



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 04:54 AM UTC

PDB ID : 9YA3 / pdb_00009ya3
EMDB ID : EMD-72719
Title : Cryo-EM structure of the apical region of subpellicular microtubule (SPMT)
from Toxoplasma gondii (8-nm repeat)
Authors : Zeng, J.; Zhang, R.
Deposited on : 2025-09-15
Resolution : 3.30 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

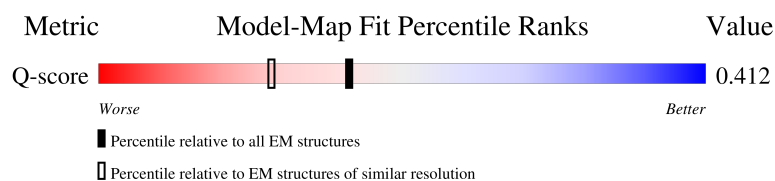
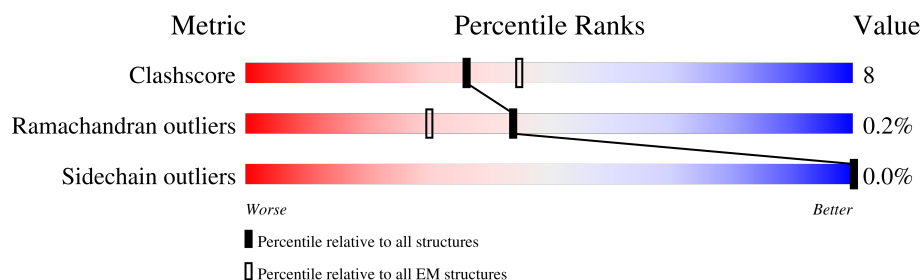
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.



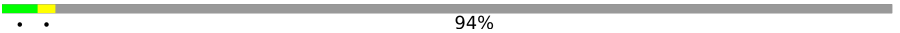
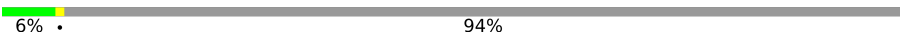
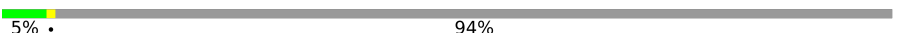
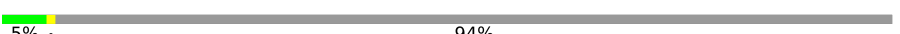
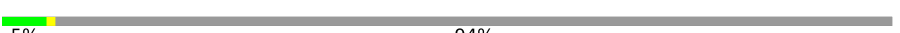
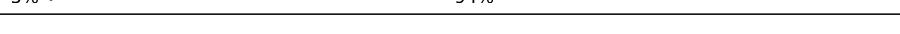
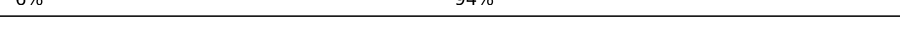
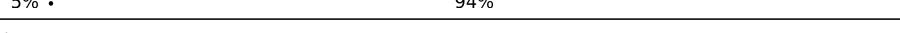
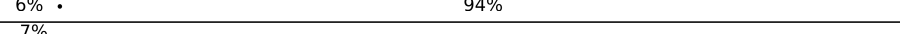
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	0	351	5% . 94%
1	1	351	5% . 94%
1	10	351	5% . 94%
1	11	351	5% . 94%

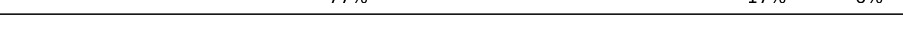
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Mol	Chain	Length	Quality of chain
1	12	351	 94%
1	13	351	 94%
1	14	351	 94%
1	15	351	 94%
1	16	351	 94%
1	17	351	 94%
1	18	351	 94%
1	19	351	 94%
1	2	351	 94%
1	22	351	 94%
1	23	351	 94%
1	3	351	 94%
1	4	351	 94%
1	5	351	 94%
1	6	351	 94%
1	7	351	 94%
1	8	351	 94%
1	9	351	 94%
2	A	583	 71%
2	B	583	 62%
2	C	583	 92%
3	A0	453	 76% 19% 6%
3	A2	453	 75% 20% 6%
3	A4	453	 83% 11% 6%
3	A6	453	 76% 19% 6%

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Mol	Chain	Length	Quality of chain
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	
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	

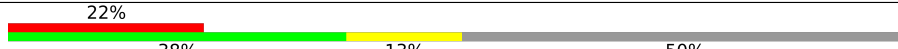
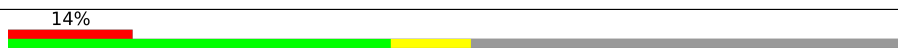
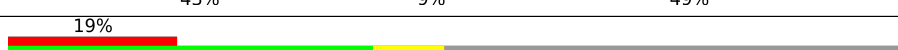
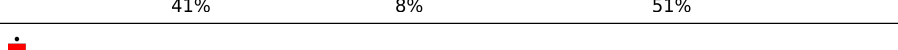
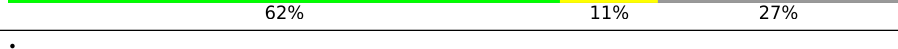
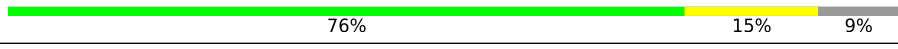
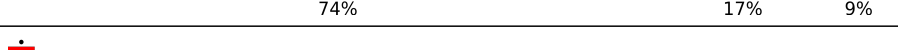
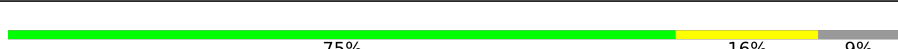
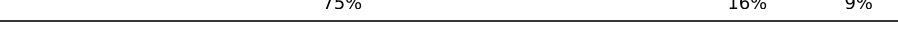
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Mol	Chain	Length	Quality of chain
4	A7	449	
4	A9	449	
4	B1	449	
4	B3	449	
4	B5	449	
4	B7	449	
4	B9	449	
4	C1	449	
4	C3	449	
4	C5	449	
4	C7	449	
4	C9	449	
4	D1	449	
4	D3	449	
4	D5	449	
4	D7	449	
4	D9	449	
4	E1	449	
4	E3	449	
4	E5	449	
4	E7	449	
4	E9	449	
4	F1	449	
5	E	336	
5	F	336	

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Mol	Chain	Length	Quality of chain
5	G	336	
6	H	446	
6	I	446	
6	J	446	
6	K	446	
7	a	220	
7	b	220	
7	c	220	
7	d	220	
7	e	220	
7	f	220	
7	g	220	
7	h	220	
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	

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Mol	Chain	Length	Quality of chain
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 228257 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Microtubule associated protein SPM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	1	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	10	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	11	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	12	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	13	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	14	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	15	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	16	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	17	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	18	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	19	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	2	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	22	20	Total	C	N	O	S	0	0
			160	105	26	28	1		
1	23	20	Total	C	N	O	S	0	0
			160	105	26	28	1		
1	3	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	4	22	Total	C	N	O	S	0	0
			174	114	28	31	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	6	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	7	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	8	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	9	22	Total	C	N	O	S	0	0
			174	114	28	31	1		

There are 22 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called TLAP3 (apical cap protein AC5), TGME49_235380.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	169	Total	C	N	O	S	0	0
			1338	829	252	255	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	220	Total	C	N	O	S	0	0
			1744	1084	329	329	2		
2	C	49	Total	C	N	O		0	0
			384	240	74	70			

- 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		
3	C8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	D0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	D2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	D4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	D6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	D8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	E0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	E2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	E4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	E6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	E8	428	Total	C	N	O	S	0	0
			3319	2102	566	625	26		
3	F0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		

- Molecule 4 is a protein called Tubulin beta chain.

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
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 TLAP4 (thioredoxin-like associated protein), TGME49_201760.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	89	Total 740	C 459	N 141	O 139	S 1	0	0
5	F	89	Total 740	C 459	N 141	O 139	S 1	0	0
5	G	67	Total 558	C 347	N 103	O 108		0	0

- Molecule 6 is a protein called TLAP2 (thioredoxin-like associated protein), TGME49_232130.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	223	Total	C	N	O	S	0	0
			1817	1173	322	319	3		
6	I	224	Total	C	N	O	S	0	0
			1817	1170	323	321	3		
6	J	229	Total	C	N	O	S	0	0
			1870	1202	334	331	3		
6	K	220	Total	C	N	O	S	0	0
			1795	1158	319	315	3		

- 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		
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		

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Mol	Chain	Residues	Atoms					AltConf	Trace
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	139	Total	C	N	O	S	0	0
			1140	738	203	195	4		
8	l	139	Total	C	N	O	S	0	0
			1140	738	203	195	4		

There are 46 discrepancies between the modelled and reference sequences:

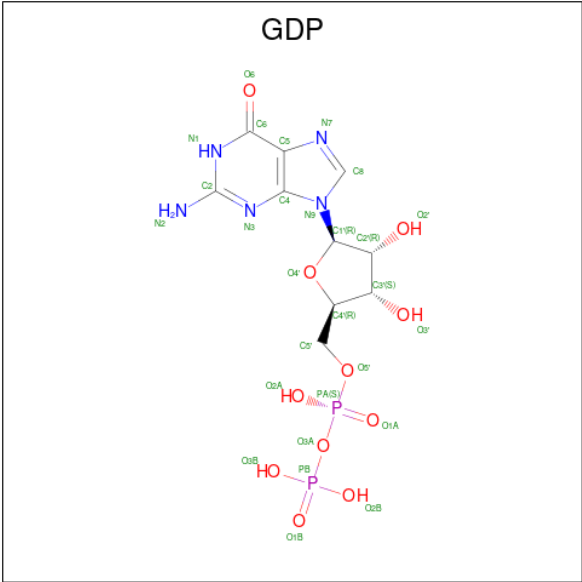
Chain	Residue	Modelled	Actual	Comment	Reference
k	167	SER	-	expression tag	UNP A0A7J6K232
k	168	ALA	-	expression tag	UNP A0A7J6K232
k	169	GLN	-	expression tag	UNP A0A7J6K232
k	170	ARG	-	expression tag	UNP A0A7J6K232
k	171	LEU	-	expression tag	UNP A0A7J6K232
k	172	ARG	-	expression tag	UNP A0A7J6K232
k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

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Chain	Residue	Modelled	Actual	Comment	Reference
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'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



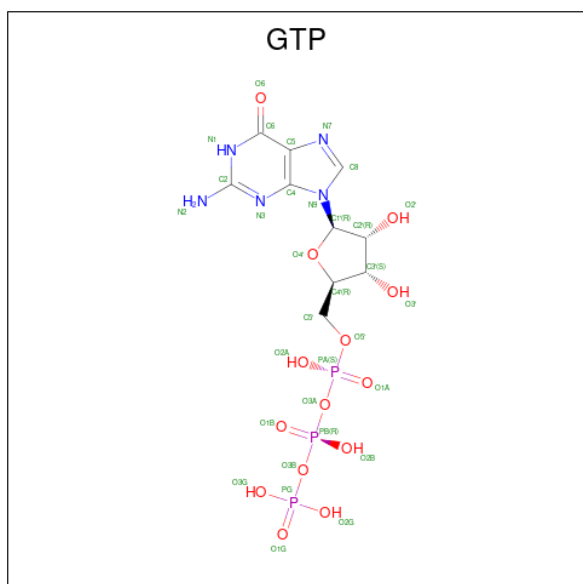
Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	A1	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	A3	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	A5	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	A7	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	B	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	B3	1	Total	C	N	O	P	0
		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

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Mol	Chain	Residues	Atoms					AltConf
9	C9	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	D1	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	D3	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	D5	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	D7	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	D9	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	E1	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	E3	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	E5	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	E7	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	E9	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	F1	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 10 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	A0	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	A2	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	A4	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	A6	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	A8	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	B0	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	B2	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	B4	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	B6	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	B8	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	C0	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	C2	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	C4	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	C6	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	C8	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	D0	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	D2	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	D4	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	D6	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	D8	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	E0	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	E2	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
10	E4	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	E6	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	E8	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	F0	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	A0	1	Total	Mg	0
			1	1	
11	A3	1	Total	Mg	0
			1	1	
11	A4	1	Total	Mg	0
			1	1	
11	A6	1	Total	Mg	0
			1	1	
11	A8	1	Total	Mg	0
			1	1	
11	B0	1	Total	Mg	0
			1	1	
11	B2	1	Total	Mg	0
			1	1	
11	B4	1	Total	Mg	0
			1	1	
11	B6	1	Total	Mg	0
			1	1	
11	B8	1	Total	Mg	0
			1	1	
11	C0	1	Total	Mg	0
			1	1	
11	C2	1	Total	Mg	0
			1	1	
11	C4	1	Total	Mg	0
			1	1	
11	C6	1	Total	Mg	0
			1	1	
11	C8	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
11	D0	1	Total 1	Mg 1	0
11	D2	1	Total 1	Mg 1	0
11	D4	1	Total 1	Mg 1	0
11	D6	1	Total 1	Mg 1	0
11	D8	1	Total 1	Mg 1	0
11	E0	1	Total 1	Mg 1	0
11	E2	1	Total 1	Mg 1	0
11	E4	1	Total 1	Mg 1	0
11	E6	1	Total 1	Mg 1	0
11	E8	1	Total 1	Mg 1	0
11	F0	1	Total 1	Mg 1	0

[illegible]

- Molecule 1: Microtubule associated protein SPM1

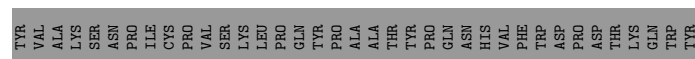
Chain 13: 6% 94%

[illegible]

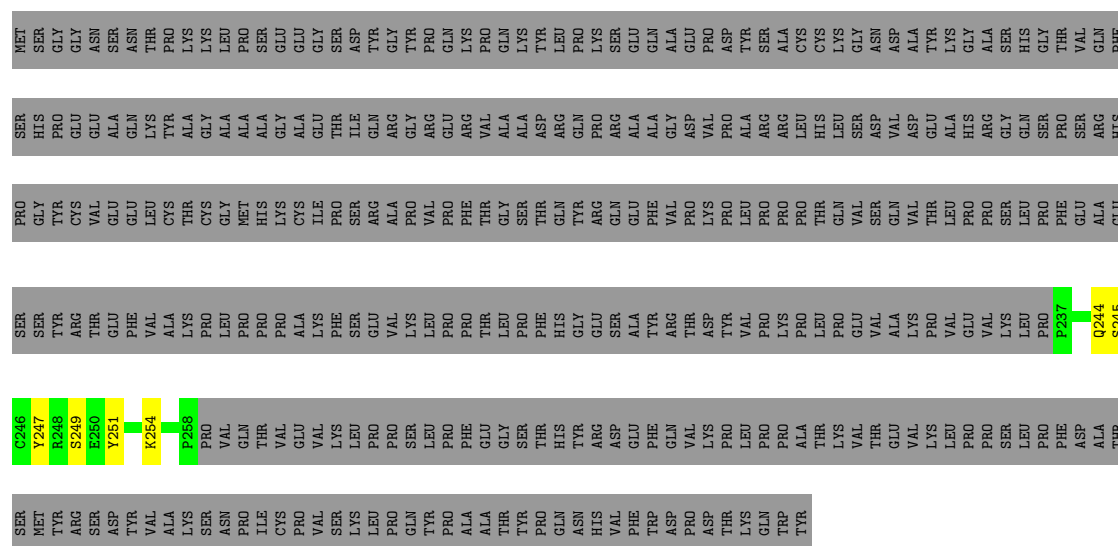
- Molecule 1: Microtubule associated protein SPM1

Chain 14: 5% . 94%

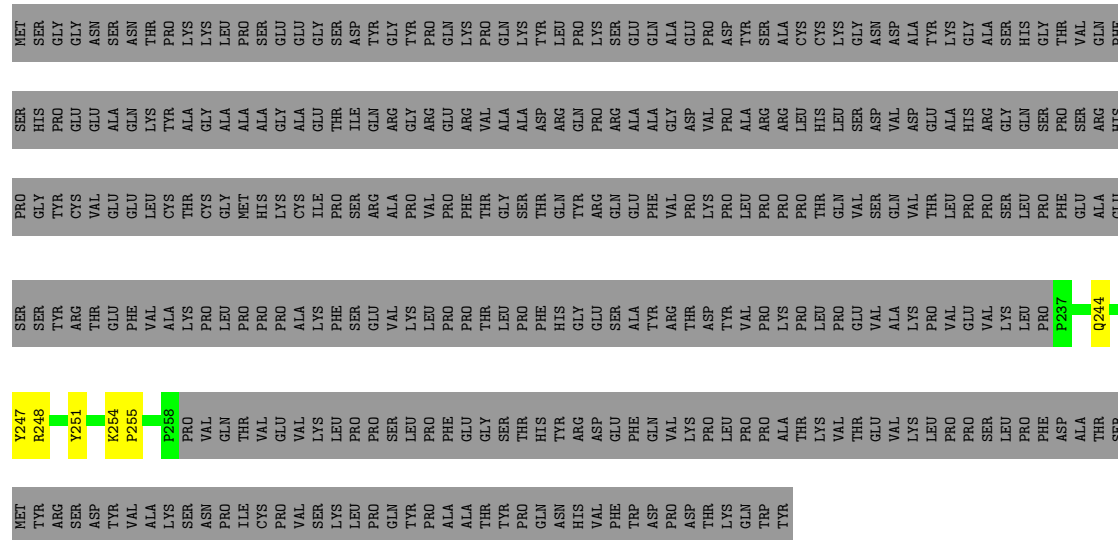
[illegible]



Chain 18: 5% 94%



Chain 19: 5% 94%



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

- Molecule 1: Microtubule associated protein SPM1

Chain 3: 5% • 94%

ASP	TYR	VAL	ALA	LYS	SER	ASN	PRO	ILE	CYS	PRO	VAL	SER	LYS	LEU	PRO	GLN	TYR	PRO	ALA	ALA	THR	TYR	PRO	GLN	ASN	HIS	VAL	PHE	TRP	ASP	PRO	ASP	THR	LYS	GLN	TRP	TYR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

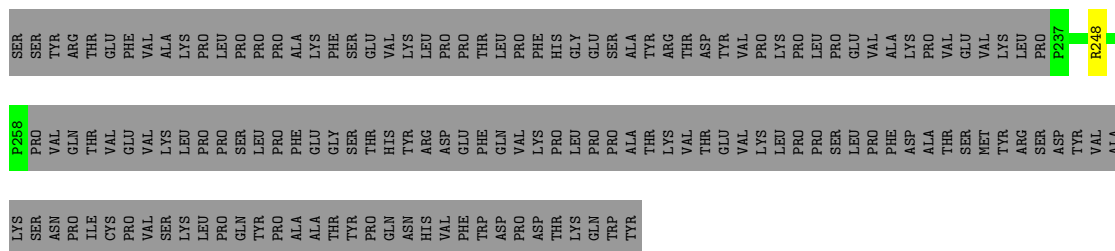
- Molecule 1: Microtubule associated protein SPM1

Chain 4: 5% • 94%

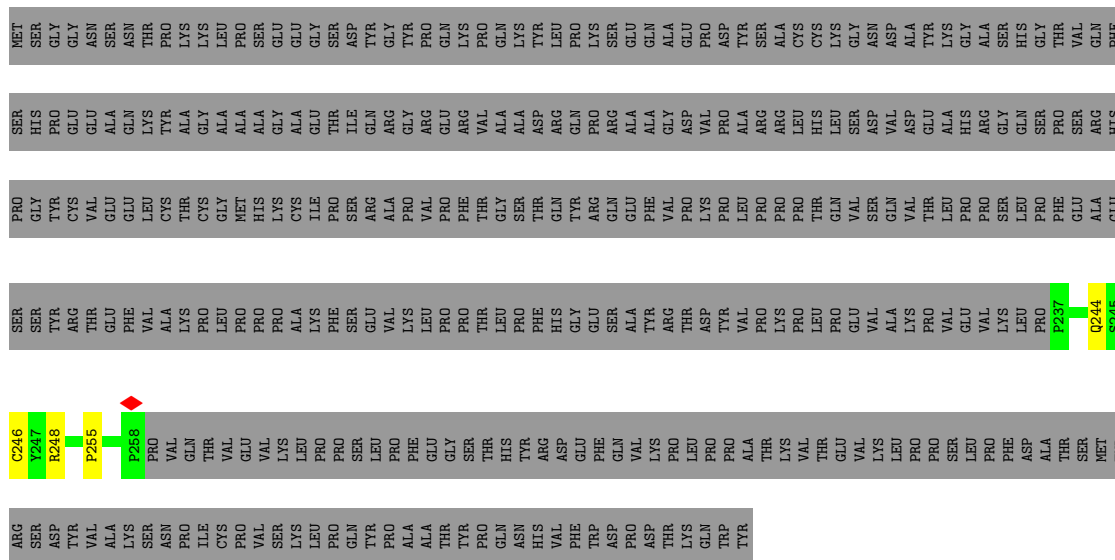
ARG	SER	ASP	TYR	VAL	ALA	LYS	SER	ASN	PRO	ILE	CYS	PRO	VAL	SER	LYS	LEU	PRO	GLN	TYR	PRO	ALA	ALA	THR	TYR	PRO	GLN	ASN	HIS	VAL	PHE	TRP	PRO	ASP	THR	ASP	LYS	GLN	TRP	TYR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----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

- Molecule 1: Microtubule associated protein SPM1

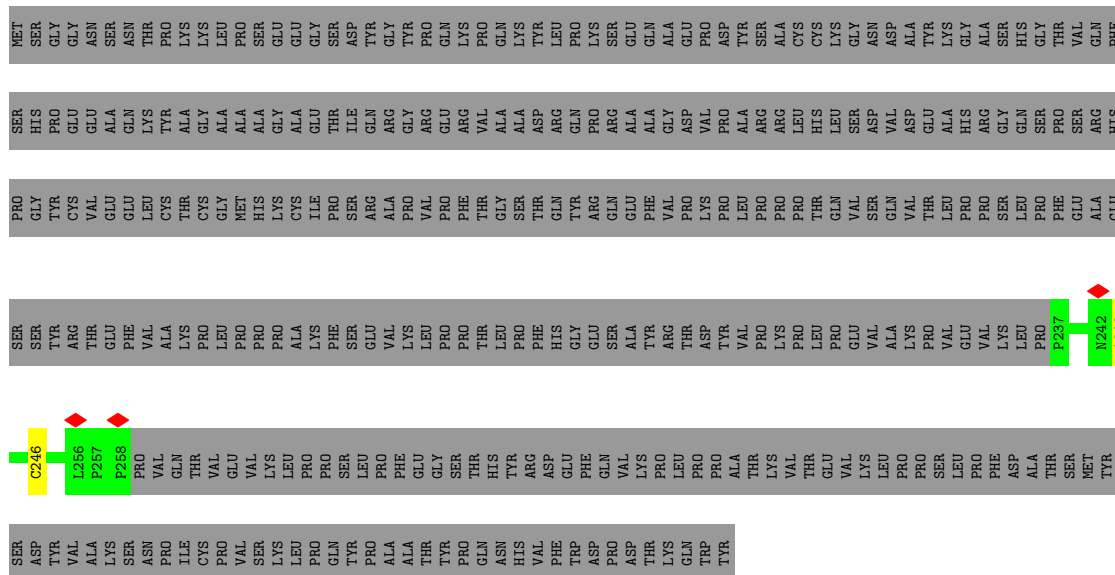


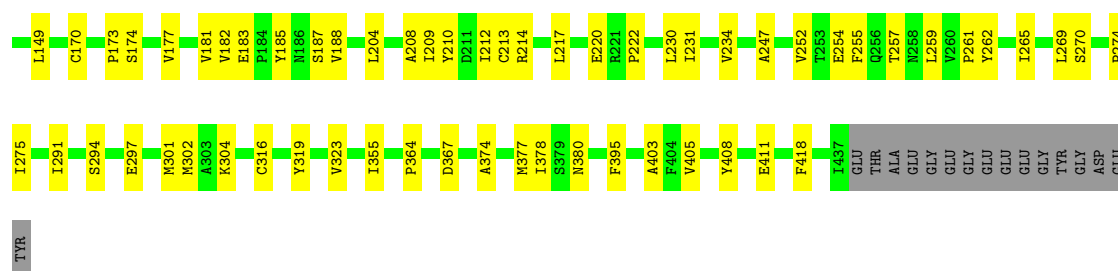


- Molecule 1: Microtubule associated protein SPM1



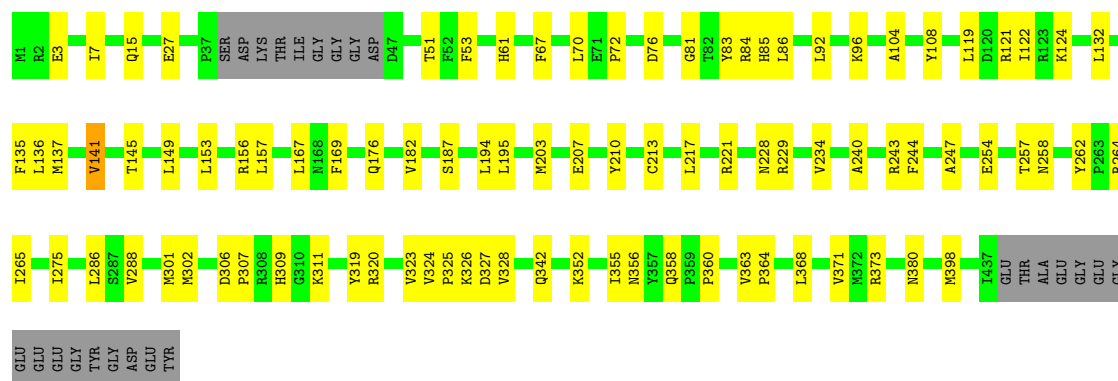
- Molecule 1: Microtubule associated protein SPM1





- Molecule 3: Tubulin alpha chain

Chain A2: 75% 20% 6%



- Molecule 3: Tubulin alpha chain

Chain A4: 83% 11% 6%



- Molecule 3: Tubulin alpha chain

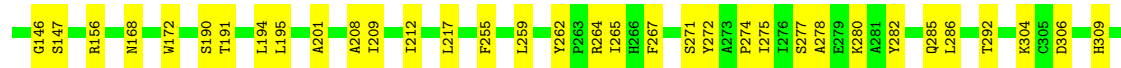
Chain A6: 76% 19% 6%





• Molecule 3: Tubulin alpha chain

Chain B6: 77% 18% 6%



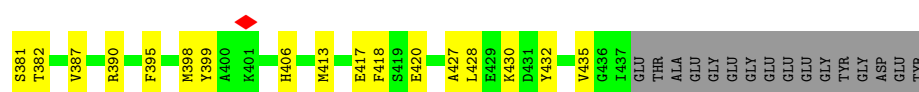
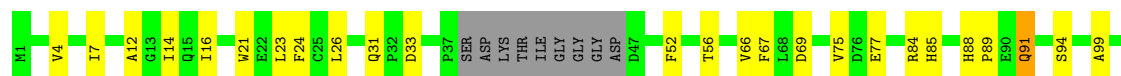
• Molecule 3: Tubulin alpha chain

Chain B8: 77% 17% 6%

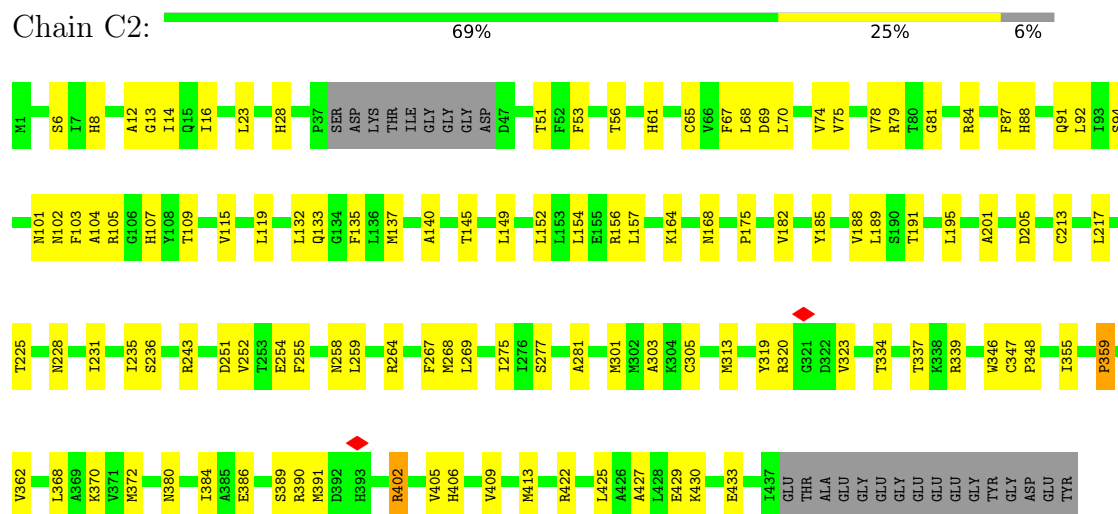


• Molecule 3: Tubulin alpha chain

Chain C0: 70% 24% 6%



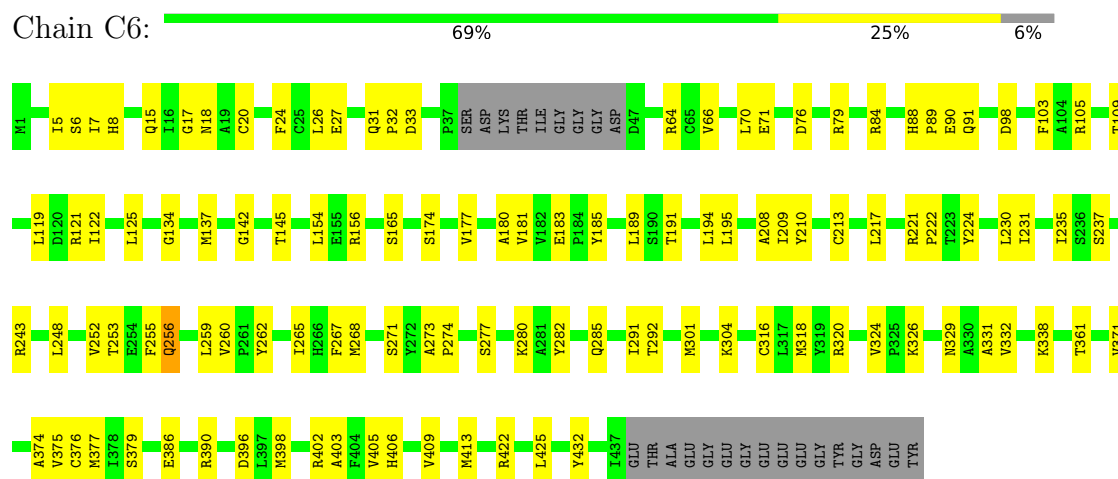
• Molecule 3: Tubulin alpha chain



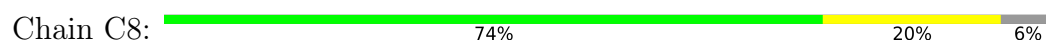
- Molecule 3: Tubulin alpha chain

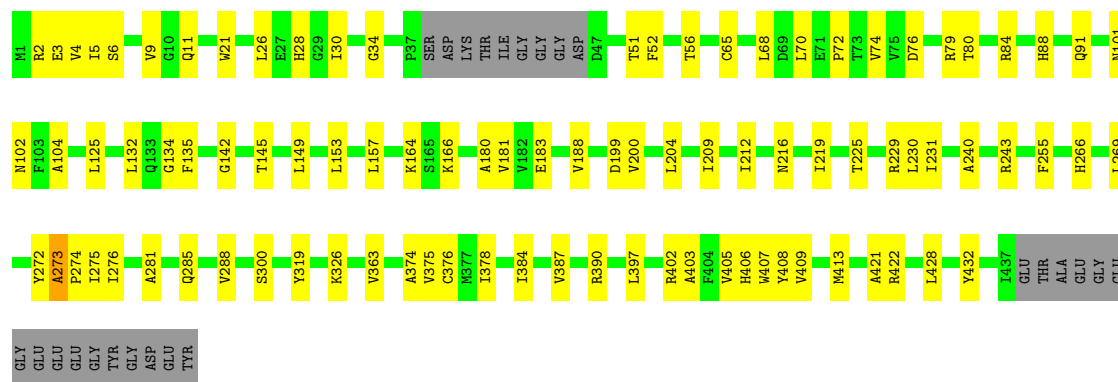


- Molecule 3: Tubulin alpha chain



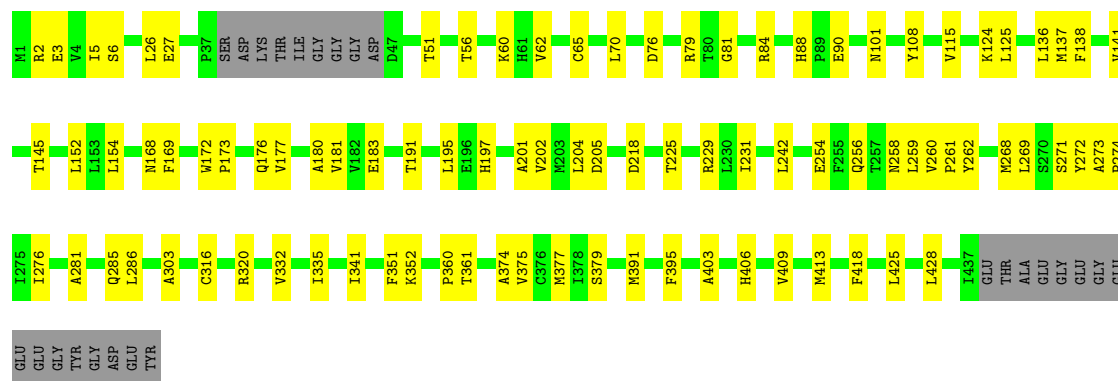
- Molecule 3: Tubulin alpha chain





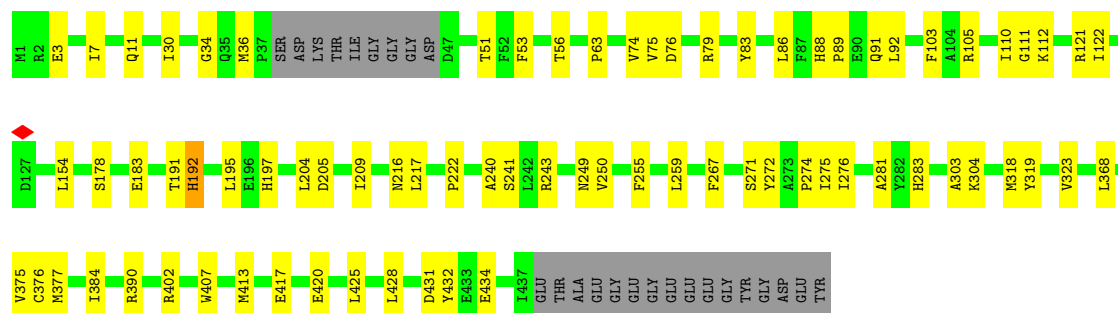
• Molecule 3: Tubulin alpha chain

Chain D0: 74% 20% 6%



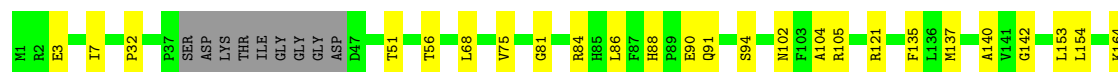
• Molecule 3: Tubulin alpha chain

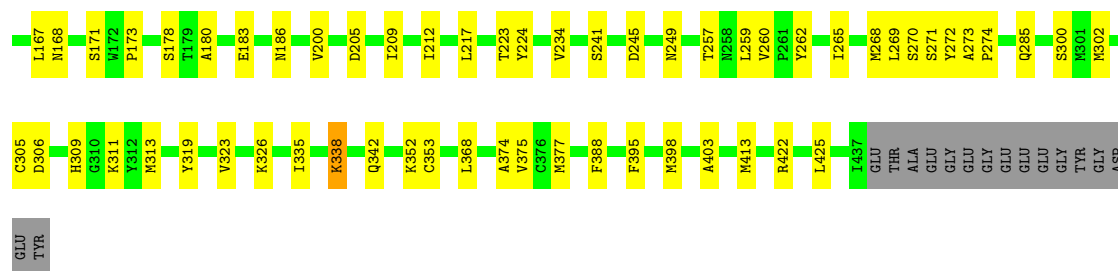
Chain D2: 78% 17% 6%



• Molecule 3: Tubulin alpha chain

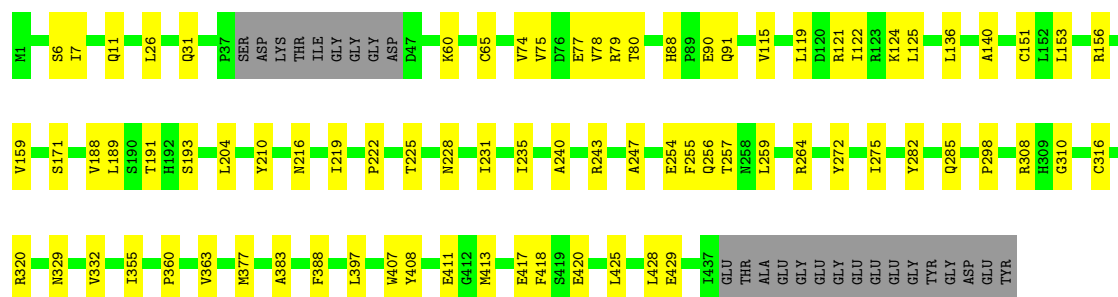
Chain D4: 76% 18% 6%





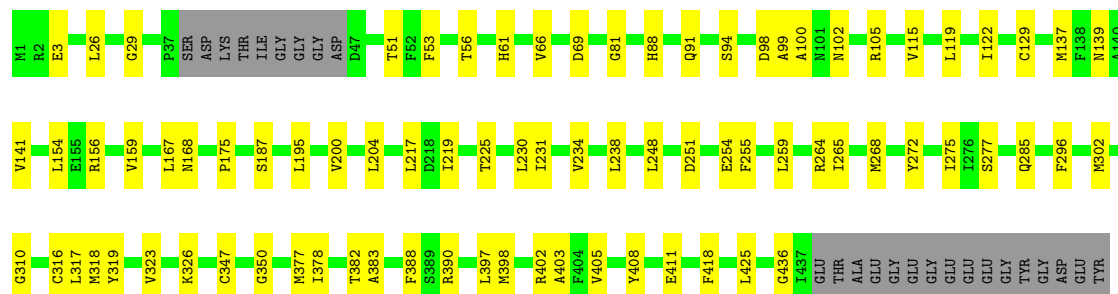
• Molecule 3: Tubulin alpha chain

Chain D6: 77% 17% 6%



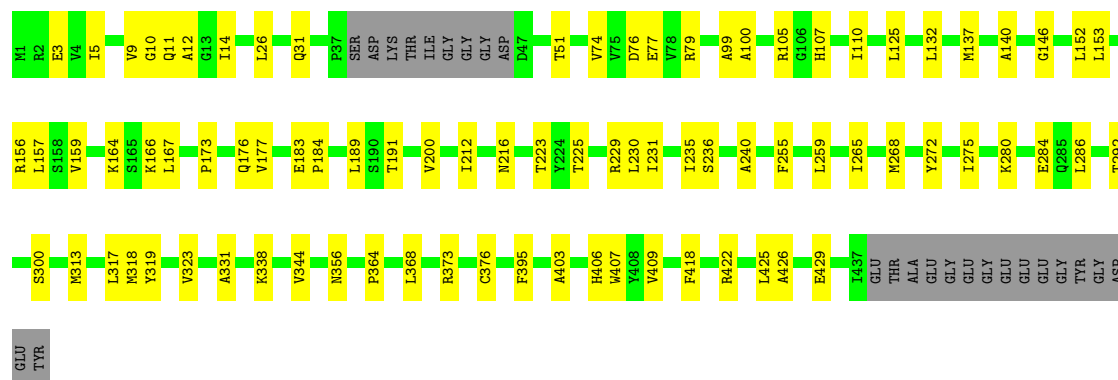
• Molecule 3: Tubulin alpha chain

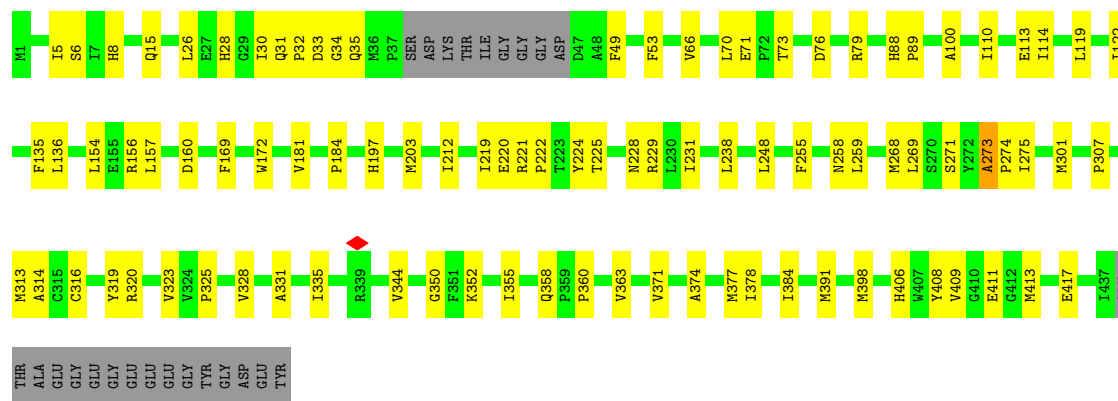
Chain D8: 77% 18% 6%



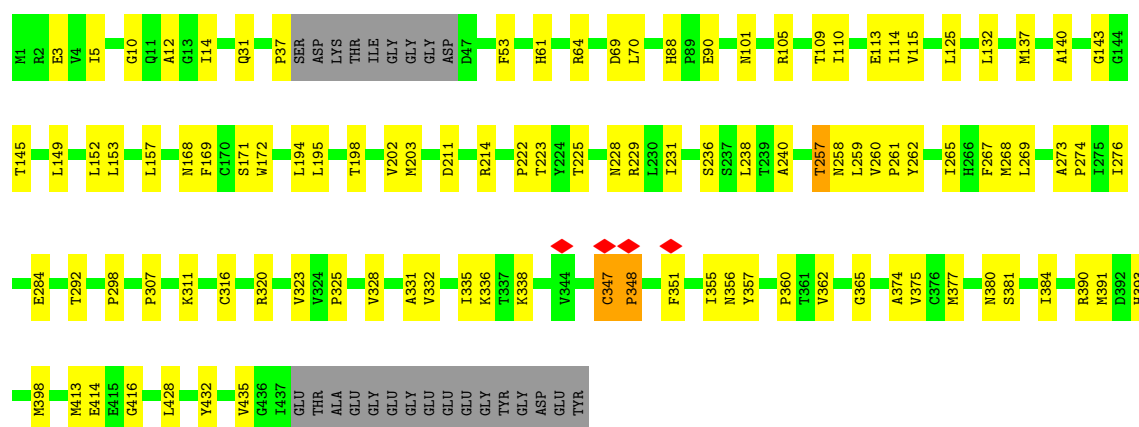
• Molecule 3: Tubulin alpha chain

Chain E0: 76% 19% 6%

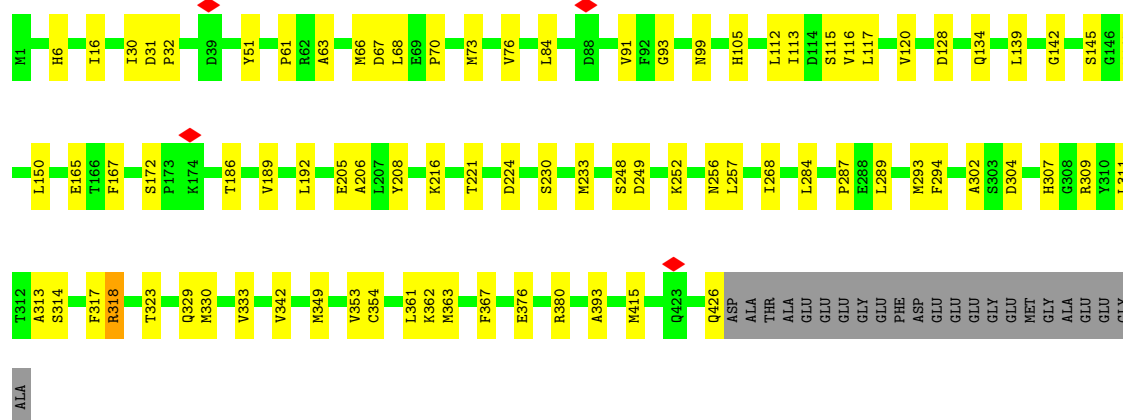
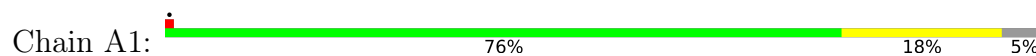




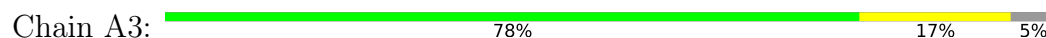
• Molecule 3: Tubulin alpha chain

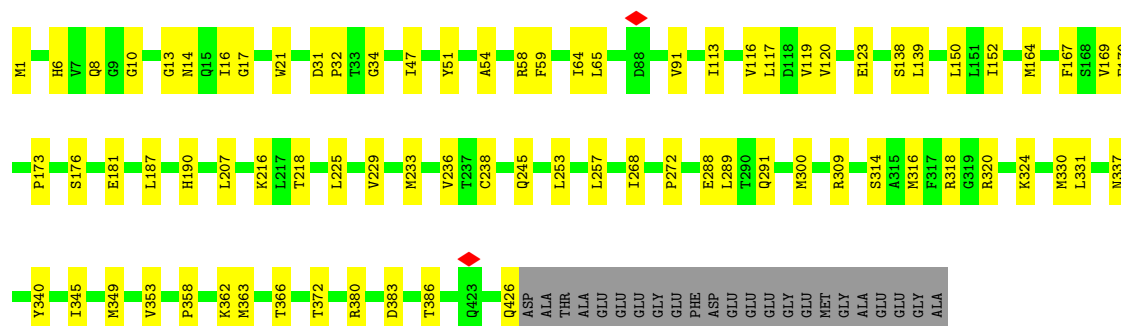


• Molecule 4: Tubulin beta chain



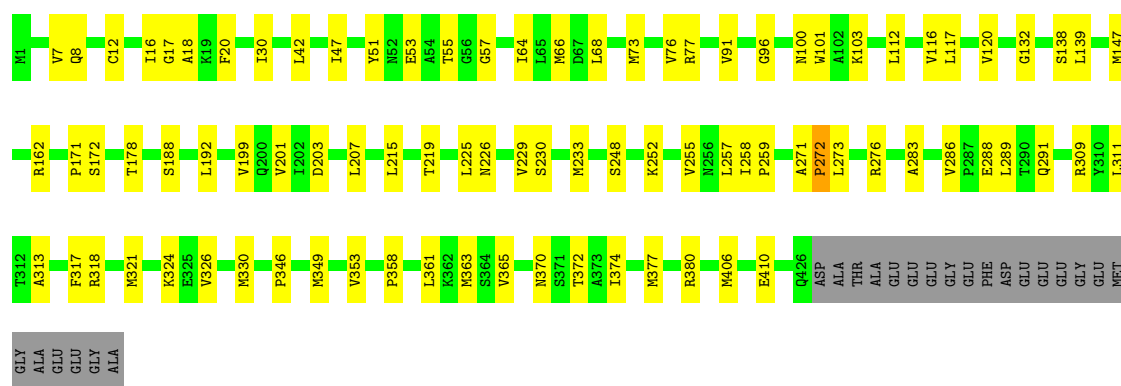
• Molecule 4: Tubulin beta chain





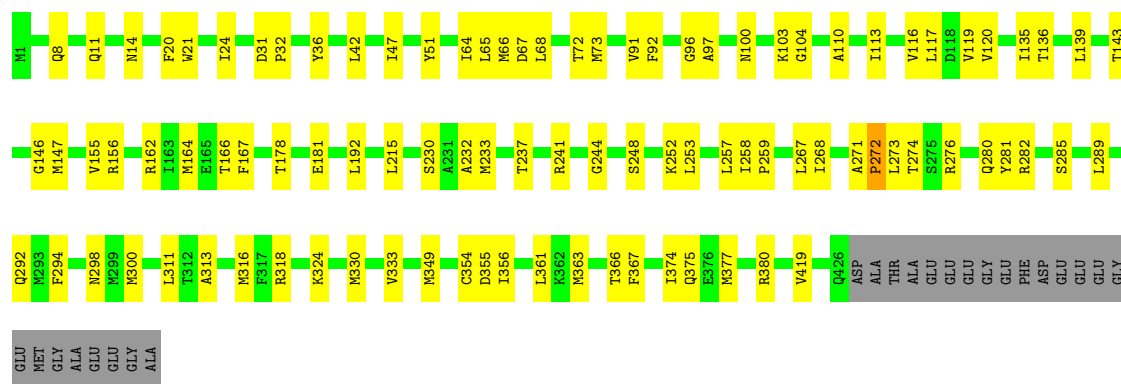
- Molecule 4: Tubulin beta chain

Chain A5: 75% 19% 5%



- Molecule 4: Tubulin beta chain

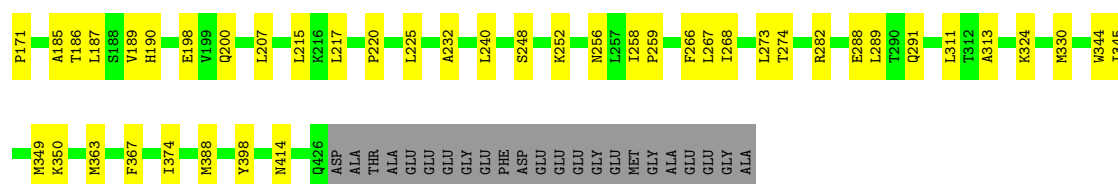
Chain A7: 73% 21% 5%



- Molecule 4: Tubulin beta chain

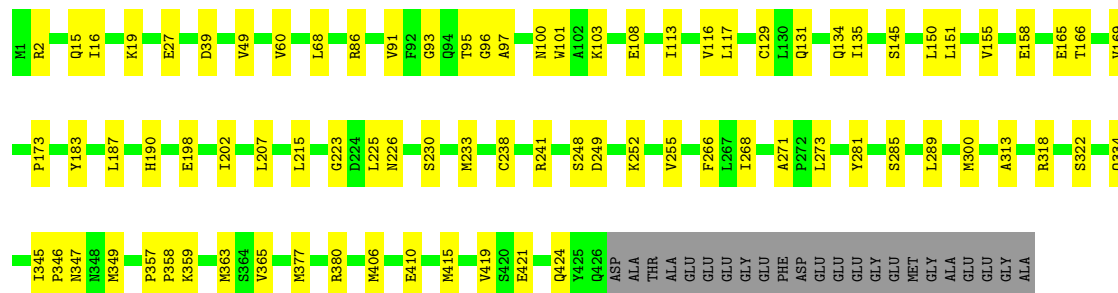
Chain A9: 78% 17% 5%





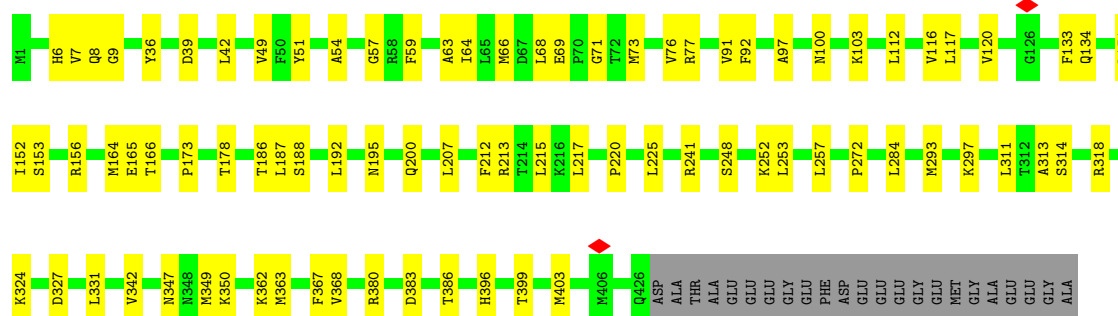
- Molecule 4: Tubulin beta chain

Chain B1: 77% 18% 5%



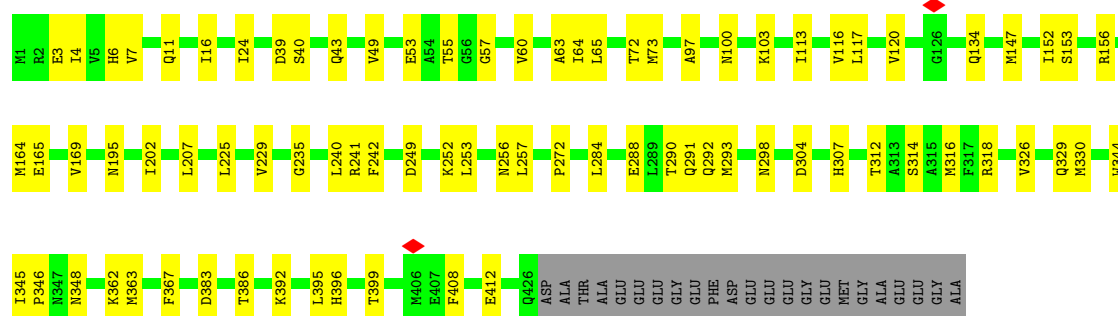
- Molecule 4: Tubulin beta chain

Chain B3: 76% 19% 5%



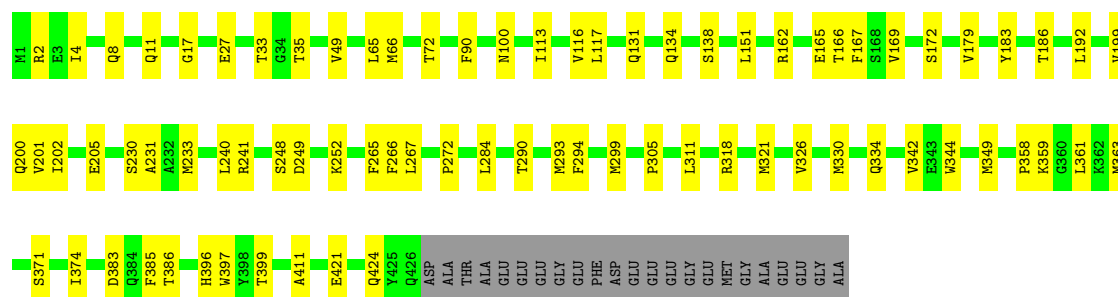
- Molecule 4: Tubulin beta chain

Chain B5: 77% 18% 5%



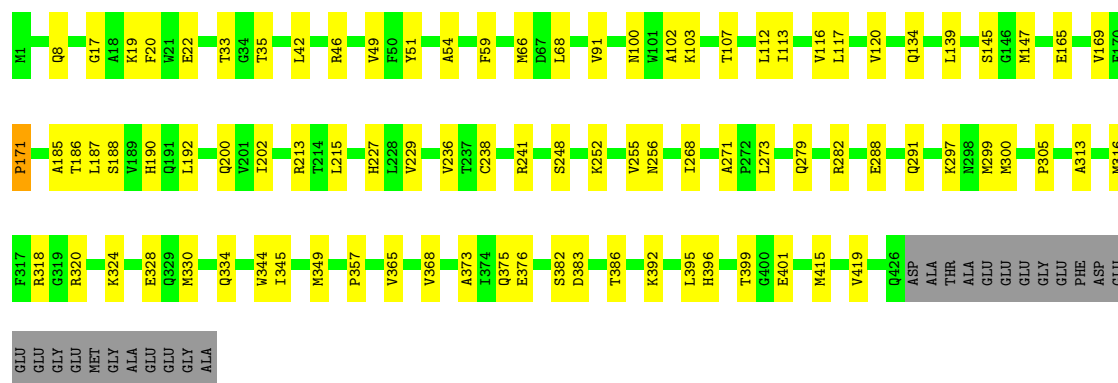
- Molecule 4: Tubulin beta chain

Chain B7:  78% 17% 5%



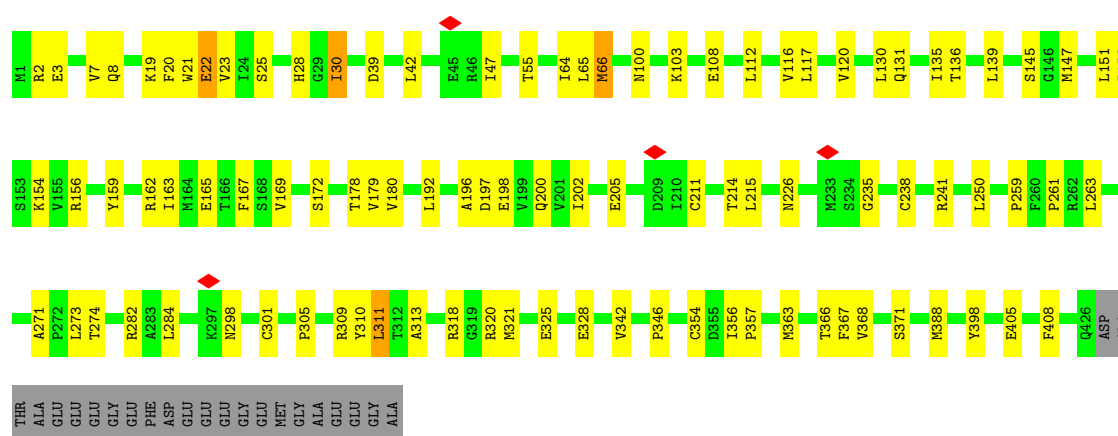
• Molecule 4: Tubulin beta chain

Chain B9:  75% 20% 5%



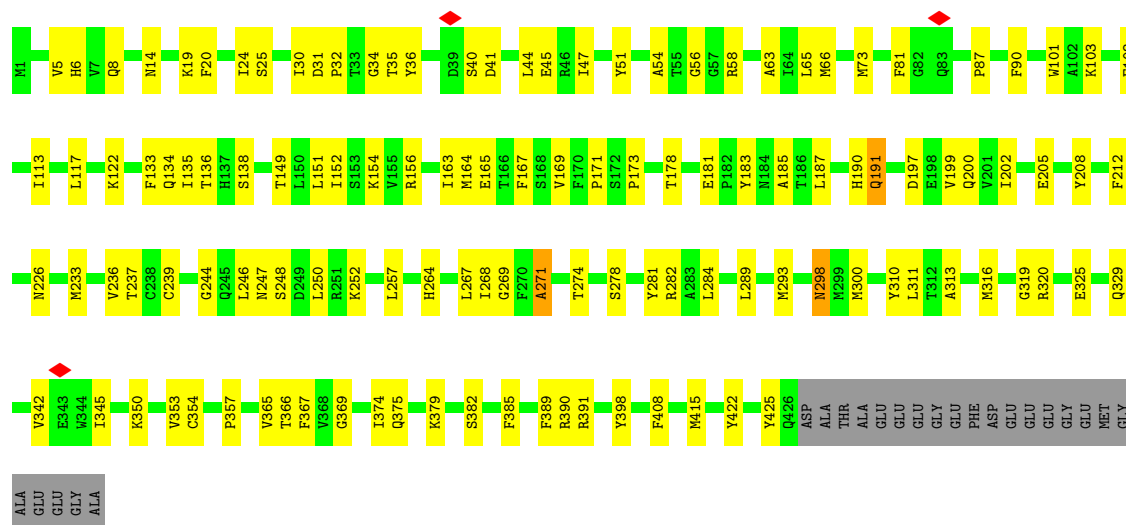
• Molecule 4: Tubulin beta chain

Chain C1:  73% 21% 5%

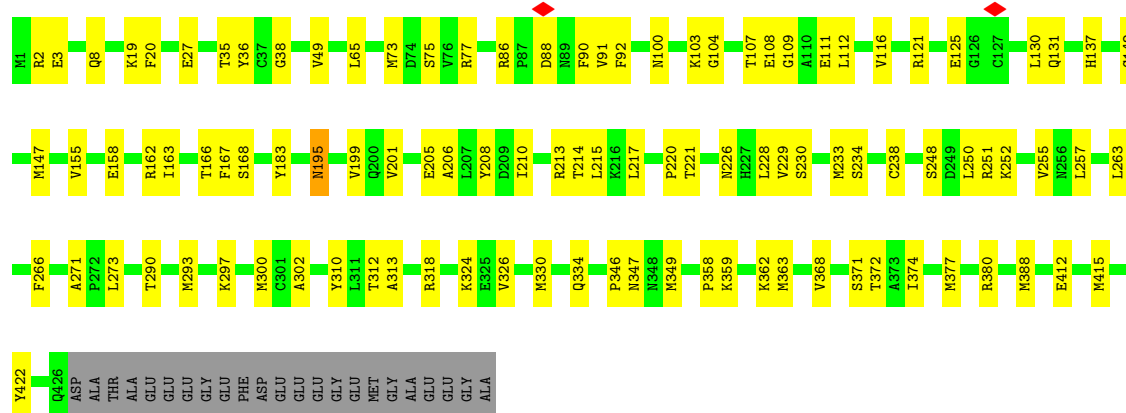


• Molecule 4: Tubulin beta chain

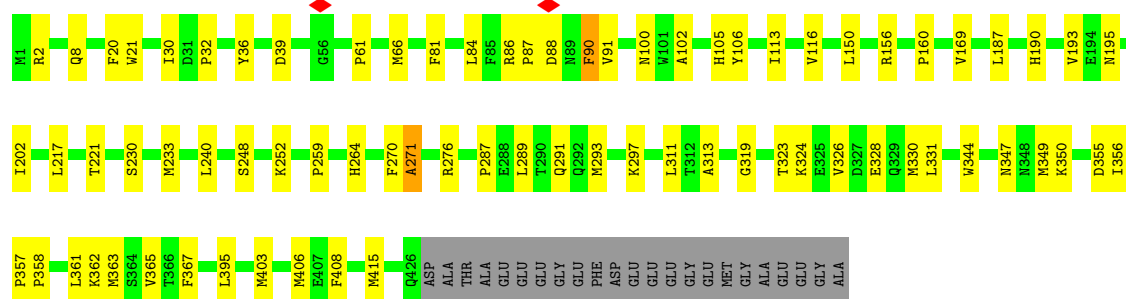
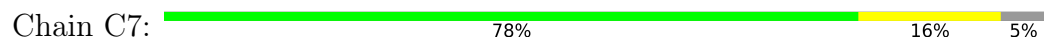
Chain C3:  67% 27% 5%



- Molecule 4: Tubulin beta chain

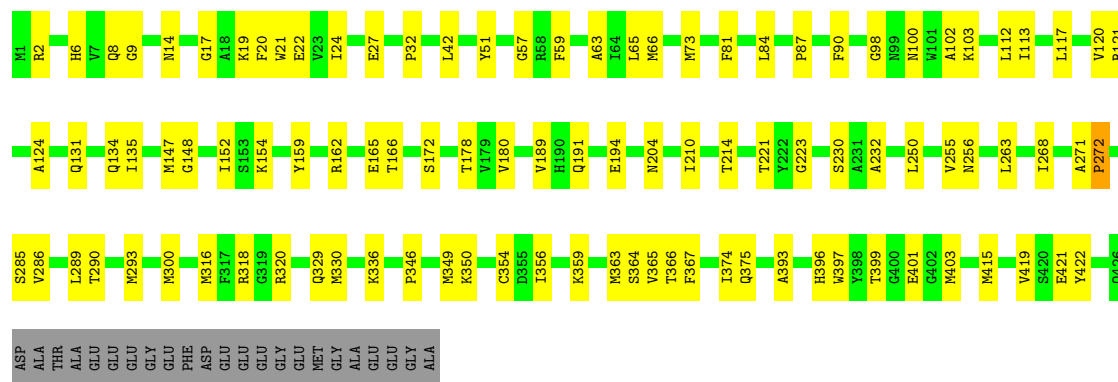


- Molecule 4: Tubulin beta chain

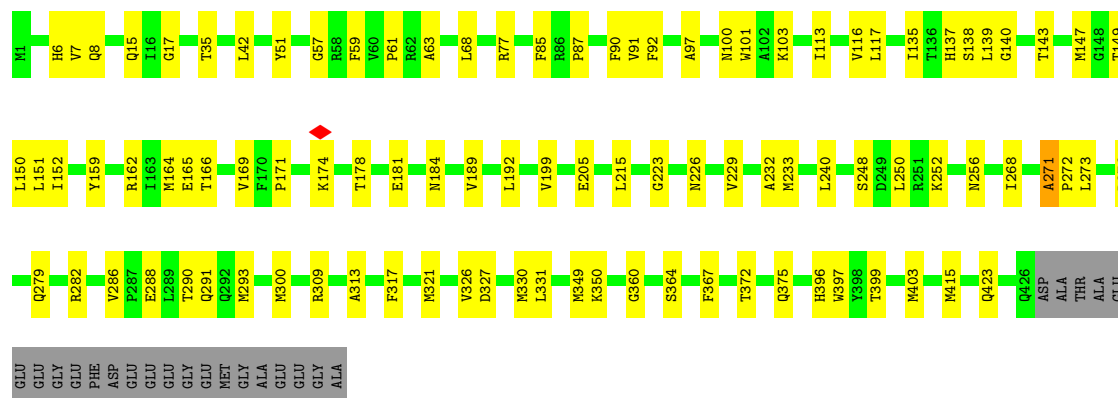


- Molecule 4: Tubulin beta chain

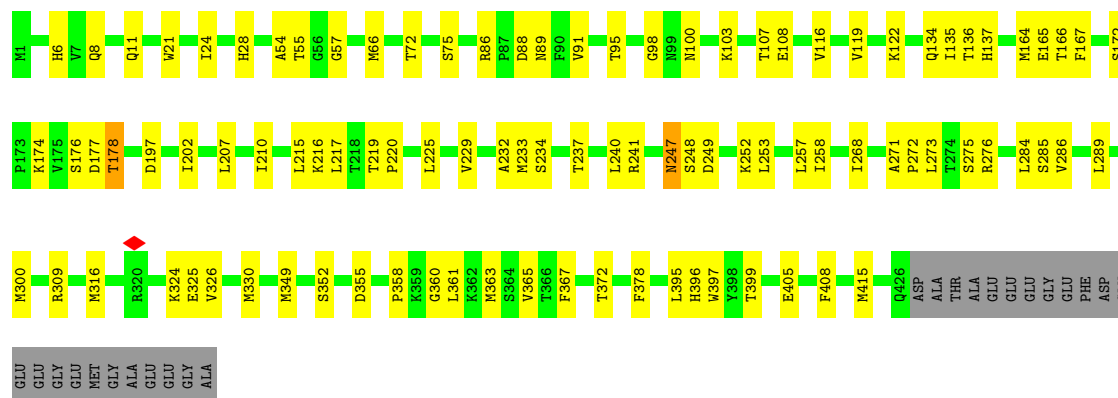
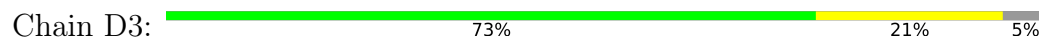




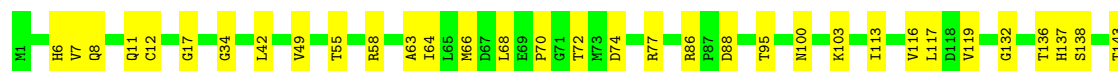
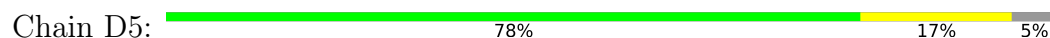
- Molecule 4: Tubulin beta chain



- Molecule 4: Tubulin beta chain

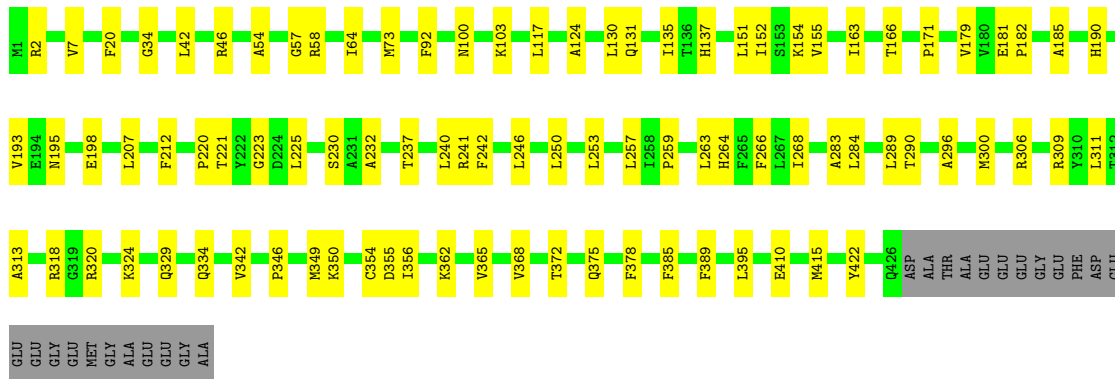


- Molecule 4: Tubulin beta chain

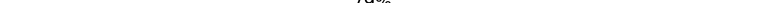


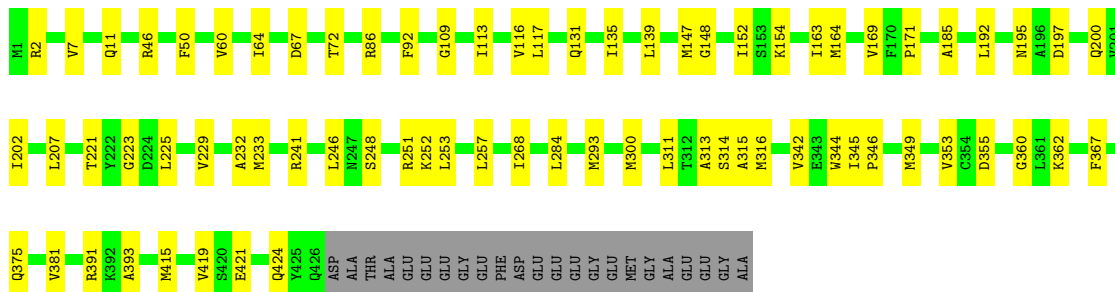
- Molecule 4: Tubulin beta chain

Chain D7: 75% 20% 5%



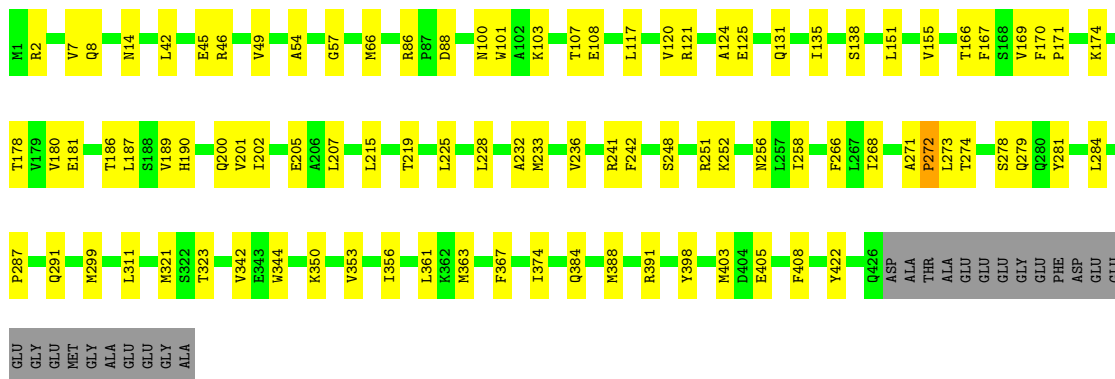
- Molecule 4: Tubulin beta chain

Chain D9:  79% 16% 5%

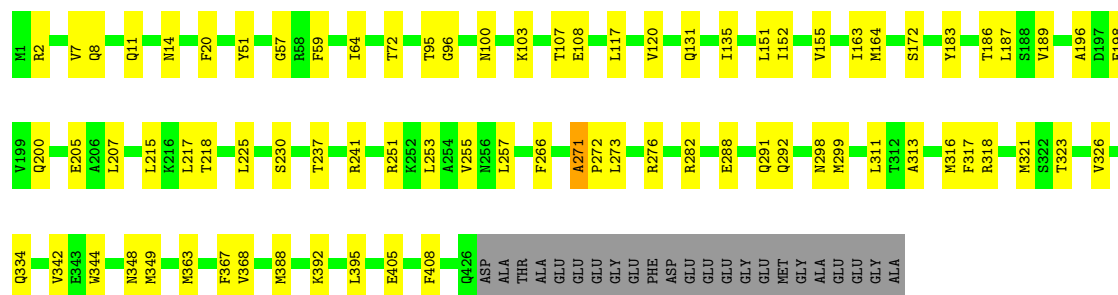


- Molecule 4: Tubulin beta chain

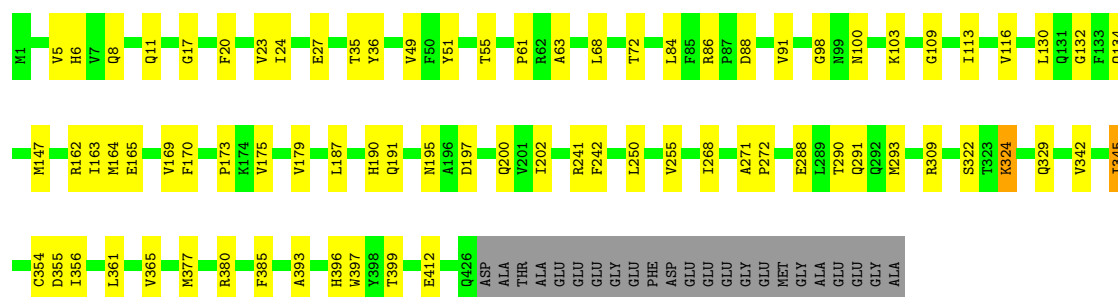
Chain E1: 74% 20% 5%



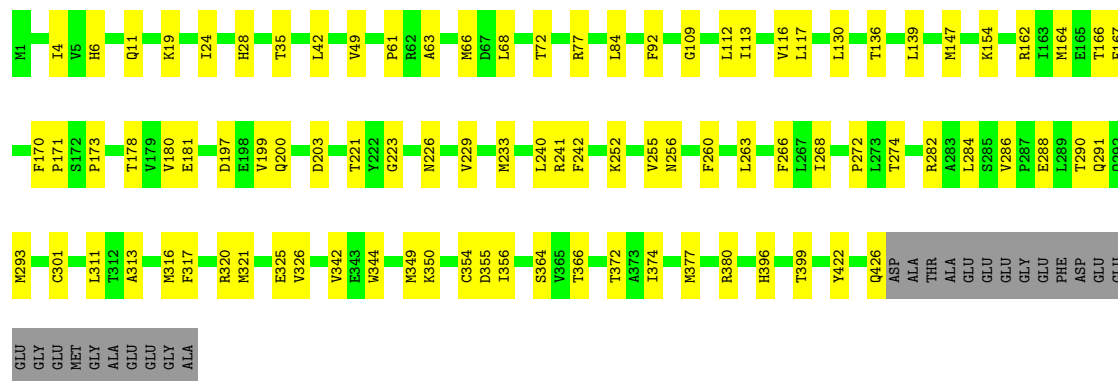
• Molecule 4: Tubulin beta chain

Chain E3: 

• Molecule 4: Tubulin beta chain

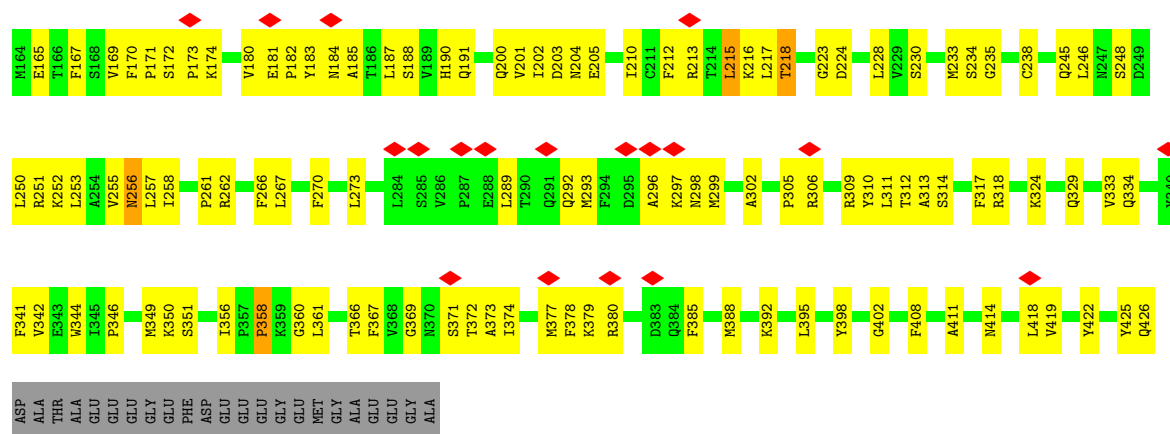
Chain E5: 

• Molecule 4: Tubulin beta chain

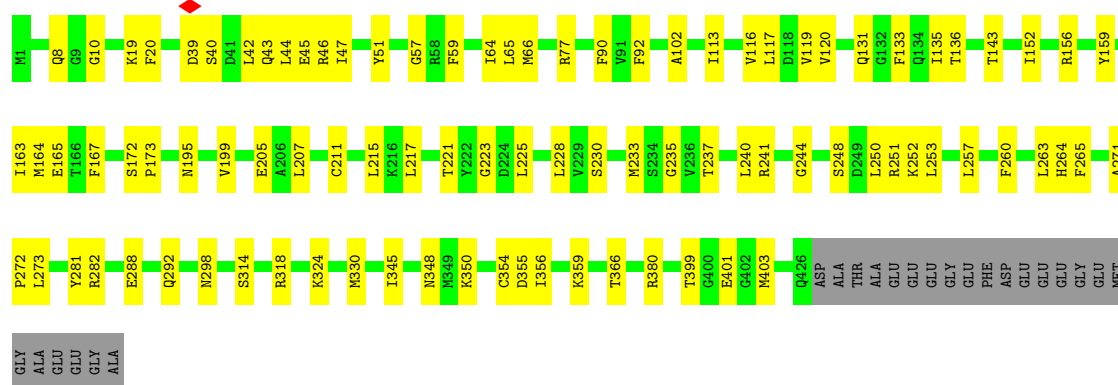
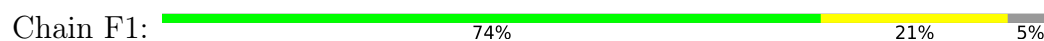
Chain E7: 

• Molecule 4: Tubulin beta chain

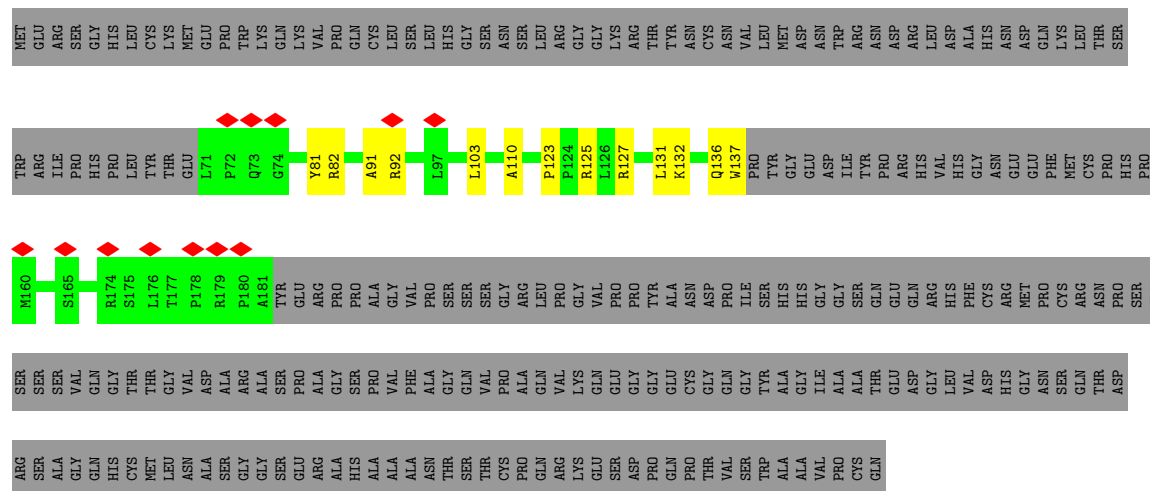
Chain E9: 



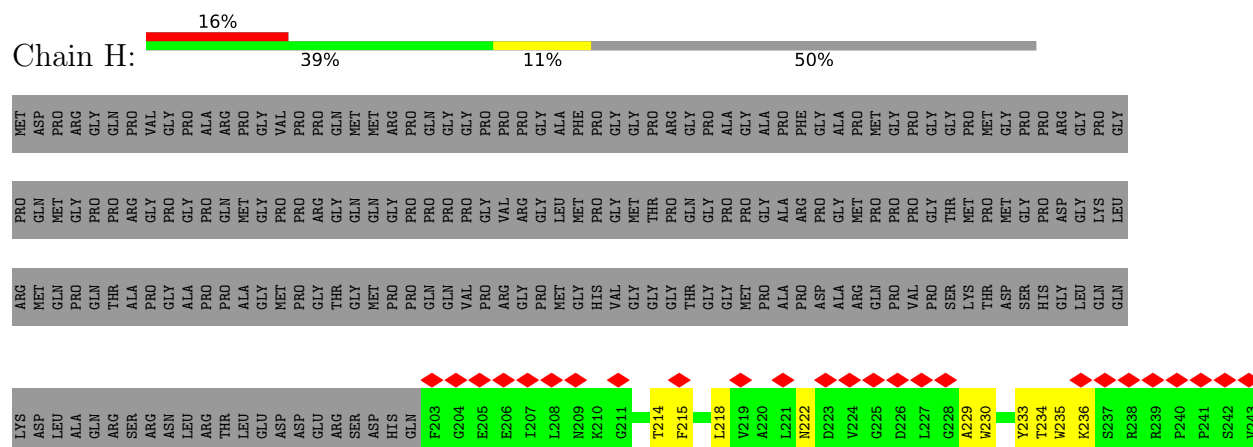
- Molecule 4: Tubulin beta chain

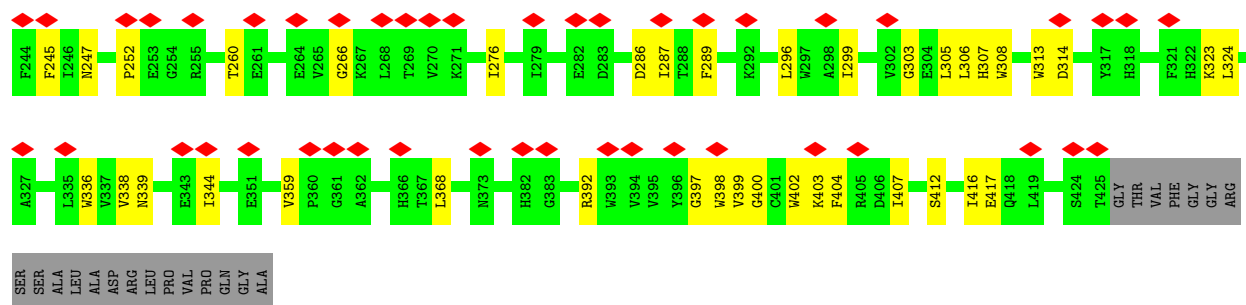


- Molecule 5: TLAP4 (thioredoxin-like associated protein), TGME49_201760

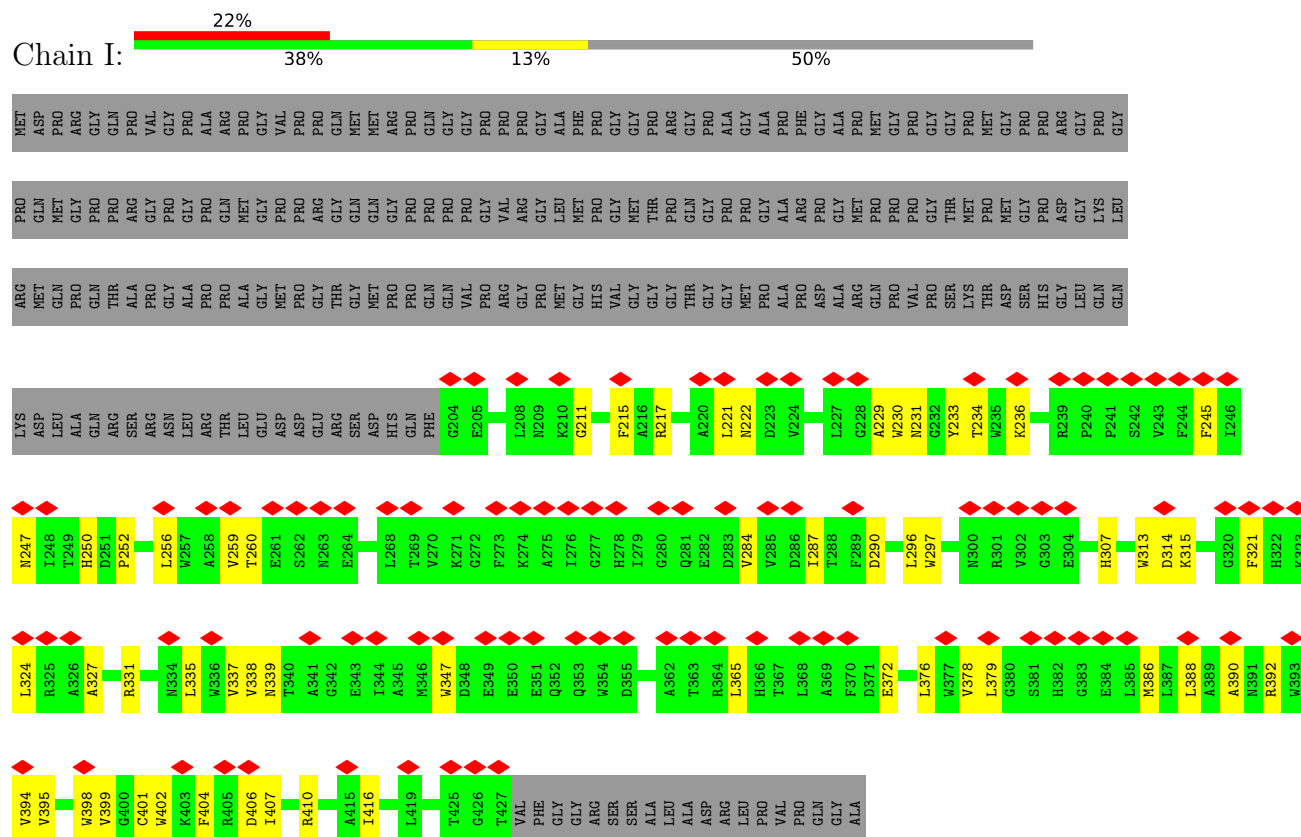


- Molecule 5: TLAP4 (thioredoxin-like associated protein), TGME49_201760

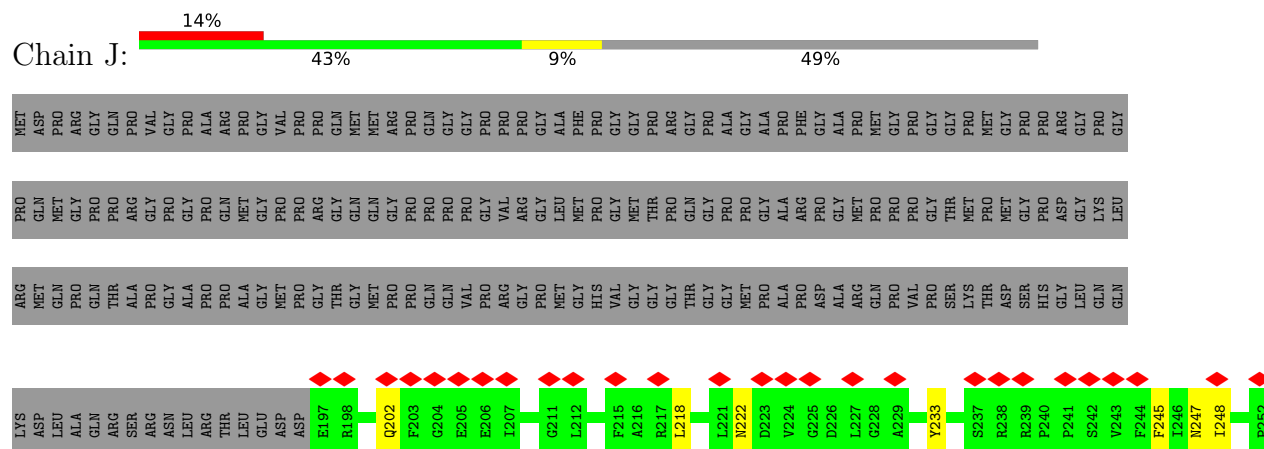


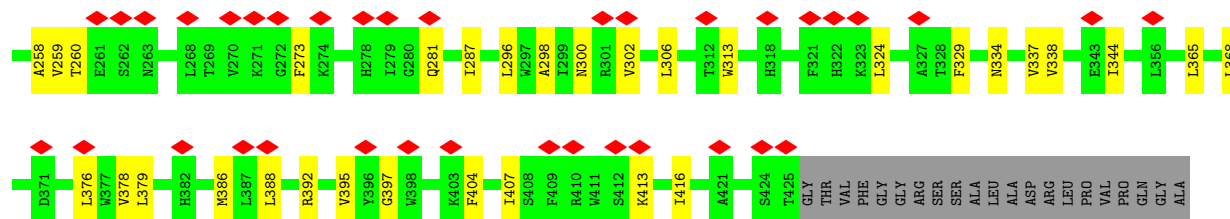


- Molecule 6: TLAP2 (thioredoxin-like associated protein), TGME49_232130

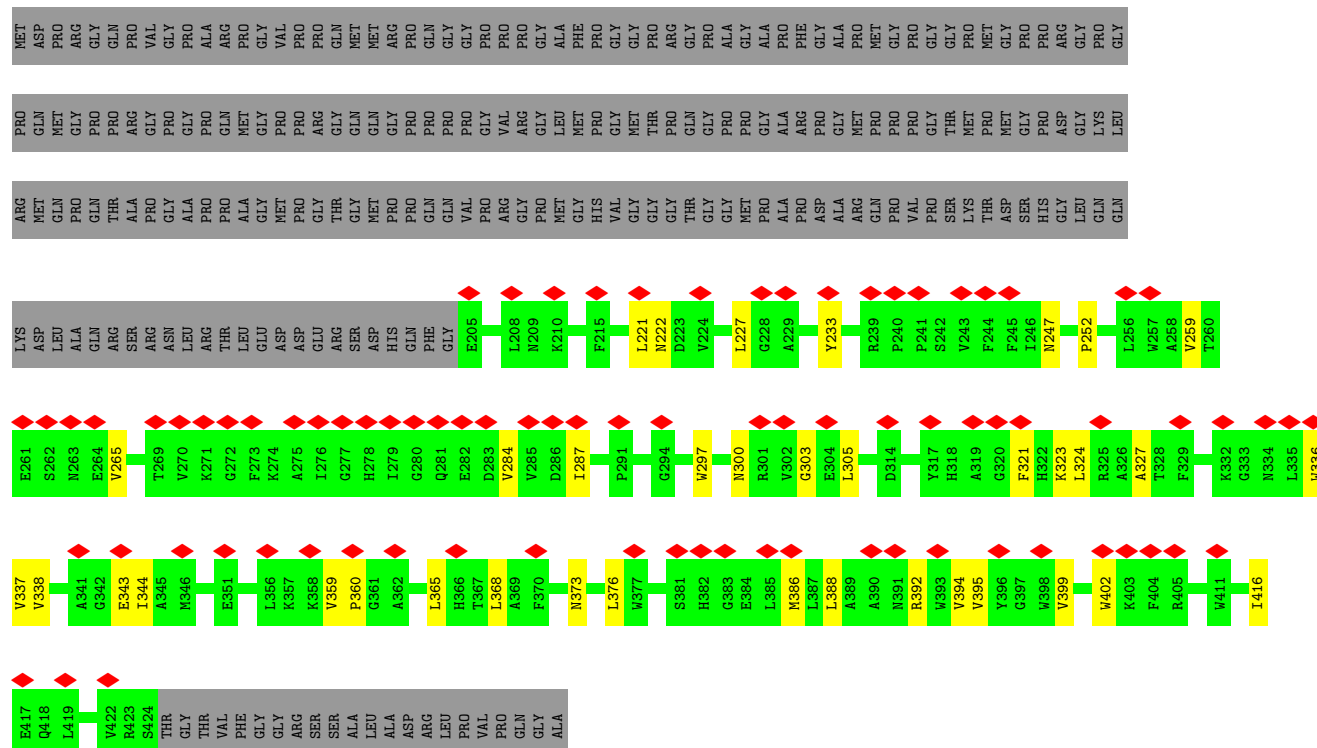
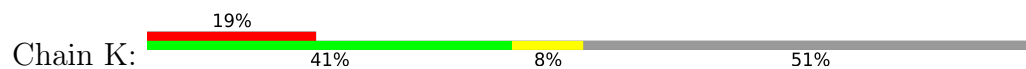


