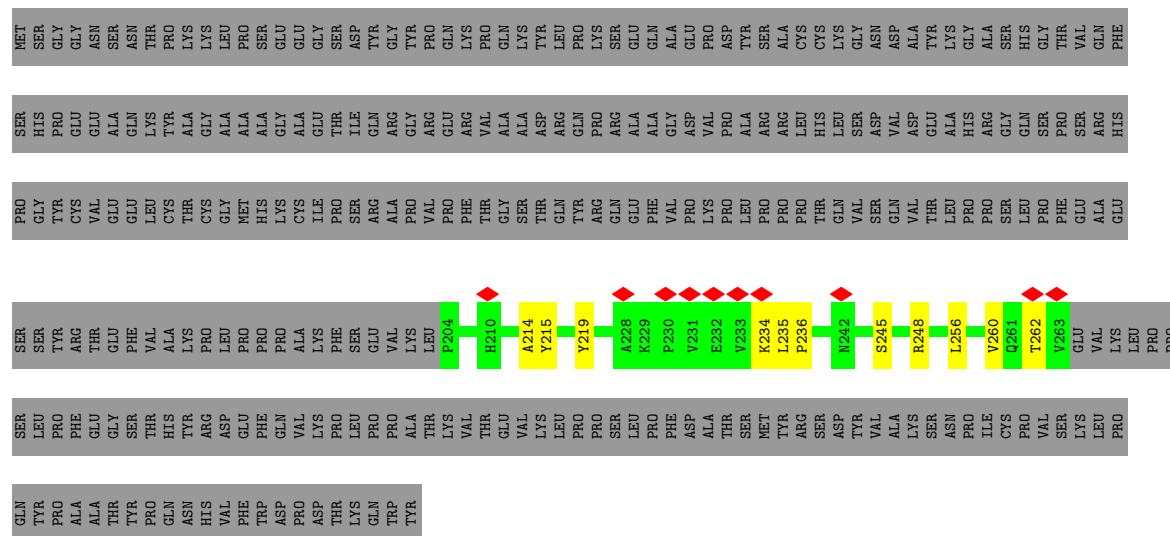
- Molecule 2: Microtubule associated protein SPM1



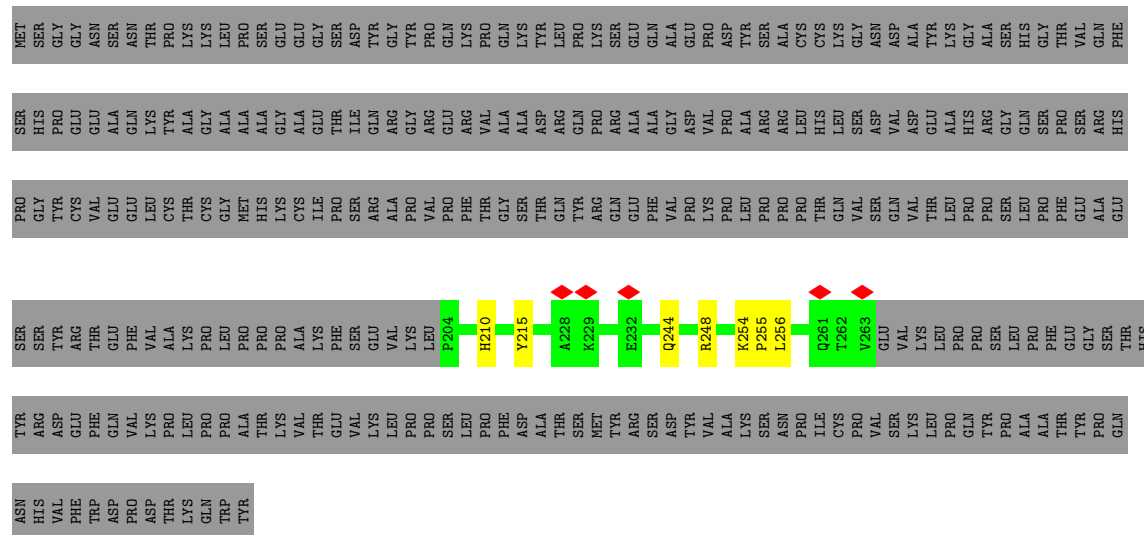
- Molecule 2: Microtubule associated protein SPM1



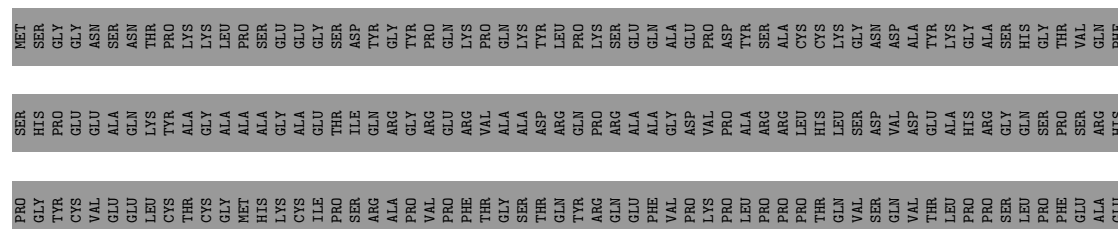
Chain I: 14% 83%

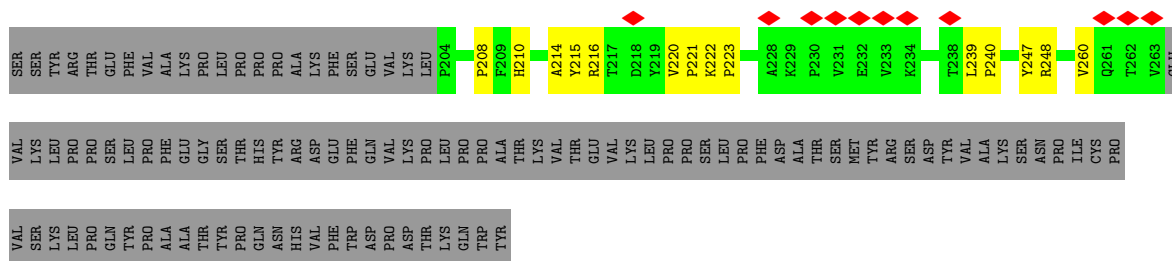


Chain J: 15% 83%

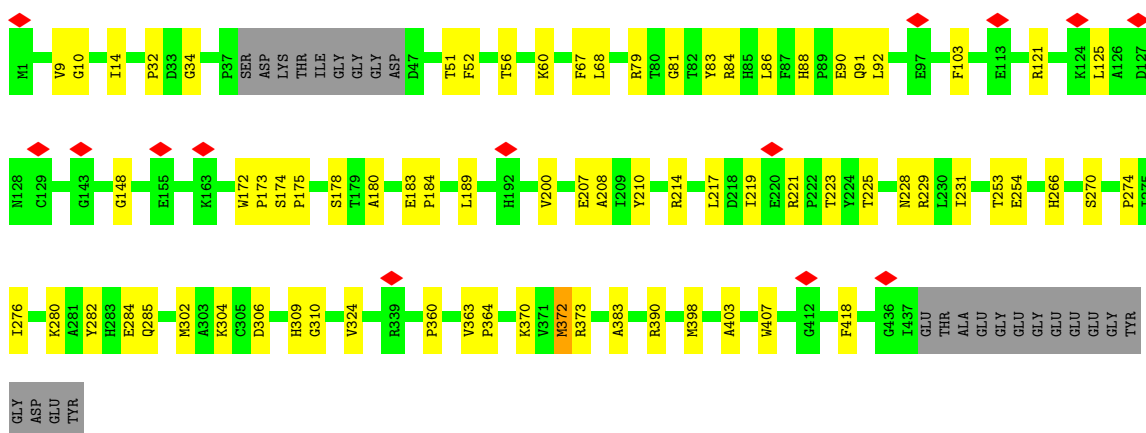
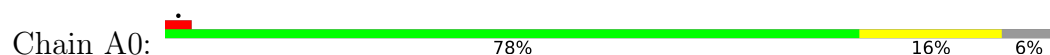


Chain K: 13% 83%

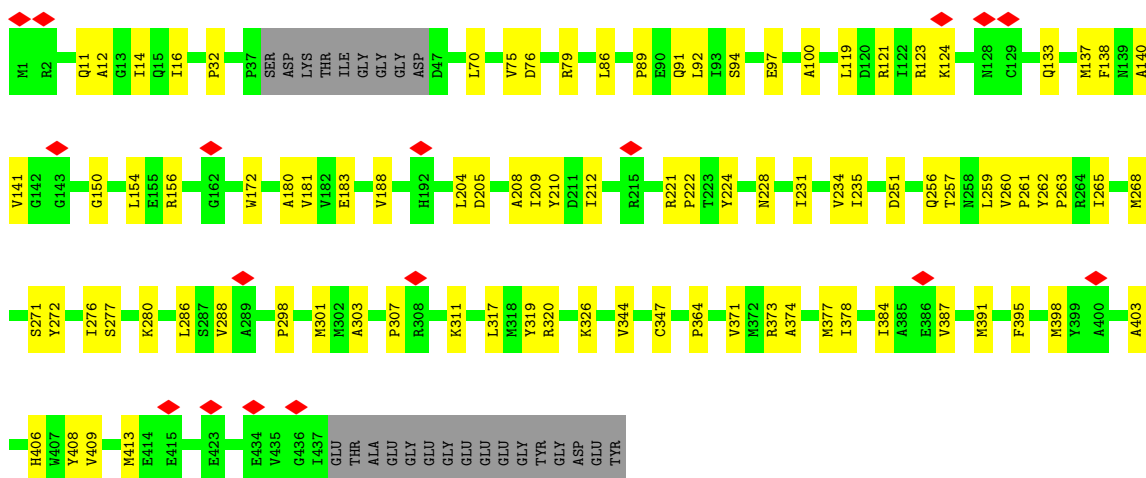
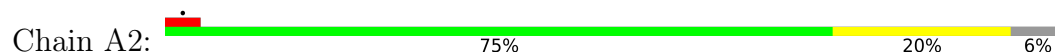




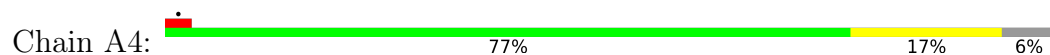
- Molecule 3: Tubulin alpha chain

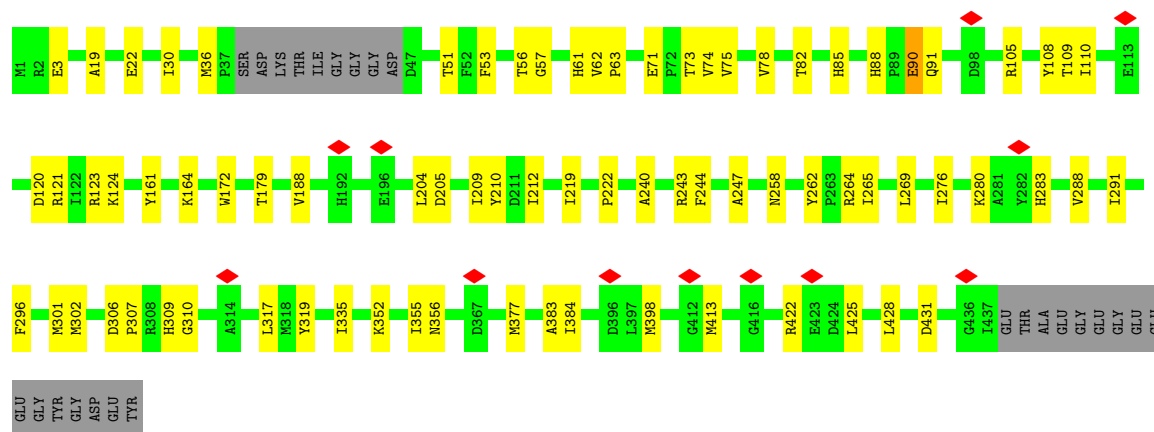


- Molecule 3: Tubulin alpha chain



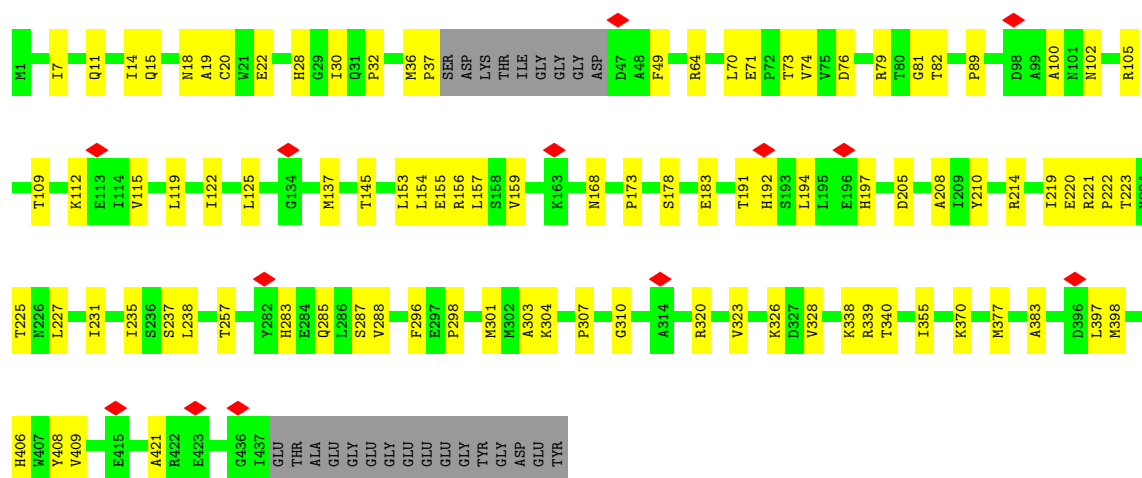
- Molecule 3: Tubulin alpha chain





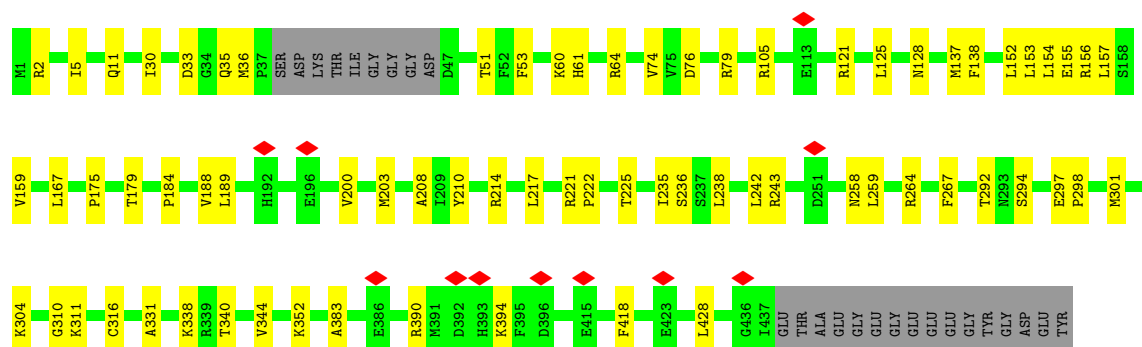
• Molecule 3: Tubulin alpha chain

Chain A6: 74% 21% 6%



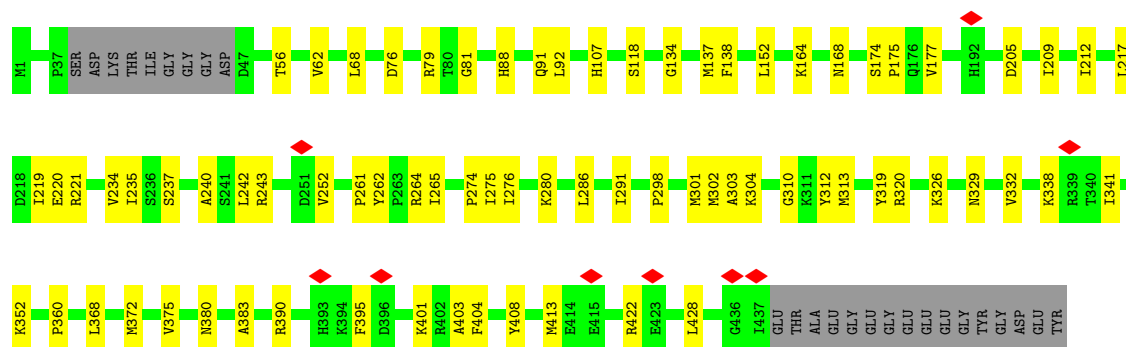
• Molecule 3: Tubulin alpha chain

Chain A8: 79% 16% 6%

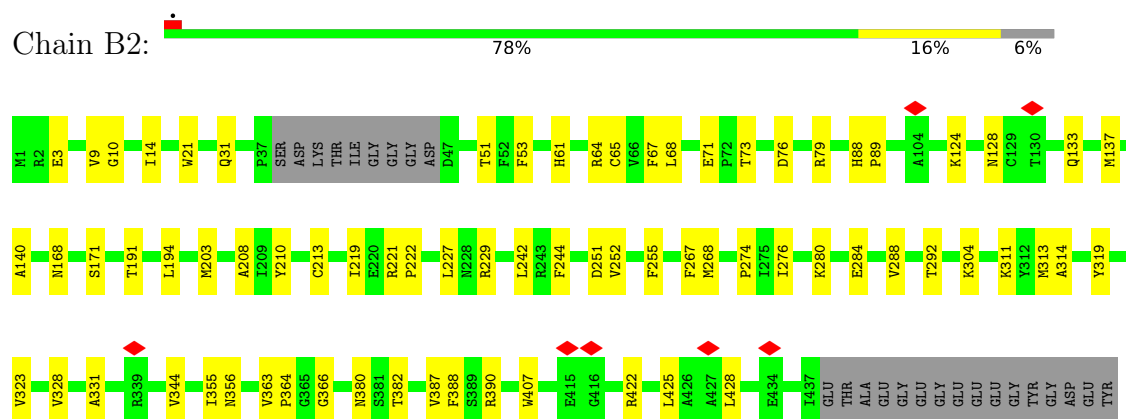


• Molecule 3: Tubulin alpha chain

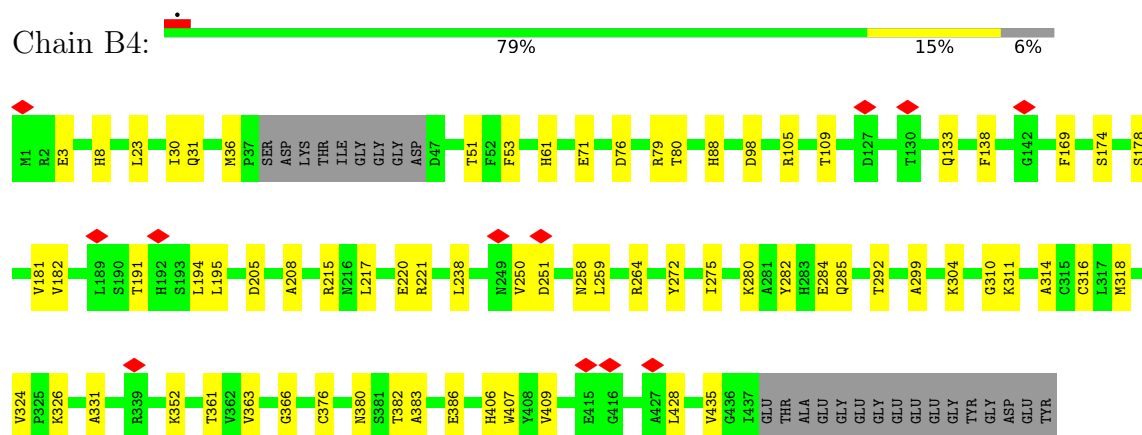
Chain B0: 78% 17% 6%



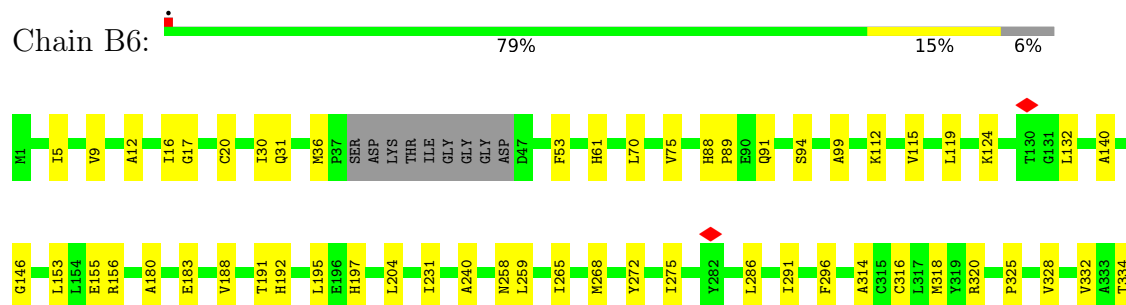
• Molecule 3: Tubulin alpha chain



• Molecule 3: Tubulin alpha chain



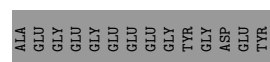
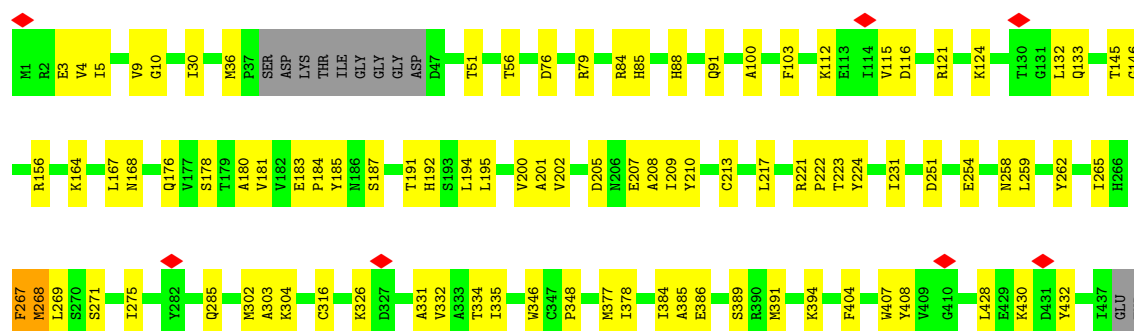
• Molecule 3: Tubulin alpha chain





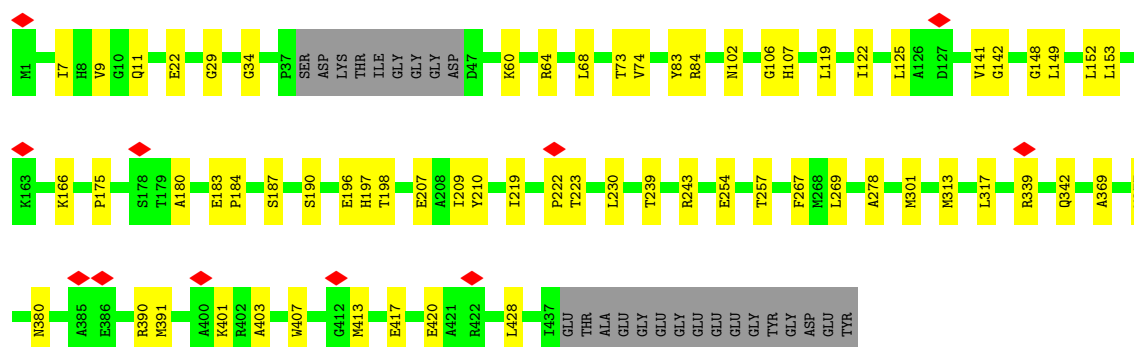
• Molecule 3: Tubulin alpha chain

Chain B8: 74% 20% 6%



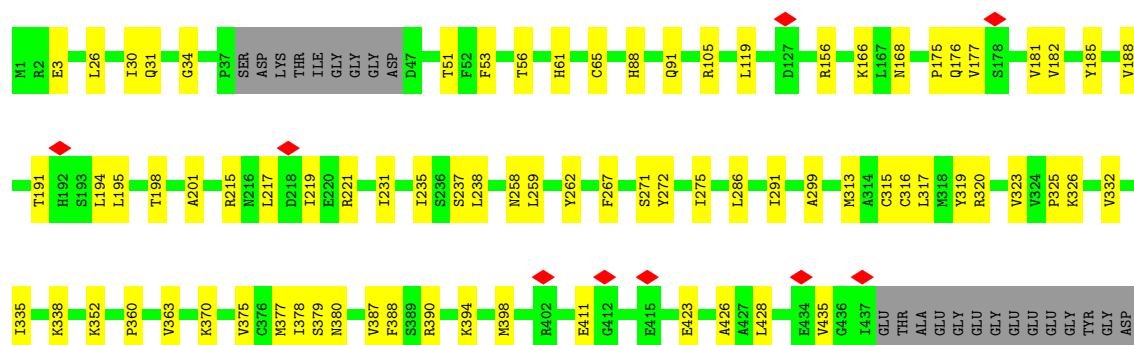
• Molecule 3: Tubulin alpha chain

Chain C0: 80% 15% 6%



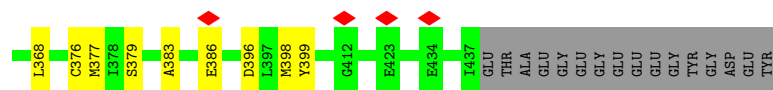
• Molecule 3: Tubulin alpha chain

Chain C2: 77% 17% 6%

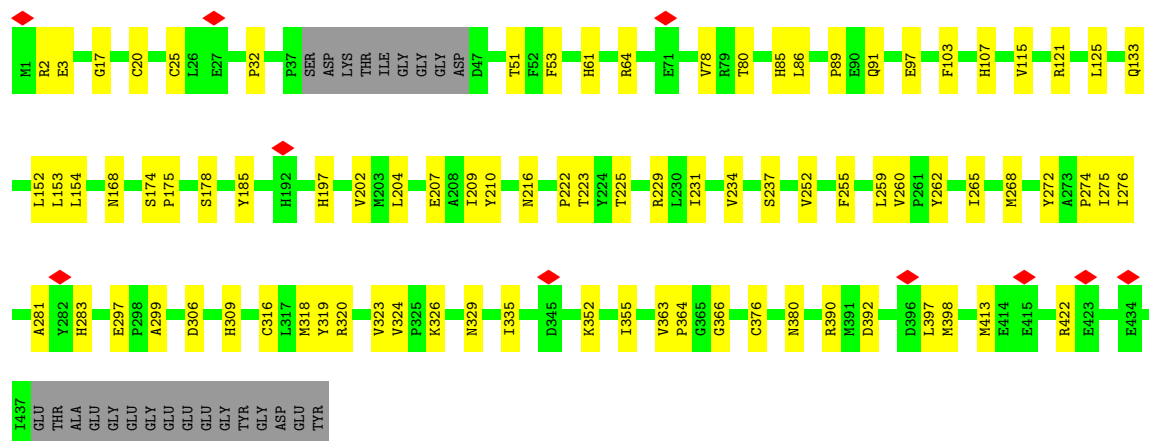
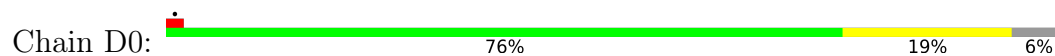


The chart displays the distribution of 250 amino acids across three categories: Green (100), Yellow (100), and Grey (50). The chart is divided into three sections. The first section (left) contains 100 amino acids, mostly in the Green category, with a few in Yellow and Grey. The second section (middle) contains 100 amino acids, mostly in the Yellow category, with a few in Green and Grey. The third section (right) contains 50 amino acids, mostly in the Green category, with a few in Yellow and Grey. The chart uses a color-coded system: Green for 100, Yellow for 100, and Grey for 50. The amino acids are listed on the x-axis, and the y-axis shows the count for each category.

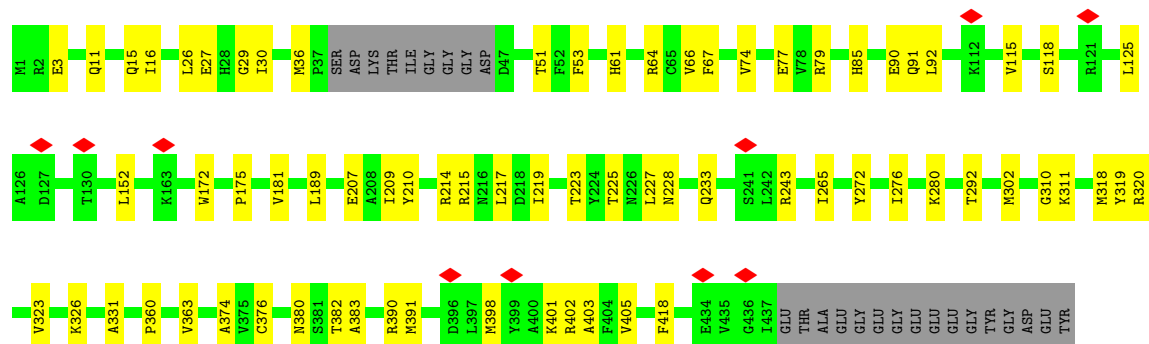
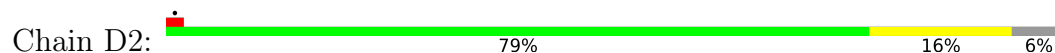
Amino Acid	Green (100)	Yellow (100)	Grey (50)
V177	1	0	0
V181	1	0	0
S190	1	0	0
T191	1	0	0
H192	1	0	0
S193	1	0	0
L194	1	0	0
L196	1	0	0
E207	1	0	0
A208	1	0	0
I209	1	0	0
Y210	1	0	0
E220	1	0	0
R221	1	0	0
P222	1	0	0
R229	1	0	0
L230	1	0	0
Q233	1	0	0
L259	1	0	0
Y262	1	0	0
I265	1	0	0
Y272	1	0	0
I275	1	0	0
K280	1	0	0
A281	1	0	0
Y282	1	0	0
H283	1	0	0
E284	1	0	0
K304	1	0	0
H309	1	0	0
G310	1	0	0
C316	1	0	0
L317	1	0	0
M318	1	0	0
Y319	1	0	0
V323	1	0	0
R339	1	0	0
D345	1	0	0
T349	1	0	0
V350	1	0	0
M1	1	0	0
A12	1	0	0
W21	1	0	0
P32	1	0	0
K36	1	0	0
F37	1	0	0
SER	1	0	0
ASP	1	0	0
LVS	1	0	0
THR	1	0	0
ILE	1	0	0
GLY	1	0	0
GLY	1	0	0
ASP	1	0	0
D47	1	0	0
H61	1	0	0
L70	1	0	0
T73	1	0	0
R79	1	0	0
T80	1	0	0
G81	1	0	0
T82	1	0	0
H88	1	0	0
S94	1	0	0
A100	1	0	0
N101	1	0	0
N102	1	0	0
R105	1	0	0
E113	1	0	0
I122	1	0	0
A140	1	0	0
T145	1	0	0
G146	1	0	0
S147	1	0	0
E155	1	0	0
L156	1	0	0
L157	1	0	0
G162	1	0	0
N168	1	0	0



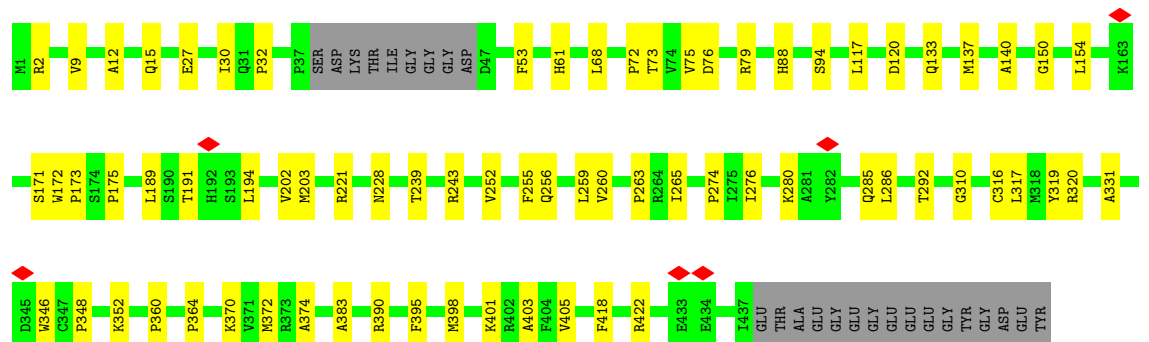
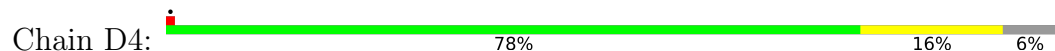
• Molecule 3: Tubulin alpha chain



• Molecule 3: Tubulin alpha chain

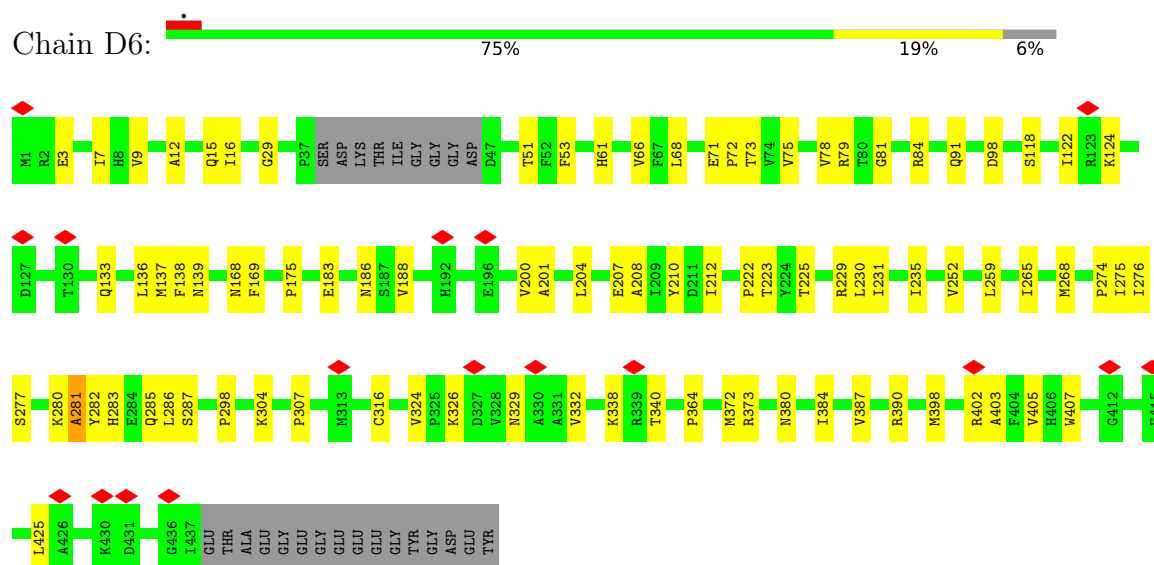


• Molecule 3: Tubulin alpha chain



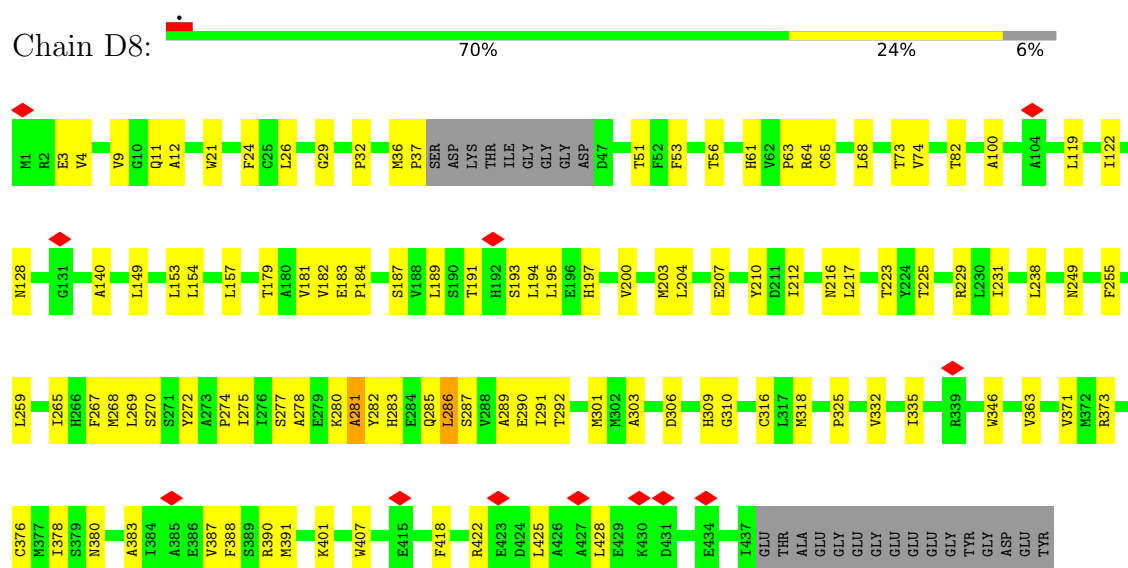
- Molecule 3: Tubulin alpha chain

Chain D6:



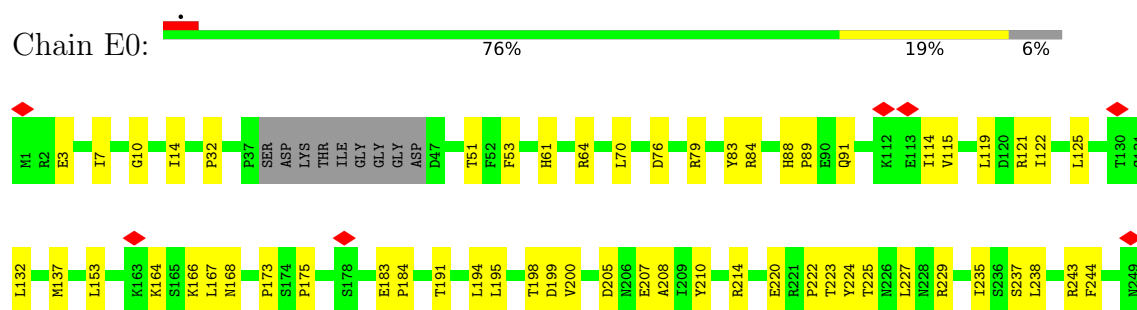
- Molecule 3: Tubulin alpha chain

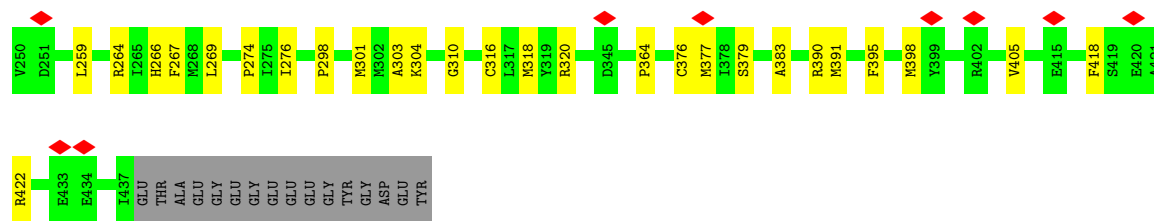
Chain D8:



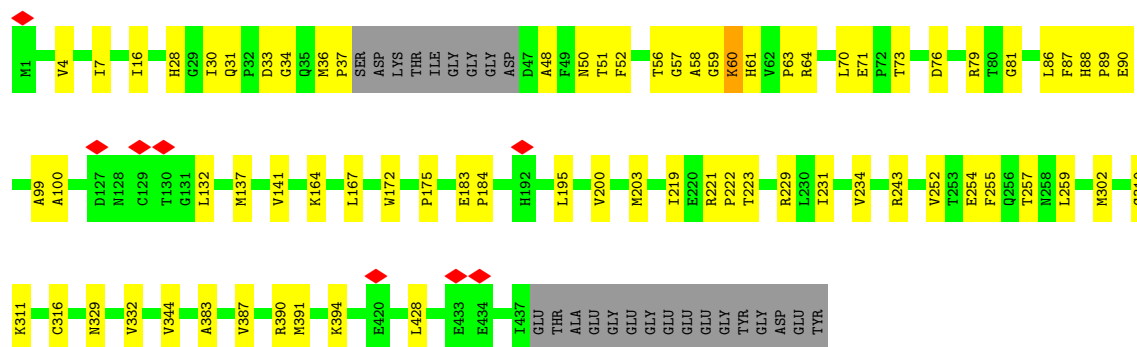
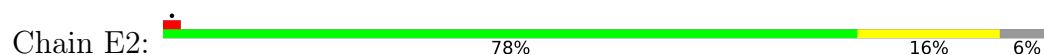
- Molecule 3: Tubulin alpha chain

Chain E0:

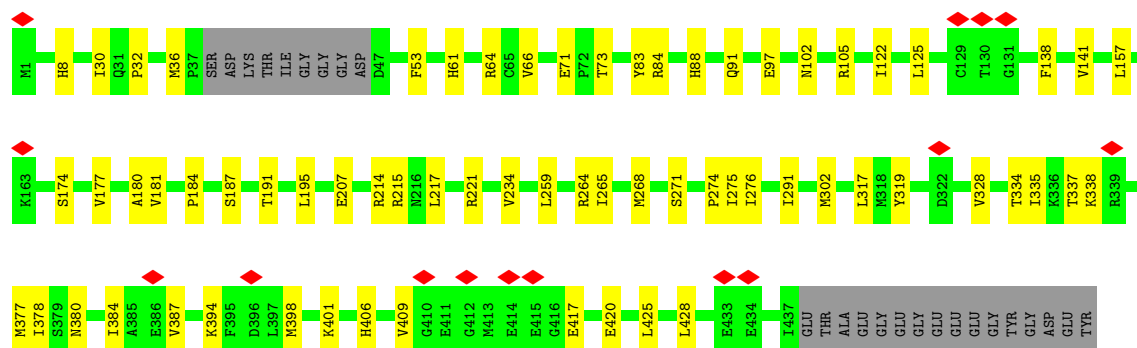
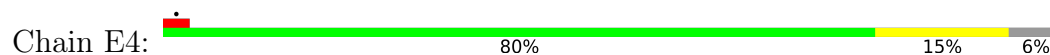




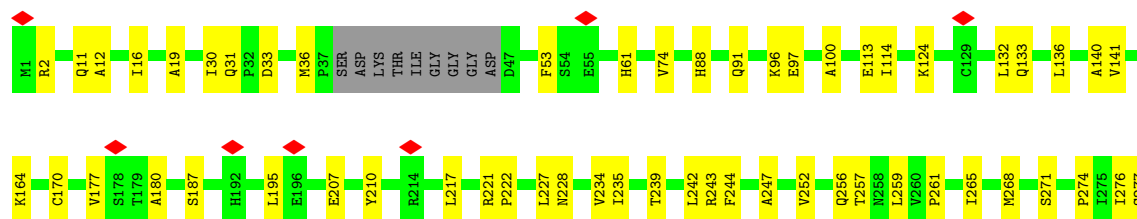
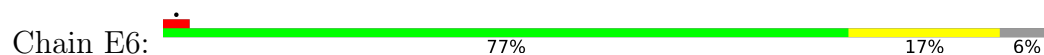
• Molecule 3: Tubulin alpha chain

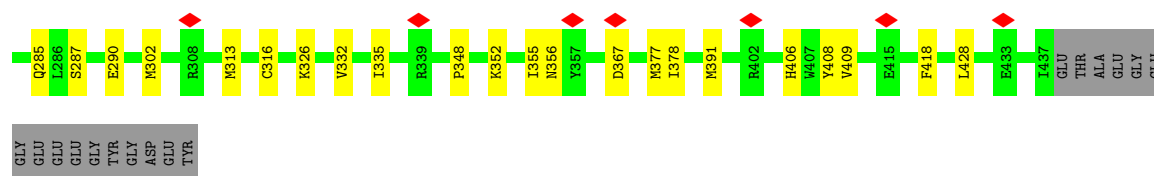


• Molecule 3: Tubulin alpha chain

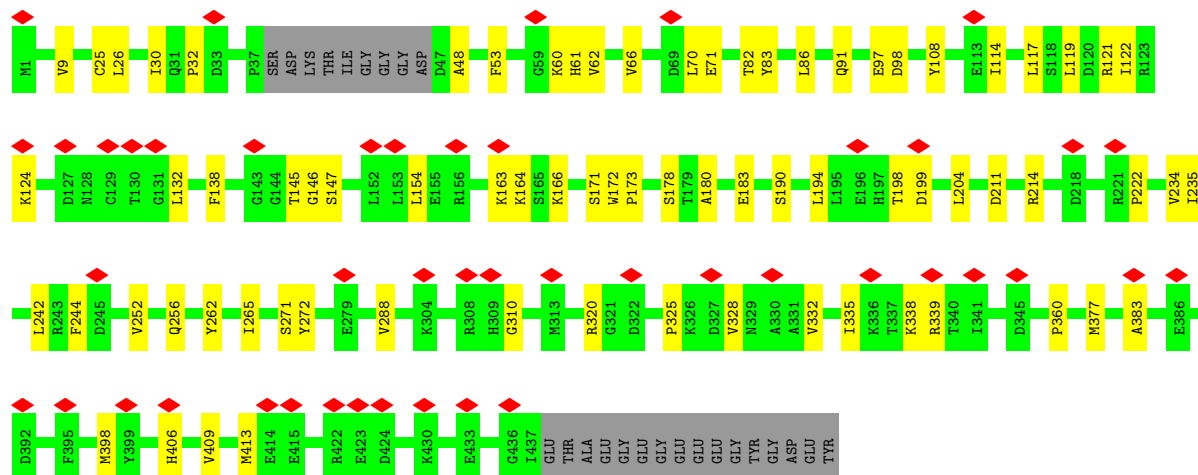
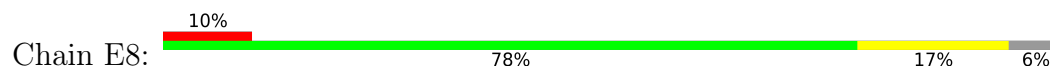


• Molecule 3: Tubulin alpha chain

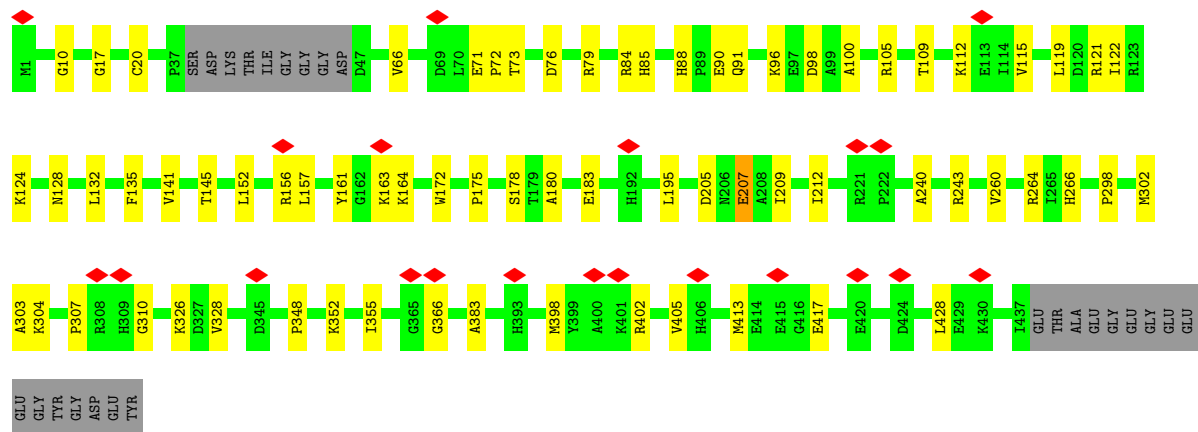
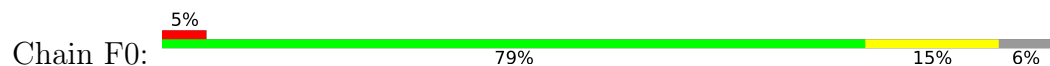




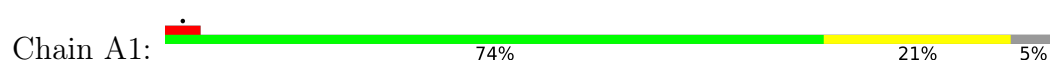
• Molecule 3: Tubulin alpha chain



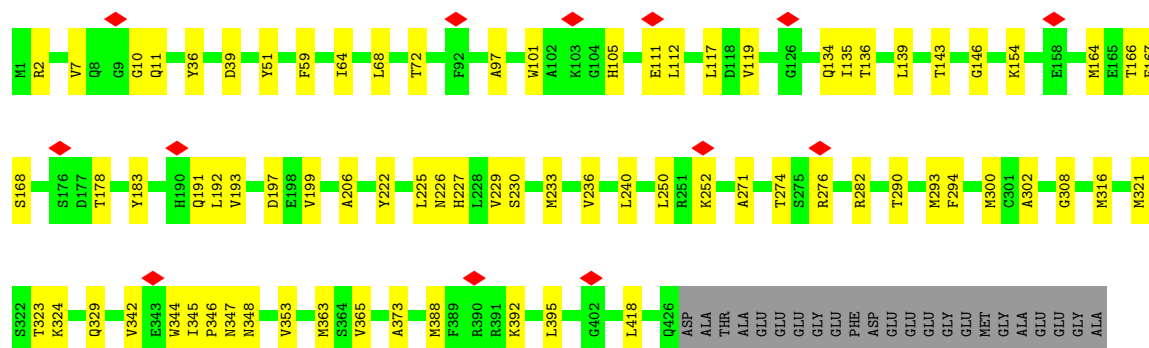
• Molecule 3: Tubulin alpha chain



• Molecule 4: Tubulin beta chain

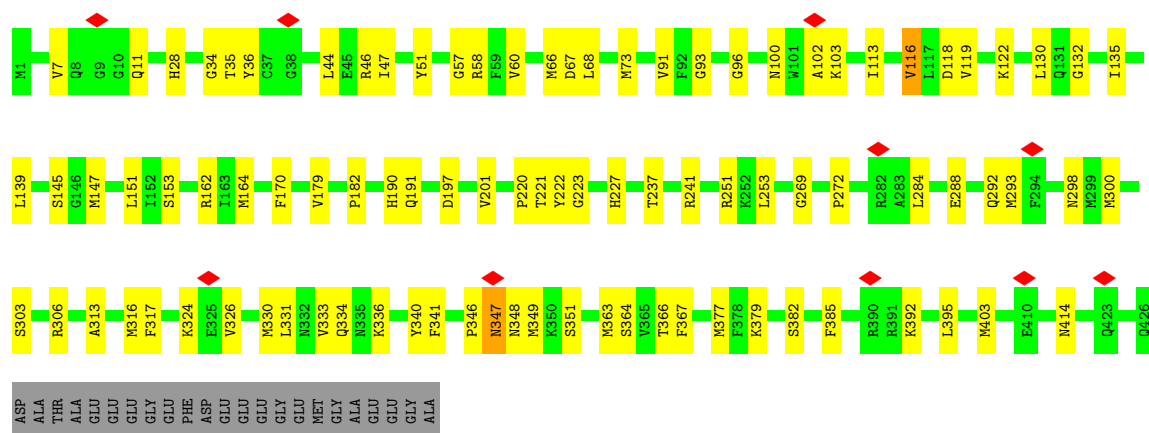


Chain A7: 



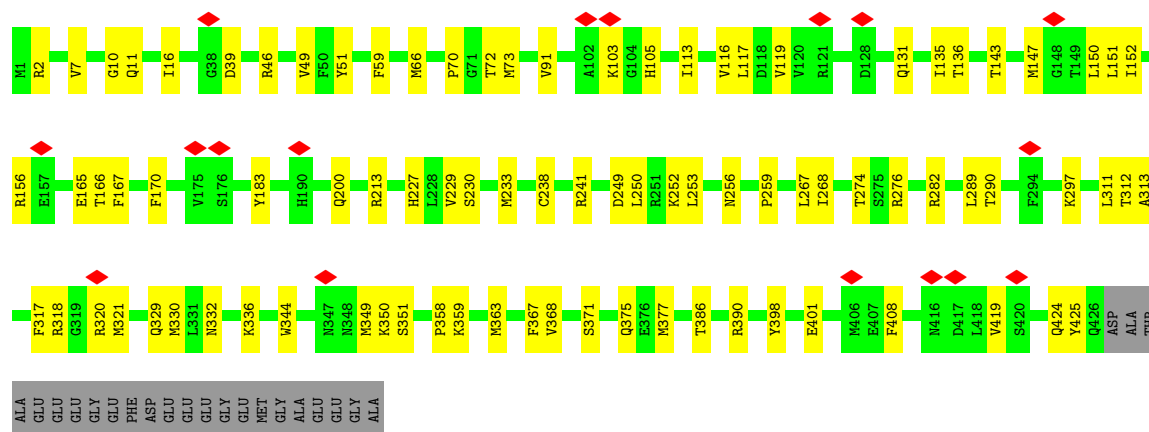
• Molecule 4: Tubulin beta chain

Chain A9: 



• Molecule 4: Tubulin beta chain

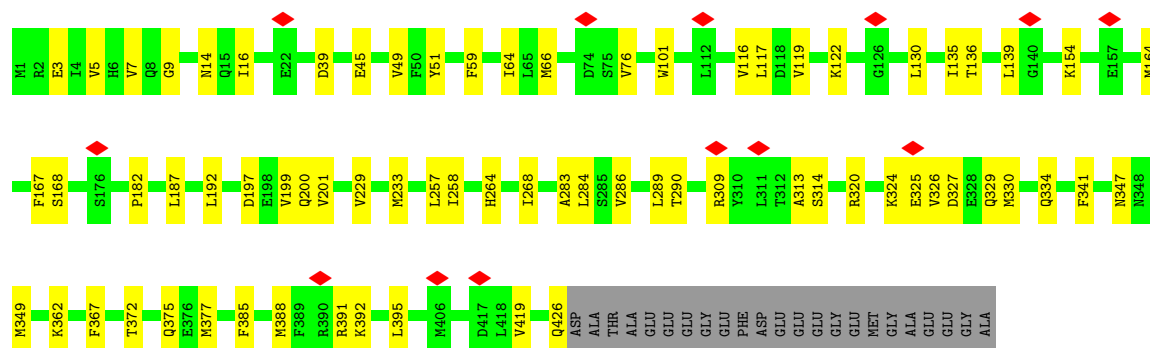
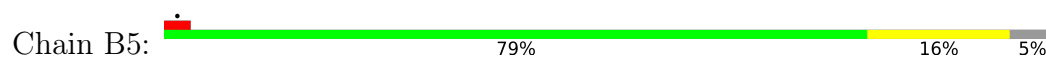
Chain B1: 



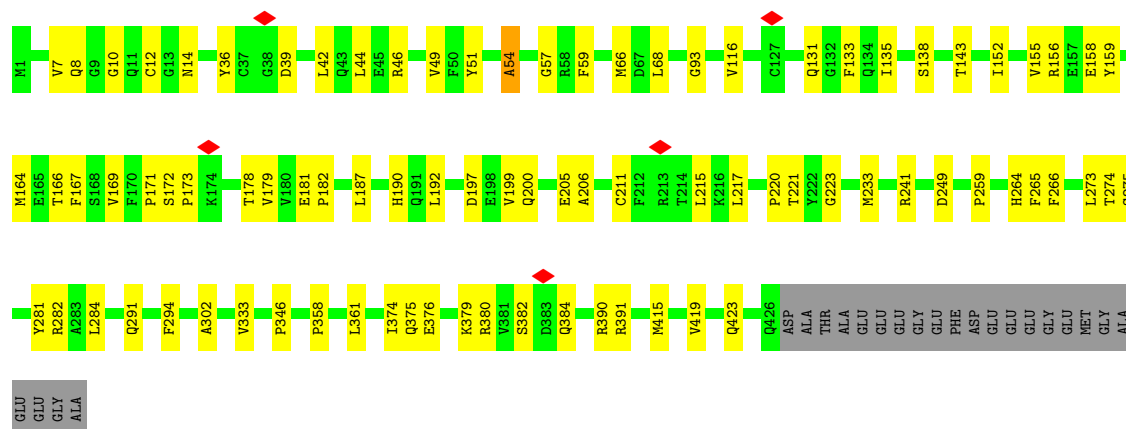
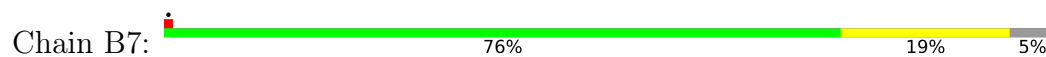
• Molecule 4: Tubulin beta chain

Chain B3: 

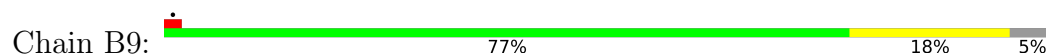
- Molecule 4: Tubulin beta chain

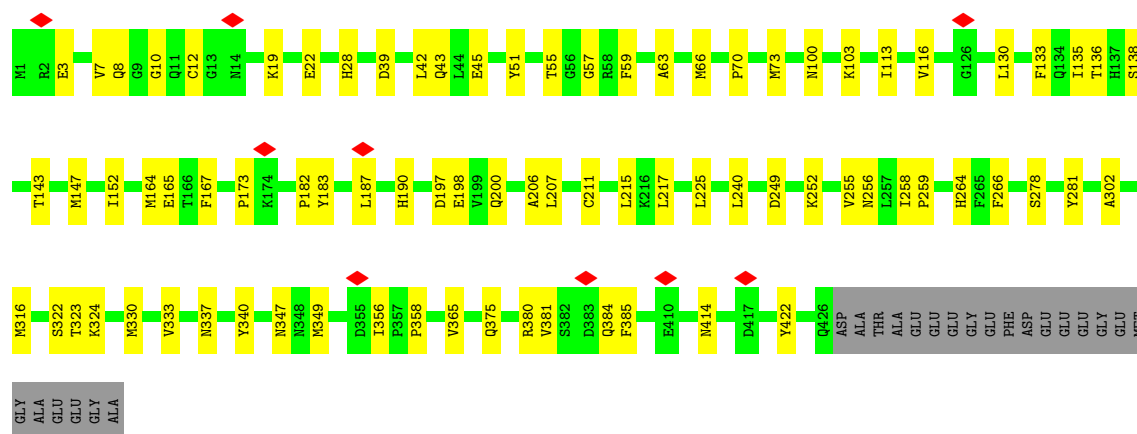


- Molecule 4: Tubulin beta chain



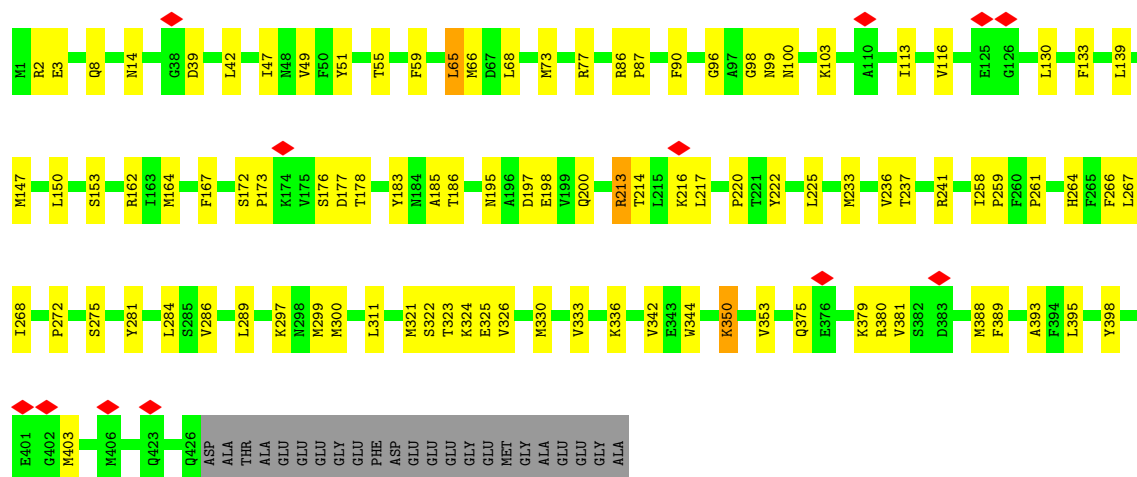
- Molecule 4: Tubulin beta chain





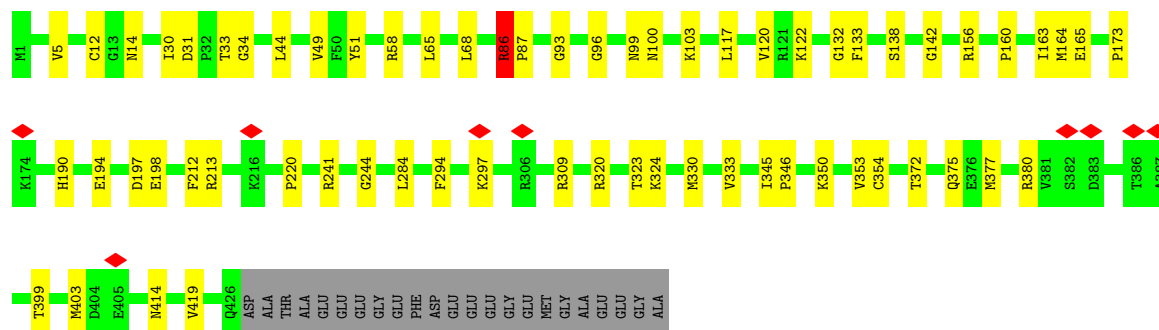
• Molecule 4: Tubulin beta chain

Chain C1: 73% 21% 5%



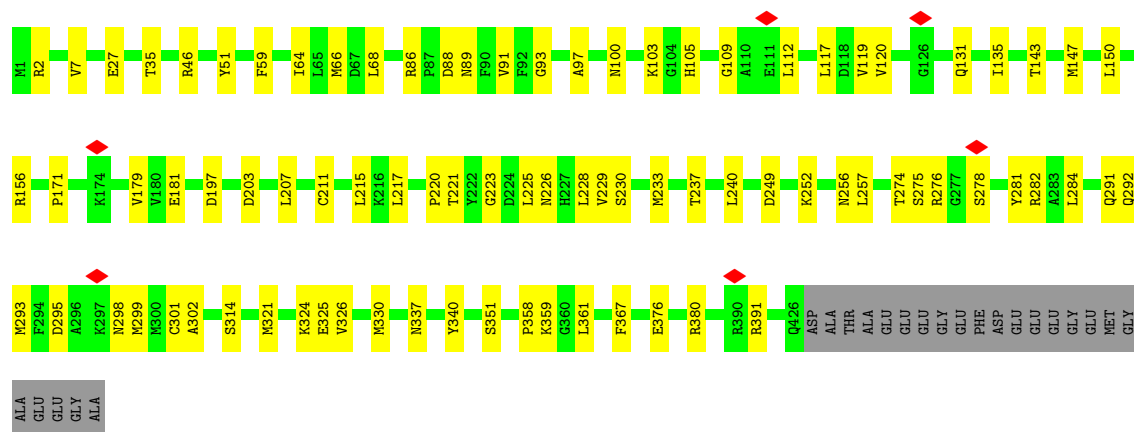
• Molecule 4: Tubulin beta chain

Chain C3: 81% 14% 5%



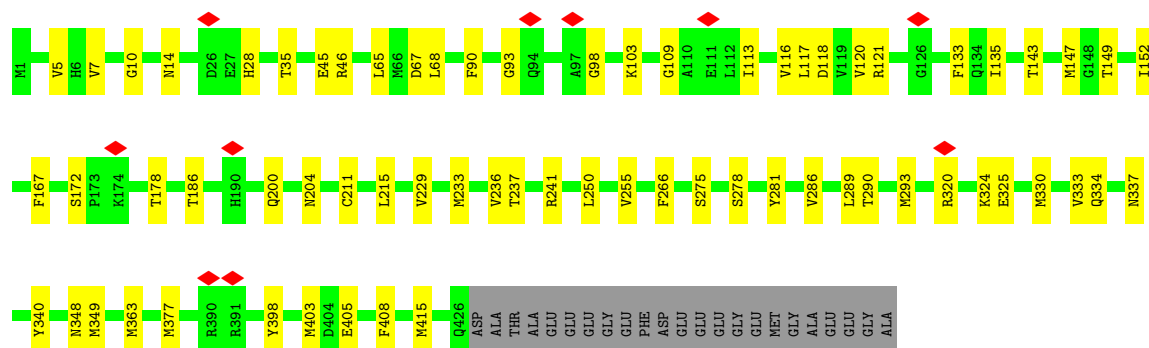
• Molecule 4: Tubulin beta chain

Chain C5: 76% 19% 5%



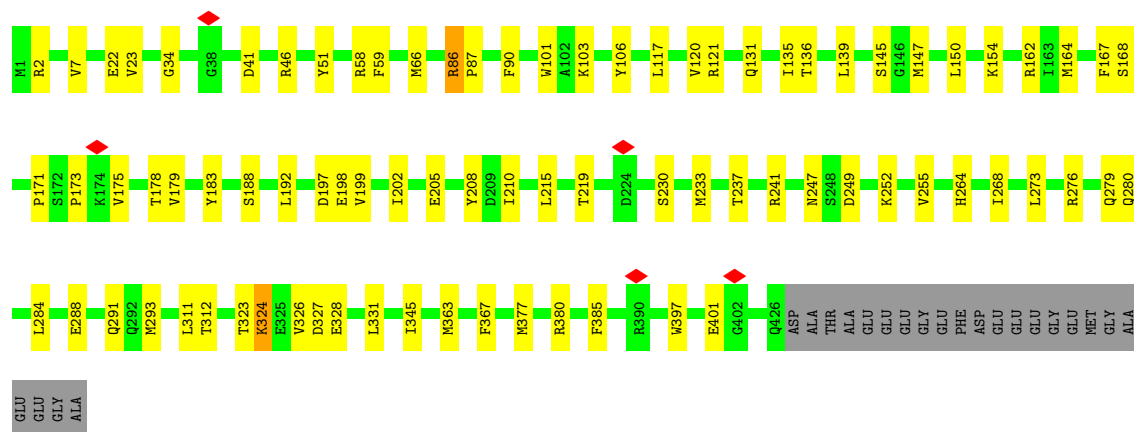
- Molecule 4: Tubulin beta chain

Chain C7: 80% 15% 5%



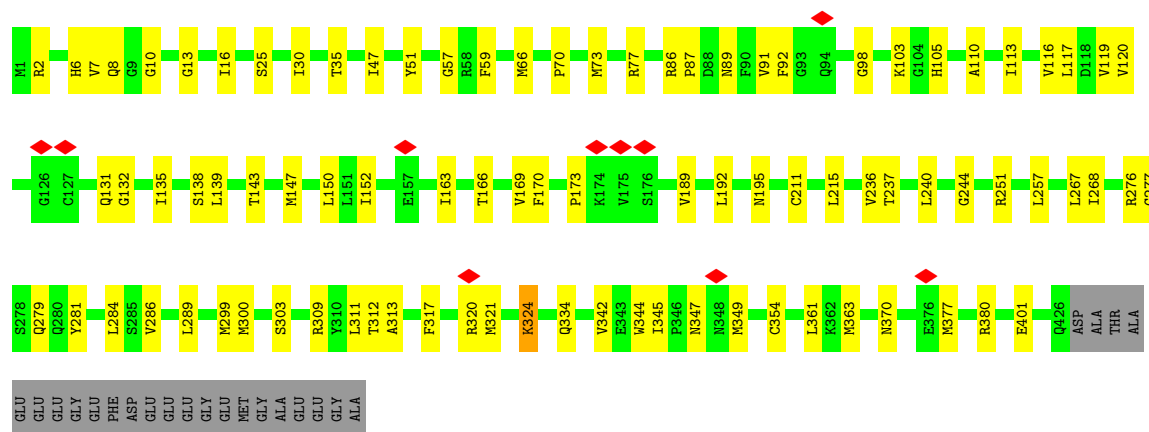
- Molecule 4: Tubulin beta chain

Chain C9: 76% 18% 5%



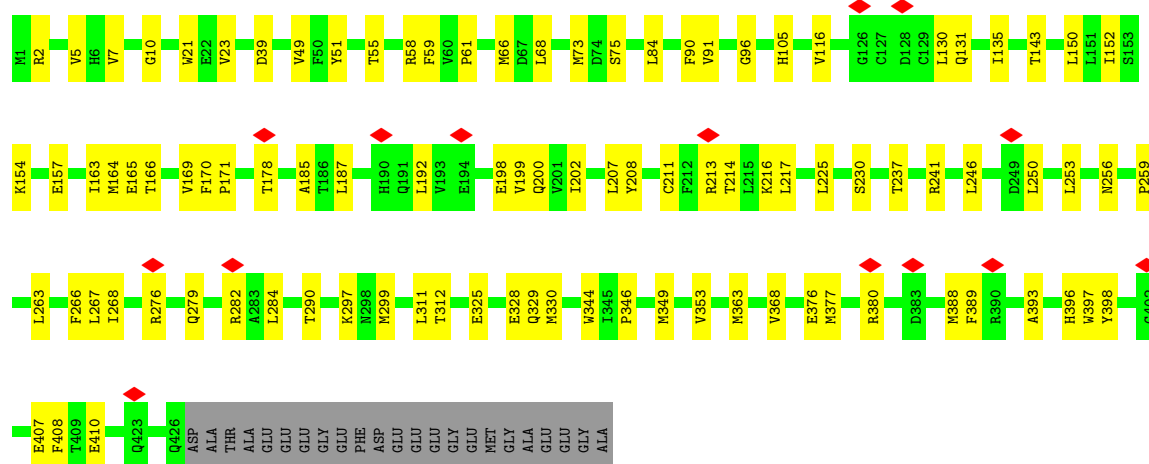
- Molecule 4: Tubulin beta chain

Chain D1: 75% 20% 5%



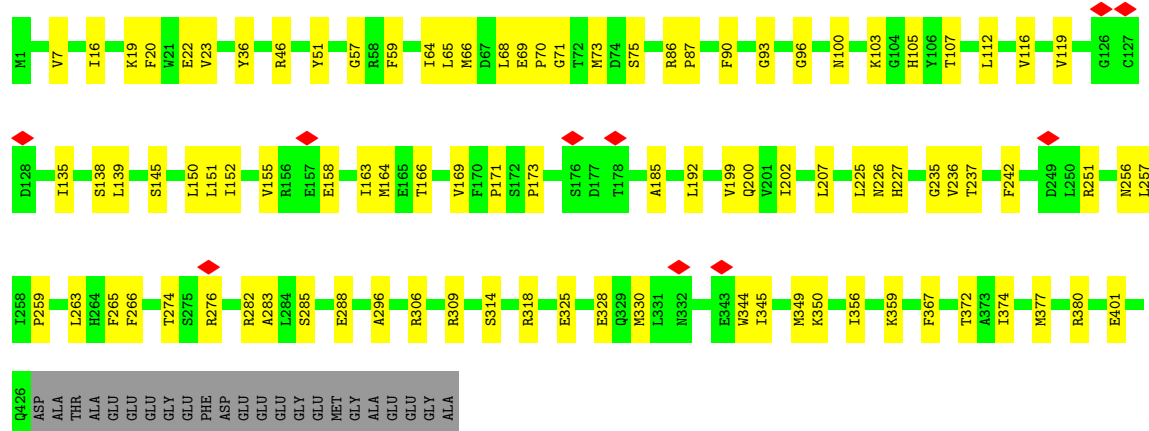
- Molecule 4: Tubulin beta chain

Chain D3: 73% 22% 5%

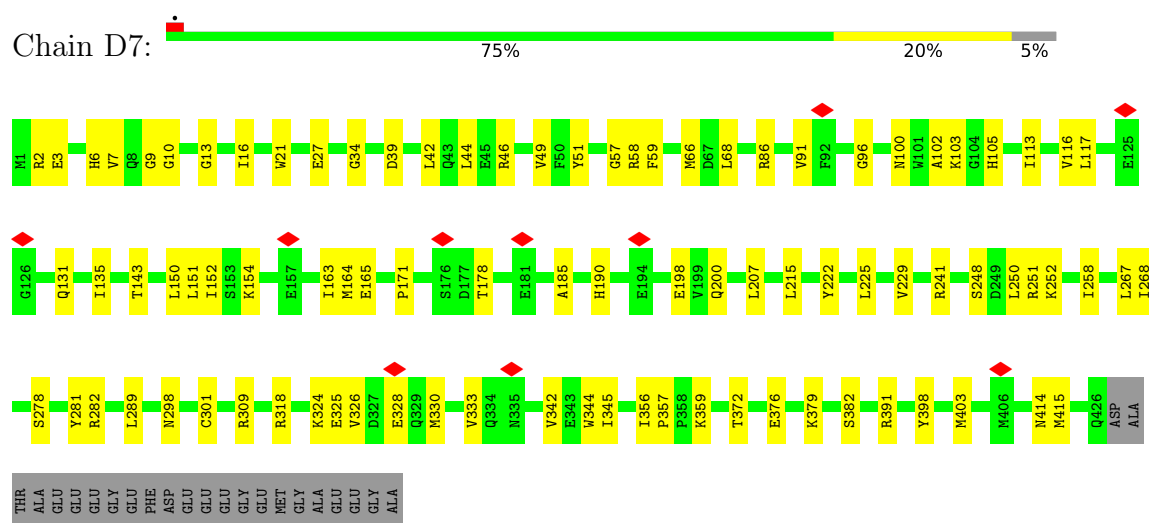


- Molecule 4: Tubulin beta chain

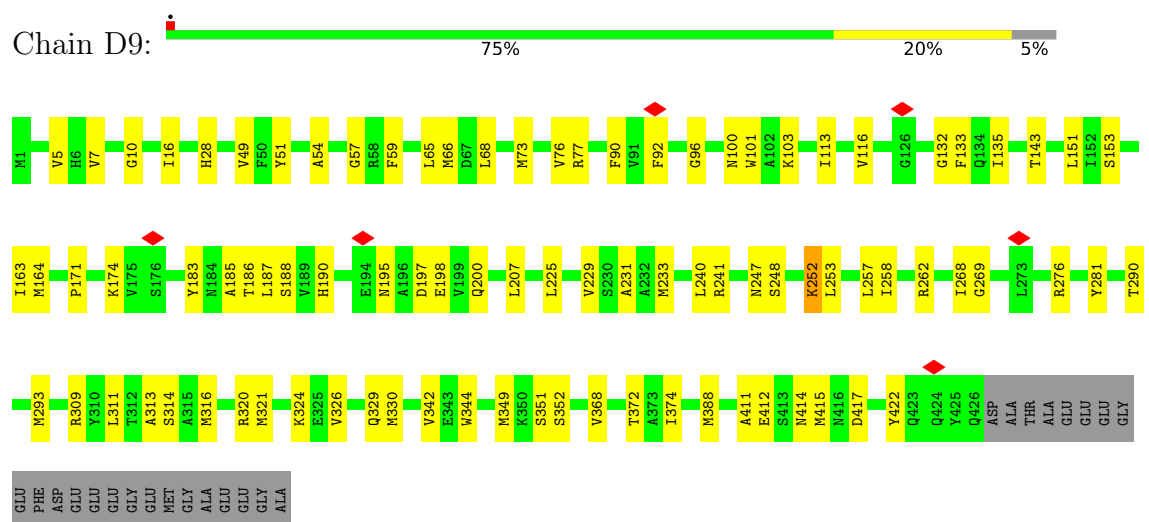
Chain D5: 74% 21% 5%



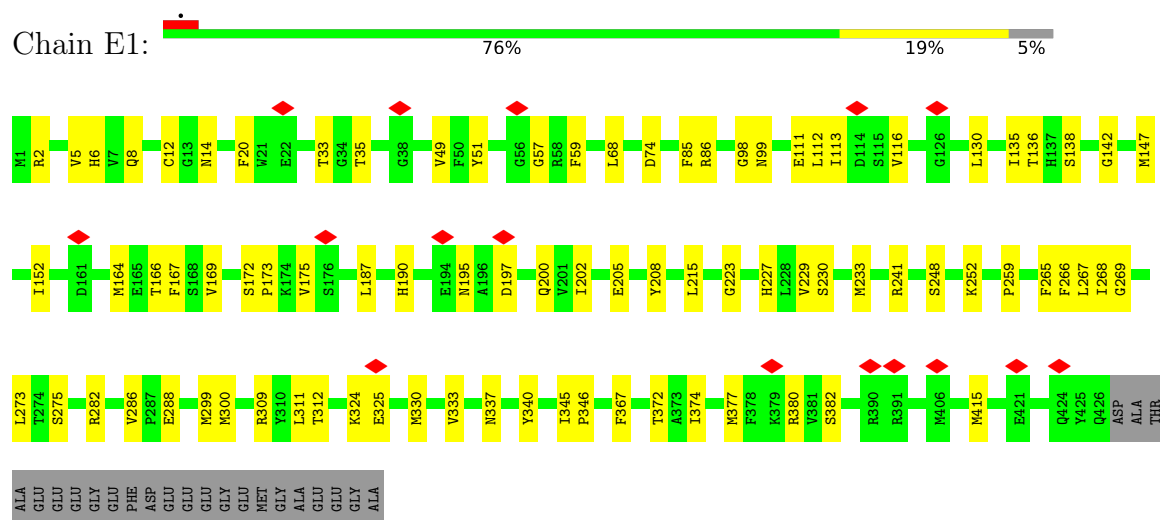
- Molecule 4: Tubulin beta chain



• Molecule 4: Tubulin beta chain

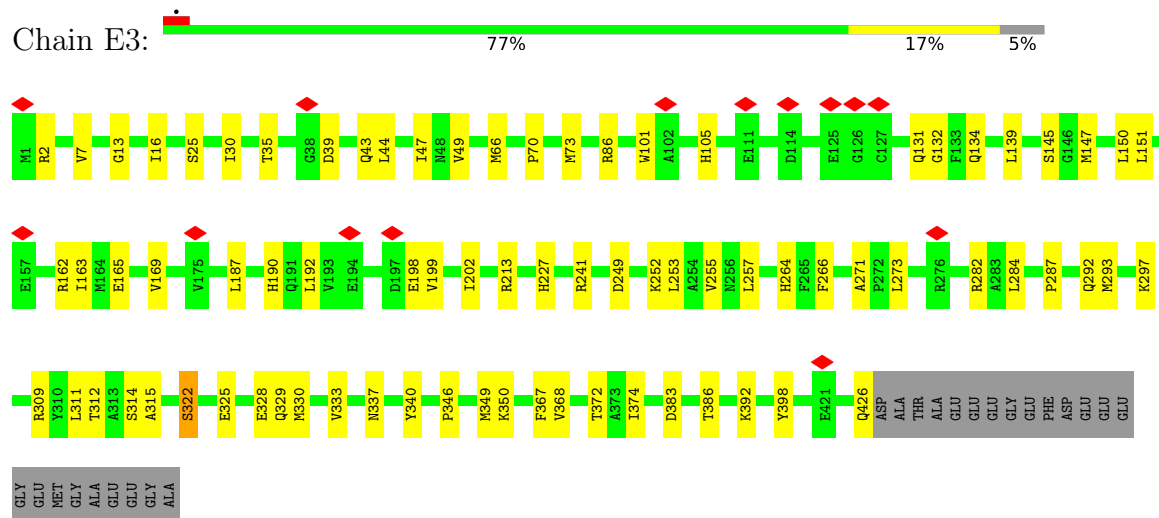


• Molecule 4: Tubulin beta chain



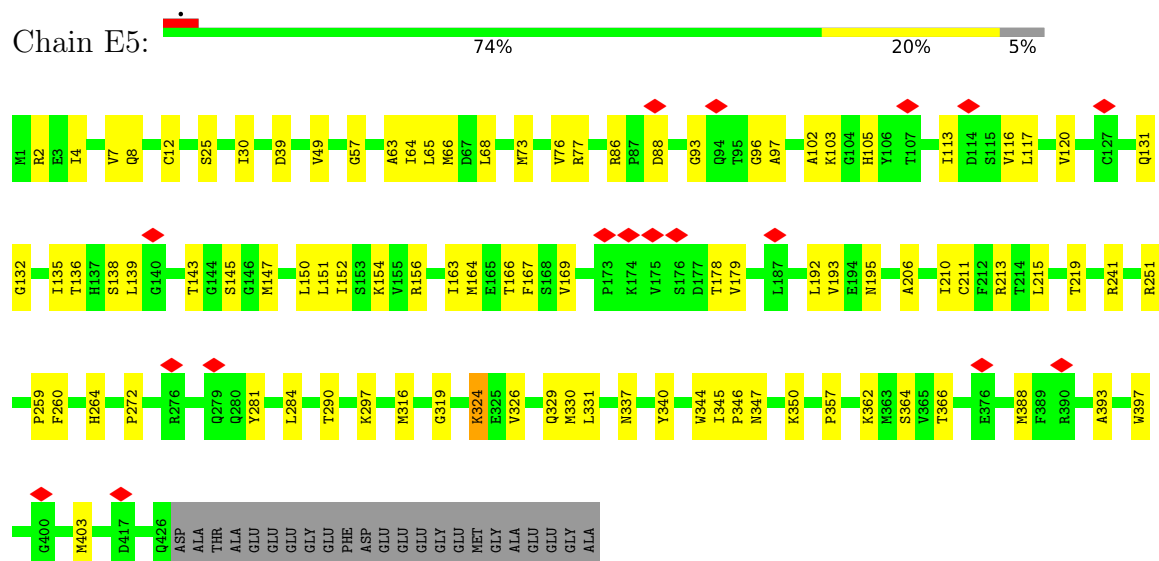
- Molecule 4: Tubulin beta chain

Chain E3:



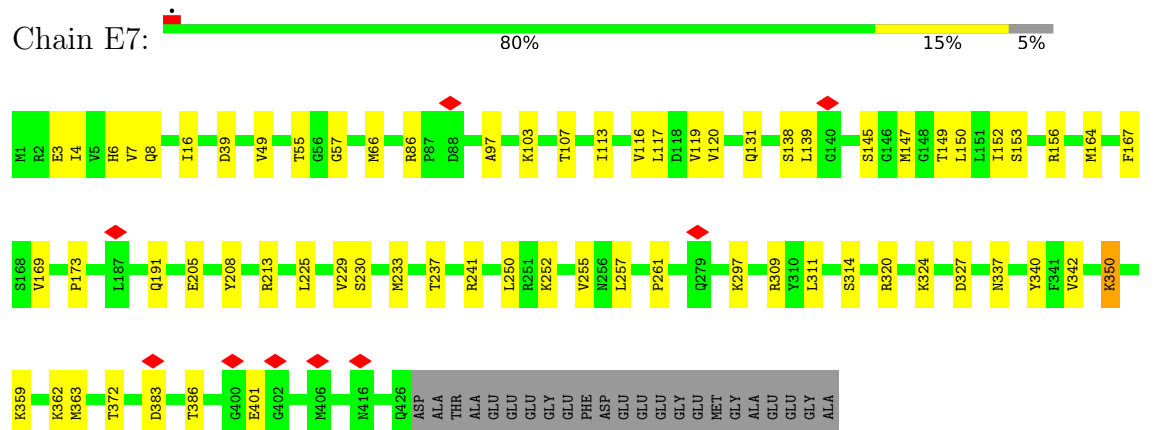
- Molecule 4: Tubulin beta chain

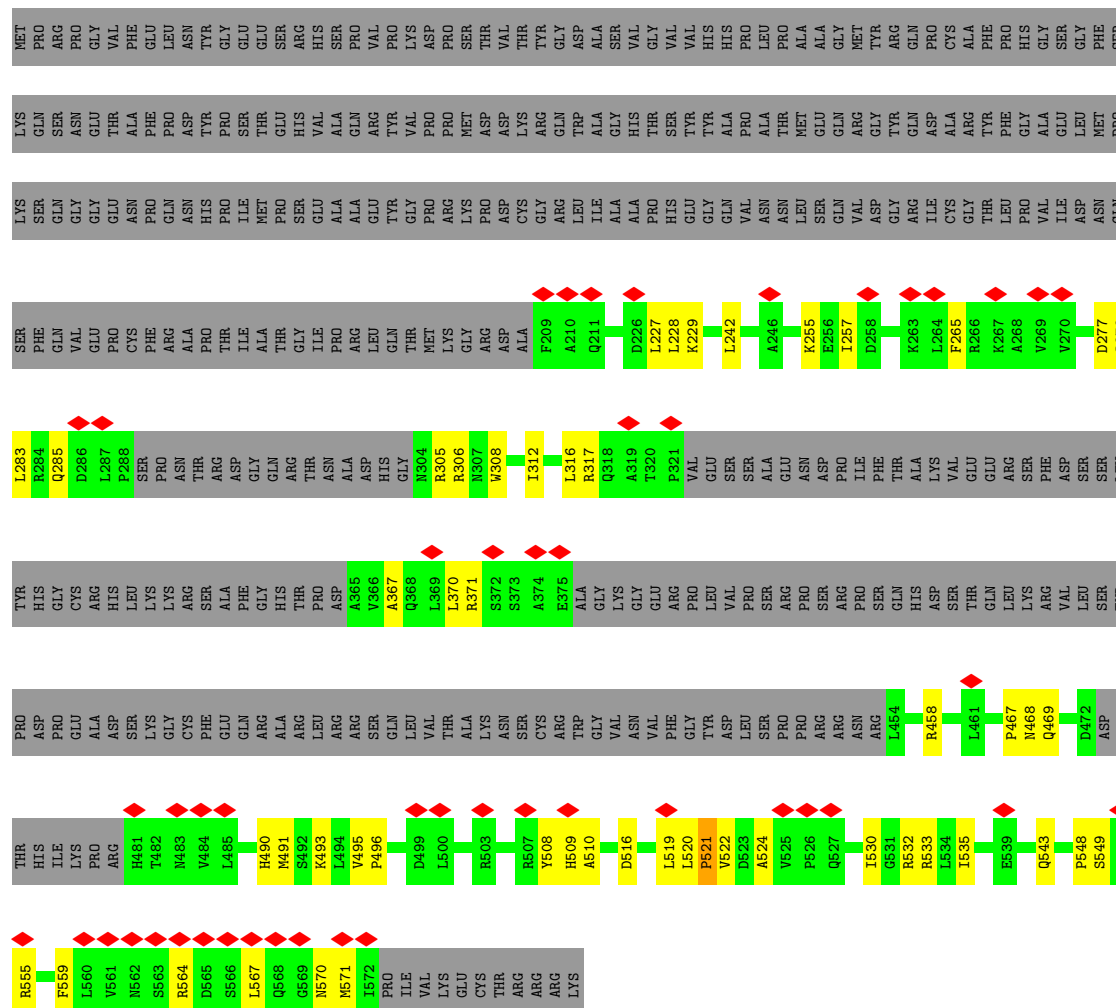
Chain E5:



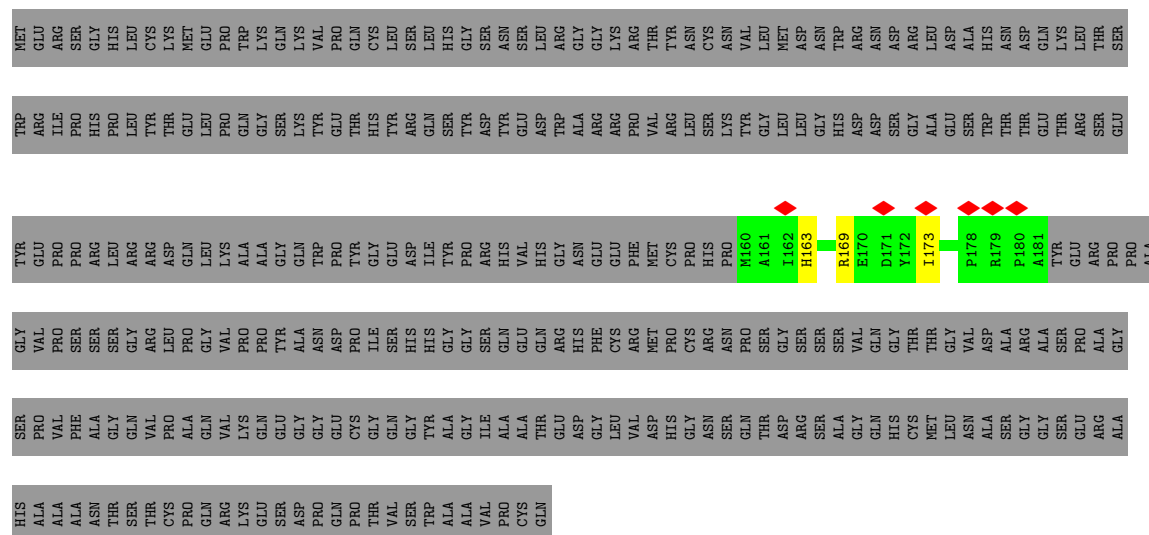
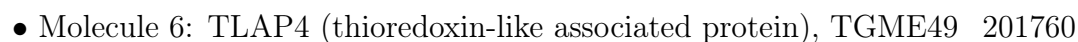
- Molecule 4: Tubulin beta chain

Chain E7:

