



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 07:02 PM UTC

PDB ID : 9EOK / pdb_00009eok
EMDB ID : EMD-19862
Title : Minus end of the vertebrate gamma-tubulin ring complex-capped microtubule
Authors : Vermeulen, B.J.A.; Pfeffer, S.
Deposited on : 2024-03-15
Resolution : 23.00 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:

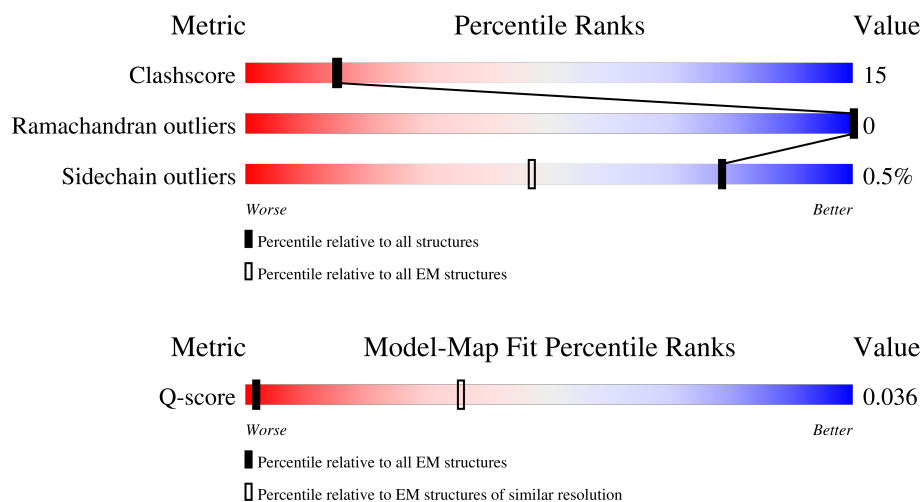
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 23.00 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	17 (22.90 - 23.50)

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	A	450	58% 89% 6% .
1	C	450	24% 88% 7% .
1	D	450	20% 85% 10% .
1	E	450	40% 84% 11% .

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Mol	Chain	Length	Quality of chain
1	G	450	
1	H	450	
1	I	450	
1	J	450	
1	K	450	
1	L	450	
1	M	450	
1	N	450	
1	O	450	
1	P	450	
1	c	450	
1	d	450	
1	e	450	
1	f	450	
1	g	450	
1	h	450	
1	i	450	
1	j	450	
1	k	450	
2	B	445	
2	F	445	
2	Q	445	
2	R	445	
2	S	445	
2	T	445	

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Mol	Chain	Length	Quality of chain
2	U	445	
2	V	445	
2	W	445	
2	X	445	
2	Y	445	
2	Z	445	
2	a	445	
2	b	445	
2	o	445	
2	p	445	
2	q	445	
2	r	445	
2	s	445	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 143457 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 Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	430	Total 3365	C 2127	N 574	O 641	S 23	0	0
1	C	430	Total 3365	C 2127	N 574	O 641	S 23	0	0
1	D	430	Total 3365	C 2127	N 574	O 641	S 23	0	0
1	E	430	Total 3365	C 2127	N 574	O 641	S 23	0	0
1	G	430	Total 3365	C 2127	N 574	O 641	S 23	0	0
1	H	430	Total 3365	C 2127	N 574	O 641	S 23	0	0
1	I	430	Total 3365	C 2127	N 574	O 641	S 23	0	0
1	J	430	Total 3365	C 2127	N 574	O 641	S 23	0	0
1	K	430	Total 3365	C 2127	N 574	O 641	S 23	0	0
1	L	430	Total 3365	C 2127	N 574	O 641	S 23	0	0
1	M	430	Total 3365	C 2127	N 574	O 641	S 23	0	0
1	N	430	Total 3365	C 2127	N 574	O 641	S 23	0	0
1	O	430	Total 3365	C 2127	N 574	O 641	S 23	0	0
1	P	430	Total 3365	C 2127	N 574	O 641	S 23	0	0
1	c	430	Total 3365	C 2127	N 574	O 641	S 23	0	0
1	d	430	Total 3365	C 2127	N 574	O 641	S 23	0	0
1	e	430	Total 3365	C 2127	N 574	O 641	S 23	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	f	430	Total	C	N	O	S	0	0
			3365	2127	574	641	23		
1	g	430	Total	C	N	O	S	0	0
			3365	2127	574	641	23		
1	h	430	Total	C	N	O	S	0	0
			3365	2127	574	641	23		
1	i	430	Total	C	N	O	S	0	0
			3365	2127	574	641	23		
1	j	430	Total	C	N	O	S	0	0
			3365	2127	574	641	23		
1	k	430	Total	C	N	O	S	0	0
			3365	2127	574	641	23		

- Molecule 2 is a protein called Tubulin beta-4 chain.

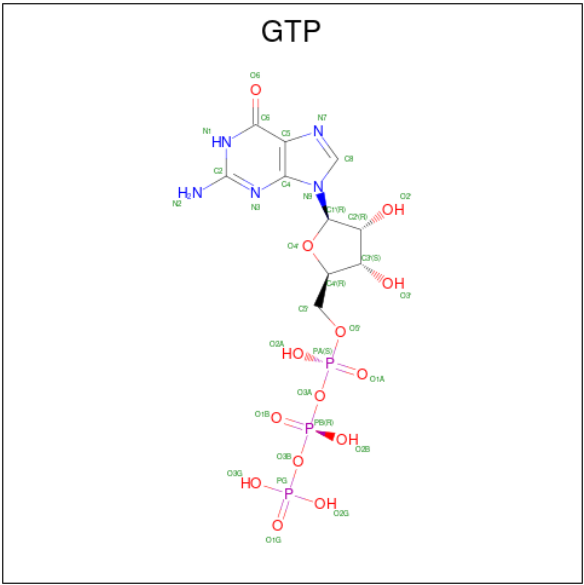
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	F	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	Q	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	R	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	S	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	T	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	U	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	V	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	W	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	X	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	Y	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	Z	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	a	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	o	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	p	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	q	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	r	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	s	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	C	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	D	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	E	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	G	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
3	H	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	I	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	J	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	K	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	L	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	M	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	N	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	O	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	P	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	c	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	d	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	e	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	f	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	g	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	h	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	i	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	j	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	k	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	

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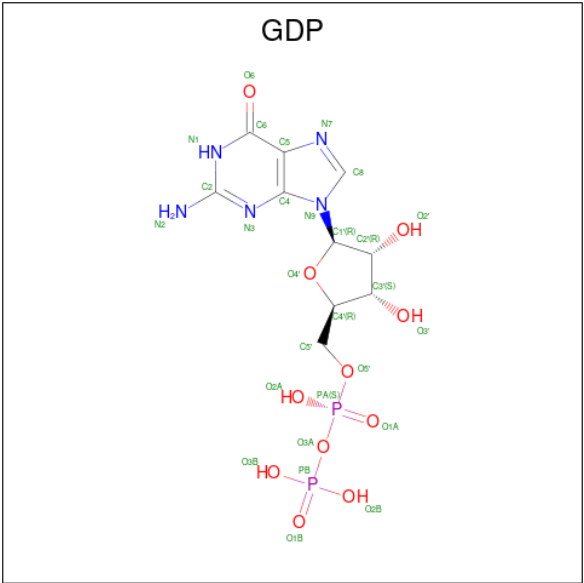
Mol	Chain	Residues	Atoms		AltConf
4	C	1	Total 1	Mg 1	0
4	D	1	Total 1	Mg 1	0
4	E	1	Total 1	Mg 1	0
4	G	1	Total 1	Mg 1	0
4	H	1	Total 1	Mg 1	0
4	I	1	Total 1	Mg 1	0
4	J	1	Total 1	Mg 1	0
4	K	1	Total 1	Mg 1	0
4	L	1	Total 1	Mg 1	0
4	M	1	Total 1	Mg 1	0
4	N	1	Total 1	Mg 1	0
4	O	1	Total 1	Mg 1	0
4	P	1	Total 1	Mg 1	0
4	c	1	Total 1	Mg 1	0
4	d	1	Total 1	Mg 1	0
4	e	1	Total 1	Mg 1	0
4	f	1	Total 1	Mg 1	0
4	g	1	Total 1	Mg 1	0
4	h	1	Total 1	Mg 1	0
4	i	1	Total 1	Mg 1	0
4	j	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
4	k	1	Total	Mg	0
			1	1	

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



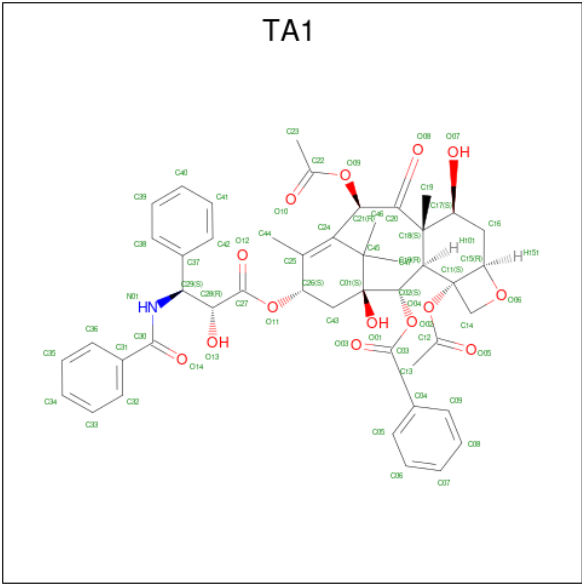
Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	F	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	Q	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	R	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	S	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	T	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	U	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	V	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	W	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	X	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
5	Y	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	Z	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	a	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	b	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	o	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	p	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	q	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	r	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	s	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 6 is TAXOL (CCD ID: TA1) (formula: C₄₇H₅₁NO₁₄).



Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			62	47	1	14	
6	F	1	Total	C	N	O	0
			62	47	1	14	

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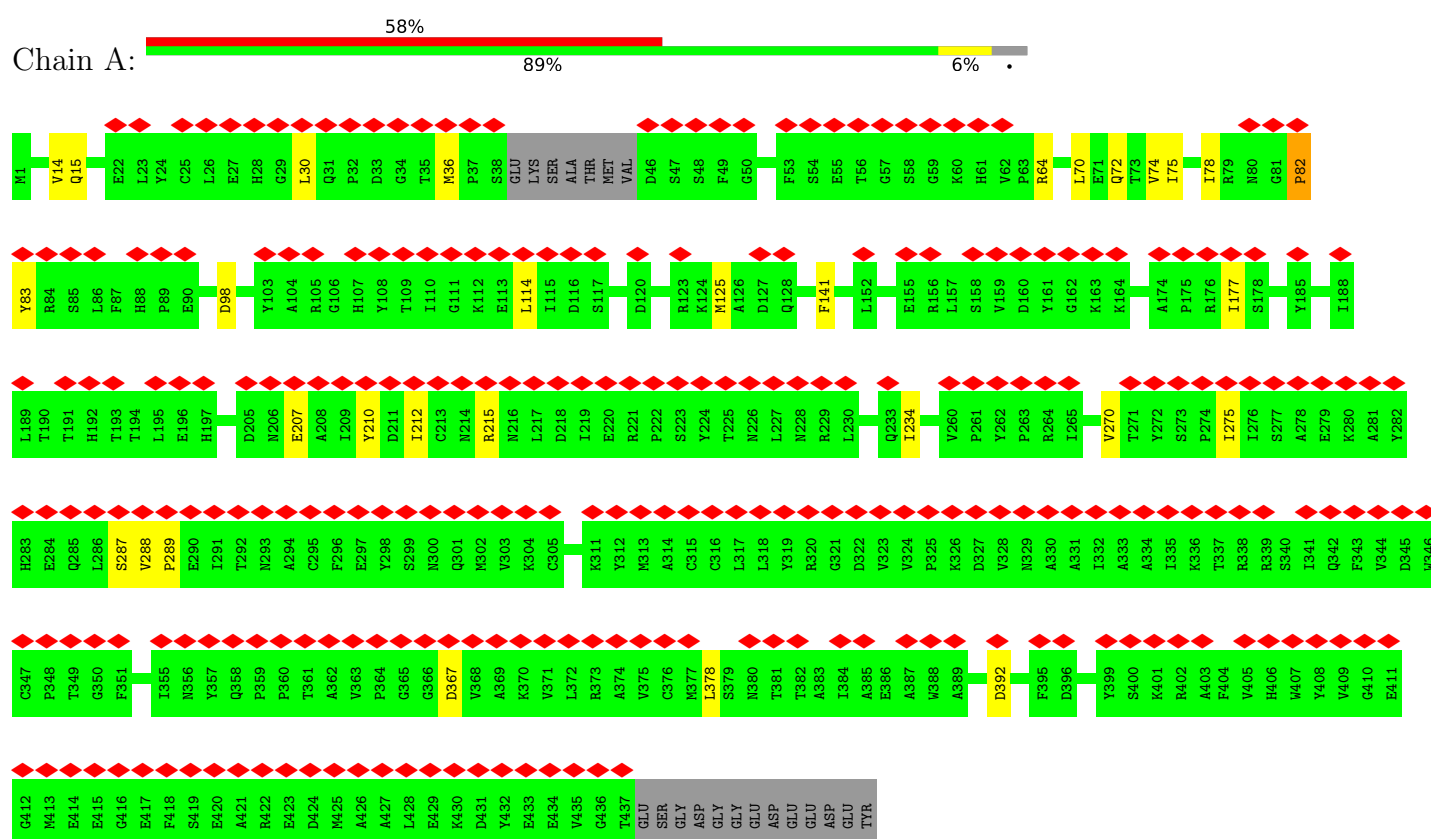
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Mol	Chain	Residues	Atoms				AltConf
6	Q	1	Total	C	N	O	0
			62	47	1	14	
6	R	1	Total	C	N	O	0
			62	47	1	14	
6	S	1	Total	C	N	O	0
			62	47	1	14	
6	T	1	Total	C	N	O	0
			62	47	1	14	
6	U	1	Total	C	N	O	0
			62	47	1	14	
6	V	1	Total	C	N	O	0
			62	47	1	14	
6	W	1	Total	C	N	O	0
			62	47	1	14	
6	X	1	Total	C	N	O	0
			62	47	1	14	
6	Y	1	Total	C	N	O	0
			62	47	1	14	
6	Z	1	Total	C	N	O	0
			62	47	1	14	
6	a	1	Total	C	N	O	0
			62	47	1	14	
6	b	1	Total	C	N	O	0
			62	47	1	14	
6	o	1	Total	C	N	O	0
			62	47	1	14	
6	p	1	Total	C	N	O	0
			62	47	1	14	
6	q	1	Total	C	N	O	0
			62	47	1	14	
6	r	1	Total	C	N	O	0
			62	47	1	14	
6	s	1	Total	C	N	O	0
			62	47	1	14	

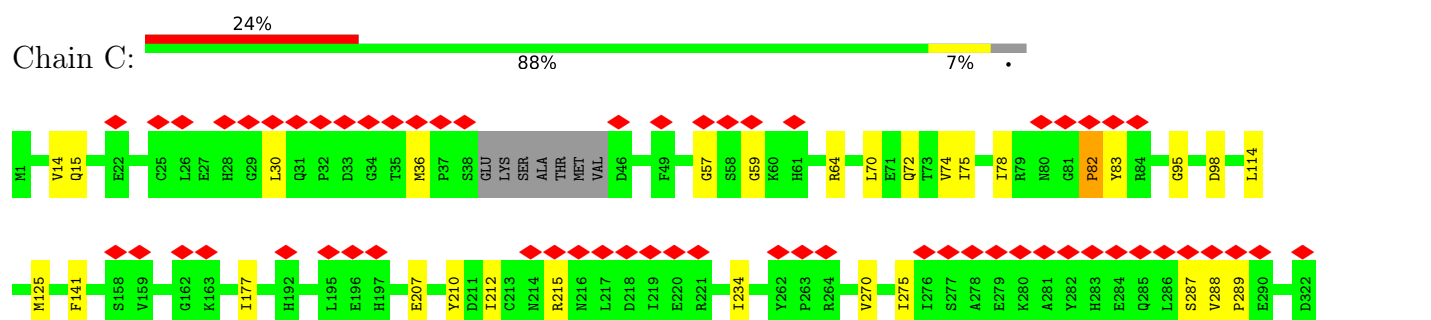
3 Residue-property plots

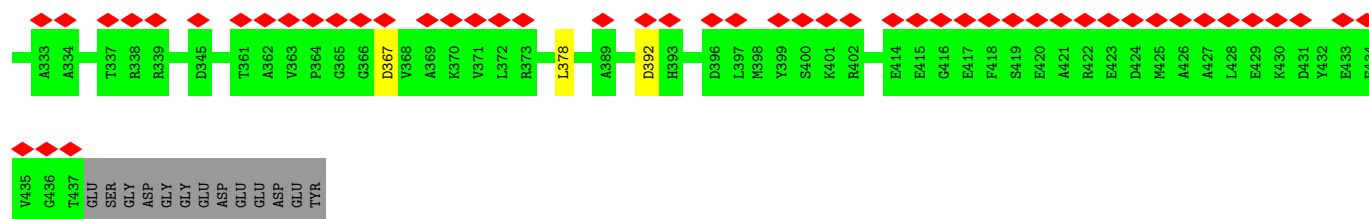
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Tubulin alpha chain

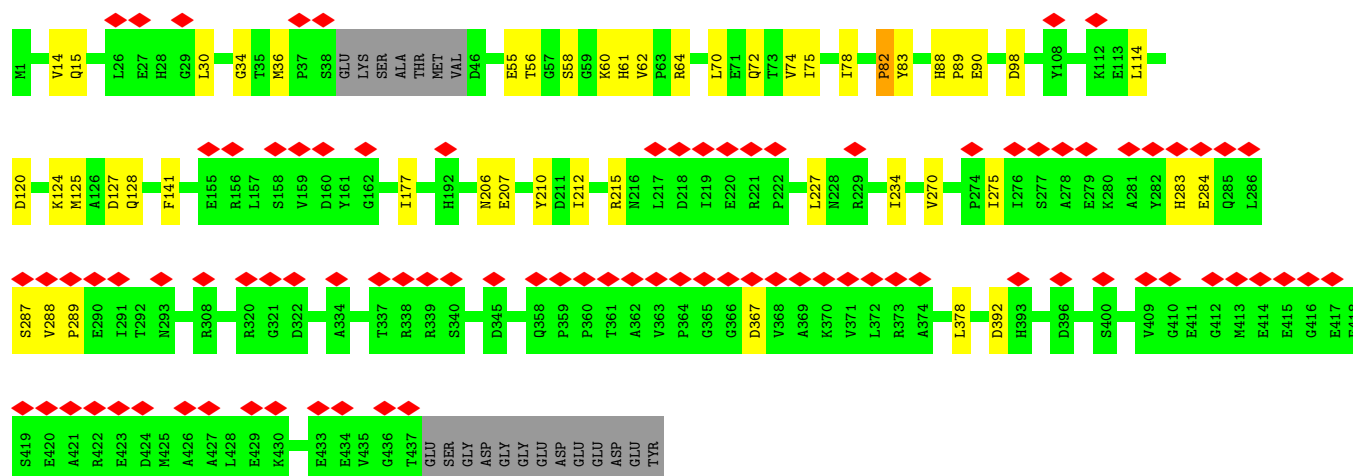
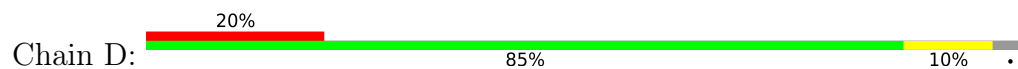


• Molecule 1: Tubulin alpha chain

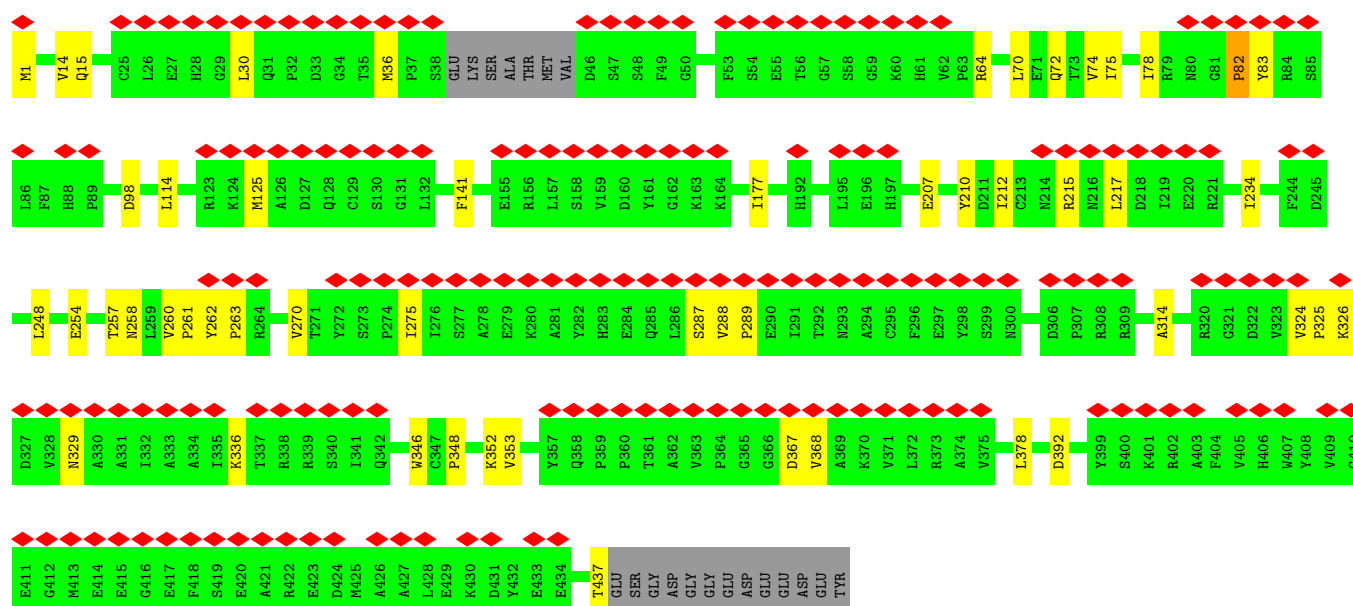
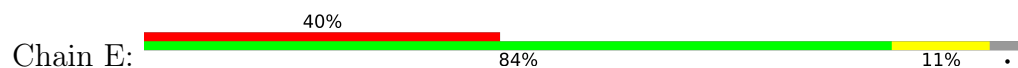




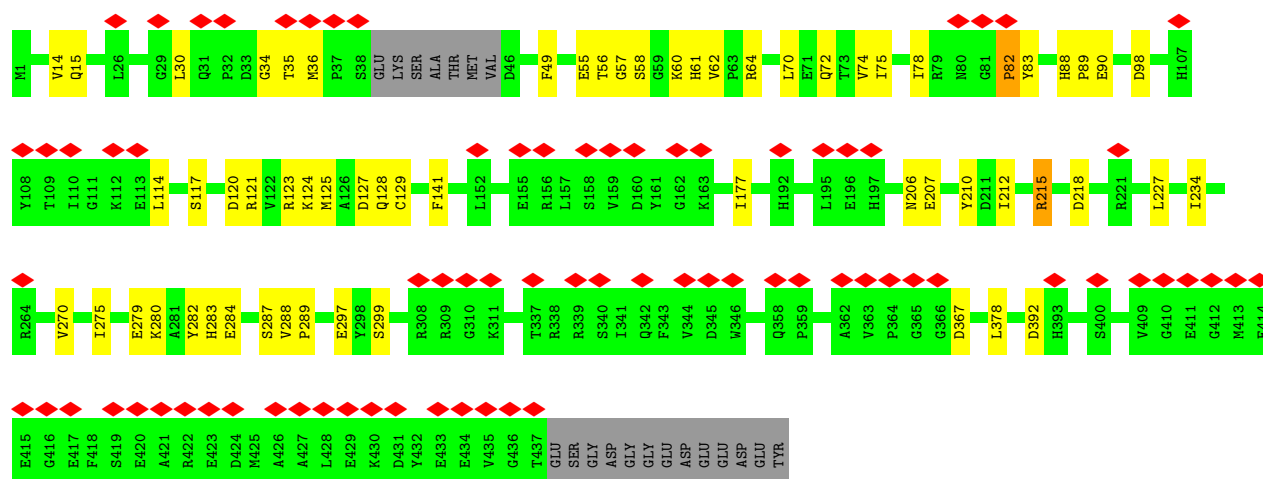
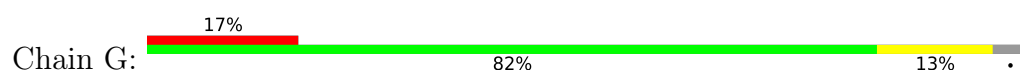
• Molecule 1: Tubulin alpha chain



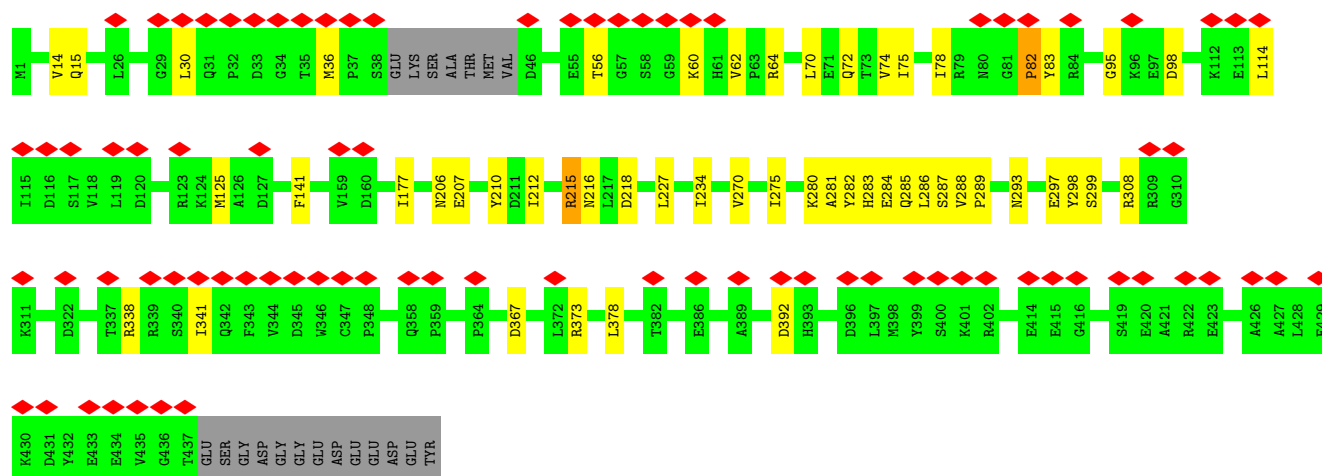
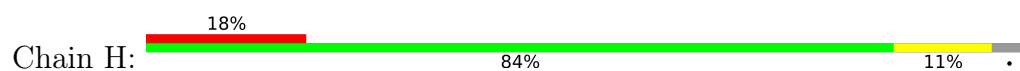
• Molecule 1: Tubulin alpha chain



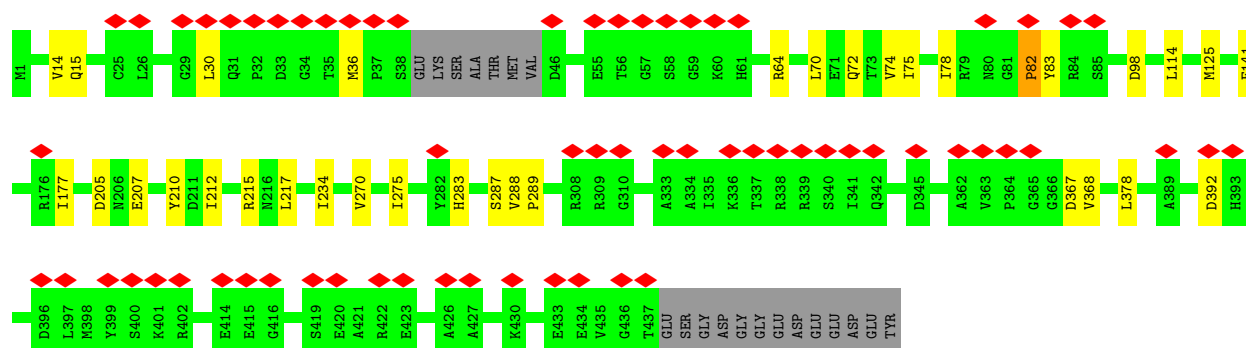
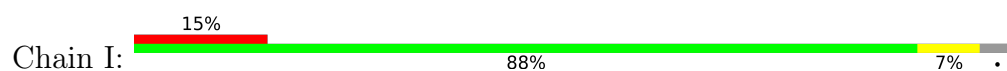
• Molecule 1: Tubulin alpha chain



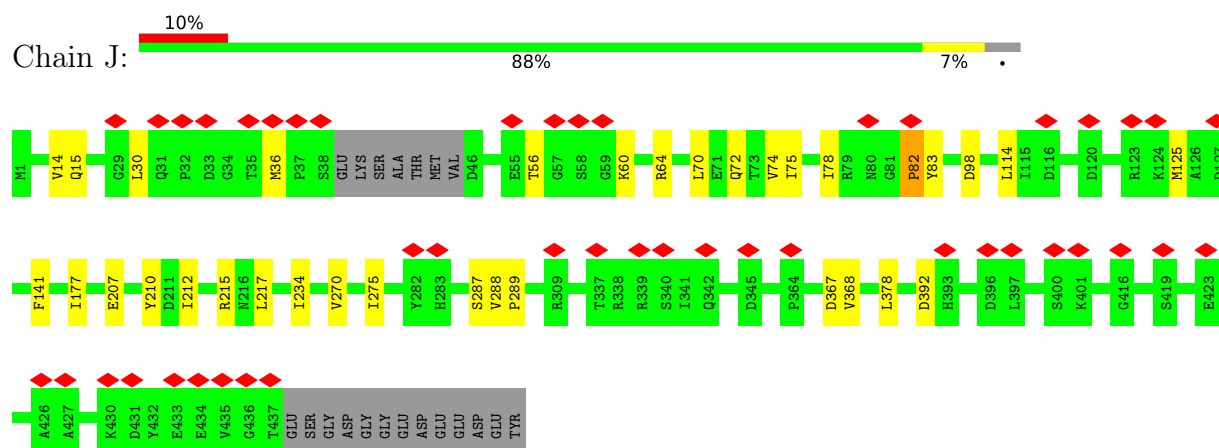
• Molecule 1: Tubulin alpha chain



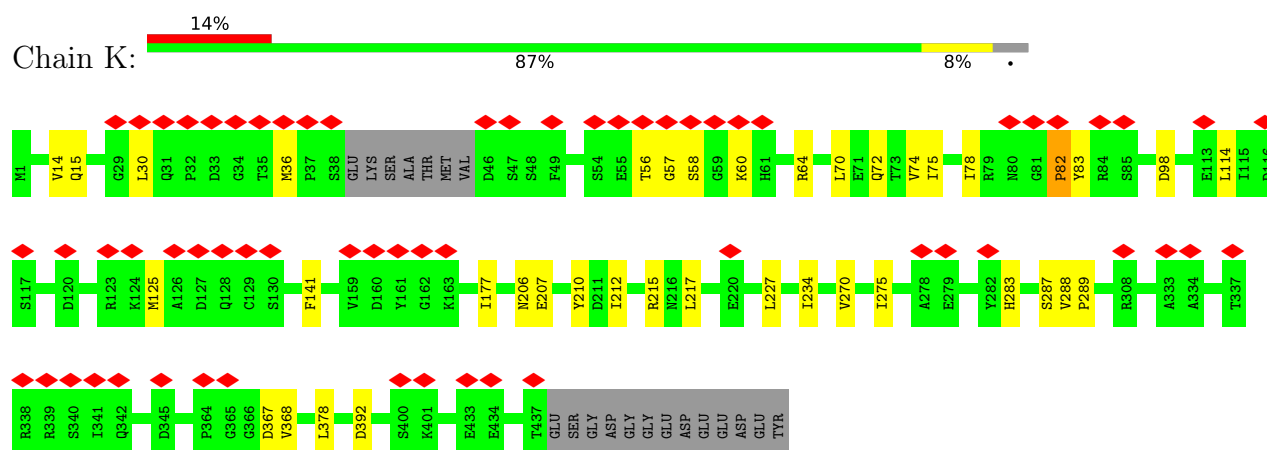
• Molecule 1: Tubulin alpha chain



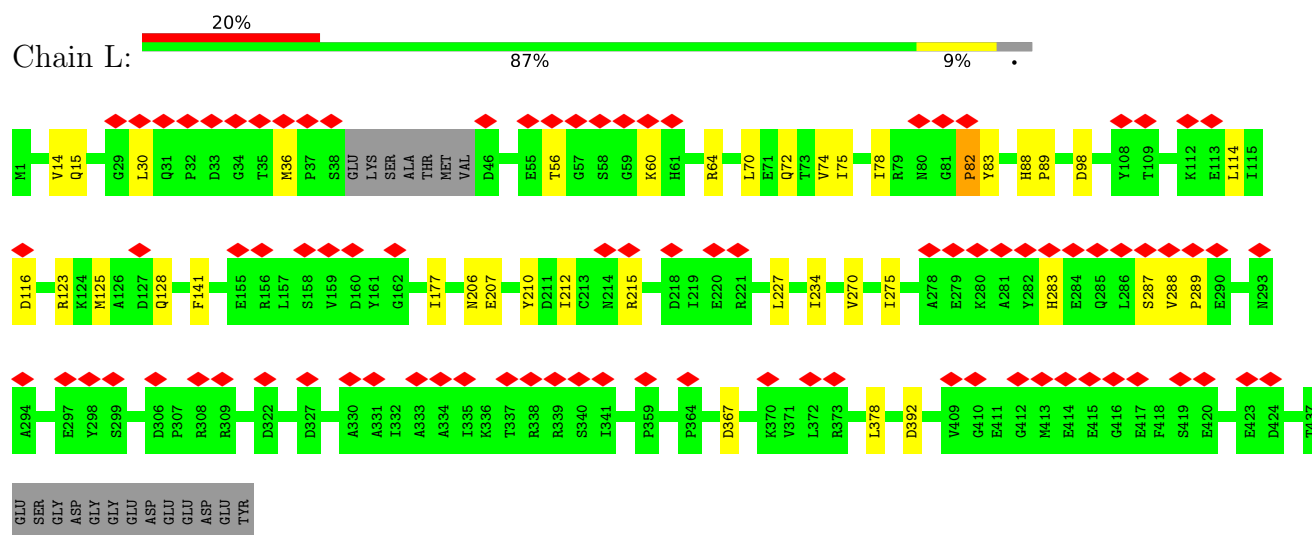
• Molecule 1: Tubulin alpha chain



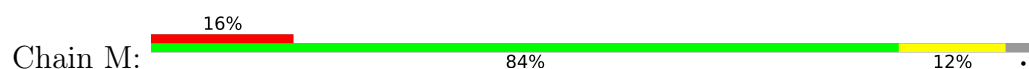
• Molecule 1: Tubulin alpha chain

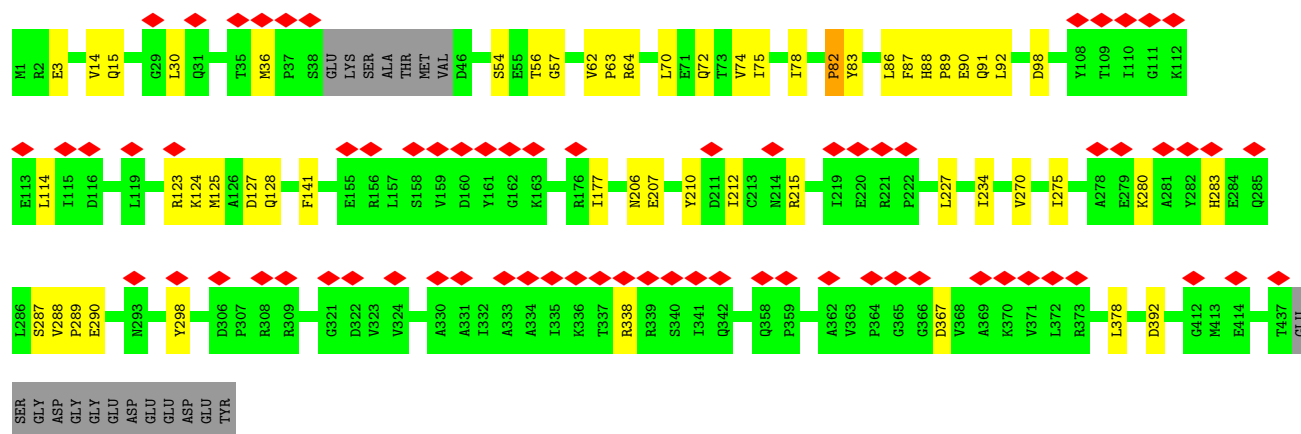


• Molecule 1: Tubulin alpha chain

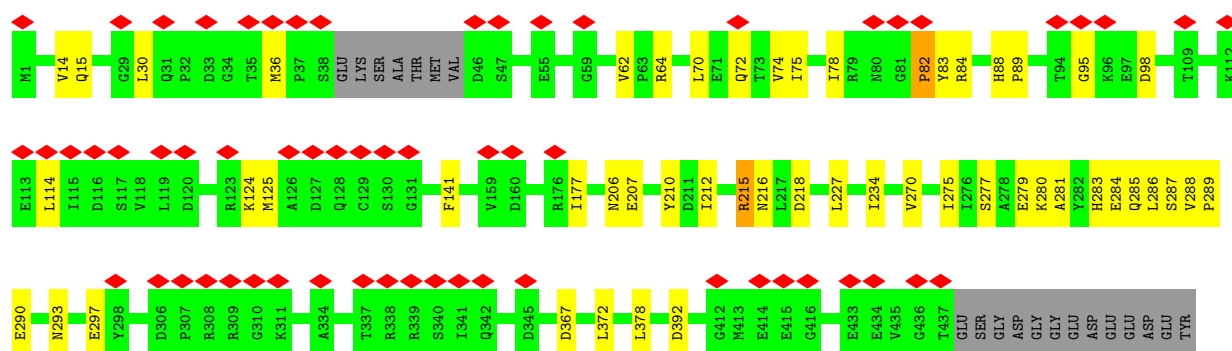
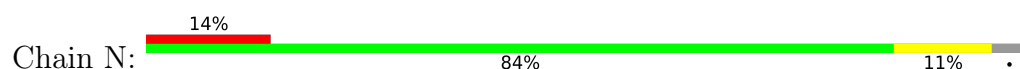


• Molecule 1: Tubulin alpha chain

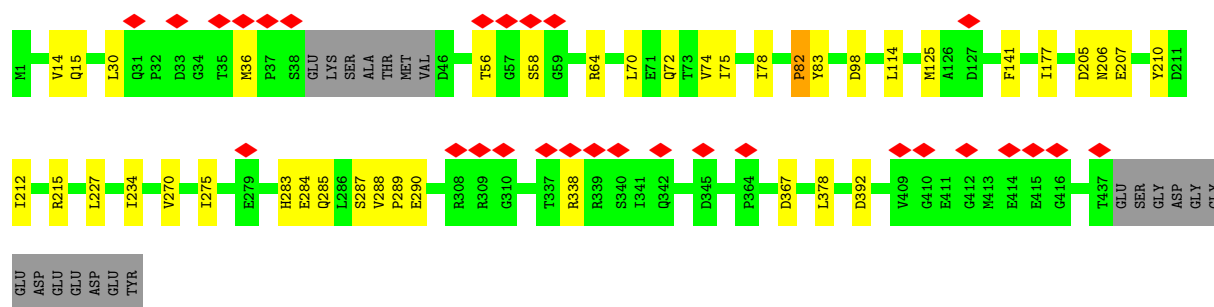
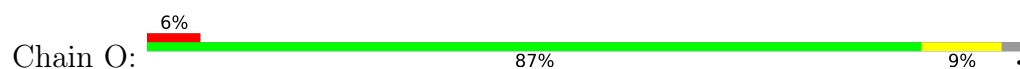




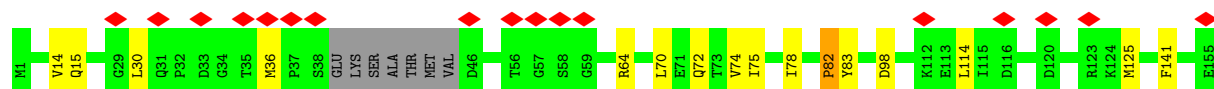
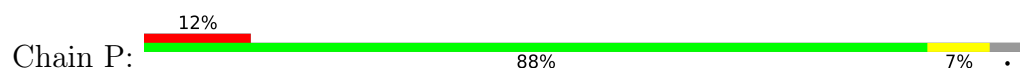
• Molecule 1: Tubulin alpha chain

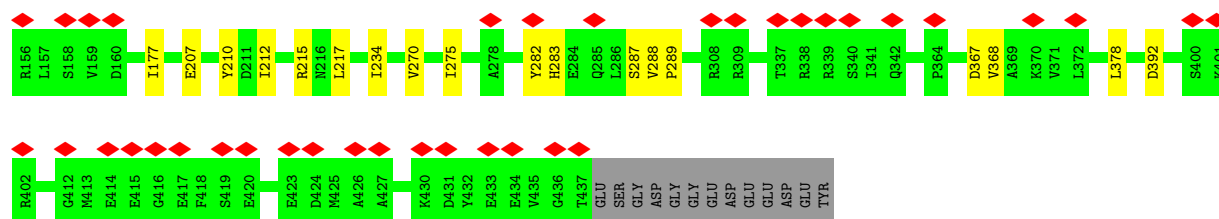


• Molecule 1: Tubulin alpha chain

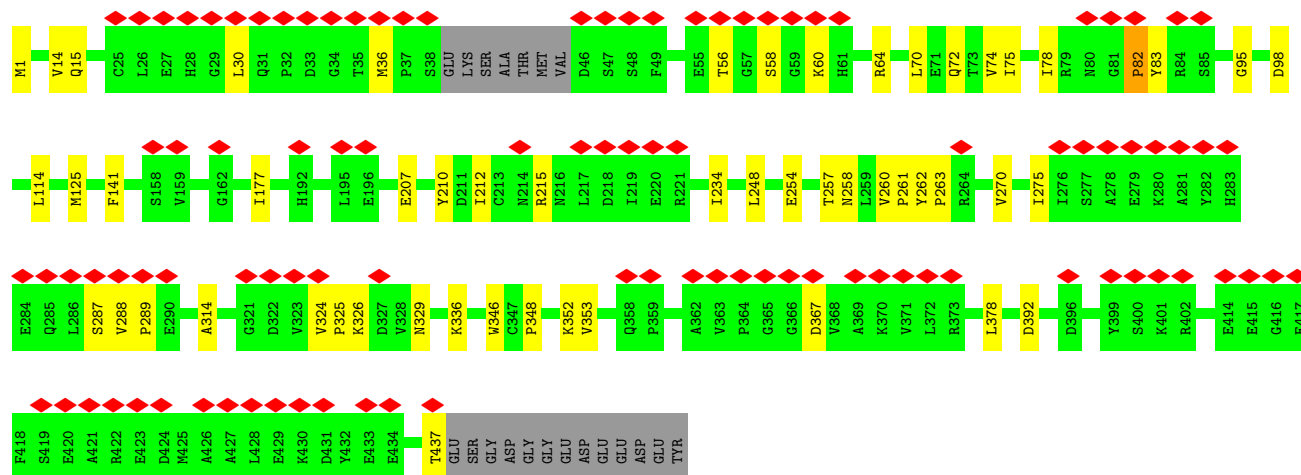
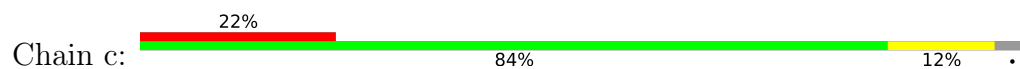


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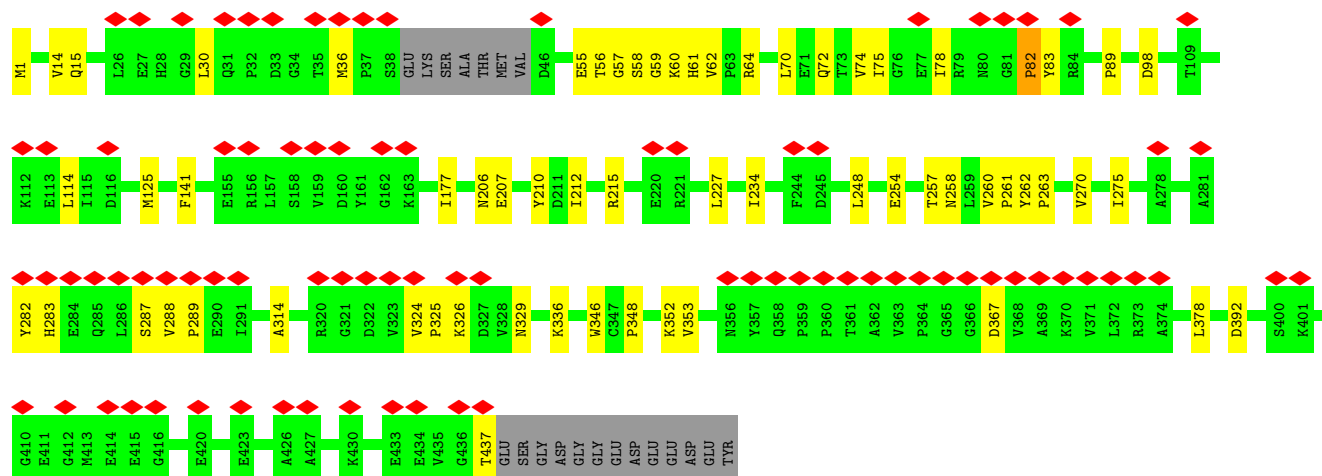
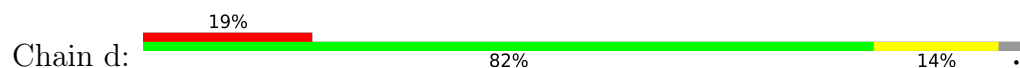




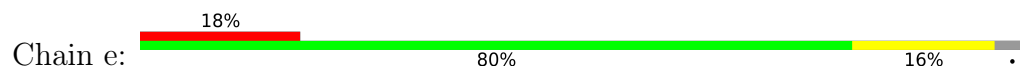
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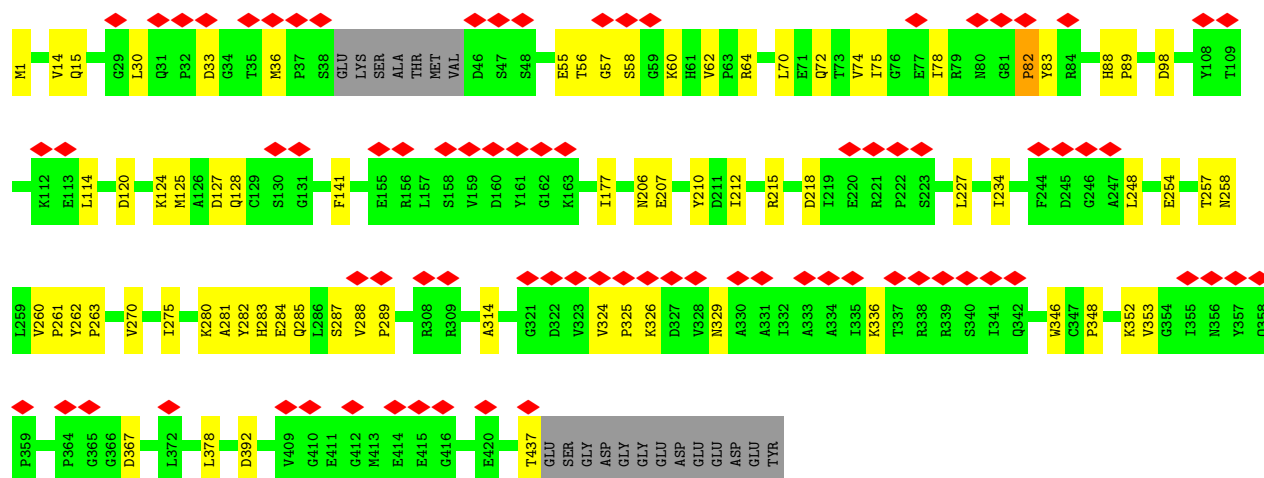


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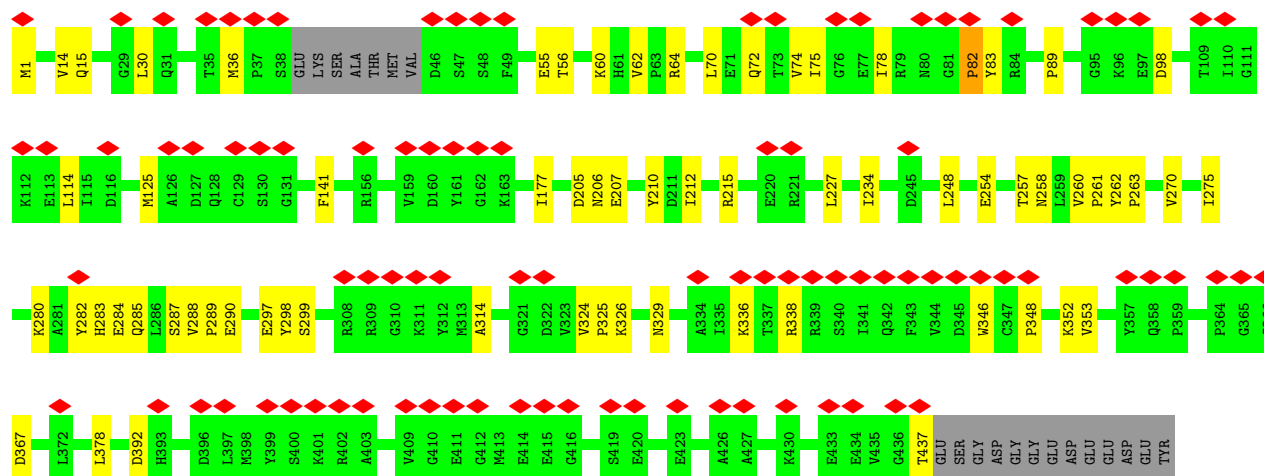
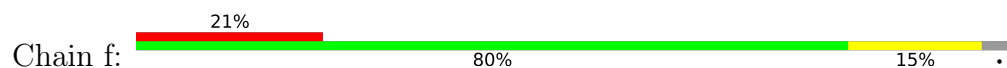


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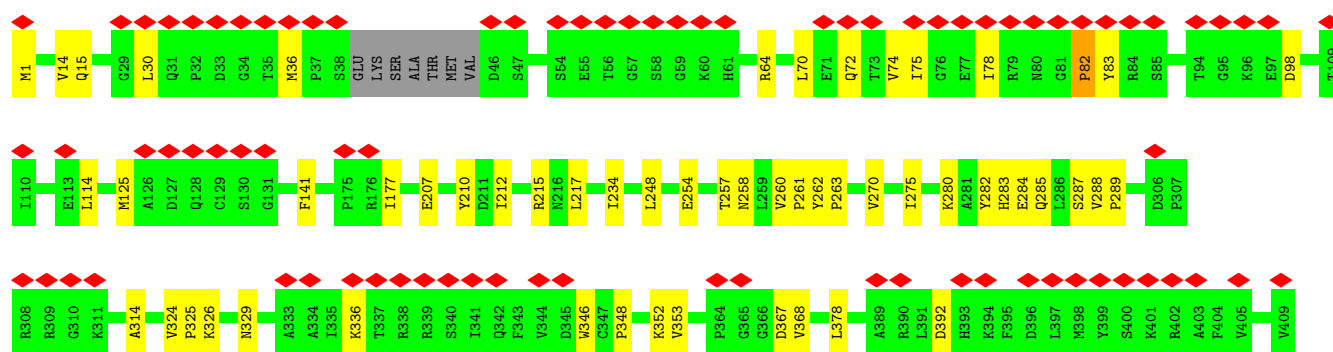
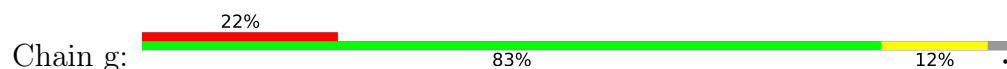


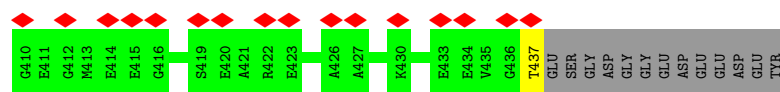


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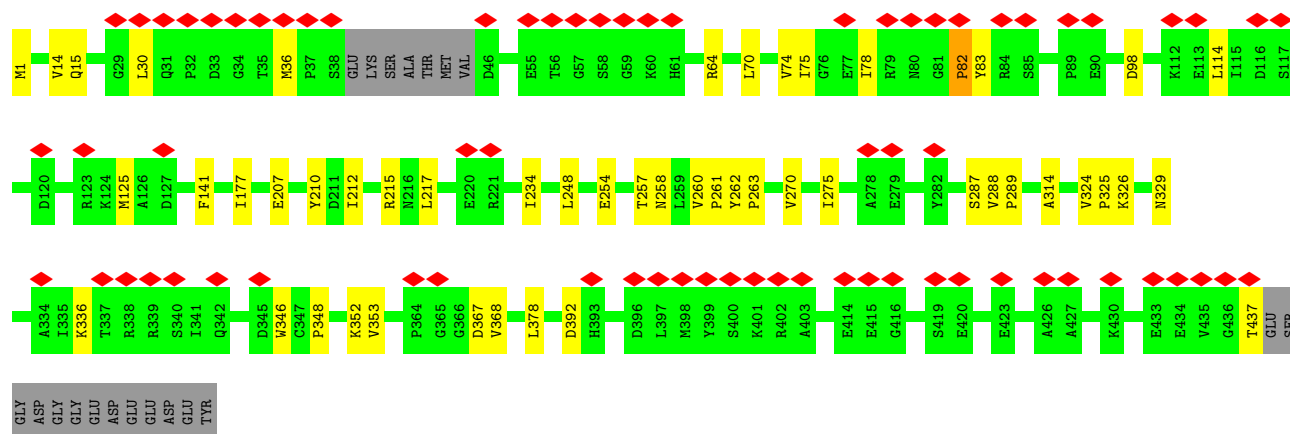
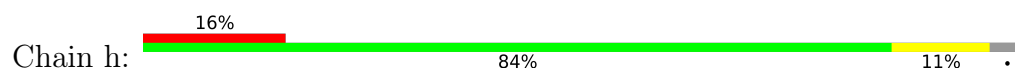


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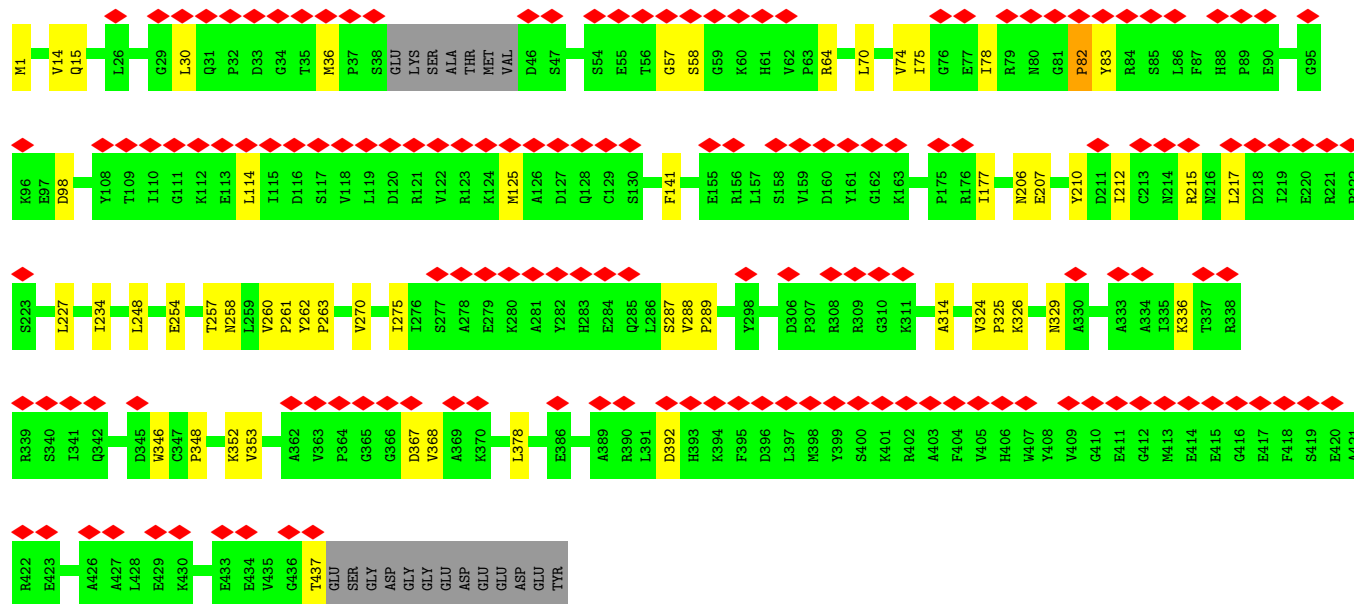
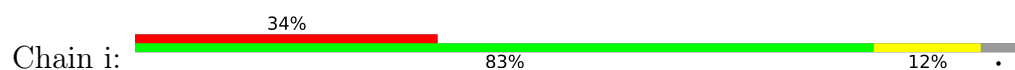




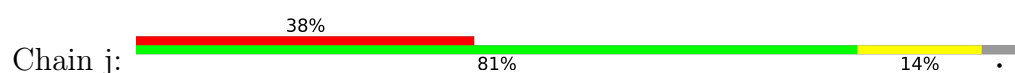
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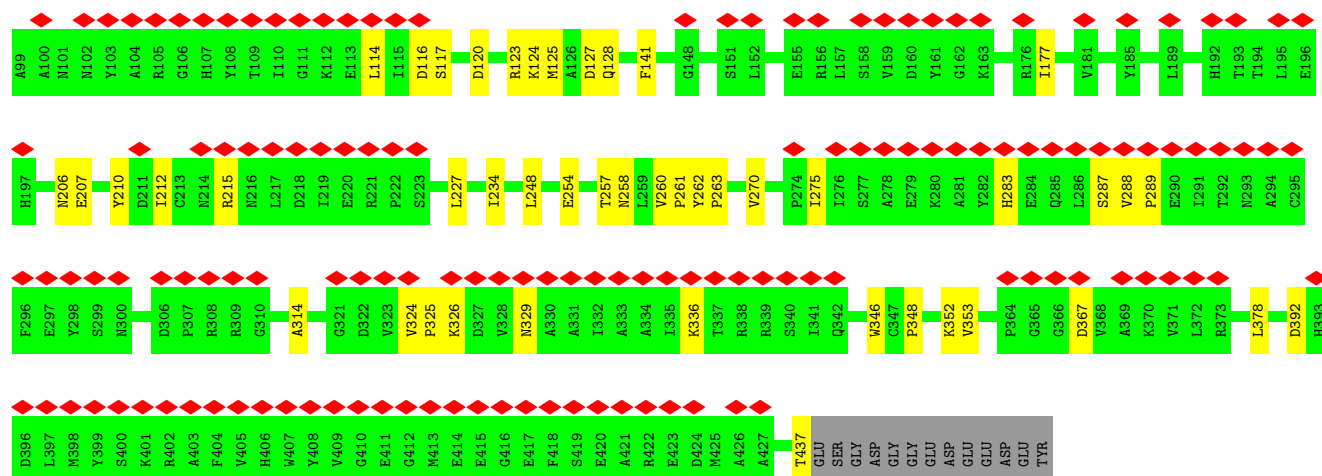


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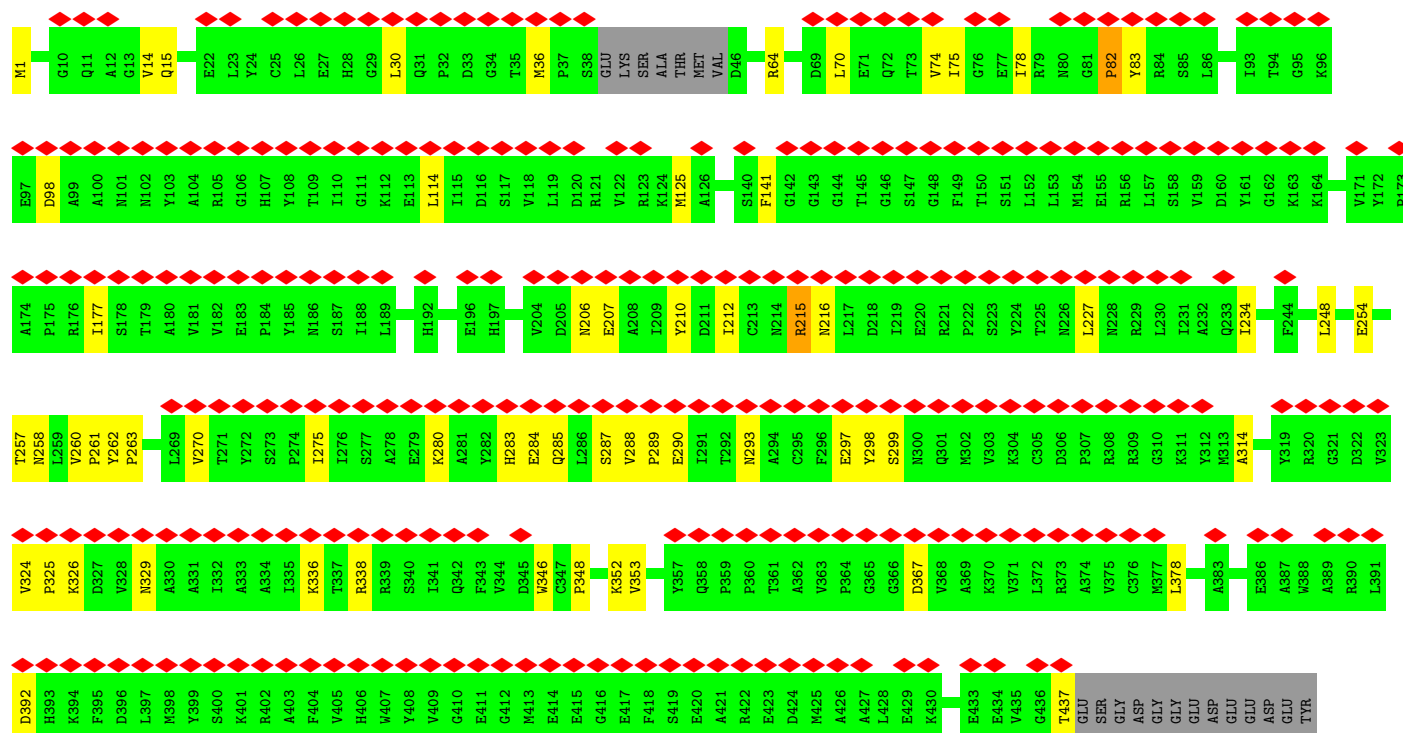
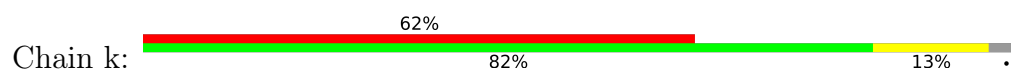


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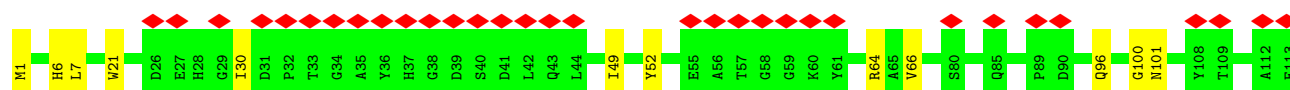
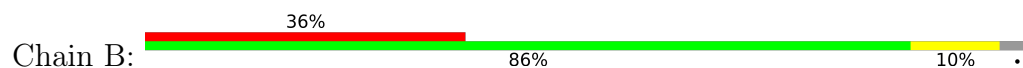


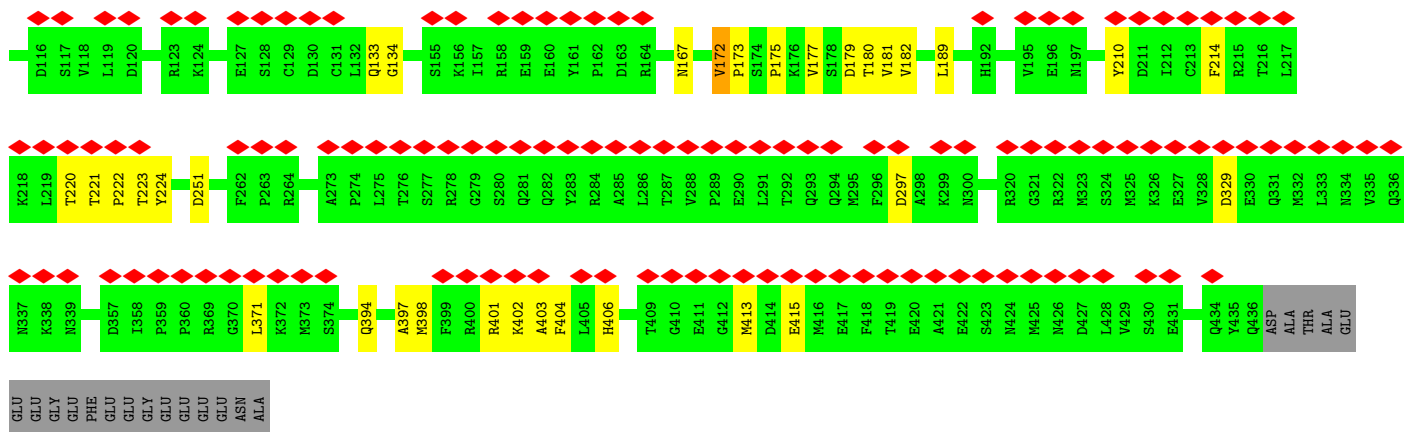


• Molecule 1: Tubulin alpha chain

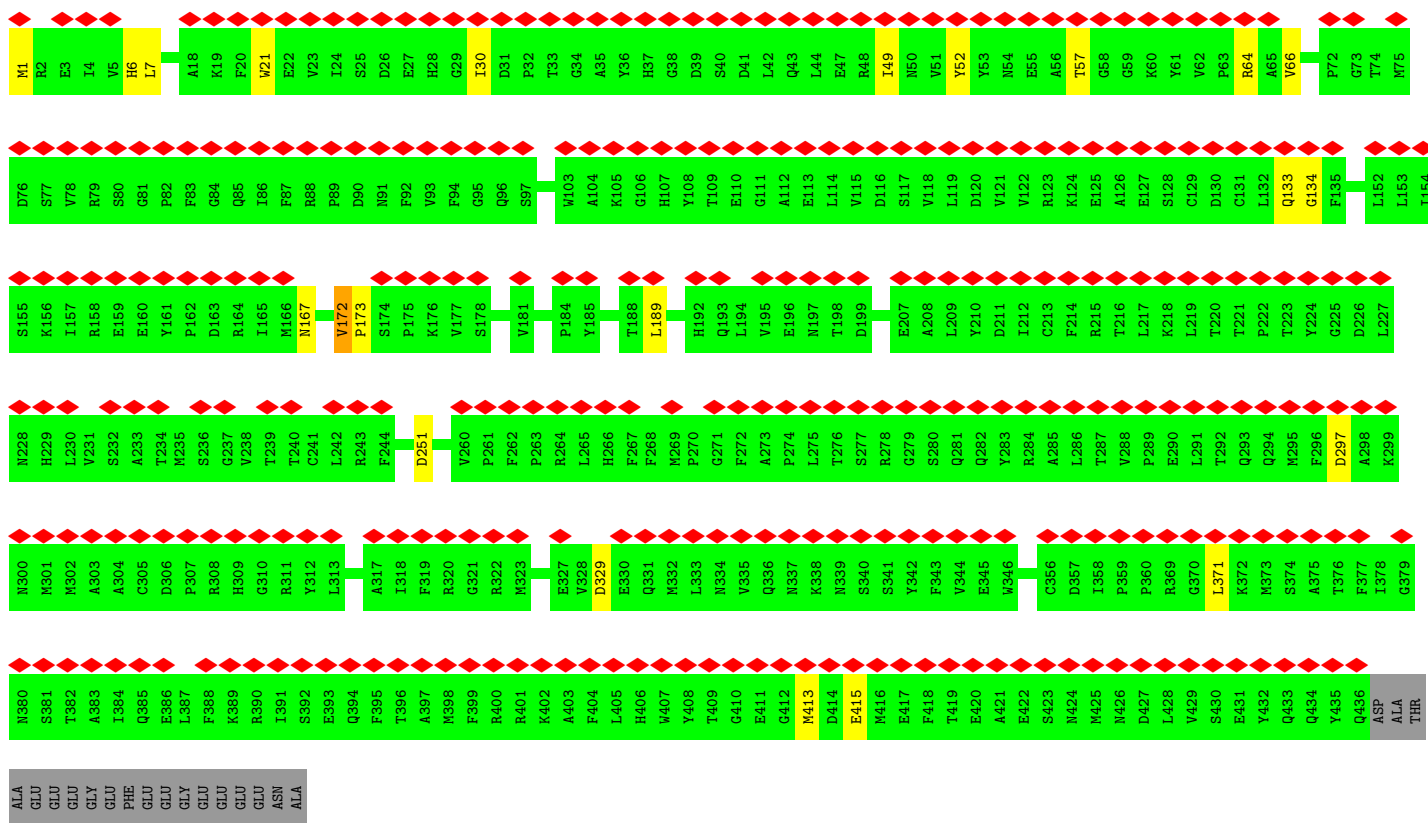
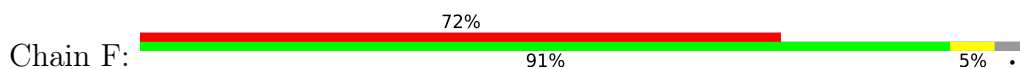


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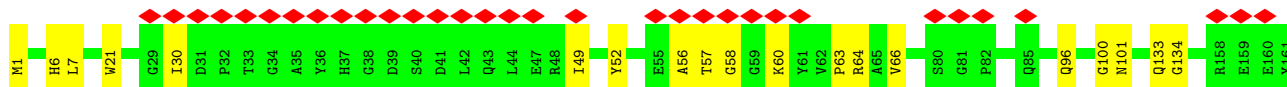
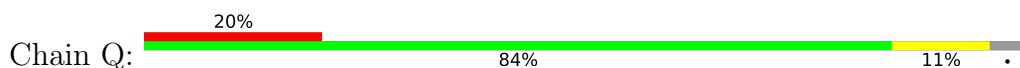


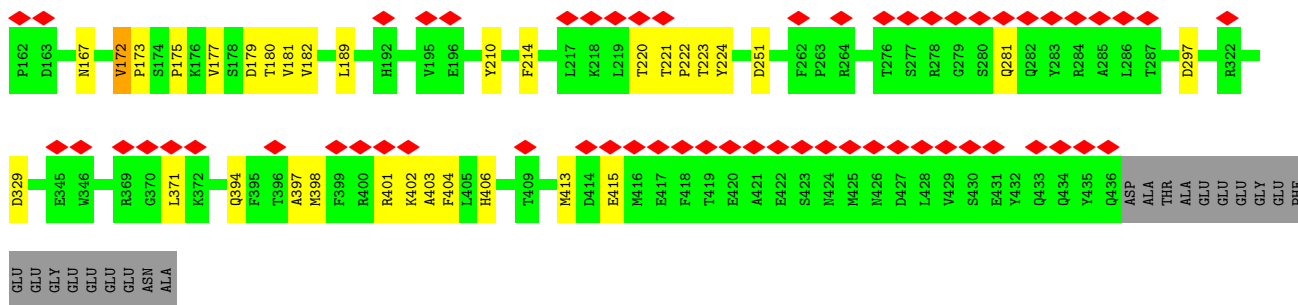


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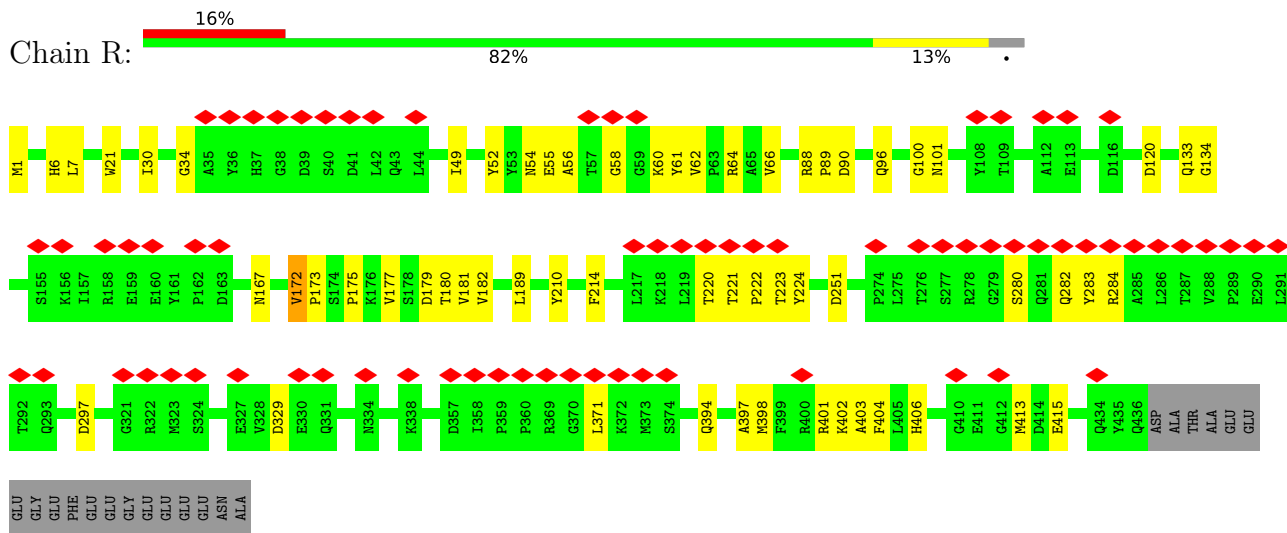


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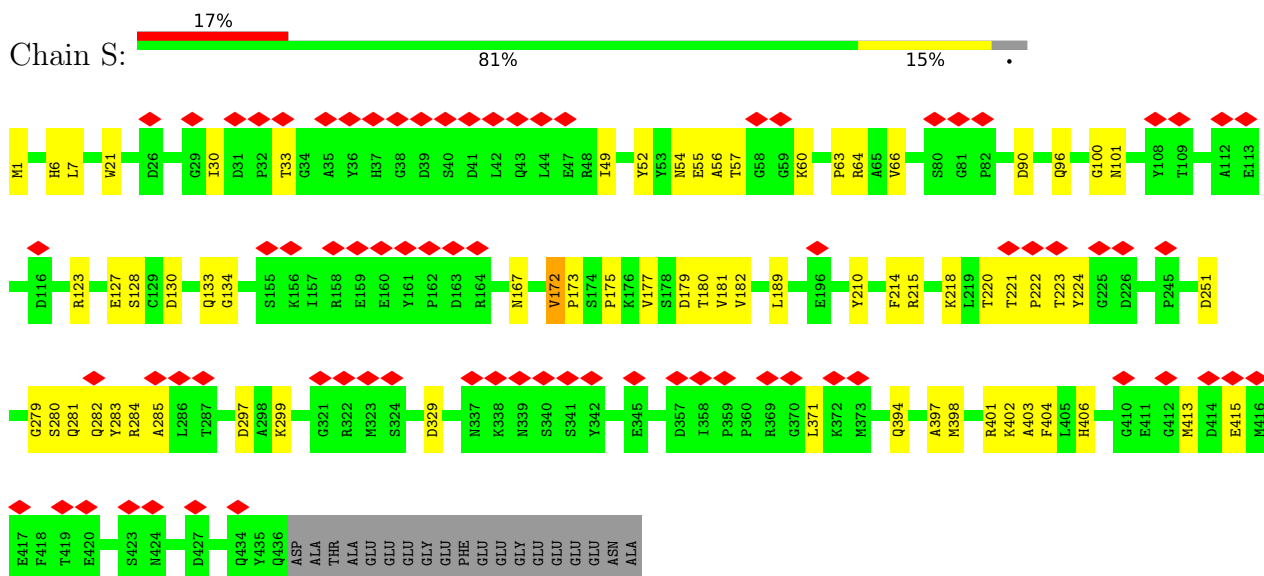




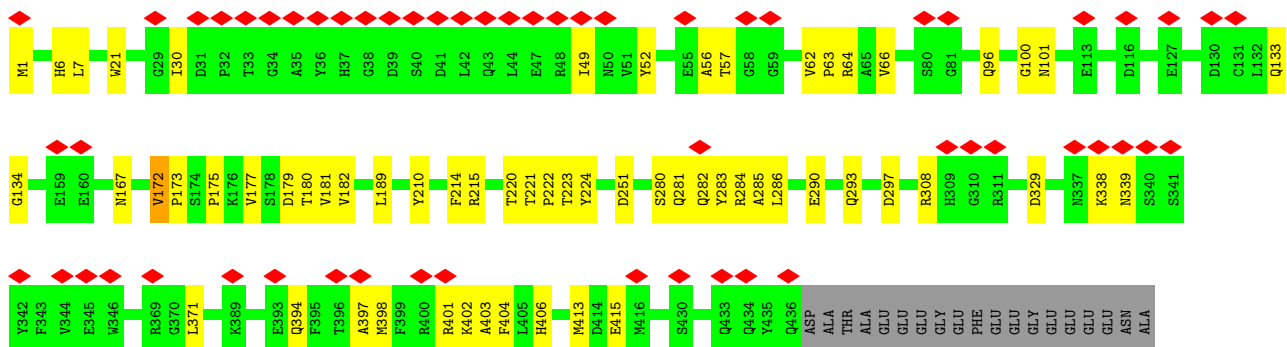
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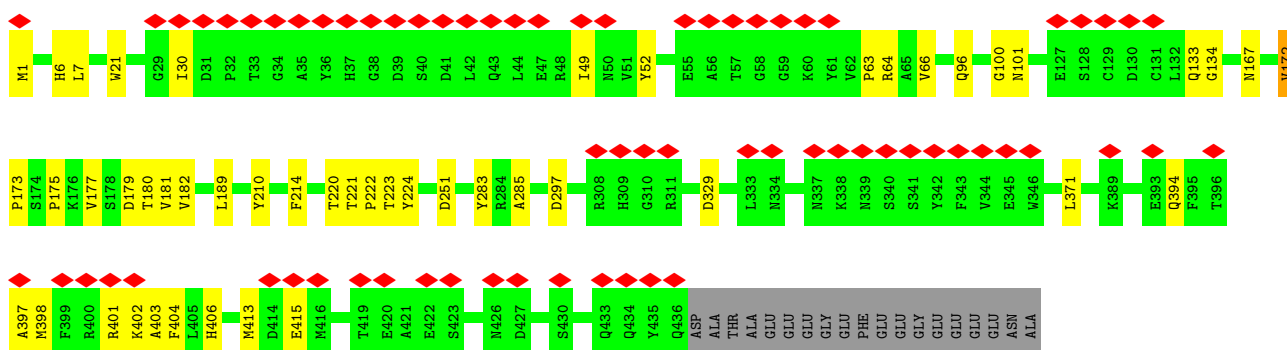
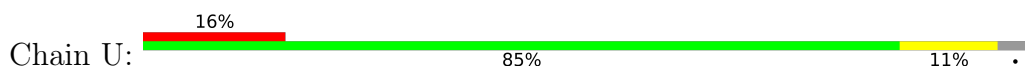
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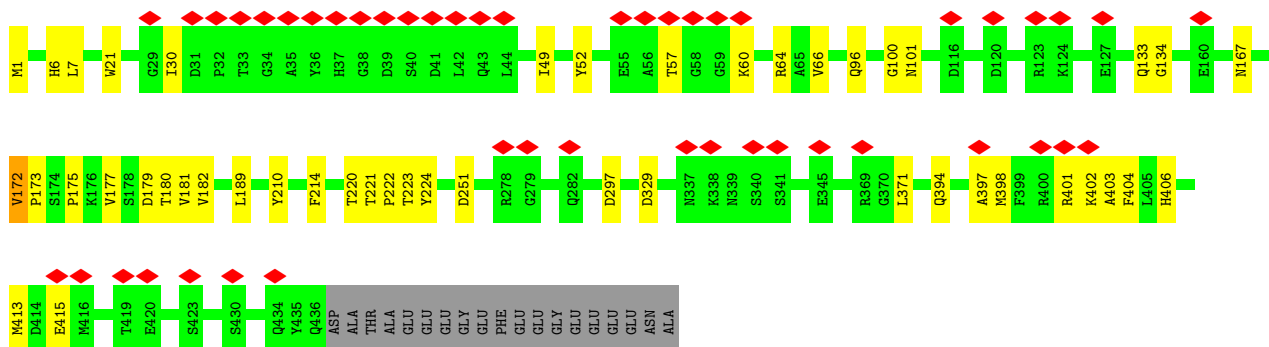
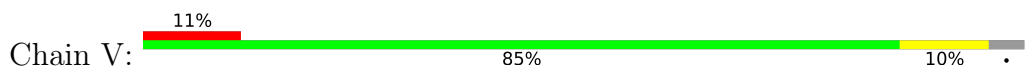
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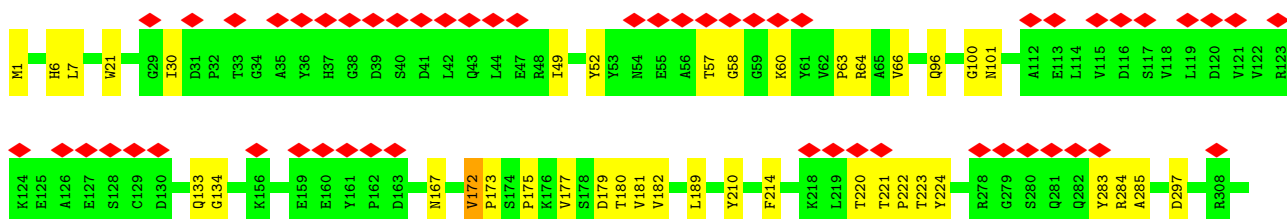
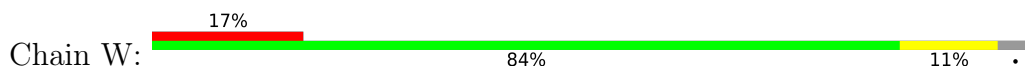
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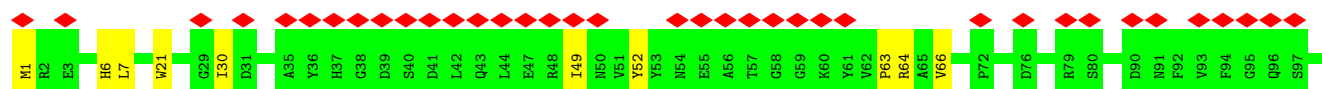