- Molecule 6: TLAP2 (thioredoxin-like associated protein), TGME49_232130

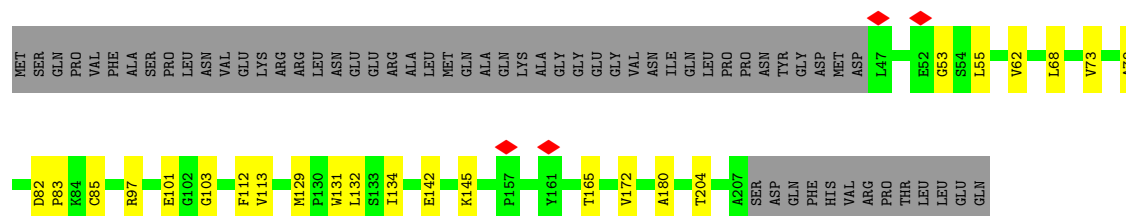




• Molecule 6: TLAP2 (thioredoxin-like associated protein), TGME49_232130

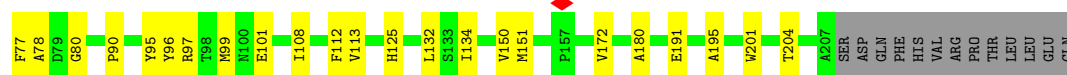
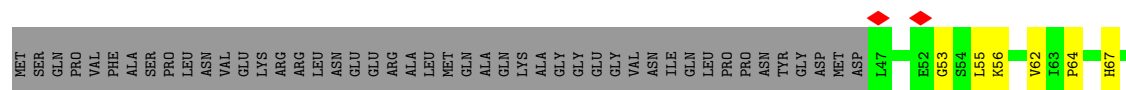


• Molecule 7: TRXL1, TGME49_232410



• Molecule 7: TRXL1, TGME49_232410





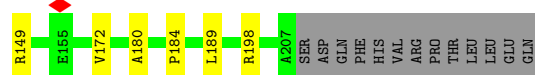
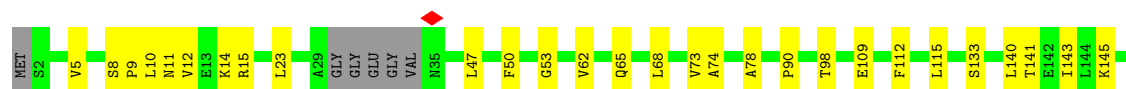
• Molecule 7: TRXL1, TGME49_232410

Chain c: 76% 15% 9%



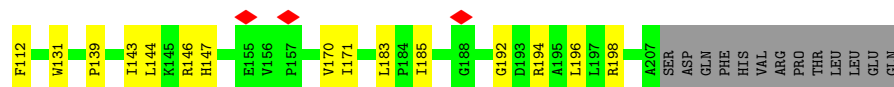
• Molecule 7: TRXL1, TGME49_232410

Chain d: 76% 15% 9%



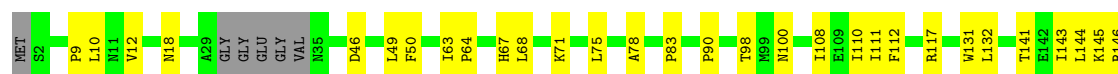
• Molecule 7: TRXL1, TGME49_232410

Chain e: 71% 20% 9%

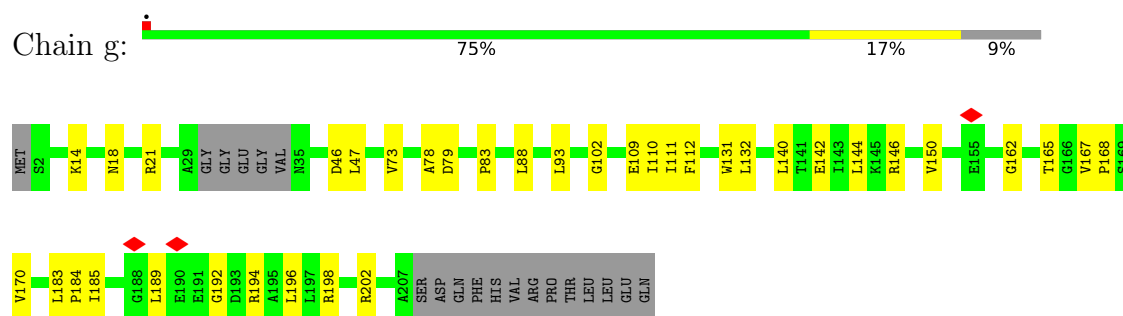


• Molecule 7: TRXL1, TGME49_232410

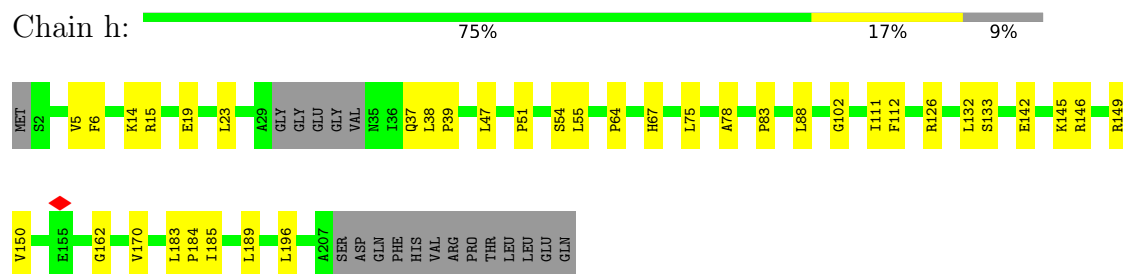
Chain f: 72% 20% 9%



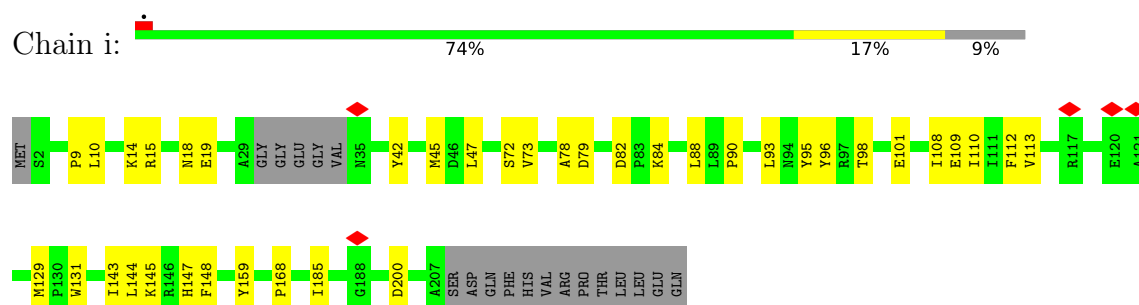
- Molecule 7: TRXL1, TGME49_232410



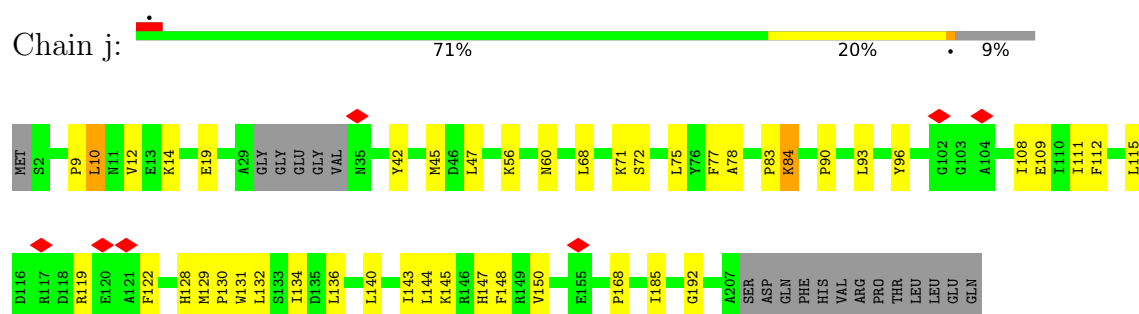
- Molecule 7: TRXL1, TGME49_232410



- Molecule 7: TRXL1, TGME49_232410

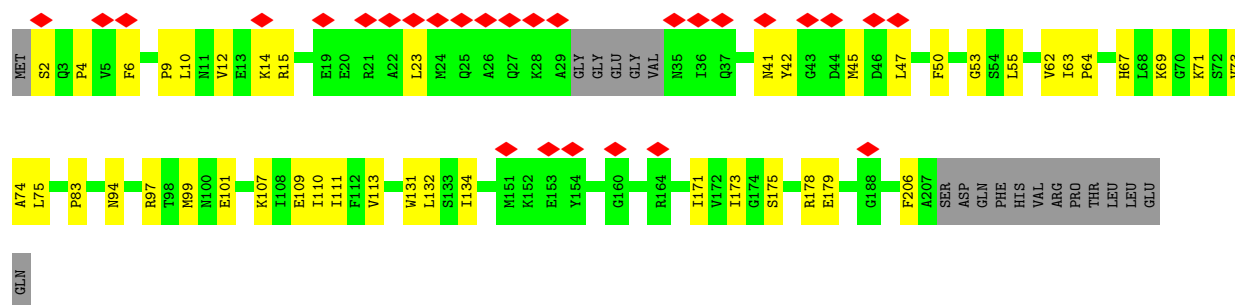


- Molecule 7: TRXL1, TGME49_232410

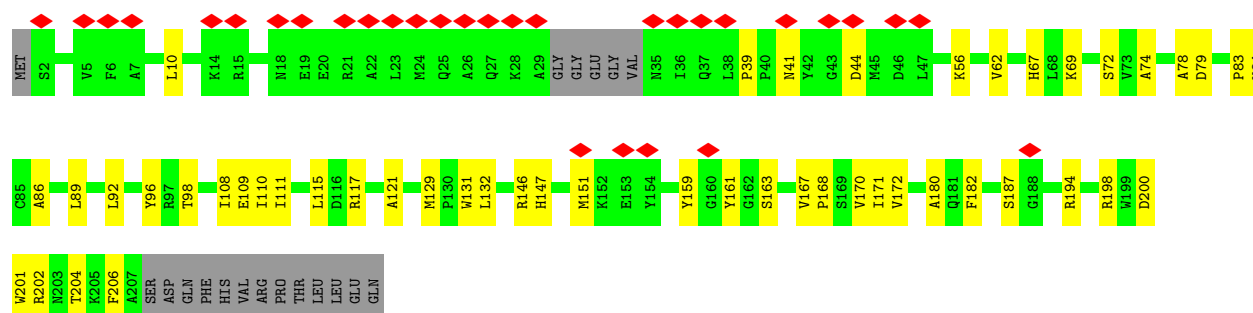


- Molecule 7: TRXL1, TGME49_232410

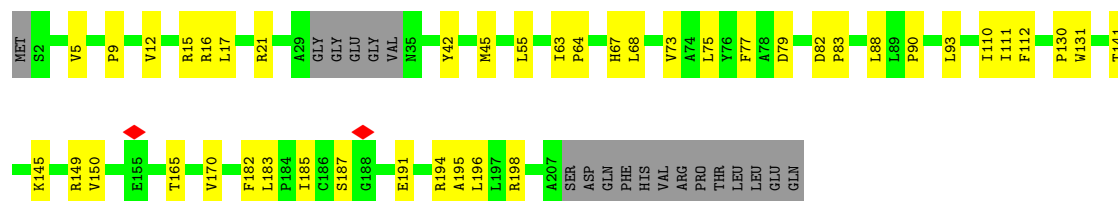




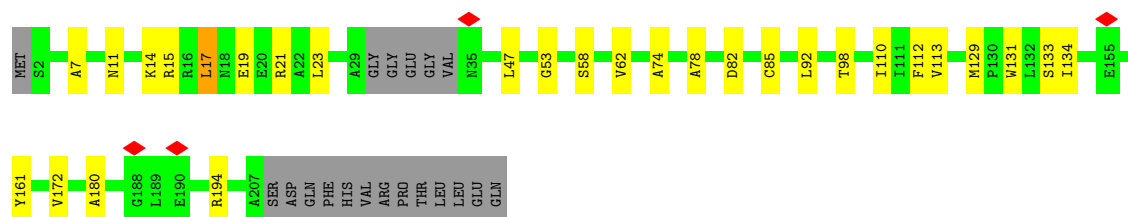
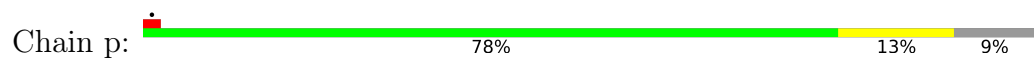
- Molecule 7: TRXL1, TGME49_232410



- Molecule 7: TRXL1, TGME49_232410

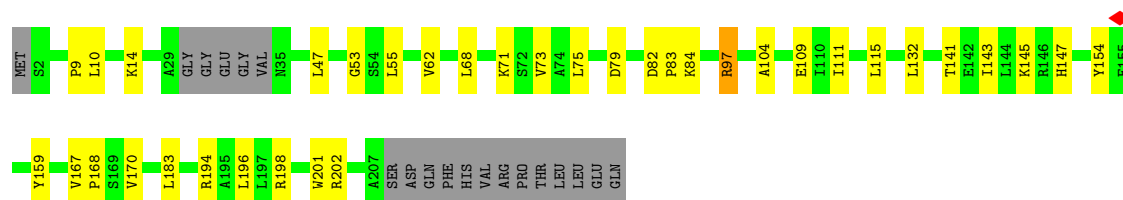


- Molecule 7: TRXL1, TGME49_232410

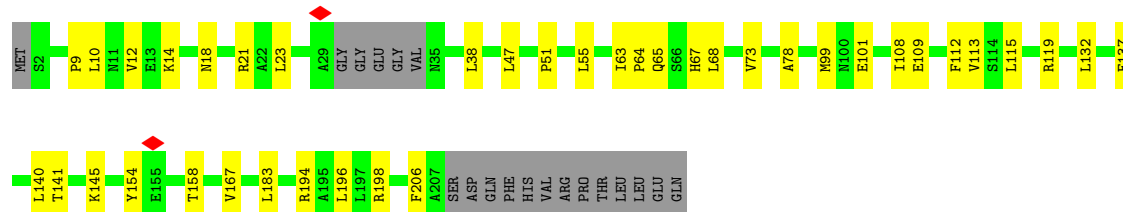


- Molecule 7: TRXL1, TGME49_232410

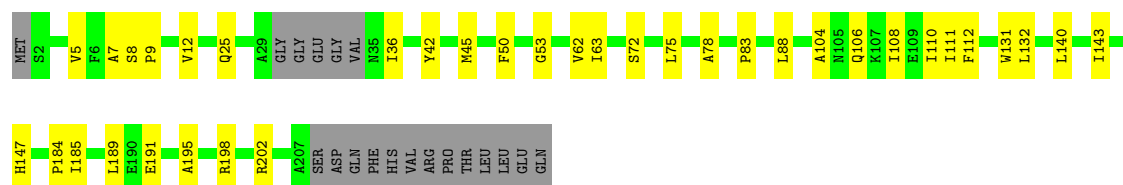




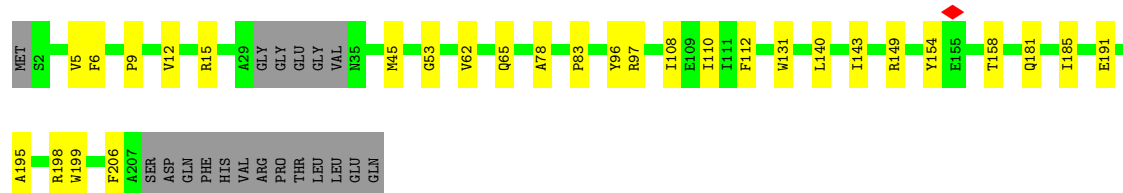
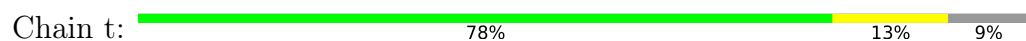
• Molecule 7: TRXL1, TGME49_232410



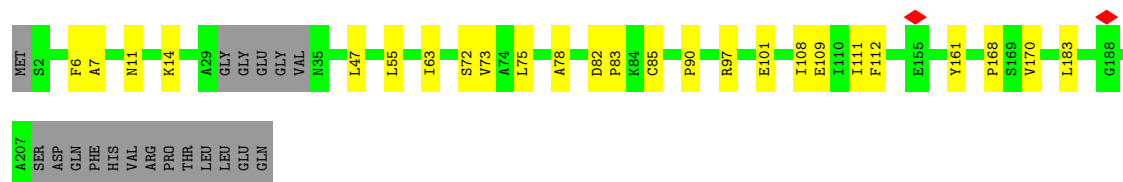
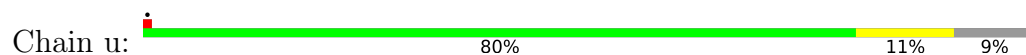
• Molecule 7: TRXL1, TGME49_232410



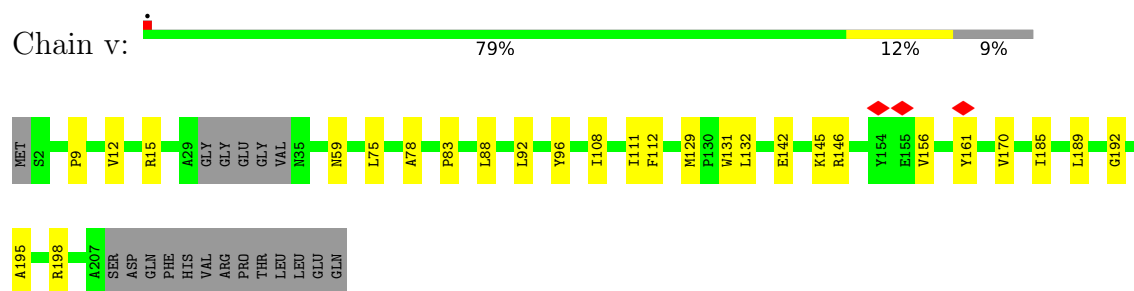
• Molecule 7: TRXL1, TGME49_232410



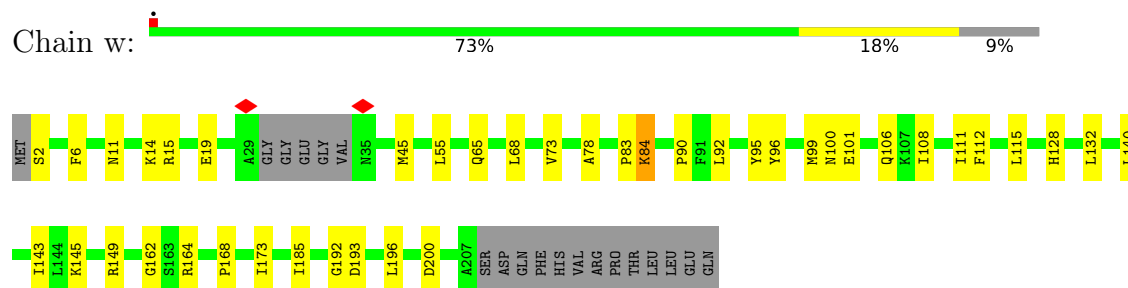
• Molecule 7: TRXL1, TGME49_232410



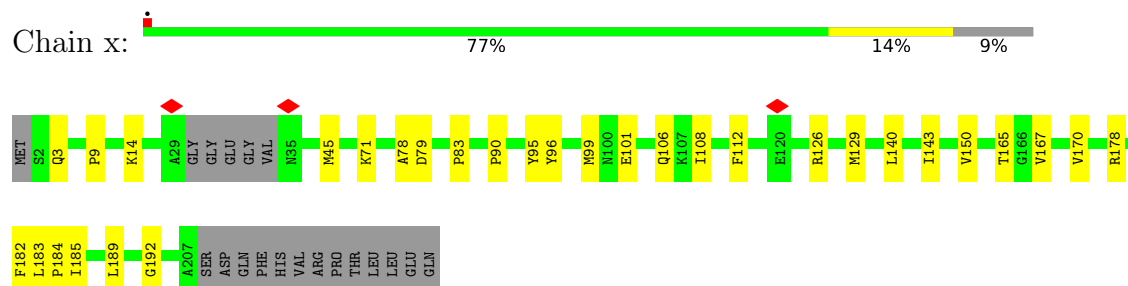
• Molecule 7: TRXL1, TGME49_232410



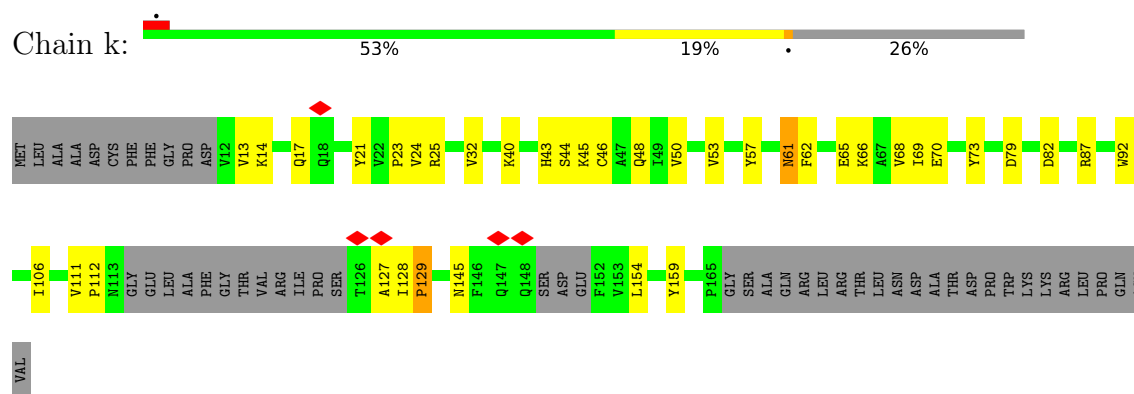
- Molecule 7: TRXL1, TGME49_232410



- Molecule 7: TRXL1, TGME49_232410

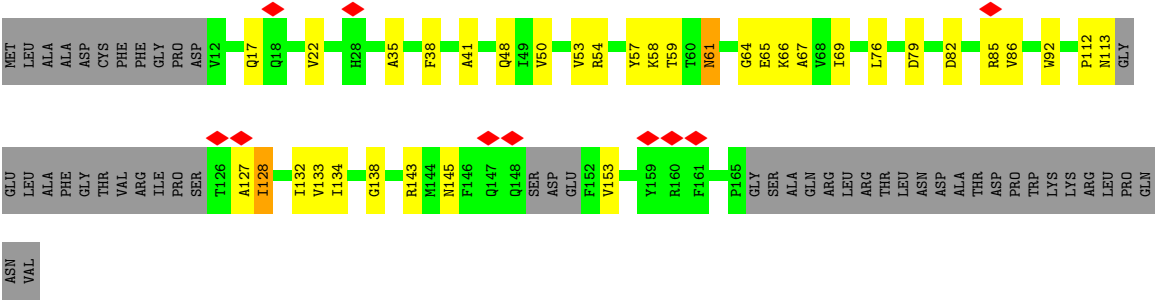


- Molecule 8: TRXL2, TGME49_225790



- 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	225207	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	2.187	Depositor
Minimum map value	0.000	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.05	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: MG, GDP, GTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.17	0/181	0.42	0/248
1	1	0.18	0/181	0.39	0/248
1	10	0.17	0/181	0.43	0/248
1	11	0.16	0/181	0.38	0/248
1	12	0.19	0/181	0.33	0/248
1	13	0.15	0/181	0.32	0/248
1	14	0.19	0/181	0.46	0/248
1	15	0.18	0/181	0.45	0/248
1	16	0.19	0/181	0.42	0/248
1	17	0.21	0/181	0.45	0/248
1	18	0.21	0/181	0.55	0/248
1	19	0.24	0/181	0.67	0/248
1	2	0.19	0/181	0.39	0/248
1	22	0.20	0/166	0.44	0/227
1	23	0.17	0/166	0.36	0/227
1	3	0.18	0/181	0.37	0/248
1	4	0.20	0/181	0.45	0/248
1	5	0.16	0/181	0.44	0/248
1	6	0.17	0/181	0.33	0/248
1	7	0.14	0/181	0.27	0/248
1	8	0.27	0/181	0.95	2/248 (0.8%)
1	9	0.23	0/181	0.79	0/248
2	A	0.26	0/1359	0.73	0/1837
2	B	0.27	0/1776	0.71	0/2403
2	C	0.30	0/392	0.75	0/529
3	A0	0.27	0/3398	0.63	1/4606 (0.0%)
3	A2	0.27	0/3398	0.68	2/4606 (0.0%)
3	A4	0.28	0/3398	0.61	1/4606 (0.0%)
3	A6	0.26	0/3398	0.61	0/4606
3	A8	0.25	0/3398	0.56	0/4606
3	B0	0.25	0/3398	0.59	0/4606
3	B2	0.25	0/3398	0.54	0/4606

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	B4	0.24	0/3398	0.53	0/4606
3	B6	0.23	0/3398	0.53	0/4606
3	B8	0.24	0/3398	0.53	0/4606
3	C0	0.29	0/3398	0.75	3/4606 (0.1%)
3	C2	0.31	0/3398	0.71	3/4606 (0.1%)
3	C4	0.25	0/3398	0.64	3/4606 (0.1%)
3	C6	0.29	0/3398	0.68	2/4606 (0.0%)
3	C8	0.27	0/3398	0.70	1/4606 (0.0%)
3	D0	0.26	0/3398	0.61	1/4606 (0.0%)
3	D2	0.25	0/3398	0.63	3/4606 (0.1%)
3	D4	0.27	0/3398	0.60	0/4606
3	D6	0.24	0/3398	0.57	0/4606
3	D8	0.25	0/3398	0.56	1/4606 (0.0%)
3	E0	0.28	1/3398 (0.0%)	0.63	3/4606 (0.1%)
3	E2	0.28	0/3398	0.59	0/4606
3	E4	0.26	0/3398	0.67	3/4606 (0.1%)
3	E6	0.27	0/3398	0.68	3/4606 (0.1%)
3	E8	0.28	0/3392	0.70	2/4599 (0.0%)
3	F0	0.32	0/3398	0.74	3/4606 (0.1%)
4	A1	0.26	0/3404	0.64	2/4606 (0.0%)
4	A3	0.24	0/3404	0.57	1/4606 (0.0%)
4	A5	0.29	0/3404	0.63	0/4606
4	A7	0.27	0/3404	0.61	0/4606
4	A9	0.27	0/3404	0.57	0/4606
4	B1	0.25	0/3404	0.60	0/4606
4	B3	0.26	0/3404	0.56	2/4606 (0.0%)
4	B5	0.24	0/3404	0.58	0/4606
4	B7	0.25	0/3404	0.57	0/4606
4	B9	0.25	0/3404	0.67	4/4606 (0.1%)
4	C1	0.27	0/3404	0.69	3/4606 (0.1%)
4	C3	0.27	0/3404	0.64	0/4606
4	C5	0.28	0/3404	0.66	0/4606
4	C7	0.29	0/3404	0.72	4/4606 (0.1%)
4	C9	0.26	0/3404	0.63	1/4606 (0.0%)
4	D1	0.27	0/3404	0.61	0/4606
4	D3	0.26	0/3404	0.65	3/4606 (0.1%)
4	D5	0.26	0/3404	0.61	0/4606
4	D7	0.25	0/3404	0.59	0/4606
4	D9	0.26	0/3404	0.55	1/4606 (0.0%)
4	E1	0.29	0/3404	0.68	0/4606
4	E3	0.27	0/3404	0.62	0/4606
4	E5	0.29	0/3404	0.68	4/4606 (0.1%)
4	E7	0.27	0/3404	0.58	2/4606 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	E9	0.35	0/3404	0.92	7/4606 (0.2%)
4	F1	0.29	0/3404	0.69	1/4606 (0.0%)
5	E	0.26	0/761	0.58	0/1031
5	F	0.24	0/761	0.58	0/1031
5	G	0.25	0/575	0.59	0/780
6	H	0.22	0/1871	0.61	2/2541 (0.1%)
6	I	0.23	0/1870	0.56	0/2540
6	J	0.18	0/1925	0.47	0/2613
6	K	0.19	0/1848	0.50	0/2510
7	a	0.25	0/1321	0.61	0/1788
7	b	0.29	0/1321	0.66	1/1788 (0.1%)
7	c	0.25	0/1645	0.60	0/2225
7	d	0.23	0/1645	0.53	0/2225
7	e	0.24	0/1645	0.51	2/2225 (0.1%)
7	f	0.25	0/1645	0.54	0/2225
7	g	0.21	0/1645	0.49	0/2225
7	h	0.22	0/1645	0.54	0/2225
7	i	0.24	0/1645	0.55	0/2225
7	j	0.24	0/1645	0.64	4/2225 (0.2%)
7	m	0.25	0/1645	0.60	0/2225
7	n	0.25	0/1645	0.59	0/2225
7	o	0.24	0/1645	0.57	0/2225
7	p	0.23	0/1645	0.55	3/2225 (0.1%)
7	q	0.26	0/1645	0.61	0/2225
7	r	0.23	0/1645	0.49	0/2225
7	s	0.21	0/1645	0.48	0/2225
7	t	0.23	0/1645	0.51	0/2225
7	u	0.21	0/1645	0.48	0/2225
7	v	0.24	0/1645	0.54	0/2225
7	w	0.27	0/1645	0.79	3/2225 (0.1%)
7	x	0.22	0/1645	0.55	0/2225
8	k	0.27	0/1168	0.72	2/1578 (0.1%)
8	l	0.27	0/1168	0.71	0/1578
All	All	0.26	1/231814 (0.0%)	0.62	89/313966 (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
2	A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
3	A0	0	1
3	A6	0	1
3	B2	0	1
3	B6	0	1
3	C0	0	2
3	C2	0	1
3	C6	0	1
3	C8	0	1
3	D0	0	2
3	D2	0	2
3	D4	0	1
3	D6	0	1
3	D8	0	1
3	E4	0	2
3	E6	0	3
3	E8	0	1
3	F0	0	3
4	A5	0	2
4	A7	0	1
4	C1	0	3
4	C3	0	2
4	C5	0	1
4	C7	0	2
4	C9	0	1
4	D1	0	3
4	D3	0	2
4	D5	0	1
4	D9	0	1
4	E1	0	1
4	E3	0	1
4	E5	0	1
4	E9	0	2
4	F1	0	2
7	q	0	1
8	k	0	1
8	l	0	1
All	All	0	56

All (1) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E0	173	PRO	C-N	-7.07	1.23	1.33

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B9	171	PRO	CA-C-N	14.91	149.28	120.94
4	B9	171	PRO	C-N-CA	14.91	149.28	120.94
7	w	128	HIS	CA-C-N	14.51	142.73	120.68
7	w	128	HIS	C-N-CA	14.51	142.73	120.68
3	E0	173	PRO	CA-C-N	8.85	134.13	120.68
3	E0	173	PRO	C-N-CA	8.85	134.13	120.68
3	A0	405	VAL	N-CA-C	-7.86	106.25	113.71
3	E6	243	ARG	CA-C-N	-7.55	113.46	122.44
3	E6	243	ARG	C-N-CA	-7.55	113.46	122.44
3	E4	182	VAL	N-CA-C	-7.47	105.44	112.83
4	A1	318	ARG	CA-C-N	7.41	131.47	121.83
4	A1	318	ARG	C-N-CA	7.41	131.47	121.83
4	F1	330	MET	CB-CG-SD	7.19	134.26	112.70
3	A2	182	VAL	N-CA-C	-6.93	105.97	112.83
3	E8	35	GLN	CA-C-N	6.92	130.01	120.39
3	E8	35	GLN	C-N-CA	6.92	130.01	120.39
3	C6	221	ARG	CB-CG-CD	6.68	126.66	111.30
1	8	255	PRO	CA-C-N	6.67	130.82	120.68
1	8	255	PRO	C-N-CA	6.67	130.82	120.68
4	A3	216	LYS	CA-CB-CG	6.52	127.14	114.10
7	w	84	LYS	CA-CB-CG	6.39	126.89	114.10
8	k	145	ASN	CA-C-N	6.31	129.60	120.38
8	k	145	ASN	C-N-CA	6.31	129.60	120.38
3	C8	405	VAL	N-CA-C	-6.29	107.73	113.71
3	A2	141	VAL	N-CA-C	-6.25	107.20	113.20
3	C4	111	GLY	N-CA-C	-6.01	106.80	114.37
7	j	128	HIS	CA-C-N	5.99	132.33	120.94
7	j	128	HIS	C-N-CA	5.99	132.33	120.94
4	C1	30	ILE	CA-C-N	5.95	128.67	120.39
4	C1	30	ILE	C-N-CA	5.95	128.67	120.39
3	F0	257	THR	CA-C-N	5.88	128.62	120.63
3	F0	257	THR	C-N-CA	5.88	128.62	120.63
7	p	17	LEU	CA-CB-CG	5.76	136.47	116.30
6	H	417	GLU	N-CA-CB	5.74	119.76	110.40
3	D8	265	ILE	N-CA-C	-5.71	106.83	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	p	58	SER	CA-C-N	5.68	136.20	126.32
7	p	58	SER	C-N-CA	5.68	136.20	126.32
7	b	151	MET	CA-CB-CG	-5.65	102.81	114.10
3	C0	91	GLN	N-CA-C	-5.62	106.24	114.39
3	D0	181	VAL	N-CA-C	-5.62	107.34	112.96
3	E6	141	VAL	N-CA-C	-5.57	106.91	113.42
4	C7	297	LYS	CA-CB-CG	5.51	125.13	114.10
4	E7	354	CYS	CA-C-N	5.51	132.07	121.54
4	E7	354	CYS	C-N-CA	5.51	132.07	121.54
3	E4	219	ILE	CA-C-N	5.50	132.05	121.54
3	E4	219	ILE	C-N-CA	5.50	132.05	121.54
3	F0	260	VAL	CA-CB-CG2	5.47	119.70	110.40
4	C7	90	PHE	CA-C-N	-5.42	114.31	122.01
4	C7	90	PHE	C-N-CA	-5.42	114.31	122.01
4	E5	345	ILE	CB-CA-C	5.40	115.61	110.16
3	C0	199	ASP	CA-C-N	5.38	127.91	120.49
3	C0	199	ASP	C-N-CA	5.38	127.91	120.49
4	D9	355	ASP	CB-CA-C	-5.36	109.42	115.79
4	E5	354	CYS	CA-C-N	5.35	131.77	121.54
4	E5	354	CYS	C-N-CA	5.35	131.77	121.54
4	D3	54	ALA	CA-C-N	5.32	131.69	121.54
4	D3	54	ALA	C-N-CA	5.32	131.69	121.54
3	C6	221	ARG	CG-CD-NE	5.30	123.66	112.00
4	C9	19	LYS	N-CA-C	-5.30	107.83	114.56
3	C4	242	LEU	CA-C-N	5.29	131.65	121.54
3	C4	242	LEU	C-N-CA	5.29	131.65	121.54
4	E5	324	LYS	CD-CE-NZ	-5.28	95.01	111.90
3	E0	429	GLU	N-CA-CB	5.26	117.95	110.16
3	C2	402	ARG	CA-CB-CG	5.22	124.54	114.10
7	e	59	ASN	CA-C-N	5.22	131.50	121.54
7	e	59	ASN	C-N-CA	5.22	131.50	121.54
4	E9	218	THR	CA-C-N	-5.19	117.14	122.85
4	E9	218	THR	C-N-CA	-5.19	117.14	122.85
7	j	84	LYS	CA-CB-CG	5.17	124.44	114.10
3	A4	155	GLU	CA-CB-CG	5.17	124.44	114.10
4	B3	54	ALA	CA-C-N	5.17	130.67	122.61
4	B3	54	ALA	C-N-CA	5.17	130.67	122.61
4	E9	180	VAL	CB-CA-C	5.17	119.77	111.29
3	D2	432	TYR	CA-C-N	-5.16	112.57	121.66
3	D2	432	TYR	C-N-CA	-5.16	112.57	121.66
4	E9	373	ALA	CA-C-N	-5.15	115.87	122.26
4	E9	373	ALA	C-N-CA	-5.15	115.87	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D2	111	GLY	N-CA-C	-5.13	107.72	114.95
4	B9	54	ALA	CA-C-N	5.11	130.58	122.61
4	B9	54	ALA	C-N-CA	5.11	130.58	122.61
6	H	214	THR	N-CA-C	-5.08	107.03	113.43
3	C2	359	PRO	O-C-N	5.06	123.53	121.15
3	C2	429	GLU	N-CA-CB	5.04	117.62	110.16
4	D3	122	LYS	CA-CB-CG	5.04	124.17	114.10
7	j	10	LEU	CA-CB-CG	5.03	133.91	116.30
4	C7	271	ALA	N-CA-C	5.02	120.91	109.81
4	C1	22	GLU	N-CA-CB	5.01	117.63	110.67
4	E9	54	ALA	CA-C-N	5.01	130.42	122.61
4	E9	54	ALA	C-N-CA	5.01	130.42	122.61

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	276	SER	Peptide
3	A0	262	TYR	Peptide
4	A5	271	ALA	Peptide
4	A5	272	PRO	Peptide
3	A6	273	ALA	Peptide
4	A7	271	ALA	Peptide
2	B	276	SER	Peptide
3	B2	284	GLU	Peptide
3	B6	90	GLU	Peptide
3	C0	258	ASN	Peptide
3	C0	273	ALA	Peptide
4	C1	21	TRP	Peptide
4	C1	271	ALA	Peptide
4	C1	66	MET	Peptide
3	C2	109	THR	Peptide
4	C3	271	ALA	Peptide
4	C3	298	ASN	Peptide
4	C5	271	ALA	Peptide
3	C6	273	ALA	Peptide
4	C7	21	TRP	Peptide
4	C7	271	ALA	Peptide
3	C8	273	ALA	Peptide
4	C9	271	ALA	Peptide
3	D0	256	GLN	Peptide
3	D0	273	ALA	Peptide