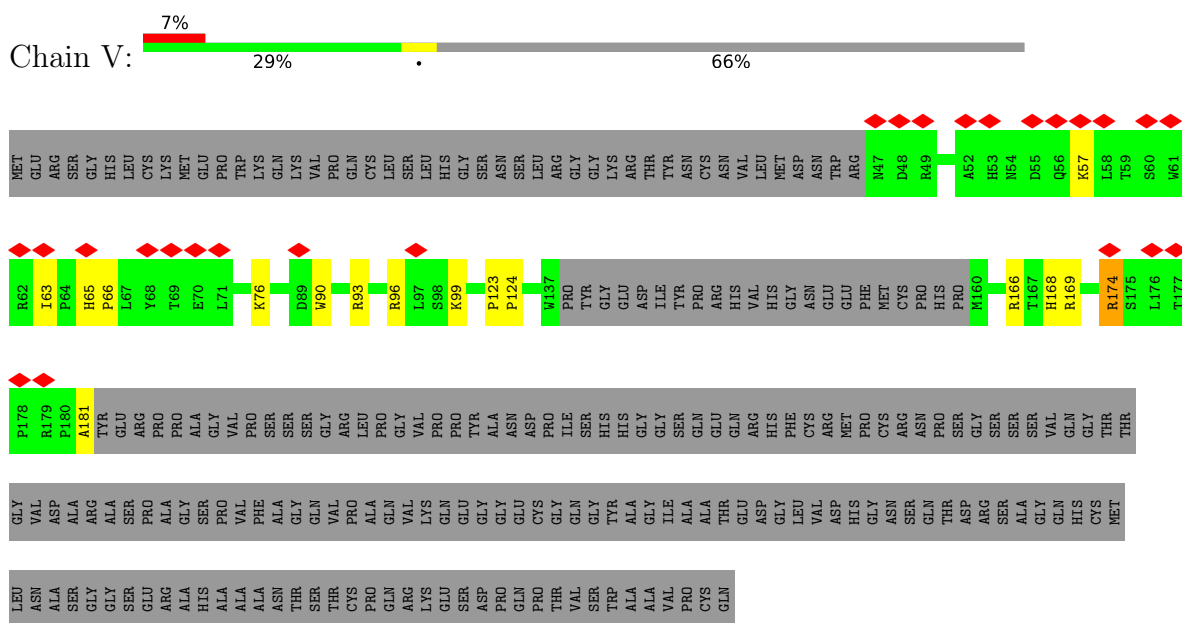




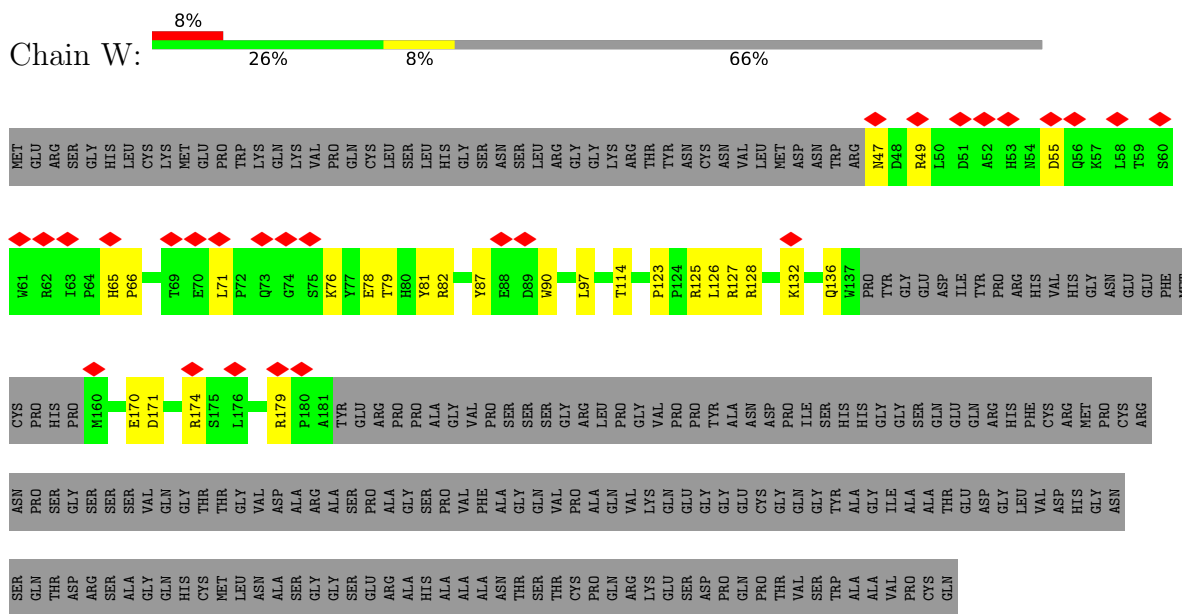
Chain R:



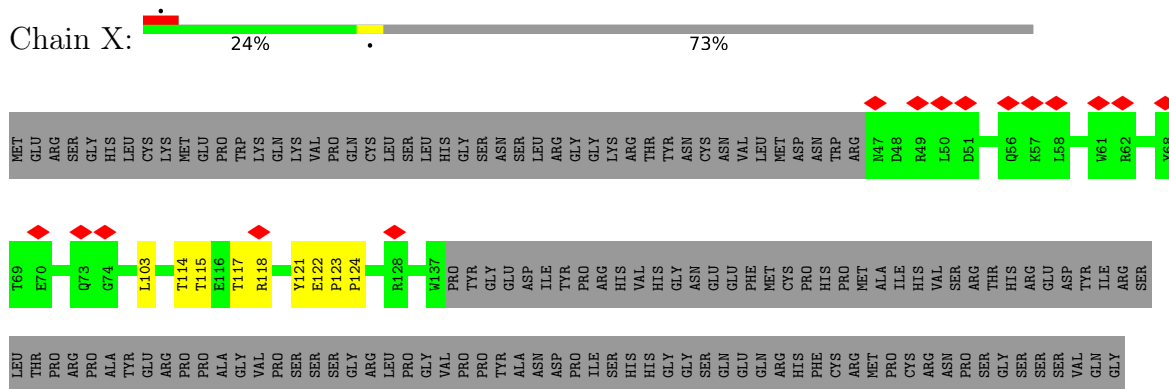
- Molecule 6: TLAP4 (thioredoxin-like associated protein), TGME49 201760



- Molecule 6: TLAP4 (thioredoxin-like associated protein), TGME49 201760



- Molecule 6: TLAP4 (thioredoxin-like associated protein), TGME49_201760



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

• Molecule 7: TRXL1, TGME49_232410

Chain a: 

ASP	GLN	PHE	HIS	VAL	ARG	PRO	THR	LEU	LEU	GLU	GLN																													ASP	GLN	PHE	HIS	VAL	ARG	PRO	THR	LEU	LEU	GLU	GLN	ASP	GLN	PHE	HIS	VAL	ARG	PRO	THR	LEU	LEU	GLU	GLN	ASP	GLN	PHE	HIS	VAL	ARG	PRO	THR	LEU	LEU	GLU	GLN																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
A78	C85	L88	L89	P90	F91	L92	Y96	R97	T98	I108	F112	R117	M151	Y154	E155	V156	P157	T158	Y159	G160	Y161	G162	S163	P168	V172	R178	E179	A180	I185	G188	L189	E190	R194	A195	L196	L197	R198	W199	D200	W201	R202	A207	SER	GLN	PRO	VAL	PHE	ALA	SER	PRO	LEU	LEU	ASN	VAL	GLU	GLY	LYS	ARG	ARG	LEU	ASN	GLU	GLU	ARG	ALA	LEU	MET																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														

• Molecule 7: TRXL1, TGME49_232410

Chain b: 

THR	LEU	LEU	GLU	GLN	Y76	F77	A78	D79	D82	A86	P90	F91	L92	Y95	T98	M99	I108	F112	R126	M129	I134	E137	N138	V150	P157	G162	S163	R164	T165	G166	V172	I173	G188	L196	T204	A207	SER	ASP	GLN	PHE	HIS	VAL	ARG	PRO																	
MET	SER	GLN	PRO	VAL	PHE	ALA	SER	SER	PRO	LEU	LEU	ASN	VAL	GLY	GLY	LYS	ARG	ARG	LEU	ASN	GLY	GLU	GLU	ARG	ALA	LEU	LEU	GLN	GLN	LYS	ALA	ALA	GLY	GLY	GLY	GLY	VAL	ASN	ASN	ILE	ILE	GLN	LEU	PRO	PRO	ASN	TYR	GLY	ASP	ASP	MET	ASP	L47	G53	K56	T61	V62	L68	K71	S72	V73

• Molecule 7: TRXL1, TGME49_232410

Chain c: 

MET	S2	V5	F6	N11	K14	R15	Q27	K28	A29	GLY	GLY	GLY	VAL	N35	M45	D46	L47	I48	L49	F50	P51	E52	G53	V62	Q65	S66	H67	L68	V73	A74	L75	A78	D79	D82	P83	A86	S87	G103	I111	F112	V113	S114	L115	R119
W131	L132	L136	E137	L140	I143	L144	K145	R146	R149	E155	G160	Y159	Y161	T165	V172	F182	L183	P184	G188	L189	A195	A207	SER	ASP	GLN	PHE	HIS	VAL	ARG	PRO	THR	LEU	LEU	GLY	GLN									

• Molecule 7: TRXL1, TGME49_232410

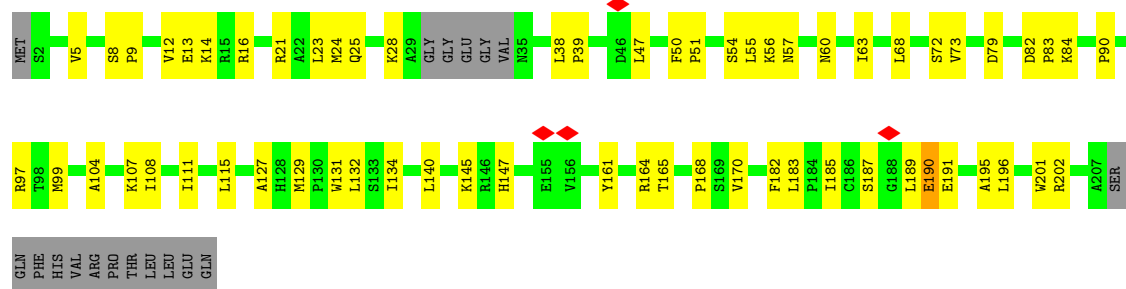
Chain d: 

MET	S2	Q3	P4	V5	F6	A7	S8	P9	V12	E13	K14	R15	R16	L17	Q27	K28	A29	GLY	GLY	GLY	VAL	N35	L47	I48	L49	F50	P51	S54	L55	S58	I63	P64	Q65	L68	K71	S72	V73	A78	K84	C85	L88	L89	P90	F91	L92	Y96
-----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



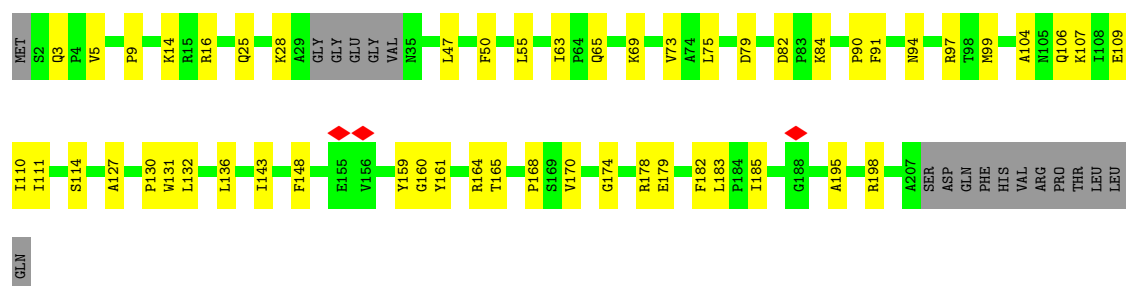
- Molecule 7: TRXL1, TGME49_232410

Chain e: 63% 28% 9%



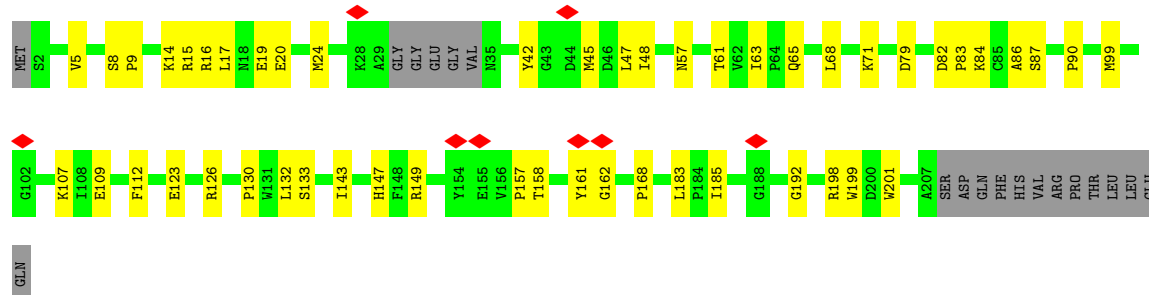
- Molecule 7: TRXL1, TGME49_232410

Chain f: 68% 24% 9%



- Molecule 7: TRXL1, TGME49_232410

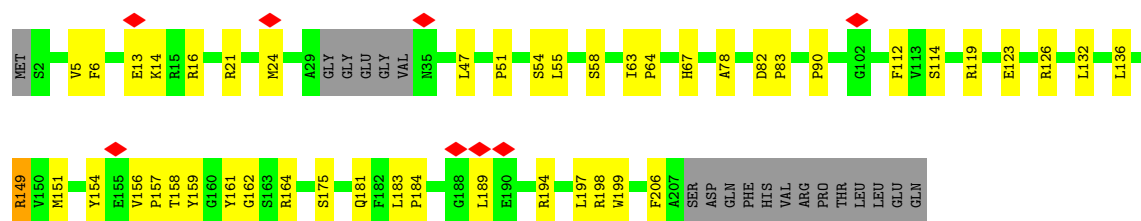
Chain g: 69% 23% 9%



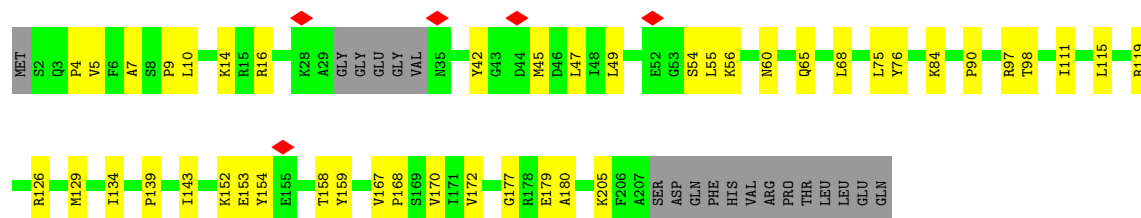
- Molecule 7: TRXL1, TGME49_232410

Chain h: 70% 20% 9%

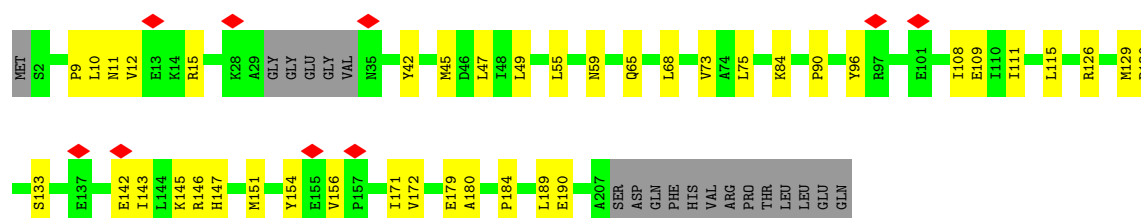




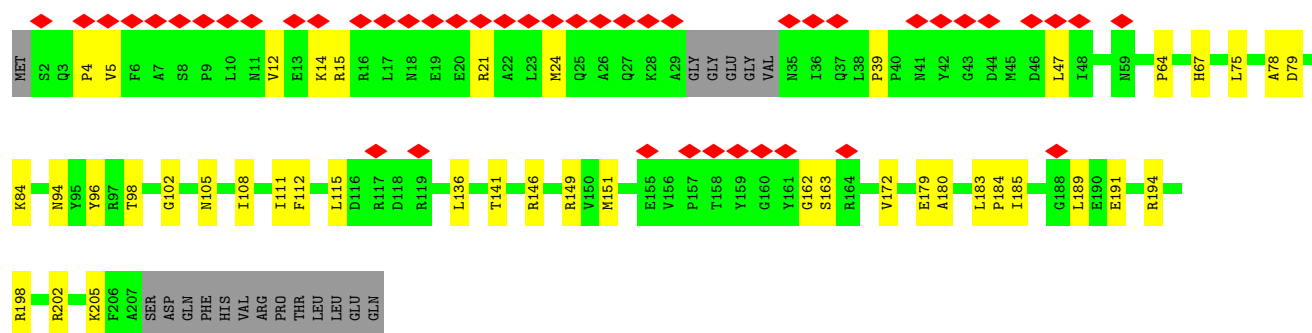
• Molecule 7: TRXL1, TGME49_232410



• Molecule 7: TRXL1, TGME49_232410

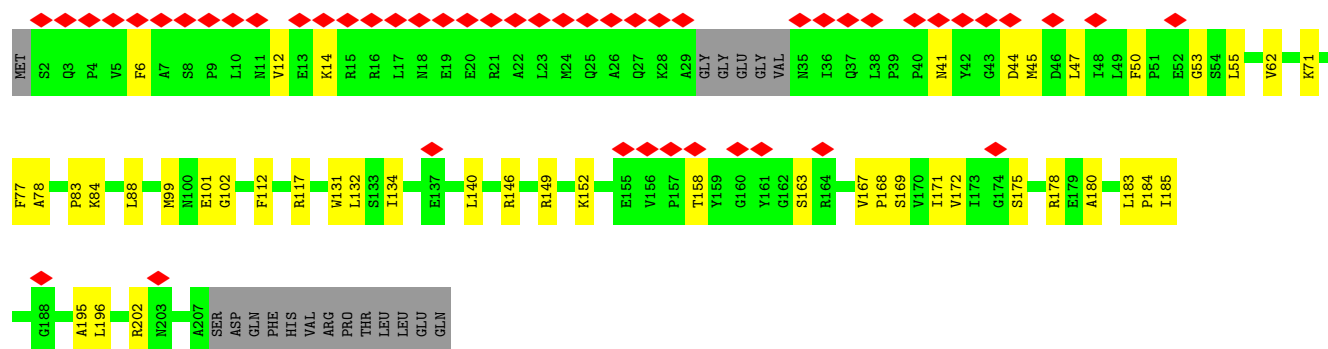


• Molecule 7: TRXL1, TGME49_232410

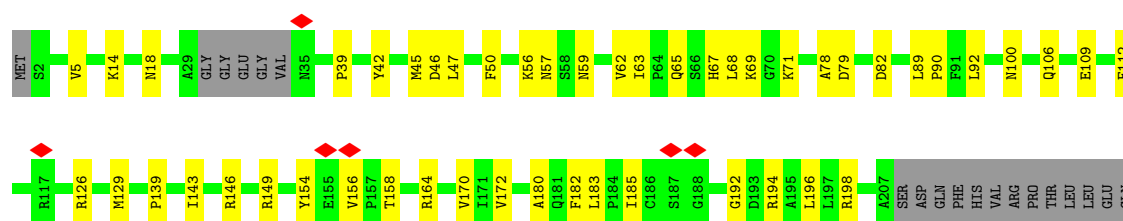


• Molecule 7: TRXL1, TGME49_232410

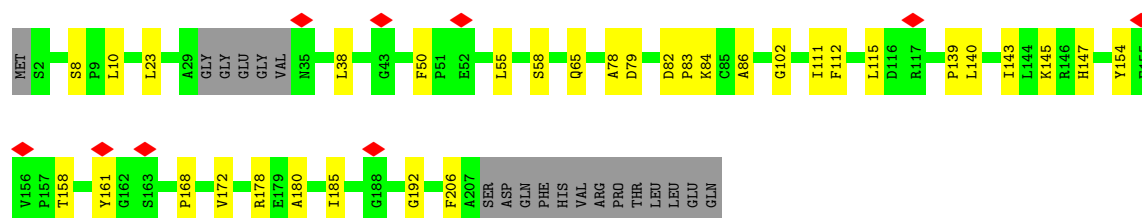
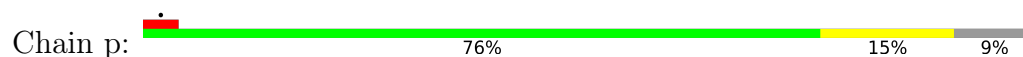




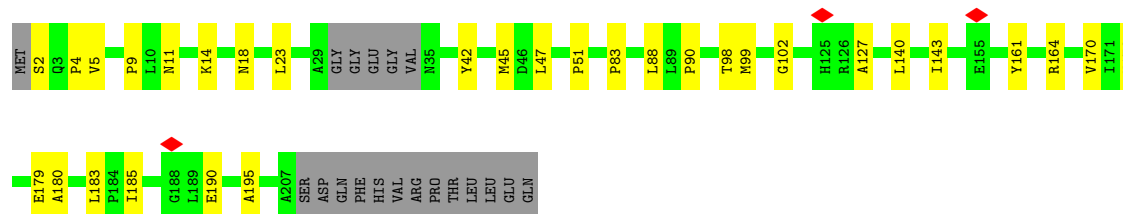
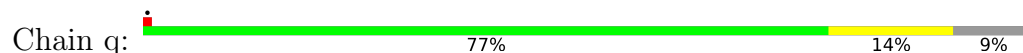
• Molecule 7: TRXL1, TGME49_232410



• Molecule 7: TRXL1, TGME49_232410

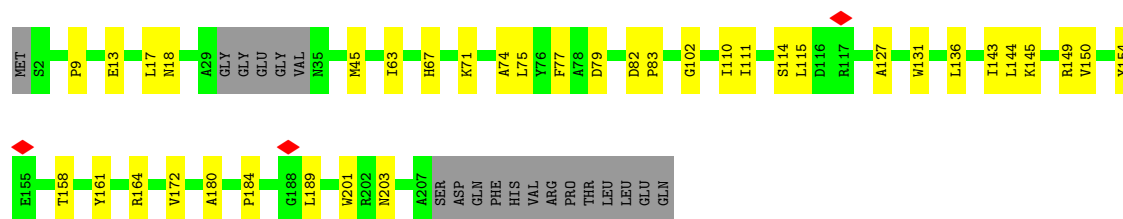


• Molecule 7: TRXL1, TGME49_232410

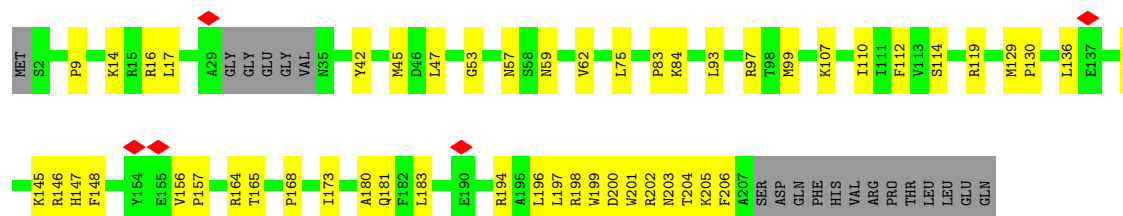


• Molecule 7: TRXL1, TGME49_232410

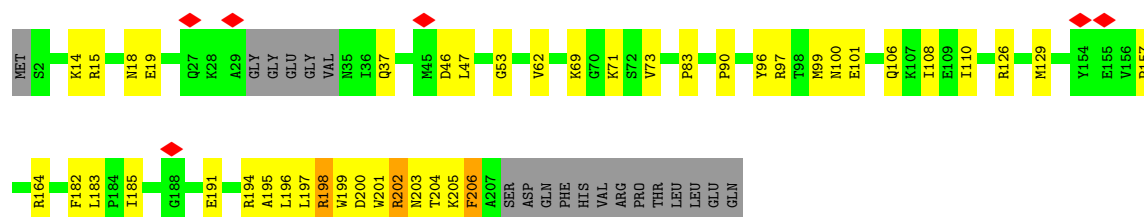




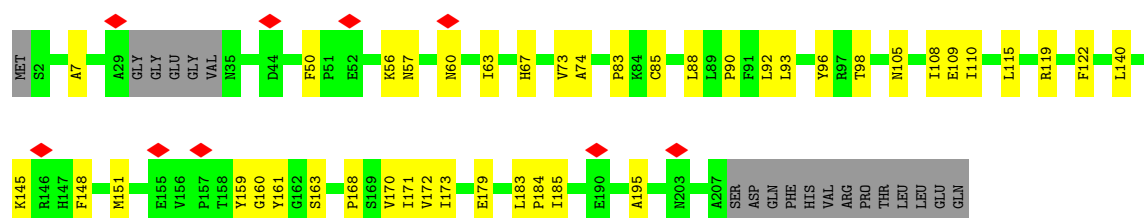
- Molecule 7: TRXL1, TGME49_232410



- Molecule 7: TRXL1, TGME49_232410

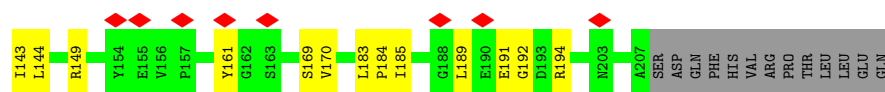


- Molecule 7: TRXL1, TGME49_232410

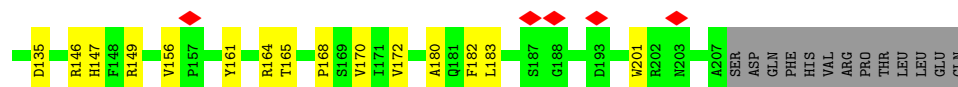
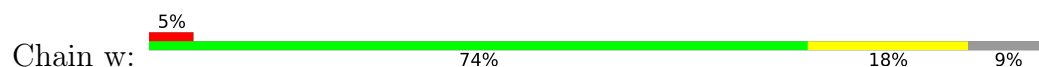


- Molecule 7: TRXL1, TGME49_232410

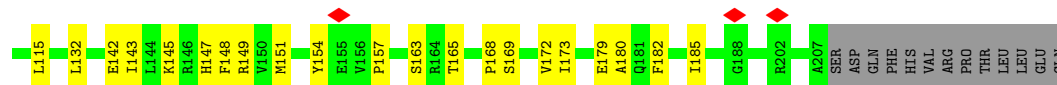




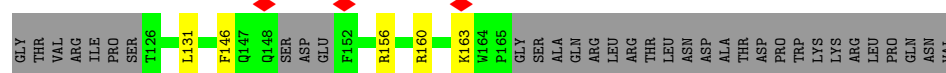
• Molecule 7: TRXL1, TGME49_232410



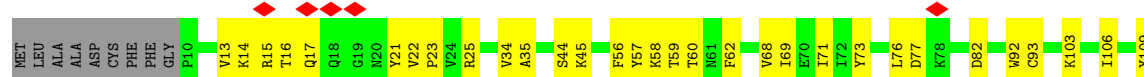
• Molecule 7: TRXL1, TGME49_232410



• Molecule 8: TRXL2, TGME49_225790



• Molecule 8: TRXL2, TGME49_225790



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55276	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	25000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.133	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.019	Depositor
Map value standard deviation	0.088	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	536.0, 536.0, 536.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.28	0/1069	0.78	1/1440 (0.1%)
1	2	0.22	0/1069	0.65	0/1440
2	A	0.20	0/483	0.51	0/667
2	B	0.20	0/491	0.51	0/679
2	C	0.21	0/483	0.53	0/667
2	D	0.37	1/484 (0.2%)	0.64	0/669
2	E	0.19	0/491	0.70	2/679 (0.3%)
2	F	0.26	0/461	0.61	0/637
2	G	0.22	0/491	0.62	2/679 (0.3%)
2	H	0.26	0/461	0.57	0/637
2	I	0.29	0/491	0.58	0/679
2	J	0.25	0/491	0.52	0/679
2	K	0.21	0/491	0.60	0/679
3	A0	0.21	0/3398	0.57	2/4606 (0.0%)
3	A2	0.23	0/3398	0.62	0/4606
3	A4	0.21	0/3398	0.53	0/4606
3	A6	0.23	0/3398	0.60	0/4606
3	A8	0.22	0/3398	0.58	2/4606 (0.0%)
3	B0	0.21	0/3398	0.57	0/4606
3	B2	0.21	0/3398	0.56	0/4606
3	B4	0.22	0/3398	0.57	0/4606
3	B6	0.20	0/3398	0.54	0/4606
3	B8	0.24	0/3398	0.58	1/4606 (0.0%)
3	C0	0.24	0/3398	0.59	0/4606
3	C2	0.24	0/3398	0.60	0/4606
3	C4	0.25	0/3398	0.62	0/4606
3	C6	0.23	0/3398	0.58	1/4606 (0.0%)
3	C8	0.22	0/3398	0.56	1/4606 (0.0%)
3	D0	0.24	0/3398	0.58	0/4606
3	D2	0.21	0/3398	0.54	0/4606
3	D4	0.23	0/3398	0.56	0/4606
3	D6	0.23	0/3398	0.55	0/4606

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	D8	0.29	0/3398	0.60	0/4606
3	E0	0.22	0/3398	0.56	0/4606
3	E2	0.32	0/3398	0.63	0/4606
3	E4	0.21	0/3398	0.54	0/4606
3	E6	0.22	0/3398	0.53	0/4606
3	E8	0.20	0/3398	0.55	0/4606
3	F0	0.22	0/3398	0.61	0/4606
4	A1	0.23	0/3404	0.61	1/4606 (0.0%)
4	A3	0.22	0/3404	0.60	1/4606 (0.0%)
4	A5	0.23	0/3404	0.59	2/4606 (0.0%)
4	A7	0.22	0/3404	0.56	0/4606
4	A9	0.23	0/3404	0.61	1/4606 (0.0%)
4	B1	0.23	0/3404	0.61	0/4606
4	B3	0.24	0/3404	0.61	0/4606
4	B5	0.23	0/3404	0.58	0/4606
4	B7	0.22	0/3404	0.58	2/4606 (0.0%)
4	B9	0.23	0/3404	0.60	0/4606
4	C1	0.27	0/3404	0.68	2/4606 (0.0%)
4	C3	0.23	0/3404	0.59	1/4606 (0.0%)
4	C5	0.26	0/3404	0.64	0/4606
4	C7	0.22	0/3404	0.56	0/4606
4	C9	0.25	0/3404	0.66	3/4606 (0.1%)
4	D1	0.22	0/3404	0.57	1/4606 (0.0%)
4	D3	0.24	0/3404	0.59	0/4606
4	D5	0.23	0/3404	0.55	0/4606
4	D7	0.22	0/3404	0.60	1/4606 (0.0%)
4	D9	0.21	0/3404	0.55	1/4606 (0.0%)
4	E1	0.22	0/3404	0.58	2/4606 (0.0%)
4	E3	0.24	0/3404	0.56	0/4606
4	E5	0.23	0/3404	0.59	1/4606 (0.0%)
4	E7	0.21	0/3404	0.56	1/4606 (0.0%)
4	E9	0.22	0/3404	0.58	0/4606
4	F1	0.24	0/3404	0.63	1/4606 (0.0%)
5	O	0.26	0/1383	0.73	0/1871
5	P	0.24	0/1776	0.73	1/2403 (0.0%)
5	R	0.22	0/1776	0.67	0/2403
6	U	0.23	0/186	0.69	0/251
6	V	0.25	0/982	0.58	0/1332
6	W	0.30	0/982	0.76	0/1332
6	X	0.22	0/796	0.61	0/1081
7	a	0.28	0/1321	0.65	0/1788
7	b	0.30	0/1321	0.66	0/1788
7	c	0.26	0/1645	0.63	0/2225

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	d	0.25	0/1645	0.64	2/2225 (0.1%)
7	e	0.25	0/1645	0.66	1/2225 (0.0%)
7	f	0.25	0/1645	0.63	0/2225
7	g	0.25	0/1645	0.63	0/2225
7	h	0.23	0/1645	0.64	1/2225 (0.0%)
7	i	0.22	0/1645	0.60	0/2225
7	j	0.23	0/1645	0.58	1/2225 (0.0%)
7	m	0.24	0/1645	0.62	0/2225
7	n	0.23	0/1645	0.59	0/2225
7	o	0.24	0/1645	0.61	0/2225
7	p	0.24	0/1645	0.60	2/2225 (0.1%)
7	q	0.25	0/1645	0.58	1/2225 (0.0%)
7	r	0.23	0/1645	0.56	0/2225
7	s	0.32	0/1645	0.66	1/2225 (0.0%)
7	t	0.32	0/1645	0.66	0/2225
7	u	0.22	0/1645	0.54	0/2225
7	v	0.24	0/1645	0.65	3/2225 (0.1%)
7	w	0.23	0/1645	0.62	0/2225
7	x	0.22	0/1645	0.59	0/2225
8	k	0.22	0/1184	0.57	1/1600 (0.1%)
8	l	0.26	0/1184	0.69	0/1600
All	All	0.24	1/230099 (0.0%)	0.60	47/311692 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	1
2	F	0	1
3	A0	0	2
3	A4	0	1
3	B2	0	1
3	B8	0	1
3	C4	0	3
3	C8	0	2
3	E2	0	1
3	F0	0	1
4	A1	0	1
4	A7	0	1
4	A9	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	C1	0	3
4	C3	0	2
4	C5	0	1
4	C9	0	2
4	E3	0	1
5	O	0	1
6	V	0	2
6	W	0	1
7	a	0	1
7	d	0	1
7	e	0	1
7	g	0	1
7	p	0	1
7	s	0	2
7	t	0	3
8	l	0	2
All	All	0	42

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	253	ALA	C-N	-5.42	1.25	1.33

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	221	PRO	CA-C-N	8.74	133.75	121.61
2	E	221	PRO	C-N-CA	8.74	133.75	121.61
4	A5	396	HIS	CA-C-N	8.30	136.63	122.26
4	A5	396	HIS	C-N-CA	8.30	136.63	122.26
4	A1	391	ARG	CA-CB-CG	6.83	127.77	114.10
7	d	58	SER	CA-C-N	6.64	136.64	124.82
7	d	58	SER	C-N-CA	6.64	136.64	124.82
4	E1	85	PHE	CA-C-N	6.54	133.37	120.94
4	E1	85	PHE	C-N-CA	6.54	133.37	120.94
4	D9	252	LYS	CB-CG-CD	6.44	126.11	111.30
4	C9	171	PRO	CA-C-N	6.30	132.91	120.94
4	C9	171	PRO	C-N-CA	6.30	132.91	120.94
7	p	58	SER	CA-C-N	6.13	136.99	126.32
7	p	58	SER	C-N-CA	6.13	136.99	126.32
7	e	190	GLU	CA-CB-CG	5.94	125.98	114.10
7	v	192	GLY	CA-C-N	5.88	132.77	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	v	192	GLY	C-N-CA	5.88	132.77	121.54
1	1	443	LYS	CA-CB-CG	5.81	125.72	114.10
7	j	84	LYS	CA-CB-CG	5.81	125.72	114.10
7	v	63	ILE	CB-CA-C	5.74	115.96	110.16
4	C9	324	LYS	CB-CG-CD	5.72	124.45	111.30
3	C6	401	LYS	CA-CB-CG	5.71	125.52	114.10
7	s	196	LEU	N-CA-C	-5.70	105.59	112.54
4	C3	86	ARG	CB-CG-CD	5.58	124.12	111.30
3	B8	268	MET	CG-SD-CE	-5.57	88.65	100.90
3	C8	181	VAL	N-CA-C	-5.54	108.44	113.71
3	A0	217	LEU	CA-C-N	5.49	130.20	122.46
3	A0	217	LEU	C-N-CA	5.49	130.20	122.46
3	A8	217	LEU	CA-C-N	5.48	132.00	121.54
3	A8	217	LEU	C-N-CA	5.48	132.00	121.54
8	k	86	VAL	N-CA-C	-5.39	107.56	112.96
4	C1	47	ILE	N-CA-C	-5.33	108.09	113.47
5	P	285	GLN	CA-CB-CG	5.29	124.67	114.10
4	B7	54	ALA	CA-C-N	5.21	131.49	121.54
4	B7	54	ALA	C-N-CA	5.21	131.49	121.54
4	F1	297	LYS	CA-CB-CG	5.20	124.50	114.10
4	E5	324	LYS	CG-CD-CE	-5.17	99.41	111.30
4	D7	326	VAL	N-CA-C	-5.17	106.86	112.80
4	A3	263	LEU	CA-CB-CG	5.15	134.33	116.30
4	E7	350	LYS	CB-CG-CD	5.12	123.09	111.30
4	D1	324	LYS	CG-CD-CE	5.11	123.05	111.30
4	A9	116	VAL	N-CA-C	-5.11	108.53	113.53
7	h	149	ARG	CG-CD-NE	5.09	123.21	112.00
7	q	190	GLU	CA-CB-CG	5.08	124.27	114.10
2	G	247	TYR	CA-C-N	5.08	131.24	121.18
2	G	247	TYR	C-N-CA	5.08	131.24	121.18
4	C1	350	LYS	CB-CG-CD	5.01	122.83	111.30

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	443	LYS	Peptide
3	A0	372	MET	Peptide
3	A0	90	GLU	Peptide
4	A1	391	ARG	Sidechain
3	A4	90	GLU	Peptide
4	A7	178	THR	Peptide