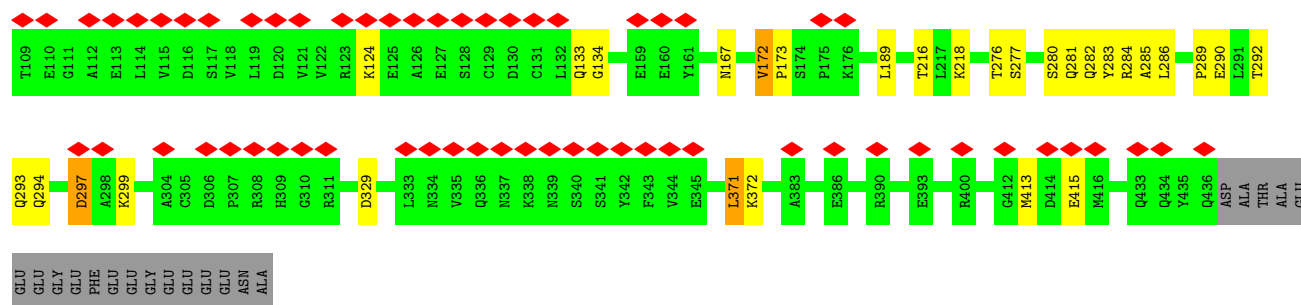
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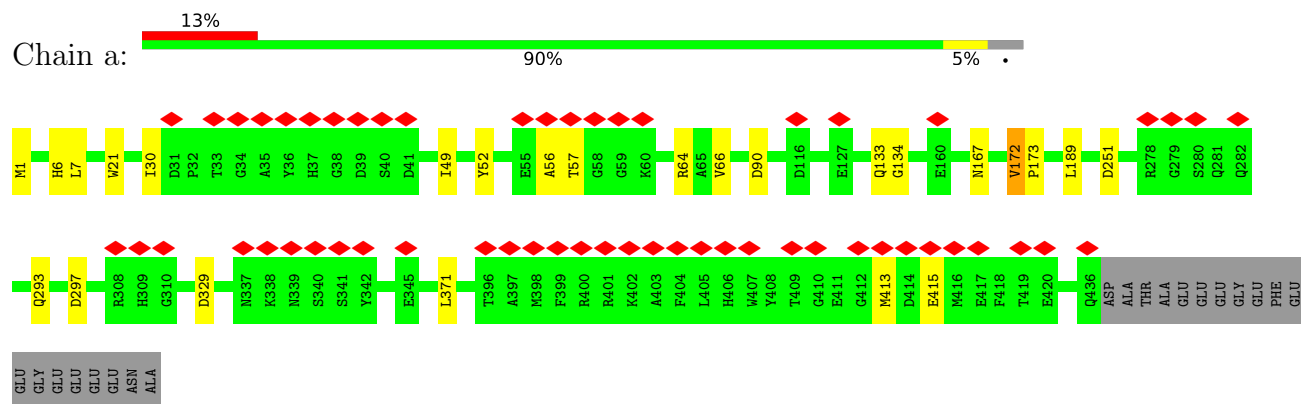
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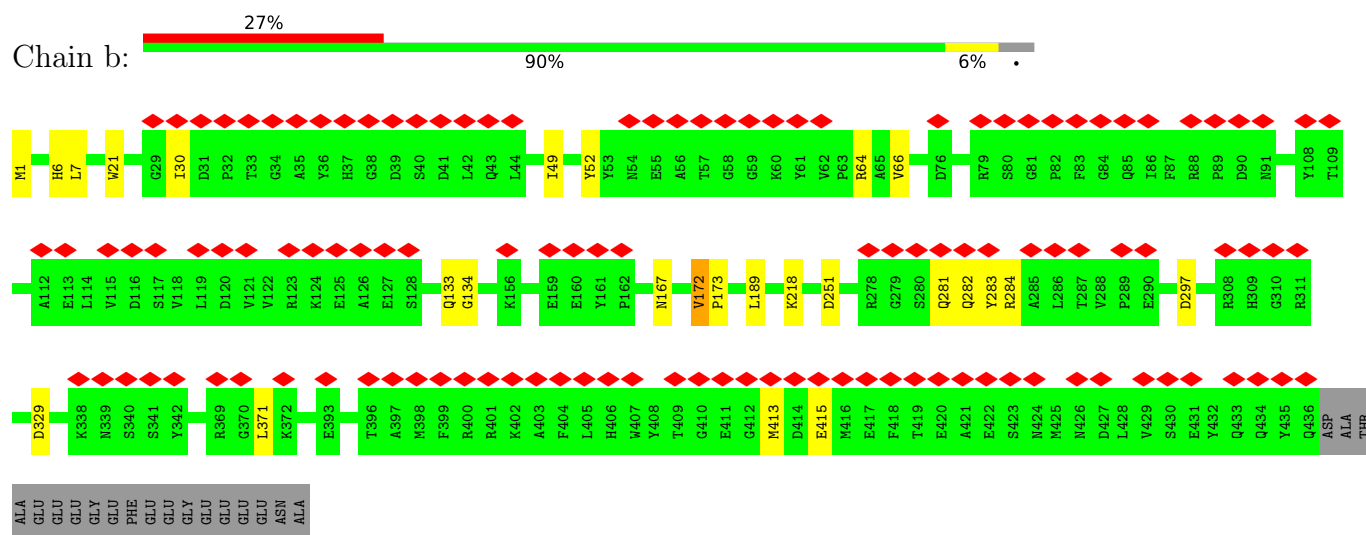




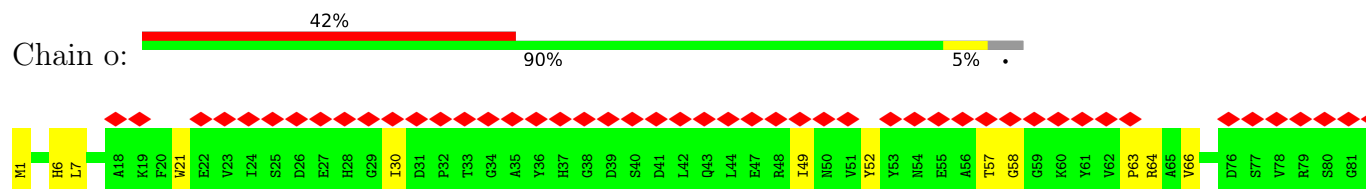
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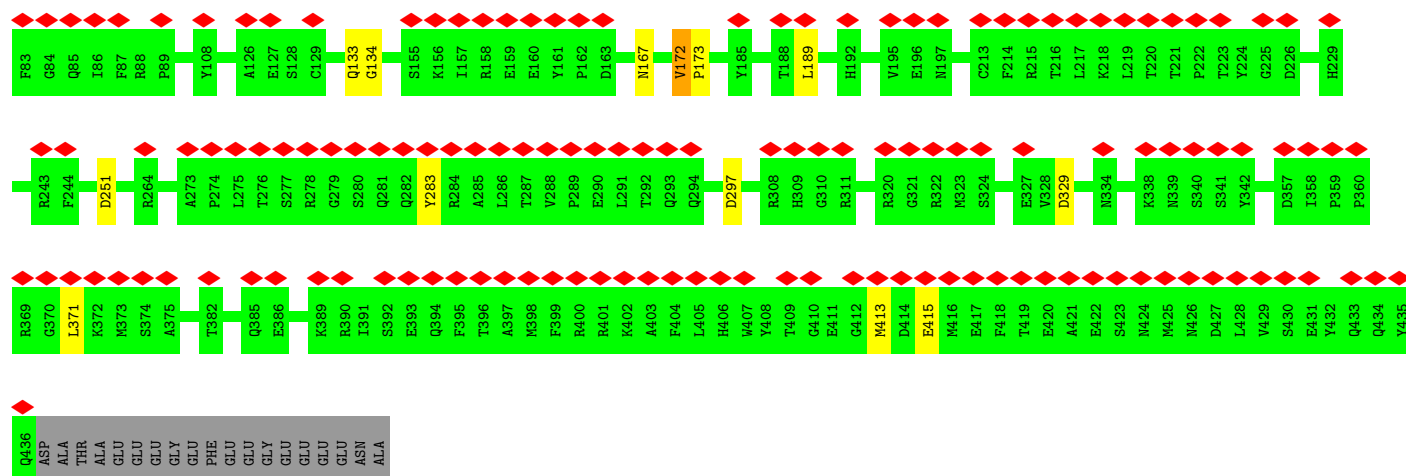


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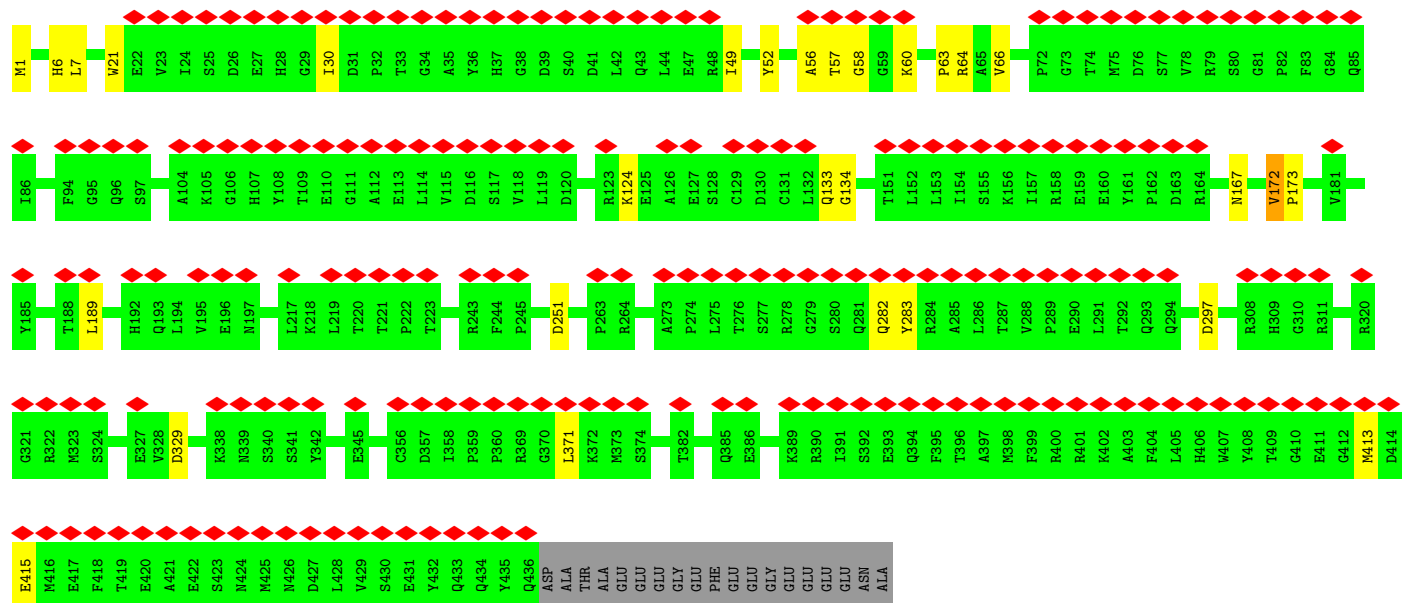
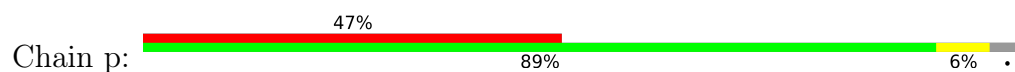


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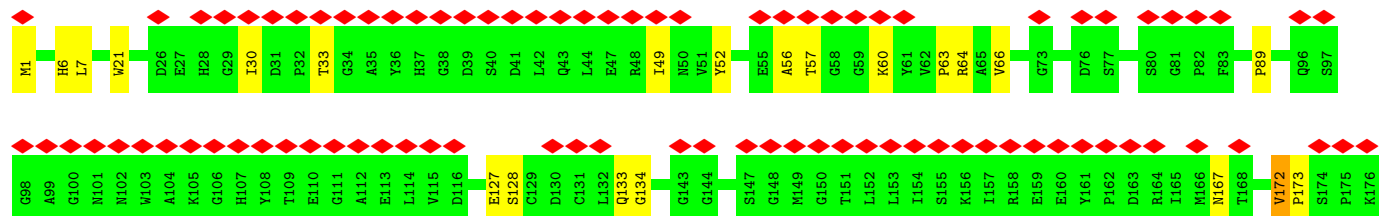
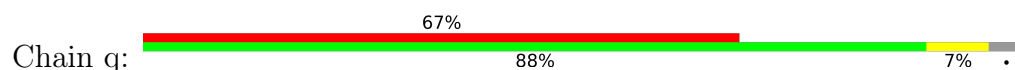


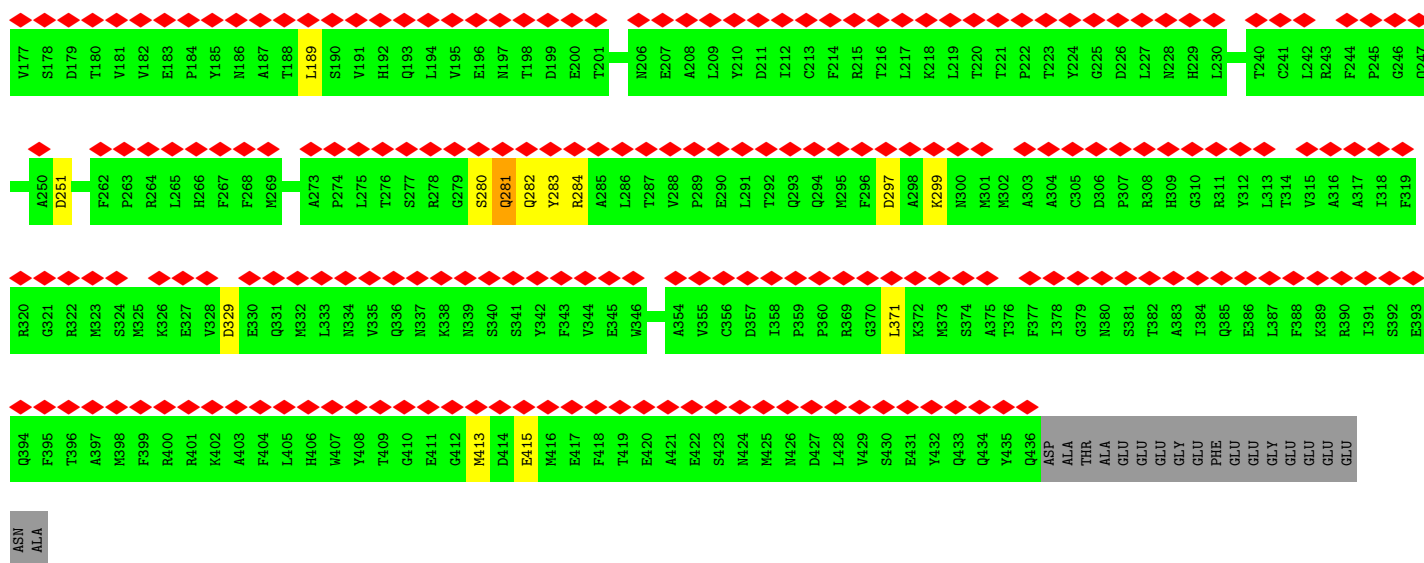


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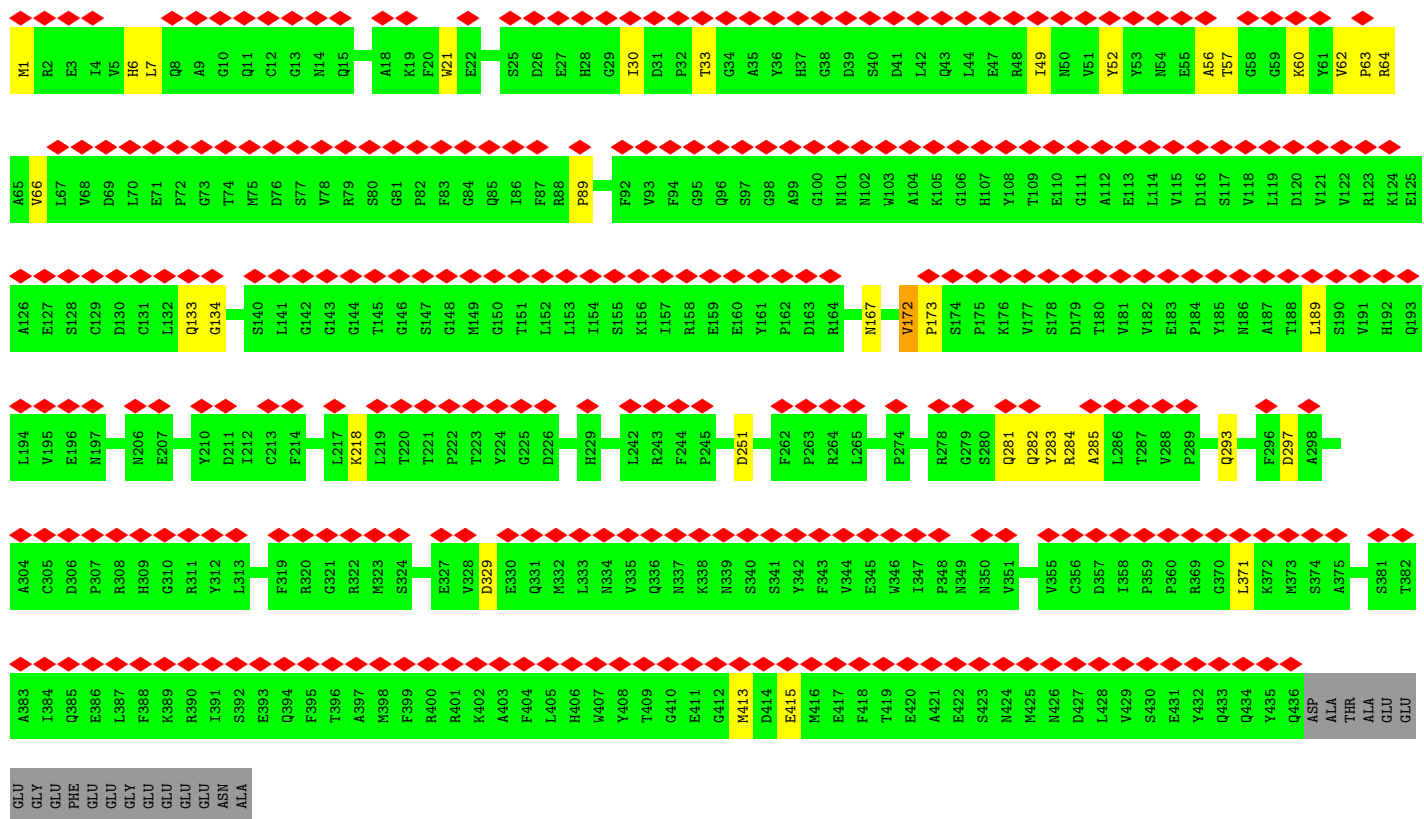
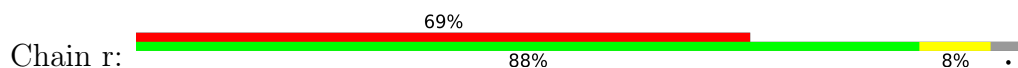


• Molecule 2: Tubulin beta-4 chain

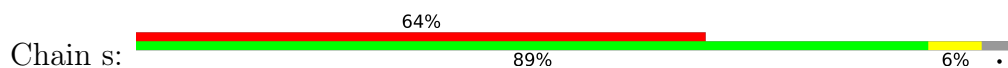




• Molecule 2: Tubulin beta-4 chain



• Molecule 2: Tubulin beta-4 chain



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D69	L70	E71	P72	G73	T74	M75	D76	A79	S77	V78	R79	S80	G81	P82	F83	G84	Q85	I86	F87	B88	P89	D90	N91	F92	V93	F94	G95	Q96	S97	G98	A99	G100	N101	N102	V103	A104	K105	G106	H107	Y108	T109	E110	G111	A112	E113	L114	V115	D116	S117	V118	L119	D120	V121	V122	R123	K124	E125	A126	E127	S128																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
C129	D130	C131	L132	Q133	G134	S140	L141	G142	G143	G144	T145	G146	S147	G148	M149	G150	T151	L152	L153	I154	S155	K156	I157	R158	E159	E160	Y161	P162	D163	R164	N167	V172	P173	S174	P175	K176	V177	S178	D179	T180	V181	V182	E183	P184	Y185	N186	A187	T188	L189	S190	V191	H192	Q193	L194	V195	E196																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
N197	D205	N206	E207	Y210	D211	F214	R215	K218	L219	T220	T221	P222	T223	Y224	L242	R243	F244	P245	D251	P261	F262	P263	R264	L265	R278	G279	S280	Q281	Q282	Y283	R284	A285	L286	D297	A298	A304	C305	D306	P307	R308	H309	G310	R311	Y312	L313	R322	D329																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
E330	Q331	M332	L333	N334	V335	Q336	N337	K338	N339	S340	S341	Y342	F343	V344	E345	W346	I347	F348	N349	N350	I358	R369	G370	L371	S381	T382	A383	I384	Q385	E386	L387	F388	K389	R390	I391	S392	E393	Q394	F395	T396	A397	M398	F399	R400	R401	K402	A403	F404	L405	H406	W407	Y408	T409	G410	E411	G412																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
M413	D414	E415	M416	E417	F418	T419	E420	A421	E422	S423	M424	M425	M426	D427	L428	V429	S430	E431	Y432	Q433	Q434	Y435	Q436	ASP	ALA	ALA	THR	ALA	GLU	GLU	GLU	GLY	PHE	GLU	GLU	GLY	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8497	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	33000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.051	Depositor
Minimum map value	-0.021	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0157	Depositor
Map size ($\text{\AA}$)	513.024, 513.024, 513.024	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.004, 2.004, 2.004	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, TA1, GTP, GDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.76	0/3442	1.36	5/4667 (0.1%)
1	C	0.76	0/3442	1.36	5/4667 (0.1%)
1	D	0.76	0/3442	1.36	5/4667 (0.1%)
1	E	0.76	0/3442	1.36	5/4667 (0.1%)
1	G	0.76	0/3442	1.36	5/4667 (0.1%)
1	H	0.76	0/3442	1.36	5/4667 (0.1%)
1	I	0.76	0/3442	1.36	6/4667 (0.1%)
1	J	0.76	0/3442	1.36	5/4667 (0.1%)
1	K	0.76	0/3442	1.36	5/4667 (0.1%)
1	L	0.76	0/3442	1.36	5/4667 (0.1%)
1	M	0.76	0/3442	1.36	5/4667 (0.1%)
1	N	0.76	0/3442	1.36	5/4667 (0.1%)
1	O	0.76	0/3442	1.36	6/4667 (0.1%)
1	P	0.76	0/3442	1.36	5/4667 (0.1%)
1	c	0.76	0/3442	1.36	5/4667 (0.1%)
1	d	0.76	0/3442	1.36	5/4667 (0.1%)
1	e	0.76	0/3442	1.36	5/4667 (0.1%)
1	f	0.76	0/3442	1.36	6/4667 (0.1%)
1	g	0.76	0/3442	1.36	5/4667 (0.1%)
1	h	0.76	0/3442	1.36	5/4667 (0.1%)
1	i	0.76	0/3442	1.36	5/4667 (0.1%)
1	j	0.76	0/3442	1.36	5/4667 (0.1%)
1	k	0.76	0/3442	1.36	5/4667 (0.1%)
2	B	0.76	0/3422	1.37	9/4636 (0.2%)
2	F	0.76	0/3422	1.37	9/4636 (0.2%)
2	Q	0.76	0/3422	1.37	10/4636 (0.2%)
2	R	0.76	0/3422	1.37	9/4636 (0.2%)
2	S	0.76	0/3422	1.37	9/4636 (0.2%)
2	T	0.76	0/3422	1.37	9/4636 (0.2%)
2	U	0.76	0/3422	1.37	9/4636 (0.2%)
2	V	0.76	0/3422	1.37	9/4636 (0.2%)
2	W	0.76	0/3422	1.37	8/4636 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	X	0.76	0/3422	1.37	10/4636 (0.2%)
2	Y	0.76	0/3422	1.37	8/4636 (0.2%)
2	Z	0.76	0/3422	1.37	8/4636 (0.2%)
2	a	0.76	0/3422	1.37	9/4636 (0.2%)
2	b	0.76	0/3422	1.37	9/4636 (0.2%)
2	o	0.76	0/3422	1.37	9/4636 (0.2%)
2	p	0.76	0/3422	1.37	9/4636 (0.2%)
2	q	0.76	0/3422	1.37	10/4636 (0.2%)
2	r	0.76	0/3422	1.37	9/4636 (0.2%)
2	s	0.76	0/3422	1.37	9/4636 (0.2%)
All	All	0.76	0/144184	1.37	289/195425 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
2	F	0	2
2	Q	0	2
2	R	0	2
2	S	0	2
2	T	0	2
2	U	0	2
2	V	0	2
2	W	0	2
2	X	0	2
2	Y	0	2
2	Z	0	2
2	a	0	2
2	b	0	2
2	o	0	2
2	p	0	2
2	q	0	2
2	r	0	2
2	s	0	2
All	All	0	38

There are no bond length outliers.

All (289) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	82	PRO	CA-N-CD	-9.90	98.14	112.00
1	G	82	PRO	CA-N-CD	-9.89	98.15	112.00
1	d	82	PRO	CA-N-CD	-9.88	98.16	112.00
1	C	82	PRO	CA-N-CD	-9.88	98.17	112.00
1	A	82	PRO	CA-N-CD	-9.87	98.18	112.00
1	K	82	PRO	CA-N-CD	-9.87	98.18	112.00
1	H	82	PRO	CA-N-CD	-9.87	98.18	112.00
1	M	82	PRO	CA-N-CD	-9.87	98.18	112.00
1	g	82	PRO	CA-N-CD	-9.87	98.18	112.00
1	e	82	PRO	CA-N-CD	-9.87	98.19	112.00
1	k	82	PRO	CA-N-CD	-9.87	98.19	112.00
1	h	82	PRO	CA-N-CD	-9.87	98.19	112.00
1	j	82	PRO	CA-N-CD	-9.87	98.19	112.00
1	L	82	PRO	CA-N-CD	-9.86	98.19	112.00
1	E	82	PRO	CA-N-CD	-9.86	98.19	112.00
1	P	82	PRO	CA-N-CD	-9.86	98.19	112.00
1	D	82	PRO	CA-N-CD	-9.86	98.20	112.00
1	i	82	PRO	CA-N-CD	-9.86	98.20	112.00
1	I	82	PRO	CA-N-CD	-9.86	98.20	112.00
1	f	82	PRO	CA-N-CD	-9.86	98.20	112.00
1	O	82	PRO	CA-N-CD	-9.85	98.22	112.00
1	c	82	PRO	CA-N-CD	-9.84	98.22	112.00
1	N	82	PRO	CA-N-CD	-9.83	98.24	112.00
2	b	297	ASP	CA-C-N	6.39	129.70	120.38
2	b	297	ASP	C-N-CA	6.39	129.70	120.38
2	p	297	ASP	CA-C-N	6.38	129.69	120.38
2	p	297	ASP	C-N-CA	6.38	129.69	120.38
2	F	297	ASP	CA-C-N	6.37	129.67	120.38
2	F	297	ASP	C-N-CA	6.37	129.67	120.38
2	Q	297	ASP	CA-C-N	6.37	129.68	120.38
2	Q	297	ASP	C-N-CA	6.37	129.68	120.38
2	U	297	ASP	CA-C-N	6.36	129.67	120.38
2	U	297	ASP	C-N-CA	6.36	129.67	120.38
2	S	297	ASP	CA-C-N	6.36	129.67	120.38
2	S	297	ASP	C-N-CA	6.36	129.67	120.38
2	s	297	ASP	CA-C-N	6.36	129.66	120.38
2	s	297	ASP	C-N-CA	6.36	129.66	120.38
2	R	297	ASP	CA-C-N	6.36	129.66	120.38
2	R	297	ASP	C-N-CA	6.36	129.66	120.38
2	T	297	ASP	CA-C-N	6.35	129.66	120.38
2	T	297	ASP	C-N-CA	6.35	129.66	120.38
2	B	297	ASP	CA-C-N	6.35	129.65	120.38
2	B	297	ASP	C-N-CA	6.35	129.65	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	297	ASP	CA-C-N	6.35	129.65	120.38
2	V	297	ASP	C-N-CA	6.35	129.65	120.38
2	X	297	ASP	CA-C-N	6.35	129.65	120.38
2	X	297	ASP	C-N-CA	6.35	129.65	120.38
2	Z	297	ASP	CA-C-N	6.35	129.65	120.38
2	Z	297	ASP	C-N-CA	6.35	129.65	120.38
2	r	297	ASP	CA-C-N	6.35	129.65	120.38
2	r	297	ASP	C-N-CA	6.35	129.65	120.38
2	o	297	ASP	CA-C-N	6.35	129.65	120.38
2	o	297	ASP	C-N-CA	6.35	129.65	120.38
2	q	297	ASP	CA-C-N	6.34	129.64	120.38
2	q	297	ASP	C-N-CA	6.34	129.64	120.38
2	a	297	ASP	CA-C-N	6.34	129.63	120.38
2	a	297	ASP	C-N-CA	6.34	129.63	120.38
2	Y	297	ASP	CA-C-N	6.33	129.63	120.38
2	Y	297	ASP	C-N-CA	6.33	129.63	120.38
2	W	297	ASP	CA-C-N	6.32	129.61	120.38
2	W	297	ASP	C-N-CA	6.32	129.61	120.38
1	M	392	ASP	CA-CB-CG	6.26	118.86	112.60
1	K	392	ASP	CA-CB-CG	6.25	118.85	112.60
1	d	392	ASP	CA-CB-CG	6.25	118.85	112.60
1	f	392	ASP	CA-CB-CG	6.25	118.84	112.60
1	N	392	ASP	CA-CB-CG	6.24	118.84	112.60
1	G	392	ASP	CA-CB-CG	6.24	118.84	112.60
1	H	392	ASP	CA-CB-CG	6.24	118.84	112.60
1	k	392	ASP	CA-CB-CG	6.24	118.84	112.60
1	J	392	ASP	CA-CB-CG	6.24	118.84	112.60
1	L	392	ASP	CA-CB-CG	6.24	118.84	112.60
1	c	392	ASP	CA-CB-CG	6.24	118.83	112.60
1	A	392	ASP	CA-CB-CG	6.23	118.83	112.60
1	E	392	ASP	CA-CB-CG	6.23	118.83	112.60
1	j	392	ASP	CA-CB-CG	6.22	118.83	112.60
1	C	392	ASP	CA-CB-CG	6.22	118.82	112.60
1	I	392	ASP	CA-CB-CG	6.22	118.82	112.60
1	O	392	ASP	CA-CB-CG	6.21	118.81	112.60
1	P	392	ASP	CA-CB-CG	6.20	118.80	112.60
1	e	392	ASP	CA-CB-CG	6.20	118.80	112.60
1	h	392	ASP	CA-CB-CG	6.20	118.80	112.60
1	g	392	ASP	CA-CB-CG	6.19	118.79	112.60
1	i	392	ASP	CA-CB-CG	6.18	118.78	112.60
1	D	392	ASP	CA-CB-CG	6.17	118.77	112.60
1	E	98	ASP	CA-CB-CG	6.15	118.75	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	98	ASP	CA-CB-CG	6.14	118.74	112.60
1	H	98	ASP	CA-CB-CG	6.14	118.74	112.60
1	d	98	ASP	CA-CB-CG	6.13	118.73	112.60
1	P	98	ASP	CA-CB-CG	6.12	118.72	112.60
1	c	98	ASP	CA-CB-CG	6.12	118.72	112.60
1	i	98	ASP	CA-CB-CG	6.12	118.72	112.60
1	f	98	ASP	CA-CB-CG	6.12	118.72	112.60
1	h	98	ASP	CA-CB-CG	6.12	118.72	112.60
1	D	98	ASP	CA-CB-CG	6.11	118.71	112.60
1	N	98	ASP	CA-CB-CG	6.11	118.71	112.60
1	e	98	ASP	CA-CB-CG	6.11	118.71	112.60
1	I	98	ASP	CA-CB-CG	6.11	118.71	112.60
1	A	98	ASP	CA-CB-CG	6.10	118.70	112.60
1	g	98	ASP	CA-CB-CG	6.10	118.70	112.60
1	G	98	ASP	CA-CB-CG	6.10	118.70	112.60
1	C	98	ASP	CA-CB-CG	6.09	118.69	112.60
1	J	98	ASP	CA-CB-CG	6.09	118.69	112.60
1	O	98	ASP	CA-CB-CG	6.09	118.69	112.60
1	j	98	ASP	CA-CB-CG	6.08	118.68	112.60
1	L	98	ASP	CA-CB-CG	6.08	118.68	112.60
1	k	98	ASP	CA-CB-CG	6.07	118.67	112.60
1	K	98	ASP	CA-CB-CG	6.03	118.63	112.60
2	Z	167	ASN	CA-CB-CG	5.96	118.56	112.60
2	W	167	ASN	CA-CB-CG	5.96	118.56	112.60
2	Y	167	ASN	CA-CB-CG	5.95	118.55	112.60
2	S	167	ASN	CA-CB-CG	5.95	118.55	112.60
2	a	167	ASN	CA-CB-CG	5.95	118.55	112.60
2	F	167	ASN	CA-CB-CG	5.94	118.54	112.60
2	b	167	ASN	CA-CB-CG	5.94	118.54	112.60
2	B	167	ASN	CA-CB-CG	5.93	118.53	112.60
2	Q	167	ASN	CA-CB-CG	5.93	118.53	112.60
2	q	167	ASN	CA-CB-CG	5.93	118.53	112.60
2	s	167	ASN	CA-CB-CG	5.93	118.53	112.60
2	U	167	ASN	CA-CB-CG	5.92	118.52	112.60
2	V	167	ASN	CA-CB-CG	5.92	118.52	112.60
2	R	167	ASN	CA-CB-CG	5.91	118.51	112.60
2	T	167	ASN	CA-CB-CG	5.91	118.51	112.60
2	X	167	ASN	CA-CB-CG	5.90	118.50	112.60
2	o	167	ASN	CA-CB-CG	5.89	118.49	112.60
2	r	167	ASN	CA-CB-CG	5.89	118.49	112.60
2	p	167	ASN	CA-CB-CG	5.87	118.47	112.60
2	Z	134	GLY	N-CA-C	5.73	118.88	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	134	GLY	N-CA-C	5.72	118.86	110.80
2	Y	134	GLY	N-CA-C	5.72	118.87	110.80
2	b	134	GLY	N-CA-C	5.71	118.86	110.80
2	U	134	GLY	N-CA-C	5.71	118.84	110.80
2	o	134	GLY	N-CA-C	5.70	118.84	110.80
2	q	134	GLY	N-CA-C	5.70	118.84	110.80
2	r	134	GLY	N-CA-C	5.70	118.83	110.80
2	B	134	GLY	N-CA-C	5.70	118.83	110.80
2	S	134	GLY	N-CA-C	5.70	118.83	110.80
2	X	134	GLY	N-CA-C	5.69	118.83	110.80
2	W	134	GLY	N-CA-C	5.69	118.82	110.80
2	a	134	GLY	N-CA-C	5.68	118.81	110.80
2	F	134	GLY	N-CA-C	5.68	118.81	110.80
2	R	134	GLY	N-CA-C	5.68	118.81	110.80
2	Q	134	GLY	N-CA-C	5.68	118.81	110.80
2	p	134	GLY	N-CA-C	5.68	118.80	110.80
2	V	134	GLY	N-CA-C	5.67	118.80	110.80
2	s	134	GLY	N-CA-C	5.67	118.79	110.80
2	V	133	GLN	OE1-CD-NE2	-5.48	117.12	122.60
1	i	215	ARG	NE-CZ-NH2	5.48	124.13	119.20
1	P	15	GLN	OE1-CD-NE2	-5.47	117.13	122.60
1	g	15	GLN	OE1-CD-NE2	-5.47	117.13	122.60
2	U	133	GLN	OE1-CD-NE2	-5.47	117.13	122.60
2	F	133	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	k	15	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	J	15	GLN	OE1-CD-NE2	-5.46	117.14	122.60
2	b	133	GLN	OE1-CD-NE2	-5.46	117.14	122.60
2	Y	133	GLN	OE1-CD-NE2	-5.45	117.15	122.60
1	L	215	ARG	NE-CZ-NH2	5.45	124.11	119.20
2	s	133	GLN	OE1-CD-NE2	-5.45	117.15	122.60
2	Q	133	GLN	OE1-CD-NE2	-5.45	117.15	122.60
2	Z	133	GLN	OE1-CD-NE2	-5.45	117.15	122.60
2	q	133	GLN	OE1-CD-NE2	-5.45	117.15	122.60
2	B	133	GLN	OE1-CD-NE2	-5.45	117.16	122.60
1	h	15	GLN	OE1-CD-NE2	-5.45	117.16	122.60
1	L	15	GLN	OE1-CD-NE2	-5.44	117.16	122.60
2	p	133	GLN	OE1-CD-NE2	-5.44	117.16	122.60
2	X	133	GLN	OE1-CD-NE2	-5.44	117.16	122.60
2	T	133	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	c	15	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	f	15	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	A	15	GLN	OE1-CD-NE2	-5.43	117.17	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	215	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	I	15	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	M	15	GLN	OE1-CD-NE2	-5.43	117.17	122.60
2	R	133	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	e	15	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	K	15	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	d	15	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	D	15	GLN	OE1-CD-NE2	-5.42	117.17	122.60
2	a	133	GLN	OE1-CD-NE2	-5.42	117.17	122.60
1	j	15	GLN	OE1-CD-NE2	-5.42	117.17	122.60
2	S	133	GLN	OE1-CD-NE2	-5.42	117.18	122.60
1	i	15	GLN	OE1-CD-NE2	-5.42	117.18	122.60
1	E	15	GLN	OE1-CD-NE2	-5.42	117.18	122.60
1	K	215	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	O	15	GLN	OE1-CD-NE2	-5.41	117.19	122.60
1	P	215	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	c	215	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	C	15	GLN	OE1-CD-NE2	-5.41	117.19	122.60
2	W	133	GLN	OE1-CD-NE2	-5.41	117.19	122.60
1	G	15	GLN	OE1-CD-NE2	-5.40	117.20	122.60
1	M	215	ARG	NE-CZ-NH2	5.40	124.06	119.20
1	h	215	ARG	NE-CZ-NH2	5.40	124.06	119.20
2	o	133	GLN	OE1-CD-NE2	-5.39	117.20	122.60
2	r	133	GLN	OE1-CD-NE2	-5.39	117.21	122.60
1	O	215	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	H	15	GLN	OE1-CD-NE2	-5.38	117.22	122.60
1	A	215	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	I	215	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	e	215	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	E	215	ARG	NE-CZ-NH2	5.37	124.04	119.20
1	G	215	ARG	NE-CZ-NH2	5.37	124.04	119.20
1	f	215	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	H	215	ARG	NE-CZ-NH2	5.36	124.03	119.20
1	N	215	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	N	15	GLN	OE1-CD-NE2	-5.36	117.24	122.60
1	C	215	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	k	215	ARG	NE-CZ-NH2	5.34	124.00	119.20
1	J	215	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	D	215	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	j	215	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	d	215	ARG	NE-CZ-NH2	5.33	124.00	119.20
2	T	329	ASP	CA-C-N	5.12	127.09	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	329	ASP	C-N-CA	5.12	127.09	120.44
2	a	329	ASP	CA-C-N	5.12	127.09	120.44
2	a	329	ASP	C-N-CA	5.12	127.09	120.44
2	X	172	VAL	N-CA-C	5.12	114.79	109.01
2	W	329	ASP	CA-C-N	5.11	127.08	120.44
2	W	329	ASP	C-N-CA	5.11	127.08	120.44
2	q	329	ASP	CA-C-N	5.11	127.08	120.44
2	q	329	ASP	C-N-CA	5.11	127.08	120.44
2	F	329	ASP	CA-C-N	5.11	127.08	120.44
2	F	329	ASP	C-N-CA	5.11	127.08	120.44
2	U	329	ASP	CA-C-N	5.11	127.08	120.44
2	U	329	ASP	C-N-CA	5.11	127.08	120.44
2	Z	172	VAL	N-CA-C	5.10	114.78	109.01
2	r	172	VAL	N-CA-C	5.10	114.78	109.01
2	W	172	VAL	N-CA-C	5.10	114.77	109.01
2	b	329	ASP	CA-C-N	5.10	127.07	120.44
2	b	329	ASP	C-N-CA	5.10	127.07	120.44
2	b	172	VAL	N-CA-C	5.09	114.77	109.01
2	s	329	ASP	CA-C-N	5.09	127.06	120.44
2	s	329	ASP	C-N-CA	5.09	127.06	120.44
2	Q	172	VAL	N-CA-C	5.09	114.76	109.01
2	V	172	VAL	N-CA-C	5.09	114.76	109.01
2	o	172	VAL	N-CA-C	5.09	114.76	109.01
2	Z	329	ASP	CA-C-N	5.09	127.06	120.44
2	Z	329	ASP	C-N-CA	5.09	127.06	120.44
2	Y	172	VAL	N-CA-C	5.09	114.76	109.01
2	B	329	ASP	CA-C-N	5.08	127.05	120.44
2	B	329	ASP	C-N-CA	5.08	127.05	120.44
2	Y	329	ASP	CA-C-N	5.08	127.05	120.44
2	Y	329	ASP	C-N-CA	5.08	127.05	120.44
2	B	172	VAL	N-CA-C	5.08	114.75	109.01
2	U	172	VAL	N-CA-C	5.08	114.75	109.01
2	o	329	ASP	CA-C-N	5.08	127.04	120.44
2	o	329	ASP	C-N-CA	5.08	127.04	120.44
2	r	329	ASP	CA-C-N	5.08	127.04	120.44
2	r	329	ASP	C-N-CA	5.08	127.04	120.44
2	R	329	ASP	CA-C-N	5.08	127.04	120.44
2	R	329	ASP	C-N-CA	5.08	127.04	120.44
2	T	172	VAL	N-CA-C	5.08	114.75	109.01
2	S	172	VAL	N-CA-C	5.08	114.74	109.01
2	a	172	VAL	N-CA-C	5.07	114.74	109.01
2	s	172	VAL	N-CA-C	5.07	114.74	109.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	329	ASP	CA-C-N	5.07	127.03	120.44
2	V	329	ASP	C-N-CA	5.07	127.03	120.44
2	R	172	VAL	N-CA-C	5.07	114.73	109.01
2	a	251	ASP	CA-CB-CG	5.07	117.67	112.60
2	Q	329	ASP	CA-C-N	5.06	127.02	120.44
2	Q	329	ASP	C-N-CA	5.06	127.02	120.44
2	S	251	ASP	CA-CB-CG	5.06	117.66	112.60
2	p	172	VAL	N-CA-C	5.06	114.72	109.01
2	F	172	VAL	N-CA-C	5.05	114.72	109.01
2	S	329	ASP	CA-C-N	5.05	127.01	120.44
2	S	329	ASP	C-N-CA	5.05	127.01	120.44
2	q	281	GLN	OE1-CD-NE2	-5.05	117.55	122.60
2	X	329	ASP	CA-C-N	5.04	127.00	120.44
2	X	329	ASP	C-N-CA	5.04	127.00	120.44
2	p	329	ASP	CA-C-N	5.04	127.00	120.44
2	p	329	ASP	C-N-CA	5.04	127.00	120.44
2	Q	251	ASP	CA-CB-CG	5.04	117.64	112.60
1	O	205	ASP	CA-CB-CG	5.04	117.64	112.60
2	q	172	VAL	N-CA-C	5.04	114.70	109.01
2	U	251	ASP	CA-CB-CG	5.04	117.64	112.60
2	X	251	ASP	CA-CB-CG	5.03	117.63	112.60
2	b	251	ASP	CA-CB-CG	5.03	117.63	112.60
2	r	251	ASP	CA-CB-CG	5.03	117.62	112.60
2	T	251	ASP	CA-CB-CG	5.02	117.62	112.60
2	q	251	ASP	CA-CB-CG	5.02	117.62	112.60
2	B	251	ASP	CA-CB-CG	5.02	117.62	112.60
2	X	281	GLN	OE1-CD-NE2	-5.02	117.58	122.60
2	p	251	ASP	CA-CB-CG	5.02	117.62	112.60
2	R	251	ASP	CA-CB-CG	5.02	117.62	112.60
2	V	251	ASP	CA-CB-CG	5.02	117.62	112.60
1	I	205	ASP	CA-CB-CG	5.01	117.61	112.60
1	f	205	ASP	CA-CB-CG	5.01	117.61	112.60
2	o	251	ASP	CA-CB-CG	5.01	117.61	112.60
2	F	251	ASP	CA-CB-CG	5.00	117.60	112.60
2	Q	281	GLN	OE1-CD-NE2	-5.00	117.60	122.60
2	s	251	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (38) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	52	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	B	64	ARG	Sidechain
2	F	52	TYR	Sidechain
2	F	64	ARG	Sidechain
2	Q	52	TYR	Sidechain
2	Q	64	ARG	Sidechain
2	R	52	TYR	Sidechain
2	R	64	ARG	Sidechain
2	S	52	TYR	Sidechain
2	S	64	ARG	Sidechain
2	T	52	TYR	Sidechain
2	T	64	ARG	Sidechain
2	U	52	TYR	Sidechain
2	U	64	ARG	Sidechain
2	V	52	TYR	Sidechain
2	V	64	ARG	Sidechain
2	W	52	TYR	Sidechain
2	W	64	ARG	Sidechain
2	X	52	TYR	Sidechain
2	X	64	ARG	Sidechain
2	Y	52	TYR	Sidechain
2	Y	64	ARG	Sidechain
2	Z	52	TYR	Sidechain
2	Z	64	ARG	Sidechain
2	a	52	TYR	Sidechain
2	a	64	ARG	Sidechain
2	b	52	TYR	Sidechain
2	b	64	ARG	Sidechain
2	o	52	TYR	Sidechain
2	o	64	ARG	Sidechain
2	p	52	TYR	Sidechain
2	p	64	ARG	Sidechain
2	q	52	TYR	Sidechain
2	q	64	ARG	Sidechain
2	r	52	TYR	Sidechain
2	r	64	ARG	Sidechain
2	s	52	TYR	Sidechain
2	s	64	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3365	0	3272	40	0
1	C	3365	0	3271	48	0
1	D	3365	0	3268	134	0
1	E	3365	0	3272	188	0
1	G	3365	0	3263	312	0
1	H	3365	0	3265	241	0
1	I	3365	0	3272	55	0
1	J	3365	0	3272	51	0
1	K	3365	0	3270	73	0
1	L	3365	0	3272	90	0
1	M	3365	0	3263	242	0
1	N	3365	0	3266	246	0
1	O	3365	0	3272	83	0
1	P	3365	0	3272	57	0
1	c	3365	0	3270	201	0
1	d	3365	0	3270	236	0
1	e	3365	0	3265	280	0
1	f	3365	0	3268	275	0
1	g	3365	0	3272	218	0
1	h	3365	0	3272	190	0
1	i	3365	0	3271	191	0
1	j	3365	0	3272	267	0
1	k	3365	0	3270	264	0
2	B	3347	0	3235	165	0
2	F	3347	0	3236	30	0
2	Q	3347	0	3234	194	0
2	R	3347	0	3229	290	0
2	S	3347	0	3232	326	0
2	T	3347	0	3226	244	0
2	U	3347	0	3235	181	0
2	V	3347	0	3235	172	0
2	W	3347	0	3234	176	0
2	X	3347	0	3234	206	0
2	Y	3347	0	3227	390	0
2	Z	3347	0	3223	208	0
2	a	3347	0	3231	37	0
2	b	3347	0	3235	34	0
2	o	3347	0	3235	41	0
2	p	3347	0	3234	55	0
2	q	3347	0	3232	67	0
2	r	3347	0	3232	116	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	s	3347	0	3235	94	0
3	A	32	0	12	0	0
3	C	32	0	12	0	0
3	D	32	0	12	0	0
3	E	32	0	12	0	0
3	G	32	0	12	0	0
3	H	32	0	12	0	0
3	I	32	0	12	0	0
3	J	32	0	12	0	0
3	K	32	0	12	0	0
3	L	32	0	12	0	0
3	M	32	0	12	0	0
3	N	32	0	12	0	0
3	O	32	0	12	0	0
3	P	32	0	12	0	0
3	c	32	0	12	0	0
3	d	32	0	12	0	0
3	e	32	0	12	0	0
3	f	32	0	12	0	0
3	g	32	0	12	0	0
3	h	32	0	12	0	0
3	i	32	0	12	0	0
3	j	32	0	12	0	0
3	k	32	0	12	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
4	c	1	0	0	0	0
4	d	1	0	0	0	0
4	e	1	0	0	0	0
4	f	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	g	1	0	0	0	0
4	h	1	0	0	0	0
4	i	1	0	0	0	0
4	j	1	0	0	0	0
4	k	1	0	0	0	0
5	B	28	0	12	0	0
5	F	28	0	12	0	0
5	Q	28	0	12	0	0
5	R	28	0	12	0	0
5	S	28	0	12	0	0
5	T	28	0	12	0	0
5	U	28	0	12	0	0
5	V	28	0	12	0	0
5	W	28	0	12	0	0
5	X	28	0	12	0	0
5	Y	28	0	12	0	0
5	Z	28	0	12	0	0
5	a	28	0	12	0	0
5	b	28	0	12	0	0
5	o	28	0	12	0	0
5	p	28	0	12	0	0
5	q	28	0	12	0	0
5	r	28	0	12	0	0
5	s	28	0	12	0	0
6	B	62	0	51	5	0
6	F	62	0	51	5	0
6	Q	62	0	51	5	0
6	R	62	0	51	5	0
6	S	62	0	51	5	0
6	T	62	0	51	5	0
6	U	62	0	51	5	0
6	V	62	0	51	5	0
6	W	62	0	51	5	0
6	X	62	0	51	5	0
6	Y	62	0	51	5	0
6	Z	62	0	51	5	0
6	a	62	0	51	5	0
6	b	62	0	51	5	0
6	o	62	0	51	5	0
6	p	62	0	51	5	0
6	q	62	0	51	5	0
6	r	62	0	51	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	s	62	0	51	5	0
All	All	143457	0	138087	4206	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 15.