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Mol	Chain	Res	Type	Group
4	D1	271	ALA	Peptide
4	D1	276	ARG	Sidechain
4	D1	282	ARG	Peptide
3	D2	390	ARG	Sidechain
3	D2	402	ARG	Sidechain
4	D3	107	THR	Peptide
4	D3	137	HIS	Peptide
3	D4	273	ALA	Peptide
4	D5	70	PRO	Peptide
3	D6	285	GLN	Peptide
3	D8	129	CYS	Peptide
4	D9	46	ARG	Sidechain
4	E1	271	ALA	Peptide
4	E3	271	ALA	Peptide
3	E4	273	ALA	Peptide
3	E4	390	ARG	Sidechain
4	E5	271	ALA	Peptide
3	E6	245	ASP	Peptide
3	E6	273	ALA	Peptide
3	E6	305	CYS	Peptide
3	E8	273	ALA	Peptide
4	E9	160	PRO	Peptide
4	E9	215	LEU	Peptide
3	F0	273	ALA	Peptide
3	F0	348	PRO	Peptide
3	F0	357	TYR	Peptide
4	F1	271	ALA	Peptide
4	F1	348	ASN	Peptide
8	k	128	ILE	Peptide
8	l	128	ILE	Peptide
7	q	97	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	174	0	171	4	0
1	1	174	0	171	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	10	174	0	171	5	0
1	11	174	0	171	3	0
1	12	174	0	171	4	0
1	13	174	0	171	3	0
1	14	174	0	171	5	0
1	15	174	0	171	6	0
1	16	174	0	171	3	0
1	17	174	0	171	2	0
1	18	174	0	171	5	0
1	19	174	0	171	7	0
1	2	174	0	171	2	0
1	22	160	0	156	1	0
1	23	160	0	156	1	0
1	3	174	0	171	4	0
1	4	174	0	171	4	0
1	5	174	0	171	2	0
1	6	174	0	171	2	0
1	7	174	0	171	1	0
1	8	174	0	171	2	0
1	9	174	0	171	1	0
2	A	1338	0	1341	28	0
2	B	1744	0	1734	41	0
2	C	384	0	379	10	0
3	A0	3325	0	3252	52	0
3	A2	3325	0	3252	55	0
3	A4	3325	0	3252	34	0
3	A6	3325	0	3252	51	0
3	A8	3325	0	3252	33	0
3	B0	3325	0	3252	48	0
3	B2	3325	0	3252	45	0
3	B4	3325	0	3252	45	0
3	B6	3325	0	3252	51	0
3	B8	3325	0	3252	48	0
3	C0	3325	0	3252	69	0
3	C2	3325	0	3251	76	0
3	C4	3325	0	3252	54	0
3	C6	3325	0	3252	79	0
3	C8	3325	0	3252	59	0
3	D0	3325	0	3252	62	0
3	D2	3325	0	3252	44	0
3	D4	3325	0	3252	55	0
3	D6	3325	0	3252	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D8	3325	0	3252	53	0
3	E0	3325	0	3252	52	0
3	E2	3325	0	3252	51	0
3	E4	3325	0	3252	63	0
3	E6	3325	0	3252	64	0
3	E8	3319	0	3241	65	0
3	F0	3325	0	3252	68	0
4	A1	3331	0	3207	56	0
4	A3	3331	0	3208	53	0
4	A5	3331	0	3207	55	0
4	A7	3331	0	3207	62	0
4	A9	3331	0	3207	52	0
4	B1	3331	0	3209	56	0
4	B3	3331	0	3207	53	0
4	B5	3331	0	3207	51	0
4	B7	3331	0	3209	53	0
4	B9	3331	0	3209	63	0
4	C1	3331	0	3209	60	0
4	C3	3331	0	3209	88	0
4	C5	3331	0	3209	61	0
4	C7	3331	0	3209	56	0
4	C9	3331	0	3209	63	0
4	D1	3331	0	3209	60	0
4	D3	3331	0	3207	62	0
4	D5	3331	0	3207	43	0
4	D7	3331	0	3207	59	0
4	D9	3331	0	3207	42	0
4	E1	3331	0	3207	61	0
4	E3	3331	0	3209	48	0
4	E5	3331	0	3207	54	0
4	E7	3331	0	3207	59	0
4	E9	3331	0	3207	113	0
4	F1	3331	0	3207	56	0
5	E	740	0	690	12	0
5	F	740	0	690	8	0
5	G	558	0	507	13	0
6	H	1817	0	1768	32	0
6	I	1817	0	1769	38	0
6	J	1870	0	1811	26	0
6	K	1795	0	1749	27	0
7	a	1289	0	1274	14	0
7	b	1289	0	1274	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	c	1608	0	1590	22	0
7	d	1608	0	1590	26	0
7	e	1608	0	1590	26	0
7	f	1608	0	1590	29	0
7	g	1608	0	1590	23	0
7	h	1608	0	1590	25	0
7	i	1608	0	1590	24	0
7	j	1608	0	1590	31	0
7	m	1608	0	1590	30	0
7	n	1608	0	1590	33	0
7	o	1608	0	1590	28	0
7	p	1608	0	1590	21	0
7	q	1608	0	1590	26	0
7	r	1608	0	1590	26	0
7	s	1608	0	1590	24	0
7	t	1608	0	1590	18	0
7	u	1608	0	1590	15	0
7	v	1608	0	1590	18	0
7	w	1608	0	1590	24	0
7	x	1608	0	1590	22	0
8	k	1140	0	1143	24	0
8	l	1140	0	1143	27	0
9	A	28	0	12	0	0
9	A1	28	0	12	0	0
9	A3	28	0	12	0	0
9	A5	28	0	12	0	0
9	A7	28	0	12	0	0
9	B	28	0	12	0	0
9	B3	28	0	12	0	0
9	B5	28	0	12	0	0
9	B7	28	0	12	0	0
9	B9	28	0	12	0	0
9	C1	28	0	12	0	0
9	C3	28	0	12	0	0
9	C5	28	0	12	0	0
9	C7	28	0	12	0	0
9	C9	28	0	12	0	0
9	D1	28	0	12	0	0
9	D3	28	0	12	0	0
9	D5	28	0	12	0	0
9	D7	28	0	12	0	0
9	D9	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	E1	28	0	12	0	0
9	E3	28	0	12	0	0
9	E5	28	0	12	0	0
9	E7	28	0	12	0	0
9	E9	28	0	12	3	0
9	F1	28	0	12	0	0
10	A0	32	0	12	0	0
10	A2	32	0	12	0	0
10	A4	32	0	12	0	0
10	A6	32	0	12	0	0
10	A8	32	0	12	0	0
10	B0	32	0	12	0	0
10	B2	32	0	12	0	0
10	B4	32	0	12	0	0
10	B6	32	0	12	0	0
10	B8	32	0	12	0	0
10	C0	32	0	11	1	0
10	C2	32	0	12	0	0
10	C4	32	0	12	0	0
10	C6	32	0	12	0	0
10	C8	32	0	12	0	0
10	D0	32	0	12	0	0
10	D2	32	0	12	0	0
10	D4	32	0	12	0	0
10	D6	32	0	12	0	0
10	D8	32	0	12	0	0
10	E0	32	0	12	0	0
10	E2	32	0	12	0	0
10	E4	32	0	12	0	0
10	E6	32	0	12	0	0
10	E8	32	0	12	0	0
10	F0	32	0	12	0	0
11	A0	1	0	0	0	0
11	A3	1	0	0	0	0
11	A4	1	0	0	0	0
11	A6	1	0	0	0	0
11	A8	1	0	0	0	0
11	B0	1	0	0	0	0
11	B2	1	0	0	0	0
11	B4	1	0	0	0	0
11	B6	1	0	0	0	0
11	B8	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	C0	1	0	0	0	0
11	C2	1	0	0	0	0
11	C4	1	0	0	0	0
11	C6	1	0	0	0	0
11	C8	1	0	0	0	0
11	D0	1	0	0	0	0
11	D2	1	0	0	0	0
11	D4	1	0	0	0	0
11	D6	1	0	0	0	0
11	D8	1	0	0	0	0
11	E0	1	0	0	0	0
11	E2	1	0	0	0	0
11	E4	1	0	0	0	0
11	E6	1	0	0	0	0
11	E8	1	0	0	0	0
11	F0	1	0	0	0	0
All	All	228257	0	221370	3461	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 (3461) 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)
3:E2:212:ILE:O	3:E2:216:ASN:HB2	1.69	0.92
4:E9:183:TYR:O	4:E9:187:LEU:HB2	1.71	0.90
1:12:247:TYR:O	1:12:251:TYR:HB2	1.72	0.89
4:C3:289:LEU:O	4:C3:293:MET:HB2	1.74	0.87
4:C1:8:GLN:O	4:C1:66:MET:HB2	1.74	0.86
3:D2:255:PHE:O	3:D2:259:LEU:HB2	1.76	0.86
2:C:224:THR:O	2:C:228:LEU:HB2	1.75	0.86
7:j:10:LEU:HD12	7:j:143:ILE:HG12	1.60	0.84
4:C1:318:ARG:HA	4:C1:354:CYS:O	1.77	0.84
4:C1:267:LEU:O	4:C1:368:VAL:HA	1.78	0.82
4:B9:8:GLN:O	4:B9:66:MET:HB3	1.81	0.81
4:E9:318:ARG:HH11	4:E9:358:PRO:HG3	1.47	0.80
3:D0:101:ASN:HD22	4:D1:256:ASN:HD21	1.30	0.79
3:D4:270:SER:HA	3:D4:377:MET:O	1.82	0.79
4:E5:164:MET:HB3	4:E5:197:ASP:H	1.48	0.79
4:D5:100:ASN:HB3	4:D5:103:LYS:HB2	1.65	0.79
3:E6:259:LEU:HD21	3:E6:316:CYS:HB2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A3:253:LEU:O	4:A3:257:LEU:HB2	1.83	0.78
4:E7:164:MET:HB3	4:E7:197:ASP:H	1.49	0.78
3:E8:184:PRO:HA	3:E8:391:MET:HE1	1.65	0.78
4:E5:191:GLN:O	4:E5:195:ASN:HB2	1.83	0.78
4:E9:418:LEU:O	4:E9:422:TYR:HB2	1.84	0.78
3:C6:259:LEU:HD21	3:C6:316:CYS:HB2	1.65	0.77
3:B8:88:HIS:HB3	3:B8:91:GLN:HG3	1.67	0.77
7:r:194:ARG:HH12	7:r:198:ARG:HH21	1.32	0.77
4:E9:139:LEU:HD12	4:E9:188:SER:HB3	1.67	0.76
1:13:247:TYR:O	1:13:251:TYR:HB2	1.84	0.76
4:C1:321:MET:HE2	4:C1:363:MET:HG3	1.67	0.75
4:B9:330:MET:HB3	4:B9:349:MET:HG3	1.69	0.75
4:D1:248:SER:HA	4:D1:252:LYS:HD2	1.67	0.75
3:E6:3:GLU:HA	3:E6:51:THR:HA	1.69	0.75
1:19:247:TYR:O	1:19:251:TYR:HB2	1.86	0.74
4:E7:166:THR:HB	4:E7:199:VAL:HG12	1.69	0.74
3:E8:274:PRO:HG2	3:E8:374:ALA:HA	1.69	0.74
4:E9:398:TYR:O	4:E9:402:GLY:HA2	1.85	0.74
4:C9:330:MET:HB3	4:C9:349:MET:HG2	1.68	0.74
4:E9:210:ILE:HD11	4:E9:273:LEU:HD21	1.70	0.74
3:F0:274:PRO:HG2	3:F0:374:ALA:HA	1.69	0.74
3:B0:136:LEU:HD13	3:B0:235:ILE:HD11	1.70	0.74
4:A7:285:SER:O	4:A7:289:LEU:HB2	1.88	0.73
4:C7:323:THR:HA	4:C7:326:VAL:HG12	1.70	0.73
4:E9:134:GLN:HA	4:E9:165:GLU:O	1.88	0.73
7:f:9:PRO:HB2	7:f:143:ILE:HG23	1.71	0.73
3:E0:292:THR:HG21	3:E0:331:ALA:HB1	1.69	0.73
3:B4:255:PHE:O	3:B4:259:LEU:HB2	1.89	0.73
7:c:9:PRO:HB2	7:c:143:ILE:HG23	1.69	0.73
3:E2:318:MET:O	3:E2:375:VAL:HA	1.89	0.72
7:e:14:LYS:HD3	7:e:47:LEU:HD23	1.70	0.72
3:C8:285:GLN:HB3	3:D2:56:THR:HA	1.70	0.72
3:A6:274:PRO:HG2	3:A6:374:ALA:HA	1.70	0.72
7:e:9:PRO:HB2	7:e:143:ILE:HG23	1.70	0.72
3:B0:3:GLU:HA	3:B0:51:THR:HA	1.71	0.72
4:D1:313:ALA:HB3	4:D1:349:MET:HG2	1.70	0.72
7:n:146:ARG:HH22	7:n:159:TYR:HE1	1.35	0.72
4:A3:320:ARG:HD2	5:F:83:GLN:HG3	1.71	0.72
7:n:84:LYS:HB3	7:n:168:PRO:HD3	1.71	0.72
3:B8:187:SER:HB2	3:B8:391:MET:HE1	1.69	0.71
3:C6:88:HIS:HB3	3:C6:91:GLN:HG2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D7:220:PRO:HD2	3:D8:326:LYS:HD3	1.73	0.71
1:1:247:TYR:O	1:1:251:TYR:HB2	1.91	0.71
4:A1:289:LEU:HD13	4:A1:363:MET:HE2	1.71	0.70
3:E6:31:GLN:HE21	3:E6:37:PRO:HG3	1.56	0.70
3:E6:274:PRO:HG2	3:E6:374:ALA:HA	1.74	0.70
4:A5:377:MET:HG3	4:A5:380:ARG:HH21	1.55	0.70
3:D0:70:LEU:HD12	3:D0:145:THR:HG22	1.72	0.70
4:D9:313:ALA:HB3	4:D9:349:MET:HG2	1.73	0.70
7:n:69:LYS:HA	7:n:206:PHE:HB3	1.72	0.70
4:D3:135:ILE:HB	4:D3:166:THR:HG22	1.73	0.70
4:B9:279:GLN:HG2	4:B9:282:ARG:HH12	1.57	0.70
4:E1:135:ILE:HB	4:E1:166:THR:HG22	1.72	0.70
4:B7:49:VAL:HG11	4:B7:241:ARG:HG2	1.73	0.70
3:C2:69:ASP:O	3:C2:94:SER:HA	1.92	0.70
3:D8:219:ILE:HG12	7:t:198:ARG:HH22	1.55	0.70
4:E5:27:GLU:HG2	4:E5:241:ARG:HH12	1.57	0.70
4:F1:156:ARG:HG2	4:F1:195:ASN:HB2	1.72	0.70
3:B2:176:GLN:HG2	4:B3:331:LEU:HD21	1.72	0.69
4:E7:117:LEU:HD11	4:E7:154:LYS:HD3	1.73	0.69
3:C6:280:LYS:HB2	3:D0:88:HIS:HE1	1.57	0.69
3:D6:219:ILE:HG12	7:s:198:ARG:HH22	1.57	0.69
4:D7:334:GLN:HE21	4:D7:349:MET:HE2	1.57	0.69
1:23:239:LEU:HD12	2:B:465:LEU:HD22	1.74	0.69
3:E4:269:LEU:HD21	3:E4:384:ILE:HD13	1.73	0.69
6:J:218:LEU:HD11	6:J:407:ILE:HB	1.73	0.69
3:C0:296:PHE:HE1	3:C0:377:MET:HG3	1.57	0.69
4:C3:54:ALA:HB3	4:C3:58:ARG:HB3	1.75	0.69
4:D5:303:SER:HB3	4:D5:377:MET:HE1	1.74	0.69
3:C6:31:GLN:HE22	8:l:65:GLU:HG2	1.58	0.69
4:E9:248:SER:HA	4:E9:252:LYS:HD3	1.75	0.69
7:i:88:LEU:HD11	7:i:185:ILE:HD13	1.75	0.69
1:18:247:TYR:O	1:18:251:TYR:HB2	1.93	0.68
1:3:239:LEU:H	2:A:317:ARG:HH22	1.41	0.68
4:A3:289:LEU:HD13	4:A3:363:MET:HE2	1.74	0.68
3:D4:32:PRO:HA	3:D4:86:LEU:HD12	1.74	0.68
4:D9:7:VAL:HB	4:D9:135:ILE:HG12	1.76	0.68
4:A9:207:LEU:HB3	4:A9:225:LEU:HD22	1.75	0.68
4:B1:49:VAL:HG21	4:B1:241:ARG:HG2	1.76	0.68
7:w:115:LEU:HD21	7:w:145:LYS:HZ2	1.58	0.68
3:B4:318:MET:O	3:B4:375:VAL:HA	1.94	0.68
3:C8:166:LYS:HB2	3:C8:199:ASP:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A4:88:HIS:HB3	3:A4:91:GLN:HG2	1.74	0.68
4:C7:289:LEU:HD23	4:C7:365:VAL:HG13	1.74	0.68
4:D7:309:ARG:H	4:D7:372:THR:HG22	1.59	0.68
3:E0:105:ARG:HG2	3:E0:110:ILE:HG12	1.75	0.68
3:A8:136:LEU:HD13	3:A8:235:ILE:HD11	1.74	0.68
4:C3:267:LEU:HD12	4:C3:374:ILE:HD11	1.74	0.68
4:E9:385:PHE:HZ	4:E9:408:PHE:HB3	1.57	0.68
3:A6:132:LEU:HD23	3:A6:164:LYS:HE3	1.76	0.68
3:D2:274:PRO:HB2	3:D2:276:ILE:HG12	1.76	0.68
4:B9:288:GLU:HG3	4:B9:291:GLN:HE21	1.58	0.67
4:C5:234:SER:O	4:C5:238:CYS:HB2	1.94	0.67
3:A4:277:SER:O	3:A4:281:ALA:HB2	1.94	0.67
4:E9:171:PRO:HG2	9:E9:501:GDP:H1'	1.76	0.67
4:B7:27:GLU:HA	4:B7:359:LYS:HD3	1.77	0.67
3:C6:142:GLY:HA2	3:C6:183:GLU:HG3	1.76	0.67
4:E7:200:GLN:HG3	4:E7:266:PHE:HB2	1.76	0.67
3:D0:180:ALA:HB3	3:D0:183:GLU:HB2	1.74	0.67
4:D1:290:THR:HA	4:D1:293:MET:HG2	1.77	0.67
5:F:79:THR:O	5:F:83:GLN:HB2	1.95	0.67
6:K:324:LEU:HD22	6:K:337:VAL:HG21	1.76	0.67
4:A9:248:SER:HA	4:A9:252:LYS:HD3	1.76	0.67
3:C8:397:LEU:HD22	4:C9:346:PRO:HD3	1.77	0.67
3:E0:212:ILE:HD11	3:E0:300:SER:HA	1.76	0.67
4:E5:293:MET:HE2	4:E5:365:VAL:HG11	1.75	0.67
4:D1:100:ASN:HB2	4:D1:103:LYS:HB2	1.77	0.67
4:D5:232:ALA:HB2	4:D5:300:MET:HE1	1.77	0.67
4:D9:232:ALA:HB2	4:D9:300:MET:HE1	1.77	0.67
4:E9:6:HIS:O	4:E9:63:ALA:HA	1.95	0.67
3:C0:319:TYR:HB2	3:C0:355:ILE:HG13	1.76	0.66
3:C4:390:ARG:HH12	3:C4:394:LYS:HZ2	1.40	0.66
4:A7:237:THR:HG23	4:A7:241:ARG:HH12	1.60	0.66
4:E1:57:GLY:HA3	7:s:83:PRO:HB2	1.77	0.66
4:C9:22:GLU:HG3	4:C9:81:PHE:HB2	1.76	0.66
4:D7:2:ARG:HB3	4:D7:131:GLN:HB2	1.77	0.66
3:C6:189:LEU:HD21	3:C6:413:MET:HE1	1.76	0.66
7:j:14:LYS:HG3	7:j:47:LEU:HB2	1.78	0.66
3:A0:102:ASN:HB3	3:A0:105:ARG:H	1.59	0.66
4:B1:249:ASP:H	4:B1:252:LYS:HB2	1.60	0.66
3:B6:102:ASN:HB3	3:B6:105:ARG:HB2	1.77	0.66
2:A:288:PRO:HG3	4:A7:280:GLN:HE21	1.61	0.66
3:B4:229:ARG:HE	3:B4:363:VAL:HG21	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B6:208:ALA:HA	3:B6:304:LYS:HE3	1.77	0.66
4:C1:180:VAL:HG22	3:C2:258:ASN:HD21	1.61	0.66
3:B6:71:GLU:HG3	4:B7:2:ARG:HH12	1.61	0.66
3:C2:101:ASN:HB3	3:C2:182:VAL:HG11	1.78	0.66
3:E0:212:ILE:O	3:E0:216:ASN:HB2	1.94	0.66
6:J:413:LYS:HA	6:J:416:ILE:HG12	1.78	0.66
4:B9:49:VAL:HG11	4:B9:241:ARG:HG2	1.78	0.66
4:C9:134:GLN:HA	4:C9:165:GLU:HB2	1.77	0.66
4:B9:334:GLN:HE21	4:B9:349:MET:HG2	1.61	0.65
3:C4:210:TYR:HB3	4:C5:324:LYS:HD2	1.77	0.65
4:D1:35:THR:HG22	7:n:83:PRO:HG3	1.78	0.65
4:E7:68:LEU:HD11	4:E7:147:MET:HE3	1.78	0.65
4:E9:310:TYR:HA	4:E9:371:SER:HA	1.77	0.65
7:d:14:LYS:HD3	7:d:47:LEU:HD23	1.77	0.65
4:A3:8:GLN:HB2	4:A3:65:LEU:HA	1.78	0.65
4:E3:253:LEU:O	4:E3:257:LEU:HB2	1.96	0.65
7:c:11:ASN:HB3	7:c:15:ARG:HH12	1.59	0.65
4:A9:207:LEU:HD23	4:A9:225:LEU:HB3	1.77	0.65
4:E1:45:GLU:HG2	4:E1:46:ARG:HG2	1.78	0.65
3:E4:222:PRO:HD2	4:E5:324:LYS:HZ3	1.59	0.65
4:E5:170:PHE:HB3	4:E5:377:MET:HE2	1.78	0.65
3:D2:417:GLU:HA	3:D2:420:GLU:HG3	1.78	0.65
4:E3:207:LEU:HD13	4:E3:225:LEU:HB3	1.78	0.65
7:x:3:GLN:HB3	7:x:178:ARG:HD3	1.76	0.65
3:E6:310:GLY:HA3	3:E6:383:ALA:HB2	1.79	0.65
4:B1:100:ASN:HB3	4:B1:103:LYS:HG2	1.79	0.65
4:B3:7:VAL:HG23	4:B3:64:ILE:HB	1.79	0.65
4:E7:272:PRO:HG3	4:E7:284:LEU:HD21	1.79	0.65
7:h:14:LYS:HB2	7:h:47:LEU:HD12	1.79	0.65
3:C0:206:ASN:HA	3:C0:209:ILE:HG22	1.79	0.65
3:C0:236:SER:O	3:C0:240:ALA:HB2	1.96	0.65
3:E2:396:ASP:HB2	3:E2:422:ARG:HH12	1.61	0.65
3:A0:8:HIS:HE1	3:A0:21:TRP:HE1	1.45	0.65
4:C1:165:GLU:HB2	4:C1:250:LEU:HD11	1.77	0.65
3:E0:105:ARG:HH12	4:E1:251:ARG:HD2	1.62	0.65
4:E5:397:TRP:HE1	3:E6:260:VAL:HG23	1.62	0.65
7:t:5:VAL:HG11	7:t:149:ARG:HD3	1.79	0.65
3:A4:387:VAL:HG22	3:A4:390:ARG:HH22	1.62	0.65
3:D8:66:VAL:HG11	3:D8:122:ILE:HD11	1.79	0.65
7:x:185:ILE:HG23	7:x:192:GLY:HA2	1.79	0.65
3:B6:137:MET:HB3	3:B6:168:ASN:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C5:91:VAL:HG21	4:C5:116:VAL:HG22	1.77	0.64
4:A5:283:ALA:HA	4:A9:55:THR:H	1.60	0.64
3:B2:234:VAL:HG21	3:B2:302:MET:HE1	1.79	0.64
3:B2:238:LEU:HD23	3:B2:318:MET:HE1	1.77	0.64
3:C0:201:ALA:HB3	3:C0:267:PHE:HA	1.78	0.64
4:C9:6:HIS:O	4:C9:63:ALA:HA	1.97	0.64
4:E9:258:ILE:HD11	4:E9:261:PRO:HA	1.79	0.64
4:A7:215:LEU:HD11	4:A7:273:LEU:HD22	1.78	0.64
4:D3:396:HIS:HA	4:D3:399:THR:HG22	1.80	0.64
3:D6:222:PRO:HD2	4:D7:324:LYS:HD2	1.79	0.64
6:I:331:ARG:HH22	6:I:372:GLU:HA	1.62	0.64
3:C0:223:THR:HG23	3:C0:225:THR:H	1.62	0.64
3:C2:406:HIS:HA	3:C2:409:VAL:HG22	1.79	0.64
4:D5:66:MET:HE1	4:D5:147:MET:HG2	1.80	0.64
3:B4:398:MET:HE2	4:B5:345:ILE:HD12	1.80	0.64
4:C5:2:ARG:HA	4:C5:130:LEU:HA	1.80	0.64
3:E6:307:PRO:HB2	3:E6:312:TYR:HE1	1.61	0.64
7:j:68:LEU:HA	7:j:71:LYS:HD3	1.78	0.64
1:6:254:LYS:HD3	3:B6:364:PRO:HD2	1.79	0.64
3:D6:264:ARG:HH12	3:D6:428:LEU:HA	1.63	0.64
3:E2:272:TYR:HB3	3:E2:275:ILE:HD11	1.80	0.64
4:A7:244:GLY:HA2	4:A7:355:ASP:HB2	1.80	0.64
3:E6:207:GLU:HA	3:E6:210:TYR:HB2	1.80	0.64
6:K:368:LEU:HB2	6:K:376:LEU:HD11	1.80	0.64
3:C2:201:ALA:HB3	3:C2:267:PHE:HA	1.80	0.64
3:E8:271:SER:HB3	3:E8:377:MET:HB3	1.80	0.64
4:E9:374:ILE:HA	4:E9:377:MET:HB2	1.80	0.64
3:A0:3:GLU:HA	3:A0:51:THR:HA	1.81	0.63
3:C2:88:HIS:HB3	3:C2:91:GLN:HG3	1.80	0.63
3:C4:212:ILE:HG23	3:C4:275:ILE:HD12	1.78	0.63
3:D2:178:SER:HB2	3:D2:183:GLU:HG2	1.80	0.63
3:C2:12:ALA:O	3:C2:16:ILE:HB	1.98	0.63
7:b:55:LEU:HG	7:b:132:LEU:HD12	1.81	0.63
3:A2:53:PHE:HB3	3:A2:61:HIS:HB3	1.81	0.63
4:D5:315:ALA:HB3	4:D5:330:MET:HE1	1.80	0.63
4:D7:232:ALA:HB2	4:D7:300:MET:HE1	1.81	0.63
3:E6:105:ARG:HG2	3:E6:411:GLU:HG2	1.79	0.63
4:E9:203:ASP:HB2	4:E9:302:ALA:H	1.64	0.63
4:C3:25:SER:HB2	4:C3:30:ILE:HB	1.78	0.63
4:C7:358:PRO:HG2	4:C7:361:LEU:HB2	1.80	0.63
4:D5:132:GLY:HA3	4:D5:163:ILE:HG22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E9:235:GLY:HA2	4:E9:318:ARG:HH22	1.63	0.63
3:F0:3:GLU:HB3	3:F0:132:LEU:HA	1.80	0.63
1:16:247:TYR:O	1:16:251:TYR:HB2	1.98	0.63
4:B3:69:GLU:HG2	4:B3:71:GLY:H	1.64	0.63
2:C:239:ARG:HH22	5:E:92:ARG:HH12	1.45	0.63
3:C0:31:GLN:HG3	3:C0:33:ASP:H	1.64	0.63
7:f:194:ARG:HH21	7:f:198:ARG:HH21	1.46	0.63
3:A0:255:PHE:O	3:A0:259:LEU:HB2	1.99	0.63
3:B4:259:LEU:HB3	3:B4:268:MET:HE1	1.81	0.63
4:E1:207:LEU:HD13	4:E1:225:LEU:HB3	1.81	0.63
4:E5:35:THR:HG22	7:u:83:PRO:HG3	1.81	0.63
3:E8:314:ALA:HA	3:E8:350:GLY:HA3	1.81	0.63
4:B9:100:ASN:HB3	4:B9:103:LYS:HG2	1.79	0.63
3:C2:70:LEU:HD23	3:C2:145:THR:HG22	1.81	0.63
7:p:17:LEU:HD12	7:p:21:ARG:HH12	1.63	0.63
1:4:247:TYR:HE2	3:B2:81:GLY:HA3	1.64	0.63
3:C4:180:ALA:HB3	3:C4:183:GLU:HB2	1.79	0.63
3:B6:320:ARG:HH21	3:B6:360:PRO:HA	1.64	0.63
4:E9:216:LYS:HG3	4:E9:218:THR:H	1.64	0.63
7:t:181:GLN:HE22	7:t:199:TRP:HA	1.63	0.63
1:0:247:TYR:O	1:0:251:TYR:HB2	1.99	0.62
4:C5:334:GLN:HE21	4:C5:349:MET:HG3	1.63	0.62
7:c:14:LYS:HB2	7:c:47:LEU:HD13	1.81	0.62
4:B3:68:LEU:HD23	4:B3:112:LEU:HD13	1.81	0.62
3:B8:255:PHE:O	3:B8:259:LEU:HB3	1.99	0.62
4:D7:171:PRO:HG2	4:D7:185:ALA:HB2	1.80	0.62
3:D8:238:LEU:HG	3:D8:318:MET:HE1	1.80	0.62
4:B3:6:HIS:O	4:B3:63:ALA:HA	1.98	0.62
3:C6:285:GLN:HE22	3:D0:56:THR:HA	1.62	0.62
4:E7:11:GLN:HA	4:E7:72:THR:HG21	1.82	0.62
3:A6:3:GLU:HA	3:A6:51:THR:HA	1.80	0.62
4:C1:30:ILE:HD11	4:C1:47:ILE:HD11	1.80	0.62
7:m:75:LEU:HD23	7:m:173:ILE:HG13	1.81	0.62
7:q:9:PRO:HB2	7:q:143:ILE:HG23	1.80	0.62
3:D0:76:ASP:HA	3:D0:79:ARG:HG2	1.81	0.62
4:D9:293:MET:HE3	4:D9:367:PHE:HB2	1.80	0.62
4:E1:207:LEU:HB3	4:E1:225:LEU:HD22	1.81	0.62
4:E1:248:SER:HA	4:E1:252:LYS:HD3	1.81	0.62
4:A5:47:ILE:HG12	4:A5:51:TYR:HB2	1.80	0.62
4:A9:100:ASN:HB3	4:A9:103:LYS:HG2	1.80	0.62
4:D3:136:THR:HG22	4:D3:167:PHE:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D7:313:ALA:HB3	4:D7:349:MET:HG2	1.80	0.62
4:C5:310:TYR:HA	4:C5:371:SER:HA	1.80	0.62
4:A3:91:VAL:HG21	4:A3:116:VAL:HG12	1.81	0.62
4:A9:134:GLN:HA	4:A9:165:GLU:O	1.99	0.62
4:C7:8:GLN:O	4:C7:66:MET:HB3	1.99	0.62
4:E9:317:PHE:HA	4:E9:366:THR:O	2.00	0.62
6:I:307:HIS:O	6:I:313:TRP:HA	2.00	0.62
4:B3:9:GLY:HA2	4:B3:66:MET:HB3	1.82	0.62
4:B3:49:VAL:HG21	4:B3:241:ARG:HG2	1.80	0.62
4:B3:66:MET:HE1	4:B3:151:LEU:HD22	1.82	0.62
3:C0:278:ALA:HA	3:C0:369:ALA:HB2	1.80	0.62
3:E6:195:LEU:HD21	3:E6:428:LEU:HD12	1.81	0.62
4:E9:163:ILE:HG21	4:E9:250:LEU:HB3	1.82	0.62
6:I:231:ASN:HB3	6:I:236:LYS:HE2	1.80	0.62
3:A0:174:SER:HB2	3:A0:177:VAL:HB	1.81	0.62
4:A5:276:ARG:HH22	2:B:282:ARG:HA	1.63	0.62
4:A7:377:MET:HG3	4:A7:380:ARG:HH21	1.64	0.62
4:F1:237:THR:HG23	4:F1:241:ARG:HH12	1.65	0.62
2:A:273:VAL:HG13	2:A:274:PHE:HD2	1.64	0.61
4:A1:287:PRO:HA	4:A1:329:GLN:HG2	1.82	0.61
2:B:278:GLN:HB3	2:B:282:ARG:HH22	1.65	0.61
4:C1:39:ASP:HA	7:i:90:PRO:HG3	1.82	0.61
3:E4:207:GLU:HA	3:E4:210:TYR:HD2	1.65	0.61
1:3:247:TYR:O	1:3:251:TYR:HB2	2.00	0.61
3:B0:212:ILE:HG12	3:B0:275:ILE:HD11	1.81	0.61
3:B4:76:ASP:HA	3:B4:79:ARG:HD2	1.81	0.61
4:E9:57:GLY:HA3	7:w:83:PRO:HB2	1.82	0.61
4:E9:139:LEU:HD23	9:E9:501:GDP:H4'	1.82	0.61
4:F1:135:ILE:HG21	4:F1:152:ILE:HD11	1.82	0.61
8:k:43:HIS:HB3	8:k:46:CYS:HB2	1.82	0.61
7:s:106:GLN:HE21	7:u:6:PHE:HZ	1.48	0.61
4:A3:330:MET:HE1	4:A3:349:MET:HE2	1.81	0.61
4:A3:362:LYS:HB3	2:B:234:TYR:HB2	1.80	0.61
4:A9:388:MET:HE3	3:B0:348:PRO:HD2	1.82	0.61
3:D8:137:MET:HB3	3:D8:168:ASN:HA	1.83	0.61
3:D8:402:ARG:HD3	3:D8:405:VAL:HG21	1.81	0.61
3:E6:318:MET:HB2	3:E6:376:CYS:HB3	1.82	0.61
7:v:88:LEU:HD11	7:v:185:ILE:HD13	1.82	0.61
4:C3:385:PHE:O	4:C3:389:PHE:HB2	2.00	0.61
3:E4:2:ARG:HB3	3:E4:242:LEU:HD12	1.82	0.61
4:E9:117:LEU:HD21	4:E9:154:LYS:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F0:325:PRO:HA	3:F0:328:VAL:HG12	1.81	0.61
7:b:96:TYR:HA	7:b:108:ILE:HD11	1.82	0.61
7:o:42:TYR:HA	7:o:45:MET:HG3	1.83	0.61
4:A1:330:MET:HG3	4:A1:349:MET:HE3	1.82	0.61
4:A3:383:ASP:HA	4:A3:386:THR:HG22	1.82	0.61
3:A6:219:ILE:HG12	7:d:198:ARG:HH22	1.64	0.61
4:B7:66:MET:HE1	4:B7:151:LEU:HD13	1.83	0.61
4:D5:7:VAL:HG22	4:D5:64:ILE:HB	1.82	0.61
8:k:17:GLN:HE22	7:m:9:PRO:HB3	1.65	0.61
1:14:245:SER:HB2	4:D7:42:LEU:HD21	1.82	0.61
4:B3:248:SER:HA	4:B3:252:LYS:HD3	1.83	0.61
3:B6:259:LEU:HD21	3:B6:316:CYS:HB2	1.83	0.61
4:E1:86:ARG:HG2	4:E1:88:ASP:H	1.65	0.61
3:A0:213:CYS:HA	3:A0:217:LEU:HD13	1.81	0.61
4:A5:286:VAL:HG22	4:A5:363:MET:HE1	1.83	0.61
4:A7:259:PRO:HG2	4:A7:311:LEU:HD23	1.83	0.61
4:C1:7:VAL:O	4:C1:135:ILE:HA	2.01	0.61
4:C3:133:PHE:O	4:C3:164:MET:HA	2.01	0.61
3:D4:102:ASN:HB2	3:D4:105:ARG:HB2	1.83	0.61
3:E2:292:THR:HG21	3:E2:331:ALA:HB1	1.82	0.61
3:D0:274:PRO:HG3	3:D0:374:ALA:HA	1.83	0.61
4:D5:6:HIS:O	4:D5:63:ALA:HA	2.01	0.61
4:D7:7:VAL:HG13	4:D7:64:ILE:HD11	1.82	0.61
4:C3:257:LEU:HD11	4:C3:369:GLY:HA2	1.82	0.61
3:E0:272:TYR:HB3	3:E0:275:ILE:HD11	1.83	0.61
3:E4:273:ALA:HA	3:E4:275:ILE:HG12	1.81	0.61
3:E8:248:LEU:HB2	3:E8:355:ILE:HG22	1.81	0.61
4:E9:187:LEU:HD12	4:E9:190:HIS:HE1	1.65	0.61
6:H:218:LEU:HD23	6:H:230:TRP:HZ3	1.66	0.61
6:I:222:ASN:HD22	6:I:402:TRP:HE1	1.48	0.61
1:6:247:TYR:O	1:6:251:TYR:HB2	2.01	0.60
4:E5:49:VAL:HG11	4:E5:241:ARG:HG2	1.83	0.60
4:F1:215:LEU:HG	4:F1:217:LEU:HD23	1.83	0.60
4:B9:139:LEU:HA	4:B9:145:SER:HB3	1.83	0.60
4:C9:268:ILE:HA	4:C9:367:PHE:O	2.02	0.60
3:D4:241:SER:HB2	3:D4:249:ASN:HB2	1.82	0.60
4:E1:178:THR:HB	4:E1:181:GLU:HB2	1.82	0.60
4:E5:11:GLN:HA	4:E5:72:THR:HG21	1.83	0.60
4:E7:61:PRO:HD3	4:E7:84:LEU:HG	1.83	0.60
6:J:245:PHE:HA	6:J:260:THR:HA	1.83	0.60
3:A0:204:LEU:HD12	3:A0:209:ILE:HD11	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C3:135:ILE:HD12	4:C3:151:LEU:HD11	1.82	0.60
3:C8:3:GLU:HA	3:C8:51:THR:HA	1.83	0.60
4:E1:174:LYS:HE2	4:E1:205:GLU:HG2	1.82	0.60
3:E8:316:CYS:HA	3:E8:352:LYS:HB2	1.83	0.60
3:C0:195:LEU:HD22	3:C0:428:LEU:HD12	1.83	0.60
3:E6:318:MET:O	3:E6:375:VAL:HA	2.00	0.60
6:H:324:LEU:HA	6:H:339:ASN:HA	1.82	0.60
6:I:324:LEU:HD13	6:I:337:VAL:HG21	1.83	0.60
3:B0:319:TYR:HB3	3:B0:323:VAL:HG21	1.84	0.60
3:B0:320:ARG:HD3	3:B0:360:PRO:HG3	1.84	0.60
3:B8:195:LEU:HD22	3:B8:428:LEU:HD12	1.84	0.60
3:A8:133:GLN:HG3	3:A8:242:LEU:HD21	1.82	0.60
2:B:491:MET:HE1	4:C9:22:GLU:HB3	1.82	0.60
4:C3:44:LEU:HA	4:C3:47:ILE:HG12	1.84	0.60
3:E4:53:PHE:HB3	3:E4:61:HIS:HB3	1.83	0.60
6:I:287:ILE:HB	6:I:296:LEU:HD11	1.84	0.60
1:2:248:ARG:HD2	7:c:97:ARG:HH22	1.66	0.60
4:C9:375:GLN:HG2	4:C9:419:VAL:HG13	1.83	0.60
3:E4:3:GLU:HA	3:E4:51:THR:HA	1.83	0.60
6:H:336:TRP:HB3	6:H:368:LEU:HD11	1.82	0.60
3:A0:364:PRO:HB2	2:C:242:LEU:HB2	1.83	0.60
3:C2:268:MET:HG2	3:C2:380:ASN:HB3	1.83	0.60
3:D6:397:LEU:HD23	4:D7:346:PRO:HD3	1.84	0.60
4:E9:163:ILE:HD11	4:E9:251:ARG:HD2	1.83	0.60
4:E9:311:LEU:HD12	4:E9:312:THR:H	1.67	0.60
4:C1:112:LEU:HB3	4:C1:147:MET:HE1	1.83	0.60
3:C2:319:TYR:HB2	3:C2:355:ILE:HG13	1.83	0.60
3:C6:274:PRO:HG2	3:C6:374:ALA:HA	1.84	0.60
3:D2:240:ALA:HA	3:D2:243:ARG:HE	1.66	0.60
4:D3:86:ARG:HD3	4:D3:88:ASP:HB2	1.84	0.60
4:E3:207:LEU:HB3	4:E3:225:LEU:HD22	1.84	0.60
4:B3:173:PRO:HB3	4:B3:380:ARG:HD3	1.83	0.59
3:B8:191:THR:HA	3:B8:194:LEU:HG	1.84	0.59
4:B9:134:GLN:HA	4:B9:165:GLU:O	2.02	0.59
3:C2:362:VAL:HB	3:C2:370:LYS:HB2	1.82	0.59
4:D9:268:ILE:HG23	4:D9:300:MET:HE3	1.84	0.59
7:r:73:VAL:HA	7:r:109:GLU:O	2.02	0.59
4:A5:288:GLU:HA	4:A5:291:GLN:HG2	1.83	0.59
3:C2:14:ILE:HD11	3:C2:75:VAL:HG22	1.83	0.59
3:C4:105:ARG:HA	3:C4:109:THR:HB	1.82	0.59
7:h:75:LEU:HD23	7:h:111:ILE:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:v:111:ILE:HG13	7:v:132:LEU:HB2	1.83	0.59
3:A6:121:ARG:HH21	3:A6:124:LYS:HG2	1.67	0.59
4:E9:181:GLU:HA	4:E9:184:ASN:HB2	1.84	0.59
4:F1:10:GLY:HA2	4:F1:143:THR:HG23	1.85	0.59
7:m:14:LYS:HB2	7:m:47:LEU:HD22	1.84	0.59
7:q:84:LYS:HB3	7:q:168:PRO:HD3	1.83	0.59
3:B4:30:ILE:HG22	3:B4:36:MET:HB3	1.83	0.59
4:B5:288:GLU:HA	4:B5:291:GLN:HG3	1.84	0.59
3:C2:301:MET:HE1	3:C2:305:CYS:H	1.67	0.59
4:C7:156:ARG:HG2	4:C7:195:ASN:HB2	1.84	0.59
4:D1:15:GLN:HB3	4:D1:226:ASN:HD21	1.67	0.59
3:F0:31:GLN:HE22	3:F0:37:PRO:HB3	1.66	0.59
3:C2:217:LEU:HD11	3:C2:275:ILE:HG12	1.84	0.59
3:C6:191:THR:HG21	3:C6:425:LEU:HD13	1.83	0.59
3:C8:88:HIS:HB3	3:C8:91:GLN:HG2	1.85	0.59
4:D5:11:GLN:HA	4:D5:72:THR:HG21	1.85	0.59
3:E8:255:PHE:O	3:E8:259:LEU:HB2	2.01	0.59
3:E8:258:ASN:HB3	3:E8:352:LYS:HG3	1.84	0.59
6:H:229:ALA:HB3	6:H:236:LYS:HB3	1.84	0.59
7:o:15:ARG:HA	7:o:45:MET:HE1	1.84	0.59
3:A4:76:ASP:HA	3:A4:79:ARG:HG2	1.83	0.59
4:A7:155:VAL:HG12	4:A7:164:MET:HE1	1.85	0.59
3:B6:191:THR:HA	3:B6:194:LEU:HG	1.85	0.59
4:D3:135:ILE:O	4:D3:166:THR:HA	2.03	0.59
4:E5:290:THR:HG21	4:E5:329:GLN:HB3	1.85	0.59
7:o:130:PRO:HG3	7:q:159:TYR:HB3	1.84	0.59
7:x:14:LYS:HD2	7:x:45:MET:HB3	1.83	0.59
4:C9:290:THR:HA	4:C9:293:MET:HE3	1.84	0.59
4:D7:253:LEU:O	4:D7:257:LEU:HB2	2.02	0.59
3:A6:283:HIS:HB3	3:B0:62:VAL:HG11	1.84	0.59
4:C1:320:ARG:HH12	4:C1:356:ILE:H	1.51	0.59
3:C4:109:THR:HG22	3:C4:110:ILE:H	1.67	0.59
4:D1:171:PRO:HB3	4:D1:181:GLU:HG2	1.85	0.59
3:F0:140:ALA:HA	3:F0:171:SER:HB3	1.85	0.59
7:p:172:VAL:HG23	7:p:180:ALA:HB3	1.85	0.59
3:A4:259:LEU:HD21	3:A4:316:CYS:HB2	1.85	0.59
4:C5:377:MET:HA	4:C5:380:ARG:HG2	1.83	0.59
4:C9:172:SER:HB2	4:C9:204:ASN:HB2	1.84	0.59
3:D4:274:PRO:HG3	3:D4:374:ALA:HA	1.85	0.59
3:E0:76:ASP:HA	3:E0:79:ARG:HD2	1.84	0.59
3:E4:64:ARG:HG3	3:E4:125:LEU:HD22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E7:167:PHE:HE2	4:E7:233:MET:HG3	1.67	0.59
3:E8:325:PRO:HA	3:E8:328:VAL:HG22	1.85	0.59
6:J:222:ASN:HA	6:J:404:PHE:HA	1.85	0.59
3:B8:274:PRO:HD3	3:B8:291:ILE:HD11	1.84	0.58
3:C4:320:ARG:HG3	3:C4:360:PRO:HD3	1.85	0.58
4:C5:35:THR:HG22	8:k:44:SER:HB3	1.85	0.58
4:D7:137:HIS:HE1	4:D7:166:THR:HB	1.68	0.58
4:C9:57:GLY:HA3	7:m:83:PRO:HB2	1.85	0.58
3:D6:121:ARG:HE	3:D6:124:LYS:HB2	1.68	0.58
3:A8:417:GLU:HA	3:A8:420:GLU:HB3	1.84	0.58
3:B2:311:LYS:H	3:B2:382:THR:HG22	1.68	0.58
3:B8:285:GLN:HB3	3:C2:56:THR:HA	1.85	0.58
4:C3:200:GLN:HB3	4:C3:268:ILE:HD11	1.84	0.58
3:C8:30:ILE:HG23	3:C8:34:GLY:HA2	1.86	0.58
7:j:10:LEU:HD13	7:j:147:HIS:HB2	1.85	0.58
3:A4:394:LYS:HG2	4:A5:346:PRO:HG3	1.84	0.58
3:C2:236:SER:HA	3:C2:243:ARG:HH22	1.68	0.58
4:D3:358:PRO:HG2	4:D3:361:LEU:HD11	1.86	0.58
8:k:68:VAL:HG12	8:k:159:TYR:HB2	1.84	0.58
4:A7:136:THR:HG22	4:A7:167:PHE:HB2	1.84	0.58
4:B5:7:VAL:HG12	4:B5:64:ILE:HB	1.86	0.58
4:C3:133:PHE:HB2	4:C3:164:MET:HG2	1.85	0.58
4:C9:263:LEU:HD21	4:C9:421:GLU:HG2	1.85	0.58
4:D3:268:ILE:HA	4:D3:367:PHE:O	2.03	0.58
3:F0:335:ILE:HD12	3:F0:338:LYS:HD3	1.85	0.58
4:F1:318:ARG:HA	4:F1:354:CYS:O	2.03	0.58
7:j:78:ALA:HB3	7:j:112:PHE:HE1	1.68	0.58
3:A2:240:ALA:HB1	3:A2:356:ASN:HD22	1.67	0.58
3:D2:205:ASP:HB2	3:D2:303:ALA:HA	1.86	0.58
4:F1:292:GLN:HE21	4:F1:298:ASN:HD21	1.51	0.58
6:I:376:LEU:HB2	6:I:388:LEU:HB2	1.85	0.58
4:A1:293:MET:HE3	4:A1:367:PHE:HD1	1.68	0.58
3:A8:271:SER:HB3	3:A8:377:MET:HE3	1.85	0.58
3:B2:177:VAL:HB	4:B3:331:LEU:HD22	1.86	0.58
4:C1:284:LEU:HD13	4:C1:363:MET:HB3	1.85	0.58
3:E0:137:MET:HE1	3:E0:153:LEU:HD23	1.86	0.58
4:E5:290:THR:HA	4:E5:293:MET:HE3	1.84	0.58
4:E7:136:THR:HG22	4:E7:167:PHE:HB2	1.84	0.58
7:u:14:LYS:HD3	7:u:47:LEU:HD23	1.84	0.58
4:A9:274:THR:HG21	4:A9:282:ARG:HG2	1.86	0.58
3:B8:255:PHE:O	3:B8:259:LEU:CB	2.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C2:255:PHE:O	3:C2:259:LEU:HB2	2.03	0.58
4:C5:86:ARG:HD2	4:C5:88:ASP:H	1.69	0.58
4:C9:285:SER:O	4:C9:289:LEU:HB2	2.04	0.58
3:E8:301:MET:HE1	3:E8:307:PRO:HG3	1.86	0.58
6:K:303:GLY:HA3	6:K:323:LYS:HA	1.85	0.58
7:b:113:VAL:HG22	7:b:134:ILE:HD12	1.85	0.58
7:h:126:ARG:HE	7:h:133:SER:HB3	1.68	0.58
3:A2:229:ARG:HD3	3:A2:363:VAL:HG11	1.86	0.58
2:B:555:ARG:HE	2:B:556:HIS:H	1.52	0.58
4:B7:267:LEU:HD23	4:B7:299:MET:HG2	1.86	0.58
3:D6:11:GLN:HG3	3:D6:74:VAL:HG21	1.85	0.58
3:D6:121:ARG:HD3	3:D6:125:LEU:HG	1.84	0.58
3:F0:194:LEU:HD12	3:F0:198:THR:HG21	1.86	0.58
4:A7:68:LEU:HB3	4:A7:96:GLY:HA2	1.84	0.58
4:D3:11:GLN:HA	4:D3:72:THR:HG21	1.85	0.58
3:D6:77:GLU:HA	3:D6:80:THR:HG22	1.86	0.58
4:D7:57:GLY:HA3	7:q:83:PRO:HB2	1.85	0.58
3:E4:395:PHE:HE2	3:E4:422:ARG:HB2	1.68	0.58
3:E6:102:ASN:HB3	3:E6:105:ARG:HG3	1.86	0.58
7:m:69:LYS:HA	7:m:206:PHE:HB3	1.85	0.58
7:q:73:VAL:HG12	7:q:109:GLU:HB3	1.86	0.58
3:A6:182:VAL:HA	3:A6:398:MET:HE1	1.85	0.57
3:C0:295:ALA:HB2	3:C0:375:VAL:HG21	1.86	0.57
3:C2:6:SER:O	3:C2:65:CYS:HA	2.04	0.57
4:E3:2:ARG:HB3	4:E3:131:GLN:HB2	1.86	0.57
7:h:38:LEU:HD12	7:h:39:PRO:HA	1.86	0.57
8:k:66:LYS:HD3	7:m:41:ASN:HA	1.85	0.57
4:C3:149:THR:HB	4:C3:191:GLN:HG2	1.85	0.57
4:E1:167:PHE:HB3	4:E1:202:ILE:HD11	1.85	0.57
4:E1:178:THR:HG23	3:E2:258:ASN:HD21	1.68	0.57
7:r:55:LEU:HD23	7:r:132:LEU:HD13	1.86	0.57
4:B3:313:ALA:HB3	4:B3:349:MET:HG2	1.85	0.57
4:B5:235:GLY:HA2	4:B5:318:ARG:HH11	1.69	0.57
3:C2:67:PHE:HB2	3:C2:92:LEU:HG	1.85	0.57
4:E9:100:ASN:HB2	3:F0:257:THR:HG21	1.86	0.57
3:F0:202:VAL:HA	3:F0:268:MET:HB2	1.87	0.57
7:e:14:LYS:HD2	7:e:45:MET:HB3	1.87	0.57
1:5:244:GLN:HG2	7:h:162:GLY:HA3	1.85	0.57
4:A1:172:SER:HB2	4:A1:205:GLU:HB2	1.87	0.57
4:C5:228:LEU:HB3	4:C5:300:MET:HE1	1.84	0.57
4:D9:248:SER:HA	4:D9:252:LYS:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E9:42:LEU:HD12	4:E9:356:ILE:HD11	1.86	0.57
4:A7:20:PHE:HA	4:A7:230:SER:HB2	1.87	0.57
3:B6:272:TYR:HB3	3:B6:275:ILE:HD11	1.85	0.57
3:E4:210:TYR:CD1	4:E5:324:LYS:HD3	2.40	0.57
3:A8:76:ASP:HA	3:A8:79:ARG:HG2	1.86	0.57
3:B6:30:ILE:HG22	3:B6:36:MET:HB3	1.86	0.57
4:B7:383:ASP:HA	4:B7:386:THR:HG22	1.86	0.57
3:D2:103:PHE:HD2	3:D2:413:MET:HE1	1.69	0.57
4:D3:397:TRP:HH2	3:D4:260:VAL:HG23	1.69	0.57
4:E9:342:VAL:HG21	4:E9:425:TYR:HD2	1.69	0.57
6:J:338:VAL:HG13	6:J:368:LEU:HD22	1.86	0.57
3:B2:184:PRO:HA	3:B2:391:MET:HE1	1.87	0.57
4:E7:396:HIS:HA	4:E7:399:THR:HG22	1.86	0.57
4:A3:64:ILE:HD11	4:A3:123:GLU:HG3	1.86	0.57
4:B1:313:ALA:O	4:B1:349:MET:HA	2.04	0.57
3:B2:177:VAL:HG21	4:B3:327:ASP:HB3	1.87	0.57
3:C0:387:VAL:HA	3:C0:390:ARG:HE	1.70	0.57
4:E7:288:GLU:HA	4:E7:291:GLN:HG2	1.87	0.57
8:l:57:TYR:HA	8:l:69:ILE:HD11	1.86	0.57
3:B6:408:TYR:HB3	3:B6:413:MET:HE2	1.85	0.57
3:B8:408:TYR:HB3	3:B8:413:MET:HE2	1.85	0.57
4:B9:8:GLN:O	4:B9:66:MET:CB	2.52	0.57
4:D7:42:LEU:HD23	4:D7:356:ILE:HD11	1.87	0.57
3:D8:230:LEU:HD22	3:D8:275:ILE:HD12	1.87	0.57
4:F1:39:ASP:HA	7:x:90:PRO:HG3	1.85	0.57
4:F1:165:GLU:HG3	4:F1:250:LEU:HD11	1.86	0.57
6:J:298:ALA:HB3	6:J:306:LEU:HB2	1.86	0.57
7:a:113:VAL:HG22	7:a:134:ILE:HD12	1.87	0.57
7:g:14:LYS:HD3	7:g:47:LEU:HB2	1.87	0.57
7:x:126:ARG:HH12	7:x:129:MET:HB2	1.70	0.57
1:15:250:GLU:HG3	3:D8:225:THR:HG21	1.86	0.57
3:A0:173:PRO:HB3	3:A0:183:GLU:HG3	1.87	0.57
3:A0:252:VAL:HA	3:A0:255:PHE:HD1	1.70	0.57
4:A5:276:ARG:HH12	2:B:282:ARG:HD3	1.70	0.57
4:B1:207:LEU:HB3	4:B1:225:LEU:HD22	1.85	0.57
3:C2:23:LEU:HD21	3:C2:236:SER:HB2	1.87	0.57
4:D7:290:THR:HG21	4:D7:329:GLN:HB3	1.85	0.57
4:E7:170:PHE:HB3	4:E7:377:MET:HE2	1.86	0.57
6:H:222:ASN:HB3	6:H:402:TRP:CZ2	2.40	0.57
6:I:217:ARG:HB3	6:I:410:ARG:HB3	1.86	0.57
8:l:66:LYS:HD2	7:n:41:ASN:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:r:65:GLN:HE21	7:r:206:PHE:HZ	1.51	0.57
4:A7:117:LEU:HA	4:A7:120:VAL:HG12	1.87	0.56
3:D8:285:GLN:HB3	3:E2:56:THR:HA	1.87	0.56
3:E6:213:CYS:HA	3:E6:217:LEU:HD13	1.86	0.56
7:e:75:LEU:O	7:e:170:VAL:HA	2.05	0.56
7:u:6:PHE:HA	7:u:11:ASN:HD22	1.70	0.56
4:B1:134:GLN:HA	4:B1:165:GLU:O	2.04	0.56
3:B4:212:ILE:O	3:B4:216:ASN:HB2	2.05	0.56
3:B8:250:VAL:HG22	3:B8:352:LYS:HE3	1.87	0.56
4:C5:166:THR:HB	4:C5:199:VAL:HA	1.86	0.56
4:D3:248:SER:HA	4:D3:252:LYS:HD3	1.85	0.56
4:E7:109:GLY:HA2	4:E7:147:MET:HE2	1.86	0.56
3:A2:81:GLY:HA2	5:F:82:ARG:HH12	1.70	0.56
3:A8:195:LEU:HD11	3:A8:428:LEU:HD21	1.86	0.56
3:B2:265:ILE:HG21	3:B2:313:MET:HE1	1.86	0.56
4:B9:91:VAL:HG21	4:B9:116:VAL:HG22	1.87	0.56
4:C1:19:LYS:HG3	4:C1:226:ASN:HB3	1.86	0.56
4:C3:248:SER:HA	4:C3:252:LYS:HD2	1.88	0.56
3:C8:408:TYR:HB3	3:C8:413:MET:HE2	1.87	0.56
4:D7:237:THR:HG23	4:D7:241:ARG:HE	1.71	0.56
4:E5:385:PHE:HE2	4:E5:412:GLU:HB2	1.70	0.56
4:E7:313:ALA:HB3	4:E7:349:MET:HG2	1.87	0.56
3:E8:406:HIS:HA	3:E8:409:VAL:HG12	1.88	0.56
4:F1:42:LEU:HG	4:F1:356:ILE:HD11	1.88	0.56
4:F1:173:PRO:HG3	4:F1:380:ARG:HD3	1.87	0.56
6:J:306:LEU:HB3	6:J:313:TRP:HB3	1.87	0.56
7:t:9:PRO:HB2	7:t:143:ILE:HG13	1.87	0.56
7:v:96:TYR:HA	7:v:108:ILE:HD11	1.86	0.56
4:B7:166:THR:HB	4:B7:199:VAL:HG22	1.87	0.56
4:C3:274:THR:HG21	4:C3:282:ARG:HD3	1.86	0.56
3:C8:104:ALA:HB2	3:C8:413:MET:HE1	1.87	0.56
4:C9:396:HIS:HA	4:C9:399:THR:HG22	1.87	0.56
3:D2:318:MET:HB2	3:D2:376:CYS:HB3	1.88	0.56
4:D3:207:LEU:HB3	4:D3:225:LEU:HG	1.88	0.56
4:D3:330:MET:HE2	4:D3:349:MET:HE2	1.87	0.56
4:E3:8:GLN:HE21	4:E3:14:ASN:HA	1.69	0.56
6:K:321:PHE:HE1	6:K:343:GLU:HG3	1.70	0.56
7:n:172:VAL:HG21	7:n:204:THR:HG21	1.87	0.56
3:A6:316:CYS:HB3	3:A6:378:ILE:HG13	1.86	0.56
3:B4:268:MET:HE2	3:B4:380:ASN:HB2	1.86	0.56
4:B7:167:PHE:HD1	4:B7:202:ILE:HD11	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E1:200:GLN:HG3	4:E1:266:PHE:HB2	1.86	0.56
2:B:454:LEU:HD22	4:C5:75:SER:HB3	1.86	0.56
3:C0:319:TYR:HD2	3:C0:323:VAL:HG11	1.69	0.56
4:C7:61:PRO:HD3	4:C7:84:LEU:HD23	1.87	0.56
3:D6:282:TYR:HD1	7:s:202:ARG:HH21	1.54	0.56
4:E9:267:LEU:HG	4:E9:369:GLY:H	1.70	0.56
7:t:15:ARG:HG2	7:t:45:MET:HE1	1.87	0.56
3:A4:3:GLU:HA	3:A4:51:THR:HA	1.88	0.56
4:A5:100:ASN:HB3	4:A5:103:LYS:HB2	1.87	0.56
3:A8:320:ARG:HD3	3:A8:360:PRO:HG3	1.86	0.56
4:C5:318:ARG:HE	4:C5:358:PRO:HD3	1.70	0.56
4:E3:163:ILE:HD11	4:E3:251:ARG:HG3	1.87	0.56
3:A6:167:LEU:HD22	3:A6:169:PHE:HE2	1.70	0.56
3:B0:88:HIS:HB3	3:B0:91:GLN:HG2	1.87	0.56
4:B1:173:PRO:HB3	4:B1:380:ARG:HD3	1.88	0.56
3:B2:203:MET:HE1	3:B2:267:PHE:HB3	1.86	0.56
4:C3:375:GLN:O	4:C3:379:LYS:HB2	2.06	0.56
3:D2:75:VAL:HG23	3:D2:92:LEU:HD12	1.88	0.56
4:E1:121:ARG:O	4:E1:124:ALA:C	2.49	0.56
3:A2:364:PRO:HB2	2:B:242:LEU:HB2	1.87	0.56
4:A3:51:TYR:HD2	4:A3:59:PHE:HB3	1.71	0.56
3:C2:430:LYS:HA	3:C2:433:GLU:HG2	1.88	0.56
4:C5:226:ASN:HA	4:C5:229:VAL:HG12	1.88	0.56
3:C6:8:HIS:CD2	3:C6:17:GLY:HA3	2.40	0.56
4:D3:91:VAL:HG21	4:D3:116:VAL:HG22	1.88	0.56
4:D9:200:GLN:HG2	4:D9:268:ILE:HD12	1.88	0.56
4:E9:172:SER:HB3	4:E9:204:ASN:HB3	1.88	0.56
4:E9:334:GLN:HA	4:E9:341:PHE:HD2	1.71	0.56
6:H:398:TRP:HB2	6:I:398:TRP:HB2	1.88	0.56
8:l:67:ALA:HB3	7:n:39:PRO:HG3	1.88	0.56
7:x:96:TYR:HA	7:x:108:ILE:HD11	1.86	0.56
3:A8:296:PHE:HE1	3:A8:377:MET:HG3	1.70	0.56
3:B2:156:ARG:HA	3:B2:159:VAL:HG12	1.88	0.56
3:C4:194:LEU:HD21	3:C4:203:MET:HE1	1.87	0.56
3:C4:402:ARG:HD3	3:C4:405:VAL:HG11	1.88	0.56
3:C6:210:TYR:HB3	4:C7:324:LYS:HD2	1.87	0.56
3:C8:6:SER:O	3:C8:65:CYS:HA	2.05	0.56
3:D4:234:VAL:HG21	3:D4:302:MET:HE1	1.88	0.56
3:D4:285:GLN:HB3	3:D8:56:THR:HA	1.88	0.56
4:E1:311:LEU:HD12	4:E1:342:VAL:HG11	1.88	0.56
4:F1:163:ILE:HD11	4:F1:251:ARG:HH11	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:132:LYS:HA	5:G:136:GLN:HB2	1.87	0.56
3:B4:53:PHE:HB3	3:B4:61:HIS:HB3	1.88	0.55
4:C1:117:LEU:HG	4:C1:154:LYS:HE3	1.87	0.55
3:D0:137:MET:O	3:D0:168:ASN:HA	2.06	0.55
4:D3:219:THR:HA	3:D4:326:LYS:HD3	1.88	0.55
3:E2:195:LEU:HD11	3:E2:428:LEU:HD13	1.87	0.55
4:E3:164:MET:HG3	4:E3:196:ALA:HA	1.88	0.55
3:A0:81:GLY:HA3	5:E:81:TYR:HE2	1.71	0.55
4:A7:268:ILE:HA	4:A7:367:PHE:O	2.06	0.55
3:B4:84:ARG:HD2	7:f:98:THR:HG21	1.88	0.55
4:B5:117:LEU:HA	4:B5:120:VAL:HG12	1.88	0.55
4:B7:230:SER:HA	4:B7:233:MET:HG2	1.88	0.55
3:B8:403:ALA:HB2	4:B9:344:TRP:HZ3	1.71	0.55
3:C8:132:LEU:HD23	3:C8:134:GLY:H	1.72	0.55
4:D5:317:PHE:HD2	4:D5:321:MET:HE2	1.72	0.55
3:E0:183:GLU:HG2	3:E0:184:PRO:HD3	1.87	0.55
4:E5:86:ARG:HG2	4:E5:88:ASP:H	1.72	0.55
3:E8:30:ILE:HD12	3:E8:34:GLY:HA2	1.89	0.55
4:E9:104:GLY:HA2	4:E9:147:MET:HE2	1.88	0.55
7:d:9:PRO:HA	7:d:12:VAL:HG22	1.88	0.55
7:s:185:ILE:HD13	7:s:195:ALA:HB3	1.88	0.55
7:s:191:GLU:HB2	7:s:195:ALA:HB2	1.88	0.55
3:A8:30:ILE:HG22	3:A8:36:MET:HG2	1.88	0.55
4:B5:257:LEU:HD21	4:B5:314:SER:HB2	1.88	0.55
3:B8:70:LEU:HD12	3:B8:99:ALA:HB2	1.89	0.55
3:C0:258:ASN:HD21	3:C0:352:LYS:HD3	1.72	0.55
3:C2:275:ILE:HG13	3:C2:368:LEU:HD21	1.87	0.55
4:D1:6:HIS:O	4:D1:63:ALA:HA	2.07	0.55
4:D3:286:VAL:HG11	4:D3:326:VAL:HA	1.88	0.55
3:F0:298:PRO:HB3	3:F0:307:PRO:HD2	1.88	0.55
7:c:149:ARG:HH11	7:c:161:TYR:HB3	1.71	0.55
1:19:247:TYR:HE2	3:E6:81:GLY:HA3	1.71	0.55
4:A7:313:ALA:HB3	4:A7:349:MET:HG3	1.89	0.55
3:C0:4:VAL:HB	3:C0:52:PHE:HE1	1.71	0.55
4:C9:102:ALA:HB2	4:C9:403:MET:HE2	1.89	0.55
4:D1:135:ILE:O	4:D1:166:THR:HA	2.06	0.55
4:D1:309:ARG:H	4:D1:372:THR:HG22	1.71	0.55
3:D2:222:PRO:HD2	4:D3:324:LYS:HG2	1.89	0.55
3:D2:250:VAL:HG13	3:D2:255:PHE:HE1	1.71	0.55
4:D9:109:GLY:HA2	4:D9:147:MET:HE1	1.87	0.55
3:E0:26:LEU:HD13	3:E0:364:PRO:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E8:398:MET:HE1	4:E9:346:PRO:HD2	1.89	0.55
6:I:379:LEU:HG	6:I:407:ILE:HD11	1.89	0.55
3:A2:213:CYS:HA	3:A2:217:LEU:HD23	1.87	0.55
3:D2:191:THR:HG21	3:D2:425:LEU:HD12	1.87	0.55
3:D6:136:LEU:HD13	3:D6:235:ILE:HD11	1.88	0.55
4:E9:139:LEU:HD11	4:E9:185:ALA:HA	1.88	0.55
7:c:53:GLY:HA2	7:c:62:VAL:HG21	1.89	0.55
7:v:185:ILE:HG23	7:v:192:GLY:HA2	1.89	0.55
3:B2:212:ILE:O	3:B2:216:ASN:HB2	2.06	0.55
4:B3:311:LEU:HD12	4:B3:342:VAL:HG11	1.87	0.55
3:B6:64:ARG:HH21	3:B6:128:ASN:HD21	1.53	0.55
3:C8:406:HIS:HA	3:C8:409:VAL:HG12	1.87	0.55
3:D0:271:SER:HB3	3:D0:377:MET:HE3	1.89	0.55
3:D4:265:ILE:HG21	3:D4:313:MET:HE1	1.89	0.55
3:D6:259:LEU:HD21	3:D6:316:CYS:HB2	1.88	0.55
4:D9:67:ASP:O	4:D9:92:PHE:HA	2.07	0.55
4:E9:299:MET:HB2	4:E9:305:PRO:HD3	1.89	0.55
6:I:247:ASN:HD22	6:I:287:ILE:H	1.54	0.55
7:b:191:GLU:HB2	7:b:195:ALA:HB2	1.87	0.55
7:h:67:HIS:HD2	7:j:19:GLU:HG2	1.72	0.55
7:w:65:GLN:HA	7:w:68:LEU:HD23	1.88	0.55
4:A7:330:MET:SD	4:A7:349:MET:HE2	2.47	0.55
4:B1:91:VAL:HG21	4:B1:116:VAL:HG22	1.89	0.55
4:C3:14:ASN:HD21	4:C3:73:MET:HE2	1.72	0.55
4:C3:19:LYS:HG3	4:C3:226:ASN:HB3	1.88	0.55
3:C4:157:LEU:HB3	3:C4:166:LYS:HZ2	1.72	0.55
3:C6:64:ARG:HG3	3:C6:125:LEU:HD22	1.89	0.55
3:C8:26:LEU:HD12	3:C8:363:VAL:HG12	1.87	0.55
4:D7:375:GLN:HB3	4:D7:422:TYR:HD2	1.71	0.55
4:E3:57:GLY:HA3	7:t:83:PRO:HB2	1.89	0.55
4:E9:342:VAL:HG22	4:E9:344:TRP:H	1.72	0.55
4:F1:20:PHE:HA	4:F1:230:SER:HB2	1.89	0.55
6:H:218:LEU:HD11	6:H:407:ILE:HB	1.89	0.55
7:d:73:VAL:HA	7:d:109:GLU:O	2.06	0.55
7:i:14:LYS:HG2	7:i:47:LEU:HB2	1.87	0.55
7:r:101:GLU:HG2	7:t:6:PHE:HB2	1.88	0.55
3:A0:83:TYR:HB3	3:A0:86:LEU:HB3	1.89	0.55
3:C4:7:ILE:HA	3:C4:66:VAL:HB	1.88	0.55
3:C6:259:LEU:HD13	3:C6:268:MET:HE2	1.89	0.55
6:H:234:THR:HG22	6:I:395:VAL:HG12	1.88	0.55
7:r:14:LYS:HD3	7:r:47:LEU:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:368:GLN:O	2:A:372:SER:HB3	2.07	0.55
3:A4:265:ILE:HG12	3:A4:432:TYR:HE1	1.71	0.55
3:B2:53:PHE:HB3	3:B2:61:HIS:HB3	1.87	0.55
4:B5:16:ILE:HD11	4:B5:229:VAL:HG11	1.89	0.55
4:B9:229:VAL:HA	4:B9:300:MET:HE1	1.89	0.55
3:D4:167:LEU:HG	3:D4:200:VAL:HB	1.89	0.55
4:E5:242:PHE:HB3	4:E5:356:ILE:HD13	1.89	0.55
4:E7:4:ILE:HD11	4:E7:240:LEU:HD13	1.89	0.55
4:E9:20:PHE:HA	4:E9:230:SER:HB2	1.89	0.55
3:A2:265:ILE:HG22	3:A2:380:ASN:HD21	1.71	0.55
3:A8:296:PHE:HZ	3:A8:317:LEU:HD21	1.71	0.55
4:B5:249:ASP:H	4:B5:252:LYS:HB3	1.72	0.55
4:B5:383:ASP:HA	4:B5:386:THR:HG22	1.88	0.55
3:C0:288:VAL:HG21	3:C0:327:ASP:HB3	1.88	0.55
3:C8:276:ILE:HD12	3:C8:281:ALA:HA	1.88	0.55
3:D0:191:THR:HG21	3:D0:425:LEU:HD13	1.89	0.55
4:E7:178:THR:HB	4:E7:181:GLU:HG3	1.87	0.55
6:I:378:VAL:HG23	6:I:386:MET:HE3	1.87	0.55
3:A4:219:ILE:HG12	7:c:198:ARG:HH22	1.73	0.54
3:A4:280:LYS:HB3	3:A8:89:PRO:HG2	1.89	0.54
4:A5:318:ARG:HH12	4:A5:358:PRO:HB3	1.72	0.54
4:B3:8:GLN:O	4:B3:66:MET:HB3	2.07	0.54
3:C2:14:ILE:HG13	3:C2:74:VAL:HG12	1.89	0.54
3:C2:269:LEU:HD23	3:C2:384:ILE:HD11	1.88	0.54
4:C3:103:LYS:HB2	4:C3:108:GLU:HG3	1.89	0.54
3:C6:134:GLY:HA3	3:C6:165:SER:HB2	1.89	0.54
4:C7:106:TYR:CD2	6:K:323:LYS:HE2	2.42	0.54
6:K:338:VAL:HG11	6:K:365:LEU:HB2	1.89	0.54
4:A1:313:ALA:O	4:A1:349:MET:HA	2.07	0.54
3:A4:234:VAL:HG21	3:A4:302:MET:HE1	1.89	0.54
3:A8:3:GLU:HA	3:A8:51:THR:HA	1.89	0.54
4:B1:97:ALA:HA	4:B1:103:LYS:HE3	1.88	0.54
4:C5:313:ALA:O	4:C5:349:MET:HA	2.07	0.54
4:C9:232:ALA:HB2	4:C9:300:MET:HE1	1.89	0.54
3:D4:212:ILE:HD11	3:D4:300:SER:HA	1.89	0.54
4:D7:198:GLU:HG2	4:D7:266:PHE:HE2	1.70	0.54
3:D8:251:ASP:H	3:D8:254:GLU:HB2	1.71	0.54
4:E5:68:LEU:HD21	4:E5:147:MET:HE1	1.89	0.54
4:E9:388:MET:HG3	3:F0:347:CYS:H	1.72	0.54
4:A5:8:GLN:OE1	4:A5:17:GLY:HA3	2.08	0.54
4:A5:18:ALA:HB2	4:A5:76:VAL:HG23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C2:68:LEU:HG	3:C2:149:LEU:HD21	1.89	0.54
3:C4:288:VAL:HG21	3:C4:327:ASP:HB3	1.89	0.54
4:C7:169:VAL:HG12	4:C7:202:ILE:HB	1.89	0.54
4:E1:107:THR:HG22	4:E1:108:GLU:H	1.72	0.54
4:E7:19:LYS:HG3	4:E7:226:ASN:HB3	1.89	0.54
3:E8:313:MET:HG3	3:E8:344:VAL:HG11	1.88	0.54
7:d:11:ASN:HD22	7:d:14:LYS:HE3	1.72	0.54
8:k:57:TYR:HA	8:k:69:ILE:HD11	1.88	0.54
7:w:73:VAL:HG13	7:w:173:ILE:HB	1.89	0.54
3:B0:217:LEU:HD21	3:B0:368:LEU:HD23	1.90	0.54
4:B1:223:GLY:HA2	4:B1:226:ASN:HB2	1.88	0.54
4:B3:188:SER:O	4:B3:192:LEU:HB2	2.07	0.54
3:C0:99:ALA:HB3	3:C0:144:GLY:HA3	1.89	0.54
4:C5:374:ILE:HG22	4:C5:422:TYR:CZ	2.42	0.54
4:D7:268:ILE:HG23	4:D7:300:MET:HE3	1.90	0.54
4:E1:117:LEU:HA	4:E1:120:VAL:HG12	1.88	0.54
7:g:73:VAL:HA	7:g:109:GLU:O	2.07	0.54
7:q:55:LEU:HD23	7:q:132:LEU:HD13	1.89	0.54
4:A7:272:PRO:HG2	4:A7:361:LEU:HD13	1.89	0.54
4:A9:282:ARG:HH22	2:B:318:GLN:HE21	1.56	0.54
4:B1:268:ILE:HB	4:B1:300:MET:HE2	1.88	0.54
4:C1:172:SER:HB2	4:C1:205:GLU:HB2	1.88	0.54
4:C1:235:GLY:HA3	4:C1:366:THR:HG21	1.89	0.54
3:C6:7:ILE:HA	3:C6:66:VAL:HB	1.88	0.54
4:D9:163:ILE:HD11	4:D9:251:ARG:HG2	1.90	0.54
4:D9:311:LEU:HD23	4:D9:342:VAL:HG21	1.88	0.54
3:E8:181:VAL:HG12	4:E9:256:ASN:HB2	1.89	0.54
2:B:368:GLN:O	2:B:372:SER:HB3	2.08	0.54
3:B6:332:VAL:HA	3:B6:335:ILE:HG22	1.89	0.54
3:C8:274:PRO:HG3	3:C8:374:ALA:HA	1.90	0.54
3:D4:388:PHE:HB3	3:D4:425:LEU:HD11	1.90	0.54
3:F0:323:VAL:HG23	3:F0:355:ILE:HG23	1.89	0.54
7:x:78:ALA:HB3	7:x:112:PHE:HE1	1.72	0.54
3:A6:84:ARG:HH21	7:b:95:TYR:HD2	1.54	0.54
4:C1:259:PRO:HG2	4:C1:311:LEU:HD21	1.89	0.54
4:D7:54:ALA:HB3	4:D7:58:ARG:HB3	1.88	0.54
3:E2:298:PRO:HB3	3:E2:307:PRO:HD2	1.89	0.54
3:E6:53:PHE:HB3	3:E6:61:HIS:HB3	1.89	0.54
3:E8:88:HIS:HD2	3:E8:89:PRO:HD2	1.72	0.54
6:H:235:TRP:HE1	6:H:400:GLY:HA3	1.72	0.54
7:b:172:VAL:HG23	7:b:180:ALA:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:p:11:ASN:HB3	7:p:15:ARG:HH12	1.72	0.54
1:22:239:LEU:HD13	2:A:465:LEU:HD23	1.90	0.54
3:A2:141:VAL:HG22	3:A2:187:SER:HA	1.89	0.54
4:B3:383:ASP:HA	4:B3:386:THR:HG22	1.89	0.54
4:B5:304:ASP:HB3	4:B5:307:HIS:CE1	2.42	0.54
4:C7:362:LYS:HD2	4:C7:363:MET:HG2	1.90	0.54
4:E1:8:GLN:HE21	4:E1:14:ASN:HA	1.73	0.54
4:E7:35:THR:HG22	7:v:83:PRO:HG3	1.89	0.54
4:E7:242:PHE:HB3	4:E7:356:ILE:HD13	1.90	0.54
4:E9:372:THR:HG22	4:E9:422:TYR:HE2	1.73	0.54
7:d:9:PRO:HB2	7:d:143:ILE:HG13	1.89	0.54
1:1:237:PRO:HD2	2:A:284:ARG:HH22	1.72	0.54
3:A2:301:MET:HE2	3:A2:307:PRO:HG3	1.90	0.54
4:A3:113:ILE:HA	4:A3:116:VAL:HG22	1.89	0.54
4:A5:91:VAL:HG21	4:A5:116:VAL:HG22	1.89	0.54
3:A8:407:TRP:HE1	4:A9:258:ILE:HB	1.72	0.54
2:B:522:VAL:HG21	4:D3:276:ARG:HD3	1.89	0.54
3:B8:5:ILE:HG12	3:B8:132:LEU:HD11	1.89	0.54
3:D6:204:LEU:HD13	3:D6:231:ILE:HD12	1.90	0.54
3:F0:202:VAL:HG22	3:F0:268:MET:HG3	1.90	0.54
7:j:9:PRO:HA	7:j:12:VAL:HG22	1.90	0.54
3:A6:49:PHE:HD2	3:A6:53:PHE:HB2	1.73	0.54
4:A7:253:LEU:O	4:A7:257:LEU:HB2	2.08	0.54
3:C8:219:ILE:HG12	7:o:198:ARG:HH21	1.73	0.54
3:D6:255:PHE:O	3:D6:259:LEU:HB2	2.08	0.54
7:a:53:GLY:HA2	7:a:62:VAL:HG21	1.90	0.54
8:l:41:ALA:HB1	8:l:86:VAL:HG21	1.89	0.54
7:q:75:LEU:HD23	7:q:111:ILE:HB	1.90	0.54
7:w:78:ALA:HB3	7:w:112:PHE:HE1	1.73	0.54
4:A1:257:LEU:HD11	4:A1:314:SER:HB2	1.90	0.53
3:B2:244:PHE:HB2	3:B2:356:ASN:HD21	1.72	0.53
4:B5:100:ASN:HB3	4:B5:103:LYS:HG2	1.90	0.53
4:C3:187:LEU:HD13	4:C3:190:HIS:HE1	1.73	0.53
3:C4:26:LEU:HD12	3:C4:363:VAL:HG12	1.90	0.53
3:C6:402:ARG:HD2	3:C6:405:VAL:HG11	1.88	0.53
4:D1:57:GLY:HA3	7:n:83:PRO:HB2	1.90	0.53
4:D1:77:ARG:HH21	4:D1:92:PHE:HZ	1.56	0.53
3:D4:262:TYR:HB2	3:D4:265:ILE:HG12	1.91	0.53
3:F0:258:ASN:HD21	3:F0:316:CYS:HB2	1.73	0.53
6:H:233:TYR:OH	6:I:392:ARG:HG2	2.08	0.53
6:I:338:VAL:HG11	6:I:365:LEU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:115:LEU:HD21	7:d:145:LYS:HD3	1.90	0.53
7:g:14:LYS:HB2	7:g:47:LEU:HD12	1.90	0.53
7:p:78:ALA:HB3	7:p:112:PHE:HE1	1.73	0.53
3:B0:208:ALA:HB2	3:B0:304:LYS:HG2	1.90	0.53
4:B5:326:VAL:O	4:B5:330:MET:HG2	2.08	0.53
4:B7:35:THR:HG22	7:g:83:PRO:HG3	1.89	0.53
3:C6:5:ILE:HD13	3:C6:64:ARG:HD3	1.90	0.53
3:D0:218:ASP:HB3	7:p:194:ARG:HH22	1.73	0.53
3:D0:276:ILE:HD12	3:D0:281:ALA:HA	1.89	0.53
4:E1:2:ARG:HB3	4:E1:131:GLN:HB2	1.88	0.53
4:E5:134:GLN:HA	4:E5:165:GLU:O	2.09	0.53
3:A8:298:PRO:HG2	3:A8:308:ARG:HE	1.73	0.53
3:B0:200:VAL:HG13	3:B0:268:MET:HE1	1.89	0.53
4:B5:290:THR:HG21	4:B5:329:GLN:HB3	1.91	0.53
4:B9:169:VAL:HG12	4:B9:202:ILE:HB	1.90	0.53
4:C9:316:MET:HB2	4:C9:366:THR:HB	1.90	0.53
4:D5:12:CYS:HB3	4:D5:138:SER:HB2	1.89	0.53
3:E8:259:LEU:HB3	3:E8:268:MET:HE1	1.89	0.53
7:t:154:TYR:HE1	7:t:158:THR:HG22	1.73	0.53
3:A6:320:ARG:HB3	3:A6:374:ALA:HB3	1.89	0.53
2:B:567:LEU:HD21	4:E1:228:LEU:HG	1.91	0.53
3:B4:203:MET:HE1	3:B4:267:PHE:HB3	1.89	0.53
3:C0:237:SER:HA	3:C0:320:ARG:HE	1.73	0.53
4:C3:281:TYR:CZ	4:C7:87:PRO:HD2	2.43	0.53
4:C5:73:MET:HB3	4:C5:90:PHE:HE2	1.72	0.53
4:D3:271:ALA:HB3	4:D3:365:VAL:HG22	1.90	0.53
4:D5:64:ILE:HD12	4:D5:119:VAL:HG12	1.90	0.53
3:D6:247:ALA:HB3	3:D6:355:ILE:HB	1.91	0.53
3:D6:254:GLU:HA	3:D6:257:THR:HG22	1.90	0.53
6:J:379:LEU:HD11	6:J:407:ILE:HG23	1.90	0.53
7:j:134:ILE:HD13	7:j:140:LEU:HD22	1.90	0.53
7:o:112:PHE:HB2	7:o:131:TRP:HE1	1.74	0.53
7:o:183:LEU:HD23	7:o:196:LEU:HA	1.89	0.53
7:s:72:SER:HB3	7:s:108:ILE:HG22	1.90	0.53
1:19:244:GLN:H	4:E7:320:ARG:NH2	2.06	0.53
4:A3:16:ILE:HD11	4:A3:229:VAL:HB	1.89	0.53
3:D2:7:ILE:HD11	3:D2:122:ILE:HD11	1.91	0.53
3:D2:272:TYR:HB3	3:D2:275:ILE:HD11	1.90	0.53
4:E3:183:TYR:O	4:E3:187:LEU:HB2	2.08	0.53
3:E8:5:ILE:HB	3:E8:135:PHE:HD1	1.73	0.53
6:J:386:MET:HE1	6:J:395:VAL:HG13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:327:ALA:HA	6:K:337:VAL:HG12	1.90	0.53
7:h:183:LEU:HD13	7:h:196:LEU:HA	1.91	0.53
7:h:184:PRO:HG3	7:h:189:LEU:HD12	1.91	0.53
1:14:244:GLN:HG2	4:D7:320:ARG:HH21	1.72	0.53
2:A:469:GLN:HE22	4:C7:276:ARG:H	1.57	0.53
4:A1:311:LEU:HD12	4:A1:342:VAL:HG11	1.90	0.53
4:C3:117:LEU:HG	4:C3:154:LYS:HD2	1.90	0.53
4:C5:137:HIS:O	4:C5:168:SER:HA	2.08	0.53
3:C6:191:THR:O	3:C6:195:LEU:HB2	2.08	0.53
3:C8:200:VAL:HA	3:C8:266:HIS:HB2	1.91	0.53
3:D0:154:LEU:HB3	3:D0:197:HIS:HB3	1.89	0.53
4:D5:113:ILE:HG13	4:D5:117:LEU:HD13	1.91	0.53
3:E0:284:GLU:HG2	3:E0:286:LEU:HD22	1.89	0.53
3:E6:5:ILE:HD13	3:E6:64:ARG:HB3	1.89	0.53
4:E9:182:PRO:HB3	4:E9:385:PHE:HA	1.91	0.53
7:h:88:LEU:HD22	7:h:185:ILE:HG21	1.91	0.53
3:A0:274:PRO:HD3	3:A0:374:ALA:HA	1.91	0.53
4:A1:248:SER:HA	4:A1:252:LYS:HG3	1.90	0.53
4:B9:215:LEU:HD21	4:B9:273:LEU:HB3	1.90	0.53
3:C0:14:ILE:HD11	3:C0:69:ASP:HB2	1.88	0.53
3:C0:259:LEU:HD21	3:C0:316:CYS:HB2	1.89	0.53
3:C2:133:GLN:HG3	3:C2:252:VAL:HB	1.90	0.53
3:C6:252:VAL:HA	3:C6:255:PHE:HB3	1.91	0.53
3:D6:90:GLU:HG3	3:D6:121:ARG:HH12	1.73	0.53
3:E0:280:LYS:HG2	3:E4:89:PRO:HD2	1.89	0.53
4:E5:8:GLN:HG2	4:E5:17:GLY:HA3	1.91	0.53
7:g:183:LEU:HD23	7:g:196:LEU:HA	1.91	0.53
3:A0:100:ALA:HA	4:A1:252:LYS:HD2	1.91	0.53
4:B5:11:GLN:HA	4:B5:72:THR:HG21	1.90	0.53
4:B5:39:ASP:HA	7:f:90:PRO:HG3	1.91	0.53
4:B5:134:GLN:HA	4:B5:165:GLU:O	2.09	0.53
4:B9:213:ARG:HH11	4:B9:297:LYS:HG2	1.73	0.53
4:C9:51:TYR:HB3	4:C9:59:PHE:HB3	1.90	0.53
3:E0:3:GLU:HA	3:E0:51:THR:HA	1.90	0.53
3:E4:167:LEU:HD22	3:E4:200:VAL:HB	1.90	0.53
3:F0:336:LYS:HE3	3:F0:348:PRO:HB3	1.89	0.53
8:k:40:LYS:HD2	8:k:43:HIS:HB2	1.91	0.53
8:l:82:ASP:HA	8:l:85:ARG:HG2	1.91	0.53
7:r:113:VAL:HG13	7:r:141:THR:HG23	1.91	0.53
3:A6:240:ALA:HA	3:A6:243:ARG:HE	1.74	0.53
3:B6:195:LEU:HD22	3:B6:428:LEU:HD12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B6:195:LEU:HD11	3:B6:264:ARG:HG3	1.90	0.53
3:B6:292:THR:HG21	3:B6:331:ALA:HB1	1.91	0.53
4:C1:179:VAL:HG12	3:C2:258:ASN:HD22	1.73	0.53
3:C6:406:HIS:HA	3:C6:409:VAL:HG12	1.90	0.53
3:D2:91:GLN:HG2	3:D2:121:ARG:HD2	1.89	0.53
3:D6:210:TYR:HA	4:D7:324:LYS:HZ2	1.73	0.53
4:E7:274:THR:HB	4:E7:282:ARG:HH21	1.74	0.53
6:K:343:GLU:HA	6:K:359:VAL:HG21	1.90	0.53
7:f:49:LEU:HD21	7:f:144:LEU:HD21	1.91	0.53
1:18:245:SER:O	1:18:249:SER:HB3	2.09	0.53
3:A2:194:LEU:HD21	3:A2:203:MET:HE1	1.90	0.53
3:A4:210:TYR:HE1	4:A5:324:LYS:HA	1.73	0.53
3:A6:406:HIS:HA	3:A6:409:VAL:HG12	1.89	0.53
3:B0:402:ARG:HD3	3:B0:405:VAL:HG21	1.91	0.53
3:C2:168:ASN:O	3:C2:201:ALA:HA	2.09	0.53
4:C3:374:ILE:HB	4:C3:422:TYR:HE2	1.74	0.53
4:C5:257:LEU:HD12	4:C5:312:THR:HG23	1.89	0.53
4:E1:272:PRO:HG2	4:E1:361:LEU:HD12	1.90	0.53
7:d:5:VAL:HG11	7:d:149:ARG:HD2	1.90	0.53
7:j:9:PRO:HB2	7:j:143:ILE:HG13	1.91	0.53
7:n:172:VAL:HG13	7:n:180:ALA:HB3	1.91	0.53
1:8:248:ARG:HH12	3:C0:77:GLU:HA	1.73	0.52
3:A2:275:ILE:HD12	3:A2:368:LEU:HD11	1.90	0.52
3:A4:30:ILE:HG22	3:A4:36:MET:HG2	1.91	0.52
4:A5:132:GLY:HA2	4:A5:162:ARG:HG3	1.91	0.52
4:B9:19:LYS:HA	4:B9:22:GLU:HB2	1.92	0.52
4:D3:247:ASN:C	4:D3:247:ASN:HD22	2.17	0.52
4:D5:200:GLN:HB3	4:D5:268:ILE:HD11	1.92	0.52
4:D7:182:PRO:HB2	4:D7:385:PHE:HB2	1.91	0.52
4:D7:296:ALA:HB2	4:D7:306:ARG:HE	1.74	0.52
3:E6:167:LEU:HD22	3:E6:200:VAL:HB	1.91	0.52
4:E7:372:THR:HG21	4:E7:426:GLN:HB2	1.90	0.52
7:d:78:ALA:HB3	7:d:112:PHE:HE1	1.74	0.52
7:f:191:GLU:HB2	7:f:195:ALA:HB2	1.91	0.52
7:q:73:VAL:HA	7:q:109:GLU:O	2.09	0.52
3:A0:182:VAL:HG22	3:A0:185:TYR:HB2	1.91	0.52
4:A7:110:ALA:HA	4:A7:113:ILE:HG22	1.92	0.52
4:A7:268:ILE:HG23	4:A7:300:MET:HE3	1.91	0.52
4:B3:213:ARG:HB3	4:B3:297:LYS:HE3	1.90	0.52
4:B5:284:LEU:HD23	4:B5:362:LYS:HB3	1.90	0.52
4:C1:325:GLU:HA	4:C1:328:GLU:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D6:88:HIS:HB3	3:D6:91:GLN:HG3	1.90	0.52
4:D7:259:PRO:HD2	4:D7:263:LEU:HD12	1.91	0.52
3:E8:319:TYR:HB3	3:E8:323:VAL:HG11	1.90	0.52
5:G:117:THR:HA	5:G:120:GLU:HB3	1.91	0.52
6:H:307:HIS:HB3	6:H:314:ASP:HB2	1.91	0.52
6:J:247:ASN:HB3	6:J:259:VAL:HB	1.91	0.52
7:b:53:GLY:HA2	7:b:62:VAL:HG11	1.92	0.52
4:A1:224:ASP:HB2	2:C:224:THR:HG23	1.91	0.52
4:A9:68:LEU:HB3	4:A9:96:GLY:HA2	1.89	0.52
4:A9:187:LEU:HA	4:A9:190:HIS:CE1	2.44	0.52
4:B1:2:ARG:HB3	4:B1:131:GLN:HB2	1.92	0.52
4:B1:113:ILE:HG12	4:B1:150:LEU:HD22	1.90	0.52
3:B2:168:ASN:O	3:B2:201:ALA:HA	2.10	0.52
4:D1:149:THR:HA	4:D1:152:ILE:HD12	1.91	0.52
3:D4:91:GLN:HG2	3:D4:121:ARG:HD2	1.92	0.52
4:D7:207:LEU:HB3	4:D7:225:LEU:HG	1.92	0.52
4:D7:311:LEU:HD23	4:D7:342:VAL:HG21	1.90	0.52
4:E3:271:ALA:HB2	4:E3:298:ASN:HD21	1.74	0.52
7:d:68:LEU:HD23	7:d:73:VAL:HG21	1.91	0.52
8:l:50:VAL:O	8:l:54:ARG:HG2	2.09	0.52
7:u:75:LEU:HD23	7:u:111:ILE:HB	1.92	0.52
2:A:312:ILE:HG23	2:A:316:LEU:HD13	1.90	0.52
3:A2:319:TYR:HB3	3:A2:323:VAL:HG21	1.91	0.52
4:A5:20:PHE:HA	4:A5:230:SER:HB2	1.91	0.52
4:A5:321:MET:HE3	4:A5:353:VAL:HG13	1.89	0.52
4:A7:281:TYR:HB3	4:B1:60:VAL:HG11	1.91	0.52
3:B0:76:ASP:HA	3:B0:79:ARG:HG2	1.91	0.52
4:B1:39:ASP:HA	7:d:90:PRO:HG3	1.91	0.52
3:B2:319:TYR:HB3	3:B2:323:VAL:HG21	1.92	0.52
4:C3:56:GLY:N	7:j:84:LYS:HZ1	2.07	0.52
3:D2:83:TYR:HD1	3:D2:86:LEU:HD13	1.73	0.52
4:D5:229:VAL:HG12	4:D5:233:MET:HE2	1.92	0.52
3:D6:417:GLU:HA	3:D6:420:GLU:HG3	1.91	0.52
3:D8:105:ARG:HG3	3:D8:411:GLU:HG3	1.92	0.52
4:E9:257:LEU:HD21	4:E9:266:PHE:HZ	1.74	0.52
7:d:140:LEU:HA	7:d:143:ILE:HG22	1.91	0.52
7:r:51:PRO:HD2	7:r:140:LEU:HD22	1.91	0.52
1:15:247:TYR:O	1:15:251:TYR:HB2	2.10	0.52
4:A9:232:ALA:HB1	4:A9:268:ILE:HG21	1.91	0.52
2:B:558:ARG:HG3	3:E2:48:ALA:HB2	1.91	0.52
3:B6:208:ALA:HB2	3:B6:304:LYS:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C2:107:HIS:CD2	3:C2:152:LEU:HB2	2.44	0.52
4:D5:207:LEU:HB3	4:D5:225:LEU:HG	1.90	0.52
3:E0:236:SER:O	3:E0:240:ALA:HB2	2.09	0.52
4:E1:278:SER:HA	4:E1:281:TYR:HD2	1.75	0.52
3:E2:11:GLN:HG3	3:E2:74:VAL:HG21	1.90	0.52
3:E8:71:GLU:HG3	3:E8:73:THR:HG22	1.92	0.52
7:o:182:PHE:HE2	7:o:187:SER:HB3	1.74	0.52
7:u:78:ALA:HB3	7:u:112:PHE:HE1	1.74	0.52
3:A0:8:HIS:HE1	3:A0:21:TRP:NE1	2.07	0.52
4:A7:232:ALA:HB2	4:A7:300:MET:HE1	1.90	0.52
3:B2:402:ARG:HG3	3:B2:405:VAL:HG11	1.92	0.52
4:B9:19:LYS:HE3	4:B9:227:HIS:HB2	1.91	0.52
3:C2:28:HIS:NE2	3:C2:243:ARG:HD2	2.24	0.52
3:C4:395:PHE:HB3	3:C4:422:ARG:HH22	1.74	0.52
3:E0:265:ILE:HG21	3:E0:313:MET:HE1	1.90	0.52
3:E4:318:MET:O	3:E4:375:VAL:HA	2.10	0.52
7:m:15:ARG:HA	7:m:45:MET:HE1	1.92	0.52
2:A:460:HIS:HB3	4:C7:221:THR:HG21	1.92	0.52
4:A1:221:THR:HG21	2:C:219:LEU:HD22	1.91	0.52
4:A3:176:SER:HB2	4:A3:181:GLU:HG3	1.92	0.52
3:A8:210:TYR:HB3	4:A9:324:LYS:HE2	1.92	0.52
3:B0:167:LEU:HG	3:B0:200:VAL:HB	1.92	0.52
3:B6:217:LEU:HD11	3:B6:275:ILE:HG22	1.92	0.52
4:B7:192:LEU:HD21	4:B7:199:VAL:HG21	1.92	0.52
3:C0:21:TRP:HA	3:C0:24:PHE:HB2	1.92	0.52
3:C0:168:ASN:O	3:C0:201:ALA:HA	2.10	0.52
4:C3:311:LEU:HD13	4:C3:342:VAL:HG21	1.91	0.52
4:D1:139:LEU:HD11	4:D1:192:LEU:HD22	1.92	0.52
4:D3:289:LEU:HD13	4:D3:365:VAL:HG13	1.91	0.52
3:D4:3:GLU:HA	3:D4:51:THR:HA	1.90	0.52
3:D6:320:ARG:HD3	3:D6:360:PRO:HG3	1.91	0.52
3:E4:195:LEU:HD13	3:E4:428:LEU:HD12	1.91	0.52
4:E9:139:LEU:HB3	9:E9:501:GDP:H5'	1.91	0.52
4:E9:266:PHE:HA	4:E9:369:GLY:O	2.10	0.52
7:b:64:PRO:HD2	7:b:67:HIS:CE1	2.45	0.52
1:19:244:GLN:H	4:E7:320:ARG:HH22	1.58	0.52
4:A3:207:LEU:HB3	4:A3:225:LEU:HG	1.92	0.52
3:A4:212:ILE:HG22	3:A4:215:ARG:HH12	1.74	0.52
3:A6:30:ILE:HG22	3:A6:36:MET:HB2	1.92	0.52
4:A7:248:SER:HA	4:A7:252:LYS:HD2	1.92	0.52
4:B9:383:ASP:HA	4:B9:386:THR:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C1:156:ARG:HH22	4:C1:197:ASP:H	1.58	0.52
4:C1:192:LEU:HD12	4:C1:196:ALA:HB2	1.91	0.52
5:E:131:LEU:HB3	5:E:136:GLN:HA	1.91	0.52
3:E8:259:LEU:HD21	3:E8:316:CYS:HB2	1.91	0.52
7:m:14:LYS:HE2	7:m:45:MET:HB3	1.91	0.52
7:o:88:LEU:HD11	7:o:185:ILE:HD13	1.91	0.52
1:19:255:PRO:HD3	7:x:178:ARG:HH21	1.74	0.52
4:B1:281:TYR:HB3	4:B5:60:VAL:HG11	1.91	0.52
4:B7:318:ARG:HD3	4:B7:358:PRO:HD3	1.91	0.52
3:C0:106:GLY:HA3	3:C0:148:GLY:HA3	1.90	0.52
4:C1:309:ARG:HG2	4:C1:342:VAL:HB	1.92	0.52
4:C3:40:SER:H	7:j:90:PRO:HB3	1.73	0.52
4:D1:232:ALA:HB2	4:D1:300:MET:HE1	1.92	0.52
3:E2:48:ALA:HB1	3:E2:243:ARG:HB3	1.92	0.52
3:E4:222:PRO:HD2	4:E5:324:LYS:NZ	2.25	0.52
4:E7:203:ASP:HB2	4:E7:301:CYS:HA	1.92	0.52
3:E8:76:ASP:HA	3:E8:79:ARG:HB2	1.90	0.52
4:E9:187:LEU:HA	4:E9:190:HIS:CE1	2.44	0.52
4:E9:293:MET:HE3	4:E9:367:PHE:HB2	1.90	0.52
8:k:45:LYS:HG3	8:k:48:GLN:HE21	1.74	0.52
7:t:65:GLN:HE21	7:t:206:PHE:HZ	1.58	0.52
7:x:126:ARG:HH11	7:x:129:MET:HE3	1.75	0.52
1:4:254:LYS:HB3	3:B2:364:PRO:HG2	1.91	0.52
2:B:469:GLN:HE22	4:C5:217:LEU:HG	1.75	0.52
4:C9:103:LYS:HB2	4:C9:401:GLU:HG3	1.92	0.52
4:D3:8:GLN:O	4:D3:66:MET:HB3	2.10	0.52
4:D5:272:PRO:HD2	4:D5:361:LEU:HD13	1.92	0.52
4:D9:257:LEU:HD11	4:D9:314:SER:HB2	1.91	0.52
4:E1:7:VAL:HB	4:E1:135:ILE:HG13	1.91	0.52
3:E4:210:TYR:HD1	4:E5:324:LYS:HD3	1.75	0.52
3:E4:219:ILE:HG13	3:E4:222:PRO:HG3	1.90	0.52
7:o:79:ASP:HB3	7:o:82:ASP:HB2	1.92	0.52
7:t:9:PRO:HA	7:t:12:VAL:HG22	1.92	0.52
4:A7:135:ILE:HB	4:A7:166:THR:HG22	1.91	0.51
3:B6:277:SER:HB3	3:B6:280:LYS:HG2	1.92	0.51
3:B6:403:ALA:HB2	4:B7:344:TRP:HZ3	1.75	0.51
4:C1:214:THR:HG21	4:C1:273:LEU:HD13	1.91	0.51
3:C2:81:GLY:H	3:C2:84:ARG:HG3	1.76	0.51
4:C3:136:THR:HG22	4:C3:167:PHE:HB2	1.92	0.51
4:E3:334:GLN:HE22	4:E3:348:ASN:N	2.08	0.51
4:E9:377:MET:HA	4:E9:380:ARG:HG3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:j:93:LEU:HA	7:j:131:TRP:HZ3	1.74	0.51
4:A1:167:PHE:HD2	4:A1:233:MET:HE2	1.74	0.51
4:B7:358:PRO:HG2	4:B7:361:LEU:HD13	1.92	0.51
3:C4:24:PHE:HA	3:C4:27:GLU:HG3	1.92	0.51
3:D0:406:HIS:HA	3:D0:409:VAL:HG12	1.92	0.51
3:D8:310:GLY:HA3	3:D8:383:ALA:HB2	1.91	0.51
4:E3:334:GLN:HE21	4:E3:349:MET:HG2	1.74	0.51
3:E4:223:THR:HG22	3:E4:224:TYR:H	1.75	0.51
3:E6:209:ILE:HG22	3:E6:227:LEU:HD22	1.92	0.51
7:d:53:GLY:HA2	7:d:62:VAL:HG11	1.92	0.51
4:A5:73:MET:HA	4:A5:76:VAL:HG12	1.92	0.51
3:B2:76:ASP:HA	3:B2:79:ARG:HG2	1.92	0.51
4:B5:53:GLU:HG3	4:B5:55:THR:H	1.75	0.51
3:C2:205:ASP:HB2	3:C2:303:ALA:HA	1.93	0.51
4:C7:156:ARG:HH21	4:C7:160:PRO:HA	1.76	0.51
4:C7:395:LEU:HD11	4:C7:408:PHE:CE2	2.45	0.51
4:D1:159:TYR:HB3	4:D1:162:ARG:HD3	1.92	0.51
4:D5:137:HIS:HE1	4:D5:166:THR:HB	1.75	0.51
3:F0:88:HIS:CD2	3:F0:90:GLU:HG2	2.46	0.51
6:K:336:TRP:HB3	6:K:368:LEU:HD11	1.92	0.51
7:c:75:LEU:O	7:c:170:VAL:HA	2.09	0.51
7:r:9:PRO:HA	7:r:12:VAL:HG22	1.93	0.51
4:A1:134:GLN:HA	4:A1:165:GLU:O	2.10	0.51
4:A5:117:LEU:HA	4:A5:120:VAL:HG12	1.92	0.51
4:B3:396:HIS:HA	4:B3:399:THR:HG22	1.92	0.51
4:B7:33:THR:HG23	4:B7:35:THR:HG23	1.93	0.51
4:C5:205:GLU:HA	4:C5:208:TYR:HB2	1.93	0.51
4:D1:137:HIS:HE1	4:D1:166:THR:HB	1.74	0.51
3:D2:283:HIS:HB2	3:D6:88:HIS:HD2	1.75	0.51
4:D9:221:THR:HG23	4:D9:223:GLY:H	1.76	0.51
3:E0:107:HIS:HD2	3:E0:152:LEU:HB2	1.76	0.51
4:E1:384:GLN:HG2	3:E2:348:PRO:HB2	1.92	0.51
3:E4:88:HIS:HB3	3:E4:91:GLN:HB2	1.93	0.51
6:K:252:PRO:HB3	6:K:416:ILE:HD13	1.92	0.51
8:l:58:LYS:HG2	7:n:161:TYR:HE2	1.75	0.51
4:A9:289:LEU:HD11	4:A9:363:MET:HG2	1.93	0.51
3:B4:311:LYS:H	3:B4:382:THR:HG22	1.74	0.51
4:B5:156:ARG:HD3	4:B5:164:MET:HG2	1.93	0.51
4:D7:221:THR:HG23	4:D7:223:GLY:H	1.76	0.51
3:E4:208:ALA:HB2	3:E4:304:LYS:HG2	1.93	0.51
3:E6:262:TYR:HB2	3:E6:265:ILE:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E9:215:LEU:HG	5:G:97:LEU:HD22	1.92	0.51
4:F1:57:GLY:HA3	7:x:83:PRO:HB2	1.92	0.51
1:9:243:ALA:HB1	4:C3:320:ARG:HH22	1.76	0.51
3:B4:230:LEU:HD22	3:B4:275:ILE:HD12	1.92	0.51
3:B8:102:ASN:HB3	3:B8:105:ARG:HB2	1.92	0.51
3:C2:195:LEU:HD11	3:C2:264:ARG:HG3	1.93	0.51
3:C4:7:ILE:HD11	3:C4:122:ILE:HD12	1.92	0.51
4:C9:180:VAL:HG22	3:D0:258:ASN:HD21	1.75	0.51
4:E9:235:GLY:HA2	4:E9:318:ARG:NH2	2.26	0.51
4:E9:385:PHE:CZ	4:E9:408:PHE:HB3	2.43	0.51
3:F0:222:PRO:HD2	4:F1:324:LYS:HZ1	1.76	0.51
4:F1:8:GLN:HB2	4:F1:65:LEU:HA	1.92	0.51
7:q:14:LYS:HD3	7:q:47:LEU:HB2	1.93	0.51
7:s:53:GLY:HA2	7:s:62:VAL:HG21	1.92	0.51
7:x:95:TYR:O	7:x:99:MET:HG2	2.11	0.51
4:A5:12:CYS:HB3	4:A5:138:SER:HB2	1.93	0.51
4:B1:377:MET:HG2	4:B1:380:ARG:HH21	1.75	0.51
4:B3:51:TYR:HB3	4:B3:59:PHE:HB3	1.92	0.51
3:B6:209:ILE:HA	3:B6:212:ILE:HG22	1.93	0.51
4:B9:288:GLU:HA	4:B9:291:GLN:HG3	1.93	0.51
4:C1:103:LYS:HB2	4:C1:108:GLU:HB3	1.91	0.51
4:C1:238:CYS:HB2	4:C1:318:ARG:HD2	1.92	0.51
4:C3:138:SER:HA	4:C3:169:VAL:HB	1.92	0.51
3:C6:180:ALA:HB3	3:C6:183:GLU:HB2	1.92	0.51
3:C6:280:LYS:HB2	3:D0:88:HIS:CE1	2.43	0.51
3:E0:5:ILE:HD12	3:E0:125:LEU:HB3	1.91	0.51
6:I:307:HIS:HB3	6:I:314:ASP:HB2	1.92	0.51
6:J:300:ASN:HB2	6:J:302:VAL:HG22	1.93	0.51
7:s:50:PHE:HD1	7:s:140:LEU:HD21	1.76	0.51
4:A9:155:VAL:HG23	4:A9:164:MET:HE1	1.93	0.51
3:B0:102:ASN:HB2	3:B0:105:ARG:HB2	1.93	0.51
3:B0:398:MET:HE2	4:B1:346:PRO:HD2	1.92	0.51
4:B3:186:THR:HG23	4:B3:187:LEU:HD12	1.93	0.51
4:D5:113:ILE:HA	4:D5:116:VAL:HG12	1.93	0.51
3:D8:217:LEU:HG	3:D8:277:SER:HB3	1.91	0.51
4:E7:6:HIS:O	4:E7:63:ALA:HA	2.10	0.51
6:I:259:VAL:HG23	6:I:287:ILE:HG12	1.93	0.51
2:A:282:ARG:HH21	4:A7:276:ARG:HE	1.57	0.51
4:A3:113:ILE:HG13	4:A3:150:LEU:HD23	1.93	0.51
4:A3:138:SER:HA	4:A3:169:VAL:HG22	1.93	0.51
2:B:458:ARG:NH1	4:C5:221:THR:HA	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B3:39:ASP:HA	7:e:90:PRO:HG3	1.93	0.51
3:B8:3:GLU:HA	3:B8:51:THR:HA	1.93	0.51
4:B9:17:GLY:HA2	4:B9:20:PHE:HB3	1.93	0.51
4:B9:318:ARG:HG2	4:B9:357:PRO:HA	1.93	0.51
3:C0:296:PHE:CE1	3:C0:377:MET:HG3	2.43	0.51
4:C1:139:LEU:HA	4:C1:145:SER:HB3	1.93	0.51
4:C5:8:GLN:HE21	4:C5:65:LEU:HG	1.75	0.51
4:D7:152:ILE:HG22	4:D7:195:ASN:HB3	1.92	0.51
3:E2:10:GLY:HA2	3:E2:145:THR:HG23	1.93	0.51
3:E4:313:MET:HE2	3:E4:382:THR:HG22	1.93	0.51
4:E7:164:MET:H	4:E7:197:ASP:HB2	1.74	0.51
4:E9:392:LYS:HA	4:E9:395:LEU:HD12	1.93	0.51
3:C0:88:HIS:HD2	3:C0:89:PRO:HD2	1.76	0.51
3:C2:188:VAL:HA	3:C2:191:THR:HG23	1.91	0.51
4:C5:104:GLY:HA2	4:C5:109:GLY:HA3	1.92	0.51
4:C9:112:LEU:HB2	4:C9:147:MET:HE1	1.93	0.51
4:D3:326:VAL:O	4:D3:330:MET:HG2	2.10	0.51
3:D4:180:ALA:HB3	3:D4:183:GLU:HB2	1.92	0.51
3:E2:319:TYR:HB3	3:E2:323:VAL:HG21	1.93	0.51
3:E4:284:GLU:HG3	3:E4:286:LEU:HD12	1.92	0.51
4:E5:169:VAL:HG12	4:E5:202:ILE:HB	1.93	0.51
6:H:247:ASN:HD21	6:H:287:ILE:H	1.59	0.51
3:A0:60:LYS:HE2	4:F1:281:TYR:HE1	1.76	0.50
4:A7:31:ASP:OD1	4:A7:32:PRO:HD2	2.11	0.50
3:B0:223:THR:HG22	4:B1:322:SER:HA	1.92	0.50
3:B2:141:VAL:HG12	3:B2:187:SER:HA	1.92	0.50
4:B7:131:GLN:HE22	4:B7:249:ASP:HB2	1.75	0.50
3:C8:80:THR:HA	3:C8:84:ARG:HH11	1.75	0.50
4:C9:120:VAL:O	4:C9:124:ALA:CB	2.59	0.50
4:C9:210:ILE:O	4:C9:214:THR:HB	2.10	0.50
3:D6:298:PRO:HG2	3:D6:308:ARG:HH11	1.74	0.50
3:E0:31:GLN:HE22	7:s:104:ALA:HB2	1.75	0.50
3:E6:153:LEU:O	3:E6:157:LEU:HB2	2.11	0.50
6:J:329:PHE:HA	6:J:334:ASN:O	2.11	0.50
7:f:64:PRO:HD2	7:f:67:HIS:CE1	2.45	0.50
7:j:140:LEU:HA	7:j:143:ILE:HG22	1.91	0.50
7:m:74:ALA:HB3	7:m:110:ILE:HD13	1.93	0.50
7:n:201:TRP:H	7:n:201:TRP:CD1	2.30	0.50
7:r:73:VAL:HG12	7:r:109:GLU:HB3	1.93	0.50
3:A2:149:LEU:O	3:A2:153:LEU:HB2	2.11	0.50
4:A3:257:LEU:HD21	4:A3:314:SER:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A5:30:ILE:HD11	4:A5:47:ILE:HD11	1.93	0.50
4:A5:77:ARG:HH22	2:B:265:PHE:HB3	1.75	0.50
3:B8:332:VAL:HA	3:B8:335:ILE:HG22	1.92	0.50
3:D6:88:HIS:CE1	3:D6:90:GLU:HG2	2.46	0.50
3:E0:99:ALA:HA	3:E0:110:ILE:HD11	1.93	0.50
4:E3:95:THR:HG22	4:E3:96:GLY:H	1.77	0.50
7:v:142:GLU:HA	7:v:145:LYS:HD3	1.93	0.50
4:A7:318:ARG:O	4:A7:363:MET:HA	2.11	0.50
4:B7:8:GLN:HE21	4:B7:17:GLY:HA3	1.76	0.50
3:C0:413:MET:HE2	3:C0:417:GLU:HB2	1.94	0.50
3:C6:71:GLU:HB3	3:C6:98:ASP:HB2	1.94	0.50
3:D0:88:HIS:CD2	3:D0:90:GLU:HG2	2.47	0.50
4:E3:107:THR:HG22	4:E3:108:GLU:H	1.76	0.50
3:E4:153:LEU:O	3:E4:157:LEU:HB2	2.12	0.50
7:c:10:LEU:HG	7:c:143:ILE:HG22	1.93	0.50
7:t:185:ILE:HD13	7:t:195:ALA:HB3	1.93	0.50
1:4:244:GLN:HG2	7:g:162:GLY:HA3	1.92	0.50
3:A2:85:HIS:HB2	5:F:93:ARG:HH22	1.76	0.50
4:A7:178:THR:HB	4:A7:181:GLU:HG3	1.92	0.50
3:C2:8:HIS:HB3	3:C2:13:GLY:HA2	1.93	0.50
4:C7:100:ASN:HD21	4:C7:102:ALA:HB3	1.77	0.50
4:D1:256:ASN:HB2	4:D1:350:LYS:HD2	1.93	0.50
3:D6:310:GLY:HA3	3:D6:383:ALA:HB2	1.93	0.50
4:E1:66:MET:HE1	4:E1:151:LEU:HG	1.93	0.50
7:e:99:MET:HE3	7:e:107:LYS:HD2	1.92	0.50
4:B1:207:LEU:HD13	4:B1:225:LEU:HB3	1.93	0.50
4:B5:253:LEU:HD12	4:B5:316:MET:HE3	1.93	0.50
4:C1:20:PHE:HA	4:C1:23:VAL:HG12	1.93	0.50
3:E2:212:ILE:HG23	3:E2:216:ASN:HD22	1.77	0.50
3:E2:238:LEU:HD11	3:E2:378:ILE:HD11	1.94	0.50
3:E4:274:PRO:HG3	3:E4:374:ALA:HA	1.91	0.50
3:E6:49:PHE:HB2	3:E6:53:PHE:HB2	1.94	0.50
3:E6:238:LEU:HD12	3:E6:318:MET:HE3	1.92	0.50
4:E7:139:LEU:HB2	4:E7:171:PRO:HD3	1.93	0.50
3:F0:12:ALA:HB3	3:F0:140:ALA:HB2	1.93	0.50
7:j:10:LEU:HD11	7:j:144:LEU:HD23	1.94	0.50
7:p:110:ILE:HB	7:p:131:TRP:CG	2.46	0.50
7:r:115:LEU:HG	7:r:167:VAL:HG11	1.94	0.50
3:A0:254:GLU:HA	3:A0:257:THR:HG22	1.94	0.50
3:A6:217:LEU:HD11	3:A6:275:ILE:HG13	1.94	0.50
4:A7:91:VAL:HG21	4:A7:116:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A8:24:PHE:HA	3:A8:27:GLU:HG2	1.94	0.50
4:B7:138:SER:HA	4:B7:169:VAL:HG22	1.93	0.50
4:C1:100:ASN:HB3	4:C1:103:LYS:HG2	1.93	0.50
4:C5:100:ASN:H	4:C5:142:GLY:HA3	1.77	0.50
3:C6:396:ASP:HB3	3:C6:422:ARG:HH12	1.77	0.50
4:C7:187:LEU:HD21	4:C7:403:MET:HE3	1.93	0.50
4:D9:113:ILE:HA	4:D9:116:VAL:HG12	1.93	0.50
4:D9:253:LEU:HD21	4:D9:316:MET:HE1	1.92	0.50
3:E4:298:PRO:HB3	3:E4:307:PRO:HD2	1.93	0.50
4:E9:190:HIS:CE1	4:E9:191:GLN:HG2	2.47	0.50
4:E9:360:GLY:HA2	5:G:108:SER:C	2.37	0.50
4:F1:248:SER:HA	4:F1:252:LYS:HD3	1.94	0.50
7:h:142:GLU:O	7:h:146:ARG:HG2	2.10	0.50
8:k:25:ARG:HB3	7:m:23:LEU:HD11	1.93	0.50
1:0:245:SER:HB3	4:A5:42:LEU:HD21	1.94	0.50
1:5:247:TYR:HE2	3:B4:81:GLY:HA3	1.77	0.50
4:A9:30:ILE:HD11	4:A9:47:ILE:HD11	1.94	0.50
3:B8:109:THR:HG22	3:B8:110:ILE:HG23	1.92	0.50
3:C2:137:MET:HE1	3:C2:154:LEU:HD11	1.94	0.50
3:D0:3:GLU:HA	3:D0:51:THR:HA	1.92	0.50
3:D0:195:LEU:HD11	3:D0:428:LEU:HD12	1.93	0.50
3:D4:395:PHE:HE2	3:D4:422:ARG:HB2	1.77	0.50
3:E0:406:HIS:HA	3:E0:409:VAL:HG12	1.94	0.50
3:E2:98:ASP:HB3	3:E2:100:ALA:H	1.77	0.50
3:E6:169:PHE:HZ	3:E6:238:LEU:HD22	1.77	0.50
3:E8:136:LEU:HD22	3:E8:169:PHE:HE1	1.76	0.50
3:F0:414:GLU:HG3	3:F0:416:GLY:H	1.77	0.50
8:k:21:TYR:CZ	8:k:87:ARG:HD2	2.45	0.50
2:A:312:ILE:HA	2:A:315:LEU:HB2	1.93	0.50
3:A8:212:ILE:HG12	3:A8:275:ILE:HD11	1.93	0.50
2:B:278:GLN:HB3	2:B:282:ARG:NH2	2.27	0.50
3:B4:68:LEU:HD22	3:B4:153:LEU:HD11	1.93	0.50
4:B9:171:PRO:HG2	4:B9:185:ALA:HB2	1.92	0.50
4:B9:236:VAL:HA	4:B9:316:MET:HE3	1.94	0.50
3:C6:329:ASN:HA	3:C6:332:VAL:HG22	1.94	0.50
3:C8:68:LEU:HD23	3:C8:153:LEU:HD11	1.93	0.50
3:D4:7:ILE:HD11	3:D4:135:PHE:HD2	1.76	0.50
4:D7:257:LEU:HD11	4:D7:368:VAL:HG13	1.93	0.50
3:D8:296:PHE:HE2	3:D8:317:LEU:HD21	1.75	0.50
3:E0:11:GLN:HG3	3:E0:74:VAL:HG21	1.94	0.50
4:E3:334:GLN:HE22	4:E3:348:ASN:H	1.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F0:113:GLU:HG2	3:F0:114:ILE:HG12	1.94	0.50
7:f:183:LEU:HD13	7:f:196:LEU:HA	1.94	0.50
7:n:151:MET:HB2	7:n:163:SER:HB3	1.92	0.50
1:3:247:TYR:HE2	3:B0:81:GLY:HA3	1.77	0.50
3:A0:26:LEU:HD21	2:C:241:ARG:HH22	1.77	0.50
3:A0:214:ARG:HG3	3:A0:220:GLU:HA	1.94	0.50
3:C0:311:LYS:H	3:C0:382:THR:HG22	1.76	0.50
3:C2:277:SER:O	3:C2:281:ALA:HB2	2.11	0.50
4:C3:113:ILE:HD11	4:C3:151:LEU:HB3	1.94	0.50
3:C6:88:HIS:HD2	3:C6:89:PRO:HD2	1.77	0.50
3:D0:259:LEU:HD21	3:D0:316:CYS:HB2	1.92	0.50
3:D8:204:LEU:HD22	3:D8:302:MET:HE2	1.93	0.50
4:E1:49:VAL:HG21	4:E1:241:ARG:HG2	1.93	0.50
4:E1:405:GLU:HA	4:E1:408:PHE:HD2	1.75	0.50
4:E5:163:ILE:HG21	4:E5:250:LEU:HB3	1.94	0.50
8:k:53:VAL:HA	8:k:154:LEU:HD21	1.93	0.50
7:m:64:PRO:HD2	7:m:67:HIS:CE1	2.47	0.50
7:t:78:ALA:HB3	7:t:112:PHE:HE1	1.76	0.50
3:A4:210:TYR:HE2	3:A4:227:LEU:HD11	1.76	0.49
3:A6:319:TYR:HD1	3:A6:375:VAL:HG22	1.77	0.49
3:A8:5:ILE:HG12	3:A8:132:LEU:HD11	1.94	0.49
3:B8:183:GLU:HG3	3:B8:184:PRO:HD3	1.93	0.49
4:C1:398:TYR:HB3	4:C1:408:PHE:HZ	1.77	0.49
3:C8:142:GLY:HA2	3:C8:183:GLU:HG3	1.94	0.49
3:C8:212:ILE:HD11	3:C8:300:SER:HA	1.93	0.49
3:D0:177:VAL:HB	4:D1:327:ASP:HB3	1.94	0.49
3:D2:3:GLU:HA	3:D2:51:THR:HA	1.93	0.49
3:D2:154:LEU:HB3	3:D2:197:HIS:HB3	1.93	0.49
3:E6:215:ARG:HH21	3:E6:299:ALA:HB1	1.77	0.49
6:K:360:PRO:HB3	6:K:392:ARG:HA	1.94	0.49
7:m:50:PHE:HZ	7:m:75:LEU:HD21	1.75	0.49
7:n:96:TYR:HE1	7:n:109:GLU:HA	1.76	0.49
7:p:129:MET:HE3	7:p:131:TRP:HE1	1.77	0.49
1:16:254:LYS:HB3	3:E0:364:PRO:HG2	1.94	0.49
4:B1:135:ILE:HB	4:B1:166:THR:HG22	1.93	0.49
4:B5:292:GLN:HG3	4:B5:298:ASN:HD22	1.76	0.49
3:B6:26:LEU:HD21	3:B6:364:PRO:HD3	1.94	0.49
4:B9:248:SER:HA	4:B9:252:LYS:HE2	1.95	0.49
4:C7:190:HIS:HA	4:C7:193:VAL:HG12	1.94	0.49
3:D0:395:PHE:HZ	3:D0:418:PHE:HB3	1.77	0.49
4:E1:274:THR:HG21	4:E1:279:GLN:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:55:LEU:HG	7:a:132:LEU:HD12	1.93	0.49
7:h:78:ALA:HB3	7:h:112:PHE:HE1	1.77	0.49
7:o:90:PRO:HA	7:o:93:LEU:HD12	1.94	0.49
7:w:140:LEU:HA	7:w:143:ILE:HG22	1.93	0.49
3:A0:234:VAL:HG21	3:A0:302:MET:HE1	1.93	0.49
3:A4:277:SER:O	3:A4:281:ALA:CB	2.60	0.49
4:B3:117:LEU:HA	4:B3:120:VAL:HG12	1.94	0.49
4:B3:215:LEU:HB3	4:B3:217:LEU:HD13	1.95	0.49
4:B7:272:PRO:HG3	4:B7:284:LEU:HD11	1.95	0.49
4:C3:202:ILE:HD11	4:C3:268:ILE:HD12	1.94	0.49
4:D3:237:THR:HG23	4:D3:241:ARG:HE	1.77	0.49
4:D9:11:GLN:HB2	4:D9:72:THR:HG21	1.92	0.49
3:E0:132:LEU:HB3	3:E0:164:LYS:HE3	1.95	0.49
3:E4:259:LEU:HD11	3:E4:316:CYS:HB2	1.94	0.49
4:E9:313:ALA:HB3	4:E9:349:MET:HE1	1.93	0.49
3:F0:195:LEU:HD12	3:F0:428:LEU:HD22	1.94	0.49
7:r:119:ARG:HH22	7:r:137:GLU:HG2	1.77	0.49
1:18:247:TYR:HE2	3:E4:81:GLY:HA3	1.77	0.49
1:8:244:GLN:HB3	1:8:248:ARG:HB2	1.94	0.49
3:A6:122:ILE:HG21	3:A6:157:LEU:HD21	1.94	0.49
3:A6:311:LYS:HE3	3:A6:344:VAL:HG12	1.93	0.49
4:A7:232:ALA:HB1	4:A7:268:ILE:HD13	1.94	0.49
4:A9:256:ASN:ND2	4:A9:350:LYS:HD3	2.27	0.49
3:B0:283:HIS:HE1	3:B4:85:HIS:O	1.94	0.49
3:B6:335:ILE:HD12	3:B6:338:LYS:HD3	1.95	0.49
4:B9:200:GLN:HG2	4:B9:268:ILE:HD11	1.94	0.49
4:C1:8:GLN:HB2	4:C1:65:LEU:HA	1.94	0.49
4:C5:201:VAL:HG21	4:C5:374:ILE:HD13	1.94	0.49
4:C9:286:VAL:HG22	4:C9:363:MET:HE1	1.93	0.49
4:D3:100:ASN:HB2	4:D3:103:LYS:HB2	1.93	0.49
4:D3:286:VAL:HB	4:D3:325:GLU:HG3	1.94	0.49
3:E2:326:LYS:HG3	3:E2:327:ASP:N	2.27	0.49
4:E9:379:LYS:HB2	4:E9:419:VAL:HG11	1.94	0.49
3:F0:236:SER:O	3:F0:240:ALA:HB2	2.12	0.49
7:g:185:ILE:HG23	7:g:192:GLY:HA2	1.93	0.49
7:r:18:ASN:HA	7:r:21:ARG:HG2	1.93	0.49
7:u:7:ALA:HB3	7:u:161:TYR:HE1	1.75	0.49
3:A0:395:PHE:HZ	3:A0:418:PHE:HB3	1.78	0.49
3:A6:28:HIS:CE1	3:A6:243:ARG:HD2	2.48	0.49
4:B7:8:GLN:OE1	4:B7:65:LEU:HG	2.11	0.49
3:B8:217:LEU:HD21	3:B8:368:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C1:42:LEU:HD21	4:C1:356:ILE:HG13	1.94	0.49
4:C3:271:ALA:HB2	4:C3:298:ASN:HD21	1.77	0.49
3:D0:204:LEU:HD22	3:D0:231:ILE:HG12	1.95	0.49
4:D3:178:THR:H	3:D4:352:LYS:HA	1.76	0.49
4:D5:34:GLY:HA3	4:D5:58:ARG:HD2	1.94	0.49
4:D7:100:ASN:HB3	4:D7:103:LYS:HB2	1.94	0.49
7:h:5:VAL:HG11	7:h:149:ARG:HD2	1.94	0.49
7:m:110:ILE:HB	7:m:131:TRP:CG	2.48	0.49
3:A2:258:ASN:ND2	3:A2:352:LYS:HE3	2.28	0.49
3:A2:398:MET:HE3	4:A3:345:ILE:HG12	1.95	0.49
3:A6:135:PHE:HB2	3:A6:166:LYS:HA	1.94	0.49
4:A7:292:GLN:HG2	4:A7:298:ASN:HD22	1.77	0.49
4:A9:130:LEU:HG	4:A9:162:ARG:HD2	1.95	0.49
4:B5:97:ALA:HA	4:B5:103:LYS:HE2	1.93	0.49
3:C2:225:THR:HA	3:C2:228:ASN:HB2	1.94	0.49
4:C3:87:PRO:HA	4:C3:90:PHE:HD2	1.78	0.49
3:C8:204:LEU:HD13	3:C8:231:ILE:HG12	1.93	0.49
4:E3:198:GLU:HG2	4:E3:266:PHE:HE2	1.77	0.49
3:E4:318:MET:HB2	3:E4:376:CYS:HB3	1.92	0.49
4:F1:77:ARG:HH22	4:F1:92:PHE:HZ	1.61	0.49
7:o:5:VAL:HG11	7:o:149:ARG:HD3	1.94	0.49
7:p:14:LYS:HD3	7:p:47:LEU:HD22	1.93	0.49
1:18:244:GLN:HE21	7:w:162:GLY:HA3	1.77	0.49
3:A0:89:PRO:HD3	4:F1:281:TYR:CD2	2.48	0.49
4:A1:105:HIS:CD2	4:A1:150:LEU:HB2	2.47	0.49
3:B4:3:GLU:HA	3:B4:51:THR:HA	1.95	0.49
3:B4:195:LEU:HD11	3:B4:428:LEU:HD12	1.95	0.49
3:B8:5:ILE:HD12	3:B8:125:LEU:HD23	1.94	0.49
4:C1:64:ILE:HD13	4:C1:120:VAL:HG22	1.95	0.49
4:C1:211:CYS:HA	4:C1:215:LEU:HB2	1.94	0.49
3:C6:292:THR:HG21	3:C6:331:ALA:HB1	1.94	0.49
4:D1:147:MET:HA	4:D1:150:LEU:HB3	1.95	0.49
4:E1:374:ILE:HD11	4:E1:422:TYR:CZ	2.47	0.49
4:A5:330:MET:SD	4:A5:349:MET:HE2	2.53	0.49
4:B7:267:LEU:HD13	4:B7:371:SER:HB3	1.95	0.49
3:C2:145:THR:O	3:C2:149:LEU:HB3	2.11	0.49
4:C9:290:THR:HG21	4:C9:329:GLN:HB3	1.94	0.49
3:D0:176:GLN:HB3	4:D1:331:LEU:HD13	1.94	0.49
4:D1:91:VAL:HG11	4:D1:116:VAL:HG22	1.94	0.49
4:D3:232:ALA:HB2	4:D3:300:MET:HE1	1.94	0.49
4:D9:207:LEU:HB3	4:D9:225:LEU:HG	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E6:69:ASP:O	3:E6:94:SER:HA	2.13	0.49
4:E7:130:LEU:HB3	4:E7:162:ARG:HE	1.77	0.49
3:E8:26:LEU:HD12	3:E8:363:VAL:HG12	1.94	0.49
5:F:132:LYS:HA	5:F:136:GLN:HB2	1.94	0.49
4:F1:314:SER:HB3	4:F1:350:LYS:HB3	1.95	0.49
7:e:8:SER:HB2	7:e:147:HIS:HA	1.95	0.49
7:q:170:VAL:HG13	7:q:183:LEU:HB2	1.94	0.49
2:B:508:TYR:HE1	4:D3:75:SER:HA	1.78	0.49
3:B0:49:PHE:HD2	3:B0:53:PHE:HB2	1.77	0.49
3:B4:238:LEU:HD12	3:B4:318:MET:HE3	1.95	0.49
4:B9:382:SER:HB2	4:B9:415:MET:HE3	1.93	0.49
4:C3:8:GLN:HB2	4:C3:65:LEU:HA	1.95	0.49
3:D6:240:ALA:HA	3:D6:243:ARG:HB2	1.95	0.49
4:D9:164:MET:H	4:D9:197:ASP:HB2	1.76	0.49
3:E4:270:SER:HA	3:E4:377:MET:O	2.13	0.49
7:d:10:LEU:HG	7:d:143:ILE:HG12	1.95	0.49
7:w:55:LEU:HD22	7:w:111:ILE:HG12	1.95	0.49
3:A0:265:ILE:HG22	3:A0:380:ASN:HD21	1.77	0.49
4:A1:70:PRO:HA	4:A1:73:MET:HE2	1.94	0.49
4:A5:361:LEU:HD23	2:B:285:GLN:HB2	1.95	0.49
4:B3:152:ILE:HG23	4:B3:164:MET:HE1	1.95	0.49
3:C0:174:SER:HB3	3:C0:177:VAL:O	2.13	0.49
4:C1:2:ARG:HD3	4:C1:131:GLN:HG3	1.95	0.49
4:C1:405:GLU:HA	4:C1:408:PHE:HD2	1.77	0.49
4:C3:236:VAL:HG13	4:C3:237:THR:HG23	1.95	0.49
3:C4:288:VAL:HA	3:C4:291:ILE:HG22	1.93	0.49
3:C4:296:PHE:HE1	3:C4:377:MET:HG3	1.77	0.49
4:D5:136:THR:HA	4:D5:167:PHE:O	2.11	0.49
3:E4:28:HIS:CE1	3:E4:243:ARG:HD2	2.48	0.49
3:F0:203:MET:HE1	3:F0:267:PHE:HB3	1.95	0.49
4:F1:260:PHE:HB2	4:F1:263:LEU:HD13	1.94	0.49
5:G:136:GLN:HG3	5:G:137:TRP:CD1	2.48	0.49
7:n:89:LEU:HD11	7:n:129:MET:HG2	1.95	0.49
2:A:571:MET:HG3	2:A:572:ILE:HG12	1.94	0.48
4:A1:128:ASP:H	5:F:169:ARG:HH22	1.61	0.48
4:A3:268:ILE:HG23	4:A3:300:MET:HE3	1.95	0.48
4:A5:57:GLY:HA3	7:a:83:PRO:HB2	1.94	0.48
3:A6:360:PRO:HG3	3:A6:374:ALA:HB2	1.95	0.48
4:A9:10:GLY:HA2	4:A9:143:THR:HG23	1.95	0.48
3:B0:219:ILE:HG22	7:f:198:ARG:NH2	2.28	0.48
4:B5:4:ILE:HD11	4:B5:240:LEU:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B5:6:HIS:O	4:B5:63:ALA:HA	2.13	0.48
4:C7:36:TYR:HD2	8:l:48:GLN:HB3	1.78	0.48
3:C8:180:ALA:HB3	3:C8:183:GLU:HB2	1.95	0.48
4:C9:256:ASN:HB2	4:C9:350:LYS:HE2	1.94	0.48
3:D4:272:TYR:HA	3:D4:375:VAL:O	2.12	0.48
4:D7:318:ARG:HG2	4:D7:354:CYS:HB3	1.95	0.48
4:D9:246:LEU:HB3	4:D9:353:VAL:H	1.78	0.48
4:E1:398:TYR:HB3	4:E1:408:PHE:HZ	1.78	0.48
4:E3:311:LEU:HD23	4:E3:342:VAL:HG11	1.95	0.48
4:E7:317:PHE:CD1	4:E7:321:MET:HE1	2.47	0.48
3:E8:157:LEU:O	3:E8:160:ASP:C	2.56	0.48
7:n:110:ILE:HB	7:n:131:TRP:CG	2.48	0.48
4:A3:337:ASN:HB3	4:A3:340:TYR:HB2	1.96	0.48
3:B4:403:ALA:HB2	4:B5:344:TRP:HZ3	1.77	0.48
3:B6:9:VAL:HG12	3:B6:146:GLY:HA2	1.95	0.48
4:C3:156:ARG:HH22	4:C3:197:ASP:N	2.10	0.48
3:C4:394:LYS:HE2	4:C5:346:PRO:HB2	1.95	0.48
3:E0:191:THR:HG21	3:E0:425:LEU:HD13	1.94	0.48
3:E8:30:ILE:HD13	3:E8:53:PHE:HE1	1.78	0.48
4:F1:64:ILE:HG12	4:F1:119:VAL:HG12	1.94	0.48
6:I:247:ASN:ND2	6:I:287:ILE:H	2.11	0.48
7:v:78:ALA:HB3	7:v:112:PHE:HE1	1.78	0.48
1:12:246:CYS:O	1:12:250:GLU:HG2	2.13	0.48
1:14:247:TYR:O	1:14:251:TYR:HB2	2.14	0.48
2:A:262:LYS:HB3	4:A3:218:THR:HB	1.95	0.48
3:A2:70:LEU:HD12	3:A2:145:THR:HG22	1.94	0.48
3:A2:195:LEU:HD21	3:A2:264:ARG:HH21	1.77	0.48
4:A5:215:LEU:HD21	4:A5:273:LEU:HD22	1.96	0.48
3:A8:403:ALA:HB2	4:A9:344:TRP:HZ3	1.79	0.48
4:B3:91:VAL:HG21	4:B3:116:VAL:HG22	1.94	0.48
4:B3:284:LEU:HD23	4:B3:362:LYS:HB2	1.95	0.48
4:B5:272:PRO:HG3	4:B5:284:LEU:HD11	1.94	0.48
4:B9:103:LYS:HA	4:B9:107:THR:HG22	1.95	0.48
4:C3:293:MET:HA	4:C3:298:ASN:HD22	1.77	0.48
3:D0:5:ILE:HD12	3:D0:125:LEU:HB3	1.95	0.48
4:D1:8:GLN:HG2	4:D1:17:GLY:HA3	1.96	0.48
5:E:137:TRP:HH2	3:F0:362:VAL:HG11	1.77	0.48
3:F0:5:ILE:HD12	3:F0:125:LEU:HB3	1.96	0.48
4:F1:199:VAL:HG13	4:F1:265:PHE:HA	1.95	0.48
6:J:287:ILE:HB	6:J:296:LEU:HD11	1.95	0.48
7:c:85:CYS:HA	7:c:168:PRO:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:m:99:MET:HE3	7:m:107:LYS:HD2	1.95	0.48
4:B7:248:SER:HA	4:B7:252:LYS:HE2	1.95	0.48
3:C6:217:LEU:HA	3:C6:277:SER:HB2	1.94	0.48
3:D6:31:GLN:HE22	7:q:104:ALA:HB2	1.77	0.48
3:D8:167:LEU:HG	3:D8:200:VAL:HB	1.94	0.48
4:F1:40:SER:HB3	4:F1:43:GLN:HE21	1.77	0.48
6:I:215:PHE:HB2	6:I:230:TRP:CD1	2.48	0.48
6:K:247:ASN:HD22	6:K:287:ILE:H	1.61	0.48
7:j:42:TYR:HD1	7:j:45:MET:HE2	1.78	0.48
3:A8:255:PHE:O	3:A8:259:LEU:HB3	2.13	0.48
4:A9:11:GLN:HG2	4:A9:72:THR:HG21	1.96	0.48
2:B:465:LEU:HD21	4:C5:359:LYS:HB3	1.94	0.48
3:B0:104:ALA:HB2	3:B0:413:MET:HE2	1.95	0.48
4:B3:257:LEU:HD21	4:B3:314:SER:HB2	1.96	0.48
3:B8:189:LEU:HD11	3:B8:418:PHE:HD1	1.79	0.48
3:C0:75:VAL:HG21	3:C0:94:SER:HB3	1.96	0.48
4:C1:267:LEU:HD23	4:C1:301:CYS:HB3	1.94	0.48
3:C2:313:MET:HE1	3:C2:346:TRP:HZ2	1.77	0.48
4:C7:293:MET:HE3	4:C7:367:PHE:HB2	1.95	0.48
4:C9:27:GLU:HA	4:C9:359:LYS:HD2	1.94	0.48
3:E4:195:LEU:HD21	3:E4:264:ARG:HH22	1.77	0.48
4:F1:45:GLU:HG2	4:F1:46:ARG:HG2	1.95	0.48
5:G:123:PRO:HG2	7:w:101:GLU:HB3	1.94	0.48
6:J:247:ASN:HD22	6:J:248:ILE:N	2.11	0.48
7:b:97:ARG:O	7:b:101:GLU:HG3	2.14	0.48
1:17:246:CYS:O	1:17:250:GLU:HG2	2.13	0.48
3:A0:316:CYS:SG	3:A0:378:ILE:HB	2.54	0.48
4:B7:134:GLN:HA	4:B7:165:GLU:O	2.14	0.48
4:B9:113:ILE:HG13	4:B9:117:LEU:HD23	1.96	0.48
4:D1:113:ILE:HG13	4:D1:117:LEU:HD23	1.94	0.48
3:D8:388:PHE:HB3	3:D8:425:LEU:HD11	1.96	0.48
3:E6:105:ARG:HA	3:E6:109:THR:OG1	2.14	0.48
3:E8:408:TYR:HB3	3:E8:413:MET:HB2	1.95	0.48
3:F0:5:ILE:HD13	3:F0:64:ARG:HD3	1.96	0.48
7:e:50:PHE:HD2	7:e:65:GLN:HG3	1.78	0.48
3:A0:247:ALA:HB3	3:A0:355:ILE:HB	1.96	0.48
3:A0:294:SER:HA	3:A0:297:GLU:HG3	1.94	0.48
4:A1:112:LEU:HD12	4:A1:115:SER:HB3	1.95	0.48
4:B1:113:ILE:HG13	4:B1:117:LEU:HD23	1.96	0.48
3:B2:3:GLU:HA	3:B2:51:THR:HA	1.95	0.48
3:B6:172:TRP:HH2	3:B6:191:THR:HB	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C0:323:VAL:HB	3:C0:355:ILE:HG12	1.95	0.48
3:C4:195:LEU:HD21	3:C4:264:ARG:HE	1.78	0.48
3:D0:205:ASP:HB2	3:D0:303:ALA:HA	1.94	0.48
4:F1:221:THR:HG23	4:F1:223:GLY:H	1.79	0.48
7:b:78:ALA:HB3	7:b:112:PHE:HE1	1.78	0.48
7:g:184:PRO:HB2	7:g:189:LEU:HB2	1.96	0.48
1:17:247:TYR:HE2	3:E2:81:GLY:HA3	1.78	0.48
4:A1:189:VAL:HA	4:A1:192:LEU:HB2	1.95	0.48
3:A2:373:ARG:HH22	2:B:257:ILE:HD11	1.79	0.48
4:A5:101:TRP:HE1	4:A5:188:SER:HB3	1.79	0.48
4:A7:113:ILE:HG13	4:A7:117:LEU:HD23	1.94	0.48
3:B4:265:ILE:HG22	3:B4:380:ASN:HD21	1.78	0.48
3:C2:102:ASN:HB3	3:C2:105:ARG:HB2	1.96	0.48
3:C4:66:VAL:HG12	3:C4:68:LEU:HD23	1.96	0.48
4:C7:20:PHE:HA	4:C7:230:SER:HB2	1.94	0.48
3:D2:30:ILE:HG22	3:D2:36:MET:HG2	1.94	0.48
3:D6:272:TYR:HB3	3:D6:275:ILE:HD11	1.96	0.48
3:E4:310:GLY:HA3	3:E4:383:ALA:HB2	1.95	0.48
4:E9:273:LEU:HD11	4:E9:298:ASN:HD21	1.78	0.48
7:j:119:ARG:HH21	7:j:136:LEU:HD23	1.78	0.48
3:A4:7:ILE:HG21	3:A4:153:LEU:HD21	1.96	0.48
3:B0:141:VAL:HB	3:B0:173:PRO:HD3	1.95	0.48
4:B3:100:ASN:HB3	4:B3:103:LYS:HG2	1.96	0.48
4:B7:200:GLN:HG2	4:B7:266:PHE:HB2	1.96	0.48
4:B9:396:HIS:HA	4:B9:399:THR:HG22	1.96	0.48
4:C1:310:TYR:HA	4:C1:371:SER:HA	1.95	0.48
3:C2:251:ASP:H	3:C2:254:GLU:HB3	1.77	0.48
3:C2:359:PRO:HB3	3:C2:372:MET:HA	1.94	0.48
4:C5:215:LEU:HD21	4:C5:273:LEU:HD22	1.95	0.48
4:C5:220:PRO:HD2	3:C6:326:LYS:HG3	1.94	0.48
4:C7:32:PRO:HB3	4:C7:81:PHE:HA	1.94	0.48
4:D3:272:PRO:HG3	4:D3:284:LEU:HD21	1.95	0.48
3:E8:269:LEU:HD21	3:E8:384:ILE:HG12	1.95	0.48
7:i:42:TYR:HD2	7:i:45:MET:HE2	1.78	0.48
7:m:113:VAL:HG22	7:m:134:ILE:HD11	1.95	0.48
1:10:245:SER:HA	4:C9:320:ARG:HH12	1.78	0.48
3:A2:136:LEU:HD22	3:A2:169:PHE:HE2	1.77	0.48
3:A2:288:VAL:HG21	3:A2:327:ASP:HB3	1.95	0.48
4:A5:53:GLU:HG3	4:A5:55:THR:H	1.78	0.48
3:A6:221:ARG:HA	4:A7:324:LYS:HG3	1.95	0.48
4:B1:421:GLU:HA	4:B1:424:GLN:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B4:156:ARG:HA	3:B4:159:VAL:HG12	1.95	0.48
3:B4:406:HIS:HA	3:B4:409:VAL:HG12	1.96	0.48
3:B8:398:MET:HE3	4:B9:345:ILE:HG23	1.96	0.48
4:B9:202:ILE:HD12	4:B9:300:MET:HE2	1.95	0.48
3:C2:402:ARG:HD2	3:C2:405:VAL:HG21	1.95	0.48
4:C7:91:VAL:HG11	4:C7:116:VAL:HG12	1.96	0.48
4:E1:215:LEU:HD21	4:E1:273:LEU:HD22	1.94	0.48
3:E2:70:LEU:HD12	3:E2:145:THR:HB	1.96	0.48
4:E5:288:GLU:HA	4:E5:291:GLN:HG3	1.96	0.48
4:E9:302:ALA:HB1	4:E9:374:ILE:HD11	1.96	0.48
7:o:9:PRO:HA	7:o:12:VAL:HG12	1.96	0.48
1:10:248:ARG:HH22	3:C8:80:THR:HG23	1.79	0.47
1:13:247:TYR:HE2	3:D4:81:GLY:HA3	1.79	0.47
4:A1:362:LYS:HG3	4:A1:363:MET:HG2	1.96	0.47
4:C3:183:TYR:O	4:C3:187:LEU:HB2	2.14	0.47
4:D5:138:SER:HA	4:D5:169:VAL:HG22	1.96	0.47
4:D9:113:ILE:HG13	4:D9:117:LEU:HD13	1.96	0.47
4:D9:293:MET:HE1	4:D9:315:ALA:HB2	1.95	0.47
3:E0:223:THR:HA	4:E1:323:THR:HG22	1.96	0.47
3:E8:119:LEU:HD22	3:E8:156:ARG:HH11	1.78	0.47
6:J:392:ARG:HD2	6:K:233:TYR:HD2	1.78	0.47
7:r:14:LYS:HD3	7:r:47:LEU:HD12	1.95	0.47
4:A1:128:ASP:HB3	5:F:160:MET:HE1	1.95	0.47
4:A9:217:LEU:HB2	4:A9:220:PRO:HG3	1.95	0.47
3:B0:32:PRO:HA	3:B0:86:LEU:HD12	1.95	0.47
3:B2:332:VAL:HA	3:B2:335:ILE:HG22	1.96	0.47
4:C1:388:MET:HG3	3:C2:347:CYS:HA	1.97	0.47
4:C7:248:SER:HA	4:C7:252:LYS:HD2	1.96	0.47
4:D5:8:GLN:HG2	4:D5:17:GLY:HA3	1.95	0.47
3:D6:26:LEU:HD12	3:D6:363:VAL:HG12	1.96	0.47
3:E6:106:GLY:HA3	3:E6:148:GLY:HA3	1.96	0.47
3:E6:298:PRO:HB2	3:E6:306:ASP:HB2	1.95	0.47
3:E8:224:TYR:HB2	4:E9:245:GLN:HE21	1.77	0.47
4:E9:224:ASP:O	4:E9:228:LEU:HD12	2.14	0.47
3:F0:225:THR:O	3:F0:229:ARG:HG2	2.14	0.47
6:I:222:ASN:HD22	6:I:402:TRP:NE1	2.10	0.47
7:a:82:ASP:HB3	7:a:85:CYS:HB3	1.96	0.47
7:f:18:ASN:HD21	7:f:46:ASP:H	1.59	0.47
7:f:63:ILE:HD11	7:f:132:LEU:HD11	1.96	0.47
8:k:73:TYR:HB2	8:k:92:TRP:HE1	1.78	0.47
4:A7:97:ALA:HB3	4:A7:143:THR:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:THR:O	2:B:228:LEU:HB2	2.13	0.47
4:B1:15:GLN:HB3	4:B1:226:ASN:HD21	1.79	0.47
4:B7:265:PHE:HB3	4:B7:374:ILE:HD13	1.95	0.47
4:C3:422:TYR:HA	4:C3:425:TYR:CE1	2.50	0.47
4:D3:215:LEU:HD11	4:D3:273:LEU:HD22	1.97	0.47
3:D4:88:HIS:CE1	3:D4:90:GLU:HG3	2.49	0.47
3:D8:3:GLU:HA	3:D8:51:THR:HA	1.95	0.47
3:D8:98:ASP:HB3	3:D8:100:ALA:H	1.79	0.47
3:E0:403:ALA:HB2	4:E1:344:TRP:HZ3	1.80	0.47
4:E3:186:THR:HA	4:E3:189:VAL:HG12	1.96	0.47
4:E5:113:ILE:HA	4:E5:116:VAL:HG12	1.96	0.47
3:E6:161:TYR:HD2	3:E6:164:LYS:HG3	1.80	0.47
3:E8:181:VAL:HG12	4:E9:350:LYS:HE3	1.95	0.47
7:m:73:VAL:HB	7:m:173:ILE:HB	1.96	0.47
7:n:111:ILE:HD13	7:n:132:LEU:HB2	1.97	0.47
7:t:97:ARG:HH22	7:v:161:TYR:HD1	1.60	0.47
3:A0:104:ALA:HB1	3:A0:411:GLU:OE2	2.15	0.47
3:A0:270:SER:HB2	3:A0:378:ILE:HG12	1.97	0.47
3:B6:407:TRP:O	3:B6:411:GLU:HB2	2.14	0.47
4:C1:259:PRO:HD2	4:C1:263:LEU:HD12	1.95	0.47
4:C5:107:THR:HG22	4:C5:108:GLU:H	1.79	0.47
3:C6:24:PHE:HA	3:C6:27:GLU:HG2	1.96	0.47
4:C9:8:GLN:HE21	4:C9:65:LEU:HG	1.78	0.47
4:C9:318:ARG:HA	4:C9:354:CYS:HB3	1.95	0.47
4:E9:143:THR:HA	4:E9:147:MET:HG2	1.96	0.47
3:F0:274:PRO:HD3	3:F0:375:VAL:HG12	1.96	0.47
5:G:116:GLU:O	5:G:120:GLU:CB	2.63	0.47
7:v:12:VAL:HG12	7:v:15:ARG:HH22	1.78	0.47
1:11:254:LYS:HB2	3:D0:26:LEU:HD21	1.96	0.47
3:A0:274:PRO:HB3	3:A0:291:ILE:HG22	1.96	0.47
3:A4:194:LEU:HG	3:A4:267:PHE:HE1	1.80	0.47
4:A5:66:MET:HE1	4:A5:147:MET:HG3	1.97	0.47
3:B4:191:THR:HA	3:B4:194:LEU:HG	1.97	0.47
3:B6:363:VAL:HG23	3:B6:366:GLY:HA3	1.96	0.47
3:C0:319:TYR:CE1	3:C0:375:VAL:HG12	2.49	0.47
3:C6:27:GLU:HB3	3:C6:361:THR:HG21	1.96	0.47
4:D1:164:MET:HB3	4:D1:164:MET:HE2	1.82	0.47
4:D3:177:ASP:HB2	3:D4:353:CYS:H	1.79	0.47
4:D3:316:MET:HG2	4:D3:352:SER:HB2	1.95	0.47
4:E5:51:TYR:HE1	4:E5:84:LEU:HD21	1.78	0.47
4:E5:272:PRO:HG2	4:E5:361:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F0:70:LEU:H	3:F0:145:THR:HG21	1.78	0.47
4:F1:19:LYS:HE3	4:F1:223:GLY:HA2	1.96	0.47
4:F1:51:TYR:HB3	4:F1:59:PHE:HB3	1.96	0.47
4:F1:167:PHE:CD2	4:F1:233:MET:HE2	2.50	0.47
6:K:259:VAL:HG22	6:K:265:VAL:HG22	1.95	0.47
8:k:45:LYS:HD2	8:k:129:PRO:HG3	1.96	0.47
8:l:38:PHE:HB3	8:l:128:ILE:HG13	1.97	0.47
7:m:55:LEU:HD22	7:m:111:ILE:HD12	1.96	0.47
7:m:111:ILE:HD13	7:m:132:LEU:HB2	1.96	0.47
7:o:110:ILE:HB	7:o:131:TRP:CG	2.49	0.47
7:r:115:LEU:HD11	7:r:145:LYS:HZ1	1.79	0.47
4:A1:73:MET:HA	4:A1:76:VAL:HG12	1.95	0.47
3:A2:234:VAL:HG21	3:A2:302:MET:HE1	1.95	0.47
3:B0:140:ALA:HA	3:B0:171:SER:HB3	1.95	0.47
4:B1:285:SER:O	4:B1:289:LEU:HB2	2.14	0.47
3:B2:280:LYS:HG2	3:B6:88:HIS:HE1	1.80	0.47
3:B6:306:ASP:HB3	3:B6:309:HIS:CE1	2.50	0.47
3:C0:270:SER:HB3	3:C0:378:ILE:HG23	1.95	0.47
4:C1:274:THR:HG21	4:C1:282:ARG:HE	1.80	0.47
4:C3:171:PRO:HG2	4:C3:185:ALA:HB2	1.95	0.47
4:C3:325:GLU:O	4:C3:329:GLN:HB2	2.14	0.47
3:C4:222:PRO:HD2	4:C5:324:LYS:HD3	1.97	0.47
4:C9:42:LEU:HD13	4:C9:356:ILE:HD11	1.96	0.47
3:D0:202:VAL:HG12	3:D0:268:MET:HB2	1.96	0.47
4:E7:290:THR:HA	4:E7:293:MET:HG2	1.96	0.47
4:E9:270:PHE:HE1	4:E9:361:LEU:HD22	1.80	0.47
7:a:142:GLU:HA	7:a:145:LYS:HG2	1.97	0.47
8:k:17:GLN:HB3	8:k:21:TYR:H	1.79	0.47
1:11:248:ARG:HH12	4:D1:42:LEU:HD13	1.80	0.47
1:15:239:LEU:HD11	4:D9:360:GLY:HA2	1.96	0.47
3:A0:210:TYR:HD1	3:A0:222:PRO:HG2	1.79	0.47
3:A2:83:TYR:HB3	3:A2:86:LEU:HB3	1.95	0.47
4:A3:117:LEU:HA	4:A3:120:VAL:HG12	1.95	0.47
4:A5:16:ILE:HA	4:A5:226:ASN:HB3	1.96	0.47
4:A7:47:ILE:HG13	4:A7:51:TYR:HB2	1.95	0.47
3:A8:167:LEU:HG	3:A8:200:VAL:HB	1.97	0.47
4:A9:313:ALA:O	4:A9:349:MET:HA	2.15	0.47
3:C0:417:GLU:HA	3:C0:420:GLU:HG3	1.97	0.47
3:C4:259:LEU:HD13	3:C4:316:CYS:HB2	1.96	0.47
3:C6:208:ALA:HB2	3:C6:304:LYS:HB2	1.96	0.47
4:C7:2:ARG:HH21	4:C7:240:LEU:HA	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C7:105:HIS:HA	4:C7:150:LEU:HD22	1.97	0.47
3:D2:204:LEU:HD23	3:D2:209:ILE:HD11	1.95	0.47
4:D3:309:ARG:H	4:D3:372:THR:HG22	1.78	0.47
4:D7:135:ILE:HB	4:D7:166:THR:HG22	1.96	0.47
3:D8:99:ALA:O	3:D8:102:ASN:HB2	2.15	0.47
3:D8:272:TYR:HB3	3:D8:275:ILE:HD11	1.96	0.47
4:E3:288:GLU:HA	4:E3:291:GLN:HG2	1.97	0.47
4:E5:91:VAL:HG21	4:E5:116:VAL:HG23	1.96	0.47
3:E8:31:GLN:HB2	5:G:125:ARG:HH22	1.80	0.47
3:E8:225:THR:O	3:E8:229:ARG:HG2	2.14	0.47
4:E9:318:ARG:NH1	4:E9:358:PRO:HG3	2.23	0.47
3:F0:169:PHE:HZ	3:F0:238:LEU:HD13	1.78	0.47
4:F1:131:GLN:HG2	4:F1:240:LEU:HD21	1.95	0.47
6:H:308:TRP:HB2	6:H:313:TRP:CZ3	2.50	0.47
7:d:172:VAL:HG23	7:d:180:ALA:HB3	1.96	0.47
7:f:141:THR:O	7:f:145:LYS:HG3	2.15	0.47
8:k:112:PRO:HD2	8:k:127:ALA:HB3	1.96	0.47
7:n:41:ASN:HB2	7:n:44:ASP:HB2	1.97	0.47
7:s:9:PRO:HA	7:s:12:VAL:HG22	1.97	0.47
7:t:53:GLY:HA2	7:t:62:VAL:HG11	1.97	0.47
7:t:96:TYR:HA	7:t:108:ILE:HD11	1.96	0.47
7:x:165:THR:HB	7:x:182:PHE:HZ	1.79	0.47
3:A0:118:SER:O	3:A0:122:ILE:HG12	2.15	0.47
4:A1:31:ASP:OD1	4:A1:32:PRO:HD2	2.14	0.47
3:A2:254:GLU:HA	3:A2:257:THR:HG22	1.96	0.47
3:B2:72:PRO:O	3:B2:76:ASP:HB3	2.15	0.47
4:C3:56:GLY:H	7:j:84:LYS:HZ1	1.62	0.47
4:C9:255:VAL:HG13	4:C9:256:ASN:OD1	2.15	0.47
4:D9:50:PHE:HD2	4:D9:241:ARG:HD3	1.78	0.47
3:E0:407:TRP:HE1	4:E1:258:ILE:HG13	1.80	0.47
3:E2:288:VAL:HG13	3:E2:319:TYR:CE2	2.50	0.47
6:J:397:GLY:HA3	6:K:399:VAL:HA	1.97	0.47
7:i:15:ARG:O	7:i:19:GLU:HG3	2.15	0.47
7:q:10:LEU:HG	7:q:143:ILE:HG22	1.97	0.47
7:w:55:LEU:HB3	7:w:132:LEU:HD13	1.97	0.47
7:x:170:VAL:HG23	7:x:183:LEU:HB2	1.97	0.47
1:15:247:TYR:HE1	3:D8:81:GLY:HA3	1.80	0.47
2:A:517:ALA:HB2	2:A:523:ASP:HB2	1.97	0.47
3:A2:210:TYR:CE1	4:A3:324:LYS:HA	2.50	0.47