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Mol	Chain	Res	Type	Group
4	A9	347	ASN	Peptide
3	B2	221	ARG	Sidechain
3	B8	267	PHE	Peptide
4	C1	213	ARG	Sidechain
4	C1	325	GLU	Peptide
4	C1	65	LEU	Peptide
4	C3	122	LYS	Peptide
4	C3	86	ARG	Sidechain
3	C4	21	TRP	Peptide
3	C4	221	ARG	Sidechain
3	C4	284	GLU	Peptide
4	C5	325	GLU	Peptide
3	C8	21	TRP	Peptide
3	C8	284	GLU	Peptide
4	C9	323	THR	Peptide
4	C9	86	ARG	Sidechain
3	E2	64	ARG	Sidechain
4	E3	322	SER	Peptide
2	F	221	PRO	Peptide
3	F0	207	GLU	Peptide
5	O	262	LYS	Peptide
6	V	174	ARG	Peptide,Sidechain
6	W	87	TYR	Peptide
7	a	159	TYR	Peptide
7	d	167	VAL	Peptide
7	e	202	ARG	Sidechain
7	g	19	GLU	Peptide
8	l	16	THR	Peptide
8	l	25	ARG	Peptide
7	p	161	TYR	Peptide
7	s	198	ARG	Sidechain
7	s	202	ARG	Sidechain
7	t	194	ARG	Sidechain
7	t	198	ARG	Sidechain
7	t	202	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1054	0	1111	15	0
1	2	1054	0	1111	15	0
2	A	464	0	469	5	0
2	B	471	0	476	6	0
2	C	464	0	469	5	0
2	D	464	0	467	11	0
2	E	471	0	476	9	0
2	F	441	0	443	9	0
2	G	471	0	476	3	0
2	H	441	0	443	5	0
2	I	471	0	476	8	0
2	J	471	0	476	6	0
2	K	471	0	476	12	0
3	A0	3325	0	3252	52	0
3	A2	3325	0	3252	66	0
3	A4	3325	0	3252	56	0
3	A6	3325	0	3252	63	0
3	A8	3325	0	3251	48	0
3	B0	3325	0	3252	53	0
3	B2	3325	0	3251	50	0
3	B4	3325	0	3252	48	0
3	B6	3325	0	3252	43	0
3	B8	3325	0	3252	72	0
3	C0	3325	0	3252	41	0
3	C2	3325	0	3252	53	0
3	C4	3325	0	3252	58	0
3	C6	3325	0	3252	56	0
3	C8	3325	0	3252	39	0
3	D0	3325	0	3252	63	0
3	D2	3325	0	3252	45	0
3	D4	3325	0	3252	50	0
3	D6	3325	0	3251	59	0
3	D8	3325	0	3251	81	0
3	E0	3325	0	3251	54	0
3	E2	3325	0	3252	51	0
3	E4	3325	0	3252	45	0
3	E6	3325	0	3252	55	0
3	E8	3325	0	3252	46	0
3	F0	3325	0	3252	50	0
4	A1	3331	0	3207	67	0
4	A3	3331	0	3209	71	0
4	A5	3331	0	3207	65	0
4	A7	3331	0	3207	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A9	3331	0	3207	71	0
4	B1	3331	0	3209	58	0
4	B3	3331	0	3207	60	0
4	B5	3331	0	3207	47	0
4	B7	3331	0	3209	63	0
4	B9	3331	0	3209	55	0
4	C1	3331	0	3209	73	0
4	C3	3331	0	3209	43	0
4	C5	3331	0	3209	59	0
4	C7	3331	0	3209	44	0
4	C9	3331	0	3209	66	0
4	D1	3331	0	3209	65	0
4	D3	3331	0	3207	77	0
4	D5	3331	0	3207	60	0
4	D7	3331	0	3207	63	0
4	D9	3331	0	3207	58	0
4	E1	3331	0	3207	57	0
4	E3	3331	0	3209	53	0
4	E5	3331	0	3207	75	0
4	E7	3331	0	3205	46	0
4	E9	3331	0	3207	70	0
4	F1	3331	0	3207	50	0
5	O	1360	0	1354	25	0
5	P	1744	0	1734	48	0
5	R	1744	0	1736	15	0
6	U	182	0	183	3	0
6	V	954	0	899	13	0
6	W	954	0	899	23	0
6	X	772	0	716	7	0
7	a	1289	0	1274	28	0
7	b	1289	0	1274	23	0
7	c	1608	0	1590	33	0
7	d	1608	0	1590	26	0
7	e	1608	0	1590	44	0
7	f	1608	0	1590	37	0
7	g	1608	0	1590	38	0
7	h	1608	0	1590	33	0
7	i	1608	0	1590	28	0
7	j	1608	0	1590	29	0
7	m	1608	0	1590	31	0
7	n	1608	0	1590	34	0
7	o	1608	0	1590	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	p	1608	0	1590	22	0
7	q	1608	0	1590	23	0
7	r	1608	0	1590	28	0
7	s	1608	0	1590	36	0
7	t	1608	0	1590	29	0
7	u	1608	0	1590	25	0
7	v	1608	0	1590	25	0
7	w	1608	0	1590	23	0
7	x	1608	0	1590	29	0
8	k	1155	0	1155	19	0
8	l	1155	0	1155	29	0
9	A0	32	0	12	0	0
9	A2	32	0	12	0	0
9	A4	32	0	12	0	0
9	A6	32	0	12	0	0
9	A8	32	0	12	0	0
9	B0	32	0	12	0	0
9	B2	32	0	12	0	0
9	B4	32	0	12	0	0
9	B6	32	0	12	0	0
9	B8	32	0	12	0	0
9	C0	32	0	12	0	0
9	C2	32	0	12	0	0
9	C4	32	0	12	0	0
9	C6	32	0	12	0	0
9	C8	32	0	12	0	0
9	D0	32	0	12	0	0
9	D2	32	0	12	0	0
9	D4	32	0	12	0	0
9	D6	32	0	12	0	0
9	D8	32	0	12	0	0
9	E0	32	0	12	0	0
9	E2	32	0	12	0	0
9	E4	32	0	12	0	0
9	E7	32	0	12	1	0
9	E8	32	0	12	0	0
9	F0	32	0	12	0	0
10	A0	1	0	0	0	0
10	A2	1	0	0	0	0
10	A4	1	0	0	0	0
10	A6	1	0	0	0	0
10	A8	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B0	1	0	0	0	0
10	B2	1	0	0	0	0
10	B4	1	0	0	0	0
10	B6	1	0	0	0	0
10	B8	1	0	0	0	0
10	C0	1	0	0	0	0
10	C2	1	0	0	0	0
10	C4	1	0	0	0	0
10	C6	1	0	0	0	0
10	C9	1	0	0	0	0
10	D1	1	0	0	0	0
10	D3	1	0	0	0	0
10	D4	1	0	0	0	0
10	D6	1	0	0	0	0
10	D8	1	0	0	0	0
10	E0	1	0	0	0	0
10	E2	1	0	0	0	0
10	E4	1	0	0	0	0
10	E6	1	0	0	0	0
10	E8	1	0	0	0	0
10	F0	1	0	0	0	0
11	A1	28	0	12	0	0
11	A3	28	0	12	0	0
11	A5	28	0	12	0	0
11	A7	28	0	12	0	0
11	B3	28	0	12	0	0
11	B5	28	0	12	0	0
11	B7	28	0	12	0	0
11	B9	28	0	12	0	0
11	C1	28	0	12	0	0
11	C3	28	0	12	0	0
11	C5	28	0	12	0	0
11	C7	28	0	12	1	0
11	C9	28	0	12	1	0
11	D1	28	0	12	0	0
11	D3	28	0	12	0	0
11	D5	28	0	12	0	0
11	D7	28	0	12	1	0
11	D9	28	0	12	0	0
11	E1	28	0	12	0	0
11	E3	28	0	12	0	0
11	E5	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	E7	28	0	12	0	0
11	E9	28	0	12	0	0
11	F1	28	0	12	0	0
11	O	28	0	12	0	0
11	P	28	0	12	0	0
All	All	226608	0	220121	3381	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (3381) 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)
7:v:100:ASN:HD21	7:v:106:GLN:HG2	1.43	0.84
4:C1:8:GLN:HE21	4:C1:14:ASN:HA	1.42	0.81
4:C5:179:VAL:H	3:C6:352:LYS:HZ1	1.29	0.81
4:A5:68:LEU:HB3	4:A5:96:GLY:HA2	1.63	0.80
4:B1:213:ARG:HH22	4:B1:297:LYS:HB3	1.47	0.79
3:E2:48:ALA:HB1	3:E2:243:ARG:HB3	1.64	0.78
3:E4:221:ARG:HA	4:E5:324:LYS:HZ1	1.44	0.78
4:B3:256:ASN:HD22	4:B3:350:LYS:HE2	1.48	0.77
3:A8:105:ARG:HH12	4:A9:251:ARG:HD2	1.50	0.77
3:C6:32:PRO:HA	3:C6:86:LEU:HD12	1.67	0.76
4:C1:198:GLU:HB2	4:C1:266:PHE:HE2	1.50	0.76
3:A6:338:LYS:HZ2	3:A6:340:THR:H	1.33	0.76
3:D4:221:ARG:HH12	4:D5:325:GLU:HB3	1.48	0.76
7:o:194:ARG:HH12	7:o:198:ARG:HH21	1.33	0.76
4:A3:200:GLN:HB3	4:A3:268:ILE:HD11	1.69	0.75
4:B9:42:LEU:HA	4:B9:45:GLU:HG2	1.69	0.75
7:i:9:PRO:HB2	7:i:143:ILE:HG23	1.67	0.75
3:B8:178:SER:HB3	4:B9:347:ASN:HB2	1.69	0.75
4:C5:275:SER:H	4:C5:278:SER:HB2	1.52	0.75
7:a:151:MET:HE1	7:a:154:TYR:H	1.53	0.74
7:d:5:VAL:HG11	7:d:149:ARG:HD3	1.69	0.74
7:f:84:LYS:HB3	7:f:168:PRO:HD3	1.70	0.74
4:A3:207:LEU:HB3	4:A3:225:LEU:HD22	1.68	0.74
7:o:14:LYS:HD3	7:o:47:LEU:HD23	1.70	0.74
4:C1:8:GLN:HG2	4:C1:65:LEU:HG	1.69	0.73
3:E6:88:HIS:HB3	3:E6:91:GLN:HB2	1.71	0.73
4:C7:330:MET:HE2	4:C7:349:MET:HB2	1.71	0.73
3:C0:207:GLU:HA	3:C0:210:TYR:HB2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A2:286:LEU:H	5:P:255:LYS:HZ1	1.35	0.73
7:h:119:ARG:HH22	7:h:136:LEU:HB2	1.54	0.72
4:A1:262:ARG:HH12	4:A1:418:LEU:HA	1.53	0.72
4:C5:391:ARG:HE	3:C6:346:TRP:HB2	1.52	0.72
4:B1:359:LYS:HG2	5:O:317:ARG:HH12	1.54	0.72
3:D0:222:PRO:HG2	4:D1:324:LYS:HE3	1.70	0.72
4:B3:287:PRO:HG3	4:B3:329:GLN:HE22	1.55	0.72
4:E1:172:SER:HB3	4:E1:205:GLU:HG2	1.71	0.72
4:D1:35:THR:HG22	7:n:83:PRO:HG3	1.70	0.71
3:A2:91:GLN:HA	3:A2:121:ARG:HH12	1.53	0.71
3:C0:180:ALA:HB3	3:C0:183:GLU:HG2	1.72	0.71
3:D8:301:MET:HG3	3:D8:303:ALA:H	1.54	0.71
3:B8:268:MET:HE1	3:B8:378:ILE:HA	1.73	0.71
3:C4:219:ILE:HG22	3:C4:221:ARG:H	1.54	0.71
3:D0:178:SER:HB2	4:D1:347:ASN:HD22	1.56	0.71
3:D2:276:ILE:HG23	3:D2:280:LYS:HB2	1.73	0.71
7:j:9:PRO:HB2	7:j:143:ILE:HG23	1.72	0.70
4:E9:244:GLY:HA2	4:E9:355:ASP:HB2	1.72	0.70
3:A6:310:GLY:HA3	3:A6:383:ALA:HB2	1.73	0.70
7:n:146:ARG:HH12	7:n:158:THR:HA	1.57	0.70
4:C7:186:THR:HG23	4:C7:415:MET:HG3	1.74	0.70
3:E2:50:ASN:HB2	5:P:555:ARG:HH21	1.56	0.70
4:C1:198:GLU:HA	4:C1:264:HIS:HB2	1.74	0.69
7:q:4:PRO:HG3	7:q:179:GLU:H	1.57	0.69
3:C0:339:ARG:HH21	3:C0:342:GLN:HG2	1.57	0.69
3:C4:219:ILE:HG13	7:m:198:ARG:HH22	1.55	0.69
3:C6:90:GLU:HB3	3:C6:121:ARG:HH21	1.57	0.69
3:D4:285:GLN:HB3	3:D8:56:THR:HA	1.73	0.69
3:A0:207:GLU:HA	3:A0:210:TYR:HB2	1.74	0.69
7:g:14:LYS:HZ1	7:g:45:MET:HB3	1.56	0.69
4:A3:289:LEU:HD22	4:A3:363:MET:HG2	1.73	0.69
3:C2:181:VAL:H	4:C3:350:LYS:HZ3	1.38	0.69
4:C9:276:ARG:HD3	5:P:496:PRO:HB2	1.73	0.69
4:E1:275:SER:HA	5:P:570:ASN:HD21	1.57	0.69
8:l:76:LEU:HD12	8:l:128:ILE:HD11	1.73	0.69
4:C1:86:ARG:HE	4:C1:87:PRO:HD2	1.57	0.69
8:l:45:LYS:HE3	8:l:148:GLN:H	1.56	0.69
3:A6:208:ALA:HB2	3:A6:304:LYS:HG2	1.75	0.69
4:B7:281:TYR:HB2	4:C1:86:ARG:HD2	1.75	0.69
7:t:69:LYS:HZ1	7:v:38:LEU:HB2	1.56	0.69
4:B9:278:SER:HA	4:C3:86:ARG:HH22	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F1:244:GLY:HA2	4:F1:355:ASP:HB2	1.75	0.69
3:B4:133:GLN:HE22	3:B4:251:ASP:HB3	1.57	0.68
3:C6:262:TYR:HB2	3:C6:265:ILE:HG22	1.75	0.68
3:C6:209:ILE:HG13	3:C6:302:MET:HG2	1.75	0.68
4:E9:163:ILE:HG21	4:E9:251:ARG:HG3	1.75	0.68
7:i:10:LEU:HD12	7:i:143:ILE:HG22	1.76	0.68
3:C6:84:ARG:HH22	8:l:56:PHE:HA	1.59	0.68
3:F0:180:ALA:HB3	3:F0:183:GLU:HG2	1.76	0.68
3:A8:208:ALA:HA	3:A8:304:LYS:HE3	1.76	0.68
4:D5:200:GLN:HG3	4:D5:266:PHE:HB2	1.75	0.68
4:D5:242:PHE:HB3	4:D5:356:ILE:HD13	1.75	0.68
4:D7:207:LEU:HD23	4:D7:225:LEU:HB2	1.76	0.68
4:D5:69:GLU:HG2	4:D5:71:GLY:H	1.58	0.68
4:D5:276:ARG:H	5:O:522:VAL:HG13	1.59	0.68
7:r:184:PRO:HG3	7:r:189:LEU:HD23	1.74	0.68
4:A3:46:ARG:HH12	6:U:169:ARG:HH21	1.41	0.68
4:E1:200:GLN:HG3	4:E1:266:PHE:HB2	1.76	0.68
3:A0:373:ARG:HG2	5:R:255:LYS:HZ3	1.58	0.67
3:C2:237:SER:HA	3:C2:320:ARG:HH21	1.59	0.67
3:B0:320:ARG:HE	3:B0:360:PRO:HG3	1.60	0.67
4:D7:68:LEU:HB3	4:D7:96:GLY:HA2	1.76	0.67
3:E6:271:SER:HB2	3:E6:377:MET:HB3	1.76	0.67
3:A4:222:PRO:HD2	4:A5:324:LYS:HG2	1.76	0.67
3:C2:168:ASN:HB2	3:C2:201:ALA:HA	1.75	0.67
3:C2:271:SER:HB3	3:C2:377:MET:HB3	1.77	0.67
4:C7:275:SER:HA	5:O:469:GLN:HE22	1.60	0.67
4:B5:3:GLU:HA	4:B5:49:VAL:HA	1.77	0.67
4:A5:98:GLY:H	4:A5:103:LYS:HD3	1.59	0.67
4:D7:6:HIS:HD2	4:D7:21:TRP:HE1	1.43	0.67
4:A9:223:GLY:HA3	5:P:308:TRP:H	1.58	0.67
7:o:18:ASN:HD22	7:o:45:MET:HE3	1.59	0.66
7:v:75:LEU:HD23	7:v:144:LEU:HD21	1.77	0.66
4:D3:23:VAL:HG21	4:D3:230:SER:HB3	1.77	0.66
3:D8:285:GLN:O	3:D8:286:LEU:C	2.38	0.66
4:E1:164:MET:HB3	4:E1:197:ASP:H	1.60	0.66
3:F0:178:SER:HB3	3:F0:183:GLU:HG3	1.75	0.66
4:B1:165:GLU:HG3	4:B1:250:LEU:HD11	1.78	0.66
3:B0:408:TYR:HB3	3:B0:413:MET:HE2	1.77	0.66
4:B1:200:GLN:HB3	4:B1:268:ILE:HD11	1.77	0.66
3:B4:314:ALA:HB3	3:B4:380:ASN:HB2	1.77	0.66
4:B5:257:LEU:HD21	4:B5:314:SER:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C7:98:GLY:H	4:C7:103:LYS:HZ1	1.41	0.66
7:h:14:LYS:HE3	7:h:47:LEU:HA	1.78	0.66
4:D3:267:LEU:HB3	4:D3:299:MET:HE1	1.78	0.66
3:E6:177:VAL:HG11	4:E7:327:ASP:HB3	1.77	0.66
7:x:14:LYS:HZ1	7:x:45:MET:HB3	1.61	0.66
4:D9:101:TRP:HE1	4:D9:188:SER:HB3	1.61	0.66
3:A2:371:VAL:HG22	3:A2:373:ARG:H	1.60	0.66
3:A8:259:LEU:HD21	3:A8:316:CYS:HB2	1.78	0.66
3:A4:269:LEU:HB3	3:A4:301:MET:HE1	1.78	0.66
4:D5:68:LEU:HB3	4:D5:96:GLY:HA2	1.78	0.66
7:e:14:LYS:HA	7:e:47:LEU:HD21	1.76	0.66
7:h:21:ARG:HA	7:h:24:MET:HE2	1.78	0.66
7:q:42:TYR:HA	7:q:45:MET:HE2	1.78	0.66
4:C7:334:GLN:HE22	4:C7:348:ASN:HB2	1.61	0.65
4:E9:216:LYS:HZ2	6:W:174:ARG:HB3	1.60	0.65
3:A8:310:GLY:HA3	3:A8:383:ALA:HB2	1.79	0.65
3:B4:31:GLN:HE22	7:f:104:ALA:HB2	1.61	0.65
4:B9:10:GLY:HA2	4:B9:143:THR:HG23	1.78	0.65
4:E3:213:ARG:HH21	4:E3:297:LYS:HD3	1.60	0.65
7:e:8:SER:HB2	7:e:147:HIS:HA	1.78	0.65
7:t:97:ARG:HH22	7:v:149:ARG:HH21	1.44	0.65
4:B5:14:ASN:HB3	4:B5:76:VAL:HG11	1.78	0.65
4:D5:155:VAL:HG23	4:D5:164:MET:HE1	1.78	0.65
4:D9:65:LEU:HB3	4:D9:73:MET:HE2	1.78	0.65
4:E7:337:ASN:HB3	4:E7:340:TYR:HB2	1.78	0.65
3:A8:175:PRO:HB3	3:A8:390:ARG:HD3	1.79	0.65
4:C1:130:LEU:HB3	4:C1:162:ARG:HH12	1.61	0.65
1:2:446:GLU:H	4:C3:194:GLU:HB2	1.60	0.65
4:D3:330:MET:HG2	4:D3:349:MET:HG2	1.76	0.65
4:D7:117:LEU:HD11	4:D7:154:LYS:HE2	1.78	0.65
4:E5:7:VAL:HG23	4:E5:64:ILE:HB	1.77	0.65
4:A5:39:ASP:HA	7:a:90:PRO:HG3	1.78	0.65
3:C6:102:ASN:HD21	4:C7:255:VAL:HG11	1.61	0.65
4:C9:311:LEU:HD23	4:C9:312:THR:HG23	1.78	0.65
3:E0:3:GLU:HA	3:E0:51:THR:HA	1.78	0.65
7:s:164:ARG:HG3	7:s:165:THR:HG23	1.79	0.65
3:B2:311:LYS:H	3:B2:382:THR:HG22	1.62	0.65
4:B3:39:ASP:HA	7:e:90:PRO:HG3	1.77	0.65
4:B7:172:SER:HB2	4:B7:205:GLU:HG2	1.78	0.65
4:D9:132:GLY:HA3	4:D9:163:ILE:HG22	1.77	0.65
4:B7:178:THR:HA	3:B8:258:ASN:HD21	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:99:MET:HE1	7:f:107:LYS:HB2	1.79	0.65
3:A0:180:ALA:HB3	3:A0:183:GLU:HB2	1.79	0.65
4:E7:257:LEU:HD21	4:E7:314:SER:HB3	1.77	0.65
3:F0:240:ALA:HA	3:F0:243:ARG:HE	1.61	0.65
4:F1:217:LEU:HB3	6:V:174:ARG:HH21	1.61	0.65
4:B9:215:LEU:HB3	4:B9:217:LEU:HD23	1.79	0.64
4:D1:7:VAL:HB	4:D1:135:ILE:HG12	1.78	0.64
4:E9:10:GLY:HA2	4:E9:143:THR:HG23	1.78	0.64
4:F1:86:ARG:HG2	4:F1:89:ASN:H	1.61	0.64
3:A6:285:GLN:HB2	3:B0:56:THR:HA	1.78	0.64
4:C3:100:ASN:HB3	4:C3:103:LYS:HG2	1.80	0.64
3:C8:73:THR:HA	4:C9:46:ARG:HH22	1.61	0.64
3:C8:229:ARG:HD3	3:C8:363:VAL:HG21	1.80	0.64
4:D1:10:GLY:HA2	4:D1:143:THR:HG23	1.78	0.64
4:D3:276:ARG:HG2	5:P:521:PRO:HB2	1.80	0.64
4:A1:258:ILE:HD12	4:A1:264:HIS:HB3	1.80	0.64
4:B9:19:LYS:HA	4:B9:22:GLU:HG2	1.78	0.64
3:D8:183:GLU:HG2	3:D8:184:PRO:HD3	1.79	0.64
4:F1:209:ASP:HB3	4:F1:213:ARG:HH22	1.62	0.64
7:t:96:TYR:HA	7:t:108:ILE:HD11	1.79	0.64
3:C4:272:TYR:HD2	3:C4:275:ILE:HG12	1.62	0.64
3:D4:259:LEU:HD21	3:D4:316:CYS:HB2	1.80	0.64
4:A3:337:ASN:HB3	4:A3:340:TYR:HB2	1.80	0.64
3:A8:225:THR:HG21	2:C:250:GLU:HG2	1.80	0.64
3:D8:269:LEU:HB3	3:D8:301:MET:HE1	1.80	0.64
2:F:221:PRO:HG3	7:t:101:GLU:HB3	1.78	0.64
7:g:42:TYR:HA	7:g:45:MET:HG2	1.80	0.64
7:g:185:ILE:HG23	7:g:192:GLY:HA2	1.78	0.64
4:A3:378:PHE:HD1	4:A3:415:MET:HE1	1.63	0.64
2:D:214:ALA:HA	4:D9:320:ARG:HH22	1.63	0.64
4:A1:42:LEU:HD21	6:W:78:GLU:H	1.63	0.63
4:B9:330:MET:HG2	4:B9:349:MET:HG2	1.80	0.63
4:E5:68:LEU:HB3	4:E5:96:GLY:HA2	1.79	0.63
7:j:10:LEU:HD12	7:j:143:ILE:HG22	1.80	0.63
3:E2:223:THR:HG22	4:E3:322:SER:HA	1.78	0.63
4:A9:220:PRO:HD2	3:B0:326:LYS:HD2	1.80	0.63
3:D6:73:THR:HG22	4:D7:46:ARG:HH12	1.63	0.63
4:E5:397:TRP:HH2	3:E6:256:GLN:HG2	1.63	0.63
2:K:221:PRO:HG3	7:n:101:GLU:HB3	1.79	0.63
3:A4:264:ARG:HH21	3:A4:431:ASP:HB3	1.64	0.63
3:B2:208:ALA:HB2	3:B2:304:LYS:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F0:76:ASP:HA	3:F0:79:ARG:HB2	1.80	0.63
4:B1:170:PHE:HD2	4:B1:377:MET:HE1	1.62	0.63
3:C0:222:PRO:HD2	4:C1:324:LYS:HZ1	1.64	0.63
7:t:73:VAL:HG12	7:t:206:PHE:HB2	1.81	0.63
3:E0:166:LYS:HB2	3:E0:199:ASP:H	1.63	0.63
7:x:42:TYR:HA	7:x:45:MET:HE2	1.79	0.63
3:B0:134:GLY:HA2	3:B0:164:LYS:HG3	1.80	0.63
4:B7:7:VAL:HB	4:B7:135:ILE:HG22	1.81	0.63
4:B7:211:CYS:HA	4:B7:215:LEU:HB2	1.80	0.63
7:g:8:SER:HB2	7:g:147:HIS:HA	1.80	0.63
4:A1:99:ASN:HA	4:A1:142:GLY:H	1.64	0.62
4:A1:211:CYS:HA	4:A1:215:LEU:HB3	1.79	0.62
4:B9:381:VAL:HA	4:B9:384:GLN:HE21	1.64	0.62
4:E1:286:VAL:HG21	4:E1:325:GLU:HB3	1.80	0.62
4:A1:9:GLY:HA2	4:A1:66:MET:HB2	1.81	0.62
3:A6:119:LEU:HD11	3:A6:156:ARG:HG2	1.81	0.62
3:B4:195:LEU:HD11	3:B4:428:LEU:HD22	1.80	0.62
3:C4:205:ASP:HB2	3:C4:303:ALA:HA	1.81	0.62
4:C5:97:ALA:HB3	4:C5:143:THR:HB	1.81	0.62
3:C6:84:ARG:HG3	8:l:59:THR:HG21	1.79	0.62
4:C9:131:GLN:HA	4:C9:162:ARG:HH21	1.63	0.62
4:C9:280:GLN:HE22	4:D3:58:ARG:HH11	1.46	0.62
3:D0:272:TYR:HB3	3:D0:275:ILE:HD11	1.81	0.62
3:D2:66:VAL:HA	3:D2:91:GLN:HB2	1.80	0.62
8:l:73:TYR:HB2	8:l:92:TRP:HE1	1.63	0.62
4:C1:113:ILE:HG13	4:C1:150:LEU:HD23	1.80	0.62
4:C9:22:GLU:HB3	5:P:491:MET:HE1	1.81	0.62
7:a:194:ARG:HH22	7:a:198:ARG:HH21	1.46	0.62
4:A7:222:TYR:HA	4:A7:225:LEU:HD12	1.80	0.62
3:B2:244:PHE:HB2	3:B2:356:ASN:HD21	1.64	0.62
4:B3:2:ARG:HB2	4:B3:131:GLN:HB2	1.81	0.62
3:B4:311:LYS:H	3:B4:382:THR:HG22	1.63	0.62
4:B7:200:GLN:HE22	4:B7:266:PHE:HD2	1.47	0.62
4:B7:215:LEU:HD12	5:P:370:LEU:HD21	1.81	0.62
4:B7:375:GLN:HE22	4:B7:419:VAL:HA	1.64	0.62
3:F0:132:LEU:HB3	3:F0:164:LYS:HZ1	1.64	0.62
3:D6:66:VAL:HG12	3:D6:91:GLN:HG3	1.81	0.62
3:E6:100:ALA:HA	4:E7:252:LYS:HD3	1.81	0.62
7:j:172:VAL:HG13	7:j:180:ALA:HB3	1.81	0.62
4:C5:179:VAL:H	3:C6:352:LYS:NZ	1.98	0.62
3:C8:318:MET:HB2	3:C8:376:CYS:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F0:207:GLU:HG2	3:F0:304:LYS:HZ2	1.65	0.62
3:D4:76:ASP:HA	3:D4:79:ARG:HB2	1.80	0.62
4:D7:325:GLU:HA	4:D7:328:GLU:HG3	1.82	0.62
4:D9:28:HIS:HE2	4:D9:241:ARG:HD2	1.64	0.62
4:D9:66:MET:HE1	4:D9:151:LEU:HD22	1.81	0.62
3:E2:63:PRO:HD3	3:E2:86:LEU:O	2.00	0.62
4:E5:179:VAL:H	3:E6:352:LYS:HE2	1.63	0.62
4:B9:164:MET:HB2	4:B9:197:ASP:H	1.65	0.62
4:C1:172:SER:HB3	4:C1:176:SER:HB3	1.81	0.62
3:D6:402:ARG:HD3	3:D6:405:VAL:HG21	1.82	0.62
7:h:194:ARG:HH11	7:h:197:LEU:HD12	1.63	0.62
3:C0:223:THR:HG22	4:C1:322:SER:HA	1.82	0.62
3:E4:30:ILE:HG22	3:E4:36:MET:HB3	1.82	0.62
3:A0:221:ARG:HA	4:A1:324:LYS:HD2	1.81	0.62
3:C0:73:THR:HB	4:C1:2:ARG:HH22	1.64	0.62
3:D4:310:GLY:HA3	3:D4:383:ALA:HB2	1.81	0.62
4:F1:10:GLY:HA2	4:F1:143:THR:HG23	1.82	0.62
4:B9:358:PRO:HB2	5:O:371:ARG:HH22	1.65	0.61
4:C7:290:THR:HA	4:C7:293:MET:HG3	1.81	0.61
5:P:493:LYS:HB3	5:P:495:VAL:HG12	1.82	0.61
3:A6:11:GLN:HB2	3:A6:74:VAL:HG21	1.82	0.61
4:B1:113:ILE:HG13	4:B1:150:LEU:HD22	1.83	0.61
4:C9:164:MET:HB3	4:C9:197:ASP:H	1.64	0.61
4:A1:268:ILE:H	4:A1:299:MET:HE1	1.64	0.61
3:C4:221:ARG:HH22	7:m:189:LEU:HB3	1.65	0.61
3:C8:398:MET:HE2	4:C9:345:ILE:HG23	1.81	0.61
4:D9:248:SER:HA	4:D9:252:LYS:HG3	1.82	0.61
8:l:109:TYR:HE1	8:l:140:GLU:HB3	1.65	0.61
4:A7:229:VAL:HA	4:A7:300:MET:HE1	1.81	0.61
4:C5:299:MET:HG3	4:C5:301:CYS:H	1.65	0.61
4:E5:132:GLY:HA3	4:E5:163:ILE:HG22	1.82	0.61
3:A8:222:PRO:HD2	4:A9:324:LYS:HD3	1.83	0.61
3:D8:280:LYS:HZ3	3:E2:90:GLU:CD	2.09	0.61
7:j:59:ASN:HD21	8:l:103:LYS:HE3	1.65	0.61
4:B3:135:ILE:HD13	4:B3:164:MET:HE2	1.83	0.61
3:D8:193:SER:HB3	3:D8:197:HIS:HE1	1.66	0.61
4:E9:135:ILE:HD13	4:E9:152:ILE:HD11	1.83	0.61
7:i:115:LEU:HD11	7:i:167:VAL:HG21	1.82	0.61
1:1:490:GLU:HA	1:1:493:ARG:HG2	1.81	0.61
4:A5:318:ARG:HA	4:A5:354:CYS:HB2	1.82	0.61
3:B4:71:GLU:HB2	3:B4:98:ASP:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B5:66:MET:HE2	4:B5:116:VAL:HG21	1.83	0.61
3:C8:309:HIS:HE1	3:C8:386:GLU:HG2	1.66	0.61
3:D0:262:TYR:HB2	3:D0:265:ILE:HG22	1.82	0.61
7:c:79:ASP:HB3	7:c:82:ASP:HB2	1.82	0.61
7:h:151:MET:HE3	7:h:154:TYR:HA	1.83	0.61
7:f:55:LEU:HD23	7:f:132:LEU:HD23	1.82	0.61
4:A9:164:MET:H	4:A9:197:ASP:HB2	1.65	0.61
3:B2:53:PHE:HB3	3:B2:61:HIS:HB3	1.82	0.61
3:D2:115:VAL:HG11	3:D2:152:LEU:HD22	1.82	0.61
4:D5:309:ARG:H	4:D5:372:THR:HG22	1.65	0.61
4:A1:221:THR:HG21	5:R:219:LEU:HD22	1.81	0.60
3:A4:188:VAL:HG11	3:A4:422:ARG:HH12	1.66	0.60
4:A9:34:GLY:HA3	4:A9:58:ARG:HG3	1.83	0.60
4:B1:7:VAL:HB	4:B1:66:MET:HE1	1.83	0.60
3:D8:181:VAL:HG23	3:D8:182:VAL:HG13	1.82	0.60
7:i:55:LEU:HD11	7:i:111:ILE:HD12	1.82	0.60
7:u:92:LEU:HD21	7:u:110:ILE:HG13	1.82	0.60
3:A2:89:PRO:HB3	6:U:173:ILE:HD13	1.81	0.60
3:A8:236:SER:HA	3:A8:243:ARG:HH22	1.66	0.60
3:C4:4:VAL:HB	3:C4:133:GLN:HE21	1.66	0.60
3:D0:174:SER:HB2	3:D0:207:GLU:HG2	1.83	0.60
3:E4:259:LEU:HB3	3:E4:268:MET:HE1	1.81	0.60
3:E8:82:THR:HG21	6:X:122:GLU:HA	1.81	0.60
7:d:9:PRO:HB2	7:d:143:ILE:HG13	1.83	0.60
4:A1:216:LYS:HB3	4:A1:275:SER:HB3	1.83	0.60
4:A9:113:ILE:HA	4:A9:116:VAL:HG12	1.81	0.60
3:C8:177:VAL:HG13	4:C9:327:ASP:HB3	1.83	0.60
3:E4:234:VAL:HG21	3:E4:302:MET:HE1	1.83	0.60
4:E5:136:THR:HG22	4:E5:167:PHE:HB2	1.81	0.60
3:E8:406:HIS:HA	3:E8:409:VAL:HG22	1.83	0.60
7:p:55:LEU:HD11	7:p:111:ILE:HD12	1.84	0.60
3:A0:83:TYR:HB3	3:A0:86:LEU:HB3	1.83	0.60
3:A2:180:ALA:HB3	3:A2:183:GLU:HB2	1.83	0.60
4:B7:39:ASP:HA	7:g:90:PRO:HG3	1.83	0.60
3:E2:28:HIS:CE1	3:E2:243:ARG:HD2	2.36	0.60
4:F1:44:LEU:HD21	7:x:87:SER:HA	1.83	0.60
3:B8:271:SER:HA	3:B8:302:MET:HG3	1.81	0.60
3:D4:398:MET:HE1	4:D5:345:ILE:HA	1.83	0.60
7:n:149:ARG:HG2	7:n:163:SER:HA	1.83	0.60
7:s:142:GLU:HA	7:s:145:LYS:HZ2	1.66	0.60
3:A0:360:PRO:HD2	3:A0:372:MET:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B9:133:PHE:HD1	4:B9:164:MET:HE1	1.67	0.60
4:C1:393:ALA:HA	3:C2:262:TYR:HE2	1.66	0.60
3:C2:191:THR:HA	3:C2:194:LEU:HG	1.83	0.60
3:C8:272:TYR:HB3	3:C8:275:ILE:HD11	1.83	0.60
3:E6:53:PHE:HB3	3:E6:61:HIS:HB3	1.84	0.60
4:E9:248:SER:HA	4:E9:252:LYS:HD2	1.83	0.60
4:F1:330:MET:HB3	4:F1:349:MET:HE3	1.83	0.60
7:g:123:GLU:HA	7:g:126:ARG:HB2	1.83	0.60
7:h:158:THR:HB	7:h:161:TYR:HB2	1.84	0.60
8:l:136:PRO:HG3	8:l:165:PRO:HD2	1.84	0.60
4:A1:284:LEU:HB2	4:A5:55:THR:HG21	1.84	0.60
3:C2:217:LEU:HB3	3:C2:219:ILE:HG13	1.82	0.60
4:C3:99:ASN:HA	4:C3:142:GLY:H	1.66	0.60
4:D1:313:ALA:HB3	4:D1:349:MET:HG2	1.83	0.60
7:b:164:ARG:HH11	7:b:166:GLY:H	1.49	0.60
3:A2:301:MET:HG2	3:A2:377:MET:HE1	1.81	0.60
4:A3:16:ILE:HD11	4:A3:229:VAL:HB	1.84	0.60
4:B5:182:PRO:HB2	4:B5:385:PHE:HD1	1.66	0.60
3:C4:271:SER:HB3	3:C4:377:MET:HB3	1.83	0.60
4:C5:276:ARG:HH12	5:P:469:GLN:HG2	1.67	0.60
3:D0:32:PRO:HG2	7:n:102:GLY:HA2	1.83	0.60
3:D2:265:ILE:HG22	3:D2:380:ASN:HD21	1.67	0.60
4:E7:314:SER:HA	4:E7:350:LYS:HB3	1.84	0.60
7:g:20:GLU:HB3	7:g:24:MET:HE1	1.84	0.60
7:i:172:VAL:HG23	7:i:180:ALA:HB3	1.83	0.60
3:A0:103:PHE:HD2	3:A0:148:GLY:HA2	1.66	0.60
4:A1:68:LEU:HD12	4:A1:97:ALA:HB2	1.83	0.60
3:A6:288:VAL:HG21	3:A6:323:VAL:HG23	1.84	0.60
3:B6:119:LEU:HG	3:B6:156:ARG:HD3	1.84	0.60
4:B9:330:MET:HA	4:B9:333:VAL:HG12	1.83	0.60
3:D8:3:GLU:HA	3:D8:51:THR:HA	1.83	0.60
3:D8:287:SER:HA	3:D8:373:ARG:HH12	1.65	0.60
4:E5:193:VAL:HA	4:E5:264:HIS:HE1	1.67	0.60
7:e:97:ARG:HH22	7:g:161:TYR:HD1	1.49	0.60
3:A0:276:ILE:HB	3:A0:280:LYS:HB2	1.84	0.60
3:A6:76:ASP:HB3	3:A6:79:ARG:HH21	1.67	0.60
4:C7:118:ASP:HA	4:C7:121:ARG:HH21	1.67	0.59
4:D5:207:LEU:HD13	4:D5:225:LEU:HB3	1.84	0.59
3:D8:289:ALA:HA	3:D8:292:THR:HG22	1.82	0.59
3:E4:191:THR:HG21	3:E4:425:LEU:HD13	1.84	0.59
2:H:222:LYS:HD2	2:H:223:PRO:HD2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A9:179:VAL:HG12	3:B0:352:LYS:HE2	1.83	0.59
4:A9:293:MET:HE2	4:A9:367:PHE:HB3	1.84	0.59
4:B9:57:GLY:HA3	7:h:83:PRO:HB2	1.85	0.59
4:D5:135:ILE:HG21	4:D5:152:ILE:HD11	1.84	0.59
3:D8:200:VAL:HG13	3:D8:268:MET:HE1	1.85	0.59
7:x:14:LYS:HD3	7:x:47:LEU:HD23	1.84	0.59
4:B1:313:ALA:HB3	4:B1:349:MET:HB3	1.83	0.59
3:D0:319:TYR:HB3	3:D0:323:VAL:HG11	1.85	0.59
4:D1:135:ILE:HB	4:D1:166:THR:HG22	1.84	0.59
4:D3:246:LEU:HB3	4:D3:353:VAL:H	1.67	0.59
4:E1:223:GLY:HA3	5:P:564:ARG:HG3	1.85	0.59
4:E3:311:LEU:HD23	4:E3:312:THR:HG23	1.83	0.59
7:a:172:VAL:HG13	7:a:180:ALA:HB3	1.84	0.59
7:g:14:LYS:HE2	7:g:47:LEU:HD22	1.84	0.59
3:A2:301:MET:HE1	3:A2:307:PRO:HD3	1.84	0.59
3:C6:199:ASP:HB3	3:C6:256:GLN:HE21	1.68	0.59
4:D3:388:MET:HE1	3:D4:348:PRO:HD2	1.83	0.59
3:D6:222:PRO:HD2	4:D7:324:LYS:HE3	1.83	0.59
4:A5:77:ARG:HH12	4:A5:87:PRO:HG3	1.66	0.59
3:B2:407:TRP:HE1	4:B3:258:ILE:HG13	1.67	0.59
4:B7:135:ILE:HD11	4:B7:166:THR:HG23	1.84	0.59
4:D1:284:LEU:HD11	4:D1:361:LEU:HD23	1.83	0.59
4:E9:180:VAL:HG13	4:E9:183:TYR:HD2	1.67	0.59
7:u:148:PHE:HZ	7:u:173:ILE:HD13	1.68	0.59
3:A8:53:PHE:HB3	3:A8:61:HIS:HB3	1.84	0.59
3:C0:239:THR:HG23	3:C0:243:ARG:HE	1.68	0.59
6:V:166:ARG:HH12	6:V:181:ALA:H	1.51	0.59
3:A0:285:GLN:HB2	3:A4:56:THR:HA	1.84	0.59
2:D:251:TYR:HE1	3:D6:229:ARG:HH12	1.51	0.59
3:D8:53:PHE:HB3	3:D8:61:HIS:HB3	1.83	0.59
6:W:79:THR:HG23	6:W:81:TYR:H	1.68	0.59
7:n:134:ILE:HG12	7:n:140:LEU:HD22	1.85	0.59
7:p:50:PHE:H	7:p:65:GLN:HG3	1.68	0.59
3:A0:208:ALA:HB2	3:A0:304:LYS:HE2	1.84	0.59
4:A5:207:LEU:HD23	4:A5:225:LEU:HB3	1.84	0.59
4:A7:39:ASP:HA	7:b:90:PRO:HG3	1.85	0.59
4:A7:323:THR:HG22	4:A7:353:VAL:HG21	1.82	0.59
3:C6:102:ASN:HB2	3:C6:105:ARG:HB2	1.85	0.59
3:C6:247:ALA:HB3	3:C6:355:ILE:HB	1.84	0.59
3:E0:70:LEU:HD21	3:E0:114:ILE:HG21	1.85	0.59
3:A4:398:MET:HE1	4:A5:345:ILE:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A5:217:LEU:HD11	5:P:278:GLN:HB3	1.85	0.59
3:A6:70:LEU:HD12	3:A6:145:THR:HG22	1.83	0.59
3:A8:184:PRO:HG2	4:A9:346:PRO:HG3	1.83	0.59
3:D4:175:PRO:HB3	3:D4:390:ARG:HD3	1.85	0.59
4:F1:66:MET:HE1	4:F1:147:MET:HG3	1.85	0.59
7:j:146:ARG:HD3	7:j:156:VAL:HG11	1.84	0.59
7:r:115:LEU:HD11	7:r:145:LYS:HZ3	1.67	0.59
7:s:114:SER:HB3	7:s:136:LEU:HD21	1.85	0.59
3:A2:79:ARG:HG3	3:A2:92:LEU:HD22	1.84	0.59
3:A8:210:TYR:CE1	4:A9:324:LYS:HG2	2.38	0.59
4:B7:57:GLY:HA3	7:g:83:PRO:HB2	1.84	0.59
4:E3:192:LEU:HD13	4:E3:199:VAL:HG21	1.85	0.59
7:w:172:VAL:HG13	7:w:180:ALA:HB3	1.84	0.59
3:A0:407:TRP:HE1	4:A1:258:ILE:HG23	1.68	0.58
4:A3:164:MET:HB2	4:A3:197:ASP:H	1.68	0.58
3:A6:30:ILE:HG22	3:A6:36:MET:HB3	1.84	0.58
4:D1:276:ARG:HE	5:O:496:PRO:HB2	1.68	0.58
4:D1:334:GLN:HE22	4:D1:347:ASN:HA	1.68	0.58
3:D2:189:LEU:HD11	3:D2:418:PHE:HA	1.85	0.58
4:D3:200:GLN:HG2	4:D3:266:PHE:HB2	1.85	0.58
7:x:96:TYR:HA	7:x:108:ILE:HD11	1.84	0.58
3:B2:313:MET:HE2	3:B2:380:ASN:HB3	1.84	0.58
4:B7:49:VAL:HG11	4:B7:241:ARG:HG2	1.84	0.58
3:D4:32:PRO:HG2	7:p:102:GLY:HA3	1.85	0.58
4:D5:100:ASN:HB3	4:D5:103:LYS:HG2	1.85	0.58
3:D6:407:TRP:HE1	4:D7:258:ILE:HG13	1.66	0.58
3:E2:70:LEU:HD12	3:E2:99:ALA:HB2	1.85	0.58
3:E8:180:ALA:HB3	3:E8:183:GLU:HG2	1.84	0.58
7:t:71:LYS:HE3	7:t:106:GLN:HG2	1.85	0.58
7:w:149:ARG:HE	7:w:161:TYR:HB3	1.69	0.58
3:A6:214:ARG:HH12	4:A7:324:LYS:HD2	1.68	0.58
3:C0:219:ILE:HD12	8:k:156:ARG:HD3	1.84	0.58
3:E2:132:LEU:HB3	3:E2:164:LYS:HZ1	1.68	0.58
4:E7:237:THR:HG23	4:E7:241:ARG:HE	1.67	0.58
7:n:168:PRO:HG2	7:n:185:ILE:HD12	1.86	0.58
7:p:84:LYS:HB3	7:p:168:PRO:HD3	1.85	0.58
4:B1:91:VAL:HG11	4:B1:116:VAL:HG12	1.85	0.58
3:C2:272:TYR:HB3	3:C2:275:ILE:HD11	1.85	0.58
4:D1:132:GLY:HA3	4:D1:163:ILE:HG22	1.85	0.58
3:E4:335:ILE:HD12	3:E4:338:LYS:HD3	1.85	0.58
8:k:15:ARG:HH21	8:k:16:THR:HG22	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:q:14:LYS:HD2	7:q:47:LEU:HB2	1.84	0.58
4:A5:219:THR:HG23	3:A6:326:LYS:HD3	1.85	0.58
4:A9:91:VAL:HG21	4:A9:116:VAL:HG23	1.85	0.58
4:B7:171:PRO:HB3	4:B7:181:GLU:HG3	1.86	0.58
3:C0:317:LEU:HG	3:C0:377:MET:HE1	1.86	0.58
3:D4:27:GLU:HG2	3:D4:243:ARG:HH12	1.68	0.58
3:D8:280:LYS:HZ2	3:E2:89:PRO:HB2	1.69	0.58
4:E5:152:ILE:HG23	4:E5:164:MET:HE3	1.84	0.58
3:A0:223:THR:HG22	4:A1:322:SER:HA	1.86	0.58
3:A6:15:GLN:HA	3:A6:18:ASN:HB2	1.85	0.58
4:B3:80:PRO:HB3	2:E:235:LEU:HD21	1.85	0.58
3:B4:31:GLN:HG2	2:E:224:LEU:HD21	1.85	0.58
4:E1:282:ARG:HD2	4:E1:288:GLU:HG3	1.84	0.58
3:E8:32:PRO:HA	3:E8:86:LEU:HD12	1.86	0.58
7:h:149:ARG:HH12	7:h:162:GLY:H	1.51	0.58
4:A1:215:LEU:HD23	4:A1:217:LEU:HD13	1.86	0.58
3:E8:178:SER:HB3	3:E8:183:GLU:HG3	1.85	0.58
3:E8:335:ILE:HA	3:E8:338:LYS:HD2	1.85	0.58
7:f:114:SER:HB3	7:f:136:LEU:HD13	1.84	0.58
3:B2:203:MET:HE1	3:B2:267:PHE:HB3	1.85	0.58
3:C4:132:LEU:HB3	3:C4:164:LYS:HZ3	1.69	0.58
3:E2:254:GLU:HA	3:E2:257:THR:HG22	1.86	0.58
6:W:128:ARG:HE	6:W:132:LYS:HE3	1.67	0.58
3:B8:262:TYR:HD2	3:B8:265:ILE:HD12	1.68	0.58
4:C5:89:ASN:HA	4:C5:119:VAL:HG21	1.86	0.58
4:D7:3:GLU:HA	4:D7:49:VAL:HA	1.85	0.58
4:E9:68:LEU:HG	4:E9:147:MET:HE2	1.85	0.58
7:b:79:ASP:HB3	7:b:82:ASP:HB2	1.85	0.58
7:f:9:PRO:HB2	7:f:143:ILE:HG23	1.86	0.58
7:i:5:VAL:HG22	7:i:7:ALA:H	1.69	0.58
7:n:14:LYS:HG3	7:n:47:LEU:HB2	1.85	0.58
3:A0:34:GLY:HA3	3:A0:60:LYS:HG3	1.86	0.58
4:A1:256:ASN:HD22	4:A1:350:LYS:HE2	1.68	0.58
4:B1:227:HIS:HB3	5:O:312:ILE:HD11	1.85	0.58
3:E0:183:GLU:HG2	3:E0:184:PRO:HD3	1.86	0.58
3:B4:191:THR:HA	3:B4:194:LEU:HG	1.86	0.57
3:B4:250:VAL:HG11	3:B4:352:LYS:HD2	1.85	0.57
7:m:151:MET:HE2	7:m:163:SER:HB3	1.86	0.57
7:u:115:LEU:HD21	7:u:145:LYS:HD3	1.85	0.57
4:A3:117:LEU:HA	4:A3:120:VAL:HG12	1.85	0.57
3:B8:285:GLN:HB3	3:C2:56:THR:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E6:31:GLN:HG2	2:H:224:LEU:HD21	1.86	0.57
7:h:123:GLU:HA	7:h:126:ARG:HB3	1.86	0.57
4:B3:44:LEU:HA	4:B3:47:ILE:HB	1.87	0.57
3:B6:112:LYS:HA	3:B6:115:VAL:HG12	1.86	0.57
3:C2:176:GLN:HG3	3:C2:177:VAL:HG23	1.87	0.57
3:C4:119:LEU:HD13	3:C4:122:ILE:HD11	1.85	0.57
4:C9:34:GLY:HA3	4:C9:58:ARG:HG3	1.87	0.57
4:D3:207:LEU:HB3	4:D3:225:LEU:HD22	1.85	0.57
3:D6:136:LEU:HD13	3:D6:235:ILE:HD11	1.86	0.57
3:E6:244:PHE:HB2	3:E6:356:ASN:HD21	1.68	0.57
4:F1:358:PRO:HG2	4:F1:361:LEU:HB3	1.85	0.57
8:k:15:ARG:HD3	7:m:15:ARG:HH21	1.69	0.57
3:B2:210:TYR:HE1	3:B2:227:LEU:HD21	1.69	0.57
3:D2:175:PRO:HB3	3:D2:390:ARG:HD3	1.86	0.57
3:D8:281:ALA:O	3:D8:283:HIS:N	2.37	0.57
7:c:111:ILE:HD13	7:c:132:LEU:HB2	1.86	0.57
4:A3:164:MET:H	4:A3:197:ASP:HB2	1.69	0.57
4:A7:135:ILE:HB	4:A7:166:THR:HG22	1.86	0.57
4:B1:51:TYR:HB3	4:B1:59:PHE:HB3	1.87	0.57
4:B7:382:SER:HB2	4:B7:415:MET:HE1	1.86	0.57
4:D3:165:GLU:HG2	4:D3:198:GLU:HG2	1.86	0.57
3:D6:9:VAL:HG12	3:D6:68:LEU:HB2	1.86	0.57
4:E3:169:VAL:HG12	4:E3:202:ILE:HB	1.86	0.57
3:E4:66:VAL:HA	3:E4:91:GLN:HE21	1.70	0.57
4:B5:258:ILE:HG21	4:B5:264:HIS:HA	1.86	0.57
4:B9:100:ASN:HB3	4:B9:103:LYS:HG2	1.87	0.57
3:E6:242:LEU:HD21	3:E6:252:VAL:HG13	1.86	0.57
4:E9:2:ARG:HD3	4:E9:131:GLN:HG3	1.85	0.57
4:E9:199:VAL:HG23	4:E9:264:HIS:CE1	2.40	0.57
7:w:84:LYS:HB2	7:w:168:PRO:HD3	1.87	0.57
3:A4:108:TYR:HE2	3:A4:413:MET:HB3	1.70	0.57
4:A9:269:GLY:HA2	4:A9:300:MET:HG3	1.86	0.57
3:B6:30:ILE:HG22	3:B6:36:MET:HB3	1.86	0.57
4:B7:164:MET:HB3	4:B7:197:ASP:H	1.69	0.57
4:B9:207:LEU:HB3	4:B9:225:LEU:HD12	1.86	0.57
4:C1:42:LEU:HD21	2:I:245:SER:HB2	1.86	0.57
3:C2:320:ARG:HD2	3:C2:360:PRO:HG3	1.86	0.57
4:D3:2:ARG:HB3	4:D3:131:GLN:HG3	1.86	0.57
3:E0:175:PRO:HB3	3:E0:390:ARG:HD3	1.86	0.57
2:F:207:LEU:HD12	2:F:208:PRO:HD2	1.87	0.57
2:K:208:PRO:HG3	7:p:154:TYR:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:q:9:PRO:HB2	7:q:143:ILE:HG13	1.87	0.57
3:A8:292:THR:HG21	3:A8:331:ALA:HB1	1.86	0.57
4:A9:164:MET:HB3	4:A9:197:ASP:H	1.68	0.57
4:C1:164:MET:HB2	4:C1:197:ASP:H	1.69	0.57
4:C1:286:VAL:HA	4:C1:289:LEU:HB2	1.87	0.57
3:C8:230:LEU:HD11	3:C8:275:ILE:HD12	1.87	0.57
4:D3:282:ARG:HA	4:D7:86:ARG:HH12	1.69	0.57
3:D6:281:ALA:O	3:D6:283:HIS:N	2.38	0.57
6:V:76:LYS:HB3	7:b:162:GLY:HA3	1.85	0.57
7:j:73:VAL:HG12	7:j:109:GLU:HB3	1.86	0.57
7:m:4:PRO:HG3	7:m:179:GLU:HB2	1.86	0.57
3:B2:191:THR:HA	3:B2:194:LEU:HG	1.85	0.57
3:B4:406:HIS:HA	3:B4:409:VAL:HG22	1.85	0.57
3:D2:318:MET:HB2	3:D2:376:CYS:HB3	1.87	0.57
3:D4:370:LYS:HD3	7:r:203:ASN:HD22	1.70	0.57
3:D8:332:VAL:HA	3:D8:335:ILE:HD12	1.86	0.57
3:E0:318:MET:HB2	3:E0:376:CYS:HB3	1.86	0.57
7:r:149:ARG:HD3	7:r:161:TYR:HD1	1.70	0.57
4:C1:222:TYR:HA	4:C1:225:LEU:HD12	1.87	0.57
3:C6:51:THR:HG23	3:C6:52:PHE:HD1	1.70	0.57
4:B5:16:ILE:HD11	4:B5:229:VAL:HG11	1.87	0.56
3:B8:202:VAL:HG22	3:B8:268:MET:HG2	1.87	0.56
3:B8:210:TYR:CG	4:B9:324:LYS:HE3	2.39	0.56
4:B9:135:ILE:HD13	4:B9:152:ILE:HD11	1.85	0.56
3:C4:229:ARG:HD3	3:C4:363:VAL:HG21	1.87	0.56
3:D2:79:ARG:HH11	3:D2:92:LEU:HB3	1.68	0.56
3:E4:394:LYS:HZ2	4:E5:346:PRO:HG2	1.70	0.56
7:v:127:ALA:HB1	7:x:157:PRO:HG3	1.85	0.56
3:A2:262:TYR:HB2	3:A2:265:ILE:HG22	1.87	0.56
4:D1:139:LEU:HD12	4:D1:170:PHE:HE1	1.70	0.56
4:F1:320:ARG:HH22	6:W:114:THR:H	1.51	0.56
7:t:202:ARG:O	7:t:204:THR:N	2.38	0.56
3:A4:240:ALA:HB1	3:A4:356:ASN:HD22	1.70	0.56
3:B0:209:ILE:HA	3:B0:212:ILE:HG12	1.87	0.56
4:B3:2:ARG:HD2	4:B3:240:LEU:HD22	1.87	0.56
4:B9:187:LEU:HA	4:B9:190:HIS:HE1	1.71	0.56
3:C4:68:LEU:HD12	3:C4:149:LEU:HD21	1.86	0.56
4:C5:211:CYS:HA	4:C5:215:LEU:HB2	1.88	0.56
3:C6:322:ASP:HB3	3:C6:373:ARG:HH21	1.69	0.56
3:C8:122:ILE:HD13	3:C8:157:LEU:HD11	1.88	0.56
4:D7:309:ARG:H	4:D7:372:THR:HG22	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E2:36:MET:O	3:E2:37:PRO:C	2.47	0.56
4:E3:282:ARG:HA	4:E7:86:ARG:HH22	1.71	0.56
3:E4:265:ILE:HG22	3:E4:380:ASN:HD21	1.69	0.56
3:E8:71:GLU:HB3	3:E8:98:ASP:HB2	1.87	0.56
3:E8:132:LEU:HB3	3:E8:164:LYS:HZ1	1.70	0.56
6:W:49:ARG:HH21	6:W:55:ASP:HB2	1.69	0.56
7:e:63:ILE:HA	7:g:16:ARG:HH12	1.69	0.56
7:g:14:LYS:NZ	7:g:45:MET:HB3	2.20	0.56
8:l:58:LYS:HZ2	7:n:6:PHE:HB3	1.71	0.56
4:B5:375:GLN:HE22	4:B5:419:VAL:HA	1.70	0.56
4:C5:217:LEU:HD13	4:C5:220:PRO:HB3	1.87	0.56
4:D5:66:MET:HE3	4:D5:151:LEU:HD22	1.88	0.56
3:D6:208:ALA:HB2	3:D6:304:LYS:HG2	1.87	0.56
4:D7:190:HIS:HB2	4:D7:414:ASN:HB3	1.87	0.56
3:A0:370:LYS:HZ1	5:R:251:GLN:HA	1.69	0.56
4:A3:316:MET:HE2	4:A3:366:THR:HG23	1.87	0.56
3:B0:88:HIS:HB3	3:B0:91:GLN:HB2	1.86	0.56
3:B2:274:PRO:HB2	3:B2:276:ILE:HG13	1.87	0.56
3:B2:319:TYR:HD1	3:B2:323:VAL:HG11	1.70	0.56
3:B6:240:ALA:HB2	3:B6:320:ARG:HH11	1.70	0.56
3:C4:207:GLU:HA	3:C4:210:TYR:HB2	1.87	0.56
7:m:79:ASP:HB3	7:m:115:LEU:HB2	1.87	0.56
7:w:122:PHE:HE2	7:w:135:ASP:HA	1.71	0.56
3:B2:31:GLN:HE22	7:e:104:ALA:HB2	1.69	0.56
3:B2:219:ILE:HG12	7:g:198:ARG:HH21	1.71	0.56
4:C1:99:ASN:HD22	4:C1:178:THR:HG23	1.70	0.56
3:C2:26:LEU:HD12	3:C2:363:VAL:HG12	1.85	0.56
4:C7:286:VAL:HG22	4:C7:363:MET:HE1	1.87	0.56
3:D0:85:HIS:HD2	7:n:99:MET:HE1	1.71	0.56
3:E4:268:MET:HE2	3:E4:378:ILE:HG22	1.88	0.56
2:I:260:VAL:HG12	2:I:262:THR:H	1.71	0.56
5:P:305:ARG:HE	5:P:308:TRP:HE1	1.53	0.56
7:g:158:THR:HB	7:g:161:TYR:HB2	1.87	0.56
4:A9:227:HIS:HB3	5:P:312:ILE:HD13	1.88	0.56
4:C1:267:LEU:HB3	4:C1:299:MET:HE2	1.87	0.56
3:D0:204:LEU:HD13	3:D0:231:ILE:HD12	1.86	0.56
4:D5:139:LEU:HA	4:D5:145:SER:HB3	1.87	0.56
4:D7:113:ILE:HG12	4:D7:154:LYS:HZ1	1.70	0.56
3:E4:274:PRO:HD3	3:E4:291:ILE:HD11	1.87	0.56
4:E5:97:ALA:HA	4:E5:103:LYS:HE2	1.88	0.56
5:P:279:VAL:HA	5:P:282:ARG:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:16:ARG:HE	7:d:17:LEU:HD12	1.71	0.56
7:j:65:GLN:HA	7:j:68:LEU:HD13	1.88	0.56
7:m:136:LEU:HA	7:m:141:THR:HG21	1.88	0.56
7:o:71:LYS:HE2	7:o:106:GLN:HB3	1.87	0.56
7:p:78:ALA:HB3	7:p:112:PHE:HE1	1.71	0.56
4:A1:232:ALA:HB2	4:A1:270:PHE:HB2	1.87	0.56
3:A2:408:TYR:HB3	3:A2:413:MET:HE3	1.87	0.56
4:A3:153:SER:HA	4:A3:195:ASN:HD22	1.71	0.56
3:A4:317:LEU:HB3	3:A4:319:TYR:HE1	1.70	0.56
4:B1:276:ARG:HH21	5:O:315:LEU:HD22	1.71	0.56
3:B2:64:ARG:HH21	3:B2:128:ASN:HD21	1.53	0.56
4:D7:39:ASP:HA	7:q:90:PRO:HG3	1.88	0.56
3:E0:266:HIS:CE1	3:E0:267:PHE:CE1	2.94	0.56
3:E2:229:ARG:HH12	2:F:219:TYR:HE1	1.52	0.56
4:E9:398:TYR:HB3	4:E9:403:MET:HG3	1.88	0.56
7:g:61:THR:HG23	7:i:16:ARG:HH21	1.71	0.56
3:A0:282:TYR:HE2	3:A4:85:HIS:HB3	1.70	0.56
4:B7:135:ILE:HG21	4:B7:152:ILE:HD11	1.88	0.56
3:C2:215:ARG:HH12	3:C2:299:ALA:HB1	1.70	0.56
4:C9:2:ARG:HB3	4:C9:131:GLN:HB2	1.87	0.56
3:D0:53:PHE:HB3	3:D0:61:HIS:HB3	1.88	0.56
3:D2:233:GLN:HG3	3:D2:272:TYR:HE2	1.71	0.56
7:n:112:PHE:HB2	7:n:131:TRP:HE1	1.71	0.56
4:A1:118:ASP:HA	4:A1:121:ARG:HE	1.70	0.56
4:A3:54:ALA:HB3	4:A3:58:ARG:HB3	1.88	0.56
4:A5:325:GLU:HA	4:A5:328:GLU:HG3	1.88	0.56
4:A5:397:TRP:CZ3	3:A6:257:THR:HA	2.41	0.56
3:A8:258:ASN:HB3	3:A8:352:LYS:HG3	1.87	0.56
4:C1:100:ASN:HB3	4:C1:103:LYS:HG2	1.88	0.56
4:C3:164:MET:HB3	4:C3:197:ASP:H	1.69	0.56
4:C3:320:ARG:HH22	2:I:214:ALA:HA	1.70	0.56
4:D1:257:LEU:HA	4:D1:312:THR:HG21	1.88	0.56
3:D8:203:MET:HE1	3:D8:267:PHE:HB3	1.88	0.56
3:E0:244:PHE:HA	5:R:558:ARG:HH12	1.71	0.56
3:E6:259:LEU:HD13	3:E6:268:MET:HE1	1.88	0.56
3:E8:114:ILE:HD12	3:E8:117:LEU:HD21	1.88	0.56
7:s:14:LYS:HD2	7:s:47:LEU:HD22	1.88	0.56
4:A3:8:GLN:HG3	4:A3:65:LEU:HD13	1.87	0.55
4:B7:220:PRO:HD2	3:B8:326:LYS:HE2	1.87	0.55
4:C1:375:GLN:HB3	4:C1:379:LYS:HE3	1.87	0.55
3:C4:280:LYS:HE3	3:C8:88:HIS:HE1	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C4:338:LYS:HG2	3:C4:340:THR:HG22	1.89	0.55
4:D3:200:GLN:HB3	4:D3:268:ILE:HD11	1.87	0.55
4:F1:333:VAL:HA	4:F1:336:LYS:HG2	1.88	0.55
8:k:103:LYS:HA	8:k:106:ILE:HG22	1.88	0.55
4:A3:299:MET:HG3	4:A3:301:CYS:H	1.71	0.55
3:A4:296:PHE:HE1	3:A4:377:MET:HG3	1.71	0.55
4:A9:139:LEU:HA	4:A9:145:SER:HB3	1.87	0.55
4:B1:330:MET:HB3	4:B1:349:MET:HE3	1.88	0.55
3:B2:292:THR:HG21	3:B2:331:ALA:HB1	1.89	0.55
3:B6:70:LEU:HD12	3:B6:99:ALA:HB2	1.87	0.55
4:C5:293:MET:HG2	4:C5:367:PHE:HB2	1.88	0.55
3:C6:76:ASP:HA	3:C6:79:ARG:HB3	1.88	0.55
4:C7:45:GLU:HG2	4:C7:46:ARG:HG2	1.88	0.55
3:E8:211:ASP:HA	3:E8:214:ARG:HG2	1.87	0.55
4:E9:117:LEU:HA	4:E9:120:VAL:HG12	1.87	0.55
7:s:119:ARG:HH12	7:s:136:LEU:HB2	1.72	0.55
1:l:415:PRO:HA	3:B6:430:LYS:HG2	1.88	0.55
4:A5:273:LEU:H	4:A5:292:GLN:HE22	1.53	0.55
3:A8:138:PHE:HZ	3:A8:235:ILE:HD12	1.71	0.55
4:D3:68:LEU:HB3	4:D3:96:GLY:HA2	1.89	0.55
4:D3:171:PRO:HG2	4:D3:185:ALA:HB2	1.89	0.55
4:D7:178:THR:HG21	11:D7:501:GDP:H5'	1.88	0.55
4:D9:253:LEU:HD21	4:D9:368:VAL:HG21	1.87	0.55
3:E4:102:ASN:HB2	4:E5:251:ARG:HH12	1.71	0.55
2:F:242:ASN:O	2:F:242:ASN:ND2	2.38	0.55
7:s:16:ARG:HE	7:s:17:LEU:HD12	1.71	0.55
1:2:418:GLN:HA	1:2:421:LEU:HD13	1.87	0.55
3:D0:97:GLU:HA	4:D1:2:ARG:HH21	1.71	0.55
4:D9:7:VAL:HB	4:D9:135:ILE:HG13	1.89	0.55
4:D9:68:LEU:HB3	4:D9:96:GLY:HA2	1.88	0.55
4:E3:44:LEU:HD12	4:E3:47:ILE:HG13	1.88	0.55
4:E5:113:ILE:HG13	4:E5:150:LEU:HD23	1.88	0.55
3:E6:217:LEU:HD21	3:E6:367:ASP:HB3	1.88	0.55
7:a:88:LEU:HD21	7:a:185:ILE:HD13	1.88	0.55
4:A5:77:ARG:HA	4:A5:82:GLY:HA3	1.88	0.55
4:B7:10:GLY:HA2	4:B7:143:THR:HG23	1.89	0.55
4:C3:68:LEU:HA	4:C3:93:GLY:HA3	1.88	0.55
3:C4:82:THR:HA	8:k:59:THR:HG23	1.87	0.55
3:E4:97:GLU:HA	4:E5:2:ARG:HH21	1.71	0.55
4:F1:217:LEU:HB3	6:V:174:ARG:NH2	2.21	0.55
7:o:18:ASN:HD21	7:o:46:ASP:H	1.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A7:10:GLY:HA2	4:A7:143:THR:HG23	1.89	0.55
4:B1:289:LEU:HD22	4:B1:363:MET:HG3	1.88	0.55
3:B2:133:GLN:HE21	3:B2:252:VAL:HG22	1.72	0.55
3:B8:167:LEU:HG	3:B8:200:VAL:HB	1.89	0.55
3:B8:185:TYR:HE2	3:B8:404:PHE:HB2	1.70	0.55
4:B9:12:CYS:HB2	4:B9:138:SER:HB2	1.88	0.55
4:B9:183:TYR:HA	4:B9:385:PHE:HE2	1.71	0.55
4:B9:200:GLN:HB3	4:B9:266:PHE:HB2	1.88	0.55
3:C6:137:MET:HB3	3:C6:168:ASN:HA	1.88	0.55
3:D0:202:VAL:HG12	3:D0:268:MET:HB2	1.89	0.55
4:E5:178:THR:HA	3:E6:352:LYS:HZ3	1.72	0.55
4:E5:319:GLY:HA2	4:E5:357:PRO:HG3	1.88	0.55
7:e:191:GLU:HG2	7:e:195:ALA:HB2	1.89	0.55
7:h:55:LEU:HB3	7:h:132:LEU:HD23	1.89	0.55
3:A4:57:GLY:HA2	5:R:253:ALA:HA	1.88	0.55
4:C5:221:THR:HG23	4:C5:223:GLY:H	1.72	0.55
4:C7:172:SER:HB2	4:C7:204:ASN:HB2	1.89	0.55
3:D2:30:ILE:HG22	3:D2:36:MET:HB3	1.89	0.55
4:D7:282:ARG:HH12	4:E1:86:ARG:HH21	1.53	0.55
4:E9:73:MET:HE1	4:E9:92:PHE:HA	1.88	0.55
7:c:51:PRO:HD2	7:c:140:LEU:HD11	1.87	0.55
7:x:79:ASP:HB2	7:x:115:LEU:HB2	1.88	0.55
4:B9:7:VAL:HB	4:B9:135:ILE:HG22	1.87	0.55
4:B9:182:PRO:HB2	4:B9:385:PHE:HD2	1.72	0.55
3:D4:239:THR:HG23	3:D4:243:ARG:HE	1.71	0.55
4:D5:51:TYR:HB3	4:D5:59:PHE:HB3	1.87	0.55
4:E3:139:LEU:HA	4:E3:145:SER:HB3	1.89	0.55
4:E5:397:TRP:HZ3	3:E6:257:THR:HG22	1.71	0.55
7:a:97:ARG:HH21	7:c:5:VAL:HG13	1.72	0.55
1:2:415:PRO:HA	3:B8:430:LYS:HD3	1.87	0.55
3:A8:137:MET:HG3	3:A8:154:LEU:HD11	1.88	0.55
4:C3:309:ARG:H	4:C3:372:THR:HG22	1.72	0.55
4:D5:325:GLU:HA	4:D5:328:GLU:HG3	1.88	0.55
4:E7:107:THR:HG21	4:E7:401:GLU:HB3	1.88	0.55
4:A7:64:ILE:HD12	4:A7:119:VAL:HG13	1.89	0.55
4:B7:138:SER:HA	4:B7:169:VAL:HG22	1.89	0.55
4:C5:171:PRO:HB3	4:C5:181:GLU:HB3	1.89	0.55
4:D1:267:LEU:HB3	4:D1:299:MET:HE2	1.88	0.55
4:D7:330:MET:HA	4:D7:333:VAL:HG12	1.87	0.55
3:E0:88:HIS:HD1	3:E0:121:ARG:HH12	1.54	0.55
4:E3:132:GLY:HA2	4:E3:162:ARG:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E9:213:ARG:HH22	4:E9:297:LYS:HB3	1.72	0.55
7:h:149:ARG:HD2	7:h:164:ARG:HG2	1.88	0.55
3:B0:174:SER:HB2	3:B0:177:VAL:HB	1.87	0.54
3:C0:209:ILE:HG23	3:C0:230:LEU:HD22	1.89	0.54
3:D0:398:MET:HE2	4:D1:345:ILE:HG23	1.88	0.54
3:E4:8:HIS:HD2	3:E4:138:PHE:HB2	1.72	0.54
5:P:367:ALA:HB1	5:P:371:ARG:HH22	1.73	0.54
7:a:78:ALA:HB3	7:a:112:PHE:HE1	1.72	0.54
7:n:84:LYS:HB3	7:n:168:PRO:HD3	1.89	0.54
3:A0:189:LEU:HD21	3:A0:418:PHE:HD1	1.71	0.54
3:A4:109:THR:HG23	3:A4:110:ILE:HG23	1.89	0.54
4:B5:117:LEU:HD22	4:B5:154:LYS:HZ2	1.72	0.54
3:C0:64:ARG:HG3	3:C0:125:LEU:HD23	1.89	0.54
3:C6:310:GLY:HA3	3:C6:383:ALA:HB2	1.88	0.54
4:C9:101:TRP:HE1	4:C9:188:SER:HB3	1.71	0.54
4:D1:320:ARG:HH22	2:K:214:ALA:HA	1.72	0.54
4:D9:276:ARG:HH21	5:O:551:GLU:HB3	1.71	0.54
3:E2:252:VAL:HA	3:E2:255:PHE:HD2	1.73	0.54
4:E5:49:VAL:HG11	4:E5:241:ARG:HG2	1.89	0.54
4:E9:215:LEU:HD11	4:E9:228:LEU:HD11	1.89	0.54
5:R:305:ARG:HB3	5:R:308:TRP:CE2	2.43	0.54
7:v:7:ALA:HB3	7:v:161:TYR:HE1	1.71	0.54
3:A6:82:THR:HA	7:b:98:THR:HB	1.90	0.54
4:B1:290:THR:HG21	4:B1:329:GLN:HB3	1.88	0.54
4:C1:86:ARG:NE	4:C1:87:PRO:HD2	2.22	0.54
4:C1:330:MET:HA	4:C1:333:VAL:HG12	1.90	0.54
3:C6:219:ILE:HD12	3:C6:222:PRO:HG3	1.89	0.54
4:D7:382:SER:HB2	4:D7:415:MET:HE1	1.89	0.54
3:E4:417:GLU:HA	3:E4:420:GLU:HG3	1.89	0.54
4:E5:117:LEU:HA	4:E5:120:VAL:HG12	1.88	0.54
3:E8:53:PHE:HB3	3:E8:61:HIS:HB3	1.89	0.54
7:o:172:VAL:HG23	7:o:180:ALA:HB3	1.88	0.54
3:A4:74:VAL:HG13	3:A4:75:VAL:HG13	1.89	0.54
3:B4:272:TYR:HB3	3:B4:275:ILE:HD11	1.90	0.54
4:B7:199:VAL:HG23	4:B7:264:HIS:CE1	2.43	0.54
3:B8:223:THR:HG22	4:B9:322:SER:HA	1.89	0.54
3:C4:392:ASP:HA	3:C4:422:ARG:HH22	1.72	0.54
4:D3:39:ASP:HA	7:o:90:PRO:HG3	1.89	0.54
3:D6:276:ILE:HD12	3:D6:280:LYS:O	2.07	0.54
3:D8:149:LEU:HG	3:D8:153:LEU:HD13	1.88	0.54
6:W:125:ARG:HH12	6:W:126:LEU:HD23	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:p:185:ILE:HG23	7:p:192:GLY:HA2	1.89	0.54
1:2:462:LEU:HD12	1:2:465:LYS:HD3	1.90	0.54
4:A9:11:GLN:HG2	5:P:306:ARG:HH12	1.72	0.54
3:B2:76:ASP:HA	3:B2:79:ARG:HG2	1.89	0.54
4:B9:375:GLN:HE21	4:B9:422:TYR:HB3	1.71	0.54
3:C2:105:ARG:HB3	3:C2:411:GLU:HG2	1.88	0.54
4:C3:330:MET:HA	4:C3:333:VAL:HG22	1.89	0.54
4:D1:311:LEU:HD12	4:D1:342:VAL:HG11	1.90	0.54
4:E1:382:SER:HB2	4:E1:415:MET:HE1	1.88	0.54
4:E5:139:LEU:HA	4:E5:145:SER:HB2	1.90	0.54
7:e:79:ASP:HB3	7:e:82:ASP:HB2	1.89	0.54
3:A8:394:LYS:HE3	4:A9:346:PRO:HB3	1.89	0.54
3:B0:234:VAL:HG21	3:B0:302:MET:HE1	1.90	0.54
3:B0:280:LYS:HG2	3:B4:88:HIS:HE1	1.73	0.54
3:B4:23:LEU:HG	3:B4:361:THR:HG21	1.90	0.54
4:C9:247:ASN:HD22	4:C9:247:ASN:C	2.15	0.54
3:D6:175:PRO:HB3	3:D6:390:ARG:HD3	1.90	0.54
7:d:49:LEU:H	7:d:65:GLN:HE22	1.56	0.54
3:A2:398:MET:HE2	4:A3:345:ILE:HG12	1.90	0.54
3:B4:215:ARG:HH12	3:B4:299:ALA:HB1	1.72	0.54
4:B7:215:LEU:HD21	4:B7:273:LEU:HB3	1.90	0.54
4:C1:236:VAL:HG13	4:C1:237:THR:HG23	1.88	0.54
4:D7:278:SER:HA	4:D7:281:TYR:HD1	1.73	0.54
3:E0:259:LEU:HD21	3:E0:316:CYS:HB2	1.88	0.54
4:E1:309:ARG:H	4:E1:372:THR:HG22	1.72	0.54
4:E9:6:HIS:CG	4:E9:8:GLN:HE22	2.26	0.54
4:E9:49:VAL:HG21	4:E9:241:ARG:HB3	1.90	0.54
2:K:223:PRO:HB3	7:p:178:ARG:HH22	1.72	0.54
7:r:127:ALA:HB1	7:t:157:PRO:HG3	1.89	0.54
7:x:169:SER:HA	7:x:185:ILE:HD11	1.90	0.54
7:x:172:VAL:HG13	7:x:180:ALA:HB3	1.90	0.54
3:A0:210:TYR:HB3	3:A0:214:ARG:HH12	1.72	0.54
4:A3:173:PRO:HD2	4:A3:205:GLU:HG2	1.89	0.54
4:A5:313:ALA:HB3	4:A5:349:MET:HG3	1.90	0.54
4:A7:392:LYS:HE2	4:A7:395:LEU:HG	1.90	0.54
4:B7:66:MET:HE2	4:B7:116:VAL:HG21	1.89	0.54
4:C1:213:ARG:NH2	4:C1:297:LYS:HG3	2.21	0.54
4:C5:230:SER:HA	4:C5:233:MET:HB3	1.89	0.54
4:D7:248:SER:HA	4:D7:252:LYS:HG3	1.88	0.54
4:E3:35:THR:HG22	7:t:83:PRO:HG3	1.89	0.54
3:E6:316:CYS:HA	3:E6:352:LYS:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A6:205:ASP:HB2	3:A6:303:ALA:HA	1.90	0.54
3:A6:222:PRO:HD2	4:A7:324:LYS:HE2	1.88	0.54
4:A7:230:SER:HA	4:A7:233:MET:HB3	1.90	0.54
4:B1:70:PRO:HA	4:B1:73:MET:HE2	1.89	0.54
4:B5:330:MET:HE3	4:B5:349:MET:HB3	1.90	0.54
3:B8:191:THR:HA	3:B8:194:LEU:HG	1.90	0.54
3:C6:247:ALA:HB1	5:P:458:ARG:HG2	1.89	0.54
3:C8:396:ASP:HA	3:C8:399:TYR:HB3	1.89	0.54
4:D9:51:TYR:HB3	4:D9:59:PHE:HB3	1.90	0.54
3:E0:310:GLY:HA3	3:E0:383:ALA:HB2	1.88	0.54
3:E2:310:GLY:HA3	3:E2:383:ALA:HB2	1.89	0.54
4:E3:66:MET:HE3	4:E3:147:MET:HG3	1.90	0.54
7:o:68:LEU:HD22	7:o:109:GLU:HG2	1.90	0.54
2:B:222:LYS:HE2	3:D4:364:PRO:HD2	1.90	0.54
4:C1:68:LEU:HB3	4:C1:96:GLY:HA2	1.89	0.54
4:C7:10:GLY:HA2	4:C7:143:THR:HG23	1.89	0.54
4:C9:397:TRP:HZ2	3:D0:260:VAL:HG23	1.73	0.54
4:D1:152:ILE:HG22	4:D1:195:ASN:HB3	1.90	0.54
4:D7:49:VAL:HG21	4:D7:241:ARG:HG3	1.90	0.54
3:D8:36:MET:HE3	3:D8:37:PRO:HD2	1.90	0.54
3:E6:406:HIS:HA	3:E6:409:VAL:HG12	1.90	0.54
3:E8:97:GLU:HA	4:E9:2:ARG:HH12	1.72	0.54
6:V:96:ARG:HH22	6:V:99:LYS:HB3	1.72	0.54
7:g:99:MET:HE3	7:g:107:LYS:HE3	1.89	0.54
7:i:14:LYS:HD2	7:i:47:LEU:HD22	1.88	0.54
8:k:160:ARG:HA	8:k:163:LYS:HE2	1.88	0.54
2:A:215:TYR:HE2	3:A6:81:GLY:HA3	1.73	0.53
3:A2:119:LEU:HD11	3:A2:156:ARG:HB3	1.90	0.53
4:A3:7:VAL:HB	4:A3:135:ILE:HG22	1.89	0.53
3:A4:276:ILE:HB	3:A4:280:LYS:HB2	1.89	0.53
3:B8:192:HIS:HD1	3:B8:192:HIS:C	2.16	0.53
4:C3:86:ARG:HH21	4:C3:87:PRO:HG2	1.73	0.53
3:C8:147:SER:HB2	3:C8:190:SER:HB3	1.89	0.53
4:D3:75:SER:HA	5:P:508:TYR:HE1	1.73	0.53
4:E1:152:ILE:HG23	4:E1:164:MET:HE2	1.90	0.53
2:F:242:ASN:C	2:F:242:ASN:HD22	2.12	0.53
4:A5:262:ARG:HH22	4:A5:417:ASP:HB3	1.74	0.53
4:B5:286:VAL:HA	4:B5:289:LEU:HB2	1.89	0.53
3:C0:278:ALA:HA	3:C0:369:ALA:HB2	1.90	0.53
4:C9:139:LEU:HD13	4:C9:168:SER:HB2	1.89	0.53
3:E0:191:THR:HA	3:E0:194:LEU:HG	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E1:265:PHE:HB3	4:E1:374:ILE:HD13	1.90	0.53
4:E7:311:LEU:HD12	4:E7:342:VAL:HG11	1.90	0.53
7:u:170:VAL:HG23	7:u:183:LEU:HB2	1.90	0.53
4:A3:91:VAL:HG21	4:A3:116:VAL:HG12	1.91	0.53
4:A5:86:ARG:HE	4:A5:87:PRO:HD2	1.73	0.53
4:A5:107:THR:HG21	4:A5:401:GLU:HB2	1.91	0.53
3:D2:311:LYS:H	3:D2:382:THR:HG22	1.74	0.53
3:D6:324:VAL:HG12	3:D6:326:LYS:H	1.73	0.53
3:E2:81:GLY:HA2	2:F:216:ARG:HE	1.74	0.53
6:V:90:TRP:HA	6:V:93:ARG:HD2	1.89	0.53
8:l:58:LYS:NZ	7:n:6:PHE:HB3	2.23	0.53
7:v:78:ALA:HB3	7:v:112:PHE:HE1	1.73	0.53
3:A6:191:THR:HA	3:A6:194:LEU:HB3	1.89	0.53
4:A7:236:VAL:HA	4:A7:316:MET:HE1	1.90	0.53
4:A7:240:LEU:HD22	4:A7:250:LEU:HD13	1.89	0.53
4:B5:136:THR:HG22	4:B5:167:PHE:HB2	1.91	0.53
4:B9:281:TYR:HB2	4:C3:86:ARG:NH1	2.24	0.53
4:D7:222:TYR:CE2	3:D8:325:PRO:HG2	2.44	0.53
4:D7:309:ARG:HH21	4:D7:342:VAL:HA	1.73	0.53
3:D8:187:SER:HB2	3:D8:391:MET:HE2	1.90	0.53
3:D8:223:THR:HG23	3:D8:225:THR:H	1.73	0.53
3:E0:53:PHE:HB3	3:E0:61:HIS:HB3	1.91	0.53
3:E4:398:MET:HE1	4:E5:346:PRO:HD2	1.89	0.53
4:E5:12:CYS:HB2	4:E5:138:SER:HB2	1.91	0.53
3:E8:398:MET:HE1	4:E9:345:ILE:HA	1.89	0.53
4:E9:7:VAL:HB	4:E9:135:ILE:HG22	1.91	0.53
6:W:170:GLU:HG3	6:W:171:ASP:H	1.72	0.53
7:u:105:ASN:HD21	7:w:39:PRO:HD2	1.73	0.53
7:v:184:PRO:HB2	7:v:189:LEU:HB2	1.89	0.53
7:x:4:PRO:HG3	7:x:179:GLU:H	1.73	0.53
1:2:487:ARG:HG3	1:2:491:LEU:HD13	1.90	0.53
4:A5:281:TYR:HA	4:A9:60:VAL:HG11	1.90	0.53
3:A6:19:ALA:HA	3:A6:22:GLU:HG2	1.90	0.53
4:A7:193:VAL:HG21	4:A7:418:LEU:HD21	1.91	0.53
3:B8:88:HIS:HB3	3:B8:91:GLN:HG3	1.90	0.53
3:C4:31:GLN:HE21	8:k:64:GLY:HA2	1.74	0.53
3:D8:119:LEU:HA	3:D8:122:ILE:HG22	1.89	0.53
7:c:68:LEU:HD23	7:c:73:VAL:HG21	1.91	0.53
4:B1:10:GLY:HA2	4:B1:143:THR:HG23	1.89	0.53
3:B2:213:CYS:HB3	3:B2:222:PRO:HG2	1.90	0.53
3:B8:202:VAL:HA	3:B8:268:MET:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D3:10:GLY:HA2	4:D3:143:THR:HG23	1.91	0.53
3:D6:212:ILE:HG22	3:D6:275:ILE:HD11	1.90	0.53
3:D8:191:THR:HA	3:D8:194:LEU:HB3	1.91	0.53
3:E4:64:ARG:HB2	3:E4:125:LEU:HD21	1.91	0.53
3:E8:288:VAL:HG11	3:E8:328:VAL:HG12	1.90	0.53
3:F0:135:PHE:HZ	3:F0:161:TYR:HD2	1.55	0.53
4:F1:133:PHE:HZ	4:F1:159:TYR:HD2	1.56	0.53
7:r:75:LEU:HD13	7:r:111:ILE:HG23	1.90	0.53
7:t:185:ILE:HD13	7:t:195:ALA:HB3	1.90	0.53
3:A2:311:LYS:HE2	3:A2:344:VAL:HG12	1.91	0.53
3:C0:401:LYS:HZ1	4:C1:344:TRP:CG	2.27	0.53
4:C1:173:PRO:HA	4:C1:380:ARG:HH12	1.74	0.53
4:C5:220:PRO:HG2	3:C6:326:LYS:HE2	1.91	0.53
4:D7:215:LEU:HD22	5:P:548:PRO:HD3	1.91	0.53
4:E9:199:VAL:HG23	4:E9:264:HIS:HE1	1.74	0.53
7:i:75:LEU:HD23	7:i:111:ILE:HB	1.89	0.53
7:v:14:LYS:HE2	7:v:47:LEU:HD23	1.90	0.53
7:w:14:LYS:HD3	7:w:47:LEU:HB3	1.90	0.53
3:A4:90:GLU:HG2	3:A4:121:ARG:HH12	1.73	0.53
3:A6:64:ARG:HG2	3:A6:125:LEU:HD22	1.91	0.53
3:B8:9:VAL:HG12	3:B8:146:GLY:HA2	1.91	0.53
3:E0:88:HIS:HD2	3:E0:89:PRO:HD2	1.74	0.53
4:F1:293:MET:HE2	4:F1:367:PHE:HB2	1.90	0.53
3:A0:270:SER:HB3	3:A0:302:MET:HE2	1.89	0.53
3:C4:104:ALA:HB2	3:C4:413:MET:HG2	1.91	0.53
3:C8:81:GLY:HA3	2:K:247:TYR:HE2	1.72	0.53
3:D8:212:ILE:HG23	3:D8:216:ASN:HD22	1.74	0.53
4:E9:113:ILE:HD11	4:E9:150:LEU:HD13	1.90	0.53
4:F1:49:VAL:HG11	4:F1:241:ARG:HB3	1.89	0.53
7:w:112:PHE:HD2	7:w:131:TRP:HE1	1.55	0.53
4:A7:2:ARG:HH21	4:A7:240:LEU:HD12	1.73	0.53
4:B3:99:ASN:HD22	4:B3:178:THR:HG23	1.74	0.53
4:B7:135:ILE:HD13	4:B7:152:ILE:HD11	1.91	0.53
3:B8:221:ARG:HH12	7:j:190:GLU:HB2	1.74	0.53
4:C1:216:LYS:HB2	4:C1:275:SER:HB2	1.91	0.53
3:C2:398:MET:HE1	4:C3:345:ILE:HG23	1.91	0.53
4:C5:249:ASP:H	4:C5:252:LYS:HB3	1.74	0.53
4:C9:150:LEU:HG	4:C9:154:LYS:HZ2	1.73	0.53
7:x:75:LEU:HD23	7:x:173:ILE:HG21	1.91	0.53
4:A9:100:ASN:HB2	4:A9:103:LYS:HG2	1.91	0.52
4:B3:8:GLN:HE22	4:B3:17:GLY:HA3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B5:309:ARG:H	4:B5:372:THR:HG22	1.73	0.52
3:B8:76:ASP:HA	3:B8:79:ARG:HD2	1.89	0.52
3:B8:207:GLU:HA	3:B8:210:TYR:HB2	1.91	0.52
3:C6:84:ARG:HH21	8:l:60:THR:HG23	1.74	0.52
3:C6:286:LEU:HB3	3:C6:291:ILE:HD11	1.90	0.52
4:C9:219:THR:HA	3:D0:326:LYS:NZ	2.24	0.52
4:D3:91:VAL:HG21	4:D3:116:VAL:HG22	1.91	0.52
4:D7:171:PRO:HG2	4:D7:185:ALA:HB2	1.90	0.52
4:D9:153:SER:HA	4:D9:195:ASN:HD21	1.72	0.52
3:E0:64:ARG:HG3	3:E0:125:LEU:HD21	1.91	0.52
4:E1:169:VAL:HG12	4:E1:202:ILE:HB	1.91	0.52
4:E5:281:TYR:HD2	4:E9:87:PRO:HD3	1.73	0.52
7:n:14:LYS:HG2	7:n:45:MET:HE2	1.91	0.52
7:o:185:ILE:HG23	7:o:192:GLY:HA2	1.90	0.52
7:x:151:MET:HE3	7:x:154:TYR:HA	1.90	0.52
4:A1:68:LEU:HA	4:A1:93:GLY:HA3	1.90	0.52
4:B9:198:GLU:HA	4:B9:264:HIS:HB2	1.92	0.52
3:D6:402:ARG:HE	3:D6:405:VAL:HG11	1.74	0.52
3:E0:173:PRO:HG2	3:E0:391:MET:HE1	1.91	0.52
7:m:78:ALA:HB3	7:m:112:PHE:HE1	1.73	0.52
7:o:63:ILE:HB	7:o:67:HIS:CD2	2.44	0.52
4:A5:23:VAL:HG11	4:A5:230:SER:HB3	1.90	0.52
4:A9:303:SER:HB3	4:A9:377:MET:HB2	1.92	0.52
3:C0:11:GLN:HE22	3:C0:74:VAL:HG21	1.73	0.52
4:C1:39:ASP:HA	7:i:90:PRO:HG3	1.92	0.52
4:D3:396:HIS:CD2	3:D4:263:PRO:HD3	2.44	0.52
3:D4:252:VAL:HA	3:D4:255:PHE:HD2	1.74	0.52
4:E9:97:ALA:HB3	4:E9:143:THR:HB	1.91	0.52
3:F0:66:VAL:HA	3:F0:91:GLN:HB2	1.91	0.52
7:i:4:PRO:HG3	7:i:179:GLU:H	1.74	0.52
7:o:78:ALA:HB3	7:o:112:PHE:HE1	1.74	0.52
7:r:114:SER:HB3	7:r:136:LEU:HD13	1.91	0.52
7:x:11:ASN:HA	7:x:14:LYS:HB2	1.91	0.52
3:A2:298:PRO:HA	3:A2:301:MET:HE2	1.90	0.52
3:A6:296:PHE:HE1	3:A6:377:MET:HG3	1.75	0.52
4:C1:133:PHE:HD2	4:C1:164:MET:HE1	1.74	0.52
4:D1:51:TYR:HB3	4:D1:59:PHE:HB3	1.91	0.52
4:E3:2:ARG:HB3	4:E3:131:GLN:HB2	1.92	0.52
7:b:172:VAL:HG22	7:b:204:THR:HG21	1.92	0.52
7:t:53:GLY:HA2	7:t:62:VAL:HG21	1.90	0.52
3:D6:137:MET:HE3	3:D6:168:ASN:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D6:298:PRO:HB3	3:D6:307:PRO:HD2	1.92	0.52
3:D6:372:MET:HG2	3:D6:373:ARG:HG2	1.91	0.52
3:D8:277:SER:O	3:D8:281:ALA:N	2.42	0.52
4:E1:12:CYS:HB2	4:E1:138:SER:HB2	1.91	0.52
4:E9:246:LEU:H	4:E9:353:VAL:HB	1.75	0.52
4:F1:228:LEU:HD23	4:F1:300:MET:HE2	1.92	0.52
7:c:50:PHE:HB2	7:c:65:GLN:HG3	1.92	0.52
7:s:194:ARG:O	7:s:197:LEU:HB2	2.09	0.52
3:A4:19:ALA:HA	3:A4:22:GLU:HG2	1.91	0.52
4:A9:222:TYR:HD2	5:P:306:ARG:HE	1.57	0.52
4:B3:97:ALA:HB3	4:B3:143:THR:HB	1.92	0.52
4:B3:207:LEU:HB3	4:B3:225:LEU:HD22	1.91	0.52
4:B9:51:TYR:HB3	4:B9:59:PHE:HB3	1.91	0.52
3:C0:7:ILE:HG21	3:C0:153:LEU:HD21	1.91	0.52
3:C4:104:ALA:HA	3:C4:413:MET:HE3	1.90	0.52
3:D0:237:SER:HA	3:D0:320:ARG:HH11	1.74	0.52
4:D7:391:ARG:HD3	3:D8:346:TRP:HB3	1.90	0.52
3:D8:195:LEU:HD12	3:D8:428:LEU:HD22	1.92	0.52
7:a:92:LEU:HD22	7:a:196:LEU:HD11	1.91	0.52
3:A4:296:PHE:HD2	3:A4:335:ILE:HG12	1.74	0.52
4:A9:317:PHE:HE1	4:A9:330:MET:HE1	1.74	0.52
3:B8:84:ARG:HH21	7:h:197:LEU:HD21	1.74	0.52
3:B8:112:LYS:HA	3:B8:115:VAL:HG12	1.90	0.52
4:C5:337:ASN:HB3	4:C5:340:TYR:HB2	1.92	0.52
3:C8:310:GLY:HA3	3:C8:383:ALA:HB2	1.91	0.52
3:D2:272:TYR:HE1	3:D2:374:ALA:HB1	1.74	0.52
4:D5:68:LEU:HA	4:D5:93:GLY:HA3	1.91	0.52
7:b:92:LEU:HD22	7:b:196:LEU:HD11	1.91	0.52
7:n:55:LEU:HB3	7:n:132:LEU:HD12	1.91	0.52
4:C9:173:PRO:HG3	4:C9:380:ARG:CZ	2.39	0.52
4:D1:117:LEU:HA	4:D1:120:VAL:HG12	1.91	0.52
4:D7:100:ASN:HB3	4:D7:103:LYS:HG2	1.91	0.52
3:E0:205:ASP:HB2	3:E0:303:ALA:HA	1.91	0.52
3:E6:30:ILE:HG22	3:E6:36:MET:HB3	1.92	0.52
7:i:84:LYS:HB3	7:i:168:PRO:HD3	1.91	0.52
8:l:76:LEU:HD21	8:l:106:ILE:HG21	1.90	0.52
7:r:172:VAL:HG23	7:r:180:ALA:HB3	1.91	0.52
4:A3:233:MET:HA	4:A3:236:VAL:HG12	1.90	0.52
4:A5:40:SER:HB3	4:A5:43:GLN:HG3	1.90	0.52
4:A5:220:PRO:HD2	3:A6:326:LYS:HZ2	1.75	0.52
3:A8:210:TYR:HB3	3:A8:214:ARG:HH21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A9:66:MET:HG3	4:A9:147:MET:HE1	1.91	0.52
4:B7:133:PHE:HB2	4:B7:164:MET:HE1	1.91	0.52
3:C0:9:VAL:HG13	3:C0:68:LEU:HD22	1.92	0.52
3:C0:267:PHE:HE2	3:C0:428:LEU:HD11	1.75	0.52
4:C1:272:PRO:HG3	4:C1:284:LEU:HD11	1.91	0.52
3:D0:392:ASP:HA	3:D0:422:ARG:HH12	1.75	0.52
3:E0:168:ASN:HD22	3:E0:198:THR:HG21	1.75	0.52
3:E6:96:LYS:HG2	3:E6:97:GLU:HG3	1.91	0.52
7:c:48:ILE:HD12	7:c:65:GLN:HE22	1.74	0.52
7:h:184:PRO:HG3	7:h:189:LEU:HD12	1.91	0.52
7:j:184:PRO:HB2	7:j:189:LEU:HB2	1.92	0.52
4:C9:377:MET:HE3	4:C9:380:ARG:HH22	1.75	0.52
4:D3:7:VAL:HG13	4:D3:66:MET:HE1	1.92	0.52
4:D7:2:ARG:HB2	4:D7:131:GLN:HB2	1.92	0.52
4:E3:187:LEU:HA	4:E3:190:HIS:CE1	2.45	0.52
7:d:14:LYS:HB2	7:d:47:LEU:HD13	1.90	0.52
7:e:38:LEU:HD12	7:e:39:PRO:HA	1.92	0.52
7:j:126:ARG:NH1	7:j:133:SER:HB3	2.24	0.52
8:k:67:ALA:HB3	7:m:39:PRO:HG3	1.92	0.52
8:l:14:LYS:HE3	8:l:21:TYR:HA	1.91	0.52
4:A3:30:ILE:HD11	4:A3:47:ILE:HD11	1.93	0.51
4:B5:164:MET:HB3	4:B5:197:ASP:H	1.75	0.51
3:B8:116:ASP:HA	3:B8:156:ARG:HH12	1.75	0.51
4:C1:49:VAL:HG11	4:C1:241:ARG:HG2	1.92	0.51
4:C9:202:ILE:HD11	4:C9:268:ILE:HD12	1.91	0.51
4:D1:303:SER:HA	4:D1:377:MET:HE3	1.92	0.51
3:D6:75:VAL:HG22	3:D6:79:ARG:HH21	1.74	0.51
3:E0:405:VAL:HG13	3:E0:418:PHE:HE2	1.74	0.51
3:E6:234:VAL:HG21	3:E6:302:MET:HE1	1.92	0.51
3:E8:271:SER:HB3	3:E8:377:MET:HB3	1.91	0.51
4:E9:337:ASN:HB3	4:E9:340:TYR:HB2	1.93	0.51
5:R:243:PRO:HG2	7:a:178:ARG:HH11	1.75	0.51
7:b:164:ARG:NH1	7:b:166:GLY:H	2.07	0.51
7:h:63:ILE:HG21	7:h:132:LEU:HD21	1.91	0.51
7:p:115:LEU:HD21	7:p:145:LYS:HE3	1.92	0.51
4:A5:132:GLY:HA3	4:A5:163:ILE:HG22	1.91	0.51
3:B4:195:LEU:HD13	3:B4:264:ARG:HH21	1.75	0.51
3:B6:9:VAL:HG12	3:B6:146:GLY:HA2	1.92	0.51
3:D2:292:THR:HG21	3:D2:331:ALA:HB1	1.91	0.51
4:D9:321:MET:HE1	4:D9:326:VAL:HG22	1.92	0.51
3:E8:325:PRO:HA	3:E8:328:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A4:179:THR:H	4:A5:347:ASN:HD21	1.58	0.51
3:A8:338:LYS:HG3	3:A8:340:THR:HG22	1.92	0.51
4:B1:318:ARG:HE	4:B1:358:PRO:HD3	1.75	0.51
3:B2:71:GLU:HG3	3:B2:73:THR:HG22	1.92	0.51
3:B6:258:ASN:HB3	3:B6:352:LYS:HG3	1.92	0.51
4:C1:258:ILE:HD12	4:C1:261:PRO:HA	1.93	0.51
3:C8:12:ALA:HB3	3:C8:140:ALA:HB2	1.92	0.51
4:E7:3:GLU:HA	4:E7:49:VAL:HA	1.93	0.51
7:h:78:ALA:HB3	7:h:112:PHE:HE1	1.75	0.51
4:A9:153:SER:HB2	4:A9:191:GLN:HE22	1.75	0.51
4:B9:240:LEU:HD11	4:B9:249:ASP:HA	1.92	0.51
4:C5:91:VAL:HB	4:C5:112:LEU:HD11	1.92	0.51
4:D3:407:GLU:HA	4:D3:410:GLU:HB3	1.91	0.51
3:D8:73:THR:HG23	4:D9:247:ASN:HD22	1.76	0.51
2:E:222:LYS:HD2	2:E:223:PRO:HD2	1.92	0.51
4:F1:16:ILE:HD11	4:F1:229:VAL:HG11	1.93	0.51
7:v:140:LEU:HA	7:v:143:ILE:HG22	1.93	0.51
7:w:146:ARG:HH12	7:w:156:VAL:HG21	1.75	0.51
3:A6:210:TYR:HE1	3:A6:227:LEU:HD11	1.74	0.51
4:A7:117:LEU:HD11	4:A7:154:LYS:HD2	1.91	0.51
3:D2:223:THR:HG23	3:D2:225:THR:H	1.76	0.51
3:D8:249:ASN:HD21	5:P:532:ARG:HH22	1.58	0.51
4:E3:315:ALA:HB3	4:E3:330:MET:HE1	1.92	0.51
4:E5:65:LEU:HD11	4:E5:76:VAL:HG11	1.92	0.51
4:E7:167:PHE:CE2	4:E7:233:MET:HG3	2.45	0.51
4:E9:60:VAL:HG11	4:E9:86:ARG:HG3	1.92	0.51
7:t:99:MET:CE	7:t:201:TRP:HB3	2.41	0.51
4:B3:208:TYR:HE1	4:B3:225:LEU:HD11	1.76	0.51
3:C6:259:LEU:HD11	3:C6:316:CYS:HB2	1.92	0.51
3:D2:27:GLU:HG3	3:D2:243:ARG:HH12	1.74	0.51
3:D8:238:LEU:HD12	3:D8:318:MET:HE1	1.92	0.51
4:F1:209:ASP:HB3	4:F1:213:ARG:NH2	2.25	0.51
7:b:68:LEU:HA	7:b:71:LYS:HE2	1.93	0.51
1:2:390:THR:HB	1:2:393:ASP:HB2	1.93	0.51
3:A6:285:GLN:HE22	3:A6:287:SER:HB3	1.76	0.51
4:A9:36:TYR:HB3	7:c:86:ALA:HB1	1.91	0.51
4:B5:372:THR:HG21	4:B5:426:GLN:HB3	1.92	0.51
4:C1:217:LEU:HD11	4:C1:220:PRO:HB3	1.92	0.51
3:C4:88:HIS:HB3	3:C4:91:GLN:OE1	2.11	0.51
4:C9:198:GLU:HA	4:C9:264:HIS:HB2	1.92	0.51
3:D0:207:GLU:HA	3:D0:210:TYR:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D2:320:ARG:HH21	3:D2:360:PRO:HA	1.76	0.51
3:E4:71:GLU:HG3	3:E4:73:THR:HG22	1.92	0.51
3:A4:3:GLU:HA	3:A4:51:THR:HA	1.93	0.51
3:A4:209:ILE:HA	3:A4:212:ILE:HG12	1.93	0.51
4:A9:28:HIS:HE1	4:A9:241:ARG:HH11	1.58	0.51
3:D6:183:GLU:HA	3:D6:186:ASN:HD22	1.76	0.51
7:e:84:LYS:HB3	7:e:168:PRO:HD3	1.93	0.51
4:A3:246:LEU:HD23	4:A3:352:SER:HA	1.93	0.51
4:A5:207:LEU:HB3	4:A5:225:LEU:HD22	1.92	0.51
3:A6:178:SER:H	4:A7:347:ASN:ND2	2.08	0.51
4:A7:139:LEU:HG	4:A7:168:SER:HB3	1.92	0.51
4:A9:7:VAL:HB	4:A9:135:ILE:HG13	1.92	0.51
3:B0:261:PRO:HD3	3:B0:313:MET:HE2	1.92	0.51
4:B7:376:GLU:HA	4:B7:379:LYS:HG2	1.92	0.51
3:C4:286:LEU:HB3	3:C4:291:ILE:HD11	1.93	0.51
3:C8:210:TYR:CE1	4:C9:324:LYS:HG3	2.46	0.51
4:D7:282:ARG:HH22	4:E1:86:ARG:HH21	1.58	0.51
3:D8:265:ILE:HG22	3:D8:380:ASN:HD21	1.76	0.51
3:D8:407:TRP:HZ2	4:D9:258:ILE:HB	1.76	0.51
4:D9:113:ILE:HA	4:D9:116:VAL:HG12	1.93	0.51
4:E5:284:LEU:HD11	4:E5:362:LYS:HB2	1.93	0.51
4:E7:39:ASP:HA	7:v:90:PRO:HG3	1.93	0.51
4:F1:20:PHE:HA	4:F1:23:VAL:HG12	1.92	0.51
7:v:136:LEU:HD12	7:v:141:THR:HG21	1.92	0.51
3:A0:324:VAL:HG13	5:R:257:ILE:HD13	1.91	0.51
3:B0:329:ASN:HA	3:B0:332:VAL:HG12	1.92	0.51
3:B2:137:MET:HE3	3:B2:168:ASN:HB2	1.92	0.51
4:B3:51:TYR:HB3	4:B3:59:PHE:HB3	1.93	0.51
4:B3:207:LEU:HA	4:B3:210:ILE:HG12	1.93	0.51
4:B9:66:MET:HG2	4:B9:147:MET:HE1	1.91	0.51
3:D2:3:GLU:HA	3:D2:51:THR:HA	1.93	0.51
3:D4:72:PRO:HA	3:D4:75:VAL:HG12	1.93	0.51
4:E1:337:ASN:HB3	4:E1:340:TYR:HB2	1.93	0.51
6:V:63:ILE:HG13	7:b:157:PRO:HA	1.93	0.51
8:k:36:LEU:HD23	8:k:72:ILE:HB	1.93	0.51
1:2:400:GLU:HA	1:2:403:LEU:HD23	1.93	0.50
3:A0:9:VAL:HG22	3:A0:68:LEU:HD22	1.93	0.50
4:A5:284:LEU:HG	4:A5:363:MET:HE2	1.93	0.50
3:A6:137:MET:HB3	3:A6:168:ASN:HA	1.93	0.50
4:B3:248:SER:HB2	4:B3:252:LYS:HG2	1.92	0.50
4:B7:221:THR:HG23	4:B7:223:GLY:H	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C6:66:VAL:HG23	3:C6:91:GLN:HB2	1.92	0.50
3:C8:377:MET:HE2	3:C8:379:SER:HB3	1.93	0.50
3:D8:277:SER:O	3:D8:278:ALA:C	2.54	0.50
3:E6:177:VAL:HB	3:E6:207:GLU:HG2	1.93	0.50
3:F0:85:HIS:HE1	7:x:98:THR:HB	1.76	0.50
1:2:431:LEU:HD23	1:2:434:ARG:HH12	1.76	0.50
3:A0:81:GLY:HA3	6:W:81:TYR:HE1	1.76	0.50
3:A2:277:SER:HB2	3:A2:280:LYS:HG2	1.93	0.50
4:A3:383:ASP:HA	4:A3:386:THR:HG22	1.92	0.50
4:B5:334:GLN:HA	4:B5:341:PHE:HE2	1.76	0.50
3:B8:195:LEU:HD11	3:B8:428:LEU:HD12	1.93	0.50
3:B8:271:SER:HB3	3:B8:377:MET:HB3	1.93	0.50
4:C1:177:ASP:HB2	3:C2:352:LYS:HA	1.92	0.50
3:C2:166:LYS:HD2	3:C2:198:THR:HA	1.92	0.50
3:C2:175:PRO:HB3	3:C2:390:ARG:HD2	1.94	0.50
3:C6:119:LEU:HD13	3:C6:122:ILE:HD11	1.93	0.50
3:C8:259:LEU:HD11	3:C8:316:CYS:HB2	1.93	0.50
4:E1:111:GLU:HG2	4:E1:112:LEU:HD12	1.93	0.50
3:E8:9:VAL:HG12	3:E8:146:GLY:HA2	1.93	0.50
4:E9:219:THR:HA	3:F0:326:LYS:HD2	1.93	0.50
7:c:112:PHE:HB2	7:c:131:TRP:HE1	1.76	0.50
7:g:149:ARG:NH2	7:g:162:GLY:H	2.09	0.50
7:j:96:TYR:HA	7:j:108:ILE:HD11	1.93	0.50
7:n:175:SER:H	7:n:178:ARG:NH2	2.09	0.50
7:s:97:ARG:HH22	7:u:160:GLY:HA3	1.75	0.50
7:x:142:GLU:HA	7:x:145:LYS:HG2	1.92	0.50
3:A0:174:SER:HB2	3:A0:304:LYS:HZ2	1.76	0.50
3:A6:220:GLU:HG3	3:A6:221:ARG:HD3	1.94	0.50
4:A9:190:HIS:HB2	4:A9:414:ASN:HB3	1.93	0.50
3:B0:205:ASP:HB2	3:B0:303:ALA:HA	1.92	0.50
3:B4:363:VAL:HG23	3:B4:366:GLY:HA3	1.93	0.50
3:B6:75:VAL:HG21	3:B6:94:SER:HB2	1.94	0.50
3:B8:187:SER:HB2	3:B8:391:MET:HE1	1.92	0.50
3:D0:178:SER:HB2	4:D1:347:ASN:ND2	2.25	0.50
4:D7:91:VAL:HG21	4:D7:116:VAL:HG22	1.93	0.50
4:E1:229:VAL:HA	4:E1:300:MET:HE1	1.92	0.50
7:c:14:LYS:HD2	7:c:47:LEU:HD13	1.92	0.50
7:c:114:SER:HB3	7:c:136:LEU:HD13	1.92	0.50
7:e:127:ALA:HB1	7:g:157:PRO:HG3	1.93	0.50
3:A2:137:MET:HG2	3:A2:154:LEU:HD21	1.94	0.50
4:A3:118:ASP:HA	4:A3:121:ARG:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A4:121:ARG:HD3	3:A4:124:LYS:HB2	1.93	0.50
4:B3:182:PRO:HB2	4:B3:385:PHE:HD1	1.75	0.50
4:B3:199:VAL:HG23	4:B3:264:HIS:CE1	2.46	0.50
3:B4:3:GLU:HA	3:B4:51:THR:HA	1.93	0.50
4:C3:30:ILE:HG13	4:C3:51:TYR:HE2	1.76	0.50
4:C9:179:VAL:HG23	3:D0:352:LYS:HB2	1.92	0.50
3:D0:175:PRO:HB3	3:D0:390:ARG:NH1	2.27	0.50
3:D8:255:PHE:HE2	3:D8:378:ILE:HD12	1.76	0.50
4:E7:66:MET:HB3	4:E7:147:MET:HE1	1.93	0.50
3:A6:237:SER:HA	3:A6:320:ARG:HD2	1.93	0.50
3:B0:220:GLU:HG2	3:B0:221:ARG:HG3	1.92	0.50
3:B4:292:THR:HG21	3:B4:331:ALA:HB1	1.94	0.50
3:B8:259:LEU:HD21	3:B8:316:CYS:HB2	1.94	0.50
3:C4:70:LEU:HD13	3:C4:110:ILE:HG23	1.93	0.50
4:D3:259:PRO:HD2	4:D3:263:LEU:HD11	1.93	0.50
4:D7:16:ILE:HD11	4:D7:229:VAL:HG21	1.92	0.50
4:E1:51:TYR:HB3	4:E1:59:PHE:HB3	1.94	0.50
3:F0:73:THR:HG22	4:F1:46:ARG:NE	2.27	0.50
7:i:56:LYS:HD2	7:i:60:ASN:HA	1.94	0.50
7:q:185:ILE:HD13	7:q:195:ALA:HB3	1.93	0.50
3:B8:3:GLU:HA	3:B8:51:THR:HA	1.94	0.50
3:B8:208:ALA:HB2	3:B8:304:LYS:HG2	1.92	0.50
3:C2:319:TYR:HD2	3:C2:323:VAL:HG11	1.77	0.50
4:D1:30:ILE:HD11	4:D1:47:ILE:HD11	1.93	0.50
3:D6:16:ILE:HD11	3:D6:138:PHE:HB3	1.94	0.50
4:D7:198:GLU:HG2	4:D7:200:GLN:HE22	1.76	0.50
4:D9:311:LEU:HD12	4:D9:342:VAL:HG11	1.92	0.50
3:E0:224:TYR:HA	3:E0:227:LEU:HD13	1.93	0.50
4:E5:166:THR:HG21	4:E5:192:LEU:HD21	1.94	0.50
4:E9:66:MET:HG2	4:E9:91:VAL:HB	1.92	0.50
7:e:72:SER:HB3	7:e:108:ILE:HG22	1.93	0.50
7:m:105:ASN:HD21	7:o:39:PRO:HD2	1.76	0.50
7:x:19:GLU:HB3	7:x:40:PRO:HD2	1.94	0.50
1:1:487:ARG:HG3	1:1:491:LEU:HD13	1.94	0.50
3:A2:228:ASN:HA	3:A2:231:ILE:HG22	1.94	0.50
3:A6:112:LYS:HA	3:A6:115:VAL:HG12	1.94	0.50
4:A7:51:TYR:HB3	4:A7:59:PHE:HB3	1.93	0.50
4:A7:164:MET:HB3	4:A7:197:ASP:H	1.76	0.50
3:B0:138:PHE:HZ	3:B0:235:ILE:HD12	1.77	0.50
4:C1:66:MET:SD	4:C1:147:MET:HE3	2.52	0.50
3:C4:7:ILE:HD13	3:C4:153:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C4:181:VAL:HG12	4:C5:256:ASN:HB2	1.94	0.50
4:C5:100:ASN:HB3	4:C5:103:LYS:HG2	1.94	0.50
4:C9:192:LEU:HD21	4:C9:199:VAL:HG11	1.93	0.50
4:D3:187:LEU:HD21	4:D3:408:PHE:HE2	1.76	0.50
3:D6:259:LEU:HD21	3:D6:316:CYS:HB2	1.94	0.50
3:E4:274:PRO:HB2	3:E4:276:ILE:HG12	1.94	0.50
4:E5:113:ILE:HA	4:E5:116:VAL:HG12	1.94	0.50
7:s:110:ILE:HD11	7:s:199:TRP:CZ3	2.47	0.50
4:A5:231:ALA:HB2	5:P:283:LEU:HD11	1.94	0.50
3:B0:137:MET:HB3	3:B0:168:ASN:HD22	1.77	0.50
3:B0:240:ALA:HA	3:B0:243:ARG:HG3	1.93	0.50
4:B3:8:GLN:HB2	4:B3:65:LEU:HA	1.94	0.50
3:B4:259:LEU:HD11	3:B4:316:CYS:HB2	1.92	0.50
3:B6:335:ILE:HD12	3:B6:338:LYS:HE3	1.92	0.50
3:C2:370:LYS:HD3	8:l:161:PHE:CE2	2.46	0.50
4:C9:117:LEU:HD13	4:C9:121:ARG:HH22	1.77	0.50
4:D1:77:ARG:HH22	4:D1:92:PHE:HZ	1.60	0.50
3:D2:398:MET:HE2	4:D3:346:PRO:HD2	1.94	0.50
4:D5:171:PRO:HG2	4:D5:185:ALA:HB2	1.94	0.50
3:D8:100:ALA:HA	4:D9:252:LYS:HD2	1.93	0.50
3:E0:377:MET:HE3	3:E0:379:SER:HB3	1.94	0.50
3:E6:187:SER:HB2	3:E6:391:MET:HE2	1.93	0.50
3:E6:268:MET:HE2	3:E6:378:ILE:HG22	1.94	0.50
7:e:99:MET:HE3	7:e:107:LYS:HE2	1.94	0.50
3:A2:181:VAL:HG23	4:A3:350:LYS:HB2	1.94	0.50
3:B0:81:GLY:HA3	2:C:215:TYR:HE2	1.77	0.50
3:C4:191:THR:HB	3:C4:425:LEU:HD21	1.94	0.50
4:C7:5:VAL:HB	4:C7:133:PHE:HD1	1.76	0.50
4:D1:103:LYS:HB3	4:D1:401:GLU:HG3	1.93	0.50
4:D5:65:LEU:HD22	4:D5:90:PHE:HE1	1.75	0.50
4:D7:2:ARG:HD3	4:D7:131:GLN:HG3	1.93	0.50
4:D9:316:MET:HG3	4:D9:352:SER:HB3	1.93	0.50
3:E2:311:LYS:HZ2	3:E2:344:VAL:HA	1.77	0.50
4:E7:117:LEU:HA	4:E7:120:VAL:HG12	1.93	0.50
3:E8:26:LEU:HD21	6:X:124:PRO:HG3	1.93	0.50
3:E8:66:VAL:HG23	3:E8:91:GLN:HB2	1.94	0.50
4:E9:183:TYR:OH	4:E9:388:MET:HB3	2.12	0.50
3:F0:100:ALA:HA	4:F1:252:LYS:HB2	1.94	0.50
7:b:73:VAL:HG13	7:b:173:ILE:HG13	1.94	0.50
7:p:172:VAL:HG23	7:p:180:ALA:HB3	1.94	0.50
7:u:7:ALA:HB1	7:u:159:TYR:HD2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:u:73:VAL:HG23	7:u:109:GLU:HG3	1.94	0.50
3:B4:53:PHE:HB3	3:B4:61:HIS:HB3	1.94	0.49
3:C2:313:MET:HB3	3:C2:380:ASN:HB3	1.93	0.49
4:C7:229:VAL:HG12	4:C7:233:MET:HE3	1.93	0.49
3:E0:132:LEU:HB3	3:E0:164:LYS:HZ1	1.76	0.49
7:e:5:VAL:HG23	7:e:8:SER:HB3	1.94	0.49
7:h:149:ARG:NH1	7:h:161:TYR:HB3	2.27	0.49
7:j:115:LEU:HD21	7:j:145:LYS:HD3	1.94	0.49
4:B3:382:SER:HB2	4:B3:415:MET:HE1	1.94	0.49
4:C1:139:LEU:HD12	4:C1:185:ALA:HA	1.95	0.49
4:C3:244:GLY:HA3	4:C3:354:CYS:HA	1.94	0.49
4:C9:7:VAL:HB	4:C9:135:ILE:HG13	1.94	0.49
4:D5:256:ASN:HB2	4:D5:350:LYS:HE2	1.94	0.49
3:D6:53:PHE:HB3	3:D6:61:HIS:HB3	1.93	0.49
3:D6:265:ILE:HG22	3:D6:380:ASN:HD21	1.77	0.49
3:E2:4:VAL:HG12	3:E2:51:THR:O	2.11	0.49
3:E2:259:LEU:HD21	3:E2:316:CYS:HB2	1.93	0.49
4:E5:86:ARG:HD3	4:E5:88:ASP:HB3	1.94	0.49
4:E5:337:ASN:HB3	4:E5:340:TYR:HB2	1.94	0.49
7:b:134:ILE:HG23	7:b:138:ASN:HD21	1.76	0.49
7:e:99:MET:HE1	7:e:201:TRP:CE2	2.47	0.49
7:m:14:LYS:HB2	7:m:47:LEU:HD22	1.94	0.49
3:A8:221:ARG:HA	4:A9:324:LYS:NZ	2.27	0.49
4:A9:28:HIS:HD2	4:A9:47:ILE:HD13	1.77	0.49
4:A9:57:GLY:HA3	7:c:83:PRO:HB2	1.94	0.49
4:B1:2:ARG:HB2	4:B1:131:GLN:HB2	1.94	0.49
4:B1:49:VAL:HG21	4:B1:241:ARG:HG2	1.94	0.49
3:B4:30:ILE:HG22	3:B4:36:MET:HB3	1.94	0.49
3:C0:313:MET:HB3	3:C0:380:ASN:HB3	1.94	0.49
3:C2:317:LEU:HD23	3:C2:375:VAL:HG21	1.94	0.49
3:C4:434:GLU:HA	3:C4:437:ILE:HG22	1.93	0.49
3:D2:217:LEU:HB2	3:D2:219:ILE:HG22	1.94	0.49
4:D3:170:PHE:HD2	4:D3:377:MET:HE1	1.77	0.49
4:D5:349:MET:HE1	4:D5:367:PHE:HE1	1.77	0.49
4:D7:27:GLU:HA	4:D7:359:LYS:HD2	1.93	0.49
4:D9:231:ALA:HB2	5:O:546:PHE:CE1	2.47	0.49
3:E8:332:VAL:HA	3:E8:335:ILE:HD12	1.94	0.49
4:A1:11:GLN:HG3	4:A1:72:THR:HG21	1.94	0.49
3:A2:16:ILE:HG12	3:A2:231:ILE:HG21	1.94	0.49
3:A2:222:PRO:HG2	4:A3:324:LYS:HD3	1.94	0.49
3:A4:161:TYR:HB3	3:A4:164:LYS:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B0:338:LYS:HG3	3:B0:341:ILE:HG22	1.95	0.49
4:B3:191:GLN:HE22	4:B3:195:ASN:HD22	1.60	0.49
3:B6:180:ALA:HB3	3:B6:183:GLU:HG2	1.94	0.49
3:B8:269:LEU:HB2	3:B8:384:ILE:HD11	1.94	0.49
4:C9:326:VAL:HG13	4:C9:327:ASP:HB2	1.94	0.49
4:D5:377:MET:HA	4:D5:380:ARG:HG2	1.92	0.49
3:D8:21:TRP:CZ3	3:D8:63:PRO:HB3	2.46	0.49
3:D8:270:SER:H	3:D8:301:MET:HE1	1.78	0.49
7:c:78:ALA:HB3	7:c:112:PHE:HE1	1.77	0.49
7:f:127:ALA:HB1	7:h:157:PRO:HG3	1.94	0.49
7:m:172:VAL:HG23	7:m:180:ALA:HB3	1.95	0.49
7:n:14:LYS:HA	7:n:47:LEU:HD13	1.94	0.49
7:w:11:ASN:HA	7:w:14:LYS:HB2	1.95	0.49
3:A0:56:THR:HA	4:F1:283:ALA:HB2	1.94	0.49
4:C3:165:GLU:HA	4:C3:198:GLU:HG2	1.95	0.49
4:C3:212:PHE:HE1	4:C3:220:PRO:HG3	1.78	0.49
4:C9:205:GLU:HA	4:C9:208:TYR:HD1	1.76	0.49
4:E1:215:LEU:HD21	4:E1:273:LEU:HD22	1.94	0.49
4:E1:330:MET:HA	4:E1:333:VAL:HG12	1.95	0.49
4:F1:314:SER:HA	4:F1:350:LYS:HB2	1.95	0.49
7:b:112:PHE:CD2	7:b:129:MET:HE1	2.47	0.49
4:A7:105:HIS:HE1	4:A7:191:GLN:HE22	1.61	0.49
4:A7:290:THR:HG21	4:A7:329:GLN:HB3	1.95	0.49
3:B0:262:TYR:HB2	3:B0:265:ILE:HD12	1.95	0.49
3:B2:3:GLU:HA	3:B2:51:THR:HA	1.93	0.49
3:C4:234:VAL:HG23	3:C4:376:CYS:HB3	1.94	0.49
3:C4:276:ILE:HB	3:C4:280:LYS:HB2	1.95	0.49
4:C7:35:THR:HG22	8:l:44:SER:HB3	1.94	0.49
4:E9:139:LEU:HA	4:E9:145:SER:HB2	1.93	0.49
4:E9:253:LEU:HD11	4:E9:368:VAL:HG11	1.94	0.49
3:F0:402:ARG:HB3	3:F0:405:VAL:HG21	1.95	0.49
5:P:229:LYS:HE3	6:V:57:LYS:HG2	1.95	0.49
7:j:126:ARG:HH11	7:j:133:SER:HB3	1.76	0.49
8:l:35:ALA:HA	8:l:133:VAL:HA	1.95	0.49
3:A8:210:TYR:HE1	4:A9:324:LYS:HG2	1.77	0.49
4:B1:253:LEU:HD11	4:B1:368:VAL:HB	1.95	0.49
3:B2:76:ASP:HB2	4:B3:46:ARG:HH22	1.78	0.49
3:B2:363:VAL:HG23	3:B2:366:GLY:HA3	1.94	0.49
4:C5:221:THR:HG23	4:C5:223:GLY:N	2.28	0.49
4:C5:358:PRO:HG2	4:C5:361:LEU:HB2	1.95	0.49
4:D1:189:VAL:HA	4:D1:192:LEU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D6:204:LEU:HD13	3:D6:231:ILE:HD12	1.95	0.49
3:D8:259:LEU:HD21	3:D8:316:CYS:HB2	1.95	0.49
4:D9:330:MET:HE2	4:D9:349:MET:HG3	1.95	0.49
4:E7:6:HIS:CE1	4:E7:8:GLN:HE21	2.30	0.49
7:a:74:ALA:HB2	7:a:199:TRP:HH2	1.77	0.49
7:f:63:ILE:HA	7:h:16:ARG:HH12	1.77	0.49
7:i:76:TYR:HD1	7:i:170:VAL:HG22	1.77	0.49
8:l:34:VAL:HG11	8:l:164:TRP:HE3	1.77	0.49
7:n:172:VAL:HG23	7:n:180:ALA:HB3	1.95	0.49
3:A4:425:LEU:HD13	3:A4:428:LEU:HD21	1.95	0.49
4:A5:333:VAL:HA	4:A5:336:LYS:HG2	1.95	0.49
3:A6:338:LYS:NZ	3:A6:340:THR:H	2.07	0.49
3:A6:398:MET:HE1	4:A7:345:ILE:HG23	1.93	0.49
3:B0:68:LEU:HD11	3:B0:118:SER:HB3	1.93	0.49
3:B0:76:ASP:HB3	4:B1:46:ARG:HH22	1.78	0.49
4:B1:183:TYR:HB3	4:B1:398:TYR:HE2	1.77	0.49
4:B7:166:THR:HG21	4:B7:192:LEU:HD21	1.94	0.49
3:D0:185:TYR:HE2	3:D0:398:MET:HG2	1.78	0.49
3:D4:137:MET:SD	3:D4:154:LEU:HD21	2.53	0.49
4:D5:16:ILE:HG13	4:D5:226:ASN:HA	1.95	0.49
3:E0:207:GLU:HA	3:E0:210:TYR:HD1	1.76	0.49
7:f:25:GLN:HG3	7:f:28:LYS:HE3	1.95	0.49
7:g:15:ARG:HA	7:g:45:MET:HE1	1.94	0.49
7:q:170:VAL:HG23	7:q:183:LEU:HB2	1.94	0.49
7:r:110:ILE:HB	7:r:131:TRP:CG	2.48	0.49
4:A3:68:LEU:HD11	4:A3:147:MET:HE1	1.94	0.49
4:A5:136:THR:HG23	4:A5:167:PHE:HB2	1.94	0.49
4:B5:167:PHE:HE2	4:B5:233:MET:HB2	1.76	0.49
3:C8:79:ARG:HH22	3:C8:94:SER:HB2	1.77	0.49
3:D4:317:LEU:HD23	3:D4:319:TYR:HE1	1.78	0.49
4:E9:316:MET:HA	4:E9:352:SER:HB3	1.94	0.49
4:F1:11:GLN:HA	4:F1:72:THR:HG21	1.94	0.49
7:e:51:PRO:HD2	7:e:140:LEU:HD22	1.95	0.49
7:f:174:GLY:HA3	7:f:178:ARG:HB2	1.94	0.49
7:o:170:VAL:HG23	7:o:183:LEU:HB2	1.95	0.49
4:A3:27:GLU:HG2	4:A3:28:HIS:HD2	1.77	0.49
3:B0:237:SER:HA	3:B0:320:ARG:HD2	1.95	0.49
3:C0:102:ASN:HD21	3:C0:407:TRP:HB3	1.78	0.49
3:C6:221:ARG:HG3	4:C7:325:GLU:HG2	1.94	0.49
3:D2:310:GLY:HA3	3:D2:383:ALA:HB2	1.93	0.49
4:D5:257:LEU:HB3	4:D5:266:PHE:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E9:113:ILE:HG23	4:E9:117:LEU:HD23	1.95	0.49
4:E9:257:LEU:HD11	4:E9:314:SER:HB2	1.95	0.49
4:E9:416:ASN:HA	4:E9:419:VAL:HG12	1.95	0.49
3:F0:310:GLY:HA3	3:F0:383:ALA:HB2	1.94	0.49
7:f:110:ILE:HB	7:f:131:TRP:CG	2.48	0.49
8:l:58:LYS:HZ3	8:l:62:PHE:HB2	1.78	0.49
7:t:99:MET:HE3	7:t:201:TRP:HB3	1.95	0.49
7:t:110:ILE:HD11	7:t:199:TRP:CZ3	2.48	0.49
7:v:170:VAL:HG23	7:v:183:LEU:HB2	1.93	0.49
4:A7:342:VAL:HG12	4:A7:348:ASN:HD21	1.78	0.48
4:B1:16:ILE:HD11	4:B1:229:VAL:HB	1.95	0.48
4:B3:416:ASN:HA	4:B3:419:VAL:HG12	1.94	0.48
4:D5:192:LEU:HD21	4:D5:199:VAL:HG11	1.95	0.48
3:D8:217:LEU:HD11	3:D8:275:ILE:HB	1.94	0.48
4:E3:293:MET:HE2	4:E3:367:PHE:HB3	1.93	0.48
4:E3:309:ARG:H	4:E3:372:THR:HG22	1.77	0.48
3:E4:406:HIS:HA	3:E4:409:VAL:HG12	1.95	0.48
4:E7:97:ALA:HA	4:E7:103:LYS:HE3	1.95	0.48
2:G:208:PRO:HG2	7:j:154:TYR:HB3	1.94	0.48
7:i:97:ARG:NH1	7:i:98:THR:HB	2.28	0.48
7:w:170:VAL:HG13	7:w:183:LEU:HD22	1.94	0.48
4:A7:111:GLU:HG2	4:A7:112:LEU:HD12	1.95	0.48
4:B1:11:GLN:HA	4:B1:72:THR:HG21	1.94	0.48
3:C0:34:GLY:HA3	3:C0:60:LYS:HE3	1.95	0.48
3:C8:262:TYR:HB2	3:C8:265:ILE:HG22	1.95	0.48
4:D1:70:PRO:HA	4:D1:73:MET:HE2	1.94	0.48
3:D4:286:LEU:HD21	3:D4:372:MET:HB2	1.95	0.48
3:F0:115:VAL:HG11	3:F0:152:LEU:HD23	1.94	0.48
7:d:92:LEU:HD13	7:d:196:LEU:HD22	1.95	0.48
7:m:12:VAL:HG12	7:m:15:ARG:HH22	1.76	0.48
7:v:9:PRO:HA	7:v:12:VAL:HG22	1.94	0.48
7:w:7:ALA:HB3	7:w:161:TYR:HE2	1.79	0.48
3:A0:364:PRO:HB2	5:R:242:LEU:HB2	1.95	0.48
3:A8:76:ASP:HA	3:A8:79:ARG:HG3	1.95	0.48
4:A9:47:ILE:HG22	4:A9:51:TYR:HB2	1.94	0.48
3:C6:222:PRO:HG2	4:C7:324:LYS:HZ1	1.79	0.48
3:D0:154:LEU:HB3	3:D0:197:HIS:HB3	1.95	0.48
4:D3:51:TYR:HB3	4:D3:59:PHE:HB3	1.93	0.48
4:D5:259:PRO:HD2	4:D5:263:LEU:HD11	1.94	0.48
3:E0:7:ILE:HG23	3:E0:137:MET:HE2	1.94	0.48
3:E0:32:PRO:HG3	3:E0:83:TYR:HE1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E0:84:ARG:HH21	7:s:197:LEU:HD11	1.78	0.48
4:E3:134:GLN:HA	4:E3:165:GLU:HB2	1.94	0.48
3:E4:122:ILE:HG21	3:E4:157:LEU:HD21	1.95	0.48
3:E6:141:VAL:HG23	3:E6:170:CYS:HB2	1.95	0.48
3:E8:70:LEU:HD21	3:E8:114:ILE:HG21	1.95	0.48
7:h:181:GLN:HE22	7:h:199:TRP:HA	1.78	0.48
7:i:126:ARG:HH11	7:i:129:MET:HB2	1.76	0.48
7:u:57:ASN:HD22	7:w:16:ARG:HH22	1.61	0.48
1:1:425:VAL:HG22	1:1:429:LYS:HG2	1.96	0.48
4:A1:105:HIS:CE1	4:A1:150:LEU:HD12	2.49	0.48
4:A1:278:SER:HA	4:A5:86:ARG:NH2	2.29	0.48
3:A8:188:VAL:HG23	3:A8:189:LEU:HD12	1.96	0.48
4:B1:274:THR:HG21	4:B1:282:ARG:HG3	1.95	0.48
3:B4:282:TYR:HE2	3:B8:85:HIS:HB3	1.78	0.48
3:B4:284:GLU:HB2	3:B8:88:HIS:HE2	1.78	0.48
3:B6:286:LEU:HB3	3:B6:291:ILE:HD11	1.95	0.48
3:B8:121:ARG:HD2	3:B8:121:ARG:HA	1.70	0.48
3:C0:68:LEU:HD21	3:C0:149:LEU:HD13	1.96	0.48
3:C4:141:VAL:HG11	3:C4:172:TRP:CE3	2.48	0.48
3:C4:311:LYS:NZ	3:C4:344:VAL:HA	2.27	0.48
3:C6:12:ALA:HB3	3:C6:140:ALA:HB2	1.96	0.48
3:D0:80:THR:HG22	2:K:216:ARG:HH22	1.78	0.48
3:D0:318:MET:HB2	3:D0:376:CYS:HB3	1.95	0.48
4:D3:276:ARG:HB2	5:P:522:VAL:HG22	1.95	0.48
3:D4:395:PHE:HD2	3:D4:422:ARG:HD2	1.78	0.48
3:E0:195:LEU:HB3	3:E0:264:ARG:HH12	1.79	0.48
4:E1:49:VAL:HG21	4:E1:241:ARG:HG2	1.94	0.48
4:E5:213:ARG:HH21	4:E5:297:LYS:HD3	1.77	0.48
7:u:7:ALA:HB3	7:u:161:TYR:HE2	1.79	0.48
3:A0:184:PRO:HD2	3:A0:398:MET:HE1	1.96	0.48
4:D3:208:TYR:HE2	4:D3:225:LEU:HD11	1.78	0.48
4:D9:171:PRO:HG2	4:D9:185:ALA:HB2	1.95	0.48
4:E1:227:HIS:HA	4:E1:230:SER:HB3	1.95	0.48
3:F0:195:LEU:HD11	3:F0:428:LEU:HD12	1.96	0.48
7:o:89:LEU:HD11	7:o:129:MET:HE1	1.96	0.48
7:s:53:GLY:HA2	7:s:62:VAL:HG21	1.96	0.48
3:A0:79:ARG:HG3	3:A0:92:LEU:HD22	1.95	0.48
4:A3:53:GLU:HG3	6:U:163:HIS:HA	1.95	0.48
3:B0:274:PRO:HD3	3:B0:291:ILE:HD11	1.95	0.48
4:B1:249:ASP:H	4:B1:252:LYS:HB3	1.77	0.48
3:B2:14:ILE:HD12	3:B2:67:PHE:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B2:407:TRP:CG	4:B3:255:VAL:HG23	2.48	0.48
4:B3:174:LYS:HD2	4:B3:175:VAL:HG23	1.95	0.48
4:B7:42:LEU:HD11	2:G:245:SER:HB2	1.94	0.48
4:B7:155:VAL:HA	4:B7:158:GLU:HG2	1.95	0.48
4:B9:173:PRO:HG3	4:B9:380:ARG:HH11	1.77	0.48
4:C5:7:VAL:HB	4:C5:135:ILE:HG13	1.96	0.48
3:C8:32:PRO:HG2	7:m:102:GLY:HA2	1.93	0.48
2:D:256:LEU:HD11	3:D6:29:GLY:HA2	1.95	0.48
4:D1:105:HIS:CD2	4:D1:150:LEU:HB2	2.48	0.48
3:E6:285:GLN:HE22	3:F0:128:ASN:HD21	1.62	0.48
7:e:165:THR:HG21	7:e:182:PHE:CZ	2.48	0.48
7:f:168:PRO:HG2	7:f:185:ILE:HG21	1.96	0.48
7:q:5:VAL:HG23	7:q:161:TYR:HE1	1.78	0.48
7:s:9:PRO:HG2	7:s:146:ARG:HH11	1.79	0.48
7:x:55:LEU:HD12	7:x:132:LEU:HD23	1.95	0.48
4:A1:113:ILE:HA	4:A1:116:VAL:HG12	1.96	0.48
4:A5:330:MET:HE1	4:A5:351:SER:HB2	1.95	0.48
3:B0:76:ASP:HA	3:B0:79:ARG:HG2	1.95	0.48
3:B4:310:GLY:HA3	3:B4:383:ALA:HB2	1.94	0.48
3:B6:115:VAL:HG23	3:B6:153:LEU:HD22	1.96	0.48
3:B8:267:PHE:HB3	3:B8:384:ILE:HG21	1.95	0.48
3:C0:141:VAL:HG12	3:C0:187:SER:HA	1.96	0.48
4:C1:213:ARG:CZ	4:C1:297:LYS:HG3	2.44	0.48
4:C3:190:HIS:HB2	4:C3:414:ASN:HD21	1.78	0.48
4:C5:326:VAL:O	4:C5:330:MET:HG2	2.14	0.48
3:D0:3:GLU:HA	3:D0:51:THR:HA	1.96	0.48
3:E2:60:LYS:HD2	3:E2:60:LYS:HA	1.58	0.48
4:E9:158:GLU:HG3	4:E9:159:TYR:CD1	2.49	0.48
7:d:78:ALA:HB3	7:d:112:PHE:HE1	1.79	0.48
7:i:49:LEU:HD21	7:i:177:GLY:HA2	1.96	0.48
7:o:56:LYS:HD2	7:o:62:VAL:HG22	1.96	0.48
4:A1:135:ILE:HB	4:A1:166:THR:HG22	1.96	0.48
4:A1:217:LEU:HD11	5:R:227:LEU:HD21	1.96	0.48
3:A2:259:LEU:HD23	3:A2:268:MET:HG3	1.96	0.48
4:A3:113:ILE:HG13	4:A3:150:LEU:HD22	1.94	0.48
3:B0:242:LEU:HD11	3:B0:252:VAL:HG23	1.96	0.48
3:B2:268:MET:HE1	3:B2:380:ASN:ND2	2.29	0.48
4:B3:171:PRO:HB3	4:B3:181:GLU:HG2	1.96	0.48
4:B5:330:MET:HB3	4:B5:349:MET:HG3	1.94	0.48
4:B9:337:ASN:HD22	4:B9:340:TYR:HD2	1.62	0.48
3:C0:175:PRO:HD3	3:C0:390:ARG:NE	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D2:319:TYR:HD1	3:D2:323:VAL:HG11	1.79	0.48
3:D8:189:LEU:HD11	3:D8:418:PHE:HE2	1.78	0.48
3:D8:287:SER:O	3:D8:291:ILE:HG12	2.13	0.48
3:E0:269:LEU:HD11	3:E0:301:MET:HB3	1.94	0.48
7:d:55:LEU:HD12	7:d:132:LEU:HD23	1.95	0.48
4:A1:21:TRP:HA	4:A1:24:ILE:HG22	1.95	0.48
3:A2:91:GLN:HG3	3:A2:121:ARG:HH22	1.78	0.48
3:A4:82:THR:HA	7:a:98:THR:HG23	1.95	0.48
4:A9:333:VAL:HA	4:A9:336:LYS:HZ3	1.79	0.48
3:B2:267:PHE:HE2	3:B2:428:LEU:HD21	1.79	0.48
3:B2:422:ARG:HH12	3:B2:425:LEU:HD23	1.79	0.48
4:C1:321:MET:HE1	4:C1:326:VAL:HG23	1.95	0.48
4:C3:44:LEU:HD12	7:j:90:PRO:HG2	1.95	0.48
3:C4:274:PRO:HG2	3:C4:371:VAL:HG11	1.95	0.48
3:D8:4:VAL:HG12	3:D8:51:THR:HB	1.96	0.48
3:E8:48:ALA:HB1	3:E8:244:PHE:HE1	1.77	0.48
4:E9:320:ARG:HH22	6:X:114:THR:HG22	1.79	0.48
5:O:277:ASP:OD2	5:O:278:GLN:HG3	2.14	0.48
6:W:76:LYS:HD2	7:a:163:SER:H	1.79	0.48
6:X:117:THR:O	6:X:121:TYR:HB2	2.12	0.48
7:a:96:TYR:HA	7:a:108:ILE:HD11	1.96	0.48
7:a:151:MET:HE3	7:a:159:TYR:HE1	1.78	0.48
7:s:99:MET:HG3	7:s:107:LYS:HD2	1.95	0.48
7:u:88:LEU:HD22	7:u:185:ILE:HG21	1.95	0.48
4:A1:149:THR:HG21	4:A1:188:SER:HB2	1.96	0.48
4:B3:27:GLU:HA	4:B3:359:LYS:HD2	1.96	0.48
3:B6:88:HIS:HB3	3:B6:91:GLN:HG3	1.96	0.48
3:C2:332:VAL:HA	3:C2:335:ILE:HG22	1.95	0.48
4:C9:162:ARG:HA	4:C9:162:ARG:HD2	1.63	0.48
4:D3:237:THR:HG23	4:D3:241:ARG:HE	1.78	0.48
4:D3:376:GLU:HB3	4:D3:380:ARG:HH21	1.77	0.48
4:D5:169:VAL:HG12	4:D5:202:ILE:HB	1.95	0.48
3:D8:274:PRO:HG2	3:D8:371:VAL:HG21	1.96	0.48
4:E5:2:ARG:HD3	4:E5:131:GLN:HG3	1.96	0.48
3:E6:239:THR:HG23	3:E6:243:ARG:HE	1.78	0.48
4:E7:49:VAL:HG11	4:E7:241:ARG:HG2	1.96	0.48
3:E8:194:LEU:HB2	3:E8:198:THR:HG23	1.95	0.48
4:E9:178:THR:HA	3:F0:352:LYS:HE2	1.96	0.48
2:F:254:LYS:HD2	2:F:255:PRO:HD2	1.95	0.48
6:W:47:ASN:HB2	7:a:117:ARG:HH21	1.79	0.48
6:W:132:LYS:HA	6:W:136:GLN:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:64:PRO:HD2	7:a:67:HIS:CE1	2.49	0.48
7:t:14:LYS:HZ3	7:t:47:LEU:HD22	1.78	0.48
3:A4:288:VAL:HA	3:A4:291:ILE:HG12	1.94	0.47
4:B1:103:LYS:HB3	4:B1:401:GLU:HG2	1.95	0.47
4:B5:135:ILE:HD11	4:B5:164:MET:HE3	1.95	0.47
4:B5:324:LYS:HA	4:B5:327:ASP:HB2	1.96	0.47
3:C0:254:GLU:HA	3:C0:257:THR:HG22	1.96	0.47
4:C5:281:TYR:CD1	4:C9:58:ARG:HD3	2.49	0.47
4:D1:91:VAL:HG21	4:D1:116:VAL:HG22	1.96	0.47
3:D6:188:VAL:HG23	3:D6:425:LEU:HD22	1.95	0.47
3:D8:318:MET:HE3	3:D8:376:CYS:SG	2.54	0.47
4:E3:132:GLY:HA3	4:E3:163:ILE:HG22	1.95	0.47
7:h:114:SER:HB3	7:h:136:LEU:HD21	1.96	0.47
3:A4:88:HIS:HB3	3:A4:91:GLN:HG2	1.95	0.47
4:A5:64:ILE:HD12	4:A5:119:VAL:HG13	1.96	0.47
3:A8:153:LEU:HG	3:A8:157:LEU:HD13	1.96	0.47
3:A8:221:ARG:HD2	7:e:189:LEU:O	2.14	0.47
4:C1:167:PHE:CE2	4:C1:233:MET:HG3	2.49	0.47
4:C3:323:THR:HG22	4:C3:353:VAL:HG21	1.96	0.47
4:C5:68:LEU:HA	4:C5:93:GLY:HA3	1.96	0.47
3:C8:168:ASN:HD21	3:C8:194:LEU:HD11	1.77	0.47
3:D6:133:GLN:HB3	3:D6:252:VAL:HG11	1.96	0.47
3:E8:25:CYS:HB2	3:E8:30:ILE:HG13	1.95	0.47
4:E9:210:ILE:HG21	4:E9:228:LEU:HD21	1.95	0.47
3:F0:209:ILE:HG12	3:F0:302:MET:HB3	1.95	0.47
7:i:152:LYS:HZ2	7:i:153:GLU:HB2	1.79	0.47
7:q:140:LEU:HA	7:q:143:ILE:HG22	1.96	0.47
7:t:164:ARG:HH22	7:t:182:PHE:HB2	1.79	0.47
3:A4:179:THR:HG23	4:A5:351:SER:HB3	1.95	0.47
3:B4:208:ALA:HB2	3:B4:304:LYS:HG2	1.95	0.47
3:B6:31:GLN:HB3	2:G:256:LEU:HD21	1.95	0.47
3:B8:176:GLN:HA	3:B8:176:GLN:NE2	2.29	0.47
3:C0:142:GLY:HA3	3:C0:183:GLU:OE1	2.14	0.47
4:C1:398:TYR:HB3	4:C1:403:MET:HG3	1.97	0.47
4:C5:64:ILE:HD13	4:C5:89:ASN:HB3	1.96	0.47
3:D4:140:ALA:HA	3:D4:171:SER:HB3	1.95	0.47
4:E1:57:GLY:HA3	7:s:83:PRO:HB2	1.96	0.47
5:R:487:THR:HB	5:R:489:LEU:HD23	1.96	0.47
7:h:151:MET:HE1	7:h:156:VAL:HG22	1.96	0.47
7:t:183:LEU:HD23	7:t:196:LEU:HD12	1.96	0.47
7:w:42:TYR:HA	7:w:45:MET:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A1:49:VAL:HG11	4:A1:241:ARG:HG2	1.95	0.47
4:A1:388:MET:HE1	3:A2:347:CYS:HA	1.96	0.47
3:A2:221:ARG:HH22	4:A3:322:SER:HB3	1.79	0.47
4:A5:334:GLN:HG3	4:A5:349:MET:HE1	1.96	0.47
3:A6:223:THR:HG23	3:A6:225:THR:H	1.78	0.47
3:A8:11:GLN:HB2	3:A8:74:VAL:HG21	1.96	0.47
3:A8:152:LEU:HA	3:A8:155:GLU:HG2	1.95	0.47
4:B1:317:PHE:HD2	4:B1:321:MET:HE1	1.78	0.47
3:B2:388:PHE:HB3	3:B2:425:LEU:HD11	1.97	0.47
3:C4:221:ARG:NH2	7:m:189:LEU:HB3	2.29	0.47
4:C7:337:ASN:HB3	4:C7:340:TYR:HB2	1.96	0.47
3:D8:21:TRP:CH2	3:D8:65:CYS:HB3	2.50	0.47
4:D9:281:TYR:HB3	4:E3:86:ARG:HG2	1.96	0.47
3:E2:28:HIS:CE1	3:E2:243:ARG:HH11	2.33	0.47
3:E4:105:ARG:HE	4:E5:251:ARG:NH2	2.11	0.47
7:f:185:ILE:HD13	7:f:195:ALA:HB3	1.96	0.47
7:g:17:LEU:HA	7:g:20:GLU:HG2	1.97	0.47
7:g:48:ILE:HD11	7:g:65:GLN:HG2	1.96	0.47
7:o:50:PHE:HB2	7:o:65:GLN:HB2	1.95	0.47
1:2:434:ARG:HH21	1:2:462:LEU:HB3	1.79	0.47
3:A0:67:PHE:HB2	3:A0:92:LEU:HG	1.95	0.47
4:A1:113:ILE:HG13	4:A1:150:LEU:HD22	1.97	0.47
4:A3:183:TYR:HA	4:A3:385:PHE:HE2	1.79	0.47
4:A7:276:ARG:HD2	5:O:282:ARG:NH2	2.30	0.47
4:B5:51:TYR:HB3	4:B5:59:PHE:HB3	1.97	0.47
3:C0:29:GLY:HA2	2:I:256:LEU:HD12	1.97	0.47
3:D8:11:GLN:HG3	3:D8:74:VAL:HG21	1.96	0.47
4:E1:2:ARG:HG3	4:E1:49:VAL:HG12	1.96	0.47
4:E1:208:TYR:HE1	3:E2:329:ASN:HD22	1.62	0.47
4:E1:248:SER:HB2	4:E1:252:LYS:HG2	1.97	0.47
4:E7:16:ILE:HD12	4:E7:229:VAL:HG11	1.96	0.47
5:R:287:LEU:HD12	5:R:288:PRO:HD2	1.97	0.47
6:W:71:LEU:HD11	7:a:160:GLY:H	1.79	0.47
7:e:9:PRO:HA	7:e:12:VAL:HG12	1.97	0.47
7:e:55:LEU:HB3	7:e:132:LEU:HD23	1.96	0.47
7:j:42:TYR:HA	7:j:45:MET:HG2	1.96	0.47
7:s:14:LYS:HZ2	7:s:47:LEU:HD22	1.79	0.47
7:s:42:TYR:HA	7:s:45:MET:HE3	1.96	0.47
7:t:15:ARG:O	7:t:19:GLU:HG3	2.14	0.47
7:u:63:ILE:HD11	7:u:67:HIS:CD2	2.49	0.47
3:A2:91:GLN:HG3	3:A2:121:ARG:NH2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A3:361:LEU:HD21	5:P:228:LEU:HD23	1.96	0.47
3:A6:119:LEU:HA	3:A6:122:ILE:HD12	1.96	0.47
4:A9:316:MET:HB2	4:A9:366:THR:HG22	1.95	0.47
4:B5:5:VAL:HG23	4:B5:130:LEU:HD11	1.96	0.47
4:C1:268:ILE:HG22	4:C1:300:MET:HE3	1.96	0.47
3:C2:181:VAL:N	4:C3:350:LYS:HZ3	2.07	0.47
4:D5:36:TYR:HB3	7:p:86:ALA:HB1	1.96	0.47
3:E2:394:LYS:HB2	4:E3:346:PRO:HG3	1.97	0.47
7:f:50:PHE:HB2	7:f:65:GLN:HB3	1.96	0.47
7:n:14:LYS:HB2	7:n:47:LEU:HD22	1.95	0.47
7:t:196:LEU:C	7:t:198:ARG:H	2.21	0.47
7:w:149:ARG:HH11	7:w:164:ARG:HB2	1.79	0.47
4:A1:337:ASN:HB3	4:A1:340:TYR:HB2	1.95	0.47
4:A3:24:ILE:HA	4:A3:27:GLU:HB3	1.97	0.47
3:A8:5:ILE:HD12	3:A8:125:LEU:HG	1.96	0.47
4:A9:331:LEU:HA	4:A9:334:GLN:HB2	1.97	0.47
4:B3:99:ASN:HD21	3:B4:258:ASN:HD21	1.61	0.47
3:B4:169:PHE:HZ	3:B4:238:LEU:HD13	1.79	0.47
3:B6:17:GLY:HA2	3:B6:20:CYS:HB3	1.95	0.47
3:B8:316:CYS:HB3	3:B8:378:ILE:HB	1.97	0.47
4:C3:375:GLN:HG3	4:C3:419:VAL:HG13	1.96	0.47
3:C4:364:PRO:HD2	2:J:254:LYS:HE3	1.96	0.47
3:C6:282:TYR:HA	7:n:202:ARG:HH22	1.79	0.47
4:C7:237:THR:HG22	4:C7:250:LEU:HD11	1.96	0.47
4:C7:286:VAL:HA	4:C7:289:LEU:HG	1.96	0.47
3:C8:220:GLU:C	3:C8:222:PRO:HD3	2.40	0.47
3:D0:364:PRO:HD2	2:K:222:LYS:HE3	1.97	0.47
4:D1:86:ARG:HB3	4:D1:89:ASN:HB2	1.97	0.47
4:D3:349:MET:HE2	4:D3:349:MET:HB2	1.63	0.47
3:D4:75:VAL:HG11	3:D4:94:SER:HB2	1.96	0.47
4:D9:374:ILE:HB	4:D9:422:TYR:HE2	1.79	0.47
4:E1:311:LEU:HD23	4:E1:312:THR:HG23	1.97	0.47
4:E3:257:LEU:HD21	4:E3:314:SER:HB2	1.95	0.47
3:E8:108:TYR:CG	3:E8:413:MET:HE1	2.50	0.47
3:E8:147:SER:HB2	3:E8:190:SER:HB3	1.96	0.47
4:F1:276:ARG:H	6:V:174:ARG:NH1	2.13	0.47
5:P:543:GLN:HE22	5:P:549:SER:HA	1.79	0.47
7:c:146:ARG:HD2	7:c:159:TYR:HE2	1.79	0.47
7:f:75:LEU:HD12	7:f:148:PHE:HE2	1.80	0.47
7:i:139:PRO:O	7:i:143:ILE:HG12	2.15	0.47
7:s:183:LEU:HD21	7:s:199:TRP:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A5:7:VAL:HG11	4:A5:151:LEU:HD21	1.97	0.47
3:B0:313:MET:HE3	3:B0:380:ASN:HB3	1.97	0.47
4:B1:135:ILE:HB	4:B1:166:THR:HG22	1.97	0.47
4:C9:86:ARG:HD2	4:C9:86:ARG:HA	1.56	0.47
4:D3:61:PRO:HD3	4:D3:84:LEU:HG	1.97	0.47
3:D8:9:VAL:HG12	3:D8:68:LEU:HB2	1.97	0.47
4:E5:138:SER:HA	4:E5:169:VAL:HG22	1.96	0.47
3:F0:298:PRO:HB3	3:F0:307:PRO:HD2	1.96	0.47
3:B4:318:MET:HB2	3:B4:376:CYS:HB3	1.96	0.47
3:B6:397:LEU:HD23	4:B7:346:PRO:HD3	1.97	0.47
4:C1:350:LYS:HA	4:C1:350:LYS:HE3	1.96	0.47
4:C3:399:THR:HA	4:C3:403:MET:HB2	1.97	0.47
4:C5:295:ASP:HB3	4:C5:298:ASN:HB2	1.97	0.47
3:D4:53:PHE:HB3	3:D4:61:HIS:HB3	1.97	0.47
4:D5:163:ILE:HD13	4:D5:251:ARG:HG2	1.95	0.47
4:D7:376:GLU:HA	4:D7:379:LYS:HG2	1.96	0.47
3:E0:88:HIS:HB3	3:E0:91:GLN:HB2	1.97	0.47
3:E0:398:MET:HE1	4:E1:345:ILE:HD13	1.96	0.47
4:E1:377:MET:HA	4:E1:380:ARG:HG2	1.96	0.47
7:d:7:ALA:HB3	7:d:161:TYR:HE2	1.78	0.47