All (4206) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:r:60:LYS:HD3	2:s:282:GLN:C	1.24	1.61
2:S:56:ALA:HB1	2:T:284:ARG:CG	1.15	1.60
2:Q:60:LYS:HB2	2:R:283:TYR:CE2	1.32	1.58
1:M:57:GLY:HA3	1:N:372:LEU:CD2	1.31	1.56
1:M:89:PRO:CA	1:N:279:GLU:HB2	1.29	1.55
2:Q:96:GLN:CD	1:c:1:MET:HE2	1.11	1.53
2:R:60:LYS:HB2	2:S:282:GLN:CB	1.35	1.53
2:B:96:GLN:CD	1:E:1:MET:HE2	1.11	1.52
2:Y:96:GLN:CD	1:k:1:MET:HE2	1.11	1.52
1:j:88:HIS:CE1	1:k:280:LYS:HB3	1.44	1.52
2:F:57:THR:HB	2:o:283:TYR:CD2	1.41	1.52
2:R:34:GLY:HA3	2:S:283:TYR:CZ	1.43	1.51
2:X:96:GLN:CD	1:j:1:MET:HE2	1.11	1.50
2:R:60:LYS:CB	2:S:282:GLN:CB	1.87	1.50
2:R:96:GLN:CD	1:d:1:MET:HE2	1.11	1.49
2:S:33:THR:CG2	2:T:283:TYR:CZ	1.82	1.49
2:S:96:GLN:CD	1:e:1:MET:HE2	1.11	1.49
2:T:96:GLN:CD	1:f:1:MET:HE2	1.11	1.49
2:V:96:GLN:CD	1:h:1:MET:HE2	1.11	1.49
2:W:96:GLN:CD	1:i:1:MET:HE2	1.11	1.49
1:e:55:GLU:H	1:f:285:GLN:NE2	1.04	1.49
2:p:57:THR:HG23	2:q:284:ARG:CB	1.06	1.48
2:Y:62:VAL:HG22	2:Z:281:GLN:C	1.05	1.48
1:M:127:ASP:C	1:N:290:GLU:HG2	1.38	1.48
2:U:96:GLN:CD	1:g:1:MET:HE2	1.11	1.47
1:M:128:GLN:N	1:N:290:GLU:CG	1.75	1.47
1:G:56:THR:CB	1:H:286:LEU:CG	1.87	1.46
2:Y:86:ILE:C	2:Z:283:TYR:CD1	1.93	1.46
2:B:96:GLN:CD	1:E:1:MET:CE	1.88	1.46
2:Q:96:GLN:CD	1:c:1:MET:CE	1.88	1.46
2:Y:117:SER:CA	2:Z:299:LYS:HZ1	1.21	1.46
2:W:96:GLN:CD	1:i:1:MET:CE	1.88	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:96:GLN:CD	1:j:1:MET:CE	1.88	1.46
2:Y:117:SER:CA	2:Z:299:LYS:NZ	1.75	1.46
1:G:89:PRO:CD	1:H:280:LYS:HZ3	1.28	1.46
2:Y:96:GLN:CD	1:k:1:MET:CE	1.88	1.45
1:j:88:HIS:HE1	1:k:280:LYS:CB	1.28	1.45
1:M:90:GLU:OE2	1:N:216:ASN:CA	1.63	1.45
1:M:127:ASP:C	1:N:290:GLU:CG	1.90	1.44
1:N:62:VAL:HG21	1:O:285:GLN:NE2	1.23	1.44
1:M:89:PRO:HD3	1:N:279:GLU:CA	1.47	1.44
2:V:96:GLN:CD	1:h:1:MET:CE	1.88	1.44
2:U:96:GLN:CD	1:g:1:MET:CE	1.88	1.43
2:T:96:GLN:CD	1:f:1:MET:CE	1.88	1.43
2:Q:60:LYS:CB	2:R:283:TYR:CE2	1.99	1.43
2:R:96:GLN:CD	1:d:1:MET:CE	1.88	1.43
2:S:96:GLN:CD	1:e:1:MET:CE	1.88	1.43
1:e:55:GLU:N	1:f:285:GLN:HE21	0.94	1.43
1:H:60:LYS:HE2	1:I:283:HIS:NE2	1.20	1.42
1:M:89:PRO:HD3	1:N:279:GLU:N	1.24	1.42
1:G:89:PRO:HD3	1:H:280:LYS:NZ	1.30	1.42
2:X:123:ARG:HH12	2:Y:308:ARG:NH1	1.05	1.42
2:r:60:LYS:HD3	2:s:283:TYR:N	1.12	1.42
1:M:128:GLN:N	1:N:290:GLU:CD	1.77	1.41
2:R:90:ASP:N	2:S:218:LYS:NZ	1.67	1.41
2:S:60:LYS:NZ	2:T:283:TYR:CD1	1.77	1.41
2:R:34:GLY:HA3	2:S:283:TYR:CE2	1.56	1.40
2:R:90:ASP:H	2:S:218:LYS:NZ	0.94	1.40
1:J:60:LYS:HE2	1:K:283:HIS:CD2	1.58	1.38
1:M:57:GLY:CA	1:N:372:LEU:HD11	1.51	1.37
2:p:57:THR:CG2	2:q:284:ARG:HB3	0.89	1.36
2:S:57:THR:CA	2:T:286:LEU:H	1.33	1.36
2:X:220:THR:O	1:j:326:LYS:HE3	1.24	1.36
2:R:90:ASP:H	2:S:218:LYS:CE	1.34	1.36
1:M:89:PRO:N	1:N:279:GLU:HB2	1.41	1.35
2:Y:90:ASP:CA	2:Z:216:THR:O	1.72	1.35
1:G:89:PRO:HG2	1:H:215:ARG:O	1.23	1.35
1:G:127:ASP:HA	1:H:338:ARG:CD	1.55	1.35
2:Y:117:SER:HA	2:Z:299:LYS:NZ	1.03	1.35
2:R:220:THR:O	1:d:326:LYS:HE3	1.24	1.35
2:r:56:ALA:HB1	2:s:284:ARG:CA	1.55	1.34
2:T:220:THR:O	1:f:326:LYS:HE3	1.24	1.34
1:G:56:THR:CB	1:H:286:LEU:HG	1.48	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:57:GLY:CA	1:N:372:LEU:HD21	1.56	1.34
2:r:57:THR:N	2:s:285:ALA:HA	1.41	1.34
2:X:123:ARG:NH1	2:Y:308:ARG:NH1	1.76	1.33
2:r:60:LYS:CD	2:s:282:GLN:C	2.01	1.33
1:G:124:LYS:CE	1:H:297:GLU:C	2.00	1.33
2:B:220:THR:O	1:E:326:LYS:HE3	1.24	1.32
2:Y:62:VAL:HA	2:Z:282:GLN:C	1.17	1.32
2:S:220:THR:O	1:e:326:LYS:HE3	1.24	1.32
1:G:90:GLU:HB3	1:H:215:ARG:CB	1.59	1.31
2:S:33:THR:HG23	2:T:283:TYR:CZ	1.53	1.31
1:K:56:THR:CB	1:L:283:HIS:HB3	1.49	1.31
1:M:89:PRO:CG	1:N:277:SER:CB	2.06	1.31
1:M:89:PRO:CB	1:N:279:GLU:HB2	1.57	1.31
2:S:56:ALA:CB	2:T:284:ARG:CG	2.08	1.31
2:Y:62:VAL:CB	2:Z:281:GLN:O	1.77	1.31
1:D:60:LYS:HG2	1:G:283:HIS:CE1	1.64	1.31
2:R:60:LYS:CB	2:S:282:GLN:HB2	1.48	1.31
2:Y:62:VAL:CA	2:Z:282:GLN:C	2.03	1.31
1:e:127:ASP:HA	1:f:338:ARG:NH2	1.40	1.31
1:N:84:ARG:NH1	1:O:283:HIS:CE1	1.98	1.31
2:Y:220:THR:O	1:k:326:LYS:HE3	1.24	1.31
2:F:57:THR:CB	2:o:283:TYR:CD2	2.14	1.30
1:G:56:THR:CG2	1:H:286:LEU:HD23	1.59	1.30
1:G:60:LYS:NZ	1:H:283:HIS:HB2	1.43	1.30
2:Y:96:GLN:CG	1:k:1:MET:CE	2.10	1.30
2:V:404:PHE:CD2	1:h:261:PRO:HA	1.67	1.29
2:R:60:LYS:HB3	2:S:282:GLN:C	1.56	1.29
2:W:96:GLN:CG	1:i:1:MET:CE	2.10	1.29
2:X:96:GLN:CG	1:j:1:MET:CE	2.11	1.29
2:Q:96:GLN:CG	1:c:1:MET:CE	2.10	1.29
2:R:96:GLN:CG	1:d:1:MET:CE	2.10	1.29
2:V:96:GLN:CG	1:h:1:MET:CE	2.10	1.29
1:M:128:GLN:CG	1:N:290:GLU:HG3	1.63	1.29
2:S:404:PHE:CD2	1:e:261:PRO:HA	1.67	1.29
2:T:404:PHE:CD2	1:f:261:PRO:HA	1.67	1.29
2:U:96:GLN:CG	1:g:1:MET:CE	2.10	1.29
2:W:404:PHE:CD2	1:i:261:PRO:HA	1.67	1.29
2:R:404:PHE:CD2	1:d:261:PRO:HA	1.67	1.29
2:B:96:GLN:CG	1:E:1:MET:CE	2.10	1.28
2:Y:127:GLU:OE2	2:Z:293:GLN:HA	1.23	1.28
2:R:62:VAL:HG23	2:S:283:TYR:CB	1.58	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:96:GLN:CG	1:e:1:MET:CE	2.10	1.28
2:Y:34:GLY:HA3	2:Z:282:GLN:CG	1.60	1.28
2:Q:220:THR:O	1:c:326:LYS:HE3	1.24	1.28
2:Q:404:PHE:CD2	1:c:261:PRO:HA	1.67	1.28
2:r:60:LYS:CB	2:s:282:GLN:O	1.81	1.28
1:D:124:LYS:NZ	1:G:215:ARG:HH21	1.29	1.28
2:U:404:PHE:CD2	1:g:261:PRO:HA	1.67	1.28
2:R:34:GLY:HA3	2:S:283:TYR:OH	1.27	1.28
2:T:96:GLN:CG	1:f:1:MET:CE	2.10	1.28
2:B:404:PHE:CD2	1:E:261:PRO:HA	1.67	1.27
1:M:89:PRO:HG2	1:N:277:SER:CB	1.61	1.27
1:D:56:THR:H	1:G:282:TYR:C	1.38	1.27
1:G:57:GLY:CA	1:H:373:ARG:HH21	1.46	1.27
2:Y:404:PHE:CD2	1:k:261:PRO:HA	1.67	1.27
1:e:120:ASP:HB2	1:f:298:TYR:OH	1.25	1.27
1:G:124:LYS:HE3	1:H:297:GLU:C	1.34	1.27
2:U:220:THR:O	1:g:326:LYS:HE3	1.24	1.26
2:W:220:THR:O	1:i:326:LYS:HE3	1.24	1.26
2:X:404:PHE:CD2	1:j:261:PRO:HA	1.67	1.26
1:M:89:PRO:CA	1:N:279:GLU:CB	2.12	1.26
1:j:88:HIS:CE1	1:k:280:LYS:CB	2.09	1.26
1:G:89:PRO:CD	1:H:280:LYS:NZ	1.90	1.26
1:M:62:VAL:C	1:N:283:HIS:HA	0.96	1.26
1:j:88:HIS:CE1	1:k:280:LYS:CG	2.18	1.26
2:S:56:ALA:CB	2:T:284:ARG:HG3	1.66	1.26
2:Y:87:PHE:N	2:Z:283:TYR:CD1	2.04	1.25
2:Y:403:ALA:HA	1:k:262:TYR:CE1	1.72	1.25
2:R:403:ALA:HA	1:d:262:TYR:CE1	1.72	1.25
2:V:220:THR:O	1:h:326:LYS:HE3	1.24	1.25
1:M:128:GLN:CD	1:N:286:LEU:H	1.45	1.24
1:O:58:SER:HB3	1:P:282:TYR:O	1.33	1.24
2:S:403:ALA:HA	1:e:262:TYR:CE1	1.72	1.24
2:X:403:ALA:HA	1:j:262:TYR:CE1	1.72	1.24
2:S:56:ALA:HB3	2:T:284:ARG:CA	1.65	1.24
2:Y:128:SER:HA	2:Z:289:PRO:C	1.61	1.24
2:R:60:LYS:HB3	2:S:282:GLN:CA	1.67	1.23
2:T:403:ALA:HA	1:f:262:TYR:CE1	1.72	1.23
2:B:96:GLN:OE1	1:E:1:MET:CE	1.82	1.23
2:Q:403:ALA:HA	1:c:262:TYR:CE1	1.72	1.23
2:W:403:ALA:HA	1:i:262:TYR:CE1	1.72	1.23
1:D:56:THR:CG2	1:G:280:LYS:O	1.84	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:129:CYS:H	1:H:338:ARG:NH2	1.35	1.23
2:S:127:GLU:OE1	2:T:339:ASN:CG	1.81	1.23
2:B:403:ALA:HA	1:E:262:TYR:CE1	1.72	1.22
2:S:96:GLN:OE1	1:e:1:MET:CE	1.82	1.22
2:B:96:GLN:CG	1:E:1:MET:HE1	1.70	1.22
2:U:403:ALA:HA	1:g:262:TYR:CE1	1.72	1.22
2:V:403:ALA:HA	1:h:262:TYR:CE1	1.72	1.22
2:Y:62:VAL:CG1	2:Z:284:ARG:HB2	1.69	1.22
2:Y:62:VAL:HG11	2:Z:284:ARG:CB	1.66	1.22
1:N:62:VAL:CG2	1:O:285:GLN:NE2	2.02	1.22
2:r:56:ALA:HB1	2:s:284:ARG:C	1.61	1.22
2:R:96:GLN:OE1	1:d:1:MET:CE	1.82	1.22
2:S:127:GLU:OE1	2:T:339:ASN:ND2	1.70	1.22
2:r:60:LYS:HD3	2:s:283:TYR:CA	1.68	1.22
1:O:58:SER:CB	1:P:282:TYR:O	1.85	1.21
2:Q:96:GLN:OE1	1:c:1:MET:CE	1.82	1.21
2:T:96:GLN:OE1	1:f:1:MET:CE	1.82	1.21
1:e:128:GLN:OE1	1:f:290:GLU:OE1	1.56	1.21
1:D:62:VAL:CG2	1:G:283:HIS:CG	2.20	1.21
2:S:55:GLU:O	2:T:290:GLU:HG3	1.33	1.21
2:q:89:PRO:HB2	2:r:218:LYS:NZ	1.54	1.21
1:G:56:THR:HB	1:H:286:LEU:CD2	1.69	1.21
1:H:60:LYS:CE	1:I:283:HIS:NE2	2.03	1.21
2:R:34:GLY:CA	2:S:283:TYR:CE2	2.22	1.21
2:T:96:GLN:CG	1:f:1:MET:HE1	1.70	1.21
2:Y:62:VAL:CG1	2:Z:284:ARG:CB	2.07	1.21
1:G:56:THR:CG2	1:H:284:GLU:HB3	1.71	1.20
1:L:56:THR:CG2	1:M:283:HIS:O	1.88	1.20
1:M:127:ASP:C	1:N:290:GLU:CD	1.88	1.20
2:V:96:GLN:CG	1:h:1:MET:HE1	1.70	1.20
2:X:96:GLN:OE1	1:j:1:MET:CE	1.82	1.20
2:S:56:ALA:CB	2:T:284:ARG:HA	1.71	1.20
2:W:96:GLN:CG	1:i:1:MET:HE1	1.70	1.20
2:Y:96:GLN:CG	1:k:1:MET:HE1	1.70	1.20
2:r:56:ALA:HA	2:s:285:ALA:CB	1.71	1.20
2:R:89:PRO:HB2	2:S:218:LYS:CD	1.70	1.20
1:D:62:VAL:HG23	1:G:283:HIS:CB	1.65	1.20
1:M:63:PRO:O	1:N:283:HIS:HB3	1.41	1.20
2:S:220:THR:O	1:e:326:LYS:CE	1.90	1.20
1:G:56:THR:HB	1:H:286:LEU:CG	1.32	1.19
1:M:62:VAL:C	1:N:283:HIS:CA	1.92	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:56:ALA:N	2:T:285:ALA:HB3	1.43	1.19
2:Y:87:PHE:N	2:Z:283:TYR:CE1	2.09	1.19
1:D:56:THR:HG23	1:G:283:HIS:N	1.54	1.19
1:e:60:LYS:HB2	1:f:282:TYR:O	1.39	1.19
2:R:89:PRO:CA	2:S:218:LYS:HZ3	1.55	1.19
2:Y:220:THR:O	1:k:326:LYS:CE	1.90	1.19
2:Z:124:LYS:HD3	2:a:293:GLN:OE1	1.04	1.19
2:R:220:THR:O	1:d:326:LYS:CE	1.90	1.19
2:T:220:THR:O	1:f:326:LYS:CE	1.90	1.19
1:D:89:PRO:HG2	1:G:218:ASP:CB	1.74	1.18
2:W:96:GLN:OE1	1:i:1:MET:CE	1.82	1.18
1:G:35:THR:HG22	1:H:282:TYR:O	1.02	1.18
1:G:128:GLN:HA	1:H:293:ASN:CG	1.63	1.18
2:S:56:ALA:CB	2:T:284:ARG:CA	2.21	1.18
2:U:96:GLN:CG	1:g:1:MET:HE1	1.70	1.18
2:Q:96:GLN:CG	1:c:1:MET:HE1	1.70	1.18
2:X:96:GLN:CG	1:j:1:MET:HE1	1.70	1.18
2:U:220:THR:O	1:g:326:LYS:CE	1.90	1.18
1:e:124:LYS:HE2	1:f:297:GLU:OE1	1.43	1.18
2:r:60:LYS:CD	2:s:283:TYR:N	2.04	1.18
2:Q:220:THR:O	1:c:326:LYS:CE	1.90	1.18
2:W:220:THR:O	1:i:326:LYS:CE	1.90	1.18
1:M:57:GLY:HA3	1:N:372:LEU:CG	1.73	1.17
2:R:96:GLN:CG	1:d:1:MET:HE1	1.70	1.17
2:Y:127:GLU:OE2	2:Z:293:GLN:CA	1.92	1.17
1:D:62:VAL:HG23	1:G:283:HIS:CG	1.77	1.17
1:K:56:THR:HB	1:L:283:HIS:CB	1.71	1.17
2:V:220:THR:O	1:h:326:LYS:CE	1.90	1.17
2:X:220:THR:O	1:j:326:LYS:CE	1.90	1.17
2:B:220:THR:O	1:E:326:LYS:CE	1.90	1.17
1:D:56:THR:HG21	1:G:280:LYS:O	1.40	1.17
1:M:89:PRO:CD	1:N:279:GLU:HB2	1.74	1.17
2:X:221:THR:HA	1:j:326:LYS:HD3	1.25	1.17
1:M:57:GLY:CA	1:N:372:LEU:CD1	2.22	1.17
2:a:57:THR:OG1	2:b:281:GLN:O	1.60	1.17
2:p:57:THR:CG2	2:q:284:ARG:CB	1.74	1.17
1:L:56:THR:HG21	1:M:283:HIS:O	1.38	1.17
2:V:96:GLN:OE1	1:h:1:MET:CE	1.82	1.17
2:Y:96:GLN:OE1	1:k:1:MET:CE	1.82	1.17
2:B:404:PHE:CG	1:E:261:PRO:HA	1.81	1.16
1:G:89:PRO:HG3	1:H:218:ASP:OD1	1.45	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:128:GLN:CB	1:N:285:GLN:HB2	1.74	1.16
2:S:96:GLN:CG	1:e:1:MET:HE1	1.70	1.16
2:r:60:LYS:CG	2:s:283:TYR:HA	1.74	1.16
1:G:57:GLY:N	1:H:286:LEU:HB2	1.44	1.16
2:Y:56:ALA:CB	2:Z:286:LEU:HG	1.74	1.16
1:c:58:SER:HB3	1:d:283:HIS:CE1	1.80	1.16
1:N:84:ARG:NH1	1:O:283:HIS:NE2	1.93	1.16
2:S:56:ALA:N	2:T:285:ALA:CB	2.05	1.16
2:T:221:THR:HA	1:f:326:LYS:HD3	1.25	1.16
2:U:96:GLN:OE1	1:g:1:MET:CE	1.82	1.16
1:D:62:VAL:CG2	1:G:283:HIS:HB2	1.41	1.16
1:G:56:THR:OG1	1:H:286:LEU:CG	1.89	1.16
2:V:96:GLN:CB	1:h:1:MET:HE1	1.76	1.16
2:r:56:ALA:HB3	2:s:283:TYR:O	1.44	1.16
2:W:96:GLN:CB	1:i:1:MET:HE1	1.76	1.16
2:X:406:HIS:CG	1:j:263:PRO:HG3	1.81	1.16
2:T:96:GLN:CB	1:f:1:MET:HE1	1.76	1.15
2:U:96:GLN:CB	1:g:1:MET:HE1	1.76	1.15
1:j:123:ARG:HG3	1:k:297:GLU:OE2	1.45	1.15
2:B:96:GLN:CB	1:E:1:MET:HE1	1.76	1.15
2:B:406:HIS:CG	1:E:263:PRO:HG3	1.81	1.15
2:W:406:HIS:CG	1:i:263:PRO:HG3	1.81	1.15
2:Y:96:GLN:HB3	1:k:1:MET:CE	1.77	1.15
1:G:127:ASP:OD2	1:H:341:ILE:HD11	1.45	1.15
1:G:128:GLN:HG2	1:H:293:ASN:HB2	1.26	1.15
2:Q:96:GLN:CB	1:c:1:MET:HE1	1.76	1.15
2:R:90:ASP:N	2:S:218:LYS:CE	2.02	1.15
2:R:96:GLN:CB	1:d:1:MET:HE1	1.76	1.15
2:R:406:HIS:CG	1:d:263:PRO:HG3	1.81	1.15
2:S:96:GLN:CB	1:e:1:MET:HE1	1.76	1.15
2:S:406:HIS:CG	1:e:263:PRO:HG3	1.81	1.15
1:G:60:LYS:HB3	1:H:284:GLU:O	1.43	1.15
2:X:96:GLN:HB3	1:j:1:MET:CE	1.77	1.15
2:Y:90:ASP:H	2:Z:277:SER:N	1.14	1.15
2:Y:404:PHE:CG	1:k:261:PRO:HA	1.81	1.15
1:G:56:THR:CB	1:H:286:LEU:CD2	2.23	1.15
2:R:96:GLN:HB3	1:d:1:MET:CE	1.77	1.15
2:T:404:PHE:CG	1:f:261:PRO:HA	1.81	1.15
2:V:404:PHE:CG	1:h:261:PRO:HA	1.81	1.15
2:W:96:GLN:HB3	1:i:1:MET:CE	1.77	1.15
2:Y:62:VAL:HG11	2:Z:284:ARG:HB2	1.16	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:96:GLN:CB	1:k:1:MET:HE1	1.76	1.15
1:G:62:VAL:CG1	1:H:284:GLU:OE2	1.89	1.14
1:G:124:LYS:HE3	1:H:298:TYR:N	1.60	1.14
1:M:89:PRO:CD	1:N:280:LYS:H	1.57	1.14
1:M:127:ASP:O	1:N:290:GLU:HG2	1.42	1.14
2:Q:404:PHE:CG	1:c:261:PRO:HA	1.81	1.14
2:U:404:PHE:CG	1:g:261:PRO:HA	1.81	1.14
2:V:406:HIS:CG	1:h:263:PRO:HG3	1.81	1.14
2:Y:221:THR:HA	1:k:326:LYS:HD3	1.25	1.14
1:G:35:THR:CG2	1:H:282:TYR:O	1.94	1.14
1:G:60:LYS:CB	1:H:284:GLU:O	1.94	1.14
2:Q:58:GLY:CA	2:R:282:GLN:O	1.93	1.14
2:S:404:PHE:CG	1:e:261:PRO:HA	1.81	1.14
2:a:57:THR:H	2:b:283:TYR:C	1.52	1.14
2:r:56:ALA:CB	2:s:283:TYR:O	1.93	1.14
2:B:96:GLN:HB3	1:E:1:MET:CE	1.77	1.14
2:B:221:THR:HA	1:E:326:LYS:HD3	1.25	1.14
1:D:127:ASP:OD2	1:G:297:GLU:OE2	1.63	1.14
2:S:96:GLN:HB3	1:e:1:MET:CE	1.77	1.14
2:T:96:GLN:HB3	1:f:1:MET:CE	1.77	1.14
2:W:404:PHE:CG	1:i:261:PRO:HA	1.81	1.14
2:Q:96:GLN:HB3	1:c:1:MET:CE	1.77	1.14
2:S:57:THR:HA	2:T:286:LEU:N	1.41	1.14
2:U:96:GLN:HB3	1:g:1:MET:CE	1.77	1.14
2:Y:406:HIS:CG	1:k:263:PRO:HG3	1.81	1.14
1:j:127:ASP:HB2	1:k:290:GLU:OE2	1.45	1.14
2:r:89:PRO:HB2	2:s:218:LYS:NZ	1.62	1.14
2:R:34:GLY:CA	2:S:283:TYR:OH	1.89	1.14
2:R:404:PHE:CG	1:d:261:PRO:HA	1.81	1.14
2:T:406:HIS:CG	1:f:263:PRO:HG3	1.81	1.14
2:X:404:PHE:CG	1:j:261:PRO:HA	1.81	1.14
1:L:60:LYS:HD3	1:M:283:HIS:CD2	1.83	1.13
2:V:96:GLN:HB3	1:h:1:MET:CE	1.77	1.13
1:G:129:CYS:N	1:H:338:ARG:HH21	1.46	1.13
1:M:128:GLN:HG3	1:N:290:GLU:HG3	1.25	1.13
2:Q:406:HIS:CG	1:c:263:PRO:HG3	1.81	1.13
2:X:96:GLN:CB	1:j:1:MET:HE1	1.76	1.13
2:Z:124:LYS:CD	2:a:293:GLN:OE1	1.95	1.13
1:D:90:GLU:N	1:G:218:ASP:OD2	1.80	1.13
1:G:90:GLU:CB	1:H:215:ARG:HB3	1.78	1.13
2:U:406:HIS:CG	1:g:263:PRO:HG3	1.81	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:33:THR:CG2	2:T:283:TYR:OH	1.76	1.13
2:F:7:LEU:CD2	2:F:66:VAL:HB	1.80	1.12
2:R:179:ASP:O	1:d:352:LYS:HD2	1.49	1.12
2:W:7:LEU:CD2	2:W:66:VAL:HB	1.80	1.12
2:Y:90:ASP:HA	2:Z:216:THR:O	0.96	1.12
2:B:7:LEU:CD2	2:B:66:VAL:HB	1.80	1.12
2:B:179:ASP:O	1:E:352:LYS:HD2	1.49	1.12
2:S:179:ASP:O	1:e:352:LYS:HD2	1.49	1.12
2:r:57:THR:N	2:s:285:ALA:CA	2.02	1.12
2:T:56:ALA:HB1	2:U:283:TYR:O	1.50	1.12
2:Y:179:ASP:O	1:k:352:LYS:HD2	1.50	1.12
1:M:57:GLY:N	1:N:372:LEU:HD11	1.63	1.12
2:V:7:LEU:CD2	2:V:66:VAL:HB	1.80	1.12
2:Y:7:LEU:CD2	2:Y:66:VAL:HB	1.80	1.12
1:M:89:PRO:HG3	1:N:277:SER:CB	1.74	1.11
1:M:128:GLN:HE22	1:N:284:GLU:HB3	1.03	1.11
2:Q:179:ASP:O	1:c:352:LYS:HD2	1.49	1.11
2:X:7:LEU:CD2	2:X:66:VAL:HB	1.80	1.11
2:b:7:LEU:CD2	2:b:66:VAL:HB	1.80	1.11
1:M:89:PRO:HD2	1:N:280:LYS:H	1.12	1.11
2:S:33:THR:HG23	2:T:283:TYR:OH	0.94	1.11
1:K:72:GLN:OE1	2:W:1:MET:HE3	1.50	1.11
1:M:89:PRO:CD	1:N:279:GLU:N	2.14	1.11
2:R:96:GLN:OE1	1:d:1:MET:HE2	0.93	1.11
2:R:179:ASP:O	1:d:352:LYS:CD	1.99	1.11
2:s:7:LEU:CD2	2:s:66:VAL:HB	1.80	1.11
1:G:57:GLY:HA2	1:H:373:ARG:HH21	1.06	1.11
1:M:128:GLN:HB3	1:N:285:GLN:CB	1.78	1.11
2:T:179:ASP:O	1:f:352:LYS:CD	1.99	1.11
2:U:7:LEU:CD2	2:U:66:VAL:HB	1.80	1.11
1:G:90:GLU:CB	1:H:215:ARG:HD2	1.80	1.11
1:G:127:ASP:HA	1:H:338:ARG:NE	1.43	1.11
2:Q:7:LEU:CD2	2:Q:66:VAL:HB	1.80	1.11
2:W:96:GLN:CB	1:i:1:MET:CE	2.29	1.11
2:Y:96:GLN:OE1	1:k:1:MET:HE2	0.93	1.11
2:a:7:LEU:CD2	2:a:66:VAL:HB	1.80	1.11
2:o:7:LEU:CD2	2:o:66:VAL:HB	1.80	1.11
2:q:57:THR:H	2:r:284:ARG:C	1.58	1.11
1:A:72:GLN:OE1	2:B:1:MET:HE3	1.50	1.10
1:C:72:GLN:OE1	2:Q:1:MET:HE3	1.50	1.10
1:E:72:GLN:OE1	2:F:1:MET:HE3	1.50	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:34:GLY:CA	2:S:283:TYR:CZ	2.34	1.10
2:U:179:ASP:O	1:g:352:LYS:HD2	1.49	1.10
2:V:96:GLN:CB	1:h:1:MET:CE	2.29	1.10
2:X:96:GLN:OE1	1:j:1:MET:HE2	0.93	1.10
2:Y:179:ASP:O	1:k:352:LYS:CD	1.99	1.10
2:r:56:ALA:CA	2:s:285:ALA:HB2	1.81	1.10
2:B:179:ASP:O	1:E:352:LYS:CD	1.99	1.10
1:M:89:PRO:CD	1:N:279:GLU:CA	2.29	1.10
1:M:90:GLU:CD	1:N:216:ASN:HA	1.74	1.10
1:N:62:VAL:HG21	1:O:285:GLN:CD	1.77	1.10
2:Q:96:GLN:CB	1:c:1:MET:CE	2.29	1.10
2:S:7:LEU:CD2	2:S:66:VAL:HB	1.80	1.10
2:S:96:GLN:OE1	1:e:1:MET:HE2	0.93	1.10
2:T:56:ALA:CB	2:U:283:TYR:O	1.99	1.10
2:T:96:GLN:OE1	1:f:1:MET:HE2	0.93	1.10
2:V:179:ASP:O	1:h:352:LYS:HD2	1.49	1.10
2:Z:7:LEU:CD2	2:Z:66:VAL:HB	1.80	1.10
1:c:72:GLN:OE1	2:o:1:MET:HE3	1.51	1.10
1:e:120:ASP:CB	1:f:298:TYR:OH	1.99	1.10
2:q:7:LEU:CD2	2:q:66:VAL:HB	1.80	1.10
2:B:96:GLN:OE1	1:E:1:MET:HE2	0.93	1.10
1:D:62:VAL:CG2	1:G:283:HIS:ND1	2.15	1.10
2:Q:179:ASP:O	1:c:352:LYS:CD	1.99	1.10
2:U:96:GLN:OE1	1:g:1:MET:HE2	0.93	1.10
2:p:58:GLY:HA3	2:q:282:GLN:CB	1.71	1.10
2:r:60:LYS:CD	2:s:283:TYR:CA	2.24	1.10
2:B:181:VAL:HG21	1:E:258:ASN:O	1.52	1.10
1:D:72:GLN:OE1	2:R:1:MET:HE3	1.50	1.10
1:G:56:THR:OG1	1:H:286:LEU:HG	0.94	1.10
1:G:57:GLY:CA	1:H:373:ARG:NH2	2.14	1.10
2:R:89:PRO:N	2:S:218:LYS:HZ3	1.48	1.10
2:S:56:ALA:HB1	2:T:284:ARG:HG3	1.10	1.10
2:W:179:ASP:O	1:i:352:LYS:CD	1.99	1.10
2:Y:56:ALA:HB2	2:Z:286:LEU:HG	1.26	1.10
2:Y:62:VAL:CG2	2:Z:281:GLN:O	0.80	1.10
1:d:72:GLN:OE1	2:p:1:MET:HE3	1.51	1.10
2:r:57:THR:HG21	2:s:286:LEU:HG	1.10	1.10
1:G:89:PRO:CG	1:H:280:LYS:HZ2	1.63	1.10
1:N:72:GLN:OE1	2:Z:1:MET:HE3	1.50	1.10
1:P:72:GLN:OE1	2:b:1:MET:HE3	1.50	1.10
2:R:181:VAL:HG21	1:d:258:ASN:O	1.52	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:96:GLN:OE1	1:i:1:MET:HE2	0.93	1.10
2:o:57:THR:HA	2:p:282:GLN:O	1.48	1.10
2:r:89:PRO:CB	2:s:218:LYS:NZ	2.15	1.10
1:G:127:ASP:CA	1:H:338:ARG:NE	2.15	1.09
2:S:55:GLU:C	2:T:285:ALA:HB3	1.77	1.09
2:T:7:LEU:CD2	2:T:66:VAL:HB	1.80	1.09
2:W:181:VAL:HG21	1:i:258:ASN:O	1.52	1.09
2:X:179:ASP:O	1:j:352:LYS:CD	1.99	1.09
1:j:62:VAL:HG21	1:k:283:HIS:HB3	1.31	1.09
2:r:7:LEU:CD2	2:r:66:VAL:HB	1.80	1.09
1:G:57:GLY:HA2	1:H:373:ARG:NH2	1.67	1.09
1:J:72:GLN:OE1	2:V:1:MET:HE3	1.50	1.09
1:M:72:GLN:OE1	2:Y:1:MET:HE3	1.51	1.09
2:Q:96:GLN:OE1	1:c:1:MET:HE2	0.93	1.09
2:S:179:ASP:O	1:e:352:LYS:CD	1.99	1.09
2:U:96:GLN:CB	1:g:1:MET:CE	2.29	1.09
2:U:221:THR:HA	1:g:326:LYS:HD3	1.25	1.09
2:X:96:GLN:CB	1:j:1:MET:CE	2.29	1.09
2:S:181:VAL:HG21	1:e:258:ASN:O	1.52	1.09
2:Y:117:SER:HA	2:Z:299:LYS:CE	1.82	1.09
2:Y:117:SER:C	2:Z:299:LYS:NZ	2.09	1.09
2:a:57:THR:H	2:b:284:ARG:N	1.49	1.09
1:e:72:GLN:OE1	2:q:1:MET:HE3	1.50	1.09
2:p:58:GLY:HA3	2:q:282:GLN:HB3	1.28	1.09
1:G:72:GLN:OE1	2:S:1:MET:HE3	1.50	1.09
1:M:89:PRO:CG	1:N:277:SER:OG	0.79	1.09
2:Q:221:THR:HA	1:c:326:LYS:HD3	1.25	1.09
2:R:7:LEU:CD2	2:R:66:VAL:HB	1.80	1.09
2:R:221:THR:HA	1:d:326:LYS:HD3	1.25	1.09
2:T:179:ASP:O	1:f:352:LYS:HD2	1.49	1.09
2:U:179:ASP:O	1:g:352:LYS:CD	1.99	1.09
2:V:96:GLN:OE1	1:h:1:MET:HE2	0.93	1.09
2:V:221:THR:HA	1:h:326:LYS:HD3	1.25	1.09
2:X:179:ASP:O	1:j:352:LYS:HD2	1.49	1.09
1:d:60:LYS:O	1:e:283:HIS:HA	1.51	1.09
2:p:7:LEU:CD2	2:p:66:VAL:HB	1.80	1.09
2:r:56:ALA:CA	2:s:285:ALA:N	2.16	1.09
2:T:181:VAL:HG21	1:f:258:ASN:O	1.52	1.09
2:W:221:THR:HA	1:i:326:LYS:HD3	1.25	1.09
2:Y:62:VAL:HG21	2:Z:281:GLN:O	1.45	1.09
2:Y:181:VAL:HG21	1:k:258:ASN:O	1.52	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:GLN:CB	1:E:1:MET:CE	2.29	1.08
1:G:124:LYS:CD	1:H:299:SER:OG	2.01	1.08
2:R:96:GLN:CB	1:d:1:MET:CE	2.29	1.08
2:S:221:THR:HA	1:e:326:LYS:HD3	1.25	1.08
2:V:179:ASP:O	1:h:352:LYS:CD	1.99	1.08
2:W:179:ASP:O	1:i:352:LYS:HD2	1.49	1.08
2:Y:90:ASP:N	2:Z:277:SER:N	1.86	1.08
2:Y:96:GLN:CB	1:k:1:MET:CE	2.29	1.08
2:B:179:ASP:O	1:E:352:LYS:HA	1.53	1.08
1:G:60:LYS:N	1:H:284:GLU:O	1.85	1.08
1:M:86:LEU:HG	1:N:283:HIS:NE2	1.67	1.08
1:O:72:GLN:OE1	2:a:1:MET:HE3	1.51	1.08
2:S:96:GLN:CB	1:e:1:MET:CE	2.29	1.08
2:V:179:ASP:O	1:h:352:LYS:HA	1.53	1.08
2:U:96:GLN:CG	1:g:1:MET:HE2	1.80	1.08
2:V:181:VAL:HG21	1:h:258:ASN:O	1.52	1.08
1:f:72:GLN:OE1	2:r:1:MET:HE3	1.50	1.08
1:H:72:GLN:OE1	2:T:1:MET:HE3	1.51	1.08
2:S:56:ALA:HB1	2:T:284:ARG:HG2	1.09	1.08
2:S:179:ASP:O	1:e:352:LYS:HA	1.53	1.08
2:X:181:VAL:HG21	1:j:258:ASN:O	1.52	1.08
1:G:60:LYS:CA	1:H:284:GLU:O	1.94	1.08
1:I:72:GLN:OE1	2:U:1:MET:HE3	1.50	1.08
2:T:96:GLN:CB	1:f:1:MET:CE	2.29	1.08
2:R:179:ASP:O	1:d:352:LYS:HA	1.53	1.07
1:e:55:GLU:N	1:f:285:GLN:NE2	1.73	1.07
1:g:72:GLN:OE1	2:s:1:MET:HE3	1.50	1.07
1:j:88:HIS:CE1	1:k:280:LYS:HD3	1.89	1.07
1:A:234:ILE:HD13	1:A:270:VAL:CG1	1.84	1.07
1:E:234:ILE:HD13	1:E:270:VAL:CG1	1.84	1.07
1:J:234:ILE:HD13	1:J:270:VAL:CG1	1.84	1.07
1:K:234:ILE:HD13	1:K:270:VAL:CG1	1.84	1.07
2:S:33:THR:HG22	2:T:283:TYR:CZ	1.60	1.07
1:g:234:ILE:HD13	1:g:270:VAL:CG1	1.84	1.07
1:i:234:ILE:HD13	1:i:270:VAL:CG1	1.85	1.07
1:I:234:ILE:HD13	1:I:270:VAL:CG1	1.85	1.07
1:J:177:ILE:HD12	1:J:207:GLU:HG3	1.37	1.07
1:L:72:GLN:OE1	2:X:1:MET:HE3	1.51	1.07
1:P:234:ILE:HD13	1:P:270:VAL:CG1	1.85	1.07
2:Q:404:PHE:CZ	1:c:261:PRO:HB3	1.90	1.07
2:U:404:PHE:CZ	1:g:261:PRO:HB3	1.90	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:179:ASP:O	1:j:352:LYS:HA	1.53	1.07
1:f:56:THR:HB	1:g:284:GLU:O	1.54	1.07
1:h:177:ILE:HD12	1:h:207:GLU:HG3	1.37	1.07
1:h:234:ILE:HD13	1:h:270:VAL:CG1	1.85	1.07
2:Q:181:VAL:HG21	1:c:258:ASN:O	1.52	1.07
2:V:404:PHE:CZ	1:h:261:PRO:HB3	1.90	1.07
2:W:404:PHE:CZ	1:i:261:PRO:HB3	1.90	1.07
2:B:404:PHE:CZ	1:E:261:PRO:HB3	1.90	1.07
1:C:57:GLY:HA3	1:D:284:GLU:HA	1.10	1.07
1:D:177:ILE:HD12	1:D:207:GLU:HG3	1.37	1.07
2:Q:179:ASP:O	1:c:352:LYS:HA	1.53	1.07
2:W:179:ASP:O	1:i:352:LYS:HA	1.53	1.07
1:G:49:PHE:CE1	1:H:285:GLN:NE2	2.20	1.06
1:I:177:ILE:HD12	1:I:207:GLU:HG3	1.37	1.06
1:N:84:ARG:HH12	1:O:283:HIS:CE1	1.66	1.06
1:d:177:ILE:HD12	1:d:207:GLU:HG3	1.37	1.06
2:r:56:ALA:HA	2:s:285:ALA:N	1.68	1.06
1:G:177:ILE:HD12	1:G:207:GLU:HG3	1.37	1.06
1:O:234:ILE:HD13	1:O:270:VAL:CG1	1.85	1.06
1:f:89:PRO:HG2	1:g:280:LYS:HE2	1.13	1.06
1:g:177:ILE:HD12	1:g:207:GLU:HG3	1.37	1.06
1:j:234:ILE:HD13	1:j:270:VAL:CG1	1.84	1.06
1:C:234:ILE:HD13	1:C:270:VAL:CG1	1.85	1.06
1:G:62:VAL:HG23	1:H:284:GLU:HA	1.34	1.06
1:G:234:ILE:HD13	1:G:270:VAL:CG1	1.85	1.06
1:L:234:ILE:HD13	1:L:270:VAL:CG1	1.85	1.06
2:T:179:ASP:O	1:f:352:LYS:HA	1.53	1.06
2:U:179:ASP:O	1:g:352:LYS:HA	1.53	1.06
2:Y:124:LYS:HG2	2:Z:294:GLN:HA	1.37	1.06
1:c:234:ILE:HD13	1:c:270:VAL:CG1	1.84	1.06
1:e:177:ILE:HD12	1:e:207:GLU:HG3	1.37	1.06
1:e:234:ILE:HD13	1:e:270:VAL:CG1	1.84	1.06
2:r:60:LYS:HG2	2:s:283:TYR:HA	1.33	1.06
1:K:177:ILE:HD12	1:K:207:GLU:HG3	1.37	1.06
1:M:89:PRO:CD	1:N:277:SER:OG	2.03	1.06
1:N:234:ILE:HD13	1:N:270:VAL:CG1	1.85	1.06
2:S:404:PHE:CZ	1:e:261:PRO:HB3	1.90	1.06
2:U:181:VAL:HG21	1:g:258:ASN:O	1.52	1.06
1:i:177:ILE:HD12	1:i:207:GLU:HG3	1.37	1.06
1:G:74:VAL:O	1:G:78:ILE:HD12	1.56	1.06
1:L:74:VAL:O	1:L:78:ILE:HD12	1.56	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:89:PRO:N	1:N:279:GLU:CB	2.19	1.06
1:M:234:ILE:HD13	1:M:270:VAL:CG1	1.85	1.06
2:T:404:PHE:CZ	1:f:261:PRO:HB3	1.90	1.06
2:V:60:LYS:NZ	2:W:283:TYR:CE2	2.23	1.06
2:X:404:PHE:CZ	1:j:261:PRO:HB3	1.90	1.06
1:e:74:VAL:O	1:e:78:ILE:HD12	1.56	1.06
1:k:234:ILE:HD13	1:k:270:VAL:CG1	1.85	1.06
1:N:74:VAL:O	1:N:78:ILE:HD12	1.56	1.05
2:R:89:PRO:N	2:S:218:LYS:NZ	2.03	1.05
1:j:74:VAL:O	1:j:78:ILE:HD12	1.56	1.05
1:G:56:THR:CB	1:H:286:LEU:HD23	1.85	1.05
1:H:234:ILE:HD13	1:H:270:VAL:CG1	1.85	1.05
1:M:57:GLY:N	1:N:372:LEU:CD1	2.18	1.05
2:V:96:GLN:CG	1:h:1:MET:HE2	1.80	1.05
2:Y:404:PHE:CZ	1:k:261:PRO:HB3	1.90	1.05
1:f:74:VAL:O	1:f:78:ILE:HD12	1.56	1.05
1:f:234:ILE:HD13	1:f:270:VAL:CG1	1.84	1.05
1:G:57:GLY:N	1:H:286:LEU:CB	2.08	1.05
1:H:74:VAL:O	1:H:78:ILE:HD12	1.56	1.05
1:P:177:ILE:HD12	1:P:207:GLU:HG3	1.37	1.05
2:R:404:PHE:CZ	1:d:261:PRO:HB3	1.90	1.05
1:j:88:HIS:NE2	1:k:280:LYS:HD3	1.69	1.05
1:j:123:ARG:CG	1:k:297:GLU:OE2	2.03	1.05
2:p:57:THR:HG23	2:q:284:ARG:HB2	1.06	1.05
1:G:56:THR:HG21	1:H:286:LEU:HD23	1.37	1.05
1:K:57:GLY:N	1:L:283:HIS:HA	1.69	1.05
1:P:74:VAL:O	1:P:78:ILE:HD12	1.56	1.05
2:W:96:GLN:CG	1:i:1:MET:HE2	1.80	1.05
2:Y:96:GLN:CG	1:k:1:MET:HE2	1.80	1.05
2:Y:179:ASP:O	1:k:352:LYS:HA	1.53	1.05
1:f:89:PRO:CG	1:g:280:LYS:HE2	1.86	1.05
1:D:234:ILE:HD13	1:D:270:VAL:CG1	1.84	1.05
1:G:90:GLU:HB2	1:H:215:ARG:CD	1.87	1.05
1:G:129:CYS:N	1:H:338:ARG:NH2	2.01	1.05
1:H:177:ILE:HD12	1:H:207:GLU:HG3	1.37	1.05
1:M:74:VAL:O	1:M:78:ILE:HD12	1.56	1.05
1:M:128:GLN:CA	1:N:290:GLU:HG3	1.87	1.05
2:Y:60:LYS:HE3	2:Z:282:GLN:HG3	1.36	1.05
2:a:57:THR:OG1	2:b:282:GLN:C	2.00	1.05
1:d:60:LYS:O	1:e:283:HIS:CA	2.05	1.05
1:f:177:ILE:HD12	1:f:207:GLU:HG3	1.37	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:270:VAL:HG22	1:J:378:LEU:HD23	1.05	1.04
2:T:56:ALA:HB1	2:U:283:TYR:C	1.81	1.04
2:W:222:PRO:HD2	1:i:326:LYS:HD2	1.38	1.04
2:X:96:GLN:CG	1:j:1:MET:HE2	1.80	1.04
1:d:234:ILE:HD13	1:d:270:VAL:CG1	1.85	1.04
1:h:270:VAL:HG22	1:h:378:LEU:HD23	1.05	1.04
1:j:88:HIS:CE1	1:k:280:LYS:CD	2.39	1.04
1:k:74:VAL:O	1:k:78:ILE:HD12	1.56	1.04
1:D:270:VAL:HG22	1:D:378:LEU:HD23	1.05	1.04
1:J:74:VAL:O	1:J:78:ILE:HD12	1.56	1.04
1:O:74:VAL:O	1:O:78:ILE:HD12	1.56	1.04
2:S:404:PHE:CE1	1:e:261:PRO:HB3	1.92	1.04
2:T:404:PHE:CE1	1:f:261:PRO:HB3	1.92	1.04
2:X:404:PHE:CE1	1:j:261:PRO:HB3	1.92	1.04
1:h:74:VAL:O	1:h:78:ILE:HD12	1.56	1.04
1:D:62:VAL:HG21	1:G:280:LYS:HA	1.40	1.04
1:D:74:VAL:O	1:D:78:ILE:HD12	1.56	1.04
1:M:57:GLY:HA2	1:N:372:LEU:HD11	1.33	1.04
1:M:89:PRO:CD	1:N:279:GLU:CB	2.35	1.04
1:O:58:SER:HB2	1:P:282:TYR:HB3	1.34	1.04
1:O:270:VAL:HG22	1:O:378:LEU:HD23	1.05	1.04
1:P:270:VAL:HG22	1:P:378:LEU:HD23	1.04	1.04
2:Y:90:ASP:N	2:Z:277:SER:H	1.43	1.04
1:d:74:VAL:O	1:d:78:ILE:HD12	1.56	1.04
1:d:270:VAL:HG22	1:d:378:LEU:HD23	1.05	1.04
1:i:270:VAL:HG22	1:i:378:LEU:HD23	1.05	1.04
1:j:56:THR:HG21	1:k:283:HIS:HA	1.36	1.04
1:A:74:VAL:O	1:A:78:ILE:HD12	1.56	1.04
2:B:222:PRO:HD2	1:E:326:LYS:HD2	1.38	1.04
1:D:56:THR:HG21	1:G:280:LYS:C	1.62	1.04
1:D:60:LYS:HG2	1:G:283:HIS:ND1	1.70	1.04
1:E:74:VAL:O	1:E:78:ILE:HD12	1.56	1.04
1:K:270:VAL:HG22	1:K:378:LEU:HD23	1.05	1.04
2:S:56:ALA:HB1	2:T:284:ARG:CB	1.87	1.04
2:T:96:GLN:HB3	1:f:1:MET:HE1	1.36	1.04
2:U:222:PRO:HD2	1:g:326:LYS:HD2	1.39	1.04
2:Y:34:GLY:CA	2:Z:282:GLN:CG	2.36	1.04
1:G:34:GLY:CA	1:H:283:HIS:HB3	1.86	1.04
1:G:57:GLY:H	1:H:286:LEU:CB	1.54	1.04
2:R:404:PHE:CE1	1:d:261:PRO:HB3	1.92	1.04
1:j:127:ASP:CB	1:k:290:GLU:OE2	2.06	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:404:PHE:CE1	1:E:261:PRO:HB3	1.92	1.03
2:Q:222:PRO:HD2	1:c:326:LYS:HD2	1.39	1.03
2:V:404:PHE:CE1	1:h:261:PRO:HB3	1.92	1.03
1:g:74:VAL:O	1:g:78:ILE:HD12	1.56	1.03
2:r:56:ALA:HB1	2:s:284:ARG:HA	1.37	1.03
1:A:177:ILE:HD12	1:A:207:GLU:HG3	1.37	1.03
1:C:57:GLY:CA	1:D:284:GLU:HA	1.84	1.03
1:D:62:VAL:CG2	1:G:283:HIS:CB	2.08	1.03
1:E:177:ILE:HD12	1:E:207:GLU:HG3	1.37	1.03
2:F:7:LEU:HD23	2:F:66:VAL:HB	1.39	1.03
1:I:74:VAL:O	1:I:78:ILE:HD12	1.56	1.03
1:L:270:VAL:CG2	1:L:378:LEU:HD23	1.89	1.03
1:M:89:PRO:CB	1:N:277:SER:OG	2.06	1.03
2:R:62:VAL:N	2:S:283:TYR:HB3	1.73	1.03
2:X:7:LEU:HD23	2:X:66:VAL:HB	1.39	1.03
2:Y:404:PHE:CE1	1:k:261:PRO:HB3	1.92	1.03
1:c:74:VAL:O	1:c:78:ILE:HD12	1.56	1.03
2:B:7:LEU:HD23	2:B:66:VAL:HB	1.39	1.03
1:C:74:VAL:O	1:C:78:ILE:HD12	1.56	1.03
1:G:60:LYS:CE	1:H:283:HIS:HB2	1.88	1.03
1:G:117:SER:O	1:H:298:TYR:OH	1.76	1.03
1:G:270:VAL:CG2	1:G:378:LEU:HD23	1.89	1.03
1:H:270:VAL:HG22	1:H:378:LEU:HD23	1.05	1.03
2:R:56:ALA:HB3	2:S:283:TYR:N	1.66	1.03
2:U:404:PHE:CE1	1:g:261:PRO:HB3	1.92	1.03
2:a:7:LEU:HD23	2:a:66:VAL:HB	1.39	1.03
1:e:270:VAL:CG2	1:e:378:LEU:HD23	1.89	1.03
1:f:270:VAL:HG22	1:f:378:LEU:HD23	1.04	1.03
1:j:270:VAL:CG2	1:j:378:LEU:HD23	1.89	1.03
1:D:234:ILE:HD13	1:D:270:VAL:HG12	1.41	1.03
1:M:90:GLU:CB	1:N:218:ASP:OD1	2.07	1.03
1:M:128:GLN:N	1:N:290:GLU:OE1	1.71	1.03
2:Q:7:LEU:HD23	2:Q:66:VAL:HB	1.39	1.03
2:Q:404:PHE:CE1	1:c:261:PRO:HB3	1.92	1.03
1:d:234:ILE:HD13	1:d:270:VAL:HG12	1.41	1.03
1:C:270:VAL:CG2	1:C:378:LEU:HD23	1.89	1.03
1:D:270:VAL:CG2	1:D:378:LEU:HD23	1.89	1.03
1:E:270:VAL:HG22	1:E:378:LEU:HD23	1.05	1.03
1:K:74:VAL:O	1:K:78:ILE:HD12	1.56	1.03
1:K:270:VAL:CG2	1:K:378:LEU:HD23	1.89	1.03
1:M:177:ILE:HD12	1:M:207:GLU:HG3	1.37	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:7:LEU:HD23	2:Y:66:VAL:HB	1.39	1.03
1:c:270:VAL:CG2	1:c:378:LEU:HD23	1.89	1.03
1:d:270:VAL:CG2	1:d:378:LEU:HD23	1.89	1.03
1:e:128:GLN:CD	1:f:290:GLU:OE1	1.92	1.03
1:i:74:VAL:O	1:i:78:ILE:HD12	1.56	1.03
1:i:270:VAL:CG2	1:i:378:LEU:HD23	1.89	1.03
1:k:177:ILE:HD12	1:k:207:GLU:HG3	1.37	1.03
2:o:7:LEU:HD23	2:o:66:VAL:HB	1.39	1.03
1:A:270:VAL:HG22	1:A:378:LEU:HD23	1.04	1.02
1:G:90:GLU:HB2	1:H:215:ARG:HD2	1.07	1.02
1:H:60:LYS:HE2	1:I:283:HIS:CE1	1.95	1.02
1:L:177:ILE:HD12	1:L:207:GLU:HG3	1.37	1.02
1:M:127:ASP:HB3	1:N:290:GLU:HA	1.37	1.02
1:M:270:VAL:CG2	1:M:378:LEU:HD23	1.89	1.02
2:W:404:PHE:CE1	1:i:261:PRO:HB3	1.92	1.02
1:f:234:ILE:HD13	1:f:270:VAL:HG12	1.41	1.02
1:g:270:VAL:HG22	1:g:378:LEU:HD23	1.04	1.02
1:h:270:VAL:CG2	1:h:378:LEU:HD23	1.89	1.02
1:j:116:ASP:HB3	1:k:298:TYR:CE1	1.94	1.02
1:k:270:VAL:CG2	1:k:378:LEU:HD23	1.89	1.02
1:H:234:ILE:HD13	1:H:270:VAL:HG12	1.41	1.02
1:I:270:VAL:HG22	1:I:378:LEU:HD23	1.04	1.02
1:J:270:VAL:CG2	1:J:378:LEU:HD23	1.89	1.02
1:O:177:ILE:HD12	1:O:207:GLU:HG3	1.37	1.02
2:R:60:LYS:CB	2:S:282:GLN:C	2.21	1.02
2:V:222:PRO:HD2	1:h:326:LYS:HD2	1.39	1.02
2:Y:222:PRO:HD2	1:k:326:LYS:HD2	1.39	1.02
1:f:270:VAL:CG2	1:f:378:LEU:HD23	1.89	1.02
1:j:56:THR:HG21	1:k:283:HIS:CA	1.90	1.02
1:j:177:ILE:HD12	1:j:207:GLU:HG3	1.37	1.02
2:p:56:ALA:HB3	2:q:283:TYR:HB3	1.39	1.02
1:C:177:ILE:HD12	1:C:207:GLU:HG3	1.37	1.02
1:G:128:GLN:HA	1:H:293:ASN:ND2	1.72	1.02
1:H:270:VAL:CG2	1:H:378:LEU:HD23	1.89	1.02
1:M:89:PRO:HG3	1:N:277:SER:OG	1.20	1.02
1:N:270:VAL:CG2	1:N:378:LEU:HD23	1.89	1.02
1:A:270:VAL:CG2	1:A:378:LEU:HD23	1.89	1.02
1:D:56:THR:HG23	1:G:283:HIS:H	0.92	1.02
1:D:120:ASP:OD2	1:G:215:ARG:HD2	1.57	1.02
1:E:270:VAL:CG2	1:E:378:LEU:HD23	1.89	1.02
1:G:34:GLY:HA3	1:H:283:HIS:HB3	1.03	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:270:VAL:HG22	1:N:378:LEU:HD23	1.05	1.02
2:R:34:GLY:CA	2:S:283:TYR:HE2	1.67	1.02
1:c:177:ILE:HD12	1:c:207:GLU:HG3	1.37	1.02
1:G:56:THR:HG23	1:H:284:GLU:HB3	1.41	1.02
1:G:60:LYS:HZ1	1:H:283:HIS:CB	1.71	1.02
1:G:234:ILE:HD13	1:G:270:VAL:HG12	1.41	1.02
1:L:234:ILE:HD13	1:L:270:VAL:HG12	1.41	1.02
1:M:87:PHE:HA	1:N:283:HIS:ND1	1.64	1.02
1:M:89:PRO:CD	1:N:280:LYS:N	2.01	1.02
2:V:224:TYR:CE2	1:h:248:LEU:HD21	1.95	1.02
2:b:7:LEU:HD23	2:b:66:VAL:HB	1.39	1.02
1:j:234:ILE:HD13	1:j:270:VAL:HG12	1.41	1.02
2:r:57:THR:HG21	2:s:286:LEU:CG	1.83	1.02
2:B:224:TYR:CE2	1:E:248:LEU:HD21	1.95	1.01
1:M:270:VAL:HG22	1:M:378:LEU:HD23	1.05	1.01
2:R:60:LYS:HB2	2:S:282:GLN:HB3	1.26	1.01
2:U:224:TYR:CE2	1:g:248:LEU:HD21	1.95	1.01
1:e:234:ILE:HD13	1:e:270:VAL:HG12	1.41	1.01
1:G:56:THR:CG2	1:H:286:LEU:CD2	2.38	1.01
1:M:62:VAL:HG21	1:N:281:ALA:C	1.58	1.01
1:P:234:ILE:HD13	1:P:270:VAL:HG12	1.41	1.01
2:T:224:TYR:CE2	1:f:248:LEU:HD21	1.95	1.01
2:W:7:LEU:HD23	2:W:66:VAL:HB	1.39	1.01
2:Z:7:LEU:HD23	2:Z:66:VAL:HB	1.39	1.01
1:k:270:VAL:HG22	1:k:378:LEU:HD23	1.05	1.01
1:C:270:VAL:HG22	1:C:378:LEU:HD23	1.04	1.01
1:G:89:PRO:CG	1:H:280:LYS:NZ	2.22	1.01
1:G:270:VAL:HG22	1:G:378:LEU:HD23	1.04	1.01
1:M:128:GLN:CA	1:N:290:GLU:CG	2.39	1.01
2:R:222:PRO:HD2	1:d:326:LYS:HD2	1.39	1.01
2:Y:96:GLN:HB3	1:k:1:MET:HE1	1.36	1.01
1:c:270:VAL:HG22	1:c:378:LEU:HD23	1.05	1.01
1:J:234:ILE:HD13	1:J:270:VAL:HG12	1.41	1.01
1:M:57:GLY:H	1:N:372:LEU:HG	1.26	1.01
2:Q:224:TYR:CE2	1:c:248:LEU:HD21	1.95	1.01
2:S:224:TYR:CE2	1:e:248:LEU:HD21	1.95	1.01
2:T:7:LEU:HD23	2:T:66:VAL:HB	1.39	1.01
2:Y:34:GLY:HA3	2:Z:282:GLN:HG2	1.03	1.01
2:Y:56:ALA:HA	2:Z:286:LEU:HB2	1.40	1.01
2:Y:128:SER:HA	2:Z:290:GLU:N	1.71	1.01
1:e:270:VAL:HG22	1:e:378:LEU:HD23	1.05	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:270:VAL:CG2	1:g:378:LEU:HD23	1.89	1.01
1:h:234:ILE:HD13	1:h:270:VAL:HG12	1.41	1.01
2:r:7:LEU:HD23	2:r:66:VAL:HB	1.39	1.01
1:l:270:VAL:CG2	1:l:378:LEU:HD23	1.89	1.01
1:l:128:GLN:CG	1:m:290:GLU:OE1	2.08	1.01
1:m:63:PRO:N	1:n:283:HIS:HA	1.76	1.01
1:p:270:VAL:CG2	1:p:378:LEU:HD23	1.89	1.01
2:r:7:LEU:HD23	2:r:66:VAL:HB	1.39	1.01
2:t:222:PRO:HD2	1:f:326:LYS:HD2	1.38	1.01
2:x:224:TYR:CE2	1:j:248:LEU:HD21	1.95	1.01
2:p:7:LEU:HD23	2:p:66:VAL:HB	1.39	1.01
2:r:60:LYS:HB3	2:s:282:GLN:O	1.57	1.01
1:l:234:ILE:HD13	1:l:270:VAL:HG12	1.41	1.00
1:m:57:GLY:CA	1:n:372:LEU:CG	2.40	1.00
1:o:270:VAL:CG2	1:o:378:LEU:HD23	1.89	1.00
2:r:90:ASP:N	2:s:218:LYS:HE2	1.73	1.00
2:r:96:GLN:CG	1:d:1:MET:HE2	1.80	1.00
1:g:234:ILE:HD13	1:g:270:VAL:HG12	1.41	1.00
1:j:270:VAL:HG22	1:j:378:LEU:HD23	1.05	1.00
1:l:270:VAL:HG22	1:l:378:LEU:HD23	1.05	1.00
2:r:224:TYR:CE2	1:d:248:LEU:HD21	1.95	1.00
2:x:222:PRO:HD2	1:j:326:LYS:HD2	1.38	1.00
2:b:96:GLN:HB3	1:e:1:MET:HE1	1.36	1.00
1:g:127:ASP:CG	1:h:341:ILE:HD11	1.86	1.00
1:n:177:ILE:HD12	1:n:207:GLU:HG3	1.37	1.00
2:u:96:GLN:HB3	1:g:1:MET:HE1	1.36	1.00
2:w:224:TYR:CE2	1:i:248:LEU:HD21	1.95	1.00
2:y:224:TYR:CE2	1:k:248:LEU:HD21	1.95	1.00
1:e:55:GLU:CA	1:f:285:GLN:NE2	2.21	1.00
2:r:60:LYS:CD	2:s:282:GLN:O	2.05	1.00
1:m:234:ILE:HD13	1:m:270:VAL:HG12	1.41	1.00
2:y:57:THR:HA	2:z:372:LYS:HB2	1.42	1.00
2:r:89:PRO:HB2	2:s:218:LYS:HD3	1.00	1.00
2:y:62:VAL:HG23	2:z:281:GLN:O	1.57	1.00
2:r:60:LYS:CD	2:s:283:TYR:HA	1.84	1.00
2:y:90:ASP:OD1	2:z:276:THR:C	2.04	1.00
1:k:234:ILE:HD13	1:k:270:VAL:HG12	1.41	1.00
1:d:89:PRO:HG2	1:g:218:ASP:CG	1.85	1.00
2:s:7:LEU:HD23	2:s:66:VAL:HB	1.39	1.00
1:d:56:THR:CA	1:e:284:GLU:O	2.09	1.00
2:q:7:LEU:HD23	2:q:66:VAL:HB	1.39	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ILE:HD13	1:A:270:VAL:HG12	1.41	0.99
1:D:124:LYS:NZ	1:G:215:ARG:NH2	2.07	0.99
1:N:234:ILE:HD13	1:N:270:VAL:HG12	1.41	0.99
2:S:222:PRO:HD2	1:e:326:LYS:HD2	1.39	0.99
1:E:234:ILE:HD13	1:E:270:VAL:HG12	1.41	0.99
1:M:89:PRO:HD3	1:N:279:GLU:H	1.27	0.99
1:c:234:ILE:HD13	1:c:270:VAL:HG12	1.41	0.99
1:C:234:ILE:HD13	1:C:270:VAL:HG12	1.41	0.99
1:D:124:LYS:HZ1	1:G:215:ARG:HH21	1.00	0.99
2:Q:96:GLN:CG	1:c:1:MET:HE2	1.80	0.99
2:r:56:ALA:HA	2:s:285:ALA:HB2	1.32	0.99
2:V:7:LEU:HD23	2:V:66:VAL:HB	1.39	0.99
2:s:7:LEU:HD23	2:s:66:VAL:HB	1.39	0.99
2:R:172:VAL:HG22	2:R:173:PRO:HD2	1.44	0.99
2:W:172:VAL:HG22	2:W:173:PRO:HD2	1.44	0.99
2:Y:172:VAL:HG22	2:Y:173:PRO:HD2	1.44	0.99
2:p:172:VAL:HG22	2:p:173:PRO:HD2	1.44	0.99
2:U:7:LEU:HD23	2:U:66:VAL:HB	1.39	0.99
1:O:234:ILE:HD13	1:O:270:VAL:HG12	1.41	0.99
2:Q:179:ASP:C	1:c:352:LYS:HA	1.88	0.99
2:R:62:VAL:CG2	2:S:283:TYR:HB2	1.92	0.99
2:X:179:ASP:C	1:j:352:LYS:HA	1.87	0.99
1:G:57:GLY:N	1:H:286:LEU:C	2.09	0.99
1:M:62:VAL:HG21	1:N:281:ALA:O	1.62	0.99
2:r:60:LYS:HB2	2:s:282:GLN:O	1.62	0.99
2:B:179:ASP:C	1:E:352:LYS:HA	1.87	0.98
2:V:172:VAL:HG22	2:V:173:PRO:HD2	1.44	0.98
1:L:128:GLN:HG2	1:M:290:GLU:OE1	1.62	0.98
2:R:179:ASP:C	1:d:352:LYS:HA	1.88	0.98
1:M:64:ARG:NH2	1:N:285:GLN:CG	1.71	0.98
2:T:179:ASP:C	1:f:352:LYS:HA	1.87	0.98
1:M:128:GLN:N	1:N:290:GLU:HG3	1.78	0.98
2:T:96:GLN:CG	1:f:1:MET:HE2	1.80	0.98
2:X:172:VAL:HG22	2:X:173:PRO:HD2	1.44	0.98
2:a:172:VAL:HG22	2:a:173:PRO:HD2	1.44	0.98
2:V:96:GLN:HB3	1:h:1:MET:HE1	1.36	0.98
2:a:57:THR:N	2:b:283:TYR:C	2.11	0.98
1:D:62:VAL:HG23	1:G:283:HIS:ND1	1.75	0.98
1:O:58:SER:CB	1:P:282:TYR:HB3	1.94	0.98
2:Q:172:VAL:HG22	2:Q:173:PRO:HD2	1.44	0.98
2:R:60:LYS:HB3	2:S:282:GLN:CB	1.73	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:179:ASP:C	1:e:352:LYS:HA	1.87	0.98
2:V:179:ASP:C	1:h:352:LYS:HA	1.88	0.98
2:o:172:VAL:HG22	2:o:173:PRO:HD2	1.44	0.98
2:W:179:ASP:C	1:i:352:LYS:HA	1.87	0.98
2:R:89:PRO:C	2:S:218:LYS:HZ3	1.70	0.97
2:U:179:ASP:C	1:g:352:LYS:HA	1.88	0.97
2:q:172:VAL:HG22	2:q:173:PRO:HD2	1.44	0.97
1:M:128:GLN:HG3	1:N:290:GLU:CG	1.94	0.97
2:S:172:VAL:HG22	2:S:173:PRO:HD2	1.44	0.97
2:Y:179:ASP:C	1:k:352:LYS:HA	1.87	0.97
2:B:96:GLN:CG	1:E:1:MET:HE2	1.80	0.97
1:G:49:PHE:HE1	1:H:285:GLN:HE22	1.04	0.97
1:M:62:VAL:O	1:N:283:HIS:HA	1.61	0.97
2:S:96:GLN:CG	1:e:1:MET:HE2	1.80	0.97
1:D:56:THR:N	1:G:282:TYR:C	2.22	0.97
1:c:58:SER:HA	1:d:282:TYR:HB3	1.45	0.97
1:K:234:ILE:HD13	1:K:270:VAL:HG12	1.41	0.97
2:R:403:ALA:CA	1:d:262:TYR:CE1	2.48	0.97
2:Y:60:LYS:HE3	2:Z:282:GLN:CG	1.95	0.97
2:Y:87:PHE:CA	2:Z:283:TYR:CD1	2.46	0.97
2:U:172:VAL:HG22	2:U:173:PRO:HD2	1.44	0.97
1:i:234:ILE:HD13	1:i:270:VAL:HG12	1.41	0.97
2:s:172:VAL:HG22	2:s:173:PRO:HD2	1.44	0.97
2:B:403:ALA:CA	1:E:262:TYR:CE1	2.48	0.97
2:Y:86:ILE:HG13	2:Z:282:GLN:CB	1.95	0.97
1:M:125:MET:SD	1:N:284:GLU:CD	2.48	0.97
2:Q:96:GLN:HB3	1:c:1:MET:HE1	1.36	0.97
2:R:60:LYS:CB	2:S:282:GLN:HB3	1.77	0.97
2:r:89:PRO:HB2	2:s:218:LYS:HZ1	1.17	0.97
2:r:172:VAL:HG22	2:r:173:PRO:HD2	1.44	0.97
2:B:406:HIS:CB	1:E:263:PRO:HG3	1.95	0.96
1:M:62:VAL:HG11	1:N:280:LYS:O	1.65	0.96
2:R:62:VAL:HG23	2:S:283:TYR:HB2	1.00	0.96
2:W:403:ALA:CA	1:i:262:TYR:CE1	2.48	0.96
2:X:406:HIS:CB	1:j:263:PRO:HG3	1.95	0.96
2:B:398:MET:CG	1:E:346:TRP:O	2.13	0.96
1:M:125:MET:SD	1:N:284:GLU:OE1	2.23	0.96
2:Q:398:MET:CG	1:c:346:TRP:O	2.13	0.96
2:Z:172:VAL:HG22	2:Z:173:PRO:HD2	1.44	0.96
2:T:172:VAL:HG22	2:T:173:PRO:HD2	1.44	0.96
1:j:116:ASP:HA	1:k:298:TYR:OH	1.65	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:403:ALA:CA	1:e:262:TYR:CE1	2.48	0.96
2:X:403:ALA:CA	1:j:262:TYR:CE1	2.48	0.96
2:Q:406:HIS:CB	1:c:263:PRO:HG3	1.95	0.96
1:G:60:LYS:HZ3	1:H:280:LYS:HA	1.28	0.96
1:L:60:LYS:CD	1:M:283:HIS:CD2	2.47	0.96
2:R:398:MET:CG	1:d:346:TRP:O	2.13	0.96
2:V:398:MET:CG	1:h:346:TRP:O	2.13	0.96
1:d:56:THR:HA	1:e:284:GLU:O	1.31	0.96
1:j:128:GLN:N	1:k:290:GLU:OE1	1.96	0.96
1:G:60:LYS:NZ	1:H:283:HIS:CB	2.27	0.96
2:W:398:MET:CG	1:i:346:TRP:O	2.13	0.96
2:W:406:HIS:CB	1:i:263:PRO:HG3	1.95	0.96
2:b:172:VAL:HG22	2:b:173:PRO:HD2	1.44	0.96
2:S:55:GLU:O	2:T:290:GLU:CG	2.13	0.96
2:Y:403:ALA:CA	1:k:262:TYR:CE1	2.48	0.96
1:M:89:PRO:HA	1:N:279:GLU:CB	1.93	0.96
2:R:89:PRO:CB	2:S:218:LYS:HD3	1.96	0.96
2:T:403:ALA:CA	1:f:262:TYR:CE1	2.48	0.96
2:X:398:MET:CG	1:j:346:TRP:O	2.13	0.96
1:G:56:THR:HG21	1:H:286:LEU:CD2	1.96	0.95
2:R:406:HIS:CB	1:d:263:PRO:HG3	1.95	0.95
2:U:398:MET:CG	1:g:346:TRP:O	2.13	0.95
2:T:398:MET:CG	1:f:346:TRP:O	2.13	0.95
2:U:403:ALA:CA	1:g:262:TYR:CE1	2.48	0.95
1:j:120:ASP:OD1	1:k:299:SER:OG	1.84	0.95
1:M:90:GLU:HB3	1:N:218:ASP:OD1	1.65	0.95
2:p:56:ALA:HB3	2:q:283:TYR:CB	1.95	0.95
1:L:60:LYS:HD3	1:M:283:HIS:HD2	1.20	0.95
2:Q:403:ALA:CA	1:c:262:TYR:CE1	2.48	0.95
2:V:403:ALA:CA	1:h:262:TYR:CE1	2.48	0.95
1:G:34:GLY:HA3	1:H:283:HIS:CB	1.95	0.95
1:G:61:HIS:CD2	1:H:285:GLN:NE2	2.34	0.95
2:S:406:HIS:CB	1:e:263:PRO:HG3	1.95	0.95
2:Y:398:MET:CG	1:k:346:TRP:O	2.13	0.95
2:Y:406:HIS:CB	1:k:263:PRO:HG3	1.95	0.95
1:e:60:LYS:CB	1:f:282:TYR:O	2.14	0.95
2:F:172:VAL:HG22	2:F:173:PRO:HD2	1.44	0.95
1:G:128:GLN:CA	1:H:293:ASN:CG	2.33	0.95
2:S:398:MET:CG	1:e:346:TRP:O	2.13	0.95
2:U:404:PHE:CE2	1:g:261:PRO:HA	2.02	0.95
2:r:62:VAL:HG22	2:s:283:TYR:HB3	1.47	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:VAL:HG22	2:B:173:PRO:HD2	1.44	0.95
1:D:60:LYS:CG	1:G:283:HIS:CE1	2.49	0.95
1:M:88:HIS:HD1	1:N:281:ALA:N	1.65	0.95
2:T:406:HIS:CB	1:f:263:PRO:HG3	1.95	0.95
2:U:406:HIS:CB	1:g:263:PRO:HG3	1.95	0.95
2:S:404:PHE:CE2	1:e:261:PRO:HA	2.02	0.95
1:M:128:GLN:CB	1:N:290:GLU:HG3	1.96	0.95
1:N:84:ARG:HH12	1:O:283:HIS:HE1	1.10	0.95
2:V:406:HIS:CB	1:h:263:PRO:HG3	1.95	0.95
1:c:60:LYS:HB3	1:d:283:HIS:NE2	1.81	0.95
2:T:404:PHE:CE2	1:f:261:PRO:HA	2.02	0.94
2:Y:117:SER:C	2:Z:299:LYS:HZ1	1.67	0.94
2:Y:404:PHE:CE2	1:k:261:PRO:HA	2.02	0.94
1:e:55:GLU:HB3	1:f:285:GLN:NE2	1.80	0.94
1:E:82:PRO:HD2	1:E:83:TYR:H	1.32	0.94
1:L:82:PRO:HD2	1:L:83:TYR:H	1.32	0.94
2:S:57:THR:CA	2:T:286:LEU:N	1.92	0.94
1:A:82:PRO:HD2	1:A:83:TYR:H	1.32	0.94
1:G:128:GLN:HG3	1:H:293:ASN:HB3	1.48	0.94
1:j:82:PRO:HD2	1:j:83:TYR:H	1.32	0.94
1:j:128:GLN:N	1:k:290:GLU:CD	2.25	0.94
1:G:128:GLN:CG	1:H:293:ASN:CB	2.46	0.94
2:R:404:PHE:CE2	1:d:261:PRO:HA	2.02	0.94
2:V:404:PHE:CE2	1:h:261:PRO:HA	2.02	0.94
1:k:82:PRO:HD2	1:k:83:TYR:H	1.32	0.94
1:G:82:PRO:HD2	1:G:83:TYR:H	1.32	0.94
1:M:82:PRO:HD2	1:M:83:TYR:H	1.32	0.94
2:X:96:GLN:HB3	1:j:1:MET:HE1	1.36	0.94
1:C:82:PRO:HD2	1:C:83:TYR:H	1.32	0.94
1:c:82:PRO:HD2	1:c:83:TYR:H	1.32	0.94
1:e:82:PRO:HD2	1:e:83:TYR:H	1.32	0.94
2:r:60:LYS:HD3	2:s:282:GLN:O	1.66	0.94
1:L:70:LEU:HD23	1:L:114:LEU:HD12	1.50	0.94
2:X:57:THR:OG1	2:Y:282:GLN:O	1.86	0.94
2:Y:87:PHE:HA	2:Z:283:TYR:CD1	2.02	0.94
1:j:70:LEU:HD23	1:j:114:LEU:HD12	1.50	0.94
2:r:57:THR:CG2	2:s:286:LEU:HG	1.98	0.94
2:B:404:PHE:CE2	1:E:261:PRO:CA	2.51	0.94
1:D:270:VAL:HG22	1:D:378:LEU:CD2	1.98	0.94
1:G:56:THR:HG21	1:H:284:GLU:HB3	1.46	0.94
1:H:64:ARG:HA	1:H:125:MET:CE	1.98	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:128:GLN:CD	1:N:286:LEU:N	2.24	0.94
2:Q:60:LYS:HB3	2:R:283:TYR:CE2	2.02	0.94
2:Q:404:PHE:CE2	1:c:261:PRO:HA	2.02	0.94
2:R:60:LYS:HB3	2:S:283:TYR:N	1.83	0.94
2:W:404:PHE:CE2	1:i:261:PRO:CA	2.51	0.94
2:W:404:PHE:CE2	1:i:261:PRO:HA	2.02	0.94
2:X:404:PHE:CE2	1:j:261:PRO:HA	2.02	0.94
1:d:270:VAL:HG22	1:d:378:LEU:CD2	1.98	0.94
1:f:64:ARG:HA	1:f:125:MET:CE	1.98	0.94
1:h:270:VAL:HG22	1:h:378:LEU:CD2	1.98	0.94
1:j:64:ARG:HA	1:j:125:MET:CE	1.98	0.94
1:k:64:ARG:HA	1:k:125:MET:CE	1.98	0.94
1:k:64:ARG:HA	1:k:125:MET:HE2	1.50	0.94
2:r:89:PRO:CB	2:s:218:LYS:HZ2	1.77	0.94
1:l:64:ARG:HA	1:l:125:MET:CE	1.98	0.94
1:J:270:VAL:HG22	1:J:378:LEU:CD2	1.98	0.94
1:K:64:ARG:HA	1:K:125:MET:HE2	1.50	0.94
1:K:270:VAL:HG22	1:K:378:LEU:CD2	1.98	0.94
1:L:64:ARG:HA	1:L:125:MET:HE2	1.50	0.94
1:L:64:ARG:HA	1:L:125:MET:CE	1.98	0.94
1:M:64:ARG:HA	1:M:125:MET:CE	1.98	0.94
1:M:64:ARG:HA	1:M:125:MET:HE2	1.50	0.94
1:N:64:ARG:HA	1:N:125:MET:CE	1.98	0.94
2:Q:58:GLY:HA2	2:R:282:GLN:O	1.09	0.94
2:R:404:PHE:CE2	1:d:261:PRO:CA	2.51	0.94
2:S:96:GLN:HB3	1:e:1:MET:HE1	1.36	0.94
2:S:128:SER:OG	2:T:293:GLN:CB	2.04	0.94
1:g:64:ARG:HA	1:g:125:MET:CE	1.98	0.94
1:i:64:ARG:HA	1:i:125:MET:HE2	1.50	0.94
1:j:64:ARG:HA	1:j:125:MET:HE2	1.50	0.94
2:B:404:PHE:CE2	1:E:261:PRO:HA	2.02	0.94
1:G:89:PRO:CG	1:H:215:ARG:O	2.14	0.94
1:J:60:LYS:CE	1:K:283:HIS:CD2	2.49	0.94
1:O:82:PRO:HD2	1:O:83:TYR:H	1.32	0.94
2:U:404:PHE:CE2	1:g:261:PRO:CA	2.51	0.94
1:i:270:VAL:HG22	1:i:378:LEU:CD2	1.98	0.94
1:C:70:LEU:HD23	1:C:114:LEU:HD12	1.50	0.93
1:N:64:ARG:HA	1:N:125:MET:HE2	1.50	0.93
1:N:70:LEU:HD23	1:N:114:LEU:HD12	1.50	0.93
1:O:64:ARG:HA	1:O:125:MET:CE	1.98	0.93
1:c:70:LEU:HD23	1:c:114:LEU:HD12	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:64:ARG:HA	1:J:125:MET:CE	1.98	0.93
1:M:70:LEU:HD23	1:M:114:LEU:HD12	1.50	0.93
1:N:30:LEU:HD21	1:N:36:MET:HE3	1.51	0.93
2:U:172:VAL:CG2	2:U:173:PRO:CD	2.47	0.93
2:X:172:VAL:CG2	2:X:173:PRO:CD	2.47	0.93
2:Y:34:GLY:CA	2:Z:282:GLN:HG2	1.94	0.93
1:h:64:ARG:HA	1:h:125:MET:CE	1.98	0.93
1:k:70:LEU:HD23	1:k:114:LEU:HD12	1.50	0.93
1:G:70:LEU:HD23	1:G:114:LEU:HD12	1.50	0.93
1:H:30:LEU:HD21	1:H:36:MET:HE3	1.51	0.93
1:M:89:PRO:HD3	1:N:279:GLU:C	1.92	0.93
2:R:404:PHE:CD2	1:d:261:PRO:CA	2.52	0.93
2:S:60:LYS:HZ3	2:T:283:TYR:HD1	1.11	0.93
2:T:404:PHE:CE2	1:f:261:PRO:CA	2.51	0.93
2:Y:63:PRO:C	2:Z:283:TYR:O	1.89	0.93
1:f:30:LEU:HD21	1:f:36:MET:HE3	1.51	0.93
1:h:64:ARG:HA	1:h:125:MET:HE2	1.50	0.93
2:s:172:VAL:CG2	2:s:173:PRO:CD	2.47	0.93
1:D:70:LEU:HD23	1:D:114:LEU:HD12	1.50	0.93
1:G:60:LYS:HZ1	1:H:283:HIS:HB2	0.97	0.93
1:J:64:ARG:HA	1:J:125:MET:HE2	1.50	0.93
1:P:82:PRO:HD2	1:P:83:TYR:H	1.32	0.93
2:R:398:MET:HG3	1:d:346:TRP:O	1.69	0.93
2:Y:54:ASN:HD22	2:Z:284:ARG:HA	1.31	0.93
2:a:172:VAL:HG22	2:a:173:PRO:CD	1.99	0.93
2:a:172:VAL:CG2	2:a:173:PRO:CD	2.47	0.93
1:d:70:LEU:HD23	1:d:114:LEU:HD12	1.50	0.93
1:e:64:ARG:HA	1:e:125:MET:CE	1.98	0.93
1:e:70:LEU:HD23	1:e:114:LEU:HD12	1.50	0.93
1:D:82:PRO:HD2	1:D:83:TYR:H	1.32	0.93
1:G:64:ARG:HA	1:G:125:MET:CE	1.98	0.93
1:j:90:GLU:H	1:k:280:LYS:HE2	1.34	0.93
1:G:57:GLY:HA3	1:H:373:ARG:HH21	1.31	0.93
1:H:70:LEU:HD23	1:H:114:LEU:HD12	1.50	0.93
1:I:64:ARG:HA	1:I:125:MET:HE2	1.50	0.93
1:K:56:THR:HB	1:L:283:HIS:HB3	0.94	0.93
1:L:30:LEU:HD21	1:L:36:MET:HE3	1.51	0.93
2:X:398:MET:HG3	1:j:346:TRP:O	1.69	0.93
1:d:82:PRO:HD2	1:d:83:TYR:H	1.32	0.93
1:f:70:LEU:HD23	1:f:114:LEU:HD12	1.50	0.93
1:g:64:ARG:HA	1:g:125:MET:HE2	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:30:LEU:HD21	1:j:36:MET:HE3	1.51	0.93
2:r:172:VAL:HG22	2:r:173:PRO:CD	1.99	0.93
1:D:64:ARG:HA	1:D:125:MET:CE	1.98	0.93
1:D:124:LYS:HZ1	1:G:215:ARG:NH2	1.64	0.93
1:G:124:LYS:HD3	1:H:299:SER:OG	1.68	0.93
2:R:96:GLN:HB3	1:d:1:MET:HE1	1.36	0.93
2:U:172:VAL:HG22	2:U:173:PRO:CD	1.99	0.93
2:Y:404:PHE:CE2	1:k:261:PRO:CA	2.51	0.93
1:d:64:ARG:HA	1:d:125:MET:CE	1.98	0.93
2:s:172:VAL:HG22	2:s:173:PRO:CD	1.99	0.93
1:H:270:VAL:HG22	1:H:378:LEU:CD2	1.98	0.93
1:O:270:VAL:HG22	1:O:378:LEU:CD2	1.98	0.93
2:Q:404:PHE:CE2	1:c:261:PRO:CA	2.51	0.93
2:T:172:VAL:HG22	2:T:173:PRO:CD	1.99	0.93
2:W:404:PHE:CD2	1:i:261:PRO:CA	2.52	0.93
1:f:270:VAL:HG22	1:f:378:LEU:CD2	1.98	0.93
1:A:70:LEU:HD23	1:A:114:LEU:HD12	1.50	0.93
2:B:404:PHE:CD2	1:E:261:PRO:CA	2.52	0.93
1:E:70:LEU:HD23	1:E:114:LEU:HD12	1.50	0.93
1:G:127:ASP:HA	1:H:338:ARG:HD2	1.51	0.93
2:S:404:PHE:CE2	1:e:261:PRO:CA	2.51	0.93
2:T:398:MET:HG3	1:f:346:TRP:O	1.69	0.93
2:T:404:PHE:CD2	1:f:261:PRO:CA	2.52	0.93
2:V:398:MET:HG3	1:h:346:TRP:O	1.69	0.93
2:V:404:PHE:CE2	1:h:261:PRO:CA	2.51	0.93
2:X:172:VAL:HG22	2:X:173:PRO:CD	1.99	0.93
2:X:404:PHE:CD2	1:j:261:PRO:CA	2.51	0.93
2:X:404:PHE:CE2	1:j:261:PRO:CA	2.51	0.93
2:b:172:VAL:HG22	2:b:173:PRO:CD	1.99	0.93
1:d:56:THR:O	1:e:282:TYR:O	1.86	0.93
1:A:177:ILE:CD1	1:A:207:GLU:HG3	1.99	0.93
1:A:270:VAL:HG22	1:A:378:LEU:CD2	1.98	0.93
1:E:177:ILE:CD1	1:E:207:GLU:HG3	1.99	0.93
1:E:270:VAL:HG22	1:E:378:LEU:CD2	1.98	0.93
1:H:82:PRO:HD2	1:H:83:TYR:H	1.32	0.93
1:N:82:PRO:HD2	1:N:83:TYR:H	1.32	0.93
2:U:404:PHE:CD2	1:g:261:PRO:CA	2.52	0.93
2:V:172:VAL:CG2	2:V:173:PRO:CD	2.47	0.93
1:f:82:PRO:HD2	1:f:83:TYR:H	1.32	0.93
1:i:64:ARG:HA	1:i:125:MET:CE	1.98	0.93
2:p:57:THR:HG22	2:q:284:ARG:HB3	0.94	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:172:VAL:HG22	2:p:173:PRO:CD	1.99	0.93
1:N:62:VAL:HG21	1:O:285:GLN:HE21	1.29	0.92
1:N:177:ILE:CD1	1:N:207:GLU:HG3	1.99	0.92
1:O:70:LEU:HD23	1:O:114:LEU:HD12	1.50	0.92
2:R:172:VAL:HG22	2:R:173:PRO:CD	1.99	0.92
2:S:127:GLU:OE1	2:T:339:ASN:OD1	1.87	0.92
2:S:172:VAL:HG22	2:S:173:PRO:CD	1.99	0.92
2:X:123:ARG:NH1	2:Y:308:ARG:HH11	1.50	0.92
2:q:172:VAL:HG22	2:q:173:PRO:CD	1.99	0.92
2:r:172:VAL:CG2	2:r:173:PRO:CD	2.47	0.92
1:K:64:ARG:HA	1:K:125:MET:CE	1.98	0.92
1:K:70:LEU:HD23	1:K:114:LEU:HD12	1.50	0.92
1:M:89:PRO:CD	1:N:279:GLU:C	2.42	0.92
1:M:177:ILE:CD1	1:M:207:GLU:HG3	1.99	0.92
2:W:398:MET:HG3	1:i:346:TRP:O	1.69	0.92
1:i:70:LEU:HD23	1:i:114:LEU:HD12	1.50	0.92
1:k:177:ILE:CD1	1:k:207:GLU:HG3	1.99	0.92
1:G:124:LYS:HE2	1:H:297:GLU:C	1.92	0.92
2:S:60:LYS:NZ	2:T:283:TYR:HD1	1.32	0.92
2:T:172:VAL:CG2	2:T:173:PRO:CD	2.47	0.92
2:X:56:ALA:CB	2:Y:283:TYR:O	2.17	0.92
2:Y:172:VAL:HG22	2:Y:173:PRO:CD	1.99	0.92
1:d:64:ARG:HA	1:d:125:MET:HE2	1.50	0.92
1:D:64:ARG:HA	1:D:125:MET:HE2	1.50	0.92
1:O:177:ILE:CD1	1:O:207:GLU:HG3	1.99	0.92
2:W:172:VAL:CG2	2:W:173:PRO:CD	2.47	0.92
2:Y:117:SER:CA	2:Z:299:LYS:HZ3	1.67	0.92
2:o:172:VAL:CG2	2:o:173:PRO:CD	2.47	0.92
1:M:30:LEU:HD21	1:M:36:MET:HE3	1.51	0.92
2:Q:172:VAL:CG2	2:Q:173:PRO:CD	2.47	0.92
2:Y:117:SER:O	2:Z:299:LYS:NZ	2.02	0.92
2:b:172:VAL:CG2	2:b:173:PRO:CD	2.47	0.92
1:h:82:PRO:HD2	1:h:83:TYR:H	1.32	0.92
1:k:30:LEU:HD21	1:k:36:MET:HE3	1.51	0.92
1:C:64:ARG:HA	1:C:125:MET:CE	1.98	0.92
1:G:90:GLU:HB3	1:H:215:ARG:HB3	0.94	0.92
1:G:128:GLN:HG2	1:H:293:ASN:CB	1.99	0.92
1:J:82:PRO:HD2	1:J:83:TYR:H	1.32	0.92
2:Q:172:VAL:HG22	2:Q:173:PRO:CD	1.99	0.92
2:S:404:PHE:CD2	1:e:261:PRO:CA	2.52	0.92
2:Z:172:VAL:HG22	2:Z:173:PRO:CD	1.99	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:64:ARG:HA	1:c:125:MET:CE	1.98	0.92
1:e:55:GLU:CB	1:f:285:GLN:NE2	2.32	0.92
1:c:64:ARG:HA	1:c:125:MET:HE2	1.50	0.92
2:o:172:VAL:HG22	2:o:173:PRO:CD	1.99	0.92
2:r:56:ALA:CB	2:s:284:ARG:C	2.41	0.92
2:B:172:VAL:CG2	2:B:173:PRO:CD	2.47	0.92
1:C:64:ARG:HA	1:C:125:MET:HE2	1.50	0.92
2:F:172:VAL:CG2	2:F:173:PRO:CD	2.47	0.92
1:I:270:VAL:HG22	1:I:378:LEU:CD2	1.98	0.92
1:L:270:VAL:HG22	1:L:378:LEU:CD2	1.98	0.92
1:P:64:ARG:HA	1:P:125:MET:CE	1.98	0.92
1:P:177:ILE:CD1	1:P:207:GLU:HG3	1.99	0.92
2:Q:404:PHE:CD2	1:c:261:PRO:CA	2.52	0.92
2:W:172:VAL:HG22	2:W:173:PRO:CD	1.99	0.92
2:Y:172:VAL:CG2	2:Y:173:PRO:CD	2.47	0.92
2:Y:404:PHE:CD2	1:k:261:PRO:CA	2.52	0.92
1:g:270:VAL:HG22	1:g:378:LEU:CD2	1.98	0.92
1:I:70:LEU:HD23	1:I:114:LEU:HD12	1.50	0.92
2:V:404:PHE:CD2	1:h:261:PRO:CA	2.52	0.92
2:Y:56:ALA:CB	2:Z:286:LEU:CG	2.48	0.92
2:Z:172:VAL:CG2	2:Z:173:PRO:CD	2.47	0.92
1:e:55:GLU:HB3	1:f:285:GLN:CD	1.94	0.92
1:g:70:LEU:HD23	1:g:114:LEU:HD12	1.50	0.92
1:j:270:VAL:HG22	1:j:378:LEU:CD2	1.98	0.92
1:G:30:LEU:HD21	1:G:36:MET:HE3	1.51	0.92
1:G:88:HIS:CE1	1:H:216:ASN:OD1	2.23	0.92
1:G:177:ILE:CD1	1:G:207:GLU:HG3	1.99	0.92
1:I:82:PRO:HD2	1:I:83:TYR:H	1.32	0.92
1:J:177:ILE:CD1	1:J:207:GLU:HG3	1.99	0.92
1:M:128:GLN:NE2	1:N:284:GLU:HB3	1.85	0.92
2:Q:60:LYS:N	2:R:283:TYR:CD2	2.37	0.92
2:U:398:MET:HG3	1:g:346:TRP:O	1.69	0.92
1:e:58:SER:CB	1:f:282:TYR:HA	1.99	0.92
1:e:177:ILE:CD1	1:e:207:GLU:HG3	1.99	0.92
1:j:177:ILE:CD1	1:j:207:GLU:HG3	1.99	0.92
1:D:62:VAL:HG22	1:G:283:HIS:ND1	1.82	0.91
2:F:172:VAL:HG22	2:F:173:PRO:CD	1.99	0.91
1:L:177:ILE:CD1	1:L:207:GLU:HG3	1.99	0.91
2:S:172:VAL:CG2	2:S:173:PRO:CD	2.47	0.91
1:e:30:LEU:HD21	1:e:36:MET:HE3	1.51	0.91
1:g:82:PRO:HD2	1:g:83:TYR:H	1.32	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:177:ILE:CD1	1:h:207:GLU:HG3	1.99	0.91
1:A:64:ARG:HA	1:A:125:MET:CE	1.98	0.91
2:B:172:VAL:HG22	2:B:173:PRO:CD	1.99	0.91
1:C:270:VAL:HG22	1:C:378:LEU:CD2	1.98	0.91
1:G:90:GLU:HB3	1:H:215:ARG:CG	1.99	0.91
1:J:60:LYS:HE2	1:K:283:HIS:HD2	1.16	0.91
1:h:70:LEU:HD23	1:h:114:LEU:HD12	1.50	0.91
2:q:172:VAL:CG2	2:q:173:PRO:CD	2.47	0.91
1:J:70:LEU:HD23	1:J:114:LEU:HD12	1.50	0.91
1:P:270:VAL:HG22	1:P:378:LEU:CD2	1.98	0.91
2:S:128:SER:OG	2:T:293:GLN:HB3	1.69	0.91
1:c:270:VAL:HG22	1:c:378:LEU:CD2	1.98	0.91
1:g:30:LEU:HD21	1:g:36:MET:HE3	1.51	0.91
2:p:172:VAL:CG2	2:p:173:PRO:CD	2.47	0.91
1:E:64:ARG:HA	1:E:125:MET:CE	1.98	0.91
2:F:57:THR:HB	2:o:283:TYR:CE2	2.05	0.91
2:F:57:THR:CB	2:o:283:TYR:HD2	1.60	0.91
1:H:177:ILE:CD1	1:H:207:GLU:HG3	1.99	0.91
1:I:30:LEU:HD21	1:I:36:MET:HE3	1.51	0.91
2:R:172:VAL:CG2	2:R:173:PRO:CD	2.47	0.91
1:c:177:ILE:CD1	1:c:207:GLU:HG3	1.99	0.91
1:f:177:ILE:CD1	1:f:207:GLU:HG3	1.99	0.91
2:X:56:ALA:HB2	2:Y:283:TYR:O	1.70	0.91
1:C:177:ILE:CD1	1:C:207:GLU:HG3	1.99	0.91
1:G:89:PRO:HG3	1:H:280:LYS:HZ2	1.35	0.91
1:O:30:LEU:HD21	1:O:36:MET:HE3	1.51	0.91
1:D:177:ILE:CD1	1:D:207:GLU:HG3	1.99	0.91
1:E:30:LEU:HD21	1:E:36:MET:HE3	1.51	0.91
2:V:172:VAL:HG22	2:V:173:PRO:CD	1.99	0.91
1:A:30:LEU:HD21	1:A:36:MET:HE3	1.51	0.91
1:P:30:LEU:HD21	1:P:36:MET:HE3	1.51	0.91
1:P:70:LEU:HD23	1:P:114:LEU:HD12	1.50	0.91
2:Q:398:MET:HG3	1:c:346:TRP:O	1.69	0.91
2:Y:398:MET:HG3	1:k:346:TRP:O	1.69	0.91
1:i:82:PRO:HD2	1:i:83:TYR:H	1.32	0.91
1:A:64:ARG:HA	1:A:125:MET:HE2	1.50	0.91
1:E:64:ARG:HA	1:E:125:MET:HE2	1.50	0.91
1:I:177:ILE:CD1	1:I:207:GLU:HG3	1.99	0.91
1:K:82:PRO:HD2	1:K:83:TYR:H	1.32	0.91
1:M:90:GLU:OE2	1:N:216:ASN:HA	0.74	0.91
2:V:60:LYS:HZ3	2:W:283:TYR:HE2	1.18	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:177:ILE:CD1	1:d:207:GLU:HG3	1.99	0.91
1:G:270:VAL:HG22	1:G:378:LEU:CD2	1.98	0.91
1:K:177:ILE:CD1	1:K:207:GLU:HG3	1.99	0.91
2:U:172:VAL:CG2	2:U:173:PRO:HD2	2.01	0.91
1:e:270:VAL:HG22	1:e:378:LEU:CD2	1.98	0.91
1:g:177:ILE:CD1	1:g:207:GLU:HG3	1.99	0.91
1:i:177:ILE:CD1	1:i:207:GLU:HG3	1.99	0.91
2:r:56:ALA:HA	2:s:285:ALA:CA	2.00	0.91
1:G:62:VAL:HG11	1:H:284:GLU:OE2	1.70	0.90
1:G:127:ASP:CA	1:H:338:ARG:CD	2.47	0.90
1:J:30:LEU:HD21	1:J:36:MET:HE3	1.51	0.90
2:R:90:ASP:H	2:S:218:LYS:HZ1	0.96	0.90
1:d:30:LEU:HD21	1:d:36:MET:HE3	1.51	0.90
1:e:64:ARG:HA	1:e:125:MET:HE2	1.50	0.90
1:h:30:LEU:HD21	1:h:36:MET:HE3	1.51	0.90
2:s:172:VAL:CG2	2:s:173:PRO:HD2	2.02	0.90
1:G:64:ARG:HA	1:G:125:MET:HE2	1.50	0.90
2:T:172:VAL:CG2	2:T:173:PRO:HD2	2.02	0.90
2:r:56:ALA:C	2:s:285:ALA:CA	2.44	0.90
2:r:172:VAL:CG2	2:r:173:PRO:HD2	2.01	0.90
1:D:30:LEU:HD21	1:D:36:MET:HE3	1.51	0.90
1:M:128:GLN:OE1	1:N:286:LEU:N	1.83	0.90
1:G:128:GLN:CG	1:H:293:ASN:HB2	2.01	0.90
1:G:57:GLY:HA3	1:H:373:ARG:NH2	1.84	0.90
1:O:58:SER:HB2	1:P:282:TYR:CB	2.01	0.90
1:O:64:ARG:HA	1:O:125:MET:HE2	1.50	0.90
2:W:172:VAL:CG2	2:W:173:PRO:HD2	2.01	0.90
1:e:124:LYS:NZ	1:f:299:SER:OG	2.04	0.90
2:T:96:GLN:HG3	1:f:1:MET:HE1	1.54	0.90
2:a:172:VAL:CG2	2:a:173:PRO:HD2	2.02	0.90
1:d:60:LYS:O	1:e:283:HIS:CB	2.04	0.90
1:C:30:LEU:HD21	1:C:36:MET:HE3	1.51	0.90
2:R:172:VAL:CG2	2:R:173:PRO:HD2	2.02	0.90
2:S:398:MET:HG3	1:e:346:TRP:O	1.69	0.90
1:c:30:LEU:HD21	1:c:36:MET:HE3	1.51	0.90
2:V:172:VAL:CG2	2:V:173:PRO:HD2	2.02	0.90
2:p:172:VAL:CG2	2:p:173:PRO:HD2	2.02	0.90
1:H:64:ARG:HA	1:H:125:MET:HE2	1.50	0.90
2:R:60:LYS:HB2	2:S:282:GLN:HB2	0.93	0.90
2:X:96:GLN:HG3	1:j:1:MET:HE1	1.54	0.90
2:Y:172:VAL:CG2	2:Y:173:PRO:HD2	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:270:VAL:HG22	1:k:378:LEU:CD2	1.98	0.90
1:M:270:VAL:HG22	1:M:378:LEU:CD2	1.98	0.89
1:P:64:ARG:HA	1:P:125:MET:HE2	1.50	0.89
2:S:60:LYS:HB2	2:T:282:GLN:O	1.72	0.89
1:f:64:ARG:HA	1:f:125:MET:HE2	1.50	0.89
1:G:89:PRO:CG	1:H:218:ASP:OD1	2.19	0.89
1:M:57:GLY:H	1:N:372:LEU:CG	1.85	0.89
2:S:96:GLN:HG3	1:e:1:MET:HE1	1.54	0.89
2:b:172:VAL:CG2	2:b:173:PRO:HD2	2.02	0.89
2:p:57:THR:HA	2:q:284:ARG:O	1.71	0.89
2:B:398:MET:HG3	1:E:346:TRP:O	1.69	0.89
1:K:30:LEU:HD21	1:K:36:MET:HE3	1.51	0.89
2:Q:172:VAL:CG2	2:Q:173:PRO:HD2	2.02	0.89
2:U:404:PHE:CD2	1:g:260:VAL:O	2.26	0.89
2:R:404:PHE:CD2	1:d:260:VAL:O	2.26	0.89
2:Y:57:THR:CB	2:Z:371:LEU:HA	1.99	0.89
1:i:30:LEU:HD21	1:i:36:MET:HE3	1.51	0.89
2:o:172:VAL:CG2	2:o:173:PRO:HD2	2.02	0.89
2:q:172:VAL:CG2	2:q:173:PRO:HD2	2.02	0.89
1:N:270:VAL:HG22	1:N:378:LEU:CD2	1.98	0.89
2:S:172:VAL:CG2	2:S:173:PRO:HD2	2.02	0.89
2:W:404:PHE:CD2	1:i:260:VAL:O	2.26	0.89
2:Z:172:VAL:CG2	2:Z:173:PRO:HD2	2.02	0.89
2:B:96:GLN:HG3	1:E:1:MET:HE1	1.54	0.89
2:U:96:GLN:HG3	1:g:1:MET:HE1	1.54	0.89
2:R:90:ASP:N	2:S:218:LYS:HZ3	1.59	0.89
2:T:404:PHE:CD2	1:f:260:VAL:O	2.26	0.89
1:M:90:GLU:HA	1:N:218:ASP:CG	1.98	0.89
2:Q:96:GLN:HG3	1:c:1:MET:HE1	1.54	0.89
2:r:57:THR:CA	2:s:285:ALA:HA	2.02	0.89
2:Q:60:LYS:HB2	2:R:283:TYR:CZ	2.08	0.88
2:S:404:PHE:CD2	1:e:260:VAL:O	2.26	0.88
2:V:404:PHE:CD2	1:h:260:VAL:O	2.26	0.88
2:Y:404:PHE:CD2	1:k:260:VAL:O	2.26	0.88
2:X:404:PHE:CD2	1:j:260:VAL:O	2.26	0.88
1:j:116:ASP:CA	1:k:298:TYR:OH	2.20	0.88
2:Q:60:LYS:HB3	2:R:283:TYR:CD2	2.08	0.88
2:R:96:GLN:HG3	1:d:1:MET:HE1	1.54	0.88
2:Y:56:ALA:HA	2:Z:286:LEU:CB	2.01	0.88
2:B:172:VAL:CG2	2:B:173:PRO:HD2	2.01	0.88
1:D:124:LYS:HZ3	1:G:215:ARG:HH21	1.13	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:60:LYS:CB	2:R:283:TYR:CD2	2.55	0.88
2:Q:404:PHE:CD2	1:c:260:VAL:O	2.26	0.88
2:F:172:VAL:CG2	2:F:173:PRO:HD2	2.02	0.88
1:G:89:PRO:HD3	1:H:280:LYS:CE	2.03	0.88
2:Y:86:ILE:O	2:Z:283:TYR:CD1	2.27	0.88
2:X:172:VAL:CG2	2:X:173:PRO:HD2	2.01	0.88
1:G:89:PRO:CB	1:H:280:LYS:NZ	2.36	0.88
1:O:56:THR:HG21	1:P:283:HIS:HB3	1.54	0.88
2:Y:221:THR:HA	1:k:326:LYS:CD	2.04	0.88
2:q:89:PRO:HB2	2:r:218:LYS:HZ1	1.34	0.88
2:B:404:PHE:CD2	1:E:260:VAL:O	2.26	0.88
2:Y:56:ALA:HA	2:Z:286:LEU:CG	2.04	0.88
2:R:58:GLY:HA3	2:S:282:GLN:HG2	1.56	0.88
2:W:221:THR:HA	1:i:326:LYS:CD	2.04	0.88
2:B:221:THR:HA	1:E:326:LYS:CD	2.04	0.88
2:W:96:GLN:HG3	1:i:1:MET:HE1	1.54	0.88
2:Y:86:ILE:C	2:Z:283:TYR:CE1	2.03	0.88
1:L:56:THR:HG22	1:M:283:HIS:O	1.72	0.87
1:M:57:GLY:HA3	1:N:372:LEU:CD1	1.97	0.87
2:Q:221:THR:HA	1:c:326:LYS:CD	2.04	0.87
1:j:123:ARG:HH12	1:k:338:ARG:CZ	1.87	0.87
2:r:62:VAL:CG2	2:s:283:TYR:HB3	2.04	0.87
1:H:56:THR:HG21	1:I:283:HIS:HA	1.55	0.87
2:Y:127:GLU:OE2	2:Z:293:GLN:N	2.05	0.87
1:d:60:LYS:N	1:e:282:TYR:O	2.07	0.87
2:R:55:GLU:HB2	2:S:285:ALA:HB2	1.56	0.87
2:R:60:LYS:N	2:S:282:GLN:HB3	1.90	0.87
2:X:221:THR:HA	1:j:326:LYS:CD	2.04	0.87
2:Y:96:GLN:HG3	1:k:1:MET:HE1	1.54	0.87
1:e:62:VAL:HG23	1:f:283:HIS:O	1.75	0.87
2:S:182:VAL:HG21	1:e:257:THR:HG22	1.57	0.87
2:V:182:VAL:HG21	1:h:257:THR:HG22	1.57	0.87
2:W:404:PHE:CE2	1:i:261:PRO:N	2.43	0.87
2:Y:86:ILE:HA	2:Z:282:GLN:HB2	1.53	0.87
2:Y:124:LYS:HA	2:Z:293:GLN:HB3	1.55	0.87
1:e:120:ASP:OD1	1:f:298:TYR:CZ	2.28	0.87
1:G:58:SER:HB3	1:H:281:ALA:O	1.74	0.87
2:R:214:PHE:HZ	1:d:326:LYS:HG3	1.39	0.87
2:U:404:PHE:CE2	1:g:261:PRO:N	2.43	0.87
2:V:221:THR:HA	1:h:326:LYS:CD	2.04	0.87
2:Y:214:PHE:HZ	1:k:326:LYS:HG3	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:182:VAL:HG21	1:f:257:THR:HG22	1.57	0.87
2:R:221:THR:HA	1:d:326:LYS:CD	2.04	0.87
2:Q:60:LYS:H	2:R:283:TYR:HD2	0.91	0.87
2:X:404:PHE:CE2	1:j:261:PRO:N	2.43	0.87
1:e:124:LYS:CE	1:f:297:GLU:OE1	2.23	0.87
2:R:182:VAL:HG21	1:d:257:THR:HG22	1.57	0.86
2:W:182:VAL:HG21	1:i:257:THR:HG22	1.57	0.86
2:Y:125:GLU:O	2:Z:290:GLU:OE1	1.91	0.86
2:B:214:PHE:HZ	1:E:326:LYS:HG3	1.39	0.86
1:G:61:HIS:HD2	1:H:285:GLN:NE2	1.70	0.86
2:S:57:THR:OG1	2:T:281:GLN:NE2	2.09	0.86
2:T:214:PHE:HZ	1:f:326:LYS:HG3	1.39	0.86
2:T:404:PHE:CE2	1:f:261:PRO:N	2.43	0.86
2:V:404:PHE:CE2	1:h:261:PRO:N	2.43	0.86
2:X:214:PHE:HZ	1:j:326:LYS:HG3	1.39	0.86
2:Y:62:VAL:HG13	2:Z:280:SER:O	1.75	0.86
1:j:90:GLU:HG2	1:k:280:LYS:CD	2.03	0.86
2:o:57:THR:C	2:p:282:GLN:OE1	2.18	0.86
2:R:404:PHE:CE2	1:d:261:PRO:N	2.43	0.86
2:U:182:VAL:HG21	1:g:257:THR:HG22	1.57	0.86
2:V:96:GLN:HG3	1:h:1:MET:HE1	1.54	0.86
2:B:404:PHE:CE2	1:E:261:PRO:N	2.43	0.86
1:G:89:PRO:HD3	1:H:280:LYS:HZ3	0.74	0.86
2:W:214:PHE:HZ	1:i:326:LYS:HG3	1.39	0.86
2:q:89:PRO:HB2	2:r:218:LYS:HZ2	1.35	0.86
2:B:222:PRO:HD2	1:E:326:LYS:CD	2.06	0.86
2:S:214:PHE:HZ	1:e:326:LYS:HG3	1.39	0.86
2:S:221:THR:HA	1:e:326:LYS:CD	2.04	0.86
2:Q:214:PHE:HZ	1:c:326:LYS:HG3	1.39	0.86
1:i:57:GLY:HA3	1:j:283:HIS:O	1.74	0.86
2:Q:404:PHE:CE2	1:c:261:PRO:N	2.43	0.86
2:Y:57:THR:H	2:Z:286:LEU:HD12	1.39	0.86
1:f:62:VAL:HG21	1:g:283:HIS:HB3	1.56	0.86
1:f:89:PRO:HG2	1:g:280:LYS:CE	2.04	0.86
1:j:88:HIS:CE1	1:k:280:LYS:HG2	2.09	0.86
2:Q:182:VAL:HG21	1:c:257:THR:HG22	1.57	0.86
2:Y:404:PHE:CE2	1:k:261:PRO:N	2.43	0.86
2:q:57:THR:N	2:r:284:ARG:C	2.33	0.86
2:U:222:PRO:HD2	1:g:326:LYS:CD	2.06	0.85
1:e:55:GLU:CB	1:f:285:GLN:CD	2.49	0.85
2:V:214:PHE:HZ	1:h:326:LYS:HG3	1.39	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:404:PHE:CE2	1:e:261:PRO:N	2.43	0.85
2:T:221:THR:HA	1:f:326:LYS:CD	2.04	0.85
2:U:214:PHE:HZ	1:g:326:LYS:HG3	1.39	0.85
2:Y:127:GLU:CD	2:Z:293:GLN:HA	2.02	0.85
1:D:89:PRO:HG2	1:G:218:ASP:HB2	1.55	0.85
2:X:222:PRO:HD2	1:j:326:LYS:CD	2.06	0.85
2:R:90:ASP:N	2:S:218:LYS:HZ1	1.50	0.85
2:q:89:PRO:CB	2:r:218:LYS:NZ	2.39	0.85
1:D:56:THR:CG2	1:G:283:HIS:H	1.85	0.85
2:Q:222:PRO:HD2	1:c:326:LYS:CD	2.06	0.85
2:U:221:THR:HA	1:g:326:LYS:CD	2.04	0.85
2:W:222:PRO:HD2	1:i:326:LYS:CD	2.06	0.85
1:d:56:THR:C	1:e:282:TYR:C	2.44	0.85
2:B:182:VAL:HG21	1:E:257:THR:HG22	1.57	0.85
1:K:58:SER:HB3	1:L:283:HIS:CE1	2.11	0.85
2:S:222:PRO:HD2	1:e:326:LYS:CD	2.06	0.85
2:r:89:PRO:HB3	2:s:218:LYS:NZ	1.90	0.85
2:X:123:ARG:HH12	2:Y:308:ARG:HH11	1.10	0.85
2:q:57:THR:N	2:r:284:ARG:O	2.03	0.85
1:D:60:LYS:HE2	1:G:279:GLU:O	1.77	0.84
2:Y:86:ILE:O	2:Z:283:TYR:HD1	1.59	0.84
2:Y:222:PRO:HD2	1:k:326:LYS:CD	2.06	0.84
1:j:116:ASP:HB3	1:k:298:TYR:HE1	1.40	0.84
1:G:61:HIS:HD2	1:H:285:GLN:HE21	1.23	0.84
1:I:177:ILE:HD12	1:I:207:GLU:CG	2.07	0.84
2:R:180:THR:CG2	1:d:258:ASN:OD1	2.26	0.84
2:V:222:PRO:HD2	1:h:326:LYS:CD	2.06	0.84
2:W:180:THR:CG2	1:i:258:ASN:OD1	2.26	0.84
1:g:177:ILE:HD12	1:g:207:GLU:CG	2.07	0.84
2:r:56:ALA:CB	2:s:285:ALA:N	2.40	0.84
1:M:86:LEU:HG	1:N:283:HIS:CE1	2.12	0.84
2:Q:221:THR:CG2	1:c:324:VAL:HG21	2.08	0.84
2:V:180:THR:CG2	1:h:258:ASN:OD1	2.26	0.84
2:Y:86:ILE:C	2:Z:283:TYR:HD1	1.51	0.84
2:Y:180:THR:CG2	1:k:258:ASN:OD1	2.26	0.84
2:Y:221:THR:CG2	1:k:324:VAL:HG21	2.08	0.84
1:e:124:LYS:NZ	1:f:299:SER:CB	2.40	0.84
1:j:62:VAL:HG21	1:k:283:HIS:CB	2.08	0.84
2:S:56:ALA:HB3	2:T:284:ARG:HA	0.89	0.84
2:T:222:PRO:HD2	1:f:326:LYS:CD	2.06	0.84
1:D:177:ILE:HD12	1:D:207:GLU:CG	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:182:VAL:HG21	1:k:257:THR:HG22	1.57	0.84
2:B:221:THR:CG2	1:E:324:VAL:HG21	2.08	0.84
1:M:177:ILE:HD12	1:M:207:GLU:CG	2.07	0.84
2:R:221:THR:CG2	1:d:324:VAL:HG21	2.08	0.84
2:S:180:THR:CG2	1:e:258:ASN:OD1	2.26	0.84
2:U:180:THR:CG2	1:g:258:ASN:OD1	2.26	0.84
2:U:221:THR:CG2	1:g:324:VAL:HG21	2.08	0.84
2:Y:86:ILE:HG13	2:Z:282:GLN:HB3	1.57	0.84
1:d:59:GLY:N	1:e:282:TYR:O	2.10	0.84
1:d:177:ILE:HD12	1:d:207:GLU:CG	2.07	0.84
1:j:127:ASP:C	1:k:290:GLU:CD	2.45	0.84
1:k:177:ILE:HD12	1:k:207:GLU:CG	2.07	0.84
1:M:127:ASP:N	1:N:290:GLU:OE1	2.10	0.84
2:S:127:GLU:HG3	2:T:339:ASN:HD21	1.40	0.84
2:V:221:THR:CG2	1:h:324:VAL:HG21	2.08	0.84
2:X:182:VAL:HG21	1:j:257:THR:HG22	1.57	0.84
1:d:62:VAL:HG23	1:e:283:HIS:HB3	1.58	0.84
2:o:57:THR:O	2:p:282:GLN:OE1	1.95	0.84
2:R:56:ALA:HB3	2:S:283:TYR:H	1.39	0.84
2:X:221:THR:CG2	1:j:324:VAL:HG21	2.08	0.84
1:A:177:ILE:HD12	1:A:207:GLU:CG	2.07	0.84
1:E:177:ILE:HD12	1:E:207:GLU:CG	2.07	0.84
1:G:62:VAL:HG13	1:H:284:GLU:OE2	1.74	0.84
1:L:128:GLN:HG3	1:M:290:GLU:OE1	1.77	0.84
2:V:179:ASP:O	1:h:352:LYS:HD3	1.78	0.84
1:f:177:ILE:HD12	1:f:207:GLU:CG	2.07	0.84
2:q:57:THR:O	2:r:282:GLN:O	1.96	0.84
1:G:60:LYS:NZ	1:H:280:LYS:HA	1.92	0.83
1:H:177:ILE:HD12	1:H:207:GLU:CG	2.07	0.83
1:M:64:ARG:NH2	1:N:285:GLN:HG3	1.92	0.83
2:R:222:PRO:HD2	1:d:326:LYS:CD	2.06	0.83
1:M:89:PRO:CG	1:N:279:GLU:HB2	2.08	0.83
1:M:90:GLU:HA	1:N:218:ASP:OD2	1.78	0.83
2:V:404:PHE:CZ	1:h:261:PRO:CB	2.62	0.83
2:W:96:GLN:HB3	1:i:1:MET:HE1	1.36	0.83
2:W:404:PHE:CZ	1:i:261:PRO:CB	2.61	0.83
2:B:180:THR:CG2	1:E:258:ASN:OD1	2.25	0.83
1:G:90:GLU:CB	1:H:215:ARG:CD	2.53	0.83
2:S:221:THR:CG2	1:e:324:VAL:HG21	2.08	0.83
2:W:179:ASP:O	1:i:352:LYS:HD3	1.78	0.83
1:i:177:ILE:HD12	1:i:207:GLU:CG	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:90:GLU:N	1:k:280:LYS:HE2	1.93	0.83
2:B:404:PHE:CZ	1:E:261:PRO:CB	2.62	0.83
1:K:177:ILE:HD12	1:K:207:GLU:CG	2.07	0.83
1:M:90:GLU:CA	1:N:218:ASP:OD1	2.27	0.83
2:R:88:ARG:HG2	2:S:218:LYS:NZ	1.93	0.83
2:T:221:THR:CG2	1:f:324:VAL:HG21	2.08	0.83
2:U:179:ASP:O	1:g:352:LYS:HD3	1.79	0.83
2:Y:117:SER:HA	2:Z:299:LYS:HZ3	1.22	0.83
1:J:177:ILE:HD12	1:J:207:GLU:CG	2.07	0.83
1:h:177:ILE:HD12	1:h:207:GLU:CG	2.07	0.83
2:r:56:ALA:CA	2:s:285:ALA:CB	2.48	0.83
1:G:177:ILE:HD12	1:G:207:GLU:CG	2.07	0.83
1:M:54:SER:CB	1:N:285:GLN:HG2	2.08	0.83
1:M:57:GLY:C	1:N:372:LEU:HD21	2.04	0.83
1:O:58:SER:HB2	1:P:282:TYR:O	1.75	0.83
2:T:180:THR:CG2	1:f:258:ASN:OD1	2.26	0.83
2:U:404:PHE:CZ	1:g:261:PRO:CB	2.62	0.83
1:c:177:ILE:HD12	1:c:207:GLU:CG	2.07	0.83
1:e:177:ILE:HD12	1:e:207:GLU:CG	2.07	0.83
1:C:177:ILE:HD12	1:C:207:GLU:CG	2.07	0.83
1:M:90:GLU:HA	1:N:218:ASP:OD1	1.78	0.83
2:r:56:ALA:CB	2:s:284:ARG:CA	2.50	0.83
1:P:177:ILE:HD12	1:P:207:GLU:CG	2.07	0.83
2:Q:180:THR:CG2	1:c:258:ASN:OD1	2.26	0.83
2:X:180:THR:CG2	1:j:258:ASN:OD1	2.26	0.83
2:Y:57:THR:N	2:Z:286:LEU:HD12	1.94	0.83
2:B:179:ASP:O	1:E:352:LYS:HD3	1.79	0.83
2:W:221:THR:CG2	1:i:324:VAL:HG21	2.08	0.83
1:G:124:LYS:CE	1:H:299:SER:OG	2.19	0.83
1:N:177:ILE:HD12	1:N:207:GLU:CG	2.07	0.83
2:S:398:MET:HG2	1:e:346:TRP:O	1.79	0.83
2:W:394:GLN:HE21	1:i:348:PRO:HB2	1.44	0.83
1:G:129:CYS:HB2	1:H:338:ARG:NH2	1.93	0.82
2:Q:394:GLN:HE21	1:c:348:PRO:HB2	1.44	0.82
2:T:398:MET:HG2	1:f:346:TRP:O	1.79	0.82
2:Y:54:ASN:O	2:Z:284:ARG:O	1.95	0.82
2:Y:86:ILE:CG1	2:Z:282:GLN:HB2	2.09	0.82
1:j:177:ILE:HD12	1:j:207:GLU:CG	2.07	0.82
1:L:177:ILE:HD12	1:L:207:GLU:CG	2.07	0.82
2:T:404:PHE:CZ	1:f:261:PRO:CB	2.62	0.82
1:N:84:ARG:HH11	1:O:283:HIS:CE1	1.81	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:177:ILE:HD12	1:O:207:GLU:CG	2.07	0.82
1:M:89:PRO:HD3	1:N:279:GLU:CB	2.04	0.82
2:X:123:ARG:HH12	2:Y:308:ARG:HH12	0.83	0.82
2:Y:89:PRO:HD3	2:Z:280:SER:H	1.45	0.82
1:i:58:SER:N	1:j:283:HIS:HA	1.94	0.82
2:Q:179:ASP:O	1:c:352:LYS:HD3	1.79	0.82
2:S:404:PHE:CZ	1:e:261:PRO:CB	2.62	0.82
2:T:62:VAL:HG22	2:U:283:TYR:HD2	1.43	0.82
2:Y:404:PHE:CZ	1:k:261:PRO:CB	2.62	0.82
1:e:120:ASP:OD1	1:f:298:TYR:CE2	2.32	0.82
2:r:56:ALA:C	2:s:285:ALA:HA	2.05	0.82
1:M:90:GLU:CG	1:N:280:LYS:HD2	2.09	0.82
2:Q:404:PHE:CZ	1:c:261:PRO:CB	2.62	0.82
2:R:404:PHE:CZ	1:d:261:PRO:CB	2.62	0.82
1:f:60:LYS:HB3	1:g:282:TYR:O	1.79	0.82
2:U:394:GLN:HE21	1:g:348:PRO:HB2	1.44	0.82
2:V:394:GLN:HE21	1:h:348:PRO:HB2	1.44	0.82
2:X:179:ASP:O	1:j:352:LYS:HD3	1.78	0.82
2:Y:125:GLU:HA	2:Z:290:GLU:OE2	1.79	0.82
1:j:234:ILE:HD13	1:j:270:VAL:HG11	1.62	0.82
1:L:234:ILE:HD13	1:L:270:VAL:HG11	1.62	0.82
1:M:57:GLY:N	1:N:372:LEU:CG	2.39	0.82
1:M:88:HIS:ND1	1:N:281:ALA:N	2.27	0.82
2:R:60:LYS:CB	2:S:282:GLN:CA	2.42	0.82
2:X:120:ASP:OD1	2:Y:297:ASP:OD1	1.98	0.82
2:X:404:PHE:CZ	1:j:261:PRO:CB	2.62	0.82
2:Y:56:ALA:HB1	2:Z:286:LEU:CD1	2.09	0.82
2:B:394:GLN:HE21	1:E:348:PRO:HB2	1.44	0.82
1:D:90:GLU:HG2	1:G:218:ASP:OD1	1.78	0.82
1:M:127:ASP:N	1:N:290:GLU:CD	2.32	0.82
2:Q:398:MET:HG2	1:c:346:TRP:O	1.79	0.81
2:r:56:ALA:HB1	2:s:285:ALA:N	1.95	0.81
2:Y:88:ARG:O	2:Z:277:SER:HB2	1.78	0.81
2:Y:394:GLN:HE21	1:k:348:PRO:HB2	1.45	0.81
1:j:56:THR:HG21	1:k:283:HIS:C	2.04	0.81
1:K:234:ILE:HD13	1:K:270:VAL:HG11	1.62	0.81
1:M:234:ILE:HD13	1:M:270:VAL:HG11	1.62	0.81
2:T:394:GLN:HE21	1:f:348:PRO:HB2	1.45	0.81
2:U:398:MET:HG2	1:g:346:TRP:O	1.80	0.81
2:X:394:GLN:HE21	1:j:348:PRO:HB2	1.44	0.81
1:i:234:ILE:HD13	1:i:270:VAL:HG11	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:234:ILE:HD13	1:k:270:VAL:HG11	1.62	0.81
1:G:58:SER:CB	1:H:281:ALA:O	2.28	0.81
1:G:128:GLN:CG	1:H:293:ASN:HB3	2.09	0.81
1:J:234:ILE:HD13	1:J:270:VAL:HG11	1.62	0.81
2:T:179:ASP:O	1:f:352:LYS:HD3	1.78	0.81
2:Y:398:MET:HG2	1:k:346:TRP:O	1.79	0.81
1:h:234:ILE:HD13	1:h:270:VAL:HG11	1.62	0.81
1:P:234:ILE:HD13	1:P:270:VAL:HG11	1.62	0.81
2:S:179:ASP:O	1:e:352:LYS:HD3	1.79	0.81
2:r:89:PRO:HB3	2:s:218:LYS:HZ2	1.43	0.81
2:Y:179:ASP:O	1:k:352:LYS:HD3	1.78	0.81
2:R:398:MET:HG2	1:d:346:TRP:O	1.80	0.81
1:M:57:GLY:HA3	1:N:372:LEU:HD21	0.81	0.81
1:O:234:ILE:HD13	1:O:270:VAL:HG11	1.62	0.81
1:c:58:SER:CA	1:d:282:TYR:HB3	2.11	0.81
1:K:58:SER:CB	1:L:283:HIS:CE1	2.64	0.81
2:V:394:GLN:HG2	1:h:348:PRO:CG	2.11	0.81
2:Y:127:GLU:OE2	2:Z:292:THR:C	2.24	0.81
2:T:56:ALA:HB2	2:U:283:TYR:O	1.81	0.80
1:A:234:ILE:HD13	1:A:270:VAL:HG11	1.62	0.80
2:B:398:MET:HG2	1:E:346:TRP:O	1.80	0.80
1:E:234:ILE:HD13	1:E:270:VAL:HG11	1.62	0.80
2:R:62:VAL:HG23	2:S:283:TYR:CG	2.16	0.80
2:S:60:LYS:C	2:T:283:TYR:O	2.10	0.80
2:X:398:MET:HG2	1:j:346:TRP:O	1.79	0.80
1:e:124:LYS:HZ1	1:f:299:SER:CB	1.95	0.80
2:p:57:THR:CG2	2:q:284:ARG:CA	2.59	0.80
2:B:403:ALA:HB2	1:E:262:TYR:OH	1.82	0.80
1:L:123:ARG:NH1	1:M:338:ARG:HH12	1.80	0.80
2:R:60:LYS:CA	2:S:282:GLN:HB3	2.12	0.80
2:R:179:ASP:O	1:d:352:LYS:HD3	1.79	0.80
2:S:127:GLU:CG	2:T:339:ASN:HD21	1.94	0.80
2:S:403:ALA:HB2	1:e:262:TYR:OH	1.82	0.80
2:X:394:GLN:HG2	1:j:348:PRO:CG	2.11	0.80
1:j:90:GLU:HG2	1:k:280:LYS:HD3	1.62	0.80
1:D:234:ILE:HD13	1:D:270:VAL:HG11	1.62	0.80
2:R:394:GLN:HG2	1:d:348:PRO:CG	2.11	0.80
2:S:394:GLN:HG2	1:e:348:PRO:CG	2.11	0.80
2:W:394:GLN:HG2	1:i:348:PRO:CG	2.11	0.80
1:C:57:GLY:HA3	1:D:284:GLU:CA	2.04	0.80
2:S:394:GLN:HE21	1:e:348:PRO:HB2	1.44	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:394:GLN:HG2	1:f:348:PRO:CG	2.12	0.80
2:Y:404:PHE:CE2	1:k:260:VAL:C	2.60	0.80
1:d:234:ILE:HD13	1:d:270:VAL:HG11	1.62	0.80
1:G:89:PRO:N	1:H:280:LYS:HZ3	1.79	0.80
2:R:34:GLY:C	2:S:283:TYR:CE2	2.60	0.80
2:Y:86:ILE:CG1	2:Z:282:GLN:CB	2.58	0.80
1:c:58:SER:CB	1:d:283:HIS:CE1	2.64	0.80
1:e:127:ASP:HA	1:f:338:ARG:HH22	1.43	0.80
1:j:123:ARG:HH12	1:k:338:ARG:NH2	1.79	0.80
2:B:394:GLN:HG2	1:E:348:PRO:CG	2.11	0.80
1:D:61:HIS:HA	1:G:283:HIS:HA	1.62	0.80
2:U:404:PHE:CE2	1:g:260:VAL:C	2.60	0.80
2:W:398:MET:HG2	1:i:346:TRP:O	1.79	0.80
2:R:54:ASN:O	2:S:283:TYR:O	1.97	0.80
2:S:404:PHE:CE2	1:e:260:VAL:C	2.60	0.80
2:W:404:PHE:CE2	1:i:260:VAL:C	2.60	0.80
1:D:56:THR:C	1:G:282:TYR:HA	2.05	0.80
1:M:89:PRO:CB	1:N:279:GLU:CB	2.23	0.80
2:R:394:GLN:HE21	1:d:348:PRO:HB2	1.45	0.80
2:Y:394:GLN:HG2	1:k:348:PRO:CG	2.11	0.80
1:e:234:ILE:HD13	1:e:270:VAL:HG11	1.62	0.80
1:G:234:ILE:HD13	1:G:270:VAL:HG11	1.62	0.80
2:V:398:MET:HG2	1:h:346:TRP:O	1.80	0.80
2:X:56:ALA:HB1	2:Y:283:TYR:C	2.06	0.80
1:c:234:ILE:HD13	1:c:270:VAL:HG11	1.62	0.80
1:f:234:ILE:HD13	1:f:270:VAL:HG11	1.62	0.80
1:g:234:ILE:HD13	1:g:270:VAL:HG11	1.62	0.80
1:G:234:ILE:HG21	1:G:270:VAL:HG11	1.65	0.79
1:L:123:ARG:HH12	1:M:338:ARG:HH12	1.30	0.79
2:R:404:PHE:CE2	1:d:260:VAL:C	2.60	0.79
2:U:403:ALA:HB2	1:g:262:TYR:OH	1.82	0.79
1:e:234:ILE:HG21	1:e:270:VAL:HG11	1.65	0.79
1:j:90:GLU:OE2	1:k:215:ARG:O	1.98	0.79
1:C:234:ILE:HD13	1:C:270:VAL:HG11	1.62	0.79
1:H:234:ILE:HD13	1:H:270:VAL:HG11	1.62	0.79
1:I:234:ILE:HD13	1:I:270:VAL:HG11	1.62	0.79
1:K:57:GLY:H	1:L:283:HIS:C	1.89	0.79
2:Q:404:PHE:CE2	1:c:260:VAL:C	2.60	0.79
2:Y:88:ARG:N	2:Z:280:SER:O	2.04	0.79
1:D:234:ILE:HG21	1:D:270:VAL:HG11	1.65	0.79
2:Q:403:ALA:HB2	1:c:262:TYR:OH	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:403:ALA:HB2	1:h:262:TYR:OH	1.82	0.79
2:Y:87:PHE:CA	2:Z:283:TYR:HD1	1.89	0.79
1:d:234:ILE:HG21	1:d:270:VAL:HG11	1.65	0.79
1:M:88:HIS:ND1	1:N:280:LYS:C	2.34	0.79
2:Q:394:GLN:HG2	1:c:348:PRO:CG	2.11	0.79
2:U:394:GLN:HG2	1:g:348:PRO:CG	2.11	0.79
2:V:404:PHE:CE2	1:h:260:VAL:C	2.60	0.79
2:r:57:THR:OG1	2:s:284:ARG:O	1.83	0.79
1:M:127:ASP:OD2	1:N:293:ASN:CB	2.30	0.79
1:N:234:ILE:HD13	1:N:270:VAL:HG11	1.62	0.79
2:Q:181:VAL:CG2	1:c:258:ASN:O	2.31	0.79
2:R:181:VAL:CG2	1:d:258:ASN:O	2.31	0.79
2:T:181:VAL:CG2	1:f:258:ASN:O	2.31	0.79
2:X:404:PHE:CE2	1:j:260:VAL:C	2.60	0.79
1:e:127:ASP:OD1	1:f:338:ARG:CZ	2.31	0.79
2:B:404:PHE:CE2	1:E:260:VAL:C	2.60	0.79
2:R:403:ALA:HB2	1:d:262:TYR:OH	1.82	0.79
2:Y:62:VAL:HB	2:Z:284:ARG:O	1.67	0.79
2:Y:403:ALA:HB2	1:k:262:TYR:OH	1.82	0.79
1:K:234:ILE:HG21	1:K:270:VAL:HG11	1.65	0.79
2:T:403:ALA:HB2	1:f:262:TYR:OH	1.82	0.79
2:T:404:PHE:CE2	1:f:260:VAL:C	2.60	0.79
2:X:120:ASP:OD2	2:Y:297:ASP:OD1	2.00	0.79
2:Y:62:VAL:HG11	2:Z:284:ARG:HB3	1.59	0.79
2:Y:88:ARG:C	2:Z:277:SER:HB2	1.68	0.79
1:i:234:ILE:HG21	1:i:270:VAL:HG11	1.65	0.79
2:F:57:THR:HB	2:o:283:TYR:HD2	0.79	0.79
1:G:57:GLY:H	1:H:286:LEU:C	1.72	0.79
1:J:234:ILE:HG21	1:J:270:VAL:HG11	1.65	0.79
1:M:128:GLN:HE22	1:N:284:GLU:CB	1.90	0.79
1:M:128:GLN:H	1:N:290:GLU:CD	1.58	0.79
1:O:234:ILE:HG21	1:O:270:VAL:HG11	1.65	0.79
1:P:234:ILE:HG21	1:P:270:VAL:HG11	1.65	0.79
2:R:60:LYS:C	2:S:283:TYR:CG	2.61	0.79
2:W:403:ALA:HB2	1:i:262:TYR:OH	1.82	0.79
2:Y:62:VAL:HG12	2:Z:284:ARG:HB2	1.65	0.79
2:Y:124:LYS:CG	2:Z:294:GLN:HA	2.12	0.79
1:d:55:GLU:O	1:e:284:GLU:C	2.25	0.79
1:e:33:ASP:O	1:f:283:HIS:NE2	2.16	0.79
1:h:234:ILE:HG21	1:h:270:VAL:HG11	1.65	0.79
2:q:56:ALA:HA	2:r:285:ALA:N	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:r:60:LYS:CG	2:s:282:GLN:O	2.31	0.79
1:M:87:PHE:CA	1:N:283:HIS:ND1	2.40	0.79
1:C:234:ILE:HG21	1:C:270:VAL:HG11	1.65	0.79
1:N:62:VAL:CB	1:O:285:GLN:NE2	2.46	0.79
2:X:120:ASP:CG	2:Y:297:ASP:OD1	2.26	0.79
2:X:403:ALA:HB2	1:j:262:TYR:OH	1.82	0.79
1:c:234:ILE:HG21	1:c:270:VAL:HG11	1.65	0.79
2:Q:60:LYS:HB2	2:R:283:TYR:HE2	0.97	0.78
1:L:123:ARG:NH1	1:M:338:ARG:NH1	2.31	0.78
1:i:57:GLY:CA	1:j:283:HIS:O	2.30	0.78
2:W:224:TYR:HE2	1:i:248:LEU:CG	1.97	0.78
2:Y:57:THR:OG1	2:Z:371:LEU:HA	1.82	0.78
2:Q:60:LYS:CB	2:R:283:TYR:HE2	1.64	0.78
2:V:210:TYR:OH	1:h:325:PRO:HB2	1.84	0.78
1:N:88:HIS:NE2	1:O:290:GLU:OE1	2.16	0.78
1:P:70:LEU:CD2	1:P:114:LEU:HD12	2.14	0.78
2:R:210:TYR:OH	1:d:325:PRO:HB2	1.83	0.78
2:U:224:TYR:HE2	1:g:248:LEU:CG	1.97	0.78
1:g:234:ILE:HG21	1:g:270:VAL:HG11	1.65	0.78
1:H:70:LEU:CD2	1:H:114:LEU:HD12	2.14	0.78
1:H:234:ILE:HG21	1:H:270:VAL:HG11	1.65	0.78
1:I:234:ILE:HG21	1:I:270:VAL:HG11	1.65	0.78
1:M:90:GLU:HG3	1:N:280:LYS:HD2	1.66	0.78
1:N:234:ILE:HG21	1:N:270:VAL:HG11	1.65	0.78
2:Q:210:TYR:OH	1:c:325:PRO:HB2	1.83	0.78
2:S:127:GLU:CD	2:T:339:ASN:HD21	1.91	0.78
2:X:224:TYR:HE2	1:j:248:LEU:CG	1.97	0.78
1:e:127:ASP:OD1	1:f:338:ARG:NH1	2.17	0.78
1:f:234:ILE:HG21	1:f:270:VAL:HG11	1.65	0.78
2:B:181:VAL:CG2	1:E:258:ASN:O	2.31	0.78
1:G:124:LYS:HE2	1:H:297:GLU:O	1.82	0.78
1:I:70:LEU:CD2	1:I:114:LEU:HD12	2.14	0.78
2:Y:62:VAL:CA	2:Z:282:GLN:O	2.29	0.78
2:Y:406:HIS:CG	1:k:263:PRO:CG	2.67	0.78
1:f:70:LEU:CD2	1:f:114:LEU:HD12	2.14	0.78
1:g:70:LEU:CD2	1:g:114:LEU:HD12	2.14	0.78
2:R:55:GLU:CB	2:S:285:ALA:HB2	2.14	0.78
2:V:181:VAL:CG2	1:h:258:ASN:O	2.31	0.78
2:V:224:TYR:HE2	1:h:248:LEU:CG	1.97	0.78
2:X:123:ARG:NH1	2:Y:308:ARG:HH12	1.59	0.78
2:X:210:TYR:OH	1:j:325:PRO:HB2	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:56:ALA:CA	2:Z:286:LEU:HD12	2.13	0.78
2:Y:128:SER:C	2:Z:290:GLU:OE1	2.25	0.78
1:D:127:ASP:OD2	1:G:297:GLU:CD	2.26	0.78
1:O:70:LEU:CD2	1:O:114:LEU:HD12	2.14	0.78
2:Y:62:VAL:CG1	2:Z:284:ARG:HB3	2.11	0.78
2:Y:124:LYS:HG2	2:Z:294:GLN:CA	2.14	0.78
1:E:70:LEU:CD2	1:E:114:LEU:HD12	2.14	0.77
2:W:210:TYR:OH	1:i:325:PRO:HB2	1.84	0.77
1:A:70:LEU:CD2	1:A:114:LEU:HD12	2.14	0.77
1:E:234:ILE:HG21	1:E:270:VAL:HG11	1.65	0.77
1:J:70:LEU:CD2	1:J:114:LEU:HD12	2.14	0.77
1:M:234:ILE:HG21	1:M:270:VAL:HG11	1.65	0.77
2:S:210:TYR:OH	1:e:325:PRO:HB2	1.84	0.77
2:Y:210:TYR:OH	1:k:325:PRO:HB2	1.84	0.77
1:h:70:LEU:CD2	1:h:114:LEU:HD12	2.14	0.77
1:k:234:ILE:HG21	1:k:270:VAL:HG11	1.65	0.77
2:p:60:LYS:H	2:q:283:TYR:HA	1.48	0.77
1:A:234:ILE:HG21	1:A:270:VAL:HG11	1.65	0.77
2:R:224:TYR:HE2	1:d:248:LEU:CG	1.97	0.77
2:T:224:TYR:HE2	1:f:248:LEU:CG	1.97	0.77
2:B:224:TYR:HE2	1:E:248:LEU:CG	1.97	0.77
1:D:70:LEU:CD2	1:D:114:LEU:HD12	2.14	0.77
2:S:404:PHE:CE1	1:e:261:PRO:CB	2.68	0.77
2:X:221:THR:HG22	1:j:324:VAL:HG11	1.67	0.77
1:d:70:LEU:CD2	1:d:114:LEU:HD12	2.14	0.77
1:O:58:SER:HB2	1:P:282:TYR:CA	2.14	0.77
2:Q:224:TYR:HE2	1:c:248:LEU:CG	1.97	0.77
2:R:88:ARG:HG2	2:S:218:LYS:HZ2	1.47	0.77
2:T:404:PHE:CE1	1:f:261:PRO:CB	2.68	0.77
2:U:210:TYR:OH	1:g:325:PRO:HB2	1.84	0.77
2:W:221:THR:HG22	1:i:324:VAL:HG11	1.67	0.77
2:Y:221:THR:HG22	1:k:324:VAL:HG11	1.67	0.77
2:B:406:HIS:CG	1:E:263:PRO:CG	2.67	0.77
1:L:70:LEU:CD2	1:L:114:LEU:HD12	2.14	0.77
2:S:224:TYR:HE2	1:e:248:LEU:CG	1.97	0.77
2:B:221:THR:HG21	1:E:324:VAL:HG21	1.67	0.77
1:K:70:LEU:CD2	1:K:114:LEU:HD12	2.14	0.77
2:Q:404:PHE:CE1	1:c:261:PRO:CB	2.68	0.77
2:S:56:ALA:HB2	2:T:284:ARG:HG3	1.66	0.77
2:Y:224:TYR:HE2	1:k:248:LEU:CG	1.97	0.77
1:i:70:LEU:CD2	1:i:114:LEU:HD12	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:70:LEU:CD2	1:j:114:LEU:HD12	2.14	0.77
2:B:210:TYR:OH	1:E:325:PRO:HB2	1.84	0.77
2:X:406:HIS:CG	1:j:263:PRO:CG	2.67	0.77
2:Y:181:VAL:CG2	1:k:258:ASN:O	2.31	0.77
1:d:56:THR:CB	1:e:280:LYS:O	2.33	0.77
1:j:234:ILE:HG21	1:j:270:VAL:HG11	1.65	0.77
1:D:89:PRO:HG2	1:G:218:ASP:OD2	1.84	0.77
1:J:60:LYS:HE2	1:K:283:HIS:NE2	2.00	0.77
1:L:234:ILE:HG21	1:L:270:VAL:HG11	1.65	0.77
2:Q:57:THR:HA	2:R:283:TYR:O	1.35	0.77
2:T:210:TYR:OH	1:f:325:PRO:HB2	1.84	0.77
2:V:221:THR:HG22	1:h:324:VAL:HG11	1.67	0.77
2:W:404:PHE:CE1	1:i:261:PRO:CB	2.68	0.77
1:G:70:LEU:CD2	1:G:114:LEU:HD12	2.14	0.77
2:Q:406:HIS:CG	1:c:263:PRO:CG	2.67	0.77
2:R:404:PHE:CE1	1:d:261:PRO:CB	2.68	0.77
1:e:70:LEU:CD2	1:e:114:LEU:HD12	2.14	0.77
1:e:124:LYS:CE	1:f:297:GLU:CD	2.58	0.77
1:K:56:THR:HB	1:L:283:HIS:CA	2.15	0.76
1:N:70:LEU:CD2	1:N:114:LEU:HD12	2.14	0.76
2:U:221:THR:HG22	1:g:324:VAL:HG11	1.67	0.76
2:X:404:PHE:CE1	1:j:261:PRO:CB	2.68	0.76
2:Y:86:ILE:HG13	2:Z:282:GLN:HB2	1.64	0.76
2:S:56:ALA:CB	2:T:284:ARG:HG2	1.96	0.76
2:W:181:VAL:CG2	1:i:258:ASN:O	2.31	0.76
1:c:70:LEU:CD2	1:c:114:LEU:HD12	2.14	0.76
1:d:56:THR:O	1:e:282:TYR:C	2.27	0.76
1:j:123:ARG:HH22	1:k:338:ARG:NH1	1.83	0.76
1:j:127:ASP:HB3	1:k:290:GLU:HA	1.68	0.76
1:C:70:LEU:CD2	1:C:114:LEU:HD12	2.14	0.76
1:M:88:HIS:CD2	1:N:280:LYS:CD	2.68	0.76
2:Q:221:THR:HG21	1:c:324:VAL:HG21	1.67	0.76
2:V:221:THR:HG21	1:h:324:VAL:HG21	1.67	0.76
1:d:62:VAL:HG23	1:e:283:HIS:CB	2.15	0.76
2:B:404:PHE:CE1	1:E:261:PRO:CB	2.68	0.76
2:R:221:THR:HG22	1:d:324:VAL:HG11	1.67	0.76
2:Y:404:PHE:CE1	1:k:261:PRO:CB	2.68	0.76
1:e:124:LYS:CE	1:f:299:SER:OG	2.34	0.76
1:M:57:GLY:CA	1:N:372:LEU:CD2	2.26	0.76
2:U:179:ASP:O	1:g:352:LYS:CA	2.33	0.76
2:X:181:VAL:CG2	1:j:258:ASN:O	2.31	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:r:56:ALA:HB3	2:s:283:TYR:C	2.10	0.76
1:D:89:PRO:HD2	1:G:280:LYS:HE3	1.68	0.76
1:M:89:PRO:HD2	1:N:280:LYS:N	1.83	0.76
2:Y:57:THR:CA	2:Z:372:LYS:HB2	2.15	0.76
2:r:60:LYS:HD2	2:s:282:GLN:C	2.09	0.76
2:B:96:GLN:CD	1:E:1:MET:SD	2.69	0.76
1:G:57:GLY:N	1:H:286:LEU:O	2.18	0.76
1:G:129:CYS:CA	1:H:338:ARG:NH2	2.48	0.76
1:M:70:LEU:CD2	1:M:114:LEU:HD12	2.14	0.76
2:R:96:GLN:CD	1:d:1:MET:SD	2.69	0.76
2:T:222:PRO:CD	1:f:326:LYS:HD2	2.16	0.76
1:k:70:LEU:CD2	1:k:114:LEU:HD12	2.14	0.76
1:E:82:PRO:HD2	1:E:83:TYR:N	2.01	0.76
1:N:82:PRO:HD2	1:N:83:TYR:N	2.01	0.76
2:S:56:ALA:H	2:T:285:ALA:CB	1.98	0.76
2:S:403:ALA:HB2	1:e:262:TYR:CZ	2.21	0.76
2:T:221:THR:HG22	1:f:324:VAL:HG11	1.67	0.76
2:U:181:VAL:CG2	1:g:258:ASN:O	2.31	0.76
2:X:222:PRO:CD	1:j:326:LYS:HD2	2.16	0.76
2:Y:96:GLN:CD	1:k:1:MET:SD	2.69	0.76
1:A:82:PRO:HD2	1:A:83:TYR:N	2.01	0.76
2:Q:224:TYR:CE2	1:c:248:LEU:CD2	2.69	0.76
2:S:96:GLN:CD	1:e:1:MET:SD	2.69	0.76
2:U:96:GLN:CD	1:g:1:MET:SD	2.69	0.76
2:V:404:PHE:CE1	1:h:261:PRO:CB	2.68	0.76
2:W:221:THR:HG21	1:i:324:VAL:HG21	1.67	0.76
1:j:88:HIS:ND1	1:k:280:LYS:HG2	2.00	0.76
2:B:403:ALA:HB2	1:E:262:TYR:CZ	2.21	0.76
2:R:222:PRO:CD	1:d:326:LYS:HD2	2.16	0.76
2:X:96:GLN:CD	1:j:1:MET:SD	2.69	0.76
2:r:56:ALA:CB	2:s:284:ARG:HA	2.13	0.76
1:K:57:GLY:H	1:L:283:HIS:HA	1.49	0.75
2:Q:179:ASP:O	1:c:352:LYS:CA	2.33	0.75
2:Q:403:ALA:HB2	1:c:262:TYR:CZ	2.21	0.75
2:T:403:ALA:HB2	1:f:262:TYR:CZ	2.21	0.75
2:U:403:ALA:HB2	1:g:262:TYR:CZ	2.21	0.75
2:W:224:TYR:CE2	1:i:248:LEU:CD2	2.69	0.75
1:O:82:PRO:HD2	1:O:83:TYR:N	2.01	0.75
2:R:221:THR:HG21	1:d:324:VAL:HG21	1.67	0.75
2:U:404:PHE:CE1	1:g:261:PRO:CB	2.68	0.75
2:V:224:TYR:CE2	1:h:248:LEU:CD2	2.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:120:ASP:CG	1:f:298:TYR:OH	2.28	0.75
2:r:56:ALA:CB	2:s:283:TYR:C	2.60	0.75
1:D:60:LYS:CE	1:G:279:GLU:O	2.34	0.75
2:Q:222:PRO:CD	1:c:326:LYS:HD2	2.16	0.75
2:S:224:TYR:CE2	1:e:248:LEU:CD2	2.69	0.75
2:Y:224:TYR:CE2	1:k:248:LEU:CD2	2.69	0.75
1:N:62:VAL:HG11	1:O:285:GLN:HE21	1.51	0.75
2:T:221:THR:HG21	1:f:324:VAL:HG21	1.67	0.75
2:T:224:TYR:CE2	1:f:248:LEU:CD2	2.69	0.75
2:U:221:THR:HG21	1:g:324:VAL:HG21	1.67	0.75
2:V:96:GLN:CD	1:h:1:MET:SD	2.69	0.75
2:B:179:ASP:O	1:E:352:LYS:CA	2.33	0.75
2:S:221:THR:HG21	1:e:324:VAL:HG21	1.67	0.75
2:V:406:HIS:CG	1:h:263:PRO:CG	2.67	0.75
2:X:224:TYR:CE2	1:j:248:LEU:CD2	2.69	0.75
1:f:62:VAL:CG2	1:g:283:HIS:HB3	2.15	0.75
1:P:82:PRO:HD2	1:P:83:TYR:N	2.01	0.75
2:Q:221:THR:HG22	1:c:324:VAL:HG11	1.67	0.75
2:S:221:THR:HG22	1:e:324:VAL:HG11	1.67	0.75
2:W:222:PRO:CD	1:i:326:LYS:HD2	2.16	0.75
2:X:221:THR:HG21	1:j:324:VAL:HG21	1.67	0.75
1:G:88:HIS:HE1	1:H:216:ASN:OD1	1.70	0.75
2:R:224:TYR:CE2	1:d:248:LEU:CD2	2.69	0.75
2:T:96:GLN:CD	1:f:1:MET:SD	2.69	0.75
2:U:214:PHE:CZ	1:g:326:LYS:HG3	2.22	0.75
2:V:404:PHE:HD2	1:h:260:VAL:O	1.70	0.75
2:Y:128:SER:CA	2:Z:289:PRO:C	2.54	0.75
2:Y:221:THR:HG21	1:k:324:VAL:HG21	1.67	0.75
2:Y:222:PRO:CD	1:k:326:LYS:HD2	2.16	0.75
1:M:89:PRO:CD	1:N:279:GLU:H	1.86	0.75
2:R:56:ALA:CB	2:S:283:TYR:N	2.49	0.75
2:S:222:PRO:CD	1:e:326:LYS:HD2	2.16	0.75
2:W:96:GLN:CD	1:i:1:MET:SD	2.69	0.75
2:X:394:GLN:HA	1:j:348:PRO:HG3	1.69	0.75
2:Q:60:LYS:N	2:R:283:TYR:CE2	2.55	0.75
2:Q:60:LYS:N	2:R:283:TYR:HD2	1.76	0.75
2:S:181:VAL:CG2	1:e:258:ASN:O	2.31	0.75
2:U:222:PRO:CD	1:g:326:LYS:HD2	2.16	0.75
2:V:406:HIS:HB3	1:h:263:PRO:HG3	1.69	0.75
2:Y:87:PHE:N	2:Z:283:TYR:HD1	1.64	0.75
2:Y:403:ALA:HB2	1:k:262:TYR:CZ	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:90:GLU:OE1	1:H:299:SER:HB2	1.87	0.74
1:I:82:PRO:HD2	1:I:83:TYR:N	2.01	0.74
2:R:403:ALA:HB2	1:d:262:TYR:CZ	2.21	0.74
2:W:406:HIS:HB3	1:i:263:PRO:HG3	1.69	0.74
2:X:179:ASP:O	1:j:352:LYS:CA	2.33	0.74
2:B:224:TYR:CE2	1:E:248:LEU:CD2	2.69	0.74
2:Q:96:GLN:CD	1:c:1:MET:SD	2.69	0.74
2:T:214:PHE:CZ	1:f:326:LYS:HG3	2.22	0.74
2:U:394:GLN:HA	1:g:348:PRO:HG3	1.69	0.74
2:V:222:PRO:CD	1:h:326:LYS:HD2	2.16	0.74
1:g:82:PRO:HD2	1:g:83:TYR:N	2.01	0.74
1:G:82:PRO:HD2	1:G:83:TYR:N	2.01	0.74
2:R:62:VAL:CG2	2:S:283:TYR:CB	2.54	0.74
2:V:214:PHE:CZ	1:h:326:LYS:HG3	2.22	0.74
2:W:214:PHE:CZ	1:i:326:LYS:HG3	2.22	0.74
2:W:403:ALA:HB2	1:i:262:TYR:CZ	2.21	0.74
2:Y:179:ASP:O	1:k:352:LYS:CA	2.33	0.74
2:B:221:THR:HG22	1:E:324:VAL:HG11	1.67	0.74
2:B:406:HIS:HB3	1:E:263:PRO:HG3	1.69	0.74
1:M:57:GLY:N	1:N:372:LEU:HG	1.98	0.74
2:U:224:TYR:CE2	1:g:248:LEU:CD2	2.69	0.74
2:X:403:ALA:HB2	1:j:262:TYR:CZ	2.21	0.74
1:e:82:PRO:HD2	1:e:83:TYR:N	2.01	0.74
2:p:56:ALA:CB	2:q:283:TYR:CB	2.64	0.74
1:K:60:LYS:HB3	1:L:283:HIS:CD2	2.22	0.74
2:R:394:GLN:HA	1:d:348:PRO:HG3	1.69	0.74
2:W:179:ASP:O	1:i:352:LYS:CA	2.33	0.74
1:M:128:GLN:HA	1:N:287:SER:OG	1.87	0.74
2:V:179:ASP:O	1:h:352:LYS:CA	2.33	0.74
2:V:403:ALA:HB2	1:h:262:TYR:CZ	2.21	0.74
2:X:214:PHE:CZ	1:j:326:LYS:HG3	2.22	0.74
2:p:57:THR:OG1	2:q:280:SER:O	2.06	0.74
2:B:394:GLN:HA	1:E:348:PRO:HG3	1.69	0.74
1:G:89:PRO:HB3	1:H:280:LYS:NZ	2.03	0.74
2:Y:90:ASP:HA	2:Z:216:THR:C	2.06	0.74
2:Y:394:GLN:HA	1:k:348:PRO:HG3	1.69	0.74
2:Y:406:HIS:HB3	1:k:263:PRO:HG3	1.69	0.74
2:B:404:PHE:HD2	1:E:260:VAL:O	1.70	0.74
2:Q:181:VAL:HG23	1:c:258:ASN:HB3	1.70	0.74
2:W:404:PHE:HD2	1:i:260:VAL:O	1.70	0.74
2:Y:88:ARG:O	2:Z:280:SER:OG	1.90	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:181:VAL:HG23	1:k:258:ASN:HB3	1.70	0.74
2:Y:56:ALA:HA	2:Z:286:LEU:HD12	1.68	0.74
2:R:88:ARG:C	2:S:218:LYS:NZ	2.45	0.74
2:U:406:HIS:HB3	1:g:263:PRO:HG3	1.69	0.74
2:W:180:THR:HG23	1:i:258:ASN:OD1	1.88	0.74
2:X:181:VAL:HG23	1:j:258:ASN:HB3	1.70	0.74
2:Y:90:ASP:OD1	2:Z:276:THR:CA	2.35	0.74
1:G:124:LYS:CE	1:H:297:GLU:O	2.35	0.73
2:R:404:PHE:HD2	1:d:260:VAL:O	1.70	0.73
2:S:127:GLU:CD	2:T:339:ASN:ND2	2.46	0.73
2:T:394:GLN:HA	1:f:348:PRO:HG3	1.69	0.73
2:U:406:HIS:CG	1:g:263:PRO:CG	2.67	0.73
2:W:394:GLN:HA	1:i:348:PRO:HG3	1.69	0.73
1:G:90:GLU:CB	1:H:215:ARG:CG	2.66	0.73
2:Q:406:HIS:HB3	1:c:263:PRO:HG3	1.69	0.73
2:X:406:HIS:HB3	1:j:263:PRO:HG3	1.69	0.73
2:Y:90:ASP:CB	2:Z:216:THR:O	2.35	0.73
2:Y:403:ALA:HA	1:k:262:TYR:CZ	2.23	0.73
1:k:82:PRO:HD2	1:k:83:TYR:N	2.01	0.73
2:B:181:VAL:HG23	1:E:258:ASN:HB3	1.70	0.73
1:G:129:CYS:CB	1:H:338:ARG:NH2	2.50	0.73
1:M:82:PRO:HD2	1:M:83:TYR:N	2.01	0.73
2:Q:404:PHE:HD2	1:c:260:VAL:O	1.70	0.73
2:R:403:ALA:HA	1:d:262:TYR:CZ	2.23	0.73
2:R:406:HIS:CG	1:d:263:PRO:CG	2.67	0.73
2:V:403:ALA:HA	1:h:262:TYR:CZ	2.23	0.73
1:e:58:SER:HB2	1:f:282:TYR:HA	1.69	0.73
1:D:127:ASP:CG	1:G:297:GLU:OE2	2.31	0.73
2:Q:214:PHE:CZ	1:c:326:LYS:HG3	2.22	0.73
2:S:57:THR:HA	2:T:286:LEU:H	0.59	0.73
2:V:180:THR:HG23	1:h:258:ASN:OD1	1.88	0.73
1:D:62:VAL:CG2	1:G:283:HIS:HD1	1.96	0.73
1:M:128:GLN:CG	1:N:290:GLU:CG	2.54	0.73
2:Q:403:ALA:HA	1:c:262:TYR:CZ	2.23	0.73
2:T:403:ALA:HA	1:f:262:TYR:CZ	2.23	0.73
2:W:403:ALA:HA	1:i:262:TYR:CZ	2.23	0.73
2:X:394:GLN:HE21	1:j:348:PRO:CB	2.02	0.73
2:Y:214:PHE:CZ	1:k:326:LYS:HG3	2.22	0.73
2:Q:60:LYS:CA	2:R:283:TYR:CE2	2.72	0.73
2:R:394:GLN:HE21	1:d:348:PRO:CB	2.02	0.73
2:T:406:HIS:HB3	1:f:263:PRO:HG3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:89:PRO:C	2:Y:218:LYS:NZ	2.46	0.73
2:X:403:ALA:HA	1:j:262:TYR:CZ	2.23	0.73
2:Y:180:THR:HG23	1:k:258:ASN:OD1	1.88	0.73
2:Q:180:THR:HG23	1:c:258:ASN:OD1	1.88	0.73
2:R:180:THR:HG23	1:d:258:ASN:OD1	1.88	0.73
2:S:394:GLN:HA	1:e:348:PRO:HG3	1.69	0.73
2:U:220:THR:O	1:g:326:LYS:CD	2.37	0.73
2:V:394:GLN:HA	1:h:348:PRO:HG3	1.69	0.73
1:j:62:VAL:HG22	1:k:283:HIS:HD2	1.53	0.73
2:B:181:VAL:N	1:E:258:ASN:OD1	2.22	0.73
2:B:214:PHE:CZ	1:E:326:LYS:HG3	2.22	0.73
1:G:60:LYS:HE2	1:H:280:LYS:CA	2.17	0.73
2:T:394:GLN:HE21	1:f:348:PRO:CB	2.02	0.73
2:W:181:VAL:HG23	1:i:258:ASN:HB3	1.70	0.73
2:Y:62:VAL:CG1	2:Z:281:GLN:O	2.37	0.73
1:D:128:GLN:NE2	1:G:284:GLU:OE2	2.18	0.73
2:S:179:ASP:O	1:e:352:LYS:CA	2.33	0.73
2:S:394:GLN:HE21	1:e:348:PRO:CB	2.02	0.73
2:r:33:THR:O	2:s:283:TYR:CE2	2.42	0.73
2:S:90:ASP:CG	2:T:215:ARG:O	2.32	0.72
2:S:180:THR:HG23	1:e:258:ASN:OD1	1.88	0.72
2:V:220:THR:O	1:h:326:LYS:CD	2.37	0.72
2:Y:56:ALA:CA	2:Z:286:LEU:CG	2.66	0.72
1:f:82:PRO:HD2	1:f:83:TYR:N	2.01	0.72
1:H:82:PRO:HD2	1:H:83:TYR:N	2.01	0.72
2:T:179:ASP:O	1:f:352:LYS:CA	2.33	0.72
2:W:220:THR:O	1:i:326:LYS:CD	2.37	0.72
2:X:181:VAL:N	1:j:258:ASN:OD1	2.22	0.72
1:c:58:SER:HB2	1:d:282:TYR:HB2	1.69	0.72
2:R:179:ASP:O	1:d:352:LYS:CA	2.33	0.72
2:S:181:VAL:HG23	1:e:258:ASN:HB3	1.70	0.72
2:T:180:THR:HG23	1:f:258:ASN:OD1	1.88	0.72
2:T:181:VAL:HG23	1:f:258:ASN:HB3	1.70	0.72
2:U:181:VAL:N	1:g:258:ASN:OD1	2.22	0.72
2:V:181:VAL:HG23	1:h:258:ASN:HB3	1.70	0.72
2:Y:404:PHE:CD1	1:k:261:PRO:HA	2.25	0.72
1:e:127:ASP:HA	1:f:338:ARG:HH21	1.51	0.72
2:B:220:THR:O	1:E:326:LYS:CD	2.37	0.72
2:R:181:VAL:HG23	1:d:258:ASN:HB3	1.70	0.72
2:R:406:HIS:HB3	1:d:263:PRO:HG3	1.69	0.72
2:T:404:PHE:CD1	1:f:261:PRO:HA	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:394:GLN:HE21	1:i:348:PRO:CB	2.02	0.72
2:W:406:HIS:CG	1:i:263:PRO:CG	2.67	0.72
2:X:180:THR:HG23	1:j:258:ASN:OD1	1.88	0.72
2:X:220:THR:O	1:j:326:LYS:CD	2.37	0.72
2:Y:220:THR:O	1:k:326:LYS:CD	2.37	0.72
1:e:120:ASP:HB2	1:f:298:TYR:HH	1.54	0.72
1:j:123:ARG:HG2	1:k:297:GLU:HG2	1.71	0.72
2:B:222:PRO:CD	1:E:326:LYS:HD2	2.16	0.72
1:D:62:VAL:HG21	1:G:280:LYS:CA	2.18	0.72
1:M:89:PRO:HG3	1:N:277:SER:HB2	1.67	0.72
2:Q:394:GLN:HA	1:c:348:PRO:HG3	1.69	0.72
2:S:214:PHE:CZ	1:e:326:LYS:HG3	2.22	0.72
2:S:406:HIS:CG	1:e:263:PRO:CG	2.67	0.72
2:U:181:VAL:HG23	1:g:258:ASN:HB3	1.70	0.72
2:V:181:VAL:N	1:h:258:ASN:OD1	2.22	0.72
2:X:128:SER:OG	2:Y:290:GLU:OE1	2.07	0.72
2:Y:181:VAL:N	1:k:258:ASN:OD1	2.22	0.72
2:a:172:VAL:HG23	2:a:173:PRO:CD	2.20	0.72
1:L:56:THR:HG21	1:M:283:HIS:C	2.15	0.72
2:Q:404:PHE:CD1	1:c:261:PRO:HA	2.25	0.72
2:S:220:THR:O	1:e:326:LYS:CD	2.37	0.72
2:S:406:HIS:HB3	1:e:263:PRO:HG3	1.69	0.72
1:j:123:ARG:NH1	1:k:338:ARG:CZ	2.51	0.72
2:R:214:PHE:CZ	1:d:326:LYS:HG3	2.22	0.72
2:S:404:PHE:HD2	1:e:260:VAL:O	1.70	0.72
2:T:406:HIS:CG	1:f:263:PRO:CG	2.67	0.72
2:V:394:GLN:HE21	1:h:348:PRO:CB	2.02	0.72
2:q:56:ALA:HB1	2:r:284:ARG:CA	2.01	0.72
2:B:394:GLN:HE21	1:E:348:PRO:CB	2.02	0.72
2:U:403:ALA:HA	1:g:262:TYR:CZ	2.23	0.72
2:X:404:PHE:CD1	1:j:261:PRO:HA	2.25	0.72
1:j:62:VAL:CG2	1:k:283:HIS:HB3	2.15	0.72
2:B:172:VAL:HG23	2:B:173:PRO:CD	2.20	0.72
2:R:404:PHE:CD1	1:d:261:PRO:HA	2.25	0.72
2:Y:54:ASN:OD1	2:Z:285:ALA:HB3	1.89	0.72
2:p:124:LYS:HE2	2:q:299:LYS:NZ	2.04	0.72
1:M:89:PRO:HA	1:N:279:GLU:HB3	1.71	0.72
2:Q:172:VAL:HG23	2:Q:173:PRO:CD	2.20	0.72
2:Q:220:THR:O	1:c:326:LYS:CD	2.37	0.72
2:S:181:VAL:N	1:e:258:ASN:OD1	2.22	0.72
2:U:394:GLN:HE21	1:g:348:PRO:CB	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:181:VAL:N	1:i:258:ASN:OD1	2.22	0.72
2:X:90:ASP:N	2:Y:218:LYS:HZ1	1.87	0.72
2:Y:56:ALA:CB	2:Z:286:LEU:CD1	2.67	0.72
2:Y:124:LYS:HG2	2:Z:293:GLN:O	1.88	0.72
2:Y:394:GLN:HE21	1:k:348:PRO:CB	2.02	0.72
2:o:172:VAL:HG23	2:o:173:PRO:CD	2.20	0.72
2:B:403:ALA:HA	1:E:262:TYR:CZ	2.23	0.71
2:F:172:VAL:HG23	2:F:173:PRO:CD	2.20	0.71
2:Q:181:VAL:N	1:c:258:ASN:OD1	2.22	0.71
2:Y:128:SER:CA	2:Z:290:GLU:N	2.46	0.71
2:b:172:VAL:HG23	2:b:173:PRO:CD	2.20	0.71
1:j:88:HIS:HE1	1:k:280:LYS:HB3	0.58	0.71
2:q:172:VAL:HG23	2:q:173:PRO:CD	2.20	0.71
2:r:56:ALA:HA	2:s:285:ALA:H	1.53	0.71
1:D:56:THR:HG23	1:G:280:LYS:O	1.86	0.71
1:D:124:LYS:HZ3	1:G:215:ARG:NH2	1.82	0.71
1:K:57:GLY:N	1:L:283:HIS:CA	2.51	0.71
2:Q:394:GLN:HE21	1:c:348:PRO:CB	2.02	0.71
2:R:172:VAL:HG23	2:R:173:PRO:CD	2.20	0.71
2:S:172:VAL:HG23	2:S:173:PRO:CD	2.20	0.71
2:S:404:PHE:CD1	1:e:261:PRO:HA	2.25	0.71
2:T:220:THR:O	1:f:326:LYS:CD	2.37	0.71
2:U:404:PHE:HD2	1:g:260:VAL:O	1.70	0.71
2:p:172:VAL:HG23	2:p:173:PRO:CD	2.20	0.71
1:J:82:PRO:HD2	1:J:83:TYR:N	2.01	0.71
2:U:180:THR:HG23	1:g:258:ASN:OD1	1.88	0.71
2:Y:89:PRO:O	2:Z:218:LYS:HG3	1.89	0.71
1:h:82:PRO:HD2	1:h:83:TYR:N	2.01	0.71
1:K:57:GLY:H	1:L:283:HIS:CA	2.03	0.71
2:T:181:VAL:N	1:f:258:ASN:OD1	2.22	0.71
2:F:57:THR:CB	2:o:283:TYR:CE2	2.69	0.71
2:V:172:VAL:HG23	2:V:173:PRO:CD	2.20	0.71
2:W:404:PHE:CD1	1:i:261:PRO:HA	2.24	0.71
2:Y:120:ASP:OD1	2:Z:297:ASP:OD2	2.07	0.71
1:j:89:PRO:HG2	1:k:280:LYS:CE	2.21	0.71
1:M:127:ASP:CB	1:N:290:GLU:HA	2.19	0.71
2:R:89:PRO:CB	2:S:218:LYS:CD	2.61	0.71
2:S:33:THR:HG23	2:T:283:TYR:HH	0.88	0.71
2:V:404:PHE:CD1	1:h:261:PRO:HA	2.25	0.71
2:Y:404:PHE:HD2	1:k:260:VAL:O	1.70	0.71
2:B:404:PHE:CD1	1:E:261:PRO:HA	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:60:LYS:NZ	2:S:279:GLY:O	2.18	0.71
2:W:172:VAL:HG23	2:W:173:PRO:CD	2.20	0.71
2:U:404:PHE:CD1	1:g:261:PRO:HA	2.25	0.71
1:e:124:LYS:HE2	1:f:297:GLU:CD	2.15	0.71
2:R:181:VAL:N	1:d:258:ASN:OD1	2.22	0.71
2:B:101:ASN:CG	1:E:254:GLU:HG3	2.16	0.70
2:T:101:ASN:CG	1:f:254:GLU:HG3	2.16	0.70
2:X:101:ASN:CG	1:j:254:GLU:HG3	2.16	0.70
1:C:57:GLY:CA	1:D:284:GLU:CA	2.65	0.70
2:R:220:THR:O	1:d:326:LYS:CD	2.37	0.70
2:B:180:THR:HG23	1:E:258:ASN:OD1	1.88	0.70
2:W:101:ASN:CG	1:i:254:GLU:HG3	2.16	0.70
2:r:172:VAL:HG23	2:r:173:PRO:CD	2.20	0.70
1:G:123:ARG:HG2	1:H:308:ARG:HD3	1.71	0.70
1:M:54:SER:CB	1:N:284:GLU:C	2.60	0.70
1:M:63:PRO:N	1:N:283:HIS:CA	2.38	0.70
1:M:89:PRO:CG	1:N:279:GLU:H	2.04	0.70
2:S:101:ASN:CG	1:e:254:GLU:HG3	2.16	0.70
2:T:404:PHE:HD2	1:f:260:VAL:O	1.70	0.70
2:U:172:VAL:HG23	2:U:173:PRO:CD	2.20	0.70
2:T:172:VAL:HG23	2:T:173:PRO:CD	2.20	0.70
2:R:56:ALA:C	2:S:284:ARG:O	2.30	0.70
2:R:60:LYS:CB	2:S:283:TYR:N	2.49	0.70
2:R:101:ASN:CG	1:d:254:GLU:HG3	2.16	0.70
2:Y:56:ALA:HA	2:Z:286:LEU:CD1	2.20	0.70
2:Y:172:VAL:HG23	2:Y:173:PRO:CD	2.20	0.70
2:s:172:VAL:HG23	2:s:173:PRO:CD	2.20	0.70
1:M:128:GLN:HB3	1:N:285:GLN:HB2	0.83	0.70
2:R:394:GLN:CG	1:d:348:PRO:CG	2.70	0.70
2:U:406:HIS:CE1	1:g:263:PRO:HA	2.27	0.70
1:e:56:THR:HG23	1:f:283:HIS:O	1.90	0.70
1:G:90:GLU:OE1	1:H:299:SER:CB	2.40	0.70
2:Q:101:ASN:CG	1:c:254:GLU:HG3	2.16	0.70
2:W:394:GLN:CG	1:i:348:PRO:CG	2.70	0.70
2:W:406:HIS:CE1	1:i:263:PRO:HA	2.27	0.70
2:X:56:ALA:HB1	2:Y:283:TYR:O	1.89	0.70
2:Y:406:HIS:CE1	1:k:263:PRO:HA	2.27	0.70
2:r:56:ALA:CA	2:s:285:ALA:CA	2.63	0.70
2:T:406:HIS:CE1	1:f:263:PRO:HA	2.27	0.70
2:X:172:VAL:HG23	2:X:173:PRO:CD	2.20	0.70
2:X:406:HIS:CE1	1:j:263:PRO:HA	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:PRO:CG	1:G:218:ASP:OD2	2.40	0.69
2:Q:404:PHE:CZ	1:c:261:PRO:CA	2.76	0.69
2:R:406:HIS:CE1	1:d:263:PRO:HA	2.27	0.69
2:S:403:ALA:HA	1:e:262:TYR:CZ	2.23	0.69
2:V:101:ASN:CG	1:h:254:GLU:HG3	2.16	0.69
2:Z:172:VAL:HG23	2:Z:173:PRO:CD	2.20	0.69
1:f:60:LYS:CB	1:g:282:TYR:O	2.39	0.69
2:R:34:GLY:O	2:S:283:TYR:CE2	2.45	0.69
2:W:403:ALA:HA	1:i:262:TYR:CD1	2.27	0.69
2:Y:127:GLU:O	2:Z:289:PRO:HB2	1.91	0.69
1:j:116:ASP:HB3	1:k:298:TYR:CZ	2.27	0.69
1:D:58:SER:N	1:G:282:TYR:CE1	2.30	0.69
2:U:101:ASN:CG	1:g:254:GLU:HG3	2.16	0.69
2:Y:101:ASN:CG	1:k:254:GLU:HG3	2.16	0.69
1:j:56:THR:CG2	1:k:283:HIS:C	2.66	0.69
2:Q:406:HIS:CE1	1:c:263:PRO:HA	2.27	0.69
2:S:406:HIS:CE1	1:e:263:PRO:HA	2.27	0.69
2:U:403:ALA:HA	1:g:262:TYR:CD1	2.27	0.69
2:Y:86:ILE:CG1	2:Z:282:GLN:HB3	2.22	0.69
2:B:394:GLN:CG	1:E:348:PRO:CG	2.70	0.69
2:B:406:HIS:CE1	1:E:263:PRO:HA	2.27	0.69
1:C:82:PRO:HD2	1:C:83:TYR:N	2.01	0.69
1:M:54:SER:HB2	1:N:285:GLN:HG2	1.75	0.69
2:T:404:PHE:CZ	1:f:261:PRO:CA	2.76	0.69
1:c:82:PRO:HD2	1:c:83:TYR:N	2.01	0.69
1:d:56:THR:HG21	1:e:280:LYS:O	1.91	0.69
2:B:404:PHE:CZ	1:E:261:PRO:CA	2.76	0.69
1:G:60:LYS:HD3	1:H:284:GLU:HG2	1.75	0.69
2:S:394:GLN:CG	1:e:348:PRO:CG	2.70	0.69
2:S:404:PHE:CZ	1:e:261:PRO:CA	2.76	0.69
2:Y:394:GLN:CG	1:k:348:PRO:CG	2.70	0.69
2:a:57:THR:HG1	2:b:281:GLN:C	1.90	0.69
1:M:127:ASP:OD2	1:N:293:ASN:HB3	1.92	0.69
2:R:404:PHE:CD2	1:d:260:VAL:C	2.71	0.69
2:U:404:PHE:CD2	1:g:260:VAL:C	2.71	0.69
2:V:406:HIS:CE1	1:h:263:PRO:HA	2.27	0.69
2:X:404:PHE:CZ	1:j:261:PRO:CA	2.75	0.69
1:L:60:LYS:HE2	1:M:283:HIS:CD2	2.28	0.69
2:R:404:PHE:CZ	1:d:261:PRO:CA	2.76	0.69
2:T:404:PHE:CD2	1:f:260:VAL:C	2.71	0.69
2:U:394:GLN:CG	1:g:348:PRO:CG	2.70	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:403:ALA:HA	1:h:262:TYR:CD1	2.27	0.69
2:V:404:PHE:CZ	1:h:261:PRO:CA	2.76	0.69
2:W:404:PHE:CD2	1:i:260:VAL:C	2.71	0.69
2:W:404:PHE:CZ	1:i:261:PRO:CA	2.75	0.69
2:X:404:PHE:HD2	1:j:260:VAL:O	1.70	0.69
2:Y:56:ALA:CA	2:Z:286:LEU:HG	2.23	0.69
1:f:56:THR:CB	1:g:284:GLU:O	2.38	0.69
1:G:61:HIS:CD2	1:H:285:GLN:HE21	2.01	0.69
2:V:394:GLN:CG	1:h:348:PRO:CG	2.70	0.69
2:X:7:LEU:HD22	2:X:66:VAL:HB	1.75	0.69
2:X:394:GLN:CG	1:j:348:PRO:CG	2.70	0.69
2:S:403:ALA:HA	1:e:262:TYR:CD1	2.27	0.69
2:T:394:GLN:CG	1:f:348:PRO:CG	2.70	0.69
2:X:404:PHE:CD2	1:j:260:VAL:C	2.71	0.69
2:Y:404:PHE:CD2	1:k:260:VAL:C	2.71	0.69
2:B:404:PHE:CD2	1:E:260:VAL:C	2.71	0.68
2:Q:394:GLN:CG	1:c:348:PRO:CG	2.70	0.68
2:Q:406:HIS:NE2	1:c:263:PRO:HA	2.09	0.68
2:o:57:THR:CA	2:p:282:GLN:O	2.21	0.68
1:G:56:THR:HG22	1:H:286:LEU:HD23	1.71	0.68
2:Q:403:ALA:HA	1:c:262:TYR:CD1	2.27	0.68
2:V:406:HIS:NE2	1:h:263:PRO:HA	2.09	0.68
2:Y:404:PHE:CZ	1:k:261:PRO:CA	2.76	0.68
1:j:56:THR:CG2	1:k:283:HIS:O	2.40	0.68
1:j:56:THR:CG2	1:k:283:HIS:HA	2.19	0.68
2:V:404:PHE:CD2	1:h:260:VAL:C	2.71	0.68
2:W:406:HIS:NE2	1:i:263:PRO:HA	2.09	0.68
2:Y:128:SER:O	2:Z:289:PRO:HG2	1.94	0.68
2:a:57:THR:N	2:b:284:ARG:N	2.33	0.68
1:e:120:ASP:CG	1:f:298:TYR:CZ	2.71	0.68
1:j:89:PRO:HD2	1:k:280:LYS:HG2	1.75	0.68
1:H:30:LEU:CD2	1:H:36:MET:HE3	2.24	0.68
2:Y:397:ALA:O	1:k:346:TRP:CB	2.42	0.68
1:f:30:LEU:CD2	1:f:36:MET:HE3	2.24	0.68
1:f:56:THR:CG2	1:g:284:GLU:C	2.67	0.68
1:D:60:LYS:CG	1:G:283:HIS:HE1	2.07	0.68