3:A2:311:LYS:HZ3	3:A2:342:GLN:HB3	1.79	0.47
4:A5:289:LEU:HD13	4:A5:365:VAL:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B0:398:MET:HE1	4:B1:345:ILE:HG23	1.97	0.47
3:B2:212:ILE:HG22	3:B2:275:ILE:HD11	1.97	0.47
4:B7:299:MET:HE3	4:B7:305:PRO:HG3	1.97	0.47
3:C0:23:LEU:HA	3:C0:26:LEU:HD12	1.96	0.47
3:C0:115:VAL:HG21	3:C0:152:LEU:HD22	1.97	0.47
4:C1:388:MET:HB2	3:C2:348:PRO:HD2	1.97	0.47
4:C3:281:TYR:CE2	4:C7:86:ARG:HG3	2.50	0.47
3:C6:265:ILE:HG23	3:C6:432:TYR:HE1	1.80	0.47
4:D3:215:LEU:HB3	4:D3:217:LEU:HD13	1.96	0.47
3:D8:204:LEU:HD13	3:D8:231:ILE:HG12	1.97	0.47
3:D8:347:CYS:SG	3:D8:350:GLY:HA3	2.55	0.47
4:E5:396:HIS:HA	4:E5:399:THR:HG22	1.95	0.47
3:F0:269:LEU:HD21	3:F0:384:ILE:HG12	1.96	0.47
7:d:50:PHE:HD2	7:d:65:GLN:HG3	1.80	0.47
7:i:113:VAL:HG12	7:i:145:LYS:HZ3	1.80	0.47
7:n:182:PHE:HE2	7:n:187:SER:HB3	1.79	0.47
4:A7:21:TRP:HA	4:A7:24:ILE:HG22	1.96	0.47
4:B7:421:GLU:HA	4:B7:424:GLN:HG2	1.96	0.47
3:C2:191:THR:HG21	3:C2:425:LEU:HD13	1.96	0.47
3:D0:108:TYR:CE2	3:D0:413:MET:HG2	2.50	0.47
4:D9:421:GLU:HA	4:D9:424:GLN:HG2	1.97	0.47
4:E1:284:LEU:HG	4:E1:363:MET:HE2	1.96	0.47
4:E9:262:ARG:HB3	4:E9:418:LEU:HA	1.97	0.47
4:F1:117:LEU:HA	4:F1:120:VAL:HG12	1.97	0.47
6:J:365:LEU:HD13	6:J:378:VAL:HG21	1.97	0.47
6:K:344:ILE:HD11	6:K:368:LEU:HD13	1.97	0.47
7:m:74:ALA:HA	7:m:171:ILE:O	2.15	0.47
7:x:150:VAL:HG13	7:x:165:THR:HG23	1.97	0.47
3:A4:231:ILE:O	3:A4:235:ILE:HG12	2.15	0.46
4:A5:7:VAL:HG23	4:A5:64:ILE:HB	1.96	0.46
4:B1:183:TYR:O	4:B1:187:LEU:HB2	2.15	0.46
4:B1:334:GLN:HE22	4:B1:347:ASN:HA	1.80	0.46
4:B3:36:TYR:HE2	4:B3:39:ASP:H	1.63	0.46
3:B6:70:LEU:HD12	3:B6:99:ALA:HB2	1.96	0.46
4:B7:66:MET:HE2	4:B7:116:VAL:HG21	1.98	0.46
3:C2:323:VAL:HB	3:C2:355:ILE:HG12	1.97	0.46
4:C3:171:PRO:HB3	4:C3:181:GLU:HG2	1.96	0.46
3:D4:137:MET:HE3	3:D4:154:LEU:HG	1.97	0.46
7:d:74:ALA:HB2	7:d:172:VAL:HG12	1.96	0.46
7:f:9:PRO:HA	7:f:12:VAL:HG22	1.97	0.46
7:j:77:PHE:CD2	7:j:150:VAL:HG11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:p:129:MET:HE3	7:p:131:TRP:NE1	2.30	0.46
7:x:79:ASP:HB2	7:x:167:VAL:HG21	1.97	0.46
4:A3:318:ARG:O	4:A3:363:MET:HA	2.15	0.46
4:A7:64:ILE:HD12	4:A7:119:VAL:HG12	1.96	0.46
4:B1:238:CYS:HB3	4:B1:318:ARG:NH1	2.30	0.46
3:C0:427:ALA:HA	3:C0:430:LYS:HZ2	1.80	0.46
3:C2:243:ARG:HH21	3:C2:320:ARG:HH21	1.63	0.46
4:C5:412:GLU:HA	4:C5:415:MET:HB2	1.96	0.46
3:D0:27:GLU:HB2	3:D0:361:THR:HG21	1.95	0.46
4:D3:405:GLU:HA	4:D3:408:PHE:HD2	1.80	0.46
3:D8:141:VAL:HG12	3:D8:187:SER:HA	1.96	0.46
5:E:125:ARG:HH22	3:F0:31:GLN:HG3	1.80	0.46
4:E1:391:ARG:HD3	3:E2:346:TRP:CD1	2.50	0.46
4:E3:135:ILE:HG21	4:E3:152:ILE:HD11	1.97	0.46
3:E4:387:VAL:HG12	3:E4:390:ARG:NH2	2.30	0.46
4:E5:187:LEU:HA	4:E5:190:HIS:CE1	2.50	0.46
3:E6:122:ILE:HG21	3:E6:157:LEU:HD11	1.97	0.46
3:E6:141:VAL:HB	3:E6:173:PRO:HD3	1.97	0.46
7:f:172:VAL:HG11	7:f:204:THR:HG21	1.97	0.46
8:l:145:ASN:H	8:l:153:VAL:HG11	1.80	0.46
7:w:185:ILE:HG23	7:w:192:GLY:HA2	1.97	0.46
3:A2:7:ILE:HG21	3:A2:137:MET:HE2	1.97	0.46
4:A7:167:PHE:CE2	4:A7:233:MET:HG2	2.51	0.46
4:B1:318:ARG:O	4:B1:363:MET:HA	2.15	0.46
3:B2:101:ASN:HB3	3:B2:182:VAL:HG11	1.97	0.46
3:C0:205:ASP:HB2	3:C0:303:ALA:HA	1.97	0.46
3:C2:334:THR:HA	3:C2:337:THR:HG22	1.98	0.46
3:C4:207:GLU:HA	3:C4:210:TYR:HB2	1.97	0.46
3:C6:318:MET:O	3:C6:375:VAL:HA	2.15	0.46
4:D3:57:GLY:HA3	7:o:83:PRO:HB2	1.98	0.46
3:D6:225:THR:HA	3:D6:228:ASN:HB2	1.98	0.46
3:E2:244:PHE:HB2	3:E2:356:ASN:HD21	1.80	0.46
4:E5:20:PHE:CZ	4:E5:24:ILE:HD11	2.51	0.46
4:E7:200:GLN:HG2	4:E7:268:ILE:HD11	1.98	0.46
3:E8:31:GLN:HG3	3:E8:33:ASP:HB2	1.97	0.46
3:F0:262:TYR:HB2	3:F0:265:ILE:HG12	1.98	0.46
6:I:259:VAL:HG13	6:I:284:VAL:HG23	1.97	0.46
7:x:184:PRO:HB2	7:x:189:LEU:HB2	1.98	0.46
1:18:254:LYS:HE3	3:E4:364:PRO:HG2	1.95	0.46
2:A:467:PRO:HD2	4:C7:361:LEU:HD11	1.96	0.46
4:A1:349:MET:HE2	4:A1:349:MET:HB3	1.90	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A3:152:ILE:HG13	4:A3:164:MET:HE1	1.97	0.46
3:B0:255:PHE:O	3:B0:259:LEU:HB2	2.15	0.46
3:B2:252:VAL:HA	3:B2:255:PHE:HD2	1.81	0.46
4:C1:313:ALA:HB1	4:C1:367:PHE:HE1	1.80	0.46
3:C2:213:CYS:HA	3:C2:217:LEU:HD13	1.98	0.46
4:C5:206:ALA:HB2	4:C5:302:ALA:HB2	1.98	0.46
3:C8:101:ASN:HD22	4:C9:256:ASN:HD21	1.63	0.46
4:C9:191:GLN:HA	4:C9:194:GLU:HG2	1.96	0.46
3:D0:88:HIS:NE2	3:D0:90:GLU:HG2	2.31	0.46
3:D4:223:THR:HG22	3:D4:224:TYR:H	1.80	0.46
5:E:82:ARG:HH12	5:E:91:ALA:HB3	1.80	0.46
3:E6:221:ARG:HD2	4:E7:325:GLU:OE2	2.16	0.46
3:E8:113:GLU:HG3	3:E8:114:ILE:HG12	1.98	0.46
3:F0:390:ARG:HD3	3:F0:393:HIS:CE1	2.51	0.46
6:I:327:ALA:HA	6:I:337:VAL:HG12	1.98	0.46
7:i:78:ALA:HB3	7:i:112:PHE:HE1	1.79	0.46
3:A2:96:LYS:HE2	4:A3:1:MET:HA	1.98	0.46
4:A9:11:GLN:HE22	2:B:306:ARG:HE	1.64	0.46
4:A9:171:PRO:HG2	4:A9:185:ALA:HB2	1.97	0.46
3:B0:3:GLU:HG3	3:B0:132:LEU:HD13	1.96	0.46
3:B6:271:SER:HB3	3:B6:377:MET:HE3	1.97	0.46
3:C0:136:LEU:HD23	3:C0:167:LEU:HB2	1.97	0.46
3:C2:277:SER:O	3:C2:281:ALA:CB	2.63	0.46
4:C5:121:ARG:O	4:C5:125:GLU:HB2	2.15	0.46
3:C6:274:PRO:HB3	3:C6:371:VAL:HG11	1.98	0.46
4:D3:172:SER:HB3	4:D3:176:SER:HB3	1.96	0.46
3:D4:164:LYS:HD3	3:D4:164:LYS:HA	1.75	0.46
6:H:392:ARG:HH21	6:I:234:THR:HG22	1.81	0.46
7:b:99:MET:HE1	7:b:201:TRP:CD2	2.51	0.46
7:g:88:LEU:HD23	7:g:168:PRO:HB2	1.98	0.46
7:n:67:HIS:ND1	7:p:19:GLU:HG3	2.30	0.46
7:n:117:ARG:NH1	7:n:121:ALA:H	2.14	0.46
7:s:42:TYR:HA	7:s:45:MET:HG2	1.97	0.46
7:t:140:LEU:HA	7:t:143:ILE:HG22	1.98	0.46
7:u:55:LEU:HB3	7:u:63:ILE:HG23	1.98	0.46
1:15:254:LYS:HB2	3:D8:26:LEU:HD21	1.97	0.46
1:2:254:LYS:HB2	3:A8:26:LEU:HD21	1.98	0.46
3:A8:255:PHE:O	3:A8:259:LEU:CB	2.64	0.46
3:A8:398:MET:HE2	4:A9:345:ILE:HG23	1.98	0.46
3:B0:96:LYS:HE2	4:B1:129:CYS:HB3	1.97	0.46
4:B9:392:LYS:HD2	4:B9:395:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C8:181:VAL:HG12	4:C9:256:ASN:HB3	1.98	0.46
4:C9:32:PRO:HA	4:C9:84:LEU:HD11	1.98	0.46
3:D0:168:ASN:O	3:D0:201:ALA:HA	2.16	0.46
4:D1:51:TYR:HB3	4:D1:59:PHE:HB3	1.97	0.46
3:E0:240:ALA:HB1	3:E0:356:ASN:HD22	1.80	0.46
3:E2:225:THR:O	3:E2:229:ARG:HG2	2.16	0.46
4:E5:342:VAL:HG23	4:E5:345:ILE:HG22	1.98	0.46
4:E7:77:ARG:HH22	4:E7:92:PHE:HZ	1.64	0.46
3:E8:28:HIS:CE1	3:E8:49:PHE:HA	2.50	0.46
3:E8:319:TYR:HB2	3:E8:355:ILE:HA	1.98	0.46
7:b:77:PHE:CD1	7:b:150:VAL:HG11	2.50	0.46
7:h:15:ARG:O	7:h:19:GLU:HG3	2.16	0.46
8:l:112:PRO:HG2	8:l:127:ALA:HB3	1.97	0.46
3:A6:53:PHE:HB3	3:A6:61:HIS:HB3	1.97	0.46
4:B5:152:ILE:HG23	4:B5:164:MET:HE2	1.96	0.46
3:B6:329:ASN:HA	3:B6:332:VAL:HG12	1.98	0.46
4:C7:20:PHE:HB2	4:C7:233:MET:HE3	1.97	0.46
3:D2:30:ILE:HB	3:D2:34:GLY:HA2	1.98	0.46
4:D5:68:LEU:HD12	4:D5:143:THR:HB	1.98	0.46
4:D7:378:PHE:HD1	4:D7:415:MET:HE3	1.81	0.46
3:D8:398:MET:HE2	4:D9:345:ILE:HG23	1.97	0.46
4:E3:313:ALA:HB3	4:E3:349:MET:SD	2.55	0.46
4:E9:212:PHE:HA	4:E9:217:LEU:HD22	1.97	0.46
4:F1:65:LEU:HB2	4:F1:90:PHE:HD1	1.81	0.46
7:b:172:VAL:HB	7:b:204:THR:HG21	1.98	0.46
7:e:78:ALA:HB3	7:e:112:PHE:HE1	1.79	0.46
7:i:96:TYR:HA	7:i:108:ILE:HD11	1.96	0.46
7:s:78:ALA:HB3	7:s:112:PHE:HE1	1.81	0.46
4:A1:139:LEU:HA	4:A1:145:SER:HB2	1.98	0.46
4:A9:259:PRO:HG2	4:A9:311:LEU:HD21	1.98	0.46
4:B1:101:TRP:CD1	4:B1:145:SER:HG	2.34	0.46
3:B6:278:ALA:HB1	7:i:200:ASP:HB3	1.98	0.46
3:C0:16:ILE:HG13	3:C0:228:ASN:HB3	1.97	0.46
4:C3:342:VAL:HG12	4:C3:345:ILE:H	1.81	0.46
4:C5:77:ARG:HH22	4:C5:92:PHE:HE1	1.62	0.46
3:D6:408:TYR:HB3	3:D6:413:MET:HE2	1.98	0.46
3:D8:53:PHE:HB3	3:D8:61:HIS:HB3	1.96	0.46
4:E1:167:PHE:HZ	4:E1:236:VAL:HG21	1.81	0.46
3:E2:259:LEU:HD21	3:E2:316:CYS:HB2	1.97	0.46
4:E3:215:LEU:HD21	4:E3:273:LEU:HD22	1.97	0.46
4:E3:323:THR:HA	4:E3:326:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E8:259:LEU:HD11	3:E8:316:CYS:HB2	1.98	0.46
4:E9:19:LYS:HZ3	4:E9:223:GLY:HA2	1.80	0.46
4:E9:19:LYS:NZ	4:E9:223:GLY:HA2	2.30	0.46
4:F1:207:LEU:HB3	4:F1:225:LEU:HG	1.97	0.46
7:g:18:ASN:HD22	7:g:46:ASP:H	1.64	0.46
7:n:56:LYS:HG2	7:n:62:VAL:HG12	1.98	0.46
2:A:496:PRO:HD3	4:D1:215:LEU:HD12	1.98	0.46
4:A5:313:ALA:HB3	4:A5:349:MET:HG3	1.97	0.46
3:B2:265:ILE:HG22	3:B2:380:ASN:HD21	1.81	0.46
3:B4:5:ILE:HB	3:B4:135:PHE:HD1	1.81	0.46
3:B4:310:GLY:HA3	3:B4:383:ALA:HB2	1.97	0.46
4:B7:169:VAL:HG12	4:B7:202:ILE:HB	1.97	0.46
4:B7:172:SER:HB2	4:B7:205:GLU:HG3	1.97	0.46
4:B7:334:GLN:HE21	4:B7:349:MET:HG2	1.81	0.46
4:B9:238:CYS:SG	4:B9:318:ARG:HD2	2.55	0.46
4:B9:324:LYS:O	4:B9:328:GLU:HG3	2.16	0.46
3:C0:188:VAL:HA	3:C0:191:THR:HG23	1.97	0.46
3:C4:390:ARG:HH21	3:C4:391:MET:HE1	1.81	0.46
3:C6:32:PRO:HG2	8:l:64:GLY:N	2.31	0.46
4:C7:30:ILE:HG12	4:C7:36:TYR:HA	1.98	0.46
4:C7:328:GLU:HA	4:C7:331:LEU:HG	1.97	0.46
4:C9:135:ILE:O	4:C9:166:THR:HA	2.16	0.46
3:D0:115:VAL:HG21	3:D0:152:LEU:HD23	1.97	0.46
3:D2:318:MET:O	3:D2:375:VAL:HA	2.16	0.46
3:D4:142:GLY:HA2	3:D4:186:ASN:HB2	1.97	0.46
3:D6:6:SER:O	3:D6:65:CYS:HA	2.15	0.46
4:D7:179:VAL:HG23	3:D8:350:GLY:HA2	1.97	0.46
3:D8:195:LEU:HD11	3:D8:264:ARG:HG3	1.98	0.46
3:E4:156:ARG:HA	3:E4:159:VAL:HG12	1.98	0.46
4:F1:292:GLN:NE2	4:F1:298:ASN:HD21	2.12	0.46
7:e:11:ASN:O	7:e:15:ARG:HG3	2.16	0.46
7:m:12:VAL:HA	7:m:15:ARG:HG2	1.98	0.46
7:o:191:GLU:HG3	7:o:195:ALA:HB2	1.98	0.46
3:A0:319:TYR:HB3	3:A0:323:VAL:HG21	1.98	0.46
4:A1:117:LEU:HA	4:A1:120:VAL:HG12	1.96	0.46
3:A2:306:ASP:HB3	3:A2:309:HIS:CE1	2.50	0.46
3:A4:33:ASP:OD2	7:a:103:GLY:HA2	2.16	0.46
4:A5:66:MET:HE2	4:A5:147:MET:HE3	1.97	0.46
4:A7:8:GLN:HG3	4:A7:14:ASN:HA	1.96	0.46
4:A9:288:GLU:HA	4:A9:291:GLN:HG3	1.98	0.46
4:B3:97:ALA:HA	4:B3:103:LYS:HE2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B3:166:THR:O	4:B3:200:GLN:HB2	2.16	0.46
3:B6:119:LEU:HG	3:B6:156:ARG:HG2	1.98	0.46
4:B7:294:PHE:HZ	4:B7:349:MET:HE2	1.81	0.46
4:C5:19:LYS:HD2	4:C5:19:LYS:HA	1.77	0.46
4:C9:9:GLY:HA2	4:C9:66:MET:HG3	1.97	0.46
4:C9:397:TRP:HZ2	3:D0:260:VAL:HB	1.81	0.46
4:D5:155:VAL:HG12	4:D5:164:MET:HE1	1.98	0.46
4:D9:169:VAL:HG22	4:D9:202:ILE:HD11	1.97	0.46
3:E2:259:LEU:HB3	3:E2:268:MET:HE3	1.97	0.46
4:E7:113:ILE:HA	4:E7:116:VAL:HG12	1.97	0.46
3:E8:119:LEU:HD22	3:E8:156:ARG:HD3	1.97	0.46
3:F0:332:VAL:HG22	3:F0:351:PHE:CG	2.51	0.46
7:g:111:ILE:HG12	7:g:132:LEU:HB2	1.97	0.46
7:r:78:ALA:HB3	7:r:112:PHE:HE1	1.80	0.46
7:w:185:ILE:HD12	7:w:193:ASP:H	1.81	0.46
4:A1:317:PHE:HE1	4:A1:330:MET:HE1	1.81	0.45
4:A3:187:LEU:HA	4:A3:190:HIS:CE1	2.51	0.45
4:A5:192:LEU:HG	4:A5:199:VAL:HG21	1.97	0.45
4:A5:406:MET:O	4:A5:410:GLU:HB2	2.16	0.45
3:A6:231:ILE:O	3:A6:235:ILE:HG12	2.16	0.45
3:B0:225:THR:O	3:B0:229:ARG:HG2	2.15	0.45
4:B9:66:MET:HG2	4:B9:147:MET:HE1	1.97	0.45
4:C3:178:THR:O	4:C3:181:GLU:HG3	2.15	0.45
3:C4:208:ALA:O	3:C4:212:ILE:HG12	2.16	0.45
3:D6:189:LEU:HD11	3:D6:418:PHE:HE1	1.81	0.45
4:E9:169:VAL:HA	4:E9:202:ILE:HD13	1.98	0.45
3:F0:137:MET:HB3	3:F0:168:ASN:HB3	1.97	0.45
7:q:79:ASP:HB3	7:q:82:ASP:HB2	1.97	0.45
7:r:154:TYR:HE2	7:r:158:THR:HG22	1.81	0.45
3:A6:270:SER:HA	3:A6:377:MET:O	2.16	0.45
4:A7:67:ASP:HB2	4:A7:73:MET:HE2	1.98	0.45
4:B1:271:ALA:HB3	4:B1:365:VAL:HB	1.97	0.45
4:B5:284:LEU:HD12	4:B5:284:LEU:HA	1.84	0.45
4:C3:135:ILE:HG21	4:C3:152:ILE:HD11	1.98	0.45
4:C5:20:PHE:HA	4:C5:230:SER:HB2	1.98	0.45
3:C6:105:ARG:HA	3:C6:109:THR:HB	1.98	0.45
3:C6:396:ASP:HB3	3:C6:422:ARG:NH1	2.31	0.45
3:D2:76:ASP:HA	3:D2:79:ARG:HG2	1.98	0.45
4:D3:164:MET:HB2	4:D3:197:ASP:H	1.82	0.45
3:D4:178:SER:HB3	4:D5:347:ASN:ND2	2.30	0.45
3:D4:413:MET:HE3	3:D4:413:MET:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E1:186:THR:HA	4:E1:189:VAL:HG12	1.97	0.45
4:E3:151:LEU:O	4:E3:155:VAL:HG12	2.16	0.45
4:E3:405:GLU:HA	4:E3:408:PHE:HD2	1.80	0.45
3:E4:5:ILE:HG13	3:E4:132:LEU:HD11	1.98	0.45
4:E7:178:THR:HG22	4:E7:180:VAL:H	1.81	0.45
4:E7:221:THR:HG23	4:E7:223:GLY:H	1.81	0.45
3:E8:154:LEU:HD12	3:E8:197:HIS:HB3	1.99	0.45
4:F1:282:ARG:HH12	4:F1:288:GLU:HB3	1.80	0.45
6:I:399:VAL:H	6:I:404:PHE:HE2	1.65	0.45
7:q:97:ARG:NH2	7:s:5:VAL:HB	2.32	0.45
4:A3:245:GLN:HB2	4:A3:353:VAL:HB	1.97	0.45
3:A4:227:LEU:O	3:A4:231:ILE:HG12	2.15	0.45
4:B1:318:ARG:HE	4:B1:358:PRO:HD3	1.80	0.45
3:B4:397:LEU:HD22	4:B5:346:PRO:HD3	1.98	0.45
4:B5:169:VAL:HG12	4:B5:202:ILE:HB	1.97	0.45
4:B5:241:ARG:HG3	4:B5:242:PHE:CD2	2.51	0.45
4:B7:290:THR:HA	4:B7:293:MET:HE2	1.98	0.45
3:B8:207:GLU:HA	3:B8:210:TYR:HB2	1.97	0.45
4:C1:135:ILE:HG21	4:C1:152:ILE:HD11	1.97	0.45
4:C3:34:GLY:HA2	4:C3:58:ARG:NH1	2.31	0.45
3:C6:17:GLY:HA2	3:C6:20:CYS:HB2	1.98	0.45
3:C8:240:ALA:HA	3:C8:243:ARG:HH21	1.80	0.45
3:E0:157:LEU:HB3	3:E0:166:LYS:HD3	1.98	0.45
3:E0:317:LEU:HD22	3:E0:319:TYR:HE1	1.81	0.45
4:E5:175:VAL:HG12	3:E6:329:ASN:HB3	1.97	0.45
3:E8:66:VAL:HG21	3:E8:122:ILE:HG13	1.97	0.45
6:H:397:GLY:HA3	6:I:401:CYS:H	1.81	0.45
7:j:144:LEU:HD22	7:j:148:PHE:HE2	1.81	0.45
7:n:83:PRO:HA	7:n:86:ALA:HB3	1.99	0.45
4:A1:99:ASN:HA	4:A1:142:GLY:H	1.80	0.45
3:A2:320:ARG:HG3	3:A2:360:PRO:HG3	1.98	0.45
4:A5:139:LEU:HB3	4:A5:171:PRO:HD3	1.99	0.45
3:A6:325:PRO:HA	3:A6:328:VAL:HB	1.99	0.45
2:B:241:ARG:HD2	2:B:241:ARG:HA	1.72	0.45
4:B5:57:GLY:HA3	7:f:83:PRO:HB2	1.98	0.45
3:B8:210:TYR:CD2	4:B9:324:LYS:HG2	2.51	0.45
4:B9:33:THR:HG23	4:B9:35:THR:HG23	1.98	0.45
3:C0:137:MET:O	3:C0:168:ASN:HA	2.16	0.45
3:C0:406:HIS:CG	4:C1:261:PRO:HG3	2.52	0.45
3:C0:432:TYR:HA	3:C0:435:VAL:HG12	1.98	0.45
4:C3:382:SER:HB2	4:C3:415:MET:HE1	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C5:112:LEU:HB2	4:C5:147:MET:HE1	1.97	0.45
3:E0:176:GLN:HG2	3:E0:177:VAL:HG23	1.98	0.45
3:E4:238:LEU:HD12	3:E4:318:MET:HE3	1.98	0.45
4:E5:5:VAL:HG23	4:E5:130:LEU:HD11	1.98	0.45
4:E9:246:LEU:HD12	4:E9:246:LEU:HA	1.82	0.45
4:E9:296:ALA:HB2	4:E9:306:ARG:HB2	1.97	0.45
7:a:172:VAL:HG23	7:a:180:ALA:HB3	1.98	0.45
7:g:170:VAL:HG23	7:g:183:LEU:HB2	1.98	0.45
7:r:183:LEU:HD23	7:r:196:LEU:HA	1.99	0.45
1:16:247:TYR:HB3	3:E0:77:GLU:OE2	2.16	0.45
4:A1:66:MET:HE1	4:A1:147:MET:HG2	1.98	0.45
3:A2:15:GLN:HG3	3:A2:228:ASN:ND2	2.31	0.45
3:A4:195:LEU:HD12	3:A4:428:LEU:HD22	1.98	0.45
4:A5:317:PHE:HB3	4:A5:321:MET:HE1	1.98	0.45
4:A9:113:ILE:HD12	4:A9:113:ILE:HA	1.88	0.45
3:B2:377:MET:HE2	3:B2:379:SER:HB3	1.98	0.45
3:B8:99:ALA:HA	3:B8:110:ILE:HD11	1.99	0.45
3:C0:132:LEU:HD23	3:C0:164:LYS:HE2	1.98	0.45
3:C6:291:ILE:HD12	3:C6:375:VAL:HG13	1.99	0.45
3:C8:11:GLN:HA	3:C8:74:VAL:HG11	1.98	0.45
4:C9:14:ASN:HD22	4:C9:73:MET:HE1	1.80	0.45
3:D2:88:HIS:CD2	3:D2:89:PRO:HD2	2.51	0.45
3:D4:84:ARG:HD3	7:p:98:THR:HG21	1.98	0.45
4:D5:180:VAL:HG13	4:D5:184:ASN:HD21	1.82	0.45
3:D6:140:ALA:HA	3:D6:171:SER:HB3	1.97	0.45
3:D6:388:PHE:HB3	3:D6:425:LEU:HD11	1.98	0.45
4:D7:20:PHE:HA	4:D7:230:SER:HB2	1.98	0.45
4:D7:253:LEU:HD12	4:D7:350:LYS:HZ1	1.82	0.45
4:D9:7:VAL:HG22	4:D9:64:ILE:HB	1.99	0.45
3:E2:53:PHE:HB3	3:E2:61:HIS:HB3	1.98	0.45
3:E4:282:TYR:HD2	3:E4:283:HIS:CE1	2.34	0.45
4:E9:44:LEU:HD13	4:E9:47:ILE:HG21	1.98	0.45
4:E9:190:HIS:HB2	4:E9:414:ASN:OD1	2.17	0.45
4:E9:377:MET:HE2	4:E9:380:ARG:HH21	1.82	0.45
7:a:78:ALA:HB3	7:a:112:PHE:HE1	1.80	0.45
7:m:97:ARG:O	7:m:101:GLU:HG3	2.17	0.45
7:o:63:ILE:HB	7:o:67:HIS:CD2	2.51	0.45
3:A0:217:LEU:HD23	3:A0:367:ASP:HB3	1.98	0.45
3:B6:147:SER:HB2	3:B6:190:SER:HB2	1.98	0.45
4:B7:186:THR:HG22	4:B7:411:ALA:HB1	1.98	0.45
3:C2:103:PHE:HD2	3:C2:413:MET:HE1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C2:104:ALA:HB2	3:C2:413:MET:HE3	1.98	0.45
4:C3:163:ILE:HD13	4:C3:250:LEU:HG	1.98	0.45
4:C5:372:THR:HA	4:C5:422:TYR:CZ	2.51	0.45
3:C6:282:TYR:HB2	7:n:202:ARG:NH2	2.32	0.45
3:C8:2:ARG:HG2	3:C8:51:THR:HG22	1.99	0.45
3:C8:200:VAL:HG11	3:C8:255:PHE:HE2	1.80	0.45
3:C8:272:TYR:HA	3:C8:375:VAL:O	2.16	0.45
3:C8:273:ALA:HA	3:C8:275:ILE:HG13	1.99	0.45
4:D3:378:PHE:HD1	4:D3:415:MET:HE3	1.81	0.45
4:D5:164:MET:HB3	4:D5:197:ASP:H	1.82	0.45
4:D7:7:VAL:HB	4:D7:135:ILE:HA	1.98	0.45
3:E2:312:TYR:HD2	3:E2:341:ILE:HG23	1.82	0.45
4:E3:200:GLN:HG2	4:E3:266:PHE:HB2	1.98	0.45
4:E3:282:ARG:HH12	4:E3:292:GLN:HE21	1.65	0.45
3:E6:71:GLU:HB3	3:E6:98:ASP:HB3	1.98	0.45
3:E8:15:GLN:HB3	3:E8:228:ASN:ND2	2.31	0.45
3:E8:220:GLU:HG2	3:E8:221:ARG:HG3	1.98	0.45
7:f:117:ARG:HH12	7:f:152:LYS:HE2	1.82	0.45
7:f:170:VAL:HG23	7:f:183:LEU:HB2	1.99	0.45
7:i:110:ILE:HB	7:i:131:TRP:CG	2.51	0.45
7:i:112:PHE:CG	7:i:129:MET:HE1	2.51	0.45
7:o:68:LEU:HB3	7:o:73:VAL:HG21	1.98	0.45
1:3:239:LEU:HB2	2:A:317:ARG:HH22	1.80	0.45
4:A1:284:LEU:HD12	4:A1:284:LEU:HA	1.79	0.45
3:A2:363:VAL:HA	3:A2:364:PRO:HD3	1.85	0.45
3:A6:174:SER:HB3	3:A6:207:GLU:H	1.82	0.45
3:A6:205:ASP:HB2	3:A6:303:ALA:HA	1.98	0.45
4:A9:65:LEU:HB3	4:A9:73:MET:HE1	1.98	0.45
4:B5:395:LEU:HD11	4:B5:408:PHE:CE2	2.51	0.45
3:B8:401:LYS:HD2	4:B9:344:TRP:CD2	2.51	0.45
3:C0:273:ALA:O	3:C0:375:VAL:HG22	2.17	0.45
3:C6:90:GLU:HB3	3:C6:121:ARG:HH11	1.82	0.45
3:C6:137:MET:SD	3:C6:154:LEU:HD11	2.57	0.45
4:C9:159:TYR:HB3	4:C9:162:ARG:HD3	1.98	0.45
4:D1:271:ALA:HA	4:D1:273:LEU:HG	1.97	0.45
3:D2:112:LYS:HD3	3:D2:112:LYS:HA	1.74	0.45
4:D3:134:GLN:HG3	4:D3:165:GLU:OE2	2.17	0.45
4:D9:2:ARG:HB3	4:D9:131:GLN:HB2	1.99	0.45
4:E1:121:ARG:O	4:E1:124:ALA:O	2.34	0.45
4:E3:64:ILE:HD13	4:E3:120:VAL:HG22	1.98	0.45
4:E9:117:LEU:O	4:E9:121:ARG:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E9:273:LEU:HD12	4:E9:292:GLN:HG2	1.99	0.45
3:F0:292:THR:HG21	3:F0:331:ALA:HB1	1.98	0.45
7:i:93:LEU:HA	7:i:131:TRP:HZ3	1.82	0.45
7:j:115:LEU:HD21	7:j:145:LYS:HZ2	1.81	0.45
3:A2:221:ARG:HA	4:A3:324:LYS:HE3	1.99	0.45
4:A7:20:PHE:HB2	4:A7:233:MET:HE3	1.99	0.45
4:A7:65:LEU:HB3	4:A7:73:MET:HE1	1.99	0.45
4:A9:39:ASP:HA	7:c:90:PRO:HG3	1.99	0.45
4:B1:68:LEU:HA	4:B1:93:GLY:HA3	1.99	0.45
4:B3:220:PRO:HD2	3:B4:326:LYS:HD3	1.98	0.45
3:B4:175:PRO:HB3	3:B4:390:ARG:NE	2.32	0.45
3:C0:107:HIS:HA	3:C0:152:LEU:HD11	1.98	0.45
3:C0:191:THR:HA	3:C0:194:LEU:HG	1.98	0.45
4:C5:155:VAL:HA	4:C5:158:GLU:HG2	1.99	0.45
3:C8:288:VAL:HG13	3:C8:319:TYR:HE2	1.82	0.45
3:D2:75:VAL:HG13	3:D2:79:ARG:HH12	1.82	0.45
4:D3:86:ARG:HG2	4:D3:88:ASP:H	1.81	0.45
4:D3:229:VAL:HG12	4:D3:233:MET:HE3	1.99	0.45
4:D5:237:THR:HG23	4:D5:241:ARG:HE	1.81	0.45
5:E:125:ARG:HH22	3:F0:31:GLN:HA	1.81	0.45
3:E8:360:PRO:HG2	3:E8:371:VAL:HG23	1.98	0.45
3:E8:408:TYR:HD2	3:E8:413:MET:HG3	1.82	0.45
4:E9:64:ILE:HD13	4:E9:120:VAL:HG22	1.99	0.45
3:F0:316:CYS:O	3:F0:377:MET:HA	2.17	0.45
7:f:9:PRO:HG3	7:f:146:ARG:HH21	1.81	0.45
8:k:14:LYS:HA	8:k:23:PRO:HA	1.98	0.45
7:n:92:LEU:HD11	7:n:170:VAL:HG11	1.99	0.45
1:0:255:PRO:HG3	7:c:178:ARG:HD3	1.98	0.45
4:A1:376:GLU:O	4:A1:380:ARG:HG2	2.16	0.45
4:A7:64:ILE:HD12	4:A7:64:ILE:HG23	1.83	0.45
4:B7:396:HIS:HA	4:B7:399:THR:HG22	1.98	0.45
3:C4:207:GLU:HA	3:C4:210:TYR:HD2	1.82	0.45
4:C9:21:TRP:HA	4:C9:24:ILE:HG22	1.97	0.45
4:D1:87:PRO:HA	4:D1:90:PHE:HD2	1.82	0.45
4:D1:313:ALA:HB1	4:D1:367:PHE:HE1	1.81	0.45
3:D6:316:CYS:O	3:D6:377:MET:HA	2.17	0.45
4:D7:34:GLY:HA3	4:D7:58:ARG:HD2	1.99	0.45
4:D7:151:LEU:O	4:D7:155:VAL:HG12	2.17	0.45
4:E9:8:GLN:HB2	4:E9:65:LEU:HG	1.99	0.45
4:E9:398:TYR:O	4:E9:402:GLY:CA	2.60	0.45
3:F0:390:ARG:HA	3:F0:393:HIS:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:215:PHE:HB3	6:H:230:TRP:CZ3	2.52	0.45
6:I:252:PRO:HB3	6:I:416:ILE:HG12	1.99	0.45
7:f:71:LYS:HG2	7:h:39:PRO:HG3	1.99	0.45
7:f:75:LEU:HD23	7:f:111:ILE:HB	1.99	0.45
7:g:18:ASN:HA	7:g:21:ARG:HB3	1.99	0.45
7:i:84:LYS:HG3	7:i:168:PRO:HD3	1.99	0.45
7:q:201:TRP:CD1	7:q:201:TRP:H	2.34	0.45
7:w:15:ARG:O	7:w:19:GLU:HG3	2.15	0.45
1:7:248:ARG:HH22	4:B9:42:LEU:HD22	1.81	0.45
3:A0:204:LEU:HD11	3:A0:231:ILE:HD13	1.99	0.45
4:A3:54:ALA:HB3	4:A3:58:ARG:HB3	1.99	0.45
4:A3:173:PRO:HB3	4:A3:380:ARG:HD3	1.98	0.45
3:B2:301:MET:HE1	3:B2:305:CYS:O	2.17	0.45
3:B8:75:VAL:HG21	3:B8:94:SER:HB2	1.99	0.45
3:C0:313:MET:HE3	3:C0:382:THR:HB	1.99	0.45
3:C2:175:PRO:HB3	3:C2:390:ARG:NH1	2.32	0.45
4:C3:134:GLN:HG3	4:C3:165:GLU:HB2	1.98	0.45
4:C5:130:LEU:HG	4:C5:162:ARG:HH12	1.83	0.45
3:C6:222:PRO:HD2	4:C7:324:LYS:HB3	1.99	0.45
4:D1:97:ALA:HA	4:D1:103:LYS:HD2	1.98	0.45
3:D4:68:LEU:HD23	3:D4:153:LEU:HD11	1.99	0.45
3:E4:172:TRP:HZ3	3:E4:194:LEU:HD21	1.82	0.45
3:E4:237:SER:HA	3:E4:320:ARG:HH11	1.81	0.45
4:E5:100:ASN:HB2	4:E5:103:LYS:HG3	1.98	0.45
6:I:221:LEU:HD21	6:I:245:PHE:HB2	1.99	0.45
6:I:386:MET:HA	6:I:394:VAL:O	2.17	0.45
7:o:55:LEU:HD11	7:o:111:ILE:HD12	1.98	0.45
1:19:248:ARG:HH21	4:E7:42:LEU:HD11	1.82	0.44
2:A:370:LEU:HD21	4:B9:215:LEU:HD22	1.98	0.44
4:A1:206:ALA:HB2	4:A1:302:ALA:HB2	1.99	0.44
3:A2:325:PRO:HA	3:A2:328:VAL:HG22	1.99	0.44
3:A6:279:GLU:OE2	7:d:198:ARG:HD2	2.17	0.44
4:B1:215:LEU:HD11	4:B1:273:LEU:HD22	1.99	0.44
3:B2:2:ARG:HG2	3:B2:51:THR:HG22	1.99	0.44
4:B3:313:ALA:O	4:B3:349:MET:HA	2.17	0.44
4:B5:392:LYS:NZ	4:B5:395:LEU:HD22	2.32	0.44
4:C1:116:VAL:HG11	4:C1:151:LEU:HD21	1.98	0.44
4:C3:187:LEU:HD13	4:C3:190:HIS:CE1	2.52	0.44
3:C6:185:TYR:O	3:C6:189:LEU:HB2	2.17	0.44
3:C6:253:THR:HA	3:C6:256:GLN:HG3	1.99	0.44
4:C7:313:ALA:O	4:C7:349:MET:HA	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C7:349:MET:HE2	4:C7:349:MET:HB2	1.56	0.44
3:C8:209:ILE:HG23	3:C8:230:LEU:HD23	1.98	0.44
3:D0:6:SER:O	3:D0:65:CYS:HA	2.17	0.44
3:D2:217:LEU:HD21	3:D2:368:LEU:HD23	1.98	0.44
3:D8:217:LEU:HB3	3:D8:219:ILE:HG13	2.00	0.44
3:E0:100:ALA:HA	4:E1:252:LYS:HG2	1.98	0.44
4:E1:171:PRO:HB3	4:E1:181:GLU:HG2	1.99	0.44
4:E1:284:LEU:HB3	4:E5:55:THR:HG21	1.97	0.44
4:E5:98:GLY:O	3:E6:257:THR:HG21	2.17	0.44
3:F0:259:LEU:HD23	3:F0:259:LEU:HA	1.88	0.44
3:F0:381:SER:HB2	3:F0:384:ILE:HG13	1.98	0.44
6:K:221:LEU:HB2	6:K:227:LEU:HD23	1.99	0.44
7:c:152:LYS:HE2	7:c:152:LYS:HB3	1.74	0.44
7:m:4:PRO:HG3	7:m:179:GLU:HB2	1.99	0.44
7:n:194:ARG:NH2	7:n:198:ARG:HE	2.15	0.44
2:A:469:GLN:HB2	4:C7:217:LEU:HD12	1.98	0.44
3:A0:181:VAL:HG22	4:A1:256:ASN:HB3	1.99	0.44
3:A2:104:ALA:O	3:A2:108:TYR:HB2	2.17	0.44
3:A4:217:LEU:HD11	3:A4:275:ILE:HG22	1.98	0.44
4:B7:4:ILE:HD11	4:B7:240:LEU:HD22	1.99	0.44
3:B8:193:SER:HA	3:B8:196:GLU:HG2	2.00	0.44
4:B9:188:SER:O	4:B9:192:LEU:HB2	2.17	0.44
4:B9:316:MET:HE1	4:B9:368:VAL:HG23	1.99	0.44
4:C1:156:ARG:HH12	4:C1:197:ASP:HB2	1.82	0.44
4:C3:173:PRO:HD2	4:C3:205:GLU:HB2	1.99	0.44
4:C3:269:GLY:HA2	4:C3:300:MET:HE3	2.00	0.44
3:C6:213:CYS:HA	3:C6:217:LEU:HD13	1.99	0.44
4:D1:61:PRO:HD2	4:D1:85:PHE:HA	1.98	0.44
4:D3:98:GLY:O	3:D4:257:THR:HG21	2.17	0.44
4:D7:124:ALA:HB1	4:D7:130:LEU:HD22	1.99	0.44
5:E:103:LEU:HD11	4:F1:228:LEU:HD23	1.99	0.44
3:E0:156:ARG:HA	3:E0:159:VAL:HG12	1.98	0.44
4:E1:242:PHE:HB3	4:E1:356:ILE:HD12	2.00	0.44
3:E4:407:TRP:CG	4:E5:255:VAL:HG23	2.52	0.44
4:E9:314:SER:HA	4:E9:350:LYS:HB2	1.99	0.44
6:K:222:ASN:HB3	6:K:402:TRP:CE2	2.52	0.44
7:i:9:PRO:HB2	7:i:143:ILE:HG23	1.99	0.44
7:i:129:MET:HE2	7:i:131:TRP:NE1	2.31	0.44
7:o:194:ARG:HH22	7:o:198:ARG:NH1	2.14	0.44
7:p:7:ALA:HB3	7:p:161:TYR:HE1	1.81	0.44
7:q:183:LEU:HD22	7:q:198:ARG:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A1:67:ASP:HB3	4:A1:73:MET:HE1	1.99	0.44
4:A1:167:PHE:CE2	4:A1:233:MET:HG3	2.52	0.44
4:A3:64:ILE:HD12	4:A3:119:VAL:HG12	1.98	0.44
3:A4:70:LEU:HD12	3:A4:145:THR:HB	1.99	0.44
3:A6:11:GLN:HG3	3:A6:74:VAL:HG21	2.00	0.44
4:A7:139:LEU:HD11	4:A7:192:LEU:HD22	2.00	0.44
4:B3:77:ARG:HH22	4:B3:92:PHE:HZ	1.65	0.44
4:B3:293:MET:HG3	4:B3:367:PHE:HB2	1.99	0.44
4:B5:396:HIS:HA	4:B5:399:THR:HG22	1.99	0.44
3:B6:398:MET:HG2	3:B6:403:ALA:HB3	1.99	0.44
4:B7:179:VAL:HG12	3:B8:258:ASN:OD1	2.16	0.44
4:B9:299:MET:HE3	4:B9:305:PRO:HG3	1.99	0.44
3:C6:31:GLN:HG3	3:C6:33:ASP:H	1.81	0.44
4:C7:193:VAL:HA	4:C7:264:HIS:CE1	2.52	0.44
3:D0:225:THR:O	3:D0:229:ARG:HG3	2.17	0.44
3:D0:320:ARG:HH12	3:D0:360:PRO:HA	1.82	0.44
3:D4:259:LEU:HB3	3:D4:268:MET:HE1	1.98	0.44
3:D6:407:TRP:O	3:D6:411:GLU:HG2	2.18	0.44
4:E1:151:LEU:O	4:E1:155:VAL:HG12	2.16	0.44
3:E2:5:ILE:HD13	3:E2:64:ARG:HB3	1.98	0.44
4:E3:317:PHE:HB3	4:E3:321:MET:SD	2.58	0.44
3:E4:275:ILE:HD12	3:E4:368:LEU:HD11	1.99	0.44
4:E5:173:PRO:HB3	4:E5:380:ARG:HD3	1.98	0.44
4:E9:173:PRO:HB3	4:E9:380:ARG:NH2	2.33	0.44
4:F1:282:ARG:NH1	4:F1:288:GLU:HB3	2.32	0.44
7:d:112:PHE:H	7:d:133:SER:HA	1.81	0.44
7:d:184:PRO:HB2	7:d:189:LEU:HB3	1.99	0.44
7:f:110:ILE:O	7:f:131:TRP:HB2	2.16	0.44
7:p:53:GLY:HA2	7:p:62:VAL:HG21	1.99	0.44
2:A:316:LEU:C	2:A:317:ARG:HG2	2.43	0.44
3:A0:208:ALA:HB2	3:A0:304:LYS:HG2	1.99	0.44
4:A1:309:ARG:HH21	4:A1:426:GLN:C	2.26	0.44
3:A2:207:GLU:HA	3:A2:210:TYR:HB2	1.99	0.44
3:A6:292:THR:HG21	3:A6:331:ALA:HB1	1.97	0.44
4:A7:267:LEU:HD21	4:A7:374:ILE:HG12	1.99	0.44
4:A7:294:PHE:CE2	4:A7:333:VAL:HG11	2.52	0.44
4:A9:267:LEU:HD21	4:A9:374:ILE:HG22	1.99	0.44
4:A9:349:MET:HB2	4:A9:349:MET:HE3	1.65	0.44
2:B:222:HIS:ND1	2:B:225:ALA:HB3	2.32	0.44
2:B:522:VAL:HG11	4:D3:276:ARG:HA	1.98	0.44
4:C3:20:PHE:CZ	4:C3:24:ILE:HG13	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C3:199:VAL:HG23	4:C3:264:HIS:CD2	2.53	0.44
3:D0:173:PRO:HB2	3:D0:391:MET:HE1	1.99	0.44
3:D0:332:VAL:HG13	3:D0:351:PHE:CD2	2.53	0.44
4:D3:21:TRP:HA	4:D3:24:ILE:HG22	1.99	0.44
3:E0:189:LEU:HD11	3:E0:418:PHE:HD1	1.82	0.44
3:E0:255:PHE:O	3:E0:259:LEU:HB2	2.18	0.44
3:E4:12:ALA:HB3	3:E4:140:ALA:HB2	1.99	0.44
6:H:266:GLY:HA2	6:H:276:ILE:HD13	2.00	0.44
3:A0:2:ARG:HA	3:A0:131:GLY:HA3	1.98	0.44
3:A0:88:HIS:H	3:A0:91:GLN:HE21	1.64	0.44
3:C0:398:MET:HB2	4:C1:346:PRO:HD2	2.00	0.44
3:C6:403:ALA:HB2	4:C7:344:TRP:HZ3	1.83	0.44
3:C8:188:VAL:O	3:C8:421:ALA:HB1	2.18	0.44
3:D4:271:SER:H	3:D4:377:MET:HB3	1.82	0.44
3:D8:88:HIS:HB3	3:D8:91:GLN:HG2	1.99	0.44
3:D8:175:PRO:HB3	3:D8:390:ARG:HD2	1.98	0.44
4:E1:299:MET:HE1	4:E1:367:PHE:HE2	1.82	0.44
3:E4:71:GLU:HB3	3:E4:98:ASP:HB3	2.00	0.44
3:E6:272:TYR:HD2	3:E6:275:ILE:HD11	1.82	0.44
4:E7:256:ASN:ND2	4:E7:350:LYS:HD3	2.33	0.44
4:E9:267:LEU:HD11	4:E9:367:PHE:HD2	1.81	0.44
3:F0:311:LYS:NZ	3:F0:347:CYS:HB2	2.32	0.44
7:h:23:LEU:HD23	7:h:38:LEU:HD21	1.99	0.44
7:q:115:LEU:HG	7:q:167:VAL:HG11	1.99	0.44
1:0:237:PRO:HD2	2:B:284:ARG:HH22	1.83	0.44
1:15:256:LEU:HD22	3:D8:29:GLY:HA2	1.99	0.44
3:B6:282:TYR:HE2	3:C0:85:HIS:HB3	1.82	0.44
4:C7:259:PRO:HG2	4:C7:311:LEU:HD23	1.99	0.44
3:D0:218:ASP:HB3	7:p:194:ARG:NH2	2.32	0.44
3:D4:75:VAL:HG11	3:D4:94:SER:HB2	2.00	0.44
4:D9:60:VAL:HG11	4:D9:86:ARG:HB2	2.00	0.44
4:E3:51:TYR:HB3	4:E3:59:PHE:HB3	2.00	0.44
4:E3:395:LEU:HD23	4:E3:395:LEU:HA	1.85	0.44
3:E6:247:ALA:HB3	3:E6:355:ILE:HB	1.99	0.44
3:E6:406:HIS:HA	3:E6:409:VAL:HG22	2.00	0.44
3:E6:425:LEU:HD12	3:E6:425:LEU:HA	1.84	0.44
4:E7:252:LYS:HE3	4:E7:350:LYS:HZ1	1.83	0.44
3:E8:222:PRO:HD2	4:E9:324:LYS:HE3	1.99	0.44
4:E9:256:ASN:O	4:E9:256:ASN:ND2	2.47	0.44
4:E9:289:LEU:O	4:E9:293:MET:HG3	2.17	0.44
3:F0:69:ASP:HA	3:F0:145:THR:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:k:13:VAL:HG13	8:k:24:VAL:HB	2.00	0.44
8:l:17:GLN:HE22	8:l:22:VAL:HG12	1.83	0.44
8:l:134:ILE:HD12	8:l:138:GLY:HA2	1.99	0.44
7:u:72:SER:HB3	7:u:108:ILE:HG22	1.98	0.44
1:11:247:TYR:HE2	3:D0:81:GLY:HA3	1.83	0.44
2:A:467:PRO:HG2	4:C7:270:PHE:HE2	1.82	0.44
3:A0:102:ASN:HD22	3:A0:104:ALA:HB3	1.82	0.44
4:B3:272:PRO:HG3	4:B3:284:LEU:HD11	2.00	0.44
4:C1:3:GLU:HB3	4:C1:130:LEU:HA	1.99	0.44
4:C3:5:VAL:HB	4:C3:133:PHE:HD1	1.82	0.44
4:C3:289:LEU:HD23	4:C3:365:VAL:HG12	2.00	0.44
3:C4:137:MET:HE3	3:C4:154:LEU:HD22	1.99	0.44
3:C4:234:VAL:HG22	3:C4:272:TYR:HB2	2.00	0.44
3:C4:269:LEU:HB2	3:C4:384:ILE:HD11	2.00	0.44
3:C6:26:LEU:HD23	3:C6:26:LEU:HA	1.89	0.44
3:C6:70:LEU:HD12	3:C6:145:THR:HG23	2.00	0.44
3:C6:237:SER:HA	3:C6:320:ARG:HD2	1.99	0.44
4:C7:86:ARG:HG2	4:C7:88:ASP:H	1.82	0.44
4:C9:117:LEU:HD21	4:C9:154:LYS:HB3	2.00	0.44
3:D8:405:VAL:HG13	3:D8:418:PHE:HE2	1.83	0.44
4:D9:381:VAL:HB	4:D9:415:MET:HE1	1.99	0.44
3:E8:32:PRO:HD2	5:G:125:ARG:NH2	2.33	0.44
3:E8:320:ARG:HH21	3:E8:358:GLN:HG3	1.83	0.44
4:E9:256:ASN:HB2	4:E9:350:LYS:HE3	2.00	0.44
4:E9:360:GLY:HA3	5:G:100:TYR:HD2	1.83	0.44
3:F0:228:ASN:HA	3:F0:231:ILE:HG22	1.98	0.44
4:F1:172:SER:OG	4:F1:205:GLU:HG3	2.18	0.44
6:I:290:ASP:HB2	6:I:297:TRP:CD1	2.53	0.44
7:c:112:PHE:HB2	7:c:131:TRP:HE1	1.82	0.44
7:g:78:ALA:HB3	7:g:112:PHE:HE1	1.82	0.44
7:i:72:SER:O	7:i:108:ILE:HA	2.18	0.44
7:i:144:LEU:HD22	7:i:148:PHE:HE1	1.83	0.44
7:m:175:SER:H	7:m:178:ARG:NH1	2.16	0.44
7:n:72:SER:HB2	7:n:108:ILE:HG22	1.99	0.44
7:q:97:ARG:HH21	7:s:7:ALA:H	1.64	0.44
2:A:490:HIS:ND1	2:A:493:LYS:HG2	2.33	0.44
4:A3:316:MET:HB2	4:A3:366:THR:HG22	1.99	0.44
4:A3:372:THR:HG21	4:A3:426:GLN:HG2	2.00	0.44
3:A6:200:VAL:HG13	3:A6:268:MET:HE2	1.99	0.44
4:A7:42:LEU:HD22	4:A7:356:ILE:HD11	1.99	0.44
3:A8:69:ASP:O	3:A8:94:SER:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B1:313:ALA:HB3	4:B1:349:MET:HB3	2.00	0.44
4:B3:73:MET:HA	4:B3:76:VAL:HG12	1.99	0.44
3:B6:318:MET:HE3	3:B6:318:MET:HB3	1.86	0.44
3:B8:168:ASN:HD22	3:B8:198:THR:HG21	1.83	0.44
3:B8:417:GLU:HA	3:B8:420:GLU:HG2	2.00	0.44
3:C2:135:PHE:HZ	3:C2:157:LEU:HD21	1.83	0.44
3:C2:386:GLU:HA	3:C2:389:SER:HB2	1.99	0.44
4:C3:293:MET:HA	4:C3:298:ASN:ND2	2.33	0.44
4:C7:39:ASP:HA	8:l:54:ARG:HH22	1.83	0.44
3:D0:335:ILE:HG23	3:D0:341:ILE:HD12	1.98	0.44
3:D2:319:TYR:HB3	3:D2:323:VAL:HG21	2.00	0.44
4:D5:42:LEU:HD13	4:D5:356:ILE:HD11	1.98	0.44
4:D7:117:LEU:HD21	4:D7:154:LYS:HG2	2.00	0.44
5:E:127:ARG:HE	3:F0:365:GLY:HA3	1.83	0.44
3:E2:100:ALA:O	4:E3:255:VAL:HG11	2.17	0.44
4:E7:24:ILE:HG23	4:E7:28:HIS:HD2	1.83	0.44
3:F0:223:THR:HG23	3:F0:225:THR:H	1.83	0.44
4:F1:44:LEU:HA	4:F1:47:ILE:HB	2.00	0.44
4:F1:399:THR:HG22	4:F1:403:MET:HG3	2.00	0.44
6:H:344:ILE:HD11	6:H:368:LEU:HD13	2.00	0.44
6:H:344:ILE:HG22	6:H:359:VAL:HG22	1.99	0.44
7:w:95:TYR:O	7:w:99:MET:HG2	2.18	0.44
1:10:250:GLU:HG3	3:C8:229:ARG:HH21	1.83	0.44
4:A9:2:ARG:HD3	4:A9:240:LEU:HD23	1.99	0.44
4:B1:16:ILE:HG22	4:B1:226:ASN:OD1	2.18	0.44
4:B3:212:PHE:HZ	3:B4:326:LYS:HG3	1.83	0.44
3:B6:255:PHE:O	3:B6:259:LEU:HB2	2.17	0.44
4:B7:321:MET:HE2	4:B7:363:MET:HE3	2.00	0.44
2:C:224:THR:O	2:C:228:LEU:CB	2.56	0.44
4:C3:156:ARG:HH22	4:C3:197:ASP:H	1.66	0.44
4:C9:148:GLY:O	4:C9:152:ILE:HG12	2.18	0.44
4:D1:101:TRP:HE3	4:D1:403:MET:HE1	1.83	0.44
4:D3:6:HIS:CE1	4:D3:8:GLN:HG2	2.53	0.44
3:E6:175:PRO:HG3	3:E6:390:ARG:CZ	2.47	0.44
5:G:115:THR:HG22	5:G:118:ARG:HG2	2.00	0.44
6:I:321:PHE:HE2	6:I:337:VAL:HG23	1.82	0.44
6:J:300:ASN:HD21	6:J:306:LEU:HD11	1.83	0.44
7:e:9:PRO:HA	7:e:12:VAL:HG22	2.00	0.44
7:e:139:PRO:O	7:e:143:ILE:HG12	2.18	0.44
4:A1:293:MET:HE3	4:A1:367:PHE:CD1	2.52	0.43
3:A2:27:GLU:CD	3:A2:243:ARG:HH12	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A2:244:PHE:CG	3:A2:358:GLN:HG3	2.53	0.43
4:A9:102:ALA:HB2	4:A9:398:TYR:HD1	1.83	0.43
4:B3:156:ARG:HA	4:B3:156:ARG:HD2	1.76	0.43
4:B3:252:LYS:HB3	4:B3:350:LYS:NZ	2.33	0.43
4:B7:100:ASN:HD21	4:B7:397:TRP:HB3	1.83	0.43
3:C0:12:ALA:HB2	10:C0:501:GTP:C5	2.53	0.43
3:C0:84:ARG:HH12	7:i:95:TYR:HD1	1.66	0.43
3:C2:53:PHE:HB3	3:C2:61:HIS:HB3	2.00	0.43
3:C6:224:TYR:CD2	4:C7:323:THR:HG21	2.52	0.43
4:C7:287:PRO:O	4:C7:291:GLN:HG2	2.17	0.43
3:C8:72:PRO:HD2	4:C9:2:ARG:HH21	1.82	0.43
4:D7:163:ILE:HG21	4:D7:250:LEU:HB3	1.99	0.43
3:E4:220:GLU:C	3:E4:222:PRO:HD3	2.43	0.43
4:E9:250:LEU:HA	4:E9:253:LEU:HG	1.99	0.43
3:F0:276:ILE:HG12	3:F0:284:GLU:OE2	2.18	0.43
6:K:284:VAL:HA	6:K:300:ASN:HA	2.00	0.43
7:a:172:VAL:HB	7:a:204:THR:HG21	2.00	0.43
7:c:15:ARG:HG2	7:c:45:MET:HE1	2.00	0.43
7:j:72:SER:HB3	7:j:108:ILE:HG22	2.00	0.43
7:x:71:LYS:HD3	7:x:106:GLN:HG2	1.99	0.43
4:A3:309:ARG:H	4:A3:372:THR:HG22	1.83	0.43
3:A4:175:PRO:HA	3:A4:390:ARG:HD2	2.01	0.43
3:A6:328:VAL:HG21	3:A6:355:ILE:HD11	2.00	0.43
4:A7:11:GLN:HA	4:A7:72:THR:HG21	1.99	0.43
4:A7:36:TYR:HE2	7:b:90:PRO:HG2	1.83	0.43
2:B:565:ASP:HB3	2:B:571:MET:HG2	2.01	0.43
3:B0:53:PHE:HB3	3:B0:61:HIS:HB3	2.00	0.43
4:B1:155:VAL:HA	4:B1:158:GLU:HG3	2.00	0.43
4:B1:230:SER:HA	4:B1:233:MET:HG2	1.99	0.43
4:B1:406:MET:O	4:B1:410:GLU:HG2	2.17	0.43
3:B6:3:GLU:HA	3:B6:51:THR:HA	2.00	0.43
4:B9:35:THR:HG22	7:h:83:PRO:HG3	2.00	0.43
3:C2:422:ARG:HH22	3:C2:425:LEU:HD23	1.83	0.43
4:C9:117:LEU:HD23	4:C9:121:ARG:HH12	1.83	0.43
4:C9:374:ILE:HD11	4:C9:422:TYR:CZ	2.54	0.43
4:D1:349:MET:HB3	4:D1:349:MET:HE2	1.74	0.43
3:D2:241:SER:HB2	3:D2:249:ASN:HB2	2.00	0.43
4:D3:66:MET:HA	4:D3:91:VAL:HG23	1.99	0.43
4:D9:229:VAL:HG12	4:D9:233:MET:HE3	1.99	0.43
4:E3:299:MET:HE1	4:E3:367:PHE:HE2	1.82	0.43
6:K:386:MET:HG2	6:K:395:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:b:67:HIS:HD2	7:d:23:LEU:HD22	1.83	0.43
7:e:56:LYS:HE2	7:e:60:ASN:HB2	2.00	0.43
7:e:64:PRO:HD2	7:e:67:HIS:CE1	2.53	0.43
7:e:110:ILE:O	7:e:131:TRP:HB2	2.18	0.43
7:f:100:ASN:HB3	7:h:6:PHE:CE1	2.54	0.43
7:g:79:ASP:HB3	7:g:167:VAL:HG21	2.00	0.43
8:k:61:ASN:HB3	8:k:62:PHE:H	1.66	0.43
7:p:74:ALA:HB2	7:p:172:VAL:HG12	2.00	0.43
2:A:469:GLN:HE22	4:C7:276:ARG:N	2.16	0.43
4:A1:16:ILE:HG13	4:A1:233:MET:HE1	1.99	0.43
4:A5:248:SER:HA	4:A5:252:LYS:HD2	1.99	0.43
4:A5:321:MET:HG2	4:A5:363:MET:HE3	1.99	0.43
3:A6:90:GLU:HB3	3:A6:121:ARG:NH1	2.33	0.43
2:B:209:PHE:HD1	2:B:211:GLN:HG3	1.82	0.43
4:B1:27:GLU:HA	4:B1:359:LYS:HD3	2.00	0.43
4:B5:3:GLU:HA	4:B5:49:VAL:HA	1.99	0.43
3:B8:181:VAL:HG22	4:B9:256:ASN:OD1	2.17	0.43
4:C1:169:VAL:HG22	4:C1:202:ILE:HD11	1.99	0.43
4:C3:208:TYR:O	4:C3:212:PHE:HB2	2.18	0.43
3:C6:181:VAL:HG23	4:C7:350:LYS:HB2	2.00	0.43
3:C8:272:TYR:HA	3:C8:376:CYS:HA	2.01	0.43
3:C8:407:TRP:CG	4:C9:255:VAL:HG23	2.53	0.43
4:C9:272:PRO:HD3	4:C9:364:SER:HB2	2.00	0.43
4:D3:253:LEU:HG	4:D3:257:LEU:HD12	1.99	0.43
4:D9:284:LEU:HD23	4:D9:362:LYS:HG2	2.01	0.43
3:E2:21:TRP:CZ3	3:E2:52:PHE:HB3	2.53	0.43
3:E2:275:ILE:HG23	3:E2:368:LEU:HD21	2.00	0.43
3:E4:405:VAL:HA	3:E4:408:TYR:CZ	2.53	0.43
4:E7:256:ASN:HD22	4:E7:350:LYS:HD3	1.83	0.43
3:E8:273:ALA:HA	3:E8:275:ILE:HG13	1.98	0.43
3:E8:313:MET:O	3:E8:350:GLY:HA3	2.19	0.43
4:E9:333:VAL:HG13	4:E9:341:PHE:CE2	2.53	0.43
7:j:111:ILE:HD13	7:j:132:LEU:HB2	2.00	0.43
3:A6:12:ALA:HB3	3:A6:140:ALA:HB2	2.00	0.43
3:A6:230:LEU:HG	3:A6:275:ILE:HD11	2.01	0.43
4:A7:282:ARG:HG2	4:B1:86:ARG:HH12	1.83	0.43
3:B6:274:PRO:HG3	3:B6:286:LEU:HD12	1.99	0.43
3:B8:21:TRP:CZ2	3:B8:65:CYS:HB2	2.53	0.43
3:C0:220:GLU:HB3	3:C0:221:ARG:HD2	1.99	0.43
3:C2:132:LEU:HD22	3:C2:164:LYS:HD2	2.00	0.43
3:D0:60:LYS:HG3	3:D0:62:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D0:276:ILE:HD13	3:D0:286:LEU:HD11	2.00	0.43
4:D1:7:VAL:HG11	4:D1:151:LEU:HD11	2.00	0.43
3:D4:140:ALA:HA	3:D4:171:SER:HB3	2.01	0.43
4:D5:167:PHE:CE2	4:D5:233:MET:HG2	2.53	0.43
4:D5:240:LEU:HD21	4:D5:249:ASP:HB2	2.00	0.43
4:D7:171:PRO:HB3	4:D7:181:GLU:HG2	2.01	0.43
3:D8:69:ASP:O	3:D8:94:SER:HA	2.18	0.43
3:E2:21:TRP:CZ2	3:E2:65:CYS:HB3	2.53	0.43
4:E5:309:ARG:HH21	4:E5:342:VAL:HA	1.84	0.43
3:E6:204:LEU:HD22	3:E6:209:ILE:HD11	2.01	0.43
7:c:105:ASN:HB2	7:e:39:PRO:HG2	2.00	0.43
7:n:200:ASP:O	7:n:204:THR:HG22	2.19	0.43
3:A8:306:ASP:HB3	3:A8:309:HIS:CE1	2.53	0.43
2:B:371:ARG:NH2	4:B7:231:ALA:HB2	2.34	0.43
2:B:506:PHE:CG	3:D4:245:ASP:HB3	2.54	0.43
3:B0:292:THR:HG21	3:B0:331:ALA:HB1	1.99	0.43
4:B1:198:GLU:HG2	4:B1:266:PHE:HE2	1.83	0.43
3:B6:201:ALA:HB3	3:B6:267:PHE:HD1	1.83	0.43
3:B8:265:ILE:HG12	3:B8:432:TYR:HE1	1.83	0.43
3:C2:115:VAL:HG21	3:C2:152:LEU:HD22	2.00	0.43
3:C4:30:ILE:HG21	3:C4:53:PHE:HE2	1.83	0.43
4:C7:102:ALA:HB2	4:C7:403:MET:SD	2.59	0.43
4:C9:293:MET:HE2	4:C9:365:VAL:HG11	2.00	0.43
4:D1:229:VAL:HG12	4:D1:233:MET:HE3	2.00	0.43
3:D6:156:ARG:HA	3:D6:159:VAL:HG12	2.00	0.43
3:E2:288:VAL:HB	3:E2:327:ASP:HB3	1.99	0.43
4:E9:309:ARG:HB2	4:E9:426:GLN:HG2	2.00	0.43
4:F1:273:LEU:HD23	4:F1:273:LEU:HA	1.92	0.43
6:I:250:HIS:CE1	6:I:256:LEU:HD13	2.53	0.43
7:m:71:LYS:HG2	7:m:109:GLU:OE1	2.19	0.43
3:A0:269:LEU:HD12	3:A0:301:MET:HE3	2.00	0.43
4:A3:272:PRO:HD3	4:A3:289:LEU:HD11	2.00	0.43
3:A6:319:TYR:HD2	3:A6:355:ILE:HG13	1.83	0.43
4:A7:274:THR:HG22	4:A7:282:ARG:HE	1.84	0.43
4:A9:156:ARG:HD3	4:A9:164:MET:HE3	2.00	0.43
3:B4:236:SER:O	3:B4:240:ALA:HB2	2.17	0.43
3:B6:75:VAL:HG13	3:B6:92:LEU:HB3	2.01	0.43
4:B7:183:TYR:HA	4:B7:385:PHE:HE2	1.83	0.43
3:C2:259:LEU:HB3	3:C2:268:MET:HE1	2.00	0.43
4:C5:290:THR:HA	4:C5:293:MET:HE2	2.00	0.43
3:C6:76:ASP:HA	3:C6:79:ARG:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C8:402:ARG:HA	3:C8:402:ARG:HD3	1.80	0.43
4:D1:396:HIS:HA	4:D1:399:THR:HG22	2.00	0.43
3:E2:168:ASN:O	3:E2:201:ALA:HA	2.19	0.43
3:E8:225:THR:HG23	5:G:120:GLU:OE2	2.18	0.43
4:F1:318:ARG:HG2	4:F1:354:CYS:HB3	2.00	0.43
4:A3:10:GLY:O	4:A3:14:ASN:HB2	2.18	0.43
4:A9:330:MET:HE2	4:A9:349:MET:HE2	2.00	0.43
3:B6:405:VAL:HG13	3:B6:418:PHE:HE2	1.82	0.43
3:B8:139:ASN:O	3:B8:170:CYS:HA	2.18	0.43
4:C3:32:PRO:HB3	4:C3:81:PHE:CG	2.53	0.43
4:C3:316:MET:HE2	4:C3:366:THR:HG23	2.01	0.43
3:C6:103:PHE:HB3	3:C6:189:LEU:HD23	2.01	0.43
4:D1:288:GLU:HA	4:D1:291:GLN:HG2	2.00	0.43
3:D2:267:PHE:HB2	3:D2:384:ILE:HD12	1.99	0.43
3:D6:377:MET:HE3	3:D6:377:MET:HB3	1.92	0.43
3:E0:323:VAL:HG22	3:E0:373:ARG:HG2	2.01	0.43
4:E1:42:LEU:HD22	4:E1:356:ILE:HD11	1.99	0.43
4:E1:187:LEU:HD21	4:E1:403:MET:HE1	2.00	0.43
4:E1:219:THR:HA	3:E2:326:LYS:NZ	2.34	0.43
3:E2:395:PHE:HD2	3:E2:422:ARG:HH11	1.67	0.43
4:E5:61:PRO:HD3	4:E5:84:LEU:HG	1.99	0.43
4:E9:296:ALA:HA	4:E9:305:PRO:HG2	2.01	0.43
6:H:299:ILE:HD11	6:H:305:LEU:HD13	2.01	0.43
6:H:306:LEU:HD22	6:H:313:TRP:HB3	2.00	0.43
6:J:376:LEU:HD23	6:J:388:LEU:HD22	2.00	0.43
7:g:142:GLU:O	7:g:146:ARG:HG2	2.19	0.43
8:l:53:VAL:HG13	8:l:92:TRP:HH2	1.84	0.43
7:q:53:GLY:HA2	7:q:62:VAL:HG21	2.01	0.43
7:r:55:LEU:HD21	7:r:68:LEU:HD11	1.99	0.43
3:A0:21:TRP:HZ3	3:A0:52:PHE:HB3	1.84	0.43
3:A0:70:LEU:HD12	3:A0:145:THR:HG22	1.99	0.43
3:A2:72:PRO:O	3:A2:76:ASP:HB2	2.19	0.43
4:A5:309:ARG:O	4:A5:372:THR:HG22	2.19	0.43
3:A6:301:MET:HE3	3:A6:301:MET:HB3	1.81	0.43
3:B0:269:LEU:HD22	3:B0:303:ALA:HB3	2.01	0.43
3:B2:154:LEU:HB3	3:B2:197:HIS:HB3	2.01	0.43
4:B3:153:SER:HA	4:B3:195:ASN:HD22	1.84	0.43
3:B8:72:PRO:HG2	4:B9:46:ARG:HH21	1.84	0.43
3:C0:189:LEU:HD11	3:C0:418:PHE:HD2	1.82	0.43
3:C0:212:ILE:HG22	3:C0:275:ILE:HD13	2.01	0.43
4:C5:108:GLU:HG2	4:C5:111:GLU:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C5:213:ARG:HD2	4:C5:297:LYS:HG2	2.01	0.43
4:C5:266:PHE:HD2	4:C5:368:VAL:HG12	1.84	0.43
3:C6:31:GLN:NE2	8:l:65:GLU:HG2	2.29	0.43
4:D1:138:SER:HA	4:D1:169:VAL:HG22	2.00	0.43
4:D1:140:GLY:HA2	4:D1:184:ASN:HB2	1.99	0.43
3:D4:306:ASP:HB3	3:D4:309:HIS:CE1	2.54	0.43
4:D5:113:ILE:HG12	4:D5:154:LYS:HD3	2.00	0.43
3:E0:275:ILE:HG23	3:E0:368:LEU:HD21	2.01	0.43
4:E1:100:ASN:HB3	4:E1:103:LYS:HB3	2.01	0.43
3:E2:174:SER:HB3	3:E2:177:VAL:O	2.18	0.43
6:J:258:ALA:HB3	6:J:273:PHE:HE1	1.84	0.43
6:K:323:LYS:HB3	6:K:323:LYS:HE3	1.78	0.43
6:K:386:MET:HA	6:K:394:VAL:O	2.19	0.43
7:o:77:PHE:CD2	7:o:150:VAL:HG21	2.54	0.43
7:q:141:THR:O	7:q:145:LYS:HG3	2.18	0.43
1:13:247:TYR:HA	1:13:251:TYR:HD1	1.84	0.43
3:A2:247:ALA:HB3	3:A2:355:ILE:HB	2.01	0.43
4:A3:6:HIS:HB3	4:A3:21:TRP:HZ2	1.84	0.43
4:A3:318:ARG:NH1	4:A3:358:PRO:HG3	2.34	0.43
4:A9:200:GLN:HB3	4:A9:268:ILE:HD11	2.01	0.43
4:B3:134:GLN:HA	4:B3:165:GLU:O	2.19	0.43
3:C0:120:ASP:O	3:C0:124:LYS:HG2	2.19	0.43
4:C1:318:ARG:HG2	4:C1:357:PRO:HA	2.00	0.43
3:C2:188:VAL:HG23	3:C2:425:LEU:HD22	2.01	0.43
4:C5:27:GLU:HA	4:C5:359:LYS:HD3	2.01	0.43
4:C5:195:ASN:C	4:C5:195:ASN:HD22	2.27	0.43
4:C5:388:MET:HE3	4:C5:388:MET:HB2	1.91	0.43
3:C6:318:MET:HB2	3:C6:376:CYS:HB3	1.99	0.43
4:C9:87:PRO:HA	4:C9:90:PHE:HD2	1.84	0.43
3:D0:136:LEU:HD23	3:D0:138:PHE:HZ	1.84	0.43
4:D1:165:GLU:HG2	4:D1:250:LEU:HD21	2.01	0.43
4:D1:326:VAL:O	4:D1:330:MET:HG2	2.19	0.43
3:D4:137:MET:O	3:D4:168:ASN:HA	2.19	0.43
3:D4:319:TYR:HB3	3:D4:323:VAL:HG21	2.01	0.43
4:D7:389:PHE:CE2	4:D7:395:LEU:HD11	2.53	0.43
4:D9:148:GLY:O	4:D9:152:ILE:HG12	2.18	0.43
3:E2:194:LEU:HD12	3:E2:198:THR:HG21	2.00	0.43
3:E6:223:THR:HG22	3:E6:225:THR:H	1.84	0.43
3:E6:250:VAL:HG21	3:E6:318:MET:HE1	2.01	0.43
4:E9:167:PHE:CE2	4:E9:233:MET:HG2	2.53	0.43
4:F1:102:ALA:HB1	4:F1:401:GLU:OE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:j:56:LYS:HD2	7:j:60:ASN:HA	2.01	0.43
8:l:61:ASN:OD1	8:l:67:ALA:HA	2.18	0.43
7:m:63:ILE:HG22	7:o:16:ARG:HD2	2.00	0.43
3:A4:407:TRP:CE3	4:A5:255:VAL:HA	2.54	0.43
4:A5:201:VAL:HG21	4:A5:374:ILE:HD11	2.01	0.43
4:B1:95:THR:HG21	4:B1:108:GLU:HG2	2.00	0.43
3:C0:296:PHE:CE2	3:C0:335:ILE:HG21	2.53	0.43
4:C9:221:THR:HG23	4:C9:223:GLY:H	1.83	0.43
4:D1:286:VAL:HG11	4:D1:326:VAL:HA	2.01	0.43
3:D2:276:ILE:HD12	3:D2:281:ALA:HA	2.01	0.43
4:D5:248:SER:HA	4:D5:252:LYS:HD3	2.00	0.43
4:D7:313:ALA:O	4:D7:349:MET:HA	2.19	0.43
4:E1:170:PHE:CD2	4:E1:201:VAL:HG13	2.54	0.43
4:E3:20:PHE:HA	4:E3:230:SER:OG	2.19	0.43
3:E4:271:SER:HB3	3:E4:301:MET:HE2	2.00	0.43
4:E5:36:TYR:HE1	7:u:90:PRO:HG2	1.83	0.43
4:E9:19:LYS:HA	4:E9:22:GLU:HB2	2.00	0.43
3:F0:265:ILE:HG13	3:F0:435:VAL:HG21	2.01	0.43
4:F1:113:ILE:HA	4:F1:116:VAL:HG12	1.99	0.43
6:H:296:LEU:HB3	6:H:308:TRP:HB3	1.99	0.43
7:c:119:ARG:HH12	7:c:137:GLU:HB3	1.83	0.43
7:i:10:LEU:HD12	7:i:147:HIS:CG	2.54	0.43
7:j:84:LYS:HB2	7:j:168:PRO:HD3	2.00	0.43
7:r:63:ILE:HD11	7:r:132:LEU:HD13	2.01	0.43
7:w:14:LYS:HD2	7:w:45:MET:HG2	2.01	0.43
3:A0:210:TYR:CD1	3:A0:222:PRO:HG2	2.54	0.42
3:A2:51:THR:OG1	3:A2:243:ARG:HG2	2.19	0.42
3:A2:286:LEU:HD22	3:A2:371:VAL:HG11	2.00	0.42
4:A5:207:LEU:HB3	4:A5:225:LEU:HG	2.00	0.42
3:A6:156:ARG:HA	3:A6:159:VAL:HG12	2.01	0.42
3:A6:185:TYR:HA	3:A6:395:PHE:HE2	1.84	0.42
4:A9:98:GLY:O	3:B0:257:THR:HG21	2.18	0.42
2:B:464:LYS:HG2	2:B:465:LEU:H	1.84	0.42
2:B:519:LEU:HB3	4:D3:360:GLY:HA3	2.00	0.42
3:B8:64:ARG:HH21	3:B8:128:ASN:HD22	1.66	0.42
4:B9:320:ARG:HA	4:B9:320:ARG:HD2	1.79	0.42
3:C0:145:THR:HG23	3:C0:149:LEU:HD22	2.00	0.42
4:C3:239:CYS:HB2	4:C3:354:CYS:HB2	2.00	0.42
3:C4:285:GLN:OE1	3:C8:56:THR:HA	2.19	0.42
3:D2:191:THR:O	3:D2:195:LEU:HB2	2.19	0.42
3:D2:304:LYS:HD2	3:D2:304:LYS:HA	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D4:88:HIS:HE1	3:D4:90:GLU:HG3	1.83	0.42
3:D8:397:LEU:HD23	4:D9:346:PRO:HD3	2.01	0.42
4:D9:139:LEU:HD11	4:D9:192:LEU:HD22	2.00	0.42
3:E2:403:ALA:HB2	4:E3:344:TRP:HZ3	1.84	0.42
4:E5:6:HIS:CE1	4:E5:8:GLN:HE21	2.37	0.42
3:E6:3:GLU:OE1	3:E6:129:CYS:HB3	2.19	0.42
3:E8:119:LEU:HA	3:E8:122:ILE:HB	2.01	0.42
3:E8:228:ASN:HA	3:E8:231:ILE:HG22	2.00	0.42
6:H:303:GLY:HA3	6:H:323:LYS:HG3	2.01	0.42
6:J:344:ILE:HD13	6:J:376:LEU:HD21	2.01	0.42
7:f:68:LEU:HA	7:f:71:LYS:HE3	2.01	0.42
7:n:78:ALA:HA	7:n:167:VAL:HG13	2.01	0.42
7:p:82:ASP:HB3	7:p:85:CYS:HB3	2.00	0.42
7:v:146:ARG:HD3	7:v:156:VAL:HG11	2.01	0.42
7:x:140:LEU:HA	7:x:143:ILE:HG22	2.00	0.42
3:A0:408:TYR:O	3:A0:411:GLU:HG3	2.19	0.42
4:A1:113:ILE:HA	4:A1:116:VAL:HG12	2.01	0.42
3:A6:234:VAL:HG21	3:A6:302:MET:HE1	2.00	0.42
3:B0:335:ILE:HG23	3:B0:341:ILE:HD11	2.00	0.42
4:B1:273:LEU:HD23	4:B1:273:LEU:HA	1.92	0.42
3:B2:174:SER:HB3	3:B2:207:GLU:HG2	2.01	0.42
4:B5:24:ILE:HD13	4:B5:24:ILE:HA	1.93	0.42
3:B8:76:ASP:HA	3:B8:79:ARG:HD2	2.00	0.42
3:C0:7:ILE:HG13	3:C0:66:VAL:HG12	2.01	0.42
4:C3:136:THR:HG21	4:C3:233:MET:HE3	2.00	0.42
4:C3:398:TYR:HD2	4:C3:408:PHE:HZ	1.68	0.42
4:C7:406:MET:HE3	4:C7:406:MET:HB3	1.89	0.42
3:C8:153:LEU:O	3:C8:157:LEU:HB3	2.19	0.42
3:D0:285:GLN:HB3	3:D4:56:THR:HA	2.01	0.42
4:D1:240:LEU:HD11	4:D1:250:LEU:H	1.85	0.42
3:D2:431:ASP:HA	3:D2:434:GLU:HG3	2.01	0.42
3:E0:395:PHE:HE2	3:E0:422:ARG:HB2	1.84	0.42
4:E3:316:MET:HE1	4:E3:368:VAL:HG21	2.01	0.42
3:E4:430:LYS:O	3:E4:434:GLU:HG2	2.19	0.42
4:E7:49:VAL:HG11	4:E7:241:ARG:HG2	2.01	0.42
3:E8:413:MET:HB3	3:E8:417:GLU:OE2	2.20	0.42
4:E9:311:LEU:HD23	4:E9:422:TYR:CZ	2.54	0.42
6:H:218:LEU:HD23	6:H:230:TRP:CZ3	2.52	0.42
7:i:14:LYS:O	7:i:18:ASN:HB2	2.20	0.42
7:p:113:VAL:HG22	7:p:134:ILE:HD12	2.01	0.42
7:q:194:ARG:HH12	7:q:198:ARG:NH1	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:u:170:VAL:HG23	7:u:183:LEU:HB2	2.01	0.42
7:v:9:PRO:HA	7:v:12:VAL:HG22	2.01	0.42
7:w:84:LYS:HB2	7:w:168:PRO:HD3	2.01	0.42
3:A4:36:MET:HE2	3:A4:36:MET:HB3	1.98	0.42
3:B0:209:ILE:HA	3:B0:212:ILE:HG22	2.00	0.42
3:B2:70:LEU:HD13	3:B2:110:ILE:HG23	2.00	0.42
3:B2:402:ARG:HD3	3:B2:402:ARG:HA	1.85	0.42
3:B4:9:VAL:HG21	3:B4:149:LEU:HB3	2.01	0.42
3:B8:246:GLY:HA2	3:B8:357:TYR:HD1	1.84	0.42
3:C0:14:ILE:HD12	3:C0:67:PHE:HB3	2.00	0.42
3:C2:79:ARG:HA	3:C2:87:PHE:HZ	1.84	0.42
3:C2:119:LEU:HG	3:C2:156:ARG:HD3	2.00	0.42
3:C2:243:ARG:NH2	3:C2:320:ARG:HH21	2.17	0.42
4:C3:31:ASP:H	4:C3:36:TYR:HB3	1.84	0.42
3:D0:141:VAL:HG21	3:D0:172:TRP:CE3	2.54	0.42
4:D3:202:ILE:HD13	4:D3:229:VAL:HG13	2.01	0.42
4:D5:49:VAL:HG21	4:D5:241:ARG:HG2	2.00	0.42
3:D6:388:PHE:HB2	3:D6:429:GLU:OE2	2.19	0.42
4:D7:193:VAL:HA	4:D7:264:HIS:CE1	2.54	0.42
4:E1:232:ALA:HB1	4:E1:268:ILE:HG21	2.00	0.42
4:E1:256:ASN:HD22	4:E1:350:LYS:HD2	1.85	0.42
3:E6:315:CYS:HB2	3:E6:377:MET:HE2	2.00	0.42
3:F0:70:LEU:HD13	3:F0:110:ILE:HG23	2.00	0.42
6:J:300:ASN:ND2	6:J:306:LEU:HD11	2.34	0.42
7:e:49:LEU:HD21	7:e:144:LEU:HD21	2.00	0.42
4:A3:31:ASP:OD1	4:A3:32:PRO:HD2	2.20	0.42
4:A5:68:LEU:HB3	4:A5:96:GLY:HA2	2.01	0.42
4:A5:358:PRO:HG2	4:A5:361:LEU:HB2	2.00	0.42
4:A9:198:GLU:HG2	4:A9:266:PHE:HE2	1.84	0.42
3:B2:240:ALA:HB1	3:B2:356:ASN:HD22	1.83	0.42
4:B3:133:PHE:O	4:B3:164:MET:HA	2.18	0.42
3:B8:269:LEU:HD21	3:B8:305:CYS:HB3	2.00	0.42
4:C1:136:THR:HG22	4:C1:167:PHE:HB2	2.01	0.42
4:C3:35:THR:HB	7:j:83:PRO:HG3	2.01	0.42
4:C3:313:ALA:HB1	4:C3:367:PHE:CZ	2.54	0.42
3:C4:147:SER:HB2	3:C4:190:SER:HB3	2.02	0.42
4:C7:356:ILE:HA	4:C7:357:PRO:HD3	1.87	0.42
4:C7:415:MET:HE3	4:C7:415:MET:HB3	1.84	0.42
3:D0:269:LEU:HD11	3:D0:303:ALA:HB2	2.00	0.42
4:D3:89:ASN:HA	4:D3:119:VAL:HG21	2.02	0.42
4:E1:180:VAL:HA	4:E1:388:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E5:6:HIS:O	4:E5:63:ALA:HA	2.20	0.42
3:E6:407:TRP:CG	4:E7:255:VAL:HG23	2.55	0.42
3:E6:425:LEU:O	3:E6:429:GLU:HG2	2.19	0.42
3:E8:70:LEU:HD22	3:E8:110:ILE:HG22	2.00	0.42
4:E9:170:PHE:HE1	4:E9:185:ALA:HB1	1.84	0.42
3:F0:53:PHE:HB3	3:F0:61:HIS:HB3	2.01	0.42
3:F0:211:ASP:HA	3:F0:214:ARG:HB3	2.00	0.42
6:I:315:LYS:HA	6:I:315:LYS:HE3	2.01	0.42
6:K:376:LEU:HD23	6:K:388:LEU:HD22	2.00	0.42
7:b:77:PHE:CD2	7:b:150:VAL:HG21	2.55	0.42
7:j:96:TYR:HE1	7:j:109:GLU:HA	1.85	0.42
8:l:79:ASP:HB3	8:l:82:ASP:HB2	2.01	0.42
8:l:132:ILE:HG12	8:l:143:ARG:HD3	2.00	0.42
7:r:64:PRO:HD2	7:r:67:HIS:CD2	2.55	0.42
3:B0:139:ASN:HD21	3:B0:168:ASN:HD21	1.68	0.42
4:B5:207:LEU:HB3	4:B5:225:LEU:HG	2.00	0.42
4:B9:186:THR:HG22	4:B9:415:MET:HE1	2.02	0.42
4:C3:8:GLN:O	4:C3:66:MET:HB3	2.20	0.42
3:C4:122:ILE:HD13	3:C4:157:LEU:HD21	2.01	0.42
3:C4:231:ILE:O	3:C4:235:ILE:HG12	2.19	0.42
3:C6:84:ARG:HE	8:l:59:THR:HG21	1.84	0.42
3:C6:231:ILE:O	3:C6:235:ILE:HG12	2.20	0.42
4:D3:28:HIS:CE1	4:D3:241:ARG:HD2	2.54	0.42
4:E1:120:VAL:O	4:E1:124:ALA:HB3	2.20	0.42
4:E5:179:VAL:HG22	3:E6:350:GLY:HA2	2.00	0.42
3:E6:189:LEU:HD21	3:E6:413:MET:HE3	2.01	0.42
4:E7:260:PHE:HB2	4:E7:263:LEU:HD13	2.00	0.42
3:E8:100:ALA:O	4:E9:255:VAL:HG11	2.19	0.42
4:E9:256:ASN:HD22	4:E9:256:ASN:C	2.24	0.42
4:F1:133:PHE:HZ	4:F1:159:TYR:HD2	1.66	0.42
7:e:79:ASP:HB3	7:e:82:ASP:HB2	2.02	0.42
7:f:49:LEU:HD22	7:f:50:PHE:CE1	2.54	0.42
7:g:110:ILE:O	7:g:131:TRP:HB2	2.19	0.42
7:i:98:THR:HA	7:i:101:GLU:HG3	2.00	0.42
8:l:85:ARG:HG3	8:l:86:VAL:HG23	2.01	0.42
4:A1:91:VAL:HB	4:A1:112:LEU:HD11	2.01	0.42
3:A2:3:GLU:HG2	3:A2:132:LEU:HD13	2.02	0.42
4:A9:19:LYS:HD3	4:A9:19:LYS:HA	1.81	0.42
4:A9:268:ILE:HA	4:A9:367:PHE:O	2.19	0.42
4:B1:19:LYS:HA	4:B1:19:LYS:HD3	1.79	0.42
4:B3:318:ARG:O	4:B3:363:MET:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B4:309:HIS:HE1	3:B4:386:GLU:HG2	1.84	0.42
3:B4:334:THR:HA	3:B4:337:THR:HG22	2.02	0.42
4:B7:113:ILE:HA	4:B7:116:VAL:HG12	2.02	0.42
3:C0:227:LEU:HD23	3:C0:227:LEU:H	1.85	0.42
3:C4:114:ILE:HD12	3:C4:117:LEU:HD12	2.01	0.42
3:C8:4:VAL:HG23	3:C8:135:PHE:HA	2.02	0.42
4:D7:212:PHE:HZ	3:D8:326:LYS:HD2	1.85	0.42
4:E1:101:TRP:CE3	4:E1:187:LEU:HD23	2.54	0.42
4:E3:318:ARG:O	4:E3:363:MET:HA	2.20	0.42
4:E5:20:PHE:HA	4:E5:23:VAL:HG22	2.01	0.42
4:E7:226:ASN:HA	4:E7:229:VAL:HG12	2.02	0.42
4:E9:200:GLN:HG3	4:E9:266:PHE:HD2	1.85	0.42
5:F:178:PRO:HB2	5:F:179:ARG:HD2	2.00	0.42
3:F0:398:MET:SD	4:F1:345:ILE:HA	2.59	0.42
4:F1:211:CYS:HA	4:F1:215:LEU:HB3	2.01	0.42
7:j:129:MET:HE2	7:j:131:TRP:CZ2	2.55	0.42
8:l:50:VAL:HA	8:l:53:VAL:HG12	2.02	0.42
7:m:2:SER:HB2	7:m:42:TYR:CZ	2.54	0.42
1:14:256:LEU:HD23	1:14:256:LEU:HA	1.87	0.42
3:A0:149:LEU:HD12	3:A0:149:LEU:HA	1.93	0.42
3:A2:67:PHE:HB2	3:A2:92:LEU:HD23	2.01	0.42
3:A4:57:GLY:H	2:C:254:GLY:H	1.67	0.42
4:A7:68:LEU:HD23	4:A7:68:LEU:HA	1.91	0.42
3:A8:71:GLU:HG2	3:A8:73:THR:H	1.85	0.42
4:B1:169:VAL:HG12	4:B1:202:ILE:HB	2.02	0.42
3:B2:198:THR:HG21	3:B2:201:ALA:HB2	2.02	0.42
3:B4:51:THR:HG21	3:B4:243:ARG:HG2	2.02	0.42
4:B5:113:ILE:HA	4:B5:116:VAL:HG12	2.01	0.42
3:B6:285:GLN:HB3	3:C0:56:THR:HA	2.01	0.42
4:B9:102:ALA:HB1	4:B9:401:GLU:HB2	2.01	0.42
2:C:238:HIS:HD2	7:a:165:THR:HG21	1.84	0.42
4:C1:28:HIS:NE2	4:C1:241:ARG:HD2	2.34	0.42
4:C3:374:ILE:HB	4:C3:422:TYR:CE2	2.55	0.42
3:C4:296:PHE:HZ	3:C4:317:LEU:HD11	1.85	0.42
3:C4:296:PHE:CD1	3:C4:377:MET:HE2	2.55	0.42
4:C7:319:GLY:HA2	4:C7:357:PRO:HG3	2.01	0.42
3:C8:216:ASN:HB3	3:C8:275:ILE:O	2.20	0.42
3:D0:60:LYS:HA	3:D0:60:LYS:HD2	1.78	0.42
4:D1:174:LYS:HE3	4:D1:205:GLU:HB2	2.00	0.42
4:D1:189:VAL:HG21	4:D1:415:MET:HE1	2.01	0.42
3:D2:105:ARG:HH12	3:D2:110:ILE:HD11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D2:407:TRP:HZ2	4:D3:258:ILE:HD12	1.85	0.42
4:D3:240:LEU:HD21	4:D3:249:ASP:HB2	2.00	0.42
4:D7:283:ALA:HB2	4:E1:54:ALA:HA	2.01	0.42
3:E0:231:ILE:O	3:E0:235:ILE:HG12	2.19	0.42
3:E2:76:ASP:HA	3:E2:79:ARG:HD2	2.02	0.42
3:E2:95:GLY:HA3	3:E2:114:ILE:HD11	2.02	0.42
4:E3:100:ASN:HB3	4:E3:103:LYS:HB3	2.01	0.42
4:E5:132:GLY:HA2	4:E5:162:ARG:HB3	2.01	0.42
4:E7:286:VAL:HG11	4:E7:326:VAL:HA	2.01	0.42
6:I:245:PHE:HA	6:I:260:THR:HA	2.01	0.42
6:J:202:GLN:HB3	6:K:373:ASN:HD21	1.83	0.42
7:e:9:PRO:HG3	7:e:146:ARG:HH21	1.84	0.42
7:f:10:LEU:HD12	7:f:147:HIS:CG	2.54	0.42
7:n:67:HIS:HA	7:p:23:LEU:HD11	2.01	0.42
7:o:141:THR:O	7:o:145:LYS:HG2	2.19	0.42
7:t:191:GLU:HB2	7:t:195:ALA:HB2	2.02	0.42
1:12:257:PRO:HA	1:12:258:PRO:HD3	1.87	0.42
2:A:495:VAL:HG21	4:D1:279:GLN:HE22	1.85	0.42
3:A2:122:ILE:HG21	3:A2:157:LEU:HD11	2.02	0.42
3:A2:324:VAL:HG12	3:A2:326:LYS:H	1.83	0.42
4:A3:139:LEU:HD12	4:A3:170:PHE:CE2	2.55	0.42
4:A7:66:MET:HE1	4:A7:147:MET:HG3	2.02	0.42
4:A9:164:MET:HE2	4:A9:164:MET:HB2	1.71	0.42
3:B8:219:ILE:HD12	3:B8:222:PRO:HG3	2.01	0.42
3:C2:78:VAL:HG12	3:C2:87:PHE:CE1	2.55	0.42
4:C5:131:GLN:HG2	4:C5:250:LEU:HD13	2.02	0.42
4:C5:210:ILE:O	4:C5:214:THR:HB	2.19	0.42
3:C6:285:GLN:NE2	3:D0:56:THR:HA	2.30	0.42
3:C6:338:LYS:HB3	3:C6:338:LYS:HE2	1.77	0.42
4:C7:113:ILE:HA	4:C7:116:VAL:HG22	2.02	0.42
3:C8:225:THR:O	3:C8:229:ARG:HG3	2.20	0.42
3:C8:255:PHE:HZ	3:C8:378:ILE:HG21	1.84	0.42
4:C9:113:ILE:HG13	4:C9:117:LEU:HD13	2.02	0.42
4:D5:86:ARG:HD3	4:D5:88:ASP:HB2	2.01	0.42
4:D5:215:LEU:HB3	4:D5:217:LEU:HD13	2.02	0.42
4:D9:113:ILE:HG12	4:D9:154:LYS:HD2	2.02	0.42
4:E5:393:ALA:HA	3:E6:262:TYR:HE1	1.85	0.42
3:E6:54:SER:HB3	3:E6:64:ARG:NH1	2.34	0.42
3:E6:210:TYR:CD1	3:E6:227:LEU:HD21	2.55	0.42
3:E6:278:ALA:HA	3:E6:369:ALA:HB2	2.01	0.42
3:E6:319:TYR:HB3	3:E6:323:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:n:10:LEU:HB2	7:n:147:HIS:ND1	2.34	0.42
7:o:64:PRO:HD2	7:o:67:HIS:CE1	2.54	0.42
7:o:75:LEU:HD13	7:o:111:ILE:HB	2.02	0.42
7:o:145:LYS:HE2	7:o:145:LYS:HB3	1.93	0.42
7:s:9:PRO:HB2	7:s:143:ILE:HG13	2.01	0.42
7:s:110:ILE:HB	7:s:131:TRP:CG	2.54	0.42
3:A0:209:ILE:HA	3:A0:212:ILE:HG12	2.01	0.42
4:A1:294:PHE:CD2	4:A1:333:VAL:HG21	2.55	0.42
4:A3:47:ILE:HG13	4:A3:51:TYR:HB2	2.01	0.42
4:A3:238:CYS:SG	4:A3:318:ARG:HD2	2.60	0.42
4:A3:288:GLU:O	4:A3:291:GLN:HG3	2.20	0.42
3:B0:180:ALA:HB3	3:B0:183:GLU:HB2	2.02	0.42
4:B1:151:LEU:O	4:B1:155:VAL:HG22	2.20	0.42
3:C0:121:ARG:HD3	3:C0:125:LEU:HD23	2.01	0.42
4:C1:156:ARG:HH22	4:C1:197:ASP:N	2.16	0.42
4:C3:156:ARG:HA	4:C3:156:ARG:HD3	1.58	0.42
4:C3:300:MET:HE2	4:C3:300:MET:HB3	1.86	0.42
4:C3:319:GLY:HA2	4:C3:357:PRO:HG3	2.01	0.42
3:C6:156:ARG:HA	3:C6:156:ARG:HD3	1.84	0.42
3:C6:248:LEU:HD12	3:C6:248:LEU:HA	1.83	0.42
3:D0:272:TYR:HA	3:D0:375:VAL:O	2.20	0.42
4:D1:272:PRO:HG3	4:D1:364:SER:HB2	2.01	0.42
4:D7:73:MET:HE1	4:D7:92:PHE:HB3	2.02	0.42
3:D8:115:VAL:HG22	3:D8:119:LEU:HD23	2.02	0.42
4:E1:167:PHE:CE2	4:E1:233:MET:HG2	2.55	0.42
3:E2:320:ARG:HH12	3:E2:360:PRO:HA	1.84	0.42
4:E3:334:GLN:NE2	4:E3:349:MET:HG2	2.35	0.42
3:E6:320:ARG:HD3	3:E6:360:PRO:HG3	2.01	0.42
3:F0:10:GLY:O	3:F0:14:ILE:HG12	2.20	0.42
4:F1:253:LEU:O	4:F1:257:LEU:HB2	2.19	0.42
7:f:78:ALA:HB3	7:f:112:PHE:HE1	1.84	0.42
8:k:106:ILE:HD11	8:k:111:VAL:HB	2.01	0.42
7:q:10:LEU:HD12	7:q:147:HIS:CG	2.54	0.42
7:r:145:LYS:HE3	7:r:145:LYS:HB3	1.83	0.42
7:w:11:ASN:O	7:w:14:LYS:HB3	2.20	0.42
4:A1:30:ILE:HG13	4:A1:51:TYR:HE2	1.85	0.42
4:A1:208:TYR:CE1	3:A2:326:LYS:HG2	2.55	0.42
3:A2:84:ARG:HG3	3:A2:85:HIS:CD2	2.55	0.42
3:A6:71:GLU:HG3	3:A6:73:THR:HG22	2.02	0.42
4:A7:156:ARG:HA	4:A7:156:ARG:HD2	1.83	0.42
3:B4:84:ARG:HB3	7:f:98:THR:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B5:147:MET:HE2	4:B5:147:MET:HB3	1.79	0.42
3:C2:12:ALA:HB3	3:C2:140:ALA:HB2	2.01	0.42
3:C2:339:ARG:HD3	6:J:281:GLN:HB3	2.02	0.42
4:C3:66:MET:HE3	4:C3:66:MET:HB2	1.78	0.42
3:C6:256:GLN:O	3:C6:260:VAL:HG22	2.20	0.42
3:C6:324:VAL:HG12	3:C6:326:LYS:H	1.84	0.42
4:D3:395:LEU:HD12	4:D3:395:LEU:HA	1.86	0.42
4:D5:284:LEU:HD23	4:D5:284:LEU:HA	1.86	0.42
3:E4:169:PHE:HZ	3:E4:238:LEU:HD22	1.85	0.42
4:E7:374:ILE:HD11	4:E7:422:TYR:CZ	2.55	0.42
3:E8:331:ALA:O	3:E8:335:ILE:HG12	2.20	0.42
4:E9:144:GLY:H	4:E9:147:MET:HB2	1.85	0.42
4:E9:234:SER:O	4:E9:238:CYS:HB3	2.19	0.42
6:H:338:VAL:HG23	6:H:368:LEU:HD22	2.01	0.42
6:I:211:GLY:HA3	6:I:233:TYR:HE1	1.85	0.42
6:I:247:ASN:HA	6:I:406:ASP:OD2	2.20	0.42
7:a:68:LEU:HD12	7:a:73:VAL:HG22	2.01	0.42
7:p:14:LYS:HA	7:p:17:LEU:HD23	2.01	0.42
7:s:110:ILE:O	7:s:131:TRP:HB2	2.20	0.42
7:x:9:PRO:HB2	7:x:143:ILE:HG13	2.02	0.42
3:A0:139:ASN:O	3:A0:170:CYS:HA	2.19	0.41
4:A1:249:ASP:OD1	4:A1:252:LYS:HG2	2.20	0.41
4:A3:167:PHE:HZ	4:A3:236:VAL:HG11	1.84	0.41
3:A4:209:ILE:HA	3:A4:212:ILE:HG12	2.02	0.41
4:A7:162:ARG:HD3	4:A7:162:ARG:HA	1.91	0.41
3:A8:298:PRO:HG2	3:A8:308:ARG:NE	2.34	0.41
4:A9:186:THR:HA	4:A9:189:VAL:HG22	2.01	0.41
4:B3:207:LEU:HB3	4:B3:225:LEU:HG	2.02	0.41
4:B5:408:PHE:O	4:B5:412:GLU:HG2	2.19	0.41
3:B6:120:ASP:O	3:B6:124:LYS:HG3	2.20	0.41
4:B7:326:VAL:O	4:B7:330:MET:HG2	2.20	0.41
4:B9:51:TYR:HB3	4:B9:59:PHE:HB3	2.00	0.41
4:B9:112:LEU:O	4:B9:116:VAL:HG23	2.19	0.41
4:C1:22:GLU:HA	4:C1:25:SER:HB2	2.02	0.41
3:C2:231:ILE:O	3:C2:235:ILE:HG12	2.19	0.41
4:C3:244:GLY:H	4:C3:247:ASN:HD21	1.67	0.41
3:C4:129:CYS:SG	3:C4:132:LEU:HB2	2.60	0.41
3:C4:141:VAL:HG21	3:C4:172:TRP:CE3	2.55	0.41
4:C5:3:GLU:HA	4:C5:49:VAL:HA	2.02	0.41
4:C5:103:LYS:HA	4:C5:107:THR:HB	2.01	0.41
4:C5:163:ILE:HD13	4:C5:251:ARG:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C6:15:GLN:HA	3:C6:18:ASN:ND2	2.35	0.41
3:C6:119:LEU:HA	3:C6:122:ILE:HG22	2.00	0.41
4:C7:81:PHE:HE2	4:C7:84:LEU:HD22	1.85	0.41
3:C8:326:LYS:HA	3:C8:326:LYS:HD3	1.92	0.41
4:D1:268:ILE:HG23	4:D1:300:MET:HE3	2.02	0.41
3:D2:271:SER:H	3:D2:377:MET:HB3	1.85	0.41
3:D4:137:MET:HE1	3:D4:153:LEU:HB3	2.02	0.41
4:D7:242:PHE:HB3	4:D7:356:ILE:HD13	2.02	0.41
3:D8:319:TYR:HB3	3:D8:323:VAL:HG21	2.02	0.41
3:E4:231:ILE:O	3:E4:235:ILE:HG12	2.19	0.41
3:E8:219:ILE:HG13	3:E8:222:PRO:HD3	2.01	0.41
4:F1:199:VAL:HG12	4:F1:264:HIS:CD2	2.55	0.41
7:e:75:LEU:HD23	7:e:111:ILE:HB	2.02	0.41
8:k:62:PHE:HB3	7:m:6:PHE:HB2	2.03	0.41
7:n:74:ALA:HA	7:n:171:ILE:O	2.20	0.41
7:n:79:ASP:HB3	7:n:115:LEU:HB2	2.02	0.41
7:o:170:VAL:HG23	7:o:183:LEU:HB2	2.02	0.41
7:q:183:LEU:HD13	7:q:196:LEU:HA	2.02	0.41
7:w:2:SER:HA	7:w:6:PHE:HA	2.02	0.41
4:A1:230:SER:HA	4:A1:233:MET:HB2	2.02	0.41
4:A1:393:ALA:HA	3:A2:262:TYR:HE1	1.84	0.41
3:A2:135:PHE:HE1	3:A2:157:LEU:HD12	1.85	0.41
3:A2:136:LEU:HD23	3:A2:167:LEU:HB2	2.02	0.41
3:A2:145:THR:O	3:A2:149:LEU:HB2	2.19	0.41
3:A6:141:VAL:HG21	3:A6:194:LEU:HD11	2.02	0.41
4:A7:73:MET:HB2	4:A7:92:PHE:HE2	1.84	0.41
4:B3:253:LEU:HD21	4:B3:368:VAL:HG11	2.02	0.41
4:B3:403:MET:HE2	4:B3:403:MET:HB3	1.97	0.41
3:B4:91:GLN:HE21	3:B4:125:LEU:HD11	1.85	0.41
3:C2:107:HIS:HD2	3:C2:152:LEU:HD12	1.85	0.41
4:C3:101:TRP:CZ3	4:C3:187:LEU:HD12	2.55	0.41
4:C5:362:LYS:HG3	4:C5:363:MET:HG2	2.02	0.41
3:C6:194:LEU:HG	3:C6:267:PHE:HE1	1.86	0.41
3:C6:209:ILE:HG23	3:C6:230:LEU:HD12	2.01	0.41
3:C6:377:MET:SD	3:C6:379:SER:HB3	2.60	0.41
4:C9:178:THR:HG22	3:D0:352:LYS:HZ2	1.86	0.41
4:D1:100:ASN:HD21	4:D1:397:TRP:HB3	1.85	0.41
4:D1:317:PHE:HB3	4:D1:321:MET:HE1	2.02	0.41
3:D2:53:PHE:HE1	3:D2:63:PRO:HG3	1.84	0.41
4:D3:216:LYS:HG2	4:D3:275:SER:HB2	2.02	0.41
3:D4:212:ILE:HD13	3:D4:212:ILE:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D4:217:LEU:HD21	3:D4:368:LEU:HD23	2.02	0.41
4:D7:246:LEU:HD12	4:D7:246:LEU:HA	1.90	0.41
3:E0:225:THR:O	3:E0:229:ARG:HG2	2.20	0.41
3:E4:276:ILE:HD12	3:E4:281:ALA:HA	2.02	0.41
4:E9:392:LYS:HD3	4:E9:395:LEU:HD12	2.01	0.41
6:J:324:LEU:HD13	6:J:337:VAL:HG11	2.02	0.41
6:K:297:TRP:HE3	6:K:305:LEU:HD11	1.85	0.41
7:a:129:MET:HE2	7:a:131:TRP:HE1	1.84	0.41
7:o:17:LEU:HD22	7:o:21:ARG:HH12	1.84	0.41
7:o:165:THR:HG21	7:o:182:PHE:CZ	2.55	0.41
4:A7:100:ASN:HB3	4:A7:103:LYS:HB2	2.01	0.41
4:A9:12:CYS:O	4:A9:16:ILE:HG12	2.19	0.41
4:A9:139:LEU:HA	4:A9:145:SER:HB2	2.03	0.41
3:B4:250:VAL:HG23	3:B4:352:LYS:HE3	2.03	0.41
4:B5:65:LEU:HB3	4:B5:73:MET:HE1	2.03	0.41
3:B8:96:LYS:HD3	3:B8:96:LYS:HA	1.85	0.41
4:B9:187:LEU:HA	4:B9:190:HIS:CD2	2.56	0.41
4:B9:375:GLN:HE21	4:B9:419:VAL:HG13	1.85	0.41
3:C8:5:ILE:HD12	3:C8:125:LEU:HB3	2.01	0.41
4:C9:17:GLY:HA2	4:C9:20:PHE:HB3	2.03	0.41
3:D0:2:ARG:HG2	3:D0:51:THR:HG22	2.02	0.41
3:D0:377:MET:SD	3:D0:379:SER:HB2	2.60	0.41
3:D2:11:GLN:HG2	3:D2:74:VAL:HG21	2.02	0.41
3:D8:102:ASN:HA	3:D8:408:TYR:HE1	1.84	0.41
3:D8:217:LEU:HD13	3:D8:275:ILE:HG22	2.02	0.41
3:D8:248:LEU:H	3:D8:248:LEU:HD12	1.85	0.41
3:D8:403:ALA:HB2	4:D9:344:TRP:HZ3	1.85	0.41
5:E:123:PRO:HG2	7:x:101:GLU:HB3	2.03	0.41
4:E5:109:GLY:HA2	4:E5:147:MET:HE2	2.01	0.41
4:E7:286:VAL:HG22	4:E7:321:MET:HE3	2.03	0.41
4:E7:317:PHE:HB3	4:E7:321:MET:SD	2.61	0.41
7:b:80:GLY:HA2	7:b:125:HIS:CD2	2.55	0.41
7:c:110:ILE:O	7:c:131:TRP:HB2	2.20	0.41
7:c:126:ARG:HE	7:c:126:ARG:HB3	1.61	0.41
7:e:185:ILE:HG23	7:e:192:GLY:HA2	2.03	0.41
7:i:79:ASP:HB3	7:i:82:ASP:HB2	2.02	0.41
7:s:88:LEU:HD22	7:s:185:ILE:HG21	2.02	0.41
4:A5:219:THR:HA	3:A6:326:LYS:HD2	2.02	0.41
4:A7:316:MET:HB2	4:A7:366:THR:HG22	2.02	0.41
2:B:217:ARG:NH1	2:B:222:HIS:HB3	2.36	0.41
3:B0:100:ALA:O	4:B1:255:VAL:HG11	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B0:134:GLY:HA2	3:B0:164:LYS:HE2	2.03	0.41
3:B2:185:TYR:HA	3:B2:395:PHE:HE2	1.85	0.41
4:B3:57:GLY:HA3	7:e:83:PRO:HB2	2.02	0.41
3:B4:132:LEU:HD23	3:B4:164:LYS:HE2	2.03	0.41
4:B7:65:LEU:HD22	4:B7:90:PHE:CE2	2.56	0.41
4:B7:113:ILE:HG13	4:B7:117:LEU:HD23	2.02	0.41
4:B9:117:LEU:HA	4:B9:120:VAL:HB	2.03	0.41
4:C1:198:GLU:CD	4:C1:200:GLN:HE22	2.28	0.41
3:C2:185:TYR:O	3:C2:189:LEU:HB2	2.20	0.41
3:C4:16:ILE:HD13	3:C4:228:ASN:HA	2.01	0.41
3:C4:268:MET:HB3	3:C4:378:ILE:HG12	2.02	0.41
4:C5:36:TYR:CZ	4:C5:38:GLY:HA3	2.55	0.41
3:C8:102:ASN:HD21	4:C9:255:VAL:HG21	1.85	0.41
3:D0:136:LEU:HB3	3:D0:138:PHE:CE2	2.56	0.41
4:D3:220:PRO:HD2	3:D4:326:LYS:HD2	2.01	0.41
4:D5:268:ILE:HA	4:D5:367:PHE:O	2.19	0.41
4:D7:375:GLN:HB3	4:D7:422:TYR:CD2	2.54	0.41
3:D8:156:ARG:HA	3:D8:159:VAL:HG12	2.01	0.41
4:D9:64:ILE:HD12	4:D9:64:ILE:HG23	1.85	0.41
3:E0:9:VAL:HG13	3:E0:146:GLY:HA2	2.03	0.41
4:E9:113:ILE:HA	4:E9:116:VAL:HG12	2.02	0.41
4:E9:190:HIS:CD2	4:E9:411:ALA:HA	2.55	0.41
3:F0:149:LEU:HD12	3:F0:149:LEU:HA	1.94	0.41
3:F0:265:ILE:HG23	3:F0:432:TYR:CE1	2.55	0.41
7:b:56:LYS:HG3	7:b:62:VAL:HG22	2.01	0.41
7:e:97:ARG:O	7:e:101:GLU:HB2	2.21	0.41
8:k:66:LYS:HA	8:k:66:LYS:HE3	2.03	0.41
7:v:189:LEU:HA	7:v:189:LEU:HD23	1.83	0.41
2:A:487:THR:HG22	4:D1:223:GLY:HA3	2.02	0.41
4:A1:361:LEU:HD23	2:C:230:THR:HG23	2.03	0.41
4:A3:113:ILE:HG23	4:A3:117:LEU:HD23	2.02	0.41
4:A5:257:LEU:HA	4:A5:257:LEU:HD23	1.80	0.41
3:A6:10:GLY:O	3:A6:14:ILE:HG12	2.21	0.41
2:B:506:PHE:CD2	3:D4:245:ASP:HB3	2.55	0.41
4:B7:11:GLN:HA	4:B7:72:THR:HG21	2.03	0.41
4:B7:311:LEU:HD12	4:B7:342:VAL:HG11	2.02	0.41
3:C0:395:PHE:O	3:C0:399:TYR:HB2	2.20	0.41
4:C9:98:GLY:HA2	3:D0:254:GLU:HG3	2.02	0.41
4:C9:120:VAL:O	4:C9:124:ALA:HB2	2.20	0.41
3:D0:124:LYS:HA	3:D0:124:LYS:HD3	1.93	0.41
3:D4:398:MET:HE2	4:D5:345:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D5:230:SER:HA	4:D5:233:MET:HE3	2.03	0.41
4:D7:46:ARG:HG2	4:D7:240:LEU:O	2.21	0.41
3:D8:259:LEU:HB3	3:D8:268:MET:SD	2.61	0.41
3:E0:10:GLY:O	3:E0:14:ILE:HG12	2.21	0.41
3:E0:12:ALA:HB3	3:E0:140:ALA:HB2	2.02	0.41
3:E2:115:VAL:HG23	3:E2:153:LEU:HD22	2.03	0.41
3:E2:188:VAL:O	3:E2:191:THR:HG22	2.20	0.41
3:E4:27:GLU:HB3	3:E4:361:THR:HG21	2.01	0.41
3:E6:296:PHE:CE2	3:E6:335:ILE:HG13	2.56	0.41
3:F0:70:LEU:HG	3:F0:145:THR:HG23	2.02	0.41
3:F0:101:ASN:HA	3:F0:143:GLY:HA2	2.02	0.41
3:F0:413:MET:HE2	3:F0:413:MET:HB2	1.97	0.41
6:H:247:ASN:ND2	6:H:286:ASP:HA	2.36	0.41
6:H:412:SER:O	6:H:416:ILE:HD12	2.21	0.41
7:d:115:LEU:HD23	7:d:115:LEU:HA	1.87	0.41
7:f:189:LEU:HD12	7:f:189:LEU:HA	1.93	0.41
7:j:75:LEU:HD13	7:j:111:ILE:HB	2.01	0.41
7:s:8:SER:HB2	7:s:147:HIS:HA	2.01	0.41
7:w:96:TYR:HA	7:w:108:ILE:HD11	2.02	0.41
1:19:254:LYS:HD2	3:E6:26:LEU:HD11	2.03	0.41
3:A0:141:VAL:HG12	3:A0:187:SER:HA	2.02	0.41
3:A0:230:LEU:HD11	3:A0:275:ILE:HD13	2.01	0.41
4:A1:68:LEU:HA	4:A1:93:GLY:HA3	2.03	0.41
4:A3:167:PHE:CG	4:A3:233:MET:HE2	2.55	0.41
4:A5:172:SER:HB2	4:A5:203:ASP:HB2	2.03	0.41
3:A8:7:ILE:HG23	3:A8:137:MET:HA	2.03	0.41
3:B0:84:ARG:HD2	7:d:98:THR:HG21	2.01	0.41
3:B6:71:GLU:HG3	4:B7:2:ARG:NH1	2.30	0.41
3:B8:407:TRP:CG	4:B9:255:VAL:HG23	2.55	0.41
4:C1:159:TYR:HB3	4:C1:162:ARG:HG2	2.03	0.41
3:C2:188:VAL:HB	3:C2:391:MET:HE2	2.01	0.41
4:C3:6:HIS:O	4:C3:63:ALA:HA	2.21	0.41
4:C3:278:SER:HA	4:C3:281:TYR:CE1	2.56	0.41
4:C3:284:LEU:HD23	4:C3:289:LEU:HD11	2.02	0.41
4:C3:390:ARG:NH1	4:C3:391:ARG:HB3	2.35	0.41
3:C4:319:TYR:HE2	3:C4:328:VAL:HG13	1.86	0.41
3:C6:271:SER:HB2	3:C6:301:MET:HG2	2.03	0.41
4:D1:256:ASN:CB	4:D1:350:LYS:HD2	2.51	0.41
4:D7:253:LEU:HD12	4:D7:350:LYS:NZ	2.35	0.41
3:D8:382:THR:HG21	3:D8:436:GLY:HA3	2.02	0.41
4:D9:152:ILE:HG22	4:D9:195:ASN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D9:391:ARG:HD2	4:D9:393:ALA:HB2	2.03	0.41
3:E0:259:LEU:HD23	3:E0:259:LEU:HA	1.86	0.41
3:E0:318:MET:HB2	3:E0:376:CYS:HB3	2.03	0.41
3:E2:10:GLY:O	3:E2:14:ILE:HG12	2.20	0.41
3:E2:237:SER:HA	3:E2:320:ARG:HD2	2.03	0.41
3:E6:181:VAL:HB	4:E7:256:ASN:OD1	2.19	0.41
4:E7:112:LEU:HD22	4:E7:147:MET:SD	2.60	0.41
7:e:194:ARG:NH2	7:e:198:ARG:HE	2.19	0.41
7:f:108:ILE:HG13	7:f:199:TRP:CZ2	2.56	0.41
7:j:129:MET:HA	7:j:130:PRO:HD3	1.77	0.41
8:k:32:VAL:HG21	8:k:70:GLU:HB3	2.01	0.41
8:l:76:LEU:HD21	8:l:113:ASN:HA	2.03	0.41
7:s:63:ILE:HD11	7:s:132:LEU:HD11	2.03	0.41
4:A1:268:ILE:HA	4:A1:367:PHE:O	2.21	0.41
4:A3:34:GLY:HA3	4:A3:58:ARG:HG3	2.03	0.41
4:A5:112:LEU:HD12	4:A5:147:MET:HE1	2.03	0.41
4:A7:375:GLN:HB2	4:A7:419:VAL:HG13	2.03	0.41
4:A9:40:SER:HB3	4:A9:43:GLN:HE21	1.85	0.41
4:B1:318:ARG:HB3	4:B1:357:PRO:HA	2.03	0.41
4:B1:415:MET:O	4:B1:419:VAL:HG23	2.20	0.41
4:B5:304:ASP:HB3	4:B5:307:HIS:ND1	2.36	0.41
3:B8:335:ILE:HD11	3:B8:341:ILE:HG13	2.01	0.41
4:C1:131:GLN:O	4:C1:163:ILE:HG22	2.20	0.41
3:C2:51:THR:HG21	3:C2:243:ARG:HB3	2.02	0.41
4:C3:187:LEU:HD21	4:C3:408:PHE:HE2	1.86	0.41
3:C4:105:ARG:NH2	3:C4:110:ILE:HD11	2.35	0.41
3:C4:151:CYS:SG	3:C4:193:SER:HB3	2.61	0.41
4:C5:326:VAL:O	4:C5:330:MET:HG2	2.20	0.41
3:C6:185:TYR:HE1	3:C6:398:MET:HG2	1.85	0.41
4:D1:68:LEU:HB2	4:D1:143:THR:HG21	2.01	0.41
3:D2:192:HIS:HD1	3:D2:192:HIS:C	2.29	0.41
3:D4:269:LEU:HD21	3:D4:305:CYS:HB3	2.02	0.41
3:D6:216:ASN:HB3	3:D6:275:ILE:O	2.21	0.41
3:E0:230:LEU:HD23	3:E0:275:ILE:HD13	2.03	0.41
4:E1:138:SER:HA	4:E1:169:VAL:HB	2.03	0.41
4:E3:217:LEU:HD23	4:E3:276:ARG:HH22	1.85	0.41
3:E4:406:HIS:HA	3:E4:409:VAL:HG12	2.02	0.41
4:E5:164:MET:H	4:E5:197:ASP:HB2	1.85	0.41
3:E8:88:HIS:CD2	3:E8:89:PRO:HD2	2.54	0.41
3:F0:153:LEU:O	3:F0:157:LEU:HB2	2.20	0.41
3:F0:172:TRP:HE1	3:F0:391:MET:HE3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:93:LEU:HD22	7:i:159:TYR:HD1	1.85	0.41
7:h:51:PRO:HD2	7:h:54:SER:HB2	2.02	0.41
8:k:79:ASP:HB3	8:k:82:ASP:HB2	2.03	0.41
7:p:112:PHE:H	7:p:133:SER:HA	1.83	0.41
7:q:68:LEU:HA	7:q:71:LYS:HE3	2.02	0.41
7:r:99:MET:HG2	7:r:108:ILE:HG12	2.03	0.41
7:s:25:GLN:HE21	7:s:36:ILE:HD11	1.85	0.41
7:v:59:ASN:ND2	7:x:9:PRO:HB3	2.35	0.41
4:A1:323:THR:HG22	4:A1:353:VAL:HG21	2.03	0.41
4:A3:139:LEU:HD12	4:A3:170:PHE:HE2	1.86	0.41
4:A3:349:MET:HE3	4:A3:349:MET:HB2	1.84	0.41
3:B0:297:GLU:HA	3:B0:298:PRO:HD3	1.96	0.41
3:B6:100:ALA:HA	4:B7:252:LYS:HD3	2.03	0.41
4:B7:201:VAL:HG11	4:B7:374:ILE:HD11	2.03	0.41
4:B9:291:GLN:NE2	4:C3:122:LYS:HE2	2.35	0.41
4:C3:246:LEU:HB3	4:C3:353:VAL:HG22	2.02	0.41
3:C8:387:VAL:HA	3:C8:390:ARG:HG2	2.02	0.41
4:C9:336:LYS:HB2	4:C9:336:LYS:HE3	1.77	0.41
3:D0:84:ARG:HD2	7:n:98:THR:HG21	2.01	0.41
4:D1:137:HIS:CE1	4:D1:166:THR:HB	2.54	0.41
3:D4:173:PRO:HG3	3:D4:183:GLU:OE2	2.21	0.41
3:D4:205:ASP:O	3:D4:209:ILE:HG13	2.21	0.41
3:D6:75:VAL:HG12	3:D6:79:ARG:HH21	1.86	0.41
3:E0:422:ARG:NH1	3:E0:426:ALA:HB2	2.35	0.41
4:E1:287:PRO:O	4:E1:291:GLN:HG2	2.20	0.41
3:E2:132:LEU:HB2	3:E2:164:LYS:HD2	2.03	0.41
3:E2:304:LYS:HD3	3:E2:304:LYS:HA	1.82	0.41
4:E3:7:VAL:HA	4:E3:64:ILE:HB	2.03	0.41
3:E4:1:MET:HA	3:E4:130:THR:HG23	2.03	0.41
4:E7:66:MET:HE2	4:E7:147:MET:HG3	2.02	0.41
3:E8:238:LEU:HD11	3:E8:378:ILE:HD11	2.03	0.41
4:E9:15:GLN:O	4:E9:19:LYS:HG2	2.20	0.41
6:I:229:ALA:H	6:I:236:LYS:HB2	1.86	0.41
7:c:164:ARG:HH21	7:c:182:PHE:HB2	1.86	0.41
7:d:8:SER:HB3	7:d:11:ASN:OD1	2.21	0.41
7:g:150:VAL:HG12	7:g:165:THR:HG23	2.03	0.41
7:h:64:PRO:HD2	7:h:67:HIS:CE1	2.55	0.41
7:h:145:LYS:HG3	7:h:150:VAL:HG23	2.02	0.41
8:l:35:ALA:HA	8:l:133:VAL:HA	2.03	0.41
7:r:23:LEU:HD12	7:r:38:LEU:HD22	2.02	0.41
7:v:129:MET:HG2	7:v:131:TRP:CZ2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:v:195:ALA:HA	7:v:198:ARG:HG3	2.02	0.41
1:10:248:ARG:HH21	7:m:94:ASN:HD21	1.67	0.41
1:4:256:LEU:HD23	1:4:256:LEU:HA	1.92	0.41
2:A:565:ASP:HB3	2:A:571:MET:HG2	2.03	0.41
4:A1:304:ASP:HB3	4:A1:307:HIS:NE2	2.36	0.41
3:A2:121:ARG:HH21	3:A2:124:LYS:HD3	1.86	0.41
3:A4:21:TRP:HZ3	3:A4:52:PHE:HB3	1.85	0.41
4:A7:318:ARG:HA	4:A7:354:CYS:HB2	2.02	0.41
4:A9:215:LEU:HD11	4:A9:273:LEU:HD22	2.02	0.41
3:B0:306:ASP:HA	3:B0:307:PRO:HD3	1.84	0.41
4:B1:68:LEU:HB3	4:B1:96:GLY:HA2	2.02	0.41
4:B1:248:SER:HA	4:B1:252:LYS:HE2	2.02	0.41
3:B2:195:LEU:HD22	3:B2:428:LEU:HD22	2.03	0.41
3:B2:222:PRO:HD2	4:B3:324:LYS:HB3	2.03	0.41
3:B4:181:VAL:H	4:B5:256:ASN:ND2	2.19	0.41
3:B6:11:GLN:HG2	3:B6:74:VAL:HG21	2.03	0.41
4:B7:284:LEU:H	4:C1:55:THR:HG23	1.86	0.41
3:B8:277:SER:H	3:B8:280:LYS:HB3	1.85	0.41
4:B9:68:LEU:HD23	4:B9:112:LEU:HD13	2.02	0.41
4:B9:279:GLN:HA	4:B9:282:ARG:NH1	2.35	0.41
3:C0:174:SER:HB2	3:C0:207:GLU:HB2	2.03	0.41
4:C3:47:ILE:HG23	4:C3:51:TYR:HB2	2.02	0.41
3:C4:30:ILE:HG21	3:C4:53:PHE:CE2	2.56	0.41
3:C4:195:LEU:HD21	3:C4:264:ARG:HH21	1.85	0.41
3:C4:230:LEU:HD23	3:C4:230:LEU:HA	1.97	0.41
3:C4:407:TRP:CD2	4:C5:255:VAL:HG22	2.56	0.41
4:C5:248:SER:HA	4:C5:252:LYS:HD2	2.03	0.41
3:C6:174:SER:HB2	3:C6:177:VAL:O	2.21	0.41
3:C6:386:GLU:O	3:C6:390:ARG:HG2	2.21	0.41
4:C7:86:ARG:HA	4:C7:87:PRO:HD3	1.96	0.41
4:C7:326:VAL:O	4:C7:330:MET:HG2	2.21	0.41
3:C8:132:LEU:HD22	3:C8:164:LYS:HD2	2.02	0.41
4:C9:189:VAL:HG11	4:C9:415:MET:SD	2.61	0.41
4:D1:192:LEU:HB3	4:D1:199:VAL:HG21	2.02	0.41
4:D3:234:SER:HA	4:D3:237:THR:HG22	2.03	0.41
3:D6:7:ILE:HG21	3:D6:153:LEU:HD21	2.03	0.41
3:D6:90:GLU:HG3	3:D6:121:ARG:NH1	2.36	0.41
3:D8:139:ASN:HD21	3:D8:168:ASN:HD21	1.68	0.41
3:E2:265:ILE:HG21	3:E2:313:MET:HE1	2.02	0.41
4:E3:11:GLN:HA	4:E3:72:THR:HG21	2.01	0.41
4:E3:117:LEU:HD23	4:E3:117:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E3:183:TYR:HE1	4:E3:388:MET:HE2	1.85	0.41
3:E4:10:GLY:O	3:E4:14:ILE:HG12	2.21	0.41
3:E4:313:MET:HG2	3:E4:344:VAL:HG21	2.03	0.41
3:E6:403:ALA:HB2	4:E7:344:TRP:HZ3	1.86	0.41
4:E7:173:PRO:HG3	4:E7:380:ARG:HH11	1.86	0.41
4:E7:272:PRO:HD3	4:E7:364:SER:HA	2.02	0.41
4:E7:282:ARG:HD3	4:E7:284:LEU:HG	2.03	0.41
4:E9:162:ARG:HD3	4:E9:162:ARG:HA	1.89	0.41
4:E9:174:LYS:HE3	4:E9:174:LYS:HB3	1.79	0.41
4:E9:296:ALA:HB2	4:E9:306:ARG:HD2	2.03	0.41
3:F0:115:VAL:HG21	3:F0:152:LEU:HD23	2.03	0.41
6:H:399:VAL:HG12	6:H:404:PHE:HZ	1.85	0.41
7:c:5:VAL:HG23	7:c:161:TYR:CE1	2.56	0.41
7:c:189:LEU:HG	7:c:191:GLU:HG3	2.02	0.41
7:h:37:GLN:HE21	7:h:37:GLN:HB3	1.75	0.41
7:h:55:LEU:HB3	7:h:132:LEU:HD13	2.02	0.41
7:i:73:VAL:HA	7:i:109:GLU:O	2.21	0.41
7:j:122:PHE:CE1	7:j:136:LEU:HB2	2.56	0.41
8:k:50:VAL:HA	8:k:53:VAL:HG12	2.03	0.41
7:q:202:ARG:HH11	7:q:202:ARG:HD3	1.77	0.41
7:r:68:LEU:HD13	7:r:73:VAL:HG11	2.02	0.41
7:t:110:ILE:HB	7:t:131:TRP:CG	2.56	0.41
7:u:82:ASP:HB3	7:u:85:CYS:SG	2.61	0.41
7:u:85:CYS:HB3	7:u:168:PRO:HB3	2.03	0.41
7:v:75:LEU:O	7:v:170:VAL:HA	2.21	0.41
7:v:92:LEU:HD11	7:v:170:VAL:HG11	2.02	0.41
7:w:92:LEU:HD12	7:w:196:LEU:HD11	2.03	0.41
7:w:100:ASN:OD1	7:w:106:GLN:HG3	2.21	0.41
1:14:247:TYR:HB3	3:D6:77:GLU:OE2	2.21	0.41
2:A:490:HIS:CG	2:A:491:MET:N	2.89	0.41
3:A0:377:MET:HE3	3:A0:377:MET:HB3	1.86	0.41
4:A3:8:GLN:HE22	4:A3:17:GLY:HA3	1.86	0.41
3:A4:108:TYR:CE1	3:A4:413:MET:HB3	2.56	0.41
3:A8:287:SER:O	3:A8:291:ILE:HG12	2.21	0.41
3:B0:282:TYR:CE2	3:B4:60:LYS:HE3	2.56	0.41
3:B2:282:TYR:HD1	7:g:202:ARG:HD2	1.85	0.41
3:B2:329:ASN:HA	3:B2:332:VAL:HG12	2.03	0.41
4:B5:312:THR:HA	4:B5:348:ASN:O	2.20	0.41
4:B7:162:ARG:HA	4:B7:162:ARG:HD3	1.94	0.41
4:B9:8:GLN:OE1	4:B9:17:GLY:HA3	2.21	0.41
4:C1:298:ASN:O	4:C1:298:ASN:ND2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C3:252:LYS:HB3	4:C3:350:LYS:HZ3	1.85	0.41
3:C4:132:LEU:HG	3:C4:164:LYS:HD3	2.03	0.41
4:C5:167:PHE:CZ	4:C5:233:MET:HG2	2.56	0.41
3:C8:28:HIS:NE2	3:C8:243:ARG:HD2	2.36	0.41
3:D0:51:THR:HG21	3:D0:242:LEU:O	2.20	0.41
4:D1:375:GLN:OE1	4:D1:423:GLN:NE2	2.45	0.41
3:D6:75:VAL:HA	3:D6:78:VAL:HG12	2.02	0.41
3:D6:151:CYS:SG	3:D6:193:SER:HB2	2.61	0.41
3:D6:188:VAL:O	3:D6:191:THR:HG22	2.20	0.41
4:D7:190:HIS:CE1	4:D7:410:GLU:HG2	2.56	0.41
4:D7:289:LEU:HD22	4:D7:365:VAL:HG12	2.02	0.41
3:D8:154:LEU:HD23	3:D8:154:LEU:HA	1.98	0.41
3:D8:255:PHE:HZ	3:D8:378:ILE:HG21	1.85	0.41
3:D8:316:CYS:O	3:D8:377:MET:HA	2.21	0.41
3:E6:138:PHE:HZ	3:E6:235:ILE:HD12	1.86	0.41
4:E7:316:MET:HB2	4:E7:366:THR:HG22	2.02	0.41
3:E8:212:ILE:HD13	3:E8:212:ILE:HA	1.92	0.41
3:F0:105:ARG:HA	3:F0:109:THR:HG22	2.02	0.41
3:F0:332:VAL:O	3:F0:336:LYS:HG2	2.21	0.41
4:F1:244:GLY:HA2	4:F1:355:ASP:HB2	2.03	0.41
6:H:245:PHE:HA	6:H:260:THR:HA	2.02	0.41
7:j:185:ILE:HA	7:j:192:GLY:HA2	2.03	0.41
7:s:184:PRO:HG3	7:s:189:LEU:HD23	2.03	0.41
4:A1:6:HIS:O	4:A1:63:ALA:HA	2.21	0.40
4:A1:61:PRO:HD3	4:A1:84:LEU:HG	2.03	0.40
4:A5:259:PRO:HG2	4:A5:311:LEU:HD23	2.04	0.40
4:A5:326:VAL:O	4:A5:330:MET:HG2	2.21	0.40
3:A6:21:TRP:HZ3	3:A6:52:PHE:HB3	1.86	0.40
3:A6:407:TRP:HE1	4:A7:258:ILE:HB	1.85	0.40
4:A9:4:ILE:HD11	4:A9:240:LEU:HD22	2.03	0.40
2:B:371:ARG:HH21	4:B7:231:ALA:HB2	1.86	0.40
3:B0:80:THR:HA	3:B0:84:ARG:HE	1.86	0.40
3:B0:276:ILE:HD12	3:B0:281:ALA:HA	2.03	0.40
3:B2:351:PHE:C	3:B2:352:LYS:HD2	2.46	0.40
4:B3:252:LYS:HB3	4:B3:350:LYS:HZ1	1.86	0.40
3:B4:154:LEU:HB3	3:B4:197:HIS:HB3	2.03	0.40
3:B4:265:ILE:HG21	3:B4:313:MET:HE1	2.02	0.40
4:B5:392:LYS:HE2	4:B5:392:LYS:HA	2.03	0.40
3:B6:262:TYR:HD2	3:B6:265:ILE:HD11	1.86	0.40
3:B8:112:LYS:HA	3:B8:115:VAL:HG12	2.03	0.40
4:B9:373:ALA:O	4:B9:376:GLU:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C0:213:CYS:HB3	3:C0:219:ILE:HG21	2.03	0.40
3:C0:296:PHE:HE2	3:C0:335:ILE:HG21	1.86	0.40
3:C2:88:HIS:H	3:C2:91:GLN:HE21	1.67	0.40
3:C2:427:ALA:HA	3:C2:430:LYS:HE2	2.02	0.40
4:C3:152:ILE:HG12	4:C3:164:MET:HE1	2.04	0.40
4:C7:313:ALA:HB1	4:C7:367:PHE:CE1	2.56	0.40
3:C8:428:LEU:O	3:C8:432:TYR:HB2	2.21	0.40
3:D2:195:LEU:HD22	3:D2:428:LEU:HD23	2.03	0.40
4:D3:174:LYS:HE2	4:D3:174:LYS:HB2	1.79	0.40
4:D3:285:SER:HA	4:D3:363:MET:HE1	2.03	0.40
3:E0:167:LEU:HG	3:E0:200:VAL:HB	2.03	0.40
3:E0:259:LEU:HD13	3:E0:268:MET:HE3	2.02	0.40
3:E0:338:LYS:HB2	3:E0:338:LYS:HE2	1.85	0.40
4:E3:276:ARG:HD3	4:E3:276:ARG:HA	1.94	0.40
3:E4:269:LEU:HD22	3:E4:303:ALA:HB2	2.04	0.40
4:E5:24:ILE:HD13	4:E5:24:ILE:HG21	1.88	0.40
4:E5:200:GLN:HG2	4:E5:268:ILE:HD11	2.03	0.40
3:E6:274:PRO:HG3	3:E6:291:ILE:HB	2.03	0.40
3:E8:26:LEU:HA	3:E8:26:LEU:HD23	1.81	0.40
3:E8:172:TRP:HB2	3:E8:203:MET:HG3	2.01	0.40
4:E9:39:ASP:HA	7:w:90:PRO:HG3	2.03	0.40
5:G:116:GLU:O	5:G:120:GLU:HB2	2.20	0.40
6:H:398:TRP:HE1	6:H:403:LYS:HG3	1.85	0.40
6:J:233:TYR:CD1	6:K:394:VAL:HG22	2.56	0.40
6:K:247:ASN:ND2	6:K:287:ILE:H	2.19	0.40
7:e:74:ALA:HA	7:e:171:ILE:O	2.21	0.40
7:g:194:ARG:NH1	7:g:198:ARG:HH12	2.18	0.40
7:w:149:ARG:NH2	7:w:164:ARG:HD3	2.37	0.40
3:A4:169:PHE:CD1	3:A4:202:VAL:HG22	2.56	0.40
4:A5:258:ILE:HG22	4:A5:370:ASN:ND2	2.35	0.40
3:A6:168:ASN:O	3:A6:201:ALA:HA	2.21	0.40
4:A7:233:MET:O	4:A7:237:THR:HG22	2.21	0.40
4:B1:187:LEU:HA	4:B1:190:HIS:CE1	2.56	0.40
3:B2:178:SER:HB2	4:B3:347:ASN:HD22	1.85	0.40
4:B5:293:MET:HE2	4:B5:367:PHE:HD1	1.86	0.40
4:B9:313:ALA:HB3	4:B9:349:MET:HE1	2.03	0.40
4:C3:41:ASP:O	4:C3:45:GLU:HB3	2.21	0.40
3:C6:6:SER:OG	3:C6:8:HIS:HE1	2.04	0.40
3:C6:262:TYR:HB2	3:C6:265:ILE:HD12	2.03	0.40
3:C8:269:LEU:HD11	3:C8:384:ILE:HD11	2.02	0.40
4:C9:20:PHE:HA	4:C9:230:SER:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D0:169:PHE:CD1	3:D0:202:VAL:HG22	2.57	0.40
3:D2:216:ASN:HD22	3:D2:275:ILE:HB	1.87	0.40
3:D4:335:ILE:O	3:D4:338:LYS:HB3	2.22	0.40
4:D5:253:LEU:HG	4:D5:257:LEU:HD12	2.03	0.40
5:E:132:LYS:HA	5:E:136:GLN:HB2	2.03	0.40
4:E3:172:SER:HB2	4:E3:205:GLU:HG2	2.04	0.40
4:E3:237:THR:HG23	4:E3:241:ARG:NH1	2.35	0.40
6:I:335:LEU:H	6:I:347:TRP:CD1	2.39	0.40
7:a:97:ARG:O	7:a:101:GLU:HG3	2.21	0.40
7:d:11:ASN:HB3	7:d:15:ARG:HH12	1.85	0.40
7:d:141:THR:O	7:d:145:LYS:HG2	2.21	0.40
7:g:140:LEU:HG	7:g:144:LEU:HD23	2.02	0.40
7:u:97:ARG:O	7:u:101:GLU:HG2	2.22	0.40
1:10:254:LYS:HB2	3:C8:26:LEU:HD21	2.03	0.40
1:12:240:PRO:HB2	7:q:154:TYR:HD2	1.87	0.40
3:A2:119:LEU:HD11	3:A2:156:ARG:HB3	2.02	0.40
3:A4:21:TRP:CZ3	3:A4:52:PHE:HB3	2.56	0.40
3:A8:180:ALA:HA	4:A9:350:LYS:HD2	2.03	0.40
4:B3:42:LEU:HD23	4:B3:42:LEU:HA	1.93	0.40
3:B8:236:SER:O	3:B8:240:ALA:HB2	2.22	0.40
3:C6:271:SER:HB3	3:C6:377:MET:HE3	2.03	0.40
3:C8:21:TRP:HZ3	3:C8:52:PHE:HB3	1.85	0.40
4:D5:74:ASP:HA	4:D5:77:ARG:HG2	2.02	0.40
3:D6:60:LYS:HA	3:D6:60:LYS:HD2	1.90	0.40
3:D6:115:VAL:HG22	3:D6:119:LEU:HD23	2.04	0.40
3:D6:329:ASN:HA	3:D6:332:VAL:HG12	2.02	0.40
3:D8:234:VAL:HG21	3:D8:302:MET:HE1	2.02	0.40
3:E0:313:MET:HG2	3:E0:344:VAL:HG11	2.03	0.40
4:E1:187:LEU:HA	4:E1:190:HIS:CE1	2.56	0.40
4:E1:321:MET:HB2	4:E1:353:VAL:HG13	2.04	0.40
3:E4:398:MET:HG2	4:E5:345:ILE:HD12	2.03	0.40
3:E6:270:SER:HA	3:E6:377:MET:O	2.21	0.40
3:E6:398:MET:HE3	3:E6:398:MET:HB2	1.79	0.40
4:E7:311:LEU:HD23	4:E7:342:VAL:HG11	2.04	0.40
3:E8:411:GLU:OE2	3:E8:413:MET:HG2	2.21	0.40
4:E9:172:SER:HB2	4:E9:205:GLU:HB3	2.02	0.40
3:F0:261:PRO:HD3	3:F0:380:ASN:ND2	2.37	0.40
3:F0:320:ARG:HA	3:F0:356:ASN:HB3	2.02	0.40
4:F1:156:ARG:NH2	4:F1:164:MET:HB2	2.36	0.40
4:F1:235:GLY:HA3	4:F1:366:THR:HG21	2.02	0.40
7:h:184:PRO:HB2	7:h:189:LEU:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:m:53:GLY:HA2	7:m:62:VAL:HG21	2.03	0.40
7:r:10:LEU:HG	7:r:47:LEU:HD11	2.04	0.40
7:s:75:LEU:HD23	7:s:111:ILE:HB	2.02	0.40
2:A:493:LYS:HD3	4:D1:360:GLY:HA3	2.03	0.40
3:A0:188:VAL:HG21	3:A0:395:PHE:HB2	2.04	0.40
4:A1:318:ARG:HA	4:A1:354:CYS:O	2.21	0.40
3:A2:176:GLN:OE1	4:A3:331:LEU:HG	2.22	0.40
3:A4:319:TYR:HB3	3:A4:323:VAL:HG21	2.02	0.40
4:A5:229:VAL:HG12	4:A5:233:MET:HE2	2.03	0.40
4:A7:104:GLY:HA3	4:A7:146:GLY:HA3	2.03	0.40
3:A8:204:LEU:HD13	3:A8:231:ILE:HD12	2.03	0.40
2:B:217:ARG:HH12	2:B:222:HIS:C	2.30	0.40
3:B0:77:GLU:HA	3:B0:80:THR:HG22	2.04	0.40
3:B0:156:ARG:HA	3:B0:159:VAL:HG22	2.03	0.40
4:B1:135:ILE:O	4:B1:166:THR:HA	2.21	0.40
4:B5:40:SER:HB3	4:B5:43:GLN:HG3	2.03	0.40
4:B5:153:SER:HA	4:B5:195:ASN:HD22	1.84	0.40
4:B5:318:ARG:O	4:B5:363:MET:HA	2.21	0.40
4:B9:271:ALA:HB3	4:B9:365:VAL:HG12	2.04	0.40
4:C1:305:PRO:HB2	4:C1:310:TYR:CE1	2.56	0.40
3:C4:286:LEU:HD13	3:C4:286:LEU:HA	1.90	0.40
3:C6:32:PRO:HG2	8:l:64:GLY:H	1.86	0.40
3:C8:9:VAL:HG13	3:C8:149:LEU:HD22	2.03	0.40
4:C9:165:GLU:OE1	4:C9:250:LEU:HD11	2.22	0.40
3:D0:154:LEU:HD23	3:D0:154:LEU:HA	1.93	0.40
4:D3:207:LEU:HD23	4:D3:207:LEU:HA	1.95	0.40
4:D3:207:LEU:HA	4:D3:210:ILE:HG22	2.04	0.40
3:D6:122:ILE:HD13	3:D6:122:ILE:HA	1.92	0.40
4:D7:284:LEU:HD23	4:D7:362:LYS:HG2	2.04	0.40
3:E4:189:LEU:HD21	3:E4:418:PHE:HE2	1.85	0.40
3:E4:222:PRO:O	4:E5:322:SER:HB2	2.21	0.40
3:E4:352:LYS:HA	3:E4:352:LYS:HD2	1.92	0.40
3:E4:417:GLU:HG2	3:E4:418:PHE:CD2	2.57	0.40
3:F0:172:TRP:HB2	3:F0:203:MET:HB3	2.02	0.40
3:F0:320:ARG:HH11	3:F0:360:PRO:HA	1.87	0.40
6:H:299:ILE:HD13	6:H:299:ILE:HA	1.92	0.40
7:e:183:LEU:HD23	7:e:196:LEU:HA	2.03	0.40
7:m:10:LEU:HD23	7:m:10:LEU:HA	1.97	0.40
7:p:92:LEU:HD12	7:p:92:LEU:HA	1.95	0.40
7:v:59:ASN:HD22	7:x:9:PRO:HB3	1.87	0.40
4:A1:186:THR:HG23	4:A1:415:MET:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A1:216:LYS:HD2	2:B:262:LYS:HD3	2.02	0.40
4:A3:13:GLY:HA2	4:A3:16:ILE:HG22	2.03	0.40
3:A6:57:GLY:H	2:B:254:GLY:H	1.69	0.40
3:A6:271:SER:HB3	3:A6:301:MET:HA	2.03	0.40
3:A8:118:SER:O	3:A8:122:ILE:HG12	2.22	0.40
4:A9:282:ARG:NH2	2:B:318:GLN:HE21	2.18	0.40
3:B2:12:ALA:HB3	3:B2:140:ALA:HB2	2.02	0.40
3:B4:288:VAL:HB	3:B4:327:ASP:HB3	2.03	0.40
3:B6:33:ASP:HB3	7:g:102:GLY:O	2.21	0.40
3:B8:33:ASP:HB3	7:h:102:GLY:O	2.21	0.40
3:C0:236:SER:HA	3:C0:243:ARG:HH21	1.86	0.40
3:C0:242:LEU:H	3:C0:242:LEU:HD23	1.86	0.40
4:C3:310:TYR:HE2	4:C3:369:GLY:HA3	1.86	0.40
3:C4:75:VAL:HB	3:C4:94:SER:HB3	2.03	0.40
3:C4:156:ARG:HA	3:C4:159:VAL:HG12	2.03	0.40
3:C4:276:ILE:HG23	3:C4:280:LYS:HG3	2.02	0.40
4:C5:183:TYR:CE2	4:C5:388:MET:HG2	2.56	0.40
4:C7:362:LYS:NZ	4:C7:363:MET:HE2	2.37	0.40
3:C8:70:LEU:HD12	3:C8:145:THR:HG22	2.03	0.40
3:C8:76:ASP:HA	3:C8:79:ARG:HB2	2.03	0.40
3:C8:422:ARG:HD2	3:C8:422:ARG:HA	1.87	0.40
4:C9:100:ASN:HB3	4:C9:103:LYS:HB3	2.03	0.40
3:D0:261:PRO:HB2	3:D0:262:TYR:CD1	2.56	0.40
3:D4:104:ALA:HB2	3:D4:413:MET:HE3	2.03	0.40
3:D4:311:LYS:NZ	3:D4:342:GLN:HG2	2.37	0.40
4:D9:171:PRO:HG2	4:D9:185:ALA:HB2	2.03	0.40
4:D9:375:GLN:HG3	4:D9:419:VAL:HG13	2.03	0.40
5:E:110:ALA:HB2	4:F1:359:LYS:HE2	2.02	0.40
4:E3:392:LYS:HD2	4:E3:395:LEU:HD12	2.04	0.40
3:E4:278:ALA:HB1	7:w:200:ASP:HB3	2.03	0.40
3:E8:6:SER:HB2	3:E8:8:HIS:CE1	2.57	0.40
4:E9:105:HIS:HA	4:E9:150:LEU:HG	2.03	0.40
4:E9:201:VAL:HG11	4:E9:378:PHE:HZ	1.87	0.40
4:E9:213:ARG:HH12	4:E9:297:LYS:HE2	1.86	0.40
4:E9:311:LEU:HD12	4:E9:312:THR:HG22	2.04	0.40
4:F1:8:GLN:O	4:F1:66:MET:HG3	2.21	0.40
4:F1:136:THR:HG22	4:F1:167:PHE:HB2	2.04	0.40
6:H:252:PRO:HD3	6:H:289:PHE:HB3	2.04	0.40
6:I:324:LEU:HA	6:I:339:ASN:HA	2.03	0.40
7:h:75:LEU:O	7:h:170:VAL:HA	2.21	0.40
7:u:73:VAL:HA	7:u:109:GLU:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	20/351 (6%)	20 (100%)	0	0	100	100
1	1	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	10	20/351 (6%)	20 (100%)	0	0	100	100
1	11	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	12	20/351 (6%)	20 (100%)	0	0	100	100
1	13	20/351 (6%)	20 (100%)	0	0	100	100
1	14	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	15	20/351 (6%)	20 (100%)	0	0	100	100
1	16	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	17	20/351 (6%)	20 (100%)	0	0	100	100
1	18	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	19	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	2	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	22	18/351 (5%)	15 (83%)	3 (17%)	0	100	100
1	23	18/351 (5%)	16 (89%)	2 (11%)	0	100	100
1	3	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	4	20/351 (6%)	20 (100%)	0	0	100	100
1	5	20/351 (6%)	20 (100%)	0	0	100	100
1	6	20/351 (6%)	20 (100%)	0	0	100	100
1	7	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	8	20/351 (6%)	17 (85%)	2 (10%)	1 (5%)	1	11
1	9	20/351 (6%)	14 (70%)	5 (25%)	1 (5%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	159/583 (27%)	132 (83%)	22 (14%)	5 (3%)	3	20
2	B	210/583 (36%)	173 (82%)	30 (14%)	7 (3%)	3	19
2	C	47/583 (8%)	41 (87%)	5 (11%)	1 (2%)	5	26
3	A0	424/453 (94%)	389 (92%)	33 (8%)	2 (0%)	24	55
3	A2	424/453 (94%)	393 (93%)	31 (7%)	0	100	100
3	A4	424/453 (94%)	400 (94%)	24 (6%)	0	100	100
3	A6	424/453 (94%)	391 (92%)	33 (8%)	0	100	100
3	A8	424/453 (94%)	411 (97%)	13 (3%)	0	100	100
3	B0	424/453 (94%)	407 (96%)	17 (4%)	0	100	100
3	B2	424/453 (94%)	409 (96%)	15 (4%)	0	100	100
3	B4	424/453 (94%)	406 (96%)	18 (4%)	0	100	100
3	B6	424/453 (94%)	405 (96%)	19 (4%)	0	100	100
3	B8	424/453 (94%)	407 (96%)	17 (4%)	0	100	100
3	C0	424/453 (94%)	353 (83%)	69 (16%)	2 (0%)	24	55
3	C2	424/453 (94%)	364 (86%)	60 (14%)	0	100	100
3	C4	424/453 (94%)	377 (89%)	46 (11%)	1 (0%)	43	71
3	C6	424/453 (94%)	384 (91%)	38 (9%)	2 (0%)	24	55
3	C8	424/453 (94%)	376 (89%)	47 (11%)	1 (0%)	43	71
3	D0	424/453 (94%)	383 (90%)	40 (9%)	1 (0%)	43	71
3	D2	424/453 (94%)	384 (91%)	40 (9%)	0	100	100
3	D4	424/453 (94%)	394 (93%)	28 (7%)	2 (0%)	24	55
3	D6	424/453 (94%)	396 (93%)	28 (7%)	0	100	100
3	D8	424/453 (94%)	393 (93%)	31 (7%)	0	100	100
3	E0	424/453 (94%)	396 (93%)	28 (7%)	0	100	100
3	E2	424/453 (94%)	385 (91%)	38 (9%)	1 (0%)	43	71
3	E4	424/453 (94%)	386 (91%)	36 (8%)	2 (0%)	24	55
3	E6	424/453 (94%)	367 (87%)	56 (13%)	1 (0%)	43	71
3	E8	424/453 (94%)	388 (92%)	36 (8%)	0	100	100
3	F0	424/453 (94%)	372 (88%)	51 (12%)	1 (0%)	43	71
4	A1	424/449 (94%)	399 (94%)	25 (6%)	0	100	100
4	A3	424/449 (94%)	403 (95%)	21 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A5	424/449 (94%)	398 (94%)	24 (6%)	2 (0%)	24	55
4	A7	424/449 (94%)	399 (94%)	24 (6%)	1 (0%)	43	71
4	A9	424/449 (94%)	401 (95%)	23 (5%)	0	100	100
4	B1	424/449 (94%)	402 (95%)	22 (5%)	0	100	100
4	B3	424/449 (94%)	408 (96%)	15 (4%)	1 (0%)	43	71
4	B5	424/449 (94%)	406 (96%)	18 (4%)	0	100	100
4	B7	424/449 (94%)	396 (93%)	28 (7%)	0	100	100
4	B9	424/449 (94%)	399 (94%)	25 (6%)	0	100	100
4	C1	424/449 (94%)	368 (87%)	54 (13%)	2 (0%)	24	55
4	C3	424/449 (94%)	386 (91%)	38 (9%)	0	100	100
4	C5	424/449 (94%)	381 (90%)	41 (10%)	2 (0%)	24	55
4	C7	424/449 (94%)	378 (89%)	43 (10%)	3 (1%)	18	49
4	C9	424/449 (94%)	378 (89%)	44 (10%)	2 (0%)	24	55
4	D1	424/449 (94%)	386 (91%)	37 (9%)	1 (0%)	43	71
4	D3	424/449 (94%)	375 (88%)	44 (10%)	5 (1%)	10	37
4	D5	424/449 (94%)	384 (91%)	37 (9%)	3 (1%)	18	49
4	D7	424/449 (94%)	402 (95%)	21 (5%)	1 (0%)	43	71
4	D9	424/449 (94%)	403 (95%)	21 (5%)	0	100	100
4	E1	424/449 (94%)	382 (90%)	40 (9%)	2 (0%)	24	55
4	E3	424/449 (94%)	390 (92%)	32 (8%)	2 (0%)	24	55
4	E5	424/449 (94%)	392 (92%)	31 (7%)	1 (0%)	43	71
4	E7	424/449 (94%)	396 (93%)	27 (6%)	1 (0%)	43	71
4	E9	424/449 (94%)	342 (81%)	79 (19%)	3 (1%)	18	49
4	F1	424/449 (94%)	377 (89%)	46 (11%)	1 (0%)	43	71
5	E	85/336 (25%)	68 (80%)	17 (20%)	0	100	100
5	F	85/336 (25%)	66 (78%)	19 (22%)	0	100	100
5	G	65/336 (19%)	53 (82%)	12 (18%)	0	100	100
6	H	221/446 (50%)	199 (90%)	22 (10%)	0	100	100
6	I	222/446 (50%)	206 (93%)	15 (7%)	1 (0%)	24	55
6	J	227/446 (51%)	206 (91%)	21 (9%)	0	100	100
6	K	218/446 (49%)	204 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	a	159/220 (72%)	144 (91%)	15 (9%)	0	100	100
7	b	159/220 (72%)	139 (87%)	20 (13%)	0	100	100
7	c	197/220 (90%)	185 (94%)	11 (6%)	1 (0%)	24	55
7	d	197/220 (90%)	188 (95%)	9 (5%)	0	100	100
7	e	197/220 (90%)	188 (95%)	9 (5%)	0	100	100
7	f	197/220 (90%)	186 (94%)	11 (6%)	0	100	100
7	g	197/220 (90%)	187 (95%)	10 (5%)	0	100	100
7	h	197/220 (90%)	185 (94%)	12 (6%)	0	100	100
7	i	197/220 (90%)	190 (96%)	7 (4%)	0	100	100
7	j	197/220 (90%)	186 (94%)	11 (6%)	0	100	100
7	m	197/220 (90%)	184 (93%)	13 (7%)	0	100	100
7	n	197/220 (90%)	185 (94%)	12 (6%)	0	100	100
7	o	197/220 (90%)	186 (94%)	11 (6%)	0	100	100
7	p	197/220 (90%)	189 (96%)	8 (4%)	0	100	100
7	q	197/220 (90%)	189 (96%)	8 (4%)	0	100	100
7	r	197/220 (90%)	191 (97%)	6 (3%)	0	100	100
7	s	197/220 (90%)	187 (95%)	10 (5%)	0	100	100
7	t	197/220 (90%)	190 (96%)	7 (4%)	0	100	100
7	u	197/220 (90%)	187 (95%)	10 (5%)	0	100	100
7	v	197/220 (90%)	183 (93%)	14 (7%)	0	100	100
7	w	197/220 (90%)	179 (91%)	18 (9%)	0	100	100
7	x	197/220 (90%)	184 (93%)	13 (7%)	0	100	100
8	k	133/189 (70%)	115 (86%)	15 (11%)	3 (2%)	5	25
8	l	133/189 (70%)	109 (82%)	23 (17%)	1 (1%)	16	45
All	All	28547/40933 (70%)	26241 (92%)	2236 (8%)	70 (0%)	44	71