7:q:2:SER:N	7:q:11:ASN:HD21	2.13	0.47
7:s:180:ALA:HB1	7:s:204:THR:HG22	1.95	0.47
1:1:450:GLN:O	1:1:454:GLU:HB2	2.15	0.47
4:A5:206:ALA:HB2	4:A5:302:ALA:HB2	1.97	0.47
3:A8:2:ARG:HG2	3:A8:51:THR:HG22	1.97	0.47
3:A8:35:GLN:HG3	3:A8:60:LYS:HB2	1.97	0.47
3:A8:76:ASP:HB3	3:A8:79:ARG:HH21	1.79	0.47
4:A9:331:LEU:HD21	4:A9:347:ASN:HD21	1.80	0.47
3:B4:174:SER:HB3	3:B4:205:ASP:HB3	1.95	0.47
3:B6:12:ALA:HB3	3:B6:140:ALA:HB2	1.97	0.47
3:C8:70:LEU:HD12	3:C8:145:THR:HG22	1.97	0.47
4:D1:66:MET:HG2	4:D1:147:MET:HE1	1.97	0.47
4:D5:20:PHE:HA	4:D5:23:VAL:HG12	1.97	0.47
4:D5:227:HIS:CD2	5:O:520:LEU:HD21	2.50	0.47
3:D6:124:LYS:HD2	3:D6:124:LYS:HA	1.71	0.47
3:D8:12:ALA:HB3	3:D8:140:ALA:HB2	1.97	0.47
3:E2:76:ASP:HA	3:E2:79:ARG:HD2	1.96	0.47
3:F0:112:LYS:HA	3:F0:115:VAL:HG22	1.97	0.47
7:a:66:SER:HA	7:a:69:LYS:HE2	1.96	0.47
7:d:68:LEU:HA	7:d:71:LYS:HE3	1.97	0.47
7:g:99:MET:HE1	7:g:201:TRP:CD1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:m:75:LEU:HD13	7:m:111:ILE:HG23	1.97	0.47
7:r:201:TRP:CD1	7:r:201:TRP:H	2.33	0.47
7:x:75:LEU:HD13	7:x:111:ILE:HG23	1.97	0.47
4:A1:117:LEU:HA	4:A1:120:VAL:HG12	1.95	0.46
4:A3:275:SER:O	4:A3:279:GLN:HG3	2.15	0.46
4:A7:227:HIS:CE1	5:O:280:ALA:HA	2.50	0.46
4:B1:256:ASN:HD22	4:B1:350:LYS:HD2	1.80	0.46
3:B2:229:ARG:HH12	2:E:251:TYR:HE1	1.63	0.46
4:B7:51:TYR:HB3	4:B7:59:PHE:HB3	1.97	0.46
3:C0:84:ARG:HD3	7:i:98:THR:HG21	1.97	0.46
4:C3:117:LEU:HA	4:C3:120:VAL:HG12	1.97	0.46
3:C4:237:SER:HB2	3:C4:376:CYS:SG	2.54	0.46
4:C7:68:LEU:HD21	4:C7:147:MET:HE3	1.97	0.46
4:C7:178:THR:HG21	11:C7:501:GDP:H5'	1.97	0.46
3:E2:59:GLY:O	3:E2:61:HIS:N	2.48	0.46
4:E5:4:ILE:HG13	4:E5:131:GLN:HB3	1.97	0.46
4:E5:397:TRP:CZ3	3:E6:257:THR:HG22	2.51	0.46
4:E7:139:LEU:HA	4:E7:145:SER:HB2	1.96	0.46
3:F0:119:LEU:HD22	3:F0:156:ARG:HD3	1.97	0.46
3:A0:189:LEU:HD21	3:A0:418:PHE:CD1	2.49	0.46
4:A1:281:TYR:HB2	4:A5:86:ARG:CZ	2.46	0.46
4:A5:91:VAL:HG11	4:A5:116:VAL:HG22	1.97	0.46
3:A6:219:ILE:HD12	3:A6:222:PRO:HG3	1.98	0.46
3:B0:280:LYS:HG2	3:B4:88:HIS:CE1	2.50	0.46
4:B1:320:ARG:HH11	2:C:212:GLU:HG3	1.80	0.46
3:B2:280:LYS:HG2	3:B6:89:PRO:HG2	1.98	0.46
4:B3:13:GLY:HA2	4:B3:16:ILE:HG22	1.96	0.46
3:C0:403:ALA:HB1	4:C1:259:PRO:HB3	1.96	0.46
3:C6:141:VAL:HA	3:C6:147:SER:HB2	1.98	0.46
3:C8:36:MET:HE1	3:C8:61:HIS:NE2	2.30	0.46
3:D0:297:GLU:HG3	3:D0:299:ALA:H	1.79	0.46
4:D1:324:LYS:HE2	4:D1:324:LYS:H	1.80	0.46
3:D2:209:ILE:HG12	3:D2:302:MET:HB2	1.96	0.46
4:D7:267:LEU:HD23	4:D7:301:CYS:HB3	1.97	0.46
3:D8:29:GLY:HA3	3:D8:36:MET:HE1	1.96	0.46
4:D9:187:LEU:HA	4:D9:190:HIS:CE1	2.50	0.46
3:E2:28:HIS:NE2	3:E2:243:ARG:HD2	2.29	0.46
4:E3:198:GLU:HA	4:E3:264:HIS:HB2	1.97	0.46
4:E7:152:ILE:HG12	4:E7:164:MET:HE2	1.95	0.46
3:F0:328:VAL:HG21	3:F0:355:ILE:HD11	1.98	0.46
7:c:140:LEU:HD23	7:c:143:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:e:185:ILE:HD13	7:e:195:ALA:HB3	1.96	0.46
7:f:170:VAL:HG23	7:f:183:LEU:HB2	1.97	0.46
7:s:205:LYS:HE3	7:s:205:LYS:HB3	1.76	0.46
3:A2:298:PRO:HG3	3:A2:307:PRO:HD2	1.98	0.46
3:A6:100:ALA:HA	4:A7:252:LYS:HD2	1.97	0.46
3:A6:192:HIS:HD2	3:A6:421:ALA:HA	1.81	0.46
4:A9:269:GLY:HA3	4:A9:293:MET:HE1	1.96	0.46
4:A9:313:ALA:HB3	4:A9:349:MET:HB3	1.97	0.46
3:C2:119:LEU:HD12	3:C2:156:ARG:HH12	1.80	0.46
3:C8:207:GLU:HA	3:C8:210:TYR:HB2	1.95	0.46
3:D0:115:VAL:HG21	3:D0:152:LEU:HD23	1.95	0.46
4:D9:207:LEU:HD21	4:D9:229:VAL:HG23	1.98	0.46
4:E3:253:LEU:HD21	4:E3:368:VAL:HG21	1.98	0.46
7:f:79:ASP:HB3	7:f:82:ASP:HB3	1.97	0.46
7:m:21:ARG:HA	7:m:24:MET:HE2	1.96	0.46
4:B3:28:HIS:HA	4:B3:43:GLN:HG2	1.96	0.46
4:C7:7:VAL:HB	4:C7:135:ILE:HG12	1.98	0.46
4:C7:167:PHE:CE2	4:C7:233:MET:HG2	2.51	0.46
4:C9:230:SER:HA	4:C9:233:MET:HE2	1.97	0.46
4:D3:290:THR:HG21	4:D3:329:GLN:HB3	1.97	0.46
4:D7:51:TYR:HB3	4:D7:59:PHE:HB3	1.97	0.46
4:D7:282:ARG:HH22	4:E1:86:ARG:NH2	2.13	0.46
4:D9:183:TYR:HE2	4:D9:388:MET:HE2	1.81	0.46
4:D9:257:LEU:HD21	4:D9:314:SER:HB2	1.97	0.46
3:E0:223:THR:HG23	3:E0:225:THR:HG22	1.98	0.46
4:E5:25:SER:HB2	4:E5:30:ILE:HB	1.98	0.46
4:E5:156:ARG:HA	4:E5:156:ARG:HD2	1.82	0.46
7:m:5:VAL:HG21	7:m:146:ARG:HH21	1.80	0.46
7:q:51:PRO:HD2	7:q:140:LEU:HD22	1.97	0.46
1:1:417:LEU:HB2	1:1:420:TRP:CD1	2.50	0.46
4:A3:77:ARG:HH22	4:A3:92:PHE:HZ	1.63	0.46
4:A9:102:ALA:HB2	4:A9:403:MET:HE2	1.97	0.46
3:B6:265:ILE:HG23	3:B6:432:TYR:CZ	2.50	0.46
4:C5:2:ARG:HB2	4:C5:131:GLN:HB2	1.98	0.46
4:C7:415:MET:HE3	4:C7:415:MET:HB3	1.74	0.46
4:C9:237:THR:HG23	4:C9:241:ARG:HH12	1.81	0.46
3:D6:207:GLU:HA	3:D6:210:TYR:HD1	1.80	0.46
3:E0:76:ASP:HA	3:E0:79:ARG:HD2	1.98	0.46
3:E4:214:ARG:HH21	3:E4:215:ARG:HB3	1.81	0.46
4:E9:205:GLU:HA	4:E9:208:TYR:HD2	1.81	0.46
7:c:75:LEU:HD23	7:c:111:ILE:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:5:VAL:HG23	7:g:8:SER:HB3	1.98	0.46
7:i:65:GLN:HA	7:i:68:LEU:HD13	1.98	0.46
7:u:74:ALA:HA	7:u:172:VAL:HA	1.97	0.46
7:v:55:LEU:HD23	7:v:134:ILE:HD11	1.96	0.46
3:A0:103:PHE:CD2	3:A0:148:GLY:HA2	2.46	0.46
3:A4:306:ASP:HB3	3:A4:309:HIS:CE1	2.50	0.46
4:A5:68:LEU:HA	4:A5:93:GLY:HA3	1.97	0.46
4:A5:193:VAL:HG11	4:A5:418:LEU:HD11	1.97	0.46
4:A9:44:LEU:HD11	7:c:87:SER:HA	1.97	0.46
3:B0:276:ILE:HG23	3:B0:280:LYS:HB2	1.97	0.46
4:B1:147:MET:HE3	4:B1:147:MET:HB3	1.77	0.46
3:B8:4:VAL:HG12	3:B8:133:GLN:HB3	1.97	0.46
4:C3:294:PHE:HE2	4:C3:333:VAL:HG21	1.80	0.46
4:C5:221:THR:HA	5:P:458:ARG:NH1	2.30	0.46
4:D3:154:LYS:O	4:D3:157:GLU:HG3	2.15	0.46
4:D5:236:VAL:HG13	4:D5:237:THR:HG23	1.98	0.46
3:D6:72:PRO:HD2	4:D7:2:ARG:HH21	1.79	0.46
4:D7:10:GLY:HA2	4:D7:143:THR:HG23	1.97	0.46
4:D9:313:ALA:HB3	4:D9:349:MET:HB3	1.98	0.46
3:E0:298:PRO:HA	3:E0:301:MET:HE3	1.97	0.46
3:E8:234:VAL:HG22	3:E8:272:TYR:HB2	1.97	0.46
6:W:76:LYS:HG2	7:a:162:GLY:HA3	1.97	0.46
7:b:95:TYR:CD2	7:b:196:LEU:HB3	2.51	0.46
7:c:53:GLY:HA2	7:c:62:VAL:HG21	1.97	0.46
8:l:77:ASP:HB3	8:l:82:ASP:HB3	1.97	0.46
1:l:429:LYS:HE3	1:l:432:GLN:HE22	1.80	0.46
4:A1:203:ASP:HB2	4:A1:301:CYS:HA	1.98	0.46
4:A5:309:ARG:H	4:A5:372:THR:HG22	1.81	0.46
4:A9:46:ARG:HA	4:A9:46:ARG:HD3	1.71	0.46
4:B3:91:VAL:HG21	4:B3:116:VAL:HG22	1.97	0.46
3:B4:80:THR:HB	7:f:94:ASN:HD21	1.80	0.46
4:B5:283:ALA:HA	4:B9:55:THR:HG22	1.98	0.46
4:C3:68:LEU:HB3	4:C3:96:GLY:HA2	1.97	0.46
4:C9:219:THR:HA	3:D0:326:LYS:HZ3	1.81	0.46
2:D:247:TYR:HE1	3:D6:81:GLY:HA3	1.80	0.46
2:D:255:PRO:HG2	3:D6:364:PRO:HG2	1.96	0.46
4:E3:315:ALA:HB2	4:E3:367:PHE:HD1	1.81	0.46
4:E3:330:MET:HB3	4:E3:349:MET:HG2	1.98	0.46
7:d:149:ARG:HH12	7:d:162:GLY:C	2.24	0.46
7:h:64:PRO:HD2	7:h:67:HIS:CE1	2.51	0.46
7:h:175:SER:HA	7:h:206:PHE:HE2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:l:35:ALA:HB2	8:l:133:VAL:HG12	1.98	0.46
7:t:18:ASN:HD21	7:t:46:ASP:H	1.64	0.46
7:u:56:LYS:NZ	7:u:60:ASN:HA	2.30	0.46
2:A:213:SER:HB3	2:A:216:ARG:HG3	1.97	0.46
3:A4:105:ARG:HA	3:A4:109:THR:HG22	1.97	0.46
4:A9:392:LYS:HD3	4:A9:395:LEU:HD11	1.98	0.46
3:B0:395:PHE:HD2	3:B0:422:ARG:HD3	1.80	0.46
3:C6:316:CYS:HA	3:C6:352:LYS:HB2	1.97	0.46
4:D3:5:VAL:HG23	4:D3:130:LEU:HD11	1.97	0.46
4:D3:259:PRO:HG3	4:D3:311:LEU:HD21	1.98	0.46
3:D6:329:ASN:HA	3:D6:332:VAL:HG12	1.97	0.46
4:D7:165:GLU:HG3	4:D7:250:LEU:HD22	1.98	0.46
4:E5:272:PRO:HD3	4:E5:364:SER:HA	1.97	0.46
4:E5:388:MET:HE1	3:E6:348:PRO:HD2	1.98	0.46
7:f:97:ARG:HH21	7:h:5:VAL:HG13	1.80	0.46
3:A2:221:ARG:HA	4:A3:324:LYS:HZ1	1.81	0.46
4:A3:4:ILE:HB	4:A3:50:PHE:HE1	1.81	0.46
3:B0:137:MET:HE3	3:B0:168:ASN:HD22	1.80	0.46
3:B0:403:ALA:HB2	4:B1:344:TRP:HZ3	1.80	0.46
4:B3:6:HIS:CD2	4:B3:134:GLN:HG3	2.51	0.46
4:B3:193:VAL:HG23	4:B3:265:PHE:HE1	1.80	0.46
3:B6:320:ARG:HH21	3:B6:360:PRO:HA	1.81	0.46
4:B7:211:CYS:HB3	4:B7:220:PRO:HG3	1.98	0.46
4:B9:206:ALA:HB2	4:B9:302:ALA:HB2	1.98	0.46
3:C4:231:ILE:O	3:C4:235:ILE:HG12	2.16	0.46
4:D7:7:VAL:HB	4:D7:135:ILE:HD13	1.98	0.46
4:D7:200:GLN:HG2	4:D7:268:ILE:HD11	1.98	0.46
3:E2:311:LYS:NZ	3:E2:344:VAL:HA	2.31	0.46
3:E6:207:GLU:HA	3:E6:210:TYR:CD2	2.51	0.46
4:E9:152:ILE:HG23	4:E9:164:MET:HE3	1.98	0.46
3:F0:105:ARG:HA	3:F0:109:THR:HG22	1.97	0.46
4:F1:259:PRO:HG3	4:F1:311:LEU:HD21	1.97	0.46
4:F1:318:ARG:HG2	4:F1:354:CYS:HB3	1.97	0.46
2:I:215:TYR:O	2:I:219:TYR:HB2	2.16	0.46
7:g:71:LYS:HD3	7:g:109:GLU:HB2	1.97	0.46
7:q:88:LEU:HD22	7:q:185:ILE:HG21	1.98	0.46
7:x:149:ARG:HG2	7:x:163:SER:HA	1.97	0.46
1:l:420:TRP:HE1	1:l:477:VAL:HG11	1.81	0.46
3:A4:310:GLY:HA3	3:A4:383:ALA:HB2	1.97	0.46
4:B5:192:LEU:HD21	4:B5:199:VAL:HG11	1.98	0.46
3:C0:391:MET:HE3	3:C0:391:MET:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C2:3:GLU:HA	3:C2:51:THR:HA	1.98	0.46
3:C2:262:TYR:HE1	3:C2:435:VAL:HG22	1.81	0.46
4:C7:275:SER:HB3	4:C7:278:SER:HB2	1.97	0.46
3:D0:274:PRO:HB2	3:D0:276:ILE:HG23	1.98	0.46
4:D1:289:LEU:HD23	4:D1:363:MET:HE2	1.97	0.46
3:D4:2:ARG:HB2	3:D4:133:GLN:HE22	1.79	0.46
3:D4:191:THR:HA	3:D4:194:LEU:HG	1.98	0.46
3:D4:401:LYS:HZ3	4:D5:344:TRP:CG	2.34	0.46
4:D5:7:VAL:HG22	4:D5:64:ILE:HB	1.98	0.46
4:E5:211:CYS:HA	4:E5:215:LEU:HB2	1.98	0.46
7:f:25:GLN:HA	7:f:28:LYS:HE3	1.98	0.46
4:A1:24:ILE:HG13	4:A1:28:HIS:HD2	1.81	0.45
3:A2:268:MET:SD	3:A2:378:ILE:HG23	2.55	0.45
3:A4:219:ILE:HD11	7:c:189:LEU:HD11	1.97	0.45
3:A6:20:CYS:SG	3:A6:235:ILE:HG13	2.56	0.45
3:B8:10:GLY:HA2	3:B8:145:THR:HG23	1.99	0.45
3:C0:196:GLU:HG2	3:C0:197:HIS:CD2	2.51	0.45
3:C0:269:LEU:HD13	3:C0:301:MET:SD	2.56	0.45
3:C4:29:GLY:HA2	2:J:256:LEU:HD22	1.98	0.45
3:C4:90:GLU:C	3:C4:121:ARG:HH12	2.25	0.45
3:D0:17:GLY:HA2	3:D0:20:CYS:HB2	1.98	0.45
4:D3:202:ILE:HD11	4:D3:268:ILE:HD12	1.98	0.45
3:D4:320:ARG:HG2	3:D4:360:PRO:HD3	1.98	0.45
3:D6:7:ILE:HG23	3:D6:137:MET:HA	1.97	0.45
3:D6:12:ALA:HA	3:D6:15:GLN:HE21	1.80	0.45
3:D6:169:PHE:HD2	3:D6:204:LEU:HD11	1.80	0.45
4:D9:207:LEU:HB3	4:D9:225:LEU:HG	1.98	0.45
3:E4:217:LEU:HB2	3:E4:275:ILE:HG22	1.98	0.45
3:E6:406:HIS:CD2	4:E7:261:PRO:HD3	2.51	0.45
4:E9:51:TYR:HB3	4:E9:59:PHE:HB3	1.98	0.45
8:k:61:ASN:HB2	8:k:69:ILE:HG12	1.98	0.45
4:A1:308:GLY:HA3	4:A1:373:ALA:HB2	1.98	0.45
3:A4:30:ILE:HG22	3:A4:36:MET:HB3	1.98	0.45
4:B1:424:GLN:HG3	4:B1:425:TYR:CD1	2.51	0.45
4:B3:16:ILE:HD11	4:B3:229:VAL:HG21	1.97	0.45
4:B3:232:ALA:HB2	4:B3:270:PHE:HB2	1.98	0.45
3:B6:53:PHE:HB3	3:B6:61:HIS:HB3	1.97	0.45
3:C4:280:LYS:HE3	3:C8:88:HIS:CE1	2.50	0.45
4:C5:257:LEU:HD11	4:C5:314:SER:HB3	1.98	0.45
4:D1:257:LEU:HD12	4:D1:370:ASN:HB2	1.97	0.45
3:D2:402:ARG:HD3	3:D2:405:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D3:284:LEU:HD21	4:D3:363:MET:H	1.81	0.45
4:D7:105:HIS:CD2	4:D7:150:LEU:HD12	2.51	0.45
4:E3:13:GLY:HA2	4:E3:16:ILE:HG22	1.97	0.45
5:R:253:ALA:O	5:R:255:LYS:HG2	2.16	0.45
7:r:154:TYR:HE1	7:r:158:THR:HG22	1.82	0.45
3:A6:397:LEU:HD11	4:A7:346:PRO:HD3	1.98	0.45
4:B3:105:HIS:CD2	4:B3:150:LEU:HD13	2.50	0.45
4:C3:14:ASN:HD22	4:C3:65:LEU:HD12	1.81	0.45
4:D5:296:ALA:HB2	4:D5:306:ARG:HH12	1.80	0.45
3:D8:306:ASP:HB3	3:D8:309:HIS:CE1	2.51	0.45
4:E3:337:ASN:HB3	4:E3:340:TYR:HB2	1.97	0.45
4:F1:399:THR:HA	4:F1:403:MET:HB2	1.97	0.45
7:b:77:PHE:CZ	7:b:150:VAL:HG21	2.52	0.45
7:e:99:MET:HG2	7:e:108:ILE:HG12	1.98	0.45
7:e:183:LEU:HD23	7:e:196:LEU:HA	1.98	0.45
7:n:77:PHE:HD2	7:n:169:SER:HB3	1.81	0.45
7:n:78:ALA:HA	7:n:167:VAL:HG13	1.99	0.45
7:x:9:PRO:HB2	7:x:143:ILE:HB	1.99	0.45
4:A1:286:VAL:HB	4:A1:325:GLU:HG2	1.99	0.45
3:A2:364:PRO:HB2	5:P:242:LEU:HD12	1.98	0.45
4:A3:257:LEU:HD21	4:A3:314:SER:HB2	1.99	0.45
3:B4:8:HIS:HD2	3:B4:138:PHE:HB2	1.81	0.45
4:B7:265:PHE:HB3	4:B7:374:ILE:HD13	1.99	0.45
4:B7:358:PRO:HG2	4:B7:361:LEU:HD11	1.98	0.45
3:B8:205:ASP:HB2	3:B8:303:ALA:HA	1.97	0.45
3:C2:286:LEU:HB2	3:C2:291:ILE:HD11	1.98	0.45
4:C3:12:CYS:HB3	4:C3:138:SER:HB2	1.98	0.45
4:C7:117:LEU:HA	4:C7:120:VAL:HG12	1.99	0.45
4:C9:139:LEU:HA	4:C9:145:SER:HB2	1.98	0.45
4:D3:49:VAL:HG21	4:D3:241:ARG:HG2	1.98	0.45
3:D8:207:GLU:HA	3:D8:210:TYR:HB2	1.97	0.45
3:D8:286:LEU:HD13	3:D8:371:VAL:HG23	1.99	0.45
7:f:130:PRO:HB3	7:h:159:TYR:CD2	2.52	0.45
8:l:14:LYS:HA	8:l:23:PRO:HA	1.99	0.45
8:l:35:ALA:HB3	8:l:71:ILE:HG22	1.99	0.45
7:n:117:ARG:HH12	7:n:152:LYS:HE2	1.81	0.45
3:A0:172:TRP:CD2	3:A0:173:PRO:HD2	2.52	0.45
4:A1:73:MET:HE1	4:A1:90:PHE:HB3	1.99	0.45
3:A2:204:LEU:HD23	3:A2:209:ILE:HD11	1.97	0.45
4:B1:313:ALA:HB1	4:B1:367:PHE:HE1	1.82	0.45
3:B2:313:MET:HG3	3:B2:344:VAL:HG11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B8:224:TYR:HD2	4:B9:323:THR:HG21	1.81	0.45
3:C0:141:VAL:HG13	3:C0:190:SER:HB3	1.98	0.45
4:C5:237:THR:HA	4:C5:240:LEU:HD13	1.98	0.45
2:D:247:TYR:CE1	3:D6:78:VAL:HA	2.51	0.45
3:D0:283:HIS:HB2	3:D4:88:HIS:HD2	1.82	0.45
3:E0:51:THR:HG21	3:E0:243:ARG:HG2	1.98	0.45
4:E3:372:THR:HG21	4:E3:426:GLN:HG2	1.98	0.45
4:E5:66:MET:HE2	4:E5:151:LEU:HD22	1.98	0.45
3:E8:320:ARG:HE	3:E8:360:PRO:HG3	1.80	0.45
3:F0:163:LYS:HD2	3:F0:163:LYS:HA	1.77	0.45
3:F0:209:ILE:HA	3:F0:212:ILE:HB	1.97	0.45
7:d:84:LYS:HZ3	7:d:88:LEU:HD22	1.82	0.45
7:o:146:ARG:HH12	7:o:156:VAL:HG21	1.81	0.45
7:r:154:TYR:HE1	7:r:158:THR:H	1.64	0.45
1:2:393:ASP:HA	1:2:396:LYS:NZ	2.31	0.45
3:A8:189:LEU:HD11	3:A8:418:PHE:HD1	1.82	0.45
3:B0:320:ARG:HH21	3:B0:360:PRO:HA	1.81	0.45
4:B1:113:ILE:HA	4:B1:116:VAL:HG22	1.99	0.45
4:B3:116:VAL:HA	4:B3:119:VAL:HG12	1.99	0.45
4:B3:257:LEU:HD21	4:B3:314:SER:HB3	1.99	0.45
3:B6:296:PHE:CD2	3:B6:377:MET:HE1	2.52	0.45
4:B7:391:ARG:HG3	3:B8:346:TRP:CD1	2.52	0.45
3:B8:217:LEU:HD21	3:B8:275:ILE:HG22	1.99	0.45
4:C1:3:GLU:HA	4:C1:49:VAL:HA	1.99	0.45
3:C2:182:VAL:HG22	3:C2:185:TYR:HB2	1.99	0.45
4:C5:27:GLU:HA	4:C5:359:LYS:HD2	1.99	0.45
4:C5:361:LEU:HD11	5:P:467:PRO:HD3	1.97	0.45
3:C6:198:THR:HG21	3:C6:201:ALA:HB2	1.99	0.45
3:D2:67:PHE:HB2	3:D2:92:LEU:HD23	1.99	0.45
4:D5:138:SER:HA	4:D5:169:VAL:HG22	1.99	0.45
4:D7:9:GLY:HA2	4:D7:66:MET:HB3	1.99	0.45
4:E5:2:ARG:HB2	4:E5:131:GLN:HB2	1.98	0.45
4:E7:57:GLY:HA3	7:v:83:PRO:HB2	1.97	0.45
4:E7:383:ASP:HA	4:E7:386:THR:HG22	1.98	0.45
5:P:458:ARG:HA	5:P:458:ARG:HD2	1.78	0.45
8:l:127:ALA:HB1	8:l:130:LEU:HD12	1.99	0.45
1:1:478:MET:HA	1:1:481:VAL:HG12	1.98	0.45
1:1:493:ARG:O	1:1:496:LYS:HG3	2.16	0.45
4:A1:268:ILE:N	4:A1:299:MET:HE1	2.31	0.45
4:A1:396:HIS:CD2	3:A2:263:PRO:HG3	2.52	0.45
4:A3:268:ILE:O	4:A3:300:MET:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B0:395:PHE:CD2	3:B0:422:ARG:HD3	2.52	0.45
4:B5:39:ASP:HA	7:f:90:PRO:HG3	1.98	0.45
3:B6:314:ALA:HB3	3:B6:380:ASN:HB2	1.99	0.45
3:C4:3:GLU:HG2	3:C4:51:THR:HA	1.98	0.45
2:D:256:LEU:HD12	2:D:257:PRO:HD2	1.98	0.45
3:D0:265:ILE:HG12	3:D0:380:ASN:HD21	1.81	0.45
4:D1:268:ILE:HG23	4:D1:300:MET:HE2	1.98	0.45
3:D2:115:VAL:HA	3:D2:118:SER:HB2	1.99	0.45
4:D3:178:THR:HA	3:D4:352:LYS:HD3	1.98	0.45
4:D3:276:ARG:HG3	5:P:524:ALA:H	1.81	0.45
4:E3:25:SER:HB2	4:E3:30:ILE:HB	1.99	0.45
4:E3:383:ASP:HA	4:E3:386:THR:HG22	1.98	0.45
3:E8:154:LEU:HD21	3:E8:198:THR:HG22	1.99	0.45
4:E9:236:VAL:HG13	4:E9:237:THR:HG23	1.97	0.45
4:F1:69:GLU:HB3	4:F1:96:GLY:HA2	1.99	0.45
7:c:67:HIS:HB3	7:e:16:ARG:HH22	1.81	0.45
7:d:97:ARG:HH22	7:f:159:TYR:C	2.25	0.45
7:f:75:LEU:HD23	7:f:111:ILE:HB	1.98	0.45
7:f:165:THR:HG21	7:f:182:PHE:CZ	2.51	0.45
7:j:11:ASN:O	7:j:15:ARG:HG3	2.17	0.45
8:k:15:ARG:HB2	8:k:24:VAL:HB	1.99	0.45
7:p:115:LEU:HD23	7:p:115:LEU:HA	1.77	0.45
7:q:127:ALA:HB1	7:s:157:PRO:HG3	1.98	0.45
3:A0:274:PRO:HB2	3:A0:276:ILE:HG23	1.98	0.45
3:A2:121:ARG:HD2	3:A2:124:LYS:HE2	1.99	0.45
4:A5:244:GLY:HA2	4:A5:355:ASP:HB2	1.98	0.45
4:A9:67:ASP:HB2	4:A9:73:MET:HE2	1.99	0.45
3:B0:310:GLY:HA3	3:B0:383:ALA:HB2	1.99	0.45
3:B2:284:GLU:HG2	3:B6:88:HIS:NE2	2.31	0.45
4:B7:12:CYS:HB3	4:B7:138:SER:HB2	1.99	0.45
3:C2:221:ARG:HA	4:C3:324:LYS:HZ1	1.81	0.45
3:C6:269:LEU:HD21	3:C6:384:ILE:HG22	1.99	0.45
3:D8:21:TRP:HD1	3:D8:24:PHE:HB2	1.82	0.45
3:E2:7:ILE:HG23	3:E2:137:MET:HA	1.99	0.45
3:E4:53:PHE:HB3	3:E4:61:HIS:HB3	1.98	0.45
3:E4:334:THR:HA	3:E4:337:THR:HG22	1.99	0.45
3:E6:195:LEU:HD21	3:E6:428:LEU:HD22	1.99	0.45
3:E6:287:SER:HB2	3:E6:290:GLU:HG3	1.98	0.45
3:E8:60:LYS:HZ2	3:E8:62:VAL:HG22	1.82	0.45
3:E8:242:LEU:HD11	3:E8:252:VAL:H	1.80	0.45
3:E8:310:GLY:HA3	3:E8:383:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E9:136:THR:HG22	4:E9:167:PHE:HB2	1.98	0.45
3:F0:72:PRO:HB2	4:F1:46:ARG:NH2	2.31	0.45
5:O:279:VAL:HA	5:O:282:ARG:HB3	1.99	0.45
7:g:130:PRO:HB3	7:i:159:TYR:CD2	2.52	0.45
7:q:172:VAL:HG12	7:q:180:ALA:HB3	1.99	0.45
7:r:164:ARG:HD2	7:r:164:ARG:HA	1.76	0.45
4:A1:208:TYR:HE2	3:A2:326:LYS:HA	1.82	0.45
4:A7:192:LEU:HD21	4:A7:199:VAL:HG11	1.98	0.45
4:B1:116:VAL:HG23	4:B1:151:LEU:HD13	1.97	0.45
4:B1:135:ILE:HG21	4:B1:152:ILE:HD11	1.99	0.45
3:B2:328:VAL:HG21	3:B2:355:ILE:HD11	1.99	0.45
4:B5:199:VAL:HG23	4:B5:264:HIS:CD2	2.52	0.45
3:B8:268:MET:SD	3:B8:378:ILE:HG23	2.57	0.45
4:D1:286:VAL:HG22	4:D1:363:MET:HE1	1.98	0.45
4:D9:164:MET:HB3	4:D9:197:ASP:H	1.81	0.45
3:E4:88:HIS:HB3	3:E4:91:GLN:HB3	1.97	0.45
4:E5:156:ARG:HG2	4:E5:195:ASN:HB2	1.98	0.45
3:F0:90:GLU:HG3	3:F0:121:ARG:HD3	1.99	0.45
3:F0:398:MET:HE1	4:F1:345:ILE:HG12	1.99	0.45
7:g:5:VAL:HG11	7:g:149:ARG:HD2	1.99	0.45
7:x:78:ALA:HB3	7:x:112:PHE:HE2	1.82	0.45
2:A:247:TYR:CE1	3:A4:78:VAL:HA	2.51	0.45
4:A1:397:TRP:CZ3	3:A2:257:THR:HA	2.52	0.45
3:A8:203:MET:HE1	3:A8:267:PHE:HB3	1.99	0.45
3:B2:210:TYR:CE1	3:B2:227:LEU:HD21	2.52	0.45
4:B3:136:THR:HG22	4:B3:167:PHE:HB2	1.98	0.45
4:B3:182:PRO:HA	4:B3:185:ALA:HB3	1.98	0.45
4:B3:398:TYR:HB3	4:B3:408:PHE:HZ	1.82	0.45
4:B5:313:ALA:HB1	4:B5:367:PHE:HE1	1.82	0.45
4:B7:8:GLN:HG2	4:B7:14:ASN:HA	1.99	0.45
4:B7:131:GLN:HE22	4:B7:249:ASP:HB2	1.81	0.45
4:B7:206:ALA:HB2	4:B7:302:ALA:HB2	1.98	0.45
3:C2:377:MET:HE3	3:C2:379:SER:HB3	1.99	0.45
3:C4:28:HIS:HE2	3:C4:243:ARG:HD2	1.82	0.45
4:C7:281:TYR:HB2	4:D1:86:ARG:NH2	2.31	0.45
4:D1:110:ALA:HA	4:D1:113:ILE:HG22	1.99	0.45
4:D3:7:VAL:HB	4:D3:135:ILE:HD13	1.99	0.45
4:D3:135:ILE:HG21	4:D3:152:ILE:HD11	1.98	0.45
3:D8:249:ASN:ND2	5:P:532:ARG:HH22	2.15	0.45
4:D9:49:VAL:HG11	4:D9:240:LEU:HB3	1.98	0.45
3:E0:395:PHE:HE2	3:E0:422:ARG:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E6:124:LYS:HD2	3:E6:124:LYS:HA	1.70	0.45
7:d:51:PRO:HD2	7:d:54:SER:HB2	1.99	0.45
7:g:68:LEU:HD22	7:g:109:GLU:HG2	1.99	0.45
7:o:5:VAL:HG11	7:o:149:ARG:HD3	1.98	0.45
7:q:18:ASN:HB3	7:q:45:MET:HG2	1.99	0.45
7:t:196:LEU:O	7:t:198:ARG:N	2.45	0.45
3:A0:88:HIS:HB3	3:A0:91:GLN:HG2	1.99	0.44
3:A0:219:ILE:HG22	7:a:198:ARG:NH2	2.32	0.44
4:A1:99:ASN:HA	4:A1:142:GLY:N	2.30	0.44
4:A5:117:LEU:HA	4:A5:120:VAL:HG12	1.99	0.44
3:A6:231:ILE:O	3:A6:235:ILE:HG12	2.17	0.44
3:B0:422:ARG:HA	3:B0:422:ARG:HD2	1.82	0.44
3:B4:181:VAL:HG23	3:B4:182:VAL:HG13	1.98	0.44
4:B9:39:ASP:HA	7:h:90:PRO:HG3	1.99	0.44
4:B9:42:LEU:HD11	4:B9:356:ILE:HD11	1.98	0.44
3:C2:88:HIS:HB3	3:C2:91:GLN:HB2	1.98	0.44
4:C5:117:LEU:HA	4:C5:120:VAL:HG12	1.99	0.44
4:C5:226:ASN:HA	4:C5:229:VAL:HG12	1.99	0.44
4:C9:293:MET:HE2	4:C9:293:MET:HB3	1.84	0.44
3:D0:259:LEU:HD21	3:D0:316:CYS:HB2	1.99	0.44
3:D2:53:PHE:HB3	3:D2:61:HIS:HB3	1.99	0.44
3:D2:401:LYS:HZ3	4:D3:344:TRP:CG	2.35	0.44
3:D4:292:THR:HG21	3:D4:331:ALA:HB1	1.97	0.44
3:D6:338:LYS:HG3	3:D6:340:THR:HG22	1.97	0.44
3:D6:403:ALA:HB2	4:D7:344:TRP:HZ3	1.81	0.44
4:E5:102:ALA:HA	4:E5:403:MET:HE3	1.99	0.44
6:W:179:ARG:HA	6:W:179:ARG:HD2	1.85	0.44
7:g:79:ASP:HB3	7:g:82:ASP:HB2	1.97	0.44
2:A:247:TYR:HE1	3:A4:78:VAL:HA	1.82	0.44
3:A4:352:LYS:HA	3:A4:352:LYS:HD3	1.80	0.44
4:A9:68:LEU:HA	4:A9:93:GLY:HA3	2.00	0.44
3:B2:242:LEU:HD21	3:B2:251:ASP:HA	1.99	0.44
3:B4:76:ASP:HA	3:B4:79:ARG:HE	1.82	0.44
4:C1:73:MET:O	4:C1:77:ARG:HG2	2.17	0.44
4:C1:213:ARG:HH22	4:C1:297:LYS:HG3	1.82	0.44
3:D0:397:LEU:HD12	4:D1:344:TRP:HA	1.99	0.44
4:D1:2:ARG:HB2	4:D1:131:GLN:HB2	1.98	0.44
4:D9:412:GLU:HA	4:D9:415:MET:HG3	1.99	0.44
3:E2:31:GLN:HG3	3:E2:37:PRO:HD3	1.99	0.44
4:E5:57:GLY:HA3	7:u:83:PRO:HB2	1.99	0.44
4:E5:135:ILE:HG21	4:E5:152:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E9:318:ARG:HG2	4:E9:354:CYS:HB3	1.99	0.44
7:c:2:SER:HA	7:c:6:PHE:HE1	1.82	0.44
7:g:84:LYS:HB2	7:g:168:PRO:HD3	1.99	0.44
7:s:57:ASN:HD21	7:s:59:ASN:HB2	1.82	0.44
7:s:107:LYS:HE2	7:s:107:LYS:HB2	1.66	0.44
3:A2:76:ASP:HA	3:A2:79:ARG:HD2	1.99	0.44
3:A4:244:PHE:HD2	3:A4:356:ASN:HD21	1.64	0.44
4:A9:326:VAL:O	4:A9:330:MET:HB2	2.17	0.44
3:B6:334:THR:HA	3:B6:337:THR:HG22	1.99	0.44
4:C1:51:TYR:HB3	4:C1:59:PHE:HB3	1.97	0.44
3:C4:210:TYR:CE1	4:C5:324:LYS:HD2	2.52	0.44
3:C6:280:LYS:HA	3:C6:283:HIS:HD2	1.81	0.44
4:C7:65:LEU:HB2	4:C7:90:PHE:HD1	1.81	0.44
4:C9:249:ASP:H	4:C9:252:LYS:HB2	1.82	0.44
3:D0:229:ARG:HD3	3:D0:363:VAL:HG21	2.00	0.44
4:D1:281:TYR:HD2	4:D5:86:ARG:HA	1.81	0.44
3:E0:244:PHE:HD1	5:R:558:ARG:HH12	1.66	0.44
4:E3:249:ASP:H	4:E3:252:LYS:HB2	1.82	0.44
3:E6:11:GLN:HB2	3:E6:74:VAL:HG11	1.99	0.44
4:E7:362:LYS:HD2	4:E7:363:MET:HB2	1.98	0.44
2:H:256:LEU:HD12	2:H:257:PRO:HD2	1.98	0.44
7:d:151:MET:HE1	7:d:154:TYR:HD1	1.83	0.44
7:e:187:SER:H	7:e:190:GLU:HB3	1.81	0.44
7:f:14:LYS:HZ3	7:f:47:LEU:HB2	1.82	0.44
3:A0:200:VAL:HA	3:A0:266:HIS:HB2	1.99	0.44
3:A0:306:ASP:HB3	3:A0:309:HIS:CE1	2.53	0.44
4:A1:131:GLN:HE22	4:A1:250:LEU:HB2	1.82	0.44
4:A5:334:GLN:HE22	4:A5:347:ASN:HA	1.81	0.44
3:A8:208:ALA:HB2	3:A8:304:LYS:HG2	1.99	0.44
3:B6:155:GLU:HG3	3:B6:197:HIS:CE1	2.52	0.44
3:B8:164:LYS:HA	3:B8:164:LYS:HD3	1.80	0.44
3:D0:252:VAL:HA	3:D0:255:PHE:HD2	1.82	0.44
4:D3:105:HIS:CD2	4:D3:150:LEU:HD12	2.51	0.44
4:D3:163:ILE:HD12	4:D3:250:LEU:HG	1.98	0.44
3:D4:260:VAL:HG23	3:D4:265:ILE:O	2.17	0.44
3:D8:387:VAL:HA	3:D8:390:ARG:NH1	2.33	0.44
3:E0:214:ARG:HE	3:E0:220:GLU:HA	1.82	0.44
4:E1:135:ILE:HB	4:E1:166:THR:HG22	1.99	0.44
3:E2:57:GLY:O	3:E2:59:GLY:N	2.49	0.44
3:E4:84:ARG:HE	7:u:98:THR:HG21	1.82	0.44
4:E5:316:MET:HE2	4:E5:366:THR:HG23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E6:265:ILE:HG21	3:E6:313:MET:HE1	2.00	0.44
3:E8:171:SER:HA	3:E8:204:LEU:HB2	1.98	0.44
4:E9:334:GLN:HE21	4:E9:334:GLN:HB3	1.59	0.44
4:F1:398:TYR:HB3	4:F1:403:MET:HG3	1.99	0.44
2:K:210:HIS:CE1	7:p:154:TYR:HB2	2.53	0.44
7:j:55:LEU:HD22	7:j:111:ILE:HD12	1.98	0.44
8:k:54:ARG:HG3	8:k:91:PRO:HG3	1.98	0.44
7:r:63:ILE:HD12	7:r:67:HIS:HB2	2.00	0.44
1:1:396:LYS:HA	1:1:396:LYS:HD3	1.72	0.44
4:A5:313:ALA:HA	4:A5:369:GLY:HA2	1.99	0.44
3:A6:122:ILE:HD13	3:A6:157:LEU:HD11	2.00	0.44
4:B1:317:PHE:CD2	4:B1:321:MET:HE1	2.52	0.44
4:B3:375:GLN:HG3	4:B3:419:VAL:HG23	2.00	0.44
4:B7:179:VAL:HG22	3:B8:258:ASN:OD1	2.18	0.44
3:B8:178:SER:HB2	3:B8:180:ALA:O	2.16	0.44
3:B8:404:PHE:HD1	4:B9:259:PRO:HA	1.82	0.44
4:C3:284:LEU:HD23	4:C3:284:LEU:HA	1.86	0.44
4:C7:377:MET:HE3	4:C7:377:MET:HB2	1.79	0.44
3:C8:233:GLN:HE21	3:C8:368:LEU:HD22	1.83	0.44
3:D0:91:GLN:HA	3:D0:121:ARG:HG2	1.99	0.44
3:D2:16:ILE:HA	3:D2:228:ASN:HD21	1.82	0.44
4:D3:253:LEU:HD21	4:D3:368:VAL:HG11	1.99	0.44
4:D3:389:PHE:HE2	4:D3:408:PHE:HD1	1.65	0.44
3:D8:280:LYS:HE2	3:D8:280:LYS:HB3	1.78	0.44
4:E5:8:GLN:HE22	4:E5:63:ALA:HB1	1.82	0.44
4:E5:393:ALA:HB1	3:E6:261:PRO:HB2	2.00	0.44
5:R:281:GLU:HG2	5:R:286:ASP:HB2	1.98	0.44
7:e:21:ARG:HA	7:e:24:MET:HG3	2.00	0.44
8:k:10:PRO:HB2	8:k:11:ASP:H	1.62	0.44
7:n:184:PRO:HD2	7:n:195:ALA:HB1	2.00	0.44
7:w:96:TYR:HA	7:w:108:ILE:HD11	1.98	0.44
3:A0:228:ASN:HA	3:A0:231:ILE:HG22	1.99	0.44
3:A2:12:ALA:HB3	3:A2:140:ALA:HB2	1.99	0.44
3:A2:231:ILE:HA	3:A2:234:VAL:HG12	1.98	0.44
3:B4:105:ARG:HD2	3:B4:109:THR:HB	1.99	0.44
3:B6:268:MET:HE2	3:B6:380:ASN:HD21	1.82	0.44
3:C2:191:THR:O	3:C2:195:LEU:HD23	2.18	0.44
3:C4:21:TRP:HE3	3:C4:87:PHE:HE1	1.66	0.44
4:C5:156:ARG:HH22	4:C5:197:ASP:CG	2.25	0.44
4:C5:281:TYR:CE1	4:C9:58:ARG:HD3	2.53	0.44
4:C9:101:TRP:HZ3	4:C9:106:TYR:HE2	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D3:178:THR:HG22	3:D4:352:LYS:HE3	2.00	0.44
4:D3:192:LEU:HD21	4:D3:199:VAL:HG21	1.98	0.44
3:D4:12:ALA:HB3	3:D4:140:ALA:HB2	1.99	0.44
4:D5:68:LEU:HD23	4:D5:112:LEU:HD13	1.99	0.44
4:D7:42:LEU:HD23	4:D7:356:ILE:HD11	1.99	0.44
4:D7:163:ILE:HD11	4:D7:251:ARG:HG2	2.00	0.44
3:D8:272:TYR:O	3:D8:275:ILE:HD13	2.18	0.44
4:D9:73:MET:HA	4:D9:76:VAL:HG22	2.00	0.44
4:E1:200:GLN:HB3	4:E1:268:ILE:HD11	2.00	0.44
3:E2:30:ILE:HG22	3:E2:34:GLY:HA2	1.98	0.44
3:E2:31:GLN:C	3:E2:33:ASP:H	2.26	0.44
4:E3:227:HIS:HB3	5:O:567:LEU:HD12	1.99	0.44
4:E3:314:SER:HB2	4:E3:350:LYS:HB3	1.99	0.44
4:E5:154:LYS:HA	4:E5:154:LYS:HD3	1.80	0.44
7:j:9:PRO:HA	7:j:12:VAL:HG22	2.00	0.44
7:o:100:ASN:HD21	7:o:106:GLN:HG3	1.83	0.44
7:s:75:LEU:HG	7:s:173:ILE:HG13	2.00	0.44
7:s:181:GLN:HE22	7:s:200:ASP:N	2.15	0.44
7:v:169:SER:HA	7:v:185:ILE:HD11	2.00	0.44
1:1:429:LYS:HE3	1:1:429:LYS:HA	2.00	0.44
1:2:429:LYS:HD3	1:2:432:GLN:HE22	1.83	0.44
4:A1:170:PHE:CD2	4:A1:201:VAL:HG13	2.52	0.44
3:A6:71:GLU:OE1	3:A6:73:THR:HG22	2.18	0.44
3:B0:401:LYS:HD2	4:B1:344:TRP:CD2	2.53	0.44
4:B1:117:LEU:HD12	4:B1:117:LEU:HA	1.89	0.44
4:B1:330:MET:HE2	4:B1:351:SER:HB3	2.00	0.44
3:B4:259:LEU:HG	3:B4:314:ALA:HB1	1.99	0.44
3:B8:209:ILE:HD11	3:B8:231:ILE:HD11	1.99	0.44
3:C0:184:PRO:HA	3:C0:391:MET:HE1	2.00	0.44
4:C1:98:GLY:H	4:C1:103:LYS:HD2	1.83	0.44
4:C1:103:LYS:HB3	4:C1:103:LYS:HE2	1.83	0.44
3:C4:88:HIS:CE1	3:C4:90:GLU:HG3	2.53	0.44
4:C5:207:LEU:HG	4:C5:228:LEU:HD11	1.99	0.44
4:D1:86:ARG:HE	4:D1:87:PRO:HD2	1.83	0.44
4:D9:200:GLN:HB3	4:D9:268:ILE:HG13	2.00	0.44
4:E9:199:VAL:CG2	4:E9:264:HIS:HE1	2.31	0.44
4:E9:253:LEU:HD12	4:E9:257:LEU:HD13	2.00	0.44
7:d:172:VAL:HG23	7:d:180:ALA:HB3	2.00	0.44
7:i:119:ARG:NH1	7:i:119:ARG:HA	2.33	0.44
7:j:96:TYR:HE1	7:j:109:GLU:HA	1.82	0.44
7:j:142:GLU:HA	7:j:145:LYS:NZ	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:r:74:ALA:HB2	7:r:172:VAL:HG12	1.99	0.44
3:A0:121:ARG:HA	3:A0:121:ARG:HD2	1.79	0.44
4:A1:7:VAL:HB	4:A1:135:ILE:HG13	1.99	0.44
3:A4:283:HIS:HA	3:A8:60:LYS:HZ3	1.82	0.44
3:B2:222:PRO:HD2	4:B3:324:LYS:HZ1	1.83	0.44
4:B3:73:MET:HA	4:B3:76:VAL:HG22	1.99	0.44
3:B4:407:TRP:CH2	4:B5:258:ILE:HG13	2.53	0.44
3:B8:132:LEU:HD23	3:B8:164:LYS:HZ3	1.82	0.44
3:B8:168:ASN:HB3	3:B8:201:ALA:HA	2.00	0.44
4:C1:323:THR:HG22	4:C1:353:VAL:HG11	1.99	0.44
3:C6:396:ASP:HB3	3:C6:422:ARG:HH12	1.81	0.44
4:C9:280:GLN:HE22	4:D3:58:ARG:HD2	1.83	0.44
3:D0:154:LEU:HD21	3:D0:168:ASN:HD21	1.83	0.44
3:D0:276:ILE:HD12	3:D0:281:ALA:HA	2.00	0.44
4:D5:57:GLY:HA3	7:p:83:PRO:HB2	1.99	0.44
3:D6:304:LYS:HE3	3:D6:304:LYS:HB2	1.79	0.44
4:D9:57:GLY:HA3	7:r:83:PRO:HB2	2.00	0.44
4:E3:271:ALA:HB1	4:E3:292:GLN:NE2	2.32	0.44
3:E8:166:LYS:HB2	3:E8:199:ASP:H	1.82	0.44
3:F0:96:LYS:HD3	3:F0:96:LYS:HA	1.83	0.44
7:f:106:GLN:HE21	7:h:6:PHE:HZ	1.65	0.44
7:g:63:ILE:HG13	7:i:16:ARG:HH22	1.83	0.44
7:i:54:SER:HB2	7:i:134:ILE:HD11	1.99	0.44
7:m:12:VAL:HA	7:m:15:ARG:NH1	2.32	0.44
3:A0:32:PRO:HG2	6:W:90:TRP:CZ3	2.52	0.44
3:A0:229:ARG:HD2	3:A0:363:VAL:HG21	1.99	0.44
3:A2:141:VAL:HG11	3:A2:172:TRP:CE3	2.53	0.44
3:A2:188:VAL:HG21	3:A2:395:PHE:CD1	2.53	0.44
3:A2:272:TYR:HE1	3:A2:374:ALA:HB1	1.83	0.44
3:A4:210:TYR:CD1	4:A5:324:LYS:HG3	2.53	0.44
4:A5:246:LEU:HD12	4:A5:246:LEU:HA	1.87	0.44
3:A6:28:HIS:CE1	3:A6:49:PHE:HA	2.53	0.44
4:A9:44:LEU:HA	4:A9:47:ILE:HD11	1.99	0.44
4:A9:68:LEU:HB3	4:A9:96:GLY:HA2	1.99	0.44
4:B3:165:GLU:OE1	4:B3:198:GLU:HG3	2.18	0.44
4:B5:388:MET:HE3	4:B5:388:MET:HB3	1.89	0.44
4:B7:44:LEU:HD21	7:g:87:SER:HA	1.99	0.44
3:C0:313:MET:HE2	3:C0:313:MET:HB2	1.84	0.44
4:C1:222:TYR:HE2	3:C2:325:PRO:HB2	1.83	0.44
4:C3:294:PHE:CE2	4:C3:333:VAL:HG21	2.53	0.44
3:C6:71:GLU:OE1	3:C6:73:THR:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C6:81:GLY:HA3	2:J:215:TYR:HE2	1.83	0.44
4:D5:135:ILE:HB	4:D5:166:THR:HG22	2.00	0.44
4:D5:257:LEU:HD21	4:D5:314:SER:HB3	1.99	0.44
3:D8:283:HIS:HB3	3:E2:88:HIS:ND1	2.33	0.44
3:D8:290:GLU:H	3:D8:290:GLU:HG2	1.65	0.44
4:E1:113:ILE:HA	4:E1:116:VAL:HG12	1.99	0.44
3:E2:221:ARG:HH21	7:v:191:GLU:HA	1.83	0.44
4:E5:219:THR:HA	3:E6:326:LYS:HE3	2.00	0.44
4:E7:113:ILE:HG13	4:E7:150:LEU:HD23	2.00	0.44
4:E7:320:ARG:HH12	2:H:217:THR:HG21	1.83	0.44
4:F1:113:ILE:HD13	4:F1:113:ILE:HA	1.86	0.44
7:o:92:LEU:HD22	7:o:196:LEU:HD11	2.00	0.44
3:A0:310:GLY:HA3	3:A0:383:ALA:HB2	1.99	0.43
4:A3:69:GLU:HA	4:A3:70:PRO:HD3	1.86	0.43
4:A3:113:ILE:HG23	4:A3:117:LEU:HD13	1.99	0.43
4:A3:113:ILE:HA	4:A3:116:VAL:HG22	1.99	0.43
3:A4:265:ILE:HD11	3:A4:384:ILE:HD11	1.99	0.43
4:A5:86:ARG:HH21	4:A5:87:PRO:HD2	1.83	0.43
3:A6:154:LEU:HB3	3:A6:197:HIS:HB3	2.00	0.43
3:B0:79:ARG:HB3	3:B0:92:LEU:HD12	1.98	0.43
4:B1:156:ARG:HD2	4:B1:156:ARG:HA	1.73	0.43
3:B4:220:GLU:C	3:B4:221:ARG:HD2	2.42	0.43
4:B9:165:GLU:HA	4:B9:198:GLU:HG2	2.00	0.43
4:D1:113:ILE:HG13	4:D1:117:LEU:HD23	2.01	0.43
4:D1:277:GLY:HA3	4:D5:87:PRO:HG2	2.00	0.43
4:D3:211:CYS:HB2	4:D3:217:LEU:HD12	2.00	0.43
3:D4:189:LEU:HD11	3:D4:418:PHE:HD1	1.83	0.43
3:D4:403:ALA:HB2	4:D5:344:TRP:HZ3	1.83	0.43
4:D9:10:GLY:HA2	4:D9:143:THR:HG23	1.99	0.43
4:D9:28:HIS:NE2	4:D9:241:ARG:HD2	2.31	0.43
3:E0:119:LEU:HA	3:E0:122:ILE:HB	2.00	0.43
3:E0:205:ASP:HB3	3:E0:208:ALA:HB3	2.00	0.43
7:g:112:PHE:HB3	7:g:133:SER:HA	1.98	0.43
7:j:171:ILE:HD11	7:j:179:GLU:HB2	1.99	0.43
8:k:57:TYR:HA	8:k:69:ILE:HD11	2.00	0.43
7:n:71:LYS:HD2	7:n:71:LYS:HA	1.71	0.43
7:t:100:ASN:HD21	7:t:108:ILE:HG12	1.83	0.43
4:A5:34:GLY:HA3	4:A5:58:ARG:HG3	1.99	0.43
3:A6:155:GLU:HA	3:A6:197:HIS:CD2	2.53	0.43
3:A8:30:ILE:HG13	3:A8:36:MET:HB3	1.99	0.43
3:B4:221:ARG:NH2	4:B5:325:GLU:HG2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B5:7:VAL:HG12	4:B5:64:ILE:HB	2.00	0.43
4:B7:158:GLU:HG3	4:B7:159:TYR:HD1	1.83	0.43
4:B7:187:LEU:HA	4:B7:190:HIS:HE1	1.83	0.43
3:B8:407:TRP:CG	4:B9:255:VAL:HG23	2.53	0.43
4:B9:3:GLU:HB2	4:B9:130:LEU:HD13	2.00	0.43
4:B9:19:LYS:HZ3	4:B9:19:LYS:HG2	1.65	0.43
3:C6:363:VAL:HG23	3:C6:366:GLY:HA3	2.00	0.43
4:D3:216:LYS:HE2	4:D3:216:LYS:HB2	1.80	0.43
3:E6:132:LEU:HD23	3:E6:164:LYS:HZ3	1.82	0.43
4:E7:153:SER:HB3	4:E7:191:GLN:HE21	1.83	0.43
4:E9:187:LEU:HD23	4:E9:190:HIS:HE1	1.83	0.43
4:F1:262:ARG:HH22	4:F1:417:ASP:HB3	1.83	0.43
5:P:305:ARG:HA	5:P:308:TRP:HE1	1.82	0.43
7:c:115:LEU:HD13	7:c:145:LYS:NZ	2.32	0.43
7:c:184:PRO:HD2	7:c:195:ALA:HB1	2.00	0.43
7:h:82:ASP:HA	7:h:83:PRO:HD3	1.87	0.43
7:n:77:PHE:HE2	7:n:171:ILE:HD12	1.83	0.43
7:v:18:ASN:HA	7:v:21:ARG:NH1	2.33	0.43
4:A1:2:ARG:H	6:V:169:ARG:NH2	2.16	0.43
4:A1:289:LEU:HD13	4:A1:363:MET:HG2	1.99	0.43
4:A5:323:THR:HG22	4:A5:353:VAL:HG21	2.00	0.43
3:A8:264:ARG:HH12	3:A8:428:LEU:HA	1.83	0.43
4:B9:136:THR:HG22	4:B9:167:PHE:HB2	1.99	0.43
4:C1:213:ARG:HD2	4:C1:214:THR:N	2.33	0.43
4:C1:213:ARG:HA	4:C1:216:LYS:HD3	2.00	0.43
4:D1:173:PRO:HG3	4:D1:380:ARG:HH11	1.82	0.43
4:D1:236:VAL:HG13	4:D1:237:THR:HG23	2.00	0.43
3:E0:115:VAL:HG22	3:E0:153:LEU:HD22	1.99	0.43
4:E1:99:ASN:C	4:E1:99:ASN:HD22	2.26	0.43
3:E2:175:PRO:HD3	3:E2:390:ARG:CZ	2.48	0.43
6:W:123:PRO:HG2	7:x:101:GLU:HB3	1.99	0.43
7:b:99:MET:HG2	7:b:108:ILE:HD11	1.99	0.43
7:e:115:LEU:HD22	7:e:145:LYS:HD3	2.00	0.43
7:h:183:LEU:HD11	7:h:199:TRP:CD1	2.53	0.43
8:k:40:LYS:HE3	8:k:40:LYS:HB3	1.87	0.43
7:p:8:SER:HB2	7:p:147:HIS:HA	2.00	0.43
7:s:129:MET:HA	7:s:130:PRO:HD3	1.94	0.43
7:s:142:GLU:HA	7:s:145:LYS:HG2	1.99	0.43
4:A1:73:MET:HA	4:A1:76:VAL:HG12	1.99	0.43
3:A4:120:ASP:HA	3:A4:123:ARG:NH2	2.33	0.43
4:A7:11:GLN:HA	4:A7:72:THR:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A8:51:THR:HG21	3:A8:242:LEU:HB3	2.01	0.43
3:B6:272:TYR:HB3	3:B6:275:ILE:HD11	1.99	0.43
4:C1:99:ASN:ND2	3:C2:258:ASN:HD22	2.16	0.43
3:C2:259:LEU:HD21	3:C2:316:CYS:HB2	2.01	0.43
3:C2:370:LYS:HA	3:C2:370:LYS:HD2	1.74	0.43
4:C5:321:MET:HE1	4:C5:326:VAL:HG22	2.01	0.43
3:C6:6:SER:HA	3:C6:136:LEU:HB2	1.99	0.43
2:D:253:ALA:HB2	7:q:102:GLY:HA2	2.01	0.43
3:D0:2:ARG:HB2	3:D0:133:GLN:HE22	1.83	0.43
4:D1:57:GLY:HA3	7:n:83:PRO:HB2	2.00	0.43
3:D2:172:TRP:HZ2	3:D2:391:MET:HG2	1.84	0.43
3:D6:118:SER:O	3:D6:122:ILE:HG12	2.18	0.43
3:D6:338:LYS:HA	3:D6:338:LYS:HD2	1.72	0.43
3:E0:225:THR:O	3:E0:229:ARG:HG2	2.17	0.43
4:E7:113:ILE:HG23	4:E7:117:LEU:HD23	2.00	0.43
4:F1:248:SER:HA	4:F1:252:LYS:HD2	2.00	0.43
7:b:53:GLY:HA2	7:b:62:VAL:HG21	2.01	0.43
7:f:164:ARG:HG3	7:f:165:THR:HG23	1.99	0.43
7:g:57:ASN:HB3	7:g:63:ILE:HD11	1.99	0.43
7:m:14:LYS:HG3	7:m:47:LEU:HB2	1.99	0.43
7:p:79:ASP:HB3	7:p:82:ASP:HB2	2.00	0.43
7:t:37:GLN:C	7:t:37:GLN:NE2	2.76	0.43
7:x:14:LYS:NZ	7:x:45:MET:HB3	2.31	0.43
4:A3:113:ILE:HD11	4:A3:147:MET:HB2	2.00	0.43
3:A6:102:ASN:HA	3:A6:408:TYR:HE1	1.84	0.43
4:A9:170:PHE:CD2	4:A9:201:VAL:HG13	2.54	0.43
4:A9:182:PRO:HB2	4:A9:385:PHE:HD1	1.83	0.43
4:A9:253:LEU:HD11	4:A9:316:MET:HE1	2.00	0.43
4:B7:167:PHE:CZ	4:B7:233:MET:HG2	2.53	0.43
4:B9:211:CYS:HA	4:B9:215:LEU:HB2	2.00	0.43
3:C4:21:TRP:CH2	3:C4:65:CYS:HB3	2.53	0.43
4:C7:68:LEU:HA	4:C7:93:GLY:HA3	2.01	0.43
4:C9:284:LEU:H	4:D3:55:THR:HB	1.84	0.43
4:D1:251:ARG:HA	4:D1:251:ARG:HD3	1.80	0.43
4:D1:320:ARG:HD3	4:D1:320:ARG:HA	1.79	0.43
3:D2:233:GLN:HG3	3:D2:272:TYR:CE2	2.52	0.43
3:E2:167:LEU:HD13	3:E2:200:VAL:HB	1.99	0.43
4:E3:70:PRO:HA	4:E3:73:MET:HE2	2.01	0.43
3:E4:32:PRO:HG3	3:E4:83:TYR:HE1	1.84	0.43
3:E4:271:SER:H	3:E4:377:MET:HB2	1.82	0.43
3:E6:113:GLU:HG3	3:E6:114:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E6:210:TYR:CE1	3:E6:227:LEU:HD11	2.54	0.43
3:E6:217:LEU:HA	3:E6:277:SER:HB2	2.00	0.43
3:E6:247:ALA:HB3	3:E6:355:ILE:HB	2.00	0.43
4:E7:131:GLN:HE22	4:E7:250:LEU:HB2	1.82	0.43
7:b:164:ARG:HG3	7:b:165:THR:N	2.33	0.43
7:f:73:VAL:HG12	7:f:109:GLU:HB2	2.01	0.43
7:g:63:ILE:HD13	7:g:132:LEU:HD22	2.00	0.43
7:m:194:ARG:HH12	7:m:198:ARG:HH21	1.66	0.43
7:r:18:ASN:ND2	7:r:45:MET:HB3	2.34	0.43
4:A3:147:MET:HA	4:A3:150:LEU:HB3	2.00	0.43
4:A7:134:GLN:CD	4:A7:233:MET:HE1	2.43	0.43
3:B0:298:PRO:HA	3:B0:301:MET:HG2	2.00	0.43
4:B3:117:LEU:HA	4:B3:120:VAL:HG12	2.01	0.43
4:B5:119:VAL:HA	4:B5:122:LYS:HB3	1.99	0.43
4:B7:384:GLN:HB2	3:B8:348:PRO:HG3	2.00	0.43
3:B8:391:MET:HA	3:B8:394:LYS:HG2	2.00	0.43
3:C2:335:ILE:HG13	3:C2:338:LYS:HE3	2.01	0.43
3:C2:398:MET:HE2	4:C3:346:PRO:HD2	2.00	0.43
4:C3:156:ARG:NH2	4:C3:160:PRO:HA	2.33	0.43
4:C3:173:PRO:HD3	4:C3:380:ARG:NH2	2.34	0.43
4:C5:86:ARG:HB3	4:C5:89:ASN:OD1	2.18	0.43
3:C6:7:ILE:HG21	3:C6:153:LEU:HD21	2.00	0.43
4:D3:398:TYR:HB3	4:D3:408:PHE:HZ	1.83	0.43
3:D8:26:LEU:HD13	3:D8:363:VAL:HG12	2.00	0.43
3:E0:244:PHE:HE2	3:E0:320:ARG:HH21	1.67	0.43
3:E2:172:TRP:HB2	3:E2:203:MET:HE2	2.01	0.43
4:E3:325:GLU:HA	4:E3:328:GLU:HG3	2.00	0.43
4:E9:167:PHE:CZ	4:E9:233:MET:HG2	2.54	0.43
3:F0:326:LYS:HB3	3:F0:326:LYS:HE2	1.82	0.43
3:F0:366:GLY:HA2	6:W:127:ARG:HH22	1.84	0.43
7:c:11:ASN:HB3	7:c:15:ARG:HH21	1.82	0.43
7:e:99:MET:HE1	7:e:201:TRP:CD2	2.54	0.43
8:l:68:VAL:HG13	8:l:69:ILE:HG23	2.00	0.43
7:r:75:LEU:HD11	7:r:144:LEU:HD13	2.00	0.43
4:A1:415:MET:HA	4:A1:418:LEU:HD23	2.01	0.43
3:A2:172:TRP:HZ2	3:A2:391:MET:HG3	1.83	0.43
4:A3:375:GLN:OE1	4:A3:422:TYR:HD2	2.01	0.43
4:A5:290:THR:HA	4:A5:293:MET:HE2	2.00	0.43
3:A6:406:HIS:HA	3:A6:409:VAL:HG12	2.00	0.43
3:A8:179:THR:HB	4:A9:351:SER:HB2	2.00	0.43
3:B0:217:LEU:HG	3:B0:275:ILE:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B6:406:HIS:HE1	4:B7:259:PRO:C	2.26	0.43
3:B8:267:PHE:HE2	3:B8:428:LEU:HD11	1.83	0.43
3:B8:385:ALA:HB2	3:B8:432:TYR:HB3	2.00	0.43
4:C1:183:TYR:HE1	4:C1:388:MET:HG3	1.83	0.43
4:C1:311:LEU:HA	4:C1:342:VAL:HB	2.00	0.43
3:C6:88:HIS:HB3	3:C6:91:GLN:OE1	2.18	0.43
4:C7:405:GLU:HA	4:C7:408:PHE:HB2	2.00	0.43
3:C8:210:TYR:CZ	4:C9:324:LYS:HG3	2.53	0.43
3:C8:280:LYS:HE2	3:D2:90:GLU:OE1	2.19	0.43
2:D:247:TYR:CE1	3:D6:81:GLY:HA3	2.53	0.43
3:D0:306:ASP:HB3	3:D0:309:HIS:CE1	2.53	0.43
3:D4:15:GLN:HG3	3:D4:228:ASN:HD21	1.84	0.43
4:D5:70:PRO:HA	4:D5:73:MET:HB3	2.00	0.43
3:D6:72:PRO:HD2	4:D7:2:ARG:NH2	2.34	0.43
3:D6:277:SER:O	3:D6:281:ALA:HB2	2.19	0.43
4:D9:290:THR:HG21	4:D9:329:GLN:HB3	2.01	0.43
3:E2:71:GLU:HG3	3:E2:73:THR:HG22	2.01	0.43
3:E4:401:LYS:HE2	4:E5:344:TRP:CD1	2.54	0.43
4:E5:105:HIS:CD2	4:E5:150:LEU:HB2	2.53	0.43
4:E9:74:ASP:HA	4:E9:77:ARG:HG2	2.01	0.43
4:F1:8:GLN:HE21	4:F1:17:GLY:HA3	1.84	0.43
7:d:9:PRO:HD3	7:d:146:ARG:HG2	2.00	0.43
7:p:154:TYR:HE1	7:p:158:THR:H	1.67	0.43
7:s:93:LEU:HB3	7:s:97:ARG:HH21	1.83	0.43
3:A0:253:THR:HG23	3:A0:254:GLU:HG2	2.00	0.43
4:A1:7:VAL:HG13	4:A1:66:MET:HE3	2.00	0.43
4:A1:424:GLN:HE21	4:A1:424:GLN:HB2	1.70	0.43
3:A2:271:SER:HB3	3:A2:301:MET:HA	2.01	0.43
4:A3:28:HIS:HE2	4:A3:241:ARG:HE	1.67	0.43
2:B:247:TYR:CD1	3:D2:77:GLU:HG2	2.54	0.43
4:B1:398:TYR:HD2	4:B1:408:PHE:HZ	1.66	0.43
4:B5:139:LEU:HG	4:B5:168:SER:HB2	2.01	0.43
4:B5:290:THR:HG21	4:B5:329:GLN:HB3	2.00	0.43
3:C4:417:GLU:HA	3:C4:420:GLU:HG3	2.01	0.43
4:D7:57:GLY:HA3	7:q:83:PRO:HB2	2.01	0.43
4:D9:190:HIS:HB2	4:D9:414:ASN:HB3	2.00	0.43
4:E5:326:VAL:O	4:E5:330:MET:HG2	2.19	0.43
3:E6:332:VAL:HA	3:E6:335:ILE:HG22	2.01	0.43
4:E7:7:VAL:HG22	4:E7:66:MET:HE2	2.00	0.43
3:E8:138:PHE:HZ	3:E8:235:ILE:HG21	1.84	0.43
3:F0:88:HIS:HB3	3:F0:91:GLN:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:533:ARG:HG2	5:P:535:ILE:HG23	1.99	0.43
7:b:126:ARG:HH11	7:b:129:MET:HE3	1.84	0.43
7:r:75:LEU:HB3	7:r:77:PHE:HE1	1.83	0.43
7:s:107:LYS:HD3	7:s:201:TRP:NE1	2.33	0.43
4:A5:285:SER:OG	4:A5:287:PRO:HD2	2.19	0.43
3:A8:238:LEU:HD23	3:A8:238:LEU:HA	1.90	0.43
4:A9:116:VAL:HA	4:A9:119:VAL:HG12	2.00	0.43
4:B5:320:ARG:HH22	2:E:217:THR:HG21	1.84	0.43
3:B8:192:HIS:C	3:B8:192:HIS:ND1	2.75	0.43
3:B8:332:VAL:HA	3:B8:335:ILE:HG22	2.01	0.43
3:C0:417:GLU:HA	3:C0:420:GLU:HG3	2.01	0.43
3:C6:67:PHE:HB2	3:C6:92:LEU:HD13	2.01	0.43
3:C8:319:TYR:HB3	3:C8:323:VAL:HG21	2.01	0.43
3:D2:181:VAL:HG22	4:D3:256:ASN:OD1	2.18	0.43
3:D8:289:ALA:C	3:D8:291:ILE:N	2.75	0.43
4:D9:65:LEU:HB2	4:D9:90:PHE:HA	1.99	0.43
3:E0:274:PRO:HB2	3:E0:276:ILE:HG12	2.00	0.43
3:E4:177:VAL:HA	4:E5:331:LEU:HD21	2.00	0.43
4:E9:294:PHE:HZ	4:E9:349:MET:HE3	1.83	0.43
4:F1:326:VAL:HG11	4:F1:351:SER:HB2	1.99	0.43
7:m:96:TYR:HA	7:m:108:ILE:HD11	2.00	0.43
7:o:194:ARG:HH12	7:o:198:ARG:NH2	2.08	0.43
2:A:221:PRO:HB3	3:A6:32:PRO:HG3	2.00	0.43
3:A2:123:ARG:NH1	3:A2:124:LYS:HB3	2.34	0.43
4:A9:132:GLY:HA2	4:A9:162:ARG:HG3	2.00	0.43
2:B:208:PRO:HG3	7:r:154:TYR:HB3	2.01	0.43
4:B1:136:THR:HG23	4:B1:167:PHE:HB2	2.00	0.43
4:B3:383:ASP:HA	4:B3:386:THR:HG22	2.01	0.43
4:B7:36:TYR:HB3	7:g:86:ALA:HB1	2.01	0.43
4:B7:182:PRO:HB3	4:B7:384:GLN:HE22	1.83	0.43
4:C9:273:LEU:HD23	4:C9:273:LEU:HA	1.82	0.43
3:D0:64:ARG:HA	3:D0:125:LEU:HD11	2.01	0.43
3:D4:172:TRP:CD2	3:D4:173:PRO:HD2	2.54	0.43
4:D7:152:ILE:HG23	4:D7:164:MET:SD	2.58	0.43
3:D8:193:SER:HB3	3:D8:197:HIS:CE1	2.49	0.43
3:D8:277:SER:O	3:D8:280:LYS:N	2.52	0.43
4:E1:173:PRO:HB3	4:E1:380:ARG:HD3	2.01	0.43
3:E2:141:VAL:HG21	3:E2:172:TRP:CE3	2.53	0.43
3:E4:180:ALA:HA	4:E5:350:LYS:HZ3	1.83	0.43
4:E7:359:LYS:HA	4:E7:359:LYS:HD3	1.79	0.43
5:P:509:HIS:CG	5:P:510:ALA:H	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:k:131:LEU:HD22	8:k:146:PHE:CZ	2.54	0.43
1:1:453:LYS:HA	1:1:456:ILE:HD13	2.01	0.42
4:A1:309:ARG:HB2	4:A1:426:GLN:HG3	2.01	0.42
4:A3:215:LEU:HD11	5:P:227:LEU:HD13	2.00	0.42
4:A3:276:ARG:HH21	5:P:227:LEU:HB3	1.84	0.42
3:A4:90:GLU:HG2	3:A4:121:ARG:NH1	2.34	0.42
3:A4:172:TRP:HB3	3:A4:205:ASP:OD1	2.19	0.42
4:A9:28:HIS:CE1	4:A9:241:ARG:HH11	2.35	0.42
4:A9:272:PRO:HD3	4:A9:364:SER:HA	2.01	0.42
4:A9:284:LEU:HG	4:A9:363:MET:HB2	2.00	0.42
3:B2:222:PRO:HD2	4:B3:324:LYS:NZ	2.34	0.42
4:B7:275:SER:HA	5:P:370:LEU:HD11	2.01	0.42
4:C1:65:LEU:HB3	4:C1:73:MET:HE1	2.00	0.42
4:C3:132:GLY:HA3	4:C3:163:ILE:HG22	2.00	0.42
4:C7:200:GLN:HG3	4:C7:266:PHE:HB2	2.01	0.42
4:C7:211:CYS:HA	4:C7:215:LEU:HB2	2.01	0.42
3:C8:73:THR:HB	4:C9:46:ARG:HH12	1.84	0.42
4:C9:288:GLU:HA	4:C9:291:GLN:HE22	1.83	0.42
4:D1:237:THR:HA	4:D1:240:LEU:HD13	2.00	0.42
3:D2:326:LYS:HA	3:D2:326:LYS:HD3	1.83	0.42
4:D3:377:MET:HA	4:D3:380:ARG:HG2	2.01	0.42
3:D4:286:LEU:HD11	3:D4:372:MET:H	1.84	0.42
4:D5:173:PRO:HG3	4:D5:380:ARG:HH11	1.84	0.42
3:D8:154:LEU:HA	3:D8:157:LEU:HG	2.00	0.42
4:D9:16:ILE:HD11	4:D9:229:VAL:HG11	2.01	0.42
4:E1:98:GLY:C	4:E1:99:ASN:HD22	2.26	0.42
4:E3:105:HIS:CE1	4:E3:150:LEU:HD13	2.53	0.42
4:E5:66:MET:HE3	4:E5:66:MET:HB3	1.91	0.42
4:E7:213:ARG:HD3	4:E7:297:LYS:HD2	2.01	0.42
4:E9:324:LYS:O	4:E9:328:GLU:HG3	2.19	0.42
2:I:235:LEU:HD12	2:I:236:PRO:HD2	2.01	0.42
5:P:316:LEU:C	5:P:317:ARG:HH11	2.27	0.42
7:d:199:TRP:HE1	7:d:201:TRP:HB3	1.83	0.42
7:e:50:PHE:HE1	7:e:134:ILE:HD11	1.84	0.42
7:j:47:LEU:HD11	7:j:49:LEU:HD23	2.00	0.42
3:A0:81:GLY:HA2	6:W:82:ARG:NH2	2.34	0.42
4:A1:268:ILE:HG22	4:A1:300:MET:HE3	2.00	0.42
3:A2:280:LYS:NZ	3:A6:89:PRO:HG2	2.34	0.42
4:A5:280:GLN:HB3	4:A9:58:ARG:HD3	2.00	0.42
4:A9:306:ARG:HG2	4:A9:340:TYR:HE2	1.84	0.42
3:B2:314:ALA:H	3:B2:380:ASN:HB2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B7:390:ARG:HD2	4:B7:391:ARG:HG2	2.01	0.42
4:B9:70:PRO:HA	4:B9:73:MET:HE2	2.00	0.42
3:C2:267:PHE:HE2	3:C2:428:LEU:HD11	1.84	0.42
3:C6:207:GLU:HA	3:C6:210:TYR:CG	2.54	0.42
4:D3:396:HIS:HD1	4:D3:397:TRP:CD1	2.35	0.42
3:D8:204:LEU:HD13	3:D8:231:ILE:HD12	2.01	0.42
4:E5:281:TYR:HB3	4:E9:86:ARG:HG2	2.01	0.42
3:E6:100:ALA:O	4:E7:255:VAL:HG11	2.20	0.42
3:E8:119:LEU:HD23	3:E8:122:ILE:HD11	2.00	0.42
7:a:194:ARG:HH12	7:a:198:ARG:NH2	2.17	0.42
7:f:3:GLN:HE22	7:f:178:ARG:HA	1.84	0.42
7:s:181:GLN:HE22	7:s:200:ASP:H	1.67	0.42
7:x:9:PRO:HA	7:x:12:VAL:HG22	2.01	0.42
1:1:449:LEU:HD12	1:1:453:LYS:HE3	2.01	0.42
4:A7:68:LEU:HD12	4:A7:97:ALA:HB2	2.01	0.42
4:B5:45:GLU:HA	7:f:91:PHE:HZ	1.83	0.42
4:B9:258:ILE:HA	4:B9:259:PRO:HD3	1.92	0.42
3:C6:283:HIS:CE1	3:D0:89:PRO:HD3	2.54	0.42
4:D1:105:HIS:CE1	4:D1:150:LEU:HD12	2.55	0.42
4:D3:135:ILE:HB	4:D3:166:THR:HG22	2.01	0.42
4:D3:214:THR:HG22	4:D3:297:LYS:HE2	2.01	0.42
4:D3:325:GLU:HA	4:D3:328:GLU:HG2	2.01	0.42
3:D8:32:PRO:HB2	7:r:102:GLY:HA3	2.01	0.42
4:E7:173:PRO:HD2	4:E7:205:GLU:HG2	2.01	0.42
3:E8:70:LEU:HD12	3:E8:145:THR:HG22	2.00	0.42
3:E8:163:LYS:HD2	3:E8:163:LYS:HA	1.78	0.42
4:F1:73:MET:HB3	4:F1:77:ARG:HH12	1.83	0.42
6:W:65:HIS:CD2	6:W:66:PRO:HD3	2.55	0.42
7:e:164:ARG:HG3	7:e:165:THR:HG23	1.99	0.42
7:r:149:ARG:HD3	7:r:161:TYR:CD1	2.53	0.42
7:u:151:MET:HE1	7:u:163:SER:HA	2.00	0.42
7:w:24:MET:HA	7:w:27:GLN:HE21	1.84	0.42
3:A2:100:ALA:O	4:A3:255:VAL:HG11	2.19	0.42
3:A2:317:LEU:HG	3:A2:319:TYR:HE1	1.84	0.42
4:A3:42:LEU:HB3	4:A3:242:PHE:HE1	1.84	0.42
4:A3:68:LEU:HA	4:A3:93:GLY:HA3	2.00	0.42
3:A4:204:LEU:HD22	3:A4:302:MET:HE1	2.01	0.42
3:A4:243:ARG:HH11	3:A4:243:ARG:HG3	1.85	0.42
3:A6:156:ARG:HA	3:A6:159:VAL:HG12	2.02	0.42
3:A6:338:LYS:NZ	3:A6:339:ARG:HD3	2.34	0.42
4:A7:7:VAL:HB	4:A7:135:ILE:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A7:36:TYR:HB3	7:b:86:ALA:HB1	2.02	0.42
3:A8:156:ARG:HA	3:A8:159:VAL:HG22	2.02	0.42
4:B1:213:ARG:NH2	4:B1:297:LYS:HB3	2.25	0.42
4:B7:46:ARG:HA	4:B7:46:ARG:HD3	1.77	0.42
3:B8:103:PHE:H	3:B8:408:TYR:HE1	1.66	0.42
3:C0:166:LYS:HD2	3:C0:198:THR:HA	2.01	0.42
4:C1:333:VAL:HA	4:C1:336:LYS:NZ	2.34	0.42
3:C8:208:ALA:HB2	3:C8:304:LYS:H	1.85	0.42
4:D1:279:GLN:HE21	4:D1:361:LEU:HD21	1.84	0.42
4:D5:283:ALA:HB2	4:D9:54:ALA:HA	2.00	0.42
4:D9:186:THR:HG22	4:D9:411:ALA:HB1	2.02	0.42
3:E0:10:GLY:O	3:E0:14:ILE:HG12	2.20	0.42
3:E2:16:ILE:HD11	3:E2:231:ILE:HB	2.01	0.42
3:E2:329:ASN:HA	3:E2:332:VAL:HG12	2.00	0.42
3:E4:184:PRO:HG3	3:E4:394:LYS:HG3	2.01	0.42
3:E8:172:TRP:CD2	3:E8:173:PRO:HD2	2.55	0.42
4:E9:40:SER:HB3	4:E9:43:GLN:HG3	2.00	0.42
6:X:115:THR:HG23	6:X:118:ARG:H	1.84	0.42
7:a:199:TRP:CD1	7:a:201:TRP:HB3	2.54	0.42
7:e:13:GLU:HA	7:e:16:ARG:HB2	2.02	0.42
7:j:10:LEU:HD13	7:j:147:HIS:HB2	2.00	0.42
8:l:15:ARG:HD2	8:l:93:CYS:SG	2.59	0.42
7:u:96:TYR:HA	7:u:108:ILE:HD11	2.01	0.42
7:x:19:GLU:HA	7:x:22:ALA:HB3	2.01	0.42
3:A0:175:PRO:HB3	3:A0:390:ARG:HD2	2.01	0.42
3:A2:32:PRO:HA	3:A2:86:LEU:HD13	2.02	0.42
4:A3:318:ARG:HB3	4:A3:357:PRO:HA	2.01	0.42
3:A4:258:ASN:HD22	3:A4:352:LYS:HB3	1.84	0.42
4:A5:232:ALA:HB1	4:A5:268:ILE:HG21	2.01	0.42
4:A5:375:GLN:O	4:A5:379:LYS:HD3	2.19	0.42
3:A6:7:ILE:HD11	3:A6:153:LEU:HD11	2.00	0.42
4:A7:321:MET:HB3	4:A7:363:MET:HE2	2.02	0.42
2:B:207:LEU:HD11	4:D5:359:LYS:HB3	2.00	0.42
4:B1:39:ASP:HA	7:d:90:PRO:HG3	2.01	0.42
4:B5:391:ARG:HA	4:B5:391:ARG:HD2	1.82	0.42
3:B8:124:LYS:HE2	3:B8:124:LYS:HB2	1.83	0.42
3:B8:181:VAL:HG22	4:B9:256:ASN:OD1	2.20	0.42
3:B8:213:CYS:SG	3:B8:222:PRO:HG3	2.59	0.42
3:C2:315:CYS:HB3	3:C2:377:MET:HE1	2.00	0.42
4:C5:326:VAL:HG11	4:C5:351:SER:HB2	2.01	0.42
4:D1:89:ASN:HA	4:D1:119:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D2:401:LYS:HZ3	4:D3:344:TRP:CD1	2.37	0.42
3:D4:405:VAL:HG13	3:D4:418:PHE:HE2	1.83	0.42
3:D8:64:ARG:HH21	3:D8:128:ASN:HD21	1.66	0.42
4:D9:100:ASN:HB3	4:D9:103:LYS:HG2	2.01	0.42
4:D9:262:ARG:HH22	4:D9:417:ASP:CG	2.28	0.42
4:D9:269:GLY:C	4:D9:293:MET:HE1	2.45	0.42
3:E0:398:MET:HE3	4:E1:346:PRO:HD2	2.01	0.42
4:E1:74:ASP:HB3	5:P:559:PHE:CE1	2.54	0.42
4:E5:347:ASN:C	4:E5:347:ASN:HD22	2.26	0.42
3:E6:222:PRO:HD2	4:E7:324:LYS:HZ1	1.85	0.42
4:E7:116:VAL:HA	4:E7:119:VAL:HG12	2.01	0.42
3:E8:121:ARG:HA	3:E8:124:LYS:NZ	2.33	0.42
3:F0:71:GLU:HB3	3:F0:98:ASP:HA	2.00	0.42
3:F0:413:MET:HE2	3:F0:417:GLU:HG3	2.01	0.42
7:i:42:TYR:HA	7:i:45:MET:HG3	2.02	0.42
7:w:165:THR:HG22	7:w:182:PHE:HZ	1.85	0.42
4:A1:313:ALA:HA	4:A1:369:GLY:HA2	2.00	0.42
4:A3:63:ALA:HB3	4:A3:85:PHE:HE1	1.83	0.42
4:A3:105:HIS:CE1	4:A3:150:LEU:HD12	2.54	0.42
4:A9:35:THR:HG22	7:c:83:PRO:HG3	2.01	0.42
4:A9:341:PHE:HB3	4:A9:348:ASN:ND2	2.35	0.42
2:B:256:LEU:HD11	3:D2:29:GLY:HA2	2.02	0.42
3:B0:217:LEU:HD21	3:B0:368:LEU:HD23	2.02	0.42
4:B1:375:GLN:NE2	4:B1:419:VAL:HG13	2.35	0.42
4:B3:57:GLY:HA3	7:e:83:PRO:HB2	2.02	0.42
4:B3:207:LEU:HD21	4:B3:229:VAL:HG23	2.02	0.42
4:B5:326:VAL:O	4:B5:330:MET:HG2	2.19	0.42
3:C0:106:GLY:HA3	3:C0:148:GLY:HA3	2.00	0.42
4:C5:35:THR:HG22	8:k:44:SER:HB3	2.02	0.42
4:C5:105:HIS:CE1	4:C5:150:LEU:HD13	2.55	0.42
3:C6:280:LYS:HA	3:C6:283:HIS:CD2	2.55	0.42
3:C8:282:TYR:CE2	3:D2:85:HIS:HB3	2.55	0.42
4:C9:103:LYS:HB3	4:C9:401:GLU:CD	2.45	0.42
3:D2:214:ARG:HH22	3:D2:215:ARG:HB2	1.85	0.42
4:D3:58:ARG:HH21	4:D3:84:LEU:HD12	1.84	0.42
4:D3:150:LEU:O	4:D3:154:LYS:HG2	2.20	0.42
3:D4:117:LEU:HA	3:D4:120:ASP:HB2	2.01	0.42
3:D6:168:ASN:OD1	3:D6:201:ALA:HA	2.20	0.42
3:D6:230:LEU:HD11	3:D6:275:ILE:HD13	2.01	0.42
3:D8:287:SER:O	3:D8:289:ALA:N	2.52	0.42
4:E1:98:GLY:O	4:E1:99:ASN:ND2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E3:101:TRP:HB3	4:E3:398:TYR:HE2	1.84	0.42
3:E4:141:VAL:HG12	3:E4:187:SER:HA	2.02	0.42
5:O:457:LEU:HA	5:O:460:HIS:ND1	2.33	0.42
7:e:68:LEU:HD23	7:e:73:VAL:HG11	2.02	0.42
7:e:170:VAL:HG13	7:e:183:LEU:HB2	2.02	0.42
7:q:99:MET:HE3	7:q:99:MET:HB2	1.91	0.42
1:2:478:MET:HA	1:2:481:VAL:HG12	2.01	0.42
3:A0:10:GLY:O	3:A0:14:ILE:HG12	2.20	0.42
3:A0:280:LYS:O	3:A0:284:GLU:HG3	2.20	0.42
4:A1:183:TYR:HE1	4:A1:388:MET:HB3	1.84	0.42
3:A2:70:LEU:HB3	3:A2:97:GLU:O	2.19	0.42
3:A2:320:ARG:HG3	3:A2:374:ALA:HB3	2.02	0.42
3:B0:175:PRO:HD3	3:B0:390:ARG:NH2	2.35	0.42
3:B4:181:VAL:HG12	4:B5:347:ASN:O	2.19	0.42
4:B5:392:LYS:HD2	4:B5:395:LEU:HD12	2.00	0.42
3:B6:191:THR:O	3:B6:195:LEU:HD23	2.20	0.42
3:B6:192:HIS:ND1	3:B6:192:HIS:C	2.77	0.42
3:B6:204:LEU:HD13	3:B6:231:ILE:HD12	2.02	0.42
3:B6:332:VAL:HB	3:B6:351:PHE:HD2	1.85	0.42
3:B8:100:ALA:O	4:B9:255:VAL:HG11	2.19	0.42
4:C1:113:ILE:HA	4:C1:116:VAL:HG12	2.02	0.42
3:C2:53:PHE:HB3	3:C2:61:HIS:HB3	2.01	0.42
4:C3:213:ARG:HH22	4:C3:297:LYS:HA	1.84	0.42
4:C5:376:GLU:O	4:C5:380:ARG:HG2	2.19	0.42
4:D1:244:GLY:HA3	4:D1:354:CYS:HA	2.01	0.42
4:D1:286:VAL:HA	4:D1:363:MET:HE1	2.02	0.42
3:D6:274:PRO:HG3	3:D6:286:LEU:HD22	2.01	0.42
4:D7:102:ALA:HB2	4:D7:398:TYR:HA	2.01	0.42
4:D9:5:VAL:HB	4:D9:133:PHE:HD2	1.85	0.42
4:D9:309:ARG:H	4:D9:372:THR:HG22	1.85	0.42
4:E1:195:ASN:C	4:E1:195:ASN:HD22	2.27	0.42
3:E4:195:LEU:HD21	3:E4:428:LEU:HD22	2.02	0.42
3:E6:12:ALA:HB3	3:E6:140:ALA:HB2	2.02	0.42
3:E8:222:PRO:HD2	4:E9:324:LYS:HE2	2.02	0.42
2:F:258:PRO:HA	2:F:259:PRO:HD3	1.87	0.42
3:F0:72:PRO:HG2	4:F1:2:ARG:HH21	1.84	0.42
7:e:68:LEU:HD21	7:e:111:ILE:HD11	2.00	0.42
7:m:149:ARG:HD2	7:m:162:GLY:O	2.19	0.42
7:m:202:ARG:H	7:m:202:ARG:HG2	1.74	0.42
7:o:63:ILE:HB	7:o:67:HIS:NE2	2.34	0.42
7:q:14:LYS:HB2	7:q:47:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A1:8:GLN:HB3	4:A1:13:GLY:C	2.44	0.42
3:A2:208:ALA:O	3:A2:212:ILE:HG12	2.20	0.42
4:A3:65:LEU:HB3	4:A3:73:MET:HE3	2.01	0.42
3:A4:262:TYR:HB2	3:A4:265:ILE:HG22	2.02	0.42
3:A6:105:ARG:HA	3:A6:109:THR:HG22	2.02	0.42
4:A7:274:THR:HG22	4:A7:282:ARG:HD2	2.02	0.42
3:B0:319:TYR:CD1	3:B0:375:VAL:HG22	2.55	0.42
3:B2:219:ILE:HG12	7:g:198:ARG:NH2	2.34	0.42
4:B3:119:VAL:HA	4:B3:122:LYS:HB2	2.02	0.42
4:B5:101:TRP:CZ3	4:B5:187:LEU:HB3	2.54	0.42
3:B6:259:LEU:HD21	3:B6:316:CYS:HB2	2.01	0.42
4:C1:284:LEU:HD12	4:C1:284:LEU:HA	1.95	0.42
3:C4:66:VAL:HA	3:C4:91:GLN:HB2	2.02	0.42
3:C4:217:LEU:HD21	3:C4:275:ILE:HG22	2.02	0.42
3:C6:5:ILE:HD13	3:C6:64:ARG:HB3	2.02	0.42
3:C6:119:LEU:HA	3:C6:122:ILE:HG12	2.01	0.42
3:C8:156:ARG:NH1	3:C8:156:ARG:HA	2.35	0.42
3:D2:15:GLN:HE21	3:D2:16:ILE:HG13	1.85	0.42
4:D5:19:LYS:HD2	4:D5:22:GLU:HG3	2.02	0.42
4:D5:235:GLY:HA2	4:D5:318:ARG:HH11	1.85	0.42
3:D8:225:THR:O	3:D8:229:ARG:HG2	2.19	0.42
3:E0:88:HIS:CD2	3:E0:89:PRO:HD2	2.53	0.42
3:E0:237:SER:HA	3:E0:320:ARG:HD3	2.02	0.42
4:E3:198:GLU:HB2	4:E3:266:PHE:HE2	1.84	0.42
3:E4:105:ARG:HE	4:E5:251:ARG:HH21	1.67	0.42
4:E5:73:MET:O	4:E5:77:ARG:HG3	2.20	0.42
4:E5:178:THR:HA	3:E6:352:LYS:NZ	2.35	0.42
4:E9:206:ALA:HB2	4:E9:302:ALA:HB2	2.01	0.42
3:F0:84:ARG:HD3	3:F0:85:HIS:CE1	2.54	0.42
3:F0:260:VAL:HG12	3:F0:266:HIS:HA	2.02	0.42
3:F0:352:LYS:HE3	3:F0:352:LYS:HB2	1.85	0.42
7:e:25:GLN:HA	7:e:28:LYS:NZ	2.34	0.42
7:h:51:PRO:HD2	7:h:54:SER:HB2	2.02	0.42
7:x:165:THR:HG22	7:x:182:PHE:HZ	1.84	0.42
4:A5:68:LEU:HD23	4:A5:93:GLY:HA3	2.02	0.42
3:A6:173:PRO:HG3	3:A6:183:GLU:OE2	2.20	0.42
3:A6:301:MET:HE1	3:A6:377:MET:HE1	2.01	0.42
3:A6:370:LYS:HA	3:A6:370:LYS:HE3	2.01	0.42
4:A7:271:ALA:HB3	4:A7:365:VAL:HG12	2.02	0.42
4:A9:28:HIS:CE1	4:A9:241:ARG:HD2	2.55	0.42
3:B4:383:ALA:O	3:B4:386:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B5:284:LEU:HD12	4:B5:284:LEU:HA	1.84	0.42
3:B8:5:ILE:HG12	3:B8:132:LEU:HD11	2.02	0.42
4:B9:190:HIS:HB2	4:B9:414:ASN:HD22	1.85	0.42
4:B9:375:GLN:NE2	4:B9:422:TYR:HB3	2.35	0.42
4:C3:377:MET:HE2	4:C3:377:MET:HB3	1.94	0.42
3:C4:107:HIS:HA	3:C4:152:LEU:HD22	2.02	0.42
4:C7:330:MET:HA	4:C7:333:VAL:HG22	2.01	0.42
4:C7:398:TYR:HB3	4:C7:403:MET:HG3	2.02	0.42
3:C8:82:THR:HA	7:m:98:THR:HG23	2.02	0.42
4:C9:51:TYR:HB3	4:C9:59:PHE:HB3	2.02	0.42
4:D1:13:GLY:HA2	4:D1:16:ILE:HG22	2.02	0.42
3:D2:26:LEU:HD21	3:D2:363:VAL:HG12	2.02	0.42
4:D7:44:LEU:HD21	7:q:90:PRO:HG2	2.01	0.42
3:E0:208:ALA:HB2	3:E0:304:LYS:HB2	2.01	0.42
3:E2:172:TRP:HZ2	3:E2:391:MET:HG3	1.84	0.42
4:E3:392:LYS:HA	4:E3:392:LYS:HD3	1.92	0.42
4:E5:97:ALA:HB3	4:E5:143:THR:HG22	2.01	0.42
3:E8:32:PRO:HG3	3:E8:83:TYR:HE1	1.85	0.42
4:E9:163:ILE:HD13	4:E9:251:ARG:HB2	2.02	0.42
4:E9:256:ASN:HB3	4:E9:257:LEU:HD12	2.02	0.42
2:H:204:PRO:HA	2:H:205:PRO:HD3	1.88	0.42
2:I:234:LYS:HA	2:I:234:LYS:HD2	1.83	0.42
7:a:74:ALA:HB2	7:a:199:TRP:CH2	2.55	0.42
7:g:183:LEU:HD11	7:g:199:TRP:NE1	2.35	0.42
7:o:126:ARG:HD2	7:o:129:MET:HB2	2.01	0.42
7:p:23:LEU:HG	7:p:38:LEU:HD11	2.02	0.42
7:u:184:PRO:HD2	7:u:195:ALA:HB1	2.02	0.42
7:w:107:LYS:HD3	7:w:201:TRP:CD2	2.55	0.42
4:A1:215:LEU:HD12	4:A1:273:LEU:HD22	2.02	0.42
4:A1:254:ALA:O	4:A1:258:ILE:HG22	2.20	0.42
3:A2:75:VAL:HG21	3:A2:94:SER:HA	2.01	0.42
3:A4:53:PHE:HB3	3:A4:61:HIS:HB3	2.02	0.42
3:A6:298:PRO:HB3	3:A6:307:PRO:HD2	2.02	0.42
3:A6:328:VAL:HG21	3:A6:355:ILE:HD11	2.01	0.42
4:A9:7:VAL:HG11	4:A9:151:LEU:HD22	2.02	0.42
3:B2:288:VAL:HG13	3:B2:319:TYR:HE1	1.84	0.42
3:B6:5:ILE:HG12	3:B6:132:LEU:HD11	2.00	0.42
3:B6:124:LYS:HB2	3:B6:124:LYS:HE2	1.76	0.42
4:C1:186:THR:HG23	4:C1:381:VAL:HG12	2.00	0.42
4:C9:276:ARG:HA	4:C9:279:GLN:HB2	2.02	0.42
3:D0:392:ASP:HA	3:D0:422:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D2:209:ILE:HB	3:D2:227:LEU:HG	2.02	0.42
4:D5:105:HIS:CD2	4:D5:150:LEU:HD12	2.55	0.42
3:D8:422:ARG:NH2	3:D8:425:LEU:HD22	2.34	0.42
3:E0:166:LYS:HA	3:E0:166:LYS:HD3	1.93	0.42
4:E1:20:PHE:CD1	4:E1:233:MET:HE2	2.54	0.42
3:E6:16:ILE:HD11	9:E7:501:GTP:HN21	1.85	0.42
3:E8:339:ARG:HA	3:E8:339:ARG:HD2	1.84	0.42
4:E9:187:LEU:HA	4:E9:190:HIS:CE1	2.54	0.42
4:E9:321:MET:HE2	4:E9:353:VAL:HG13	2.01	0.42
4:F1:276:ARG:NH2	6:W:97:LEU:HA	2.34	0.42
4:F1:299:MET:HE2	4:F1:299:MET:HB2	1.89	0.42
5:P:516:ASP:HB3	5:P:520:LEU:HD23	2.01	0.42
7:d:9:PRO:HA	7:d:12:VAL:HG22	2.01	0.42
7:o:139:PRO:O	7:o:143:ILE:HG12	2.20	0.42
7:o:154:TYR:HE1	7:o:158:THR:HG22	1.85	0.42
7:q:164:ARG:HD2	7:q:164:ARG:HA	1.78	0.42
7:u:85:CYS:HA	7:u:168:PRO:HG3	2.02	0.42
7:u:119:ARG:NH2	7:u:122:PHE:HD1	2.17	0.42
7:w:75:LEU:HD23	7:w:111:ILE:HB	2.01	0.42
7:x:90:PRO:HA	7:x:93:LEU:HD12	2.01	0.42
3:A0:282:TYR:HD1	7:a:202:ARG:HH11	1.67	0.41
3:A2:205:ASP:HB2	3:A2:303:ALA:HA	2.01	0.41
4:A3:358:PRO:HB2	4:A3:361:LEU:HD23	2.01	0.41
3:A6:238:LEU:HD12	3:A6:238:LEU:HA	1.78	0.41
4:A7:183:TYR:HE1	4:A7:388:MET:HB2	1.85	0.41
3:A8:294:SER:HA	3:A8:297:GLU:HG2	2.01	0.41
3:B0:137:MET:HB3	3:B0:168:ASN:ND2	2.34	0.41
3:B0:264:ARG:HH12	3:B0:428:LEU:HA	1.85	0.41
4:B1:230:SER:HA	4:B1:233:MET:HG2	2.02	0.41
3:B2:9:VAL:HG12	3:B2:68:LEU:HB2	2.01	0.41
4:B3:259:PRO:HD2	4:B3:263:LEU:HD11	2.01	0.41
3:B4:280:LYS:HB2	3:B4:280:LYS:HE2	1.81	0.41
3:B6:12:ALA:O	3:B6:16:ILE:HG12	2.20	0.41
3:B8:251:ASP:H	3:B8:254:GLU:HG3	1.85	0.41
3:C0:107:HIS:HA	3:C0:152:LEU:HD11	2.01	0.41
4:C1:220:PRO:HD2	3:C2:326:LYS:NZ	2.35	0.41
4:C9:23:VAL:HG11	4:C9:230:SER:HB3	2.01	0.41
2:D:218:ASP:HB2	3:D8:225:THR:HG21	2.02	0.41
3:D0:78:VAL:HA	2:K:215:TYR:CE2	2.55	0.41
3:D0:207:GLU:HA	3:D0:210:TYR:HB2	2.02	0.41
3:D0:223:THR:OG1	3:D0:225:THR:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D1:6:HIS:CE1	4:D1:8:GLN:HE21	2.38	0.41
4:D1:309:ARG:HH11	4:D1:342:VAL:HA	1.85	0.41
4:D3:397:TRP:CZ3	3:D4:256:GLN:HB3	2.55	0.41
3:D4:30:ILE:HD12	3:D4:61:HIS:CD2	2.54	0.41
3:D6:84:ARG:HH11	7:q:98:THR:HG21	1.85	0.41
4:D7:34:GLY:HA3	4:D7:58:ARG:HG2	2.01	0.41
4:D7:282:ARG:NH1	4:E1:86:ARG:HH21	2.18	0.41
4:E1:267:LEU:HD12	4:E1:374:ILE:HD12	2.02	0.41
3:E2:100:ALA:O	4:E3:255:VAL:HG11	2.20	0.41
3:E4:174:SER:OG	3:E4:207:GLU:HG2	2.20	0.41
3:E6:136:LEU:HD23	3:E6:235:ILE:HD11	2.02	0.41
4:E9:198:GLU:HA	4:E9:264:HIS:HD1	1.85	0.41
3:F0:175:PRO:HD2	3:F0:304:LYS:HE2	2.01	0.41
2:J:210:HIS:NE2	7:n:163:SER:HB2	2.35	0.41
7:e:99:MET:HE2	7:e:108:ILE:HG23	2.02	0.41
7:e:129:MET:HE2	7:e:131:TRP:HE1	1.85	0.41
7:f:5:VAL:HB	7:f:161:TYR:CE2	2.54	0.41
8:l:17:GLN:HE22	7:n:12:VAL:C	2.28	0.41
7:m:64:PRO:HD2	7:m:67:HIS:CE1	2.55	0.41
7:p:10:LEU:HD23	7:p:147:HIS:CE1	2.55	0.41
7:s:147:HIS:HD2	7:s:148:PHE:CZ	2.38	0.41
1:2:461:ALA:O	1:2:465:LYS:HD2	2.20	0.41
3:A2:403:ALA:HA	4:A3:260:PHE:CE1	2.56	0.41
4:A3:187:LEU:HD11	4:A3:408:PHE:HE1	1.85	0.41
4:A3:316:MET:HG3	4:A3:352:SER:HB3	2.00	0.41
3:A4:222:PRO:HG2	4:A5:324:LYS:HE2	2.02	0.41
3:A8:311:LYS:HE3	3:A8:344:VAL:HG12	2.02	0.41
3:B0:107:HIS:HA	3:B0:152:LEU:HD22	2.02	0.41
4:B1:332:ASN:O	4:B1:336:LYS:HG2	2.19	0.41
4:B3:283:ALA:HB2	4:B7:54:ALA:HA	2.01	0.41
4:B7:274:THR:HG21	4:B7:282:ARG:HE	1.85	0.41
4:B7:284:LEU:HG	4:C1:55:THR:HG21	2.02	0.41
4:B7:294:PHE:CE1	4:B7:333:VAL:HG11	2.55	0.41
2:C:233:VAL:HG21	5:P:308:TRP:HH2	1.85	0.41
4:C1:66:MET:HG3	4:C1:116:VAL:HG21	2.03	0.41
4:C1:200:GLN:OE1	4:C1:266:PHE:HB2	2.20	0.41
3:C2:31:GLN:HE21	3:C2:31:GLN:HB2	1.71	0.41
3:C4:104:ALA:HB1	3:C4:411:GLU:HB3	2.02	0.41
4:C5:66:MET:HE1	4:C5:147:MET:HG3	2.02	0.41
3:C6:102:ASN:ND2	4:C7:255:VAL:HG11	2.32	0.41
3:C6:254:GLU:O	3:C6:258:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D4:274:PRO:HD2	3:D4:374:ALA:HA	2.01	0.41
4:D5:155:VAL:HA	4:D5:158:GLU:HB2	2.01	0.41
3:D6:398:MET:HG3	4:D7:345:ILE:HD13	2.01	0.41
3:E2:48:ALA:O	3:E2:51:THR:HG23	2.19	0.41
3:E2:195:LEU:HD11	3:E2:428:LEU:HD22	2.02	0.41
4:E5:290:THR:HG21	4:E5:329:GLN:HB3	2.02	0.41
4:E7:149:THR:HA	4:E7:152:ILE:HD12	2.01	0.41
4:E9:57:GLY:HA3	7:w:83:PRO:HB2	2.02	0.41
5:O:464:LYS:HD2	5:O:465:LEU:H	1.85	0.41
7:a:155:GLU:HG2	7:a:156:VAL:HG23	2.02	0.41
7:d:3:GLN:HG3	7:d:178:ARG:HB2	2.02	0.41
7:r:82:ASP:HA	7:r:83:PRO:HD3	1.94	0.41
7:t:108:ILE:HB	7:t:199:TRP:CH2	2.55	0.41
3:A2:256:GLN:O	3:A2:260:VAL:HG12	2.20	0.41
4:A3:398:TYR:HB3	4:A3:403:MET:HG3	2.03	0.41
3:A4:62:VAL:HA	3:A4:63:PRO:HD3	1.95	0.41
3:A8:33:ASP:HB3	7:c:103:GLY:HA2	2.01	0.41
4:A9:288:GLU:C	4:A9:292:GLN:HE22	2.28	0.41
4:B1:116:VAL:HA	4:B1:119:VAL:HG12	2.01	0.41
4:B3:70:PRO:HA	4:B3:73:MET:HE2	2.03	0.41
3:B6:296:PHE:CD2	3:B6:335:ILE:HG12	2.55	0.41
4:B9:8:GLN:HE22	4:B9:63:ALA:HB1	1.85	0.41
3:C2:65:CYS:H	3:C2:91:GLN:HE21	1.68	0.41
3:C4:101:ASN:HB3	3:C4:182:VAL:HG21	2.01	0.41
3:D0:107:HIS:HD2	3:D0:152:LEU:HB2	1.85	0.41
4:D3:311:LEU:HD23	4:D3:312:THR:HG23	2.02	0.41
4:D7:135:ILE:HG21	4:D7:152:ILE:HD11	2.02	0.41
3:D8:310:GLY:HA3	3:D8:383:ALA:HB2	2.01	0.41
3:E0:222:PRO:HD2	4:E1:324:LYS:HZ1	1.85	0.41
4:E3:7:VAL:HG11	4:E3:151:LEU:HD23	2.01	0.41
4:E3:330:MET:HA	4:E3:333:VAL:HG12	2.03	0.41
3:E4:181:VAL:H	4:E5:350:LYS:HZ3	1.67	0.41
3:E6:221:ARG:HA	4:E7:324:LYS:HZ1	1.85	0.41
4:E7:4:ILE:HD13	4:E7:4:ILE:HA	1.95	0.41
4:E7:156:ARG:HA	4:E7:156:ARG:HD2	1.79	0.41
4:E7:309:ARG:O	4:E7:372:THR:HG22	2.20	0.41
3:F0:205:ASP:HB3	3:F0:303:ALA:HA	2.02	0.41
4:F1:222:TYR:HA	4:F1:225:LEU:HD12	2.02	0.41
2:K:239:LEU:HD13	2:K:240:PRO:HD2	2.02	0.41
7:r:79:ASP:HB3	7:r:82:ASP:HB2	2.02	0.41
3:A2:406:HIS:HA	3:A2:409:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A3:192:LEU:HD21	4:A3:199:VAL:HG21	2.02	0.41
3:A4:247:ALA:HB3	3:A4:355:ILE:HB	2.03	0.41
4:A7:101:TRP:CD1	4:A7:146:GLY:HA2	2.55	0.41
4:A7:136:THR:HG22	4:A7:167:PHE:HB2	2.01	0.41
4:A7:308:GLY:HA3	4:A7:373:ALA:HB2	2.03	0.41
3:A8:64:ARG:HH21	3:A8:128:ASN:ND2	2.18	0.41
4:B1:311:LEU:HD23	4:B1:312:THR:HG23	2.01	0.41
3:B2:21:TRP:CH2	3:B2:65:CYS:HB2	2.56	0.41
3:B2:387:VAL:HG12	3:B2:390:ARG:HH22	1.85	0.41
4:B3:289:LEU:HD23	4:B3:289:LEU:HA	1.93	0.41
3:B4:285:GLN:HB3	3:B8:56:THR:HA	2.03	0.41
4:B7:173:PRO:HG3	4:B7:380:ARG:NH2	2.35	0.41
3:C0:119:LEU:HD23	3:C0:122:ILE:HG13	2.03	0.41
4:C5:284:LEU:HD12	4:C5:284:LEU:HA	1.91	0.41
4:C9:117:LEU:HA	4:C9:120:VAL:HG12	2.03	0.41
4:C9:117:LEU:HA	4:C9:117:LEU:HD23	1.89	0.41
4:C9:173:PRO:HD2	4:C9:205:GLU:OE2	2.21	0.41
2:D:221:PRO:HD3	3:D8:82:THR:HG21	2.01	0.41
3:D0:319:TYR:HB2	3:D0:355:ILE:HG22	2.00	0.41
4:D1:138:SER:HA	4:D1:169:VAL:HG22	2.02	0.41
3:D4:252:VAL:HA	3:D4:255:PHE:CD2	2.55	0.41
4:D5:274:THR:HG21	4:D5:282:ARG:HG3	2.02	0.41
3:D6:3:GLU:HA	3:D6:51:THR:HA	2.03	0.41
3:D6:137:MET:HE1	3:D6:139:ASN:CG	2.46	0.41
3:D6:384:ILE:HA	3:D6:387:VAL:HG12	2.03	0.41
4:E1:33:THR:HG23	4:E1:35:THR:HG23	2.03	0.41
3:E4:195:LEU:HB3	3:E4:264:ARG:HH21	1.84	0.41
4:E5:66:MET:SD	4:E5:147:MET:HE3	2.60	0.41
3:F0:17:GLY:HA2	3:F0:20:CYS:HB2	2.02	0.41
6:X:123:PRO:HG2	7:w:101:GLU:HG2	2.02	0.41
7:e:57:ASN:HB3	7:e:63:ILE:HD11	2.02	0.41
7:s:14:LYS:HB2	7:s:47:LEU:HD13	2.02	0.41
7:s:146:ARG:HH21	7:s:156:VAL:HG21	1.85	0.41
7:u:50:PHE:CD1	7:u:140:LEU:HD21	2.56	0.41
3:A0:398:MET:HB3	3:A0:403:ALA:HB3	2.03	0.41
4:A1:183:TYR:CE1	4:A1:388:MET:HB3	2.55	0.41
4:A3:356:ILE:HD12	4:A3:357:PRO:HD2	2.02	0.41
4:A5:77:ARG:HD3	5:P:265:PHE:CG	2.54	0.41
3:A6:36:MET:HA	3:A6:37:PRO:HD3	1.88	0.41
4:A9:130:LEU:HB3	4:A9:162:ARG:NH1	2.35	0.41
3:B4:178:SER:HB3	4:B5:347:ASN:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B4:280:LYS:HG2	3:B8:88:HIS:CE1	2.56	0.41
2:C:207:LEU:HD21	5:O:317:ARG:NH1	2.36	0.41
3:C0:413:MET:HE2	3:C0:413:MET:HB3	1.85	0.41
4:C1:8:GLN:HB3	4:C1:65:LEU:HA	2.03	0.41
3:C4:73:THR:HG22	4:C5:46:ARG:CZ	2.51	0.41
3:C4:338:LYS:HB2	3:C4:338:LYS:HE3	1.75	0.41
3:C6:213:CYS:HA	3:C6:217:LEU:HD13	2.03	0.41
4:C9:268:ILE:HA	4:C9:367:PHE:O	2.21	0.41
3:D2:11:GLN:HG2	3:D2:74:VAL:HG21	2.03	0.41
4:D3:164:MET:HE2	4:D3:164:MET:HB2	1.79	0.41
4:D3:279:GLN:HE21	5:P:519:LEU:HD21	1.85	0.41
4:D5:330:MET:H	4:D5:330:MET:HG2	1.60	0.41
4:E1:167:PHE:CD1	4:E1:200:GLN:HB2	2.55	0.41
4:E1:172:SER:HB2	4:E1:175:VAL:HG12	2.01	0.41
4:E3:66:MET:HE1	4:E3:151:LEU:HD22	2.01	0.41
4:E5:68:LEU:HA	4:E5:93:GLY:HA3	2.03	0.41
3:E6:33:ASP:HB2	7:v:102:GLY:O	2.21	0.41
4:E7:208:TYR:CE1	4:E7:225:LEU:HD11	2.55	0.41
4:E7:230:SER:HA	4:E7:233:MET:HB3	2.03	0.41
3:F0:141:VAL:HG21	3:F0:172:TRP:HE3	1.84	0.41
5:P:555:ARG:HD2	5:P:555:ARG:HA	1.92	0.41
6:V:123:PRO:HA	6:V:124:PRO:HD3	1.94	0.41
7:a:53:GLY:HA2	7:a:62:VAL:HG21	2.01	0.41
7:c:119:ARG:HH22	7:c:137:GLU:HB3	1.85	0.41
8:l:17:GLN:HG3	8:l:22:VAL:HG12	2.02	0.41
7:m:84:LYS:HE3	7:m:84:LYS:HB3	1.98	0.41
7:p:65:GLN:NE2	7:p:206:PHE:HZ	2.18	0.41
7:w:126:ARG:HH11	7:w:129:MET:HB2	1.85	0.41
3:A0:51:THR:HG23	3:A0:52:PHE:HD1	1.85	0.41
4:A1:3:GLU:HB3	4:A1:130:LEU:HB2	2.02	0.41
3:A2:133:GLN:NE2	3:A2:251:ASP:HB2	2.36	0.41
4:A3:211:CYS:HA	4:A3:215:LEU:HB3	2.03	0.41
4:A7:134:GLN:NE2	4:A7:136:THR:HG23	2.36	0.41
4:A9:118:ASP:O	4:A9:122:LYS:HG2	2.21	0.41
4:B1:238:CYS:HB3	4:B1:318:ARG:NH1	2.35	0.41
3:B2:124:LYS:HD3	3:B2:124:LYS:HA	1.79	0.41
4:B7:291:GLN:NE2	4:B7:291:GLN:C	2.78	0.41
4:B9:249:ASP:H	4:B9:252:LYS:HB3	1.85	0.41
4:C1:153:SER:HA	4:C1:195:ASN:HD21	1.86	0.41
4:C1:389:PHE:HD1	4:C1:395:LEU:HD21	1.86	0.41
3:C2:423:GLU:HA	3:C2:426:ALA:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C3:34:GLY:HA3	4:C3:58:ARG:HB2	2.03	0.41
3:C4:133:GLN:HE22	3:C4:242:LEU:HG	1.86	0.41
4:C5:86:ARG:HG2	4:C5:88:ASP:H	1.86	0.41
3:C6:229:ARG:HD3	3:C6:363:VAL:HG21	2.02	0.41
4:C7:236:VAL:HG13	4:C7:237:THR:HG23	2.02	0.41
3:C8:102:ASN:HB3	3:C8:105:ARG:HB2	2.03	0.41
3:D0:103:PHE:HD2	3:D0:413:MET:HE1	1.86	0.41
3:D2:64:ARG:HA	3:D2:125:LEU:HD11	2.02	0.41
4:D3:75:SER:HA	5:P:508:TYR:CE1	2.53	0.41
4:D7:398:TYR:HB3	4:D7:403:MET:HE2	2.03	0.41
4:D9:174:LYS:HD2	4:D9:174:LYS:HA	1.91	0.41
3:E0:167:LEU:HD13	3:E0:200:VAL:HG13	2.03	0.41
4:E3:287:PRO:HB3	4:E3:329:GLN:HE22	1.86	0.41
3:E8:262:TYR:HB2	3:E8:265:ILE:HG12	2.02	0.41
7:c:14:LYS:NZ	7:c:45:MET:HB3	2.36	0.41
7:d:85:CYS:HA	7:d:168:PRO:HG3	2.02	0.41
7:e:99:MET:HE3	7:e:107:LYS:HG3	2.03	0.41
7:n:41:ASN:HB2	7:n:44:ASP:HB2	2.02	0.41
7:p:139:PRO:O	7:p:143:ILE:HG12	2.21	0.41
7:s:112:PHE:HE1	7:s:114:SER:HB2	1.85	0.41
7:u:90:PRO:HA	7:u:93:LEU:HD12	2.03	0.41
4:A1:167:PHE:CZ	4:A1:233:MET:HG2	2.56	0.41
3:A4:398:MET:HE2	4:A5:346:PRO:HD2	2.02	0.41
3:A6:283:HIS:HB3	3:B0:62:VAL:HG11	2.03	0.41
4:A7:206:ALA:HB2	4:A7:302:ALA:HB2	2.03	0.41
3:A8:121:ARG:HA	3:A8:121:ARG:HD2	1.83	0.41
3:B2:140:ALA:HA	3:B2:171:SER:HB3	2.02	0.41
4:B3:356:ILE:HD12	2:E:241:PHE:HE2	1.85	0.41
4:B5:9:GLY:HA2	4:B5:66:MET:HB2	2.01	0.41
4:C3:5:VAL:HB	4:C3:133:PHE:HD1	1.85	0.41
4:C3:49:VAL:HG11	4:C3:241:ARG:HG2	2.03	0.41
4:C3:86:ARG:HH21	4:C3:87:PRO:HD2	1.85	0.41
4:C7:113:ILE:HA	4:C7:116:VAL:HG12	2.03	0.41
4:C9:328:GLU:HA	4:C9:331:LEU:HB3	2.02	0.41
3:D0:209:ILE:HD13	3:D0:231:ILE:HD11	2.03	0.41
3:E0:167:LEU:HA	3:E0:200:VAL:HG13	2.03	0.41
4:E3:43:GLN:H	4:E3:43:GLN:HG2	1.72	0.41
3:F0:122:ILE:HG21	3:F0:157:LEU:HD11	2.03	0.41
5:O:317:ARG:HA	5:O:317:ARG:HD3	1.80	0.41
7:a:85:CYS:SG	7:a:168:PRO:HB3	2.61	0.41
7:d:97:ARG:HH12	7:f:160:GLY:HA3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:i:154:TYR:HE2	7:i:158:THR:HG22	1.86	0.41
8:l:58:LYS:HE2	8:l:58:LYS:HA	2.02	0.41
7:o:42:TYR:HA	7:o:45:MET:SD	2.61	0.41
7:r:71:LYS:HE2	7:r:71:LYS:HB2	1.82	0.41
7:t:191:GLU:O	7:t:195:ALA:HB2	2.21	0.41
7:x:147:HIS:HD2	7:x:148:PHE:CE2	2.39	0.41
3:A2:11:GLN:HA	3:A2:14:ILE:HG22	2.02	0.41
4:A3:249:ASP:H	4:A3:252:LYS:HB3	1.85	0.41
3:A8:11:GLN:HB3	3:A8:74:VAL:HG11	2.01	0.41
4:A9:298:ASN:O	4:A9:298:ASN:ND2	2.51	0.41
3:C4:311:LYS:HB3	3:C4:382:THR:OG1	2.20	0.41
4:C5:291:GLN:NE2	4:C5:292:GLN:HG3	2.36	0.41
4:C7:149:THR:HA	4:C7:152:ILE:HG22	2.03	0.41
4:C9:66:MET:HE1	4:C9:147:MET:SD	2.60	0.41
3:D0:335:ILE:HD13	3:D0:335:ILE:HA	1.93	0.41
4:D3:73:MET:HE3	4:D3:90:PHE:HD2	1.85	0.41
3:D6:280:LYS:HB3	3:D6:280:LYS:HE3	1.88	0.41
4:D7:289:LEU:HD23	4:D7:289:LEU:HA	1.87	0.41
3:D8:401:LYS:HD2	4:D9:344:TRP:CD2	2.56	0.41
4:E1:5:VAL:HG21	4:E1:130:LEU:HD22	2.01	0.41
4:E1:8:GLN:HE21	4:E1:14:ASN:HA	1.86	0.41
4:E1:259:PRO:HG2	4:E1:311:LEU:HD21	2.02	0.41
3:E2:73:THR:HB	4:E3:2:ARG:HH22	1.86	0.41
4:E3:39:ASP:HA	7:t:90:PRO:HG3	2.03	0.41
4:E5:66:MET:HG3	4:E5:116:VAL:HG21	2.03	0.41
3:F0:124:LYS:HE2	3:F0:124:LYS:HB2	1.79	0.41
4:F1:28:HIS:CE1	4:F1:241:ARG:HD2	2.55	0.41
4:F1:86:ARG:HD3	4:F1:88:ASP:HB3	2.03	0.41
4:F1:424:GLN:HE21	4:F1:424:GLN:HB2	1.65	0.41
5:O:464:LYS:HE3	5:O:466:VAL:HG22	2.01	0.41
7:f:3:GLN:HE22	7:f:179:GLU:H	1.68	0.41
7:i:205:LYS:HA	7:i:205:LYS:HD2	1.92	0.41
7:m:183:LEU:HA	7:m:184:PRO:HD3	1.88	0.41
7:o:57:ASN:ND2	7:o:59:ASN:H	2.19	0.41
7:t:37:GLN:C	7:t:37:GLN:HE21	2.29	0.41
7:t:126:ARG:HA	7:t:129:MET:HE1	2.01	0.41
7:v:112:PHE:HD2	7:v:133:SER:HB2	1.85	0.41
3:A0:91:GLN:HE22	3:A0:125:LEU:HD22	1.86	0.41
4:A1:393:ALA:HB1	3:A2:261:PRO:HB2	2.03	0.41
3:A2:286:LEU:HD13	3:A2:286:LEU:HA	1.84	0.41
4:A3:6:HIS:CD2	4:A3:134:GLN:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A4:71:GLU:OE1	3:A4:73:THR:HG22	2.21	0.41
3:A4:108:TYR:CE2	3:A4:413:MET:HB3	2.54	0.41
4:A5:89:ASN:HA	4:A5:119:VAL:HG21	2.02	0.41
4:A5:267:LEU:HG	4:A5:301:CYS:HB3	2.03	0.41
3:A8:167:LEU:HD13	3:A8:200:VAL:HB	2.03	0.41
4:A9:237:THR:HG23	4:A9:241:ARG:HH21	1.86	0.41
3:B0:304:LYS:HD3	3:B0:304:LYS:HA	1.80	0.41
3:B0:312:TYR:CE1	3:B0:341:ILE:HG13	2.55	0.41
4:B1:267:LEU:HD23	4:B1:371:SER:HB3	2.02	0.41
4:B1:386:THR:HB	4:B1:390:ARG:NH1	2.35	0.41
3:B2:10:GLY:O	3:B2:14:ILE:HG12	2.21	0.41
3:B2:88:HIS:HA	3:B2:89:PRO:HD3	1.92	0.41
3:B2:364:PRO:HG2	2:E:254:LYS:HB3	2.03	0.41
3:B6:188:VAL:HA	3:B6:191:THR:HG22	2.01	0.41
4:B7:375:GLN:HG2	4:B7:423:GLN:HE21	1.86	0.41
4:C5:207:LEU:HB3	4:C5:225:LEU:HD11	2.03	0.41
4:C5:281:TYR:HB2	4:C9:86:ARG:CZ	2.50	0.41
3:C6:177:VAL:HG11	3:C6:210:TYR:HE2	1.86	0.41
3:C6:262:TYR:HE2	3:C6:435:VAL:HG22	1.86	0.41
4:C9:247:ASN:C	4:C9:247:ASN:ND2	2.78	0.41
3:D0:25:CYS:SG	3:D0:86:LEU:HD11	2.61	0.41
3:D0:32:PRO:HA	3:D0:86:LEU:HD12	2.03	0.41
3:D0:216:ASN:HB3	3:D0:275:ILE:O	2.20	0.41
3:D0:398:MET:HG3	4:D1:345:ILE:HD13	2.03	0.41
4:D1:317:PHE:CD2	4:D1:321:MET:HE1	2.56	0.41
3:D4:150:GLY:O	3:D4:154:LEU:HD23	2.20	0.41
3:D6:200:VAL:HG13	3:D6:268:MET:HE2	2.03	0.41
3:D8:287:SER:C	3:D8:289:ALA:N	2.78	0.41
3:D8:388:PHE:HB3	3:D8:425:LEU:HD21	2.02	0.41
2:E:254:LYS:HA	2:E:254:LYS:HE3	2.02	0.41
3:E0:235:ILE:HD12	3:E0:238:LEU:HB3	2.02	0.41
3:E0:364:PRO:HB2	2:F:254:LYS:HZ1	1.84	0.41
4:E1:68:LEU:HD11	4:E1:147:MET:HG3	2.03	0.41
4:E1:99:ASN:HA	4:E1:142:GLY:N	2.36	0.41
3:E2:63:PRO:HG2	3:E2:87:PHE:CD1	2.56	0.41
3:E2:183:GLU:CD	3:E2:184:PRO:HD3	2.46	0.41
4:E3:273:LEU:HD23	4:E3:273:LEU:HA	1.88	0.41
4:E5:39:ASP:HA	7:u:90:PRO:HG3	2.03	0.41
4:E5:193:VAL:HA	4:E5:264:HIS:CE1	2.51	0.41
3:E6:2:ARG:HA	3:E6:133:GLN:HE22	1.85	0.41
3:E6:180:ALA:HA	4:E7:350:LYS:NZ	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E7:138:SER:HA	4:E7:169:VAL:HB	2.03	0.41
4:E9:294:PHE:CZ	4:E9:349:MET:HE3	2.56	0.41
4:E9:388:MET:HE1	3:F0:348:PRO:HD2	2.01	0.41
4:F1:86:ARG:HG2	4:F1:89:ASN:N	2.33	0.41
5:O:516:ASP:HB2	5:O:520:LEU:HD23	2.03	0.41
7:b:56:LYS:HZ3	7:b:61:THR:N	2.18	0.41
7:b:129:MET:HE2	7:b:129:MET:HB3	1.87	0.41
7:e:51:PRO:HG2	7:e:54:SER:HB3	2.03	0.41
7:j:68:LEU:HD23	7:j:73:VAL:HG11	2.01	0.41
7:j:151:MET:HE1	7:j:154:TYR:HA	2.02	0.41
8:k:25:ARG:HE	8:k:27:ASP:CG	2.29	0.41
7:n:50:PHE:HE2	7:n:140:LEU:HD21	1.86	0.41
7:n:88:LEU:HD11	7:n:196:LEU:HD11	2.01	0.41
7:o:79:ASP:HB3	7:o:82:ASP:HB2	2.03	0.41
7:r:13:GLU:HG2	7:r:17:LEU:HD23	2.02	0.41
7:s:84:LYS:HB3	7:s:168:PRO:HD3	2.01	0.41
7:s:129:MET:HE3	7:s:129:MET:HB2	1.99	0.41
7:v:191:GLU:OE1	7:v:194:ARG:HB3	2.21	0.41
1:2:425:VAL:O	1:2:429:LYS:HG2	2.21	0.41
3:A2:138:PHE:CZ	3:A2:235:ILE:HD13	2.56	0.41
3:A2:150:GLY:O	3:A2:154:LEU:HD23	2.21	0.41
4:A7:226:ASN:HD22	5:O:274:PHE:HE1	1.68	0.41
4:A9:379:LYS:HA	4:A9:382:SER:HB3	2.03	0.41
2:B:212:GLU:OE1	2:B:216:ARG:HG3	2.21	0.41
4:B5:200:GLN:HG2	4:B5:268:ILE:HD11	2.03	0.41
4:B7:173:PRO:HG3	4:B7:380:ARG:HH22	1.86	0.41
3:B8:30:ILE:HG22	3:B8:36:MET:HB3	2.03	0.41
3:B8:386:GLU:HA	3:B8:389:SER:HB2	2.02	0.41
3:C0:22:GLU:HG2	3:C0:83:TYR:CZ	2.56	0.41
4:C1:65:LEU:HD22	4:C1:90:PHE:CZ	2.56	0.41
3:C2:30:ILE:HD11	3:C2:34:GLY:HA2	2.02	0.41
4:C3:31:ASP:OD1	4:C3:33:THR:HG22	2.21	0.41
4:C5:109:GLY:HA2	4:C5:147:MET:SD	2.61	0.41
4:C5:203:ASP:OD1	4:C5:302:ALA:HB2	2.21	0.41
4:C5:274:THR:HG22	4:C5:282:ARG:HH11	1.86	0.41
3:C6:338:LYS:HD3	3:C6:341:ILE:HD12	2.02	0.41
4:C7:28:HIS:NE2	4:C7:241:ARG:HD2	2.36	0.41
3:D0:153:LEU:HD12	3:D0:153:LEU:HA	1.81	0.41
4:D1:98:GLY:H	4:D1:103:LYS:NZ	2.19	0.41
3:D2:403:ALA:HB2	4:D3:344:TRP:CH2	2.56	0.41
4:D5:116:VAL:HA	4:D5:119:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D6:223:THR:HG23	3:D6:225:THR:H	1.86	0.41
4:E1:187:LEU:HA	4:E1:190:HIS:CE1	2.56	0.41
3:E2:387:VAL:HG23	3:E2:390:ARG:CZ	2.51	0.41
4:E3:187:LEU:HA	4:E3:190:HIS:HE1	1.86	0.41
4:E3:374:ILE:H	4:E3:374:ILE:HG13	1.69	0.41
3:E4:319:TYR:CE2	3:E4:328:VAL:HG22	2.56	0.41
3:E4:384:ILE:HA	3:E4:387:VAL:HG12	2.02	0.41
3:E6:19:ALA:HB2	3:E6:228:ASN:HB3	2.02	0.41
2:I:245:SER:HB3	2:I:248:ARG:HG2	2.03	0.41
5:O:490:HIS:HB3	5:O:493:LYS:O	2.21	0.41
7:d:96:TYR:HA	7:d:108:ILE:HD11	2.02	0.41
7:f:69:LYS:HE3	7:f:69:LYS:HB3	1.90	0.41
7:h:58:SER:HA	7:h:126:ARG:HH21	1.85	0.41
7:h:194:ARG:HH22	7:h:198:ARG:NH2	2.19	0.41
7:m:94:ASN:O	7:m:94:ASN:ND2	2.54	0.41
7:m:205:LYS:HA	7:m:205:LYS:HE3	2.02	0.41
7:o:69:LYS:HD3	7:q:23:LEU:HD21	2.03	0.41
3:A0:178:SER:HB3	3:A0:183:GLU:HG2	2.03	0.40
3:A2:224:TYR:CD2	4:A3:323:THR:HG21	2.56	0.40
3:A2:384:ILE:HA	3:A2:387:VAL:HG12	2.02	0.40
3:A8:298:PRO:HA	3:A8:301:MET:HG2	2.02	0.40
4:B1:105:HIS:CE1	4:B1:150:LEU:HB2	2.56	0.40
4:B3:100:ASN:HB3	4:B3:103:LYS:HG2	2.02	0.40
4:B3:391:ARG:HH22	3:B4:435:VAL:HA	1.86	0.40
3:B4:217:LEU:HG	3:B4:275:ILE:HG22	2.02	0.40
4:B5:284:LEU:HD23	4:B5:362:LYS:HG2	2.03	0.40
3:B6:318:MET:HE1	3:B6:378:ILE:HG12	2.03	0.40
4:B7:156:ARG:HA	4:B7:156:ARG:HD2	1.89	0.40
4:B7:217:LEU:HD23	4:B7:220:PRO:HB3	2.02	0.40
4:B9:28:HIS:C	4:B9:43:GLN:HE21	2.29	0.40
4:C1:281:TYR:CD2	4:C5:86:ARG:HA	2.56	0.40
4:C5:86:ARG:HG2	4:C5:88:ASP:HB2	2.04	0.40
4:C7:14:ASN:HD21	4:C7:67:ASP:HB2	1.86	0.40
3:C8:100:ALA:O	4:C9:255:VAL:HG11	2.21	0.40
4:D3:169:VAL:HG12	4:D3:202:ILE:HB	2.02	0.40
3:D4:202:VAL:C	3:D4:203:MET:HE2	2.45	0.40
4:D5:75:SER:HA	5:O:508:TYR:HE1	1.85	0.40
4:D5:265:PHE:HB3	4:D5:374:ILE:HD13	2.03	0.40
4:D7:13:GLY:HA2	4:D7:16:ILE:HG22	2.03	0.40
4:D9:183:TYR:CE2	4:D9:388:MET:HE2	2.57	0.40
4:E1:6:HIS:HE2	4:E1:136:THR:HG22	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E4:180:ALA:HA	4:E5:350:LYS:NZ	2.36	0.40
3:E8:166:LYS:H	3:E8:199:ASP:HB3	1.86	0.40
4:E9:231:ALA:HB2	6:X:103:LEU:HD11	2.03	0.40
4:E9:276:ARG:H	6:W:174:ARG:HE	1.68	0.40
7:c:74:ALA:HB2	7:c:172:VAL:HG12	2.03	0.40
7:p:50:PHE:HD1	7:p:140:LEU:HD11	1.86	0.40
7:x:85:CYS:HA	7:x:168:PRO:HG3	2.03	0.40
1:1:420:TRP:HE1	1:1:477:VAL:CG1	2.35	0.40
3:A0:84:ARG:H	3:A0:84:ARG:HG2	1.70	0.40
3:A0:225:THR:O	3:A0:229:ARG:HG2	2.21	0.40
4:A1:109:GLY:O	4:A1:113:ILE:HG12	2.20	0.40
4:A1:298:ASN:O	4:A1:298:ASN:ND2	2.53	0.40
4:A3:237:THR:HG22	4:A3:250:LEU:HD21	2.02	0.40
3:A4:306:ASP:HA	3:A4:307:PRO:HD3	1.88	0.40
4:A5:228:LEU:HD23	4:A5:228:LEU:HA	1.91	0.40
4:A5:242:PHE:HB3	4:A5:356:ILE:HD13	2.03	0.40
3:A6:397:LEU:HD12	4:A7:344:TRP:HA	2.03	0.40
3:B0:219:ILE:HG22	7:f:198:ARG:NH2	2.37	0.40
3:B2:252:VAL:HA	3:B2:255:PHE:HD2	1.86	0.40
3:B4:324:VAL:HG22	3:B4:326:LYS:H	1.85	0.40
4:B5:201:VAL:HG11	4:B5:377:MET:HE3	2.04	0.40
4:B7:152:ILE:HD13	4:B7:152:ILE:HA	1.85	0.40
4:B9:316:MET:O	4:B9:365:VAL:HG23	2.21	0.40
4:C5:51:TYR:HB3	4:C5:59:PHE:HB3	2.01	0.40
3:C6:6:SER:HB3	3:C6:136:LEU:HD12	2.02	0.40
4:C7:109:GLY:HA2	4:C7:147:MET:HE1	2.02	0.40
3:C8:195:LEU:HD23	3:C8:195:LEU:HA	1.97	0.40
4:C9:41:ASP:HB3	2:K:248:ARG:HH12	1.85	0.40
3:D0:324:VAL:HG21	3:D0:326:LYS:HE2	2.03	0.40
3:D4:9:VAL:HG12	3:D4:68:LEU:HB2	2.03	0.40
3:D6:285:GLN:C	3:D6:287:SER:H	2.29	0.40
4:D7:318:ARG:HB3	4:D7:357:PRO:HA	2.03	0.40
4:E1:299:MET:HE2	4:E1:299:MET:HA	2.02	0.40
3:E2:219:ILE:HG22	3:E2:222:PRO:HD3	2.03	0.40
4:E5:86:ARG:HG2	4:E5:88:ASP:H	1.86	0.40
4:F1:313:ALA:HB3	4:F1:349:MET:HG3	2.03	0.40
7:e:56:LYS:HD2	7:e:60:ASN:HA	2.04	0.40
8:l:57:TYR:HA	8:l:69:ILE:HD11	2.03	0.40
7:n:183:LEU:HA	7:n:184:PRO:HD3	1.77	0.40
7:r:9:PRO:HB2	7:r:143:ILE:HD12	2.03	0.40
7:r:77:PHE:CD2	7:r:150:VAL:HG21	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:v:8:SER:HA	7:v:9:PRO:HD3	1.96	0.40
1:2:428:TRP:CD1	1:2:432:GLN:HE21	2.40	0.40
4:A3:162:ARG:HA	4:A3:162:ARG:HD3	1.73	0.40
3:A4:36:MET:HE3	3:A4:61:HIS:NE2	2.36	0.40
4:A5:230:SER:HA	4:A5:233:MET:HB2	2.03	0.40
4:A7:293:MET:HG3	4:A7:294:PHE:HD2	1.86	0.40
3:B8:183:GLU:HG2	3:B8:184:PRO:HD3	2.03	0.40
4:C1:99:ASN:HD21	3:C2:258:ASN:HD22	1.68	0.40
3:C4:208:ALA:HA	3:C4:304:LYS:HZ2	1.85	0.40
4:C9:87:PRO:HA	4:C9:90:PHE:HD2	1.85	0.40
4:C9:136:THR:HG22	4:C9:167:PHE:HB2	2.03	0.40
4:C9:178:THR:HG21	11:C9:502:GDP:H5'	2.03	0.40
4:C9:210:ILE:HG22	4:C9:215:LEU:HD13	2.03	0.40
4:C9:363:MET:HB3	4:C9:363:MET:HE2	1.79	0.40
3:D0:231:ILE:HA	3:D0:234:VAL:HG12	2.03	0.40
4:D3:213:ARG:HD2	4:D3:297:LYS:HE3	2.03	0.40
3:D8:210:TYR:HE2	4:D9:324:LYS:HA	1.87	0.40
4:D9:77:ARG:HH22	4:D9:92:PHE:HZ	1.67	0.40
4:D9:198:GLU:HB3	4:D9:200:GLN:HE22	1.87	0.40
2:E:244:GLN:HG3	2:E:249:SER:HB3	2.03	0.40
4:E1:269:GLY:H	4:E1:367:PHE:HB3	1.87	0.40
3:E2:234:VAL:HG21	3:E2:302:MET:HE2	2.02	0.40
3:E4:317:LEU:HD12	3:E4:319:TYR:CE1	2.56	0.40
4:E5:259:PRO:HB2	4:E5:260:PHE:HD1	1.86	0.40
3:E6:408:TYR:HB2	3:E6:418:PHE:HZ	1.86	0.40
3:E8:199:ASP:OD2	3:E8:256:GLN:HG2	2.21	0.40
4:E9:147:MET:HG2	4:E9:150:LEU:HD12	2.03	0.40
3:F0:141:VAL:HG11	3:F0:172:TRP:CZ3	2.57	0.40
4:F1:97:ALA:HB3	4:F1:143:THR:HB	2.04	0.40
7:c:14:LYS:NZ	7:c:47:LEU:HB2	2.37	0.40
7:c:67:HIS:CE1	7:e:23:LEU:HD12	2.55	0.40
7:c:165:THR:HB	7:c:182:PHE:HZ	1.86	0.40
7:g:9:PRO:HB2	7:g:143:ILE:HG23	2.03	0.40
7:j:142:GLU:HA	7:j:145:LYS:HZ3	1.86	0.40
8:k:17:GLN:HB3	8:k:20:ASN:O	2.21	0.40
7:u:171:ILE:HD11	7:u:179:GLU:HB2	2.01	0.40
7:v:10:LEU:HB2	7:v:143:ILE:HG13	2.03	0.40
4:A1:45:GLU:HB2	6:V:168:HIS:NE2	2.37	0.40
4:A1:237:THR:HG23	4:A1:240:LEU:HD13	2.04	0.40
3:A2:210:TYR:CE1	4:A3:324:LYS:HB3	2.57	0.40
3:A2:276:ILE:HB	3:A2:280:LYS:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A2:288:VAL:HG13	3:A2:319:TYR:CE2	2.56	0.40
4:A3:218:THR:HG23	4:A3:219:THR:HG22	2.03	0.40
4:A9:221:THR:HG23	4:A9:223:GLY:N	2.36	0.40
4:B3:152:ILE:O	4:B3:156:ARG:HG2	2.20	0.40
3:B6:325:PRO:HA	3:B6:328:VAL:HG12	2.03	0.40
3:B6:356:ASN:HD22	3:B6:358:GLN:HE21	1.68	0.40
3:C2:231:ILE:O	3:C2:235:ILE:HG12	2.21	0.40
3:C2:387:VAL:HG13	3:C2:388:PHE:CD1	2.57	0.40
4:C7:320:ARG:HA	4:C7:320:ARG:HD3	1.87	0.40
4:C9:175:VAL:HG11	3:D0:329:ASN:HA	2.02	0.40
4:C9:183:TYR:HA	4:C9:385:PHE:HE2	1.85	0.40
4:D1:25:SER:HB2	4:D1:30:ILE:HB	2.04	0.40
4:D1:211:CYS:HA	4:D1:215:LEU:HB2	2.02	0.40
3:D2:207:GLU:HA	3:D2:210:TYR:HD2	1.86	0.40
4:D3:393:ALA:HA	3:D4:346:TRP:HZ3	1.86	0.40
4:D3:396:HIS:HD1	4:D3:397:TRP:CG	2.40	0.40
3:D4:73:THR:HA	4:D5:46:ARG:HH22	1.86	0.40
3:D4:276:ILE:HG23	3:D4:280:LYS:HB2	2.03	0.40
4:D5:285:SER:O	4:D5:288:GLU:HG3	2.21	0.40
3:D6:71:GLU:HG2	3:D6:98:ASP:HB3	2.03	0.40
3:D8:285:GLN:HG3	3:E2:56:THR:HA	2.03	0.40
4:D9:229:VAL:O	4:D9:233:MET:HG2	2.20	0.40
3:E6:274:PRO:HB2	3:E6:276:ILE:HD11	2.03	0.40
3:F0:10:GLY:HA2	3:F0:145:THR:HG23	2.02	0.40
4:F1:206:ALA:O	4:F1:210:ILE:HD12	2.21	0.40
2:J:244:GLN:HE21	2:J:248:ARG:HB2	1.85	0.40
2:K:220:VAL:O	2:K:222:LYS:HG2	2.21	0.40
5:O:521:PRO:HB2	5:O:522:VAL:H	1.76	0.40
5:P:490:HIS:CG	5:P:493:LYS:HB2	2.57	0.40
6:V:65:HIS:CD2	6:V:66:PRO:HD3	2.56	0.40
7:a:97:ARG:HH22	7:c:149:ARG:NH2	2.20	0.40
7:b:76:TYR:HB3	7:b:112:PHE:HA	2.03	0.40
7:d:63:ILE:HA	7:f:16:ARG:HH12	1.86	0.40
7:d:68:LEU:HD13	7:d:73:VAL:HG21	2.04	0.40
7:e:5:VAL:HB	7:e:161:TYR:CE2	2.57	0.40
7:j:129:MET:HA	7:j:130:PRO:HD3	1.93	0.40
7:m:185:ILE:HA	7:m:191:GLU:O	2.20	0.40
7:o:164:ARG:HH22	7:o:182:PHE:HB2	1.86	0.40
7:s:181:GLN:HE22	7:s:199:TRP:HA	1.85	0.40
7:t:204:THR:O	7:t:205:LYS:HG2	2.21	0.40
7:v:79:ASP:HB3	7:v:82:ASP:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:w:10:LEU:HD23	7:w:147:HIS:HB2	2.03	0.40
3:A6:14:ILE:HG21	3:A6:74:VAL:HG22	2.03	0.40
3:B0:286:LEU:HD21	3:B0:372:MET:HE3	2.04	0.40
3:B0:404:PHE:CZ	4:B1:259:PRO:HG3	2.56	0.40
4:B7:68:LEU:HA	4:B7:93:GLY:HA3	2.04	0.40
3:B8:185:TYR:CE2	3:B8:404:PHE:HB2	2.53	0.40
3:B8:331:ALA:HA	3:B8:334:THR:HG22	2.02	0.40
4:B9:113:ILE:HA	4:B9:116:VAL:HG12	2.04	0.40
3:C2:188:VAL:HA	3:C2:191:THR:HG23	2.03	0.40
3:C2:238:LEU:HD13	3:C2:378:ILE:HD12	2.03	0.40
3:C2:394:LYS:HB3	4:C3:346:PRO:HG3	2.02	0.40
3:C4:28:HIS:NE2	3:C4:243:ARG:HD2	2.37	0.40
3:C4:328:VAL:HG21	3:C4:355:ILE:HD11	2.03	0.40
3:C4:364:PRO:HG2	2:J:255:PRO:HG2	2.04	0.40
3:D0:363:VAL:HG23	3:D0:366:GLY:HA3	2.03	0.40
4:D3:21:TRP:CZ3	4:D3:61:PRO:HB3	2.57	0.40
4:D5:107:THR:HG21	4:D5:401:GLU:HB2	2.03	0.40
4:D5:207:LEU:HB3	4:D5:225:LEU:HD22	2.04	0.40
4:D7:113:ILE:HD11	4:D7:151:LEU:HB2	2.03	0.40
4:D7:298:ASN:O	4:D7:298:ASN:ND2	2.54	0.40
3:D8:179:THR:OG1	4:D9:351:SER:HB3	2.21	0.40
3:D8:286:LEU:H	3:D8:286:LEU:HG	1.80	0.40
4:E3:49:VAL:HG21	4:E3:241:ARG:HG2	2.03	0.40
4:E3:284:LEU:H	4:E7:55:THR:HG21	1.87	0.40
3:E4:398:MET:HE1	4:E5:345:ILE:HA	2.02	0.40
4:E5:206:ALA:O	4:E5:210:ILE:HG12	2.21	0.40
4:E9:216:LYS:HD2	6:W:174:ARG:HB3	2.03	0.40
3:F0:96:LYS:HD2	4:F1:1:MET:HA	2.02	0.40
3:F0:195:LEU:HD22	3:F0:264:ARG:HG2	2.03	0.40
7:h:13:GLU:O	7:h:16:ARG:HB3	2.22	0.40
7:j:75:LEU:HD23	7:j:111:ILE:HB	2.03	0.40
7:n:53:GLY:HA2	7:n:62:VAL:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1	128/2041 (6%)	120 (94%)	8 (6%)	0	100	100
1	2	128/2041 (6%)	122 (95%)	6 (5%)	0	100	100
2	A	57/351 (16%)	46 (81%)	11 (19%)	0	100	100
2	B	58/351 (16%)	54 (93%)	4 (7%)	0	100	100
2	C	57/351 (16%)	48 (84%)	9 (16%)	0	100	100
2	D	57/351 (16%)	49 (86%)	7 (12%)	1 (2%)	6	34
2	E	58/351 (16%)	51 (88%)	7 (12%)	0	100	100
2	F	54/351 (15%)	48 (89%)	6 (11%)	0	100	100
2	G	58/351 (16%)	55 (95%)	3 (5%)	0	100	100
2	H	54/351 (15%)	48 (89%)	5 (9%)	1 (2%)	6	33
2	I	58/351 (16%)	54 (93%)	4 (7%)	0	100	100
2	J	58/351 (16%)	48 (83%)	10 (17%)	0	100	100
2	K	58/351 (16%)	52 (90%)	5 (9%)	1 (2%)	7	35
3	A0	424/453 (94%)	405 (96%)	19 (4%)	0	100	100
3	A2	424/453 (94%)	403 (95%)	21 (5%)	0	100	100
3	A4	424/453 (94%)	410 (97%)	14 (3%)	0	100	100
3	A6	424/453 (94%)	401 (95%)	23 (5%)	0	100	100
3	A8	424/453 (94%)	407 (96%)	17 (4%)	0	100	100
3	B0	424/453 (94%)	404 (95%)	20 (5%)	0	100	100
3	B2	424/453 (94%)	413 (97%)	11 (3%)	0	100	100
3	B4	424/453 (94%)	411 (97%)	13 (3%)	0	100	100
3	B6	424/453 (94%)	406 (96%)	18 (4%)	0	100	100
3	B8	424/453 (94%)	405 (96%)	19 (4%)	0	100	100
3	C0	424/453 (94%)	408 (96%)	16 (4%)	0	100	100
3	C2	424/453 (94%)	405 (96%)	19 (4%)	0	100	100
3	C4	424/453 (94%)	402 (95%)	22 (5%)	0	100	100
3	C6	424/453 (94%)	394 (93%)	30 (7%)	0	100	100
3	C8	424/453 (94%)	401 (95%)	23 (5%)	0	100	100
3	D0	424/453 (94%)	406 (96%)	18 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D2	424/453 (94%)	411 (97%)	13 (3%)	0	100	100
3	D4	424/453 (94%)	404 (95%)	20 (5%)	0	100	100
3	D6	424/453 (94%)	408 (96%)	14 (3%)	2 (0%)	24	58
3	D8	424/453 (94%)	401 (95%)	20 (5%)	3 (1%)	18	52
3	E0	424/453 (94%)	409 (96%)	15 (4%)	0	100	100
3	E2	424/453 (94%)	400 (94%)	21 (5%)	3 (1%)	18	52
3	E4	424/453 (94%)	404 (95%)	20 (5%)	0	100	100
3	E6	424/453 (94%)	408 (96%)	16 (4%)	0	100	100
3	E8	424/453 (94%)	404 (95%)	20 (5%)	0	100	100
3	F0	424/453 (94%)	395 (93%)	29 (7%)	0	100	100
4	A1	424/449 (94%)	394 (93%)	30 (7%)	0	100	100
4	A3	424/449 (94%)	399 (94%)	25 (6%)	0	100	100
4	A5	424/449 (94%)	398 (94%)	26 (6%)	0	100	100
4	A7	424/449 (94%)	403 (95%)	21 (5%)	0	100	100
4	A9	424/449 (94%)	401 (95%)	23 (5%)	0	100	100
4	B1	424/449 (94%)	403 (95%)	21 (5%)	0	100	100
4	B3	424/449 (94%)	403 (95%)	21 (5%)	0	100	100
4	B5	424/449 (94%)	402 (95%)	22 (5%)	0	100	100
4	B7	424/449 (94%)	403 (95%)	21 (5%)	0	100	100
4	B9	424/449 (94%)	398 (94%)	26 (6%)	0	100	100
4	C1	424/449 (94%)	391 (92%)	33 (8%)	0	100	100
4	C3	424/449 (94%)	401 (95%)	23 (5%)	0	100	100
4	C5	424/449 (94%)	404 (95%)	20 (5%)	0	100	100
4	C7	424/449 (94%)	394 (93%)	30 (7%)	0	100	100
4	C9	424/449 (94%)	398 (94%)	26 (6%)	0	100	100
4	D1	424/449 (94%)	403 (95%)	21 (5%)	0	100	100
4	D3	424/449 (94%)	404 (95%)	20 (5%)	0	100	100
4	D5	424/449 (94%)	401 (95%)	23 (5%)	0	100	100
4	D7	424/449 (94%)	405 (96%)	19 (4%)	0	100	100
4	D9	424/449 (94%)	407 (96%)	17 (4%)	0	100	100
4	E1	424/449 (94%)	402 (95%)	22 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E3	424/449 (94%)	406 (96%)	18 (4%)	0	100	100
4	E5	424/449 (94%)	402 (95%)	22 (5%)	0	100	100
4	E7	424/449 (94%)	401 (95%)	23 (5%)	0	100	100
4	E9	424/449 (94%)	394 (93%)	30 (7%)	0	100	100
4	F1	424/449 (94%)	395 (93%)	29 (7%)	0	100	100
5	O	161/583 (28%)	125 (78%)	31 (19%)	5 (3%)	3	24
5	P	210/583 (36%)	169 (80%)	34 (16%)	7 (3%)	3	23
5	R	210/583 (36%)	172 (82%)	33 (16%)	5 (2%)	4	29
6	U	20/336 (6%)	16 (80%)	4 (20%)	0	100	100
6	V	109/336 (32%)	91 (84%)	18 (16%)	0	100	100
6	W	109/336 (32%)	81 (74%)	28 (26%)	0	100	100
6	X	89/336 (26%)	75 (84%)	14 (16%)	0	100	100
7	a	159/220 (72%)	139 (87%)	19 (12%)	1 (1%)	21	55
7	b	159/220 (72%)	140 (88%)	19 (12%)	0	100	100
7	c	197/220 (90%)	185 (94%)	12 (6%)	0	100	100
7	d	197/220 (90%)	183 (93%)	14 (7%)	0	100	100
7	e	197/220 (90%)	184 (93%)	13 (7%)	0	100	100
7	f	197/220 (90%)	183 (93%)	14 (7%)	0	100	100
7	g	197/220 (90%)	184 (93%)	13 (7%)	0	100	100
7	h	197/220 (90%)	185 (94%)	12 (6%)	0	100	100
7	i	197/220 (90%)	185 (94%)	12 (6%)	0	100	100
7	j	197/220 (90%)	187 (95%)	10 (5%)	0	100	100
7	m	197/220 (90%)	182 (92%)	15 (8%)	0	100	100
7	n	197/220 (90%)	177 (90%)	20 (10%)	0	100	100
7	o	197/220 (90%)	185 (94%)	12 (6%)	0	100	100
7	p	197/220 (90%)	182 (92%)	15 (8%)	0	100	100
7	q	197/220 (90%)	185 (94%)	12 (6%)	0	100	100
7	r	197/220 (90%)	190 (96%)	7 (4%)	0	100	100
7	s	197/220 (90%)	181 (92%)	14 (7%)	2 (1%)	12	45
7	t	197/220 (90%)	181 (92%)	12 (6%)	4 (2%)	6	32
7	u	197/220 (90%)	186 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	v	197/220 (90%)	179 (91%)	18 (9%)	0	100	100
7	w	197/220 (90%)	188 (95%)	9 (5%)	0	100	100
7	x	197/220 (90%)	182 (92%)	15 (8%)	0	100	100
8	k	135/189 (71%)	129 (96%)	6 (4%)	0	100	100
8	l	135/189 (71%)	113 (84%)	21 (16%)	1 (1%)	18	52
All	All	28367/39706 (71%)	26656 (94%)	1675 (6%)	36 (0%)	49	79