2:F:57:THR:CG2	2:o:283:TYR:CD2	2.76	0.68
1:M:89:PRO:N	1:N:279:GLU:C	2.36	0.68
2:Q:60:LYS:CA	2:R:283:TYR:HE2	2.07	0.68
2:W:397:ALA:O	1:i:346:TRP:CB	2.42	0.68
2:X:397:ALA:O	1:j:346:TRP:CB	2.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:56:THR:HB	1:H:286:LEU:HD23	1.52	0.68
1:G:62:VAL:HG23	1:H:284:GLU:CA	2.02	0.68
1:I:30:LEU:CD2	1:I:36:MET:HE3	2.24	0.68
1:M:90:GLU:OE2	1:N:216:ASN:CB	2.42	0.68
1:d:57:GLY:N	1:e:281:ALA:O	2.26	0.68
1:j:30:LEU:CD2	1:j:36:MET:HE3	2.24	0.68
2:B:406:HIS:NE2	1:E:263:PRO:HA	2.09	0.68
1:L:30:LEU:CD2	1:L:36:MET:HE3	2.24	0.68
2:R:90:ASP:OD2	2:S:215:ARG:O	2.11	0.68
2:S:397:ALA:O	1:e:346:TRP:CB	2.42	0.68
1:g:30:LEU:CD2	1:g:36:MET:HE3	2.24	0.68
1:M:54:SER:HB3	1:N:284:GLU:C	2.19	0.68
2:R:397:ALA:O	1:d:346:TRP:CB	2.42	0.68
2:S:404:PHE:CD2	1:e:260:VAL:C	2.71	0.68
2:T:397:ALA:O	1:f:346:TRP:CB	2.42	0.68
2:Y:63:PRO:C	2:Z:283:TYR:HB3	1.95	0.68
2:Y:403:ALA:HA	1:k:262:TYR:CD1	2.27	0.68
1:D:30:LEU:CD2	1:D:36:MET:HE3	2.24	0.68
1:M:30:LEU:CD2	1:M:36:MET:HE3	2.24	0.68
2:S:406:HIS:NE2	1:e:263:PRO:HA	2.09	0.68
2:V:397:ALA:O	1:h:346:TRP:CB	2.42	0.68
2:Y:7:LEU:HD22	2:Y:66:VAL:HB	1.75	0.68
2:Y:86:ILE:CA	2:Z:282:GLN:HB2	2.23	0.68
1:d:30:LEU:CD2	1:d:36:MET:HE3	2.24	0.68
1:k:30:LEU:CD2	1:k:36:MET:HE3	2.24	0.68
2:U:404:PHE:CZ	1:g:261:PRO:CA	2.76	0.68
1:K:56:THR:CB	1:L:283:HIS:CB	2.31	0.67
2:Q:397:ALA:O	1:c:346:TRP:CB	2.42	0.67
2:T:403:ALA:HA	1:f:262:TYR:CD1	2.27	0.67
2:T:406:HIS:NE2	1:f:263:PRO:HA	2.09	0.67
2:X:406:HIS:NE2	1:j:263:PRO:HA	2.09	0.67
2:Y:34:GLY:HA3	2:Z:282:GLN:CB	2.23	0.67
2:Y:406:HIS:NE2	1:k:263:PRO:HA	2.09	0.67
2:Q:403:ALA:CA	1:c:262:TYR:CZ	2.77	0.67
2:r:56:ALA:HB1	2:s:284:ARG:N	2.09	0.67
1:N:30:LEU:CD2	1:N:36:MET:HE3	2.24	0.67
2:Q:404:PHE:CD2	1:c:260:VAL:C	2.71	0.67
2:R:403:ALA:HA	1:d:262:TYR:CD1	2.27	0.67
2:U:397:ALA:O	1:g:346:TRP:CB	2.42	0.67
2:U:406:HIS:NE2	1:g:263:PRO:HA	2.09	0.67
2:B:397:ALA:O	1:E:346:TRP:CB	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:403:ALA:CA	1:e:262:TYR:CZ	2.77	0.67
2:W:403:ALA:CA	1:i:262:TYR:CZ	2.77	0.67
1:D:120:ASP:OD2	1:G:215:ARG:CD	2.39	0.67
1:G:60:LYS:HZ1	1:H:283:HIS:CG	2.12	0.67
1:G:89:PRO:HB3	1:H:280:LYS:HZ1	1.59	0.67
2:F:7:LEU:HD22	2:F:66:VAL:HB	1.75	0.67
1:O:56:THR:HG21	1:P:283:HIS:CB	2.16	0.67
1:I:234:ILE:CD1	1:I:270:VAL:HG12	2.23	0.67
1:J:30:LEU:CD2	1:J:36:MET:HE3	2.24	0.67
2:R:406:HIS:NE2	1:d:263:PRO:HA	2.09	0.67
2:S:130:ASP:O	2:T:338:LYS:NZ	2.26	0.67
2:V:57:THR:CG2	2:W:285:ALA:HA	2.24	0.67
1:g:234:ILE:CD1	1:g:270:VAL:HG12	2.23	0.67
1:h:30:LEU:CD2	1:h:36:MET:HE3	2.24	0.67
2:B:7:LEU:HD22	2:B:66:VAL:HB	1.75	0.67
1:j:90:GLU:H	1:k:280:LYS:CE	2.07	0.67
2:B:403:ALA:HA	1:E:262:TYR:CD1	2.27	0.67
1:O:30:LEU:CD2	1:O:36:MET:HE3	2.24	0.67
2:S:33:THR:HG22	2:T:283:TYR:CE1	2.24	0.67
1:d:56:THR:C	1:e:284:GLU:O	2.37	0.67
1:G:30:LEU:CD2	1:G:36:MET:HE3	2.24	0.67
1:L:82:PRO:HD2	1:L:83:TYR:N	2.01	0.67
2:Y:86:ILE:HD13	2:Z:283:TYR:CE2	2.31	0.67
2:Y:403:ALA:CA	1:k:262:TYR:CZ	2.78	0.67
1:j:82:PRO:HD2	1:j:83:TYR:N	2.01	0.67
2:q:56:ALA:HB1	2:r:284:ARG:HA	1.76	0.67
1:M:90:GLU:HG3	1:N:280:LYS:CD	2.23	0.66
2:R:7:LEU:HD22	2:R:66:VAL:HB	1.75	0.66
2:S:57:THR:CG2	2:T:286:LEU:N	2.54	0.66
1:d:89:PRO:HG2	1:e:218:ASP:OD2	1.94	0.66
1:e:30:LEU:CD2	1:e:36:MET:HE3	2.24	0.66
1:f:60:LYS:HD3	1:g:283:HIS:CA	2.25	0.66
1:D:62:VAL:HG23	1:G:283:HIS:HB2	1.35	0.66
1:G:90:GLU:CD	1:H:299:SER:HB2	2.20	0.66
1:O:58:SER:HB2	1:P:282:TYR:C	2.20	0.66
2:R:403:ALA:CA	1:d:262:TYR:CZ	2.77	0.66
2:p:7:LEU:HD22	2:p:66:VAL:HB	1.75	0.66
1:C:30:LEU:CD2	1:C:36:MET:HE3	2.24	0.66
2:B:403:ALA:CA	1:E:262:TYR:CZ	2.78	0.66
1:c:30:LEU:CD2	1:c:36:MET:HE3	2.24	0.66
1:M:88:HIS:HD1	1:N:281:ALA:H	1.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:q:89:PRO:CB	2:r:218:LYS:HZ2	2.05	0.66
1:G:60:LYS:HE2	1:H:280:LYS:HB3	1.78	0.66
2:S:33:THR:CG2	2:T:283:TYR:HH	1.84	0.66
1:A:30:LEU:CD2	1:A:36:MET:HE3	2.24	0.66
1:E:30:LEU:CD2	1:E:36:MET:HE3	2.24	0.66
1:G:56:THR:CG2	1:H:284:GLU:CB	2.64	0.66
2:S:394:GLN:HG2	1:e:348:PRO:CB	2.26	0.66
1:K:234:ILE:CD1	1:K:270:VAL:HG12	2.23	0.66
2:V:60:LYS:NZ	2:W:283:TYR:HE2	1.78	0.66
2:X:394:GLN:HG2	1:j:348:PRO:CB	2.26	0.66
1:j:89:PRO:HG2	1:k:280:LYS:HE3	1.76	0.66
2:R:394:GLN:HG2	1:d:348:PRO:CB	2.26	0.66
2:X:403:ALA:CA	1:j:262:TYR:CZ	2.77	0.66
2:Y:406:HIS:CE1	1:k:263:PRO:N	2.64	0.66
1:i:234:ILE:CD1	1:i:270:VAL:HG12	2.23	0.66
2:B:96:GLN:HG3	1:E:1:MET:CE	2.17	0.66
1:G:89:PRO:HD3	1:H:280:LYS:CD	2.25	0.66
2:q:172:VAL:HG23	2:q:173:PRO:HD3	1.79	0.66
1:G:60:LYS:HD3	1:H:284:GLU:CB	2.26	0.65
2:S:172:VAL:HG23	2:S:173:PRO:HD3	1.79	0.65
2:U:403:ALA:CA	1:g:262:TYR:CZ	2.77	0.65
2:X:403:ALA:HA	1:j:262:TYR:CD1	2.27	0.65
1:D:62:VAL:CG2	1:G:280:LYS:HA	2.24	0.65
2:R:403:ALA:CB	1:d:262:TYR:CZ	2.80	0.65
2:S:403:ALA:CB	1:e:262:TYR:CZ	2.80	0.65
2:V:7:LEU:HD22	2:V:66:VAL:HB	1.75	0.65
2:W:7:LEU:HD22	2:W:66:VAL:HB	1.75	0.65
1:D:89:PRO:C	1:G:218:ASP:OD2	2.39	0.65
2:U:406:HIS:CE1	1:g:263:PRO:N	2.65	0.65
2:V:403:ALA:CA	1:h:262:TYR:CZ	2.77	0.65
2:W:394:GLN:HG2	1:i:348:PRO:CB	2.26	0.65
2:W:403:ALA:CB	1:i:262:TYR:CZ	2.80	0.65
2:X:406:HIS:CE1	1:j:263:PRO:N	2.65	0.65
2:Y:403:ALA:CB	1:k:262:TYR:CZ	2.80	0.65
2:Q:57:THR:HB	2:R:284:ARG:N	2.11	0.65
2:T:403:ALA:CB	1:f:262:TYR:CZ	2.80	0.65
2:W:406:HIS:CE1	1:i:263:PRO:N	2.65	0.65
2:Y:92:PHE:CE1	2:Z:280:SER:OG	2.49	0.65
2:Z:172:VAL:HG23	2:Z:173:PRO:HD3	1.79	0.65
1:G:121:ARG:N	1:H:298:TYR:OH	2.29	0.65
1:K:58:SER:HB3	1:L:283:HIS:NE2	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:30:LEU:CD2	1:P:36:MET:HE3	2.24	0.65
2:Q:406:HIS:CE1	1:c:263:PRO:N	2.65	0.65
2:X:403:ALA:CB	1:j:262:TYR:CZ	2.80	0.65
1:d:57:GLY:N	1:e:284:GLU:O	2.29	0.65
1:D:62:VAL:HG23	1:G:283:HIS:HD1	1.53	0.65
2:R:56:ALA:O	2:S:282:GLN:C	2.40	0.65
2:R:172:VAL:HG23	2:R:173:PRO:HD3	1.79	0.65
2:T:394:GLN:HG2	1:f:348:PRO:CB	2.26	0.65
2:V:394:GLN:HG2	1:h:348:PRO:CB	2.26	0.65
2:V:406:HIS:CE1	1:h:263:PRO:N	2.64	0.65
2:Y:394:GLN:HG2	1:k:348:PRO:CB	2.26	0.65
2:p:172:VAL:HG23	2:p:173:PRO:HD3	1.79	0.65
2:B:406:HIS:CE1	1:E:263:PRO:N	2.65	0.65
1:N:234:ILE:CD1	1:N:270:VAL:HG12	2.23	0.65
2:T:406:HIS:CE1	1:f:263:PRO:N	2.65	0.65
2:r:172:VAL:HG23	2:r:173:PRO:HD3	1.78	0.65
2:B:403:ALA:CB	1:E:262:TYR:CZ	2.80	0.65
2:T:172:VAL:HG23	2:T:173:PRO:HD3	1.79	0.65
2:U:172:VAL:HG23	2:U:173:PRO:HD3	1.79	0.65
2:U:394:GLN:HG2	1:g:348:PRO:CB	2.26	0.65
2:X:172:VAL:HG23	2:X:173:PRO:HD3	1.79	0.65
2:Y:172:VAL:HG23	2:Y:173:PRO:HD3	1.79	0.65
1:e:127:ASP:CA	1:f:338:ARG:NH2	2.37	0.65
1:G:124:LYS:C	1:H:297:GLU:OE2	2.37	0.65
1:L:234:ILE:CD1	1:L:270:VAL:HG12	2.23	0.65
2:Q:394:GLN:HG2	1:c:348:PRO:CB	2.26	0.65
2:Q:403:ALA:CB	1:c:262:TYR:CZ	2.80	0.65
2:R:120:ASP:OD2	2:S:299:LYS:HE3	1.96	0.65
2:S:406:HIS:CE1	1:e:263:PRO:N	2.64	0.65
2:U:403:ALA:CB	1:g:262:TYR:CZ	2.80	0.65
1:j:90:GLU:N	1:k:280:LYS:CE	2.57	0.65
1:j:234:ILE:CD1	1:j:270:VAL:HG12	2.23	0.65
2:s:172:VAL:HG23	2:s:173:PRO:HD3	1.79	0.65
2:B:96:GLN:HB3	1:E:1:MET:HE3	1.78	0.64
1:M:89:PRO:HD3	1:N:280:LYS:N	1.92	0.64
2:V:403:ALA:CB	1:h:262:TYR:CZ	2.80	0.64
2:a:57:THR:OG1	2:b:282:GLN:CA	2.44	0.64
2:B:394:GLN:HG2	1:E:348:PRO:CB	2.26	0.64
1:D:56:THR:H	1:G:282:TYR:CA	2.10	0.64
1:P:234:ILE:CD1	1:P:270:VAL:HG12	2.23	0.64
2:Q:7:LEU:HD22	2:Q:66:VAL:HB	1.75	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:406:HIS:CE1	1:d:263:PRO:N	2.65	0.64
2:o:7:LEU:HD22	2:o:66:VAL:HB	1.75	0.64
2:Y:87:PHE:HA	2:Z:283:TYR:HD1	1.49	0.64
1:i:74:VAL:O	1:i:78:ILE:CD1	2.42	0.64
1:A:72:GLN:OE1	2:B:1:MET:CE	2.39	0.64
1:D:89:PRO:HG2	1:G:218:ASP:HB3	1.77	0.64
1:K:74:VAL:O	1:K:78:ILE:CD1	2.42	0.64
1:L:60:LYS:CE	1:M:283:HIS:CD2	2.80	0.64
1:M:63:PRO:C	1:N:283:HIS:HB3	2.19	0.64
1:d:82:PRO:HD2	1:d:83:TYR:N	2.01	0.64
1:j:177:ILE:HD12	1:j:207:GLU:CB	2.28	0.64
2:o:172:VAL:HG23	2:o:173:PRO:HD3	1.79	0.64
1:D:82:PRO:HD2	1:D:83:TYR:N	2.01	0.64
1:E:72:GLN:OE1	2:F:1:MET:CE	2.39	0.64
1:L:177:ILE:HD12	1:L:207:GLU:CB	2.28	0.64
1:O:177:ILE:HD12	1:O:207:GLU:CB	2.28	0.64
2:Q:172:VAL:HG23	2:Q:173:PRO:HD3	1.79	0.64
2:T:403:ALA:CA	1:f:262:TYR:CZ	2.77	0.64
2:a:172:VAL:HG23	2:a:173:PRO:HD3	1.78	0.64
2:r:56:ALA:C	2:s:285:ALA:HB2	2.22	0.64
2:s:7:LEU:HD22	2:s:66:VAL:HB	1.75	0.64
1:N:177:ILE:HD12	1:N:207:GLU:CB	2.28	0.64
2:U:7:LEU:HD22	2:U:66:VAL:HB	1.75	0.64
2:V:96:GLN:HB3	1:h:1:MET:HE3	1.78	0.64
1:d:56:THR:HG22	1:e:284:GLU:HG2	1.79	0.64
1:A:234:ILE:CD1	1:A:270:VAL:HG12	2.23	0.64
1:J:234:ILE:CD1	1:J:270:VAL:HG12	2.23	0.64
1:M:127:ASP:OD2	1:N:293:ASN:HB2	1.97	0.64
1:O:234:ILE:CD1	1:O:270:VAL:HG12	2.23	0.64
2:Y:406:HIS:ND1	1:k:263:PRO:CD	2.61	0.64
1:E:234:ILE:CD1	1:E:270:VAL:HG12	2.23	0.64
1:K:30:LEU:CD2	1:K:36:MET:HE3	2.24	0.64
2:X:406:HIS:ND1	1:j:263:PRO:CD	2.61	0.64
1:f:177:ILE:HD12	1:f:207:GLU:CB	2.28	0.64
1:h:234:ILE:CD1	1:h:270:VAL:HG12	2.23	0.64
1:i:30:LEU:CD2	1:i:36:MET:HE3	2.24	0.64
2:B:172:VAL:HG23	2:B:173:PRO:HD3	1.78	0.64
1:D:89:PRO:CG	1:G:218:ASP:CB	2.65	0.64
1:G:89:PRO:HG2	1:H:215:ARG:C	2.19	0.64
1:H:177:ILE:HD12	1:H:207:GLU:CB	2.28	0.64
1:K:82:PRO:HD2	1:K:83:TYR:N	2.01	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:54:SER:HB2	1:N:285:GLN:CG	2.28	0.64
2:U:406:HIS:ND1	1:g:263:PRO:CD	2.61	0.64
2:W:172:VAL:HG23	2:W:173:PRO:HD3	1.79	0.64
1:i:82:PRO:HD2	1:i:83:TYR:N	2.01	0.64
2:F:172:VAL:HG23	2:F:173:PRO:HD3	1.79	0.64
1:K:177:ILE:HD12	1:K:207:GLU:CB	2.28	0.64
1:M:177:ILE:HD12	1:M:207:GLU:CB	2.28	0.64
2:U:96:GLN:HG3	1:g:1:MET:CE	2.17	0.64
2:V:406:HIS:ND1	1:h:263:PRO:CD	2.61	0.64
2:W:406:HIS:ND1	1:i:263:PRO:CD	2.61	0.64
2:Y:62:VAL:HG12	2:Z:284:ARG:CB	2.11	0.64
1:i:177:ILE:HD12	1:i:207:GLU:CB	2.28	0.64
1:k:177:ILE:HD12	1:k:207:GLU:CB	2.28	0.64
1:D:234:ILE:CD1	1:D:270:VAL:HG12	2.23	0.63
1:G:90:GLU:OE2	1:H:299:SER:HB2	1.98	0.63
2:R:96:GLN:HG3	1:d:1:MET:CE	2.17	0.63
2:T:62:VAL:CG2	2:U:283:TYR:HD2	2.11	0.63
2:Y:117:SER:CB	2:Z:299:LYS:HZ3	2.10	0.63
1:e:177:ILE:HD12	1:e:207:GLU:CB	2.28	0.63
1:L:60:LYS:CD	1:M:283:HIS:HD2	1.96	0.63
1:M:128:GLN:CA	1:N:290:GLU:HG2	2.19	0.63
2:T:96:GLN:HB3	1:f:1:MET:HE3	1.78	0.63
1:c:177:ILE:HD12	1:c:207:GLU:CB	2.28	0.63
1:d:234:ILE:CD1	1:d:270:VAL:HG12	2.23	0.63
1:j:123:ARG:CB	1:k:297:GLU:OE2	2.46	0.63
2:B:406:HIS:ND1	1:E:263:PRO:CD	2.61	0.63
1:D:74:VAL:O	1:D:78:ILE:CD1	2.42	0.63
1:G:177:ILE:HD12	1:G:207:GLU:CB	2.28	0.63
2:Q:96:GLN:HB3	1:c:1:MET:HE3	1.79	0.63
2:T:406:HIS:ND1	1:f:263:PRO:CD	2.61	0.63
2:Y:127:GLU:C	2:Z:289:PRO:O	2.41	0.63
1:d:74:VAL:O	1:d:78:ILE:CD1	2.42	0.63
2:B:181:VAL:HG21	1:E:314:ALA:HB1	1.80	0.63
1:C:177:ILE:HD12	1:C:207:GLU:CB	2.28	0.63
1:D:177:ILE:HD12	1:D:207:GLU:CB	2.28	0.63
2:V:172:VAL:HG23	2:V:173:PRO:HD3	1.79	0.63
1:d:60:LYS:O	1:e:283:HIS:HB3	1.96	0.63
1:d:177:ILE:HD12	1:d:207:GLU:CB	2.28	0.63
1:N:84:ARG:NH1	1:O:283:HIS:HE1	1.67	0.63
1:N:124:LYS:HG3	1:O:338:ARG:NH2	2.14	0.63
2:Q:406:HIS:ND1	1:c:263:PRO:CD	2.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:181:VAL:HG21	1:h:314:ALA:HB1	1.80	0.63
1:C:72:GLN:OE1	2:Q:1:MET:CE	2.39	0.63
1:J:177:ILE:HD12	1:J:207:GLU:CB	2.28	0.63
2:R:406:HIS:ND1	1:d:263:PRO:CD	2.61	0.63
2:Y:56:ALA:CA	2:Z:286:LEU:CD1	2.74	0.63
1:f:72:GLN:OE1	2:r:1:MET:CE	2.39	0.63
1:h:177:ILE:HD12	1:h:207:GLU:CB	2.28	0.63
2:r:89:PRO:CB	2:s:218:LYS:HZ1	1.94	0.63
1:A:177:ILE:HD12	1:A:207:GLU:CB	2.28	0.63
1:E:177:ILE:HD12	1:E:207:GLU:CB	2.28	0.63
1:H:72:GLN:OE1	2:T:1:MET:CE	2.39	0.63
1:M:74:VAL:O	1:M:78:ILE:CD1	2.42	0.63
2:S:406:HIS:ND1	1:e:263:PRO:CD	2.61	0.63
2:U:181:VAL:HG21	1:g:314:ALA:HB1	1.80	0.63
2:W:96:GLN:HG3	1:i:1:MET:CE	2.17	0.63
2:W:177:VAL:HG13	1:i:329:ASN:OD1	1.99	0.63
2:Y:90:ASP:OD1	2:Z:277:SER:N	2.32	0.63
1:c:72:GLN:OE1	2:o:1:MET:CE	2.39	0.63
1:k:74:VAL:O	1:k:78:ILE:CD1	2.42	0.63
2:B:177:VAL:HG13	1:E:329:ASN:OD1	1.99	0.63
1:P:177:ILE:HD12	1:P:207:GLU:CB	2.28	0.63
2:T:57:THR:CG2	2:U:285:ALA:HA	2.29	0.63
2:W:181:VAL:HG21	1:i:314:ALA:HB1	1.80	0.63
2:Y:177:VAL:HG13	1:k:329:ASN:OD1	1.99	0.63
1:G:61:HIS:CD2	1:H:285:GLN:CD	2.77	0.63
2:Q:177:VAL:HG13	1:c:329:ASN:OD1	1.99	0.63
2:b:7:LEU:HD22	2:b:66:VAL:HB	1.75	0.63
1:I:177:ILE:HD12	1:I:207:GLU:CB	2.28	0.62
2:V:177:VAL:HG13	1:h:329:ASN:OD1	1.99	0.62
2:Y:60:LYS:CE	2:Z:282:GLN:HG3	2.22	0.62
2:b:172:VAL:HG23	2:b:173:PRO:HD3	1.79	0.62
1:P:75:ILE:HA	1:P:78:ILE:HD13	1.81	0.62
2:R:177:VAL:HG13	1:d:329:ASN:OD1	1.99	0.62
2:S:177:VAL:HG13	1:e:329:ASN:OD1	1.99	0.62
2:X:96:GLN:HB3	1:j:1:MET:HE3	1.78	0.62
1:f:62:VAL:HG22	1:g:283:HIS:HD2	1.64	0.62
1:g:75:ILE:HA	1:g:78:ILE:HD13	1.81	0.62
1:g:177:ILE:HD12	1:g:207:GLU:CB	2.28	0.62
1:J:75:ILE:HA	1:J:78:ILE:HD13	1.82	0.62
2:S:33:THR:CB	2:T:283:TYR:OH	2.37	0.62
2:Y:89:PRO:O	2:Z:218:LYS:CG	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:75:ILE:HA	1:I:78:ILE:HD13	1.82	0.62
1:M:234:ILE:CD1	1:M:270:VAL:HG12	2.23	0.62
2:T:180:THR:HG22	1:f:258:ASN:OD1	2.00	0.62
2:U:177:VAL:HG13	1:g:329:ASN:OD1	1.99	0.62
1:h:75:ILE:HA	1:h:78:ILE:HD13	1.82	0.62
1:C:30:LEU:HD23	1:C:36:MET:HB2	1.82	0.62
1:H:74:VAL:O	1:H:78:ILE:CD1	2.42	0.62
1:M:54:SER:HB3	1:N:284:GLU:O	1.98	0.62
1:M:125:MET:C	1:N:290:GLU:OE1	2.41	0.62
2:r:56:ALA:CA	2:s:284:ARG:C	2.71	0.62
1:G:127:ASP:OD1	1:H:338:ARG:HD3	1.99	0.62
1:K:75:ILE:HA	1:K:78:ILE:HD13	1.81	0.62
2:Q:181:VAL:HG21	1:c:314:ALA:HB1	1.80	0.62
2:T:177:VAL:HG13	1:f:329:ASN:OD1	1.99	0.62
2:X:180:THR:HG22	1:j:258:ASN:OD1	2.00	0.62
1:f:74:VAL:O	1:f:78:ILE:CD1	2.42	0.62
1:k:234:ILE:CD1	1:k:270:VAL:HG12	2.23	0.62
2:p:60:LYS:N	2:q:283:TYR:HA	2.13	0.62
2:Y:86:ILE:O	2:Z:282:GLN:N	2.33	0.62
1:c:30:LEU:HD23	1:c:36:MET:HB2	1.82	0.62
1:d:56:THR:CG2	1:e:280:LYS:O	2.48	0.62
1:i:75:ILE:HA	1:i:78:ILE:HD13	1.81	0.62
2:R:55:GLU:HB2	2:S:285:ALA:CB	2.27	0.62
2:R:181:VAL:HG21	1:d:314:ALA:HB1	1.80	0.62
2:T:7:LEU:HD22	2:T:66:VAL:HB	1.75	0.62
1:J:30:LEU:HD23	1:J:36:MET:HB2	1.82	0.62
2:Q:180:THR:HG22	1:c:258:ASN:OD1	2.00	0.62
2:R:34:GLY:HA2	2:S:283:TYR:HE2	1.59	0.62
2:S:181:VAL:HG21	1:e:314:ALA:HB1	1.80	0.62
1:h:30:LEU:HD23	1:h:36:MET:HB2	1.82	0.62
1:C:234:ILE:CD1	1:C:270:VAL:HG12	2.23	0.62
1:D:60:LYS:HG2	1:G:283:HIS:HD1	1.63	0.62
1:D:62:VAL:HG23	1:G:283:HIS:N	2.15	0.62
1:G:30:LEU:HD23	1:G:36:MET:HB2	1.82	0.62
1:M:75:ILE:HA	1:M:78:ILE:HD13	1.81	0.62
2:S:180:THR:HG22	1:e:258:ASN:OD1	2.00	0.62
2:X:177:VAL:HG13	1:j:329:ASN:OD1	1.99	0.62
1:d:55:GLU:O	1:e:285:GLN:N	2.33	0.62
2:R:89:PRO:CD	2:S:218:LYS:NZ	2.62	0.61
2:T:181:VAL:HG21	1:f:314:ALA:HB1	1.80	0.61
2:Y:181:VAL:HG21	1:k:314:ALA:HB1	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:234:ILE:CD1	1:c:270:VAL:HG12	2.23	0.61
1:e:30:LEU:HD23	1:e:36:MET:HB2	1.82	0.61
1:k:75:ILE:HA	1:k:78:ILE:HD13	1.82	0.61
2:r:7:LEU:HD22	2:r:66:VAL:HB	1.75	0.61
1:A:30:LEU:HD23	1:A:36:MET:HB2	1.82	0.61
1:A:74:VAL:O	1:A:78:ILE:CD1	2.42	0.61
1:E:30:LEU:HD23	1:E:36:MET:HB2	1.82	0.61
1:E:74:VAL:O	1:E:78:ILE:CD1	2.42	0.61
1:j:62:VAL:HG22	1:k:283:HIS:CD2	2.35	0.61
1:L:75:ILE:HA	1:L:78:ILE:HD13	1.82	0.61
2:R:90:ASP:CA	2:S:218:LYS:HE2	2.06	0.61
2:R:96:GLN:HB3	1:d:1:MET:HE3	1.78	0.61
2:W:180:THR:HG22	1:i:258:ASN:OD1	2.00	0.61
2:X:128:SER:HG	2:Y:290:GLU:CD	2.09	0.61
1:e:72:GLN:OE1	2:q:1:MET:CE	2.39	0.61
1:j:75:ILE:HA	1:j:78:ILE:HD13	1.82	0.61
1:G:72:GLN:OE1	2:S:1:MET:CE	2.39	0.61
2:X:181:VAL:HG21	1:j:314:ALA:HB1	1.80	0.61
1:g:30:LEU:HD23	1:g:36:MET:HB2	1.82	0.61
1:D:75:ILE:HA	1:D:78:ILE:HD13	1.82	0.61
1:I:30:LEU:HD23	1:I:36:MET:HB2	1.82	0.61
1:M:128:GLN:N	1:N:290:GLU:HG2	1.65	0.61
1:O:58:SER:CB	1:P:282:TYR:C	2.72	0.61
2:Y:96:GLN:HB3	1:k:1:MET:HE3	1.78	0.61
1:c:75:ILE:HA	1:c:78:ILE:HD13	1.81	0.61
1:d:75:ILE:HA	1:d:78:ILE:HD13	1.82	0.61
1:e:75:ILE:HA	1:e:78:ILE:HD13	1.81	0.61
1:C:75:ILE:HA	1:C:78:ILE:HD13	1.81	0.61
1:H:75:ILE:HA	1:H:78:ILE:HD13	1.82	0.61
1:H:234:ILE:CD1	1:H:270:VAL:HG12	2.23	0.61
1:N:75:ILE:HA	1:N:78:ILE:HD13	1.81	0.61
2:X:123:ARG:CZ	2:Y:308:ARG:HH11	2.12	0.61
1:f:75:ILE:HA	1:f:78:ILE:HD13	1.82	0.61
1:f:234:ILE:CD1	1:f:270:VAL:HG12	2.23	0.61
2:r:33:THR:O	2:s:283:TYR:CZ	2.53	0.61
1:G:60:LYS:CE	1:H:280:LYS:CA	2.78	0.61
1:L:30:LEU:HD23	1:L:36:MET:HB2	1.82	0.61
1:M:89:PRO:O	1:N:218:ASP:OD2	2.19	0.61
1:j:30:LEU:HD23	1:j:36:MET:HB2	1.82	0.61
1:D:30:LEU:HD23	1:D:36:MET:HB2	1.82	0.61
1:G:75:ILE:HA	1:G:78:ILE:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:90:GLU:CG	1:H:215:ARG:HB3	2.30	0.61
1:M:212:ILE:HG21	1:M:275:ILE:HD13	1.83	0.61
2:R:89:PRO:CA	2:S:218:LYS:NZ	2.43	0.61
2:S:7:LEU:HD22	2:S:66:VAL:HB	1.75	0.61
2:T:406:HIS:CE1	1:f:262:TYR:C	2.79	0.61
1:d:30:LEU:HD23	1:d:36:MET:HB2	1.82	0.61
1:i:57:GLY:N	1:j:283:HIS:O	2.34	0.61
1:k:212:ILE:HG21	1:k:275:ILE:HD13	1.83	0.61
1:D:212:ILE:HG21	1:D:275:ILE:HD13	1.83	0.61
1:P:212:ILE:HG21	1:P:275:ILE:HD13	1.83	0.61
2:R:406:HIS:CE1	1:d:262:TYR:C	2.79	0.61
2:W:406:HIS:CE1	1:i:262:TYR:C	2.79	0.61
2:q:7:LEU:HD22	2:q:66:VAL:HB	1.75	0.61
1:D:56:THR:H	1:G:283:HIS:N	1.93	0.61
2:S:406:HIS:CE1	1:e:262:TYR:C	2.79	0.61
2:U:180:THR:HG22	1:g:258:ASN:OD1	2.00	0.61
2:V:180:THR:HG22	1:h:258:ASN:OD1	2.00	0.61
2:Y:120:ASP:OD1	2:Z:297:ASP:CG	2.25	0.61
2:r:89:PRO:HB2	2:s:218:LYS:HZ2	1.48	0.61
1:H:212:ILE:HG21	1:H:275:ILE:HD13	1.83	0.60
1:K:30:LEU:HD23	1:K:36:MET:HB2	1.82	0.60
1:O:75:ILE:HA	1:O:78:ILE:HD13	1.82	0.60
2:Q:406:HIS:CE1	1:c:262:TYR:C	2.79	0.60
2:R:180:THR:HG22	1:d:258:ASN:OD1	2.00	0.60
2:V:406:HIS:CE1	1:h:262:TYR:C	2.79	0.60
1:d:212:ILE:HG21	1:d:275:ILE:HD13	1.83	0.60
1:f:212:ILE:HG21	1:f:275:ILE:HD13	1.83	0.60
1:i:30:LEU:HD23	1:i:36:MET:HB2	1.82	0.60
2:p:57:THR:HG22	2:q:284:ARG:CB	1.79	0.60
2:B:406:HIS:CE1	1:E:262:TYR:C	2.79	0.60
1:O:30:LEU:HD23	1:O:36:MET:HB2	1.82	0.60
1:O:212:ILE:HG21	1:O:275:ILE:HD13	1.83	0.60
1:P:72:GLN:OE1	2:b:1:MET:CE	2.39	0.60
2:Y:180:THR:HG22	1:k:258:ASN:OD1	2.00	0.60
2:Y:406:HIS:CE1	1:k:262:TYR:C	2.79	0.60
1:e:124:LYS:HZ2	1:f:299:SER:CB	2.12	0.60
1:G:60:LYS:HE2	1:H:280:LYS:CB	2.31	0.60
1:I:74:VAL:O	1:I:78:ILE:CD1	2.42	0.60
1:P:30:LEU:HD23	1:P:36:MET:HB2	1.82	0.60
2:Q:96:GLN:HG3	1:c:1:MET:CE	2.17	0.60
2:Y:92:PHE:HE1	2:Z:280:SER:OG	1.85	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:62:VAL:HG22	1:g:283:HIS:CD2	2.36	0.60
1:g:74:VAL:O	1:g:78:ILE:CD1	2.42	0.60
1:E:75:ILE:HA	1:E:78:ILE:HD13	1.81	0.60
1:G:56:THR:HG21	1:H:284:GLU:CB	2.28	0.60
1:G:212:ILE:HG21	1:G:275:ILE:HD13	1.83	0.60
1:M:30:LEU:HD23	1:M:36:MET:HB2	1.82	0.60
1:M:89:PRO:HG3	1:N:279:GLU:H	1.66	0.60
1:N:212:ILE:HG21	1:N:275:ILE:HD13	1.83	0.60
2:Q:394:GLN:CA	1:c:348:PRO:HG3	2.32	0.60
2:R:89:PRO:C	2:S:218:LYS:NZ	2.34	0.60
2:R:394:GLN:CA	1:d:348:PRO:HG3	2.32	0.60
2:U:406:HIS:CE1	1:g:262:TYR:C	2.79	0.60
2:X:127:GLU:O	2:Y:293:GLN:NE2	2.24	0.60
1:e:212:ILE:HG21	1:e:275:ILE:HD13	1.83	0.60
1:k:30:LEU:HD23	1:k:36:MET:HB2	1.82	0.60
1:A:75:ILE:HA	1:A:78:ILE:HD13	1.82	0.60
1:G:60:LYS:HD3	1:H:284:GLU:CG	2.31	0.60
2:S:394:GLN:CA	1:e:348:PRO:HG3	2.32	0.60
2:T:394:GLN:CA	1:f:348:PRO:HG3	2.32	0.60
1:H:56:THR:HG21	1:I:283:HIS:CA	2.30	0.60
2:Q:406:HIS:ND1	1:c:263:PRO:HD3	2.17	0.60
2:T:182:VAL:CG2	1:f:257:THR:HG22	2.31	0.60
2:X:406:HIS:CE1	1:j:262:TYR:C	2.79	0.60
2:Y:56:ALA:HB1	2:Z:286:LEU:HD11	1.82	0.60
2:Y:124:LYS:O	2:Z:290:GLU:OE2	2.19	0.60
1:C:74:VAL:O	1:C:78:ILE:CD1	2.42	0.60
1:E:212:ILE:HG21	1:E:275:ILE:HD13	1.83	0.60
1:K:72:GLN:OE1	2:W:1:MET:CE	2.39	0.60
2:R:54:ASN:C	2:S:283:TYR:O	2.43	0.60
2:a:56:ALA:CB	2:b:283:TYR:HB3	2.31	0.60
6:b:502:TA1:H261	6:b:502:TA1:H463	1.84	0.60
1:H:30:LEU:HD23	1:H:36:MET:HB2	1.82	0.60
1:M:72:GLN:OE1	2:Y:1:MET:CE	2.39	0.60
1:N:62:VAL:CG1	1:O:285:GLN:HE21	2.15	0.60
2:R:406:HIS:ND1	1:d:263:PRO:HD3	2.17	0.60
2:S:397:ALA:O	1:e:346:TRP:HB3	2.02	0.60
2:U:406:HIS:ND1	1:g:263:PRO:HD3	2.17	0.60
2:V:406:HIS:ND1	1:h:263:PRO:HD3	2.17	0.60
2:W:397:ALA:O	1:i:346:TRP:HB3	2.02	0.60
6:W:502:TA1:H261	6:W:502:TA1:H463	1.84	0.60
2:Y:89:PRO:O	2:Z:218:LYS:CD	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:74:VAL:O	1:c:78:ILE:CD1	2.42	0.60
1:A:212:ILE:HG21	1:A:275:ILE:HD13	1.83	0.60
2:B:406:HIS:ND1	1:E:263:PRO:HD3	2.17	0.60
1:P:82:PRO:CD	1:P:83:TYR:H	2.13	0.60
2:R:89:PRO:HB2	2:S:218:LYS:HD2	1.79	0.60
2:T:57:THR:HG22	2:U:285:ALA:HA	1.83	0.60
2:Y:62:VAL:CB	2:Z:284:ARG:O	2.47	0.60
6:a:502:TA1:H463	6:a:502:TA1:H261	1.84	0.60
1:M:62:VAL:HG13	1:N:283:HIS:ND1	2.17	0.60
2:Q:57:THR:CB	2:R:283:TYR:C	2.57	0.60
2:R:182:VAL:CG2	1:d:257:THR:HG22	2.31	0.60
2:R:397:ALA:O	1:d:346:TRP:HB3	2.02	0.60
2:T:397:ALA:O	1:f:346:TRP:HB3	2.02	0.60
6:V:502:TA1:H463	6:V:502:TA1:H261	1.84	0.60
2:W:182:VAL:CG2	1:i:257:THR:HG22	2.31	0.60
2:Z:7:LEU:HD22	2:Z:66:VAL:HB	1.75	0.60
1:f:30:LEU:HD23	1:f:36:MET:HB2	1.82	0.60
1:g:212:ILE:HG21	1:g:275:ILE:HD13	1.83	0.60
2:B:224:TYR:CZ	1:E:248:LEU:HD21	2.37	0.59
1:I:212:ILE:HG21	1:I:275:ILE:HD13	1.83	0.59
1:N:30:LEU:HD23	1:N:36:MET:HB2	1.82	0.59
2:R:56:ALA:C	2:S:282:GLN:C	2.70	0.59
2:S:406:HIS:ND1	1:e:263:PRO:HD3	2.17	0.59
6:s:502:TA1:H261	6:s:502:TA1:H463	1.84	0.59
1:G:60:LYS:HB2	1:H:282:TYR:C	2.25	0.59
1:G:129:CYS:CA	1:H:338:ARG:HH21	2.11	0.59
1:J:72:GLN:OE1	2:V:1:MET:CE	2.39	0.59
1:M:54:SER:CB	1:N:285:GLN:CG	2.79	0.59
2:U:394:GLN:CA	1:g:348:PRO:HG3	2.32	0.59
6:U:501:TA1:H261	6:U:501:TA1:H463	1.84	0.59
2:B:397:ALA:O	1:E:346:TRP:HB3	2.02	0.59
6:B:502:TA1:H261	6:B:502:TA1:H463	1.84	0.59
1:D:56:THR:O	1:G:282:TYR:HA	2.01	0.59
1:M:128:GLN:HA	1:N:290:GLU:CG	2.31	0.59
2:Q:57:THR:OG1	2:R:280:SER:O	2.19	0.59
2:X:397:ALA:O	1:j:346:TRP:HB3	2.02	0.59
2:X:406:HIS:ND1	1:j:263:PRO:HD3	2.17	0.59
2:Y:90:ASP:CG	2:Z:216:THR:C	2.69	0.59
2:Y:406:HIS:ND1	1:k:263:PRO:HD3	2.17	0.59
1:f:56:THR:HB	1:g:284:GLU:C	2.27	0.59
1:j:116:ASP:CB	1:k:298:TYR:OH	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:GLN:OE1	2:R:1:MET:CE	2.39	0.59
6:F:501:TA1:H463	6:F:501:TA1:H261	1.84	0.59
2:Q:224:TYR:CE2	1:c:248:LEU:CG	2.84	0.59
2:S:96:GLN:HB3	1:e:1:MET:HE3	1.78	0.59
6:X:502:TA1:H261	6:X:502:TA1:H463	1.84	0.59
2:Y:90:ASP:H	2:Z:277:SER:H	0.60	0.59
1:j:123:ARG:NH1	1:k:338:ARG:NH2	2.51	0.59
2:r:56:ALA:C	2:s:285:ALA:CB	2.74	0.59
2:U:224:TYR:CZ	1:g:248:LEU:HD21	2.37	0.59
2:W:224:TYR:CE2	1:i:248:LEU:CG	2.84	0.59
2:a:57:THR:OG1	2:b:283:TYR:N	2.36	0.59
1:d:72:GLN:OE1	2:p:1:MET:CE	2.39	0.59
1:j:127:ASP:C	1:k:290:GLU:OE2	2.44	0.59
2:B:224:TYR:CE2	1:E:248:LEU:CG	2.84	0.59
2:B:394:GLN:CA	1:E:348:PRO:HG3	2.32	0.59
1:L:212:ILE:HG21	1:L:275:ILE:HD13	1.83	0.59
2:V:182:VAL:CG2	1:h:257:THR:HG22	2.31	0.59
2:Y:397:ALA:O	1:k:346:TRP:HB3	2.02	0.59
6:Y:502:TA1:H463	6:Y:502:TA1:H261	1.84	0.59
1:j:212:ILE:HG21	1:j:275:ILE:HD13	1.83	0.59
2:p:56:ALA:CB	2:q:283:TYR:HB2	2.32	0.59
2:r:57:THR:CG2	2:s:286:LEU:CG	2.70	0.59
1:M:87:PHE:HA	1:N:283:HIS:CG	2.33	0.59
2:W:406:HIS:CE1	1:i:263:PRO:CA	2.86	0.59
1:h:212:ILE:HG21	1:h:275:ILE:HD13	1.83	0.59
2:q:128:SER:HA	2:r:293:GLN:OE1	2.02	0.59
1:C:212:ILE:HG21	1:C:275:ILE:HD13	1.83	0.59
1:D:62:VAL:HG23	1:G:283:HIS:CA	2.32	0.59
1:J:212:ILE:HG21	1:J:275:ILE:HD13	1.83	0.59
2:Q:179:ASP:OD1	1:c:353:VAL:HB	2.03	0.59
2:S:56:ALA:CB	2:T:284:ARG:CB	2.58	0.59
6:S:502:TA1:H261	6:S:502:TA1:H463	1.84	0.59
2:V:394:GLN:CA	1:h:348:PRO:HG3	2.32	0.59
6:Z:502:TA1:H261	6:Z:502:TA1:H463	1.84	0.59
2:a:7:LEU:HD22	2:a:66:VAL:HB	1.75	0.59
2:p:56:ALA:HB3	2:q:283:TYR:HB2	1.83	0.59
1:D:124:LYS:HZ2	1:G:215:ARG:HB3	1.67	0.59
1:I:72:GLN:OE1	2:U:1:MET:CE	2.39	0.59
2:W:394:GLN:CA	1:i:348:PRO:HG3	2.32	0.59
2:X:394:GLN:CA	1:j:348:PRO:HG3	2.32	0.59
2:Y:124:LYS:HA	2:Z:293:GLN:CB	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:394:GLN:CA	1:k:348:PRO:HG3	2.32	0.59
1:c:212:ILE:HG21	1:c:275:ILE:HD13	1.83	0.59
1:g:72:GLN:OE1	2:s:1:MET:CE	2.39	0.59
6:q:502:TA1:H463	6:q:502:TA1:H261	1.84	0.59
2:Q:397:ALA:O	1:c:346:TRP:HB3	2.02	0.59
2:U:397:ALA:O	1:g:346:TRP:HB3	2.02	0.59
2:W:406:HIS:ND1	1:i:263:PRO:HD3	2.17	0.59
1:e:56:THR:OG1	1:f:283:HIS:C	2.46	0.59
2:B:179:ASP:OD1	1:E:353:VAL:HB	2.03	0.58
1:M:57:GLY:H	1:N:372:LEU:CD1	1.97	0.58
2:S:224:TYR:CZ	1:e:248:LEU:HD21	2.37	0.58
2:X:406:HIS:CE1	1:j:263:PRO:CA	2.86	0.58
2:Y:63:PRO:O	2:Z:283:TYR:HB3	2.01	0.58
2:Y:179:ASP:OD1	1:k:353:VAL:HB	2.03	0.58
1:N:72:GLN:OE1	2:Z:1:MET:CE	2.39	0.58
1:N:124:LYS:HG3	1:O:338:ARG:HH22	1.66	0.58
1:O:72:GLN:OE1	2:a:1:MET:CE	2.39	0.58
2:Q:224:TYR:CZ	1:c:248:LEU:HD21	2.37	0.58
2:T:406:HIS:CE1	1:f:263:PRO:CA	2.86	0.58
2:X:90:ASP:N	2:Y:218:LYS:NZ	2.51	0.58
2:X:128:SER:HA	2:Y:293:GLN:HE22	1.68	0.58
2:B:180:THR:HG22	1:E:258:ASN:OD1	2.00	0.58
2:B:224:TYR:HE2	1:E:248:LEU:HG	1.68	0.58
1:G:82:PRO:CD	1:G:83:TYR:H	2.13	0.58
1:L:72:GLN:OE1	2:X:1:MET:CE	2.39	0.58
6:Q:502:TA1:H463	6:Q:502:TA1:H261	1.84	0.58
2:R:55:GLU:OE1	2:S:285:ALA:HB2	2.03	0.58
2:R:406:HIS:CE1	1:d:263:PRO:CA	2.86	0.58
2:U:224:TYR:HE2	1:g:248:LEU:HG	1.68	0.58
2:Y:128:SER:HA	2:Z:289:PRO:O	1.99	0.58
2:Y:224:TYR:CZ	1:k:248:LEU:HD21	2.37	0.58
2:p:124:LYS:HE2	2:q:299:LYS:HZ1	1.67	0.58
2:B:406:HIS:CE1	1:E:263:PRO:CA	2.86	0.58
2:Y:406:HIS:CE1	1:k:263:PRO:CA	2.86	0.58
1:d:56:THR:HB	1:e:280:LYS:O	2.03	0.58
1:e:57:GLY:N	1:f:285:GLN:O	2.35	0.58
1:e:82:PRO:CD	1:e:83:TYR:H	2.13	0.58
1:h:74:VAL:O	1:h:78:ILE:CD1	2.42	0.58
6:o:502:TA1:H261	6:o:502:TA1:H463	1.84	0.58
6:p:502:TA1:H261	6:p:502:TA1:H463	1.84	0.58
2:B:182:VAL:CG2	1:E:257:THR:HG22	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:74:VAL:O	1:J:78:ILE:CD1	2.42	0.58
1:K:56:THR:CG2	1:L:283:HIS:HB3	2.29	0.58
6:R:502:TA1:H261	6:R:502:TA1:H463	1.84	0.58
2:S:179:ASP:OD1	1:e:353:VAL:HB	2.03	0.58
2:S:406:HIS:CE1	1:e:263:PRO:CA	2.86	0.58
2:T:406:HIS:ND1	1:f:263:PRO:HD3	2.17	0.58
2:V:406:HIS:CE1	1:h:263:PRO:CA	2.86	0.58
2:X:224:TYR:CE2	1:j:248:LEU:CG	2.84	0.58
2:Y:182:VAL:CG2	1:k:257:THR:HG22	2.31	0.58
1:c:58:SER:CA	1:d:282:TYR:CB	2.80	0.58
1:i:212:ILE:HG21	1:i:275:ILE:HD13	1.83	0.58
2:B:401:ARG:HH12	1:E:437:THR:HB	1.69	0.58
1:K:212:ILE:HG21	1:K:275:ILE:HD13	1.83	0.58
2:R:224:TYR:HE2	1:d:248:LEU:HG	1.68	0.58
2:S:401:ARG:HH12	1:e:437:THR:HB	1.69	0.58
2:T:398:MET:HA	1:f:346:TRP:HB2	1.86	0.58
2:U:182:VAL:CG2	1:g:257:THR:HG22	2.32	0.58
2:V:397:ALA:O	1:h:346:TRP:HB3	2.02	0.58
2:o:7:LEU:CD2	2:o:66:VAL:CB	2.71	0.58
1:M:82:PRO:CD	1:M:83:TYR:H	2.13	0.58
2:Q:7:LEU:CD2	2:Q:66:VAL:CB	2.71	0.58
2:R:179:ASP:OD1	1:d:353:VAL:HB	2.03	0.58
2:T:401:ARG:HH12	1:f:437:THR:HB	1.69	0.58
2:V:394:GLN:CG	1:h:348:PRO:HG2	2.34	0.58
2:W:401:ARG:HH12	1:i:437:THR:HB	1.69	0.58
1:d:56:THR:HG22	1:e:284:GLU:CG	2.31	0.58
1:k:82:PRO:CD	1:k:83:TYR:H	2.13	0.58
2:s:7:LEU:CD2	2:s:66:VAL:CB	2.71	0.58
1:G:120:ASP:OD2	1:H:299:SER:N	2.36	0.58
2:R:401:ARG:HH12	1:d:437:THR:HB	1.69	0.58
2:S:224:TYR:HE2	1:e:248:LEU:HG	1.68	0.58
2:S:403:ALA:N	1:e:262:TYR:CE1	2.72	0.58
6:T:502:TA1:H261	6:T:502:TA1:H463	1.84	0.58
2:V:179:ASP:OD1	1:h:353:VAL:HB	2.03	0.58
2:X:179:ASP:OD1	1:j:353:VAL:HB	2.03	0.58
2:X:398:MET:HA	1:j:346:TRP:HB2	1.86	0.58
2:B:394:GLN:CG	1:E:348:PRO:HG2	2.34	0.58
1:G:60:LYS:NZ	1:H:283:HIS:CG	2.69	0.58
1:N:74:VAL:O	1:N:78:ILE:CD1	2.42	0.58
2:R:398:MET:HA	1:d:346:TRP:HB2	1.86	0.58
2:S:398:MET:HA	1:e:346:TRP:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:179:ASP:OD1	1:f:353:VAL:HB	2.03	0.58
2:U:7:LEU:CD2	2:U:66:VAL:CB	2.71	0.58
2:U:406:HIS:CE1	1:g:263:PRO:CA	2.86	0.58
2:V:224:TYR:HE2	1:h:248:LEU:HG	1.68	0.58
2:X:401:ARG:HH12	1:j:437:THR:HB	1.69	0.58
1:c:82:PRO:CD	1:c:83:TYR:H	2.13	0.58
6:r:502:TA1:H261	6:r:502:TA1:H463	1.84	0.58
1:C:82:PRO:CD	1:C:83:TYR:H	2.13	0.58
1:G:57:GLY:H	1:H:286:LEU:HB2	1.17	0.58
1:G:234:ILE:CD1	1:G:270:VAL:HG12	2.23	0.58
1:L:74:VAL:O	1:L:78:ILE:CD1	2.42	0.58
2:Q:398:MET:HA	1:c:346:TRP:HB2	1.86	0.58
2:S:394:GLN:CG	1:e:348:PRO:HG2	2.34	0.58
2:V:224:TYR:CZ	1:h:248:LEU:HD21	2.37	0.58
2:V:403:ALA:N	1:h:262:TYR:CE1	2.72	0.58
2:W:224:TYR:HE2	1:i:248:LEU:HG	1.68	0.58
2:W:224:TYR:CZ	1:i:248:LEU:HD21	2.37	0.58
2:W:403:ALA:N	1:i:262:TYR:CE1	2.72	0.58
2:Y:398:MET:HA	1:k:346:TRP:HB2	1.86	0.58
2:a:90:ASP:OD1	2:b:218:LYS:NZ	2.31	0.58
1:G:74:VAL:O	1:G:78:ILE:CD1	2.42	0.57
1:M:91:GLN:HE22	1:N:283:HIS:CB	2.16	0.57
2:Q:406:HIS:CE1	1:c:263:PRO:CA	2.86	0.57
2:T:62:VAL:HG22	2:U:283:TYR:CD2	2.31	0.57
2:Y:90:ASP:N	2:Z:216:THR:O	2.36	0.57
1:e:74:VAL:O	1:e:78:ILE:CD1	2.42	0.57
1:e:234:ILE:CD1	1:e:270:VAL:HG12	2.23	0.57
1:j:74:VAL:O	1:j:78:ILE:CD1	2.42	0.57
1:G:34:GLY:CA	1:H:283:HIS:CB	2.61	0.57
2:Q:57:THR:HB	2:R:283:TYR:C	2.28	0.57
2:Q:394:GLN:CG	1:c:348:PRO:HG2	2.34	0.57
2:R:224:TYR:CZ	1:d:248:LEU:HD21	2.37	0.57
2:W:179:ASP:OD1	1:i:353:VAL:HB	2.03	0.57
2:Y:172:VAL:CG2	2:Y:173:PRO:HD3	2.34	0.57
1:G:127:ASP:CG	1:H:341:ILE:CD1	2.70	0.57
2:W:398:MET:HA	1:i:346:TRP:HB2	1.86	0.57
2:X:394:GLN:CG	1:j:348:PRO:HG2	2.34	0.57
1:L:82:PRO:CD	1:L:83:TYR:H	2.13	0.57
2:Q:224:TYR:HE2	1:c:248:LEU:HG	1.68	0.57
2:R:403:ALA:N	1:d:262:TYR:CE1	2.72	0.57
2:V:224:TYR:CE2	1:h:248:LEU:CG	2.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:63:PRO:O	2:Z:283:TYR:CB	2.52	0.57
2:Y:224:TYR:CE2	1:k:248:LEU:CG	2.84	0.57
2:Y:224:TYR:HE2	1:k:248:LEU:HG	1.68	0.57
1:j:82:PRO:CD	1:j:83:TYR:H	2.13	0.57
2:Q:403:ALA:N	1:c:262:TYR:CE1	2.72	0.57
2:R:172:VAL:CG2	2:R:173:PRO:HD3	2.34	0.57
2:U:96:GLN:HB3	1:g:1:MET:HE3	1.78	0.57
2:U:179:ASP:OD1	1:g:353:VAL:HB	2.03	0.57
2:W:60:LYS:HB2	2:X:283:TYR:HE2	1.68	0.57
2:Y:124:LYS:CA	2:Z:293:GLN:HB3	2.31	0.57
2:p:172:VAL:CG2	2:p:173:PRO:HD3	2.34	0.57
2:B:403:ALA:N	1:E:262:TYR:CE1	2.72	0.57
2:Q:401:ARG:HH12	1:c:437:THR:HB	1.69	0.57
2:T:224:TYR:CZ	1:f:248:LEU:HD21	2.37	0.57
2:U:403:ALA:N	1:g:262:TYR:CE1	2.72	0.57
2:V:401:ARG:HH12	1:h:437:THR:HB	1.69	0.57
2:Y:401:ARG:HH12	1:k:437:THR:HB	1.69	0.57
2:V:398:MET:HA	1:h:346:TRP:HB2	1.86	0.57
2:X:224:TYR:HE2	1:j:248:LEU:HG	1.68	0.57
2:Y:60:LYS:HE3	2:Z:282:GLN:HG2	1.81	0.57
2:U:394:GLN:CG	1:g:348:PRO:HG2	2.34	0.57
2:U:398:MET:HA	1:g:346:TRP:HB2	1.86	0.57
2:Y:87:PHE:N	2:Z:283:TYR:HE1	1.77	0.57
2:Y:120:ASP:CG	2:Z:297:ASP:OD2	2.41	0.57
2:Y:394:GLN:CG	1:k:348:PRO:HG2	2.34	0.57
2:F:7:LEU:CD2	2:F:66:VAL:CB	2.71	0.57
1:O:82:PRO:CD	1:O:83:TYR:H	2.13	0.57
2:X:224:TYR:CZ	1:j:248:LEU:HD21	2.38	0.57
2:X:403:ALA:N	1:j:262:TYR:CE1	2.72	0.57
1:j:123:ARG:HG2	1:k:297:GLU:CG	2.34	0.57
1:O:58:SER:OG	1:P:282:TYR:HB3	2.05	0.57
1:f:82:PRO:CD	1:f:83:TYR:H	2.13	0.57
2:B:7:LEU:CD2	2:B:66:VAL:CB	2.71	0.56
1:G:60:LYS:CE	1:H:280:LYS:HA	2.35	0.56
1:H:82:PRO:CD	1:H:83:TYR:H	2.13	0.56
1:K:56:THR:HB	1:L:283:HIS:C	2.29	0.56
2:T:394:GLN:CG	1:f:348:PRO:HG2	2.34	0.56
2:B:398:MET:HA	1:E:346:TRP:HB2	1.86	0.56
1:G:89:PRO:CB	1:H:218:ASP:OD1	2.53	0.56
1:G:124:LYS:HD3	1:H:297:GLU:OE1	2.05	0.56
1:M:124:LYS:HE3	1:N:297:GLU:OE1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:57:THR:HG21	2:W:284:ARG:O	2.06	0.56
2:Y:403:ALA:N	1:k:262:TYR:CE1	2.72	0.56
2:T:403:ALA:N	1:f:262:TYR:CE1	2.72	0.56
1:d:56:THR:CG2	1:e:284:GLU:HG2	2.34	0.56
1:f:60:LYS:HD3	1:g:283:HIS:HA	1.86	0.56
2:Y:221:THR:CG2	1:k:324:VAL:HG11	2.36	0.56
1:j:123:ARG:HB3	1:k:297:GLU:OE2	2.05	0.56
1:E:212:ILE:CG2	1:E:275:ILE:HD13	2.36	0.56
1:J:212:ILE:CG2	1:J:275:ILE:HD13	2.36	0.56
1:M:90:GLU:OE2	1:N:216:ASN:OD1	2.24	0.56
2:R:224:TYR:CE2	1:d:248:LEU:CG	2.84	0.56
2:U:401:ARG:HH12	1:g:437:THR:HB	1.69	0.56
2:W:394:GLN:CG	1:i:348:PRO:HG2	2.34	0.56
2:X:56:ALA:HB1	2:Y:283:TYR:HA	1.87	0.56
1:h:212:ILE:CG2	1:h:275:ILE:HD13	2.36	0.56
1:M:212:ILE:CG2	1:M:275:ILE:HD13	2.36	0.56
1:P:212:ILE:CG2	1:P:275:ILE:HD13	2.36	0.56
2:R:394:GLN:CG	1:d:348:PRO:HG2	2.34	0.56
2:Y:89:PRO:HD2	2:Z:276:THR:C	2.31	0.56
1:A:212:ILE:CG2	1:A:275:ILE:HD13	2.36	0.56
1:G:56:THR:OG1	1:H:284:GLU:C	2.48	0.56
1:I:212:ILE:CG2	1:I:275:ILE:HD13	2.36	0.56
1:K:212:ILE:CG2	1:K:275:ILE:HD13	2.36	0.56
1:M:3:GLU:HG2	1:N:285:GLN:NE2	2.20	0.56
1:M:54:SER:CB	1:N:284:GLU:O	2.54	0.56
2:R:58:GLY:CA	2:S:282:GLN:HG2	2.33	0.56
1:g:212:ILE:CG2	1:g:275:ILE:HD13	2.36	0.56
1:i:212:ILE:CG2	1:i:275:ILE:HD13	2.36	0.56
2:B:224:TYR:CE2	1:E:248:LEU:HD11	2.41	0.56
1:M:3:GLU:HG2	1:N:285:GLN:HE22	1.69	0.56
1:M:128:GLN:HA	1:N:290:GLU:HG2	1.88	0.56
2:Y:224:TYR:CE2	1:k:248:LEU:HD11	2.41	0.56
1:k:212:ILE:CG2	1:k:275:ILE:HD13	2.36	0.56
1:J:60:LYS:CE	1:K:283:HIS:HD2	2.03	0.56
2:Q:224:TYR:CE2	1:c:248:LEU:HD11	2.41	0.56
2:W:224:TYR:CE2	1:i:248:LEU:HD11	2.41	0.56
2:Y:62:VAL:CA	2:Z:281:GLN:O	2.52	0.56
1:N:212:ILE:CG2	1:N:275:ILE:HD13	2.36	0.56
2:S:60:LYS:NZ	2:T:280:SER:O	2.38	0.55
2:S:404:PHE:CZ	1:e:261:PRO:HA	2.41	0.55
1:L:212:ILE:CG2	1:L:275:ILE:HD13	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:182:VAL:HG21	1:d:257:THR:CG2	2.34	0.55
2:S:182:VAL:CG2	1:e:257:THR:HG22	2.31	0.55
2:T:224:TYR:CE2	1:f:248:LEU:HD11	2.41	0.55
2:V:394:GLN:HG2	1:h:348:PRO:HB2	1.88	0.55
2:W:221:THR:CG2	1:i:324:VAL:HG11	2.36	0.55
2:X:224:TYR:CE2	1:j:248:LEU:HD11	2.41	0.55
1:f:60:LYS:CD	1:g:282:TYR:O	2.54	0.55
1:j:212:ILE:CG2	1:j:275:ILE:HD13	2.36	0.55
2:B:182:VAL:HG21	1:E:257:THR:CG2	2.34	0.55
1:I:82:PRO:CD	1:I:83:TYR:H	2.13	0.55
1:L:60:LYS:CD	1:M:283:HIS:NE2	2.68	0.55
2:T:224:TYR:HE2	1:f:248:LEU:HG	1.68	0.55
2:T:96:GLN:CB	1:f:1:MET:HE2	2.21	0.55
2:W:394:GLN:HG2	1:i:348:PRO:HB2	1.88	0.55
2:Y:394:GLN:HG2	1:k:348:PRO:HB2	1.89	0.55
1:g:82:PRO:CD	1:g:83:TYR:H	2.13	0.55
1:j:128:GLN:NE2	1:k:284:GLU:OE1	2.39	0.55
1:C:212:ILE:CG2	1:C:275:ILE:HD13	2.36	0.55
1:D:212:ILE:CG2	1:D:275:ILE:HD13	2.36	0.55
2:T:221:THR:CG2	1:f:324:VAL:HG11	2.36	0.55
2:a:7:LEU:CD2	2:a:66:VAL:CB	2.71	0.55
1:c:212:ILE:CG2	1:c:275:ILE:HD13	2.36	0.55
2:r:62:VAL:HG23	2:s:283:TYR:O	2.07	0.55
1:J:56:THR:HG21	1:K:283:HIS:O	2.07	0.55
1:J:82:PRO:CD	1:J:83:TYR:H	2.13	0.55
1:M:63:PRO:O	1:N:283:HIS:CB	2.34	0.55
1:M:82:PRO:CD	1:M:83:TYR:N	2.70	0.55
1:O:212:ILE:CG2	1:O:275:ILE:HD13	2.36	0.55
1:d:212:ILE:CG2	1:d:275:ILE:HD13	2.36	0.55
1:f:56:THR:HA	1:g:285:GLN:HG2	1.87	0.55
1:k:82:PRO:CD	1:k:83:TYR:N	2.70	0.55
1:N:82:PRO:CD	1:N:83:TYR:N	2.70	0.55
2:Q:404:PHE:CZ	1:c:261:PRO:HA	2.41	0.55
2:R:394:GLN:HG2	1:d:348:PRO:HB2	1.88	0.55
2:R:404:PHE:CZ	1:d:261:PRO:HA	2.41	0.55
2:V:96:GLN:HG3	1:h:1:MET:CE	2.17	0.55
2:b:7:LEU:CD2	2:b:66:VAL:CB	2.71	0.55
1:h:82:PRO:CD	1:h:83:TYR:H	2.13	0.55
1:H:212:ILE:CG2	1:H:275:ILE:HD13	2.36	0.55
1:M:62:VAL:HG13	1:N:283:HIS:HD1	1.72	0.55
2:Q:57:THR:CB	2:R:280:SER:O	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:224:TYR:CE2	1:d:248:LEU:HD11	2.41	0.55
2:S:224:TYR:CE2	1:e:248:LEU:HD11	2.41	0.55
2:Y:124:LYS:CD	2:Z:294:GLN:HA	2.36	0.55
1:e:124:LYS:HZ2	1:f:299:SER:HB3	1.72	0.55
1:f:212:ILE:CG2	1:f:275:ILE:HD13	2.36	0.55
1:G:212:ILE:CG2	1:G:275:ILE:HD13	2.36	0.55
1:L:82:PRO:CD	1:L:83:TYR:N	2.70	0.55
2:Q:182:VAL:CG2	1:c:257:THR:HG22	2.31	0.55
2:Q:221:THR:CG2	1:c:324:VAL:HG11	2.36	0.55
2:R:89:PRO:N	2:S:218:LYS:HZ2	1.96	0.55
2:R:89:PRO:CD	2:S:218:LYS:HZ2	2.20	0.55
2:S:394:GLN:HG2	1:e:348:PRO:HB2	1.88	0.55
1:K:60:LYS:HB3	1:L:283:HIS:NE2	2.22	0.55
1:M:125:MET:SD	1:N:284:GLU:OE2	2.65	0.55
1:N:82:PRO:CD	1:N:83:TYR:H	2.13	0.55
2:Q:182:VAL:HG21	1:c:257:THR:CG2	2.34	0.55
2:T:404:PHE:CZ	1:f:261:PRO:HA	2.41	0.55
2:U:224:TYR:CE2	1:g:248:LEU:HD11	2.41	0.55
2:Y:129:CYS:N	2:Z:290:GLU:OE1	2.39	0.55
1:e:212:ILE:CG2	1:e:275:ILE:HD13	2.36	0.55
1:j:82:PRO:CD	1:j:83:TYR:N	2.70	0.55
2:r:56:ALA:HB2	2:s:283:TYR:O	2.02	0.55
2:B:221:THR:CG2	1:E:324:VAL:HG11	2.36	0.54
1:C:82:PRO:CD	1:C:83:TYR:N	2.70	0.54
1:I:82:PRO:CD	1:I:83:TYR:N	2.70	0.54
1:O:74:VAL:O	1:O:78:ILE:CD1	2.42	0.54
2:Q:394:GLN:HG2	1:c:348:PRO:HB2	1.88	0.54
2:S:60:LYS:HB2	2:T:282:GLN:C	2.22	0.54
2:W:394:GLN:CB	1:i:348:PRO:HG3	2.37	0.54
2:X:182:VAL:CG2	1:j:257:THR:HG22	2.31	0.54
1:D:89:PRO:CG	1:G:218:ASP:HB2	2.33	0.54
1:J:82:PRO:CD	1:J:83:TYR:N	2.70	0.54
1:M:125:MET:O	1:N:290:GLU:OE1	2.26	0.54
2:R:394:GLN:HE21	1:d:348:PRO:C	2.16	0.54
2:U:394:GLN:HG2	1:g:348:PRO:HB2	1.88	0.54
2:X:128:SER:CB	2:Y:290:GLU:OE1	2.56	0.54
1:c:82:PRO:CD	1:c:83:TYR:N	2.70	0.54
1:g:82:PRO:CD	1:g:83:TYR:N	2.70	0.54
1:h:82:PRO:CD	1:h:83:TYR:N	2.70	0.54
2:R:61:TYR:CA	2:S:283:TYR:CB	2.84	0.54
2:V:224:TYR:CE2	1:h:248:LEU:HD11	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:394:GLN:HE21	1:i:348:PRO:C	2.16	0.54
2:X:90:ASP:HA	2:Y:218:LYS:NZ	2.22	0.54
2:Y:394:GLN:CB	1:k:348:PRO:HG3	2.37	0.54
1:M:91:GLN:NE2	1:N:283:HIS:HB2	2.22	0.54
2:Q:394:GLN:HE21	1:c:348:PRO:C	2.16	0.54
2:R:394:GLN:CB	1:d:348:PRO:HG3	2.37	0.54
2:U:394:GLN:CB	1:g:348:PRO:HG3	2.37	0.54
2:X:394:GLN:HE21	1:j:348:PRO:C	2.16	0.54
2:Y:83:PHE:O	2:Z:283:TYR:OH	2.25	0.54
2:Y:394:GLN:HE21	1:k:348:PRO:C	2.16	0.54
1:e:58:SER:CB	1:f:282:TYR:CA	2.81	0.54
1:G:62:VAL:CG2	1:H:284:GLU:HA	2.23	0.54
1:G:127:ASP:C	1:H:338:ARG:NE	2.65	0.54
2:V:394:GLN:HE21	1:h:348:PRO:C	2.16	0.54
2:V:394:GLN:CB	1:h:348:PRO:HG3	2.37	0.54
2:B:394:GLN:HE21	1:E:348:PRO:C	2.16	0.54
1:D:124:LYS:NZ	1:G:215:ARG:HB3	2.22	0.54
1:H:82:PRO:CD	1:H:83:TYR:N	2.70	0.54
2:Q:394:GLN:CB	1:c:348:PRO:HG3	2.37	0.54
1:f:82:PRO:CD	1:f:83:TYR:N	2.70	0.54
2:R:62:VAL:H	2:S:283:TYR:HB3	1.65	0.54
2:S:90:ASP:OD2	2:T:215:ARG:O	2.26	0.54
2:S:394:GLN:CB	1:e:348:PRO:HG3	2.37	0.54
2:r:7:LEU:CD2	2:r:66:VAL:CB	2.71	0.54
1:N:88:HIS:CE1	1:O:290:GLU:OE1	2.61	0.54
2:T:7:LEU:CD2	2:T:66:VAL:CB	2.71	0.54
2:T:394:GLN:CB	1:f:348:PRO:HG3	2.37	0.54
6:Q:502:TA1:C20	6:Q:502:TA1:H472	2.38	0.54
2:S:57:THR:CB	2:T:286:LEU:N	2.68	0.54
2:T:394:GLN:HG2	1:f:348:PRO:HB2	1.89	0.54
2:Y:127:GLU:O	2:Z:289:PRO:O	2.25	0.54
1:G:49:PHE:HE1	1:H:285:GLN:NE2	1.83	0.54
2:T:394:GLN:HE21	1:f:348:PRO:C	2.16	0.54
2:U:182:VAL:HG21	1:g:257:THR:CG2	2.34	0.54
6:Y:502:TA1:C20	6:Y:502:TA1:H472	2.38	0.54
1:e:75:ILE:HA	1:e:78:ILE:CD1	2.38	0.54
6:o:502:TA1:C20	6:o:502:TA1:H472	2.38	0.54
2:B:394:GLN:HG2	1:E:348:PRO:HB2	1.88	0.53
1:H:56:THR:CG2	1:I:283:HIS:O	2.56	0.53
1:O:82:PRO:CD	1:O:83:TYR:N	2.70	0.53
2:X:394:GLN:HG2	1:j:348:PRO:HB2	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:502:TA1:H472	6:X:502:TA1:C20	2.38	0.53
2:q:128:SER:CA	2:r:293:GLN:OE1	2.56	0.53
1:A:75:ILE:HA	1:A:78:ILE:CD1	2.39	0.53
1:D:55:GLU:HA	1:G:283:HIS:HA	1.89	0.53
1:E:75:ILE:HA	1:E:78:ILE:CD1	2.39	0.53
1:L:116:ASP:O	1:M:298:TYR:OH	2.26	0.53
2:R:221:THR:CG2	1:d:324:VAL:HG11	2.36	0.53
2:T:62:VAL:HG21	2:U:283:TYR:HB3	1.90	0.53
2:Y:90:ASP:CG	2:Z:216:THR:O	2.51	0.53
2:Y:182:VAL:HG21	1:k:257:THR:CG2	2.34	0.53
2:Y:394:GLN:HG2	1:k:348:PRO:HG3	1.91	0.53
1:i:57:GLY:C	1:j:283:HIS:HA	2.33	0.53
1:j:127:ASP:CA	1:k:290:GLU:OE2	2.55	0.53
2:B:394:GLN:CB	1:E:348:PRO:HG3	2.37	0.53
1:G:34:GLY:C	1:H:283:HIS:HA	2.33	0.53
1:G:75:ILE:HA	1:G:78:ILE:CD1	2.39	0.53
1:H:56:THR:HG21	1:I:283:HIS:O	2.08	0.53
6:T:502:TA1:C20	6:T:502:TA1:H472	2.38	0.53
2:V:394:GLN:HG2	1:h:348:PRO:HG3	1.91	0.53
2:W:58:GLY:N	2:X:282:GLN:O	2.41	0.53
2:W:96:GLN:HB3	1:i:1:MET:HE3	1.78	0.53
2:W:394:GLN:HG2	1:i:348:PRO:HG3	1.90	0.53
2:Y:96:GLN:CB	1:k:1:MET:HE2	2.21	0.53
1:d:75:ILE:HA	1:d:78:ILE:CD1	2.39	0.53
6:r:502:TA1:H472	6:r:502:TA1:C20	2.38	0.53
1:D:75:ILE:HA	1:D:78:ILE:CD1	2.39	0.53
1:D:82:PRO:CD	1:D:83:TYR:N	2.70	0.53
1:M:62:VAL:CG1	1:N:280:LYS:O	2.49	0.53
2:S:7:LEU:CD2	2:S:66:VAL:CB	2.71	0.53
2:W:7:LEU:CD2	2:W:66:VAL:CB	2.71	0.53
2:X:394:GLN:CB	1:j:348:PRO:HG3	2.37	0.53
1:d:82:PRO:CD	1:d:83:TYR:N	2.70	0.53
1:f:89:PRO:CG	1:g:280:LYS:CE	2.74	0.53
2:q:7:LEU:CD2	2:q:66:VAL:CB	2.71	0.53
1:D:89:PRO:HG3	1:G:279:GLU:OE2	2.09	0.53
1:L:60:LYS:HE2	1:M:283:HIS:NE2	2.22	0.53
1:M:89:PRO:HD2	1:N:277:SER:O	2.09	0.53
2:S:33:THR:CG2	2:T:283:TYR:CE1	2.76	0.53
2:Z:7:LEU:CD2	2:Z:66:VAL:CB	2.71	0.53
2:a:172:VAL:HG22	2:a:173:PRO:N	2.24	0.53
6:B:502:TA1:H472	6:B:502:TA1:C20	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:ILE:HA	1:C:78:ILE:CD1	2.38	0.53
1:P:82:PRO:CD	1:P:83:TYR:N	2.70	0.53
2:R:224:TYR:HE2	1:d:248:LEU:CD1	2.22	0.53
2:T:224:TYR:HE2	1:f:248:LEU:CD1	2.22	0.53
2:W:172:VAL:HG22	2:W:173:PRO:N	2.24	0.53
2:X:89:PRO:C	2:Y:218:LYS:HZ1	2.15	0.53
6:F:501:TA1:C20	6:F:501:TA1:H472	2.38	0.53
1:G:58:SER:OG	1:H:281:ALA:O	2.26	0.53
1:G:61:HIS:CD2	1:H:285:GLN:CG	2.92	0.53
1:L:89:PRO:HG2	1:M:280:LYS:HE2	1.91	0.53
1:P:75:ILE:HA	1:P:78:ILE:CD1	2.39	0.53
2:W:57:THR:N	2:X:283:TYR:O	2.33	0.53
6:W:502:TA1:H472	6:W:502:TA1:C20	2.38	0.53
2:Y:57:THR:HG1	2:Z:371:LEU:HA	1.71	0.53
6:Z:502:TA1:H472	6:Z:502:TA1:C20	2.38	0.53
1:c:75:ILE:HA	1:c:78:ILE:CD1	2.39	0.53
1:k:75:ILE:HA	1:k:78:ILE:CD1	2.39	0.53
2:B:181:VAL:HB	1:E:258:ASN:HA	1.91	0.53
1:E:82:PRO:CD	1:E:83:TYR:H	2.13	0.53
1:K:82:PRO:CD	1:K:83:TYR:H	2.13	0.53
1:M:75:ILE:HA	1:M:78:ILE:CD1	2.39	0.53
2:R:62:VAL:CG2	2:S:283:TYR:CG	2.90	0.53
2:S:224:TYR:HE2	1:e:248:LEU:CD1	2.22	0.53
2:U:394:GLN:HE21	1:g:348:PRO:C	2.16	0.53
2:W:100:GLY:O	1:i:257:THR:OG1	2.27	0.53
2:X:224:TYR:HE2	1:j:248:LEU:CD1	2.22	0.53
1:d:60:LYS:H	1:e:282:TYR:C	2.12	0.53
1:i:82:PRO:CD	1:i:83:TYR:H	2.13	0.53
1:A:82:PRO:CD	1:A:83:TYR:H	2.13	0.53
1:G:82:PRO:CD	1:G:83:TYR:N	2.70	0.53
2:S:394:GLN:HE21	1:e:348:PRO:C	2.16	0.53
2:Y:89:PRO:CD	2:Z:280:SER:H	2.18	0.53
1:e:58:SER:HB3	1:f:282:TYR:HA	1.84	0.53
1:e:82:PRO:CD	1:e:83:TYR:N	2.70	0.53
1:g:75:ILE:HA	1:g:78:ILE:CD1	2.39	0.53
1:L:75:ILE:HA	1:L:78:ILE:CD1	2.39	0.53
6:S:502:TA1:H472	6:S:502:TA1:C20	2.38	0.53
2:Y:62:VAL:CG2	2:Z:281:GLN:C	1.98	0.53
1:j:75:ILE:HA	1:j:78:ILE:CD1	2.39	0.53
2:r:56:ALA:N	2:s:285:ALA:HB2	2.21	0.53
1:D:89:PRO:CA	1:G:218:ASP:OD2	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:75:ILE:HA	1:I:78:ILE:CD1	2.39	0.52
1:J:75:ILE:HA	1:J:78:ILE:CD1	2.39	0.52
1:K:75:ILE:HA	1:K:78:ILE:CD1	2.39	0.52
2:R:89:PRO:HD2	2:S:218:LYS:HZ2	1.74	0.52
2:S:57:THR:CA	2:T:285:ALA:HA	2.27	0.52
2:S:221:THR:CG2	1:e:324:VAL:HG11	2.36	0.52
2:Y:57:THR:H	2:Z:286:LEU:CD1	2.16	0.52
1:c:58:SER:HA	1:d:282:TYR:CB	2.30	0.52
1:i:75:ILE:HA	1:i:78:ILE:CD1	2.38	0.52
6:q:502:TA1:C20	6:q:502:TA1:H472	2.38	0.52
1:H:75:ILE:HA	1:H:78:ILE:CD1	2.39	0.52
1:K:60:LYS:CB	1:L:283:HIS:NE2	2.73	0.52
1:O:75:ILE:HA	1:O:78:ILE:CD1	2.39	0.52
6:U:501:TA1:H472	6:U:501:TA1:C20	2.38	0.52
2:V:181:VAL:HB	1:h:258:ASN:HA	1.91	0.52
2:Y:87:PHE:N	2:Z:280:SER:HA	1.86	0.52
2:Y:172:VAL:HG22	2:Y:173:PRO:N	2.24	0.52
2:Y:181:VAL:HB	1:k:258:ASN:HA	1.91	0.52
6:a:502:TA1:C20	6:a:502:TA1:H472	2.38	0.52
6:b:502:TA1:H472	6:b:502:TA1:C20	2.38	0.52
1:h:75:ILE:HA	1:h:78:ILE:CD1	2.39	0.52
6:p:502:TA1:H472	6:p:502:TA1:C20	2.38	0.52
6:s:502:TA1:H472	6:s:502:TA1:C20	2.38	0.52
2:Q:58:GLY:C	2:R:283:TYR:CD2	2.87	0.52
2:Q:172:VAL:CG2	2:Q:173:PRO:HD3	2.34	0.52
6:R:502:TA1:H472	6:R:502:TA1:C20	2.38	0.52
2:T:224:TYR:CE2	1:f:248:LEU:CG	2.84	0.52
6:V:502:TA1:C20	6:V:502:TA1:H472	2.38	0.52
2:X:56:ALA:HB1	2:Y:283:TYR:CA	2.39	0.52
1:f:75:ILE:HA	1:f:78:ILE:CD1	2.39	0.52
1:K:82:PRO:CD	1:K:83:TYR:N	2.70	0.52
2:Q:181:VAL:HB	1:c:258:ASN:HA	1.91	0.52
2:R:181:VAL:HB	1:d:258:ASN:HA	1.91	0.52
2:R:394:GLN:HG2	1:d:348:PRO:HG3	1.91	0.52
2:S:224:TYR:CE2	1:e:248:LEU:CG	2.84	0.52
2:U:172:VAL:HG22	2:U:173:PRO:N	2.24	0.52
2:Y:56:ALA:C	2:Z:286:LEU:HD12	2.34	0.52
2:o:172:VAL:CG2	2:o:173:PRO:HD3	2.34	0.52
2:s:172:VAL:HG22	2:s:173:PRO:N	2.24	0.52
1:H:60:LYS:CD	1:I:283:HIS:NE2	2.69	0.52
2:Q:224:TYR:HE2	1:c:248:LEU:CD1	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:221:THR:CG2	1:g:324:VAL:HG11	2.36	0.52
2:b:172:VAL:HG22	2:b:173:PRO:N	2.24	0.52
1:i:82:PRO:CD	1:i:83:TYR:N	2.70	0.52
2:r:60:LYS:HD2	2:s:282:GLN:HB3	1.91	0.52
2:B:404:PHE:CZ	1:E:261:PRO:HA	2.41	0.52
1:D:82:PRO:CD	1:D:83:TYR:H	2.13	0.52
1:G:89:PRO:HB3	1:H:218:ASP:OD2	2.09	0.52
2:U:181:VAL:HB	1:g:258:ASN:HA	1.91	0.52
2:X:7:LEU:CD2	2:X:66:VAL:CB	2.71	0.52
1:d:82:PRO:CD	1:d:83:TYR:H	2.13	0.52
2:o:57:THR:N	2:p:283:TYR:CG	2.71	0.52
2:B:394:GLN:CB	1:E:348:PRO:CG	2.88	0.52
2:V:394:GLN:CB	1:h:348:PRO:CG	2.88	0.52
2:X:172:VAL:HG22	2:X:173:PRO:N	2.24	0.52
2:X:181:VAL:HB	1:j:258:ASN:HA	1.91	0.52
1:G:56:THR:HG1	1:H:284:GLU:C	2.18	0.52
1:G:128:GLN:CA	1:H:293:ASN:CB	2.88	0.52
1:H:64:ARG:HA	1:H:125:MET:HE1	1.89	0.52
2:S:181:VAL:HB	1:e:258:ASN:HA	1.91	0.52
2:U:224:TYR:HE2	1:g:248:LEU:CD1	2.22	0.52
2:U:394:GLN:CB	1:g:348:PRO:CG	2.88	0.52
2:W:224:TYR:HE2	1:i:248:LEU:CD1	2.22	0.52
2:X:182:VAL:HG21	1:j:257:THR:CG2	2.34	0.52
2:Y:91:ASN:N	2:Z:277:SER:OG	2.41	0.52
2:Y:224:TYR:HE2	1:k:248:LEU:CD1	2.22	0.52
2:r:57:THR:HG23	2:s:284:ARG:C	2.34	0.52
1:E:82:PRO:CD	1:E:83:TYR:N	2.70	0.52
1:N:75:ILE:HA	1:N:78:ILE:CD1	2.39	0.52
2:Q:100:GLY:O	1:c:257:THR:OG1	2.27	0.52
2:T:181:VAL:HB	1:f:258:ASN:HA	1.91	0.52
2:T:394:GLN:HG2	1:f:348:PRO:HG3	1.91	0.52
2:W:394:GLN:CB	1:i:348:PRO:CG	2.88	0.52
2:Z:172:VAL:HG22	2:Z:173:PRO:N	2.24	0.52
2:a:172:VAL:CG2	2:a:173:PRO:HD3	2.34	0.52
1:f:64:ARG:HA	1:f:125:MET:HE1	1.89	0.52
1:A:82:PRO:CD	1:A:83:TYR:N	2.70	0.52
2:B:224:TYR:HE2	1:E:248:LEU:CD1	2.22	0.52
1:D:127:ASP:OD2	1:G:297:GLU:CG	2.58	0.52
2:Q:394:GLN:HG2	1:c:348:PRO:HG3	1.90	0.52
2:R:56:ALA:CB	2:S:280:SER:O	2.58	0.52
2:T:182:VAL:HG21	1:f:257:THR:CG2	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:404:PHE:CZ	1:j:261:PRO:HA	2.41	0.52
2:q:60:LYS:HD3	2:r:283:TYR:CA	2.38	0.52
2:S:181:VAL:CG2	1:e:314:ALA:HB1	2.41	0.51
2:T:181:VAL:CG2	1:f:314:ALA:HB1	2.41	0.51
2:W:181:VAL:HB	1:i:258:ASN:HA	1.91	0.51
1:j:116:ASP:O	1:k:298:TYR:OH	2.29	0.51
1:C:234:ILE:CG2	1:C:270:VAL:HG11	2.39	0.51
1:M:127:ASP:HB3	1:N:290:GLU:CA	2.26	0.51
2:R:100:GLY:O	1:d:257:THR:OG1	2.27	0.51
2:R:181:VAL:CG2	1:d:314:ALA:HB1	2.41	0.51
2:Y:394:GLN:CB	1:k:348:PRO:CG	2.88	0.51
1:c:234:ILE:CG2	1:c:270:VAL:HG11	2.39	0.51
1:I:64:ARG:HA	1:I:125:MET:HE1	1.89	0.51
1:I:287:SER:HB2	1:I:289:PRO:HD2	1.93	0.51
1:M:89:PRO:CG	1:N:279:GLU:CB	2.76	0.51
1:O:64:ARG:HA	1:O:125:MET:HE1	1.89	0.51
2:R:56:ALA:O	2:S:282:GLN:O	2.28	0.51
2:V:224:TYR:HE2	1:h:248:LEU:CD1	2.22	0.51
2:W:404:PHE:CZ	1:i:261:PRO:HA	2.41	0.51
2:X:394:GLN:HG2	1:j:348:PRO:HG3	1.91	0.51
1:g:64:ARG:HA	1:g:125:MET:HE1	1.89	0.51
1:g:287:SER:HB2	1:g:289:PRO:HD2	1.93	0.51
1:D:56:THR:OG1	1:G:282:TYR:CD1	2.63	0.51
1:G:55:GLU:O	1:H:287:SER:N	2.27	0.51
2:T:394:GLN:CB	1:f:348:PRO:CG	2.88	0.51
2:V:7:LEU:CD2	2:V:66:VAL:CB	2.71	0.51
2:W:181:VAL:CG2	1:i:314:ALA:HB1	2.41	0.51
2:X:181:VAL:CG2	1:j:314:ALA:HB1	2.41	0.51
2:X:394:GLN:CB	1:j:348:PRO:CG	2.88	0.51
2:a:56:ALA:HB3	2:b:283:TYR:HB3	1.93	0.51
1:f:60:LYS:HD3	1:g:282:TYR:O	2.10	0.51
2:p:172:VAL:HG22	2:p:173:PRO:N	2.24	0.51
1:A:287:SER:HB2	1:A:289:PRO:HD2	1.93	0.51
1:E:287:SER:HB2	1:E:289:PRO:HD2	1.93	0.51
1:G:128:GLN:HA	1:H:293:ASN:CB	2.37	0.51
1:K:234:ILE:CG2	1:K:270:VAL:HG11	2.39	0.51
1:P:287:SER:HB2	1:P:289:PRO:HD2	1.93	0.51
2:Q:96:GLN:CB	1:c:1:MET:HE2	2.21	0.51
2:Q:394:GLN:CB	1:c:348:PRO:CG	2.88	0.51
2:R:60:LYS:O	2:S:282:GLN:O	2.03	0.51
2:X:221:THR:CG2	1:j:324:VAL:HG11	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:234:ILE:CG2	1:i:270:VAL:HG11	2.39	0.51
1:D:60:LYS:HE2	1:G:279:GLU:C	2.35	0.51
1:K:287:SER:HB2	1:K:289:PRO:HD2	1.93	0.51
2:V:221:THR:CG2	1:h:324:VAL:HG11	2.36	0.51
1:G:62:VAL:CG2	1:H:284:GLU:CA	2.80	0.51
1:J:287:SER:HB2	1:J:289:PRO:HD2	1.93	0.51
1:N:270:VAL:CG2	1:N:378:LEU:CD2	2.76	0.51
2:R:56:ALA:HB1	2:S:280:SER:O	2.10	0.51
2:R:394:GLN:CB	1:d:348:PRO:CG	2.88	0.51
2:S:394:GLN:CB	1:e:348:PRO:CG	2.88	0.51
1:h:287:SER:HB2	1:h:289:PRO:HD2	1.93	0.51
1:j:64:ARG:HA	1:j:125:MET:HE1	1.89	0.51
1:C:287:SER:HB2	1:C:289:PRO:HD2	1.93	0.51
1:G:287:SER:HB2	1:G:289:PRO:HD2	1.93	0.51
1:L:64:ARG:HA	1:L:125:MET:HE1	1.89	0.51
1:P:74:VAL:O	1:P:78:ILE:CD1	2.42	0.51
2:S:394:GLN:HG2	1:e:348:PRO:HG3	1.91	0.51
2:X:100:GLY:O	1:j:257:THR:OG1	2.27	0.51
1:i:287:SER:HB2	1:i:289:PRO:HD2	1.93	0.51
2:Q:181:VAL:CG2	1:c:314:ALA:HB1	2.41	0.51
2:U:181:VAL:CG2	1:g:314:ALA:HB1	2.41	0.51
2:V:181:VAL:CG2	1:h:314:ALA:HB1	2.41	0.51
2:W:394:GLN:NE2	1:i:348:PRO:C	2.69	0.51
2:B:394:GLN:HG2	1:E:348:PRO:HG3	1.91	0.51
1:M:91:GLN:HE22	1:N:283:HIS:HB2	1.76	0.51
2:Q:56:ALA:O	2:R:283:TYR:HB3	1.95	0.51
2:Y:62:VAL:HG22	2:Z:282:GLN:N	2.03	0.51
2:Y:100:GLY:O	1:k:257:THR:OG1	2.27	0.51
2:Y:404:PHE:CZ	1:k:261:PRO:HA	2.41	0.51
1:c:287:SER:HB2	1:c:289:PRO:HD2	1.93	0.51
1:e:287:SER:HB2	1:e:289:PRO:HD2	1.93	0.51
2:F:57:THR:HG21	2:o:283:TYR:HB3	1.92	0.50
2:S:182:VAL:HG21	1:e:257:THR:CG2	2.34	0.50
2:Y:127:GLU:OE2	2:Z:292:THR:O	2.28	0.50
1:j:123:ARG:NH2	1:k:338:ARG:NH1	2.56	0.50
2:p:57:THR:H	2:q:284:ARG:CB	2.07	0.50
2:Q:394:GLN:NE2	1:c:348:PRO:C	2.69	0.50
2:Y:7:LEU:CD2	2:Y:66:VAL:CB	2.71	0.50
2:r:57:THR:HG23	2:s:284:ARG:O	2.11	0.50
1:H:287:SER:HB2	1:H:289:PRO:HD2	1.93	0.50
1:J:64:ARG:HA	1:J:125:MET:HE1	1.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:234:ILE:CG2	1:J:270:VAL:HG11	2.39	0.50
2:S:172:VAL:CG2	2:S:173:PRO:HD3	2.34	0.50
2:T:100:GLY:O	1:f:257:THR:OG1	2.27	0.50
2:Y:54:ASN:O	2:Z:284:ARG:C	2.53	0.50
1:h:234:ILE:CG2	1:h:270:VAL:HG11	2.39	0.50
2:p:7:LEU:CD2	2:p:66:VAL:CB	2.71	0.50
2:B:172:VAL:HG22	2:B:173:PRO:N	2.24	0.50
1:D:56:THR:HG23	1:G:282:TYR:C	2.27	0.50
2:F:172:VAL:HG22	2:F:173:PRO:N	2.24	0.50
1:G:124:LYS:O	1:H:297:GLU:OE2	2.29	0.50
1:f:287:SER:HB2	1:f:289:PRO:HD2	1.93	0.50
1:h:64:ARG:HA	1:h:125:MET:HE1	1.89	0.50
1:j:89:PRO:HG2	1:k:280:LYS:HE2	1.93	0.50
2:q:128:SER:N	2:r:293:GLN:OE1	2.44	0.50
2:q:172:VAL:CG2	2:q:173:PRO:HD3	2.34	0.50
1:G:35:THR:H	1:H:283:HIS:CD2	2.30	0.50
1:G:234:ILE:CG2	1:G:270:VAL:HG11	2.39	0.50
2:R:7:LEU:CD2	2:R:66:VAL:CB	2.71	0.50
2:T:172:VAL:HG22	2:T:173:PRO:N	2.24	0.50
2:W:182:VAL:HG21	1:i:257:THR:CG2	2.34	0.50
2:X:96:GLN:CB	1:j:1:MET:HE2	2.21	0.50
1:e:234:ILE:CG2	1:e:270:VAL:HG11	2.39	0.50
1:k:287:SER:HB2	1:k:289:PRO:HD2	1.93	0.50
2:r:172:VAL:HG22	2:r:173:PRO:N	2.24	0.50
2:B:394:GLN:NE2	1:E:348:PRO:C	2.69	0.50
1:M:128:GLN:NE2	1:N:284:GLU:OE1	2.45	0.50
1:O:287:SER:HB2	1:O:289:PRO:HD2	1.93	0.50
2:S:172:VAL:HG22	2:S:173:PRO:N	2.24	0.50
2:X:394:GLN:NE2	1:j:348:PRO:C	2.69	0.50
2:Y:124:LYS:HG2	2:Z:293:GLN:C	2.37	0.50
2:Y:181:VAL:CG2	1:k:314:ALA:HB1	2.41	0.50
2:Z:124:LYS:CE	2:a:293:GLN:OE1	2.59	0.50
1:f:56:THR:HG22	1:g:284:GLU:C	2.36	0.50
2:q:172:VAL:HG22	2:q:173:PRO:N	2.24	0.50
2:B:100:GLY:O	1:E:257:THR:OG1	2.27	0.50
1:D:120:ASP:OD1	1:G:299:SER:HB3	2.11	0.50
1:M:287:SER:HB2	1:M:289:PRO:HD2	1.93	0.50
1:N:287:SER:HB2	1:N:289:PRO:HD2	1.93	0.50
2:T:56:ALA:CB	2:U:283:TYR:C	2.62	0.50
2:T:394:GLN:NE2	1:f:348:PRO:C	2.69	0.50
2:V:182:VAL:HG21	1:h:257:THR:CG2	2.34	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:SER:HB2	1:D:289:PRO:HD2	1.93	0.50
1:O:56:THR:CG2	1:P:283:HIS:HB3	2.34	0.50
2:Q:394:GLN:NE2	1:c:348:PRO:HG2	2.27	0.50
2:S:394:GLN:NE2	1:e:348:PRO:HG2	2.27	0.50
2:T:394:GLN:NE2	1:f:348:PRO:HG2	2.27	0.50
6:U:501:TA1:H463	6:U:501:TA1:C26	2.42	0.50
2:X:394:GLN:NE2	1:j:348:PRO:HG2	2.27	0.50
1:j:287:SER:HB2	1:j:289:PRO:HD2	1.93	0.50
6:s:502:TA1:H463	6:s:502:TA1:C26	2.42	0.50
1:G:89:PRO:CB	1:H:280:LYS:HZ2	2.09	0.50
1:K:56:THR:C	1:L:283:HIS:HA	2.32	0.50
1:L:234:ILE:CG2	1:L:270:VAL:HG11	2.39	0.50
1:L:287:SER:HB2	1:L:289:PRO:HD2	1.93	0.50
2:S:100:GLY:O	1:e:257:THR:OG1	2.27	0.50
2:S:394:GLN:NE2	1:e:348:PRO:C	2.69	0.50
2:U:394:GLN:NE2	1:g:348:PRO:C	2.69	0.50
2:U:404:PHE:CZ	1:g:261:PRO:HA	2.41	0.50
2:V:394:GLN:NE2	1:h:348:PRO:C	2.69	0.50
2:W:60:LYS:CB	2:X:283:TYR:HE2	2.24	0.50
2:W:394:GLN:NE2	1:i:348:PRO:HG2	2.27	0.50
1:d:287:SER:HB2	1:d:289:PRO:HD2	1.93	0.50
1:j:234:ILE:CG2	1:j:270:VAL:HG11	2.39	0.50
2:B:397:ALA:O	1:E:346:TRP:HB2	2.12	0.49
1:G:288:VAL:N	1:G:289:PRO:CD	2.76	0.49
1:I:270:VAL:CG2	1:I:378:LEU:CD2	2.75	0.49
1:J:288:VAL:N	1:J:289:PRO:CD	2.75	0.49
1:P:288:VAL:N	1:P:289:PRO:CD	2.75	0.49
2:R:172:VAL:HG22	2:R:173:PRO:N	2.24	0.49
6:S:502:TA1:H463	6:S:502:TA1:C26	2.42	0.49
2:Y:124:LYS:HA	2:Z:293:GLN:C	2.37	0.49
2:Y:394:GLN:NE2	1:k:348:PRO:C	2.69	0.49
2:a:57:THR:H	2:b:284:ARG:CA	2.21	0.49
1:e:288:VAL:N	1:e:289:PRO:CD	2.75	0.49
1:h:288:VAL:N	1:h:289:PRO:CD	2.76	0.49
6:q:502:TA1:H463	6:q:502:TA1:C26	2.42	0.49
1:I:288:VAL:N	1:I:289:PRO:CD	2.76	0.49
1:M:90:GLU:OE2	1:N:215:ARG:O	2.29	0.49
2:Q:397:ALA:O	1:c:346:TRP:HB2	2.12	0.49
2:R:394:GLN:NE2	1:d:348:PRO:C	2.69	0.49
2:S:224:TYR:HE2	1:e:248:LEU:HD11	1.78	0.49
2:U:394:GLN:NE2	1:g:348:PRO:HG2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:397:ALA:O	1:g:346:TRP:HB2	2.12	0.49
2:Y:54:ASN:ND2	2:Z:284:ARG:HA	2.14	0.49
2:Y:394:GLN:NE2	1:k:348:PRO:HG2	2.27	0.49
1:g:270:VAL:CG2	1:g:378:LEU:CD2	2.76	0.49
1:D:270:VAL:CG2	1:D:378:LEU:CD2	2.75	0.49
1:I:234:ILE:CG2	1:I:270:VAL:HG11	2.39	0.49
1:K:288:VAL:N	1:K:289:PRO:CD	2.75	0.49
2:W:224:TYR:HE2	1:i:248:LEU:HD11	1.78	0.49
1:g:234:ILE:CG2	1:g:270:VAL:HG11	2.39	0.49
1:g:288:VAL:N	1:g:289:PRO:CD	2.76	0.49
2:B:394:GLN:NE2	1:E:348:PRO:HG2	2.27	0.49
1:G:90:GLU:OE2	1:H:215:ARG:HD2	2.13	0.49
1:N:288:VAL:N	1:N:289:PRO:CD	2.76	0.49
2:R:56:ALA:CB	2:S:281:GLN:O	2.60	0.49
2:V:404:PHE:CZ	1:h:261:PRO:HA	2.41	0.49
6:W:502:TA1:H463	6:W:502:TA1:C26	2.42	0.49
6:Z:502:TA1:H463	6:Z:502:TA1:C26	2.42	0.49
1:i:288:VAL:N	1:i:289:PRO:CD	2.76	0.49
2:o:58:GLY:N	2:p:282:GLN:OE1	2.45	0.49
6:B:502:TA1:H463	6:B:502:TA1:C26	2.42	0.49
1:K:57:GLY:N	1:L:283:HIS:O	2.41	0.49
1:O:288:VAL:N	1:O:289:PRO:CD	2.76	0.49
2:Q:57:THR:CB	2:R:284:ARG:N	2.74	0.49
2:R:394:GLN:NE2	1:d:348:PRO:HG2	2.27	0.49
2:T:172:VAL:CG2	2:T:173:PRO:HD3	2.34	0.49
2:V:224:TYR:HE2	1:h:248:LEU:HD11	1.78	0.49
1:d:270:VAL:CG2	1:d:378:LEU:CD2	2.76	0.49
2:r:172:VAL:CG2	2:r:173:PRO:HD3	2.34	0.49
6:F:501:TA1:H463	6:F:501:TA1:C26	2.42	0.49
1:M:91:GLN:HE22	1:N:283:HIS:HB3	1.76	0.49
1:M:91:GLN:NE2	1:N:283:HIS:CB	2.76	0.49
2:R:224:TYR:HE2	1:d:248:LEU:CD2	2.18	0.49
2:V:100:GLY:O	1:h:257:THR:OG1	2.27	0.49
1:e:58:SER:HB3	1:f:282:TYR:C	2.38	0.49
2:o:57:THR:N	2:p:282:GLN:C	2.54	0.49
2:B:181:VAL:CG2	1:E:314:ALA:HB1	2.41	0.49
1:D:56:THR:N	1:G:283:HIS:N	2.55	0.49
1:D:234:ILE:CG2	1:D:270:VAL:HG11	2.39	0.49
1:D:288:VAL:N	1:D:289:PRO:CD	2.76	0.49
1:G:124:LYS:HD2	1:H:299:SER:OG	2.07	0.49
1:H:288:VAL:N	1:H:289:PRO:CD	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:502:TA1:H463	6:V:502:TA1:C26	2.42	0.49
6:Y:502:TA1:H463	6:Y:502:TA1:C26	2.42	0.49
1:d:234:ILE:CG2	1:d:270:VAL:HG11	2.39	0.49
1:d:288:VAL:N	1:d:289:PRO:CD	2.75	0.49
1:f:288:VAL:N	1:f:289:PRO:CD	2.75	0.49
1:G:60:LYS:CD	1:H:284:GLU:HG2	2.40	0.49
2:R:224:TYR:HE2	1:d:248:LEU:HD11	1.78	0.49
6:a:502:TA1:H463	6:a:502:TA1:C26	2.42	0.49
6:b:502:TA1:H463	6:b:502:TA1:C26	2.42	0.49
2:Y:402:LYS:C	1:k:262:TYR:HE1	2.21	0.49
1:e:62:VAL:CG2	1:f:283:HIS:O	2.54	0.49
1:D:72:GLN:CD	2:R:1:MET:HE3	2.35	0.48
2:F:57:THR:OG1	2:o:283:TYR:CD2	2.65	0.48
1:H:234:ILE:CG2	1:H:270:VAL:HG11	2.39	0.48
1:K:58:SER:HB3	1:L:283:HIS:CD2	2.48	0.48
2:S:397:ALA:O	1:e:346:TRP:HB2	2.12	0.48
2:T:224:TYR:HE2	1:f:248:LEU:HD11	1.78	0.48
2:U:224:TYR:HE2	1:g:248:LEU:HD11	1.78	0.48
2:U:402:LYS:C	1:g:262:TYR:HE1	2.21	0.48
2:Y:123:ARG:O	2:Z:293:GLN:HB3	2.12	0.48
2:Y:397:ALA:O	1:k:346:TRP:HB2	2.12	0.48
1:f:234:ILE:CG2	1:f:270:VAL:HG11	2.39	0.48
1:k:64:ARG:HA	1:k:125:MET:HE1	1.89	0.48
1:C:288:VAL:N	1:C:289:PRO:CD	2.76	0.48
1:J:270:VAL:CG2	1:J:378:LEU:CD2	2.76	0.48
6:Q:502:TA1:H463	6:Q:502:TA1:C26	2.42	0.48
2:T:402:LYS:C	1:f:262:TYR:HE1	2.21	0.48
2:V:394:GLN:NE2	1:h:348:PRO:HG2	2.27	0.48
6:X:502:TA1:H463	6:X:502:TA1:C26	2.42	0.48
2:Y:179:ASP:CG	1:k:353:VAL:HB	2.39	0.48
2:a:172:VAL:HG23	2:a:173:PRO:HD2	1.88	0.48
1:c:288:VAL:N	1:c:289:PRO:CD	2.76	0.48
1:h:270:VAL:CG2	1:h:378:LEU:CD2	2.75	0.48
2:o:58:GLY:HA3	2:p:282:GLN:OE1	2.13	0.48
6:B:502:TA1:H101	6:B:502:TA1:C24	2.44	0.48
6:F:501:TA1:H101	6:F:501:TA1:C24	2.44	0.48
1:M:64:ARG:HA	1:M:125:MET:HE1	1.89	0.48
2:R:55:GLU:C	2:S:285:ALA:N	2.47	0.48
6:R:502:TA1:H463	6:R:502:TA1:C26	2.42	0.48
2:V:397:ALA:O	1:h:346:TRP:HB2	2.12	0.48
2:o:57:THR:HG23	2:p:283:TYR:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:o:502:TA1:H463	6:o:502:TA1:C26	2.42	0.48
6:p:502:TA1:H463	6:p:502:TA1:C26	2.42	0.48
2:q:60:LYS:HD3	2:r:283:TYR:HA	1.95	0.48
1:A:288:VAL:N	1:A:289:PRO:CD	2.75	0.48
1:E:288:VAL:N	1:E:289:PRO:CD	2.76	0.48
1:P:72:GLN:CD	2:b:1:MET:HE3	2.35	0.48
2:R:61:TYR:CA	2:S:283:TYR:HB3	2.41	0.48
2:R:90:ASP:OD2	2:S:215:ARG:C	2.57	0.48
2:U:394:GLN:HG2	1:g:348:PRO:HG3	1.90	0.48
2:V:179:ASP:CG	1:h:353:VAL:HB	2.39	0.48
2:W:180:THR:HA	1:i:352:LYS:HD3	1.96	0.48
6:b:502:TA1:H101	6:b:502:TA1:C24	2.44	0.48
1:d:72:GLN:CD	2:p:1:MET:HE3	2.35	0.48
2:B:175:PRO:O	1:E:336:LYS:NZ	2.47	0.48
1:M:288:VAL:N	1:M:289:PRO:CD	2.75	0.48
2:Q:172:VAL:HG22	2:Q:173:PRO:N	2.24	0.48
2:R:96:GLN:CB	1:d:1:MET:HE2	2.21	0.48
2:R:179:ASP:CG	1:d:353:VAL:HB	2.39	0.48
2:S:402:LYS:C	1:e:262:TYR:HE1	2.22	0.48
6:T:502:TA1:H463	6:T:502:TA1:C26	2.42	0.48
2:U:175:PRO:O	1:g:336:LYS:NZ	2.47	0.48
2:V:175:PRO:O	1:h:336:LYS:NZ	2.47	0.48
2:W:397:ALA:O	1:i:346:TRP:HB2	2.12	0.48
2:X:402:LYS:C	1:j:262:TYR:HE1	2.21	0.48
1:e:56:THR:OG1	1:f:284:GLU:N	2.46	0.48
6:r:502:TA1:H463	6:r:502:TA1:C26	2.42	0.48
2:B:180:THR:HA	1:E:352:LYS:HD3	1.96	0.48
1:D:56:THR:CG2	1:G:283:HIS:N	2.49	0.48
1:P:234:ILE:CG2	1:P:270:VAL:HG11	2.39	0.48
6:R:502:TA1:H101	6:R:502:TA1:C24	2.44	0.48
2:S:96:GLN:CB	1:e:1:MET:HE2	2.21	0.48
6:W:502:TA1:H101	6:W:502:TA1:C24	2.44	0.48
2:X:179:ASP:CG	1:j:353:VAL:HB	2.39	0.48
2:Y:86:ILE:HG12	2:Z:282:GLN:CB	2.40	0.48
2:Y:89:PRO:O	2:Z:218:LYS:HD2	2.13	0.48
1:j:116:ASP:HB3	1:k:298:TYR:OH	2.12	0.48
1:k:288:VAL:N	1:k:289:PRO:CD	2.76	0.48
2:B:402:LYS:C	1:E:262:TYR:HE1	2.21	0.48
1:I:212:ILE:HG21	1:I:275:ILE:CD1	2.44	0.48
1:L:288:VAL:N	1:L:289:PRO:CD	2.75	0.48
2:Q:175:PRO:O	1:c:336:LYS:NZ	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:402:LYS:C	1:d:262:TYR:HE1	2.21	0.48
2:Y:87:PHE:C	2:Z:280:SER:O	2.14	0.48
2:Y:180:THR:HA	1:k:352:LYS:HD3	1.96	0.48
1:g:212:ILE:HG21	1:g:275:ILE:CD1	2.44	0.48
1:h:212:ILE:HG21	1:h:275:ILE:CD1	2.44	0.48
2:o:172:VAL:HG22	2:o:173:PRO:N	2.24	0.48
1:J:212:ILE:HG21	1:J:275:ILE:CD1	2.44	0.48
1:O:212:ILE:HG21	1:O:275:ILE:CD1	2.44	0.48
2:Q:180:THR:HA	1:c:352:LYS:HD3	1.95	0.48
2:S:30:ILE:HD11	2:S:49:ILE:HD11	1.96	0.48
2:T:96:GLN:HG3	1:f:1:MET:CE	2.17	0.48
2:V:172:VAL:HG22	2:V:173:PRO:N	2.24	0.48
2:V:402:LYS:C	1:h:262:TYR:HE1	2.21	0.48
2:W:402:LYS:C	1:i:262:TYR:HE1	2.21	0.48
2:X:62:VAL:HG21	2:Y:283:TYR:HB3	1.96	0.48
2:Y:406:HIS:HB3	1:k:263:PRO:CG	2.43	0.48
1:j:288:VAL:N	1:j:289:PRO:CD	2.76	0.48
6:p:502:TA1:H101	6:p:502:TA1:C24	2.44	0.48
1:G:212:ILE:HG21	1:G:275:ILE:CD1	2.44	0.48
1:H:270:VAL:CG2	1:H:378:LEU:CD2	2.76	0.48
1:M:54:SER:CA	1:N:285:GLN:HG2	2.43	0.48
1:M:234:ILE:CG2	1:M:270:VAL:HG11	2.39	0.48
2:R:406:HIS:HB3	1:d:263:PRO:CG	2.43	0.48
2:U:100:GLY:O	1:g:257:THR:OG1	2.27	0.48
6:V:502:TA1:C24	6:V:502:TA1:H101	2.44	0.48
2:X:120:ASP:OD1	2:Y:297:ASP:CG	2.56	0.48
2:X:397:ALA:O	1:j:346:TRP:HB2	2.12	0.48
6:Y:502:TA1:H101	6:Y:502:TA1:C24	2.44	0.48
1:e:33:ASP:O	1:f:283:HIS:CD2	2.67	0.48
1:e:212:ILE:HG21	1:e:275:ILE:CD1	2.44	0.48
1:f:212:ILE:HG21	1:f:275:ILE:CD1	2.44	0.48
1:f:270:VAL:CG2	1:f:378:LEU:CD2	2.76	0.48
2:q:30:ILE:HD11	2:q:49:ILE:HD11	1.96	0.48
2:B:179:ASP:CG	1:E:353:VAL:HB	2.39	0.48
1:C:59:GLY:C	1:D:283:HIS:HD2	2.21	0.48
1:C:212:ILE:HG21	1:C:275:ILE:CD1	2.44	0.48
1:H:212:ILE:HG21	1:H:275:ILE:CD1	2.44	0.48
1:M:92:LEU:H	1:N:280:LYS:HE2	1.77	0.48
2:Q:402:LYS:C	1:c:262:TYR:HE1	2.21	0.48
2:S:179:ASP:CG	1:e:353:VAL:HB	2.39	0.48
2:T:397:ALA:O	1:f:346:TRP:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:179:ASP:CG	1:i:353:VAL:HB	2.39	0.48
2:X:128:SER:N	2:Y:293:GLN:HE22	2.12	0.48
1:c:212:ILE:HG21	1:c:275:ILE:CD1	2.44	0.48
1:k:234:ILE:CG2	1:k:270:VAL:HG11	2.39	0.48
1:H:177:ILE:HD13	1:H:210:TYR:CD2	2.49	0.47
1:P:177:ILE:HD13	1:P:210:TYR:CD2	2.49	0.47
6:Q:502:TA1:H101	6:Q:502:TA1:C24	2.44	0.47
2:T:175:PRO:O	1:f:336:LYS:NZ	2.47	0.47
6:Z:502:TA1:H101	6:Z:502:TA1:C24	2.44	0.47
1:f:72:GLN:CD	2:r:1:MET:HE3	2.35	0.47
1:f:177:ILE:HD13	1:f:210:TYR:CD2	2.49	0.47
6:o:502:TA1:H101	6:o:502:TA1:C24	2.44	0.47
1:G:127:ASP:HA	1:H:338:ARG:HD3	1.75	0.47
1:H:72:GLN:CD	2:T:1:MET:HE3	2.35	0.47
1:I:177:ILE:HD13	1:I:210:TYR:CD2	2.49	0.47
1:O:177:ILE:HD13	1:O:210:TYR:CD2	2.49	0.47
2:Q:179:ASP:CG	1:c:353:VAL:HB	2.39	0.47
2:U:179:ASP:CG	1:g:353:VAL:HB	2.39	0.47
2:W:175:PRO:O	1:i:336:LYS:NZ	2.47	0.47
2:X:172:VAL:CG2	2:X:173:PRO:HD3	2.34	0.47
2:Y:86:ILE:HG12	2:Z:282:GLN:HB2	1.95	0.47
2:b:172:VAL:CG2	2:b:173:PRO:HD3	2.34	0.47
1:g:177:ILE:HD13	1:g:210:TYR:CD2	2.49	0.47
1:C:177:ILE:HD13	1:C:210:TYR:CD2	2.49	0.47
1:G:177:ILE:HD13	1:G:210:TYR:CD2	2.49	0.47
1:G:270:VAL:CG2	1:G:378:LEU:CD2	2.75	0.47
1:M:177:ILE:HD13	1:M:210:TYR:CD2	2.49	0.47
1:N:64:ARG:HA	1:N:125:MET:HE1	1.89	0.47
1:N:212:ILE:HG21	1:N:275:ILE:CD1	2.44	0.47
1:P:212:ILE:HG21	1:P:275:ILE:CD1	2.44	0.47
2:R:180:THR:HA	1:d:352:LYS:HD3	1.96	0.47
2:S:175:PRO:O	1:e:336:LYS:NZ	2.47	0.47
6:S:502:TA1:C24	6:S:502:TA1:H101	2.44	0.47
6:T:502:TA1:H101	6:T:502:TA1:C24	2.44	0.47
2:X:175:PRO:O	1:j:336:LYS:NZ	2.47	0.47
2:X:221:THR:CG2	1:j:324:VAL:CG2	2.89	0.47
2:a:30:ILE:HD11	2:a:49:ILE:HD11	1.96	0.47
2:b:30:ILE:HD11	2:b:49:ILE:HD11	1.96	0.47
1:c:177:ILE:HD13	1:c:210:TYR:CD2	2.49	0.47
1:e:177:ILE:HD13	1:e:210:TYR:CD2	2.49	0.47
1:k:177:ILE:HD13	1:k:210:TYR:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:q:502:TA1:C24	6:q:502:TA1:H101	2.44	0.47
2:r:62:VAL:CG2	2:s:283:TYR:O	2.62	0.47
6:r:502:TA1:H101	6:r:502:TA1:C24	2.44	0.47
2:s:30:ILE:HD11	2:s:49:ILE:HD11	1.96	0.47
2:B:101:ASN:OD1	1:E:254:GLU:HG3	2.15	0.47
2:F:57:THR:OG1	2:o:283:TYR:CE2	2.66	0.47
1:N:177:ILE:HD13	1:N:210:TYR:CD2	2.49	0.47
1:O:234:ILE:CG2	1:O:270:VAL:HG11	2.39	0.47
2:Q:394:GLN:NE2	1:c:348:PRO:HB2	2.23	0.47
2:T:221:THR:CG2	1:f:324:VAL:CG2	2.89	0.47
2:U:30:ILE:HD11	2:U:49:ILE:HD11	1.96	0.47
2:W:406:HIS:HB3	1:i:263:PRO:CG	2.43	0.47
2:X:180:THR:HA	1:j:352:LYS:HD3	1.95	0.47
2:Y:175:PRO:O	1:k:336:LYS:NZ	2.47	0.47
1:d:89:PRO:CG	1:e:218:ASP:OD2	2.62	0.47
1:D:212:ILE:HG21	1:D:275:ILE:CD1	2.44	0.47
2:F:57:THR:CG2	2:o:283:TYR:HB3	2.45	0.47
1:G:60:LYS:HE3	1:H:283:HIS:HB2	1.89	0.47
1:G:120:ASP:N	1:H:298:TYR:OH	2.32	0.47
1:M:128:GLN:HG3	1:N:290:GLU:CB	2.44	0.47
2:R:175:PRO:O	1:d:336:LYS:NZ	2.47	0.47
1:e:270:VAL:CG2	1:e:378:LEU:CD2	2.76	0.47
2:o:30:ILE:HD11	2:o:49:ILE:HD11	1.96	0.47
1:G:56:THR:HG21	1:H:286:LEU:HD21	1.92	0.47
1:K:212:ILE:HG21	1:K:275:ILE:CD1	2.44	0.47
1:M:56:THR:HG21	1:N:281:ALA:O	2.15	0.47
1:N:234:ILE:CG2	1:N:270:VAL:HG11	2.39	0.47
2:Q:30:ILE:HD11	2:Q:49:ILE:HD11	1.96	0.47
2:R:30:ILE:HD11	2:R:49:ILE:HD11	1.96	0.47
2:U:96:GLN:CB	1:g:1:MET:HE2	2.21	0.47
2:V:101:ASN:OD1	1:h:254:GLU:HG3	2.15	0.47
2:W:101:ASN:OD1	1:i:254:GLU:HG3	2.15	0.47
2:Y:124:LYS:O	2:Z:293:GLN:HB2	2.14	0.47
1:d:212:ILE:HG21	1:d:275:ILE:CD1	2.44	0.47
1:i:212:ILE:HG21	1:i:275:ILE:CD1	2.44	0.47
1:M:57:GLY:HA2	1:N:372:LEU:CD1	2.20	0.47
1:O:270:VAL:CG2	1:O:378:LEU:CD2	2.76	0.47
2:Q:224:TYR:HE2	1:c:248:LEU:HD11	1.78	0.47
2:T:30:ILE:HD11	2:T:49:ILE:HD11	1.96	0.47
2:T:180:THR:HA	1:f:352:LYS:HD3	1.95	0.47
2:V:96:GLN:CB	1:h:1:MET:HE2	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:502:TA1:C24	6:X:502:TA1:H101	2.44	0.47
2:Y:30:ILE:HD11	2:Y:49:ILE:HD11	1.96	0.47
1:f:55:GLU:O	1:g:285:GLN:HG2	2.15	0.47
2:p:30:ILE:HD11	2:p:49:ILE:HD11	1.96	0.47
2:q:56:ALA:CB	2:r:284:ARG:HA	2.43	0.47
2:r:30:ILE:HD11	2:r:49:ILE:HD11	1.96	0.47
2:R:60:LYS:HB3	2:S:282:GLN:HB2	1.51	0.47
2:U:180:THR:HA	1:g:352:LYS:HD3	1.96	0.47
2:Y:101:ASN:OD1	1:k:254:GLU:HG3	2.15	0.47
6:a:502:TA1:C24	6:a:502:TA1:H101	2.44	0.47
1:E:212:ILE:HG21	1:E:275:ILE:CD1	2.44	0.47
2:T:179:ASP:CG	1:f:353:VAL:HB	2.39	0.47
2:V:30:ILE:HD11	2:V:49:ILE:HD11	1.96	0.47
2:X:128:SER:CA	2:Y:293:GLN:HE22	2.28	0.47
2:Y:54:ASN:HD22	2:Z:284:ARG:CA	2.17	0.47
2:Y:86:ILE:O	2:Z:280:SER:C	2.58	0.47
1:d:177:ILE:HD13	1:d:210:TYR:CD2	2.49	0.47
1:A:212:ILE:HG21	1:A:275:ILE:CD1	2.44	0.47
2:B:172:VAL:CG2	2:B:173:PRO:HD3	2.34	0.47
2:F:172:VAL:CG2	2:F:173:PRO:HD3	2.34	0.47
2:R:60:LYS:N	2:S:282:GLN:CB	2.63	0.47
2:U:180:THR:HA	1:g:258:ASN:OD1	2.15	0.47
2:V:180:THR:HA	1:h:352:LYS:HD3	1.96	0.47
2:Y:96:GLN:HG3	1:k:1:MET:CE	2.17	0.47
1:e:60:LYS:CB	1:f:282:TYR:C	2.86	0.47
1:A:177:ILE:HD13	1:A:210:TYR:CD2	2.49	0.46
1:D:177:ILE:HD13	1:D:210:TYR:CD2	2.49	0.46
1:E:177:ILE:HD13	1:E:210:TYR:CD2	2.49	0.46
1:J:177:ILE:HD13	1:J:210:TYR:CD2	2.49	0.46
2:V:180:THR:HA	1:h:258:ASN:OD1	2.16	0.46
2:W:394:GLN:NE2	1:i:348:PRO:HB2	2.23	0.46
1:f:60:LYS:HD3	1:g:282:TYR:C	2.40	0.46
1:j:177:ILE:HD13	1:j:210:TYR:CD2	2.49	0.46
1:L:177:ILE:HD13	1:L:210:TYR:CD2	2.49	0.46
2:U:101:ASN:OD1	1:g:254:GLU:HG3	2.15	0.46
2:X:30:ILE:HD11	2:X:49:ILE:HD11	1.96	0.46
1:h:177:ILE:HD13	1:h:210:TYR:CD2	2.49	0.46
1:i:177:ILE:HD13	1:i:210:TYR:CD2	2.49	0.46
2:p:57:THR:H	2:q:284:ARG:HB2	1.81	0.46
1:K:177:ILE:HD13	1:K:210:TYR:CD2	2.49	0.46
1:N:89:PRO:HG3	1:O:284:GLU:HG2	1.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:397:ALA:O	1:d:346:TRP:HB2	2.12	0.46
2:S:180:THR:HA	1:e:352:LYS:HD3	1.96	0.46
2:T:101:ASN:OD1	1:f:254:GLU:HG3	2.15	0.46
2:W:30:ILE:HD11	2:W:49:ILE:HD11	1.96	0.46
2:W:180:THR:HA	1:i:258:ASN:OD1	2.15	0.46
2:X:89:PRO:C	2:Y:218:LYS:HZ3	2.23	0.46
2:Y:34:GLY:CA	2:Z:282:GLN:HB3	2.45	0.46
2:Z:30:ILE:HD11	2:Z:49:ILE:HD11	1.96	0.46
1:k:212:ILE:HG21	1:k:275:ILE:CD1	2.44	0.46
2:r:56:ALA:HB1	2:s:283:TYR:C	2.37	0.46
1:M:212:ILE:HG21	1:M:275:ILE:CD1	2.44	0.46
1:N:62:VAL:CG2	1:O:285:GLN:HE21	2.00	0.46
2:R:88:ARG:HG2	2:S:218:LYS:HZ1	1.79	0.46
2:R:180:THR:CA	1:d:258:ASN:OD1	2.64	0.46
2:S:101:ASN:OD1	1:e:254:GLU:HG3	2.15	0.46
2:S:180:THR:CA	1:e:258:ASN:OD1	2.64	0.46
2:Y:88:ARG:O	2:Z:277:SER:CB	2.53	0.46
6:s:502:TA1:C24	6:s:502:TA1:H101	2.44	0.46
1:M:88:HIS:CD2	1:N:280:LYS:HD2	2.48	0.46
1:P:270:VAL:CG2	1:P:378:LEU:CD2	2.76	0.46
2:Q:101:ASN:OD1	1:c:254:GLU:HG3	2.15	0.46
6:U:501:TA1:C24	6:U:501:TA1:H101	2.44	0.46
2:Y:86:ILE:HG13	2:Z:282:GLN:OE1	2.16	0.46
1:j:124:LYS:NZ	1:k:216:ASN:OD1	2.49	0.46
2:B:30:ILE:HD11	2:B:49:ILE:HD11	1.96	0.46
2:F:30:ILE:HD11	2:F:49:ILE:HD11	1.96	0.46
1:L:212:ILE:HG21	1:L:275:ILE:CD1	2.44	0.46
2:W:180:THR:CA	1:i:258:ASN:OD1	2.64	0.46
1:j:212:ILE:HG21	1:j:275:ILE:CD1	2.44	0.46
1:D:88:HIS:HB2	1:G:280:LYS:HG2	1.61	0.46
1:K:270:VAL:CG2	1:K:378:LEU:CD2	2.76	0.46
2:V:404:PHE:CE1	1:h:261:PRO:HA	2.51	0.46
2:Y:180:THR:HA	1:k:258:ASN:OD1	2.15	0.46
1:j:120:ASP:OD1	1:k:297:GLU:OE1	2.33	0.46
2:B:180:THR:HA	1:E:258:ASN:OD1	2.16	0.46
1:G:127:ASP:OD2	1:H:341:ILE:CD1	2.38	0.46
2:Q:180:THR:CA	1:c:258:ASN:OD1	2.64	0.46
2:Q:394:GLN:CD	1:c:348:PRO:HG2	2.41	0.46
2:S:123:ARG:NH1	2:T:308:ARG:HD2	2.31	0.46
2:T:180:THR:CA	1:f:258:ASN:OD1	2.64	0.46
2:W:404:PHE:CE1	1:i:261:PRO:HA	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:56:ALA:CA	2:Z:286:LEU:HB2	2.29	0.46
2:a:57:THR:OG1	2:b:281:GLN:C	2.48	0.46
2:B:404:PHE:CE1	1:E:261:PRO:HA	2.51	0.46
1:G:64:ARG:HA	1:G:125:MET:HE1	1.89	0.46
2:R:180:THR:HA	1:d:258:ASN:OD1	2.16	0.46
2:S:406:HIS:HB3	1:e:263:PRO:CG	2.43	0.46
2:U:224:TYR:CE2	1:g:248:LEU:CG	2.84	0.46
2:U:404:PHE:CE1	1:g:261:PRO:HA	2.51	0.46
2:X:101:ASN:OD1	1:j:254:GLU:HG3	2.15	0.46
2:X:180:THR:HA	1:j:258:ASN:OD1	2.16	0.46
2:Y:404:PHE:CE1	1:k:261:PRO:HA	2.51	0.46
1:e:64:ARG:HA	1:e:125:MET:HE1	1.89	0.46
1:i:270:VAL:CG2	1:i:378:LEU:CD2	2.76	0.46
1:j:116:ASP:C	1:k:298:TYR:OH	2.59	0.46
1:j:123:ARG:HH12	1:k:338:ARG:NH1	2.14	0.46
2:r:60:LYS:HD2	2:s:282:GLN:CB	2.46	0.46
2:r:60:LYS:HD2	2:s:282:GLN:O	2.09	0.46
1:G:60:LYS:NZ	1:H:280:LYS:CA	2.72	0.46
1:I:72:GLN:CD	2:U:1:MET:HE3	2.35	0.46
2:S:394:GLN:CD	1:e:348:PRO:HG2	2.41	0.46
1:g:72:GLN:CD	2:s:1:MET:HE3	2.35	0.46
1:A:234:ILE:CG2	1:A:270:VAL:HG11	2.39	0.45
2:B:180:THR:CA	1:E:258:ASN:OD1	2.64	0.45
1:E:234:ILE:CG2	1:E:270:VAL:HG11	2.39	0.45
1:G:117:SER:C	1:H:298:TYR:HH	2.16	0.45
2:Q:180:THR:HA	1:c:258:ASN:OD1	2.16	0.45
2:T:180:THR:HA	1:f:258:ASN:OD1	2.16	0.45
2:T:394:GLN:CD	1:f:348:PRO:HG2	2.41	0.45
2:X:180:THR:CA	1:j:258:ASN:OD1	2.64	0.45
2:X:406:HIS:HB3	1:j:263:PRO:CG	2.43	0.45
2:Y:223:THR:HG22	1:k:324:VAL:HG13	1.98	0.45
2:Y:394:GLN:CD	1:k:348:PRO:HG2	2.41	0.45
1:e:60:LYS:O	1:f:283:HIS:O	2.34	0.45
1:j:117:SER:OG	1:k:215:ARG:HD3	2.15	0.45
1:K:58:SER:HB2	1:L:283:HIS:CE1	2.49	0.45
2:R:223:THR:HG22	1:d:324:VAL:HG13	1.98	0.45
2:R:394:GLN:CD	1:d:348:PRO:HG2	2.41	0.45
2:B:394:GLN:CD	1:E:348:PRO:HG2	2.41	0.45
1:G:127:ASP:CA	1:H:338:ARG:HD3	2.41	0.45
1:K:56:THR:CB	1:L:283:HIS:CA	2.87	0.45
2:S:54:ASN:HB3	2:T:290:GLU:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:123:ARG:HH11	2:T:308:ARG:HD2	1.80	0.45
2:U:180:THR:CA	1:g:258:ASN:OD1	2.64	0.45
2:V:180:THR:CA	1:h:258:ASN:OD1	2.64	0.45
1:M:90:GLU:HG2	1:N:216:ASN:O	2.17	0.45
2:S:180:THR:HA	1:e:258:ASN:OD1	2.15	0.45
2:T:223:THR:HG22	1:f:324:VAL:HG13	1.98	0.45
2:V:404:PHE:CE1	1:h:261:PRO:CA	3.00	0.45
2:a:189:LEU:HD22	2:a:413:MET:HE1	1.99	0.45
2:B:189:LEU:HD22	2:B:413:MET:HE1	1.99	0.45
1:G:35:THR:N	1:H:283:HIS:CD2	2.84	0.45
1:K:72:GLN:CD	2:W:1:MET:HE3	2.35	0.45
1:L:70:LEU:HD23	1:L:114:LEU:CD1	2.36	0.45
2:S:96:GLN:HG3	1:e:1:MET:CE	2.17	0.45
2:U:394:GLN:CD	1:g:348:PRO:HG2	2.41	0.45
2:V:394:GLN:NE2	1:h:348:PRO:HB2	2.23	0.45
2:W:221:THR:CG2	1:i:324:VAL:CG2	2.89	0.45
2:X:394:GLN:CD	1:j:348:PRO:HG2	2.41	0.45
2:Y:180:THR:CA	1:k:258:ASN:OD1	2.64	0.45
2:F:189:LEU:HD22	2:F:413:MET:HE1	1.99	0.45
1:M:88:HIS:CD2	1:N:280:LYS:HD3	2.51	0.45
2:S:223:THR:HG22	1:e:324:VAL:HG13	1.98	0.45
2:U:404:PHE:CE1	1:g:261:PRO:CA	3.00	0.45
2:W:404:PHE:CE1	1:i:261:PRO:CA	3.00	0.45
2:Y:56:ALA:HB1	2:Z:286:LEU:CG	2.35	0.45
1:j:70:LEU:HD23	1:j:114:LEU:CD1	2.36	0.45
2:B:223:THR:HG22	1:E:324:VAL:HG13	1.98	0.45
1:C:72:GLN:CD	2:Q:1:MET:HE3	2.35	0.45
1:J:72:GLN:CD	2:V:1:MET:HE3	2.35	0.45
2:Q:404:PHE:CE1	1:c:261:PRO:HA	2.51	0.45
2:R:101:ASN:OD1	1:d:254:GLU:HG3	2.15	0.45
2:R:404:PHE:CE1	1:d:261:PRO:HA	2.51	0.45
2:X:404:PHE:CE1	1:j:261:PRO:HA	2.51	0.45
2:b:189:LEU:HD22	2:b:413:MET:HE1	1.99	0.45
1:d:56:THR:OG1	1:e:280:LYS:O	2.35	0.45
1:e:56:THR:CG2	1:f:283:HIS:O	2.59	0.45
2:B:96:GLN:CB	1:E:1:MET:HE2	2.21	0.45
1:D:64:ARG:HA	1:D:125:MET:HE1	1.89	0.45
2:Q:57:THR:HB	2:R:280:SER:O	2.16	0.45
2:R:221:THR:CG2	1:d:324:VAL:CG2	2.89	0.45
2:T:404:PHE:CE1	1:f:261:PRO:HA	2.51	0.45
2:U:223:THR:HG22	1:g:324:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:128:SER:N	2:Z:289:PRO:O	2.50	0.45
1:c:56:THR:HA	1:d:283:HIS:HB3	1.68	0.45
1:c:58:SER:HB3	1:d:283:HIS:HE1	1.63	0.45
1:c:72:GLN:CD	2:o:1:MET:HE3	2.35	0.45
1:d:64:ARG:HA	1:d:125:MET:HE1	1.89	0.45
1:i:64:ARG:HA	1:i:125:MET:HE1	1.89	0.45
2:X:394:GLN:CG	1:j:348:PRO:HG3	2.47	0.45
2:Y:404:PHE:CE1	1:k:261:PRO:CA	3.00	0.45
2:a:57:THR:OG1	2:b:284:ARG:N	2.50	0.45
1:D:89:PRO:N	1:G:218:ASP:OD2	2.49	0.45
1:G:127:ASP:HA	1:H:338:ARG:HE	1.64	0.45
1:K:64:ARG:HA	1:K:125:MET:HE1	1.89	0.45
2:Q:172:VAL:HG23	2:Q:173:PRO:HD2	1.88	0.45
2:Q:404:PHE:CE1	1:c:261:PRO:CA	3.00	0.45
2:R:89:PRO:CB	2:S:218:LYS:HZ3	2.22	0.45
2:S:404:PHE:CE1	1:e:261:PRO:HA	2.51	0.45
2:V:189:LEU:HD22	2:V:413:MET:HE1	1.99	0.45
2:W:394:GLN:CD	1:i:348:PRO:HG2	2.41	0.45
2:Z:189:LEU:HD22	2:Z:413:MET:HE1	1.99	0.45
1:D:58:SER:N	1:G:282:TYR:HE1	2.03	0.44
6:F:501:TA1:C20	6:F:501:TA1:C47	2.95	0.44
1:L:88:HIS:CE1	1:M:280:LYS:HD3	2.52	0.44
2:S:221:THR:CG2	1:e:324:VAL:CG2	2.89	0.44
2:S:404:PHE:CE1	1:e:261:PRO:CA	3.00	0.44
2:V:394:GLN:CD	1:h:348:PRO:HG2	2.41	0.44
2:o:172:VAL:HG23	2:o:173:PRO:HD2	1.88	0.44
6:B:502:TA1:C20	6:B:502:TA1:C47	2.95	0.44
1:M:92:LEU:N	1:N:280:LYS:HE2	2.33	0.44
2:Q:394:GLN:CG	1:c:348:PRO:HG3	2.47	0.44
6:Q:502:TA1:C20	6:Q:502:TA1:C47	2.95	0.44
2:V:223:THR:HG22	1:h:324:VAL:HG13	1.98	0.44
1:e:58:SER:HB3	1:f:282:TYR:O	2.16	0.44
2:Q:189:LEU:HD22	2:Q:413:MET:HE1	1.99	0.44
2:Q:223:THR:HG22	1:c:324:VAL:HG13	1.98	0.44
2:R:404:PHE:CE1	1:d:261:PRO:CA	3.00	0.44
2:W:189:LEU:HD22	2:W:413:MET:HE1	1.99	0.44
2:X:96:GLN:HG3	1:j:1:MET:CE	2.17	0.44
2:o:189:LEU:HD22	2:o:413:MET:HE1	1.99	0.44
6:o:502:TA1:C20	6:o:502:TA1:C47	2.96	0.44
1:L:72:GLN:CD	2:X:1:MET:HE3	2.35	0.44
6:R:502:TA1:C20	6:R:502:TA1:C47	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:394:GLN:CG	1:g:348:PRO:HG3	2.47	0.44
6:U:501:TA1:C20	6:U:501:TA1:C47	2.95	0.44
2:X:189:LEU:HD22	2:X:413:MET:HE1	1.99	0.44
2:X:223:THR:HG22	1:j:324:VAL:HG13	1.98	0.44
6:X:502:TA1:C20	6:X:502:TA1:C47	2.95	0.44
2:Y:189:LEU:HD22	2:Y:413:MET:HE1	1.99	0.44
2:p:124:LYS:HE2	2:q:299:LYS:HZ2	1.80	0.44
6:p:502:TA1:C20	6:p:502:TA1:C47	2.95	0.44
6:s:502:TA1:C20	6:s:502:TA1:C47	2.95	0.44
1:D:60:LYS:HE3	1:G:283:HIS:CE1	2.52	0.44
1:I:70:LEU:HD23	1:I:114:LEU:CD1	2.36	0.44
2:S:189:LEU:HD22	2:S:413:MET:HE1	1.99	0.44
6:S:502:TA1:C20	6:S:502:TA1:C47	2.95	0.44
2:X:90:ASP:HA	2:Y:218:LYS:HZ3	1.82	0.44
1:g:70:LEU:HD23	1:g:114:LEU:CD1	2.36	0.44
1:j:127:ASP:OD1	1:k:293:ASN:CG	2.61	0.44
6:q:502:TA1:C20	6:q:502:TA1:C47	2.95	0.44
2:r:57:THR:HA	2:s:285:ALA:HA	1.93	0.44
1:C:64:ARG:HA	1:C:125:MET:HE1	1.89	0.44
2:F:57:THR:HG21	2:o:283:TYR:CD2	2.53	0.44
1:M:127:ASP:O	1:N:289:PRO:HB2	2.18	0.44
2:T:404:PHE:CD2	1:f:261:PRO:N	2.82	0.44
6:V:502:TA1:C20	6:V:502:TA1:C47	2.96	0.44
2:W:223:THR:HG22	1:i:324:VAL:HG13	1.98	0.44
6:Z:502:TA1:C20	6:Z:502:TA1:C47	2.95	0.44
1:c:64:ARG:HA	1:c:125:MET:HE1	1.89	0.44
1:A:64:ARG:HA	1:A:125:MET:HE1	1.89	0.44
2:B:404:PHE:CE1	1:E:261:PRO:CA	3.00	0.44
1:G:60:LYS:HZ2	1:H:283:HIS:CB	2.28	0.44
1:N:72:GLN:CD	2:Z:1:MET:HE3	2.35	0.44
2:S:57:THR:H	2:T:284:ARG:HG2	1.83	0.44
6:T:502:TA1:C20	6:T:502:TA1:C47	2.95	0.44
2:V:221:THR:HG22	1:h:324:VAL:HG21	1.98	0.44
2:W:403:ALA:N	1:i:262:TYR:HE1	2.16	0.44
2:Z:172:VAL:CG2	2:Z:173:PRO:HD3	2.34	0.44
2:q:189:LEU:HD22	2:q:413:MET:HE1	1.99	0.44
6:r:502:TA1:C20	6:r:502:TA1:C47	2.95	0.44
1:E:64:ARG:HA	1:E:125:MET:HE1	1.89	0.44
1:N:124:LYS:CG	1:O:338:ARG:NH2	2.80	0.44
2:T:404:PHE:CE1	1:f:261:PRO:CA	3.00	0.44
1:e:88:HIS:ND1	1:f:280:LYS:HD3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:116:ASP:C	1:k:298:TYR:HH	2.25	0.44
2:r:189:LEU:HD22	2:r:413:MET:HE1	1.99	0.44
1:L:60:LYS:CE	1:M:283:HIS:NE2	2.80	0.44
2:R:56:ALA:HB1	2:S:281:GLN:O	2.18	0.44
2:T:189:LEU:HD22	2:T:413:MET:HE1	1.99	0.44
2:W:180:THR:HG23	1:i:258:ASN:HD21	1.83	0.44
6:Y:502:TA1:C20	6:Y:502:TA1:C47	2.95	0.44
2:B:180:THR:HG23	1:E:258:ASN:HD21	1.83	0.43
1:D:62:VAL:HG21	1:G:280:LYS:C	2.43	0.43
2:Q:60:LYS:CA	2:R:283:TYR:CD2	3.00	0.43
2:X:180:THR:HG23	1:j:258:ASN:HD21	1.83	0.43
2:Y:34:GLY:CA	2:Z:282:GLN:CB	2.87	0.43
2:Y:394:GLN:NE2	1:k:348:PRO:HB2	2.23	0.43
1:d:58:SER:N	1:e:282:TYR:HD1	2.12	0.43
1:M:72:GLN:CD	2:Y:1:MET:HE3	2.35	0.43
2:S:394:GLN:CG	1:e:348:PRO:HG3	2.47	0.43
2:Y:180:THR:HG23	1:k:258:ASN:HD21	1.83	0.43
6:a:502:TA1:C20	6:a:502:TA1:C47	2.96	0.43
6:b:502:TA1:C20	6:b:502:TA1:C47	2.95	0.43
1:d:61:HIS:C	1:e:283:HIS:HD2	2.23	0.43
1:f:14:VAL:CG1	1:f:78:ILE:HD11	2.49	0.43
2:r:6:HIS:CD2	2:r:21:TRP:HE1	2.37	0.43
2:B:401:ARG:O	1:E:262:TYR:CE1	2.72	0.43
1:H:14:VAL:CG1	1:H:78:ILE:HD11	2.49	0.43
2:R:180:THR:HG23	1:d:258:ASN:HD21	1.83	0.43
2:T:6:HIS:CD2	2:T:21:TRP:HE1	2.37	0.43
2:V:100:GLY:O	1:h:257:THR:CB	2.67	0.43
6:W:502:TA1:C20	6:W:502:TA1:C47	2.95	0.43
2:Y:100:GLY:O	1:k:257:THR:CB	2.67	0.43
1:D:14:VAL:CG1	1:D:78:ILE:HD11	2.49	0.43
1:G:127:ASP:OD1	1:H:338:ARG:CD	2.66	0.43
1:H:60:LYS:HD3	1:I:283:HIS:CD2	2.54	0.43
1:H:70:LEU:HD23	1:H:114:LEU:CD1	2.36	0.43
1:M:128:GLN:HG2	1:N:290:GLU:HG3	1.82	0.43
1:O:70:LEU:HD23	1:O:114:LEU:CD1	2.36	0.43
2:Q:100:GLY:O	1:c:257:THR:CB	2.67	0.43
2:R:6:HIS:CD2	2:R:21:TRP:HE1	2.37	0.43
2:R:401:ARG:O	1:d:262:TYR:CE1	2.72	0.43
2:S:6:HIS:CD2	2:S:21:TRP:HE1	2.37	0.43
2:T:100:GLY:O	1:f:257:THR:CB	2.67	0.43
2:T:394:GLN:NE2	1:f:348:PRO:HB2	2.23	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:406:HIS:HB3	1:f:263:PRO:CG	2.43	0.43
2:W:401:ARG:O	1:i:262:TYR:CE1	2.72	0.43
2:X:401:ARG:O	1:j:262:TYR:CE1	2.72	0.43
2:Y:401:ARG:O	1:k:262:TYR:CE1	2.72	0.43
1:d:14:VAL:CG1	1:d:78:ILE:HD11	2.49	0.43
2:p:60:LYS:O	2:q:283:TYR:HB3	2.17	0.43
2:s:189:LEU:HD22	2:s:413:MET:HE1	1.99	0.43
1:D:60:LYS:HE2	1:G:279:GLU:HA	2.00	0.43
1:I:30:LEU:CD2	1:I:36:MET:HB2	2.48	0.43
1:L:14:VAL:CG1	1:L:78:ILE:HD11	2.49	0.43
1:M:128:GLN:CG	1:N:286:LEU:H	2.25	0.43
2:Q:180:THR:HG23	1:c:258:ASN:HD21	1.83	0.43
2:R:189:LEU:HD22	2:R:413:MET:HE1	1.99	0.43
2:S:100:GLY:O	1:e:257:THR:CB	2.67	0.43
2:S:394:GLN:NE2	1:e:348:PRO:HB2	2.23	0.43
2:T:403:ALA:N	1:f:262:TYR:HE1	2.16	0.43
2:W:6:HIS:CD2	2:W:21:TRP:HE1	2.37	0.43
1:f:70:LEU:HD23	1:f:114:LEU:CD1	2.36	0.43
2:p:6:HIS:CD2	2:p:21:TRP:HE1	2.37	0.43
2:p:189:LEU:HD22	2:p:413:MET:HE1	1.99	0.43
2:q:6:HIS:CD2	2:q:21:TRP:HE1	2.37	0.43
1:M:14:VAL:CG1	1:M:78:ILE:HD11	2.49	0.43
1:M:128:GLN:CG	1:N:286:LEU:N	2.81	0.43
2:Q:406:HIS:HB3	1:c:263:PRO:CG	2.43	0.43
2:W:96:GLN:CB	1:i:1:MET:HE2	2.21	0.43
2:X:100:GLY:O	1:j:257:THR:CB	2.67	0.43
2:X:120:ASP:OD2	2:Y:297:ASP:CG	2.62	0.43
2:X:404:PHE:CE1	1:j:261:PRO:CA	3.00	0.43
2:Y:88:ARG:HD3	2:Z:284:ARG:HH11	1.84	0.43
2:b:6:HIS:CD2	2:b:21:TRP:HE1	2.37	0.43
1:g:30:LEU:CD2	1:g:36:MET:HB2	2.48	0.43
1:j:14:VAL:CG1	1:j:78:ILE:HD11	2.49	0.43
1:k:14:VAL:CG1	1:k:78:ILE:HD11	2.49	0.43
1:A:30:LEU:CD2	1:A:36:MET:HB2	2.48	0.43
2:B:100:GLY:O	1:E:257:THR:CB	2.67	0.43
1:E:30:LEU:CD2	1:E:36:MET:HB2	2.48	0.43
1:J:70:LEU:HD23	1:J:114:LEU:CD1	2.36	0.43
1:M:54:SER:HA	1:N:285:GLN:HG2	2.01	0.43
1:N:14:VAL:CG1	1:N:78:ILE:HD11	2.49	0.43
2:R:403:ALA:N	1:d:262:TYR:HE1	2.16	0.43
2:U:180:THR:HG23	1:g:258:ASN:HD21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:189:LEU:HD22	2:U:413:MET:HE1	1.99	0.43
2:V:401:ARG:O	1:h:262:TYR:CE1	2.72	0.43
1:e:89:PRO:HD2	1:f:280:LYS:HD3	1.91	0.43
1:f:56:THR:CB	1:g:284:GLU:C	2.89	0.43
1:C:14:VAL:CG1	1:C:78:ILE:HD11	2.49	0.43
1:C:30:LEU:CD2	1:C:36:MET:HB2	2.48	0.43
1:N:62:VAL:HB	1:O:285:GLN:HE22	1.84	0.43
2:Q:6:HIS:CD2	2:Q:21:TRP:HE1	2.37	0.43
2:R:62:VAL:HG23	2:S:283:TYR:HB3	1.80	0.43
2:R:100:GLY:O	1:d:257:THR:CB	2.66	0.43
2:T:180:THR:HG23	1:f:258:ASN:HD21	1.83	0.43
2:U:394:GLN:NE2	1:g:348:PRO:HB2	2.23	0.43
2:V:403:ALA:N	1:h:262:TYR:HE1	2.16	0.43
2:X:403:ALA:N	1:j:262:TYR:HE1	2.16	0.43
2:Y:88:ARG:HD3	2:Z:284:ARG:NH1	2.33	0.43
2:Y:117:SER:HA	2:Z:299:LYS:HZ1	0.74	0.43
1:c:30:LEU:CD2	1:c:36:MET:HB2	2.48	0.43
1:h:14:VAL:CG1	1:h:78:ILE:HD11	2.49	0.43
1:h:70:LEU:HD23	1:h:114:LEU:CD1	2.36	0.43
2:o:6:HIS:CD2	2:o:21:TRP:HE1	2.37	0.43
1:J:14:VAL:CG1	1:J:78:ILE:HD11	2.49	0.43
1:J:60:LYS:CD	1:K:283:HIS:CD2	3.01	0.43
2:Q:401:ARG:O	1:c:262:TYR:CE1	2.72	0.43
2:U:401:ARG:O	1:g:262:TYR:CE1	2.72	0.43
2:X:90:ASP:CA	2:Y:218:LYS:NZ	2.82	0.43
2:Y:128:SER:CA	2:Z:289:PRO:O	2.64	0.43
1:c:14:VAL:CG1	1:c:78:ILE:HD11	2.49	0.43
1:H:62:VAL:CG2	1:I:283:HIS:HD2	2.32	0.43
1:N:62:VAL:CG2	1:O:285:GLN:CD	2.67	0.43
1:P:14:VAL:CG1	1:P:78:ILE:HD11	2.49	0.43
2:S:401:ARG:O	1:e:262:TYR:CE1	2.72	0.43
2:V:57:THR:CG2	2:W:284:ARG:O	2.67	0.43
2:X:6:HIS:CD2	2:X:21:TRP:HE1	2.37	0.43
2:Y:6:HIS:CD2	2:Y:21:TRP:HE1	2.37	0.43
1:c:58:SER:N	1:d:282:TYR:HB3	2.34	0.43
1:e:14:VAL:CG1	1:e:78:ILE:HD11	2.49	0.43
1:G:14:VAL:CG1	1:G:78:ILE:HD11	2.49	0.42
1:J:30:LEU:CD2	1:J:36:MET:HB2	2.48	0.42
1:O:14:VAL:CG1	1:O:78:ILE:HD11	2.49	0.42
2:U:220:THR:O	1:g:326:LYS:NZ	2.50	0.42
2:V:6:HIS:CD2	2:V:21:TRP:HE1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:30:LEU:CD2	1:h:36:MET:HB2	2.48	0.42
2:r:57:THR:CG2	2:s:284:ARG:O	2.58	0.42
1:K:14:VAL:CG1	1:K:78:ILE:HD11	2.49	0.42
2:S:403:ALA:N	1:e:262:TYR:HE1	2.16	0.42
2:U:221:THR:CG2	1:g:324:VAL:CG2	2.89	0.42
2:W:100:GLY:O	1:i:257:THR:CB	2.67	0.42
2:Z:6:HIS:CD2	2:Z:21:TRP:HE1	2.37	0.42
2:s:6:HIS:CD2	2:s:21:TRP:HE1	2.37	0.42
1:N:30:LEU:CD2	1:N:36:MET:HB2	2.48	0.42
2:R:221:THR:HG22	1:d:324:VAL:HG21	1.98	0.42
2:S:180:THR:HG23	1:e:258:ASN:HD21	1.83	0.42
2:U:6:HIS:CD2	2:U:21:TRP:HE1	2.37	0.42
2:U:100:GLY:O	1:g:257:THR:CB	2.67	0.42
2:V:180:THR:HG23	1:h:258:ASN:HD21	1.83	0.42
2:a:6:HIS:CD2	2:a:21:TRP:HE1	2.37	0.42
1:e:58:SER:HB3	1:f:282:TYR:CA	2.49	0.42
1:j:62:VAL:CG2	1:k:283:HIS:CD2	3.02	0.42
2:q:33:THR:O	2:r:283:TYR:HE2	2.02	0.42
1:G:30:LEU:CD2	1:G:36:MET:HB2	2.48	0.42
1:L:56:THR:HG21	1:M:283:HIS:CA	2.48	0.42
1:N:62:VAL:CG2	1:O:285:GLN:HE22	2.18	0.42
1:P:30:LEU:CD2	1:P:36:MET:HB2	2.48	0.42
2:R:34:GLY:C	2:S:283:TYR:CZ	2.91	0.42
2:T:57:THR:HG23	2:U:285:ALA:HA	2.00	0.42
2:T:394:GLN:HB3	1:f:348:PRO:HG2	2.02	0.42
2:U:394:GLN:HB3	1:g:348:PRO:HG2	2.02	0.42
2:Y:221:THR:CG2	1:k:324:VAL:CG2	2.89	0.42
1:e:30:LEU:CD2	1:e:36:MET:HB2	2.48	0.42
1:i:14:VAL:CG1	1:i:78:ILE:HD11	2.49	0.42
2:B:222:PRO:HD2	1:E:326:LYS:HB2	2.02	0.42
1:G:89:PRO:CA	1:H:280:LYS:NZ	2.82	0.42
1:M:90:GLU:OE2	1:N:216:ASN:N	2.44	0.42
2:Q:222:PRO:HD2	1:c:326:LYS:HB2	2.02	0.42
2:p:57:THR:HG22	2:q:284:ARG:CA	2.42	0.42
1:D:62:VAL:HG21	1:G:280:LYS:O	2.19	0.42
2:S:222:PRO:HD2	1:e:326:LYS:HB2	2.02	0.42
2:X:394:GLN:HB3	1:j:348:PRO:HG2	2.02	0.42
2:q:57:THR:OG1	2:r:281:GLN:O	2.38	0.42
1:A:14:VAL:CG1	1:A:78:ILE:HD11	2.49	0.42
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.37	0.42
2:B:404:PHE:CD2	1:E:261:PRO:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:HIS:CE1	1:G:218:ASP:OD1	2.73	0.42
1:D:89:PRO:CD	1:G:218:ASP:OD2	2.67	0.42
1:G:60:LYS:CE	1:H:284:GLU:HG2	2.50	0.42
1:K:56:THR:HA	1:L:283:HIS:O	2.19	0.42
1:M:70:LEU:HD23	1:M:114:LEU:CD1	2.36	0.42
2:Q:58:GLY:CA	2:R:283:TYR:CD2	3.02	0.42
2:R:394:GLN:NE2	1:d:348:PRO:HB2	2.23	0.42
2:S:221:THR:HG22	1:e:324:VAL:HG21	1.98	0.42
2:U:222:PRO:HD2	1:g:326:LYS:HB2	2.02	0.42
2:U:404:PHE:CD1	1:g:261:PRO:CA	3.01	0.42
1:c:58:SER:N	1:d:282:TYR:CB	2.83	0.42
1:i:58:SER:N	1:j:283:HIS:CA	2.73	0.42
1:j:128:GLN:HG2	1:k:290:GLU:HG3	1.69	0.42
1:E:14:VAL:CG1	1:E:78:ILE:HD11	2.49	0.42
2:F:6:HIS:CD2	2:F:21:TRP:HE1	2.37	0.42
2:Q:403:ALA:N	1:c:262:TYR:HE1	2.16	0.42
2:W:60:LYS:CB	2:X:283:TYR:CE2	3.02	0.42
2:Y:403:ALA:N	1:k:262:TYR:HE1	2.16	0.42
1:k:70:LEU:HD23	1:k:114:LEU:CD1	2.36	0.42
2:B:406:HIS:HB3	1:E:263:PRO:CG	2.43	0.42
1:D:30:LEU:CD2	1:D:36:MET:HB2	2.48	0.42
1:H:30:LEU:CD2	1:H:36:MET:HB2	2.48	0.42
1:H:60:LYS:CE	1:I:283:HIS:CD2	2.95	0.42
1:P:64:ARG:HA	1:P:125:MET:HE1	1.89	0.42
2:Q:220:THR:O	1:c:326:LYS:NZ	2.50	0.42
2:S:394:GLN:HB3	1:e:348:PRO:HG2	2.02	0.42
2:T:222:PRO:HD2	1:f:326:LYS:HB2	2.02	0.42
2:T:401:ARG:O	1:f:262:TYR:CE1	2.72	0.42
2:Y:221:THR:HG22	1:k:324:VAL:HG21	1.98	0.42
1:M:30:LEU:CD2	1:M:36:MET:HB2	2.48	0.42
1:M:90:GLU:OE2	1:N:216:ASN:CG	2.63	0.42
2:R:222:PRO:HD2	1:d:326:LYS:HB2	2.02	0.42
2:R:394:GLN:HB3	1:d:348:PRO:HG2	2.02	0.42
2:S:55:GLU:CA	2:T:285:ALA:HB3	2.46	0.42
2:Y:92:PHE:HB2	2:Z:218:LYS:HD2	1.02	0.42
1:d:30:LEU:CD2	1:d:36:MET:HB2	2.48	0.42
1:f:30:LEU:CD2	1:f:36:MET:HB2	2.48	0.42
1:j:56:THR:HG22	1:k:283:HIS:O	2.20	0.42
1:k:30:LEU:CD2	1:k:36:MET:HB2	2.48	0.42
2:B:394:GLN:HB3	1:E:348:PRO:HG2	2.02	0.41
1:L:270:VAL:CG2	1:L:378:LEU:CD2	2.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:394:GLN:HB3	1:i:348:PRO:HG2	2.02	0.41
1:f:62:VAL:HG21	1:g:283:HIS:CB	2.40	0.41
1:G:127:ASP:C	1:H:338:ARG:HE	2.27	0.41
1:I:14:VAL:CG1	1:I:78:ILE:HD11	2.49	0.41
2:V:404:PHE:CD1	1:h:261:PRO:CA	3.01	0.41
2:W:394:GLN:CB	1:i:348:PRO:HG2	2.51	0.41
2:X:224:TYR:HE2	1:j:248:LEU:HD11	1.78	0.41
1:g:14:VAL:CG1	1:g:78:ILE:HD11	2.49	0.41
1:j:270:VAL:CG2	1:j:378:LEU:CD2	2.76	0.41
2:p:56:ALA:HA	2:q:284:ARG:HA	1.53	0.41
1:L:30:LEU:CD2	1:L:36:MET:HB2	2.48	0.41
2:U:224:TYR:CE2	1:g:248:LEU:HG	2.53	0.41
2:U:406:HIS:HB3	1:g:263:PRO:CG	2.43	0.41
2:Y:63:PRO:HD3	2:Z:282:GLN:O	2.16	0.41
2:Y:181:VAL:HG21	1:k:314:ALA:CB	2.50	0.41
1:j:30:LEU:CD2	1:j:36:MET:HB2	2.48	0.41
1:j:123:ARG:CG	1:k:297:GLU:CD	2.89	0.41
1:D:34:GLY:HA3	1:G:283:HIS:CE1	2.55	0.41
1:H:56:THR:HG21	1:I:283:HIS:C	2.45	0.41
2:V:222:PRO:HD2	1:h:326:LYS:HB2	2.02	0.41
2:V:394:GLN:HB3	1:h:348:PRO:HG2	2.02	0.41
2:W:222:PRO:HD2	1:i:326:LYS:HB2	2.02	0.41
2:Y:224:TYR:HE2	1:k:248:LEU:HD11	1.78	0.41
1:e:72:GLN:CD	2:q:1:MET:HE3	2.35	0.41
2:B:224:TYR:CE2	1:E:248:LEU:HG	2.53	0.41
2:B:403:ALA:N	1:E:262:TYR:HE1	2.16	0.41
1:G:72:GLN:CD	2:S:1:MET:HE3	2.35	0.41
1:M:123:ARG:HG3	1:N:297:GLU:OE2	2.21	0.41
2:U:177:VAL:HG13	1:g:329:ASN:CG	2.46	0.41
2:V:406:HIS:HB3	1:h:263:PRO:CG	2.43	0.41
2:X:120:ASP:CG	2:Y:297:ASP:CG	2.89	0.41
2:X:224:TYR:CE2	1:j:248:LEU:HG	2.53	0.41
2:Y:394:GLN:CB	1:k:348:PRO:HG2	2.51	0.41
1:D:62:VAL:O	1:G:283:HIS:HB3	2.12	0.41
1:M:62:VAL:O	1:N:283:HIS:O	2.38	0.41
1:M:91:GLN:HG2	1:N:280:LYS:HG2	2.02	0.41
2:S:404:PHE:CD1	1:e:261:PRO:CA	3.01	0.41
2:V:394:GLN:CB	1:h:348:PRO:HG2	2.50	0.41
2:W:172:VAL:CG2	2:W:173:PRO:HD3	2.34	0.41
2:Y:124:LYS:CG	2:Z:293:GLN:O	2.62	0.41
1:j:54:SER:OG	1:k:285:GLN:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:q:127:GLU:C	2:r:293:GLN:OE1	2.64	0.41
2:V:394:GLN:CG	1:h:348:PRO:HG3	2.47	0.41
2:W:177:VAL:HG13	1:i:329:ASN:CG	2.46	0.41
2:X:394:GLN:CB	1:j:348:PRO:HG2	2.51	0.41
1:e:128:GLN:HB3	1:f:290:GLU:OE1	2.21	0.41
1:A:72:GLN:CD	2:B:1:MET:HE3	2.35	0.41
1:D:89:PRO:HG3	1:G:279:GLU:CD	2.45	0.41
1:E:72:GLN:CD	2:F:1:MET:HE3	2.35	0.41
1:O:58:SER:CB	1:P:282:TYR:CB	2.78	0.41
2:R:60:LYS:CD	2:S:282:GLN:HB2	2.51	0.41
2:T:220:THR:O	1:f:326:LYS:NZ	2.50	0.41
2:T:394:GLN:CB	1:f:348:PRO:HG2	2.51	0.41
2:U:404:PHE:CD2	1:g:261:PRO:N	2.82	0.41
2:V:177:VAL:HG13	1:h:329:ASN:CG	2.46	0.41
2:V:221:THR:CG2	1:h:324:VAL:CG2	2.89	0.41
2:a:56:ALA:CB	2:b:283:TYR:CB	2.87	0.41
1:C:287:SER:CB	1:C:289:PRO:HD2	2.51	0.41
1:H:287:SER:CB	1:H:289:PRO:HD2	2.51	0.41
1:N:62:VAL:CB	1:O:285:GLN:HE22	2.28	0.41
1:N:287:SER:CB	1:N:289:PRO:HD2	2.51	0.41
2:R:394:GLN:CB	1:d:348:PRO:HG2	2.51	0.41
2:U:394:GLN:CB	1:g:348:PRO:HG2	2.51	0.41
1:D:287:SER:CB	1:D:289:PRO:HD2	2.51	0.41
1:J:217:LEU:HD21	1:J:368:VAL:HG22	2.03	0.41
1:K:206:ASN:HD22	1:K:227:LEU:CD2	2.34	0.41
1:N:62:VAL:HG21	1:O:285:GLN:CG	2.46	0.41
1:O:30:LEU:CD2	1:O:36:MET:HB2	2.48	0.41
2:Q:394:GLN:CB	1:c:348:PRO:HG2	2.51	0.41
2:Q:394:GLN:HB3	1:c:348:PRO:HG2	2.02	0.41
2:T:221:THR:HG22	1:f:324:VAL:HG21	1.98	0.41
2:W:21:TRP:CZ3	2:W:63:PRO:HB3	2.56	0.41
2:W:404:PHE:CD1	1:i:261:PRO:CA	3.01	0.41
2:Y:34:GLY:HA2	2:Z:282:GLN:HB3	2.02	0.41
2:Y:125:GLU:CA	2:Z:290:GLU:OE2	2.61	0.41
2:Y:222:PRO:HD2	1:k:326:LYS:HB2	2.02	0.41
1:c:287:SER:CB	1:c:289:PRO:HD2	2.51	0.41
1:d:58:SER:HB2	1:e:282:TYR:N	2.22	0.41
1:d:287:SER:CB	1:d:289:PRO:HD2	2.51	0.41
1:f:287:SER:CB	1:f:289:PRO:HD2	2.51	0.41
1:i:206:ASN:HD22	1:i:227:LEU:CD2	2.34	0.41
2:B:221:THR:CG2	1:E:324:VAL:CG2	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:206:ASN:HD22	1:N:227:LEU:CD2	2.34	0.40
2:S:128:SER:HG	2:T:293:GLN:HB3	1.78	0.40
2:T:394:GLN:CG	1:f:348:PRO:HG3	2.47	0.40
2:X:177:VAL:HG13	1:j:329:ASN:CG	2.46	0.40
2:Y:56:ALA:CB	2:Z:281:GLN:HE21	2.34	0.40
2:Y:394:GLN:HB3	1:k:348:PRO:HG2	2.02	0.40
1:h:217:LEU:HD21	1:h:368:VAL:HG22	2.03	0.40
2:r:56:ALA:CB	2:s:285:ALA:H	2.25	0.40
2:B:100:GLY:HA2	1:E:254:GLU:N	2.37	0.40
1:C:95:GLY:HA3	1:C:114:LEU:HD11	2.03	0.40
1:D:206:ASN:HD22	1:D:227:LEU:CD2	2.34	0.40
1:G:60:LYS:HD3	1:H:284:GLU:HB2	2.01	0.40
1:G:206:ASN:HD22	1:G:227:LEU:CD2	2.34	0.40
1:K:217:LEU:HD21	1:K:368:VAL:HG22	2.03	0.40
2:Q:21:TRP:CZ3	2:Q:63:PRO:HB3	2.57	0.40
2:Q:221:THR:CG2	1:c:324:VAL:CG2	2.89	0.40
2:T:100:GLY:HA2	1:f:254:GLU:N	2.37	0.40
2:X:21:TRP:CZ3	2:X:63:PRO:HB3	2.56	0.40
2:X:222:PRO:HD2	1:j:326:LYS:HB2	2.02	0.40
2:Y:406:HIS:ND1	1:k:263:PRO:N	2.69	0.40
2:Z:21:TRP:CZ3	2:Z:63:PRO:HB3	2.57	0.40
1:c:95:GLY:HA3	1:c:114:LEU:HD11	2.04	0.40
1:e:206:ASN:HD22	1:e:227:LEU:CD2	2.34	0.40
1:i:217:LEU:HD21	1:i:368:VAL:HG22	2.03	0.40
2:o:21:TRP:CZ3	2:o:63:PRO:HB3	2.57	0.40
1:I:217:LEU:HD21	1:I:368:VAL:HG22	2.03	0.40
1:J:287:SER:CB	1:J:289:PRO:HD2	2.51	0.40
1:M:206:ASN:HD22	1:M:227:LEU:CD2	2.34	0.40
1:O:206:ASN:HD22	1:O:227:LEU:CD2	2.34	0.40
2:S:21:TRP:CZ3	2:S:63:PRO:HB3	2.56	0.40
2:S:100:GLY:HA2	1:e:254:GLU:N	2.37	0.40
2:S:394:GLN:CB	1:e:348:PRO:HG2	2.51	0.40
2:U:96:GLN:NE2	1:g:1:MET:SD	2.95	0.40
2:U:406:HIS:ND1	1:g:263:PRO:N	2.69	0.40
2:Y:21:TRP:CZ3	2:Y:63:PRO:HB3	2.56	0.40
2:Y:96:GLN:NE2	1:k:1:MET:SD	2.95	0.40
1:d:206:ASN:HD22	1:d:227:LEU:CD2	2.35	0.40
1:j:62:VAL:HG21	1:k:283:HIS:CA	2.51	0.40
1:j:206:ASN:HD22	1:j:227:LEU:CD2	2.34	0.40
1:k:206:ASN:HD22	1:k:227:LEU:CD2	2.34	0.40
2:p:57:THR:HG21	2:q:281:GLN:CD	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:GLN:NE2	1:E:1:MET:SD	2.95	0.40
2:B:394:GLN:CB	1:E:348:PRO:HG2	2.51	0.40
2:B:406:HIS:ND1	1:E:263:PRO:N	2.69	0.40
1:C:270:VAL:CG2	1:C:378:LEU:CD2	2.75	0.40
1:L:206:ASN:HD22	1:L:227:LEU:CD2	2.34	0.40
1:N:95:GLY:HA3	1:N:114:LEU:HD11	2.03	0.40
1:O:287:SER:CB	1:O:289:PRO:HD2	2.51	0.40
2:R:177:VAL:HG13	1:d:329:ASN:CG	2.46	0.40
2:R:406:HIS:ND1	1:d:263:PRO:N	2.69	0.40
2:S:220:THR:O	1:e:326:LYS:NZ	2.50	0.40
2:T:96:GLN:NE2	1:f:1:MET:SD	2.95	0.40
2:T:177:VAL:HG13	1:f:329:ASN:CG	2.46	0.40
2:U:21:TRP:CZ3	2:U:63:PRO:HB3	2.57	0.40
2:Y:177:VAL:HG13	1:k:329:ASN:CG	2.46	0.40
1:f:206:ASN:HD22	1:f:227:LEU:CD2	2.34	0.40
1:g:217:LEU:HD21	1:g:368:VAL:HG22	2.03	0.40
1:h:287:SER:CB	1:h:289:PRO:HD2	2.51	0.40
2:p:21:TRP:CZ3	2:p:63:PRO:HB3	2.56	0.40
2:q:21:TRP:CZ3	2:q:63:PRO:HB3	2.57	0.40
2:s:21:TRP:CZ3	2:s:63:PRO:HB3	2.57	0.40
1:E:217:LEU:HD21	1:E:368:VAL:HG22	2.03	0.40
1:H:95:GLY:HA3	1:H:114:LEU:HD11	2.03	0.40
1:H:206:ASN:HD22	1:H:227:LEU:CD2	2.34	0.40
1:O:58:SER:N	1:P:282:TYR:O	2.53	0.40
1:P:217:LEU:HD21	1:P:368:VAL:HG22	2.03	0.40
2:R:100:GLY:HA2	1:d:254:GLU:N	2.37	0.40
2:S:224:TYR:CE2	1:e:248:LEU:HG	2.53	0.40
2:T:21:TRP:CZ3	2:T:63:PRO:HB3	2.57	0.40
2:V:181:VAL:HG21	1:h:314:ALA:CB	2.50	0.40
2:Y:62:VAL:O	2:Z:284:ARG:C	2.55	0.40
1:c:270:VAL:CG2	1:c:378:LEU:CD2	2.76	0.40
1:k:287:SER:CB	1:k:289:PRO:HD2	2.51	0.40
2:r:21:TRP:CZ3	2:r:63:PRO:HB3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	A	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	C	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	D	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	E	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	G	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	H	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	I	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	J	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	K	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	L	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	M	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	N	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	O	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	P	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	c	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	d	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	e	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	f	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	g	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	h	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	i	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	j	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	k	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
2	B	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
2	F	424/445 (95%)	414 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Q	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
2	R	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
2	S	424/445 (95%)	415 (98%)	9 (2%)	0	100	100
2	T	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
2	U	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
2	V	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
2	W	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
2	X	424/445 (95%)	415 (98%)	9 (2%)	0	100	100
2	Y	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
2	Z	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
2	a	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
2	b	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
2	o	424/445 (95%)	415 (98%)	9 (2%)	0	100	100
2	p	424/445 (95%)	415 (98%)	9 (2%)	0	100	100
2	q	424/445 (95%)	415 (98%)	9 (2%)	0	100	100
2	r	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
2	s	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
All	All	17854/18805 (95%)	17554 (98%)	300 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	A	366/382 (96%)	364 (100%)	2 (0%)	81	83
1	C	366/382 (96%)	364 (100%)	2 (0%)	81	83
1	D	366/382 (96%)	364 (100%)	2 (0%)	81	83
1	E	366/382 (96%)	364 (100%)	2 (0%)	81	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	366/382 (96%)	364 (100%)	2 (0%)	81	83
1	H	366/382 (96%)	364 (100%)	2 (0%)	81	83
1	I	366/382 (96%)	364 (100%)	2 (0%)	81	83
1	J	366/382 (96%)	364 (100%)	2 (0%)	81	83
1	K	366/382 (96%)	364 (100%)	2 (0%)	81	83
1	L	366/382 (96%)	364 (100%)	2 (0%)	81	83
1	M	366/382 (96%)	364 (100%)	2 (0%)	81	83
1	N	366/382 (96%)	364 (100%)	2 (0%)	81	83
1	O	366/382 (96%)	364 (100%)	2 (0%)	81	83
1	P	366/382 (96%)	364 (100%)	2 (0%)	81	83
1	c	366/382 (96%)	364 (100%)	2 (0%)	81	83
1	d	366/382 (96%)	364 (100%)	2 (0%)	81	83
1	e	366/382 (96%)	364 (100%)	2 (0%)	81	83
1	f	366/382 (96%)	364 (100%)	2 (0%)	81	83
1	g	366/382 (96%)	364 (100%)	2 (0%)	81	83
1	h	366/382 (96%)	364 (100%)	2 (0%)	81	83
1	i	366/382 (96%)	364 (100%)	2 (0%)	81	83
1	j	366/382 (96%)	364 (100%)	2 (0%)	81	83
1	k	366/382 (96%)	364 (100%)	2 (0%)	81	83
2	B	365/379 (96%)	363 (100%)	2 (0%)	81	83
2	F	365/379 (96%)	363 (100%)	2 (0%)	81	83
2	Q	365/379 (96%)	363 (100%)	2 (0%)	81	83
2	R	365/379 (96%)	363 (100%)	2 (0%)	81	83
2	S	365/379 (96%)	363 (100%)	2 (0%)	81	83
2	T	365/379 (96%)	363 (100%)	2 (0%)	81	83
2	U	365/379 (96%)	363 (100%)	2 (0%)	81	83
2	V	365/379 (96%)	363 (100%)	2 (0%)	81	83
2	W	365/379 (96%)	363 (100%)	2 (0%)	81	83
2	X	365/379 (96%)	363 (100%)	2 (0%)	81	83
2	Y	365/379 (96%)	363 (100%)	2 (0%)	81	83
2	Z	365/379 (96%)	363 (100%)	2 (0%)	81	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	a	365/379 (96%)	363 (100%)	2 (0%)	81	83
2	b	365/379 (96%)	363 (100%)	2 (0%)	81	83
2	o	365/379 (96%)	363 (100%)	2 (0%)	81	83
2	p	365/379 (96%)	363 (100%)	2 (0%)	81	83
2	q	365/379 (96%)	363 (100%)	2 (0%)	81	83
2	r	365/379 (96%)	363 (100%)	2 (0%)	81	83
2	s	365/379 (96%)	363 (100%)	2 (0%)	81	83
All	All	15353/15987 (96%)	15269 (100%)	84 (0%)	78	83