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	277	ASP
2	B	277	ASP
2	B	468	ASN
3	C4	218	ASP
3	C6	243	ARG

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Mol	Chain	Res	Type
3	C6	256	GLN
4	C7	355	ASP
4	D3	55	THR
4	D3	95	THR
4	D5	95	THR
4	D7	355	ASP
4	E5	355	ASP
4	E7	355	ASP
3	F0	347	CYS
7	c	36	ILE
8	k	65	GLU
8	l	61	ASN
1	9	246	CYS
2	A	278	GLN
2	A	521	PRO
2	B	521	PRO
3	C0	381	SER
4	C5	347	ASN
3	D0	403	ALA
4	D5	55	THR
4	D5	355	ASP
3	E2	112	LYS
3	E4	313	MET
8	k	61	ASN
1	8	246	CYS
3	A0	403	ALA
3	C8	403	ALA
4	C9	272	PRO
3	D4	338	LYS
3	E6	145	THR
4	A5	178	THR
2	B	278	GLN
2	B	567	LEU
2	C	253	ALA
4	C1	311	LEU
4	C7	90	PHE
4	C7	347	ASN
4	C9	393	ALA
4	D3	355	ASP
4	E1	125	GLU
4	E3	218	THR
4	F1	272	PRO

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Mol	Chain	Res	Type
2	B	257	ILE
2	B	571	MET
4	C1	178	THR
4	C5	263	LEU
4	D1	178	THR
4	E1	272	PRO
3	E4	220	GLU
4	E9	101	TRP
4	E9	351	SER
2	A	468	ASN
4	B3	178	THR
4	D3	108	GLU
4	D3	178	THR
3	D4	403	ALA
6	I	390	ALA
8	k	129	PRO
3	A0	261	PRO
4	A7	272	PRO
4	E3	272	PRO
4	E9	358	PRO
2	A	530	ILE
4	A5	272	PRO
3	C0	173	PRO

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	20/305 (7%)	20 (100%)	0	100	100
1	1	20/305 (7%)	20 (100%)	0	100	100
1	10	20/305 (7%)	20 (100%)	0	100	100
1	11	20/305 (7%)	20 (100%)	0	100	100
1	12	20/305 (7%)	20 (100%)	0	100	100
1	13	20/305 (7%)	20 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	14	20/305 (7%)	20 (100%)	0	100	100
1	15	20/305 (7%)	20 (100%)	0	100	100
1	16	20/305 (7%)	20 (100%)	0	100	100
1	17	20/305 (7%)	20 (100%)	0	100	100
1	18	20/305 (7%)	20 (100%)	0	100	100
1	19	20/305 (7%)	20 (100%)	0	100	100
1	2	20/305 (7%)	20 (100%)	0	100	100
1	22	18/305 (6%)	18 (100%)	0	100	100
1	23	18/305 (6%)	18 (100%)	0	100	100
1	3	20/305 (7%)	20 (100%)	0	100	100
1	4	20/305 (7%)	20 (100%)	0	100	100
1	5	20/305 (7%)	19 (95%)	1 (5%)	22	50
1	6	20/305 (7%)	20 (100%)	0	100	100
1	7	20/305 (7%)	20 (100%)	0	100	100
1	8	20/305 (7%)	20 (100%)	0	100	100
1	9	20/305 (7%)	20 (100%)	0	100	100
2	A	154/502 (31%)	154 (100%)	0	100	100
2	B	194/502 (39%)	194 (100%)	0	100	100
2	C	38/502 (8%)	38 (100%)	0	100	100
3	A0	359/379 (95%)	359 (100%)	0	100	100
3	A2	359/379 (95%)	359 (100%)	0	100	100
3	A4	359/379 (95%)	359 (100%)	0	100	100
3	A6	359/379 (95%)	359 (100%)	0	100	100
3	A8	359/379 (95%)	359 (100%)	0	100	100
3	B0	359/379 (95%)	359 (100%)	0	100	100
3	B2	359/379 (95%)	359 (100%)	0	100	100
3	B4	359/379 (95%)	359 (100%)	0	100	100
3	B6	359/379 (95%)	359 (100%)	0	100	100
3	B8	359/379 (95%)	359 (100%)	0	100	100
3	C0	359/379 (95%)	358 (100%)	1 (0%)	86	86
3	C2	359/379 (95%)	359 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C4	359/379 (95%)	359 (100%)	0	100	100
3	C6	359/379 (95%)	359 (100%)	0	100	100
3	C8	359/379 (95%)	359 (100%)	0	100	100
3	D0	359/379 (95%)	359 (100%)	0	100	100
3	D2	359/379 (95%)	358 (100%)	1 (0%)	86	86
3	D4	359/379 (95%)	359 (100%)	0	100	100
3	D6	359/379 (95%)	358 (100%)	1 (0%)	86	86
3	D8	359/379 (95%)	359 (100%)	0	100	100
3	E0	359/379 (95%)	359 (100%)	0	100	100
3	E2	359/379 (95%)	359 (100%)	0	100	100
3	E4	359/379 (95%)	359 (100%)	0	100	100
3	E6	359/379 (95%)	359 (100%)	0	100	100
3	E8	358/379 (94%)	358 (100%)	0	100	100
3	F0	359/379 (95%)	359 (100%)	0	100	100
4	A1	364/381 (96%)	364 (100%)	0	100	100
4	A3	364/381 (96%)	364 (100%)	0	100	100
4	A5	364/381 (96%)	364 (100%)	0	100	100
4	A7	364/381 (96%)	364 (100%)	0	100	100
4	A9	364/381 (96%)	363 (100%)	1 (0%)	86	86
4	B1	364/381 (96%)	364 (100%)	0	100	100
4	B3	364/381 (96%)	364 (100%)	0	100	100
4	B5	364/381 (96%)	364 (100%)	0	100	100
4	B7	364/381 (96%)	364 (100%)	0	100	100
4	B9	364/381 (96%)	364 (100%)	0	100	100
4	C1	364/381 (96%)	364 (100%)	0	100	100
4	C3	364/381 (96%)	363 (100%)	1 (0%)	86	86
4	C5	364/381 (96%)	363 (100%)	1 (0%)	86	86
4	C7	364/381 (96%)	364 (100%)	0	100	100
4	C9	364/381 (96%)	363 (100%)	1 (0%)	86	86
4	D1	364/381 (96%)	364 (100%)	0	100	100
4	D3	364/381 (96%)	363 (100%)	1 (0%)	86	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D5	364/381 (96%)	364 (100%)	0	100	100
4	D7	364/381 (96%)	364 (100%)	0	100	100
4	D9	364/381 (96%)	364 (100%)	0	100	100
4	E1	364/381 (96%)	364 (100%)	0	100	100
4	E3	364/381 (96%)	364 (100%)	0	100	100
4	E5	364/381 (96%)	364 (100%)	0	100	100
4	E7	364/381 (96%)	364 (100%)	0	100	100
4	E9	364/381 (96%)	362 (100%)	2 (0%)	81	83
4	F1	364/381 (96%)	364 (100%)	0	100	100
5	E	76/280 (27%)	76 (100%)	0	100	100
5	F	76/280 (27%)	76 (100%)	0	100	100
5	G	56/280 (20%)	56 (100%)	0	100	100
6	H	185/345 (54%)	185 (100%)	0	100	100
6	I	185/345 (54%)	185 (100%)	0	100	100
6	J	191/345 (55%)	191 (100%)	0	100	100
6	K	183/345 (53%)	183 (100%)	0	100	100
7	a	139/190 (73%)	139 (100%)	0	100	100
7	b	139/190 (73%)	139 (100%)	0	100	100
7	c	174/190 (92%)	174 (100%)	0	100	100
7	d	174/190 (92%)	174 (100%)	0	100	100
7	e	174/190 (92%)	174 (100%)	0	100	100
7	f	174/190 (92%)	174 (100%)	0	100	100
7	g	174/190 (92%)	174 (100%)	0	100	100
7	h	174/190 (92%)	174 (100%)	0	100	100
7	i	174/190 (92%)	174 (100%)	0	100	100
7	j	174/190 (92%)	174 (100%)	0	100	100
7	m	174/190 (92%)	174 (100%)	0	100	100
7	n	174/190 (92%)	174 (100%)	0	100	100
7	o	174/190 (92%)	174 (100%)	0	100	100
7	p	174/190 (92%)	174 (100%)	0	100	100
7	q	174/190 (92%)	174 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	r	174/190 (92%)	174 (100%)	0	100	100
7	s	174/190 (92%)	174 (100%)	0	100	100
7	t	174/190 (92%)	174 (100%)	0	100	100
7	u	174/190 (92%)	174 (100%)	0	100	100
7	v	174/190 (92%)	174 (100%)	0	100	100
7	w	174/190 (92%)	174 (100%)	0	100	100
7	x	174/190 (92%)	174 (100%)	0	100	100
8	k	122/164 (74%)	122 (100%)	0	100	100
8	l	122/164 (74%)	122 (100%)	0	100	100
All	All	24573/34704 (71%)	24562 (100%)	11 (0%)	100	100

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	5	244	GLN
4	A9	414	ASN
3	C0	91	GLN
4	C3	191	GLN
4	C5	195	ASN
4	C9	131	GLN
3	D2	192	HIS
4	D3	247	ASN
3	D6	256	GLN
4	E9	256	ASN
4	E9	329	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (312) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	244	GLN
1	13	244	GLN
1	14	242	ASN
1	4	244	GLN
2	A	469	GLN
3	A0	31	GLN
3	A0	50	ASN
3	A0	91	GLN
3	A0	102	ASN

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Mol	Chain	Res	Type
4	A1	256	ASN
4	A1	334	GLN
4	A1	348	ASN
3	A2	18	ASN
3	A2	329	ASN
3	A2	380	ASN
4	A3	94	GLN
4	A3	195	ASN
4	A3	334	GLN
3	A4	216	ASN
3	A4	258	ASN
3	A4	406	HIS
4	A5	83	GLN
4	A5	348	ASN
4	A5	370	ASN
3	A6	31	GLN
3	A6	285	GLN
3	A6	380	ASN
4	A7	11	GLN
4	A7	14	ASN
4	A7	15	GLN
4	A7	43	GLN
4	A7	280	GLN
4	A7	291	GLN
3	A8	15	GLN
3	A8	61	HIS
3	A8	85	HIS
3	A8	393	HIS
4	A9	195	ASN
4	A9	279	GLN
4	A9	335	ASN
4	A9	375	GLN
2	B	543	GLN
3	B0	85	HIS
3	B0	88	HIS
3	B0	128	ASN
3	B0	139	ASN
3	B0	206	ASN
4	B1	15	GLN
4	B1	48	ASN
4	B1	99	ASN
4	B1	204	ASN

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Mol	Chain	Res	Type
4	B1	245	GLN
4	B1	279	GLN
4	B1	329	GLN
4	B1	375	GLN
3	B2	309	HIS
3	B2	356	ASN
3	B2	380	ASN
4	B3	14	ASN
4	B3	94	GLN
4	B3	247	ASN
4	B3	280	GLN
4	B3	337	ASN
3	B4	133	GLN
4	B5	227	HIS
4	B5	329	GLN
4	B5	334	GLN
3	B6	15	GLN
3	B6	88	HIS
3	B6	186	ASN
3	B6	256	GLN
3	B6	329	ASN
3	B6	393	HIS
4	B7	15	GLN
4	B7	131	GLN
4	B7	329	GLN
4	B7	348	ASN
4	B7	414	ASN
3	B8	128	ASN
3	B8	168	ASN
3	B8	285	GLN
3	B8	329	ASN
3	B8	406	HIS
4	B9	247	ASN
4	B9	291	GLN
4	B9	375	GLN
3	C0	11	GLN
3	C0	15	GLN
3	C0	18	ASN
3	C0	206	ASN
3	C0	258	ASN
3	C0	293	ASN
4	C1	14	ASN

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Mol	Chain	Res	Type
4	C1	200	GLN
4	C1	247	ASN
4	C1	335	ASN
4	C1	424	GLN
3	C2	91	GLN
3	C2	102	ASN
3	C2	107	HIS
3	C2	133	GLN
3	C2	206	ASN
3	C2	258	ASN
4	C3	89	ASN
4	C3	247	ASN
4	C3	256	ASN
4	C3	292	GLN
4	C3	298	ASN
3	C4	31	GLN
3	C4	85	HIS
3	C4	133	GLN
3	C4	192	HIS
3	C4	216	ASN
3	C4	233	GLN
3	C4	258	ASN
4	C5	52	ASN
4	C5	195	ASN
4	C5	298	ASN
4	C5	416	ASN
3	C6	8	HIS
3	C6	88	HIS
3	C6	107	HIS
3	C6	216	ASN
4	C7	8	GLN
4	C7	256	ASN
4	C7	292	GLN
4	C7	348	ASN
4	C7	370	ASN
4	C7	375	GLN
3	C8	102	ASN
3	C8	186	ASN
3	C8	329	ASN
3	C8	406	HIS
4	C9	28	HIS
4	C9	89	ASN

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Mol	Chain	Res	Type
4	C9	94	GLN
4	C9	131	GLN
4	C9	245	GLN
4	C9	256	ASN
4	C9	348	ASN
4	C9	426	GLN
3	D0	101	ASN
3	D0	258	ASN
4	D1	14	ASN
4	D1	100	ASN
4	D1	264	HIS
4	D1	292	GLN
4	D1	329	GLN
4	D1	348	ASN
3	D2	168	ASN
3	D2	216	ASN
3	D2	228	ASN
3	D2	256	GLN
3	D2	329	ASN
4	D3	184	ASN
4	D3	247	ASN
4	D3	292	GLN
4	D3	348	ASN
4	D3	384	GLN
3	D4	197	HIS
3	D4	380	ASN
4	D5	11	GLN
4	D5	195	ASN
4	D5	227	HIS
4	D5	334	GLN
4	D5	347	ASN
4	D5	375	GLN
4	D5	384	GLN
4	D5	414	ASN
3	D6	15	GLN
3	D6	35	GLN
3	D6	88	HIS
3	D6	91	GLN
3	D6	216	ASN
3	D6	258	ASN
3	D6	293	ASN
3	D6	329	ASN

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Mol	Chain	Res	Type
3	D6	342	GLN
4	D7	137	HIS
4	D7	247	ASN
4	D7	279	GLN
4	D7	334	GLN
4	D7	423	GLN
3	D8	31	GLN
3	D8	91	GLN
3	D8	139	ASN
3	D8	256	GLN
3	D8	329	ASN
4	D9	8	GLN
4	D9	204	ASN
4	D9	348	ASN
4	D9	424	GLN
3	E0	8	HIS
3	E0	91	GLN
3	E0	107	HIS
3	E0	216	ASN
3	E0	256	GLN
3	E0	329	ASN
3	E0	406	HIS
4	E1	8	GLN
4	E1	100	ASN
4	E1	191	GLN
4	E1	195	ASN
4	E1	279	GLN
4	E1	332	ASN
4	E1	348	ASN
4	E1	424	GLN
3	E2	15	GLN
3	E2	133	GLN
3	E2	216	ASN
3	E2	258	ASN
4	E3	191	GLN
4	E3	292	GLN
4	E3	298	ASN
4	E3	334	GLN
4	E3	337	ASN
4	E3	348	ASN
4	E3	384	GLN
4	E3	423	GLN