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D6	281	ALA
3	D8	286	LEU
5	O	277	ASP
5	O	468	ASN
5	P	277	ASP
5	P	468	ASN
5	P	571	MET
5	R	277	ASP
5	R	468	ASN
8	l	13	VAL
2	D	227	VAL
3	E2	60	LYS
5	O	521	PRO
5	P	521	PRO
5	R	521	PRO
7	a	160	GLY
7	s	206	PHE
7	t	203	ASN
3	D8	281	ALA
3	D8	282	TYR
3	E2	58	ALA
2	H	227	VAL
5	O	278	GLN
5	P	567	LEU
7	s	203	ASN
3	D6	282	TYR
5	P	257	ILE
7	t	197	LEU
3	E2	52	PHE
2	K	260	VAL

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Mol	Chain	Res	Type
5	R	257	ILE
5	R	287	LEU
7	t	200	ASP
7	t	206	PHE
5	P	530	ILE
5	O	530	ILE

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	$\# Z > 2$
9	GTP	E2	501	10	33,34,34	0.91	1 (3%)	50,54,54	1.61	9 (18%)
9	GTP	C0	501	10	33,34,34	0.97	3 (9%)	50,54,54	1.61	10 (20%)
9	GTP	D2	501	10	33,34,34	0.90	2 (6%)	50,54,54	1.69	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GTP	C4	501	10	33,34,34	0.97	1 (3%)	50,54,54	1.52	8 (16%)
9	GTP	A0	501	10	33,34,34	0.91	1 (3%)	50,54,54	1.59	8 (16%)
11	GDP	D3	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	6 (13%)
11	GDP	B7	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)
9	GTP	B2	501	10	33,34,34	0.88	1 (3%)	50,54,54	1.63	9 (18%)
11	GDP	A5	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	7 (15%)
11	GDP	C5	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
11	GDP	E9	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.80	7 (15%)
11	GDP	C1	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	6 (13%)
9	GTP	D4	501	10	33,34,34	0.94	1 (3%)	50,54,54	1.66	9 (18%)
11	GDP	E7	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	7 (15%)
11	GDP	A1	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.80	8 (17%)
9	GTP	E7	501	-	33,34,34	0.89	1 (3%)	50,54,54	1.67	10 (20%)
11	GDP	D7	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.79	7 (15%)
9	GTP	B8	502	10	33,34,34	0.89	1 (3%)	50,54,54	1.62	9 (18%)
11	GDP	A3	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.81	7 (15%)
9	GTP	E8	501	10	33,34,34	0.89	1 (3%)	50,54,54	1.62	9 (18%)
11	GDP	E1	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.81	9 (20%)
9	GTP	D8	501	10	33,34,34	0.92	1 (3%)	50,54,54	1.62	8 (16%)
9	GTP	C2	501	10	33,34,34	0.91	1 (3%)	50,54,54	1.60	10 (20%)
11	GDP	C3	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.78	7 (15%)
9	GTP	D0	501	10	33,34,34	0.85	1 (3%)	50,54,54	1.62	9 (18%)
11	GDP	B3	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.68	5 (11%)
11	GDP	E3	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.80	7 (15%)
11	GDP	F1	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.81	7 (15%)
11	GDP	C7	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.81	8 (17%)
11	GDP	O	601	-	29,30,30	1.18	2 (6%)	45,47,47	1.76	7 (15%)
11	GDP	D5	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	7 (15%)
9	GTP	C6	501	10	33,34,34	0.93	1 (3%)	50,54,54	1.60	9 (18%)
11	GDP	A7	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.74	8 (17%)
11	GDP	C9	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	7 (15%)
11	GDP	D9	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
11	GDP	E5	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.81	6 (13%)
9	GTP	A2	502	-	33,34,34	0.87	1 (3%)	50,54,54	1.61	8 (16%)
9	GTP	B4	501	10	33,34,34	0.89	1 (3%)	50,54,54	1.59	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GTP	C8	501	10	33,34,34	0.90	1 (3%)	50,54,54	1.59	9 (18%)
9	GTP	B0	501	10	33,34,34	0.92	1 (3%)	50,54,54	1.63	9 (18%)
11	GDP	B9	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	7 (15%)
9	GTP	E4	501	10	33,34,34	0.93	1 (3%)	50,54,54	1.65	12 (24%)
11	GDP	D1	502	-	29,30,30	1.14	2 (6%)	45,47,47	1.77	7 (15%)
9	GTP	A8	501	10	33,34,34	0.91	1 (3%)	50,54,54	1.61	10 (20%)
9	GTP	A6	501	10	33,34,34	0.86	1 (3%)	50,54,54	1.58	8 (16%)
11	GDP	P	601	-	29,30,30	1.17	2 (6%)	45,47,47	1.73	6 (13%)
11	GDP	B5	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.81	7 (15%)
9	GTP	E0	501	10	33,34,34	0.91	1 (3%)	50,54,54	1.59	8 (16%)
9	GTP	A4	501	10	33,34,34	0.91	1 (3%)	50,54,54	1.57	8 (16%)
9	GTP	F0	501	10	33,34,34	0.97	1 (3%)	50,54,54	1.59	9 (18%)
9	GTP	D6	501	10	33,34,34	0.87	1 (3%)	50,54,54	1.62	9 (18%)
9	GTP	B6	501	10	33,34,34	0.92	1 (3%)	50,54,54	1.60	9 (18%)

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
9	GTP	E2	501	10	-	5/22/38/38	0/3/3/3
9	GTP	C0	501	10	-	9/22/38/38	0/3/3/3
9	GTP	D2	501	10	-	8/22/38/38	0/3/3/3
9	GTP	C4	501	10	-	4/22/38/38	0/3/3/3
9	GTP	A0	501	10	-	6/22/38/38	0/3/3/3
11	GDP	D3	502	-	-	4/16/32/32	0/3/3/3
11	GDP	B7	501	-	-	3/16/32/32	0/3/3/3
9	GTP	B2	501	10	-	5/22/38/38	0/3/3/3
11	GDP	A5	501	-	-	2/16/32/32	0/3/3/3
11	GDP	C5	501	-	-	1/16/32/32	0/3/3/3
11	GDP	E9	501	-	-	8/16/32/32	0/3/3/3
11	GDP	C1	501	-	-	0/16/32/32	0/3/3/3
9	GTP	D4	501	10	-	3/22/38/38	0/3/3/3
11	GDP	E7	502	-	-	2/16/32/32	0/3/3/3
11	GDP	A1	501	-	-	7/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GTP	E7	501	-	-	9/22/38/38	0/3/3/3
11	GDP	D7	501	-	-	5/16/32/32	0/3/3/3
9	GTP	B8	502	10	-	6/22/38/38	0/3/3/3
11	GDP	A3	501	-	-	8/16/32/32	0/3/3/3
9	GTP	E8	501	10	-	8/22/38/38	0/3/3/3
11	GDP	E1	501	-	-	0/16/32/32	0/3/3/3
9	GTP	D8	501	10	-	5/22/38/38	0/3/3/3
9	GTP	C2	501	10	-	4/22/38/38	0/3/3/3
11	GDP	C3	501	-	-	3/16/32/32	0/3/3/3
9	GTP	D0	501	10	-	3/22/38/38	0/3/3/3
11	GDP	B3	501	-	-	3/16/32/32	0/3/3/3
11	GDP	E3	501	-	-	3/16/32/32	0/3/3/3
11	GDP	F1	501	-	-	3/16/32/32	0/3/3/3
11	GDP	C7	501	-	-	5/16/32/32	0/3/3/3
11	GDP	O	601	-	-	5/16/32/32	0/3/3/3
11	GDP	D5	501	-	-	3/16/32/32	0/3/3/3
9	GTP	C6	501	10	-	5/22/38/38	0/3/3/3
11	GDP	A7	501	-	-	7/16/32/32	0/3/3/3
11	GDP	C9	502	-	-	2/16/32/32	0/3/3/3
11	GDP	D9	501	-	-	3/16/32/32	0/3/3/3
11	GDP	E5	501	-	-	0/16/32/32	0/3/3/3
9	GTP	A2	502	-	-	9/22/38/38	0/3/3/3
9	GTP	B4	501	10	-	6/22/38/38	0/3/3/3
9	GTP	C8	501	10	-	3/22/38/38	0/3/3/3
9	GTP	B0	501	10	-	7/22/38/38	0/3/3/3
11	GDP	B9	501	-	-	6/16/32/32	0/3/3/3
9	GTP	E4	501	10	-	10/22/38/38	0/3/3/3
11	GDP	D1	502	-	-	3/16/32/32	0/3/3/3
9	GTP	A8	501	10	-	5/22/38/38	0/3/3/3
9	GTP	A6	501	10	-	6/22/38/38	0/3/3/3
11	GDP	P	601	-	-	6/16/32/32	0/3/3/3
11	GDP	B5	501	-	-	2/16/32/32	0/3/3/3
9	GTP	E0	501	10	-	3/22/38/38	0/3/3/3
9	GTP	A4	501	10	-	8/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GTP	F0	501	10	-	7/22/38/38	0/3/3/3
9	GTP	D6	501	10	-	6/22/38/38	0/3/3/3
9	GTP	B6	501	10	-	4/22/38/38	0/3/3/3