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	PHE
1	A	367	ASP
2	B	371	LEU
2	B	415	GLU
1	C	141	PHE
1	C	367	ASP
1	D	141	PHE
1	D	367	ASP
1	E	141	PHE
1	E	367	ASP
2	F	371	LEU
2	F	415	GLU
1	G	141	PHE
1	G	367	ASP
1	H	141	PHE
1	H	367	ASP
1	I	141	PHE
1	I	367	ASP
1	J	141	PHE
1	J	367	ASP
1	K	141	PHE
1	K	367	ASP
1	L	141	PHE
1	L	367	ASP
1	M	141	PHE
1	M	367	ASP
1	N	141	PHE
1	N	367	ASP

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Mol	Chain	Res	Type
1	O	141	PHE
1	O	367	ASP
1	P	141	PHE
1	P	367	ASP
2	Q	371	LEU
2	Q	415	GLU
2	R	371	LEU
2	R	415	GLU
2	S	371	LEU
2	S	415	GLU
2	T	371	LEU
2	T	415	GLU
2	U	371	LEU
2	U	415	GLU
2	V	371	LEU
2	V	415	GLU
2	W	371	LEU
2	W	415	GLU
2	X	371	LEU
2	X	415	GLU
2	Y	371	LEU
2	Y	415	GLU
2	Z	371	LEU
2	Z	415	GLU
2	a	371	LEU
2	a	415	GLU
2	b	371	LEU
2	b	415	GLU
1	c	141	PHE
1	c	367	ASP
1	d	141	PHE
1	d	367	ASP
1	e	141	PHE
1	e	367	ASP
1	f	141	PHE
1	f	367	ASP
1	g	141	PHE
1	g	367	ASP
1	h	141	PHE
1	h	367	ASP
1	i	141	PHE
1	i	367	ASP