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Mol	Chain	Res	Type
4	E3	426	GLN
3	E4	256	GLN
3	E4	266	HIS
4	E5	105	HIS
4	E5	191	GLN
4	E5	291	GLN
4	E5	329	GLN
3	E6	8	HIS
3	E6	31	GLN
3	E6	168	ASN
3	E6	342	GLN
4	E7	28	HIS
4	E7	99	ASN
4	E7	100	ASN
4	E7	247	ASN
4	E7	334	GLN
3	E8	35	GLN
3	E8	139	ASN
3	E8	228	ASN
4	E9	245	GLN
4	E9	280	GLN
4	E9	424	GLN
5	F	136	GLN
3	F0	31	GLN
3	F0	91	GLN
3	F0	197	HIS
4	F1	6	HIS
4	F1	8	GLN
4	F1	137	HIS
4	F1	191	GLN
4	F1	292	GLN
4	F1	335	ASN
5	G	136	GLN
6	H	247	ASN
6	H	250	HIS
6	I	213	GLN
6	J	201	HIS
6	J	247	ASN
6	J	391	ASN
6	K	352	GLN
6	K	418	GLN
7	a	59	ASN

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Mol	Chain	Res	Type
7	a	67	HIS
7	a	147	HIS
7	b	94	ASN
7	b	125	HIS
7	c	41	ASN
7	c	60	ASN
7	c	125	HIS
7	c	203	ASN
7	d	125	HIS
7	e	11	ASN
7	e	37	GLN
7	e	125	HIS
7	f	11	ASN
7	f	37	GLN
7	f	125	HIS
7	g	125	HIS
7	h	67	HIS
7	h	128	HIS
7	i	37	GLN
7	i	41	ASN
7	j	67	HIS
7	j	94	ASN
8	k	17	GLN
8	k	48	GLN
8	l	113	ASN
8	l	147	GLN
8	l	148	GLN
7	m	41	ASN
7	m	94	ASN
7	m	147	HIS
7	n	60	ASN
7	o	18	ASN
7	o	67	HIS
7	o	94	ASN
7	o	181	GLN
7	p	11	ASN
7	q	25	GLN
7	q	94	ASN
7	r	181	GLN
7	s	25	GLN
7	s	59	ASN
7	s	125	HIS

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Mol	Chain	Res	Type
7	s	128	HIS
7	t	37	GLN
7	t	60	ASN
7	t	106	GLN
7	u	11	ASN
7	u	128	HIS
7	w	11	ASN
7	w	128	HIS
7	w	181	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	GDP	C3	501	-	29,30,30	1.20	3 (10%)	45,47,47	1.80	7 (15%)
9	GDP	B7	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	6 (13%)
10	GTP	E2	501	11	33,34,34	0.91	1 (3%)	50,54,54	1.60	9 (18%)
10	GTP	D6	501	11	33,34,34	0.91	1 (3%)	50,54,54	1.62	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	GTP	D8	501	11	33,34,34	0.92	1 (3%)	50,54,54	1.61	11 (22%)
9	GDP	A7	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.80	7 (15%)
10	GTP	A6	501	11	33,34,34	0.92	1 (3%)	50,54,54	1.64	11 (22%)
10	GTP	A8	501	11	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
9	GDP	A3	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	6 (13%)
10	GTP	D0	501	11	33,34,34	0.89	1 (3%)	50,54,54	1.61	10 (20%)
10	GTP	C0	501	11	33,34,34	1.00	2 (6%)	50,54,54	1.63	11 (22%)
10	GTP	E4	501	11	33,34,34	0.88	1 (3%)	50,54,54	1.61	9 (18%)
10	GTP	F0	501	11	33,34,34	0.94	0	50,54,54	1.58	9 (18%)
9	GDP	D5	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.81	7 (15%)
9	GDP	E3	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	7 (15%)
9	GDP	B3	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	7 (15%)
9	GDP	A5	501	-	29,30,30	1.14	4 (13%)	45,47,47	1.72	6 (13%)
9	GDP	B9	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
9	GDP	F1	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	7 (15%)
9	GDP	A1	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.89	8 (17%)
9	GDP	A	601	-	29,30,30	1.15	2 (6%)	45,47,47	1.79	6 (13%)
10	GTP	B4	501	11	33,34,34	0.93	1 (3%)	50,54,54	1.62	11 (22%)
9	GDP	E9	501	-	29,30,30	1.12	3 (10%)	45,47,47	1.74	7 (15%)
10	GTP	E6	501	11	33,34,34	0.90	1 (3%)	50,54,54	1.61	9 (18%)
10	GTP	C4	501	11	33,34,34	0.90	0	50,54,54	1.53	9 (18%)
9	GDP	D3	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	7 (15%)
10	GTP	C8	501	11	33,34,34	0.88	1 (3%)	50,54,54	1.54	8 (16%)
9	GDP	D1	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
10	GTP	A2	501	11	33,34,34	0.89	2 (6%)	50,54,54	1.66	10 (20%)
9	GDP	B5	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.72	6 (13%)
9	GDP	B	601	-	29,30,30	1.18	3 (10%)	45,47,47	1.77	9 (20%)
10	GTP	B8	501	11	33,34,34	0.90	1 (3%)	50,54,54	1.59	8 (16%)
9	GDP	E5	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.72	5 (11%)
10	GTP	D4	501	11	33,34,34	0.91	0	50,54,54	1.55	8 (16%)
9	GDP	E1	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.73	7 (15%)
9	GDP	C7	501	-	29,30,30	1.17	2 (6%)	45,47,47	1.86	9 (20%)
10	GTP	D2	501	11	33,34,34	0.89	1 (3%)	50,54,54	1.59	8 (16%)
9	GDP	D9	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
10	GTP	A0	501	11	33,34,34	1.00	2 (6%)	50,54,54	1.67	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	GTP	B0	501	11	33,34,34	0.91	1 (3%)	50,54,54	1.60	9 (18%)
10	GTP	B6	501	11	33,34,34	0.91	1 (3%)	50,54,54	1.57	8 (16%)
10	GTP	C6	501	11	33,34,34	0.91	1 (3%)	50,54,54	1.61	9 (18%)
10	GTP	E0	501	11	33,34,34	0.90	1 (3%)	50,54,54	1.61	9 (18%)
9	GDP	C9	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
10	GTP	E8	501	11	33,34,34	0.91	1 (3%)	50,54,54	1.61	9 (18%)
9	GDP	E7	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.74	6 (13%)
9	GDP	C5	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.72	7 (15%)
10	GTP	C2	501	11	33,34,34	0.95	1 (3%)	50,54,54	1.63	11 (22%)
9	GDP	D7	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	8 (17%)
10	GTP	B2	501	11	33,34,34	0.92	1 (3%)	50,54,54	1.61	9 (18%)
9	GDP	C1	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.89	10 (22%)
10	GTP	A4	501	11	33,34,34	0.86	1 (3%)	50,54,54	1.58	8 (16%)

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	GDP	C3	501	-	-	3/16/32/32	0/3/3/3
9	GDP	B7	501	-	-	3/16/32/32	0/3/3/3
10	GTP	E2	501	11	-	1/22/38/38	0/3/3/3
10	GTP	D6	501	11	-	7/22/38/38	0/3/3/3
10	GTP	D8	501	11	-	6/22/38/38	0/3/3/3
9	GDP	A7	501	-	-	3/16/32/32	0/3/3/3
10	GTP	A6	501	11	-	6/22/38/38	0/3/3/3
10	GTP	A8	501	11	-	7/22/38/38	0/3/3/3
9	GDP	A3	502	-	-	6/16/32/32	0/3/3/3
10	GTP	D0	501	11	-	6/22/38/38	0/3/3/3
10	GTP	C0	501	11	-	7/22/38/38	0/3/3/3
10	GTP	E4	501	11	-	8/22/38/38	0/3/3/3
10	GTP	F0	501	11	-	7/22/38/38	0/3/3/3
9	GDP	D5	501	-	-	9/16/32/32	0/3/3/3
9	GDP	E3	501	-	-	5/16/32/32	0/3/3/3
9	GDP	B3	501	-	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GDP	A5	501	-	-	2/16/32/32	0/3/3/3
9	GDP	B9	501	-	-	3/16/32/32	0/3/3/3
9	GDP	F1	501	-	-	4/16/32/32	0/3/3/3
9	GDP	A1	501	-	-	5/16/32/32	0/3/3/3
9	GDP	A	601	-	-	5/16/32/32	0/3/3/3
10	GTP	B4	501	11	-	8/22/38/38	0/3/3/3
9	GDP	E9	501	-	-	5/16/32/32	0/3/3/3
10	GTP	E6	501	11	-	7/22/38/38	0/3/3/3
10	GTP	C4	501	11	-	7/22/38/38	0/3/3/3
9	GDP	D3	501	-	-	3/16/32/32	0/3/3/3
10	GTP	C8	501	11	-	4/22/38/38	0/3/3/3
9	GDP	D1	501	-	-	2/16/32/32	0/3/3/3
10	GTP	A2	501	11	-	9/22/38/38	0/3/3/3
9	GDP	B5	501	-	-	5/16/32/32	0/3/3/3
9	GDP	B	601	-	-	4/16/32/32	0/3/3/3
10	GTP	B8	501	11	-	8/22/38/38	0/3/3/3
9	GDP	E5	501	-	-	1/16/32/32	0/3/3/3
10	GTP	D4	501	11	-	5/22/38/38	0/3/3/3
9	GDP	E1	501	-	-	4/16/32/32	0/3/3/3
9	GDP	C7	501	-	-	2/16/32/32	0/3/3/3
10	GTP	D2	501	11	-	9/22/38/38	0/3/3/3
9	GDP	D9	501	-	-	4/16/32/32	0/3/3/3
10	GTP	A0	501	11	-	3/22/38/38	0/3/3/3
10	GTP	B0	501	11	-	8/22/38/38	0/3/3/3
10	GTP	B6	501	11	-	7/22/38/38	0/3/3/3
10	GTP	C6	501	11	-	9/22/38/38	0/3/3/3
10	GTP	E0	501	11	-	2/22/38/38	0/3/3/3
9	GDP	C9	501	-	-	3/16/32/32	0/3/3/3
10	GTP	E8	501	11	-	5/22/38/38	0/3/3/3
9	GDP	E7	501	-	-	6/16/32/32	0/3/3/3
9	GDP	C5	501	-	-	4/16/32/32	0/3/3/3
10	GTP	C2	501	11	-	6/22/38/38	0/3/3/3
9	GDP	D7	501	-	-	4/16/32/32	0/3/3/3
10	GTP	B2	501	11	-	6/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GDP	C1	501	-	-	2/16/32/32	0/3/3/3
10	GTP	A4	501	11	-	3/22/38/38	0/3/3/3

All (103) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C7	501	GDP	C5-C4	3.12	1.47	1.38
9	A3	502	GDP	C5-C4	3.11	1.47	1.38
9	C3	501	GDP	C5-C4	3.09	1.47	1.38
9	D5	501	GDP	C5-C4	3.09	1.47	1.38
9	A7	501	GDP	C5-C4	3.07	1.47	1.38
9	A	601	GDP	C5-C4	3.04	1.47	1.38
9	F1	501	GDP	C5-C4	3.04	1.47	1.38
9	B7	501	GDP	C5-C4	3.03	1.47	1.38
9	D9	501	GDP	C5-C4	3.02	1.47	1.38
9	B9	501	GDP	C5-C4	3.02	1.47	1.38
9	E5	501	GDP	C5-C4	3.01	1.47	1.38
9	B3	501	GDP	C5-C4	3.00	1.47	1.38
9	B5	501	GDP	C5-C4	3.00	1.47	1.38
9	E3	501	GDP	C5-C4	3.00	1.47	1.38
9	D1	501	GDP	C5-C4	2.99	1.46	1.38
9	E7	501	GDP	C5-C4	2.98	1.46	1.38
9	D7	501	GDP	C5-C4	2.97	1.46	1.38
9	A1	501	GDP	C5-C4	2.96	1.46	1.38
9	E1	501	GDP	C5-C4	2.95	1.46	1.38
9	C1	501	GDP	C5-C4	2.95	1.46	1.38
9	A5	501	GDP	C5-C4	2.94	1.46	1.38
9	D3	501	GDP	C5-C4	2.94	1.46	1.38
9	B	601	GDP	C5-C4	2.92	1.46	1.38
9	C9	501	GDP	C5-C4	2.87	1.46	1.38
9	E7	501	GDP	C6-N1	-2.85	1.33	1.38
9	C5	501	GDP	C5-C4	2.84	1.46	1.38
9	E9	501	GDP	C5-C4	2.79	1.46	1.38
9	A1	501	GDP	C6-N1	-2.76	1.33	1.38
9	E3	501	GDP	C6-N1	-2.73	1.33	1.38
9	B	601	GDP	C6-N1	-2.72	1.33	1.38
9	C5	501	GDP	C6-N1	-2.71	1.33	1.38
9	B3	501	GDP	C6-N1	-2.70	1.33	1.38
9	E5	501	GDP	C6-N1	-2.70	1.33	1.38
9	B5	501	GDP	C6-N1	-2.67	1.33	1.38
9	A7	501	GDP	C6-N1	-2.64	1.33	1.38
9	B9	501	GDP	C6-N1	-2.64	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D9	501	GDP	C6-N1	-2.64	1.33	1.38
9	F1	501	GDP	C6-N1	-2.63	1.33	1.38
9	D7	501	GDP	C6-N1	-2.63	1.33	1.38
9	C9	501	GDP	C6-N1	-2.62	1.33	1.38
9	C7	501	GDP	C6-N1	-2.62	1.33	1.38
9	C3	501	GDP	C6-N1	-2.61	1.34	1.38
9	B7	501	GDP	C6-N1	-2.60	1.34	1.38
9	D1	501	GDP	C6-N1	-2.60	1.34	1.38
9	D5	501	GDP	C6-N1	-2.60	1.34	1.38
9	E1	501	GDP	C6-N1	-2.59	1.34	1.38
9	D3	501	GDP	C6-N1	-2.58	1.34	1.38
9	C1	501	GDP	C6-N1	-2.57	1.34	1.38
9	A3	502	GDP	C6-N1	-2.57	1.34	1.38
9	A5	501	GDP	C6-N1	-2.52	1.34	1.38
9	A	601	GDP	C6-N1	-2.48	1.34	1.38
9	E9	501	GDP	C6-N1	-2.45	1.34	1.38
10	C0	501	GTP	PA-O3A	2.44	1.62	1.59
10	C0	501	GTP	PB-O3A	2.30	1.62	1.59
10	A0	501	GTP	C2-N3	2.25	1.38	1.33
9	A1	501	GDP	C5-N7	-2.24	1.34	1.39
10	D2	501	GTP	C2-N3	2.22	1.38	1.33
9	B	601	GDP	C4-N9	-2.21	1.32	1.38
9	E7	501	GDP	C5-N7	-2.19	1.34	1.39
9	B7	501	GDP	C5-N7	-2.18	1.34	1.39
9	C5	501	GDP	C5-N7	-2.18	1.34	1.39
9	D1	501	GDP	C5-N7	-2.17	1.34	1.39
9	E3	501	GDP	C5-N7	-2.17	1.34	1.39
10	A2	501	GTP	C2-N3	2.16	1.38	1.33
9	C9	501	GDP	C5-N7	-2.16	1.34	1.39
10	E8	501	GTP	C2-N3	2.16	1.38	1.33
10	A0	501	GTP	C5-N7	-2.16	1.34	1.39
10	E6	501	GTP	C2-N3	2.15	1.38	1.33
9	D5	501	GDP	C5-N7	-2.15	1.34	1.39
10	B4	501	GTP	C2-N3	2.15	1.38	1.33
10	B2	501	GTP	C2-N3	2.15	1.38	1.33
9	D7	501	GDP	C5-N7	-2.14	1.34	1.39
9	E9	501	GDP	C4-N9	-2.14	1.32	1.38
10	D6	501	GTP	C2-N3	2.13	1.38	1.33
9	A3	502	GDP	C4-N9	-2.13	1.32	1.38
9	B3	501	GDP	C5-N7	-2.13	1.34	1.39
10	D8	501	GTP	C2-N3	2.12	1.38	1.33
9	E1	501	GDP	C5-N7	-2.12	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C2	501	GTP	C2-N3	2.12	1.38	1.33
10	B8	501	GTP	C2-N3	2.11	1.38	1.33
10	E4	501	GTP	C2-N3	2.10	1.38	1.33
10	B6	501	GTP	C2-N3	2.10	1.38	1.33
9	C1	501	GDP	C5-N7	-2.09	1.34	1.39
9	A7	501	GDP	C5-N7	-2.09	1.34	1.39
9	D3	501	GDP	C5-N7	-2.08	1.34	1.39
9	B9	501	GDP	C5-N7	-2.08	1.34	1.39
9	E5	501	GDP	C5-N7	-2.07	1.34	1.39
10	E2	501	GTP	C2-N3	2.07	1.38	1.33
10	A6	501	GTP	C2-N3	2.06	1.38	1.33
10	D0	501	GTP	C2-N3	2.06	1.38	1.33
10	C6	501	GTP	C2-N3	2.06	1.38	1.33
9	C3	501	GDP	C5-N7	-2.06	1.34	1.39
10	B0	501	GTP	C2-N3	2.06	1.38	1.33
9	A5	501	GDP	C4-N9	-2.05	1.32	1.38
9	B5	501	GDP	C5-N7	-2.05	1.35	1.39
10	E0	501	GTP	C2-N3	2.05	1.38	1.33
10	A8	501	GTP	C2-N3	2.04	1.38	1.33
9	A5	501	GDP	C5-N7	-2.04	1.35	1.39
9	D9	501	GDP	C5-N7	-2.04	1.35	1.39
10	C8	501	GTP	C2-N3	2.03	1.38	1.33
10	A4	501	GTP	C2-N3	2.03	1.38	1.33
9	F1	501	GDP	C5-N7	-2.03	1.35	1.39
10	A2	501	GTP	C5-N7	-2.02	1.35	1.39

All (423) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A1	501	GDP	C5-C4-N3	-6.52	118.01	128.39
9	D5	501	GDP	C5-C4-N3	-6.32	118.33	128.39
9	A7	501	GDP	C5-C4-N3	-6.19	118.54	128.39
9	F1	501	GDP	C5-C4-N3	-6.16	118.59	128.39
9	C7	501	GDP	C5-C4-N3	-6.13	118.63	128.39
9	E3	501	GDP	C5-C4-N3	-6.13	118.64	128.39
9	B3	501	GDP	C5-C4-N3	-6.12	118.66	128.39
9	D1	501	GDP	C5-C4-N3	-6.10	118.68	128.39
9	C3	501	GDP	C5-C4-N3	-6.06	118.75	128.39
9	C1	501	GDP	C5-C4-N3	-6.04	118.77	128.39
9	D3	501	GDP	C5-C4-N3	-6.03	118.79	128.39
9	E1	501	GDP	C5-C4-N3	-5.95	118.92	128.39
9	C9	501	GDP	C5-C4-N3	-5.95	118.93	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B5	501	GDP	C5-C4-N3	-5.94	118.93	128.39
9	A	601	GDP	C5-C4-N3	-5.91	118.99	128.39
9	D9	501	GDP	C5-C4-N3	-5.91	118.99	128.39
9	E5	501	GDP	C5-C4-N3	-5.88	119.03	128.39
9	E7	501	GDP	C5-C4-N3	-5.88	119.04	128.39
9	B7	501	GDP	C5-C4-N3	-5.87	119.05	128.39
9	D7	501	GDP	C5-C4-N3	-5.86	119.06	128.39
9	B9	501	GDP	C5-C4-N3	-5.84	119.10	128.39
9	C5	501	GDP	C5-C4-N3	-5.82	119.13	128.39
9	A3	502	GDP	C5-C4-N3	-5.59	119.49	128.39
9	A5	501	GDP	C5-C4-N3	-5.59	119.49	128.39
9	E9	501	GDP	C5-C4-N3	-5.49	119.66	128.39
10	A0	501	GTP	C5-C4-N3	-5.41	119.78	128.39
9	B	601	GDP	C5-C4-N3	-5.30	119.96	128.39
10	E6	501	GTP	C5-C4-N3	-5.28	119.99	128.39
10	A2	501	GTP	C5-C4-N3	-5.21	120.10	128.39
10	E2	501	GTP	C5-C4-N3	-5.21	120.10	128.39
9	A1	501	GDP	C2-N3-C4	5.20	121.25	112.30
10	D6	501	GTP	C5-C4-N3	-5.16	120.19	128.39
9	A	601	GDP	C2-N3-C4	5.15	121.18	112.30
10	B4	501	GTP	C5-C4-N3	-5.14	120.22	128.39
10	E8	501	GTP	C5-C4-N3	-5.13	120.22	128.39
9	C1	501	GDP	C2-N3-C4	5.13	121.13	112.30
10	D2	501	GTP	C5-C4-N3	-5.13	120.23	128.39
9	B	601	GDP	C2-N3-C4	5.12	121.13	112.30
10	E4	501	GTP	C5-C4-N3	-5.10	120.27	128.39
10	D8	501	GTP	C5-C4-N3	-5.10	120.27	128.39
9	D5	501	GDP	C2-N3-C4	5.09	121.07	112.30
10	B2	501	GTP	C5-C4-N3	-5.09	120.29	128.39
10	A8	501	GTP	C5-C4-N3	-5.08	120.30	128.39
10	B0	501	GTP	C5-C4-N3	-5.06	120.33	128.39
10	B8	501	GTP	C5-C4-N3	-5.06	120.34	128.39
10	E0	501	GTP	C5-C4-N3	-5.04	120.36	128.39
9	D3	501	GDP	C2-N3-C4	5.03	120.97	112.30
9	C9	501	GDP	C2-N3-C4	5.02	120.94	112.30
10	C6	501	GTP	C5-C4-N3	-5.02	120.41	128.39
9	D1	501	GDP	C2-N3-C4	5.02	120.94	112.30
9	E3	501	GDP	C2-N3-C4	5.02	120.94	112.30
9	A1	501	GDP	N9-C4-N3	5.01	135.97	125.95
9	C7	501	GDP	C2-N3-C4	4.99	120.90	112.30
10	B6	501	GTP	C5-C4-N3	-4.99	120.44	128.39
9	B3	501	GDP	C2-N3-C4	4.99	120.90	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A6	501	GTP	C5-C4-N3	-4.98	120.46	128.39
9	F1	501	GDP	C2-N3-C4	4.98	120.87	112.30
9	A7	501	GDP	C2-N3-C4	4.97	120.87	112.30
9	C5	501	GDP	C2-N3-C4	4.96	120.85	112.30
9	E5	501	GDP	C2-N3-C4	4.96	120.84	112.30
9	B7	501	GDP	C2-N3-C4	4.95	120.83	112.30
9	B9	501	GDP	C2-N3-C4	4.95	120.83	112.30
10	A4	501	GTP	C5-C4-N3	-4.94	120.52	128.39
9	C3	501	GDP	C2-N3-C4	4.94	120.81	112.30
9	D7	501	GDP	C2-N3-C4	4.94	120.81	112.30
9	B5	501	GDP	C2-N3-C4	4.94	120.81	112.30
9	A5	501	GDP	C2-N3-C4	4.94	120.80	112.30
9	D9	501	GDP	C2-N3-C4	4.92	120.78	112.30
9	E1	501	GDP	C2-N3-C4	4.92	120.77	112.30
9	E7	501	GDP	C2-N3-C4	4.91	120.76	112.30
9	E9	501	GDP	C2-N3-C4	4.90	120.74	112.30
10	C0	501	GTP	C5-C4-N3	-4.88	120.62	128.39
10	D0	501	GTP	C5-C4-N3	-4.87	120.64	128.39
10	D4	501	GTP	C5-C4-N3	-4.83	120.70	128.39
10	F0	501	GTP	C5-C4-N3	-4.82	120.71	128.39
10	C2	501	GTP	C5-C4-N3	-4.79	120.77	128.39
9	D5	501	GDP	N9-C4-N3	4.78	135.50	125.95
10	E8	501	GTP	C2-N3-C4	4.77	120.51	112.30
10	C8	501	GTP	C5-C4-N3	-4.75	120.82	128.39
10	C6	501	GTP	C2-N3-C4	4.73	120.45	112.30
10	C4	501	GTP	C5-C4-N3	-4.73	120.86	128.39
10	A2	501	GTP	C2-N3-C4	4.70	120.39	112.30
10	A0	501	GTP	C2-N3-C4	4.69	120.38	112.30
9	C1	501	GDP	N9-C4-N3	4.68	135.31	125.95
10	E4	501	GTP	C2-N3-C4	4.66	120.33	112.30
10	E6	501	GTP	C2-N3-C4	4.65	120.31	112.30
10	A8	501	GTP	C2-N3-C4	4.65	120.31	112.30
10	D2	501	GTP	C2-N3-C4	4.65	120.30	112.30
10	B8	501	GTP	C2-N3-C4	4.64	120.30	112.30
10	D6	501	GTP	C2-N3-C4	4.64	120.30	112.30
10	E2	501	GTP	C2-N3-C4	4.63	120.28	112.30
10	C0	501	GTP	C2-N3-C4	4.63	120.27	112.30
9	A7	501	GDP	N9-C4-N3	4.60	135.16	125.95
10	D4	501	GTP	C2-N3-C4	4.60	120.22	112.30
10	B4	501	GTP	C2-N3-C4	4.60	120.22	112.30
10	B0	501	GTP	C2-N3-C4	4.59	120.21	112.30
10	E0	501	GTP	C2-N3-C4	4.59	120.21	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A6	501	GTP	C2-N3-C4	4.59	120.20	112.30
10	D0	501	GTP	C2-N3-C4	4.59	120.20	112.30
10	D8	501	GTP	C2-N3-C4	4.58	120.19	112.30
10	A4	501	GTP	C2-N3-C4	4.57	120.18	112.30
10	B6	501	GTP	C2-N3-C4	4.57	120.17	112.30
10	F0	501	GTP	C2-N3-C4	4.55	120.13	112.30
10	B2	501	GTP	C2-N3-C4	4.54	120.12	112.30
9	F1	501	GDP	N9-C4-N3	4.53	135.01	125.95
9	D1	501	GDP	N9-C4-N3	4.53	135.00	125.95
9	B3	501	GDP	N9-C4-N3	4.49	134.93	125.95
9	C3	501	GDP	N9-C4-N3	4.49	134.93	125.95
9	A3	502	GDP	C2-N3-C4	4.47	119.99	112.30
10	C2	501	GTP	C2-N3-C4	4.46	119.98	112.30
9	E3	501	GDP	N9-C4-N3	4.46	134.87	125.95
10	C8	501	GTP	C2-N3-C4	4.45	119.97	112.30
9	C7	501	GDP	N9-C4-N3	4.45	134.84	125.95
9	D3	501	GDP	N9-C4-N3	4.42	134.78	125.95
9	C9	501	GDP	N9-C4-N3	4.41	134.77	125.95
9	D9	501	GDP	N9-C4-N3	4.41	134.76	125.95
10	C4	501	GTP	C2-N3-C4	4.39	119.87	112.30
9	B5	501	GDP	N9-C4-N3	4.39	134.74	125.95
9	E7	501	GDP	N9-C4-N3	4.39	134.73	125.95
9	B7	501	GDP	N9-C4-N3	4.36	134.67	125.95
9	E5	501	GDP	N9-C4-N3	4.36	134.66	125.95
9	D7	501	GDP	N9-C4-N3	4.35	134.66	125.95
9	E1	501	GDP	N9-C4-N3	4.31	134.58	125.95
9	C5	501	GDP	N9-C4-N3	4.30	134.55	125.95
9	B9	501	GDP	N9-C4-N3	4.27	134.50	125.95
9	B	601	GDP	C6-C5-N7	4.07	137.69	130.29
9	A	601	GDP	N9-C4-N3	4.03	134.01	125.95
9	E9	501	GDP	N9-C4-N3	3.97	133.89	125.95
9	A5	501	GDP	N9-C4-N3	3.93	133.82	125.95
9	A3	502	GDP	N9-C4-N3	3.89	133.74	125.95
10	A0	501	GTP	N9-C4-N3	3.85	133.66	125.95
9	E9	501	GDP	C6-C5-N7	3.69	137.00	130.29
9	A	601	GDP	C6-C5-N7	3.67	136.97	130.29
9	A3	502	GDP	C6-C5-N7	3.65	136.94	130.29
9	A5	501	GDP	C6-C5-N7	3.59	136.82	130.29
10	E6	501	GTP	N9-C4-N3	3.54	133.03	125.95
9	B	601	GDP	N9-C4-N3	3.50	132.95	125.95
10	A2	501	GTP	N9-C4-N3	3.49	132.93	125.95
10	E2	501	GTP	N9-C4-N3	3.48	132.92	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B2	501	GTP	N9-C4-N3	3.47	132.90	125.95
9	B9	501	GDP	C6-C5-N7	3.46	136.59	130.29
10	B4	501	GTP	N9-C4-N3	3.44	132.83	125.95
9	E5	501	GDP	C6-C5-N7	3.43	136.53	130.29
10	D6	501	GTP	N9-C4-N3	3.43	132.81	125.95
10	D8	501	GTP	N9-C4-N3	3.43	132.80	125.95
9	C7	501	GDP	C6-C5-N7	3.38	136.45	130.29
9	B7	501	GDP	C6-C5-N7	3.37	136.43	130.29
9	D7	501	GDP	C6-C5-N7	3.36	136.41	130.29
9	D9	501	GDP	C6-C5-N7	3.35	136.38	130.29
9	E7	501	GDP	C6-C5-N7	3.33	136.35	130.29
9	B5	501	GDP	C6-C5-N7	3.33	136.35	130.29
10	D2	501	GTP	N9-C4-N3	3.32	132.60	125.95
9	D3	501	GDP	C6-C5-N7	3.32	136.33	130.29
9	C5	501	GDP	C6-C5-N7	3.32	136.33	130.29
9	E1	501	GDP	C6-C5-N7	3.30	136.30	130.29
9	C1	501	GDP	C6-C5-N7	3.30	136.30	130.29
9	E3	501	GDP	C6-C5-N7	3.29	136.28	130.29
10	E0	501	GTP	N9-C4-N3	3.28	132.52	125.95
10	B6	501	GTP	N9-C4-N3	3.28	132.52	125.95
10	A8	501	GTP	N9-C4-N3	3.28	132.51	125.95
9	C3	501	GDP	C6-C5-N7	3.28	136.25	130.29
9	C9	501	GDP	C6-C5-N7	3.26	136.22	130.29
10	A0	501	GTP	C2-N1-C6	-3.25	119.21	125.11
10	B8	501	GTP	N9-C4-N3	3.25	132.46	125.95
10	B0	501	GTP	N9-C4-N3	3.24	132.43	125.95
9	B3	501	GDP	C6-C5-N7	3.24	136.18	130.29
10	A4	501	GTP	N9-C4-N3	3.23	132.41	125.95
9	F1	501	GDP	C6-C5-N7	3.20	136.11	130.29
10	E8	501	GTP	N9-C4-N3	3.19	132.34	125.95
10	E4	501	GTP	N9-C4-N3	3.18	132.31	125.95
10	D0	501	GTP	N9-C4-N3	3.17	132.30	125.95
9	A7	501	GDP	C6-C5-N7	3.17	136.06	130.29
9	D1	501	GDP	C6-C5-N7	3.17	136.05	130.29
10	A6	501	GTP	N9-C4-N3	3.14	132.24	125.95
10	C4	501	GTP	N9-C4-N3	3.12	132.19	125.95
10	C0	501	GTP	C2-N1-C6	-3.11	119.48	125.11
10	C2	501	GTP	N9-C4-N3	3.10	132.16	125.95
10	C6	501	GTP	N9-C4-N3	3.09	132.14	125.95
10	A2	501	GTP	C2-N1-C6	-3.09	119.51	125.11
10	C6	501	GTP	C2-N1-C6	-3.08	119.52	125.11
10	E6	501	GTP	C2-N1-C6	-3.07	119.54	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D4	501	GTP	N9-C4-N3	3.07	132.10	125.95
10	C8	501	GTP	N9-C4-N3	3.07	132.09	125.95
9	D5	501	GDP	C6-C5-N7	3.04	135.82	130.29
10	F0	501	GTP	C2-N1-C6	-3.01	119.65	125.11
10	D2	501	GTP	C2-N1-C6	-3.00	119.66	125.11
10	B2	501	GTP	C2-N1-C6	-3.00	119.67	125.11
10	E4	501	GTP	C2-N1-C6	-2.97	119.72	125.11
10	A8	501	GTP	C2-N1-C6	-2.97	119.72	125.11
10	B0	501	GTP	C2-N1-C6	-2.97	119.72	125.11
10	D6	501	GTP	C2-N1-C6	-2.96	119.73	125.11
10	B4	501	GTP	C2-N1-C6	-2.94	119.78	125.11
10	E2	501	GTP	C2-N1-C6	-2.93	119.80	125.11
9	A1	501	GDP	C6-C5-N7	2.92	135.61	130.29
10	B6	501	GTP	C2-N1-C6	-2.92	119.82	125.11
10	E8	501	GTP	C2-N1-C6	-2.92	119.82	125.11
10	B8	501	GTP	C2-N1-C6	-2.92	119.82	125.11
10	A6	501	GTP	C2-N1-C6	-2.91	119.84	125.11
10	E0	501	GTP	C2-N1-C6	-2.90	119.84	125.11
10	D8	501	GTP	C2-N1-C6	-2.86	119.92	125.11
10	A0	501	GTP	O6-C6-C5	-2.86	118.98	126.53
10	A0	501	GTP	C5-C6-N1	2.85	120.51	113.25
10	A4	501	GTP	C2-N1-C6	-2.84	119.95	125.11
10	C0	501	GTP	N9-C4-N3	2.83	131.62	125.95
9	A3	502	GDP	C4-C5-N7	-2.83	106.19	110.67
10	C8	501	GTP	C2-N1-C6	-2.81	120.01	125.11
10	D0	501	GTP	C2-N1-C6	-2.80	120.04	125.11
9	C7	501	GDP	C4-C5-N7	-2.80	106.24	110.67
10	D4	501	GTP	N9-C8-N7	-2.79	108.23	113.40
10	C4	501	GTP	N9-C8-N7	-2.77	108.25	113.40
10	C0	501	GTP	N9-C8-N7	-2.75	108.30	113.40
10	C6	501	GTP	N9-C8-N7	-2.75	108.31	113.40
10	C8	501	GTP	N9-C8-N7	-2.74	108.32	113.40
10	C6	501	GTP	C5-C6-N1	2.73	120.21	113.25
10	B2	501	GTP	N9-C8-N7	-2.73	108.33	113.40
10	A8	501	GTP	N9-C8-N7	-2.73	108.33	113.40
10	C2	501	GTP	C2-N1-C6	-2.73	120.16	125.11
10	A6	501	GTP	N9-C8-N7	-2.73	108.34	113.40
10	A4	501	GTP	N9-C8-N7	-2.73	108.34	113.40
10	D4	501	GTP	C2-N1-C6	-2.73	120.16	125.11
10	F0	501	GTP	N9-C4-N3	2.71	131.38	125.95
10	F0	501	GTP	N9-C8-N7	-2.71	108.37	113.40
10	B2	501	GTP	C5-C6-N1	2.70	120.11	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B6	501	GTP	N9-C8-N7	-2.69	108.41	113.40
10	B8	501	GTP	N9-C8-N7	-2.68	108.43	113.40
10	D8	501	GTP	N9-C8-N7	-2.67	108.45	113.40
10	E8	501	GTP	N9-C8-N7	-2.67	108.46	113.40
10	E0	501	GTP	N9-C8-N7	-2.66	108.47	113.40
9	A5	501	GDP	C4-C5-N7	-2.65	106.47	110.67
10	D0	501	GTP	N9-C8-N7	-2.65	108.49	113.40
10	E8	501	GTP	C8-N7-C5	2.64	108.97	104.26
10	E6	501	GTP	C5-C6-N1	2.64	119.98	113.25
9	A	601	GDP	C4-C5-N7	-2.63	106.50	110.67
10	D6	501	GTP	N9-C8-N7	-2.63	108.52	113.40
10	D2	501	GTP	N9-C8-N7	-2.63	108.53	113.40
10	A2	501	GTP	C5-C6-N1	2.62	119.93	113.25
10	B6	501	GTP	C5-C6-N1	2.62	119.93	113.25
10	B4	501	GTP	N9-C8-N7	-2.62	108.54	113.40
10	E4	501	GTP	N9-C8-N7	-2.62	108.55	113.40
10	C2	501	GTP	O6-C6-C5	-2.61	119.64	126.53
9	D3	501	GDP	C4-C5-N7	-2.61	106.53	110.67
10	F0	501	GTP	C8-N7-C5	2.60	108.90	104.26
10	C4	501	GTP	C2-N1-C6	-2.60	120.39	125.11
10	B4	501	GTP	C5-C6-N1	2.60	119.86	113.25
10	A0	501	GTP	N9-C8-N7	-2.60	108.58	113.40
10	C0	501	GTP	C8-N7-C5	2.59	108.88	104.26
9	A1	501	GDP	C3'-C2'-C1'	2.59	106.36	101.46
10	A8	501	GTP	C5-C6-N1	2.59	119.85	113.25
9	A7	501	GDP	C4-C5-N7	-2.59	106.57	110.67
10	E4	501	GTP	C5-C6-N1	2.59	119.84	113.25
9	F1	501	GDP	C4-C5-N7	-2.59	106.57	110.67
10	B0	501	GTP	C5-C6-N1	2.58	119.83	113.25
10	B0	501	GTP	N9-C8-N7	-2.58	108.61	113.40
10	E6	501	GTP	N9-C8-N7	-2.58	108.61	113.40
10	D6	501	GTP	C5-C6-N1	2.58	119.83	113.25
10	E2	501	GTP	N9-C8-N7	-2.58	108.61	113.40
9	F1	501	GDP	C3'-C2'-C1'	2.58	106.34	101.46
10	C6	501	GTP	O6-C6-C5	-2.58	119.73	126.53
10	A2	501	GTP	N9-C8-N7	-2.58	108.62	113.40
9	C7	501	GDP	O2A-PA-O3A	2.57	114.23	107.27
9	B9	501	GDP	C4-C5-N7	-2.57	106.59	110.67
9	C3	501	GDP	C4-C5-N7	-2.57	106.59	110.67
10	B8	501	GTP	C5-C6-N1	2.57	119.79	113.25
10	D2	501	GTP	C5-C6-N1	2.57	119.79	113.25
10	C2	501	GTP	O2A-PA-O3A	2.57	114.21	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B3	501	GDP	C4-C5-N7	-2.57	106.61	110.67
9	E1	501	GDP	C4-C5-N7	-2.56	106.61	110.67
10	A8	501	GTP	C8-N7-C5	2.56	108.82	104.26
10	A6	501	GTP	C8-N7-C5	2.56	108.82	104.26
9	E3	501	GDP	C4-C5-N7	-2.55	106.62	110.67
10	A2	501	GTP	O6-C6-C5	-2.55	119.79	126.53
10	D0	501	GTP	C5-C6-N1	2.55	119.75	113.25
9	D9	501	GDP	C4-C5-N7	-2.55	106.63	110.67
10	D6	501	GTP	O6-C6-C5	-2.55	119.80	126.53
9	B5	501	GDP	C4-C5-N7	-2.55	106.63	110.67
10	E8	501	GTP	C5-C6-N1	2.55	119.74	113.25
10	F0	501	GTP	C5-C6-N1	2.55	119.73	113.25
10	D4	501	GTP	C8-N7-C5	2.55	108.79	104.26
9	E5	501	GDP	C4-C5-N7	-2.54	106.64	110.67
10	D8	501	GTP	C5-C6-N1	2.54	119.71	113.25
9	B7	501	GDP	C4-C5-N7	-2.53	106.66	110.67
10	E2	501	GTP	C5-C6-N1	2.53	119.69	113.25
10	E6	501	GTP	O6-C6-C5	-2.53	119.86	126.53
10	A4	501	GTP	C8-N7-C5	2.53	108.76	104.26
9	E9	501	GDP	C4-C5-N7	-2.52	106.67	110.67
10	D2	501	GTP	C8-N7-C5	2.52	108.75	104.26
10	B2	501	GTP	C8-N7-C5	2.52	108.74	104.26
9	D7	501	GDP	C4-C5-N7	-2.51	106.69	110.67
10	C2	501	GTP	N9-C8-N7	-2.51	108.74	113.40
9	C1	501	GDP	O2A-PA-O3A	2.51	114.06	107.27
10	B6	501	GTP	C8-N7-C5	2.51	108.73	104.26
10	B8	501	GTP	C8-N7-C5	2.51	108.73	104.26
10	E0	501	GTP	C5-C6-N1	2.51	119.63	113.25
10	A6	501	GTP	C5-C6-N1	2.50	119.63	113.25
9	D1	501	GDP	C4-C5-N7	-2.50	106.71	110.67
10	B0	501	GTP	O6-C6-C5	-2.50	119.93	126.53
10	C0	501	GTP	C5-C6-N1	2.50	119.62	113.25
10	A4	501	GTP	C5-C6-N1	2.50	119.61	113.25
9	C9	501	GDP	C4-C5-N7	-2.50	106.71	110.67
9	D1	501	GDP	C3'-C2'-C1'	2.50	106.19	101.46
10	E4	501	GTP	C8-N7-C5	2.50	108.71	104.26
10	D8	501	GTP	C8-N7-C5	2.49	108.70	104.26
10	E0	501	GTP	C8-N7-C5	2.49	108.69	104.26
9	B	601	GDP	C6-C5-C4	-2.49	115.08	118.83
10	B8	501	GTP	O6-C6-C5	-2.49	119.97	126.53
9	C5	501	GDP	C4-C5-N7	-2.49	106.73	110.67
10	D4	501	GTP	C5-C6-N1	2.48	119.58	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C7	501	GDP	C3'-C2'-C1'	2.48	106.16	101.46
10	A6	501	GTP	O2A-PA-O3A	2.48	113.98	107.27
10	D6	501	GTP	C8-N7-C5	2.48	108.68	104.26
10	B4	501	GTP	C8-N7-C5	2.48	108.67	104.26
9	D5	501	GDP	C3'-C2'-C1'	2.48	106.14	101.46
10	B6	501	GTP	O6-C6-C5	-2.47	120.00	126.53
10	C8	501	GTP	C5-C6-N1	2.47	119.55	113.25
10	E0	501	GTP	O6-C6-C5	-2.46	120.03	126.53
10	C8	501	GTP	C8-N7-C5	2.46	108.64	104.26
10	A6	501	GTP	O6-C6-C5	-2.46	120.04	126.53
10	E6	501	GTP	C8-N7-C5	2.46	108.64	104.26
9	C1	501	GDP	O6-C6-C5	-2.45	120.06	126.53
10	E4	501	GTP	O6-C6-C5	-2.45	120.06	126.53
10	E2	501	GTP	C8-N7-C5	2.45	108.63	104.26
9	A7	501	GDP	C3'-C2'-C1'	2.45	106.10	101.46
10	D2	501	GTP	O6-C6-C5	-2.45	120.06	126.53
10	C6	501	GTP	C8-N7-C5	2.45	108.63	104.26
10	C0	501	GTP	O6-C6-C5	-2.45	120.07	126.53
10	D0	501	GTP	O6-C6-C5	-2.45	120.08	126.53
10	B0	501	GTP	C8-N7-C5	2.45	108.62	104.26
9	D5	501	GDP	C4-C5-N7	-2.44	106.80	110.67
10	C2	501	GTP	C5-C6-N1	2.44	119.47	113.25
9	E7	501	GDP	C4-C5-N7	-2.44	106.81	110.67
10	D4	501	GTP	O6-C6-C5	-2.43	120.11	126.53
10	A4	501	GTP	O6-C6-C5	-2.43	120.11	126.53
10	E2	501	GTP	O6-C6-C5	-2.43	120.11	126.53
10	A8	501	GTP	O6-C6-C5	-2.43	120.11	126.53
9	B3	501	GDP	C3'-C2'-C1'	2.43	106.06	101.46
10	C4	501	GTP	C8-N7-C5	2.43	108.58	104.26
10	B4	501	GTP	O6-C6-C5	-2.42	120.15	126.53
10	D0	501	GTP	C8-N7-C5	2.42	108.57	104.26
10	C8	501	GTP	O6-C6-C5	-2.41	120.16	126.53
10	C4	501	GTP	O6-C6-C5	-2.41	120.17	126.53
9	E9	501	GDP	O6-C6-C5	-2.41	120.17	126.53
10	D8	501	GTP	O6-C6-C5	-2.41	120.18	126.53
10	B2	501	GTP	O6-C6-C5	-2.40	120.19	126.53
10	A2	501	GTP	C8-N7-C5	2.40	108.53	104.26
10	C4	501	GTP	C5-C6-N1	2.39	119.34	113.25
9	A1	501	GDP	O6-C6-C5	-2.38	120.26	126.53
10	A2	501	GTP	O2B-PB-O3A	2.37	113.68	107.27
10	A0	501	GTP	C8-N7-C5	2.36	108.46	104.26
9	E7	501	GDP	C3'-C2'-C1'	2.35	105.92	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B4	501	GTP	O2B-PB-O3A	2.35	113.64	107.27
9	C1	501	GDP	C4-C5-N7	-2.33	106.97	110.67
9	C3	501	GDP	O2A-PA-O3A	2.32	113.56	107.27
9	A1	501	GDP	C4-C5-N7	-2.31	107.01	110.67
10	E8	501	GTP	O6-C6-C5	-2.31	120.43	126.53
10	C2	501	GTP	C8-N7-C5	2.31	108.38	104.26
9	C5	501	GDP	C3'-C2'-C1'	2.30	105.82	101.46
9	D3	501	GDP	C3'-C2'-C1'	2.30	105.81	101.46
10	E2	501	GTP	C3'-C2'-C1'	2.30	105.81	101.46
10	A2	501	GTP	C3'-C2'-C1'	2.29	105.80	101.46
9	B	601	GDP	C5-C6-N1	2.27	119.04	113.25
10	C2	501	GTP	O2B-PB-O3A	2.27	113.40	107.27
9	C1	501	GDP	C3'-C2'-C1'	2.26	105.75	101.46
9	B9	501	GDP	C3'-C2'-C1'	2.26	105.74	101.46
10	A6	501	GTP	C3'-C2'-C1'	2.25	105.71	101.46
10	D0	501	GTP	O2B-PB-O3A	2.24	113.32	107.27
9	E1	501	GDP	C3'-C2'-C1'	2.23	105.68	101.46
10	B4	501	GTP	O2A-PA-O3A	2.23	113.30	107.27
9	E3	501	GDP	C3'-C2'-C1'	2.23	105.68	101.46
10	E0	501	GTP	C3'-C2'-C1'	2.23	105.67	101.46
10	B0	501	GTP	C3'-C2'-C1'	2.21	105.65	101.46
9	B	601	GDP	O2A-PA-O3A	2.20	113.22	107.27
10	C0	501	GTP	N2-C2-N1	2.20	121.41	116.76
10	F0	501	GTP	O6-C6-C5	-2.19	120.74	126.53
10	D0	501	GTP	C3'-C2'-C1'	2.19	105.60	101.46
10	B2	501	GTP	O2B-PB-O3A	2.19	113.18	107.27
9	B	601	GDP	C4-C5-N7	-2.18	107.21	110.67
9	D5	501	GDP	O6-C6-C5	-2.18	120.78	126.53
10	C0	501	GTP	O2B-PB-O3A	2.17	113.15	107.27
10	C0	501	GTP	C3'-C2'-C1'	2.17	105.58	101.46
9	A	601	GDP	O2A-PA-O3A	2.17	113.14	107.27
9	C5	501	GDP	O6-C6-C5	-2.17	120.82	126.53
9	C1	501	GDP	C5-C6-N1	2.16	118.76	113.25
9	A7	501	GDP	O6-C6-C5	-2.16	120.83	126.53
9	C9	501	GDP	O6-C6-C5	-2.16	120.84	126.53
9	D9	501	GDP	C3'-C2'-C1'	2.15	105.53	101.46
10	B4	501	GTP	C3'-C2'-C1'	2.14	105.51	101.46
10	D8	501	GTP	C3'-C2'-C1'	2.13	105.50	101.46
9	A3	502	GDP	C3'-C2'-C1'	2.13	105.50	101.46
9	D1	501	GDP	O6-C6-C5	-2.13	120.91	126.53
9	C9	501	GDP	C3'-C2'-C1'	2.13	105.49	101.46
9	A5	501	GDP	C3'-C2'-C1'	2.13	105.49	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A6	501	GTP	O2B-PB-O3A	2.12	113.01	107.27
9	E1	501	GDP	O6-C6-C5	-2.12	120.94	126.53
9	D3	501	GDP	O6-C6-C5	-2.12	120.95	126.53
10	D8	501	GTP	O2A-PA-O3A	2.12	112.99	107.27
9	C3	501	GDP	C3'-C2'-C1'	2.12	105.46	101.46
9	A1	501	GDP	C5-C6-N1	2.11	118.62	113.25
10	D6	501	GTP	C3'-C2'-C1'	2.10	105.44	101.46
9	C7	501	GDP	C2'-C1'-N9	-2.10	107.41	113.25
10	A8	501	GTP	C3'-C2'-C1'	2.09	105.42	101.46
10	E8	501	GTP	C3'-C2'-C1'	2.09	105.41	101.46
10	A0	501	GTP	O2B-PB-O3A	2.08	112.90	107.27
9	E3	501	GDP	O6-C6-C5	-2.08	121.05	126.53
10	F0	501	GTP	C4-C5-N7	-2.07	107.39	110.67
9	C7	501	GDP	O3B-PB-O3A	2.07	111.58	104.64
9	E9	501	GDP	C5-C6-N1	2.07	118.51	113.25
9	D7	501	GDP	O6-C6-C5	-2.06	121.11	126.53
10	C6	501	GTP	C3'-C2'-C1'	2.05	105.35	101.46
9	B7	501	GDP	O6-C6-C5	-2.04	121.14	126.53
9	D7	501	GDP	C2'-C3'-C4'	2.04	106.55	102.61
10	E4	501	GTP	C3'-C2'-C1'	2.03	105.31	101.46
10	C2	501	GTP	C3'-C2'-C1'	2.03	105.31	101.46
9	B5	501	GDP	O6-C6-C5	-2.03	121.18	126.53
9	F1	501	GDP	O6-C6-C5	-2.03	121.18	126.53
9	B	601	GDP	O3B-PB-O3A	2.03	111.43	104.64
10	A0	501	GTP	C3'-C2'-C1'	2.03	105.29	101.46
10	E6	501	GTP	C3'-C2'-C1'	2.01	105.27	101.46
9	B3	501	GDP	O6-C6-C5	-2.01	121.22	126.53
9	D9	501	GDP	O6-C6-C5	-2.01	121.22	126.53
10	C4	501	GTP	C3'-C2'-C1'	2.01	105.27	101.46
10	D8	501	GTP	O2B-PB-O3A	2.01	112.69	107.27
9	C1	501	GDP	C2'-C3'-C4'	2.00	106.48	102.61
9	D7	501	GDP	C3'-C2'-C1'	2.00	105.25	101.46

There are no chirality outliers.

All (261) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	601	GDP	C5'-O5'-PA-O3A
9	A	601	GDP	C5'-O5'-PA-O1A
9	A	601	GDP	C5'-O5'-PA-O2A
9	A1	501	GDP	C5'-O5'-PA-O3A
9	A1	501	GDP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
9	A1	501	GDP	C5'-O5'-PA-O2A
9	A3	502	GDP	PA-O3A-PB-O3B
9	A5	501	GDP	PA-O3A-PB-O2B
9	A7	501	GDP	C5'-O5'-PA-O3A
9	A7	501	GDP	C5'-O5'-PA-O1A
9	A7	501	GDP	C5'-O5'-PA-O2A
9	B	601	GDP	C5'-O5'-PA-O3A
9	B	601	GDP	C5'-O5'-PA-O1A
9	B	601	GDP	C5'-O5'-PA-O2A
9	B3	501	GDP	C5'-O5'-PA-O3A
9	B3	501	GDP	C5'-O5'-PA-O2A
9	B5	501	GDP	PA-O3A-PB-O3B
9	B5	501	GDP	C5'-O5'-PA-O3A
9	B5	501	GDP	C5'-O5'-PA-O2A
9	B7	501	GDP	C5'-O5'-PA-O3A
9	B7	501	GDP	C5'-O5'-PA-O1A
9	B7	501	GDP	C5'-O5'-PA-O2A
9	B9	501	GDP	C5'-O5'-PA-O3A
9	B9	501	GDP	C5'-O5'-PA-O1A
9	B9	501	GDP	C5'-O5'-PA-O2A
9	C3	501	GDP	C5'-O5'-PA-O3A
9	C5	501	GDP	C5'-O5'-PA-O3A
9	C5	501	GDP	C5'-O5'-PA-O2A
9	C9	501	GDP	C5'-O5'-PA-O3A
9	D1	501	GDP	C5'-O5'-PA-O3A
9	D1	501	GDP	C5'-O5'-PA-O2A
9	D3	501	GDP	C5'-O5'-PA-O3A
9	D3	501	GDP	C5'-O5'-PA-O1A
9	D3	501	GDP	C5'-O5'-PA-O2A
9	D5	501	GDP	PA-O3A-PB-O3B
9	D5	501	GDP	C5'-O5'-PA-O3A
9	D5	501	GDP	C5'-O5'-PA-O1A
9	D5	501	GDP	C5'-O5'-PA-O2A
9	D7	501	GDP	C5'-O5'-PA-O3A
9	D7	501	GDP	C5'-O5'-PA-O2A
9	D9	501	GDP	PA-O3A-PB-O2B
9	E1	501	GDP	PA-O3A-PB-O3B
9	E1	501	GDP	C5'-O5'-PA-O3A
9	E1	501	GDP	C5'-O5'-PA-O1A
9	E1	501	GDP	C5'-O5'-PA-O2A
9	E3	501	GDP	C5'-O5'-PA-O3A
9	E3	501	GDP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
9	E5	501	GDP	C5'-O5'-PA-O3A
9	E7	501	GDP	C5'-O5'-PA-O3A
9	E7	501	GDP	C5'-O5'-PA-O1A
9	E7	501	GDP	C5'-O5'-PA-O2A
9	E9	501	GDP	C5'-O5'-PA-O1A
9	F1	501	GDP	C5'-O5'-PA-O3A
9	F1	501	GDP	C5'-O5'-PA-O2A
10	A2	501	GTP	C5'-O5'-PA-O3A
10	A2	501	GTP	C5'-O5'-PA-O1A
10	A2	501	GTP	C5'-O5'-PA-O2A
10	A4	501	GTP	C5'-O5'-PA-O3A
10	A4	501	GTP	C5'-O5'-PA-O2A
10	A6	501	GTP	PB-O3B-PG-O3G
10	A6	501	GTP	C5'-O5'-PA-O3A
10	A6	501	GTP	C5'-O5'-PA-O2A
10	A8	501	GTP	C5'-O5'-PA-O3A
10	A8	501	GTP	C5'-O5'-PA-O1A
10	B0	501	GTP	C5'-O5'-PA-O3A
10	B0	501	GTP	C5'-O5'-PA-O1A
10	B2	501	GTP	C5'-O5'-PA-O3A
10	B2	501	GTP	C5'-O5'-PA-O1A
10	B4	501	GTP	C5'-O5'-PA-O3A
10	B4	501	GTP	C5'-O5'-PA-O1A
10	B4	501	GTP	C5'-O5'-PA-O2A
10	B6	501	GTP	C5'-O5'-PA-O3A
10	B6	501	GTP	C5'-O5'-PA-O1A
10	B6	501	GTP	C5'-O5'-PA-O2A
10	B8	501	GTP	C5'-O5'-PA-O3A
10	B8	501	GTP	C5'-O5'-PA-O1A
10	B8	501	GTP	C5'-O5'-PA-O2A
10	C0	501	GTP	C5'-O5'-PA-O3A
10	C0	501	GTP	C5'-O5'-PA-O2A
10	C2	501	GTP	C5'-O5'-PA-O3A
10	C2	501	GTP	C5'-O5'-PA-O2A
10	C4	501	GTP	C5'-O5'-PA-O3A
10	C4	501	GTP	C5'-O5'-PA-O1A
10	C4	501	GTP	O4'-C4'-C5'-O5'
10	C6	501	GTP	C5'-O5'-PA-O3A
10	C6	501	GTP	C5'-O5'-PA-O1A
10	C6	501	GTP	C5'-O5'-PA-O2A
10	C8	501	GTP	C5'-O5'-PA-O3A
10	C8	501	GTP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
10	C8	501	GTP	C5'-O5'-PA-O2A
10	D0	501	GTP	C5'-O5'-PA-O3A
10	D0	501	GTP	C5'-O5'-PA-O1A
10	D0	501	GTP	C5'-O5'-PA-O2A
10	D2	501	GTP	PB-O3A-PA-O5'
10	D2	501	GTP	C5'-O5'-PA-O3A
10	D2	501	GTP	C5'-O5'-PA-O1A
10	D2	501	GTP	C5'-O5'-PA-O2A
10	D6	501	GTP	C5'-O5'-PA-O3A
10	D6	501	GTP	C5'-O5'-PA-O1A
10	D6	501	GTP	C5'-O5'-PA-O2A
10	D8	501	GTP	C5'-O5'-PA-O3A
10	D8	501	GTP	C5'-O5'-PA-O1A
10	D8	501	GTP	C5'-O5'-PA-O2A
10	E0	501	GTP	C5'-O5'-PA-O1A
10	E4	501	GTP	C5'-O5'-PA-O3A
10	E4	501	GTP	C5'-O5'-PA-O1A
10	E4	501	GTP	C5'-O5'-PA-O2A
10	E6	501	GTP	C5'-O5'-PA-O3A
10	E6	501	GTP	C5'-O5'-PA-O1A
10	E6	501	GTP	C5'-O5'-PA-O2A
10	E8	501	GTP	C5'-O5'-PA-O3A
10	E8	501	GTP	C5'-O5'-PA-O1A
10	E8	501	GTP	C5'-O5'-PA-O2A
10	F0	501	GTP	C5'-O5'-PA-O3A
10	F0	501	GTP	C5'-O5'-PA-O1A
10	F0	501	GTP	C5'-O5'-PA-O2A
9	B5	501	GDP	O4'-C4'-C5'-O5'
9	B5	501	GDP	C3'-C4'-C5'-O5'
9	D9	501	GDP	C3'-C4'-C5'-O5'
9	E7	501	GDP	C3'-C4'-C5'-O5'
10	A0	501	GTP	C3'-C4'-C5'-O5'
10	B6	501	GTP	O4'-C4'-C5'-O5'
10	B6	501	GTP	C3'-C4'-C5'-O5'
10	B8	501	GTP	O4'-C4'-C5'-O5'
10	B8	501	GTP	C3'-C4'-C5'-O5'
10	C4	501	GTP	C3'-C4'-C5'-O5'
10	D4	501	GTP	O4'-C4'-C5'-O5'
10	D4	501	GTP	C3'-C4'-C5'-O5'
10	A0	501	GTP	O4'-C4'-C5'-O5'
10	B0	501	GTP	O4'-C4'-C5'-O5'
10	B0	501	GTP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
10	C6	501	GTP	O4'-C4'-C5'-O5'
10	C6	501	GTP	C3'-C4'-C5'-O5'
9	D9	501	GDP	O4'-C4'-C5'-O5'
9	E9	501	GDP	O4'-C4'-C5'-O5'
9	E7	501	GDP	C4'-C5'-O5'-PA
9	F1	501	GDP	C4'-C5'-O5'-PA
9	E7	501	GDP	O4'-C4'-C5'-O5'
9	D5	501	GDP	C3'-C4'-C5'-O5'
10	D2	501	GTP	C3'-C4'-C5'-O5'
10	D6	501	GTP	C3'-C4'-C5'-O5'
10	C8	501	GTP	C4'-C5'-O5'-PA
10	B2	501	GTP	PB-O3A-PA-O1A
10	B4	501	GTP	PB-O3A-PA-O1A
10	C2	501	GTP	PB-O3A-PA-O1A
10	C6	501	GTP	PA-O3A-PB-O1B
10	A6	501	GTP	C4'-C5'-O5'-PA
10	A4	501	GTP	C4'-C5'-O5'-PA
10	C6	501	GTP	PB-O3A-PA-O5'
10	D4	501	GTP	PB-O3A-PA-O5'
9	D7	501	GDP	C3'-C4'-C5'-O5'
9	A3	502	GDP	PA-O3A-PB-O1B
9	C5	501	GDP	PA-O3A-PB-O2B
9	E3	501	GDP	C3'-C4'-C5'-O5'
9	F1	501	GDP	C3'-C4'-C5'-O5'
10	B8	501	GTP	C4'-C5'-O5'-PA
10	C4	501	GTP	C4'-C5'-O5'-PA
9	E9	501	GDP	PB-O3A-PA-O2A
10	D2	501	GTP	PA-O3A-PB-O1B
10	E6	501	GTP	PA-O3A-PB-O2B
10	A2	501	GTP	C3'-C4'-C5'-O5'
10	D2	501	GTP	O4'-C4'-C5'-O5'
10	B4	501	GTP	C4'-C5'-O5'-PA
10	B6	501	GTP	C4'-C5'-O5'-PA
10	D2	501	GTP	C4'-C5'-O5'-PA
10	D6	501	GTP	C4'-C5'-O5'-PA
10	E4	501	GTP	C4'-C5'-O5'-PA
10	E8	501	GTP	C4'-C5'-O5'-PA
9	E9	501	GDP	C3'-C4'-C5'-O5'
10	D6	501	GTP	O4'-C4'-C5'-O5'
9	A3	502	GDP	C5'-O5'-PA-O2A
9	B3	501	GDP	C5'-O5'-PA-O1A
9	C5	501	GDP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
9	C9	501	GDP	C5'-O5'-PA-O2A
10	A8	501	GTP	C5'-O5'-PA-O2A
10	B0	501	GTP	C5'-O5'-PA-O2A
10	B2	501	GTP	C5'-O5'-PA-O2A
10	C4	501	GTP	C5'-O5'-PA-O2A
10	D4	501	GTP	C5'-O5'-PA-O1A
9	A5	501	GDP	C4'-C5'-O5'-PA
9	D5	501	GDP	C4'-C5'-O5'-PA
9	D7	501	GDP	C4'-C5'-O5'-PA
10	A2	501	GTP	C4'-C5'-O5'-PA
10	C0	501	GTP	C4'-C5'-O5'-PA
10	C2	501	GTP	C4'-C5'-O5'-PA
10	C6	501	GTP	C4'-C5'-O5'-PA
10	D0	501	GTP	C4'-C5'-O5'-PA
10	D4	501	GTP	C4'-C5'-O5'-PA
10	D8	501	GTP	C4'-C5'-O5'-PA
10	E0	501	GTP	C4'-C5'-O5'-PA
10	E2	501	GTP	C4'-C5'-O5'-PA
10	E6	501	GTP	C4'-C5'-O5'-PA
10	F0	501	GTP	C4'-C5'-O5'-PA
10	B0	501	GTP	C4'-C5'-O5'-PA
9	C3	501	GDP	PB-O3A-PA-O2A
9	C7	501	GDP	PB-O3A-PA-O1A
9	C7	501	GDP	PB-O3A-PA-O2A
10	A8	501	GTP	PB-O3A-PA-O2A
10	B0	501	GTP	PA-O3A-PB-O2B
10	C2	501	GTP	PA-O3A-PB-O1B
10	D0	501	GTP	PB-O3A-PA-O2A
10	D8	501	GTP	PB-O3A-PA-O1A
10	E4	501	GTP	PA-O3A-PB-O2B
10	E4	501	GTP	C3'-C4'-C5'-O5'
10	F0	501	GTP	C3'-C4'-C5'-O5'
10	A8	501	GTP	C4'-C5'-O5'-PA
10	B2	501	GTP	C4'-C5'-O5'-PA
9	A3	502	GDP	C2'-C1'-N9-C4
9	A1	501	GDP	PB-O3A-PA-O2A
9	E3	501	GDP	PB-O3A-PA-O1A
10	A2	501	GTP	PB-O3A-PA-O1A
10	A8	501	GTP	PB-O3A-PA-O1A
10	B0	501	GTP	PA-O3A-PB-O1B
10	C0	501	GTP	PB-O3A-PA-O1A
9	A3	502	GDP	C2'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
10	A0	501	GTP	PB-O3A-PA-O5'
9	B	601	GDP	C4'-C5'-O5'-PA
9	E9	501	GDP	C4'-C5'-O5'-PA
9	E3	501	GDP	O4'-C4'-C5'-O5'
9	A	601	GDP	C4'-C5'-O5'-PA
10	A2	501	GTP	O4'-C4'-C5'-O5'
10	E6	501	GTP	C3'-C4'-C5'-O5'
10	A6	501	GTP	PB-O3B-PG-O1G
9	D5	501	GDP	PA-O3A-PB-O2B
9	D9	501	GDP	PA-O3A-PB-O3B
10	D0	501	GTP	C3'-C4'-C5'-O5'
9	A1	501	GDP	PB-O3A-PA-O1A
9	C1	501	GDP	PB-O3A-PA-O1A
9	C1	501	GDP	PB-O3A-PA-O2A
9	C3	501	GDP	PB-O3A-PA-O1A
10	A2	501	GTP	PA-O3A-PB-O1B
10	A2	501	GTP	PA-O3A-PB-O2B
10	B2	501	GTP	PB-O3A-PA-O2A
10	B4	501	GTP	PA-O3A-PB-O1B
10	B4	501	GTP	PA-O3A-PB-O2B
10	B4	501	GTP	PB-O3A-PA-O2A
10	B6	501	GTP	PA-O3A-PB-O2B
10	B8	501	GTP	PA-O3A-PB-O2B
10	C0	501	GTP	PA-O3A-PB-O1B
10	C0	501	GTP	PA-O3A-PB-O2B
10	C0	501	GTP	PB-O3A-PA-O2A
10	C2	501	GTP	PA-O3A-PB-O2B
10	C4	501	GTP	PA-O3A-PB-O2B
10	C6	501	GTP	PA-O3A-PB-O2B
10	D2	501	GTP	PA-O3A-PB-O2B
10	D6	501	GTP	PA-O3A-PB-O2B
10	D8	501	GTP	PB-O3A-PA-O2A
10	E4	501	GTP	PA-O3A-PB-O1B
10	E6	501	GTP	PA-O3A-PB-O1B
10	F0	501	GTP	PA-O3A-PB-O1B
10	F0	501	GTP	PA-O3A-PB-O2B
9	C9	501	GDP	C3'-C4'-C5'-O5'
10	A8	501	GTP	C3'-C4'-C5'-O5'
9	D5	501	GDP	PA-O3A-PB-O1B
10	E4	501	GTP	O4'-C4'-C5'-O5'
9	A3	502	GDP	C4'-C5'-O5'-PA
9	A	601	GDP	PB-O3A-PA-O2A

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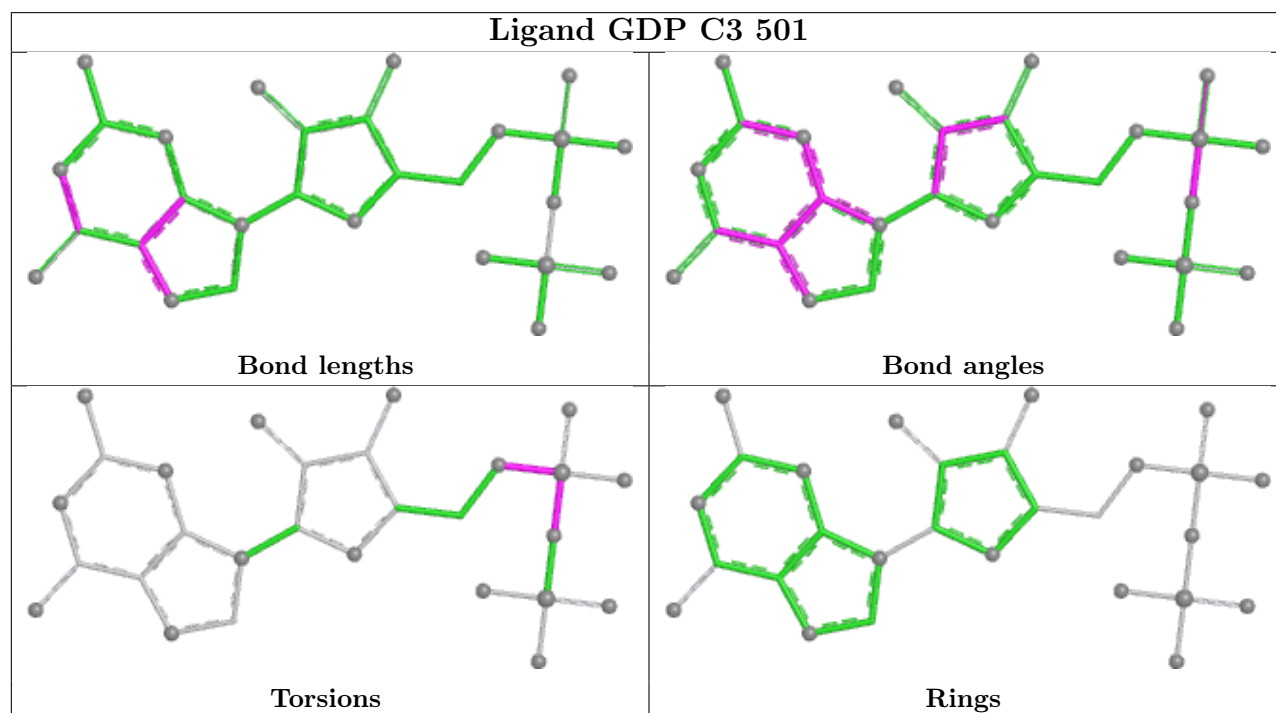
Mol	Chain	Res	Type	Atoms
10	A6	501	GTP	PA-O3A-PB-O2B
10	B8	501	GTP	PA-O3A-PB-O1B
10	E8	501	GTP	PG-O3B-PB-O2B
9	D5	501	GDP	O4'-C4'-C5'-O5'

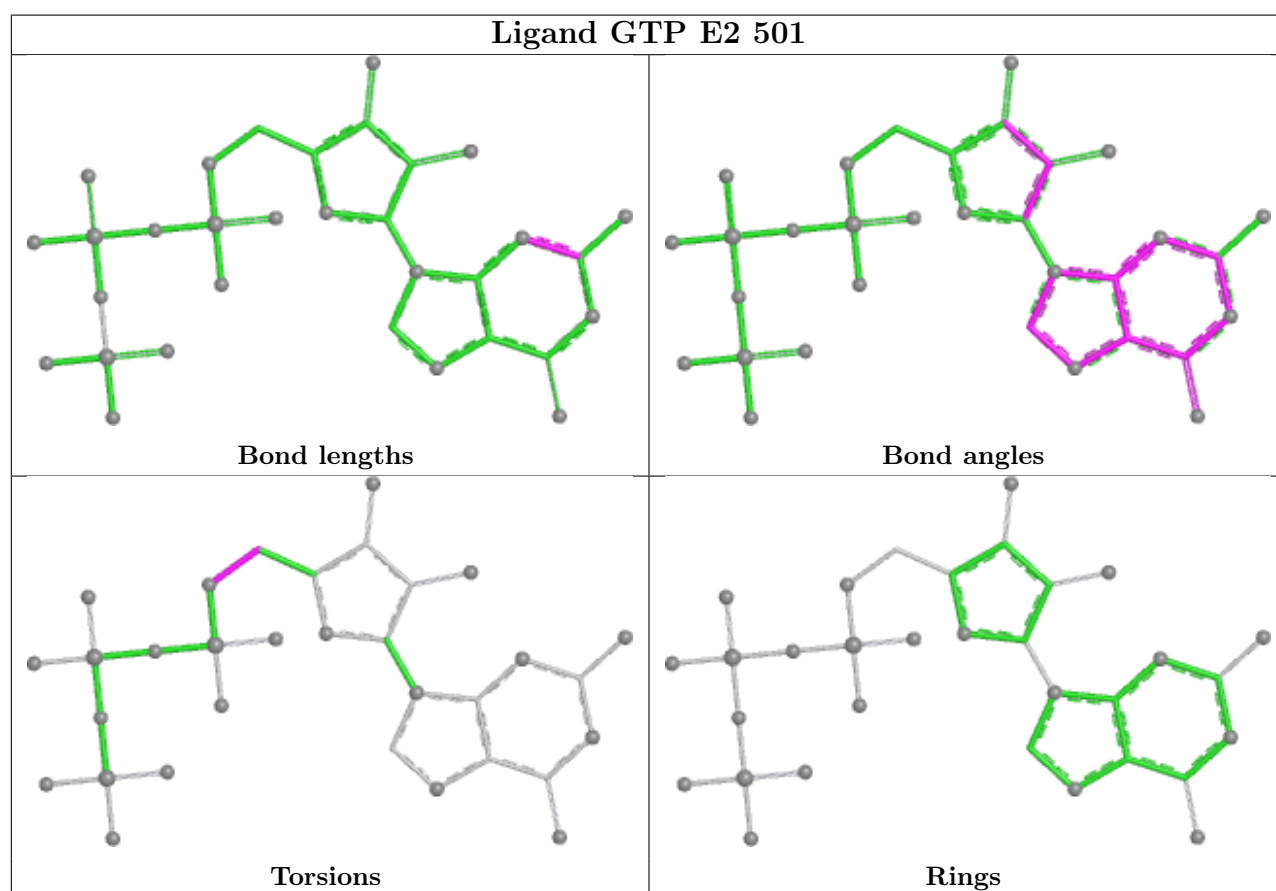
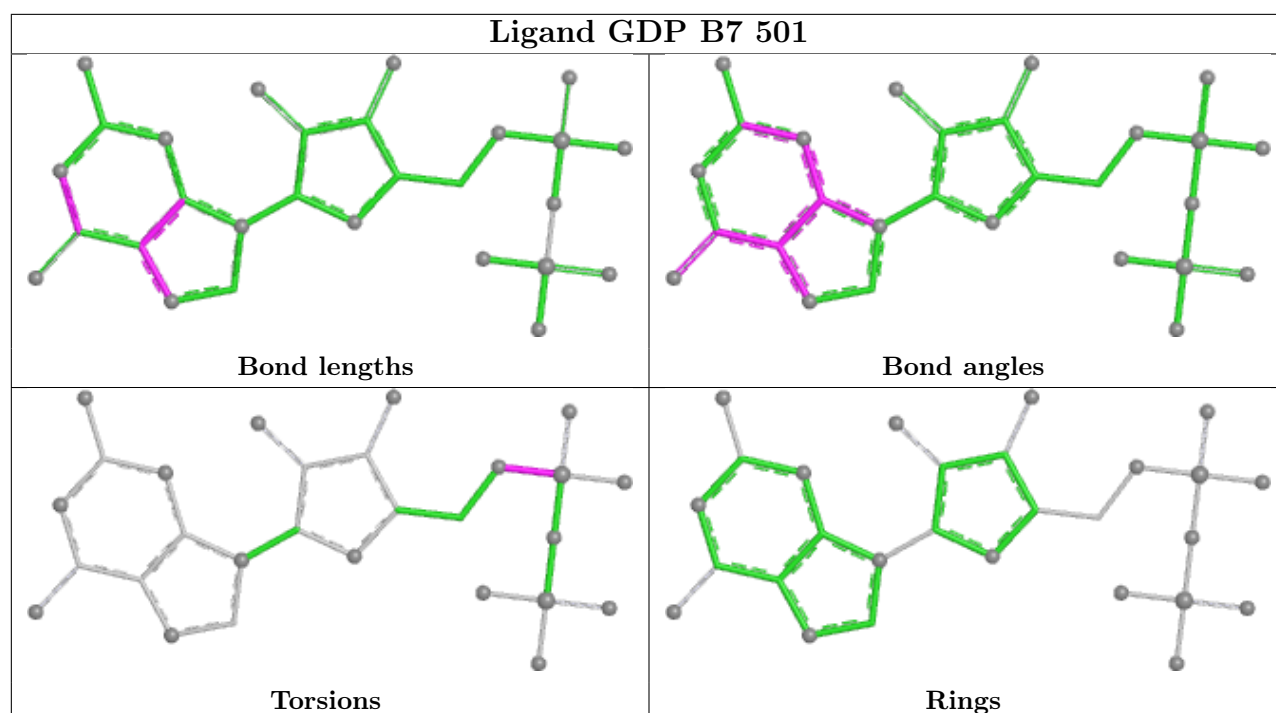
There are no ring outliers.

2 monomers are involved in 4 short contacts:

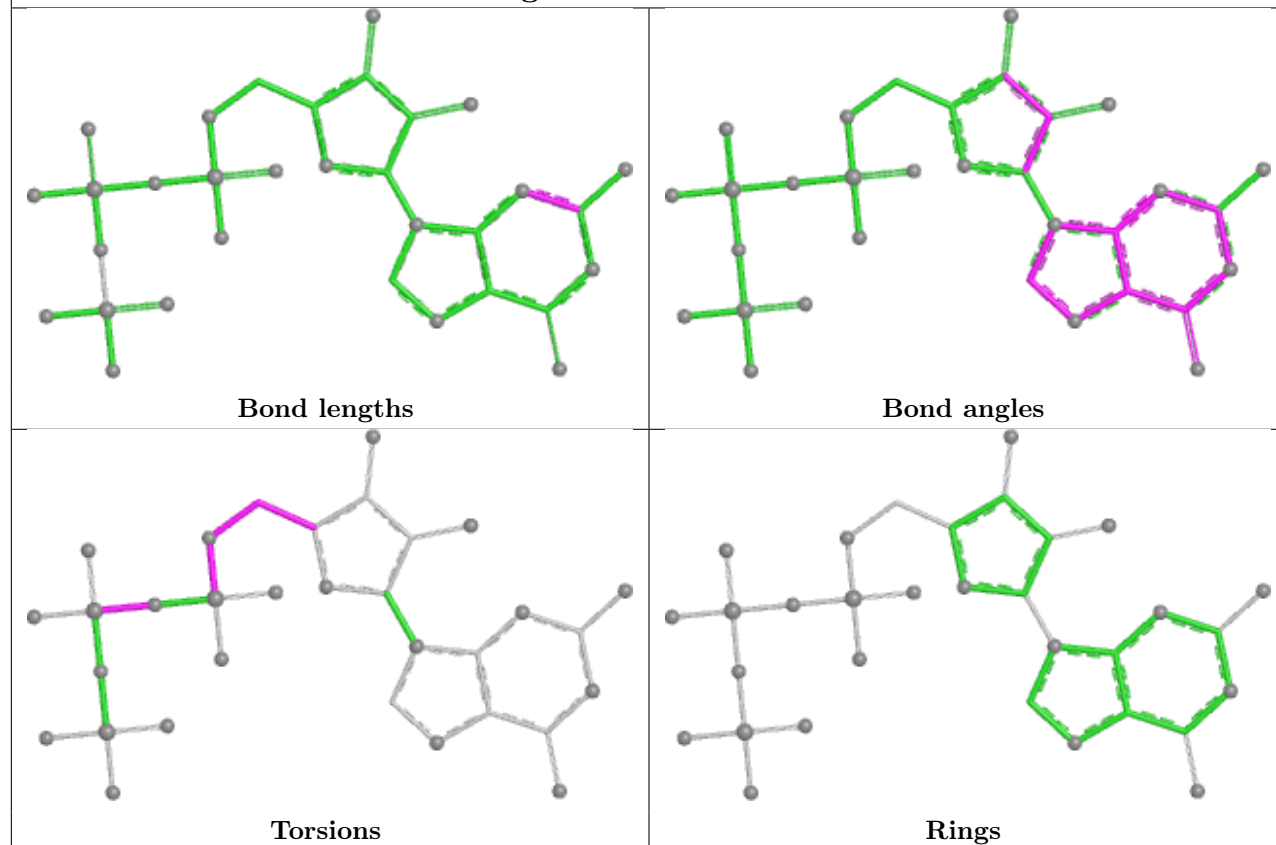
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C0	501	GTP	1	0
9	E9	501	GDP	3	0

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

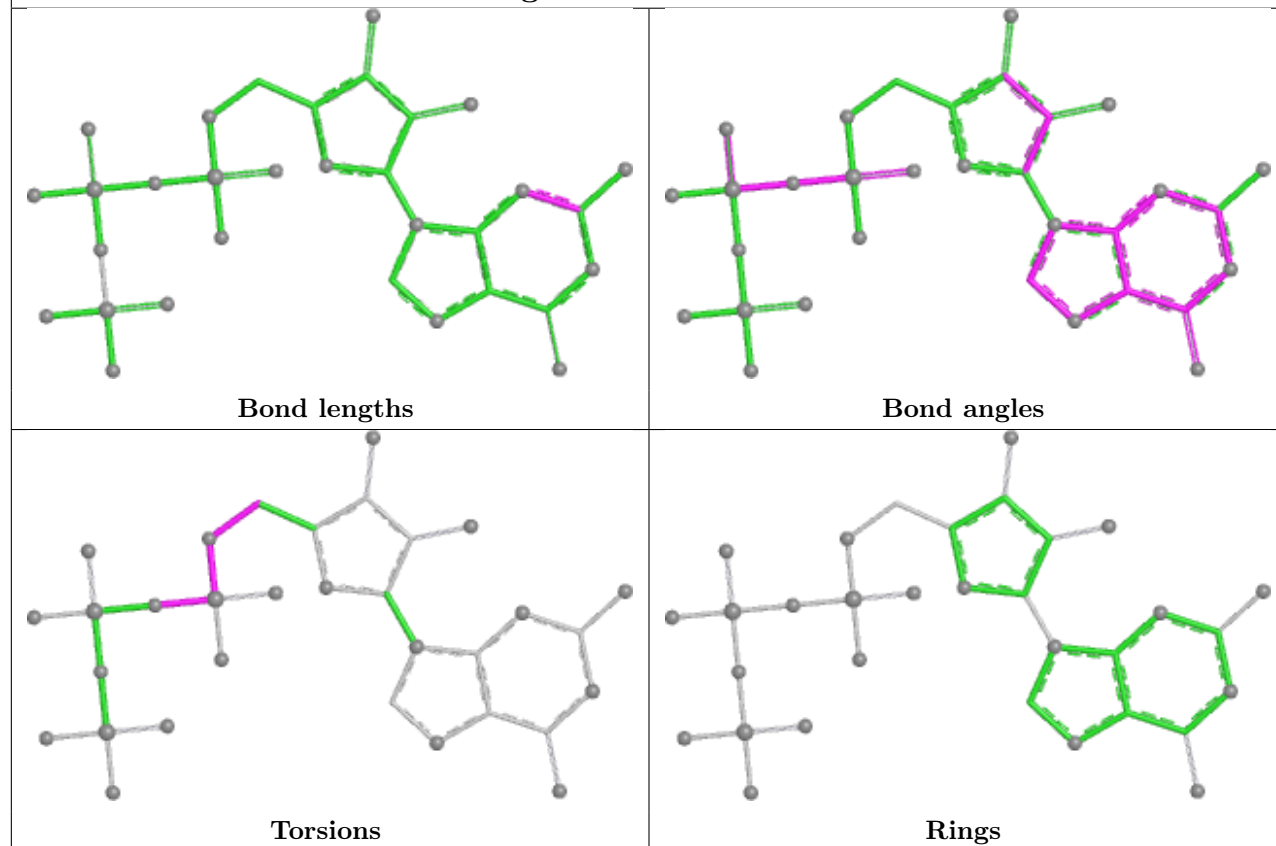


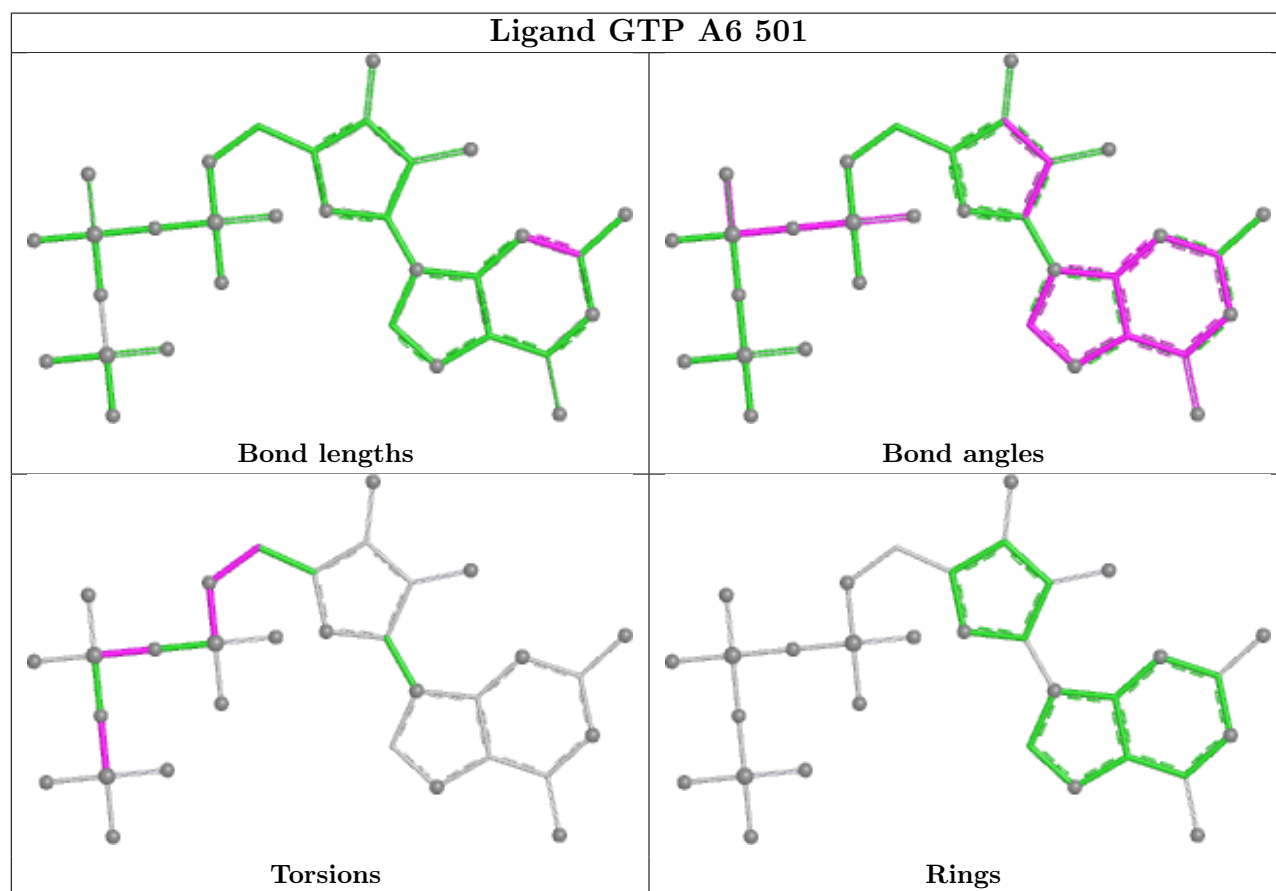
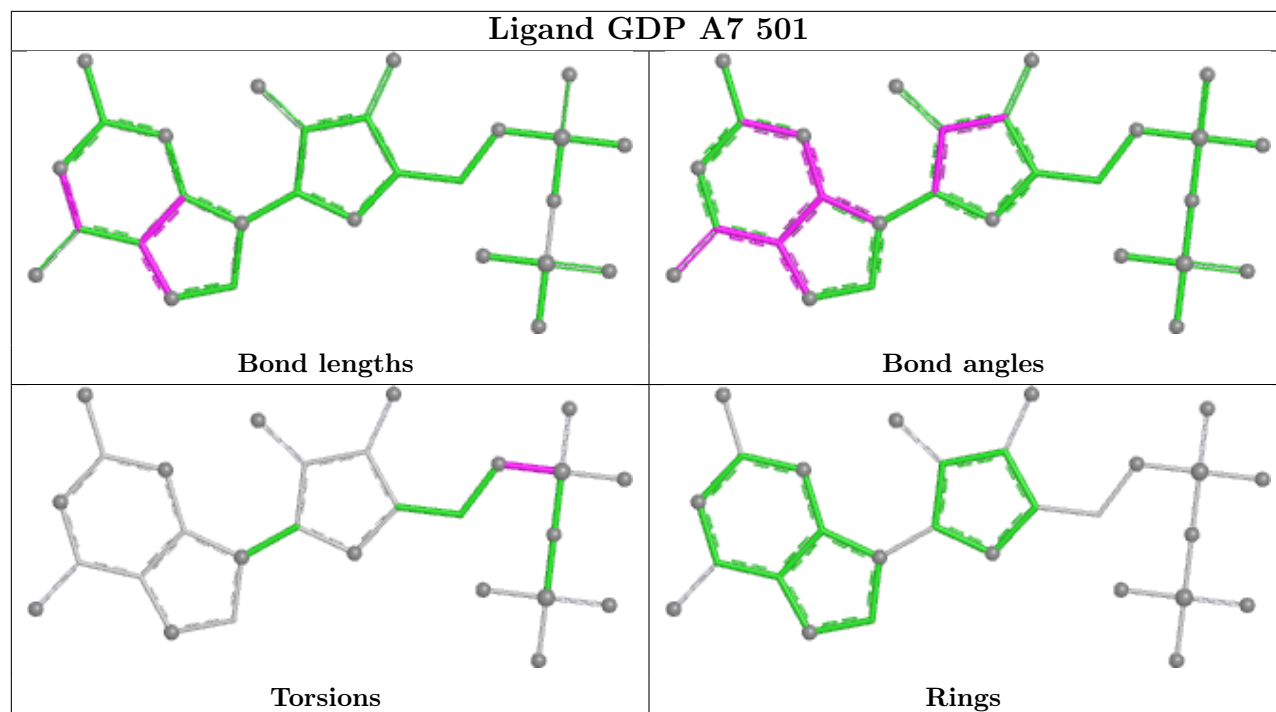


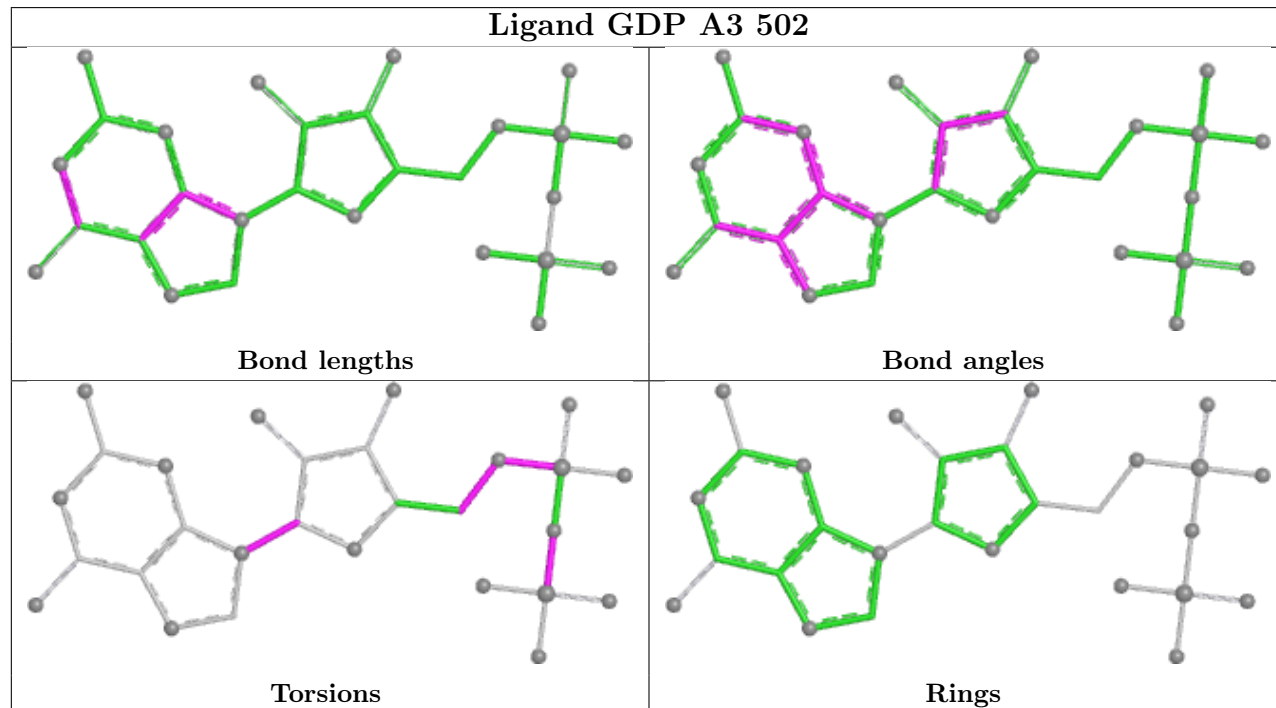
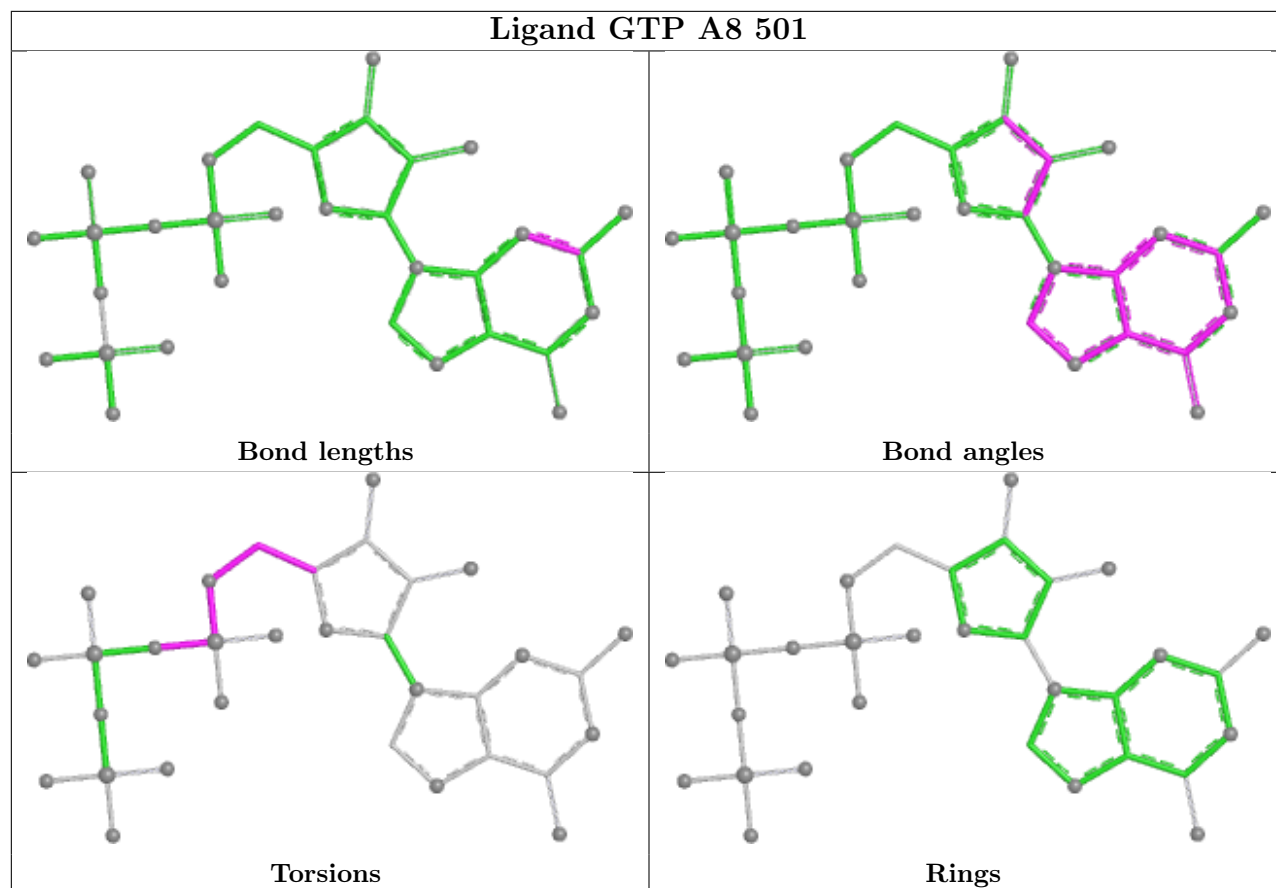
Ligand GTP D6 501