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A3	501	GDP	C5-C4	3.14	1.47	1.38
11	D7	501	GDP	C5-C4	3.13	1.47	1.38
11	O	601	GDP	C5-C4	3.13	1.47	1.38
11	D9	501	GDP	C5-C4	3.11	1.47	1.38
11	P	601	GDP	C5-C4	3.10	1.47	1.38
11	A1	501	GDP	C5-C4	3.09	1.47	1.38
11	D5	501	GDP	C5-C4	3.08	1.47	1.38
11	B3	501	GDP	C5-C4	3.08	1.47	1.38
11	A7	501	GDP	C5-C4	3.07	1.47	1.38
11	E3	501	GDP	C5-C4	3.06	1.47	1.38
11	D3	502	GDP	C5-C4	3.06	1.47	1.38
11	C7	501	GDP	C5-C4	3.06	1.47	1.38
11	C9	502	GDP	C5-C4	3.06	1.47	1.38
11	C3	501	GDP	C5-C4	3.05	1.47	1.38
11	C5	501	GDP	C5-C4	3.04	1.47	1.38
11	E5	501	GDP	C5-C4	3.04	1.47	1.38
11	C1	501	GDP	C5-C4	3.04	1.47	1.38
11	E9	501	GDP	C5-C4	3.04	1.47	1.38
11	A5	501	GDP	C5-C4	3.03	1.47	1.38
11	B5	501	GDP	C5-C4	3.02	1.47	1.38
11	E7	502	GDP	C5-C4	3.02	1.47	1.38
11	F1	501	GDP	C5-C4	3.01	1.47	1.38
11	B9	501	GDP	C5-C4	3.00	1.47	1.38
11	D1	502	GDP	C5-C4	2.99	1.46	1.38
11	E1	501	GDP	C5-C4	2.98	1.46	1.38
11	B7	501	GDP	C5-C4	2.95	1.46	1.38
11	E3	501	GDP	C6-N1	-2.80	1.33	1.38
11	A7	501	GDP	C6-N1	-2.73	1.33	1.38
11	B3	501	GDP	C6-N1	-2.72	1.33	1.38
11	D7	501	GDP	C6-N1	-2.69	1.33	1.38
11	B9	501	GDP	C6-N1	-2.67	1.33	1.38
11	A1	501	GDP	C6-N1	-2.66	1.33	1.38
11	F1	501	GDP	C6-N1	-2.64	1.33	1.38
11	P	601	GDP	C6-N1	-2.63	1.33	1.38
11	B7	501	GDP	C6-N1	-2.63	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	E1	501	GDP	C6-N1	-2.61	1.34	1.38
11	A5	501	GDP	C6-N1	-2.58	1.34	1.38
11	D9	501	GDP	C6-N1	-2.58	1.34	1.38
11	B5	501	GDP	C6-N1	-2.58	1.34	1.38
11	O	601	GDP	C6-N1	-2.57	1.34	1.38
11	D3	502	GDP	C6-N1	-2.56	1.34	1.38
11	E7	502	GDP	C6-N1	-2.56	1.34	1.38
11	E5	501	GDP	C6-N1	-2.56	1.34	1.38
11	C3	501	GDP	C6-N1	-2.55	1.34	1.38
11	E9	501	GDP	C6-N1	-2.55	1.34	1.38
11	D5	501	GDP	C6-N1	-2.54	1.34	1.38
11	C9	502	GDP	C6-N1	-2.53	1.34	1.38
11	C1	501	GDP	C6-N1	-2.53	1.34	1.38
11	C7	501	GDP	C6-N1	-2.52	1.34	1.38
11	C5	501	GDP	C6-N1	-2.51	1.34	1.38
11	D1	502	GDP	C6-N1	-2.47	1.34	1.38
11	A3	501	GDP	C6-N1	-2.39	1.34	1.38
9	D2	501	GTP	C2-N3	2.27	1.38	1.33
9	E4	501	GTP	C2-N3	2.22	1.38	1.33
9	B8	502	GTP	C2-N3	2.21	1.38	1.33
9	D8	501	GTP	C2-N3	2.21	1.38	1.33
9	E2	501	GTP	C2-N3	2.20	1.38	1.33
9	E7	501	GTP	C2-N3	2.20	1.38	1.33
9	E8	501	GTP	C2-N3	2.19	1.38	1.33
9	B0	501	GTP	C2-N3	2.17	1.38	1.33
9	A4	501	GTP	C2-N3	2.17	1.38	1.33
9	C2	501	GTP	C2-N3	2.17	1.38	1.33
11	D9	501	GDP	C5-N7	-2.17	1.34	1.39
11	B9	501	GDP	C5-N7	-2.16	1.34	1.39
9	F0	501	GTP	C2-N3	2.15	1.38	1.33
9	E0	501	GTP	C2-N3	2.15	1.38	1.33
9	A2	502	GTP	C2-N3	2.15	1.38	1.33
11	A1	501	GDP	C5-N7	-2.15	1.34	1.39
11	C7	501	GDP	C5-N7	-2.15	1.34	1.39
9	A8	501	GTP	C2-N3	2.14	1.38	1.33
11	E7	502	GDP	C5-N7	-2.14	1.34	1.39
9	C6	501	GTP	C2-N3	2.14	1.38	1.33
11	B7	501	GDP	C5-N7	-2.14	1.34	1.39
11	C3	501	GDP	C5-N7	-2.13	1.34	1.39
11	A5	501	GDP	C5-N7	-2.13	1.34	1.39
11	B5	501	GDP	C5-N7	-2.13	1.34	1.39
11	D7	501	GDP	C5-N7	-2.12	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	E9	501	GDP	C5-N7	-2.12	1.34	1.39
9	D6	501	GTP	C2-N3	2.12	1.38	1.33
9	A0	501	GTP	C2-N3	2.12	1.38	1.33
11	A7	501	GDP	C5-N7	-2.12	1.34	1.39
11	D5	501	GDP	C5-N7	-2.12	1.34	1.39
11	C9	502	GDP	C5-N7	-2.11	1.34	1.39
9	C0	501	GTP	PA-O3A	2.11	1.61	1.59
11	E3	501	GDP	C5-N7	-2.10	1.34	1.39
9	C0	501	GTP	C2-N3	2.10	1.38	1.33
9	D4	501	GTP	C2-N3	2.10	1.38	1.33
11	E5	501	GDP	C5-N7	-2.10	1.34	1.39
11	C5	501	GDP	C5-N7	-2.10	1.34	1.39
9	A6	501	GTP	C2-N3	2.09	1.38	1.33
11	C1	501	GDP	C5-N7	-2.09	1.34	1.39
9	C0	501	GTP	PB-O3A	2.08	1.61	1.59
11	B3	501	GDP	C5-N7	-2.08	1.34	1.39
11	E1	501	GDP	C5-N7	-2.08	1.34	1.39
11	D3	502	GDP	C5-N7	-2.08	1.34	1.39
9	C8	501	GTP	C2-N3	2.07	1.38	1.33
9	B2	501	GTP	C2-N3	2.07	1.38	1.33
9	D2	501	GTP	C5-N7	-2.06	1.34	1.39
9	C4	501	GTP	C2-N3	2.06	1.38	1.33
9	B4	501	GTP	C2-N3	2.05	1.38	1.33
11	F1	501	GDP	C5-N7	-2.05	1.35	1.39
9	B6	501	GTP	C2-N3	2.05	1.38	1.33
9	D0	501	GTP	C2-N3	2.02	1.38	1.33
11	A3	501	GDP	C5-N7	-2.01	1.35	1.39

All (413) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	E3	501	GDP	C5-C4-N3	-6.38	118.24	128.39
11	D9	501	GDP	C5-C4-N3	-6.33	118.32	128.39
11	E5	501	GDP	C5-C4-N3	-6.25	118.44	128.39
11	B5	501	GDP	C5-C4-N3	-6.24	118.46	128.39
11	E1	501	GDP	C5-C4-N3	-6.18	118.56	128.39
11	F1	501	GDP	C5-C4-N3	-6.17	118.57	128.39
11	A3	501	GDP	C5-C4-N3	-6.17	118.57	128.39
11	C9	502	GDP	C5-C4-N3	-6.16	118.59	128.39
11	D7	501	GDP	C5-C4-N3	-6.15	118.61	128.39
11	D3	502	GDP	C5-C4-N3	-6.15	118.61	128.39
11	E7	502	GDP	C5-C4-N3	-6.13	118.64	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	E9	501	GDP	C5-C4-N3	-6.11	118.66	128.39
11	B9	501	GDP	C5-C4-N3	-6.09	118.69	128.39
11	D5	501	GDP	C5-C4-N3	-6.09	118.70	128.39
11	O	601	GDP	C5-C4-N3	-6.04	118.77	128.39
11	C5	501	GDP	C5-C4-N3	-6.03	118.79	128.39
11	A1	501	GDP	C5-C4-N3	-6.03	118.79	128.39
11	C7	501	GDP	C5-C4-N3	-6.03	118.80	128.39
11	C3	501	GDP	C5-C4-N3	-6.01	118.82	128.39
11	A7	501	GDP	C5-C4-N3	-5.95	118.92	128.39
11	C1	501	GDP	C5-C4-N3	-5.95	118.92	128.39
11	A5	501	GDP	C5-C4-N3	-5.95	118.92	128.39
11	B7	501	GDP	C5-C4-N3	-5.93	118.95	128.39
11	D1	502	GDP	C5-C4-N3	-5.85	119.07	128.39
11	P	601	GDP	C5-C4-N3	-5.77	119.21	128.39
11	B3	501	GDP	C5-C4-N3	-5.69	119.34	128.39
9	D2	501	GTP	C5-C4-N3	-5.37	119.84	128.39
9	B8	502	GTP	C5-C4-N3	-5.36	119.86	128.39
9	B2	501	GTP	C5-C4-N3	-5.34	119.89	128.39
9	E7	501	GTP	C5-C4-N3	-5.32	119.93	128.39
9	B0	501	GTP	C5-C4-N3	-5.25	120.03	128.39
9	E2	501	GTP	C5-C4-N3	-5.24	120.04	128.39
11	B5	501	GDP	C2-N3-C4	5.24	121.33	112.30
9	E4	501	GTP	C5-C4-N3	-5.23	120.07	128.39
9	A4	501	GTP	C5-C4-N3	-5.18	120.14	128.39
11	E5	501	GDP	C2-N3-C4	5.18	121.22	112.30
11	A3	501	GDP	C2-N3-C4	5.14	121.15	112.30
9	D6	501	GTP	C5-C4-N3	-5.12	120.24	128.39
9	C6	501	GTP	C5-C4-N3	-5.11	120.26	128.39
9	D8	501	GTP	C5-C4-N3	-5.10	120.27	128.39
9	C2	501	GTP	C5-C4-N3	-5.09	120.29	128.39
11	O	601	GDP	C2-N3-C4	5.09	121.06	112.30
9	B4	501	GTP	C5-C4-N3	-5.08	120.30	128.39
11	E1	501	GDP	C2-N3-C4	5.06	121.01	112.30
11	E7	502	GDP	C2-N3-C4	5.05	121.00	112.30
11	E3	501	GDP	C2-N3-C4	5.04	120.99	112.30
9	B6	501	GTP	C5-C4-N3	-5.04	120.37	128.39
11	D9	501	GDP	C2-N3-C4	5.04	120.97	112.30
9	E8	501	GTP	C5-C4-N3	-5.03	120.39	128.39
11	D5	501	GDP	C2-N3-C4	5.02	120.95	112.30
11	C5	501	GDP	C2-N3-C4	5.01	120.94	112.30
11	E9	501	GDP	C2-N3-C4	5.00	120.92	112.30
9	A0	501	GTP	C5-C4-N3	-5.00	120.43	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F1	501	GDP	C2-N3-C4	5.00	120.91	112.30
11	C9	502	GDP	C2-N3-C4	5.00	120.91	112.30
11	C7	501	GDP	C2-N3-C4	4.99	120.89	112.30
9	D4	501	GTP	C5-C4-N3	-4.99	120.45	128.39
11	D1	502	GDP	C2-N3-C4	4.98	120.88	112.30
9	A8	501	GTP	C5-C4-N3	-4.98	120.47	128.39
11	D3	502	GDP	C2-N3-C4	4.98	120.87	112.30
9	F0	501	GTP	C5-C4-N3	-4.97	120.47	128.39
9	A2	502	GTP	C5-C4-N3	-4.97	120.48	128.39
11	P	601	GDP	C2-N3-C4	4.97	120.86	112.30
11	C3	501	GDP	C2-N3-C4	4.97	120.85	112.30
9	C0	501	GTP	C5-C4-N3	-4.94	120.52	128.39
11	B9	501	GDP	C2-N3-C4	4.94	120.81	112.30
11	A5	501	GDP	C2-N3-C4	4.94	120.81	112.30
11	D7	501	GDP	C2-N3-C4	4.93	120.80	112.30
11	B7	501	GDP	C2-N3-C4	4.93	120.79	112.30
11	C1	501	GDP	C2-N3-C4	4.93	120.78	112.30
9	D0	501	GTP	C5-C4-N3	-4.91	120.57	128.39
9	C8	501	GTP	C5-C4-N3	-4.90	120.59	128.39
9	B2	501	GTP	C2-N3-C4	4.90	120.74	112.30
9	A6	501	GTP	C5-C4-N3	-4.87	120.65	128.39
9	E0	501	GTP	C5-C4-N3	-4.85	120.66	128.39
11	A7	501	GDP	C2-N3-C4	4.83	120.63	112.30
9	E7	501	GTP	C2-N3-C4	4.78	120.53	112.30
9	D2	501	GTP	C2-N3-C4	4.78	120.53	112.30
9	D4	501	GTP	C2-N3-C4	4.74	120.46	112.30
9	B4	501	GTP	C2-N3-C4	4.72	120.44	112.30
11	B3	501	GDP	C2-N3-C4	4.72	120.44	112.30
11	E3	501	GDP	N9-C4-N3	4.72	135.39	125.95
11	A1	501	GDP	C2-N3-C4	4.71	120.42	112.30
11	D9	501	GDP	N9-C4-N3	4.71	135.37	125.95
9	D6	501	GTP	C2-N3-C4	4.70	120.40	112.30
9	B8	502	GTP	C2-N3-C4	4.70	120.39	112.30
11	D7	501	GDP	N9-C4-N3	4.70	135.34	125.95
9	C4	501	GTP	C5-C4-N3	-4.69	120.92	128.39
9	A2	502	GTP	C2-N3-C4	4.68	120.37	112.30
9	B0	501	GTP	C2-N3-C4	4.68	120.35	112.30
9	A4	501	GTP	C2-N3-C4	4.66	120.33	112.30
9	E2	501	GTP	C2-N3-C4	4.66	120.33	112.30
9	E4	501	GTP	C2-N3-C4	4.65	120.31	112.30
9	A0	501	GTP	C2-N3-C4	4.65	120.31	112.30
9	A6	501	GTP	C2-N3-C4	4.64	120.29	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A8	501	GTP	C2-N3-C4	4.63	120.28	112.30
9	D8	501	GTP	C2-N3-C4	4.63	120.27	112.30
9	F0	501	GTP	C2-N3-C4	4.62	120.27	112.30
9	C6	501	GTP	C2-N3-C4	4.62	120.26	112.30
9	E8	501	GTP	C2-N3-C4	4.62	120.26	112.30
11	D3	502	GDP	N9-C4-N3	4.62	135.20	125.95
9	C0	501	GTP	C2-N3-C4	4.61	120.24	112.30
9	C2	501	GTP	C2-N3-C4	4.60	120.22	112.30
9	C8	501	GTP	C2-N3-C4	4.59	120.21	112.30
11	E1	501	GDP	N9-C4-N3	4.58	135.11	125.95
11	B5	501	GDP	N9-C4-N3	4.58	135.10	125.95
9	D0	501	GTP	C2-N3-C4	4.57	120.18	112.30
11	F1	501	GDP	N9-C4-N3	4.57	135.10	125.95
9	E0	501	GTP	C2-N3-C4	4.57	120.18	112.30
9	B6	501	GTP	C2-N3-C4	4.57	120.17	112.30
11	B9	501	GDP	N9-C4-N3	4.56	135.06	125.95
11	E9	501	GDP	N9-C4-N3	4.55	135.05	125.95
11	D5	501	GDP	N9-C4-N3	4.54	135.04	125.95
11	C9	502	GDP	N9-C4-N3	4.53	135.02	125.95
9	C4	501	GTP	C2-N3-C4	4.51	120.06	112.30
11	E7	502	GDP	N9-C4-N3	4.50	134.96	125.95
11	A3	501	GDP	N9-C4-N3	4.50	134.95	125.95
11	C3	501	GDP	N9-C4-N3	4.49	134.93	125.95
11	E5	501	GDP	N9-C4-N3	4.49	134.93	125.95
11	A5	501	GDP	N9-C4-N3	4.48	134.92	125.95
11	C5	501	GDP	N9-C4-N3	4.45	134.84	125.95
11	A7	501	GDP	N9-C4-N3	4.45	134.84	125.95
11	C7	501	GDP	N9-C4-N3	4.42	134.79	125.95
11	A1	501	GDP	N9-C4-N3	4.42	134.78	125.95
11	C1	501	GDP	N9-C4-N3	4.37	134.69	125.95
11	B7	501	GDP	N9-C4-N3	4.36	134.67	125.95
11	O	601	GDP	N9-C4-N3	4.26	134.47	125.95
11	B3	501	GDP	N9-C4-N3	4.26	134.46	125.95
11	D1	502	GDP	N9-C4-N3	4.18	134.31	125.95
11	P	601	GDP	N9-C4-N3	3.91	133.78	125.95
9	D2	501	GTP	N9-C4-N3	3.81	133.57	125.95
11	P	601	GDP	C6-C5-N7	3.58	136.81	130.29
9	E4	501	GTP	N9-C4-N3	3.52	132.99	125.95
11	D1	502	GDP	C6-C5-N7	3.51	136.67	130.29
9	B8	502	GTP	N9-C4-N3	3.46	132.87	125.95
9	E2	501	GTP	N9-C4-N3	3.44	132.83	125.95
9	B2	501	GTP	N9-C4-N3	3.38	132.71	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D8	501	GTP	N9-C4-N3	3.38	132.70	125.95
9	B0	501	GTP	N9-C4-N3	3.37	132.69	125.95
9	E7	501	GTP	N9-C4-N3	3.36	132.68	125.95
11	A3	501	GDP	C6-C5-N7	3.33	136.35	130.29
11	E5	501	GDP	C6-C5-N7	3.33	136.35	130.29
11	C1	501	GDP	C6-C5-N7	3.31	136.31	130.29
11	B5	501	GDP	C6-C5-N7	3.30	136.30	130.29
9	A4	501	GTP	N9-C4-N3	3.29	132.53	125.95
11	B7	501	GDP	C6-C5-N7	3.29	136.27	130.29
9	C2	501	GTP	N9-C4-N3	3.29	132.52	125.95
11	B3	501	GDP	C6-C5-N7	3.28	136.27	130.29
9	B6	501	GTP	N9-C4-N3	3.28	132.51	125.95
11	F1	501	GDP	C6-C5-N7	3.26	136.22	130.29
11	C5	501	GDP	C6-C5-N7	3.26	136.22	130.29
11	D7	501	GDP	C6-C5-N7	3.26	136.22	130.29
11	E9	501	GDP	C6-C5-N7	3.25	136.20	130.29
9	D6	501	GTP	N9-C4-N3	3.25	132.44	125.95
11	E7	502	GDP	C6-C5-N7	3.25	136.20	130.29
11	C3	501	GDP	C6-C5-N7	3.24	136.19	130.29
11	E1	501	GDP	C6-C5-N7	3.24	136.18	130.29
9	D2	501	GTP	C2-N1-C6	-3.23	119.25	125.11
11	C7	501	GDP	C6-C5-N7	3.23	136.17	130.29
11	O	601	GDP	C6-C5-N7	3.22	136.15	130.29
9	C6	501	GTP	N9-C4-N3	3.22	132.39	125.95
11	A5	501	GDP	C6-C5-N7	3.21	136.12	130.29
11	E3	501	GDP	C6-C5-N7	3.20	136.12	130.29
11	D3	502	GDP	C6-C5-N7	3.20	136.12	130.29
11	D5	501	GDP	C6-C5-N7	3.19	136.09	130.29
11	C9	502	GDP	C6-C5-N7	3.18	136.07	130.29
9	E7	501	GTP	C2-N1-C6	-3.15	119.40	125.11
9	E8	501	GTP	N9-C4-N3	3.15	132.25	125.95
9	B4	501	GTP	N9-C4-N3	3.15	132.25	125.95
9	A8	501	GTP	N9-C4-N3	3.15	132.24	125.95
9	A2	502	GTP	N9-C4-N3	3.14	132.24	125.95
11	B9	501	GDP	C6-C5-N7	3.14	136.00	130.29
9	F0	501	GTP	N9-C4-N3	3.13	132.22	125.95
11	A1	501	GDP	C6-C5-N7	3.13	135.98	130.29
9	B8	502	GTP	C2-N1-C6	-3.11	119.47	125.11
9	E0	501	GTP	N9-C4-N3	3.10	132.15	125.95
11	A7	501	GDP	C6-C5-N7	3.09	135.91	130.29
9	A0	501	GTP	N9-C4-N3	3.09	132.12	125.95
9	E4	501	GTP	C2-N1-C6	-3.07	119.54	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C8	501	GTP	N9-C4-N3	3.07	132.09	125.95
9	D4	501	GTP	C2-N1-C6	-3.05	119.58	125.11
9	C2	501	GTP	C2-N1-C6	-3.04	119.59	125.11
9	B2	501	GTP	C2-N1-C6	-3.04	119.59	125.11
9	B4	501	GTP	C2-N1-C6	-3.04	119.61	125.11
9	E2	501	GTP	C2-N1-C6	-3.03	119.62	125.11
9	D2	501	GTP	O6-C6-C5	-3.02	118.56	126.53
9	D0	501	GTP	N9-C4-N3	3.01	131.98	125.95
11	D9	501	GDP	C6-C5-N7	3.01	135.77	130.29
9	A6	501	GTP	N9-C4-N3	3.00	131.96	125.95
9	D8	501	GTP	C2-N1-C6	-2.98	119.71	125.11
9	F0	501	GTP	C2-N1-C6	-2.97	119.72	125.11
9	C6	501	GTP	C2-N1-C6	-2.97	119.72	125.11
9	A4	501	GTP	C2-N1-C6	-2.97	119.72	125.11
9	C4	501	GTP	N9-C4-N3	2.96	131.87	125.95
9	B0	501	GTP	C2-N1-C6	-2.96	119.74	125.11
9	A2	502	GTP	C2-N1-C6	-2.96	119.75	125.11
9	D6	501	GTP	C2-N1-C6	-2.96	119.75	125.11
9	E8	501	GTP	C2-N1-C6	-2.95	119.75	125.11
9	D4	501	GTP	N9-C4-N3	2.95	131.86	125.95
9	A0	501	GTP	C2-N1-C6	-2.95	119.76	125.11
9	D4	501	GTP	N9-C8-N7	-2.94	107.95	113.40
9	C0	501	GTP	N9-C4-N3	2.93	131.82	125.95
9	B6	501	GTP	C2-N1-C6	-2.90	119.86	125.11
9	A8	501	GTP	C2-N1-C6	-2.89	119.86	125.11
9	C0	501	GTP	C2-N1-C6	-2.87	119.90	125.11
9	E0	501	GTP	N9-C8-N7	-2.87	108.08	113.40
9	E0	501	GTP	C2-N1-C6	-2.86	119.93	125.11
9	A6	501	GTP	C2-N1-C6	-2.84	119.96	125.11
9	D0	501	GTP	C2-N1-C6	-2.83	119.98	125.11
9	D0	501	GTP	N9-C8-N7	-2.83	108.16	113.40
9	C4	501	GTP	C2-N1-C6	-2.82	119.99	125.11
9	C8	501	GTP	C2-N1-C6	-2.81	120.01	125.11
9	E7	501	GTP	N9-C8-N7	-2.80	108.20	113.40
9	A2	502	GTP	N9-C8-N7	-2.80	108.22	113.40
9	D2	501	GTP	C5-C6-N1	2.79	120.34	113.25
9	D8	501	GTP	N9-C8-N7	-2.78	108.24	113.40
9	B0	501	GTP	C8-N7-C5	2.76	109.18	104.26
9	D4	501	GTP	C8-N7-C5	2.76	109.17	104.26
9	D6	501	GTP	N9-C8-N7	-2.76	108.29	113.40
9	B4	501	GTP	N9-C8-N7	-2.75	108.30	113.40
9	A0	501	GTP	N9-C8-N7	-2.74	108.32	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A6	501	GTP	N9-C8-N7	-2.74	108.32	113.40
9	C2	501	GTP	N9-C8-N7	-2.74	108.32	113.40
9	B0	501	GTP	N9-C8-N7	-2.73	108.33	113.40
9	D0	501	GTP	C8-N7-C5	2.73	109.12	104.26
9	E7	501	GTP	C8-N7-C5	2.73	109.12	104.26
9	A2	502	GTP	C8-N7-C5	2.71	109.09	104.26
11	E5	501	GDP	C4-C5-N7	-2.71	106.37	110.67
9	E2	501	GTP	N9-C8-N7	-2.71	108.38	113.40
9	E8	501	GTP	N9-C8-N7	-2.69	108.41	113.40
9	D8	501	GTP	C8-N7-C5	2.69	109.06	104.26
9	E0	501	GTP	C8-N7-C5	2.69	109.06	104.26
9	F0	501	GTP	N9-C8-N7	-2.68	108.42	113.40
11	D1	502	GDP	C4-C5-N7	-2.68	106.42	110.67
9	C6	501	GTP	N9-C8-N7	-2.68	108.43	113.40
9	C0	501	GTP	N9-C8-N7	-2.68	108.44	113.40
9	C8	501	GTP	N9-C8-N7	-2.67	108.44	113.40
9	D6	501	GTP	C8-N7-C5	2.66	109.00	104.26
9	A8	501	GTP	N9-C8-N7	-2.66	108.47	113.40
11	A3	501	GDP	C4-C5-N7	-2.66	106.46	110.67
9	E7	501	GTP	C5-C6-N1	2.66	120.01	113.25
9	E4	501	GTP	C5-C6-N1	2.64	119.96	113.25
9	B6	501	GTP	N9-C8-N7	-2.63	108.52	113.40
9	B8	502	GTP	C5-C6-N1	2.63	119.95	113.25
9	E8	501	GTP	C8-N7-C5	2.62	108.94	104.26
11	F1	501	GDP	C4-C5-N7	-2.62	106.52	110.67
9	A0	501	GTP	C8-N7-C5	2.61	108.91	104.26
9	C6	501	GTP	C8-N7-C5	2.61	108.91	104.26
11	E9	501	GDP	C4-C5-N7	-2.61	106.53	110.67
11	C1	501	GDP	C4-C5-N7	-2.60	106.54	110.67
9	C2	501	GTP	C5-C6-N1	2.60	119.86	113.25
11	E3	501	GDP	C4-C5-N7	-2.60	106.56	110.67
9	C4	501	GTP	N9-C8-N7	-2.60	108.59	113.40
9	C4	501	GTP	C5-C6-N1	2.60	119.86	113.25
9	A2	502	GTP	C5-C6-N1	2.59	119.85	113.25
9	B2	501	GTP	N9-C8-N7	-2.59	108.59	113.40
9	B8	502	GTP	N9-C8-N7	-2.59	108.60	113.40
11	P	601	GDP	C4-C5-N7	-2.59	106.57	110.67
9	B4	501	GTP	C5-C6-N1	2.59	119.83	113.25
11	A1	501	GDP	C4-C5-N7	-2.59	106.57	110.67
9	A6	501	GTP	C5-C6-N1	2.58	119.83	113.25
9	E4	501	GTP	N9-C8-N7	-2.58	108.61	113.40
11	B5	501	GDP	C4-C5-N7	-2.58	106.58	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C9	502	GDP	C3'-C2'-C1'	2.58	106.34	101.46
9	D4	501	GTP	C5-C6-N1	2.58	119.81	113.25
9	E2	501	GTP	C5-C6-N1	2.58	119.81	113.25
9	D6	501	GTP	C5-C6-N1	2.58	119.81	113.25
9	D8	501	GTP	C5-C6-N1	2.57	119.80	113.25
9	A6	501	GTP	C8-N7-C5	2.57	108.84	104.26
9	F0	501	GTP	C5-C6-N1	2.57	119.79	113.25
11	C3	501	GDP	C4-C5-N7	-2.57	106.60	110.67
9	A8	501	GTP	O2B-PB-O3A	2.57	114.21	107.27
11	D3	502	GDP	C4-C5-N7	-2.56	106.61	110.67
9	D2	501	GTP	N9-C8-N7	-2.56	108.65	113.40
11	C5	501	GDP	C4-C5-N7	-2.56	106.61	110.67
11	C7	501	GDP	C4-C5-N7	-2.56	106.62	110.67
11	E7	502	GDP	C4-C5-N7	-2.56	106.62	110.67
9	A8	501	GTP	C5-C6-N1	2.55	119.75	113.25
9	B4	501	GTP	C8-N7-C5	2.55	108.80	104.26
9	B2	501	GTP	C5-C6-N1	2.55	119.74	113.25
9	B8	502	GTP	C8-N7-C5	2.55	108.80	104.26
11	C9	502	GDP	C4-C5-N7	-2.55	106.64	110.67
9	E2	501	GTP	C8-N7-C5	2.54	108.79	104.26
9	D4	501	GTP	O6-C6-C5	-2.54	119.82	126.53
9	C2	501	GTP	C8-N7-C5	2.54	108.78	104.26
9	C6	501	GTP	C5-C6-N1	2.53	119.70	113.25
9	E4	501	GTP	O6-C6-C5	-2.53	119.86	126.53
9	A4	501	GTP	C5-C6-N1	2.52	119.68	113.25
9	E8	501	GTP	C5-C6-N1	2.52	119.67	113.25
9	A0	501	GTP	C5-C6-N1	2.52	119.66	113.25
9	F0	501	GTP	C8-N7-C5	2.52	108.74	104.26
9	E0	501	GTP	C5-C6-N1	2.51	119.65	113.25
9	B2	501	GTP	C8-N7-C5	2.51	108.74	104.26
11	B7	501	GDP	C4-C5-N7	-2.51	106.69	110.67
11	E1	501	GDP	C4-C5-N7	-2.51	106.69	110.67
9	A8	501	GTP	C8-N7-C5	2.50	108.72	104.26
11	D7	501	GDP	C4-C5-N7	-2.50	106.71	110.67
9	C8	501	GTP	C8-N7-C5	2.50	108.71	104.26
9	C8	501	GTP	C5-C6-N1	2.50	119.61	113.25
11	D9	501	GDP	C4-C5-N7	-2.50	106.72	110.67
11	B5	501	GDP	C3'-C2'-C1'	2.49	106.18	101.46
9	C0	501	GTP	C8-N7-C5	2.49	108.70	104.26
9	D8	501	GTP	O6-C6-C5	-2.49	119.96	126.53
9	A4	501	GTP	N9-C8-N7	-2.49	108.78	113.40
9	A4	501	GTP	C8-N7-C5	2.48	108.69	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C0	501	GTP	C5-C6-N1	2.48	119.57	113.25
11	D5	501	GDP	C4-C5-N7	-2.48	106.74	110.67
9	B0	501	GTP	C5-C6-N1	2.47	119.55	113.25
11	E7	502	GDP	C3'-C2'-C1'	2.47	106.14	101.46
9	D0	501	GTP	C5-C6-N1	2.47	119.54	113.25
11	A3	501	GDP	C3'-C2'-C1'	2.46	106.12	101.46
9	E2	501	GTP	O6-C6-C5	-2.46	120.03	126.53
9	B6	501	GTP	C5-C6-N1	2.46	119.53	113.25
9	B6	501	GTP	C8-N7-C5	2.46	108.65	104.26
9	C4	501	GTP	O6-C6-C5	-2.46	120.04	126.53
9	C2	501	GTP	O6-C6-C5	-2.46	120.05	126.53
9	F0	501	GTP	O6-C6-C5	-2.45	120.07	126.53
11	O	601	GDP	C3'-C2'-C1'	2.45	106.09	101.46
11	A1	501	GDP	C3'-C2'-C1'	2.45	106.09	101.46
9	D6	501	GTP	O6-C6-C5	-2.44	120.08	126.53
11	B9	501	GDP	C4-C5-N7	-2.44	106.81	110.67
11	F1	501	GDP	C3'-C2'-C1'	2.44	106.07	101.46
11	D9	501	GDP	C3'-C2'-C1'	2.44	106.07	101.46
11	D5	501	GDP	C3'-C2'-C1'	2.43	106.07	101.46
9	A8	501	GTP	O6-C6-C5	-2.43	120.12	126.53
9	A4	501	GTP	O6-C6-C5	-2.43	120.13	126.53
9	B8	502	GTP	O6-C6-C5	-2.43	120.13	126.53
11	A5	501	GDP	C4-C5-N7	-2.42	106.83	110.67
9	B2	501	GTP	O6-C6-C5	-2.42	120.14	126.53
11	C7	501	GDP	C3'-C2'-C1'	2.41	106.03	101.46
11	B3	501	GDP	C4-C5-N7	-2.41	106.85	110.67
9	B4	501	GTP	O6-C6-C5	-2.41	120.18	126.53
9	B6	501	GTP	O6-C6-C5	-2.40	120.20	126.53
9	A0	501	GTP	O6-C6-C5	-2.40	120.21	126.53
11	A7	501	GDP	C4-C5-N7	-2.39	106.88	110.67
9	C6	501	GTP	O6-C6-C5	-2.39	120.22	126.53
9	E7	501	GTP	O6-C6-C5	-2.39	120.23	126.53
9	E4	501	GTP	C8-N7-C5	2.39	108.51	104.26
9	E8	501	GTP	O6-C6-C5	-2.38	120.24	126.53
9	C0	501	GTP	O6-C6-C5	-2.38	120.26	126.53
11	E5	501	GDP	C3'-C2'-C1'	2.37	105.94	101.46
11	D1	502	GDP	C3'-C2'-C1'	2.35	105.91	101.46
9	D2	501	GTP	C8-N7-C5	2.33	108.41	104.26
9	C8	501	GTP	O6-C6-C5	-2.33	120.38	126.53
9	E0	501	GTP	O6-C6-C5	-2.33	120.39	126.53
11	A7	501	GDP	C3'-C2'-C1'	2.33	105.87	101.46
11	A1	501	GDP	O3B-PB-O3A	2.33	112.44	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	O	601	GDP	C4-C5-N7	-2.33	106.98	110.67
9	A2	502	GTP	O6-C6-C5	-2.32	120.40	126.53
9	E4	501	GTP	O3G-PG-O3B	2.31	112.39	104.64
9	B0	501	GTP	O6-C6-C5	-2.31	120.44	126.53
11	C5	501	GDP	C3'-C2'-C1'	2.31	105.83	101.46
9	C4	501	GTP	C8-N7-C5	2.30	108.35	104.26
9	A6	501	GTP	O6-C6-C5	-2.30	120.47	126.53
9	D0	501	GTP	C3'-C2'-C1'	2.28	105.77	101.46
11	E1	501	GDP	C3'-C2'-C1'	2.27	105.76	101.46
11	B9	501	GDP	C3'-C2'-C1'	2.24	105.70	101.46
9	E7	501	GTP	O2B-PB-O3A	2.22	113.27	107.27
9	D0	501	GTP	O6-C6-C5	-2.21	120.70	126.53
11	E9	501	GDP	C3'-C2'-C1'	2.20	105.62	101.46
9	B2	501	GTP	C3'-C2'-C1'	2.20	105.62	101.46
11	C7	501	GDP	O2A-PA-O3A	2.20	113.21	107.27
9	C2	501	GTP	O2A-PA-O3A	2.19	113.20	107.27
11	A5	501	GDP	C3'-C2'-C1'	2.18	105.59	101.46
9	B0	501	GTP	C3'-C2'-C1'	2.17	105.58	101.46
11	E3	501	GDP	C3'-C2'-C1'	2.17	105.58	101.46
11	C3	501	GDP	C3'-C2'-C1'	2.17	105.56	101.46
11	E1	501	GDP	O6-C6-C5	-2.17	120.81	126.53
11	A5	501	GDP	O6-C6-C5	-2.16	120.83	126.53
9	E8	501	GTP	C3'-C2'-C1'	2.16	105.55	101.46
9	C6	501	GTP	C3'-C2'-C1'	2.14	105.50	101.46
9	C8	501	GTP	C3'-C2'-C1'	2.13	105.50	101.46
11	D5	501	GDP	O6-C6-C5	-2.13	120.92	126.53
11	D1	502	GDP	O6-C6-C5	-2.12	120.94	126.53
11	E7	502	GDP	O6-C6-C5	-2.12	120.94	126.53
11	A1	501	GDP	O2A-PA-O3A	2.12	113.00	107.27
11	D3	502	GDP	C2'-C3'-C4'	2.12	106.70	102.61
11	E9	501	GDP	O6-C6-C5	-2.12	120.95	126.53
9	E4	501	GTP	C3'-C2'-C1'	2.11	105.46	101.46
11	C3	501	GDP	O6-C6-C5	-2.11	120.96	126.53
11	B9	501	GDP	O6-C6-C5	-2.11	120.96	126.53
11	D7	501	GDP	C3'-C2'-C1'	2.11	105.46	101.46
9	A8	501	GTP	C3'-C2'-C1'	2.11	105.45	101.46
11	C9	502	GDP	O6-C6-C5	-2.10	120.98	126.53
11	B5	501	GDP	O6-C6-C5	-2.10	121.00	126.53
11	P	601	GDP	O4'-C1'-N9	2.10	113.11	108.36
9	D2	501	GTP	C3'-C2'-C1'	2.09	105.42	101.46
11	A7	501	GDP	C2'-C3'-C4'	2.09	106.64	102.61
11	D9	501	GDP	O6-C6-C5	-2.08	121.03	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C1	501	GDP	C3'-C2'-C1'	2.08	105.39	101.46
9	C0	501	GTP	O2A-PA-O3A	2.07	112.88	107.27
11	O	601	GDP	O6-C6-C5	-2.07	121.06	126.53
9	B8	502	GTP	C3'-C2'-C1'	2.07	105.38	101.46
9	E2	501	GTP	C3'-C2'-C1'	2.07	105.38	101.46
11	E1	501	GDP	O3B-PB-O3A	2.07	111.57	104.64
11	A3	501	GDP	O6-C6-C5	-2.07	121.08	126.53
11	C5	501	GDP	O6-C6-C5	-2.06	121.08	126.53
11	B7	501	GDP	O6-C6-C5	-2.06	121.10	126.53
11	C7	501	GDP	O6-C6-C5	-2.06	121.10	126.53
11	D7	501	GDP	O6-C6-C5	-2.06	121.11	126.53
11	F1	501	GDP	O6-C6-C5	-2.05	121.13	126.53
9	C2	501	GTP	C3'-C2'-C1'	2.04	105.32	101.46
11	E1	501	GDP	C5-C6-N1	2.03	118.42	113.25
9	E4	501	GTP	O2B-PB-O3A	2.03	112.76	107.27
9	C0	501	GTP	O2G-PG-O3B	2.03	111.43	104.64
9	B6	501	GTP	C3'-C2'-C1'	2.03	105.30	101.46
9	F0	501	GTP	C3'-C2'-C1'	2.03	105.29	101.46
9	E7	501	GTP	O3G-PG-O3B	2.02	111.41	104.64
9	D4	501	GTP	C4-C5-N7	-2.01	107.48	110.67
11	A7	501	GDP	O6-C6-C5	-2.01	121.23	126.53
9	E4	501	GTP	O2A-PA-O3A	2.01	112.70	107.27
11	E3	501	GDP	C5-C6-N1	2.00	118.35	113.25
9	D6	501	GTP	C3'-C2'-C1'	2.00	105.25	101.46

There are no chirality outliers.

All (248) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A0	501	GTP	PB-O3A-PA-O5'
9	A2	502	GTP	C5'-O5'-PA-O3A
9	A2	502	GTP	C5'-O5'-PA-O1A
9	A2	502	GTP	C5'-O5'-PA-O2A
9	A4	501	GTP	C5'-O5'-PA-O3A
9	A4	501	GTP	C5'-O5'-PA-O1A
9	A4	501	GTP	C5'-O5'-PA-O2A
9	A6	501	GTP	C5'-O5'-PA-O3A
9	A6	501	GTP	C5'-O5'-PA-O1A
9	A8	501	GTP	C5'-O5'-PA-O3A
9	A8	501	GTP	C5'-O5'-PA-O1A
9	A8	501	GTP	C5'-O5'-PA-O2A
9	B0	501	GTP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
9	B0	501	GTP	C5'-O5'-PA-O1A
9	B0	501	GTP	C5'-O5'-PA-O2A
9	B4	501	GTP	C5'-O5'-PA-O3A
9	B4	501	GTP	C5'-O5'-PA-O1A
9	B4	501	GTP	O4'-C4'-C5'-O5'
9	B6	501	GTP	C5'-O5'-PA-O3A
9	B8	502	GTP	C5'-O5'-PA-O3A
9	B8	502	GTP	C5'-O5'-PA-O1A
9	B8	502	GTP	O4'-C4'-C5'-O5'
9	B8	502	GTP	C3'-C4'-C5'-O5'
9	C0	501	GTP	C5'-O5'-PA-O3A
9	C0	501	GTP	C5'-O5'-PA-O1A
9	C0	501	GTP	C5'-O5'-PA-O2A
9	C2	501	GTP	C5'-O5'-PA-O3A
9	C2	501	GTP	C5'-O5'-PA-O2A
9	C4	501	GTP	PB-O3A-PA-O5'
9	C4	501	GTP	O4'-C4'-C5'-O5'
9	C6	501	GTP	PB-O3B-PG-O2G
9	C6	501	GTP	PB-O3A-PA-O5'
9	C8	501	GTP	C5'-O5'-PA-O1A
9	D0	501	GTP	C5'-O5'-PA-O3A
9	D0	501	GTP	C5'-O5'-PA-O2A
9	D2	501	GTP	C5'-O5'-PA-O3A
9	D2	501	GTP	C5'-O5'-PA-O1A
9	D2	501	GTP	C5'-O5'-PA-O2A
9	D4	501	GTP	C5'-O5'-PA-O3A
9	D4	501	GTP	C5'-O5'-PA-O2A
9	D6	501	GTP	C5'-O5'-PA-O3A
9	D6	501	GTP	C5'-O5'-PA-O1A
9	D8	501	GTP	C5'-O5'-PA-O3A
9	D8	501	GTP	C5'-O5'-PA-O2A
9	E0	501	GTP	C5'-O5'-PA-O1A
9	E2	501	GTP	C5'-O5'-PA-O3A
9	E2	501	GTP	C5'-O5'-PA-O2A
9	E4	501	GTP	PB-O3B-PG-O3G
9	E4	501	GTP	C5'-O5'-PA-O3A
9	E4	501	GTP	C5'-O5'-PA-O1A
9	E4	501	GTP	C5'-O5'-PA-O2A
9	E7	501	GTP	C5'-O5'-PA-O3A
9	E7	501	GTP	C5'-O5'-PA-O1A
9	E7	501	GTP	C5'-O5'-PA-O2A
9	E7	501	GTP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
9	E8	501	GTP	C5'-O5'-PA-O3A
9	E8	501	GTP	C5'-O5'-PA-O1A
9	E8	501	GTP	C5'-O5'-PA-O2A
9	F0	501	GTP	C5'-O5'-PA-O3A
9	F0	501	GTP	C5'-O5'-PA-O1A
9	F0	501	GTP	C5'-O5'-PA-O2A
11	A1	501	GDP	C5'-O5'-PA-O3A
11	A1	501	GDP	C5'-O5'-PA-O1A
11	A1	501	GDP	C5'-O5'-PA-O2A
11	A3	501	GDP	C5'-O5'-PA-O3A
11	A3	501	GDP	C5'-O5'-PA-O1A
11	A3	501	GDP	C5'-O5'-PA-O2A
11	A3	501	GDP	O4'-C4'-C5'-O5'
11	A3	501	GDP	C3'-C4'-C5'-O5'
11	A7	501	GDP	C5'-O5'-PA-O3A
11	A7	501	GDP	C5'-O5'-PA-O1A
11	A7	501	GDP	C5'-O5'-PA-O2A
11	B3	501	GDP	C5'-O5'-PA-O3A
11	B3	501	GDP	C5'-O5'-PA-O2A
11	B7	501	GDP	C5'-O5'-PA-O3A
11	B7	501	GDP	C5'-O5'-PA-O1A
11	B7	501	GDP	C5'-O5'-PA-O2A
11	B9	501	GDP	PA-O3A-PB-O3B
11	B9	501	GDP	C5'-O5'-PA-O3A
11	B9	501	GDP	C5'-O5'-PA-O2A
11	C3	501	GDP	PA-O3A-PB-O3B
11	C7	501	GDP	C5'-O5'-PA-O3A
11	C7	501	GDP	C5'-O5'-PA-O1A
11	C7	501	GDP	C5'-O5'-PA-O2A
11	C9	502	GDP	C5'-O5'-PA-O3A
11	C9	502	GDP	C5'-O5'-PA-O2A
11	D3	502	GDP	C5'-O5'-PA-O3A
11	D3	502	GDP	C5'-O5'-PA-O1A
11	D3	502	GDP	C5'-O5'-PA-O2A
11	D5	501	GDP	C5'-O5'-PA-O3A
11	D5	501	GDP	C5'-O5'-PA-O1A
11	D5	501	GDP	C5'-O5'-PA-O2A
11	D7	501	GDP	C5'-O5'-PA-O3A
11	D7	501	GDP	C5'-O5'-PA-O1A
11	D7	501	GDP	C5'-O5'-PA-O2A
11	D9	501	GDP	C5'-O5'-PA-O3A
11	D9	501	GDP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
11	D9	501	GDP	C5'-O5'-PA-O2A
11	E3	501	GDP	C5'-O5'-PA-O3A
11	E3	501	GDP	C5'-O5'-PA-O2A
11	E9	501	GDP	C5'-O5'-PA-O3A
11	E9	501	GDP	C5'-O5'-PA-O1A
11	E9	501	GDP	C5'-O5'-PA-O2A
11	F1	501	GDP	C5'-O5'-PA-O3A
11	F1	501	GDP	C5'-O5'-PA-O1A
11	O	601	GDP	C5'-O5'-PA-O3A
11	O	601	GDP	C5'-O5'-PA-O1A
11	O	601	GDP	C5'-O5'-PA-O2A
11	P	601	GDP	C5'-O5'-PA-O3A
11	P	601	GDP	C5'-O5'-PA-O1A
11	P	601	GDP	C5'-O5'-PA-O2A
9	A0	501	GTP	O4'-C4'-C5'-O5'
9	A0	501	GTP	C3'-C4'-C5'-O5'
9	A2	502	GTP	O4'-C4'-C5'-O5'
9	A2	502	GTP	C3'-C4'-C5'-O5'
9	A4	501	GTP	O4'-C4'-C5'-O5'
9	A4	501	GTP	C3'-C4'-C5'-O5'
9	A6	501	GTP	O4'-C4'-C5'-O5'
9	B0	501	GTP	O4'-C4'-C5'-O5'
9	B0	501	GTP	C3'-C4'-C5'-O5'
9	B4	501	GTP	C3'-C4'-C5'-O5'
9	C4	501	GTP	C3'-C4'-C5'-O5'
9	C6	501	GTP	O4'-C4'-C5'-O5'
9	C6	501	GTP	C3'-C4'-C5'-O5'
9	E4	501	GTP	O4'-C4'-C5'-O5'
9	E7	501	GTP	C3'-C4'-C5'-O5'
9	E8	501	GTP	C3'-C4'-C5'-O5'
9	F0	501	GTP	O4'-C4'-C5'-O5'
9	F0	501	GTP	C3'-C4'-C5'-O5'
11	B5	501	GDP	O4'-C4'-C5'-O5'
9	A6	501	GTP	C3'-C4'-C5'-O5'
9	D2	501	GTP	O4'-C4'-C5'-O5'
9	D2	501	GTP	C3'-C4'-C5'-O5'
9	E4	501	GTP	C3'-C4'-C5'-O5'
9	E8	501	GTP	O4'-C4'-C5'-O5'
11	B5	501	GDP	C3'-C4'-C5'-O5'
9	B2	501	GTP	C3'-C4'-C5'-O5'
11	A7	501	GDP	C3'-C4'-C5'-O5'
11	E9	501	GDP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
11	A3	501	GDP	O4'-C1'-N9-C4
11	A5	501	GDP	C3'-C4'-C5'-O5'
11	O	601	GDP	C3'-C4'-C5'-O5'
11	A7	501	GDP	PA-O3A-PB-O1B
11	E9	501	GDP	PA-O3A-PB-O1B
9	B2	501	GTP	O4'-C4'-C5'-O5'
9	C0	501	GTP	PB-O3A-PA-O1A
9	B6	501	GTP	C4'-C5'-O5'-PA
9	D0	501	GTP	C4'-C5'-O5'-PA
9	A2	502	GTP	PB-O3A-PA-O5'
9	E7	501	GTP	PB-O3A-PA-O5'
11	B9	501	GDP	C3'-C4'-C5'-O5'
11	D1	502	GDP	C3'-C4'-C5'-O5'
11	E7	502	GDP	C3'-C4'-C5'-O5'
11	A7	501	GDP	PA-O3A-PB-O3B
11	E9	501	GDP	PA-O3A-PB-O3B
11	E3	501	GDP	C3'-C4'-C5'-O5'
9	A6	501	GTP	C4'-C5'-O5'-PA
9	A8	501	GTP	PB-O3A-PA-O1A
9	B0	501	GTP	PA-O3A-PB-O2B
9	C2	501	GTP	PB-O3A-PA-O2A
9	D2	501	GTP	PA-O3A-PB-O2B
9	D8	501	GTP	PA-O3A-PB-O2B
9	E2	501	GTP	PB-O3A-PA-O2A
11	P	601	GDP	C3'-C4'-C5'-O5'
9	A4	501	GTP	C4'-C5'-O5'-PA
9	D8	501	GTP	C4'-C5'-O5'-PA
9	E2	501	GTP	C4'-C5'-O5'-PA
9	E4	501	GTP	C4'-C5'-O5'-PA
9	E8	501	GTP	C4'-C5'-O5'-PA
9	F0	501	GTP	C4'-C5'-O5'-PA
11	A5	501	GDP	O4'-C4'-C5'-O5'
9	A6	501	GTP	C5'-O5'-PA-O2A
9	B4	501	GTP	C5'-O5'-PA-O2A
9	B8	502	GTP	C5'-O5'-PA-O2A
9	C8	501	GTP	C5'-O5'-PA-O3A
9	D4	501	GTP	C5'-O5'-PA-O1A
9	D6	501	GTP	C5'-O5'-PA-O2A
9	E0	501	GTP	C5'-O5'-PA-O3A
11	C5	501	GDP	C5'-O5'-PA-O3A
11	D1	502	GDP	C5'-O5'-PA-O1A
11	F1	501	GDP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
9	A2	502	GTP	C4'-C5'-O5'-PA
9	A8	501	GTP	C4'-C5'-O5'-PA
9	B0	501	GTP	C4'-C5'-O5'-PA
9	B4	501	GTP	C4'-C5'-O5'-PA
9	B8	502	GTP	C4'-C5'-O5'-PA
9	C0	501	GTP	C4'-C5'-O5'-PA
9	C2	501	GTP	C4'-C5'-O5'-PA
9	C8	501	GTP	C4'-C5'-O5'-PA
9	E0	501	GTP	C4'-C5'-O5'-PA
9	E7	501	GTP	C4'-C5'-O5'-PA
11	E9	501	GDP	C4'-C5'-O5'-PA
11	A7	501	GDP	O4'-C4'-C5'-O5'
9	C6	501	GTP	C4'-C5'-O5'-PA
9	A2	502	GTP	PA-O3A-PB-O2B
9	A4	501	GTP	PA-O3A-PB-O2B
9	B2	501	GTP	PB-O3A-PA-O2A
9	B6	501	GTP	PB-O3A-PA-O2A
9	D6	501	GTP	PB-O3A-PA-O1A
9	E7	501	GTP	PA-O3A-PB-O2B
9	E8	501	GTP	PA-O3A-PB-O2B
9	F0	501	GTP	PA-O3A-PB-O2B
11	A1	501	GDP	PB-O3A-PA-O2A
11	A3	501	GDP	O4'-C1'-N9-C8
9	B2	501	GTP	C4'-C5'-O5'-PA
11	B9	501	GDP	PA-O3A-PB-O1B
9	A0	501	GTP	C4'-C5'-O5'-PA
9	D2	501	GTP	C4'-C5'-O5'-PA
11	B9	501	GDP	O4'-C4'-C5'-O5'
11	D1	502	GDP	O4'-C4'-C5'-O5'
11	E7	502	GDP	O4'-C4'-C5'-O5'
9	C0	501	GTP	PB-O3A-PA-O2A
11	A1	501	GDP	C2'-C1'-N9-C4
11	P	601	GDP	C4'-C5'-O5'-PA
9	E4	501	GTP	PB-O3B-PG-O2G
11	C3	501	GDP	PA-O3A-PB-O2B
9	C4	501	GTP	C4'-C5'-O5'-PA
9	D6	501	GTP	C4'-C5'-O5'-PA
11	A1	501	GDP	C2'-C1'-N9-C8
9	A4	501	GTP	PA-O3A-PB-O1B
9	C0	501	GTP	PA-O3A-PB-O1B
9	C0	501	GTP	PA-O3A-PB-O2B
9	D2	501	GTP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
9	D8	501	GTP	PA-O3A-PB-O1B
9	E2	501	GTP	PB-O3A-PA-O1A
9	E4	501	GTP	PA-O3A-PB-O1B
9	E4	501	GTP	PA-O3A-PB-O2B
9	E8	501	GTP	PA-O3A-PB-O1B
11	C7	501	GDP	PB-O3A-PA-O1A
11	C7	501	GDP	PB-O3A-PA-O2A
11	D3	502	GDP	PB-O3A-PA-O2A
11	D7	501	GDP	PB-O3A-PA-O1A
11	D7	501	GDP	PB-O3A-PA-O2A
9	C0	501	GTP	C3'-C4'-C5'-O5'
9	D6	501	GTP	C3'-C4'-C5'-O5'
11	E9	501	GDP	O4'-C4'-C5'-O5'
11	C3	501	GDP	PA-O3A-PB-O1B
11	O	601	GDP	O4'-C4'-C5'-O5'
11	P	601	GDP	O4'-C4'-C5'-O5'
11	A3	501	GDP	C4'-C5'-O5'-PA
9	A0	501	GTP	PB-O3A-PA-O1A
9	A0	501	GTP	PB-O3A-PA-O2A
9	A2	502	GTP	PA-O3A-PB-O1B
9	B2	501	GTP	PB-O3A-PA-O1A
9	B6	501	GTP	PB-O3A-PA-O1A
9	E7	501	GTP	PA-O3A-PB-O1B
11	A1	501	GDP	PB-O3A-PA-O1A
11	B3	501	GDP	PB-O3A-PA-O2A

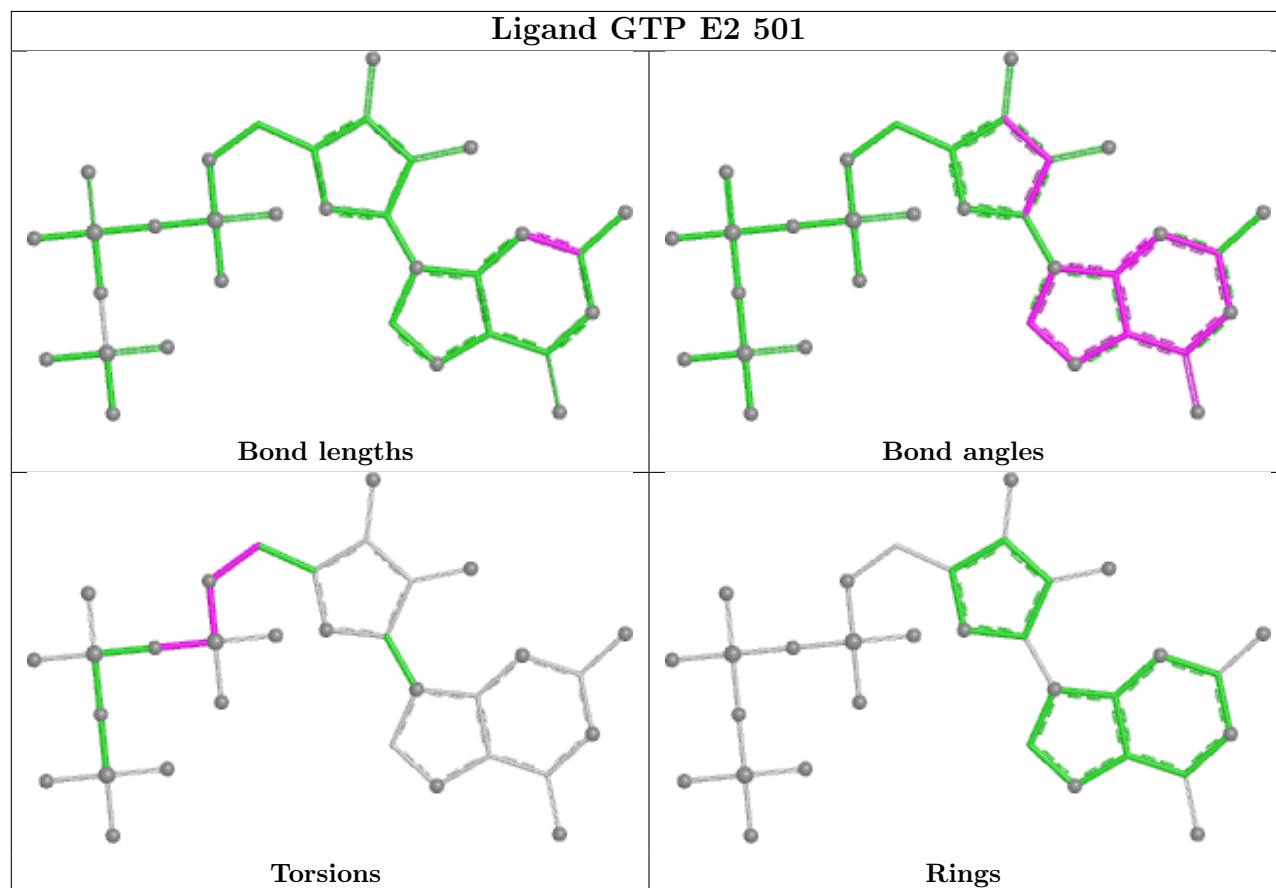
There are no ring outliers.

4 monomers are involved in 4 short contacts:

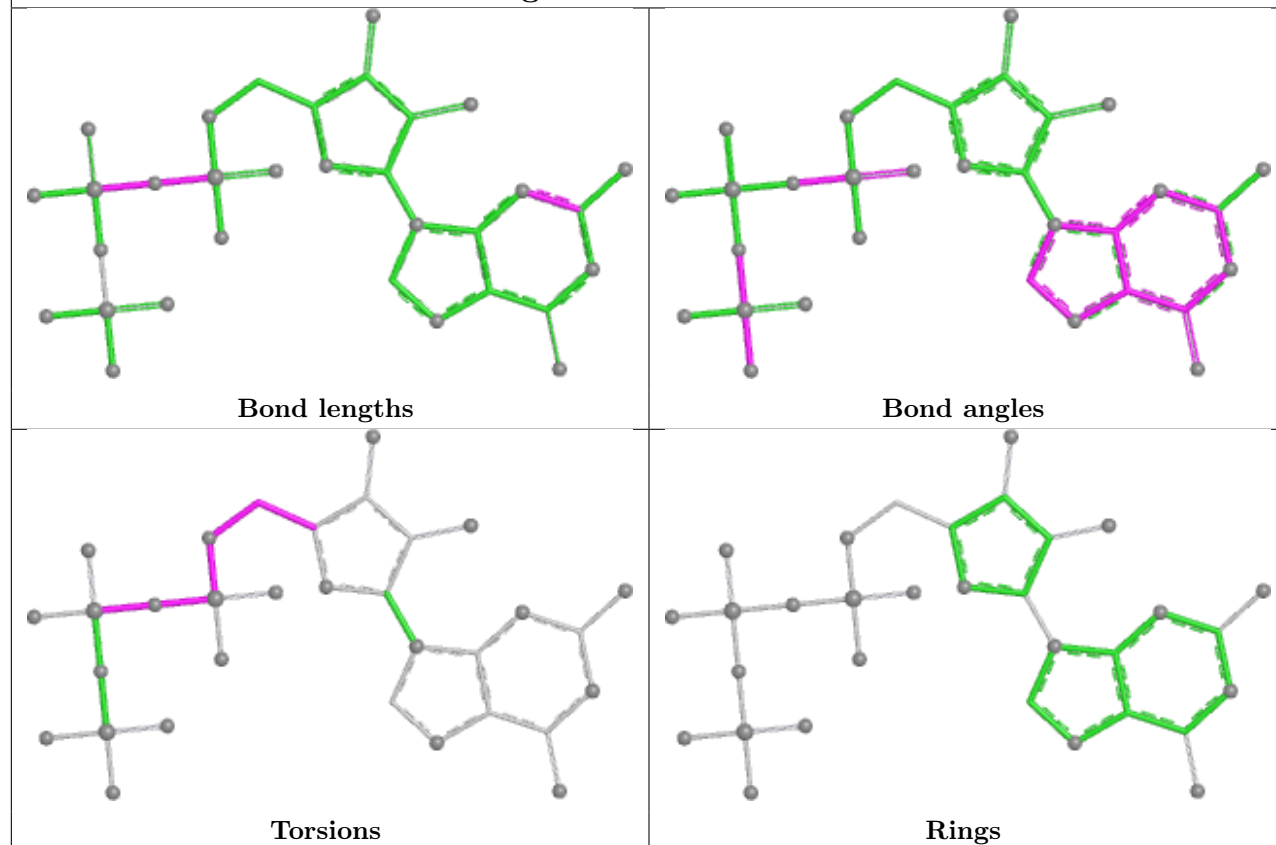
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E7	501	GTP	1	0
11	D7	501	GDP	1	0
11	C7	501	GDP	1	0
11	C9	502	GDP	1	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

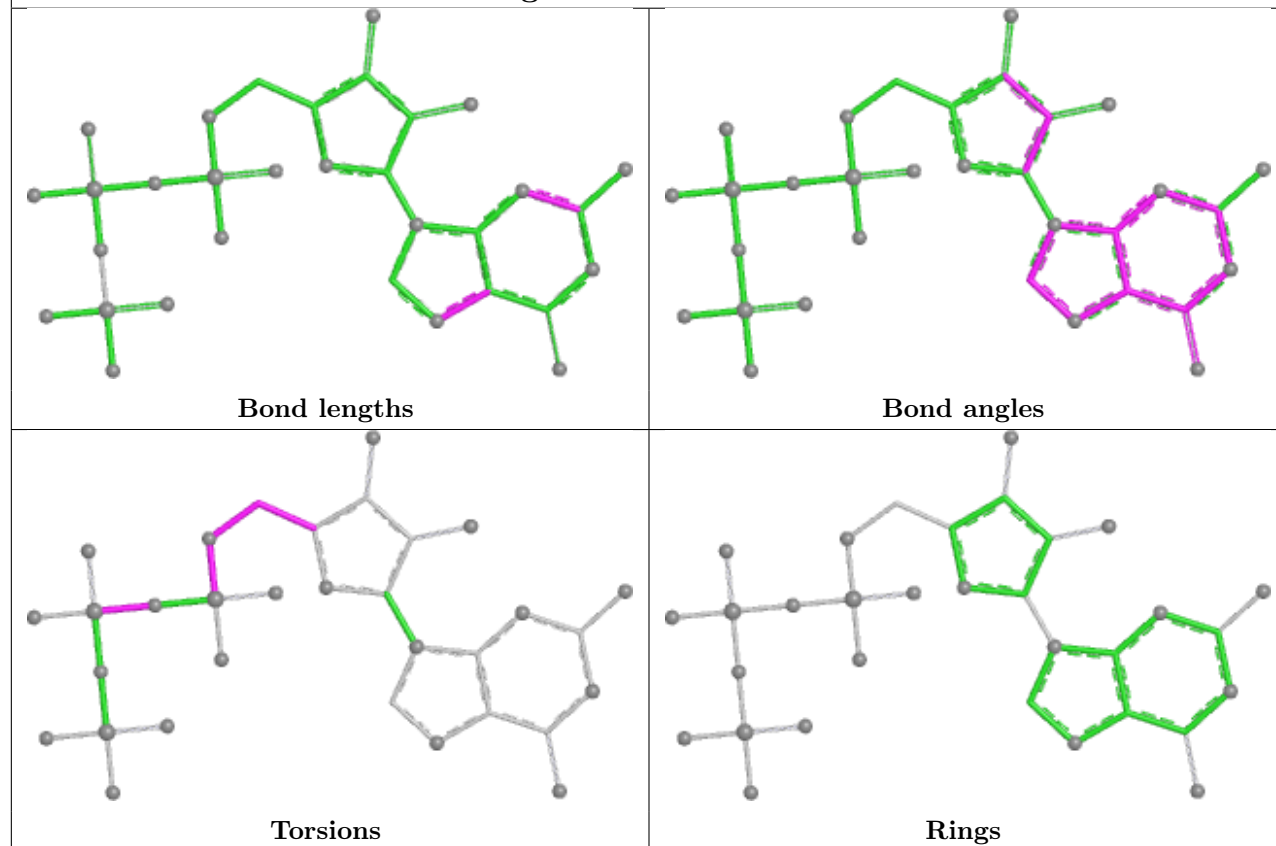
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



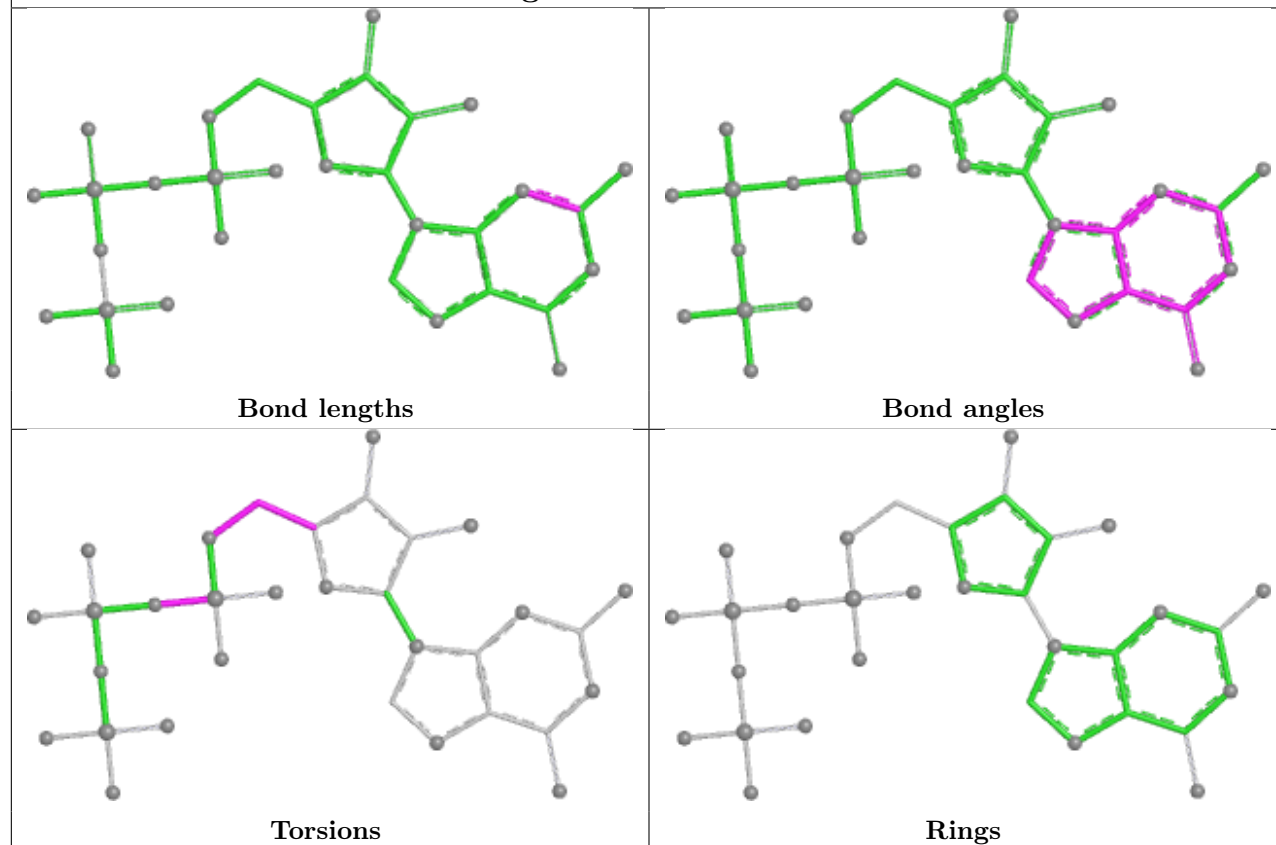
Ligand GTP C0 501



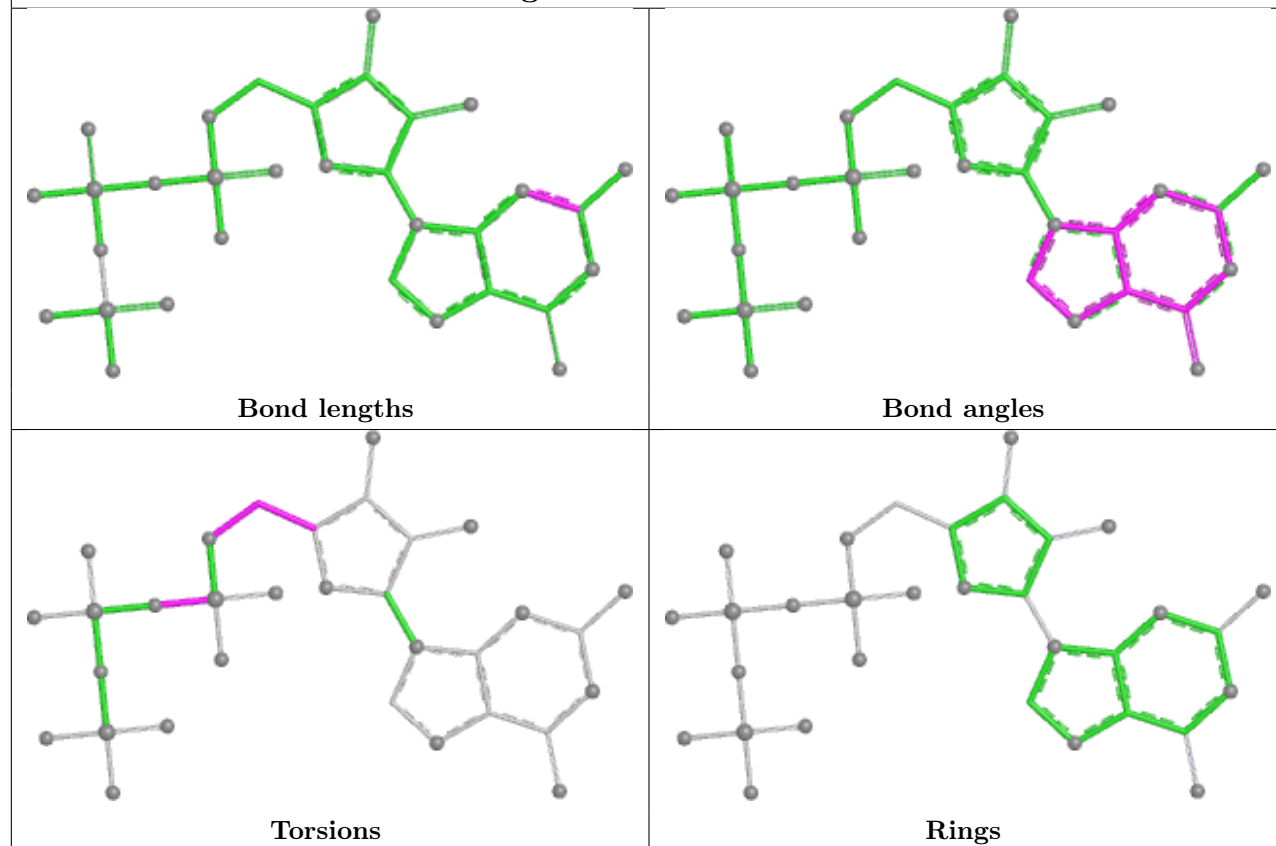
Ligand GTP D2 501

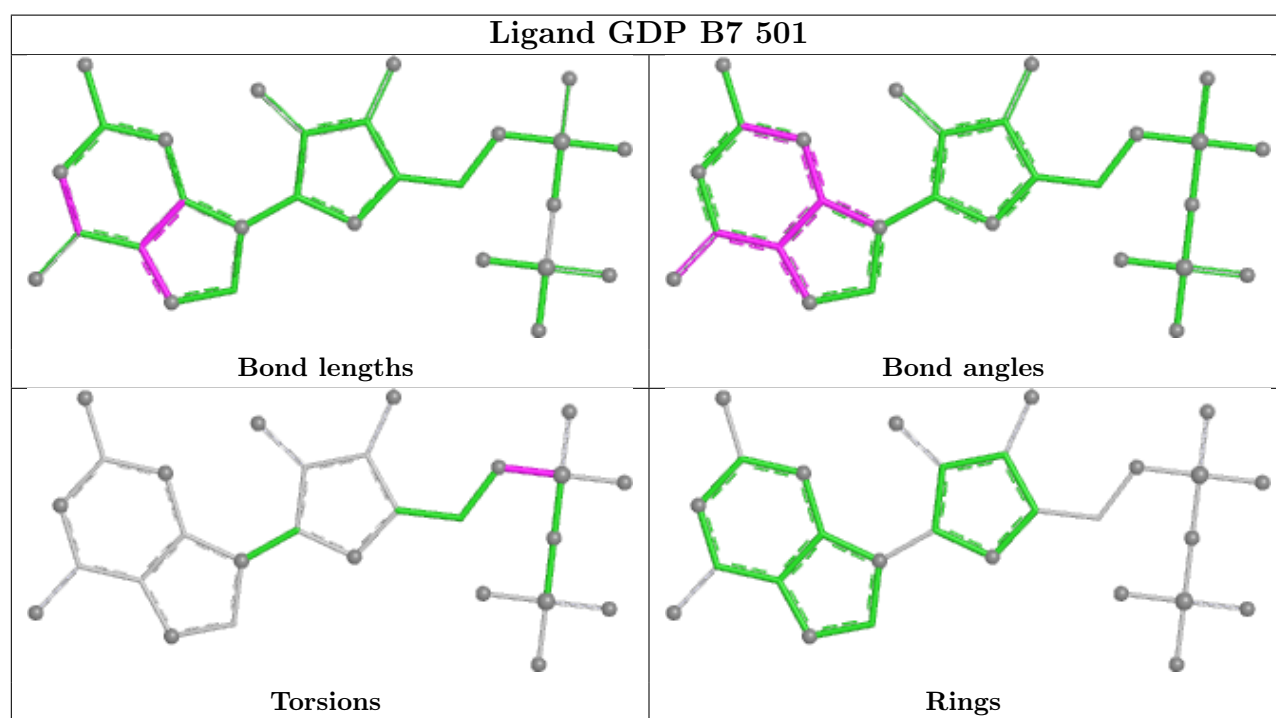
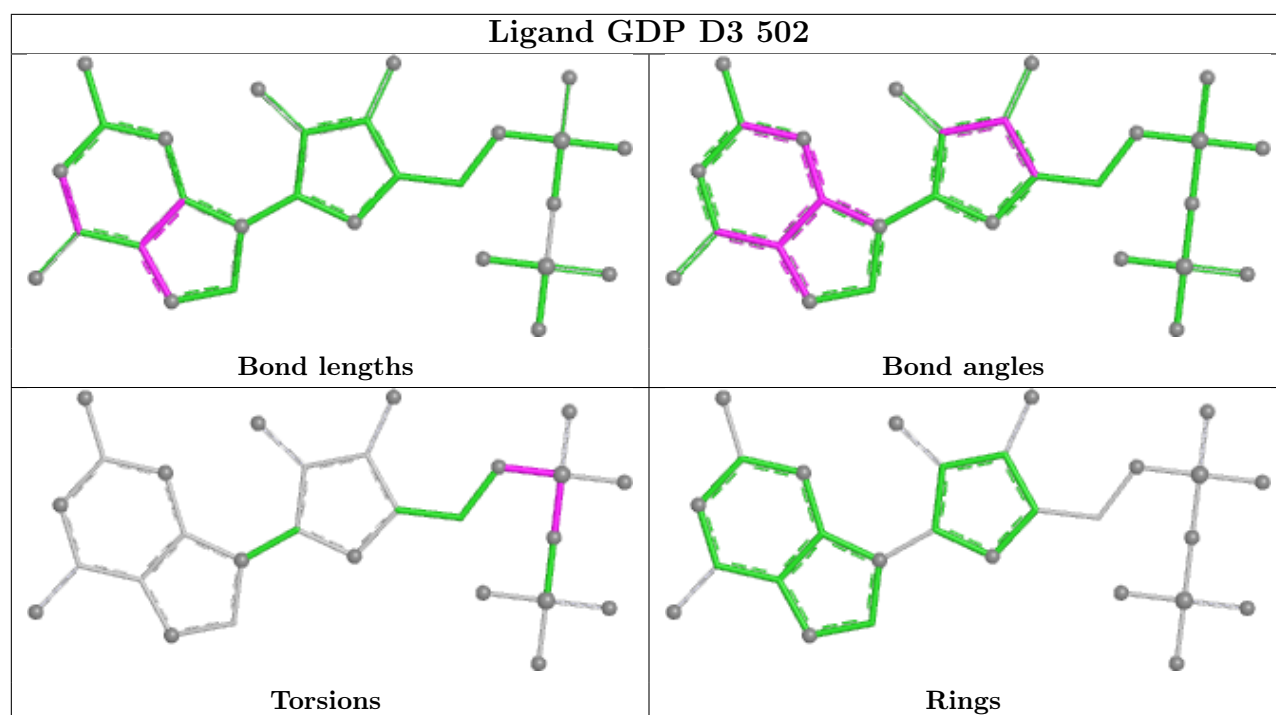


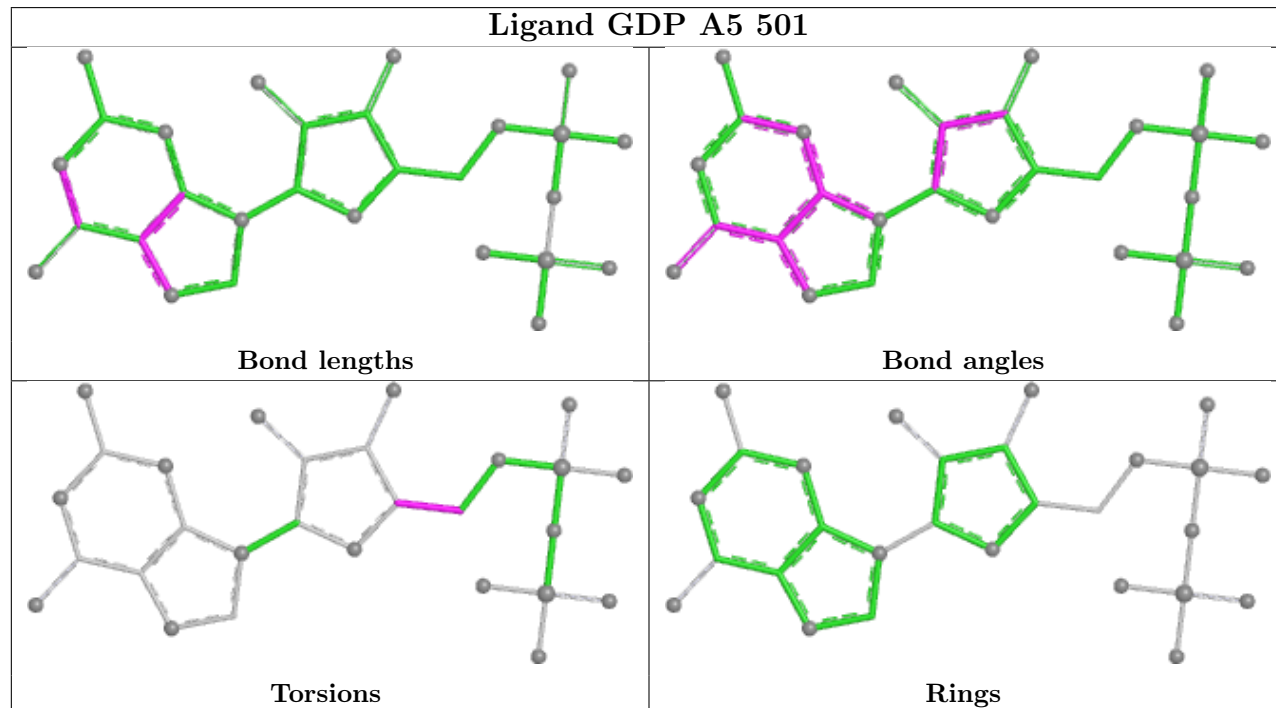
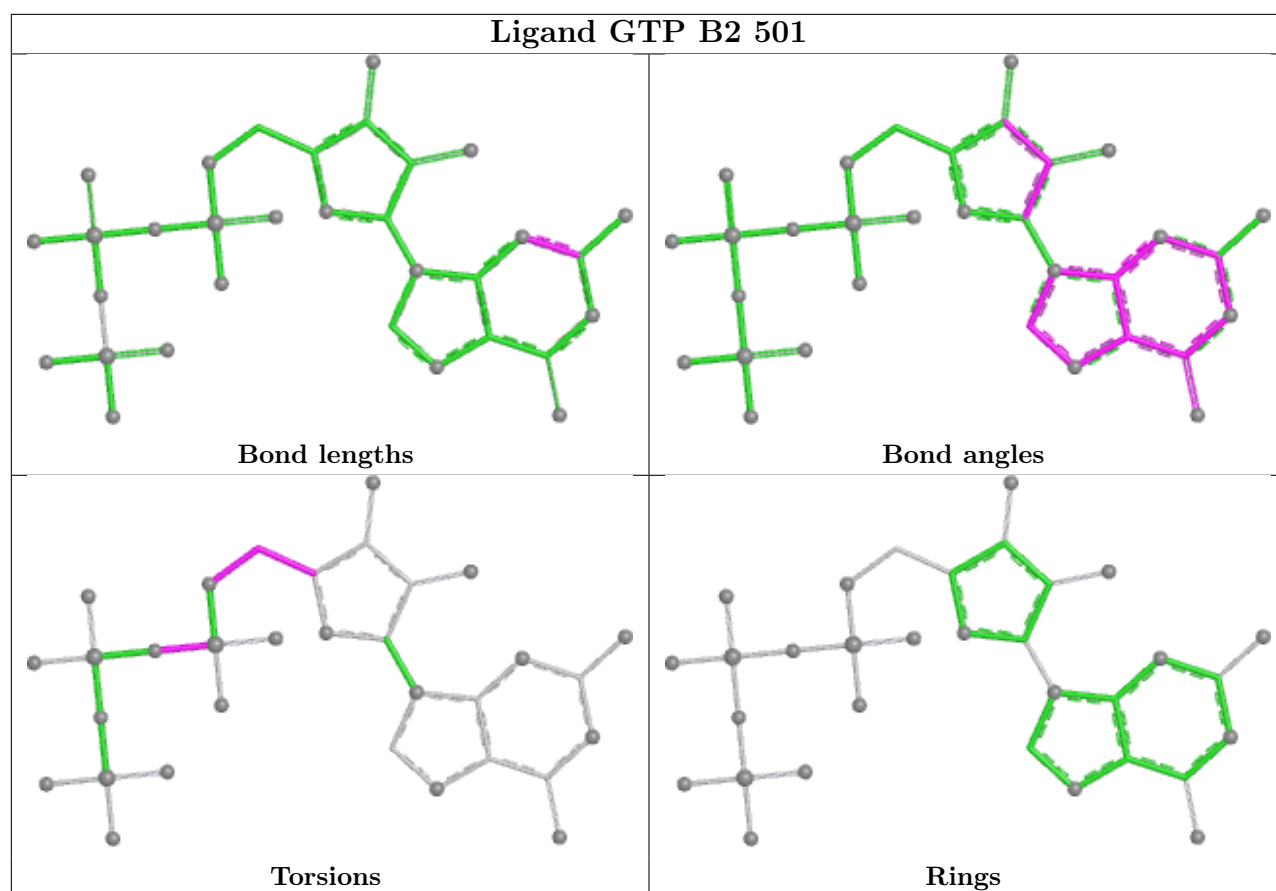
Ligand GTP C4 501

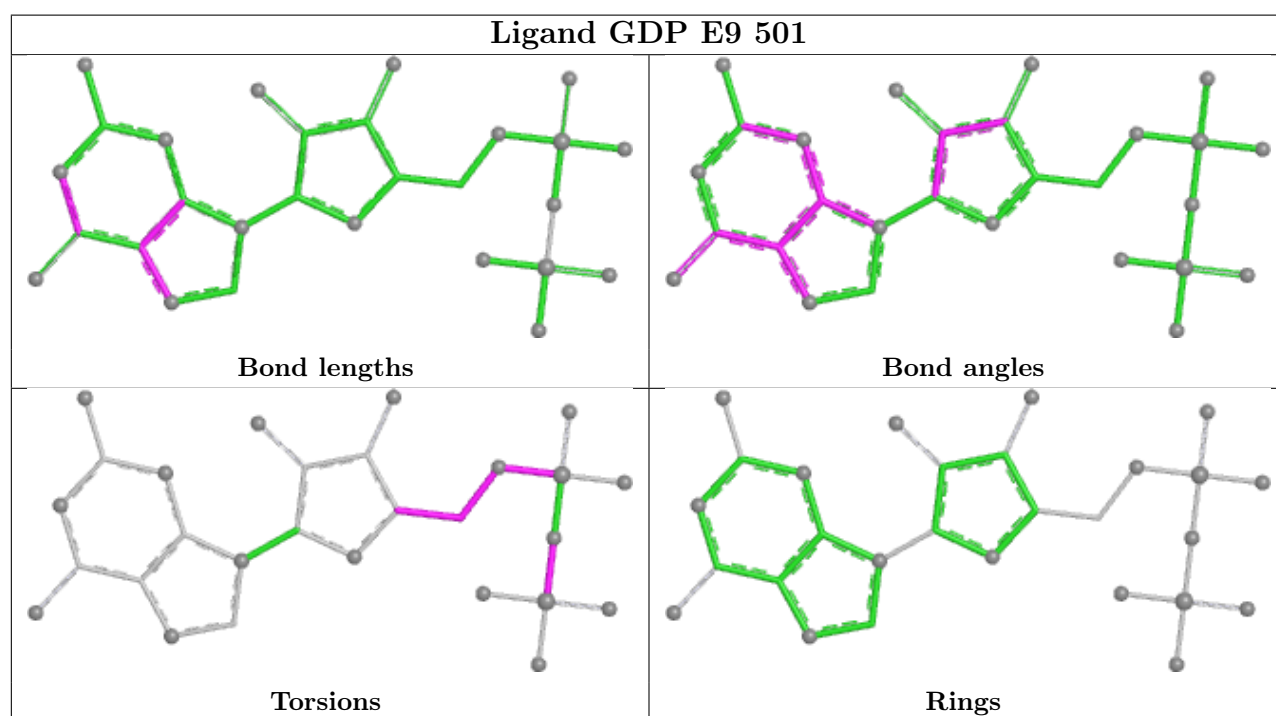
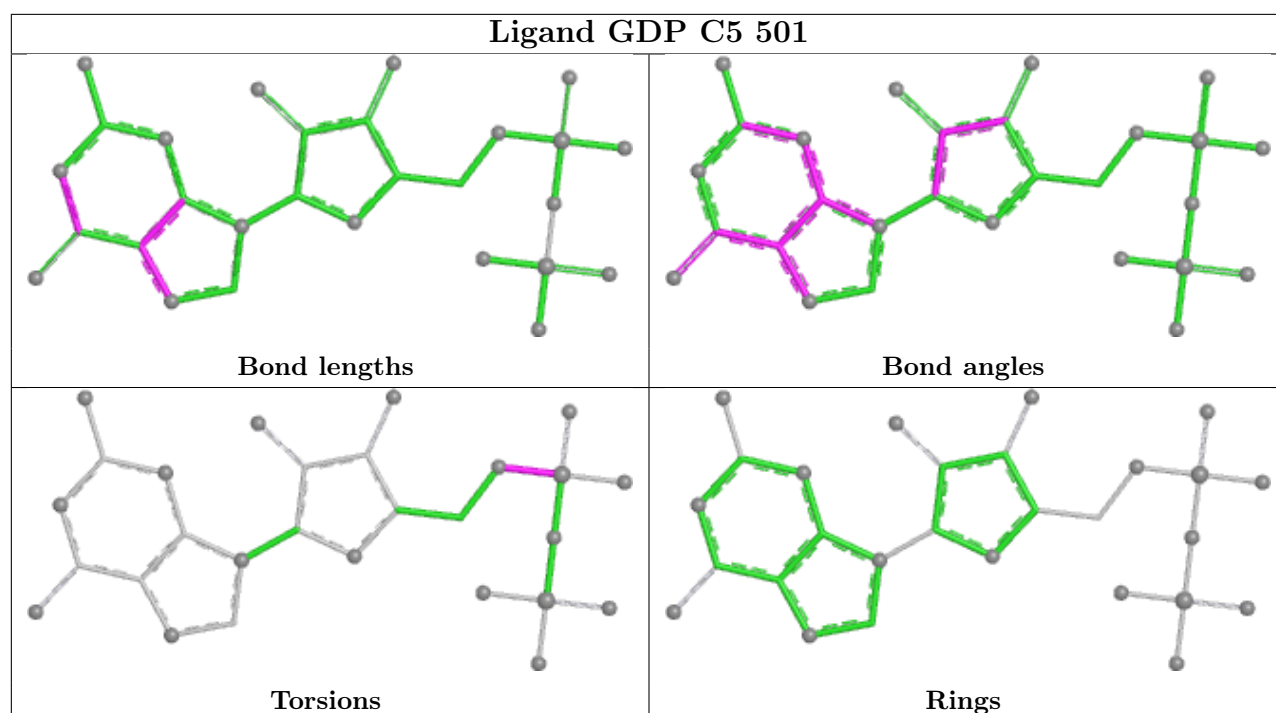