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Mol	Chain	Res	Type
1	j	141	PHE
1	j	367	ASP
1	k	141	PHE
1	k	367	ASP
2	o	371	LEU
2	o	415	GLU
2	p	371	LEU
2	p	415	GLU
2	q	371	LEU
2	q	415	GLU
2	r	371	LEU
2	r	415	GLU
2	s	371	LEU
2	s	415	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (330) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	206	ASN
1	A	249	ASN
1	A	293	ASN
1	A	356	ASN
1	A	380	ASN
2	B	136	GLN
2	B	167	ASN
2	B	206	ASN
2	B	300	ASN
2	B	309	HIS
2	B	380	ASN
2	B	385	GLN
2	B	394	GLN
2	B	433	GLN
1	C	101	ASN
1	C	206	ASN
1	C	293	ASN
1	C	301	GLN
1	C	380	ASN
1	D	101	ASN
1	D	206	ASN
1	D	249	ASN
1	D	283	HIS

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Mol	Chain	Res	Type
1	D	293	ASN
1	D	356	ASN
1	E	101	ASN
1	E	206	ASN
1	E	249	ASN
1	E	293	ASN
1	E	356	ASN
1	E	380	ASN
2	F	136	GLN
2	F	167	ASN
2	F	206	ASN
2	F	300	ASN
2	F	309	HIS
2	F	380	ASN
2	F	385	GLN
2	F	433	GLN
1	G	61	HIS
1	G	88	HIS
1	G	101	ASN
1	G	128	GLN
1	G	206	ASN
1	G	249	ASN
1	G	293	ASN
1	G	356	ASN
1	G	380	ASN
1	H	101	ASN
1	H	206	ASN
1	H	249	ASN
1	H	285	GLN
1	H	293	ASN
1	H	301	GLN
1	H	356	ASN
1	H	380	ASN
1	I	101	ASN
1	I	206	ASN
1	I	249	ASN
1	I	293	ASN
1	I	356	ASN
1	J	101	ASN
1	J	206	ASN
1	J	249	ASN
1	J	293	ASN

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Mol	Chain	Res	Type
1	J	356	ASN
1	J	380	ASN
1	K	101	ASN
1	K	206	ASN
1	K	249	ASN
1	K	293	ASN
1	K	356	ASN
1	L	101	ASN
1	L	206	ASN
1	L	249	ASN
1	L	283	HIS
1	L	293	ASN
1	L	356	ASN
1	M	91	GLN
1	M	101	ASN
1	M	206	ASN
1	M	249	ASN
1	M	283	HIS
1	M	293	ASN
1	M	356	ASN
1	N	101	ASN
1	N	206	ASN
1	N	249	ASN
1	N	283	HIS
1	N	293	ASN
1	N	356	ASN
1	O	101	ASN
1	O	206	ASN
1	O	249	ASN
1	O	283	HIS
1	O	285	GLN
1	O	293	ASN
1	O	356	ASN
1	P	101	ASN
1	P	206	ASN
1	P	249	ASN
1	P	293	ASN
1	P	356	ASN
1	P	380	ASN
2	Q	8	GLN
2	Q	14	ASN
2	Q	136	GLN

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Mol	Chain	Res	Type
2	Q	167	ASN
2	Q	206	ASN
2	Q	300	ASN
2	Q	309	HIS
2	Q	380	ASN
2	Q	385	GLN
2	Q	394	GLN
2	Q	433	GLN
2	R	8	GLN
2	R	14	ASN
2	R	136	GLN
2	R	167	ASN
2	R	206	ASN
2	R	300	ASN
2	R	309	HIS
2	R	380	ASN
2	R	385	GLN
2	R	394	GLN
2	R	433	GLN
2	S	8	GLN
2	S	14	ASN
2	S	136	GLN
2	S	167	ASN
2	S	206	ASN
2	S	293	GLN
2	S	300	ASN
2	S	380	ASN
2	S	385	GLN
2	S	394	GLN
2	T	8	GLN
2	T	14	ASN
2	T	136	GLN
2	T	167	ASN
2	T	206	ASN
2	T	281	GLN
2	T	300	ASN
2	T	309	HIS
2	T	339	ASN
2	T	380	ASN
2	T	385	GLN
2	T	394	GLN
2	T	433	GLN

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Mol	Chain	Res	Type
2	U	8	GLN
2	U	14	ASN
2	U	136	GLN
2	U	167	ASN
2	U	206	ASN
2	U	300	ASN
2	U	380	ASN
2	U	385	GLN
2	U	394	GLN
2	U	433	GLN
2	V	8	GLN
2	V	14	ASN
2	V	136	GLN
2	V	167	ASN
2	V	206	ASN
2	V	300	ASN
2	V	309	HIS
2	V	380	ASN
2	V	385	GLN
2	V	394	GLN
2	V	433	GLN
2	W	8	GLN
2	W	14	ASN
2	W	136	GLN
2	W	167	ASN
2	W	206	ASN
2	W	300	ASN
2	W	309	HIS
2	W	380	ASN
2	W	385	GLN
2	W	394	GLN
2	W	433	GLN
2	X	136	GLN
2	X	167	ASN
2	X	206	ASN
2	X	300	ASN
2	X	309	HIS
2	X	380	ASN
2	X	385	GLN
2	X	394	GLN
2	X	433	GLN
2	Y	8	GLN

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Mol	Chain	Res	Type
2	Y	14	ASN
2	Y	54	ASN
2	Y	136	GLN
2	Y	167	ASN
2	Y	206	ASN
2	Y	300	ASN
2	Y	380	ASN
2	Y	385	GLN
2	Y	394	GLN
2	Y	433	GLN
2	Z	85	GLN
2	Z	136	GLN
2	Z	167	ASN
2	Z	206	ASN
2	Z	281	GLN
2	Z	300	ASN
2	Z	309	HIS
2	Z	380	ASN
2	Z	385	GLN
2	Z	433	GLN
2	a	136	GLN
2	a	167	ASN
2	a	206	ASN
2	a	300	ASN
2	a	380	ASN
2	a	385	GLN
2	a	433	GLN
2	b	8	GLN
2	b	14	ASN
2	b	136	GLN
2	b	167	ASN
2	b	206	ASN
2	b	300	ASN
2	b	380	ASN
2	b	385	GLN
1	c	101	ASN
1	c	206	ASN
1	c	293	ASN
1	c	301	GLN
1	c	380	ASN
1	d	101	ASN
1	d	206	ASN

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Mol	Chain	Res	Type
1	d	249	ASN
1	d	293	ASN
1	d	356	ASN
1	e	101	ASN
1	e	128	GLN
1	e	206	ASN
1	e	249	ASN
1	e	293	ASN
1	e	356	ASN
1	e	380	ASN
1	f	101	ASN
1	f	206	ASN
1	f	249	ASN
1	f	285	GLN
1	f	301	GLN
1	f	356	ASN
1	g	101	ASN
1	g	206	ASN
1	g	249	ASN
1	g	293	ASN
1	g	356	ASN
1	h	11	GLN
1	h	15	GLN
1	h	206	ASN
1	h	249	ASN
1	h	293	ASN
1	h	356	ASN
1	i	11	GLN
1	i	15	GLN
1	i	206	ASN
1	i	249	ASN
1	i	293	ASN
1	i	356	ASN
1	j	11	GLN
1	j	15	GLN
1	j	88	HIS
1	j	128	GLN
1	j	206	ASN
1	j	249	ASN
1	j	293	ASN
1	j	356	ASN
1	k	11	GLN

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Mol	Chain	Res	Type
1	k	15	GLN
1	k	101	ASN
1	k	206	ASN
1	k	249	ASN
1	k	285	GLN
1	k	293	ASN
1	k	356	ASN
2	o	8	GLN
2	o	14	ASN
2	o	136	GLN
2	o	167	ASN
2	o	206	ASN
2	o	300	ASN
2	o	309	HIS
2	o	380	ASN
2	o	385	GLN
2	o	433	GLN
2	p	8	GLN
2	p	14	ASN
2	p	136	GLN
2	p	167	ASN
2	p	206	ASN
2	p	300	ASN
2	p	309	HIS
2	p	380	ASN
2	p	385	GLN
2	p	433	GLN
2	q	8	GLN
2	q	14	ASN
2	q	136	GLN
2	q	167	ASN
2	q	206	ASN
2	q	300	ASN
2	q	380	ASN
2	q	385	GLN
2	r	8	GLN
2	r	14	ASN
2	r	136	GLN
2	r	167	ASN
2	r	206	ASN
2	r	300	ASN
2	r	309	HIS

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Mol	Chain	Res	Type
2	r	380	ASN
2	r	385	GLN
2	r	433	GLN
2	s	8	GLN
2	s	14	ASN
2	s	136	GLN
2	s	167	ASN
2	s	206	ASN
2	s	300	ASN
2	s	380	ASN
2	s	385	GLN
2	s	433	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 84 ligands modelled in this entry, 23 are monoatomic - leaving 61 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	$\# Z > 2$
5	GDP	U	502	-	29,30,30	0.68	0	45,47,47	0.99	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GTP	K	501	4	33,34,34	0.91	2 (6%)	50,54,54	1.40	8 (16%)
5	GDP	b	501	-	29,30,30	0.69	0	45,47,47	0.99	1 (2%)
6	TA1	B	502	-	68,68,68	0.86	0	105,105,105	0.77	2 (1%)
3	GTP	G	501	4	33,34,34	0.91	2 (6%)	50,54,54	1.40	8 (16%)
6	TA1	X	502	-	68,68,68	0.87	0	105,105,105	0.77	2 (1%)
6	TA1	a	502	-	68,68,68	0.86	0	105,105,105	0.77	2 (1%)
3	GTP	L	501	4	33,34,34	0.90	2 (6%)	50,54,54	1.40	8 (16%)
6	TA1	q	502	-	68,68,68	0.86	0	105,105,105	0.77	2 (1%)
3	GTP	h	501	4	33,34,34	0.91	2 (6%)	50,54,54	1.40	8 (16%)
3	GTP	J	501	4	33,34,34	0.91	2 (6%)	50,54,54	1.40	8 (16%)
3	GTP	d	501	4	33,34,34	0.91	2 (6%)	50,54,54	1.40	8 (16%)
3	GTP	C	501	4	33,34,34	0.91	2 (6%)	50,54,54	1.40	8 (16%)
6	TA1	T	502	-	68,68,68	0.86	0	105,105,105	0.77	2 (1%)
3	GTP	I	501	4	33,34,34	0.90	2 (6%)	50,54,54	1.40	8 (16%)
6	TA1	s	502	-	68,68,68	0.86	0	105,105,105	0.77	2 (1%)
5	GDP	B	501	-	29,30,30	0.68	0	45,47,47	0.99	1 (2%)
6	TA1	r	502	-	68,68,68	0.86	0	105,105,105	0.77	2 (1%)
3	GTP	D	501	4	33,34,34	0.90	2 (6%)	50,54,54	1.40	8 (16%)
6	TA1	V	502	-	68,68,68	0.86	0	105,105,105	0.77	2 (1%)
5	GDP	Y	501	-	29,30,30	0.68	0	45,47,47	0.99	1 (2%)
5	GDP	R	501	-	29,30,30	0.68	0	45,47,47	0.99	1 (2%)
6	TA1	p	502	-	68,68,68	0.86	0	105,105,105	0.77	2 (1%)
6	TA1	F	501	-	68,68,68	0.86	0	105,105,105	0.77	2 (1%)
6	TA1	S	502	-	68,68,68	0.86	0	105,105,105	0.77	2 (1%)
3	GTP	A	501	4	33,34,34	0.91	2 (6%)	50,54,54	1.40	8 (16%)
3	GTP	c	501	4	33,34,34	0.91	2 (6%)	50,54,54	1.40	8 (16%)
5	GDP	V	501	-	29,30,30	0.68	0	45,47,47	0.99	1 (2%)
3	GTP	E	501	4	33,34,34	0.91	2 (6%)	50,54,54	1.40	8 (16%)
5	GDP	p	501	-	29,30,30	0.68	0	45,47,47	0.99	1 (2%)
3	GTP	g	501	4	33,34,34	0.91	2 (6%)	50,54,54	1.40	8 (16%)
5	GDP	Z	501	-	29,30,30	0.68	0	45,47,47	0.99	1 (2%)
6	TA1	Y	502	-	68,68,68	0.86	0	105,105,105	0.77	2 (1%)
3	GTP	e	501	4	33,34,34	0.90	2 (6%)	50,54,54	1.40	8 (16%)
3	GTP	N	501	4	33,34,34	0.90	2 (6%)	50,54,54	1.40	8 (16%)
3	GTP	H	501	4	33,34,34	0.91	2 (6%)	50,54,54	1.40	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GDP	o	501	-	29,30,30	0.68	0	45,47,47	0.99	1 (2%)
5	GDP	S	501	-	29,30,30	0.68	0	45,47,47	0.99	1 (2%)
3	GTP	k	501	4	33,34,34	0.90	2 (6%)	50,54,54	1.40	8 (16%)
6	TA1	Q	502	-	68,68,68	0.86	0	105,105,105	0.77	2 (1%)
5	GDP	s	501	-	29,30,30	0.69	0	45,47,47	0.99	1 (2%)
3	GTP	f	501	4	33,34,34	0.91	2 (6%)	50,54,54	1.41	8 (16%)
5	GDP	X	501	-	29,30,30	0.69	0	45,47,47	0.99	1 (2%)
3	GTP	j	501	4	33,34,34	0.91	2 (6%)	50,54,54	1.40	8 (16%)
5	GDP	r	501	-	29,30,30	0.69	0	45,47,47	0.99	1 (2%)
6	TA1	W	502	-	68,68,68	0.86	0	105,105,105	0.77	2 (1%)
3	GTP	O	501	4	33,34,34	0.90	2 (6%)	50,54,54	1.40	8 (16%)
5	GDP	T	501	-	29,30,30	0.68	0	45,47,47	0.99	1 (2%)
6	TA1	U	501	-	68,68,68	0.86	0	105,105,105	0.77	2 (1%)
6	TA1	Z	502	-	68,68,68	0.86	0	105,105,105	0.77	2 (1%)
6	TA1	o	502	-	68,68,68	0.86	0	105,105,105	0.77	2 (1%)
6	TA1	b	502	-	68,68,68	0.86	0	105,105,105	0.77	2 (1%)
5	GDP	F	502	-	29,30,30	0.69	0	45,47,47	0.99	1 (2%)
5	GDP	a	501	-	29,30,30	0.69	0	45,47,47	0.99	1 (2%)
5	GDP	W	501	-	29,30,30	0.69	0	45,47,47	0.99	1 (2%)
5	GDP	q	501	-	29,30,30	0.68	0	45,47,47	0.99	1 (2%)
3	GTP	M	501	4	33,34,34	0.90	2 (6%)	50,54,54	1.40	8 (16%)
3	GTP	i	501	4	33,34,34	0.90	2 (6%)	50,54,54	1.40	8 (16%)
6	TA1	R	502	-	68,68,68	0.86	0	105,105,105	0.77	2 (1%)
3	GTP	P	501	4	33,34,34	0.90	2 (6%)	50,54,54	1.40	8 (16%)
5	GDP	Q	501	-	29,30,30	0.68	0	45,47,47	0.99	1 (2%)