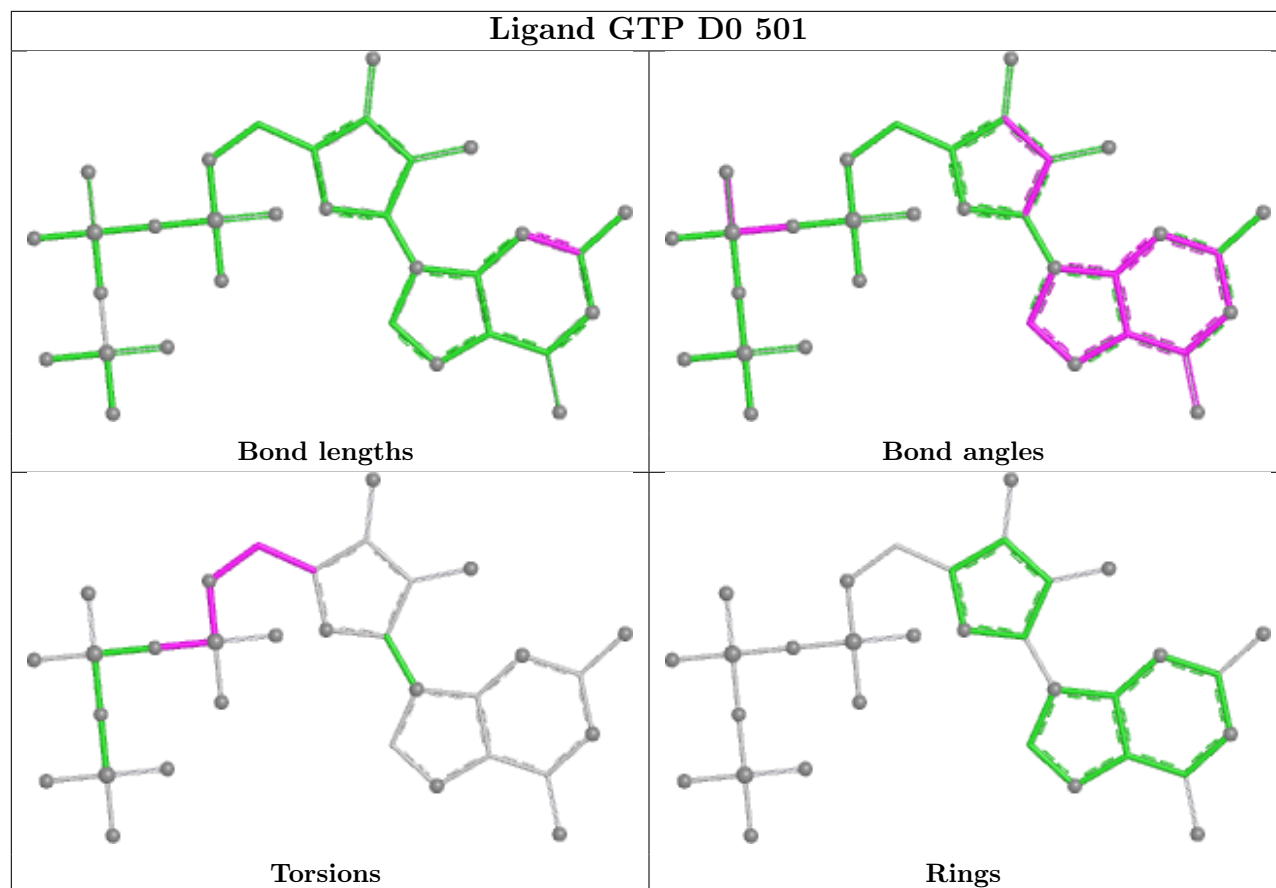
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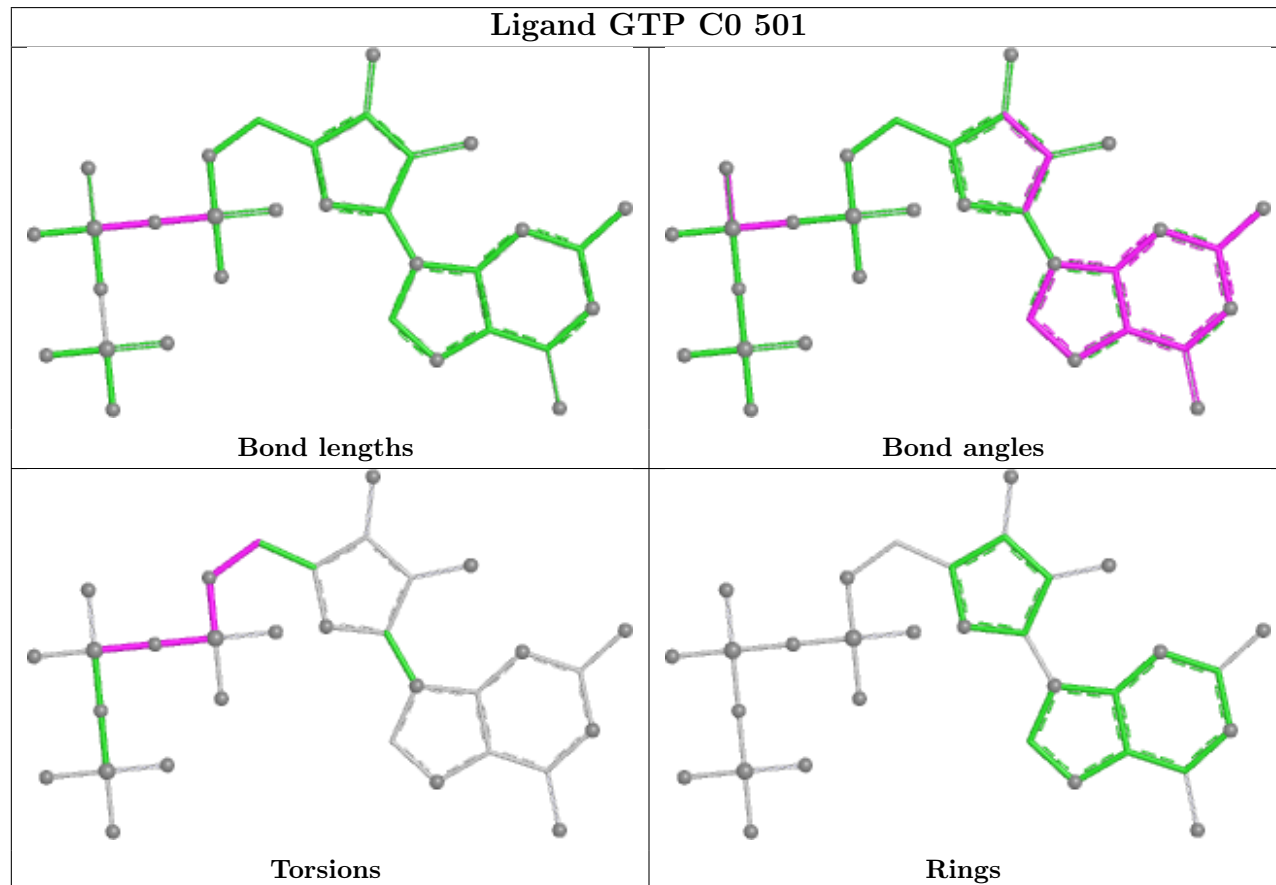




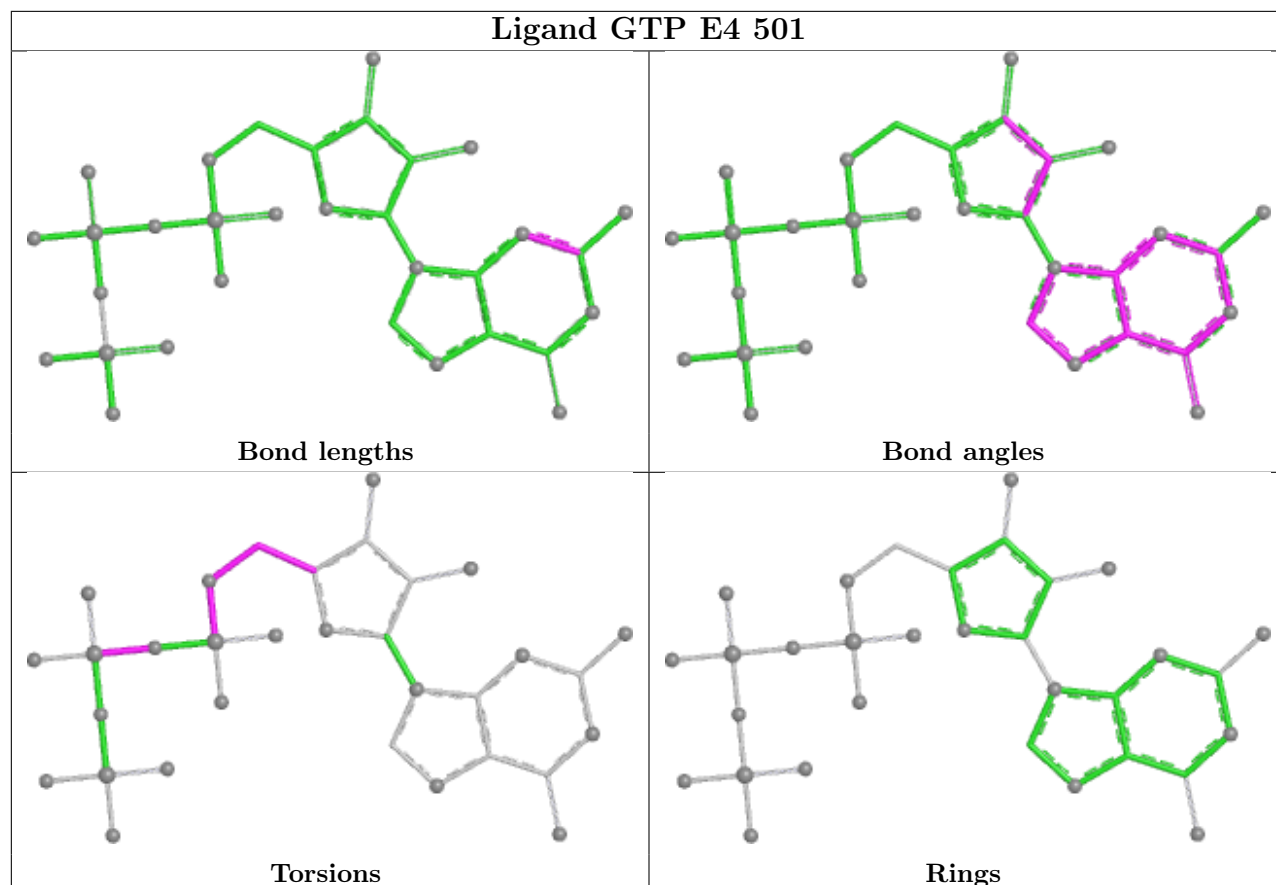
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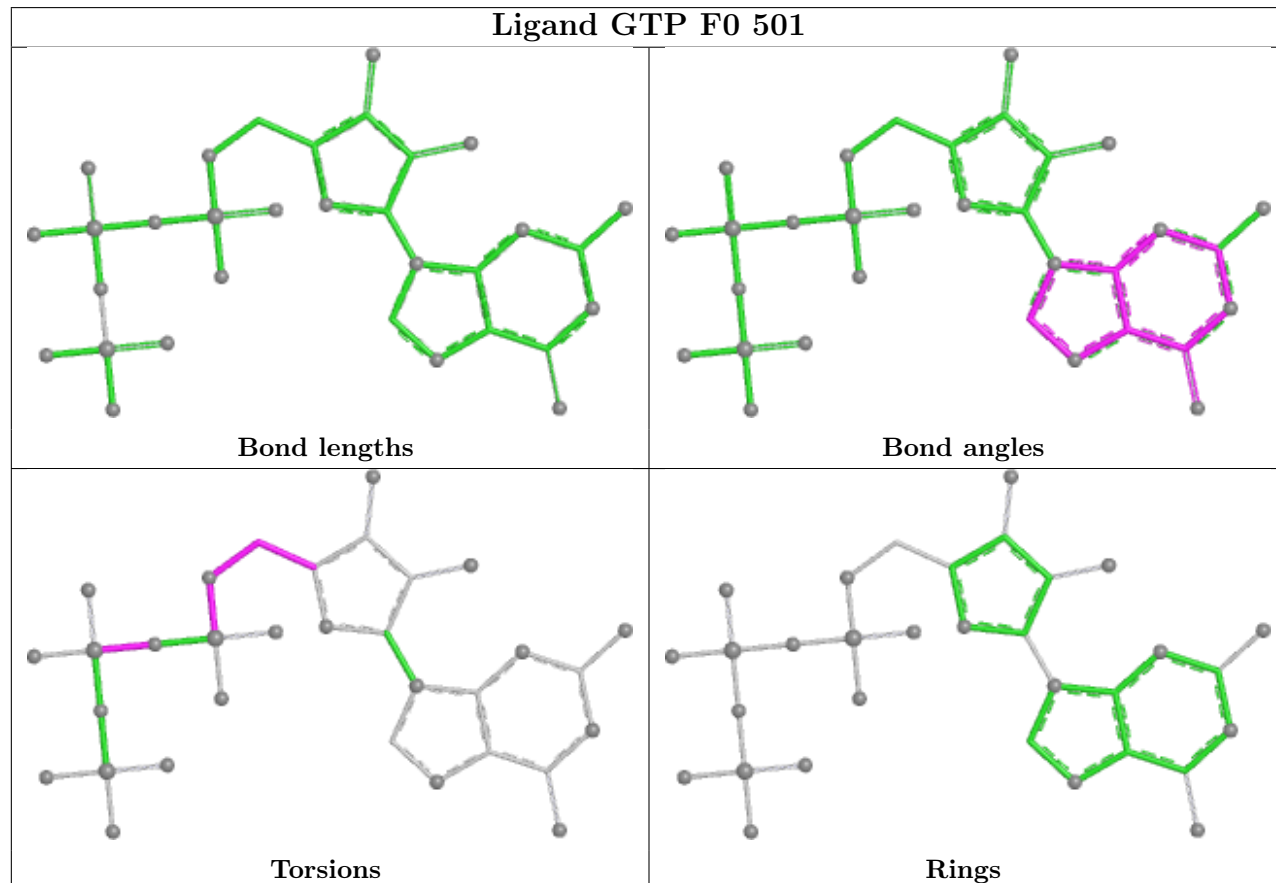
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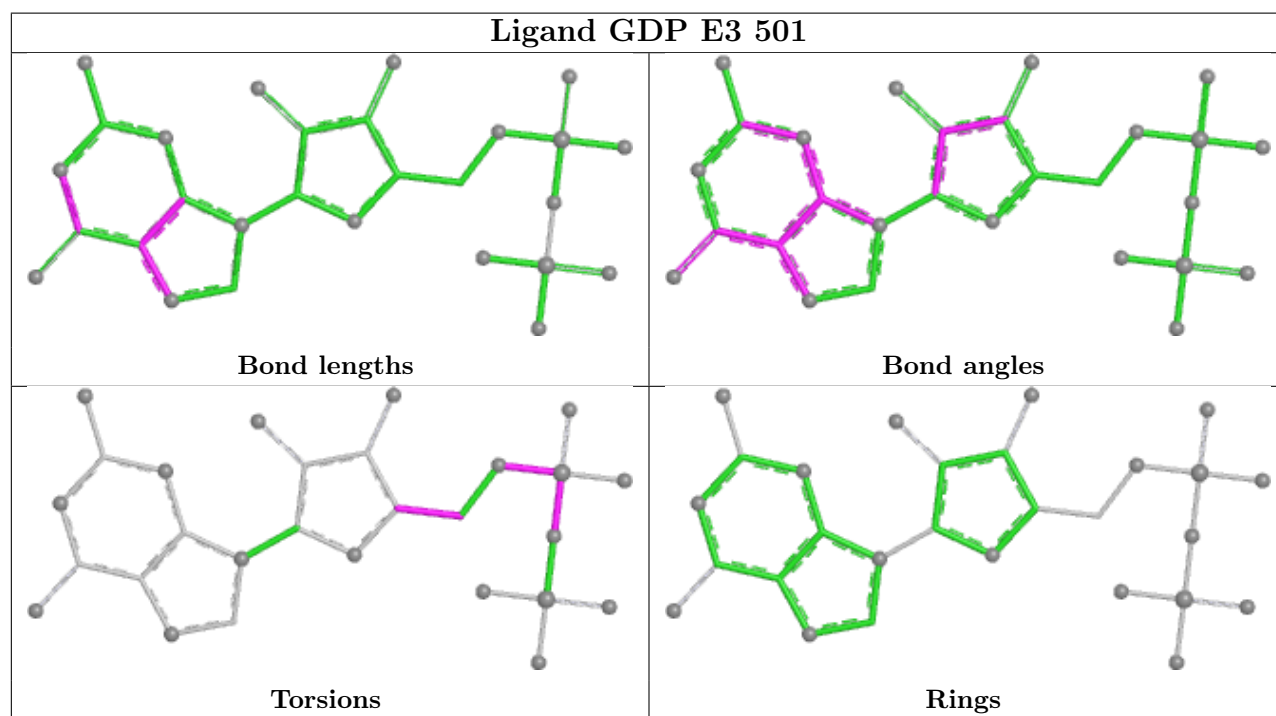
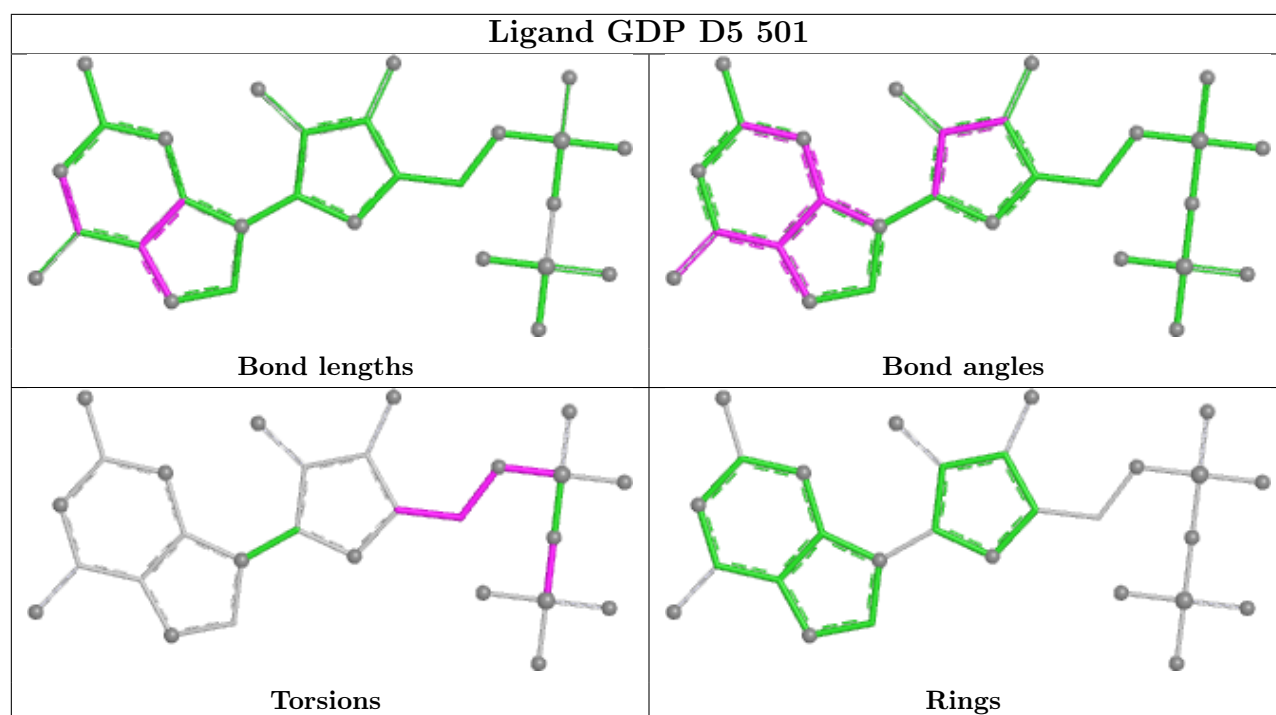


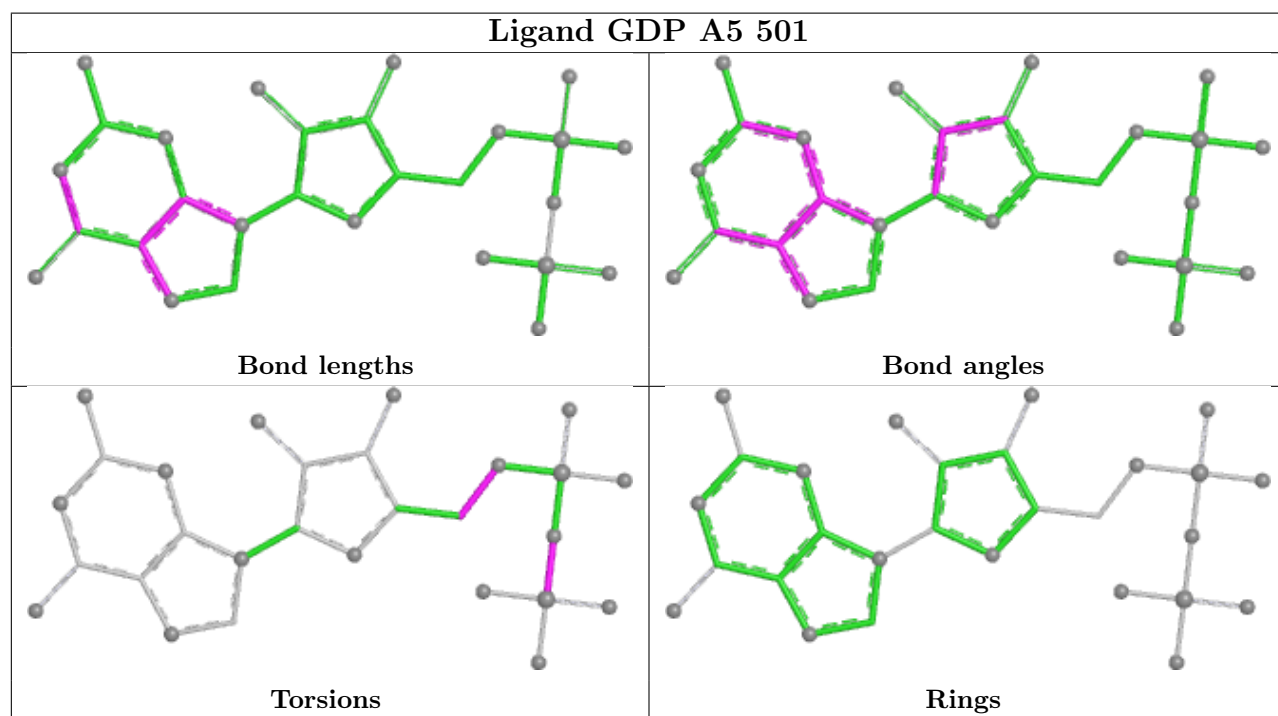
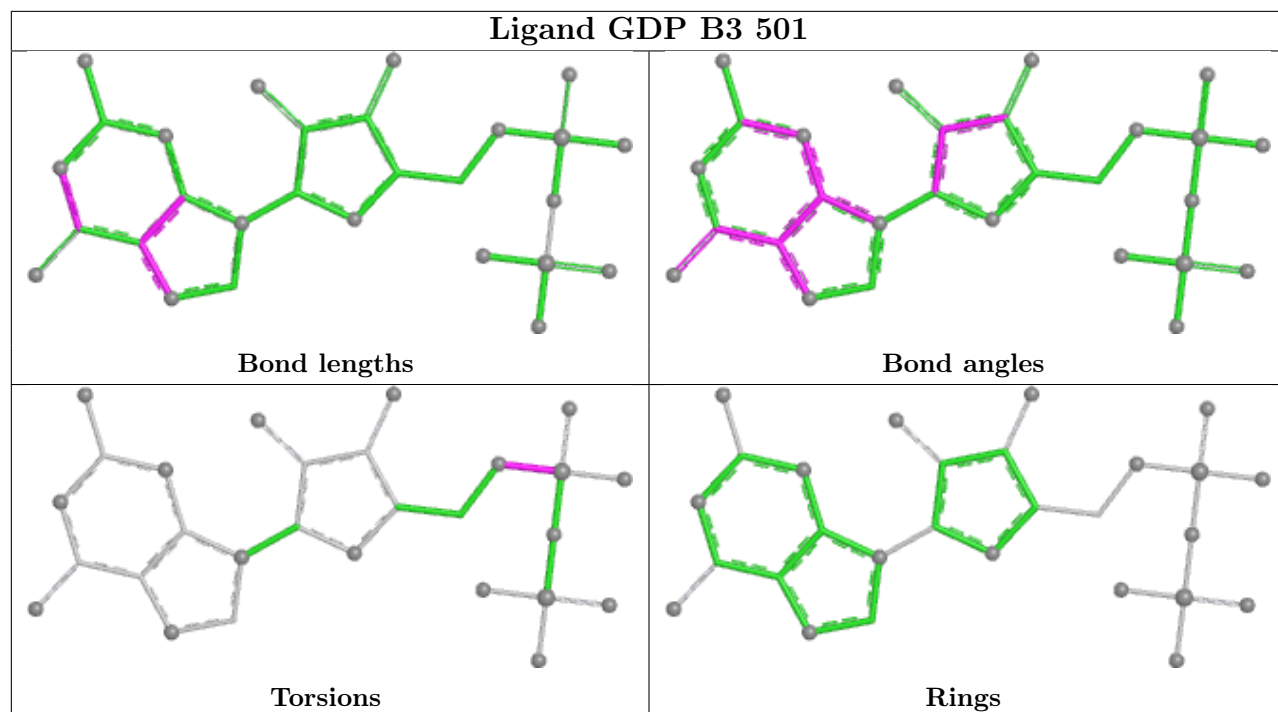
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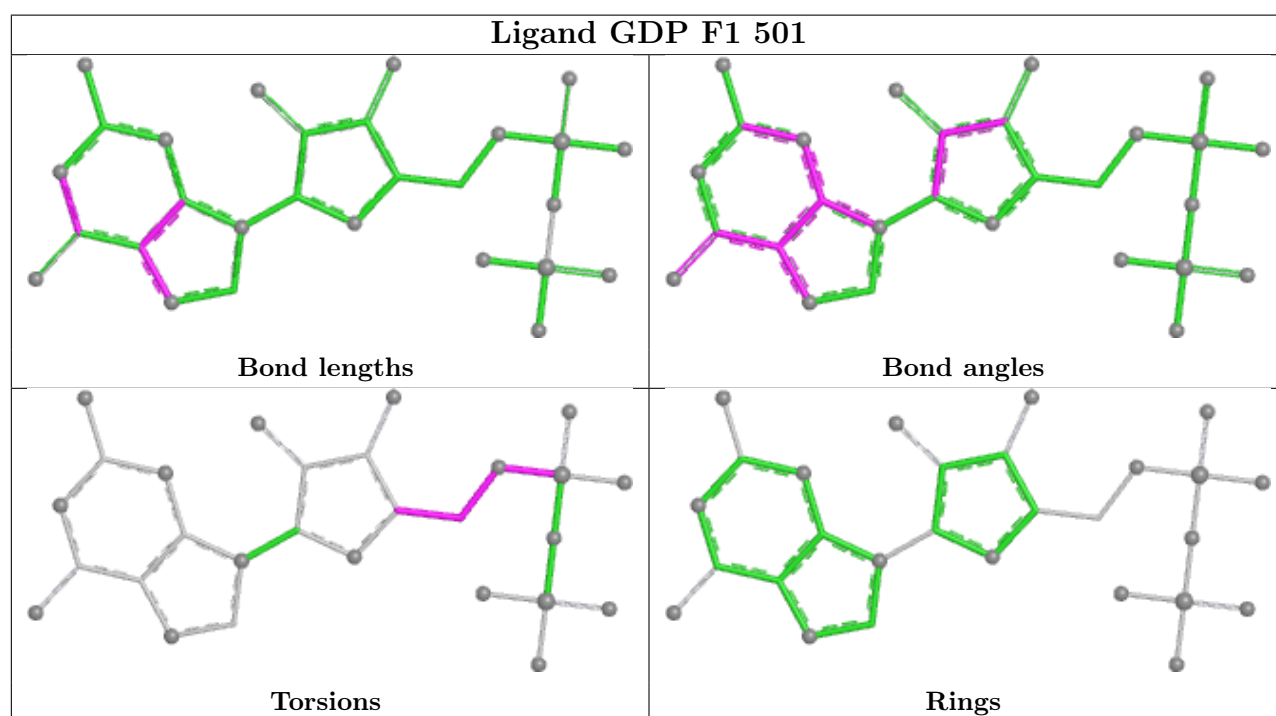
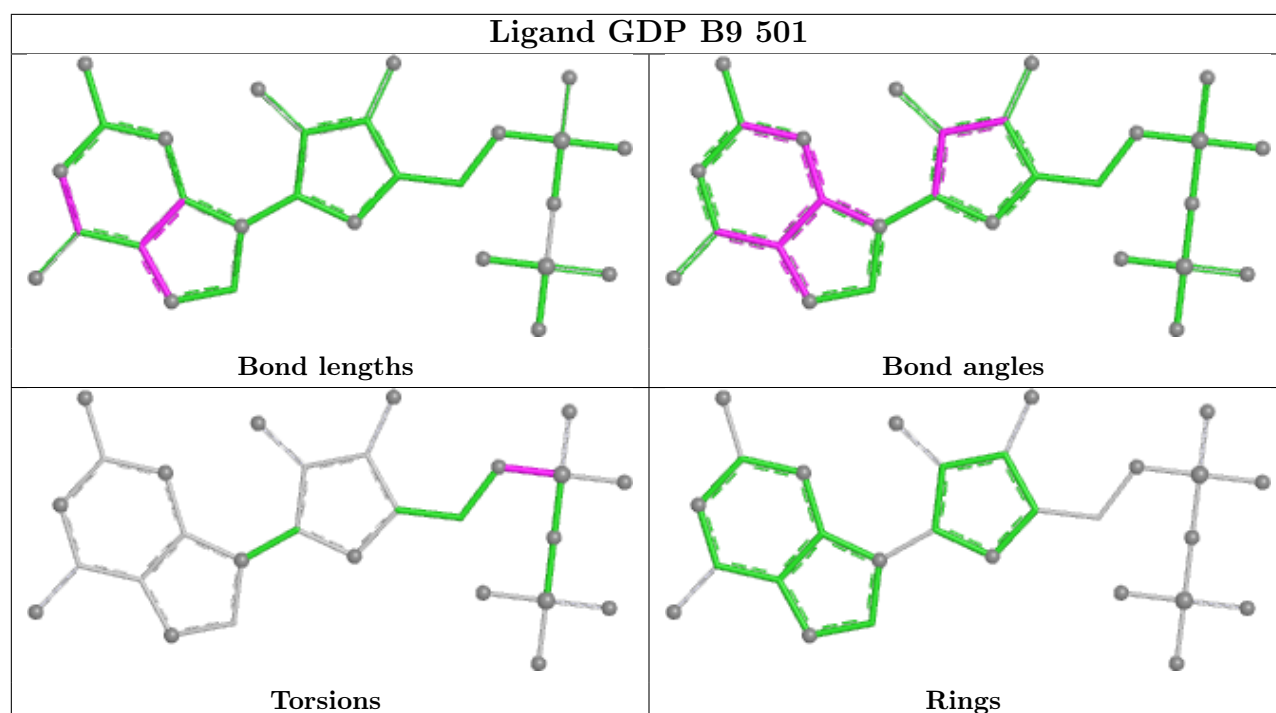


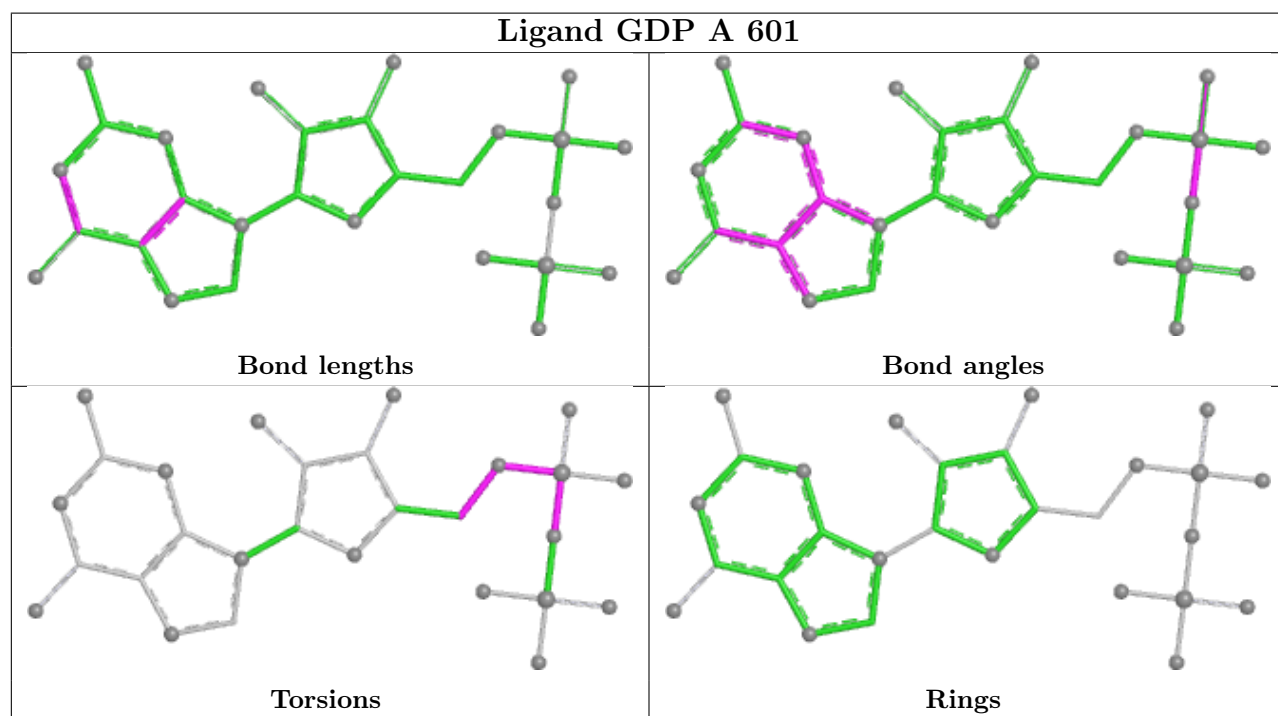
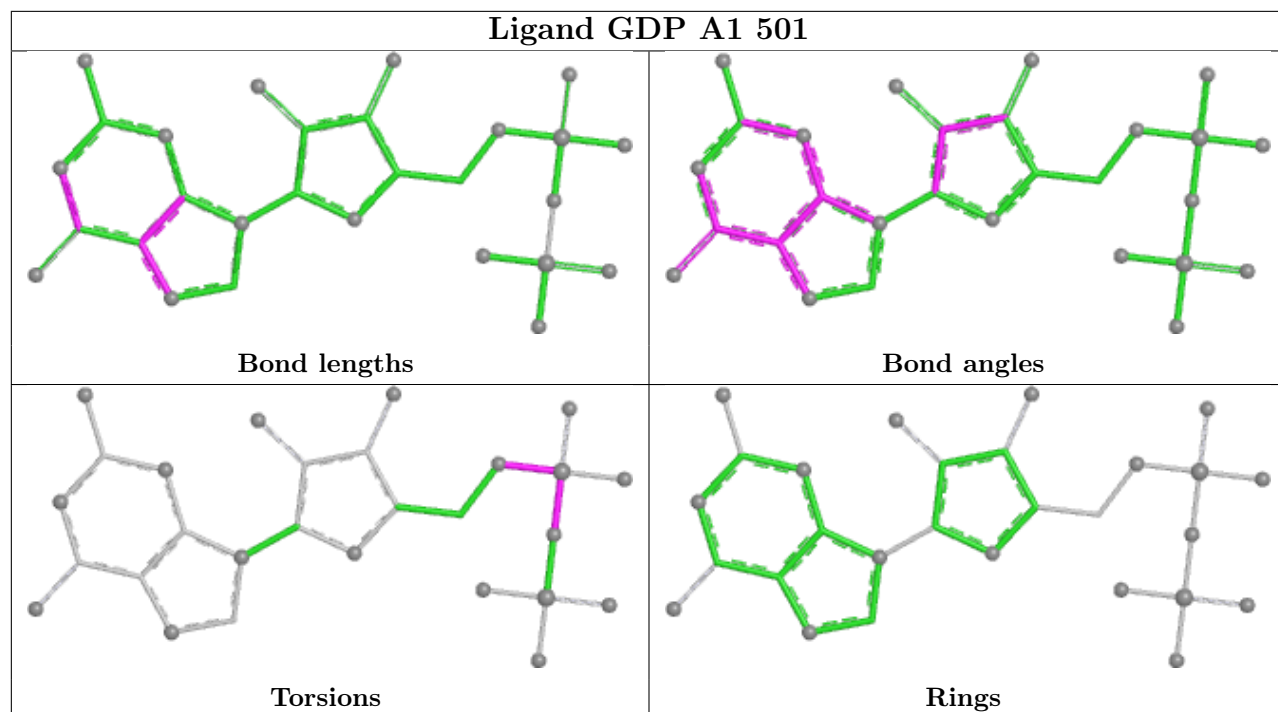
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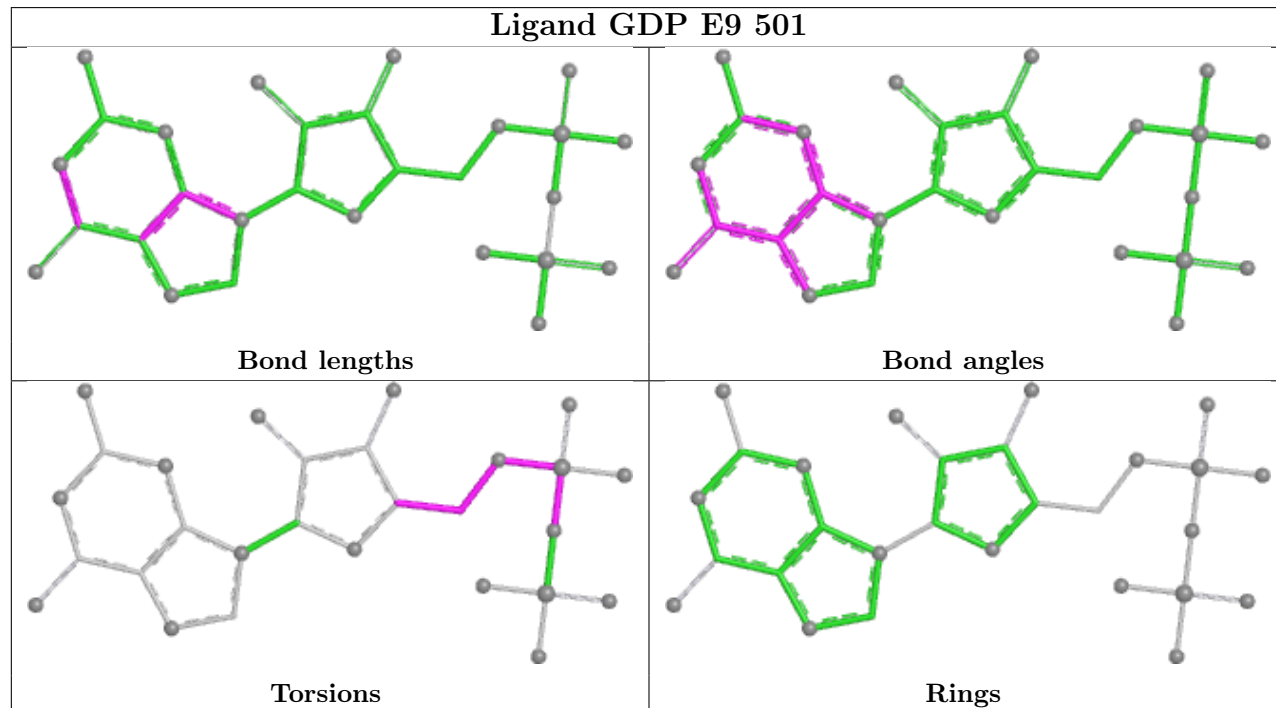
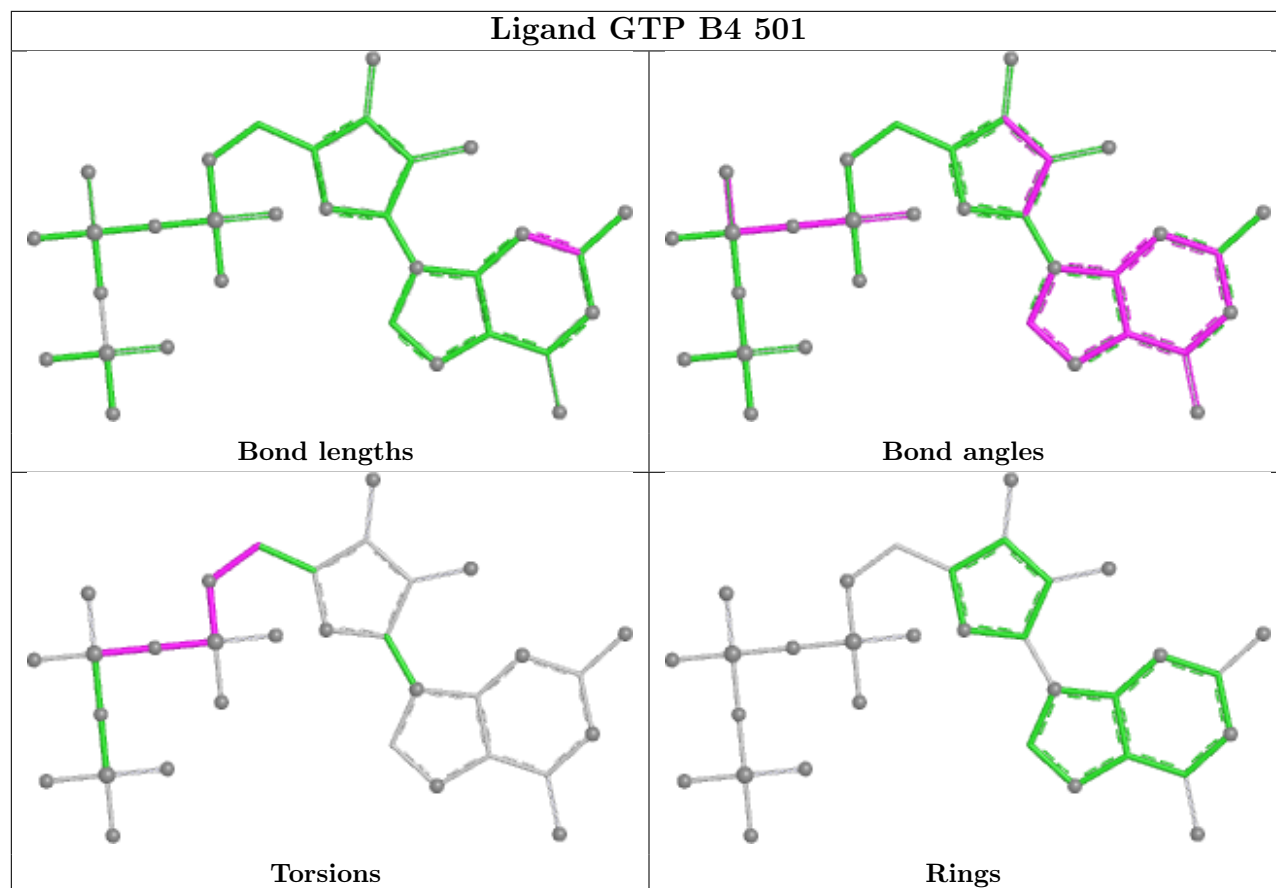




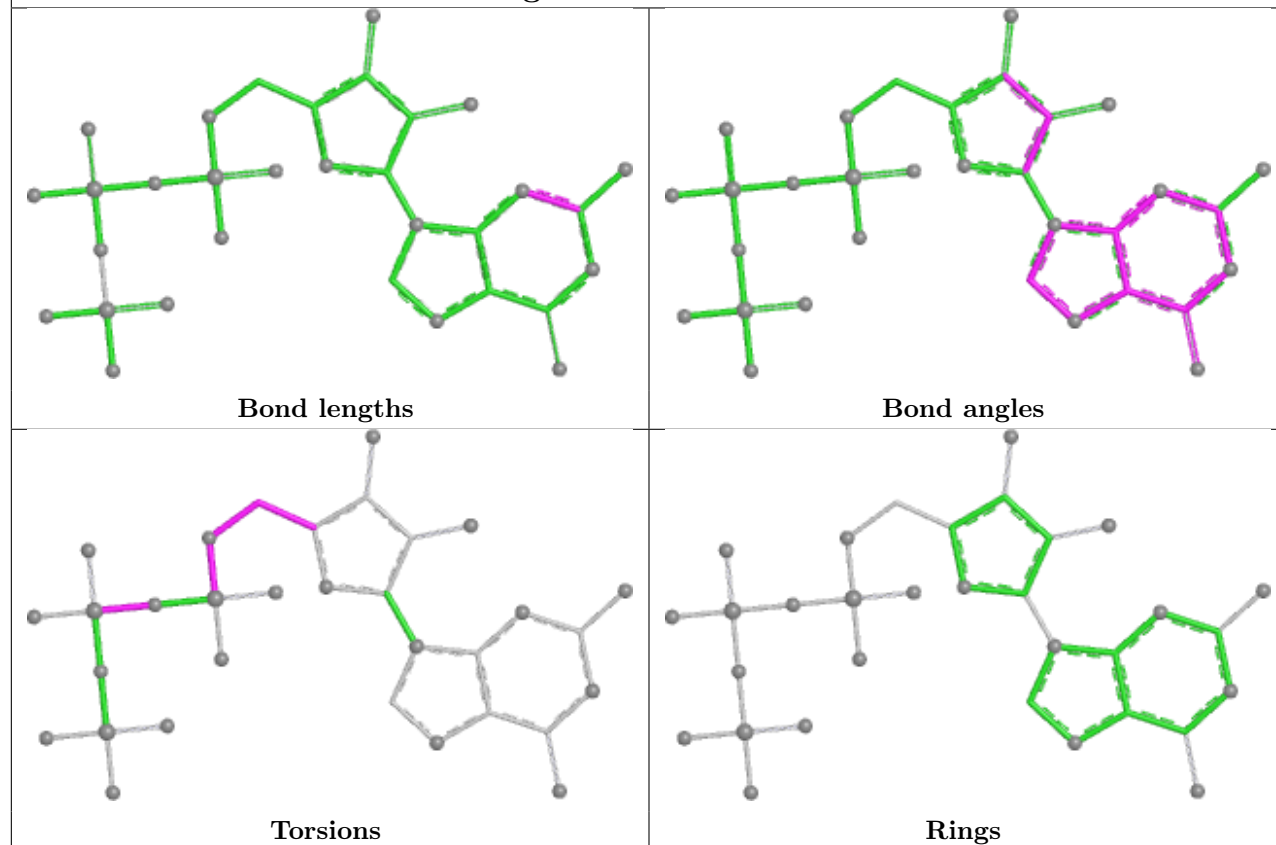




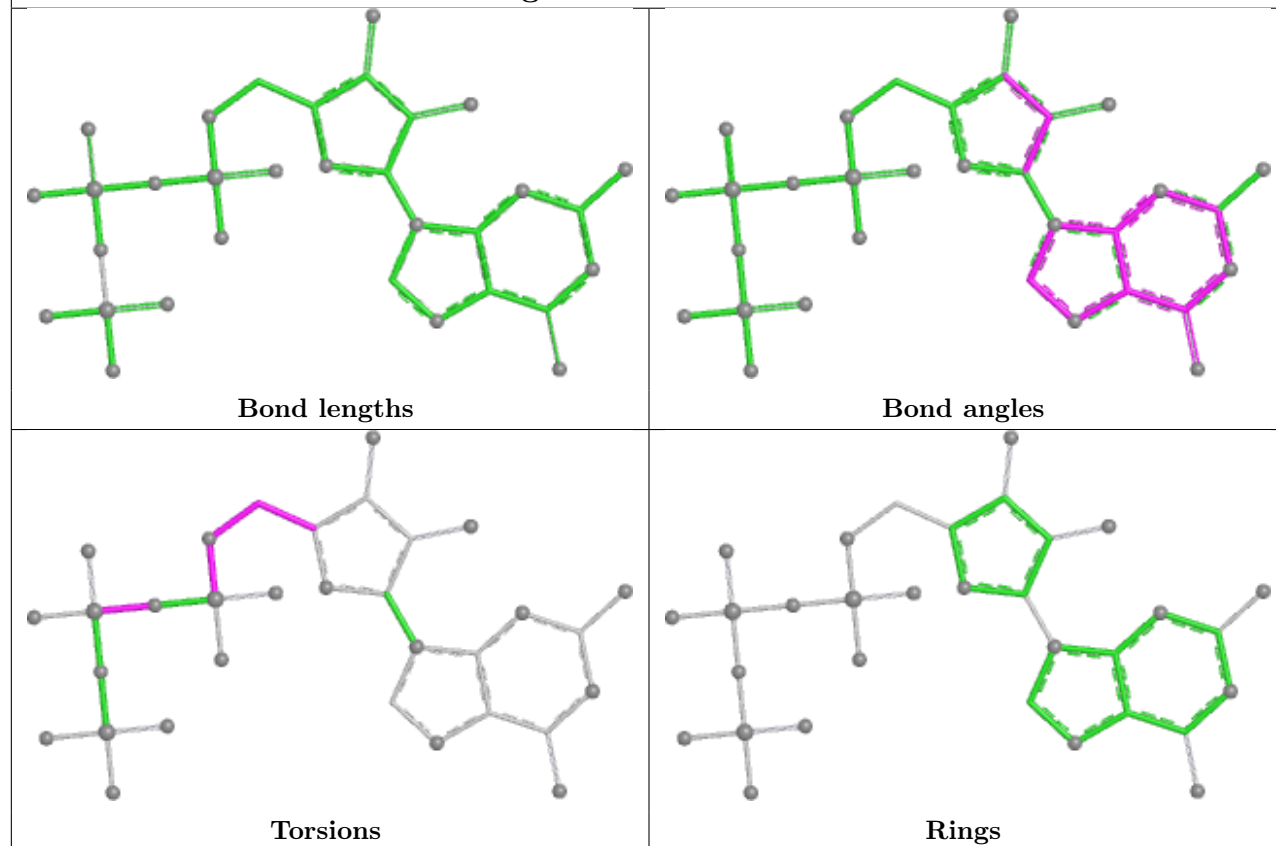


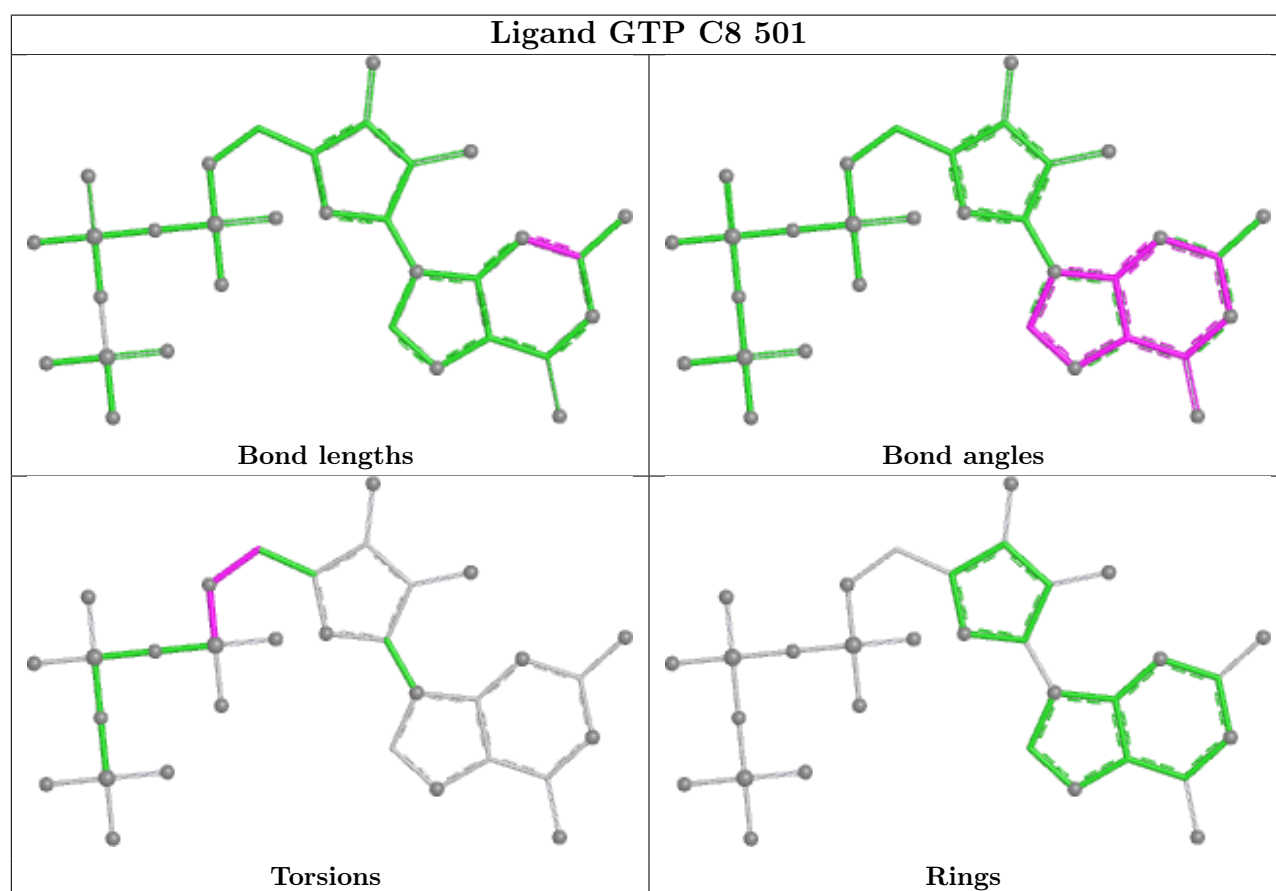
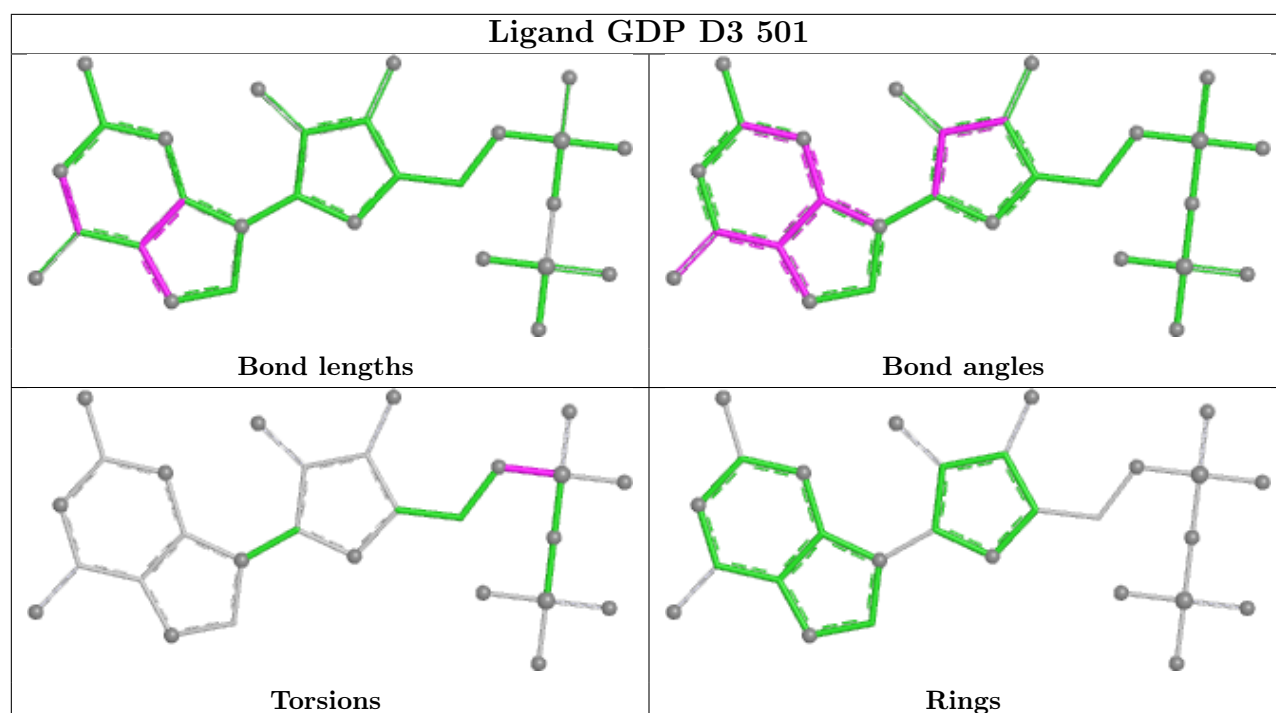


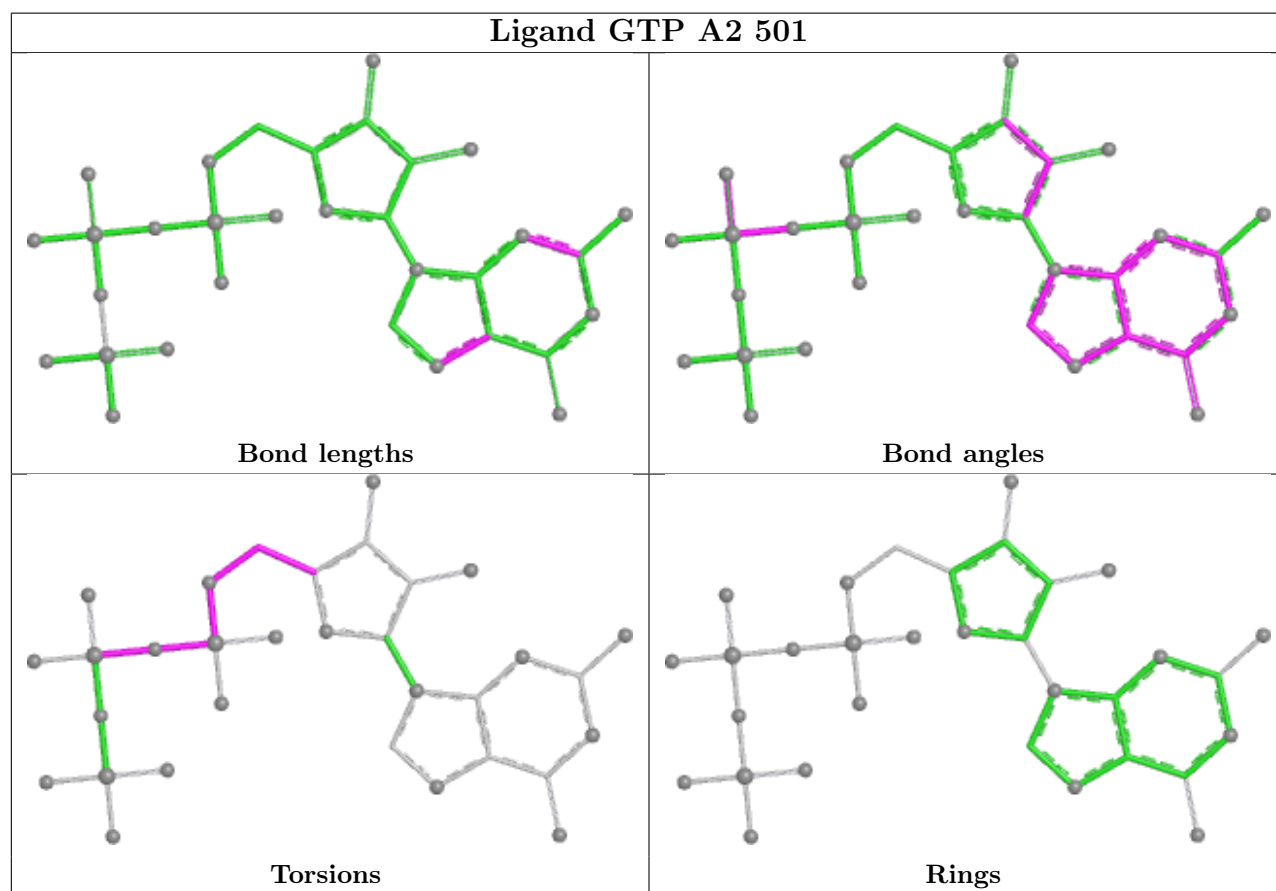
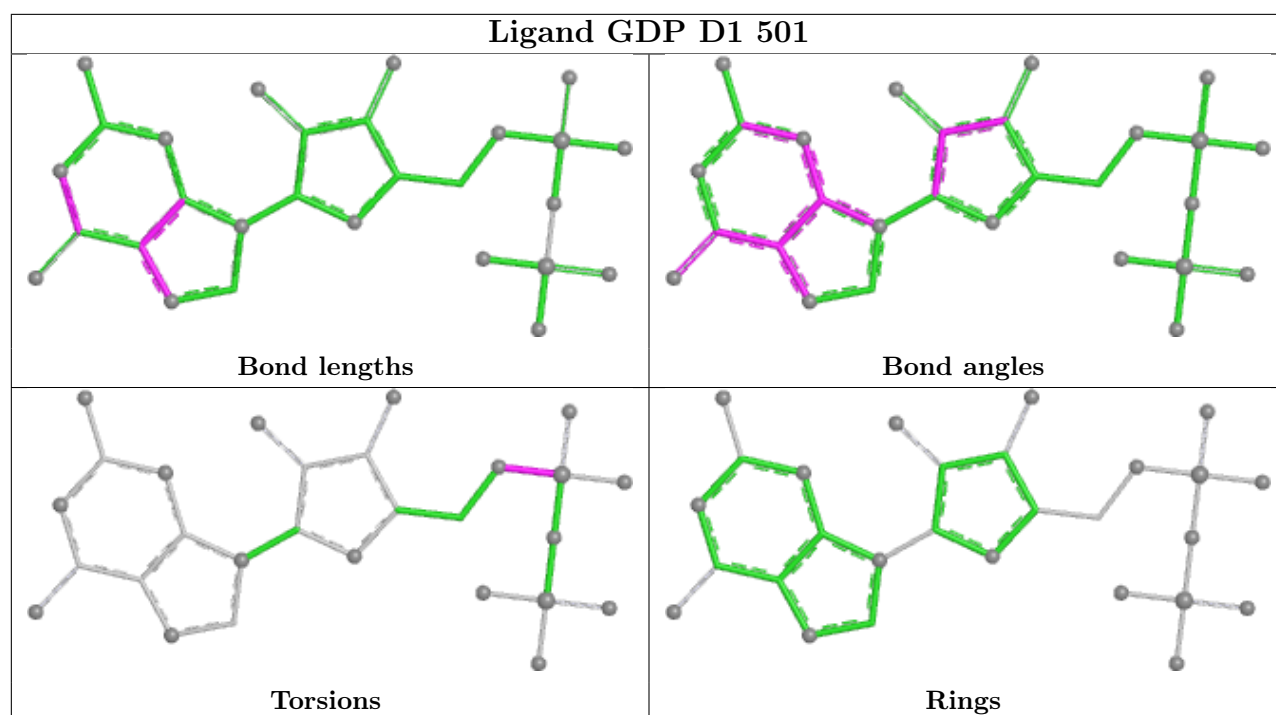
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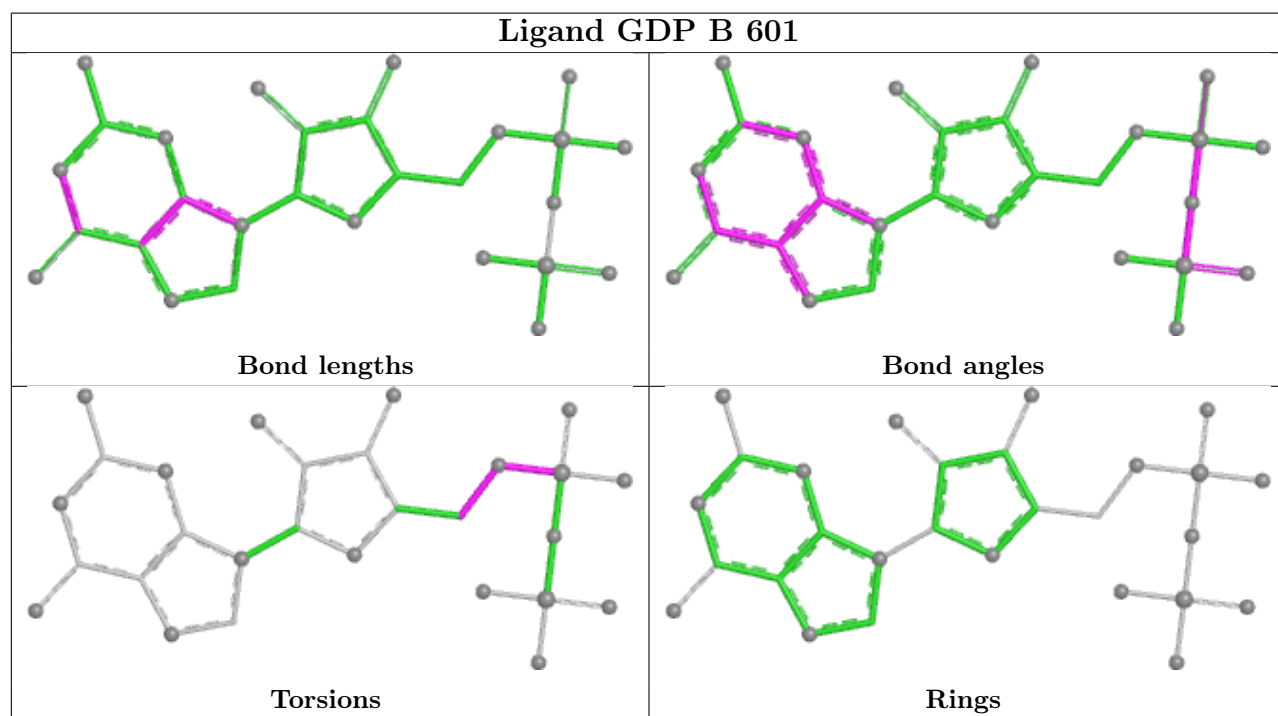
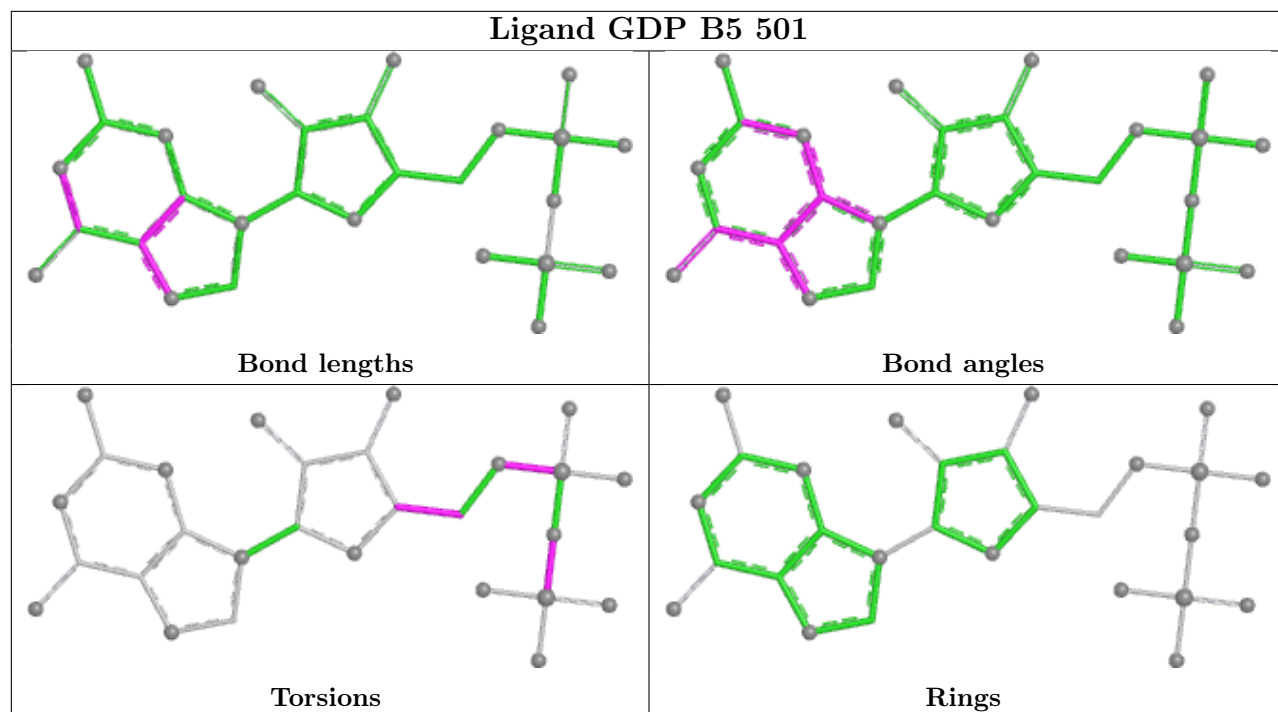


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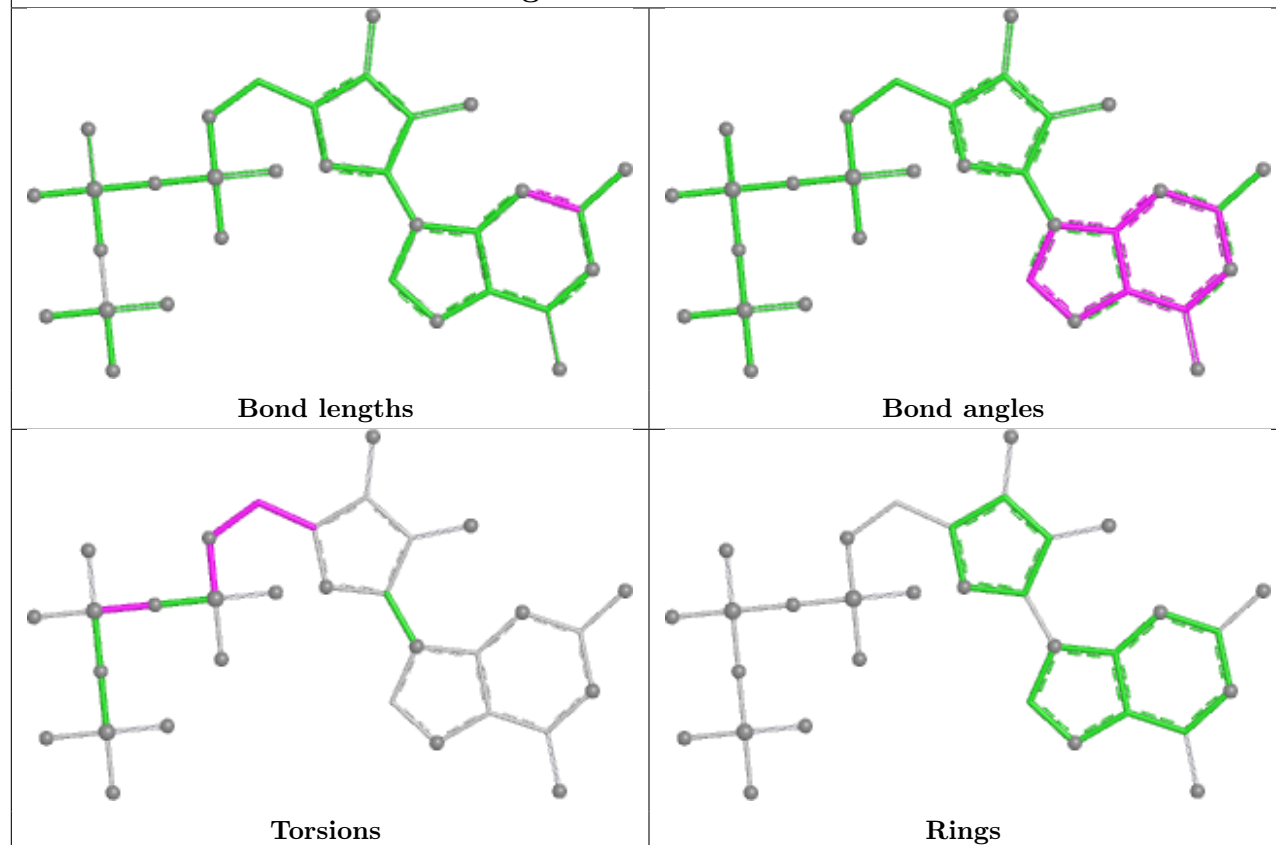




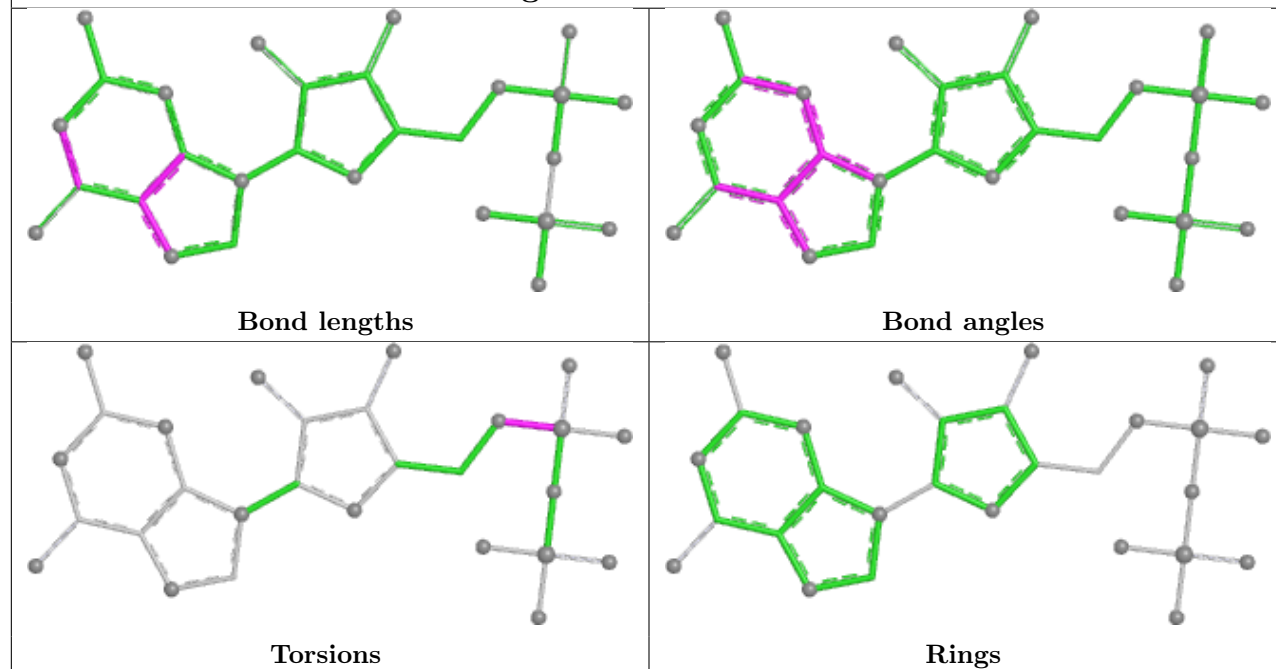


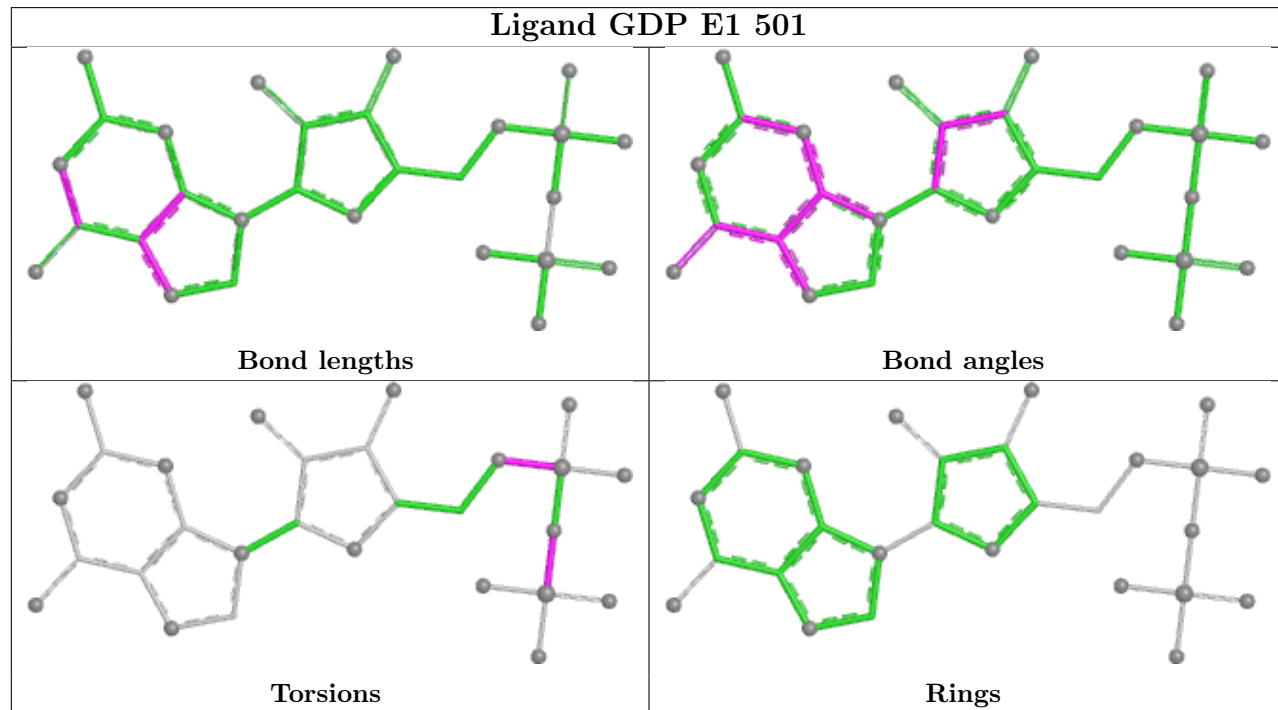
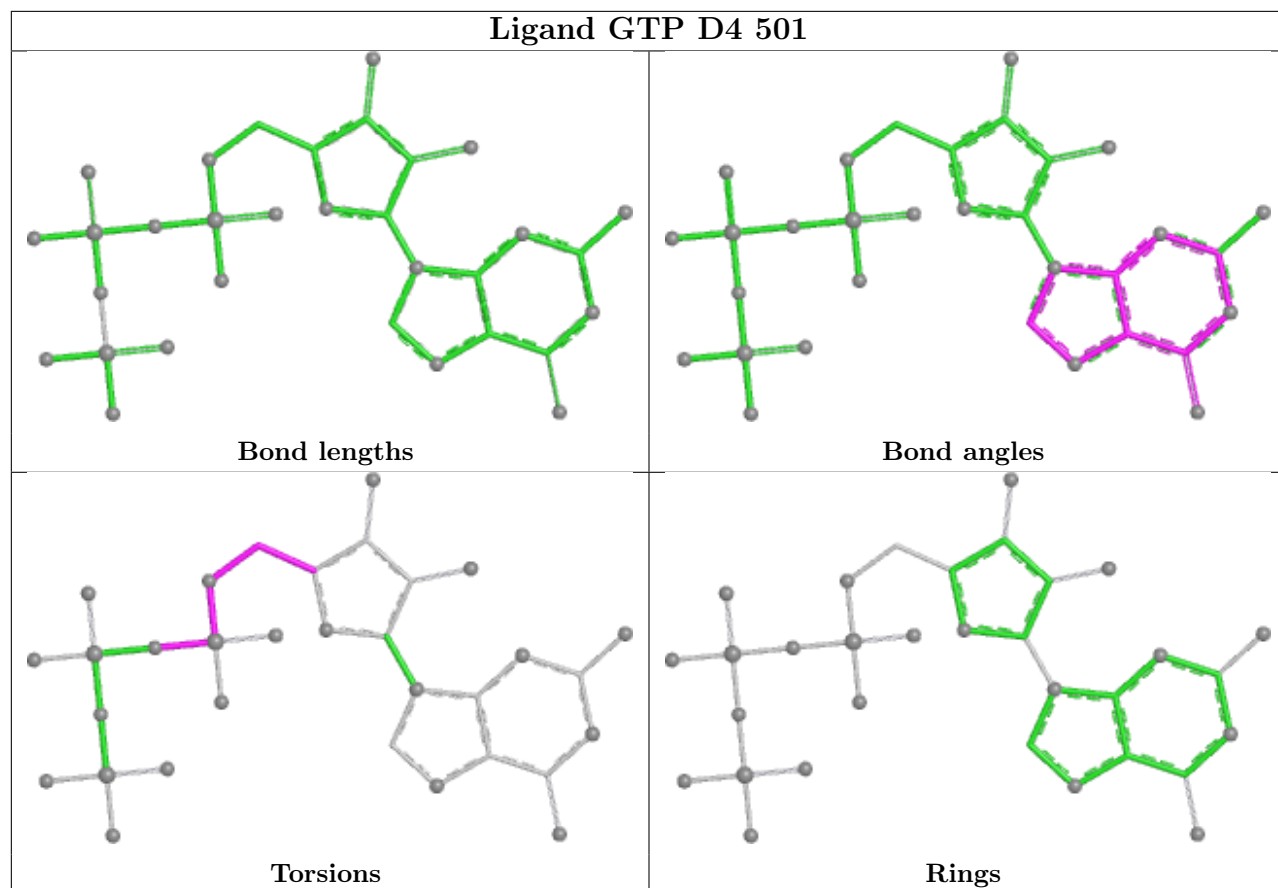


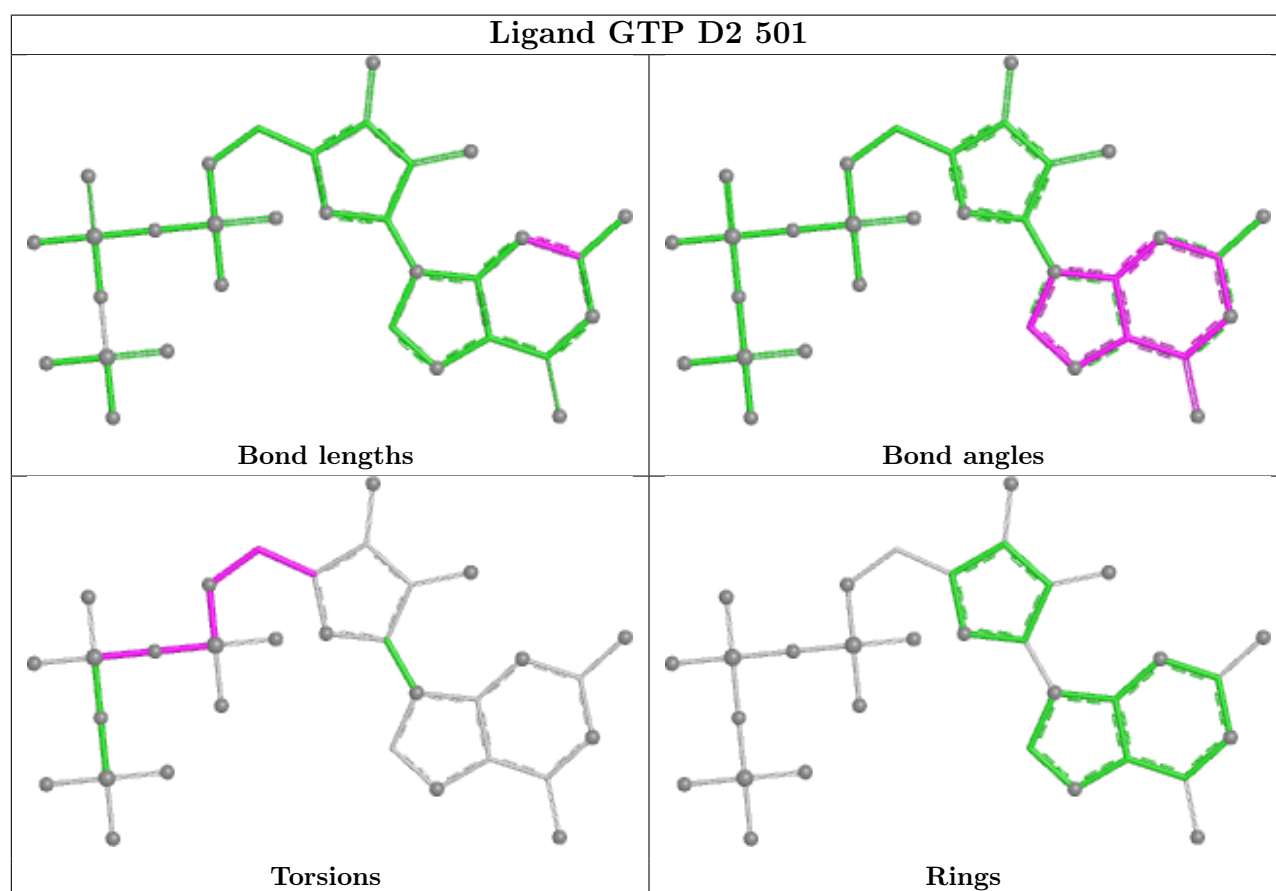
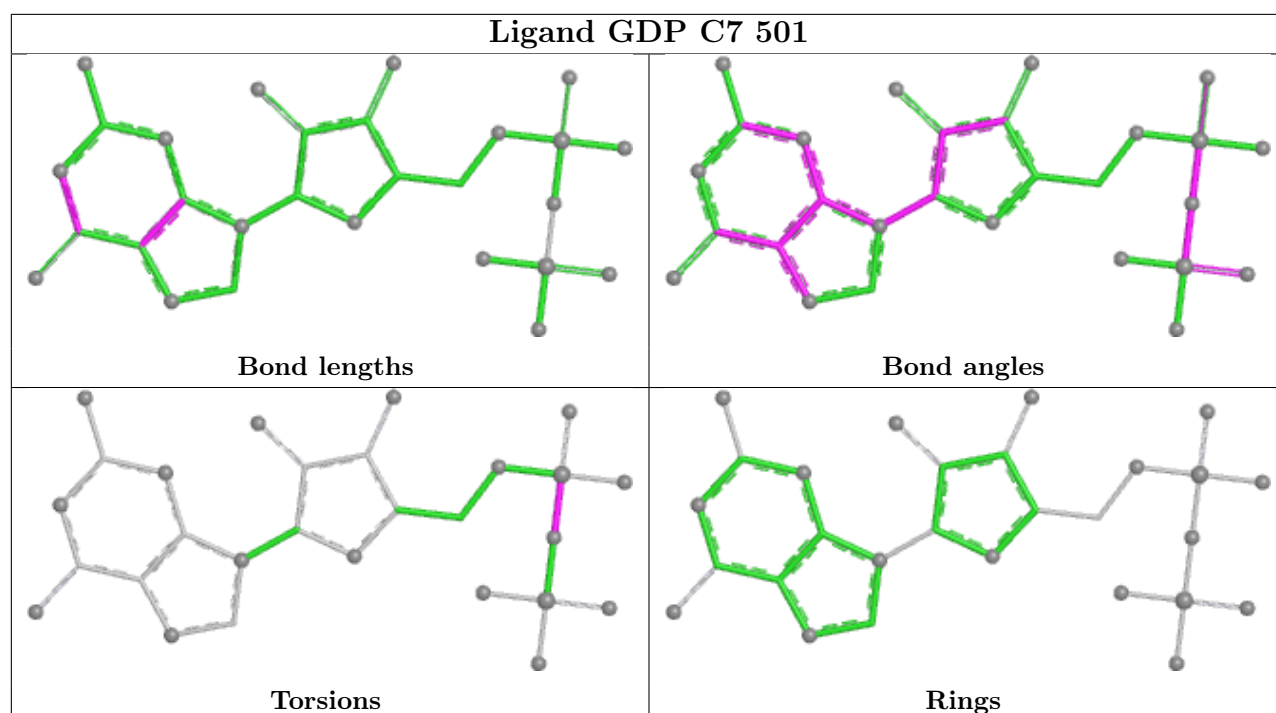
Ligand GTP B8 501