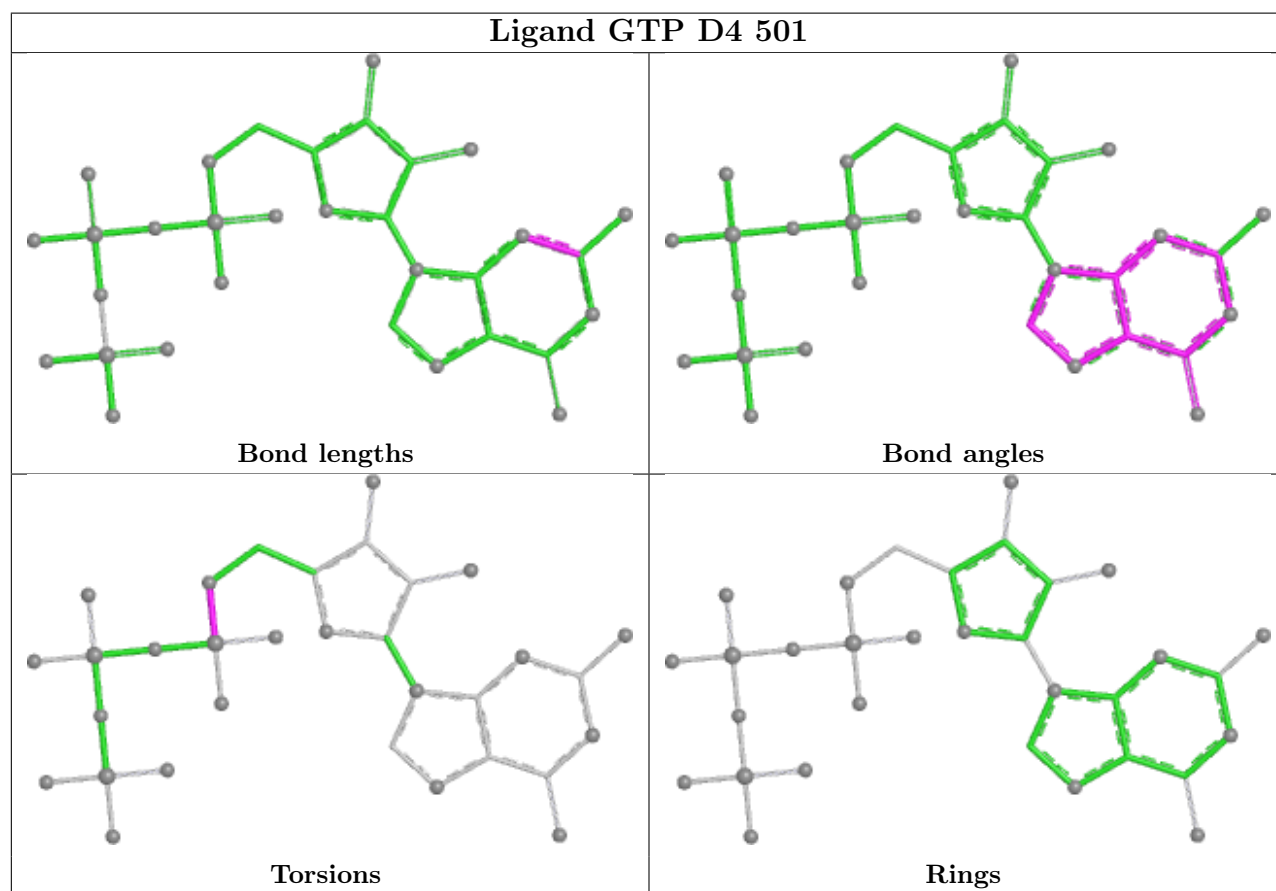
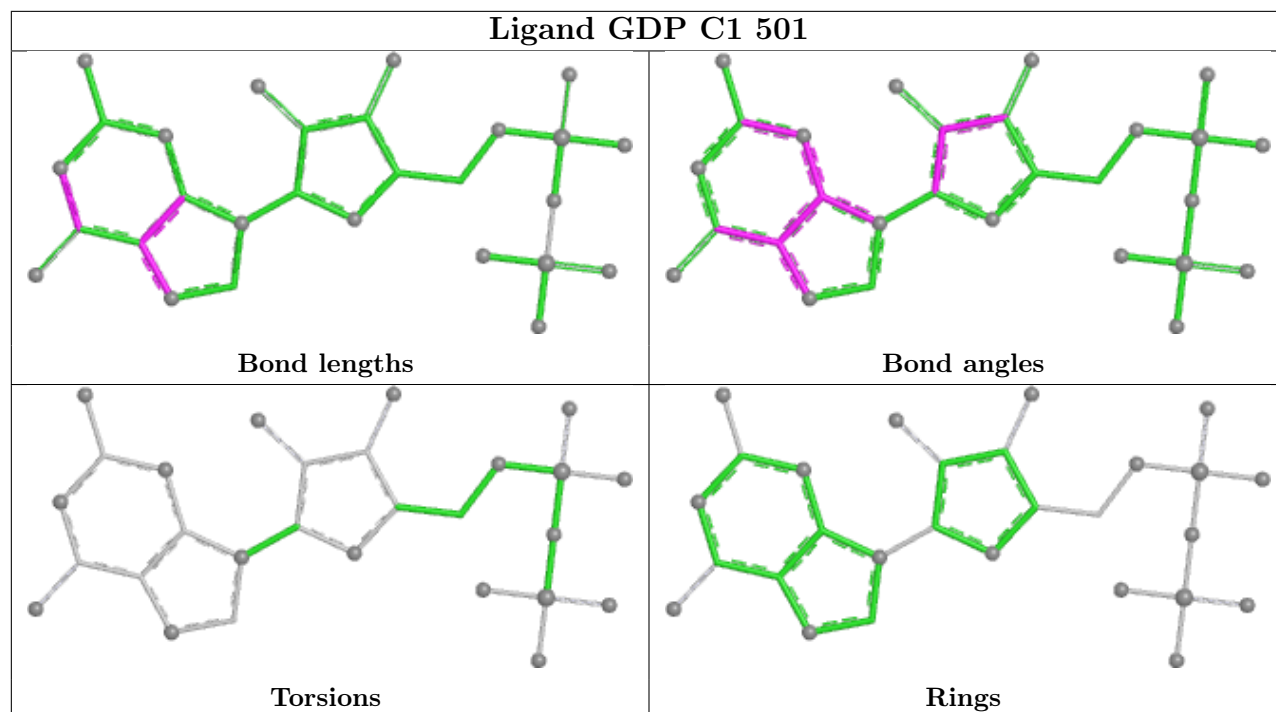
Ligand GTP A0 501

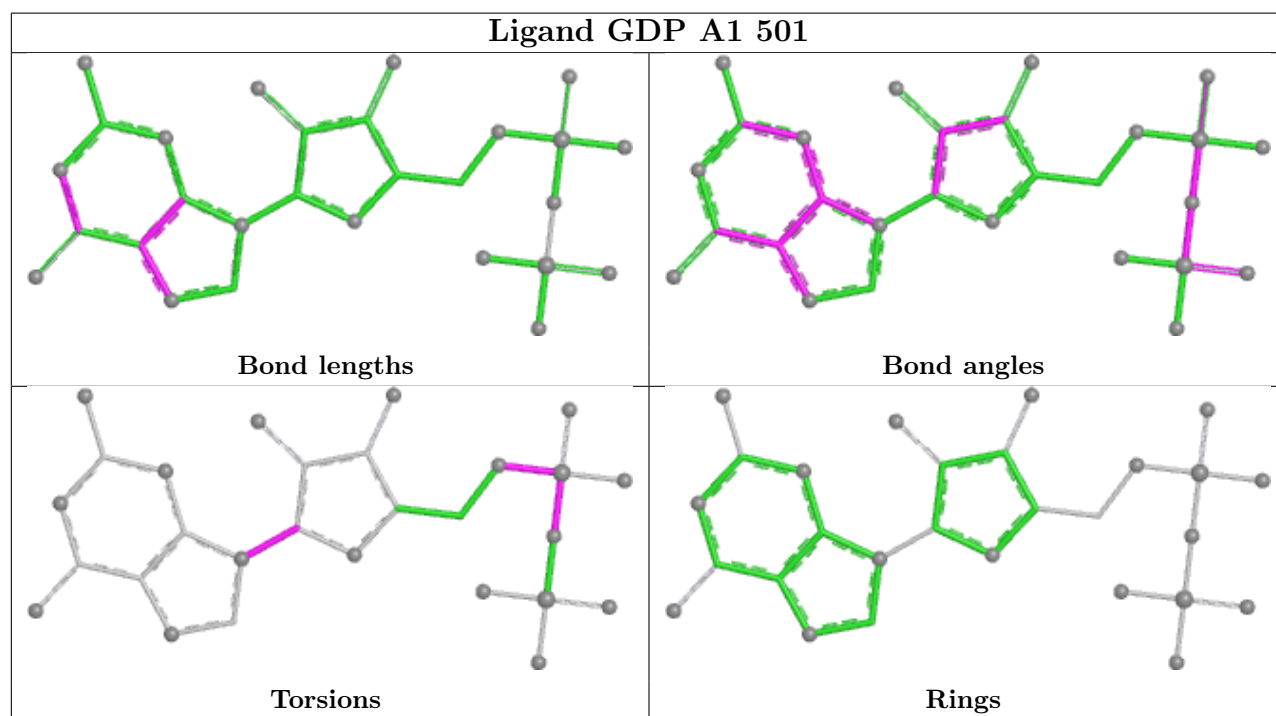
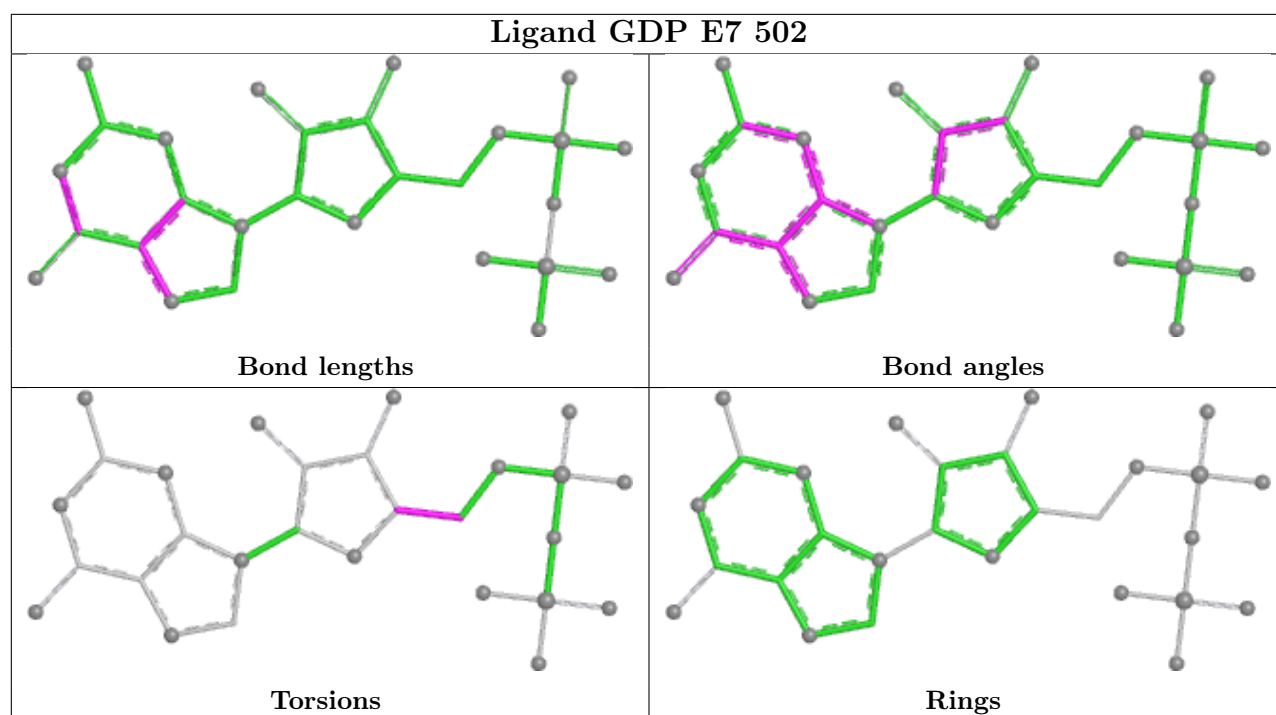


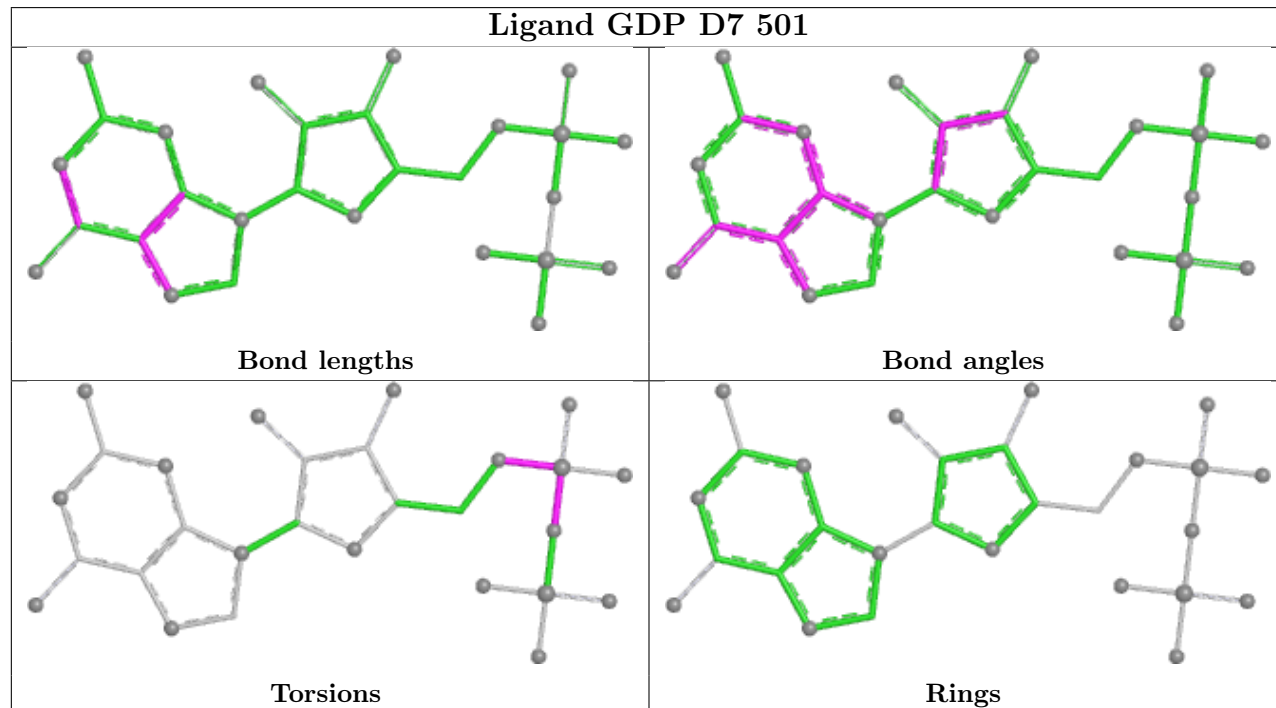
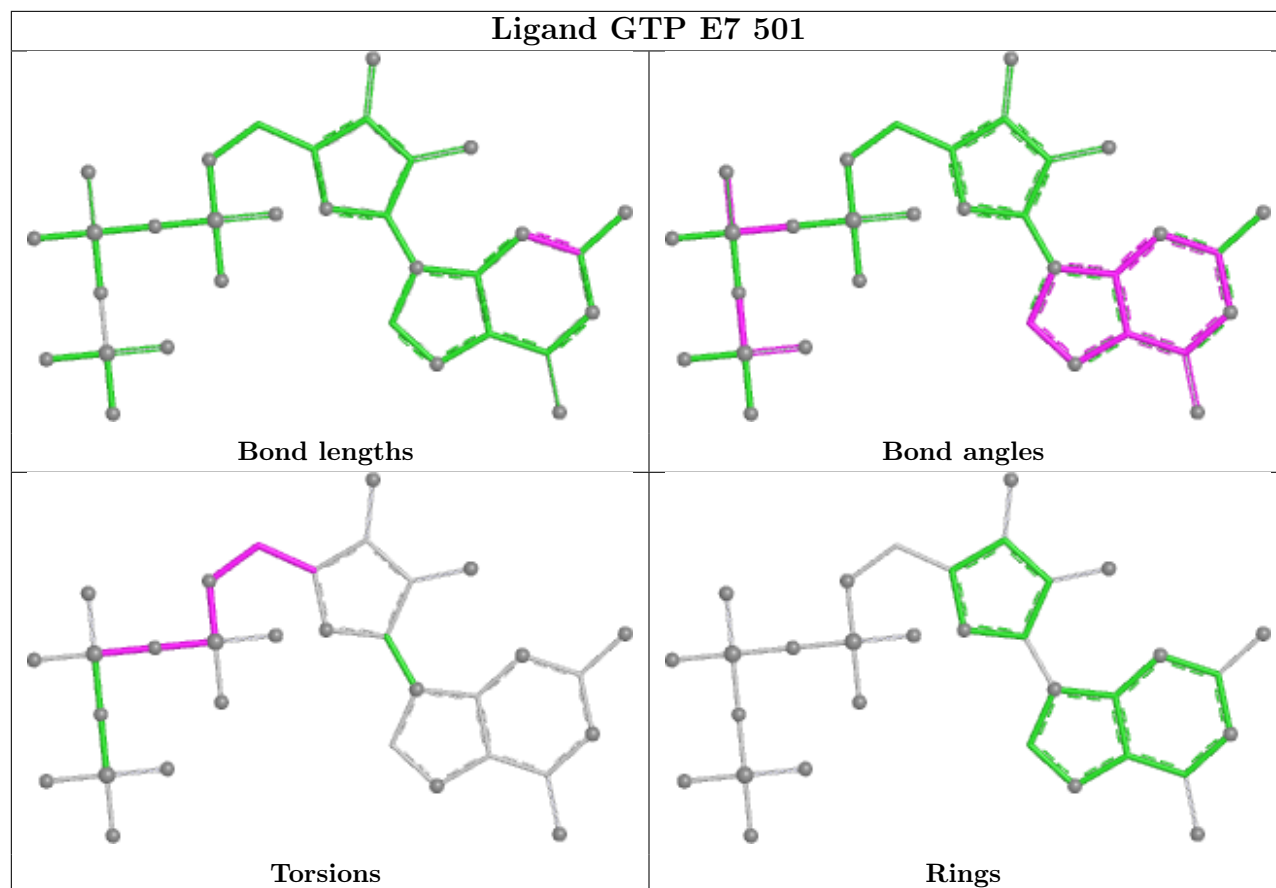


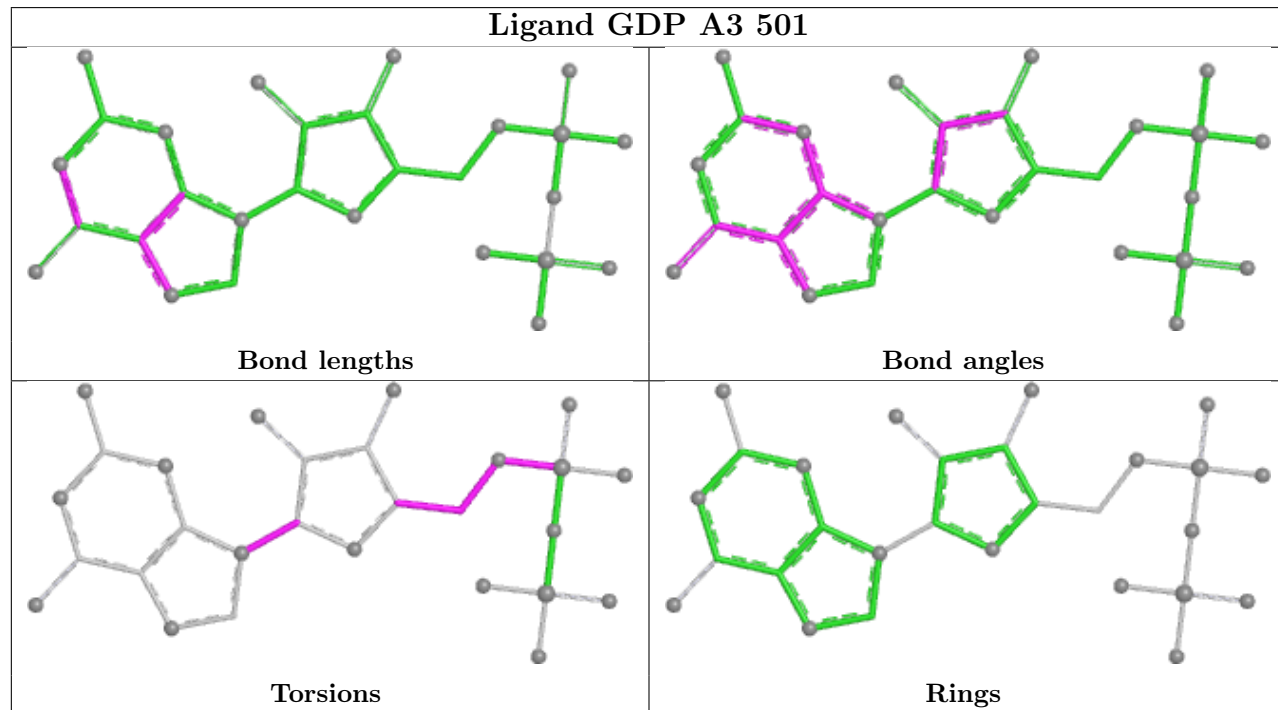
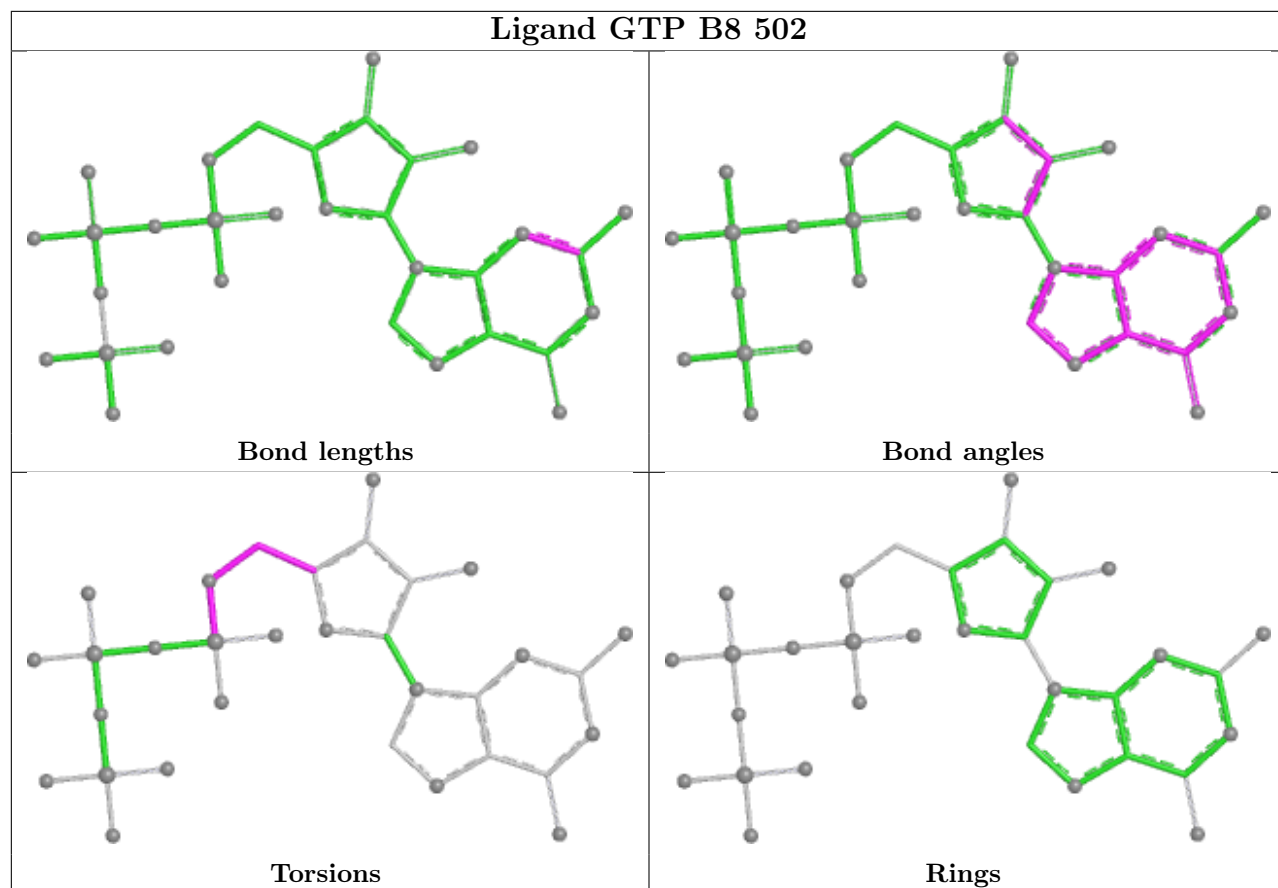


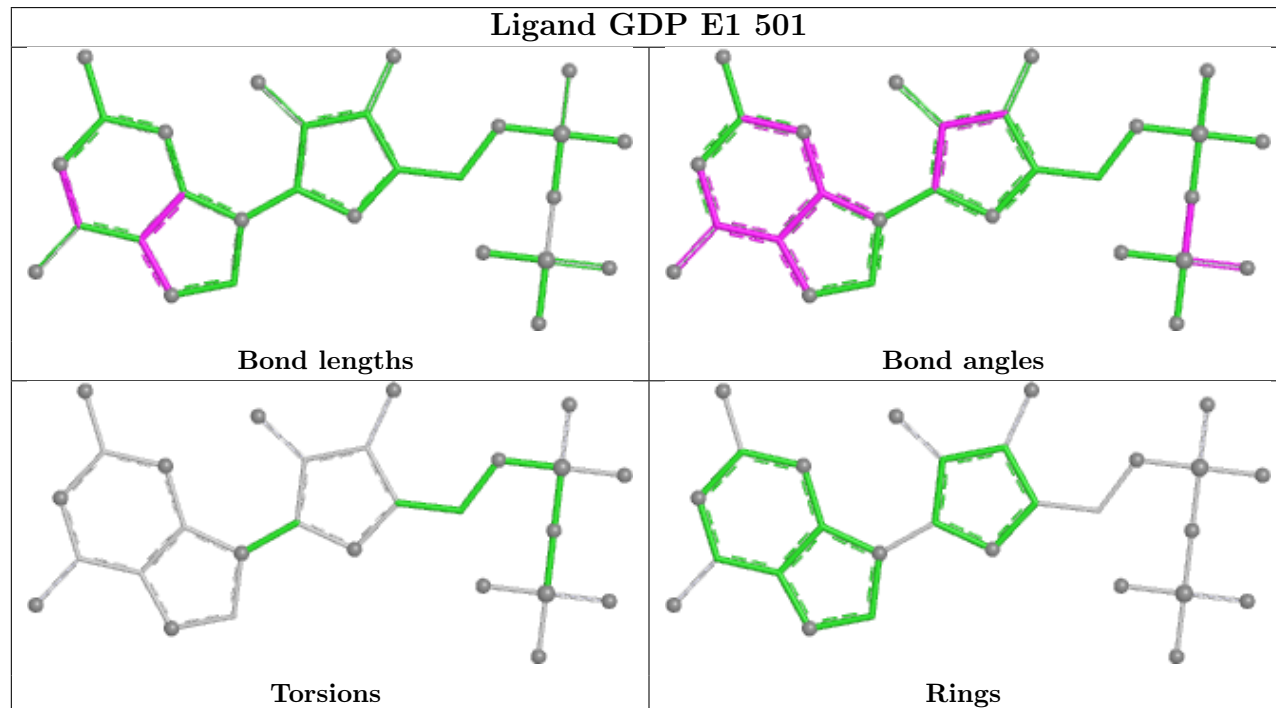
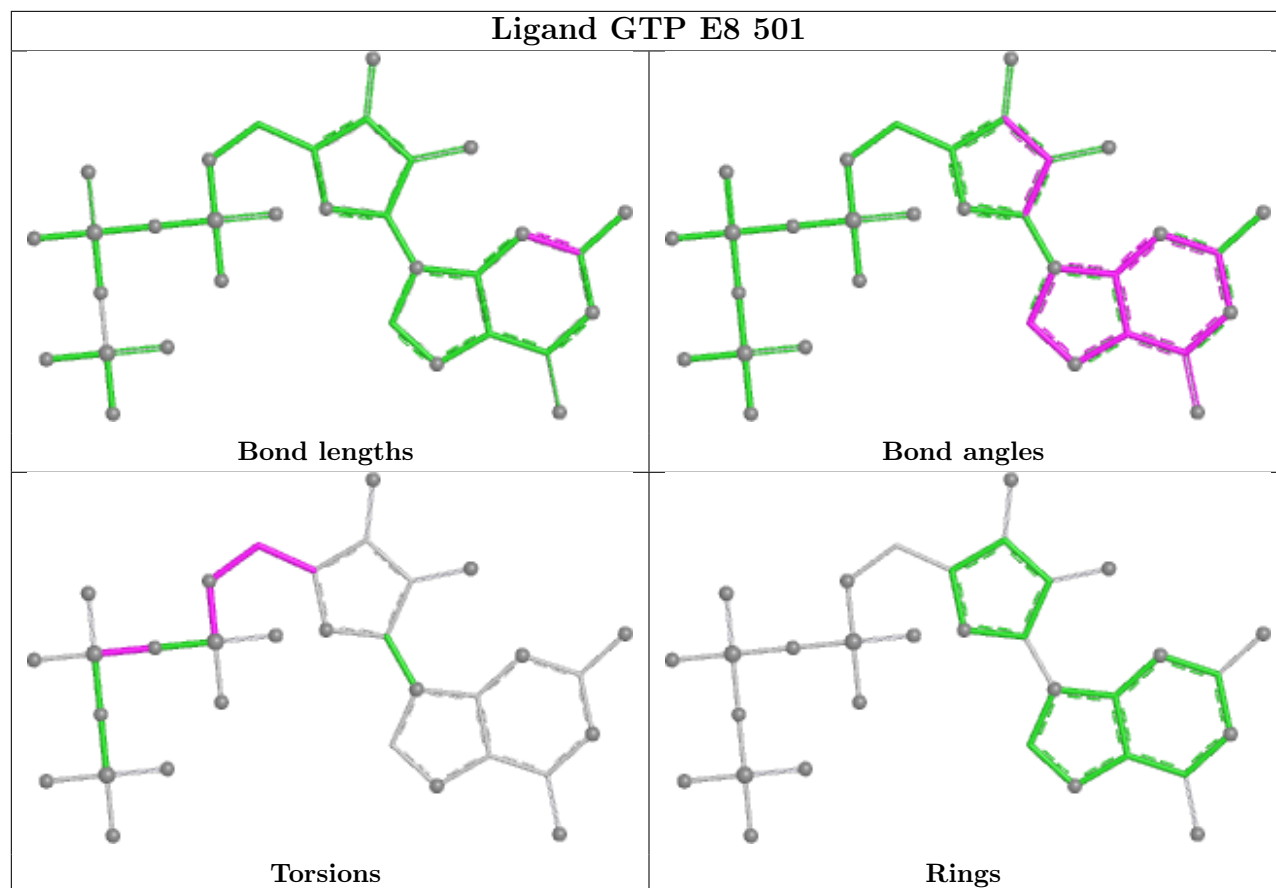




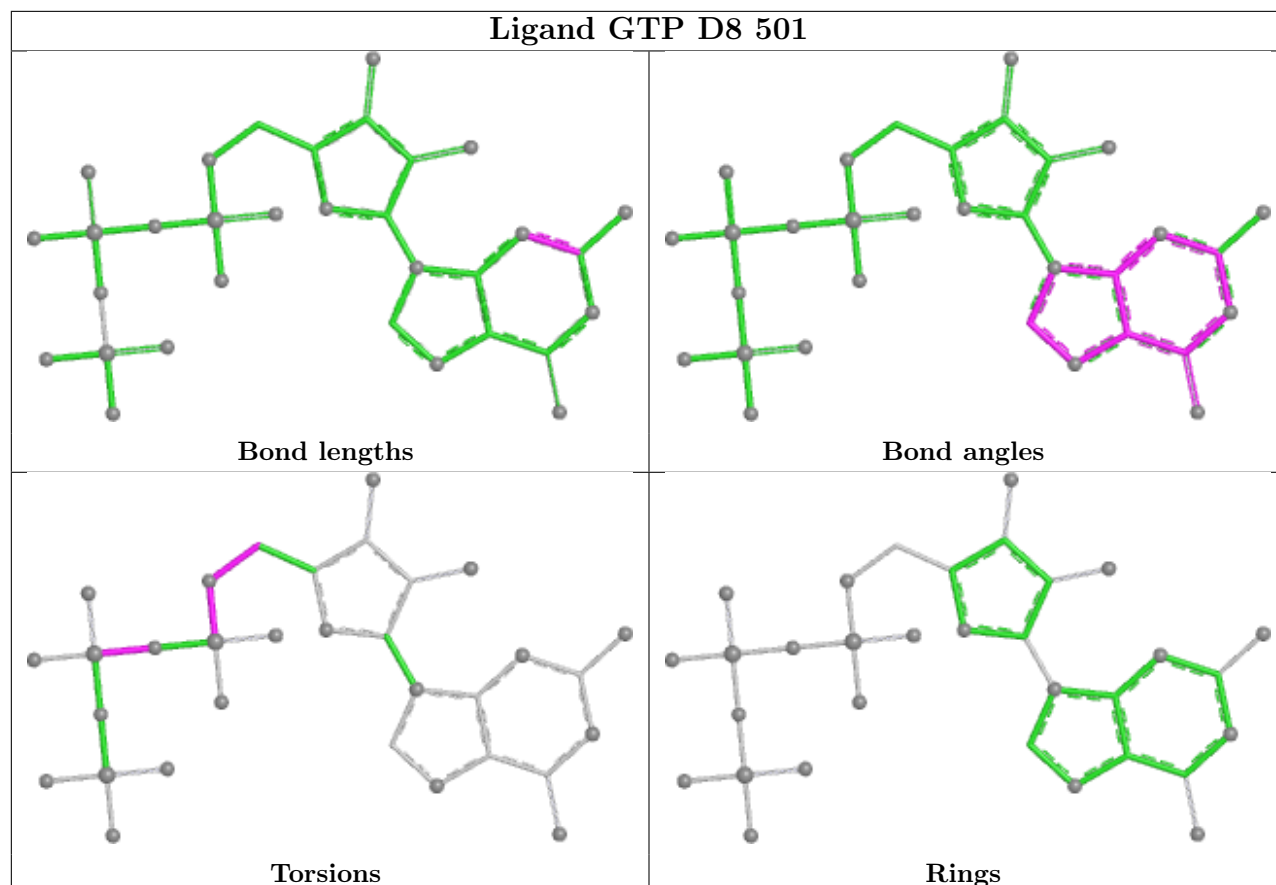




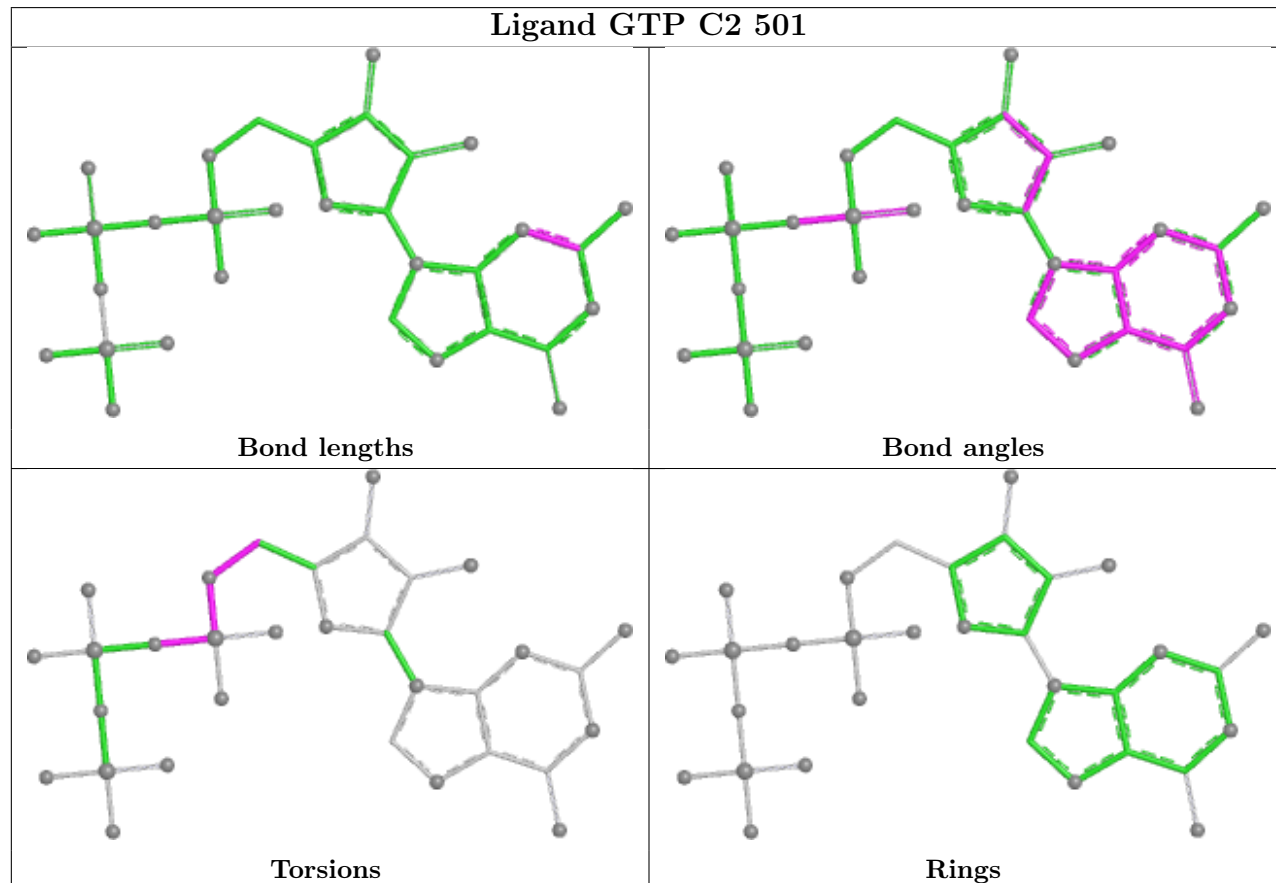


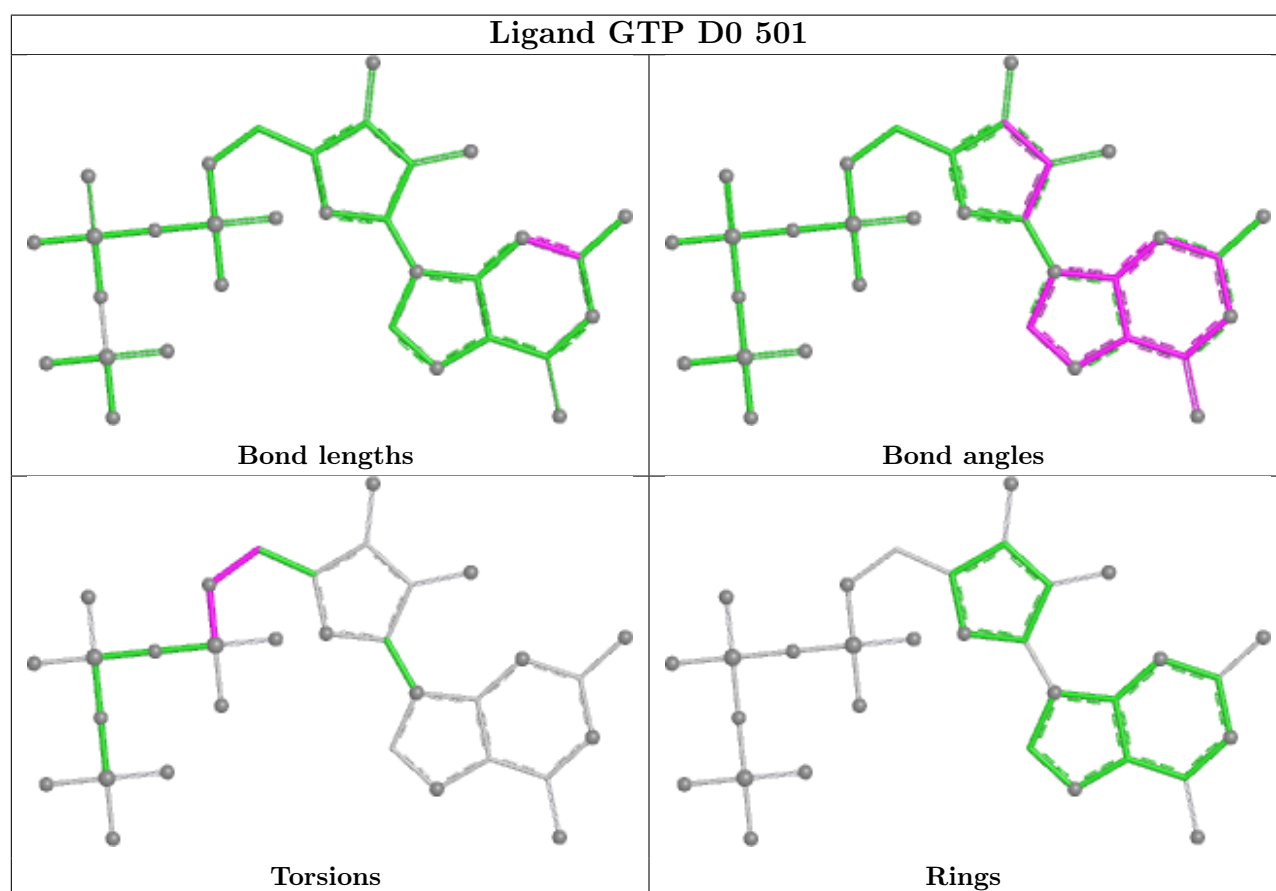
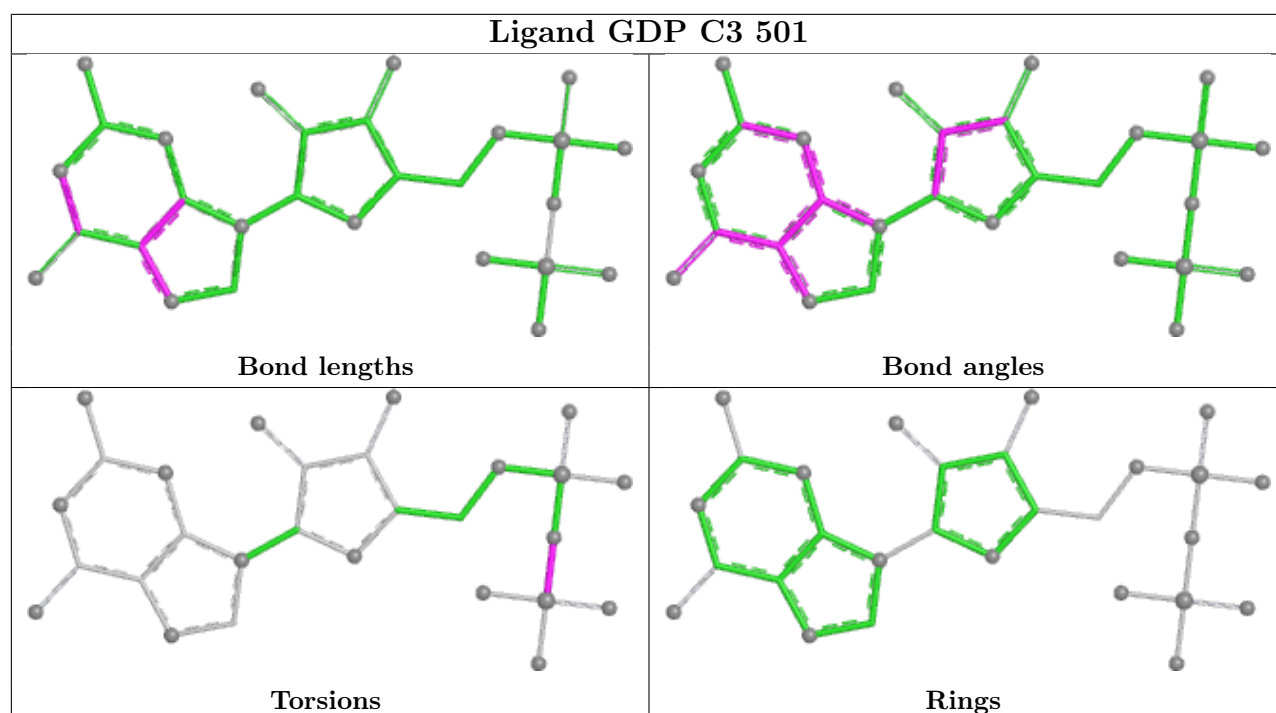


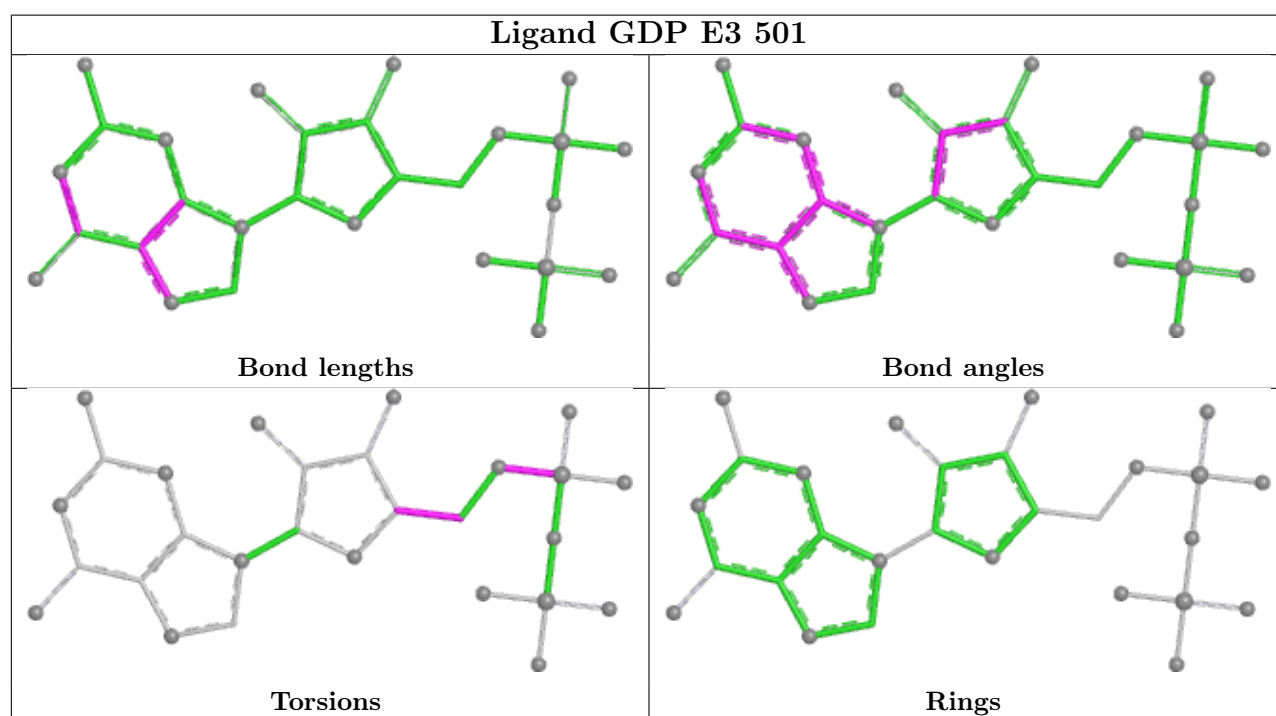
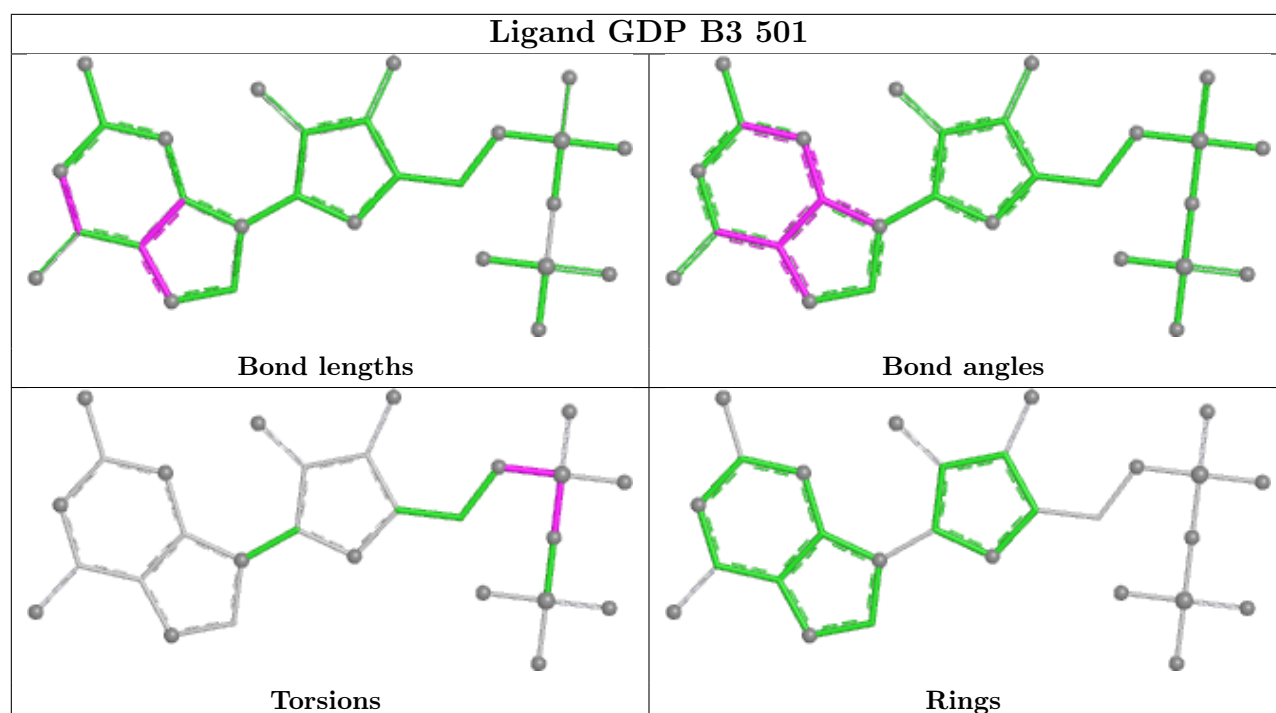
Ligand GTP D8 501

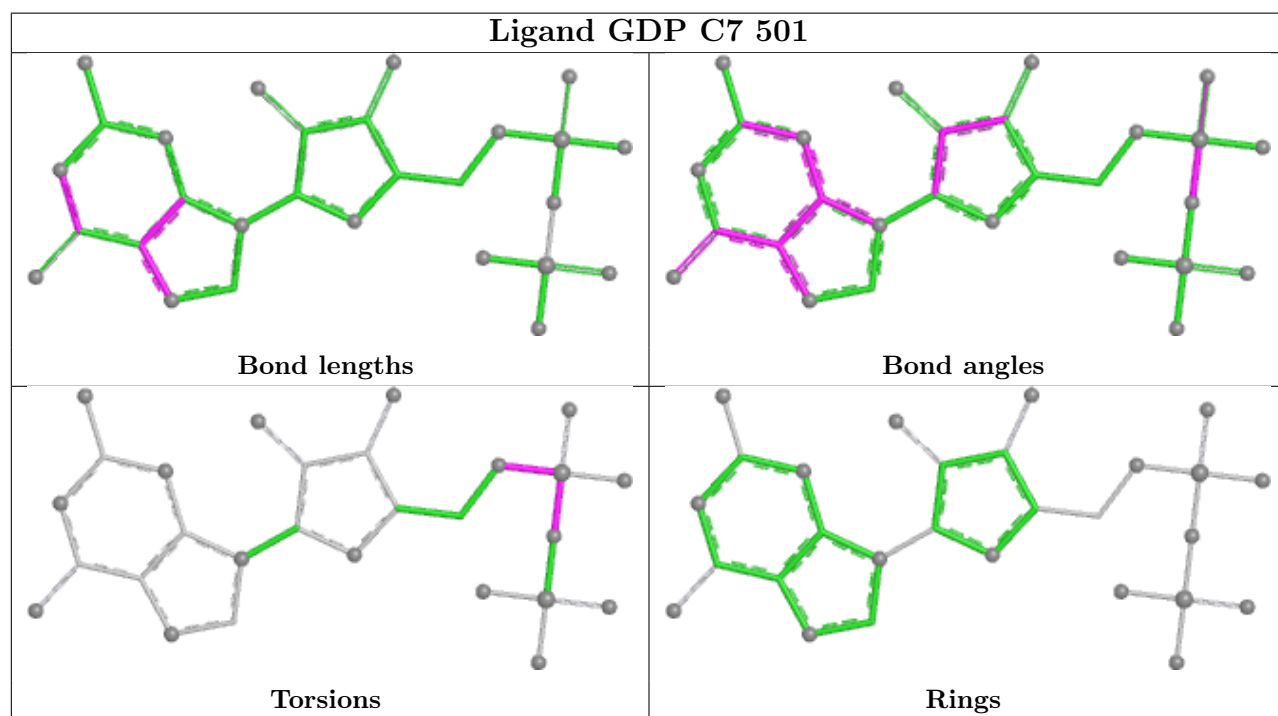
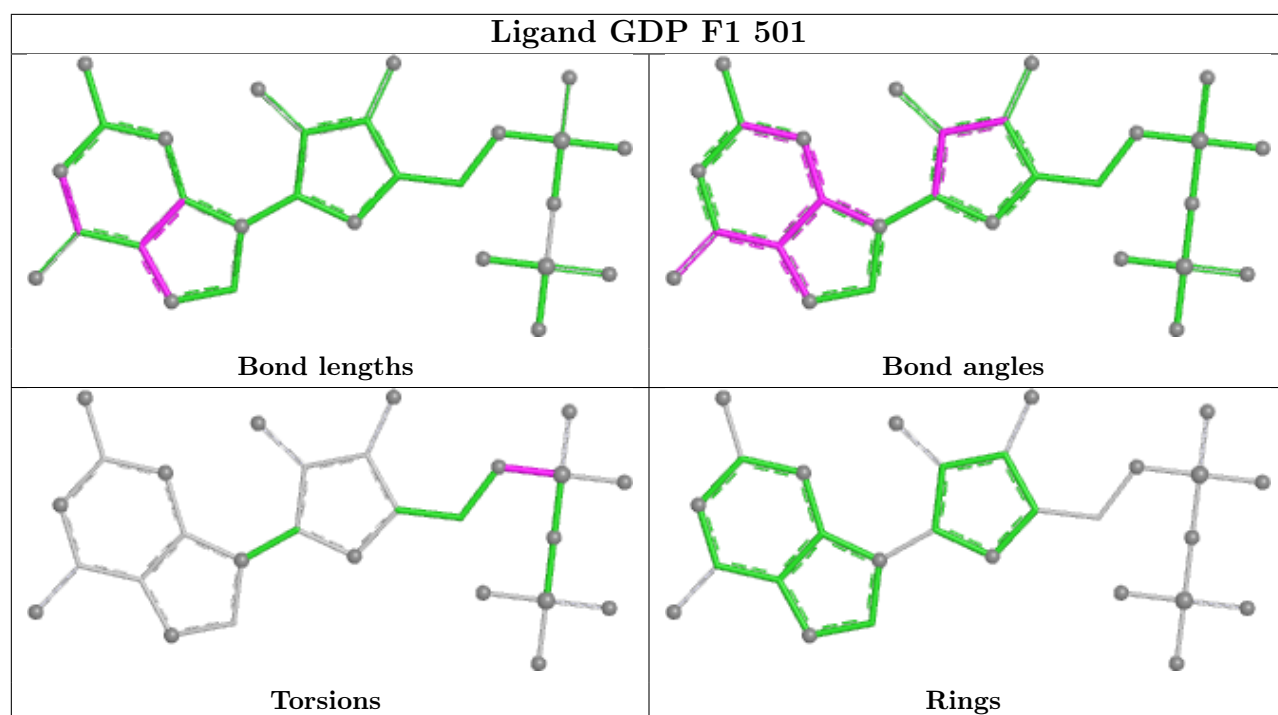


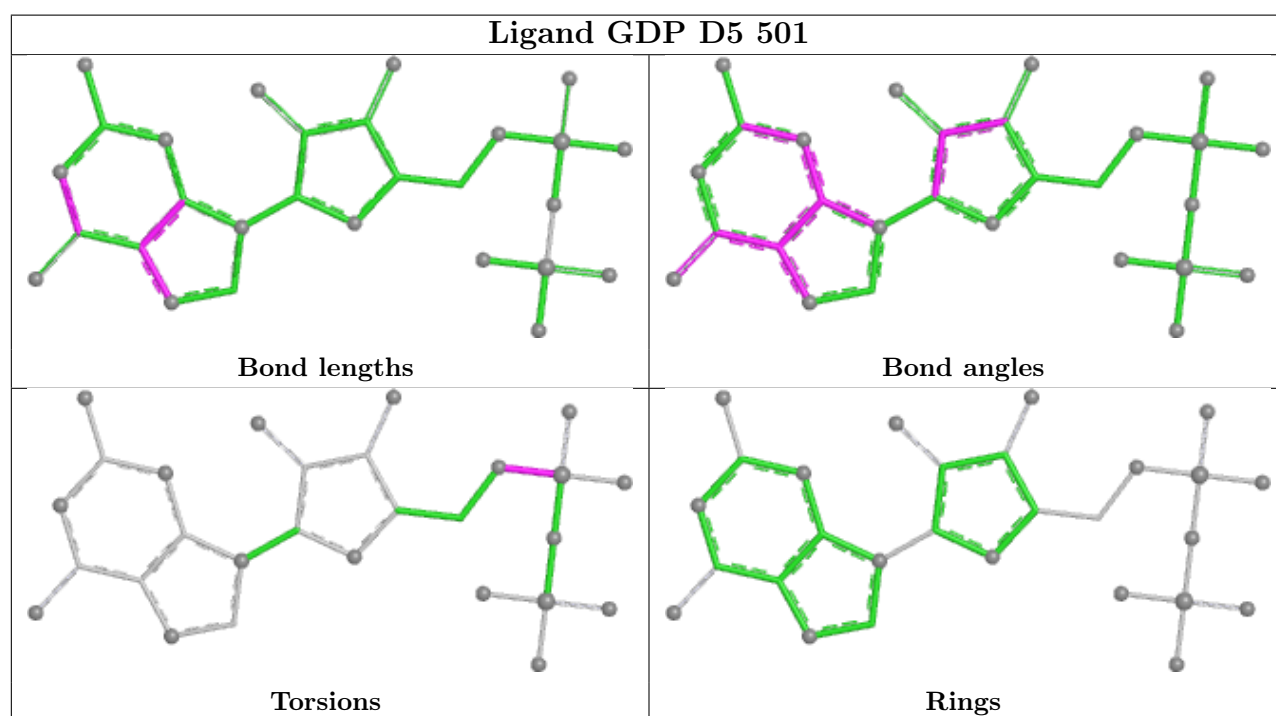
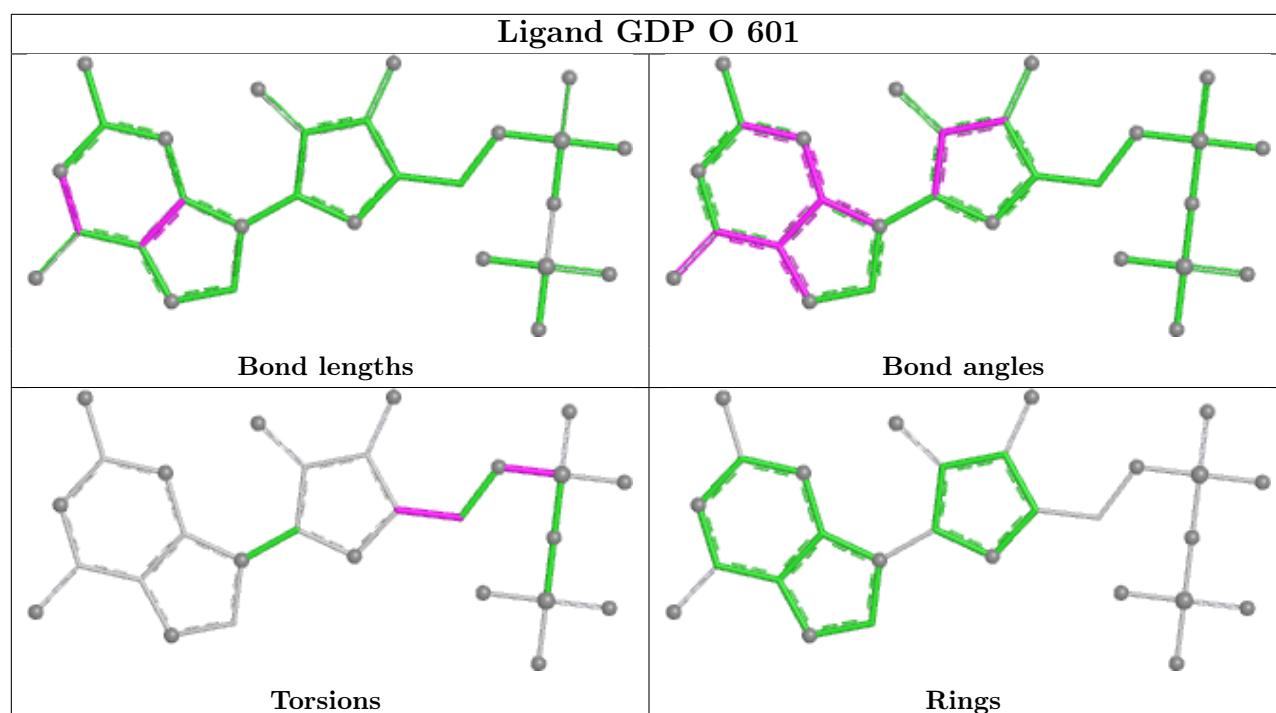
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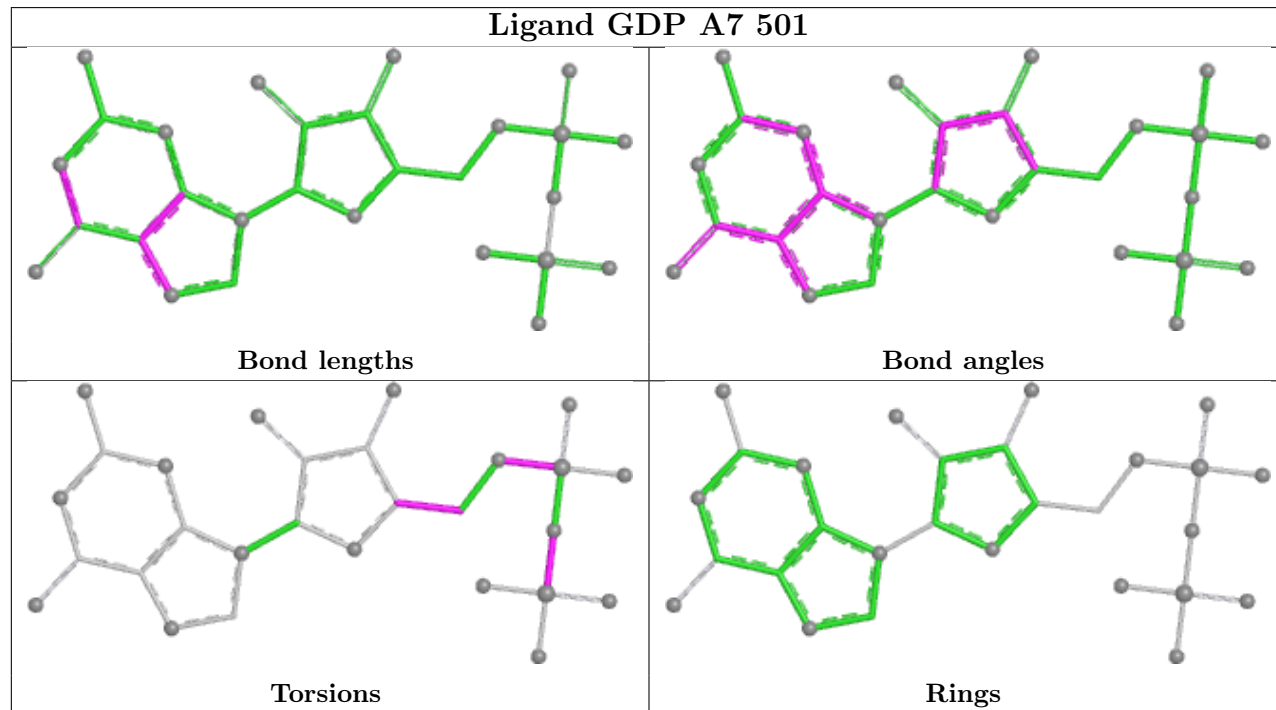
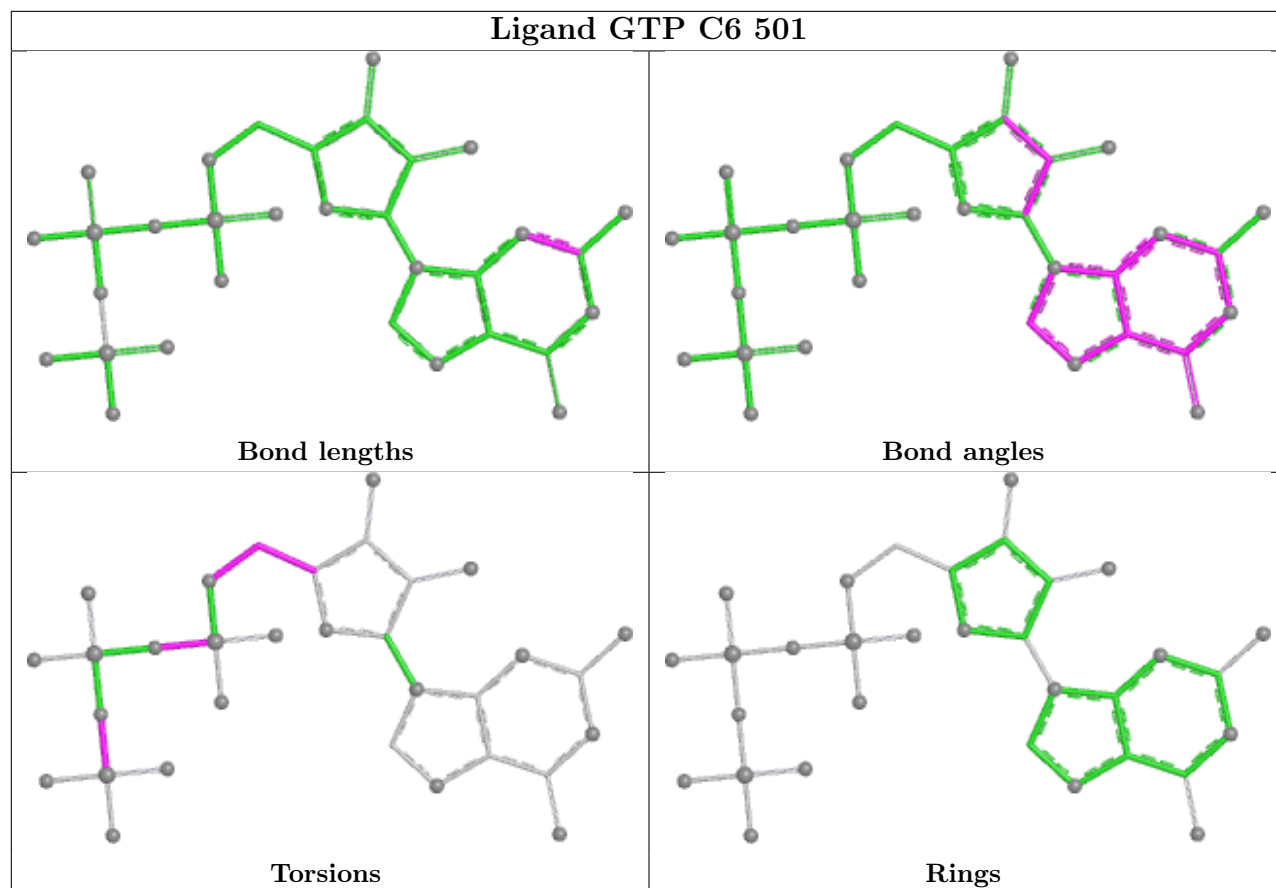


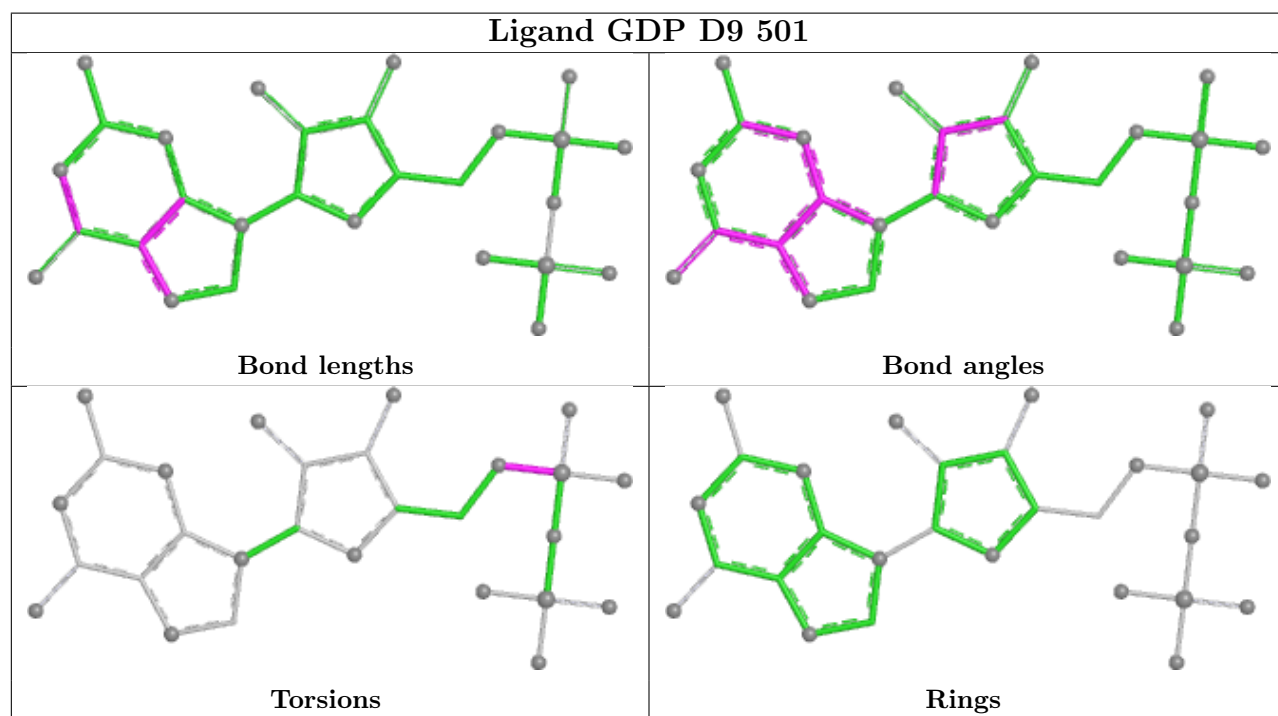
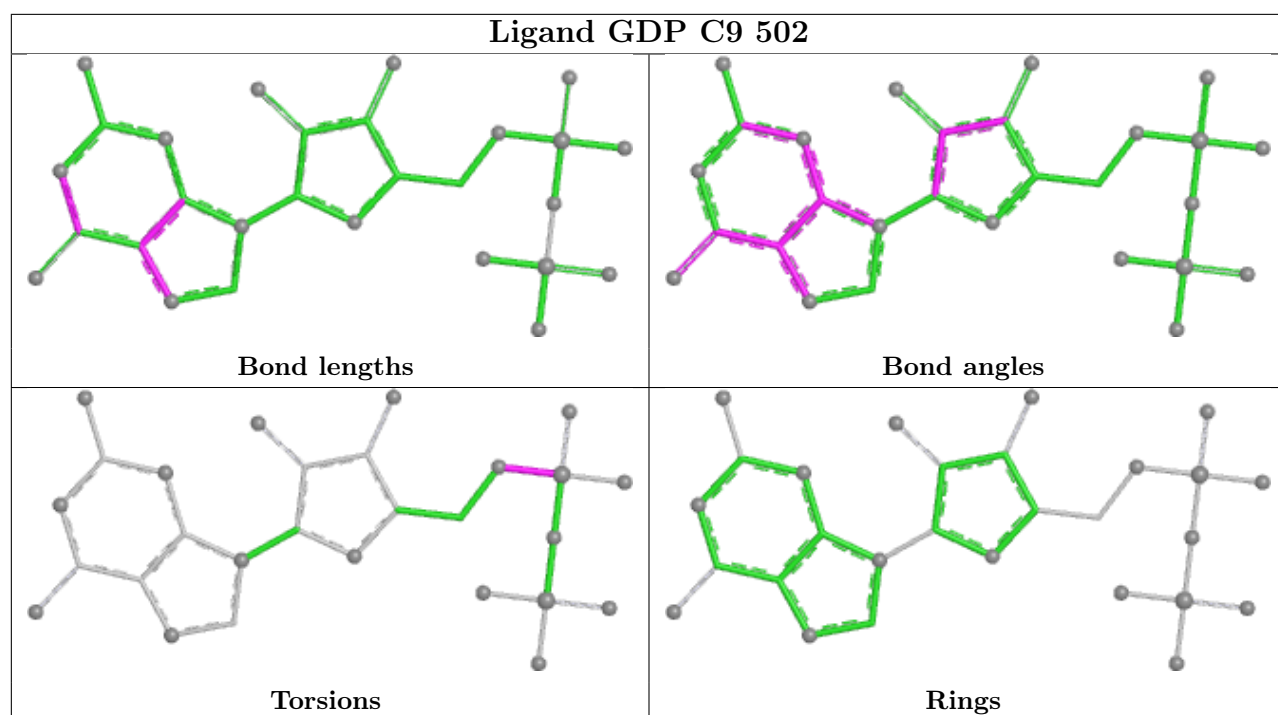


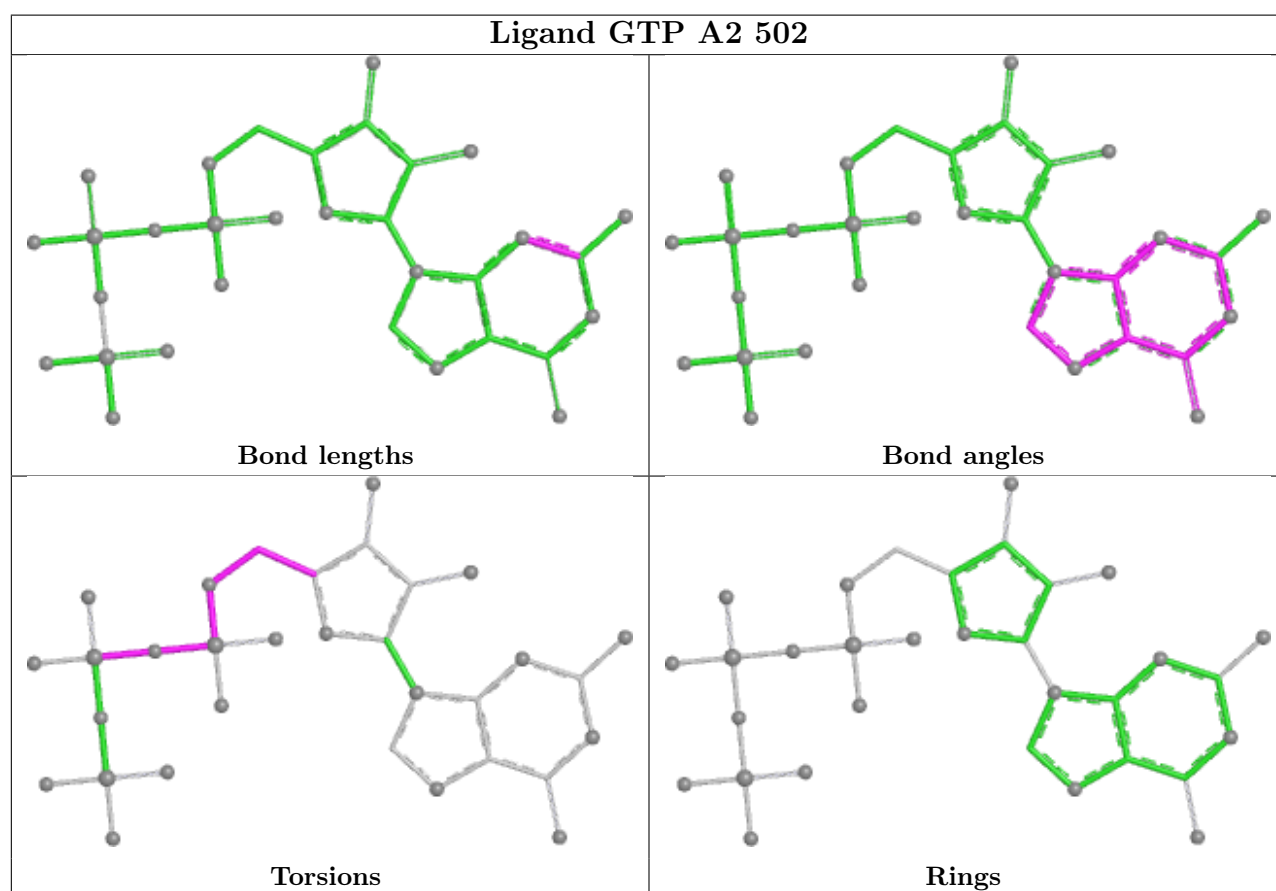
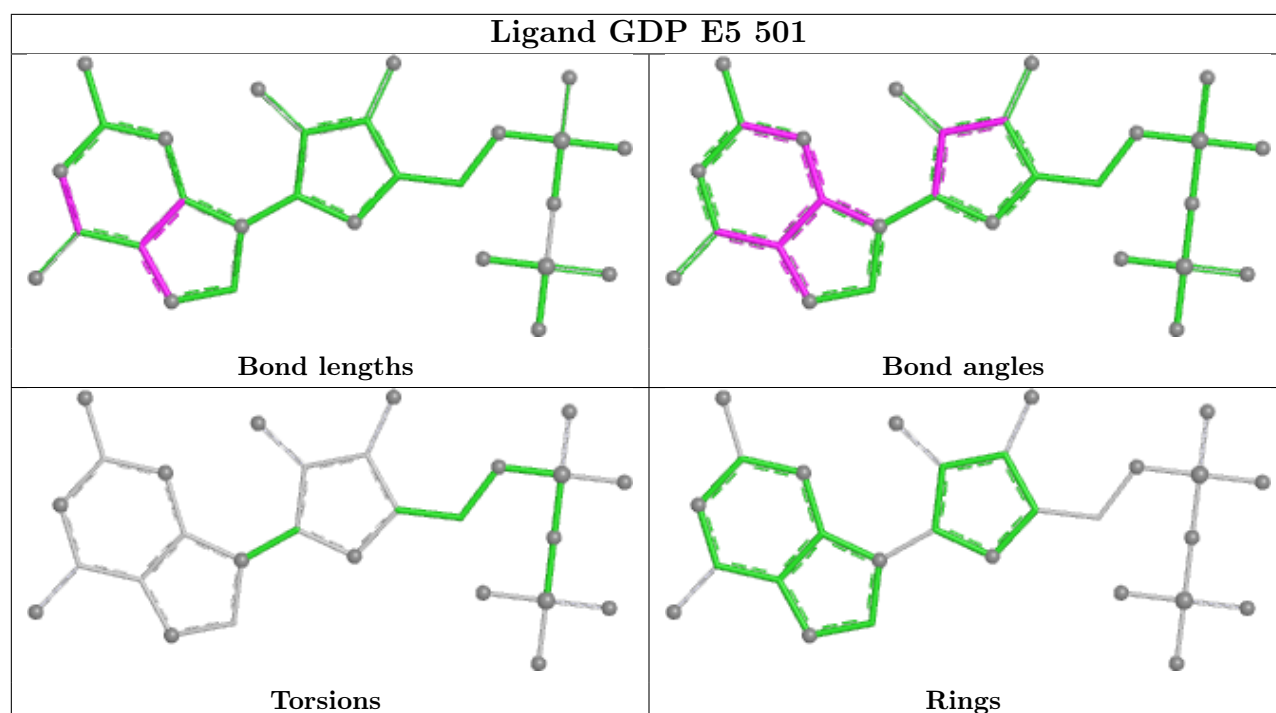




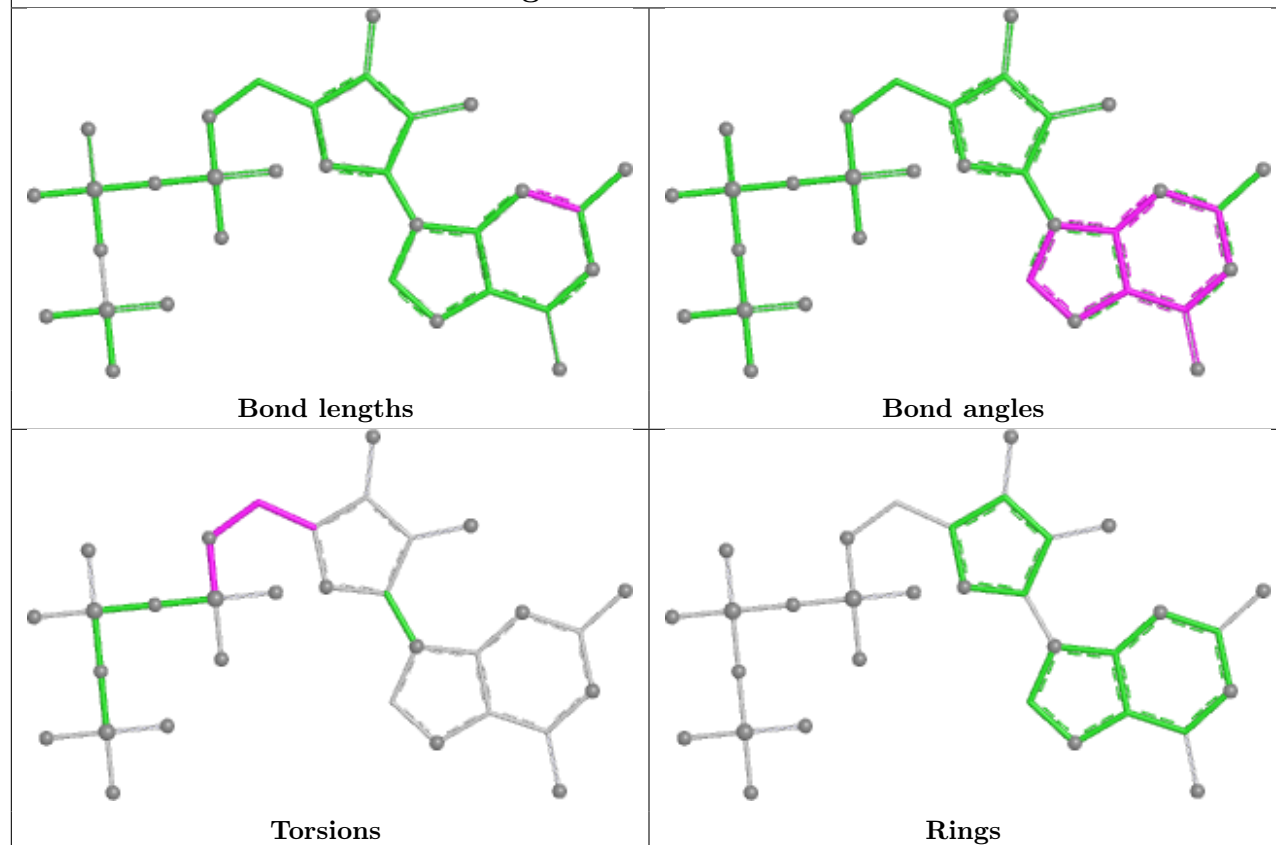




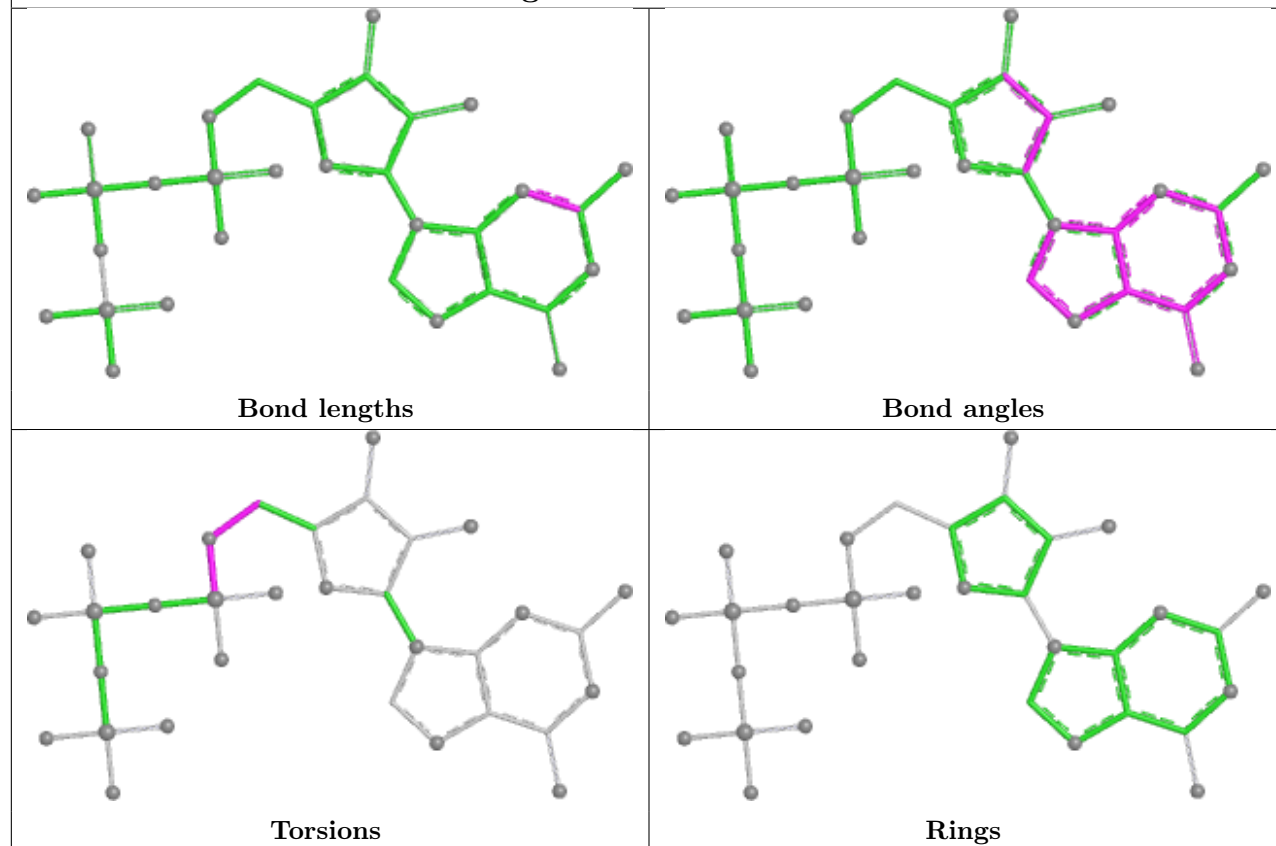


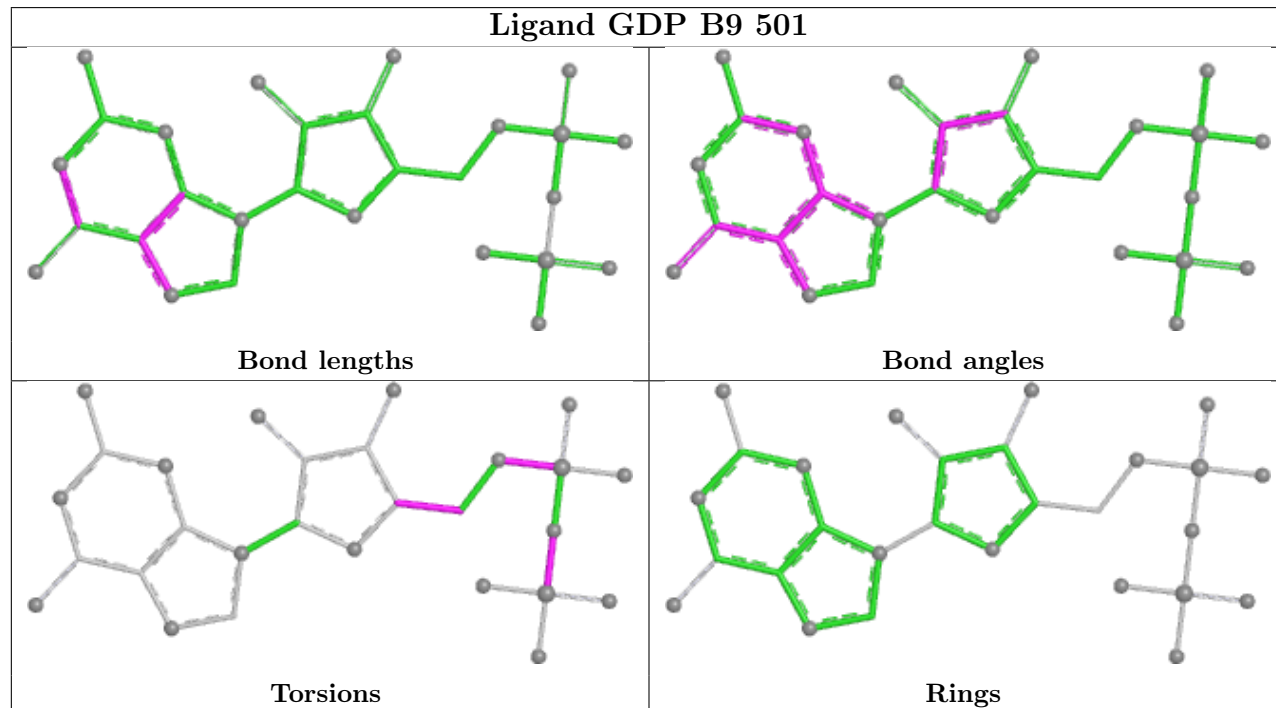
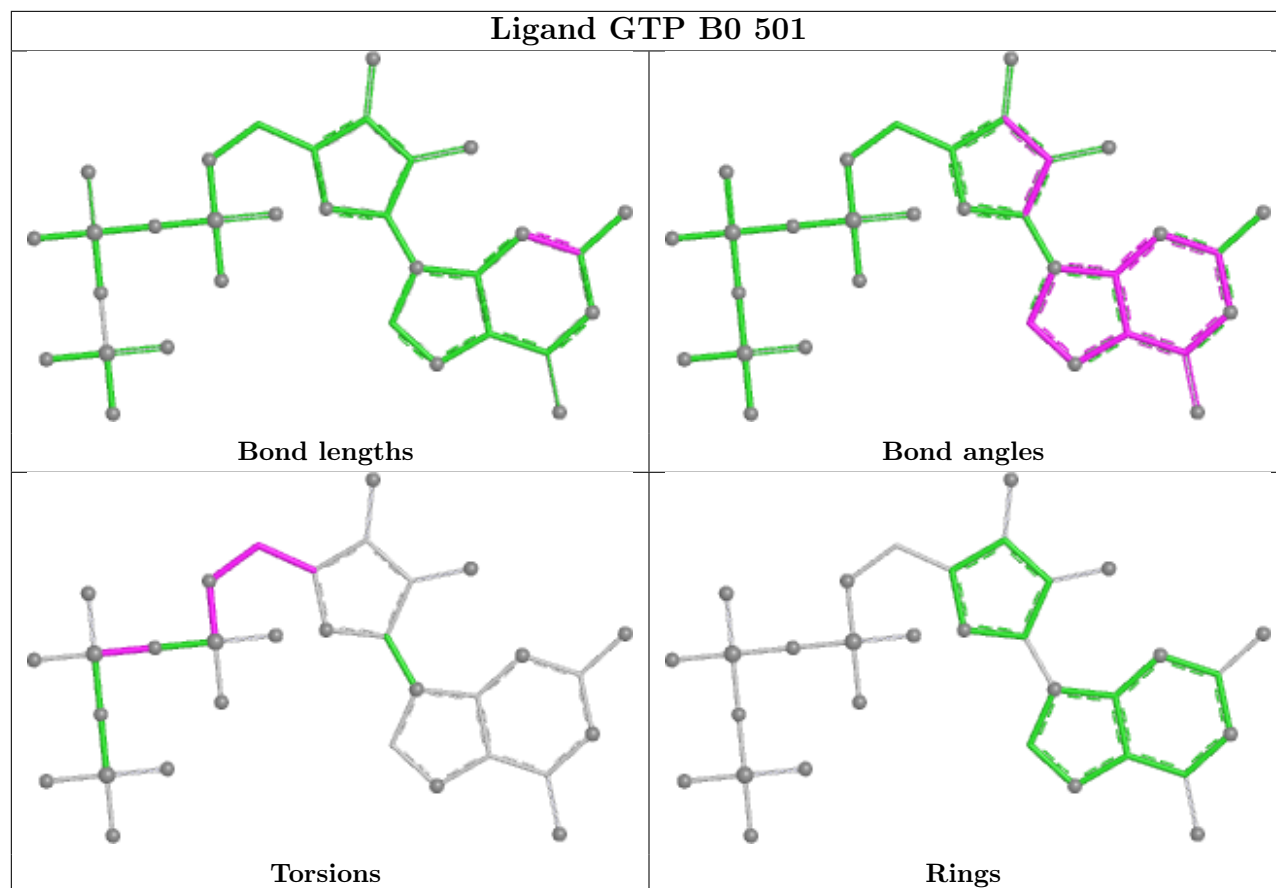