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
5	GDP	U	502	-	-	2/16/32/32	0/3/3/3
3	GTP	K	501	4	-	2/22/38/38	0/3/3/3
5	GDP	b	501	-	-	2/16/32/32	0/3/3/3
6	TA1	B	502	-	-	1/41/127/127	0/7/7/7

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	G	501	4	-	2/22/38/38	0/3/3/3
6	TA1	X	502	-	-	1/41/127/127	0/7/7/7
6	TA1	a	502	-	-	2/41/127/127	0/7/7/7
3	GTP	L	501	4	-	2/22/38/38	0/3/3/3
6	TA1	q	502	-	-	1/41/127/127	0/7/7/7
3	GTP	h	501	4	-	2/22/38/38	0/3/3/3
3	GTP	J	501	4	-	2/22/38/38	0/3/3/3
3	GTP	d	501	4	-	2/22/38/38	0/3/3/3
3	GTP	C	501	4	-	2/22/38/38	0/3/3/3
6	TA1	T	502	-	-	1/41/127/127	0/7/7/7
3	GTP	I	501	4	-	2/22/38/38	0/3/3/3
6	TA1	s	502	-	-	1/41/127/127	0/7/7/7
5	GDP	B	501	-	-	2/16/32/32	0/3/3/3
6	TA1	r	502	-	-	1/41/127/127	0/7/7/7
3	GTP	D	501	4	-	2/22/38/38	0/3/3/3
6	TA1	V	502	-	-	1/41/127/127	0/7/7/7
5	GDP	Y	501	-	-	2/16/32/32	0/3/3/3
5	GDP	R	501	-	-	2/16/32/32	0/3/3/3
6	TA1	p	502	-	-	2/41/127/127	0/7/7/7
6	TA1	F	501	-	-	1/41/127/127	0/7/7/7
6	TA1	S	502	-	-	2/41/127/127	0/7/7/7
3	GTP	A	501	4	-	2/22/38/38	0/3/3/3
3	GTP	c	501	4	-	2/22/38/38	0/3/3/3
5	GDP	V	501	-	-	2/16/32/32	0/3/3/3
3	GTP	E	501	4	-	2/22/38/38	0/3/3/3
5	GDP	p	501	-	-	2/16/32/32	0/3/3/3
3	GTP	g	501	4	-	2/22/38/38	0/3/3/3
5	GDP	Z	501	-	-	2/16/32/32	0/3/3/3
6	TA1	Y	502	-	-	2/41/127/127	0/7/7/7
3	GTP	e	501	4	-	2/22/38/38	0/3/3/3
3	GTP	N	501	4	-	2/22/38/38	0/3/3/3
3	GTP	H	501	4	-	2/22/38/38	0/3/3/3
5	GDP	o	501	-	-	2/16/32/32	0/3/3/3
5	GDP	S	501	-	-	2/16/32/32	0/3/3/3
3	GTP	k	501	4	-	2/22/38/38	0/3/3/3
6	TA1	Q	502	-	-	1/41/127/127	0/7/7/7

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GDP	s	501	-	-	2/16/32/32	0/3/3/3
3	GTP	f	501	4	-	2/22/38/38	0/3/3/3
5	GDP	X	501	-	-	2/16/32/32	0/3/3/3
3	GTP	j	501	4	-	2/22/38/38	0/3/3/3
5	GDP	r	501	-	-	2/16/32/32	0/3/3/3
6	TA1	W	502	-	-	1/41/127/127	0/7/7/7
3	GTP	O	501	4	-	2/22/38/38	0/3/3/3
5	GDP	T	501	-	-	2/16/32/32	0/3/3/3
6	TA1	U	501	-	-	1/41/127/127	0/7/7/7
6	TA1	Z	502	-	-	1/41/127/127	0/7/7/7
6	TA1	o	502	-	-	1/41/127/127	0/7/7/7
6	TA1	b	502	-	-	1/41/127/127	0/7/7/7
5	GDP	F	502	-	-	2/16/32/32	0/3/3/3
5	GDP	a	501	-	-	2/16/32/32	0/3/3/3
5	GDP	W	501	-	-	2/16/32/32	0/3/3/3
5	GDP	q	501	-	-	2/16/32/32	0/3/3/3
3	GTP	M	501	4	-	2/22/38/38	0/3/3/3
3	GTP	i	501	4	-	2/22/38/38	0/3/3/3
6	TA1	R	502	-	-	1/41/127/127	0/7/7/7
3	GTP	P	501	4	-	2/22/38/38	0/3/3/3
5	GDP	Q	501	-	-	2/16/32/32	0/3/3/3

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	501	GTP	C6-N1	-2.53	1.34	1.38
3	N	501	GTP	C6-N1	-2.52	1.34	1.38
3	e	501	GTP	C6-N1	-2.52	1.34	1.38
3	E	501	GTP	C6-N1	-2.50	1.34	1.38
3	j	501	GTP	C6-N1	-2.50	1.34	1.38
3	G	501	GTP	C6-N1	-2.50	1.34	1.38
3	P	501	GTP	C6-N1	-2.50	1.34	1.38
3	h	501	GTP	C6-N1	-2.50	1.34	1.38
3	C	501	GTP	C6-N1	-2.49	1.34	1.38
3	J	501	GTP	C6-N1	-2.49	1.34	1.38
3	f	501	GTP	C6-N1	-2.49	1.34	1.38
3	L	501	GTP	C6-N1	-2.49	1.34	1.38
3	D	501	GTP	C6-N1	-2.49	1.34	1.38
3	A	501	GTP	C6-N1	-2.48	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	501	GTP	C6-N1	-2.48	1.34	1.38
3	M	501	GTP	C6-N1	-2.48	1.34	1.38
3	g	501	GTP	C6-N1	-2.48	1.34	1.38
3	H	501	GTP	C6-N1	-2.48	1.34	1.38
3	d	501	GTP	C6-N1	-2.48	1.34	1.38
3	I	501	GTP	C6-N1	-2.47	1.34	1.38
3	k	501	GTP	C6-N1	-2.47	1.34	1.38
3	i	501	GTP	C6-N1	-2.44	1.34	1.38
3	O	501	GTP	C6-N1	-2.44	1.34	1.38
3	E	501	GTP	C4-N3	2.37	1.39	1.34
3	I	501	GTP	C4-N3	2.37	1.39	1.34
3	g	501	GTP	C4-N3	2.36	1.39	1.34
3	O	501	GTP	C4-N3	2.36	1.39	1.34
3	h	501	GTP	C4-N3	2.36	1.39	1.34
3	j	501	GTP	C4-N3	2.36	1.39	1.34
3	K	501	GTP	C4-N3	2.35	1.39	1.34
3	c	501	GTP	C4-N3	2.35	1.39	1.34
3	H	501	GTP	C4-N3	2.35	1.39	1.34
3	f	501	GTP	C4-N3	2.35	1.39	1.34
3	A	501	GTP	C4-N3	2.35	1.39	1.34
3	M	501	GTP	C4-N3	2.35	1.39	1.34
3	e	501	GTP	C4-N3	2.34	1.39	1.34
3	d	501	GTP	C4-N3	2.34	1.39	1.34
3	P	501	GTP	C4-N3	2.33	1.39	1.34
3	k	501	GTP	C4-N3	2.33	1.39	1.34
3	i	501	GTP	C4-N3	2.33	1.39	1.34
3	J	501	GTP	C4-N3	2.33	1.39	1.34
3	N	501	GTP	C4-N3	2.33	1.39	1.34
3	D	501	GTP	C4-N3	2.33	1.39	1.34
3	C	501	GTP	C4-N3	2.32	1.39	1.34
3	L	501	GTP	C4-N3	2.32	1.39	1.34
3	G	501	GTP	C4-N3	2.32	1.39	1.34

All (241) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	501	GTP	O2B-PB-O3B	4.16	118.52	107.27
3	M	501	GTP	O2B-PB-O3B	4.16	118.51	107.27
3	N	501	GTP	O2B-PB-O3B	4.16	118.50	107.27
3	k	501	GTP	O2B-PB-O3B	4.16	118.50	107.27
3	d	501	GTP	O2B-PB-O3B	4.15	118.50	107.27
3	h	501	GTP	O2B-PB-O3B	4.15	118.50	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	501	GTP	O2B-PB-O3B	4.15	118.50	107.27
3	E	501	GTP	O2B-PB-O3B	4.15	118.49	107.27
3	K	501	GTP	O2B-PB-O3B	4.15	118.49	107.27
3	i	501	GTP	O2B-PB-O3B	4.15	118.49	107.27
3	H	501	GTP	O2B-PB-O3B	4.15	118.48	107.27
3	f	501	GTP	O2B-PB-O3B	4.15	118.48	107.27
3	g	501	GTP	O2B-PB-O3B	4.15	118.48	107.27
3	A	501	GTP	O2B-PB-O3B	4.15	118.48	107.27
3	e	501	GTP	O2B-PB-O3B	4.15	118.48	107.27
3	G	501	GTP	O2B-PB-O3B	4.14	118.47	107.27
3	j	501	GTP	O2B-PB-O3B	4.14	118.46	107.27
3	P	501	GTP	O2B-PB-O3B	4.14	118.46	107.27
3	J	501	GTP	O2B-PB-O3B	4.14	118.45	107.27
3	D	501	GTP	O2B-PB-O3B	4.13	118.44	107.27
3	I	501	GTP	O2B-PB-O3B	4.13	118.44	107.27
3	O	501	GTP	O2B-PB-O3B	4.13	118.44	107.27
3	C	501	GTP	O2B-PB-O3B	4.13	118.44	107.27
3	f	501	GTP	C5-C4-N3	-3.61	122.64	128.39
3	e	501	GTP	C5-C4-N3	-3.59	122.67	128.39
3	J	501	GTP	C5-C4-N3	-3.59	122.68	128.39
3	I	501	GTP	C5-C4-N3	-3.58	122.69	128.39
3	c	501	GTP	C5-C4-N3	-3.58	122.69	128.39
3	j	501	GTP	C5-C4-N3	-3.58	122.69	128.39
3	L	501	GTP	C5-C4-N3	-3.58	122.69	128.39
3	h	501	GTP	C5-C4-N3	-3.58	122.69	128.39
3	O	501	GTP	C5-C4-N3	-3.57	122.70	128.39
3	i	501	GTP	C5-C4-N3	-3.57	122.70	128.39
3	P	501	GTP	C5-C4-N3	-3.57	122.70	128.39
3	G	501	GTP	C5-C4-N3	-3.57	122.71	128.39
3	M	501	GTP	C5-C4-N3	-3.57	122.71	128.39
3	K	501	GTP	C5-C4-N3	-3.57	122.71	128.39
3	A	501	GTP	C5-C4-N3	-3.56	122.72	128.39
3	g	501	GTP	C5-C4-N3	-3.56	122.72	128.39
3	k	501	GTP	C5-C4-N3	-3.56	122.72	128.39
3	D	501	GTP	C5-C4-N3	-3.56	122.73	128.39
3	N	501	GTP	C5-C4-N3	-3.56	122.73	128.39
3	H	501	GTP	C5-C4-N3	-3.55	122.73	128.39
3	E	501	GTP	C5-C4-N3	-3.55	122.74	128.39
3	d	501	GTP	C5-C4-N3	-3.54	122.75	128.39
3	C	501	GTP	C5-C4-N3	-3.54	122.75	128.39
3	D	501	GTP	O2G-PG-O3B	2.91	114.39	104.64
3	O	501	GTP	O2G-PG-O3B	2.90	114.38	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	501	GTP	O2G-PG-O3B	2.90	114.37	104.64
3	c	501	GTP	O2G-PG-O3B	2.90	114.36	104.64
3	I	501	GTP	O2G-PG-O3B	2.90	114.36	104.64
3	L	501	GTP	O2G-PG-O3B	2.90	114.36	104.64
3	j	501	GTP	O2G-PG-O3B	2.90	114.36	104.64
3	H	501	GTP	O2G-PG-O3B	2.90	114.36	104.64
3	K	501	GTP	O2G-PG-O3B	2.90	114.36	104.64
3	f	501	GTP	O2G-PG-O3B	2.90	114.35	104.64
3	C	501	GTP	O2G-PG-O3B	2.90	114.35	104.64
3	A	501	GTP	O2G-PG-O3B	2.90	114.35	104.64
3	k	501	GTP	O2G-PG-O3B	2.90	114.35	104.64
3	d	501	GTP	O2G-PG-O3B	2.89	114.33	104.64
3	N	501	GTP	O2G-PG-O3B	2.89	114.33	104.64
3	E	501	GTP	O2G-PG-O3B	2.89	114.33	104.64
3	h	501	GTP	O2G-PG-O3B	2.89	114.33	104.64
3	g	501	GTP	O2G-PG-O3B	2.89	114.33	104.64
3	P	501	GTP	O2G-PG-O3B	2.89	114.32	104.64
3	e	501	GTP	O2G-PG-O3B	2.89	114.32	104.64
3	i	501	GTP	O2G-PG-O3B	2.89	114.32	104.64
3	M	501	GTP	O2G-PG-O3B	2.88	114.31	104.64
3	J	501	GTP	O3A-PA-O1A	2.88	119.37	110.70
3	k	501	GTP	O3A-PA-O1A	2.88	119.37	110.70
3	j	501	GTP	O3A-PA-O1A	2.88	119.37	110.70
3	J	501	GTP	O2G-PG-O3B	2.88	114.29	104.64
3	i	501	GTP	O3A-PA-O1A	2.88	119.37	110.70
3	K	501	GTP	O3A-PA-O1A	2.88	119.36	110.70
3	G	501	GTP	O3A-PA-O1A	2.88	119.36	110.70
3	C	501	GTP	O3A-PA-O1A	2.88	119.36	110.70
3	d	501	GTP	O3A-PA-O1A	2.88	119.36	110.70
3	L	501	GTP	O3A-PA-O1A	2.88	119.35	110.70
3	P	501	GTP	O3A-PA-O1A	2.87	119.35	110.70
3	H	501	GTP	O3A-PA-O1A	2.87	119.34	110.70
3	h	501	GTP	O3A-PA-O1A	2.87	119.34	110.70
3	M	501	GTP	O3A-PA-O1A	2.87	119.34	110.70
3	A	501	GTP	O3A-PA-O1A	2.87	119.34	110.70
3	f	501	GTP	O3A-PA-O1A	2.87	119.33	110.70
3	g	501	GTP	O3A-PA-O1A	2.87	119.33	110.70
3	E	501	GTP	O3A-PA-O1A	2.87	119.33	110.70
3	c	501	GTP	O3A-PA-O1A	2.87	119.33	110.70
3	N	501	GTP	O3A-PA-O1A	2.87	119.32	110.70
3	O	501	GTP	O3A-PA-O1A	2.86	119.32	110.70
3	I	501	GTP	O3A-PA-O1A	2.86	119.31	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	e	501	GTP	O3A-PA-O1A	2.86	119.31	110.70
3	D	501	GTP	O3A-PA-O1A	2.86	119.31	110.70
5	V	501	GDP	O4'-C1'-N9	2.75	114.59	108.36
5	r	501	GDP	O4'-C1'-N9	2.75	114.59	108.36
5	R	501	GDP	O4'-C1'-N9	2.75	114.58	108.36
5	T	501	GDP	O4'-C1'-N9	2.75	114.58	108.36
5	Q	501	GDP	O4'-C1'-N9	2.74	114.57	108.36
5	U	502	GDP	O4'-C1'-N9	2.74	114.56	108.36
5	b	501	GDP	O4'-C1'-N9	2.74	114.56	108.36
5	W	501	GDP	O4'-C1'-N9	2.73	114.55	108.36
5	a	501	GDP	O4'-C1'-N9	2.73	114.55	108.36
5	B	501	GDP	O4'-C1'-N9	2.73	114.55	108.36
5	q	501	GDP	O4'-C1'-N9	2.73	114.54	108.36
5	o	501	GDP	O4'-C1'-N9	2.73	114.54	108.36
5	s	501	GDP	O4'-C1'-N9	2.73	114.54	108.36
5	Z	501	GDP	O4'-C1'-N9	2.72	114.53	108.36
5	Y	501	GDP	O4'-C1'-N9	2.72	114.53	108.36
5	X	501	GDP	O4'-C1'-N9	2.72	114.53	108.36
5	p	501	GDP	O4'-C1'-N9	2.72	114.53	108.36
5	S	501	GDP	O4'-C1'-N9	2.72	114.52	108.36
5	F	502	GDP	O4'-C1'-N9	2.71	114.51	108.36
6	a	502	TA1	C02-O02-C03	2.69	122.71	117.80
6	F	501	TA1	C02-O02-C03	2.68	122.70	117.80
6	R	502	TA1	C02-O02-C03	2.68	122.70	117.80
6	S	502	TA1	C02-O02-C03	2.68	122.69	117.80
6	V	502	TA1	C02-O02-C03	2.68	122.69	117.80
6	b	502	TA1	C02-O02-C03	2.67	122.69	117.80
6	Y	502	TA1	C02-O02-C03	2.67	122.69	117.80
6	r	502	TA1	C02-O02-C03	2.67	122.68	117.80
6	B	502	TA1	C02-O02-C03	2.67	122.68	117.80
6	T	502	TA1	C02-O02-C03	2.67	122.68	117.80
6	p	502	TA1	C02-O02-C03	2.66	122.66	117.80
6	X	502	TA1	C02-O02-C03	2.66	122.66	117.80
6	Z	502	TA1	C02-O02-C03	2.66	122.66	117.80
6	o	502	TA1	C02-O02-C03	2.66	122.66	117.80
6	W	502	TA1	C02-O02-C03	2.65	122.65	117.80
6	q	502	TA1	C02-O02-C03	2.65	122.65	117.80
6	Q	502	TA1	C02-O02-C03	2.65	122.65	117.80
6	U	501	TA1	C02-O02-C03	2.65	122.64	117.80
6	s	502	TA1	C02-O02-C03	2.64	122.63	117.80
3	H	501	GTP	O4'-C1'-C2'	-2.57	101.11	106.62
3	J	501	GTP	O4'-C1'-C2'	-2.57	101.11	106.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	501	GTP	O4'-C1'-C2'	-2.57	101.11	106.62
3	O	501	GTP	O4'-C1'-C2'	-2.57	101.11	106.62
3	P	501	GTP	O4'-C1'-C2'	-2.57	101.12	106.62
3	G	501	GTP	O4'-C1'-C2'	-2.57	101.12	106.62
3	N	501	GTP	O4'-C1'-C2'	-2.57	101.12	106.62
3	i	501	GTP	O4'-C1'-C2'	-2.57	101.12	106.62
3	C	501	GTP	O4'-C1'-C2'	-2.56	101.13	106.62
3	K	501	GTP	O4'-C1'-C2'	-2.56	101.13	106.62
3	h	501	GTP	O4'-C1'-C2'	-2.56	101.13	106.62
3	e	501	GTP	O4'-C1'-C2'	-2.56	101.13	106.62
3	A	501	GTP	O4'-C1'-C2'	-2.56	101.14	106.62
3	g	501	GTP	O4'-C1'-C2'	-2.56	101.14	106.62
3	M	501	GTP	O4'-C1'-C2'	-2.56	101.14	106.62
3	f	501	GTP	O4'-C1'-C2'	-2.56	101.14	106.62
3	d	501	GTP	O4'-C1'-C2'	-2.56	101.14	106.62
3	c	501	GTP	O4'-C1'-C2'	-2.56	101.15	106.62
3	I	501	GTP	O4'-C1'-C2'	-2.55	101.15	106.62
3	k	501	GTP	O4'-C1'-C2'	-2.55	101.16	106.62
3	L	501	GTP	O4'-C1'-C2'	-2.55	101.16	106.62
3	j	501	GTP	O4'-C1'-C2'	-2.54	101.18	106.62
3	D	501	GTP	O4'-C1'-C2'	-2.54	101.18	106.62
3	h	501	GTP	O2A-PA-O3A	2.37	113.68	107.27
3	g	501	GTP	O2A-PA-O3A	2.37	113.67	107.27
3	C	501	GTP	O2A-PA-O3A	2.37	113.67	107.27
3	j	501	GTP	O2A-PA-O3A	2.37	113.67	107.27
3	O	501	GTP	O2A-PA-O3A	2.37	113.67	107.27
3	J	501	GTP	O2A-PA-O3A	2.36	113.66	107.27
3	k	501	GTP	O2A-PA-O3A	2.36	113.66	107.27
3	H	501	GTP	O2A-PA-O3A	2.36	113.66	107.27
3	c	501	GTP	O2A-PA-O3A	2.36	113.66	107.27
3	L	501	GTP	O2A-PA-O3A	2.36	113.66	107.27
3	P	501	GTP	O2A-PA-O3A	2.36	113.66	107.27
3	D	501	GTP	O2B-PB-O3A	2.36	113.65	107.27
3	G	501	GTP	O2A-PA-O3A	2.36	113.65	107.27
3	D	501	GTP	O2A-PA-O3A	2.36	113.65	107.27
3	e	501	GTP	O2A-PA-O3A	2.36	113.65	107.27
3	P	501	GTP	O2B-PB-O3A	2.36	113.65	107.27
3	A	501	GTP	O2A-PA-O3A	2.36	113.64	107.27
3	f	501	GTP	O2A-PA-O3A	2.36	113.64	107.27
3	h	501	GTP	O2B-PB-O3A	2.36	113.64	107.27
3	N	501	GTP	O2A-PA-O3A	2.35	113.63	107.27
3	E	501	GTP	O2A-PA-O3A	2.35	113.63	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	i	501	GTP	O2B-PB-O3A	2.35	113.63	107.27
3	c	501	GTP	O2B-PB-O3A	2.35	113.63	107.27
3	H	501	GTP	O2B-PB-O3A	2.35	113.62	107.27
3	I	501	GTP	O2B-PB-O3A	2.35	113.62	107.27
3	M	501	GTP	O2A-PA-O3A	2.35	113.62	107.27
3	E	501	GTP	O2B-PB-O3A	2.35	113.62	107.27
3	j	501	GTP	O2B-PB-O3A	2.35	113.62	107.27
3	C	501	GTP	O2B-PB-O3A	2.35	113.62	107.27
3	J	501	GTP	O2B-PB-O3A	2.35	113.62	107.27
3	O	501	GTP	O2B-PB-O3A	2.35	113.61	107.27
3	A	501	GTP	O2B-PB-O3A	2.35	113.61	107.27
3	I	501	GTP	O2A-PA-O3A	2.34	113.61	107.27
3	M	501	GTP	O2B-PB-O3A	2.34	113.61	107.27
3	g	501	GTP	O2B-PB-O3A	2.34	113.61	107.27
3	i	501	GTP	O2A-PA-O3A	2.34	113.61	107.27
3	K	501	GTP	O2B-PB-O3A	2.34	113.60	107.27
3	L	501	GTP	O2B-PB-O3A	2.34	113.60	107.27
3	e	501	GTP	O2B-PB-O3A	2.34	113.60	107.27
3	G	501	GTP	O2B-PB-O3A	2.34	113.60	107.27
3	K	501	GTP	O2A-PA-O3A	2.34	113.60	107.27
3	d	501	GTP	O2A-PA-O3A	2.34	113.60	107.27
3	k	501	GTP	O2B-PB-O3A	2.34	113.60	107.27
3	f	501	GTP	O2B-PB-O3A	2.34	113.59	107.27
3	N	501	GTP	O2B-PB-O3A	2.33	113.58	107.27
3	d	501	GTP	O2B-PB-O3A	2.33	113.57	107.27
6	Y	502	TA1	O09-C21-C20	2.18	113.61	108.66
6	T	502	TA1	O09-C21-C20	2.16	113.56	108.66
6	F	501	TA1	O09-C21-C20	2.16	113.56	108.66
6	o	502	TA1	O09-C21-C20	2.16	113.56	108.66
6	Z	502	TA1	O09-C21-C20	2.16	113.56	108.66
6	q	502	TA1	O09-C21-C20	2.16	113.56	108.66
6	b	502	TA1	O09-C21-C20	2.16	113.55	108.66
6	B	502	TA1	O09-C21-C20	2.16	113.55	108.66
6	Q	502	TA1	O09-C21-C20	2.16	113.55	108.66
6	R	502	TA1	O09-C21-C20	2.16	113.55	108.66
6	S	502	TA1	O09-C21-C20	2.16	113.55	108.66
6	V	502	TA1	O09-C21-C20	2.15	113.54	108.66
6	W	502	TA1	O09-C21-C20	2.15	113.54	108.66
6	X	502	TA1	O09-C21-C20	2.15	113.53	108.66
6	s	502	TA1	O09-C21-C20	2.15	113.53	108.66
6	r	502	TA1	O09-C21-C20	2.15	113.53	108.66
6	a	502	TA1	O09-C21-C20	2.15	113.53	108.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	U	501	TA1	O09-C21-C20	2.14	113.51	108.66
6	p	502	TA1	O09-C21-C20	2.14	113.51	108.66
3	k	501	GTP	N1-C2-N3	2.12	127.21	123.32
3	M	501	GTP	N1-C2-N3	2.12	127.21	123.32
3	g	501	GTP	N1-C2-N3	2.12	127.20	123.32
3	I	501	GTP	N1-C2-N3	2.12	127.19	123.32
3	D	501	GTP	N1-C2-N3	2.11	127.18	123.32
3	j	501	GTP	N1-C2-N3	2.11	127.18	123.32
3	P	501	GTP	N1-C2-N3	2.10	127.17	123.32
3	E	501	GTP	N1-C2-N3	2.10	127.17	123.32
3	f	501	GTP	N1-C2-N3	2.10	127.16	123.32
3	K	501	GTP	N1-C2-N3	2.10	127.16	123.32
3	G	501	GTP	N1-C2-N3	2.09	127.15	123.32
3	O	501	GTP	N1-C2-N3	2.09	127.15	123.32
3	h	501	GTP	N1-C2-N3	2.09	127.15	123.32
3	L	501	GTP	N1-C2-N3	2.09	127.15	123.32
3	d	501	GTP	N1-C2-N3	2.09	127.15	123.32
3	A	501	GTP	N1-C2-N3	2.09	127.14	123.32
3	c	501	GTP	N1-C2-N3	2.09	127.14	123.32
3	i	501	GTP	N1-C2-N3	2.08	127.13	123.32
3	J	501	GTP	N1-C2-N3	2.07	127.11	123.32
3	e	501	GTP	N1-C2-N3	2.06	127.10	123.32
3	C	501	GTP	N1-C2-N3	2.06	127.09	123.32
3	N	501	GTP	N1-C2-N3	2.06	127.09	123.32
3	H	501	GTP	N1-C2-N3	2.05	127.08	123.32

There are no chirality outliers.

All (107) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	501	GDP	C5'-O5'-PA-O3A
5	B	501	GDP	C5'-O5'-PA-O2A
5	F	502	GDP	C5'-O5'-PA-O3A
5	F	502	GDP	C5'-O5'-PA-O2A
5	Q	501	GDP	C5'-O5'-PA-O3A
5	Q	501	GDP	C5'-O5'-PA-O2A
5	R	501	GDP	C5'-O5'-PA-O3A
5	R	501	GDP	C5'-O5'-PA-O2A
5	S	501	GDP	C5'-O5'-PA-O3A
5	S	501	GDP	C5'-O5'-PA-O2A
5	T	501	GDP	C5'-O5'-PA-O3A
5	T	501	GDP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
5	U	502	GDP	C5'-O5'-PA-O3A
5	U	502	GDP	C5'-O5'-PA-O2A
5	V	501	GDP	C5'-O5'-PA-O3A
5	V	501	GDP	C5'-O5'-PA-O2A
5	W	501	GDP	C5'-O5'-PA-O3A
5	W	501	GDP	C5'-O5'-PA-O2A
5	X	501	GDP	C5'-O5'-PA-O3A
5	X	501	GDP	C5'-O5'-PA-O2A
5	Y	501	GDP	C5'-O5'-PA-O3A
5	Y	501	GDP	C5'-O5'-PA-O2A
5	Z	501	GDP	C5'-O5'-PA-O3A
5	Z	501	GDP	C5'-O5'-PA-O2A
5	a	501	GDP	C5'-O5'-PA-O3A
5	a	501	GDP	C5'-O5'-PA-O2A
5	b	501	GDP	C5'-O5'-PA-O3A
5	b	501	GDP	C5'-O5'-PA-O2A
5	o	501	GDP	C5'-O5'-PA-O3A
5	o	501	GDP	C5'-O5'-PA-O2A
5	p	501	GDP	C5'-O5'-PA-O3A
5	p	501	GDP	C5'-O5'-PA-O2A
5	q	501	GDP	C5'-O5'-PA-O3A
5	q	501	GDP	C5'-O5'-PA-O2A
5	r	501	GDP	C5'-O5'-PA-O3A
5	r	501	GDP	C5'-O5'-PA-O2A
5	s	501	GDP	C5'-O5'-PA-O3A
5	s	501	GDP	C5'-O5'-PA-O2A
3	A	501	GTP	C4'-C5'-O5'-PA
3	C	501	GTP	C4'-C5'-O5'-PA
3	D	501	GTP	C4'-C5'-O5'-PA
3	E	501	GTP	C4'-C5'-O5'-PA
3	G	501	GTP	C4'-C5'-O5'-PA
3	H	501	GTP	C4'-C5'-O5'-PA
3	I	501	GTP	C4'-C5'-O5'-PA
3	J	501	GTP	C4'-C5'-O5'-PA
3	K	501	GTP	C4'-C5'-O5'-PA
3	L	501	GTP	C4'-C5'-O5'-PA
3	M	501	GTP	C4'-C5'-O5'-PA
3	N	501	GTP	C4'-C5'-O5'-PA
3	O	501	GTP	C4'-C5'-O5'-PA
3	P	501	GTP	C4'-C5'-O5'-PA
3	c	501	GTP	C4'-C5'-O5'-PA
3	d	501	GTP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
3	e	501	GTP	C4'-C5'-O5'-PA
3	f	501	GTP	C4'-C5'-O5'-PA
3	g	501	GTP	C4'-C5'-O5'-PA
3	h	501	GTP	C4'-C5'-O5'-PA
3	i	501	GTP	C4'-C5'-O5'-PA
3	j	501	GTP	C4'-C5'-O5'-PA
3	k	501	GTP	C4'-C5'-O5'-PA
3	A	501	GTP	C3'-C4'-C5'-O5'
3	C	501	GTP	C3'-C4'-C5'-O5'
3	D	501	GTP	C3'-C4'-C5'-O5'
3	E	501	GTP	C3'-C4'-C5'-O5'
3	G	501	GTP	C3'-C4'-C5'-O5'
3	H	501	GTP	C3'-C4'-C5'-O5'
3	I	501	GTP	C3'-C4'-C5'-O5'
3	J	501	GTP	C3'-C4'-C5'-O5'
3	K	501	GTP	C3'-C4'-C5'-O5'
3	L	501	GTP	C3'-C4'-C5'-O5'
3	M	501	GTP	C3'-C4'-C5'-O5'
3	N	501	GTP	C3'-C4'-C5'-O5'
3	O	501	GTP	C3'-C4'-C5'-O5'
3	P	501	GTP	C3'-C4'-C5'-O5'
3	c	501	GTP	C3'-C4'-C5'-O5'
3	d	501	GTP	C3'-C4'-C5'-O5'
3	e	501	GTP	C3'-C4'-C5'-O5'
3	f	501	GTP	C3'-C4'-C5'-O5'
3	g	501	GTP	C3'-C4'-C5'-O5'
3	h	501	GTP	C3'-C4'-C5'-O5'
3	i	501	GTP	C3'-C4'-C5'-O5'
3	j	501	GTP	C3'-C4'-C5'-O5'
3	k	501	GTP	C3'-C4'-C5'-O5'
6	B	502	TA1	C28-C29-N01-C30
6	F	501	TA1	C28-C29-N01-C30
6	Q	502	TA1	C28-C29-N01-C30
6	R	502	TA1	C28-C29-N01-C30
6	S	502	TA1	C28-C29-N01-C30
6	T	502	TA1	C28-C29-N01-C30
6	U	501	TA1	C28-C29-N01-C30
6	V	502	TA1	C28-C29-N01-C30
6	W	502	TA1	C28-C29-N01-C30
6	X	502	TA1	C28-C29-N01-C30
6	Y	502	TA1	C28-C29-N01-C30
6	a	502	TA1	C28-C29-N01-C30

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Mol	Chain	Res	Type	Atoms
6	b	502	TA1	C28-C29-N01-C30
6	o	502	TA1	C28-C29-N01-C30
6	p	502	TA1	C28-C29-N01-C30
6	q	502	TA1	C28-C29-N01-C30
6	r	502	TA1	C28-C29-N01-C30
6	s	502	TA1	C28-C29-N01-C30
6	S	502	TA1	O12-C27-C28-C29
6	Y	502	TA1	O12-C27-C28-C29
6	Z	502	TA1	O12-C27-C28-C29
6	a	502	TA1	O12-C27-C28-C29
6	p	502	TA1	O12-C27-C28-C29

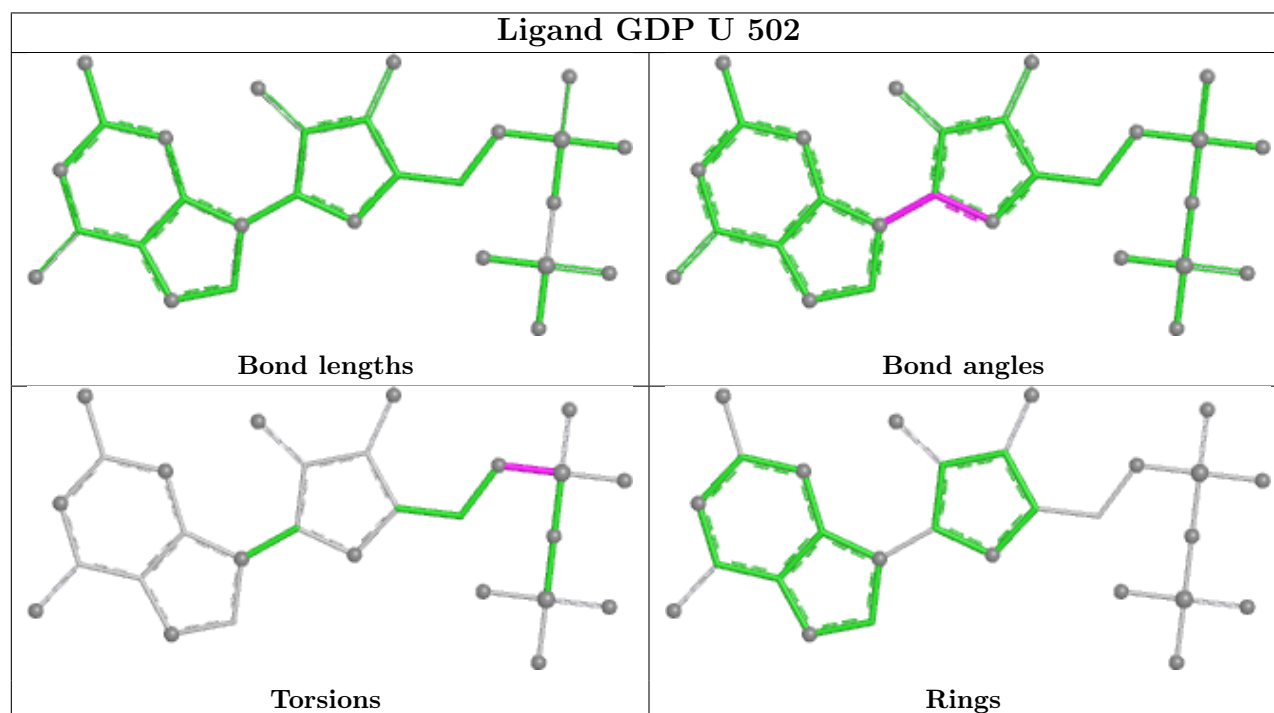
There are no ring outliers.

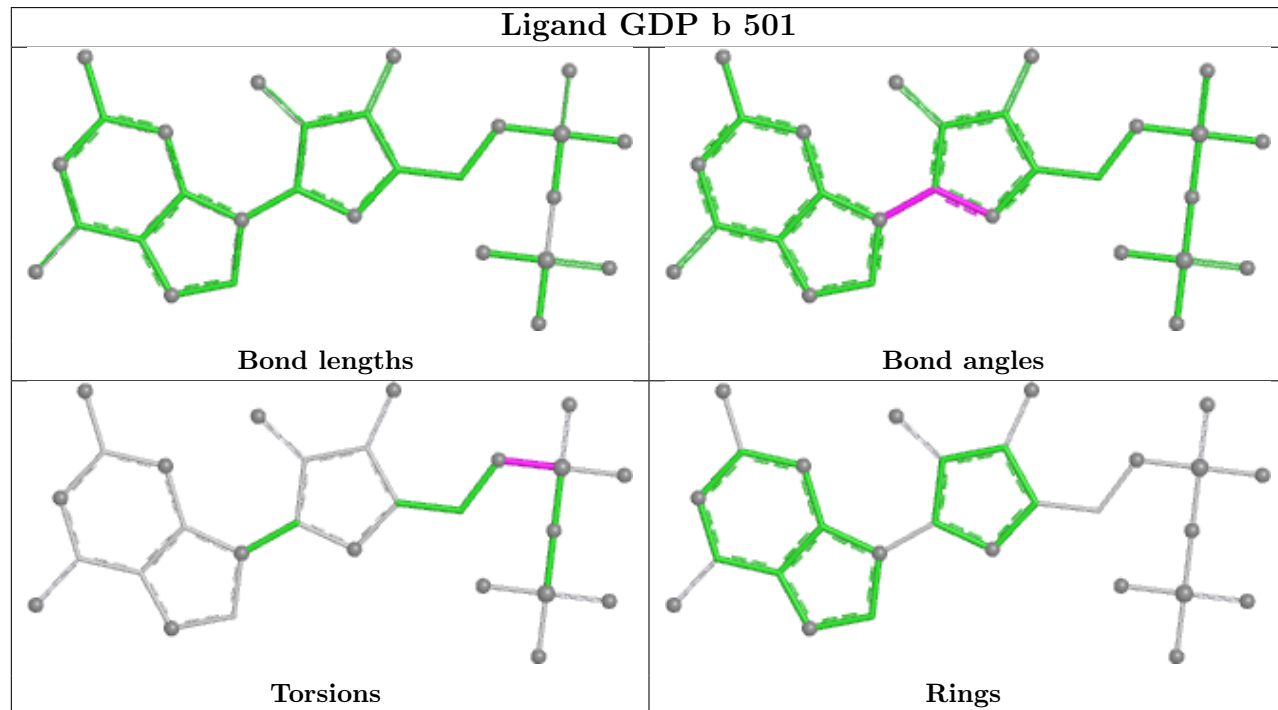
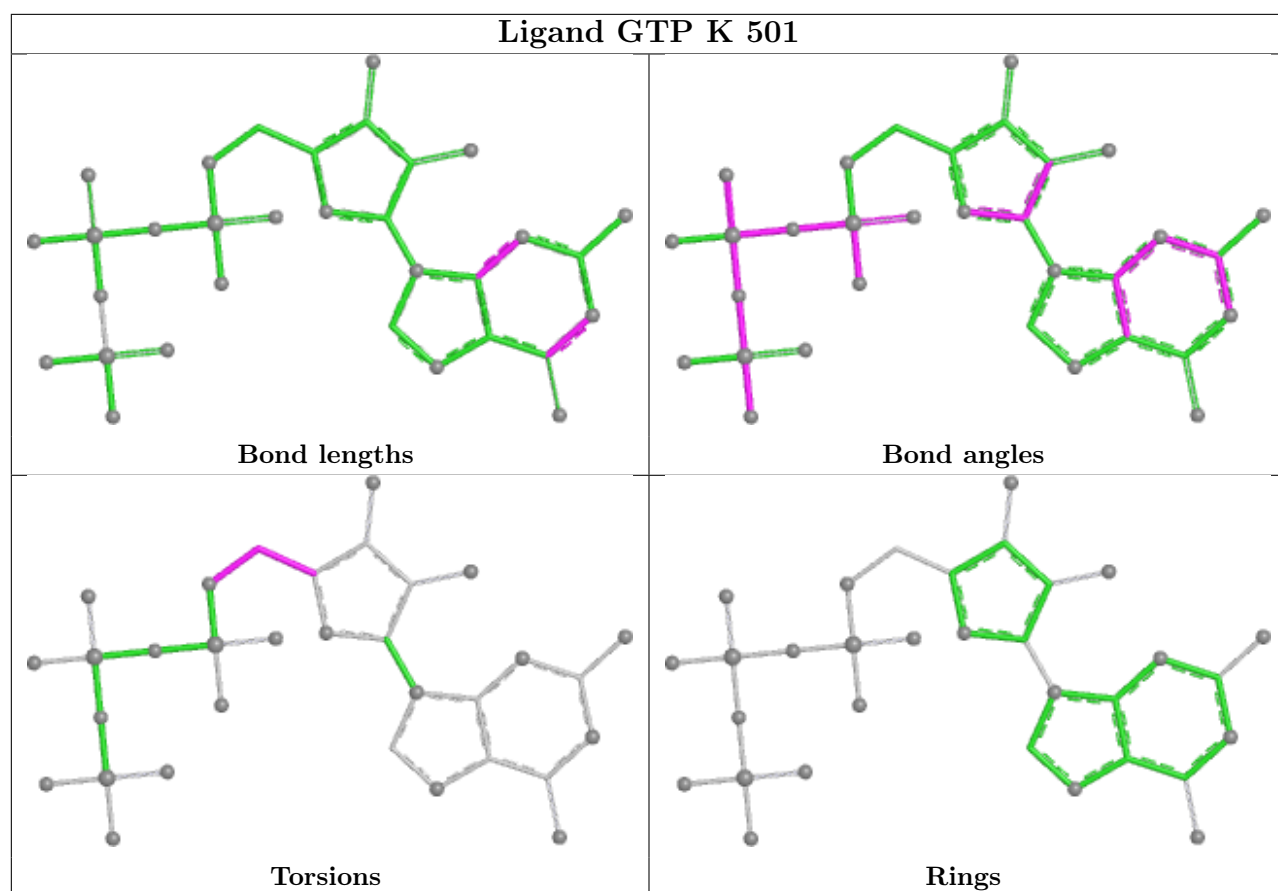
19 monomers are involved in 95 short contacts:

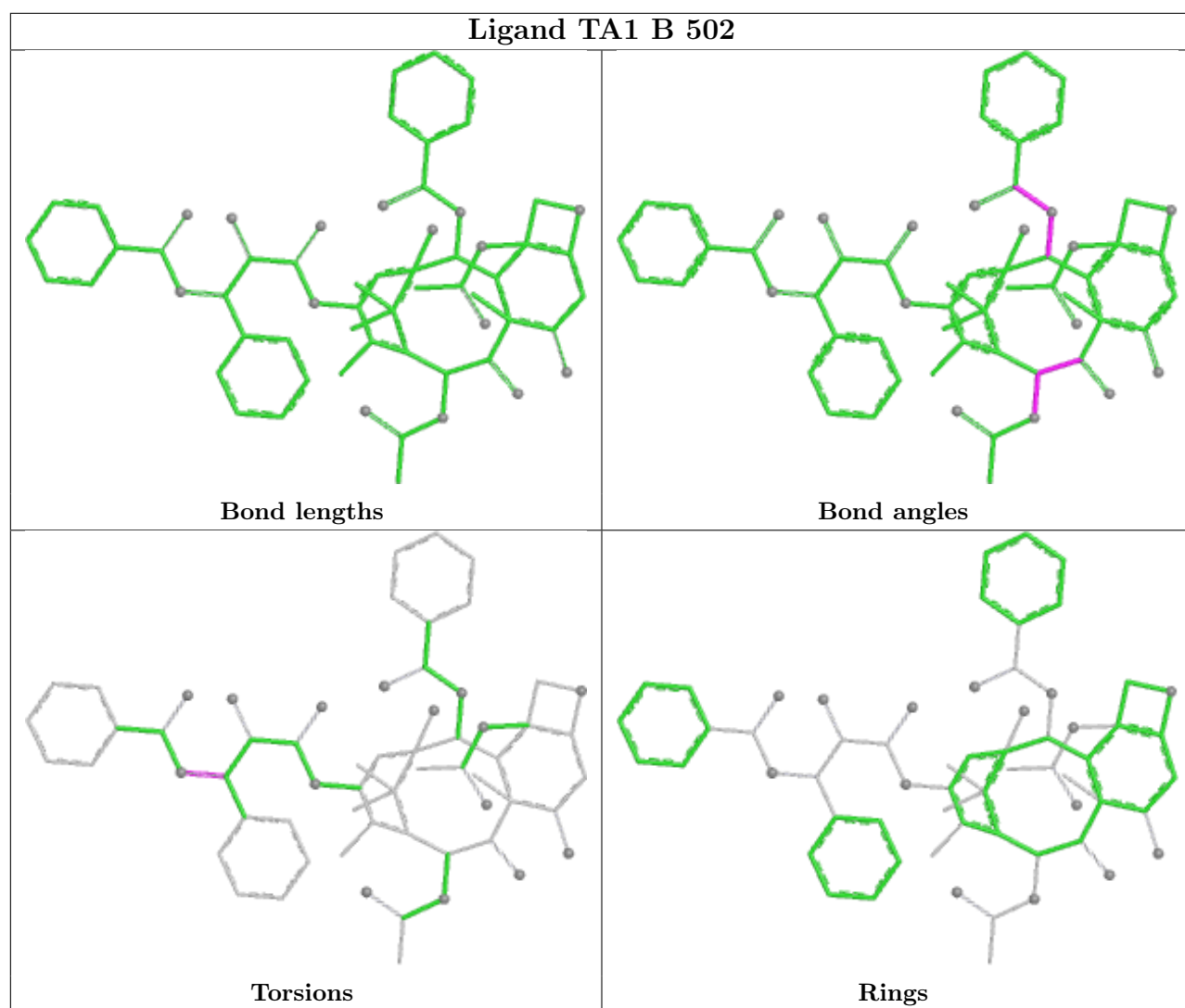
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	502	TA1	5	0
6	X	502	TA1	5	0
6	a	502	TA1	5	0
6	q	502	TA1	5	0
6	T	502	TA1	5	0
6	s	502	TA1	5	0
6	r	502	TA1	5	0
6	V	502	TA1	5	0
6	p	502	TA1	5	0
6	F	501	TA1	5	0
6	S	502	TA1	5	0
6	Y	502	TA1	5	0
6	Q	502	TA1	5	0
6	W	502	TA1	5	0
6	U	501	TA1	5	0
6	Z	502	TA1	5	0
6	o	502	TA1	5	0
6	b	502	TA1	5	0
6	R	502	TA1	5	0

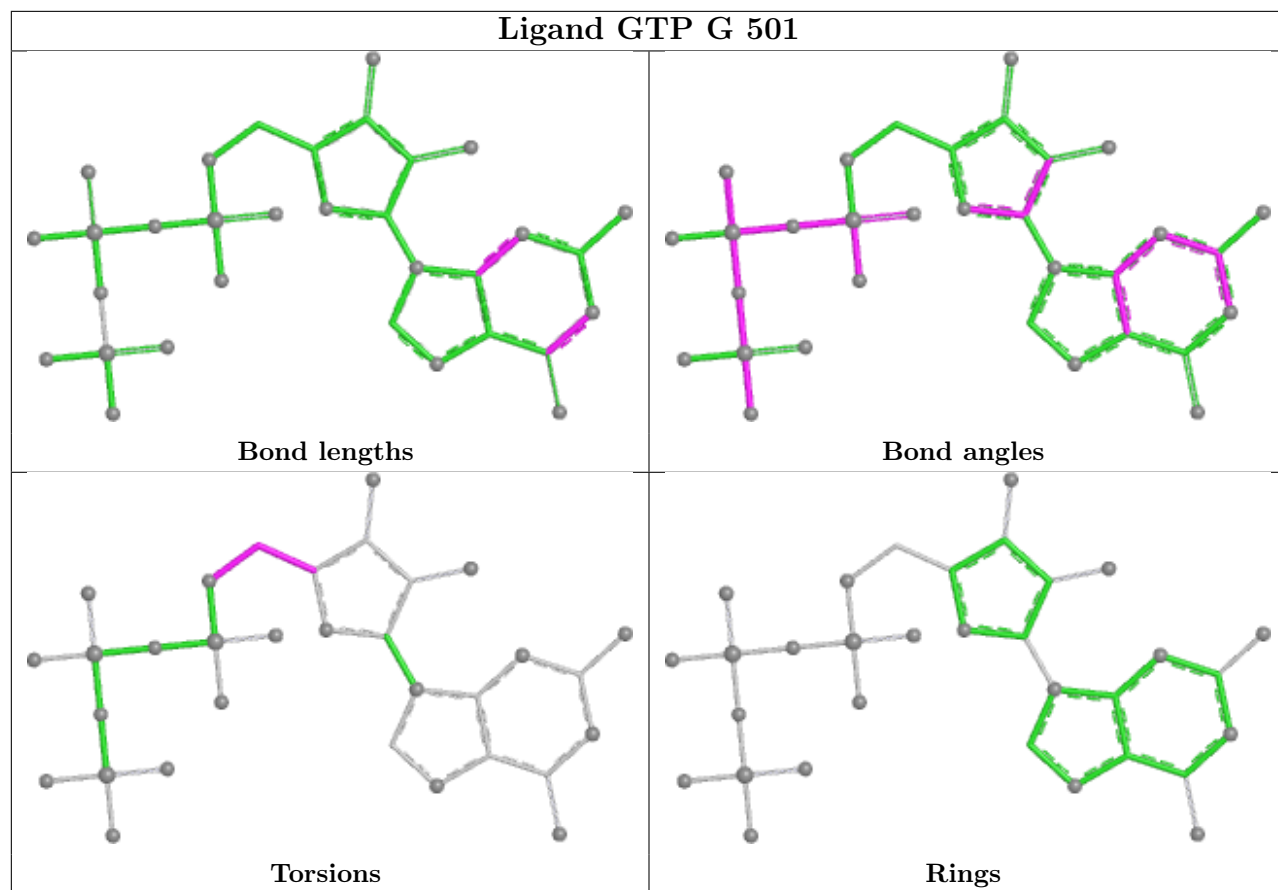
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