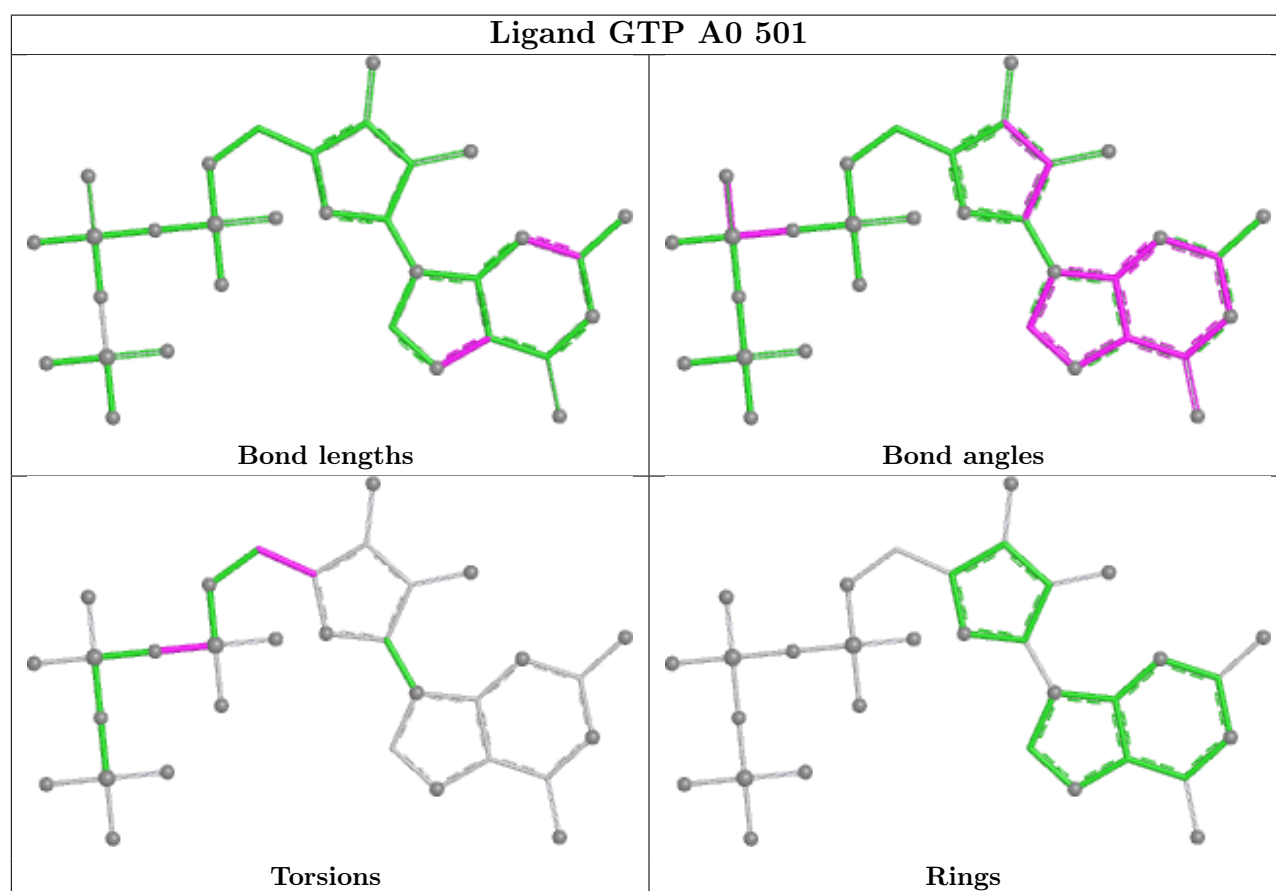
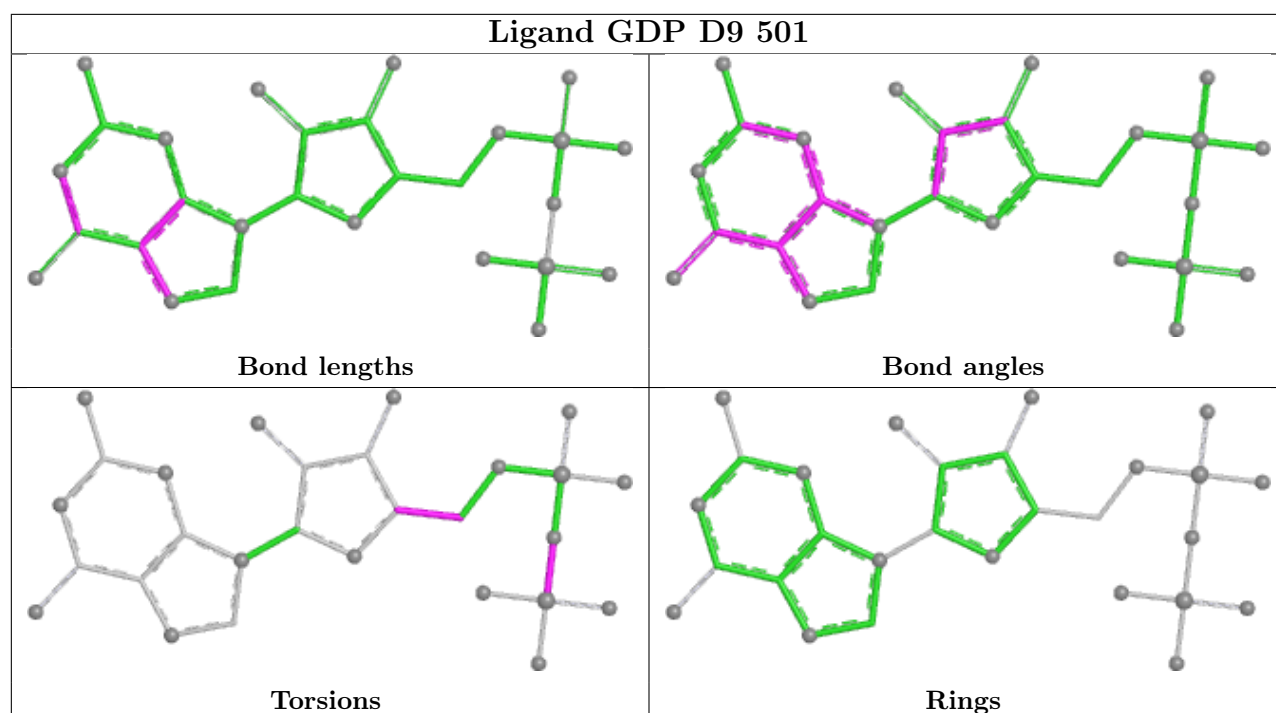


Ligand GDP E5 501

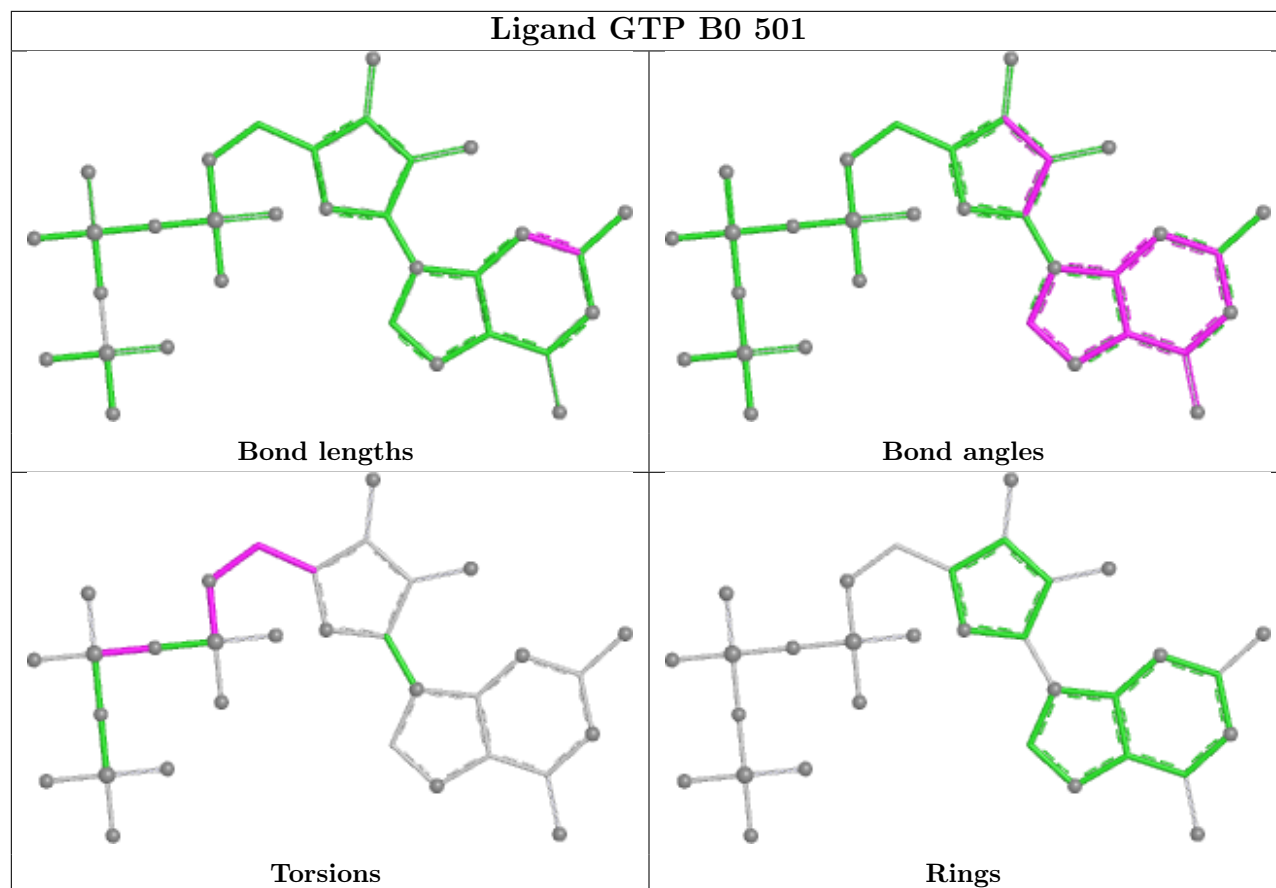




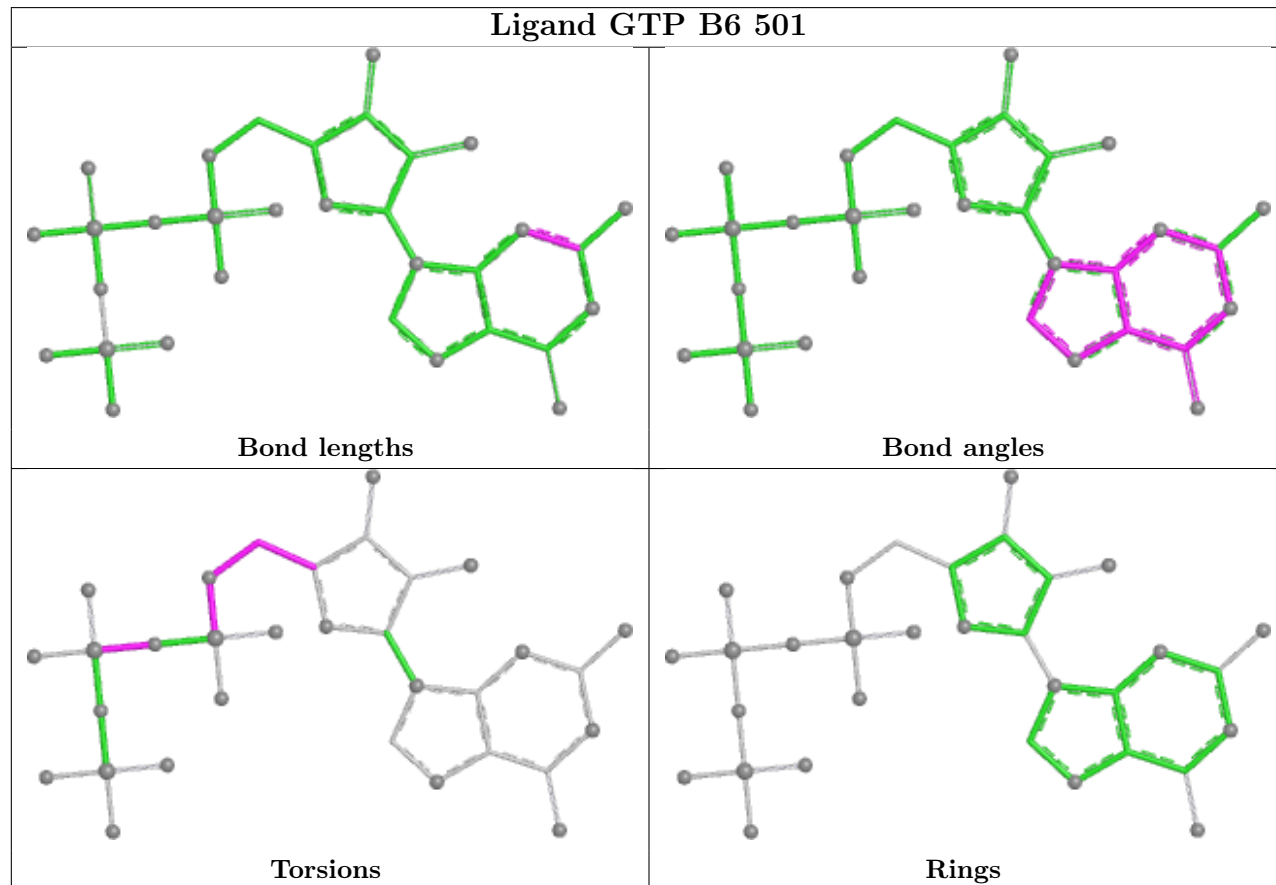




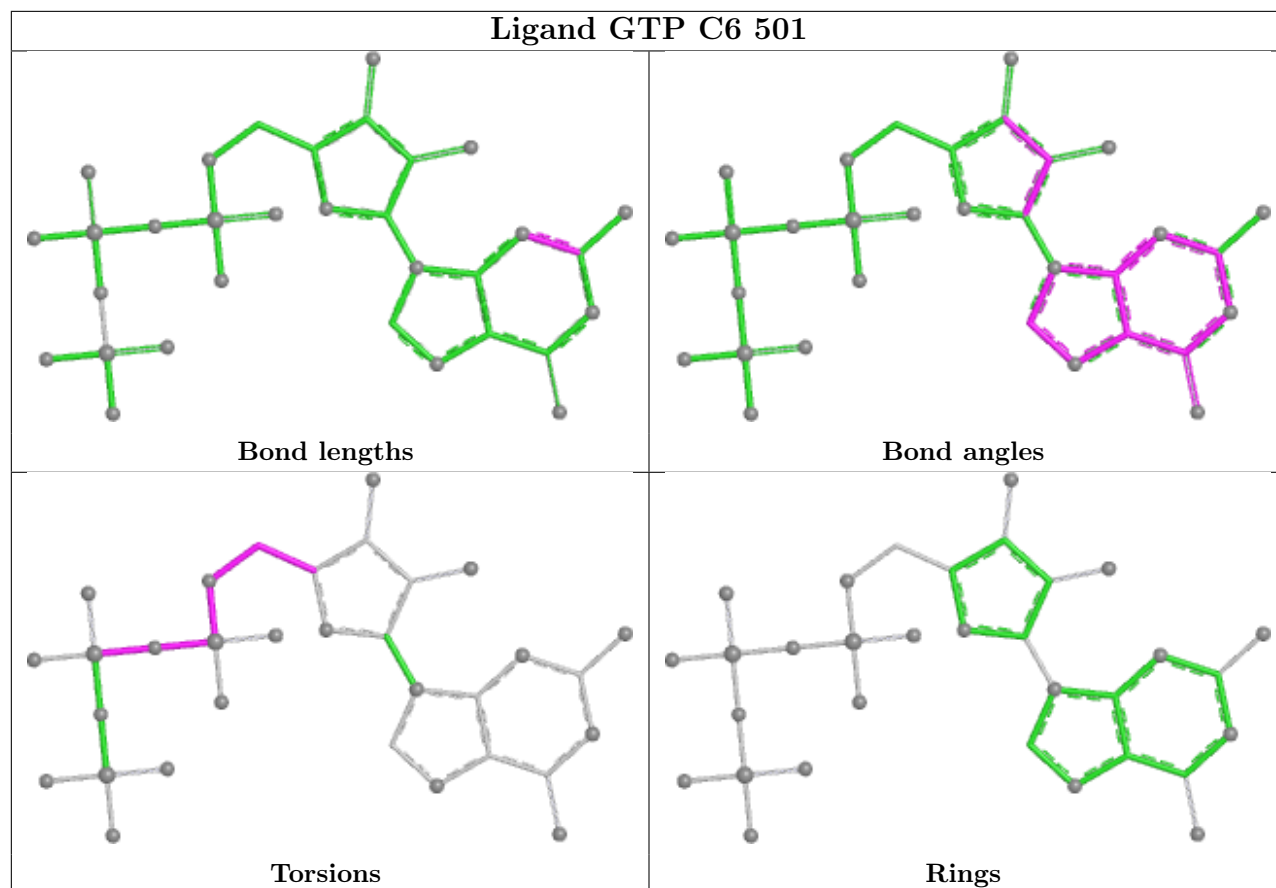
Ligand GTP B0 501



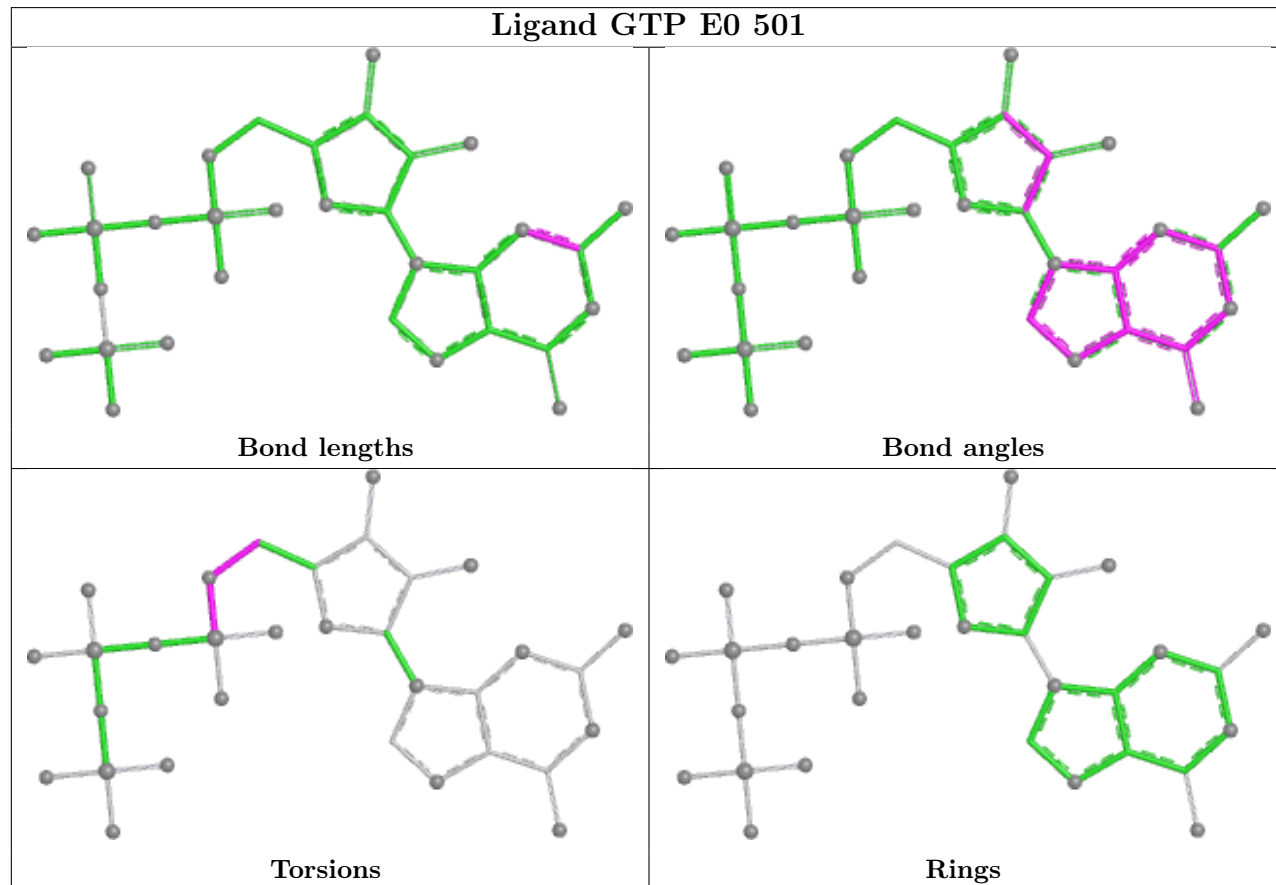
Ligand GTP B6 501

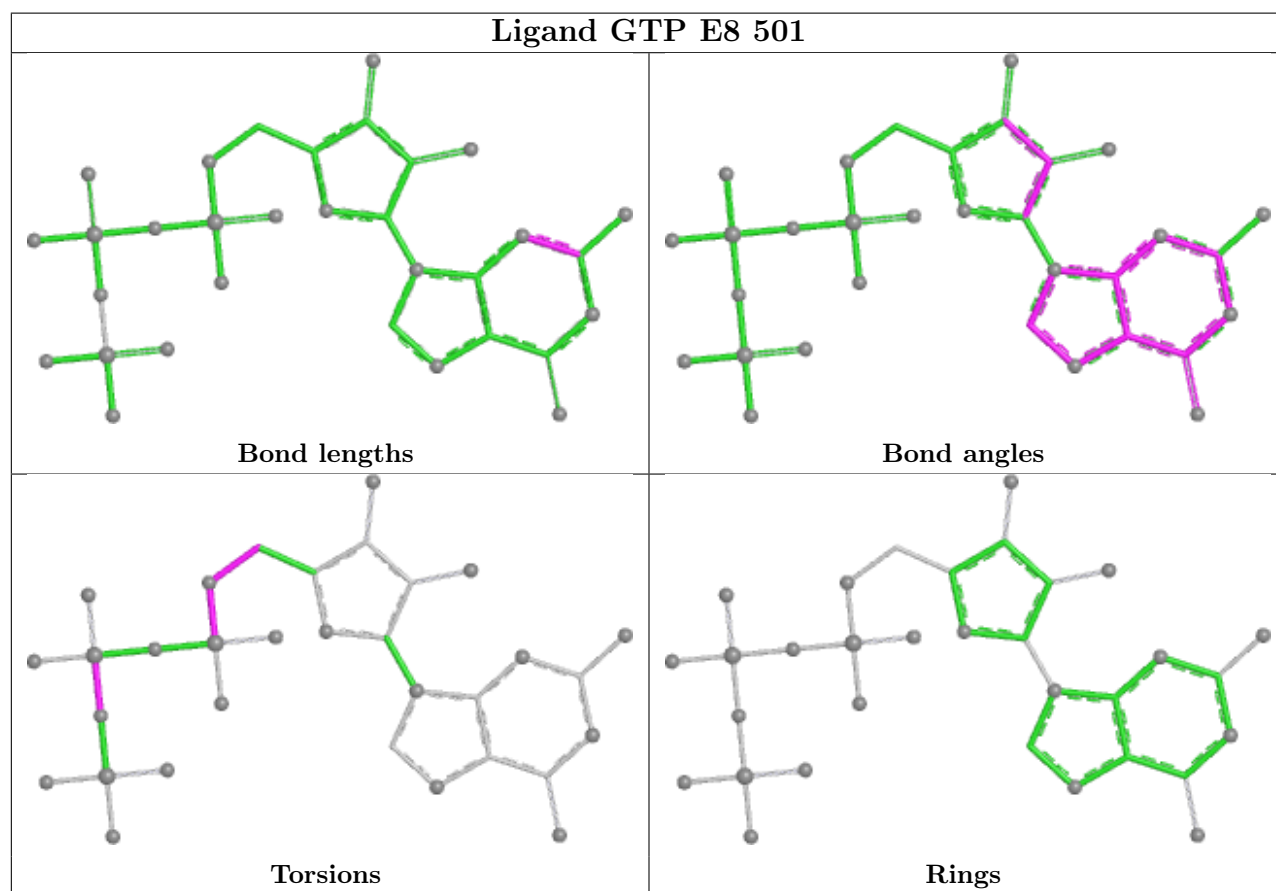
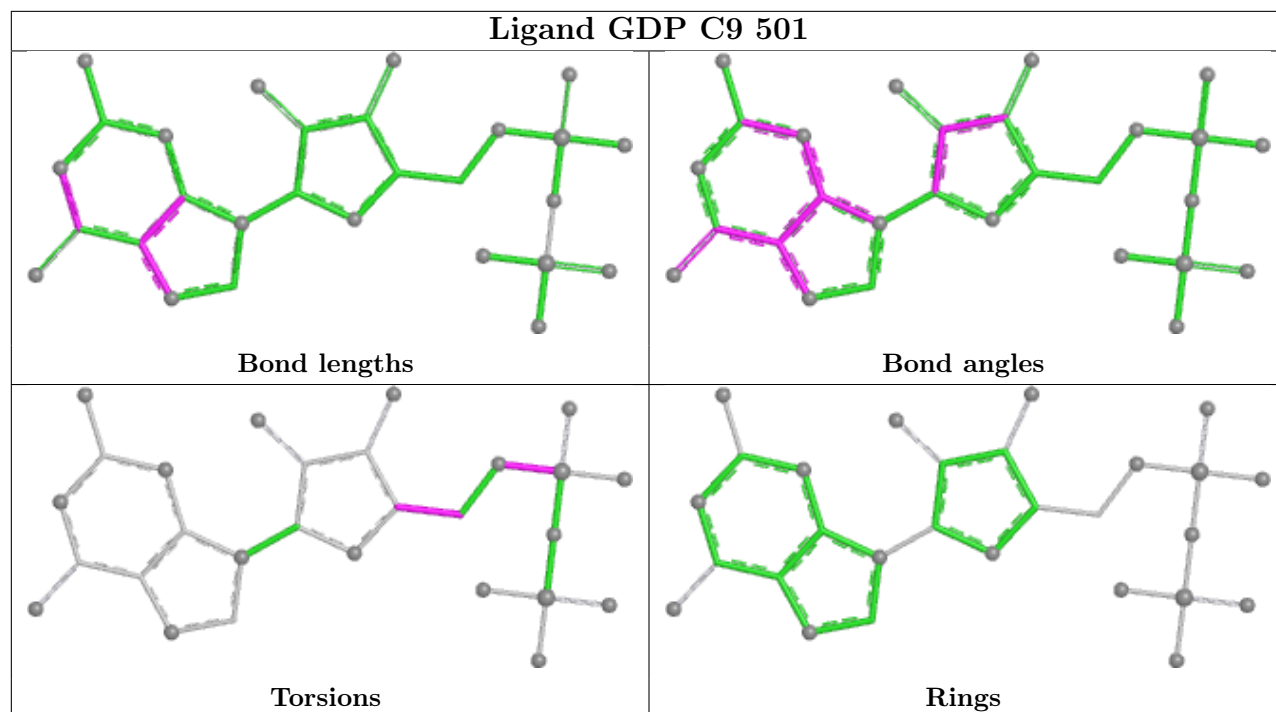


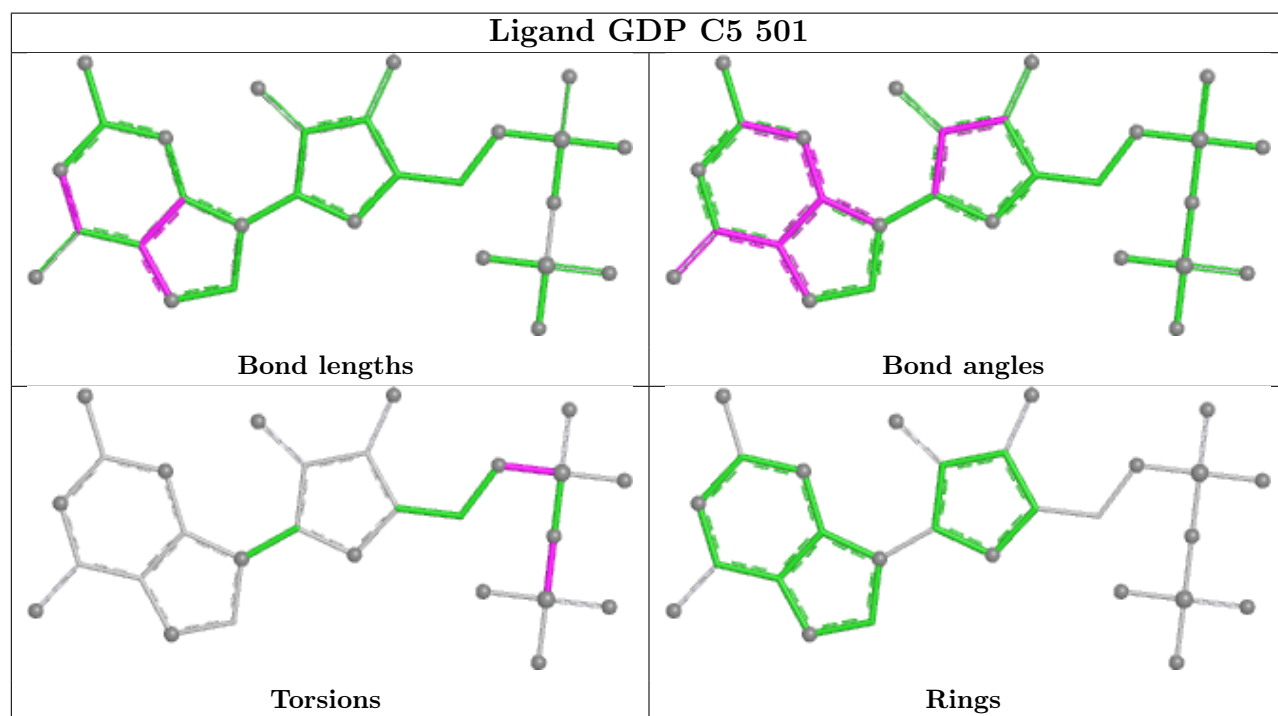
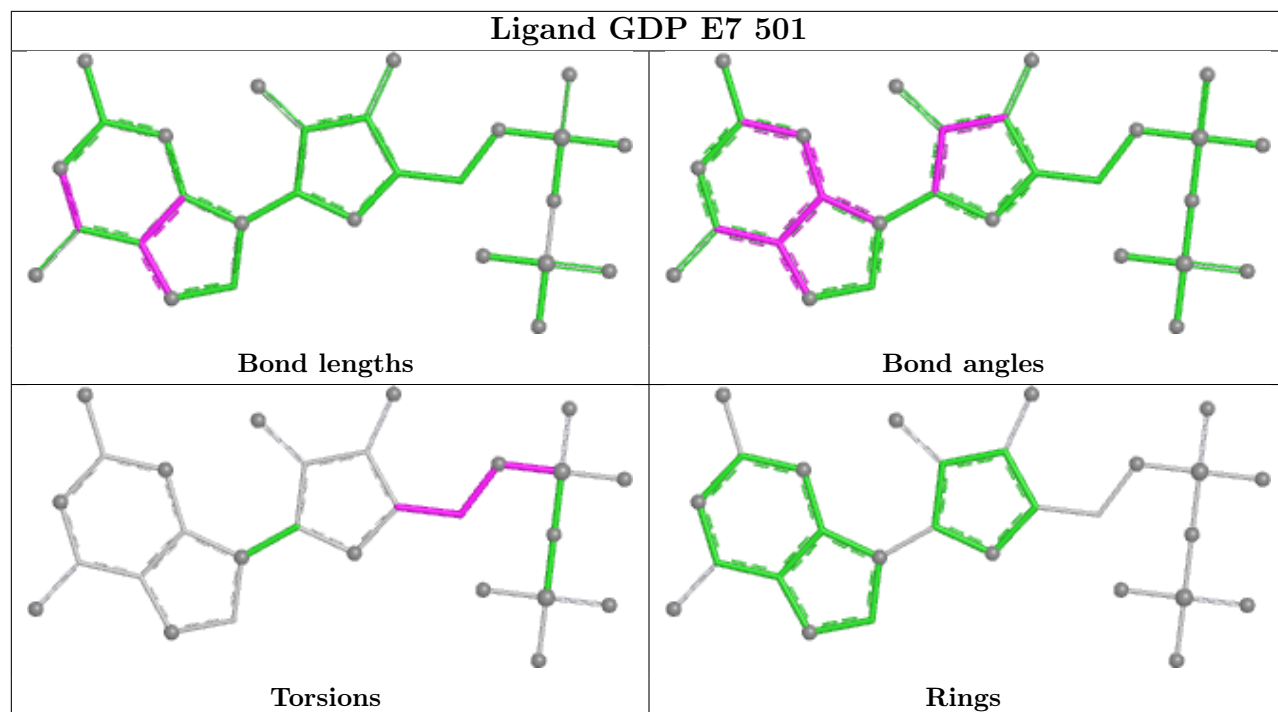
Ligand GTP C6 501

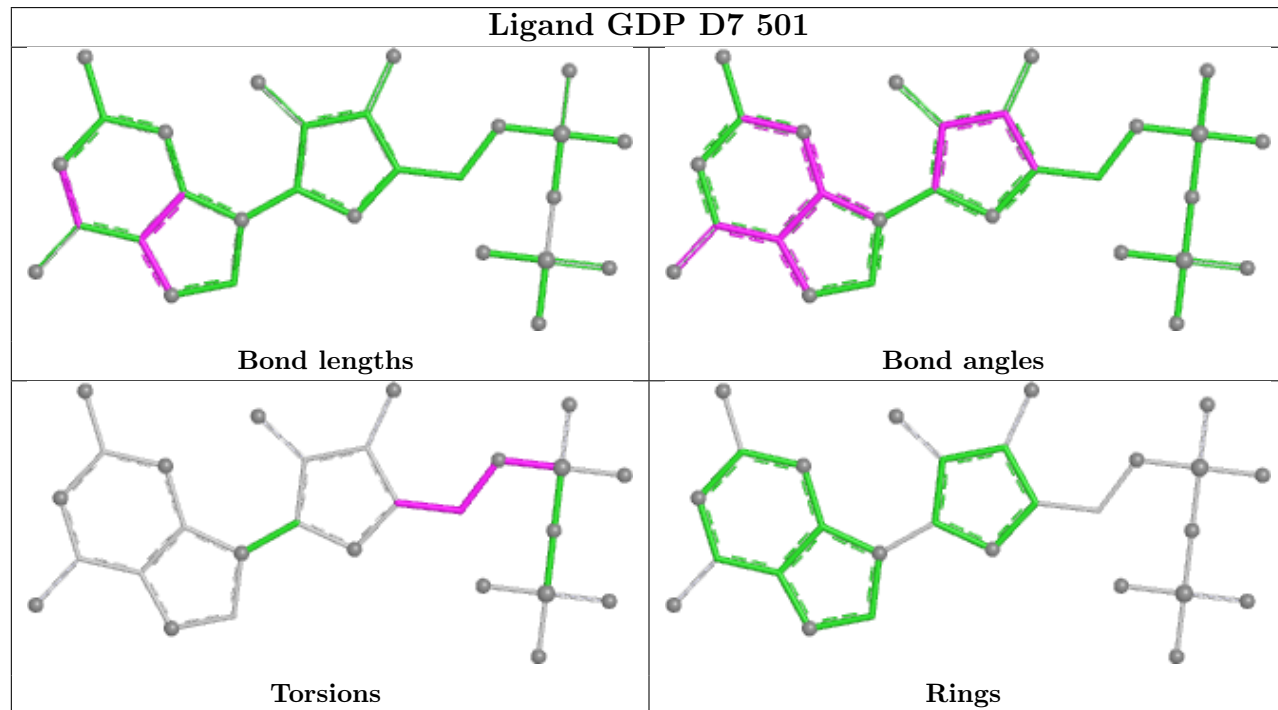
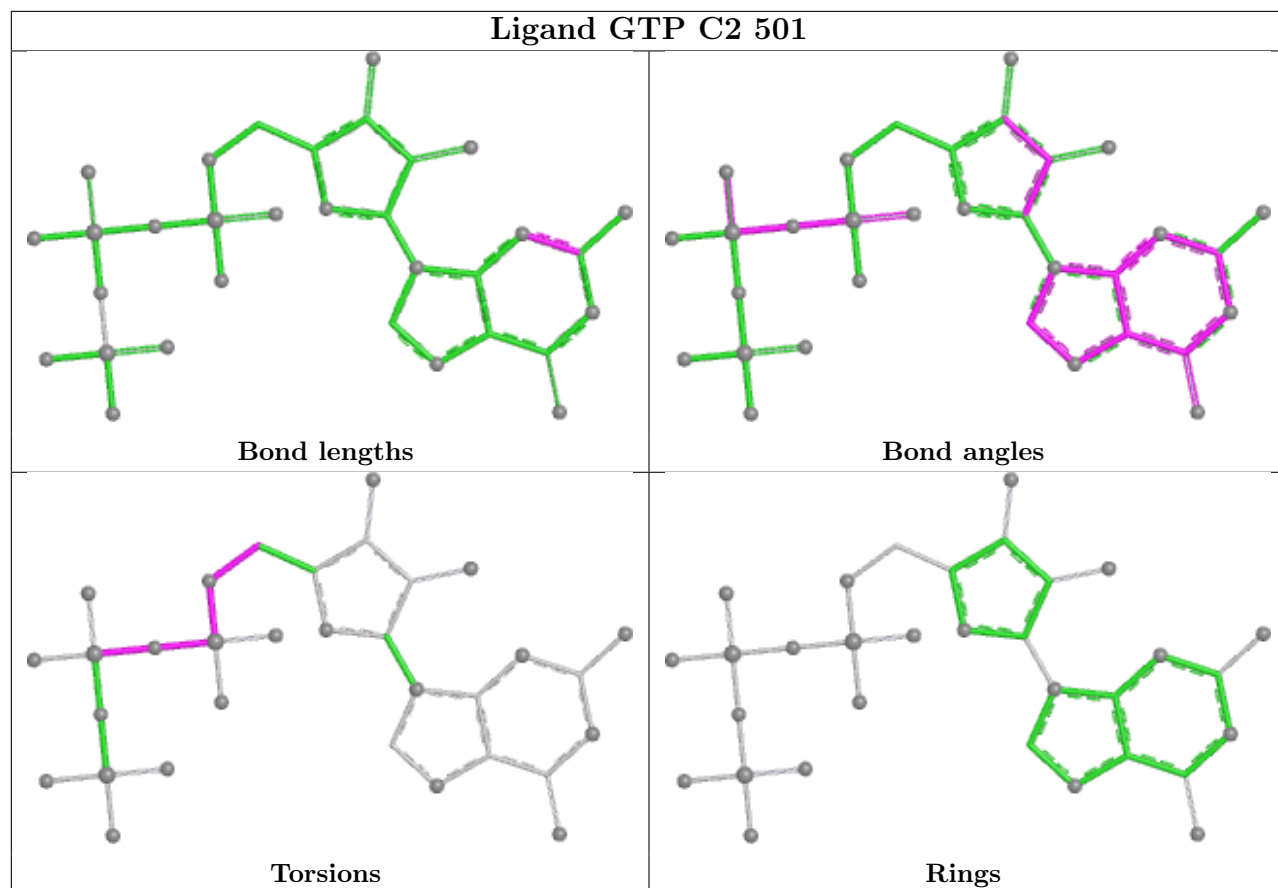


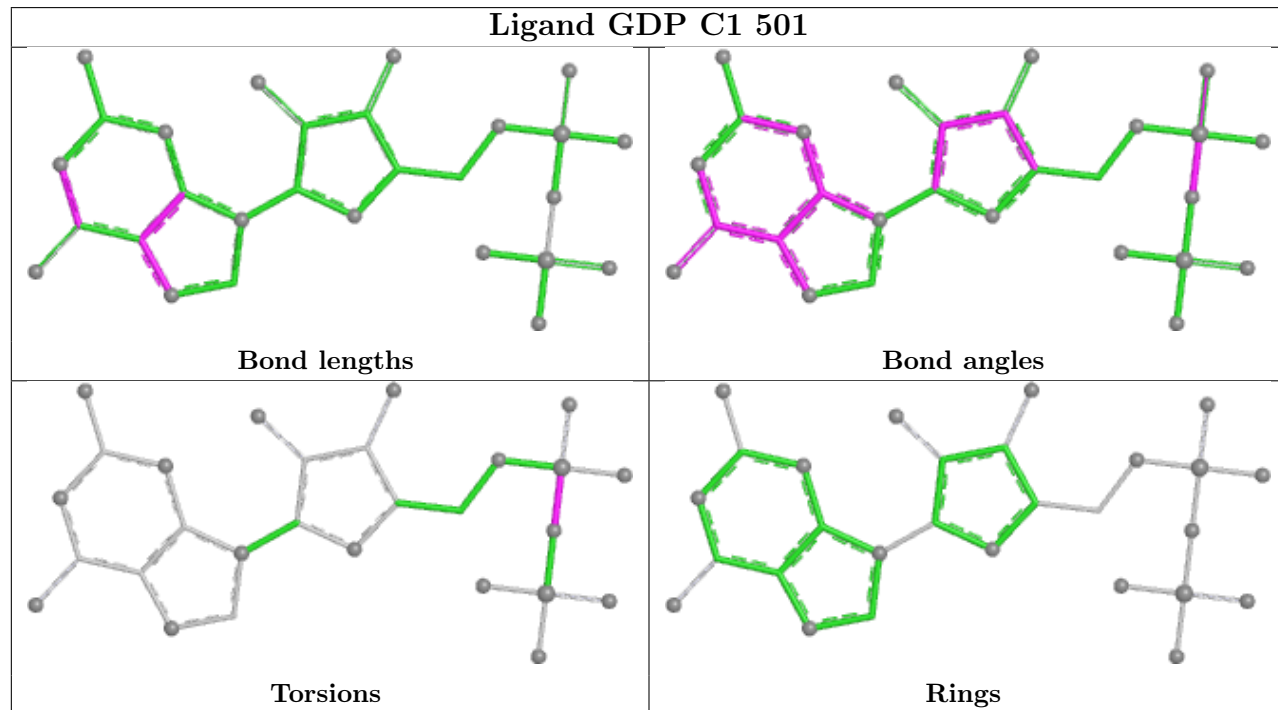
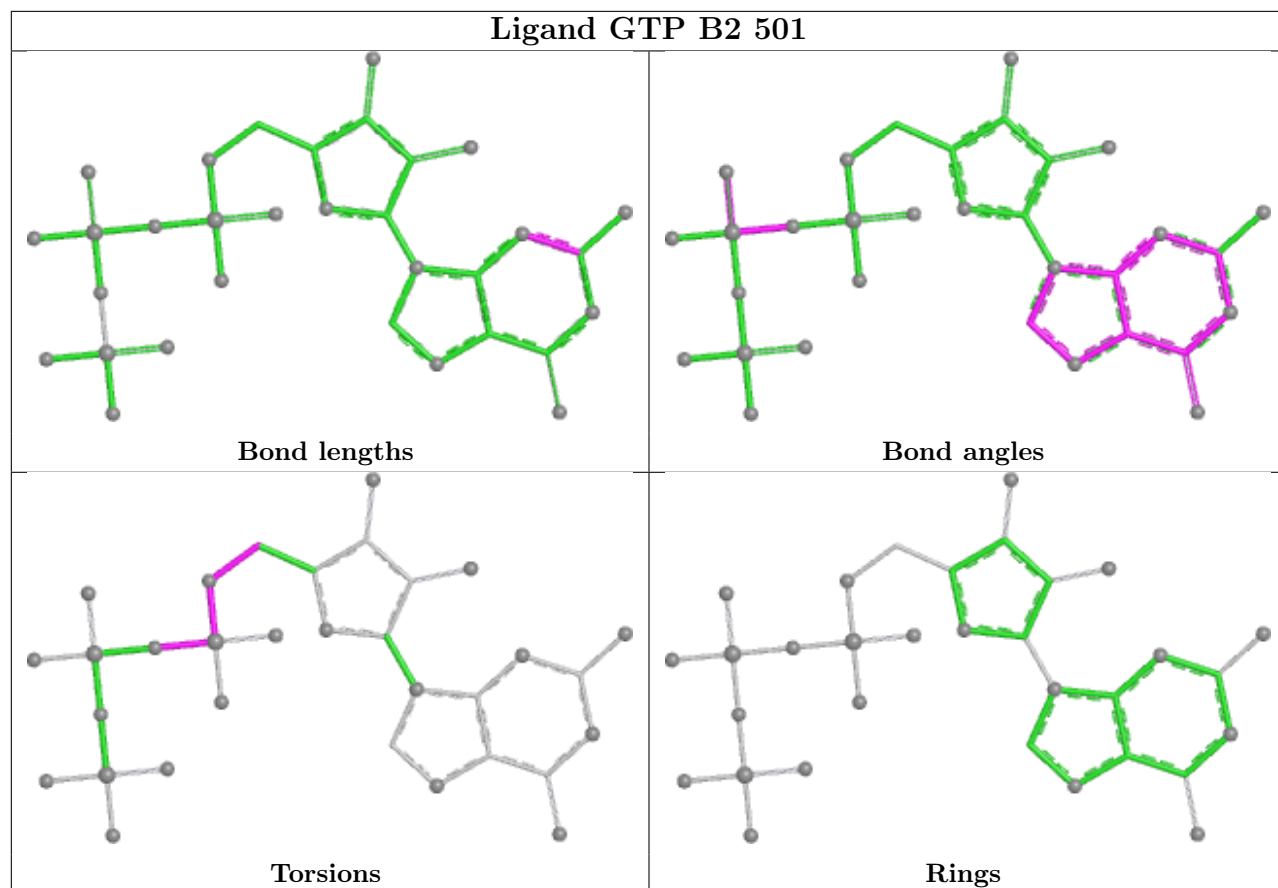
Ligand GTP E0 501

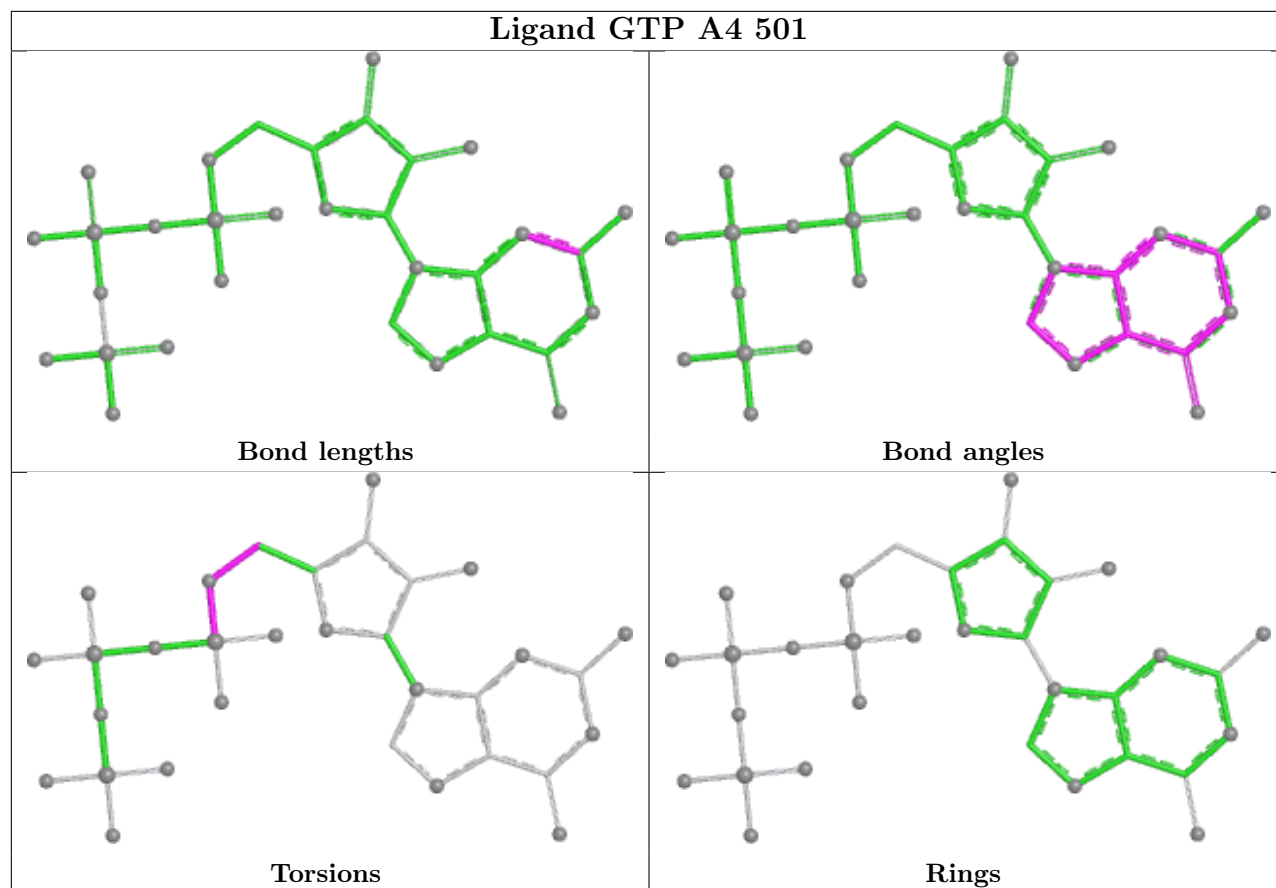












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

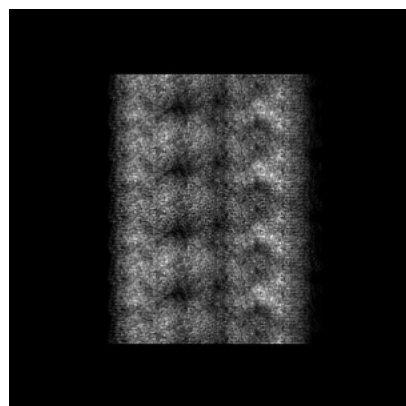
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72719. These allow visual inspection of the internal detail of the map and identification of artifacts.

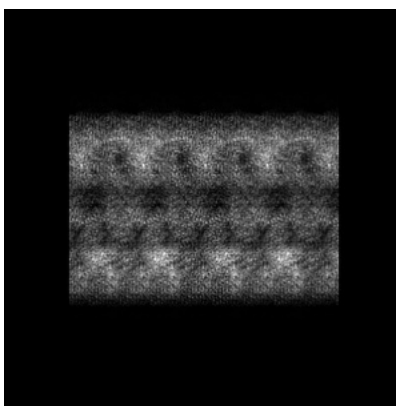
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

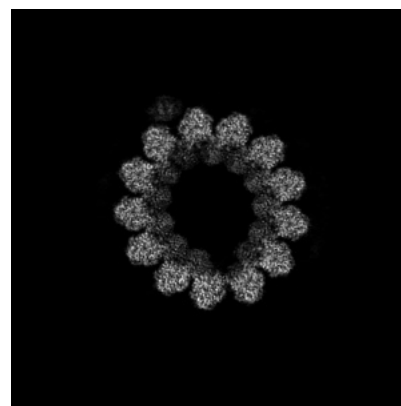
6.1.1 Primary map



X

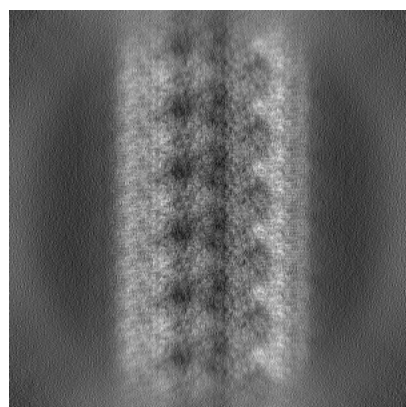


Y

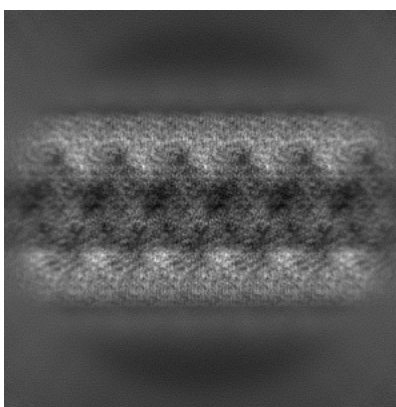


Z

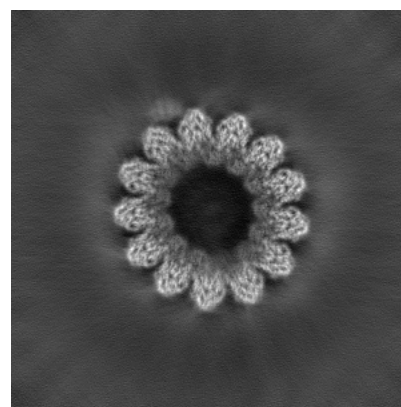
6.1.2 Raw map



X



Y

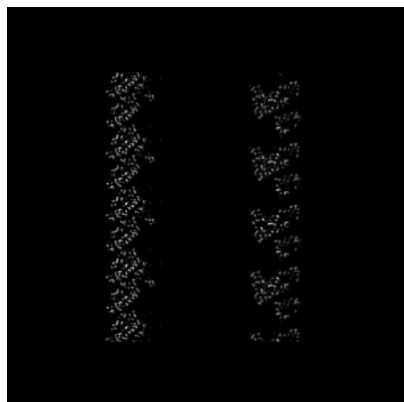


Z

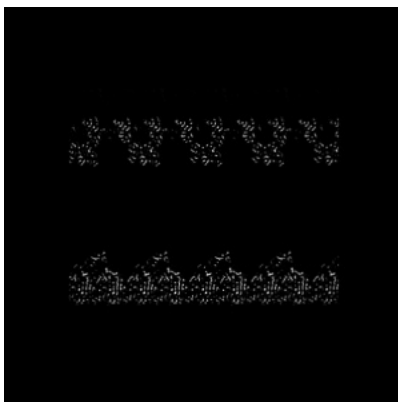
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

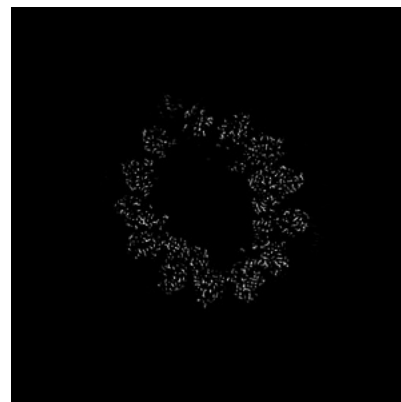
6.2.1 Primary map



X Index: 200

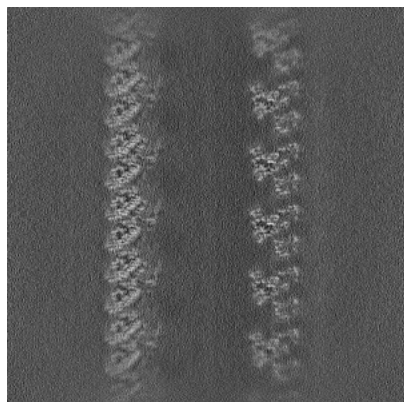


Y Index: 200

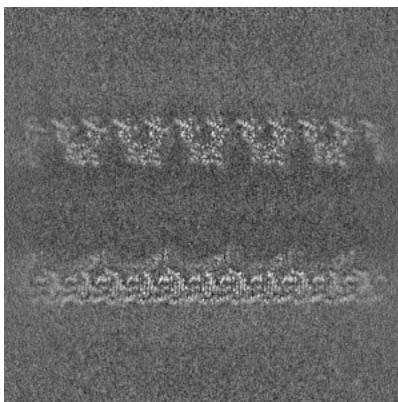


Z Index: 200

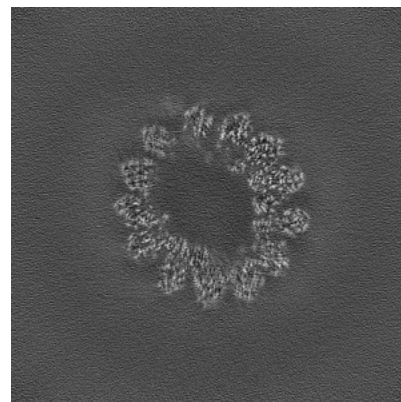
6.2.2 Raw map



X Index: 200



Y Index: 200

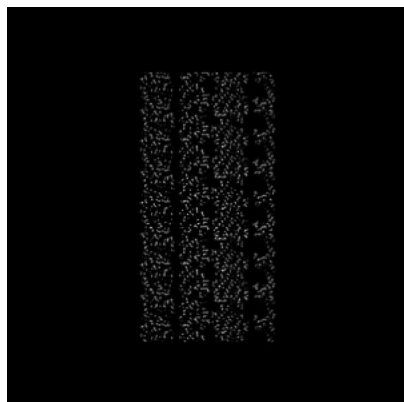


Z Index: 200

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

6.3 Largest variance slices [i](#)

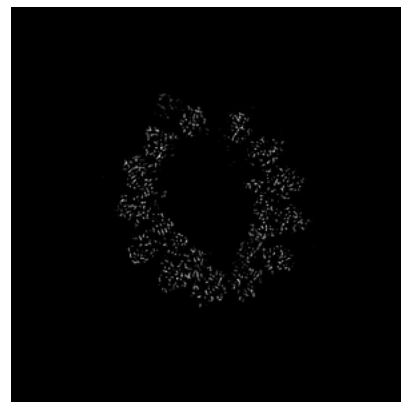
6.3.1 Primary map



X Index: 270

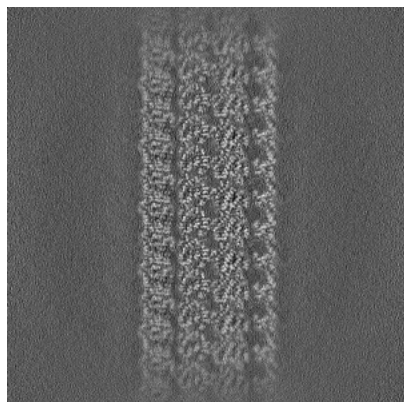


Y Index: 126

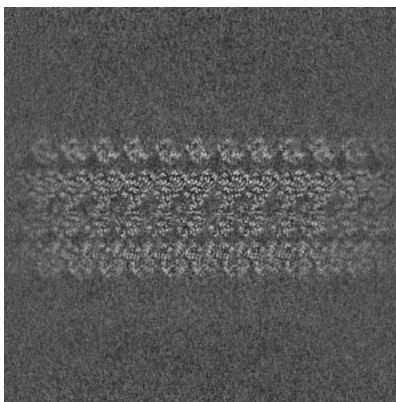


Z Index: 206

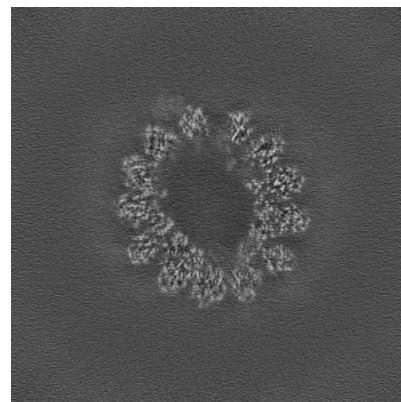
6.3.2 Raw map



X Index: 270



Y Index: 270

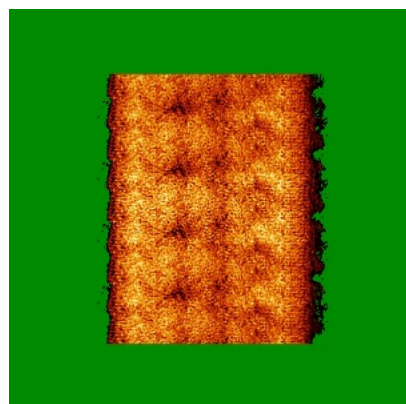


Z Index: 206

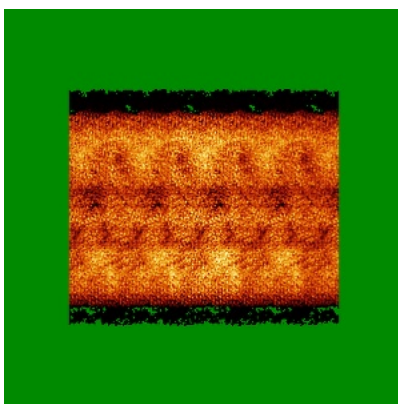
The images above show the largest variance slices of the map in three orthogonal directions.

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

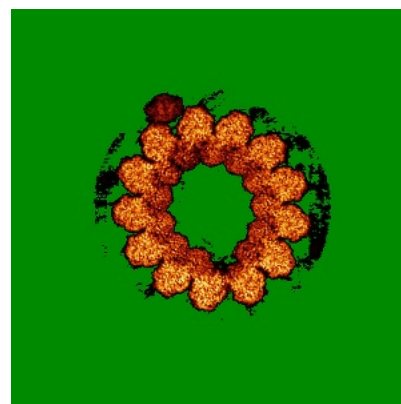
6.4.1 Primary map



X

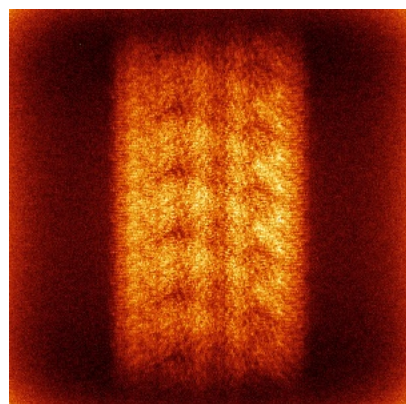


Y

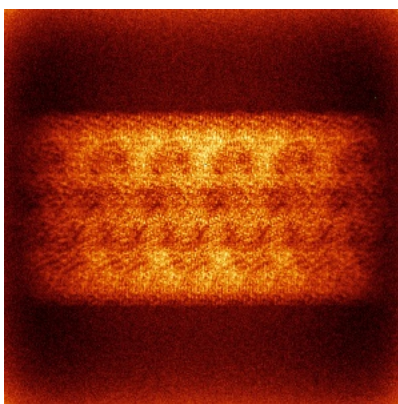


Z

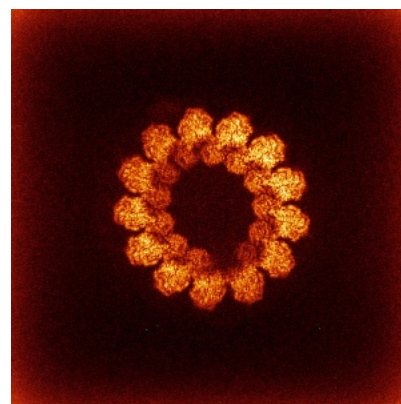
6.4.2 Raw map



X



Y

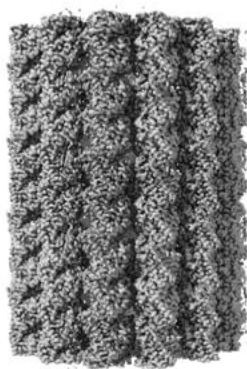


Z

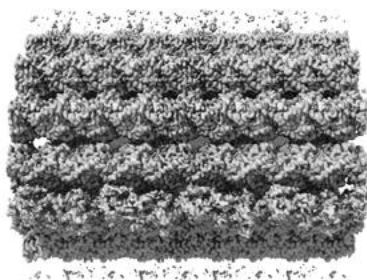
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

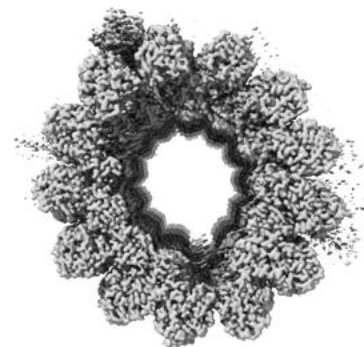
6.5.1 Primary map



X



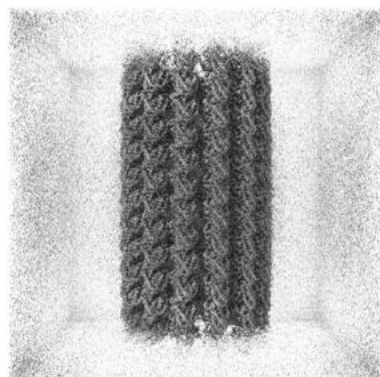
Y



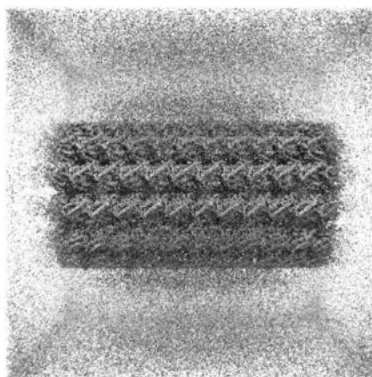
Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

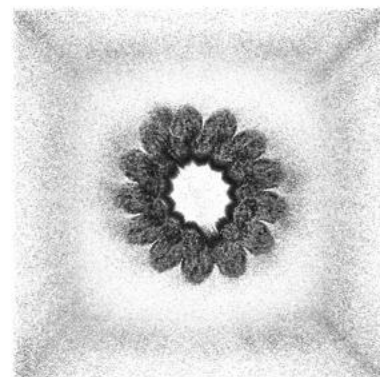
6.5.2 Raw map



X



Y



Z

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.

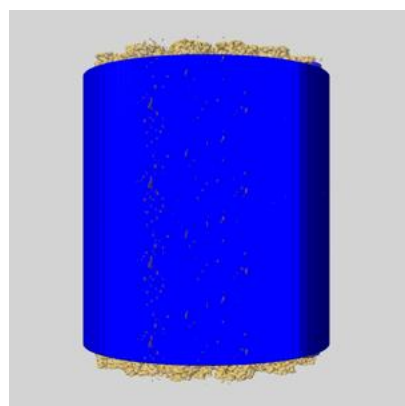
6.6 Mask visualisation [i](#)

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

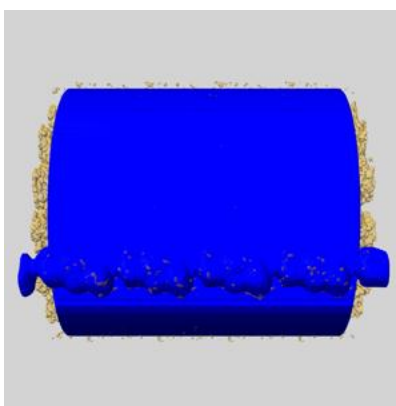
A mask typically either:

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

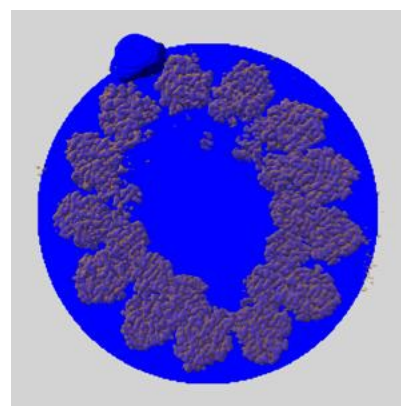
6.6.1 emd_72719_msk_1.map [i](#)



X



Y

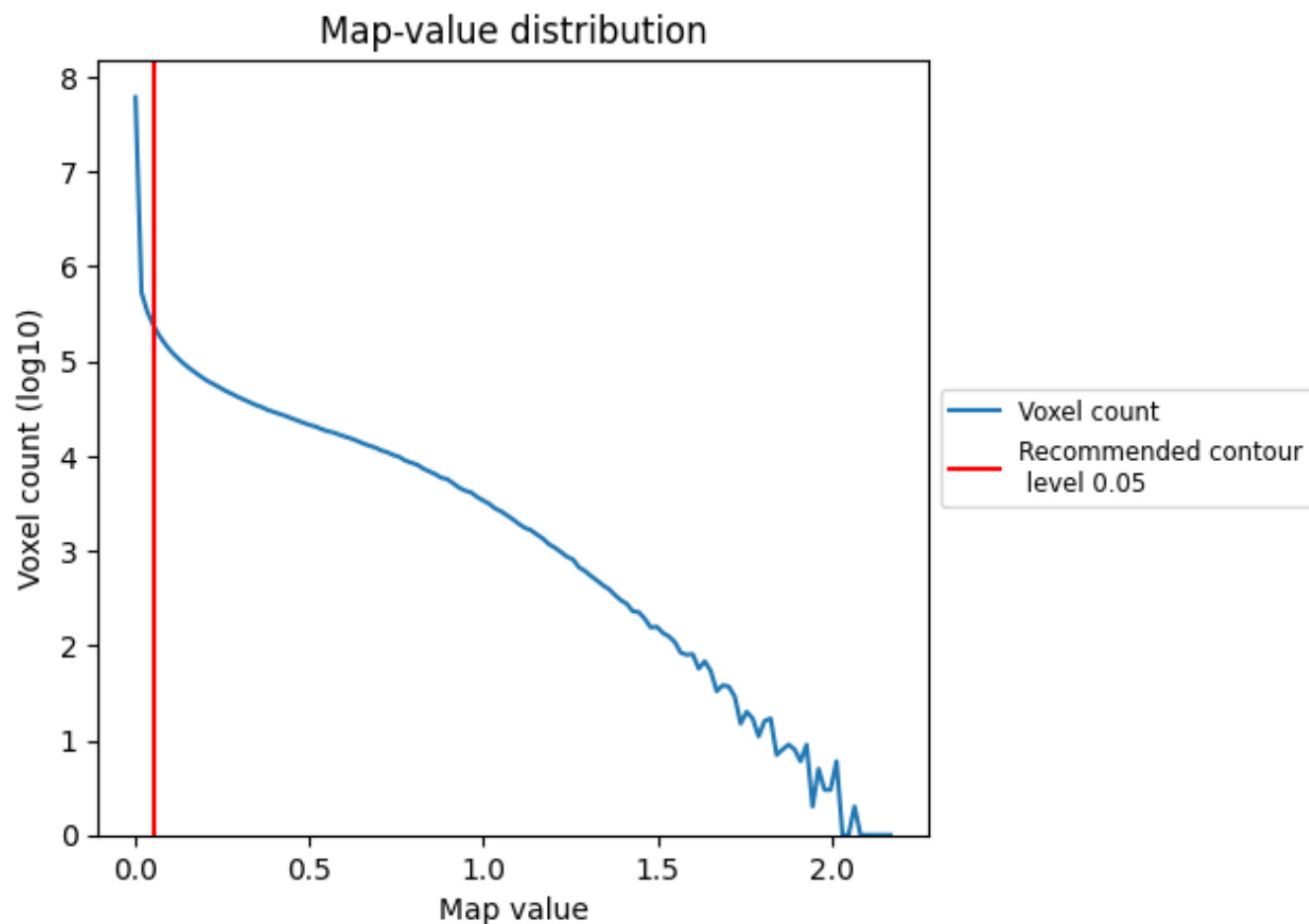


Z

7 Map analysis [i](#)

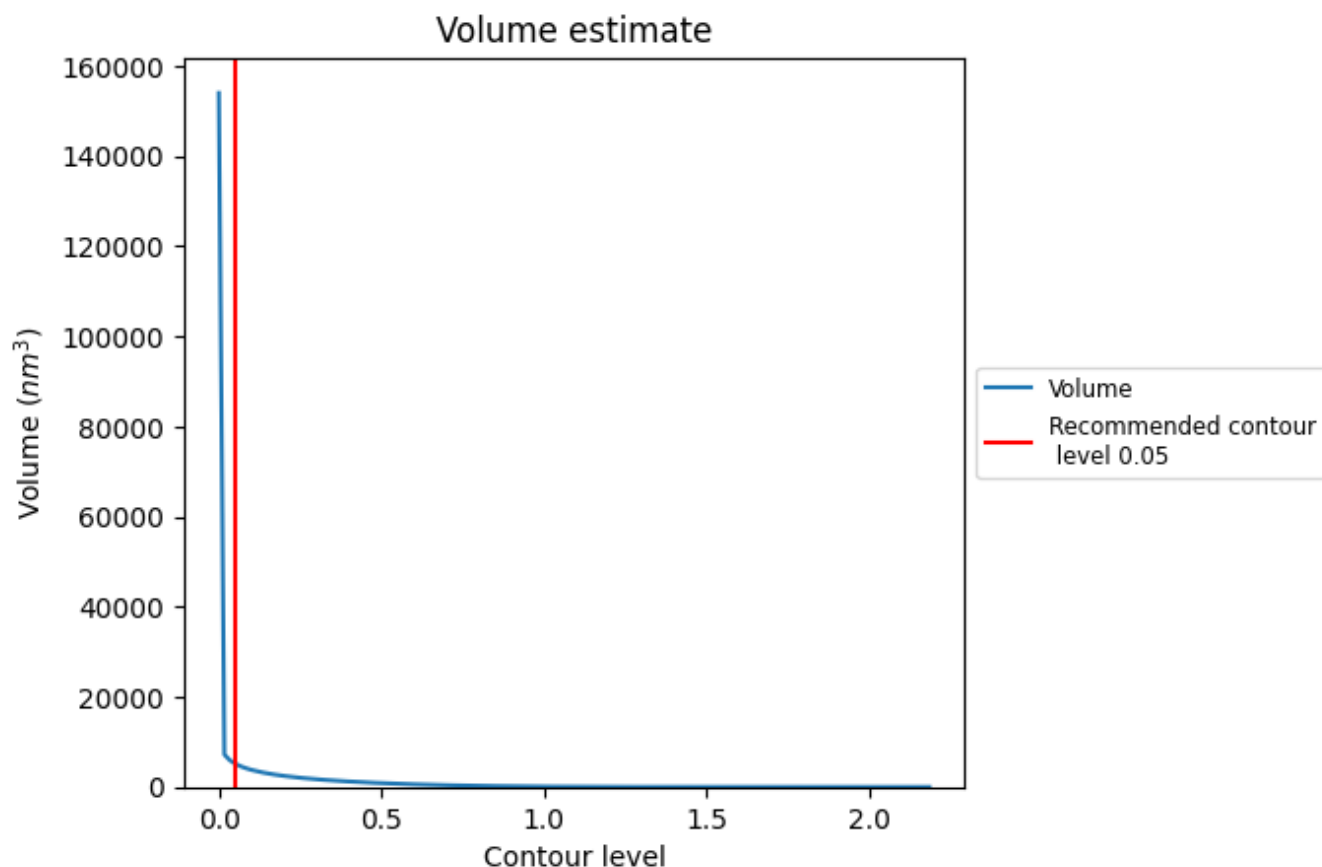
This section contains the results of statistical analysis of the map.

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.

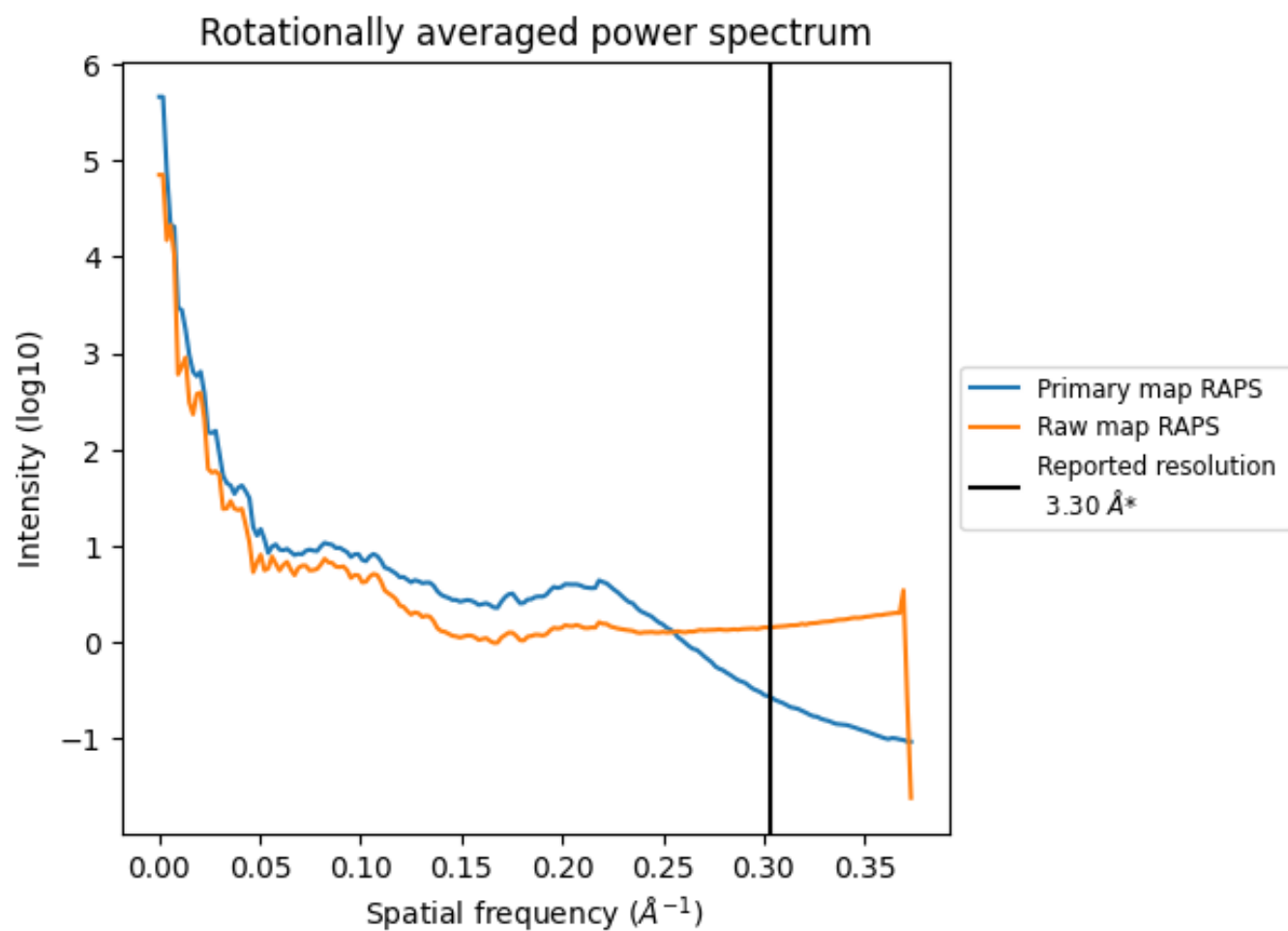
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5187 nm³; this corresponds to an approximate mass of 4686 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 ⓘ

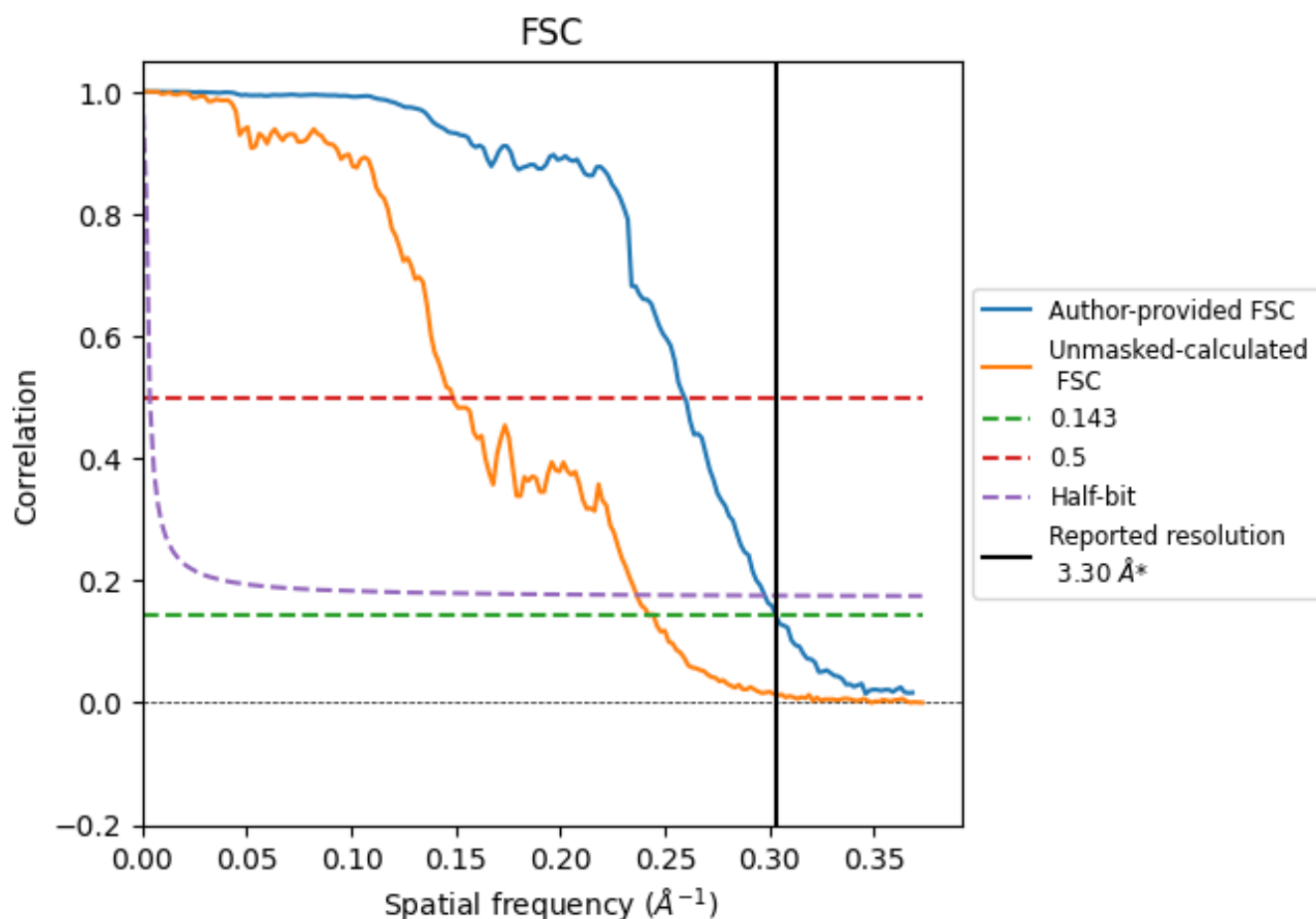


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

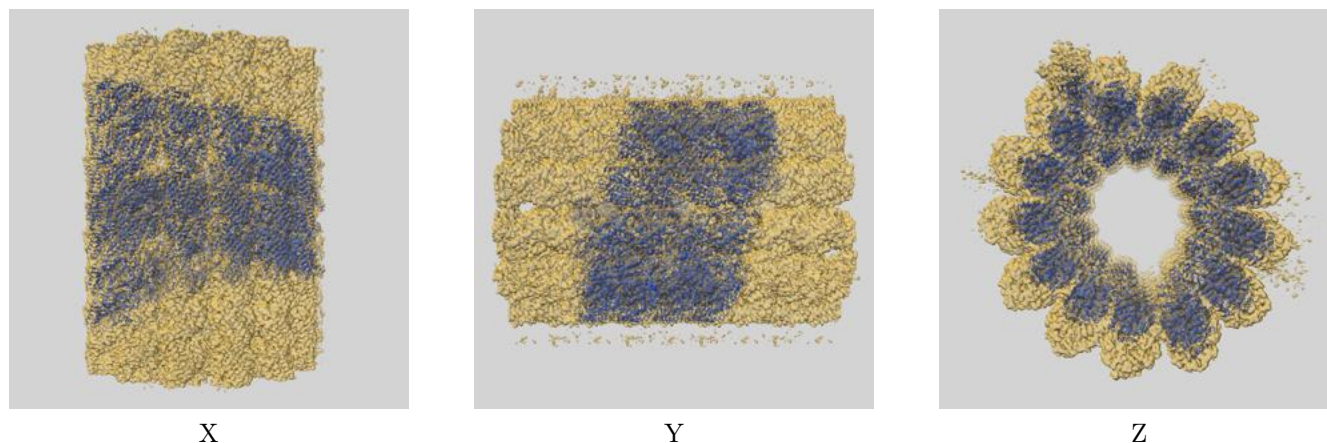
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	3.86	3.36
Unmasked-calculated*	4.13	6.73	4.23

*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 4.13 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

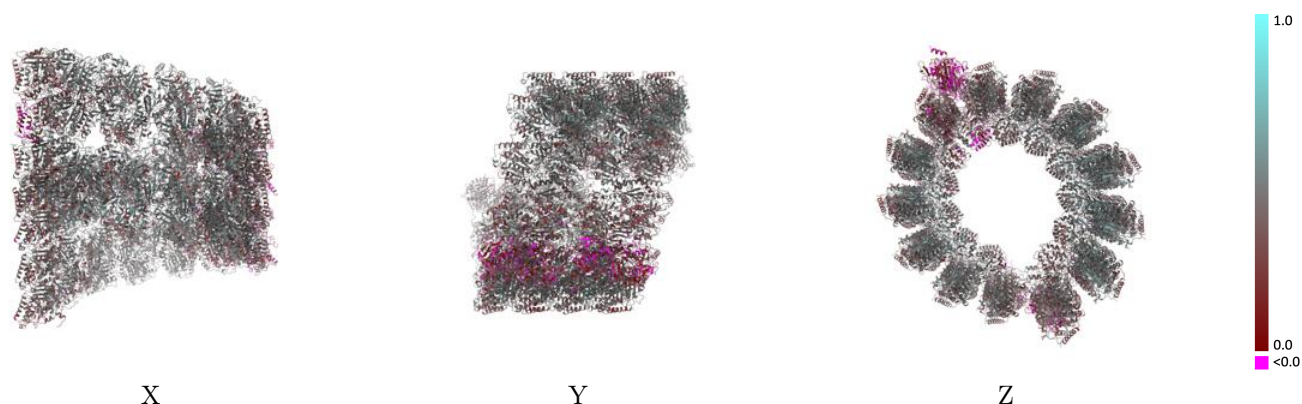
This section contains information regarding the fit between EMDB map EMD-72719 and PDB model 9YA3. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



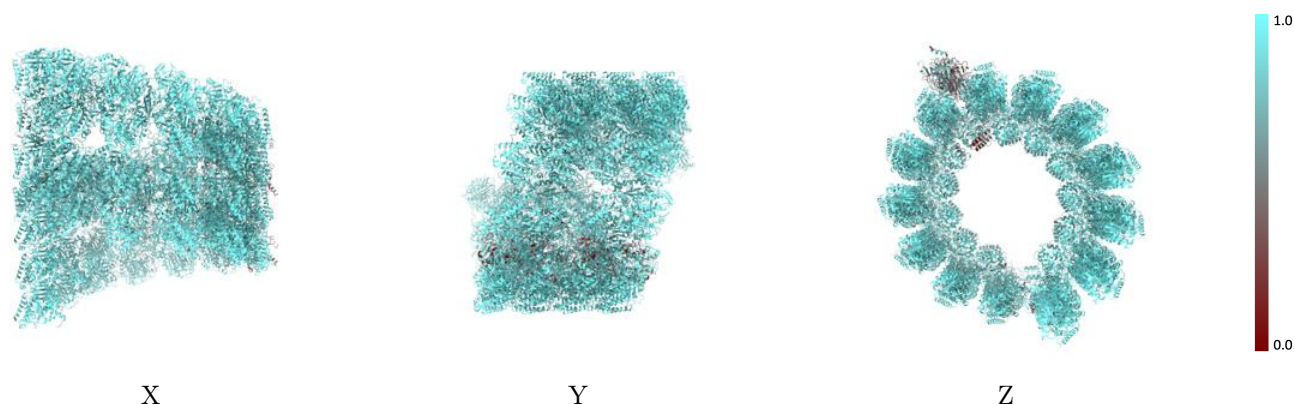
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



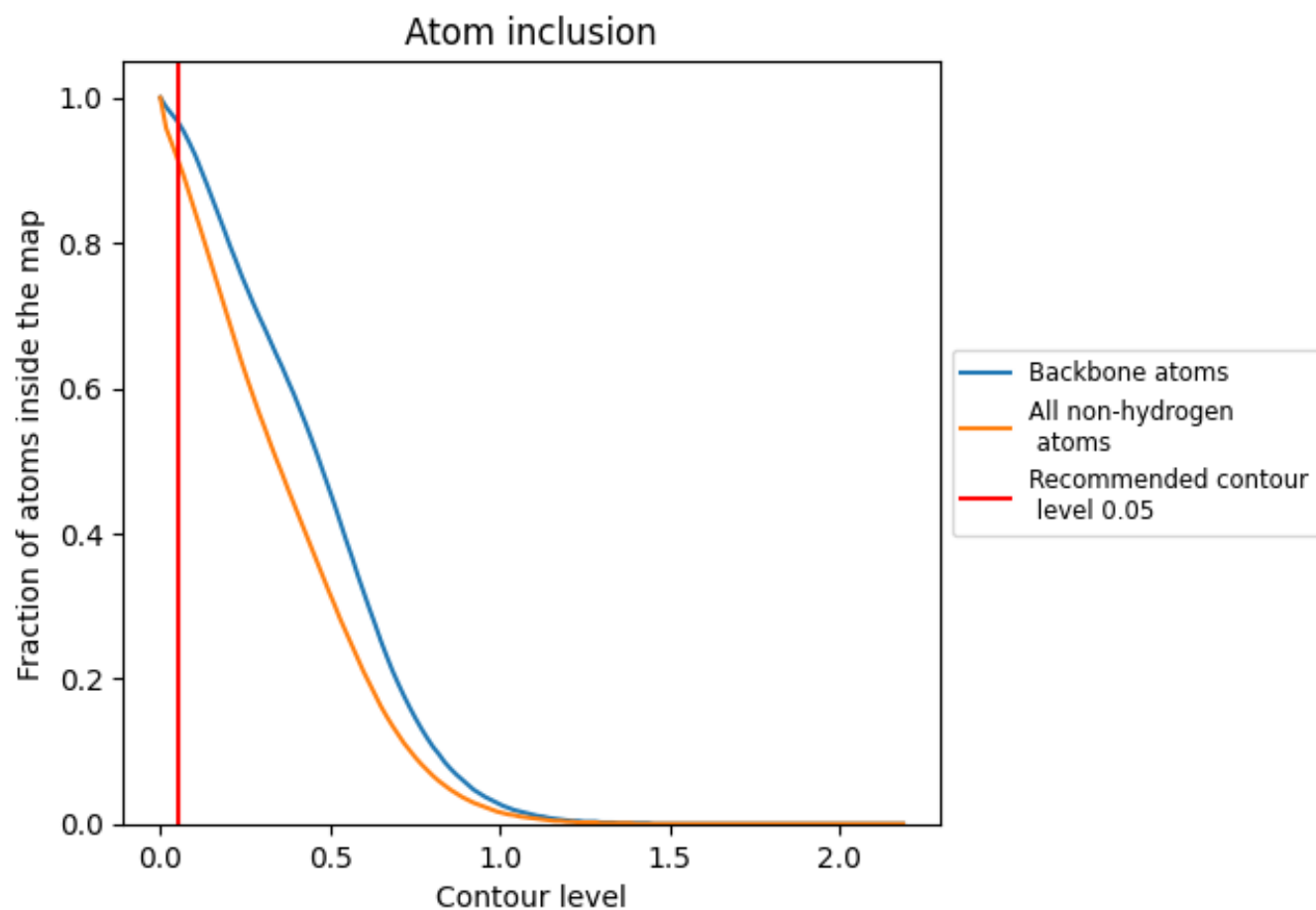
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 92% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9170	 0.4120
0	 0.8470	 0.4210
1	 0.8530	 0.4230
10	 0.9180	 0.4590
11	 0.9180	 0.4680
12	 0.9470	 0.4760
13	 0.9350	 0.4780
14	 0.9470	 0.4770
15	 0.9230	 0.4990
16	 0.9410	 0.4740
17	 0.9120	 0.4700
18	 0.9650	 0.4100
19	 0.9230	 0.4330
2	 0.9060	 0.4730
22	 0.9360	 0.4810
23	 0.9420	 0.4320
3	 0.9180	 0.4630
4	 0.8940	 0.4740
5	 0.9180	 0.4600
6	 0.9230	 0.4720
7	 0.9180	 0.4660
8	 0.7880	 0.3050
9	 0.7820	 0.2750
A	 0.6500	 0.2470
A0	 0.9120	 0.4060
A1	 0.9360	 0.3940
A2	 0.9550	 0.4070
A3	 0.9450	 0.3940
A4	 0.9430	 0.4490
A5	 0.9450	 0.4460
A6	 0.9640	 0.4440
A7	 0.9660	 0.4390
A8	 0.9390	 0.4460
A9	 0.9250	 0.4420
B	 0.6980	 0.2810



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Chain	Atom inclusion	Q-score
B0	 0.9600	 0.4450
B1	 0.9490	 0.4340
B2	 0.9410	 0.4370
B3	 0.9160	 0.4400
B4	 0.9520	 0.4380
B5	 0.9460	 0.4360
B6	 0.9530	 0.4440
B7	 0.9350	 0.4630
B8	 0.9480	 0.4480
B9	 0.9540	 0.4450
C	 0.8770	 0.3180
C0	 0.9370	 0.3360
C1	 0.8720	 0.3410
C2	 0.8960	 0.3380
C3	 0.9240	 0.3290
C4	 0.9560	 0.3900
C5	 0.9190	 0.3990
C6	 0.9250	 0.3970
C7	 0.9580	 0.3960
C8	 0.9630	 0.4350
C9	 0.9410	 0.4390
D0	 0.9260	 0.4490
D1	 0.9580	 0.4440
D2	 0.9620	 0.4590
D3	 0.9550	 0.4620
D4	 0.9370	 0.4740
D5	 0.9560	 0.4700
D6	 0.9670	 0.4650
D7	 0.9680	 0.4620
D8	 0.9430	 0.4800
D9	 0.9580	 0.4730
E	 0.7780	 0.2920
E0	 0.9600	 0.4670
E1	 0.9550	 0.4580
E2	 0.9310	 0.4700
E3	 0.9370	 0.4690
E4	 0.9690	 0.4580
E5	 0.9610	 0.4560
E6	 0.9500	 0.4700
E7	 0.9450	 0.4740
E8	 0.9480	 0.3900
E9	 0.8830	 0.2960

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Chain	Atom inclusion	Q-score
F	 0.8360	 0.3380
F0	 0.9300	 0.3890
F1	 0.9210	 0.4150
G	 0.8860	 0.3530
H	 0.5310	 0.1180
I	 0.4610	 0.0870
J	 0.5580	 0.1260
K	 0.5050	 0.1020
a	 0.8850	 0.3930
b	 0.9240	 0.3980
c	 0.9140	 0.4570
d	 0.9210	 0.4250
e	 0.9190	 0.4560
f	 0.9420	 0.4500
g	 0.9060	 0.4440
h	 0.9360	 0.4420
i	 0.8730	 0.3100
j	 0.8890	 0.3200
k	 0.8430	 0.3060
l	 0.8140	 0.2870
m	 0.8040	 0.3000
n	 0.7860	 0.3100
o	 0.9360	 0.4220
p	 0.9160	 0.4500
q	 0.9420	 0.4460
r	 0.9260	 0.4640
s	 0.9500	 0.4680
t	 0.9390	 0.4830
u	 0.9400	 0.4460
v	 0.9170	 0.4430
w	 0.9040	 0.3460
x	 0.8780	 0.3570