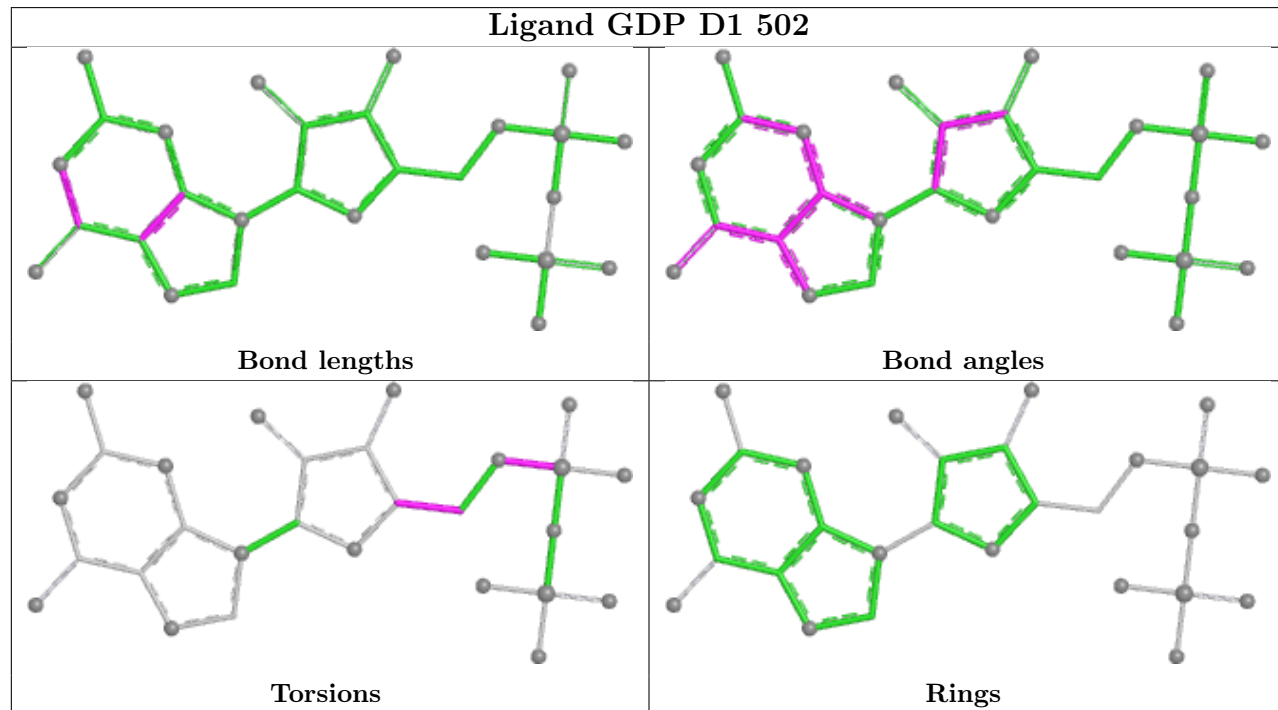
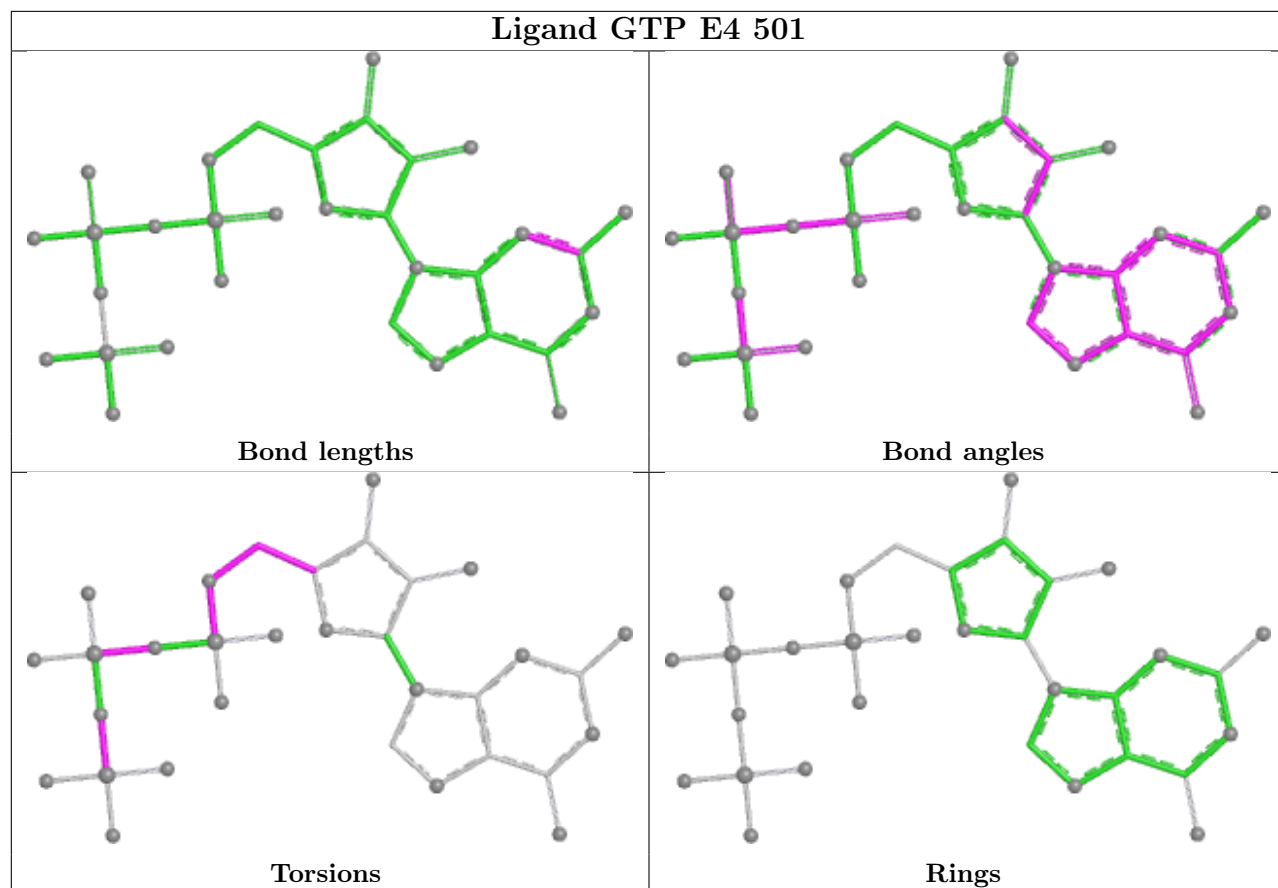
Ligand GTP B4 501



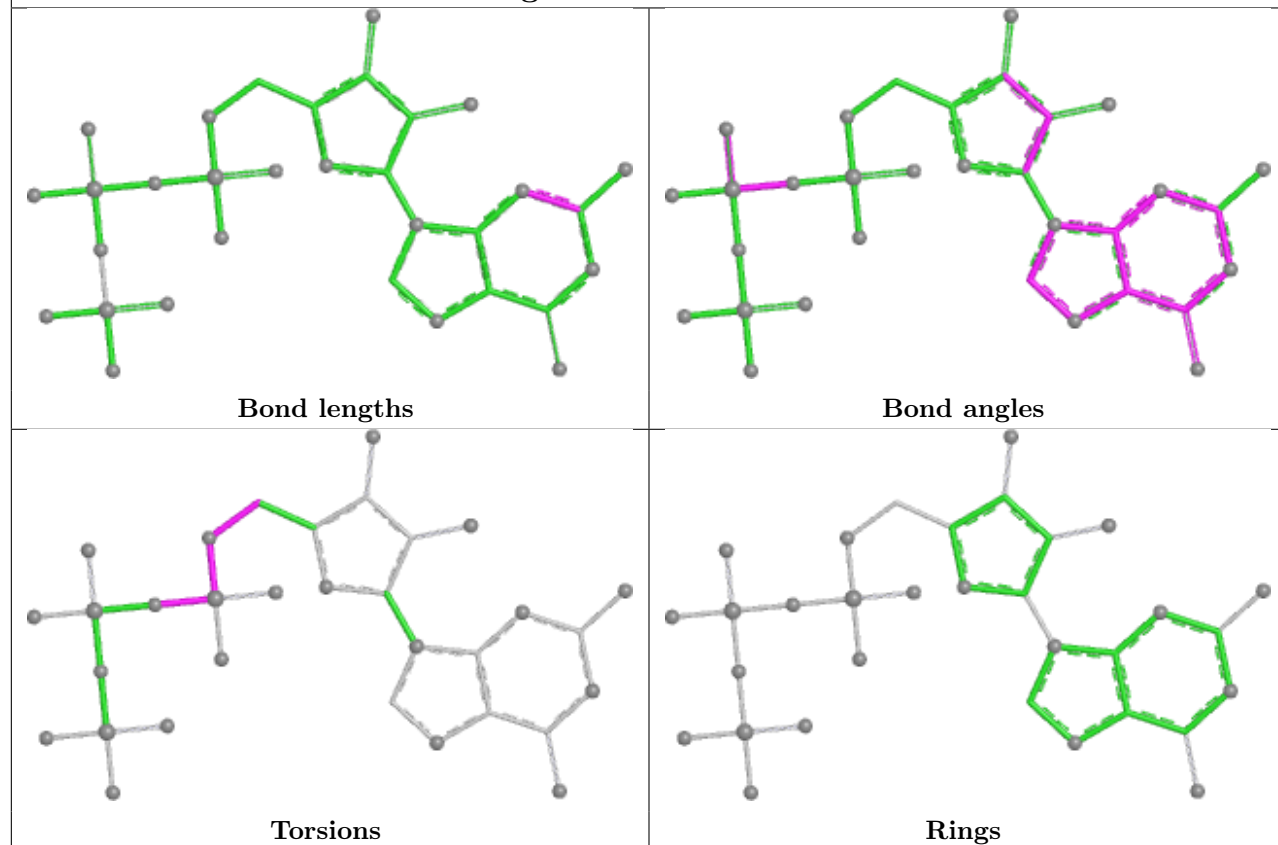
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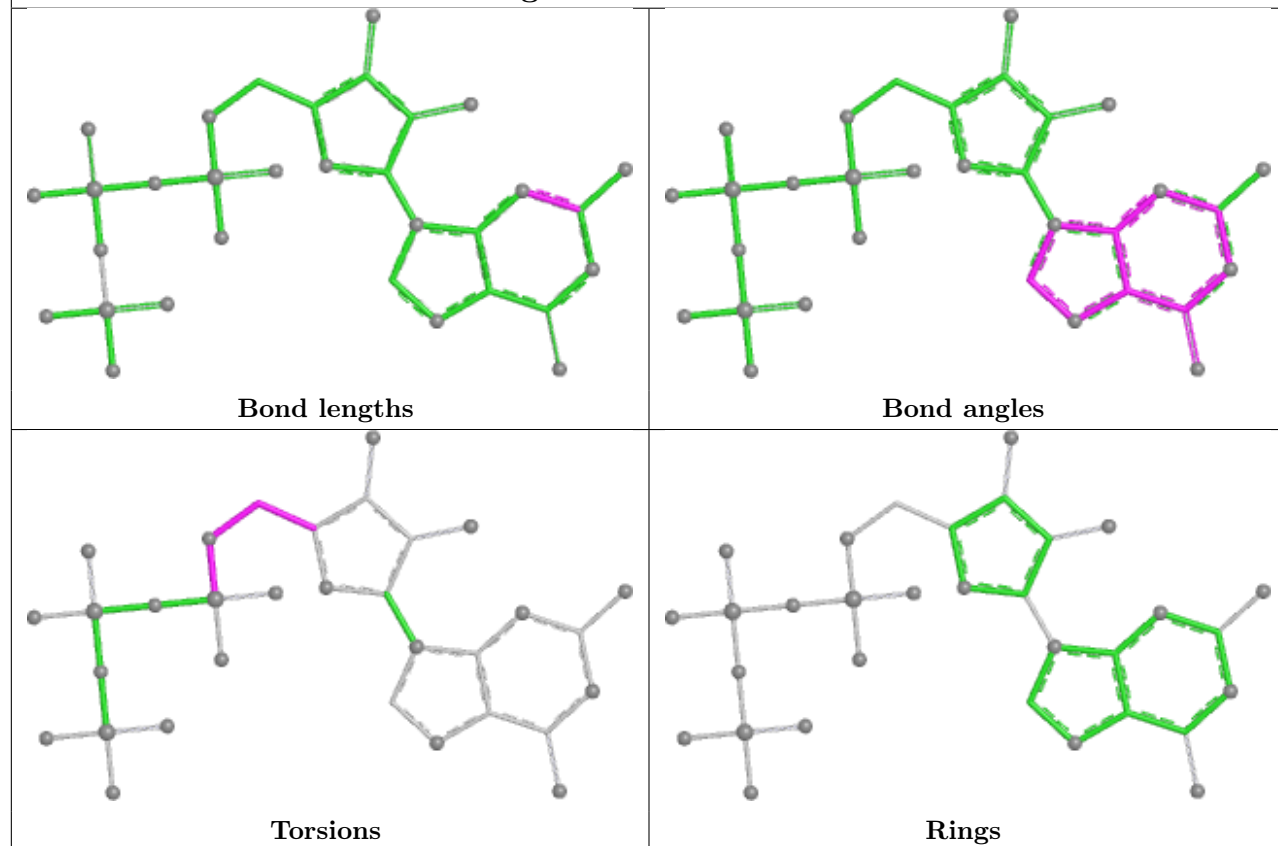


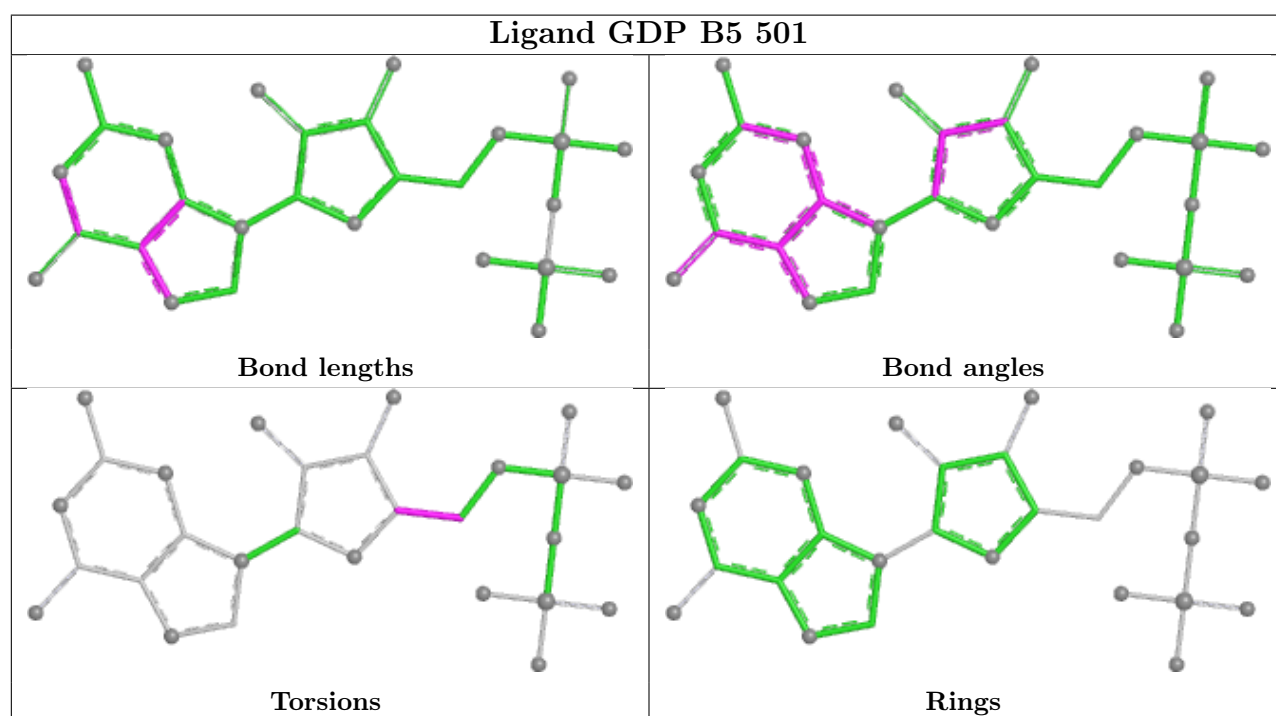
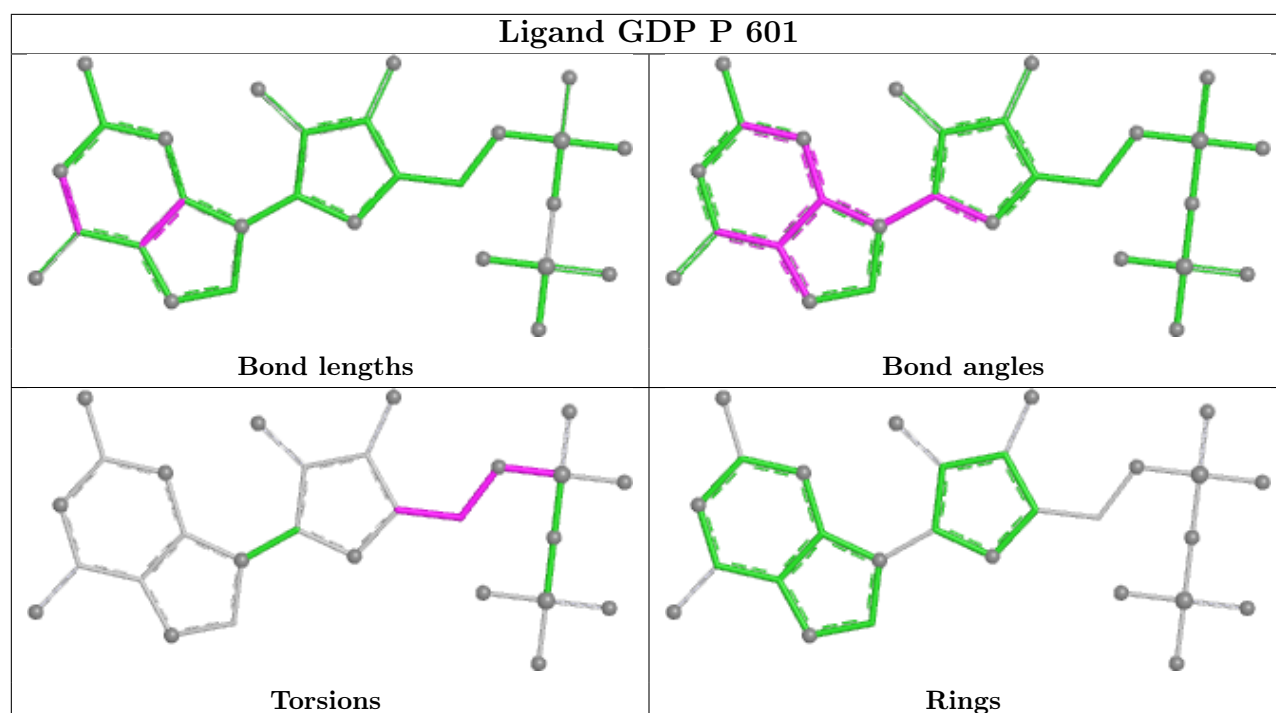


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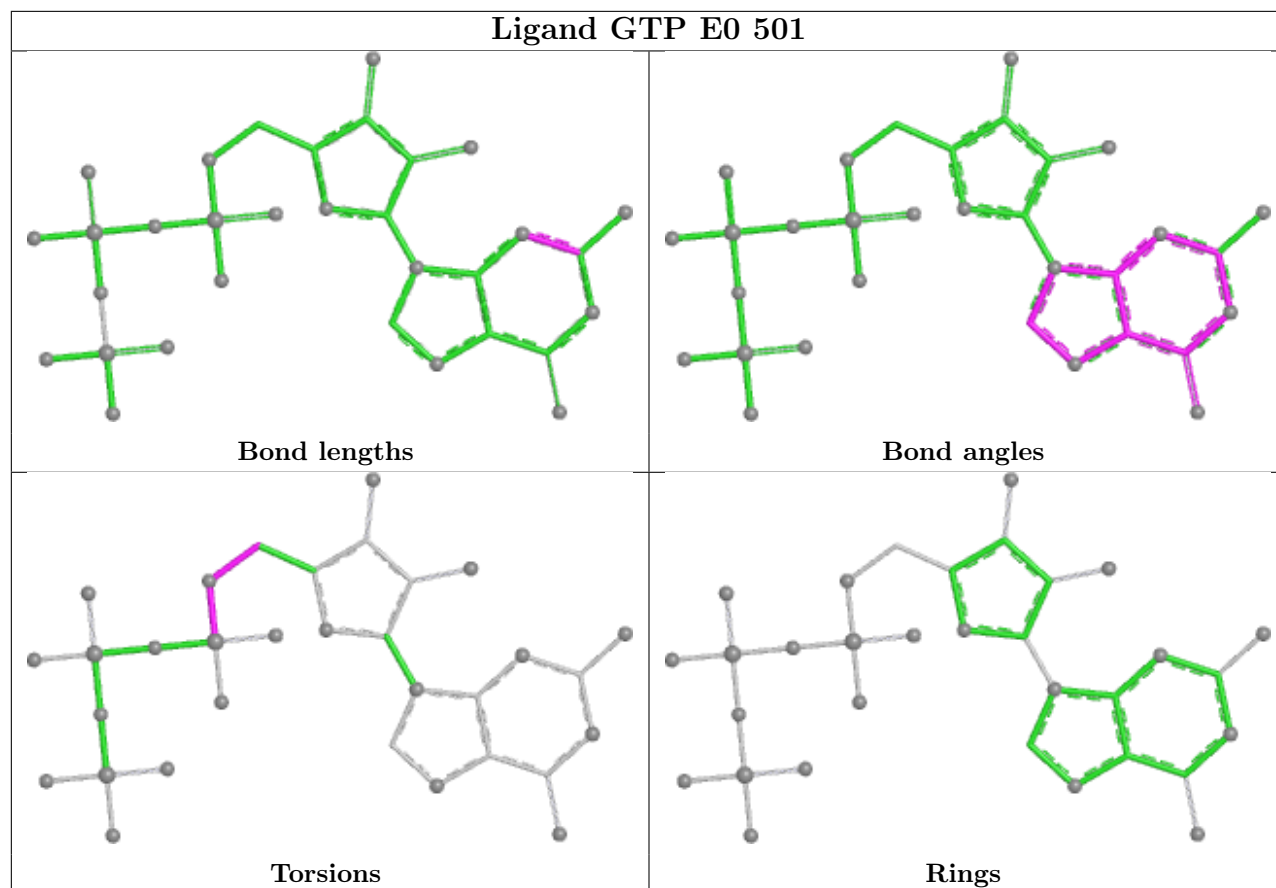


Ligand GTP A6 501

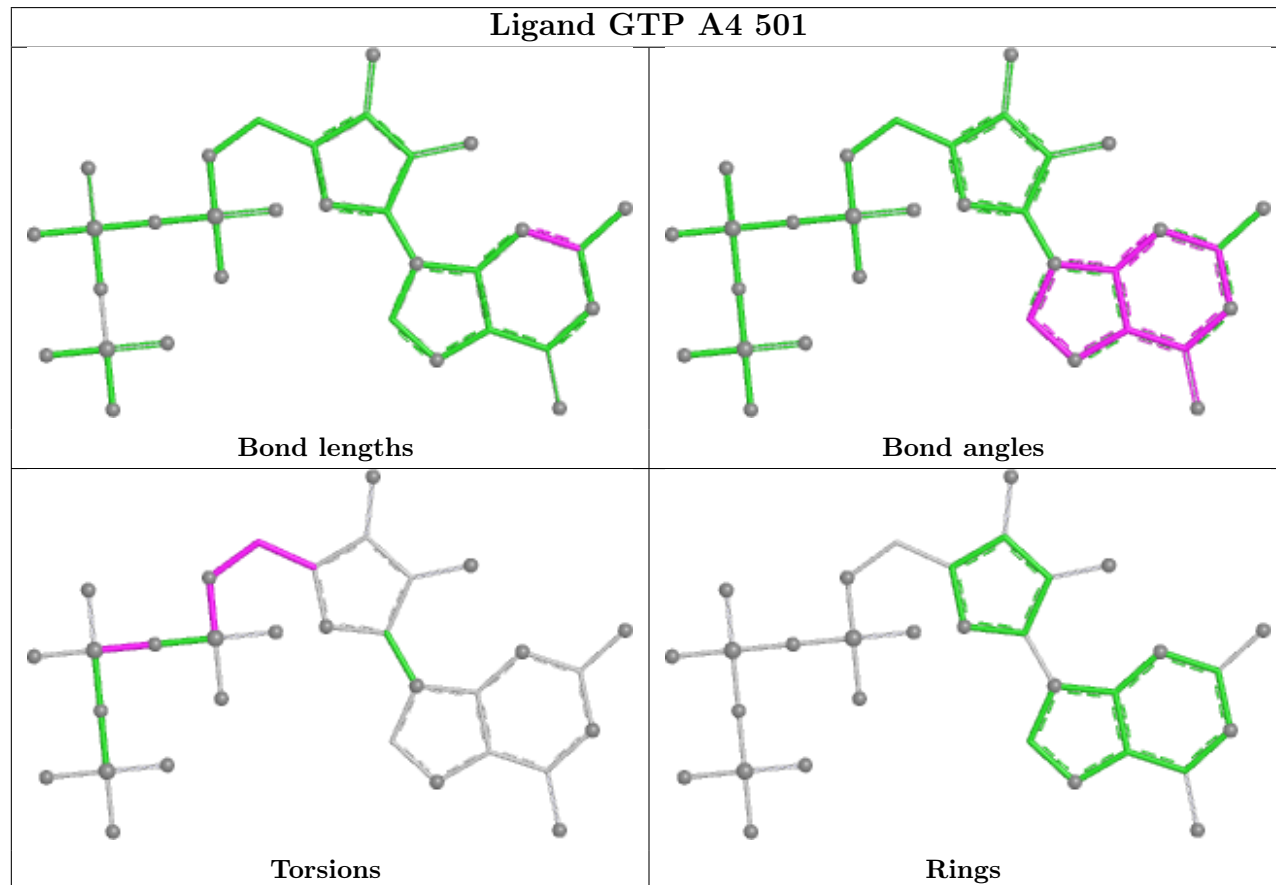




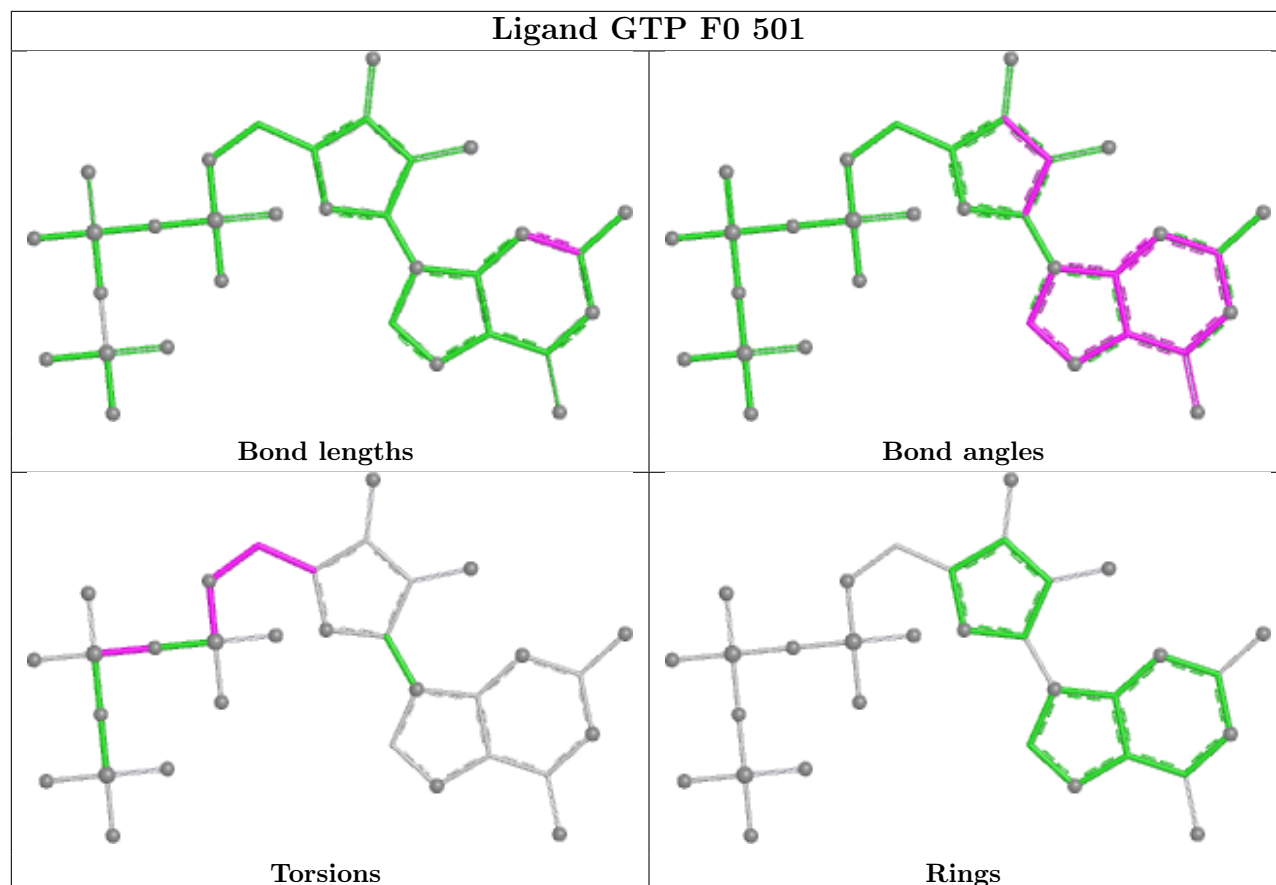
Ligand GTP E0 501



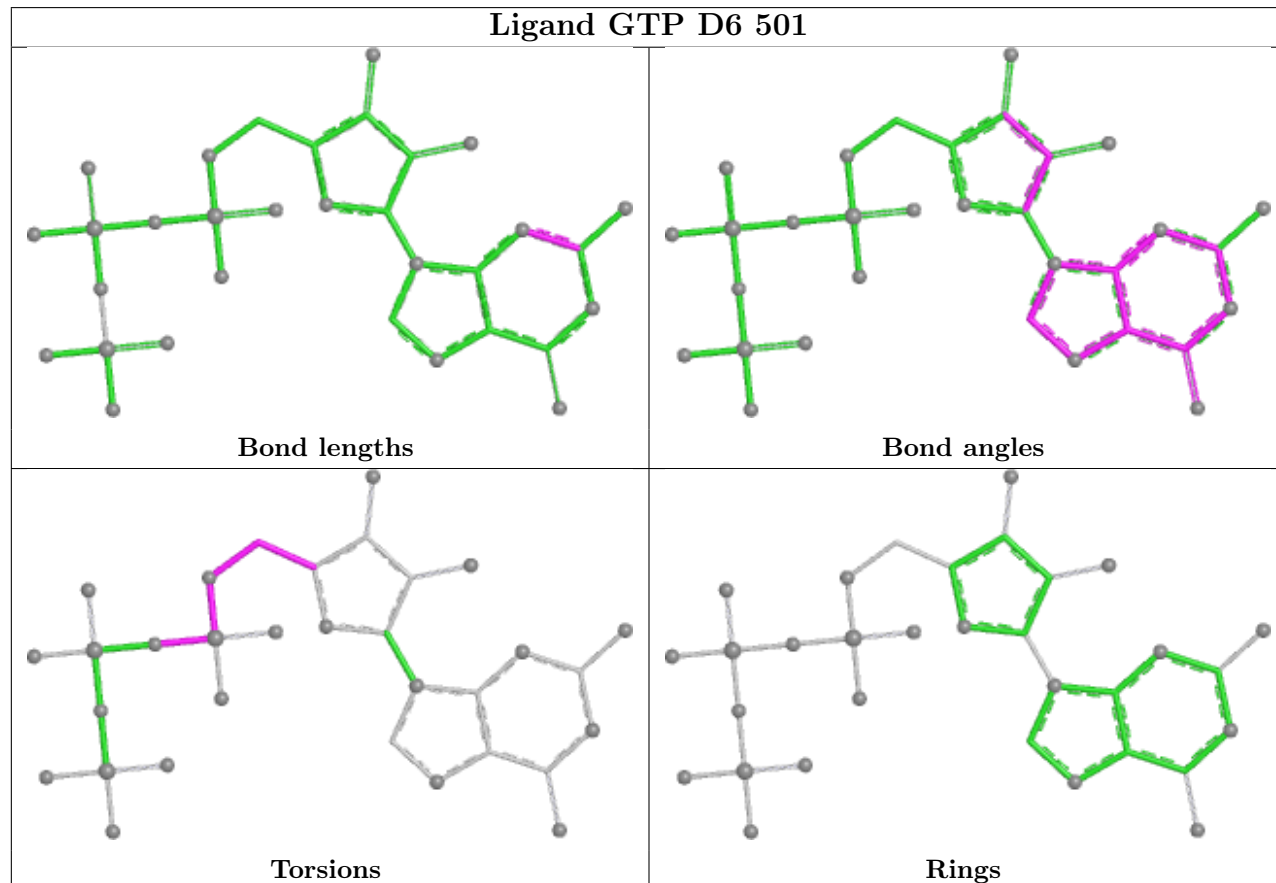
Ligand GTP A4 501

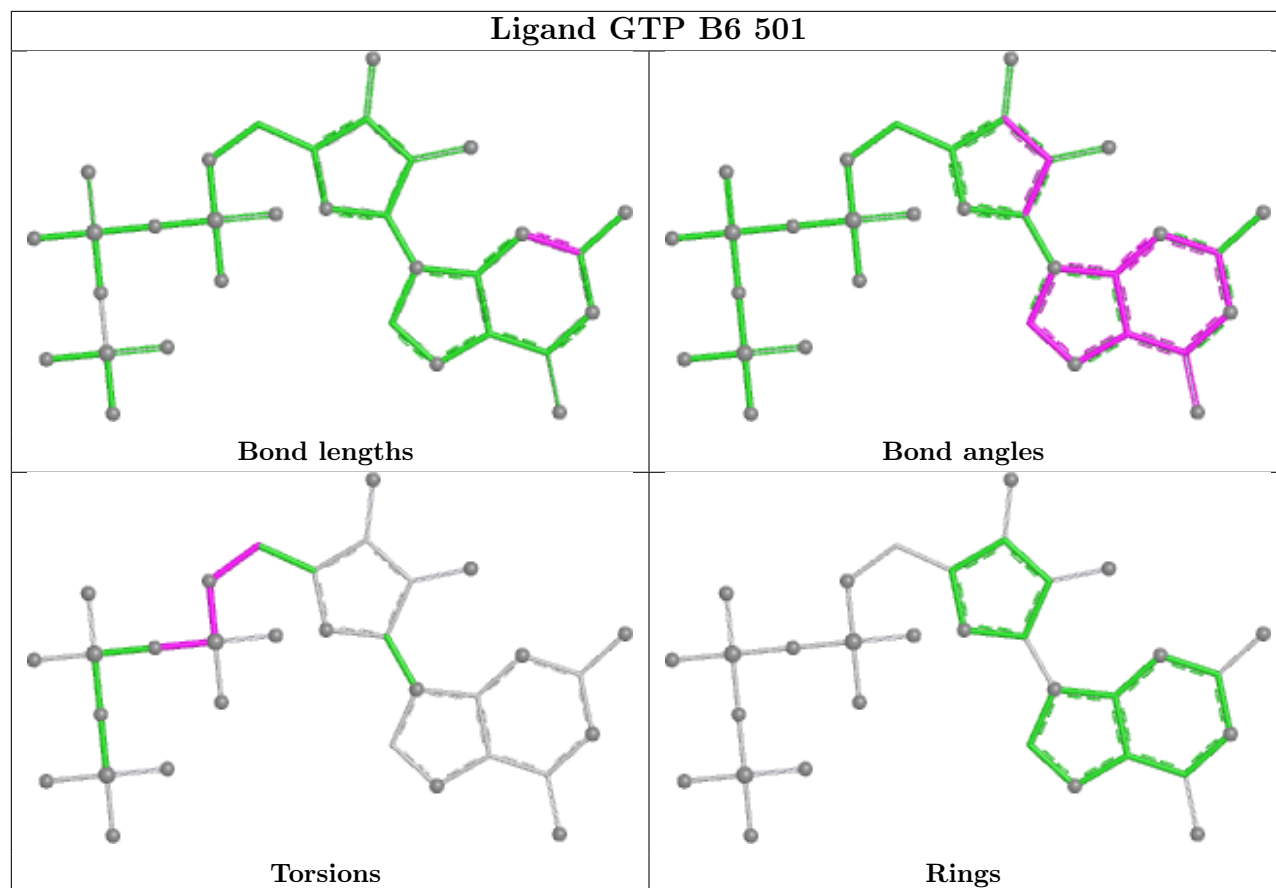


Ligand GTP F0 501



Ligand GTP D6 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

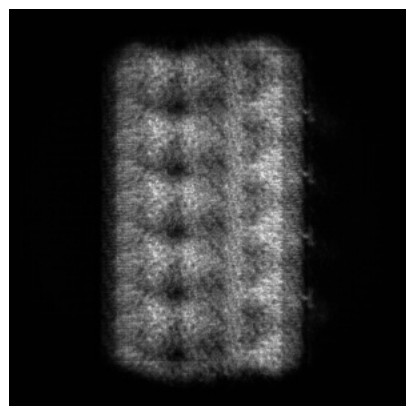
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72717. These allow visual inspection of the internal detail of the map and identification of artifacts.

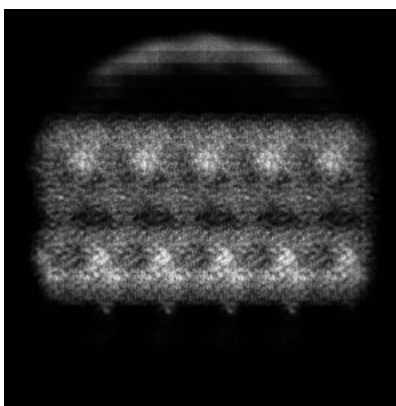
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

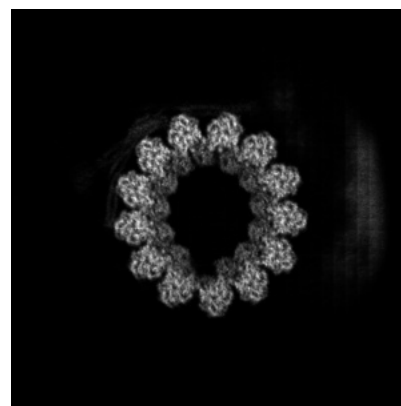
6.1.1 Primary map



X

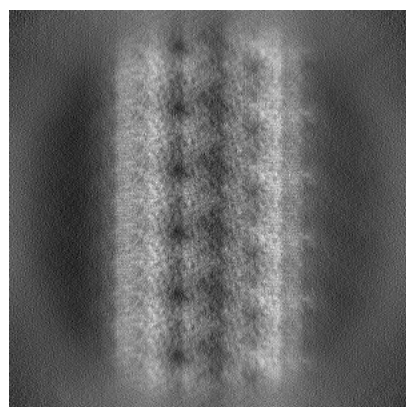


Y

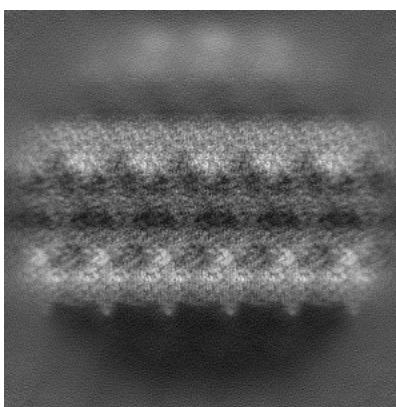


Z

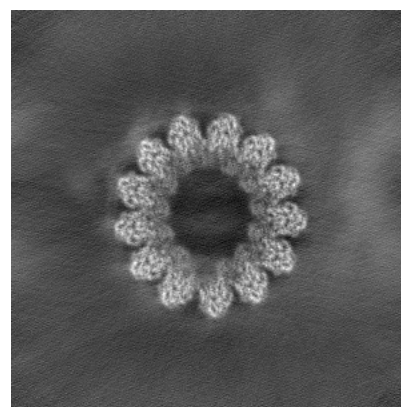
6.1.2 Raw map



X



Y

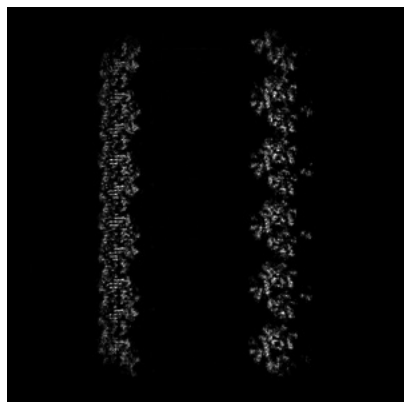


Z

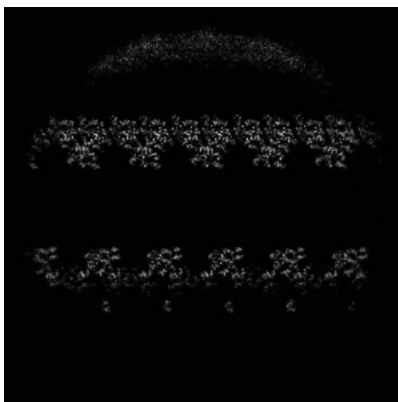
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

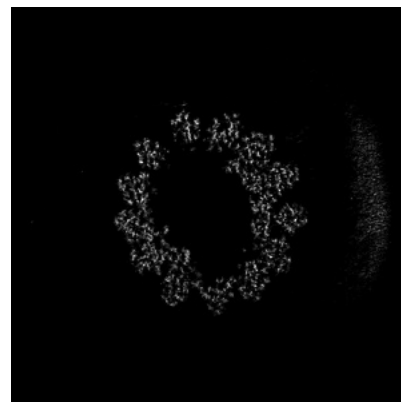
6.2.1 Primary map



X Index: 200

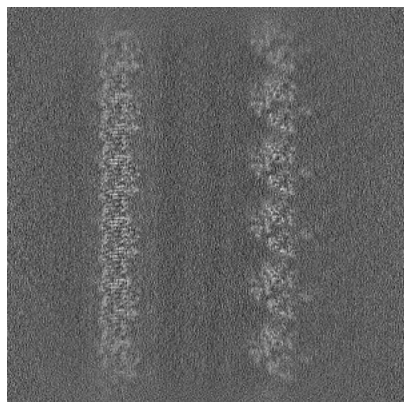


Y Index: 200

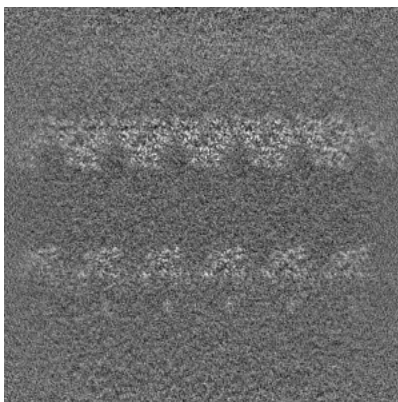


Z Index: 200

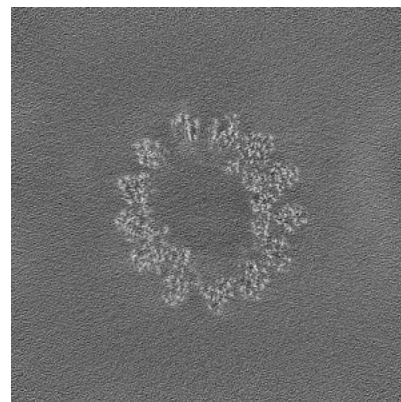
6.2.2 Raw map



X Index: 200



Y Index: 200

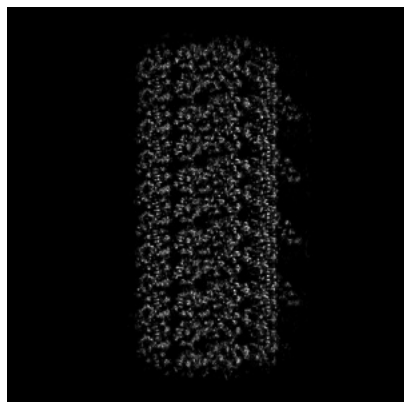


Z Index: 200

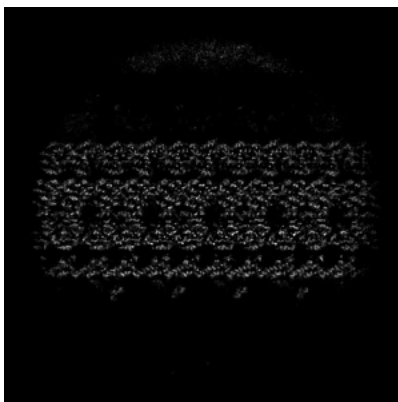
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

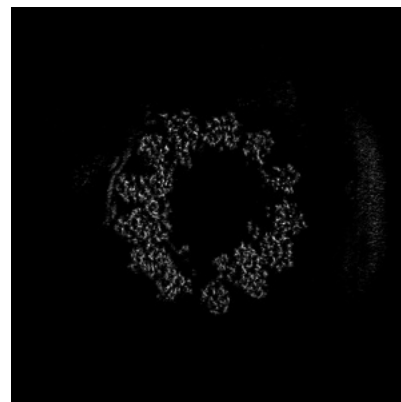
6.3.1 Primary map



X Index: 133

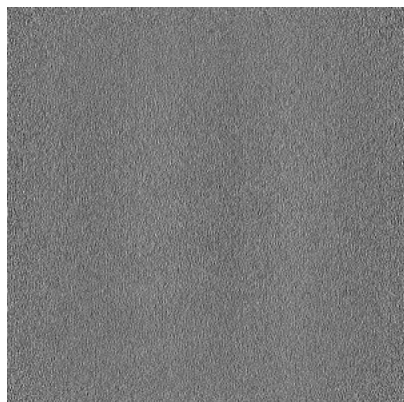


Y Index: 267

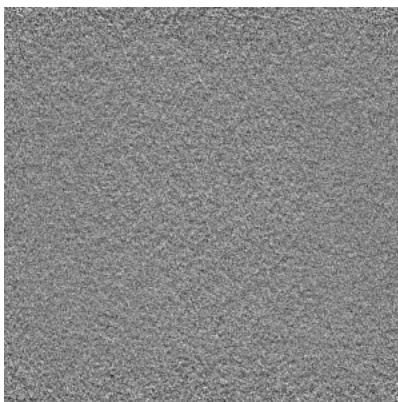


Z Index: 223

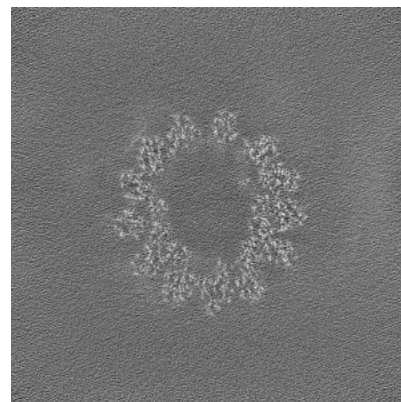
6.3.2 Raw map



X Index: 0



Y Index: 0

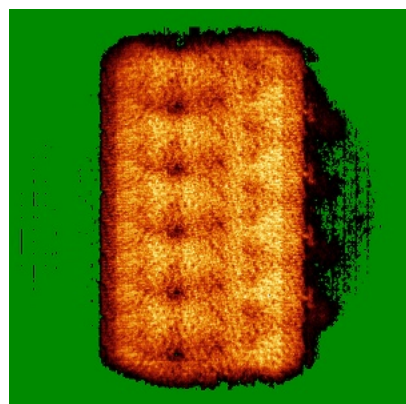


Z Index: 211

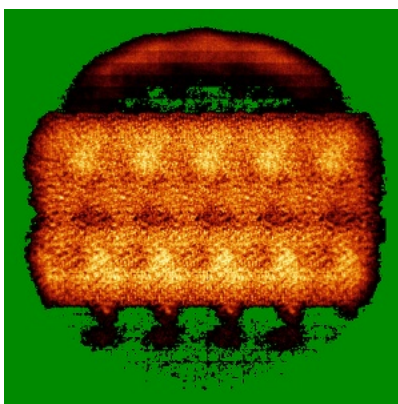
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

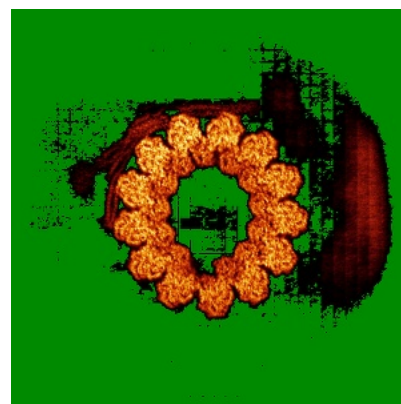
6.4.1 Primary map



X

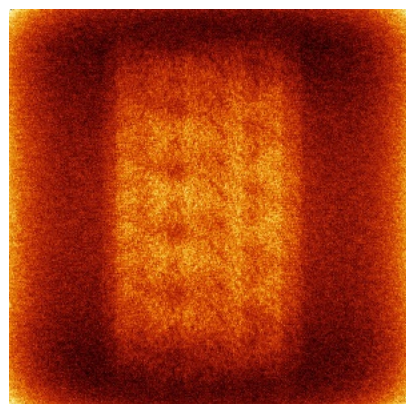


Y

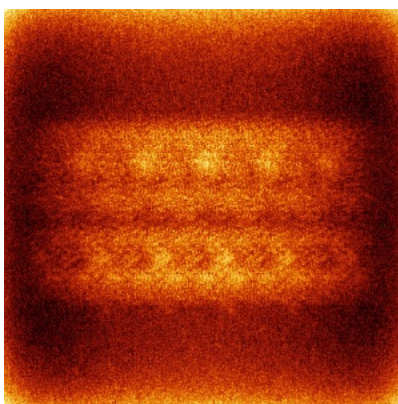


Z

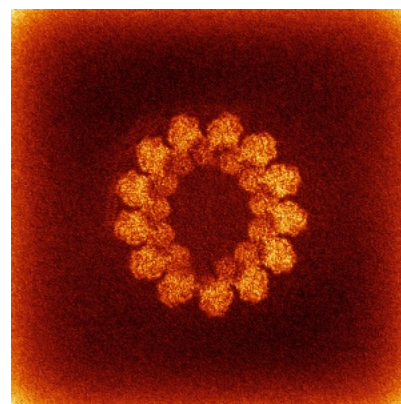
6.4.2 Raw map



X



Y

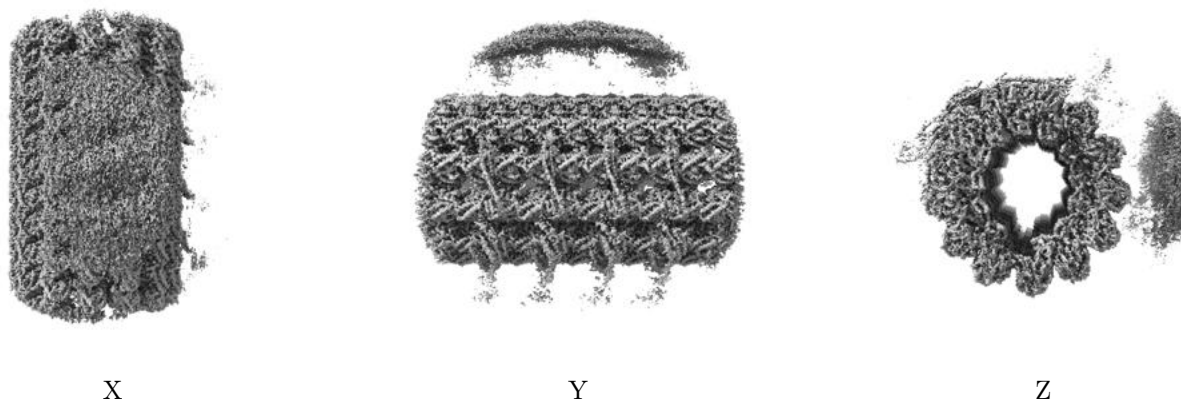


Z

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.

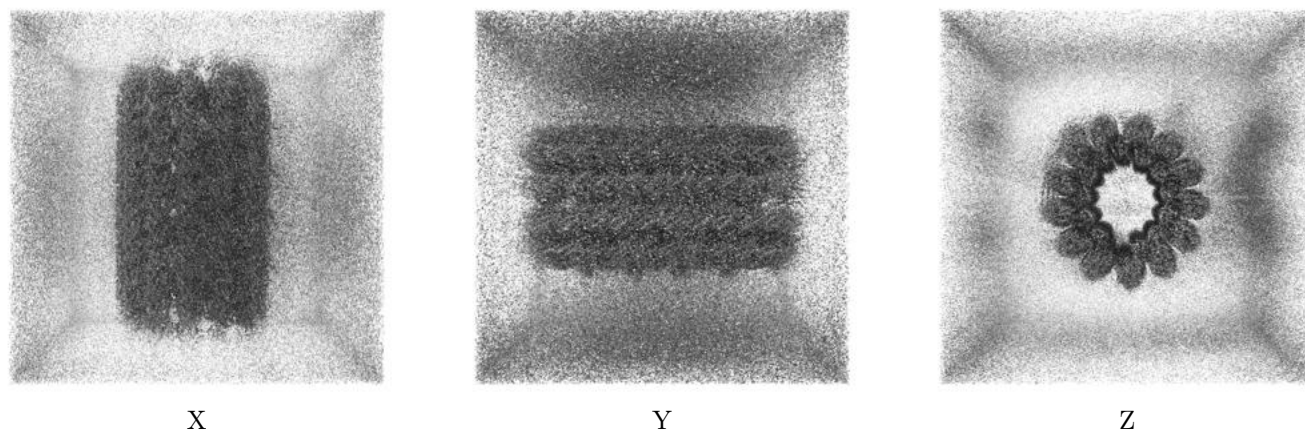
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

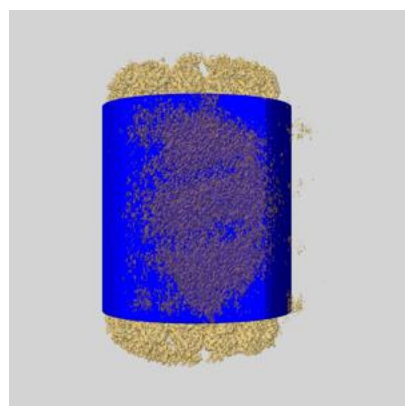
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

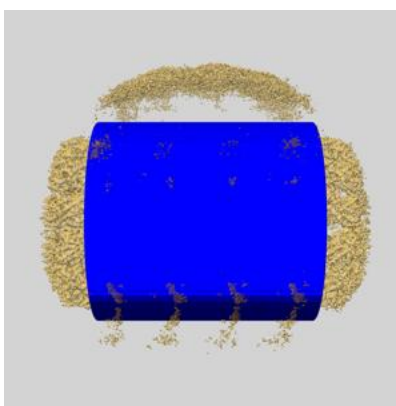
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

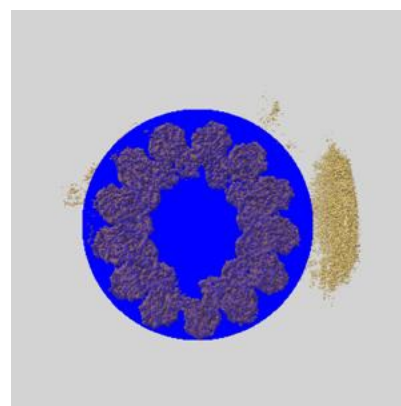
6.6.1 emd_72717_msk_1.map [i](#)



X



Y

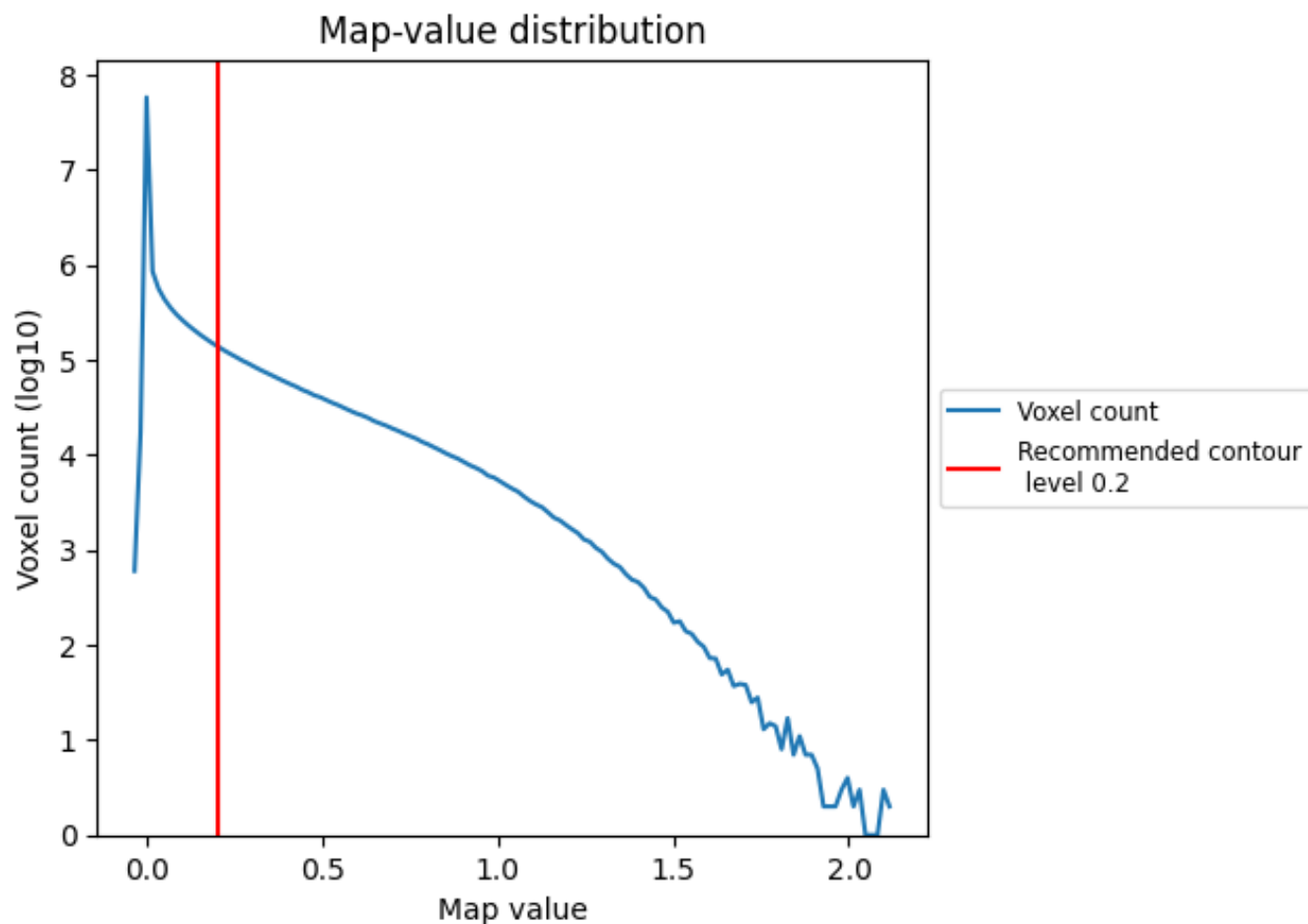


Z

7 Map analysis [i](#)

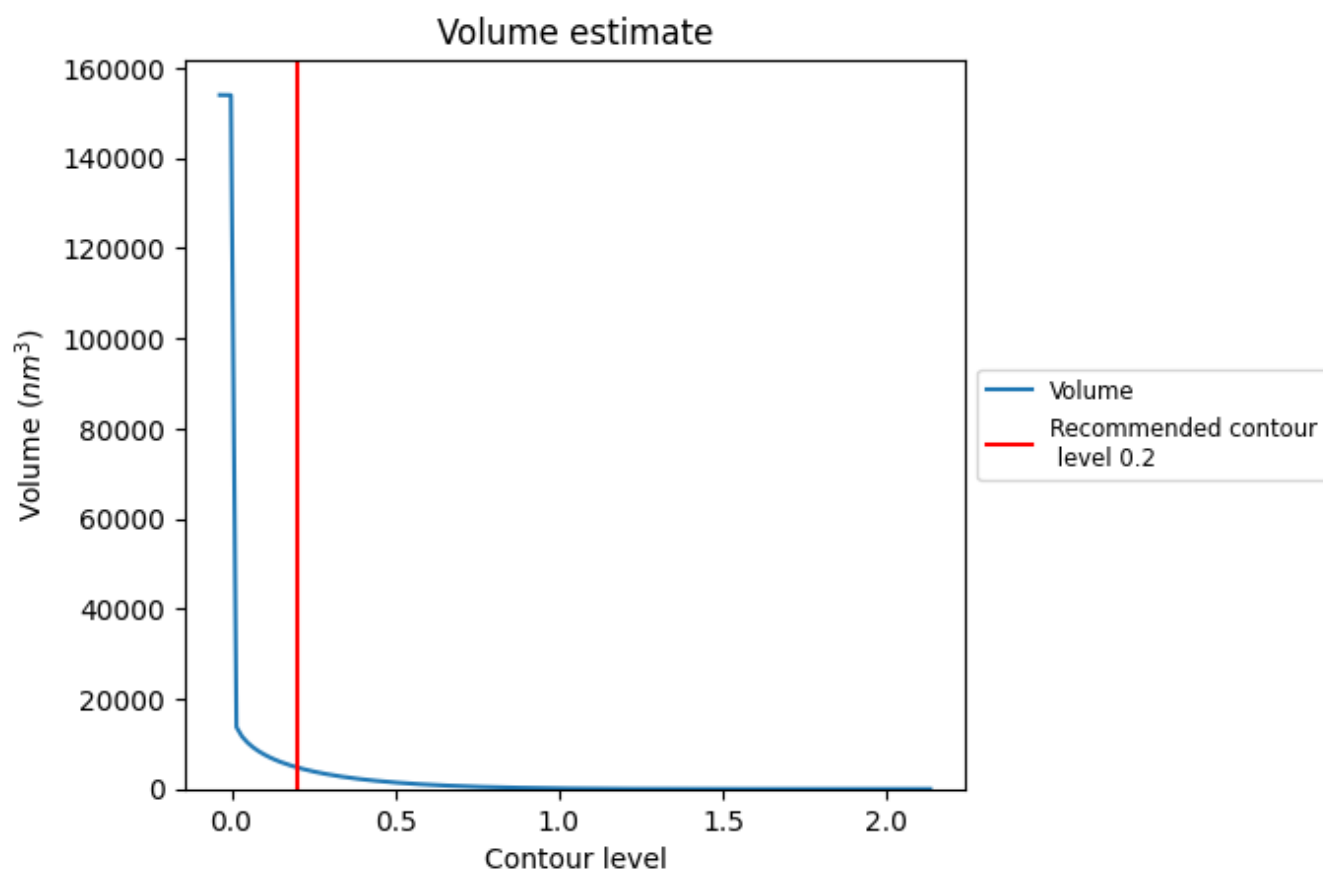
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

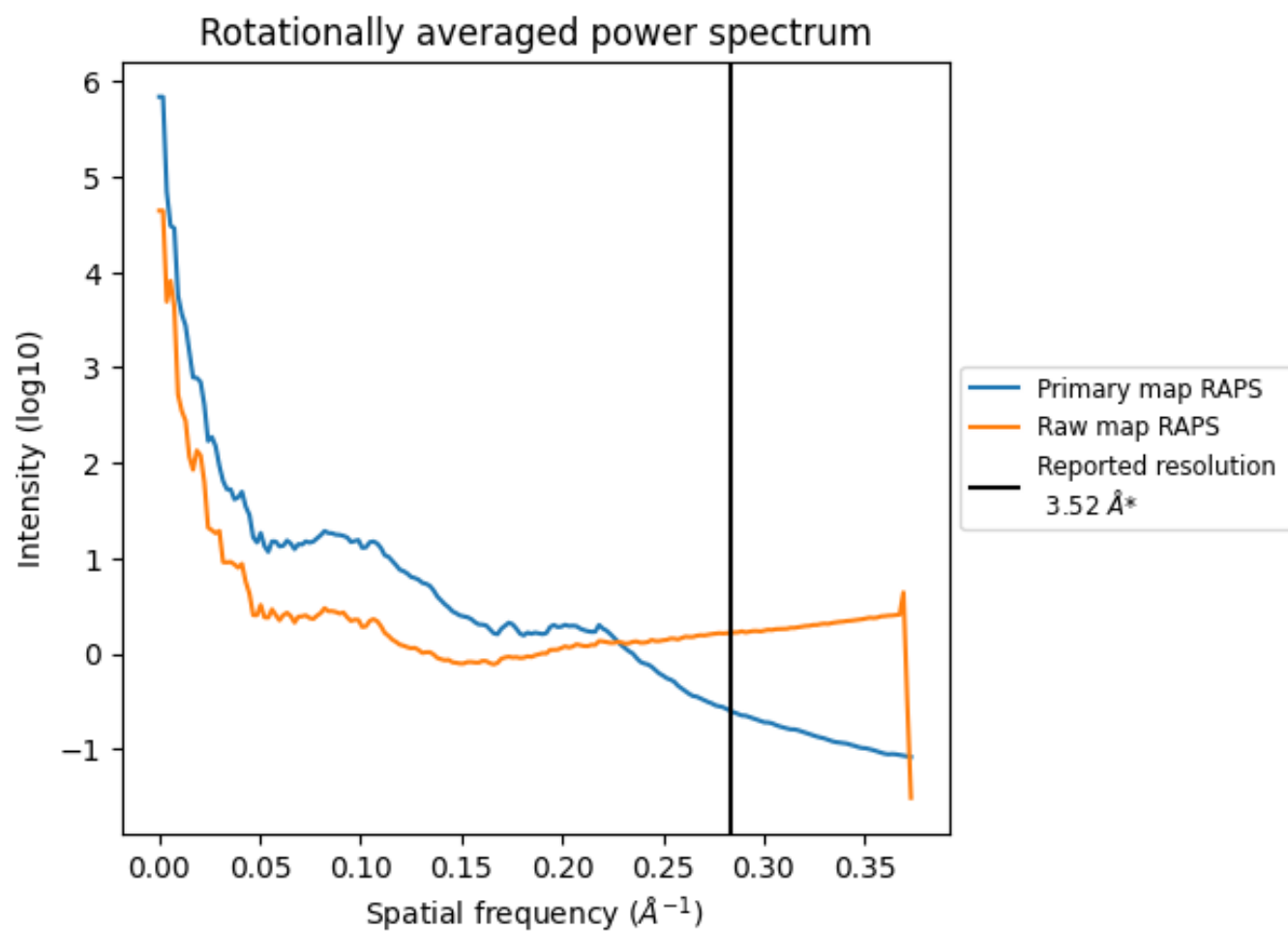
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4802 nm^3 ; this corresponds to an approximate mass of 4337 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 ⓘ

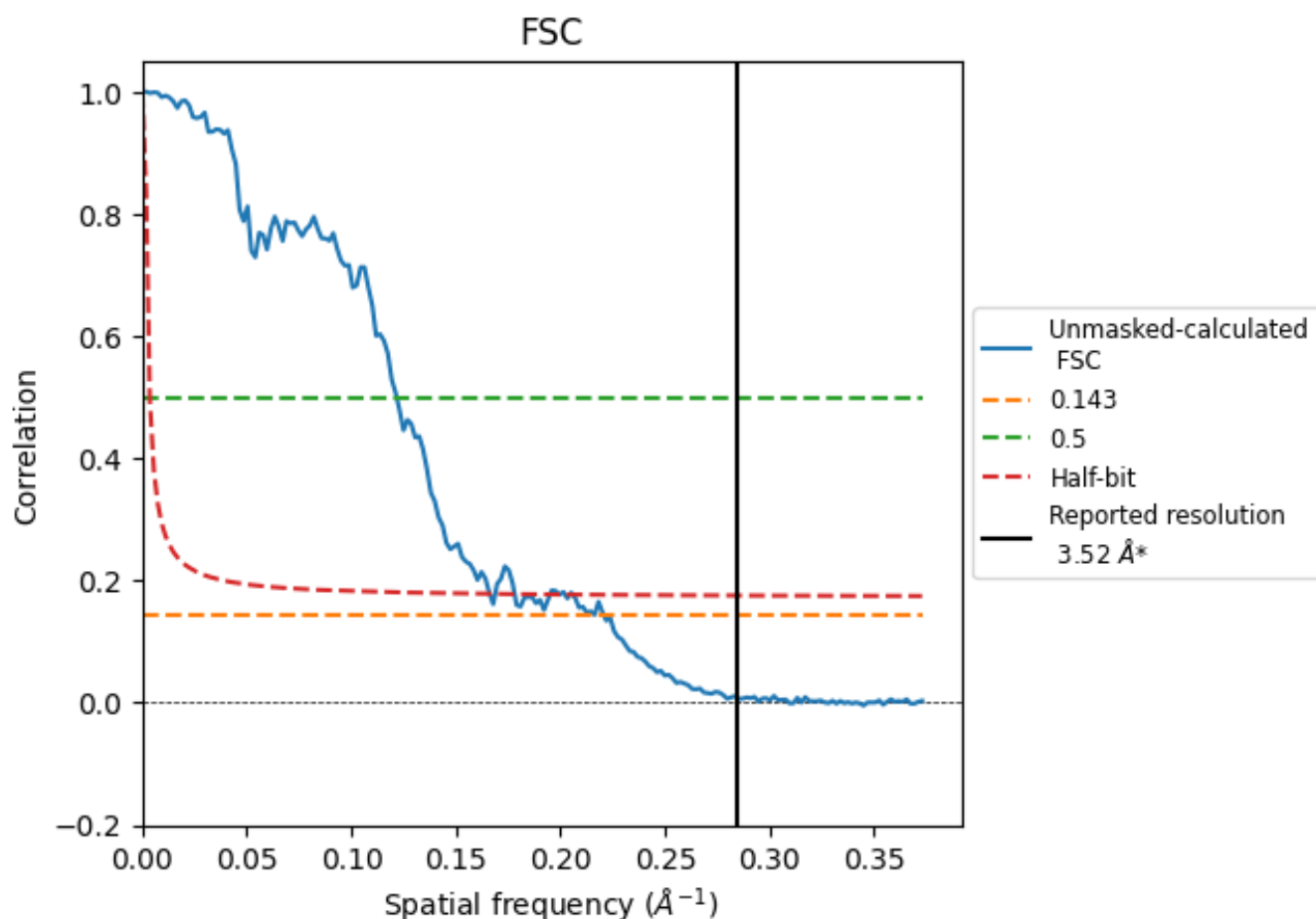


*Reported resolution corresponds to spatial frequency of 0.284 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.284 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

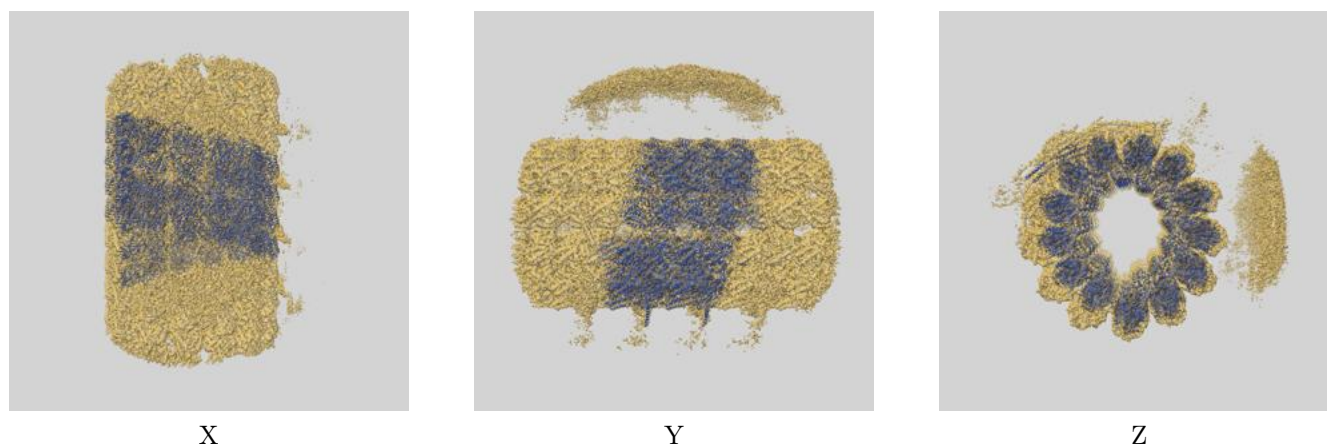
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.52	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.53	8.22	6.01

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.53 differs from the reported value 3.52 by more than 10 %

9 Map-model fit [i](#)

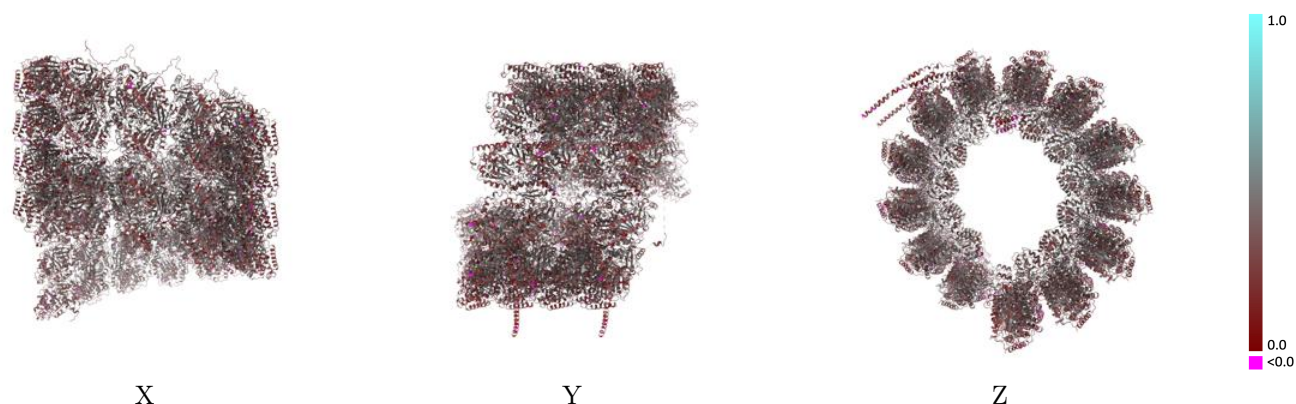
This section contains information regarding the fit between EMDB map EMD-72717 and PDB model 9YA1. Per-residue inclusion information can be found in section [3](#) on page [19](#).

9.1 Map-model overlay [i](#)



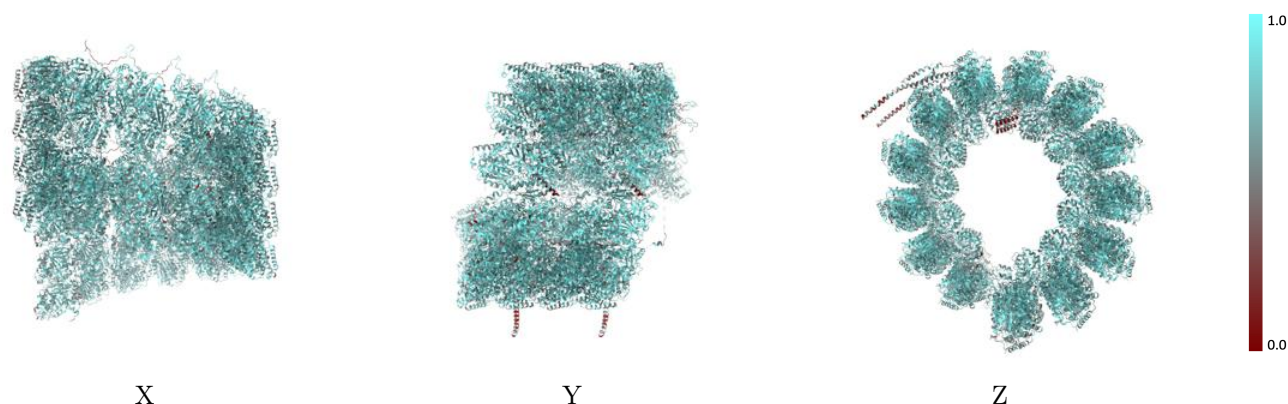
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



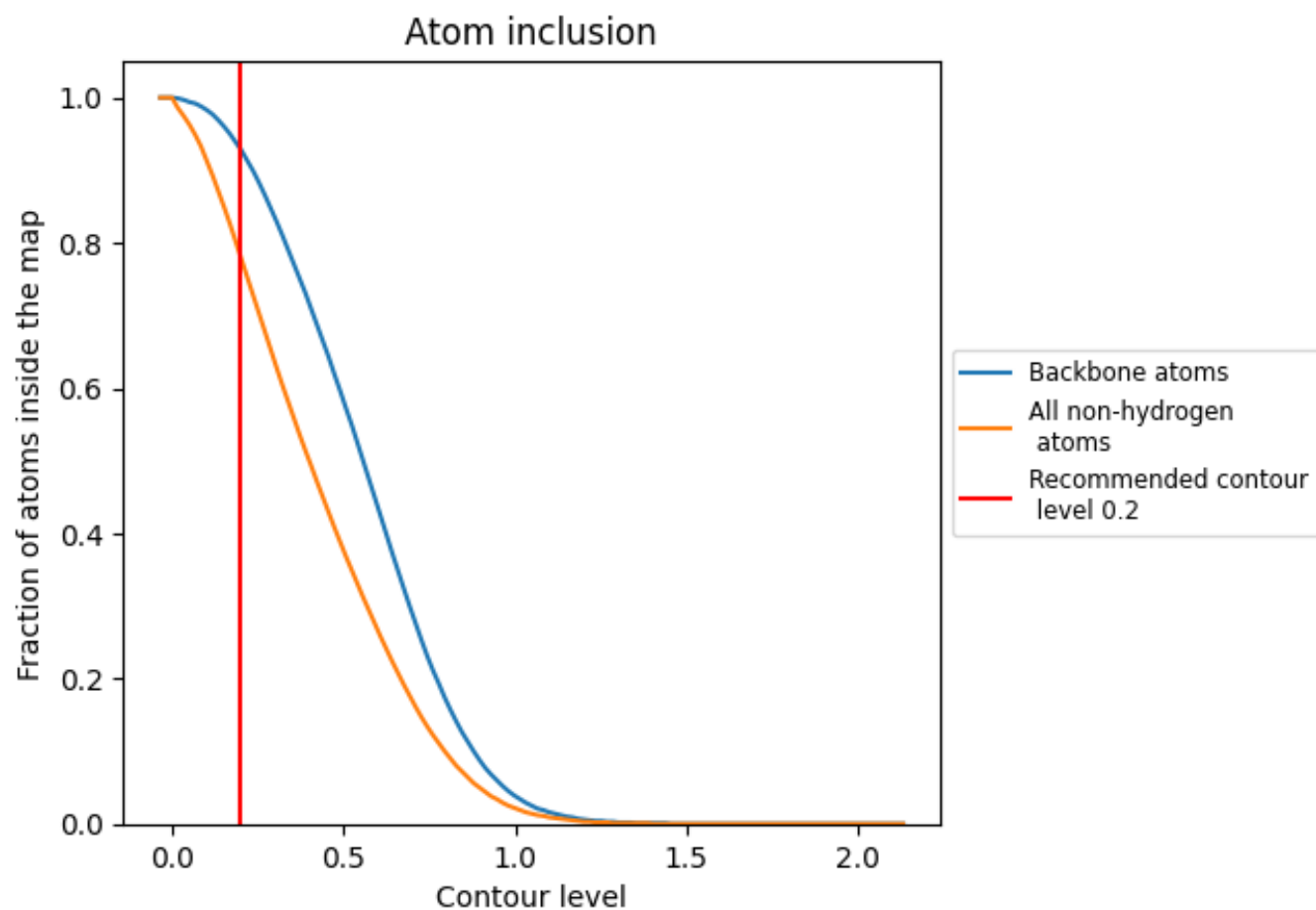
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 [i](#)



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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 78% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7800	 0.3490
1	 0.5160	 0.2480
2	 0.4690	 0.2140
A	 0.6640	 0.3540
A0	 0.7760	 0.3430
A1	 0.7730	 0.3460
A2	 0.7630	 0.3250
A3	 0.7330	 0.3260
A4	 0.8020	 0.3530
A5	 0.7760	 0.3470
A6	 0.7980	 0.3510
A7	 0.7720	 0.3460
A8	 0.8170	 0.3360
A9	 0.7900	 0.3400
B	 0.7450	 0.3720
B0	 0.8010	 0.3340
B1	 0.7910	 0.3340
B2	 0.8310	 0.3570
B3	 0.8060	 0.3460
B4	 0.8200	 0.3400
B5	 0.7920	 0.3270
B6	 0.8320	 0.3670
B7	 0.8190	 0.3670
B8	 0.8290	 0.3650
B9	 0.7980	 0.3470
C	 0.7460	 0.3350
C0	 0.8260	 0.3490
C1	 0.8000	 0.3460
C2	 0.8250	 0.3580
C3	 0.8080	 0.3490
C4	 0.8210	 0.3410
C5	 0.7950	 0.3380
C6	 0.8260	 0.3460
C7	 0.8060	 0.3480
C8	 0.7980	 0.3480



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Chain	Atom inclusion	Q-score
C9	 0.7910	 0.3630
D	 0.6730	 0.3600
D0	 0.8050	 0.3650
D1	 0.7830	 0.3650
D2	 0.8140	 0.3730
D3	 0.7950	 0.3870
D4	 0.8190	 0.3830
D5	 0.7910	 0.3790
D6	 0.8030	 0.3620
D7	 0.7910	 0.3720
D8	 0.8210	 0.3740
D9	 0.7980	 0.3770
E	 0.6780	 0.3690
E0	 0.7750	 0.3450
E1	 0.7770	 0.3620
E2	 0.8150	 0.3750
E3	 0.7840	 0.3710
E4	 0.7420	 0.3370
E5	 0.7360	 0.3420
E6	 0.7680	 0.3600
E7	 0.7700	 0.3730
E8	 0.6790	 0.3060
E9	 0.7150	 0.3240
F	 0.6980	 0.3550
F0	 0.7410	 0.3520
F1	 0.7440	 0.3470
G	 0.5790	 0.3380
H	 0.7110	 0.3730
I	 0.7620	 0.3640
J	 0.7860	 0.3710
K	 0.6800	 0.3570
O	 0.5930	 0.2810
P	 0.6190	 0.2860
R	 0.6260	 0.3020
U	 0.5900	 0.2840
V	 0.6420	 0.2780
W	 0.6330	 0.2740
X	 0.6840	 0.3020
a	 0.8030	 0.3610
b	 0.7900	 0.3490
c	 0.8130	 0.3450
d	 0.8310	 0.3650

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Chain	Atom inclusion	Q-score
e	 0.8350	 0.3530
f	 0.8410	 0.3540
g	 0.8220	 0.3500
h	 0.8190	 0.3440
i	 0.8000	 0.3550
j	 0.7950	 0.3530
k	 0.7580	 0.3250
l	 0.7600	 0.3170
m	 0.6250	 0.2830
n	 0.6190	 0.2840
o	 0.8130	 0.3750
p	 0.7980	 0.3770
q	 0.8200	 0.3920
r	 0.8380	 0.4010
s	 0.8290	 0.3750
t	 0.8380	 0.3930
u	 0.8060	 0.3520
v	 0.8120	 0.3620
w	 0.7480	 0.3360
x	 0.7610	 0.3450