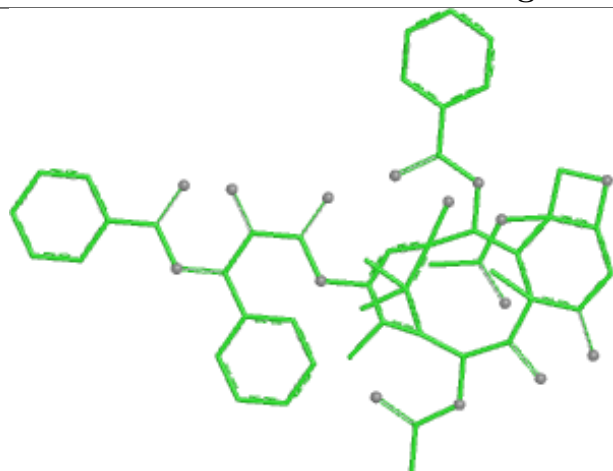




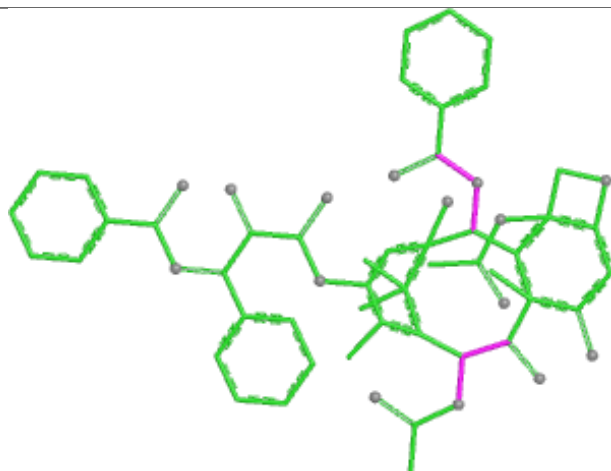




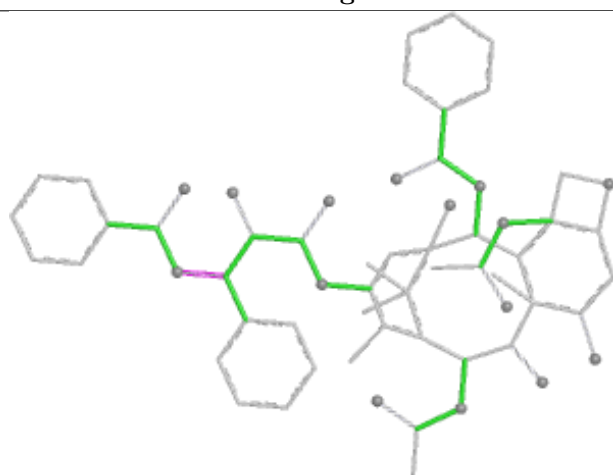
Ligand TA1 X 502



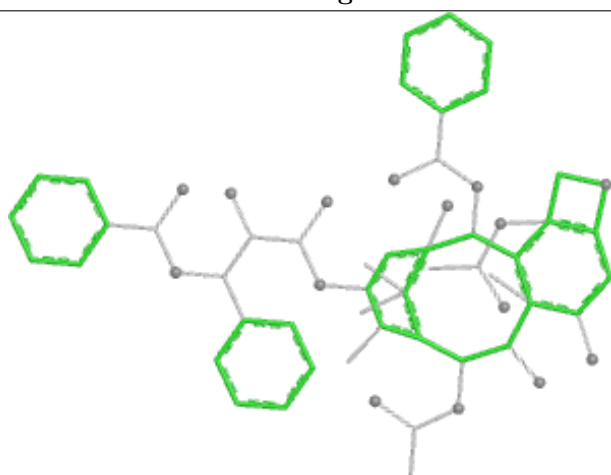
Bond lengths



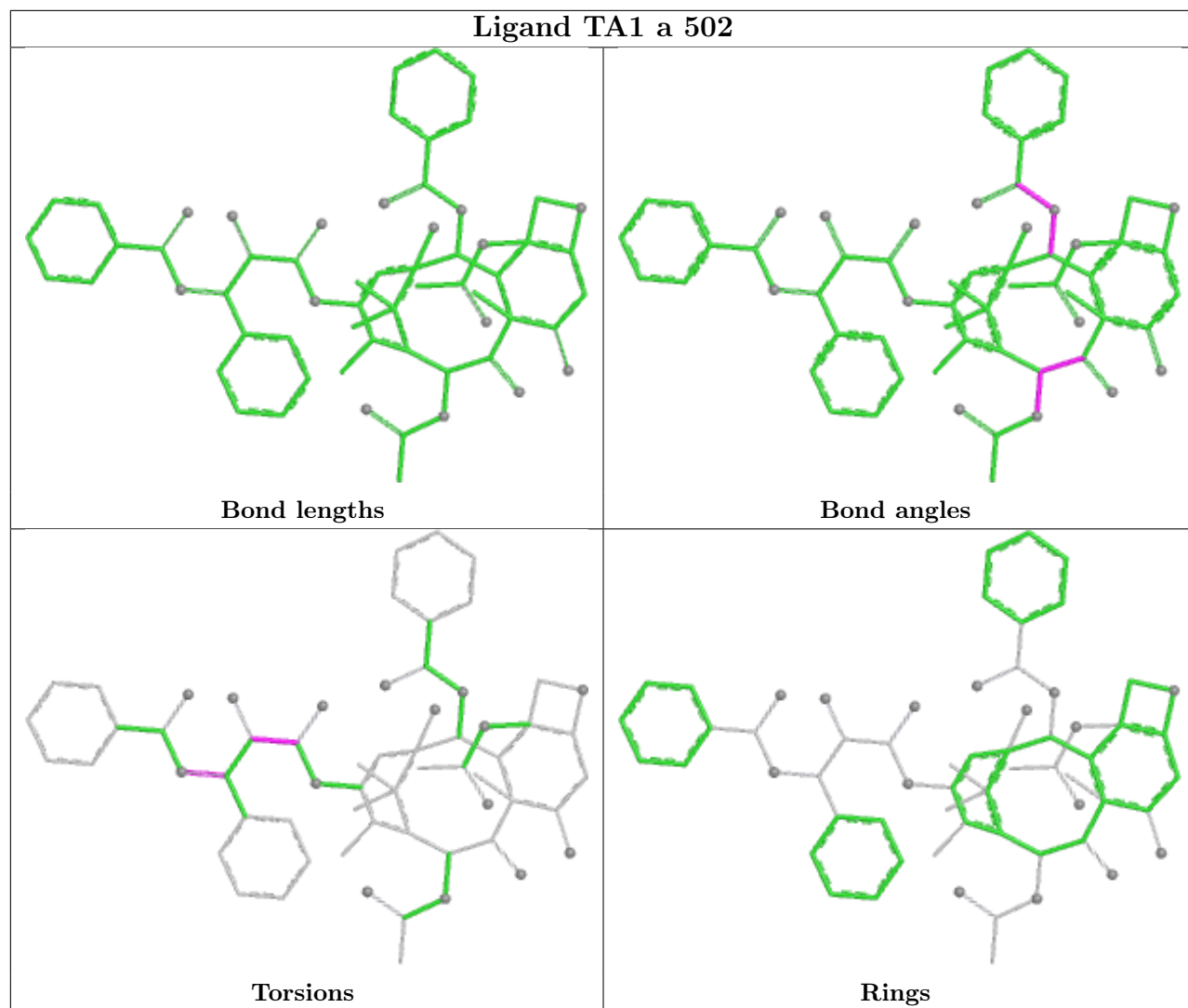
Bond angles

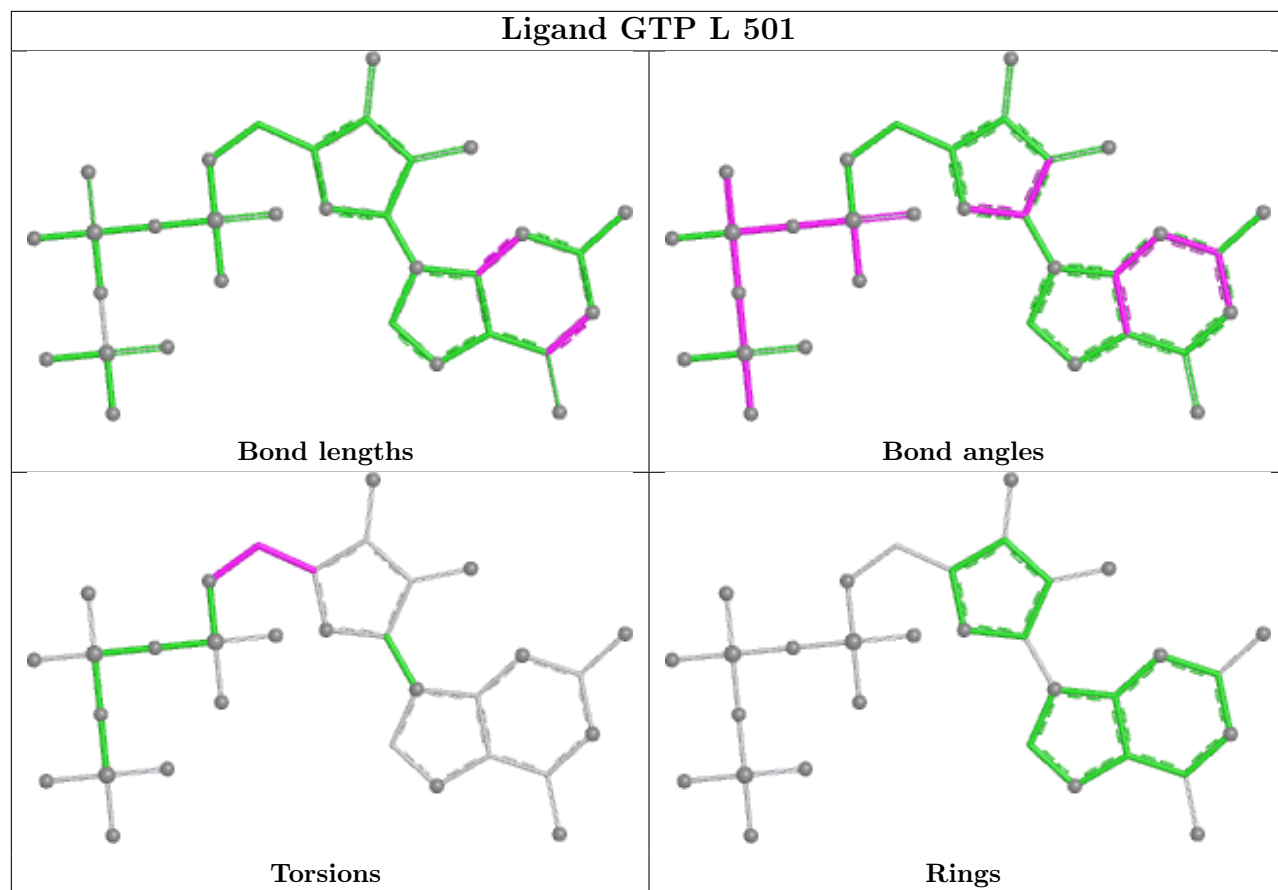


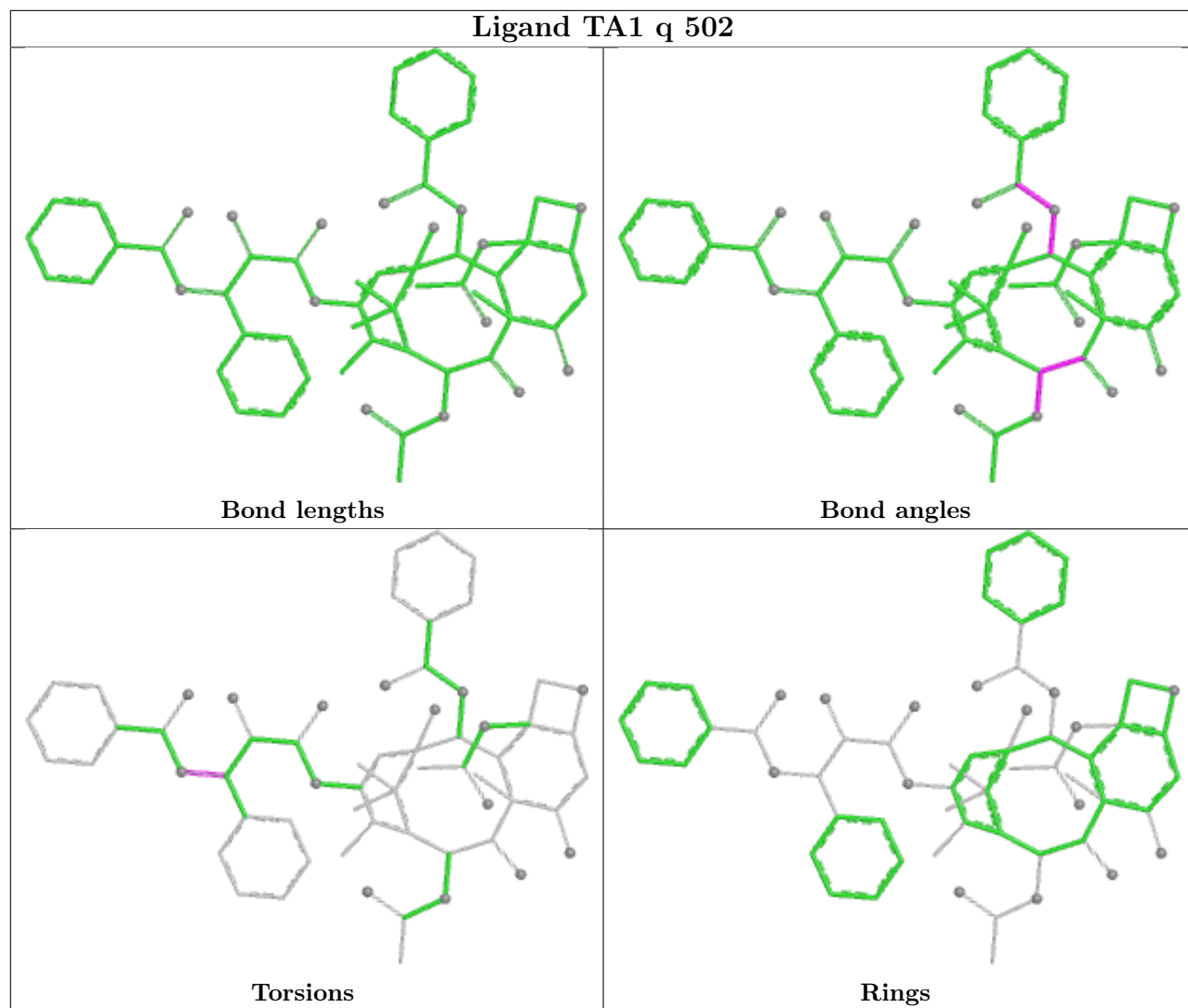
Torsions



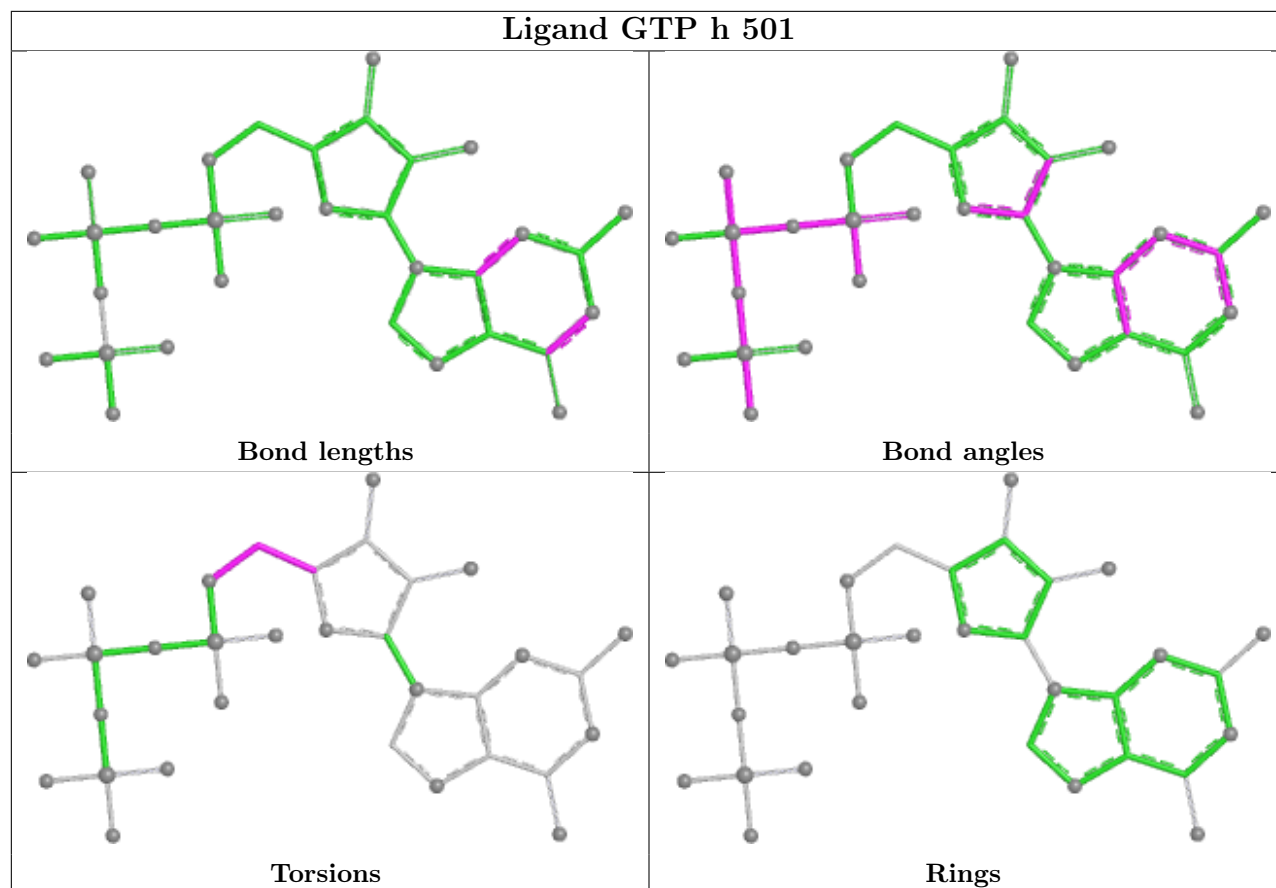
Rings



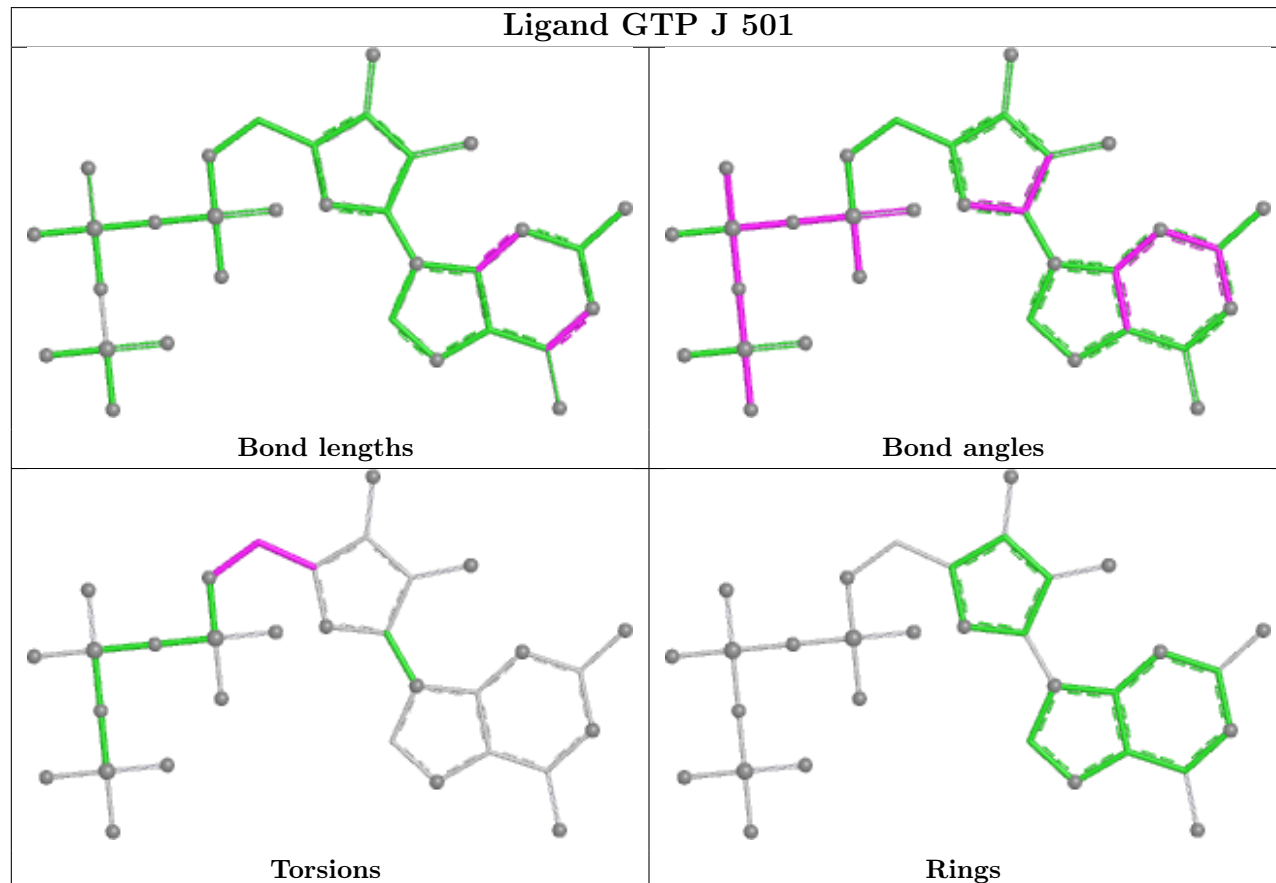




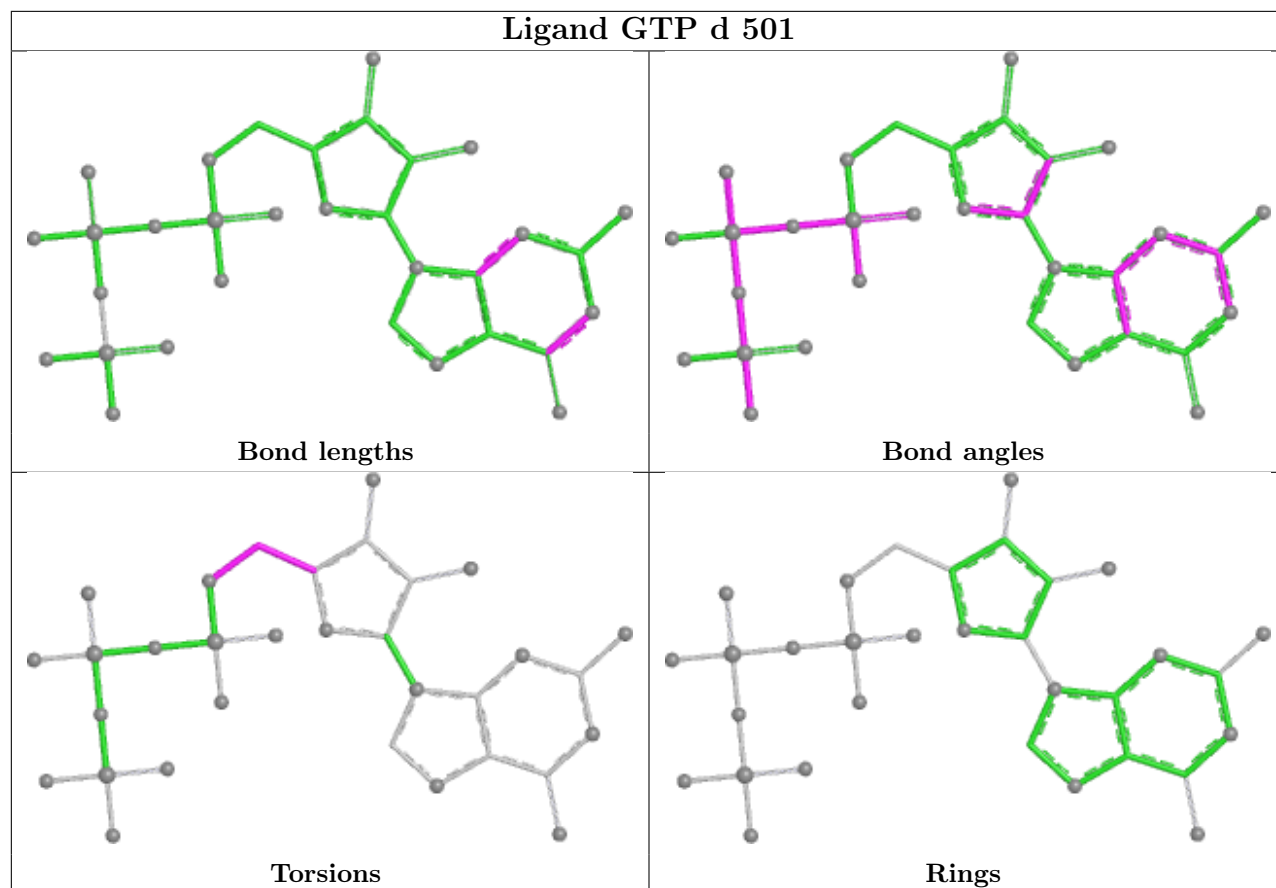
Ligand GTP h 501



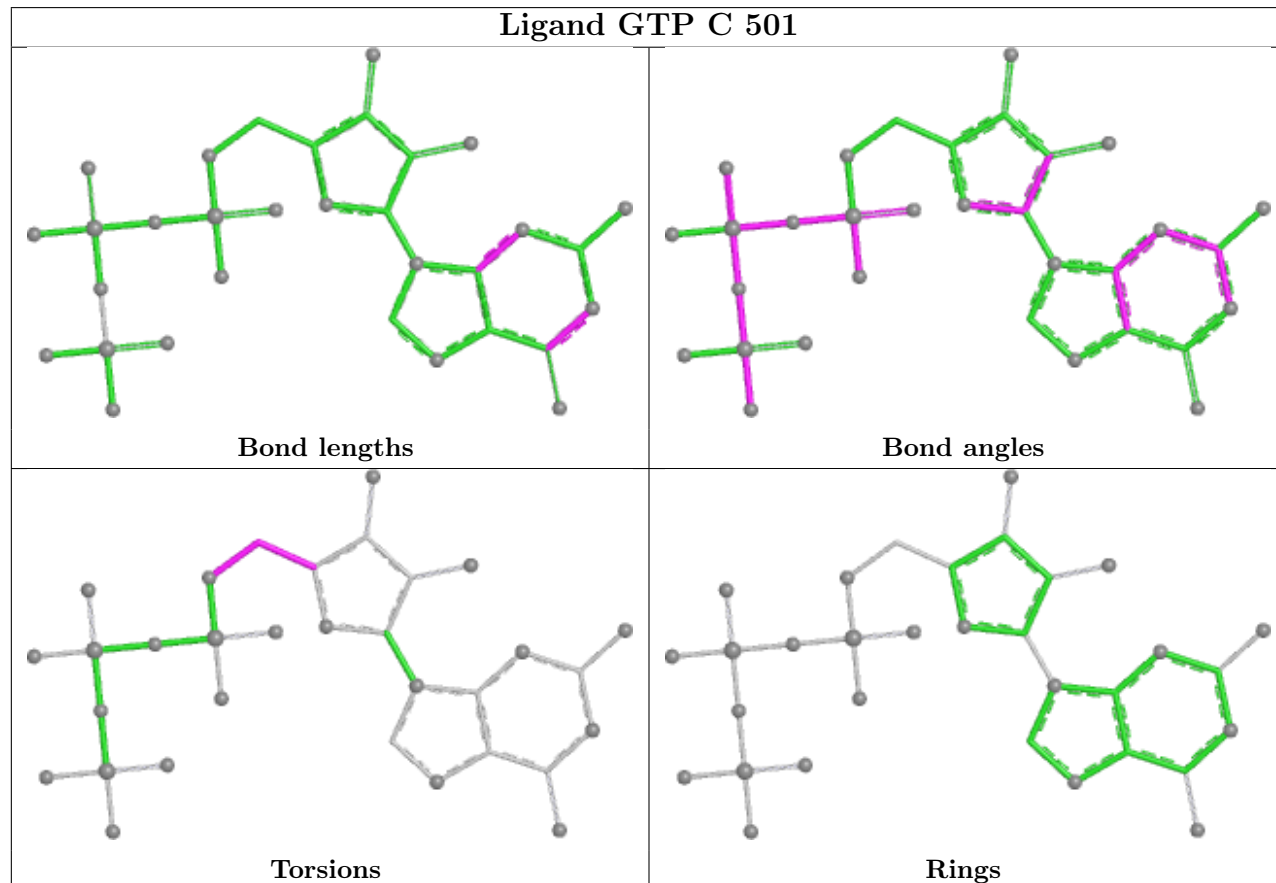
Ligand GTP J 501

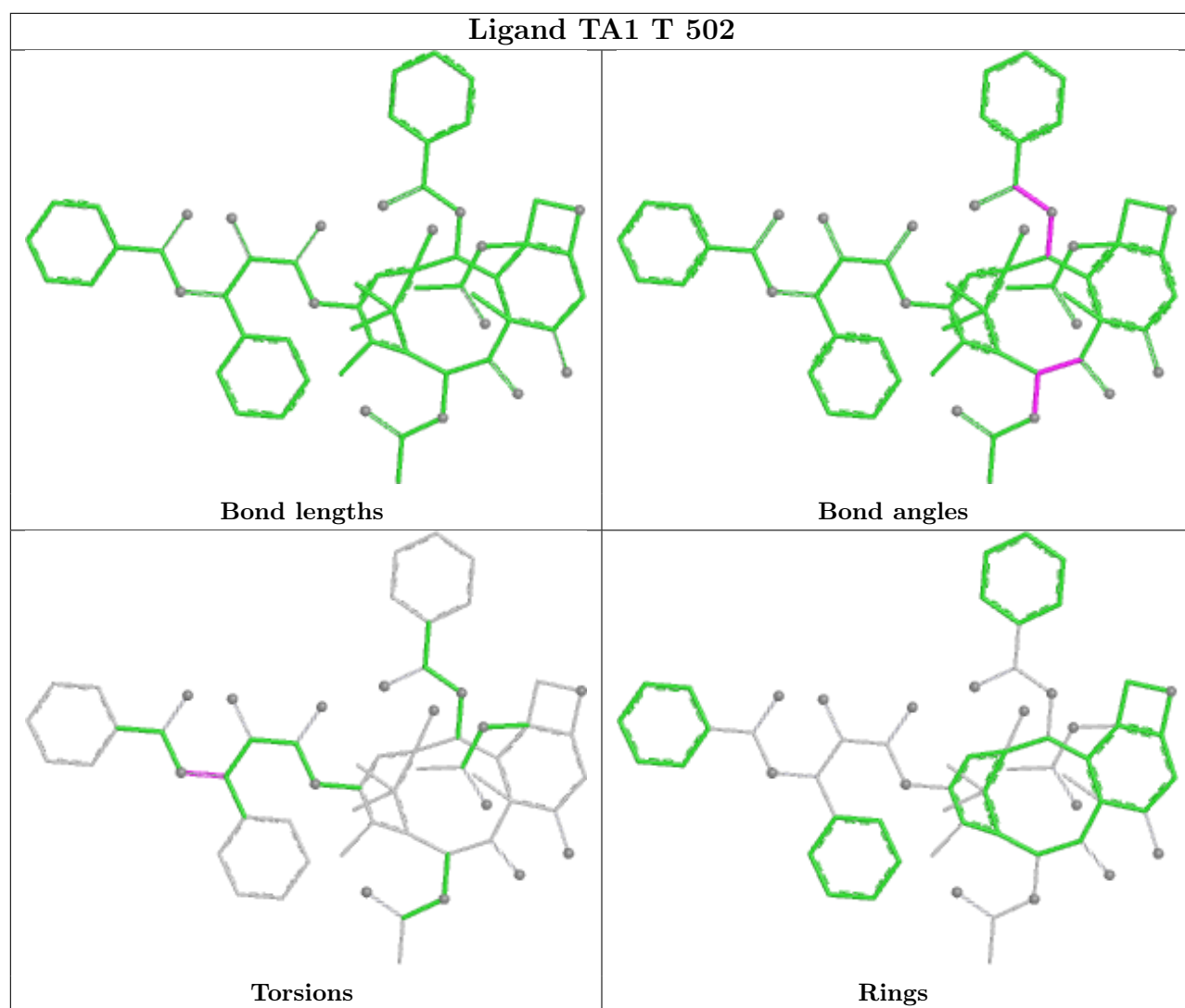


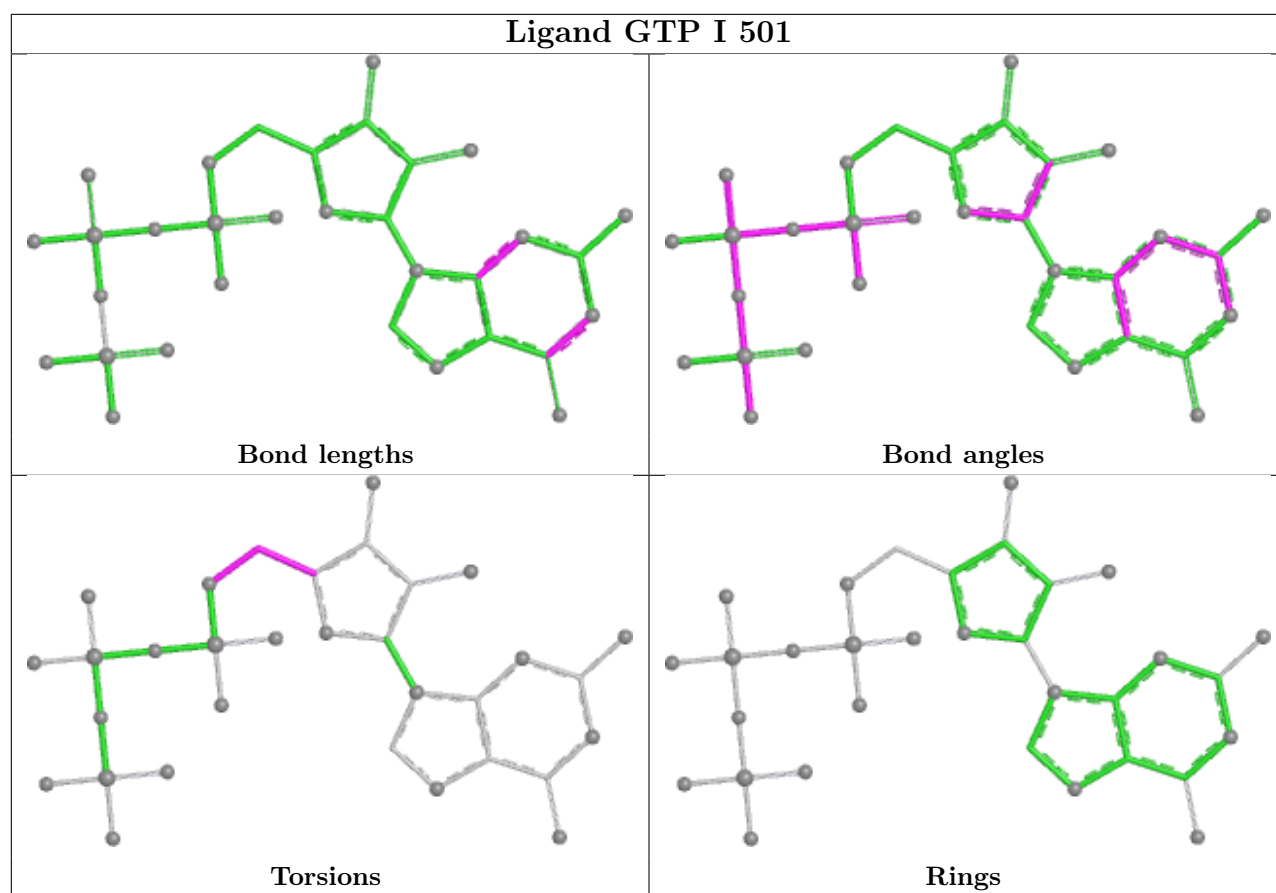
Ligand GTP d 501

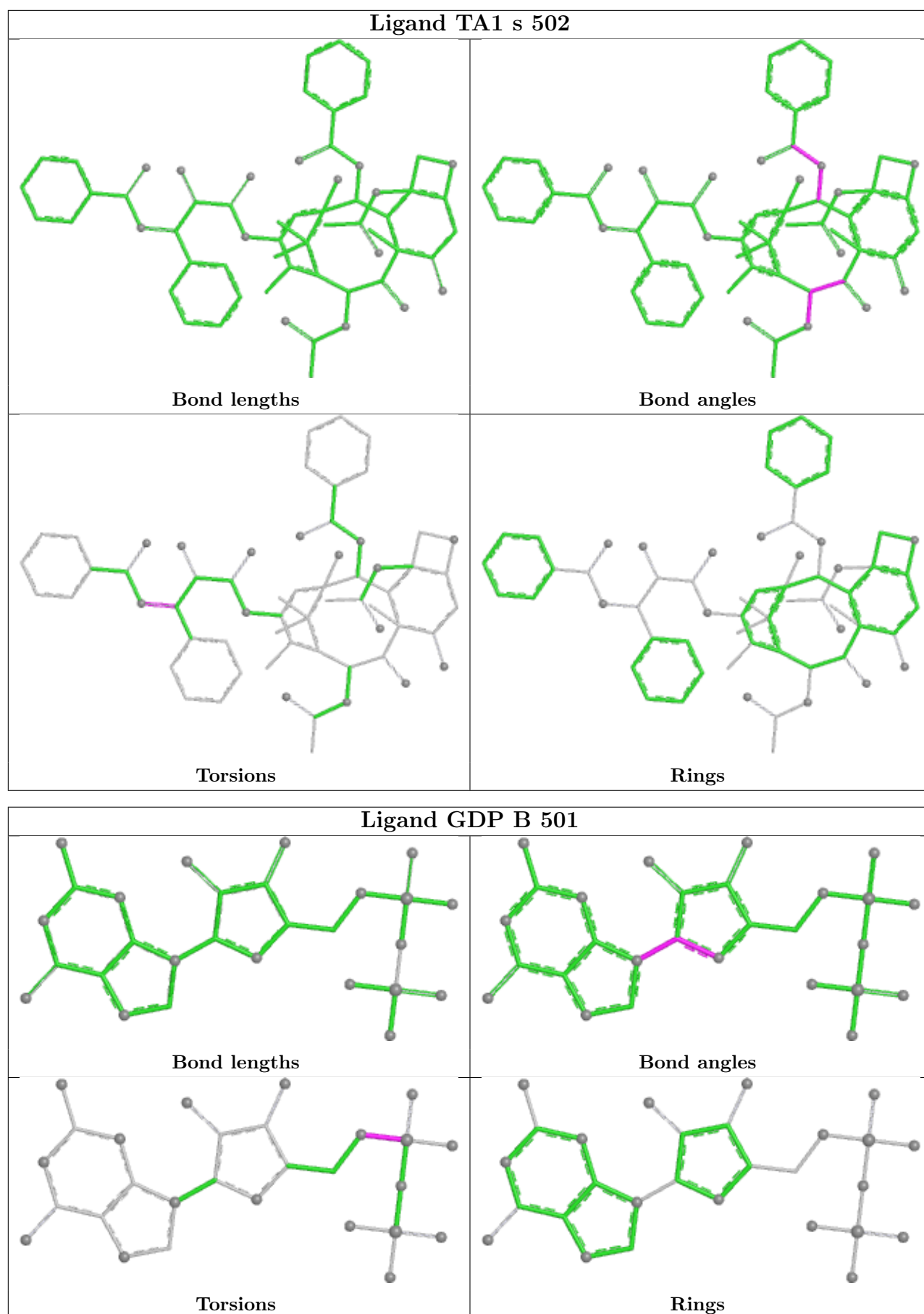


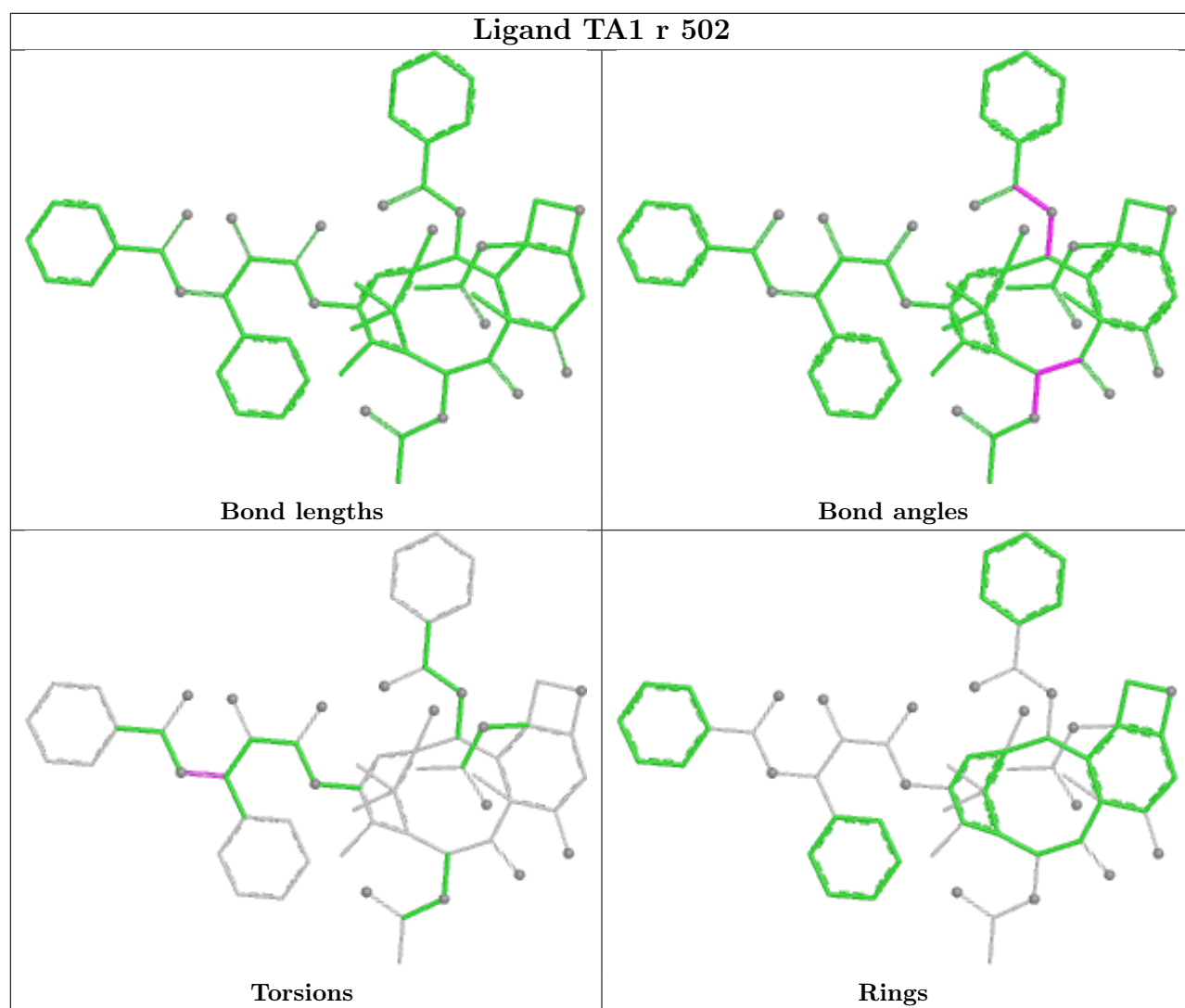
Ligand GTP C 501

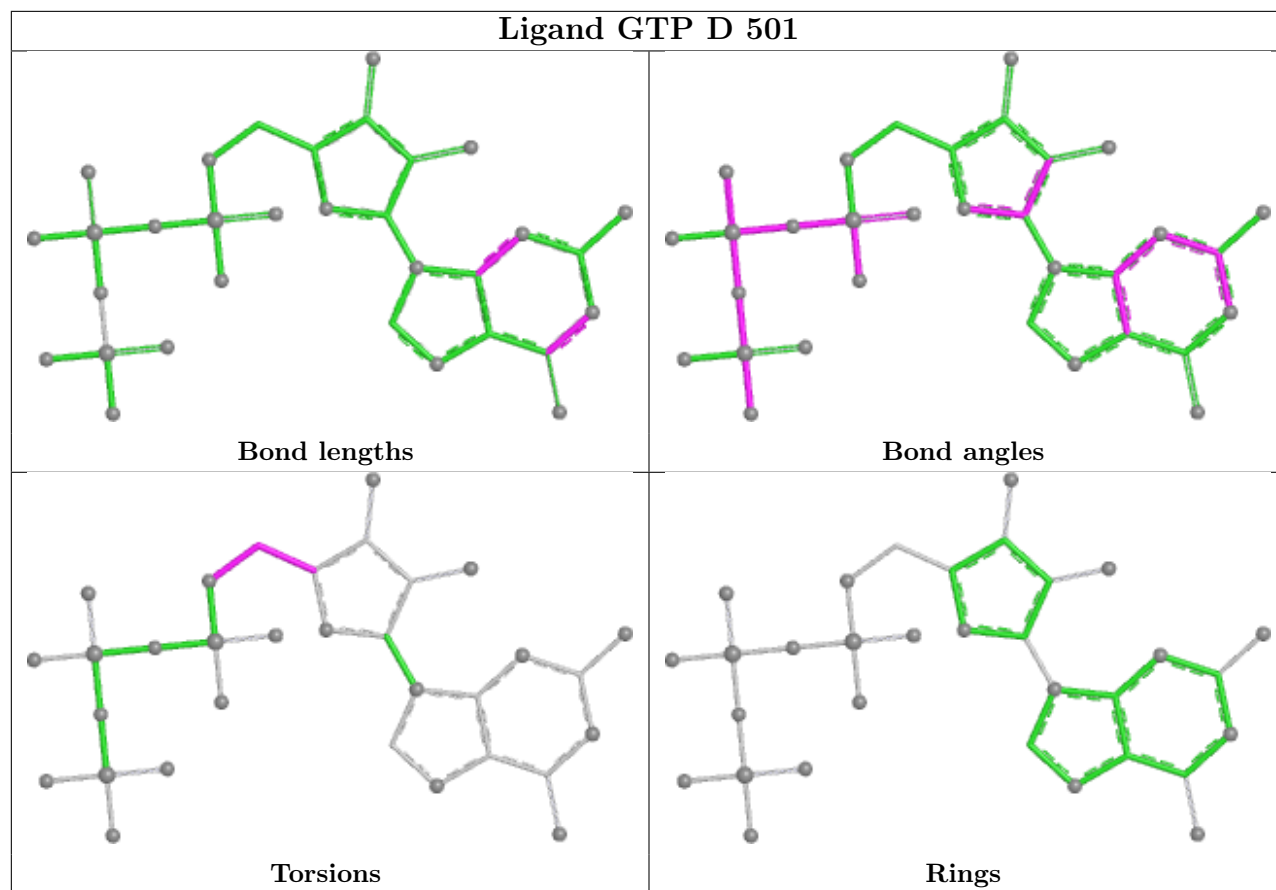




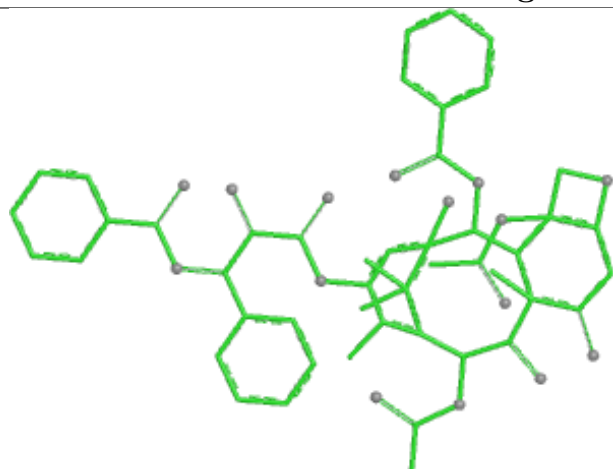




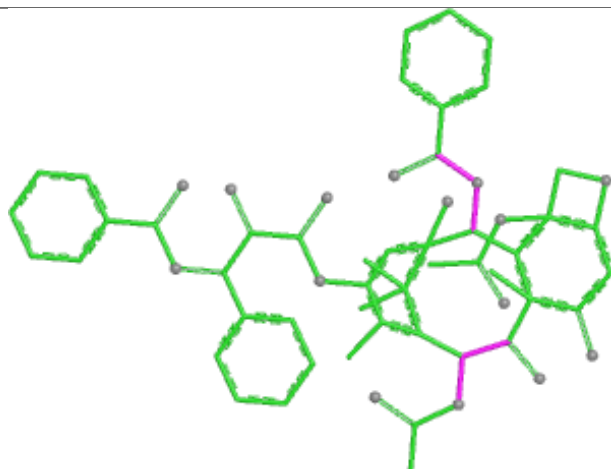




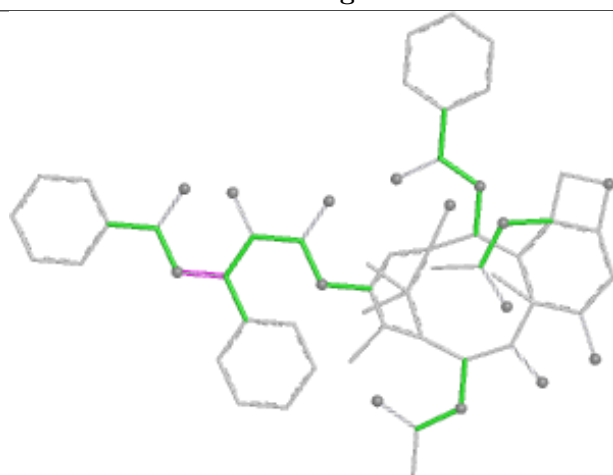
Ligand TA1 V 502



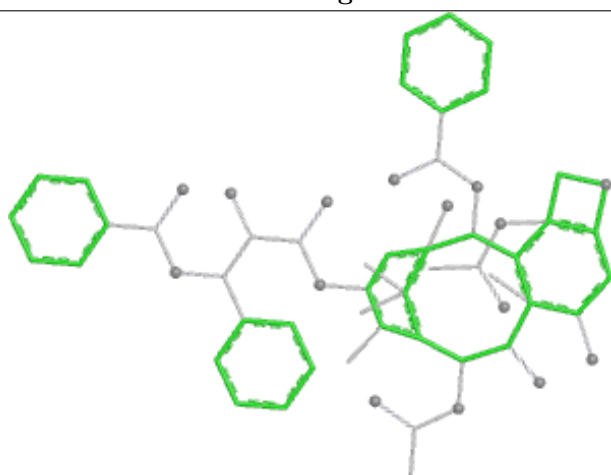
Bond lengths



Bond angles

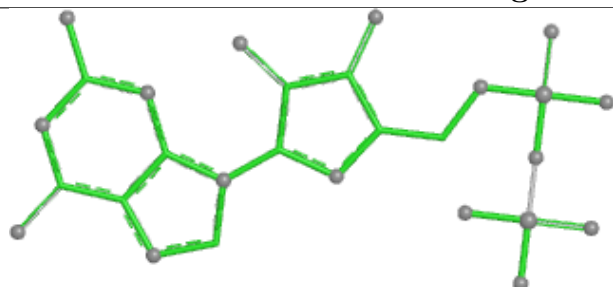


Torsions

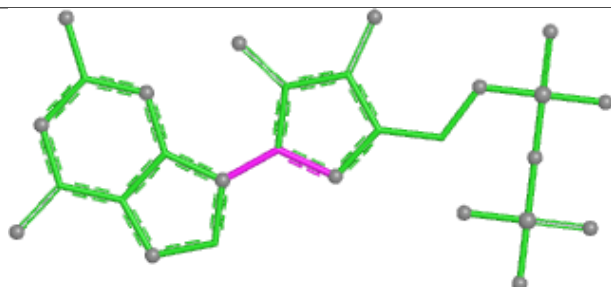


Rings

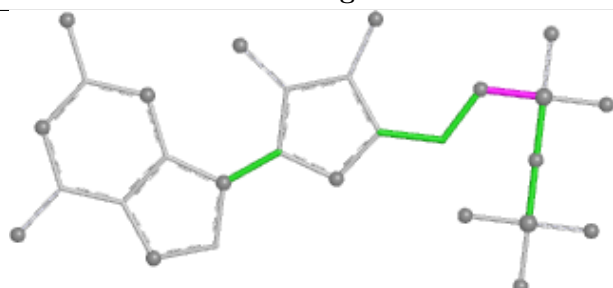
Ligand GDP Y 501



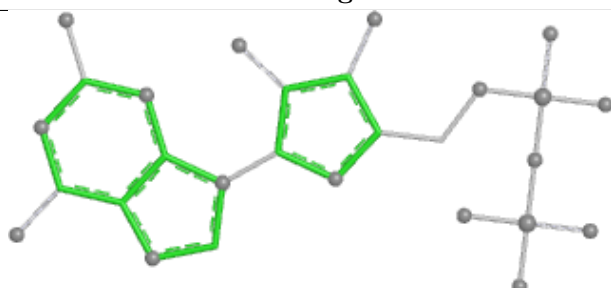
Bond lengths



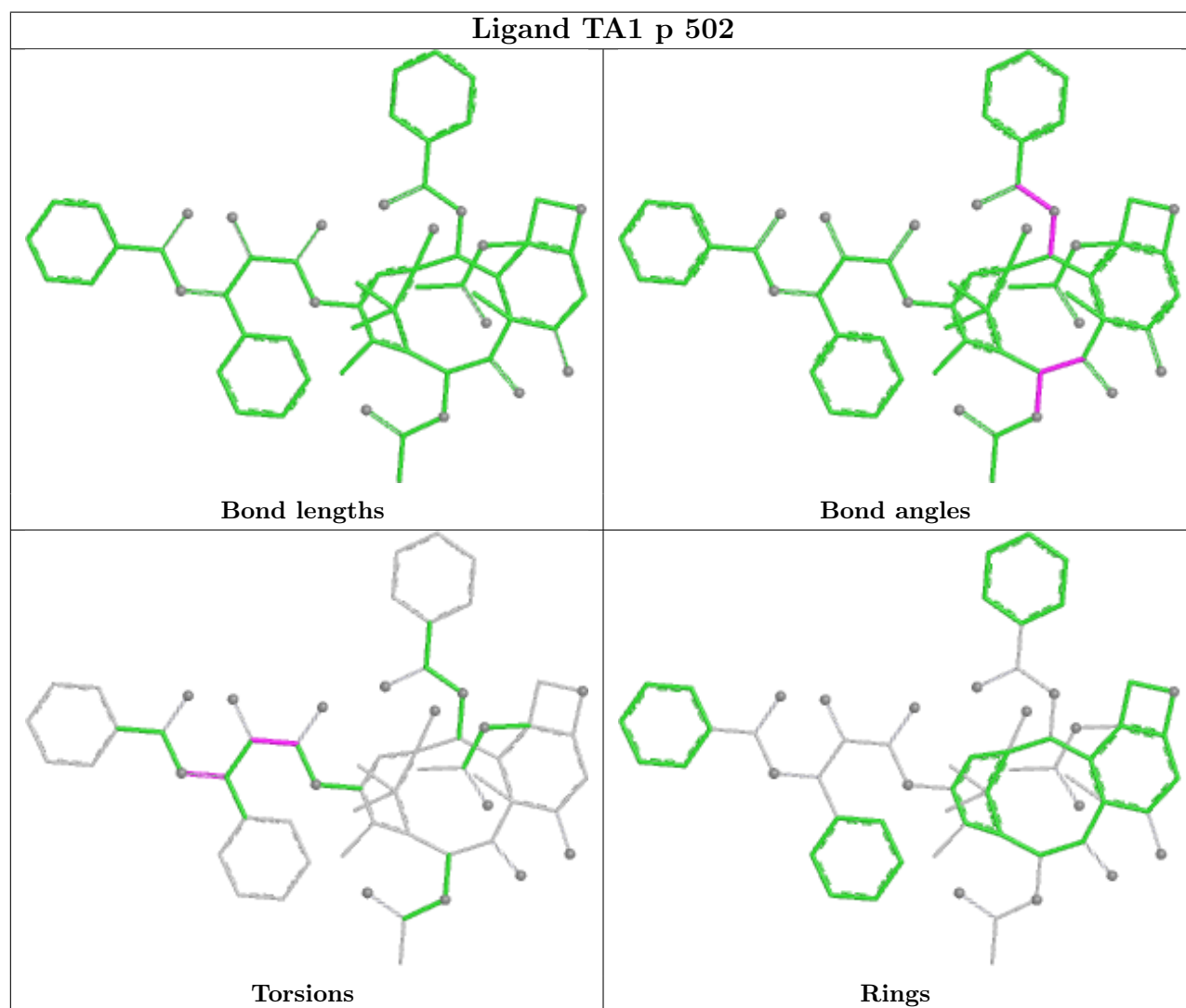
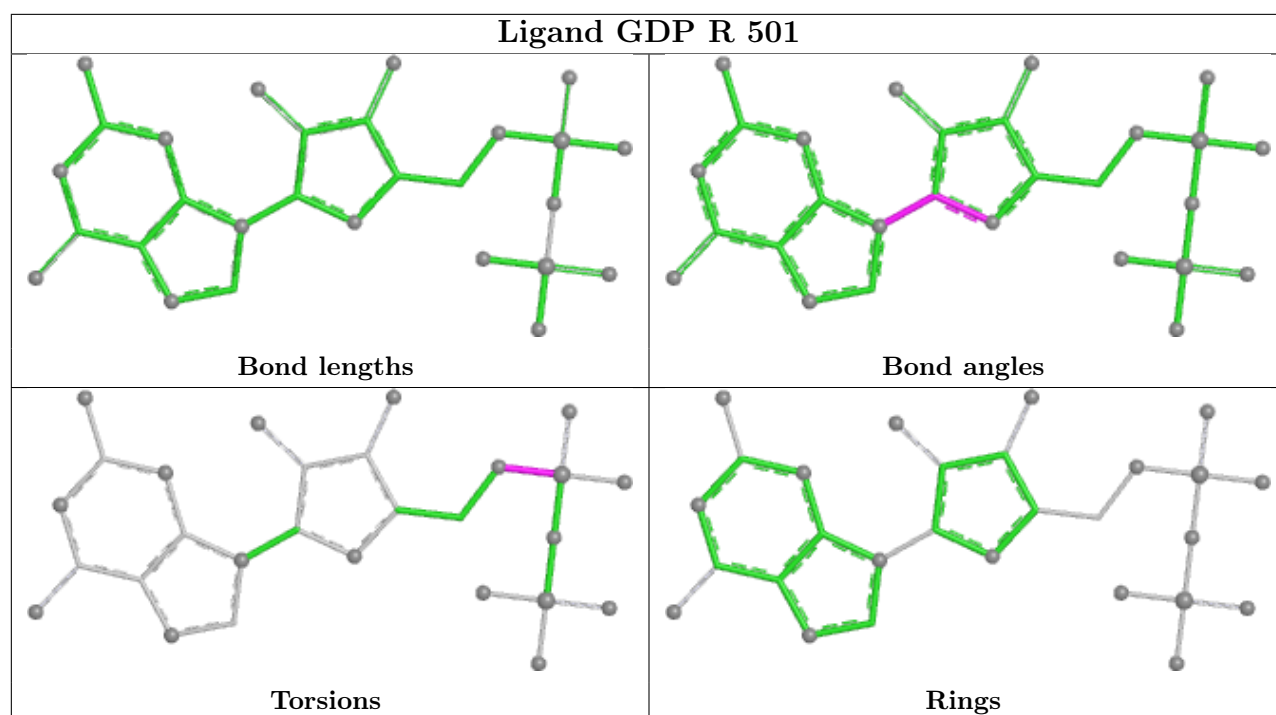
Bond angles



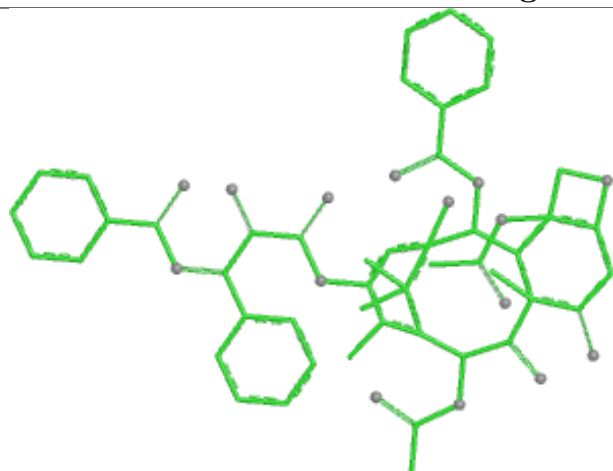
Torsions



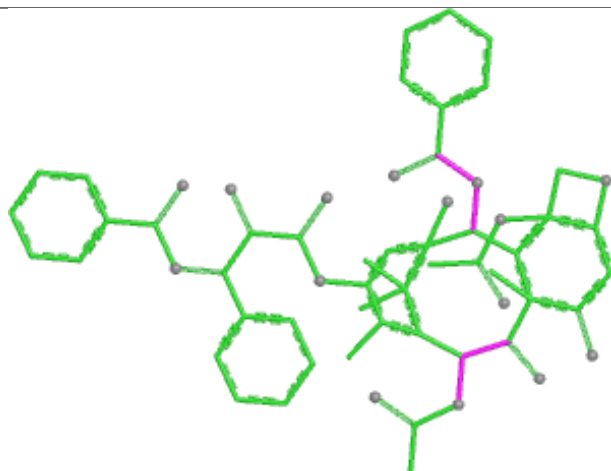
Rings



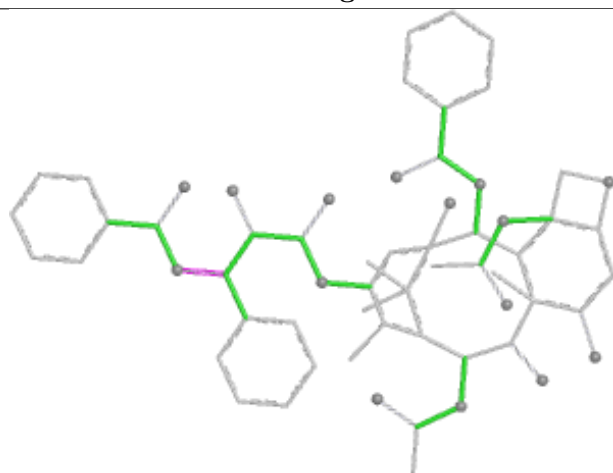
Ligand TA1 F 501



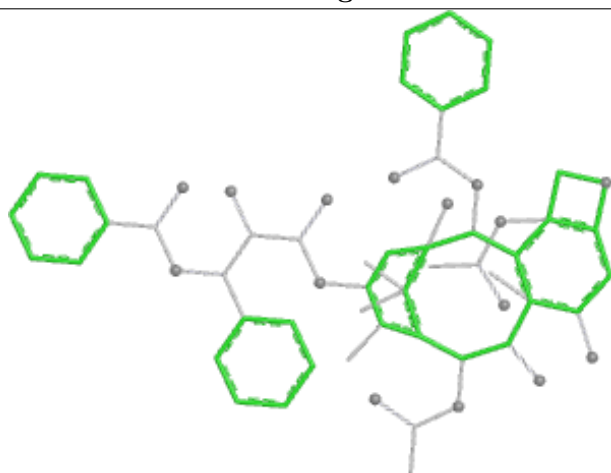
Bond lengths



Bond angles

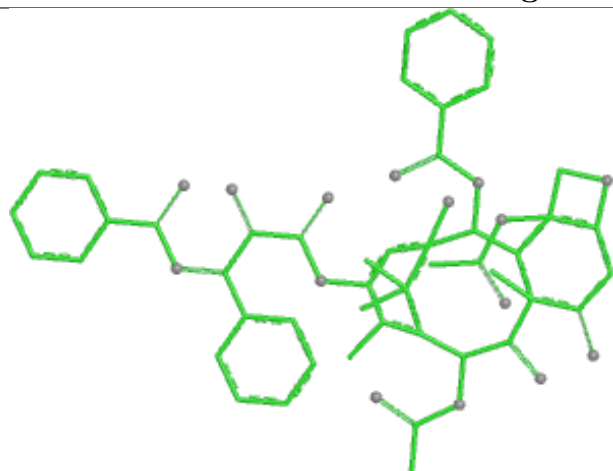


Torsions

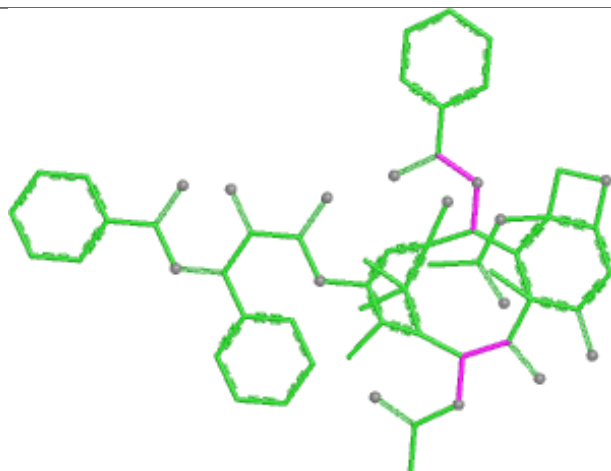


Rings

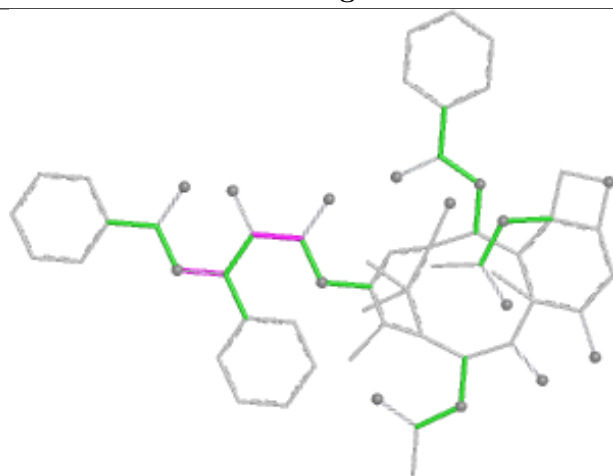
Ligand TA1 S 502



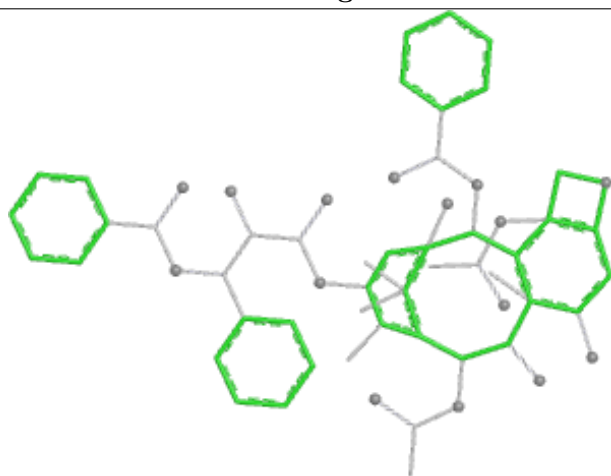
Bond lengths



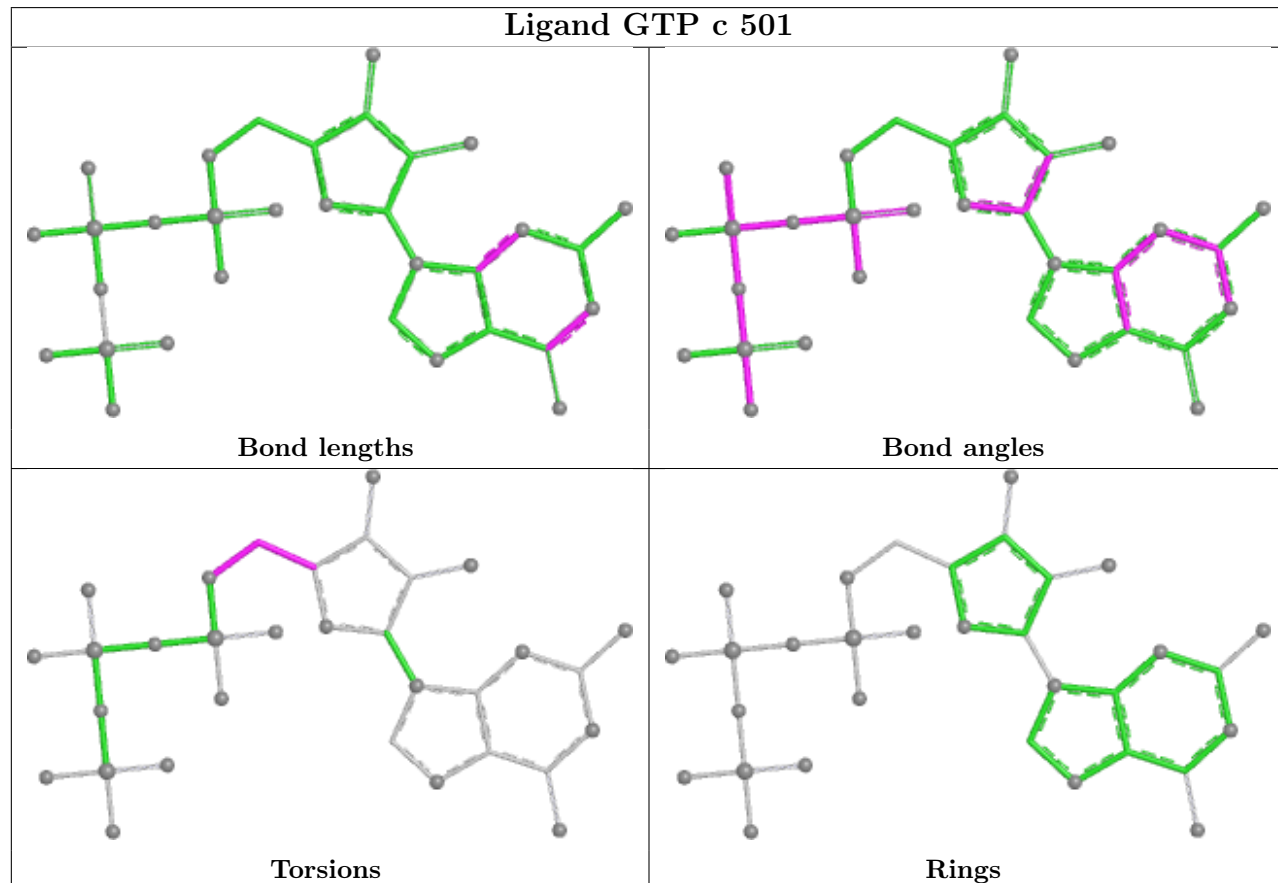
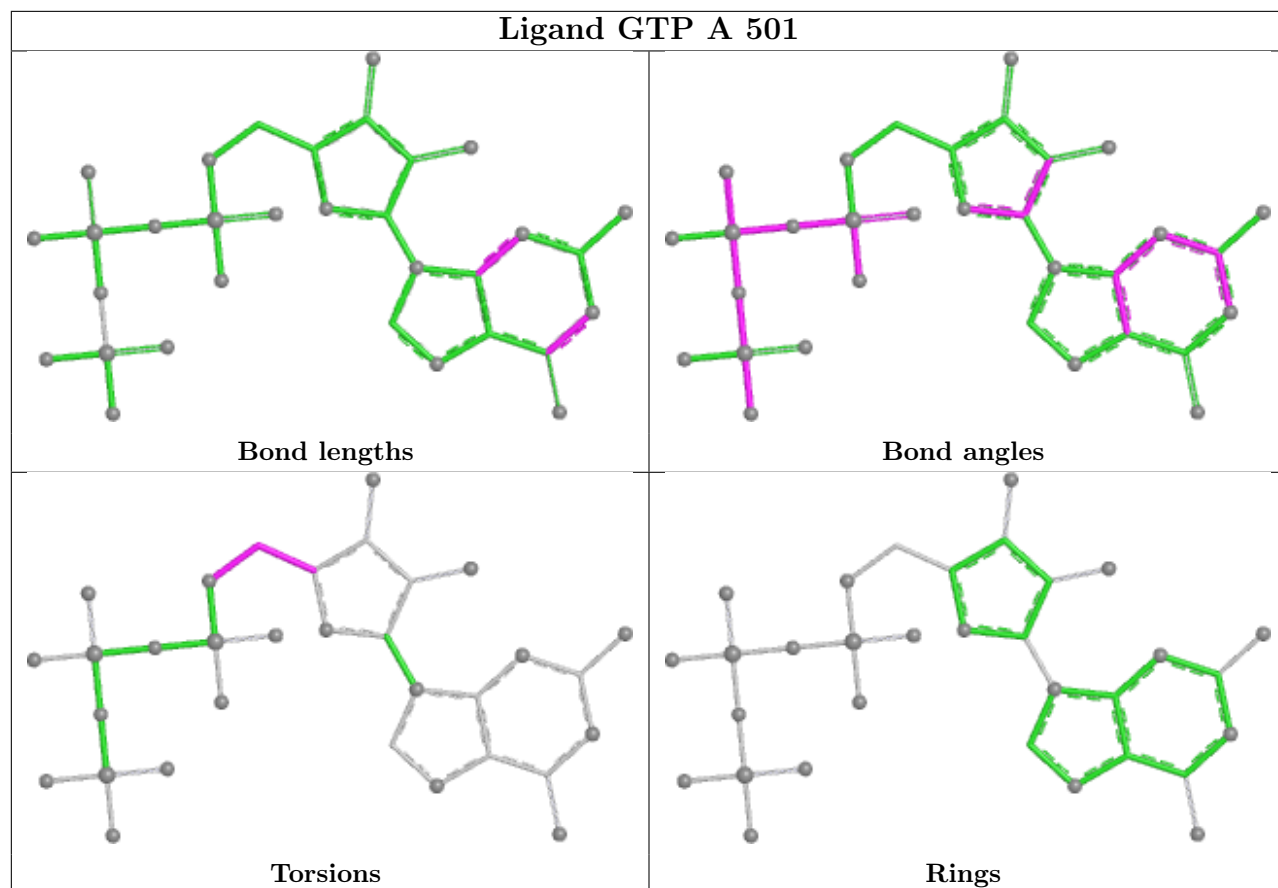
Bond angles

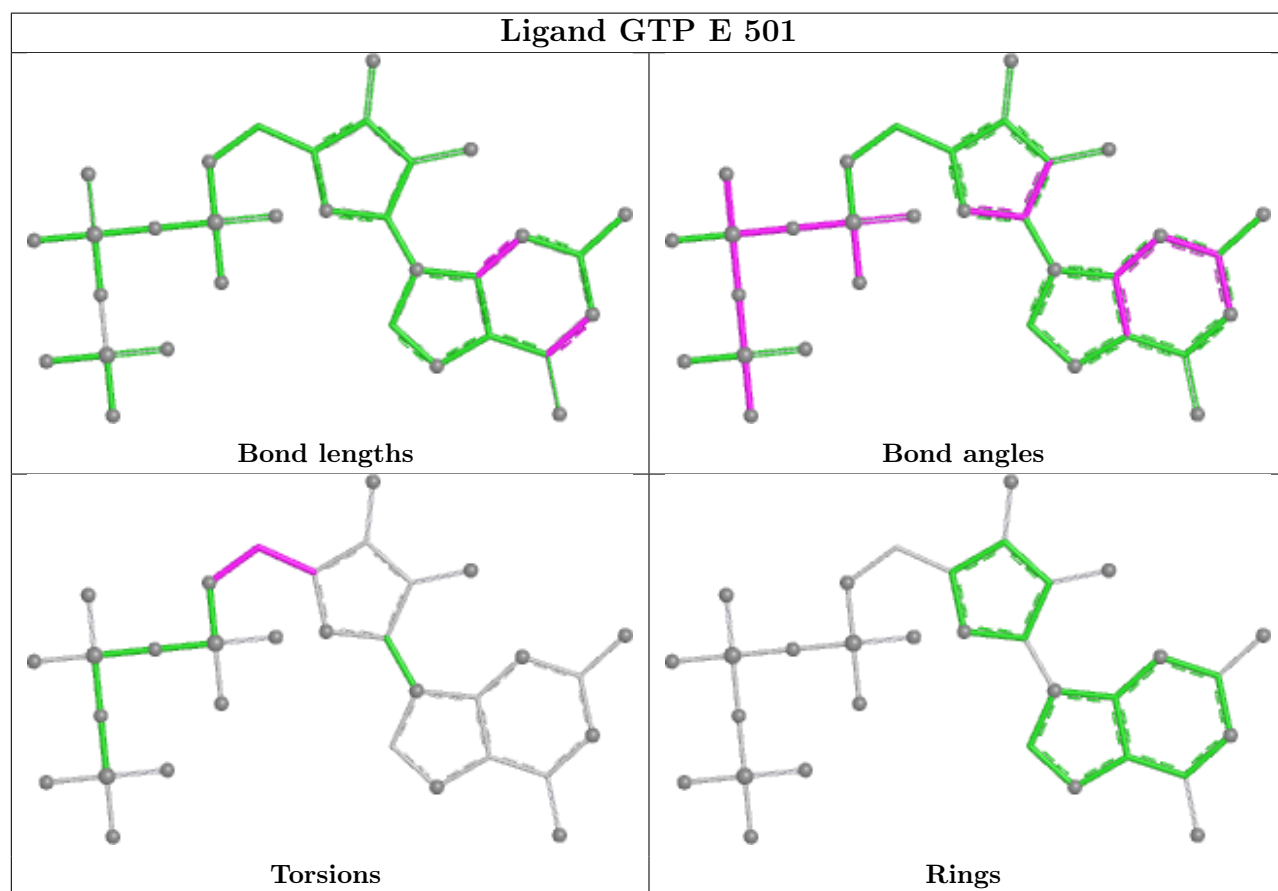
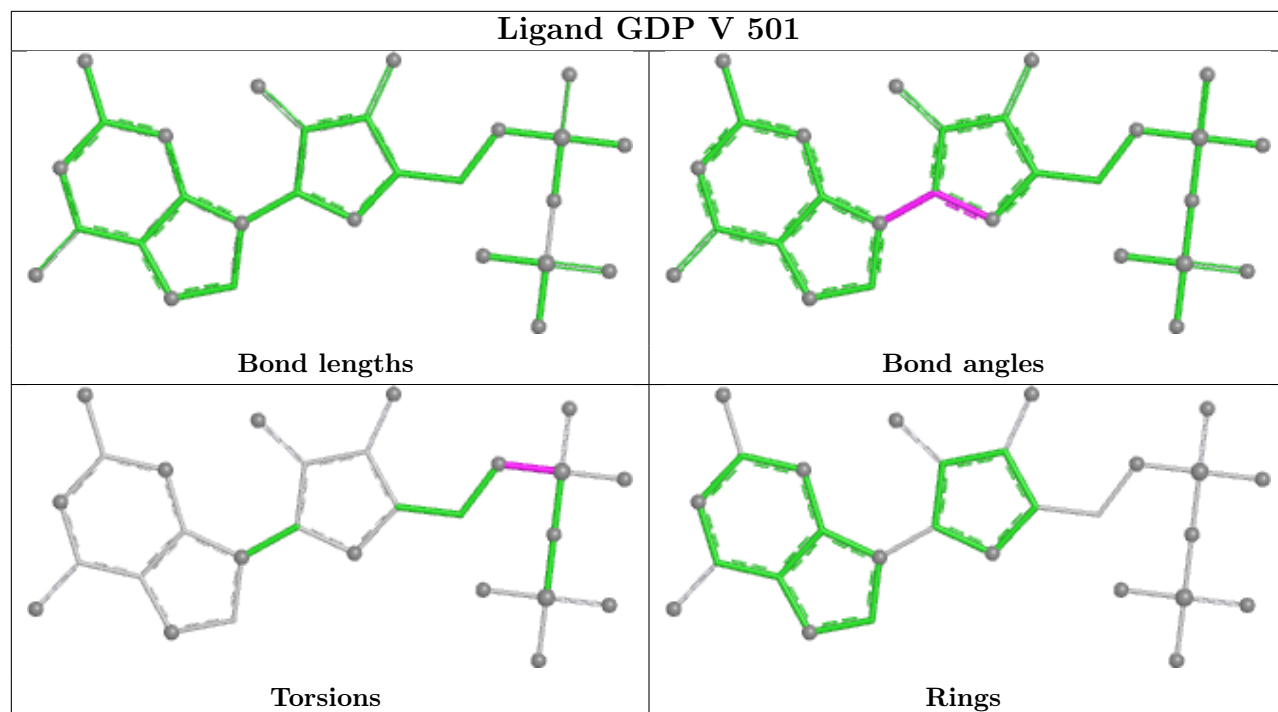


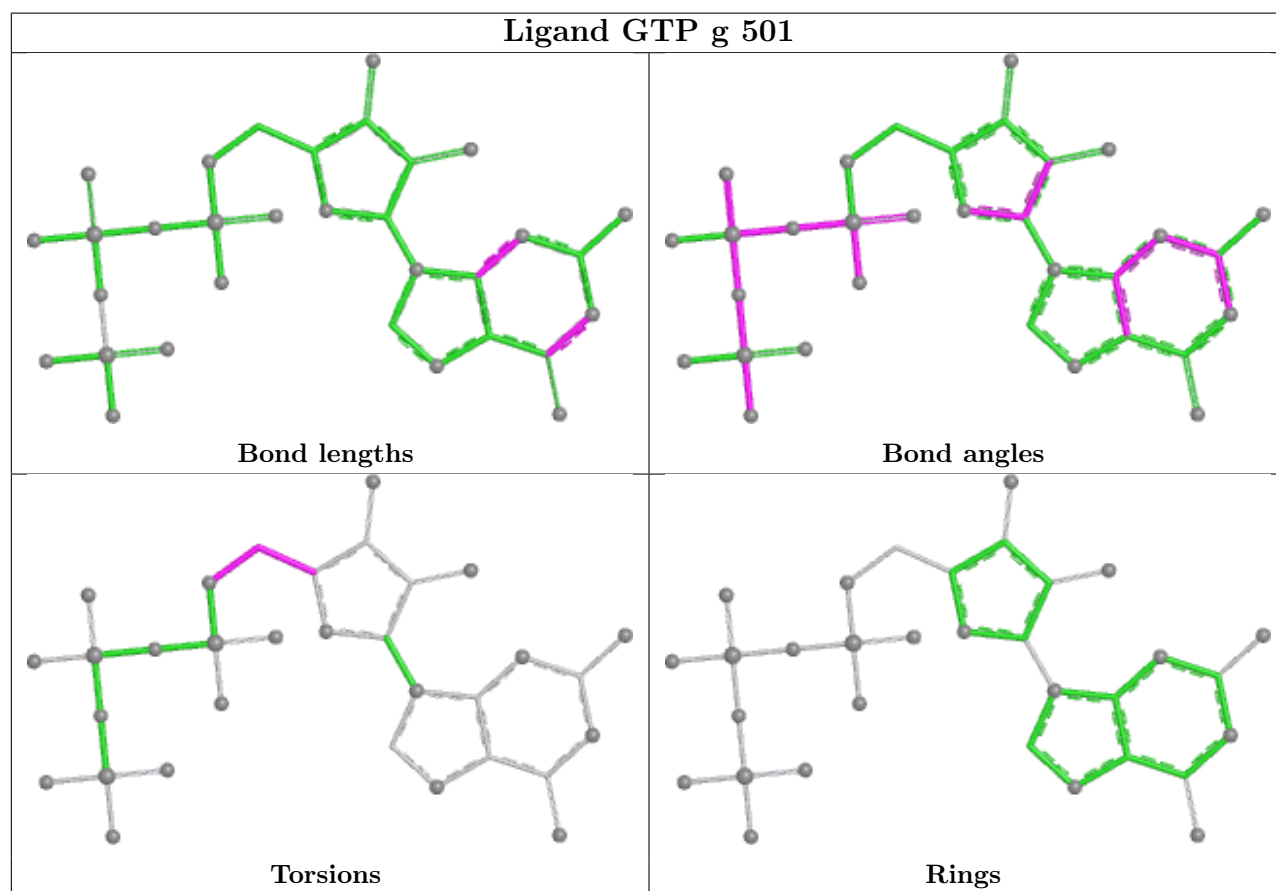
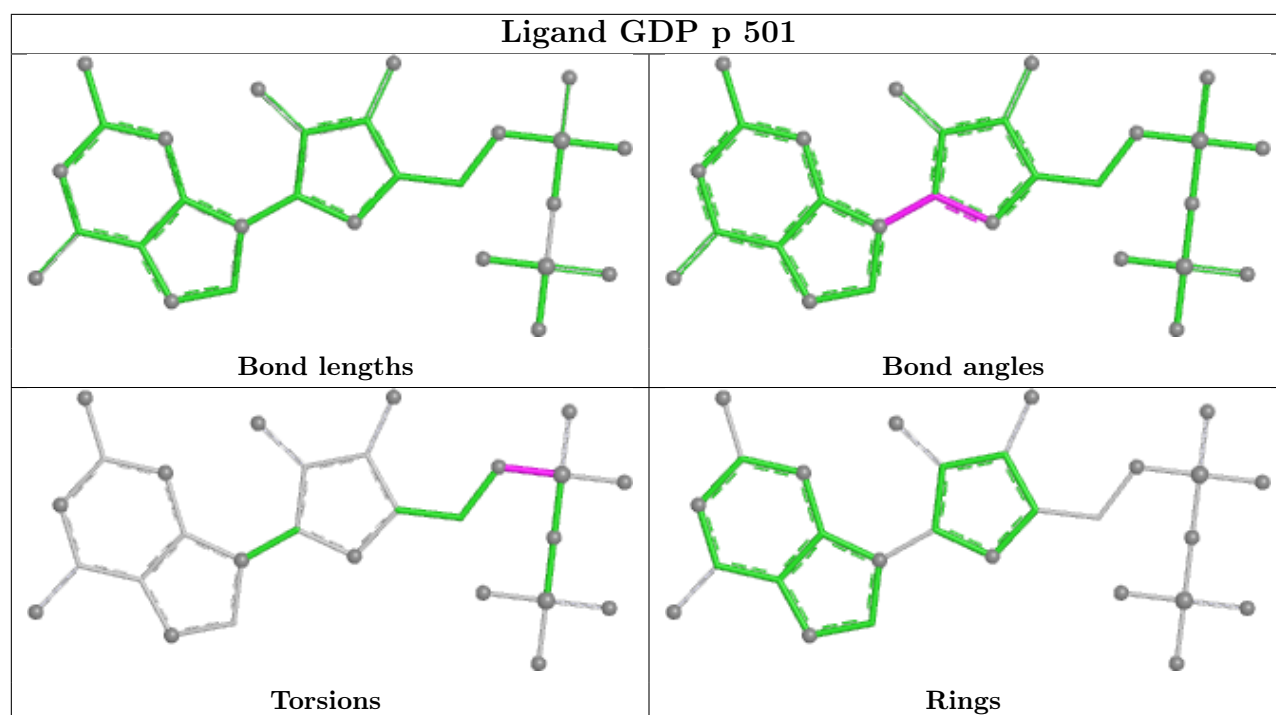
Torsions

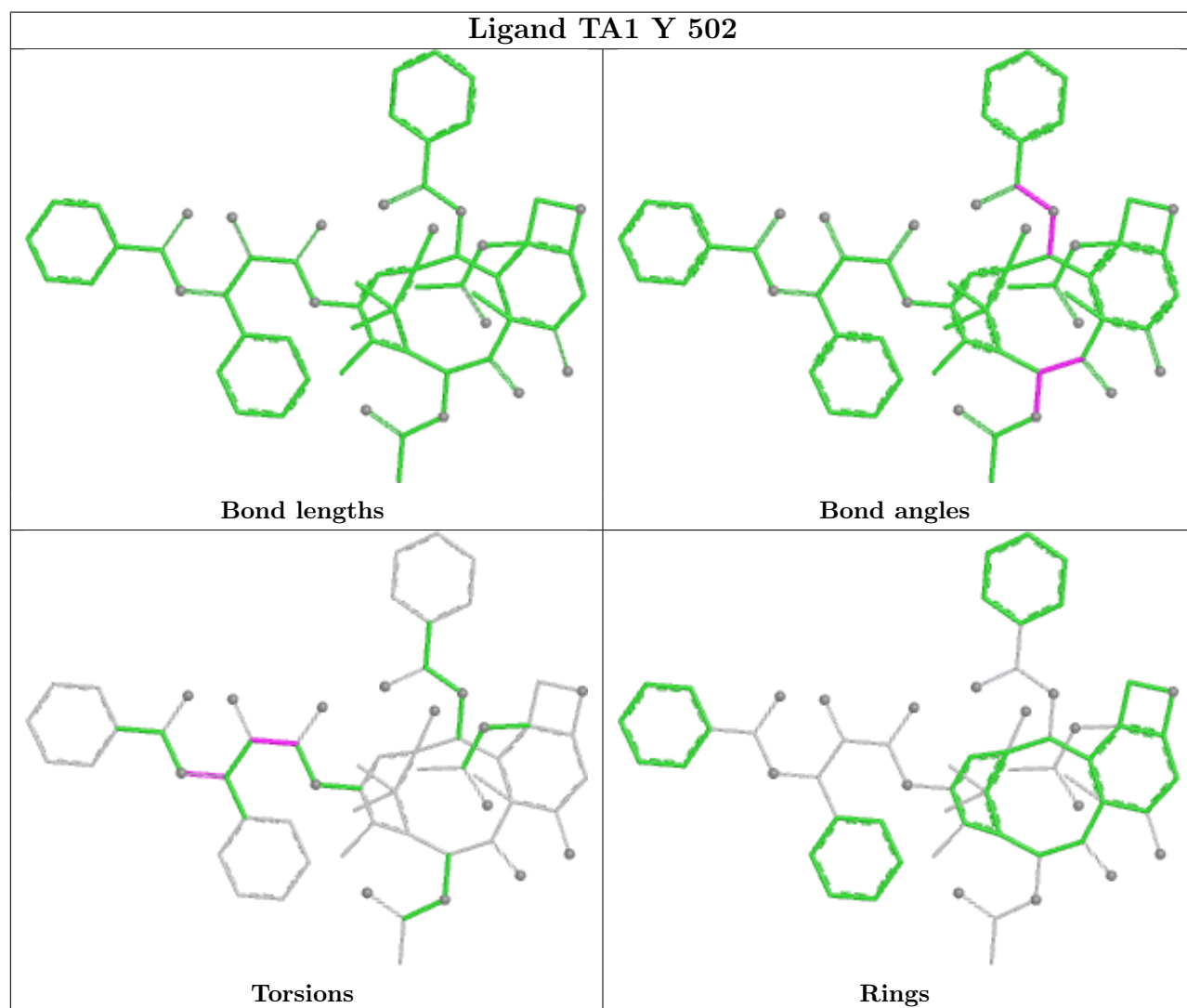
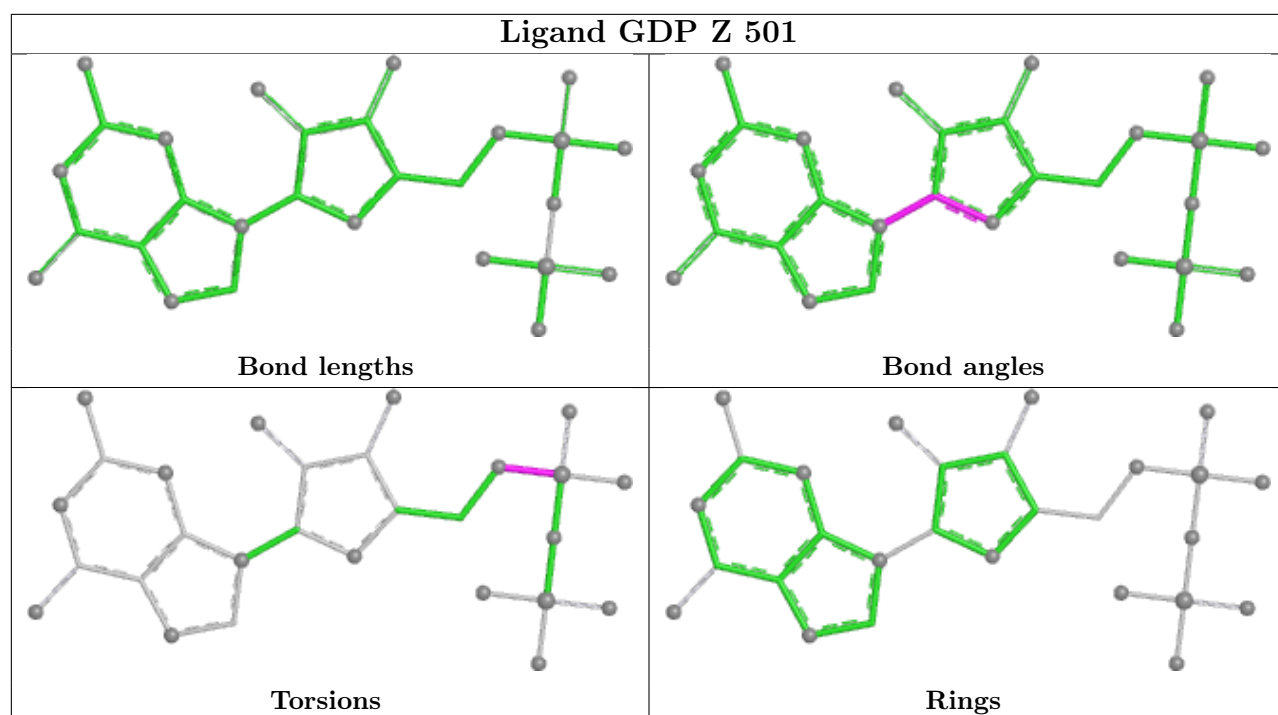


Rings

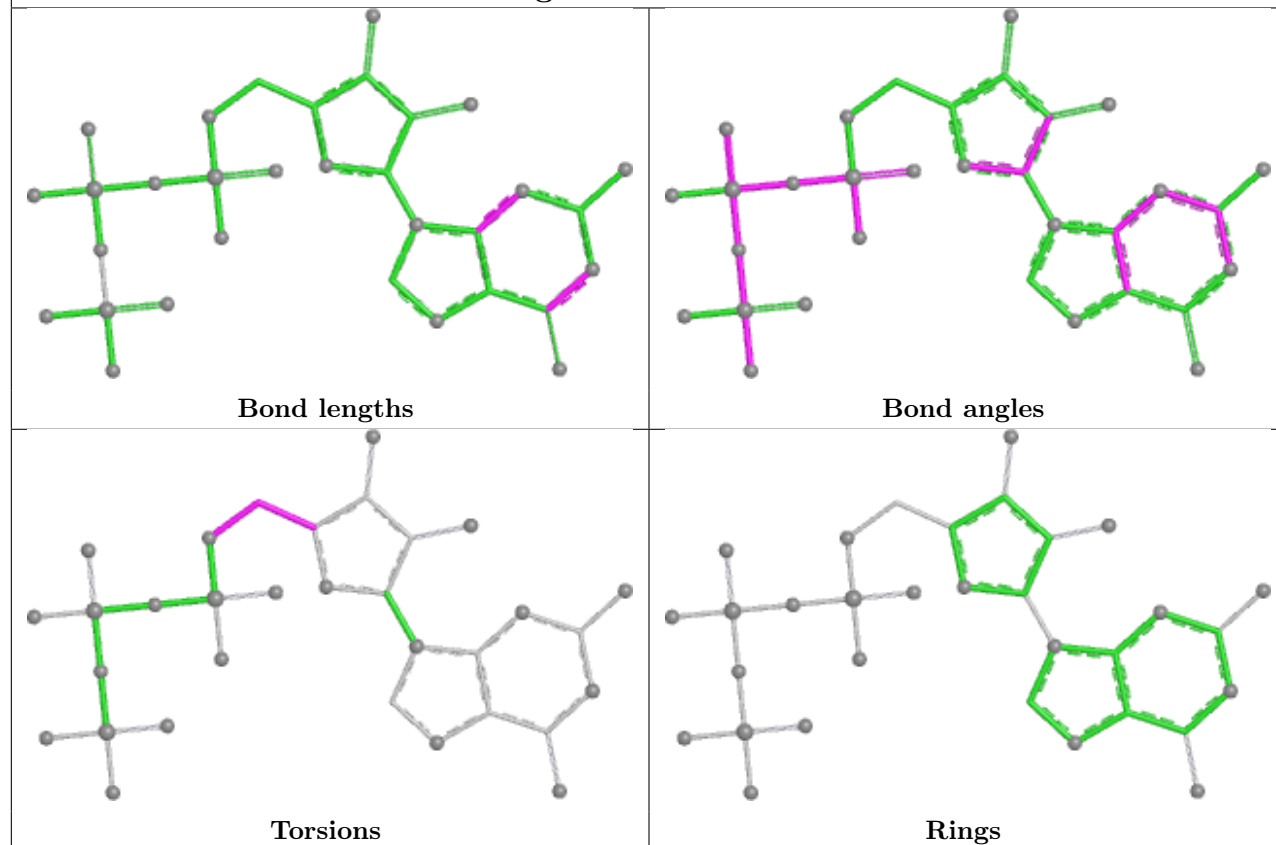




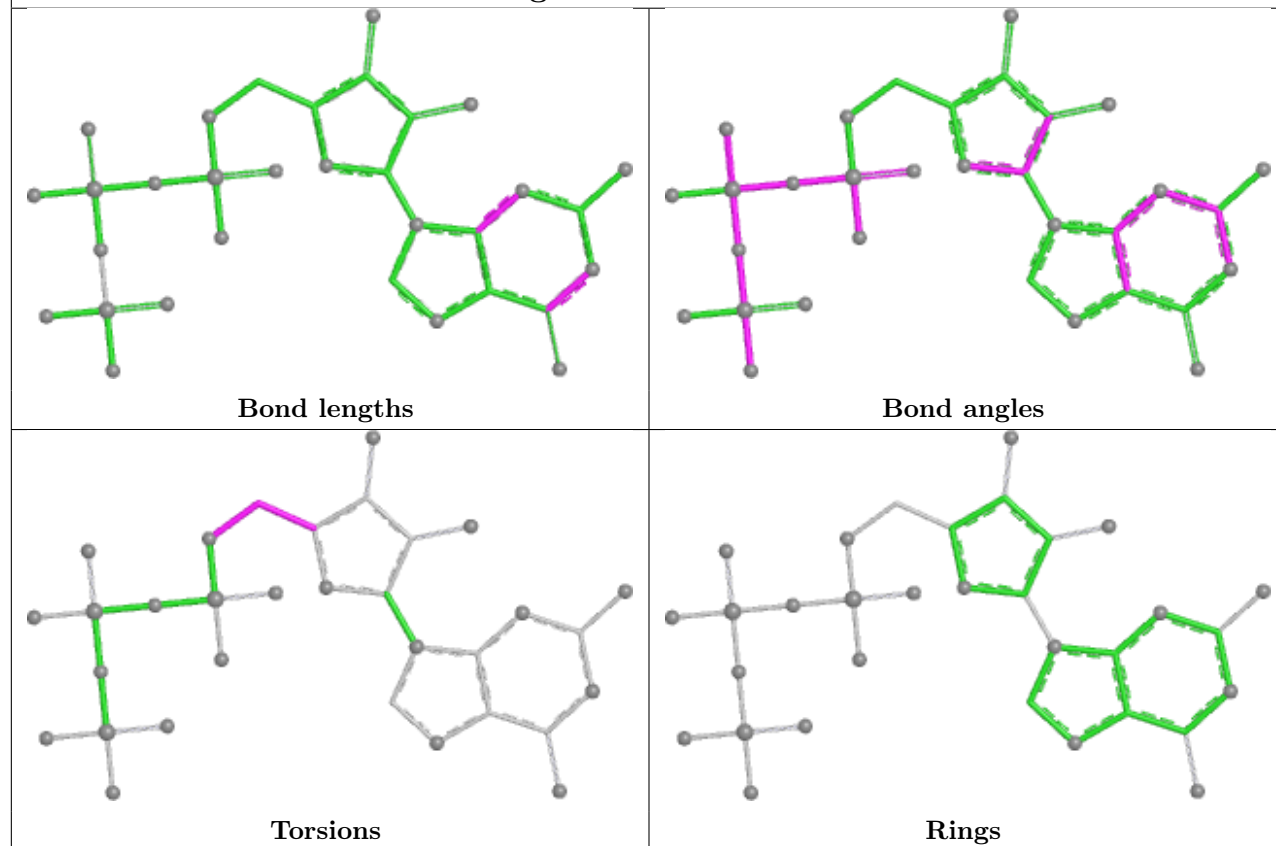


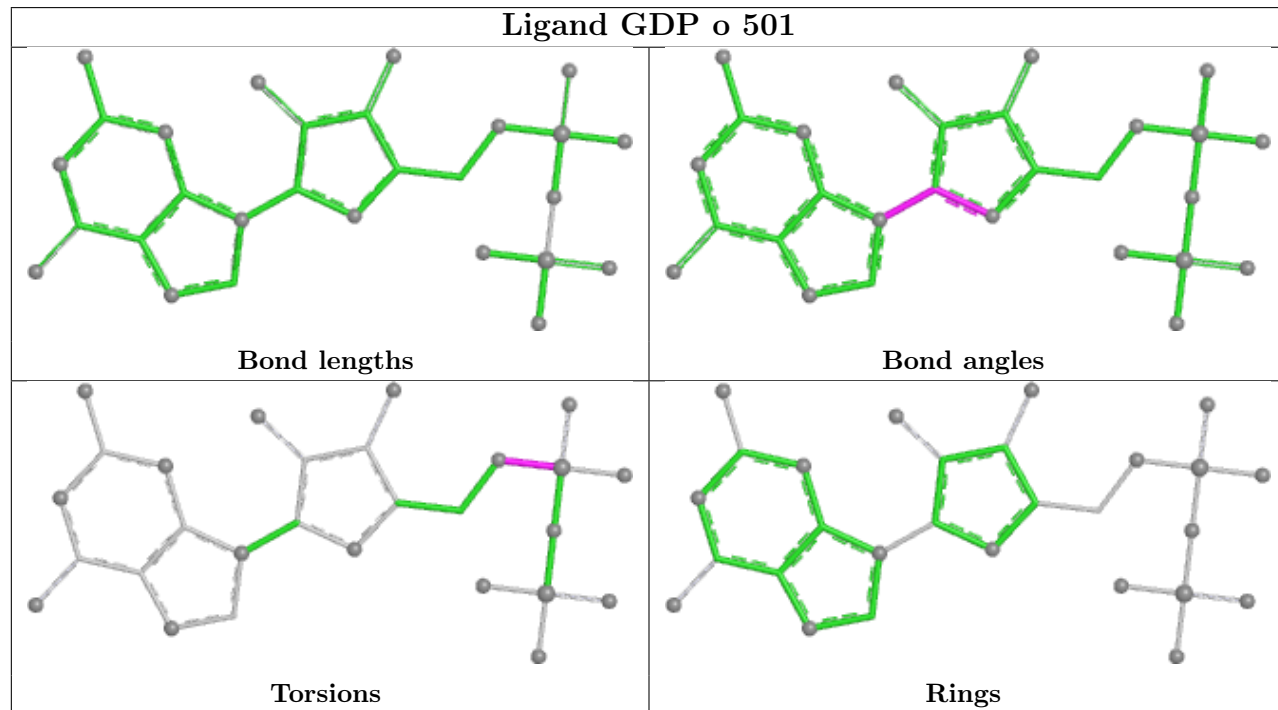
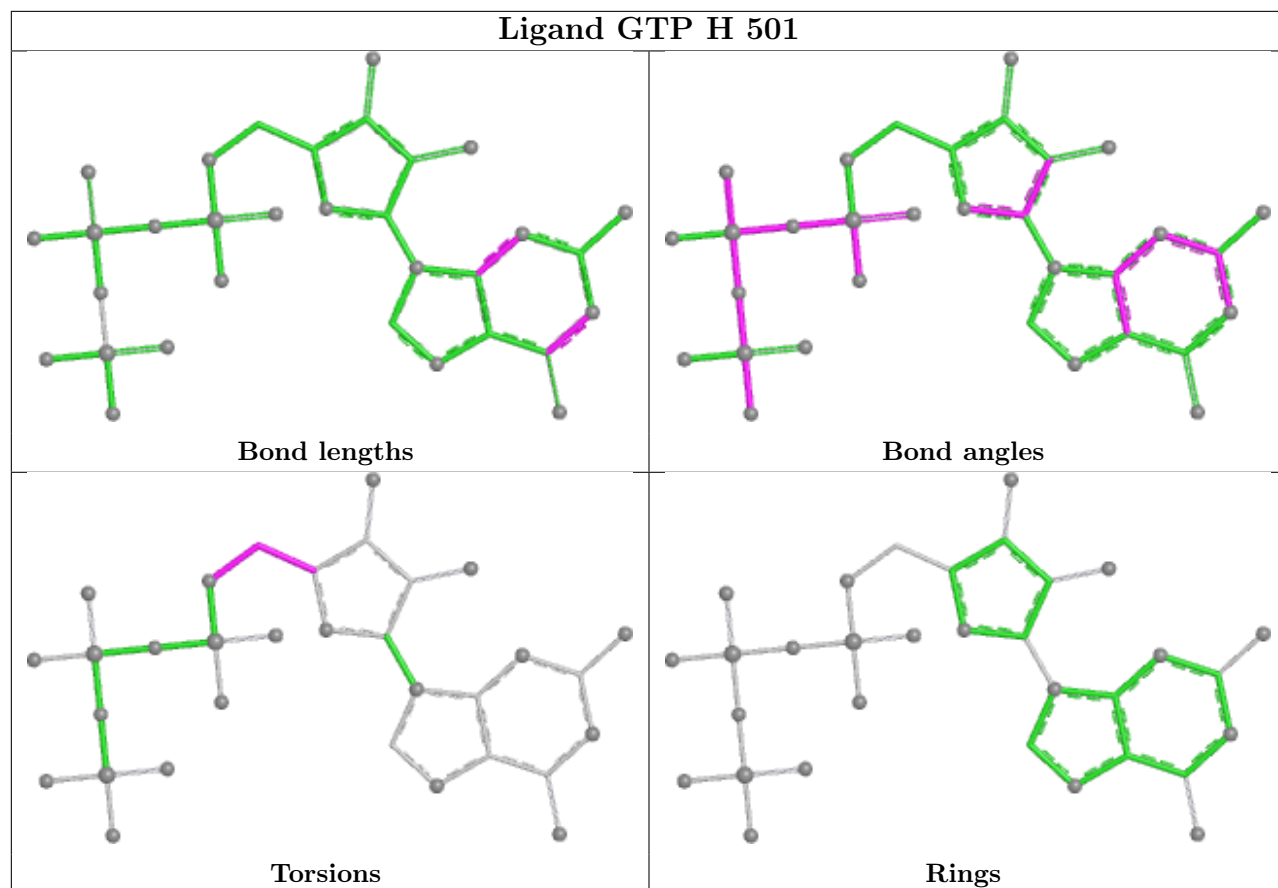


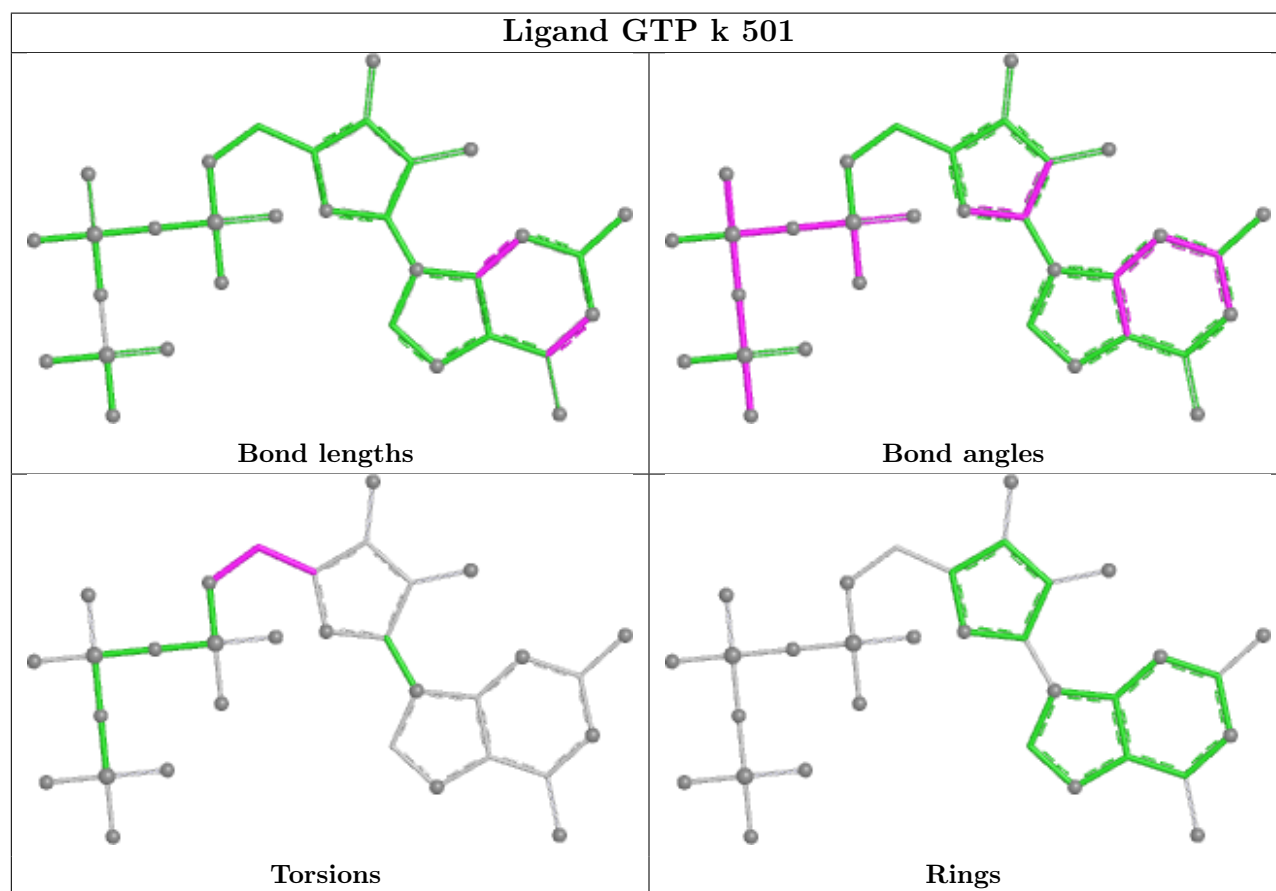
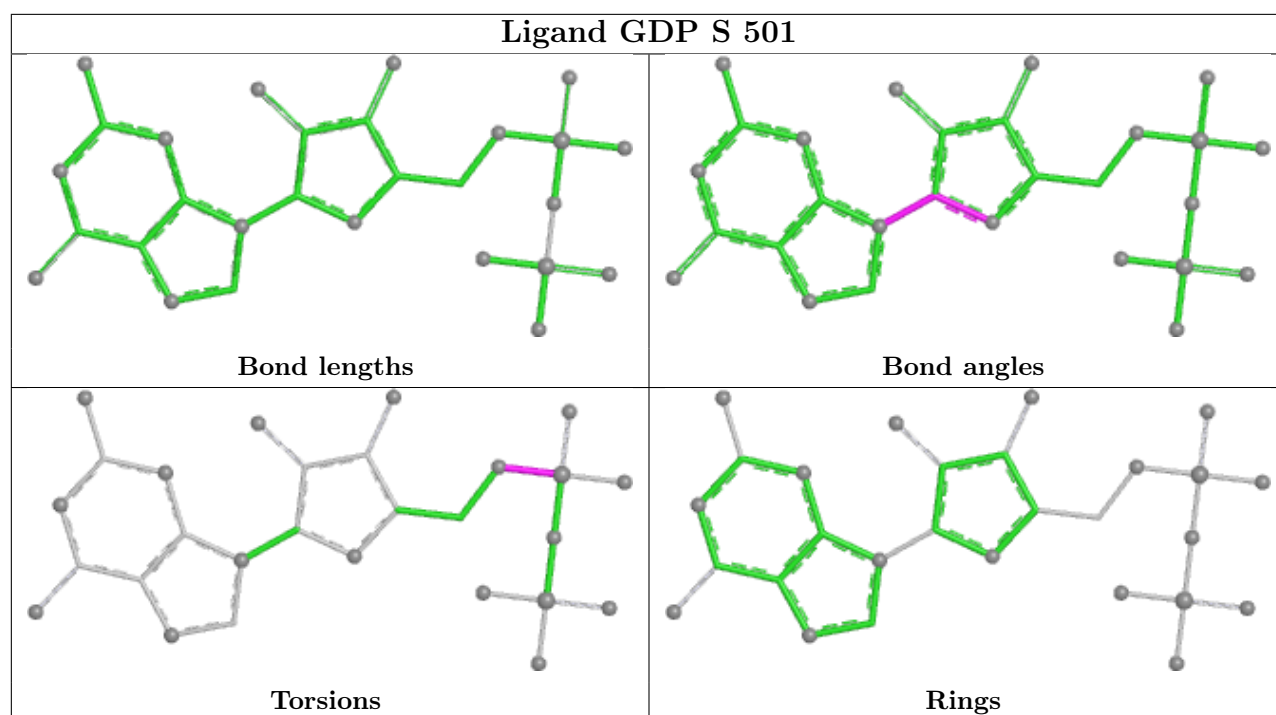
Ligand GTP e 501



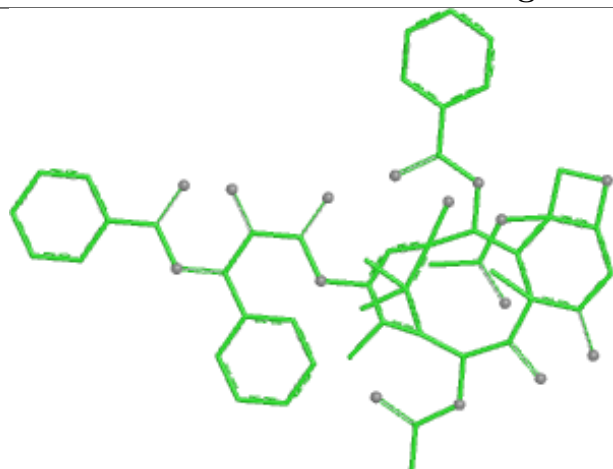
Ligand GTP N 501



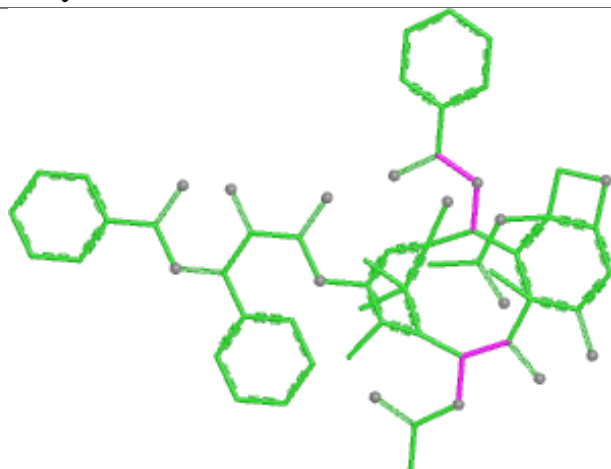




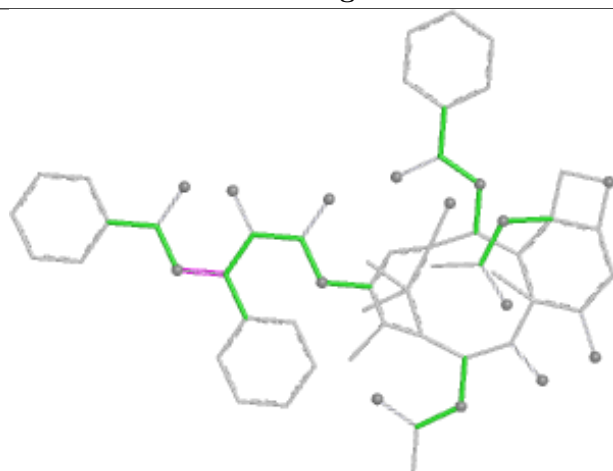
Ligand TA1 Q 502



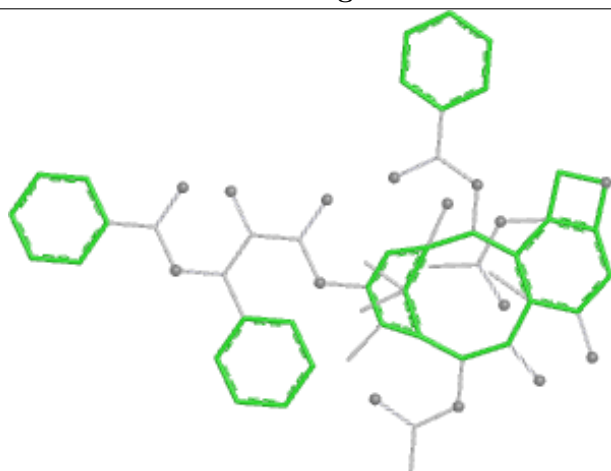
Bond lengths



Bond angles

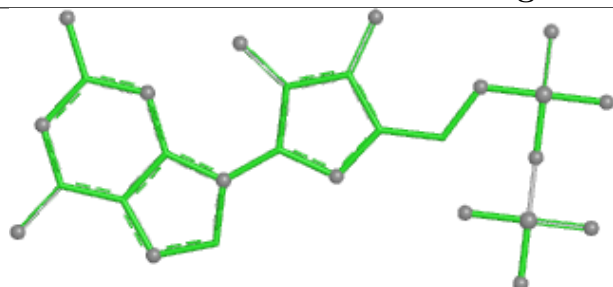


Torsions

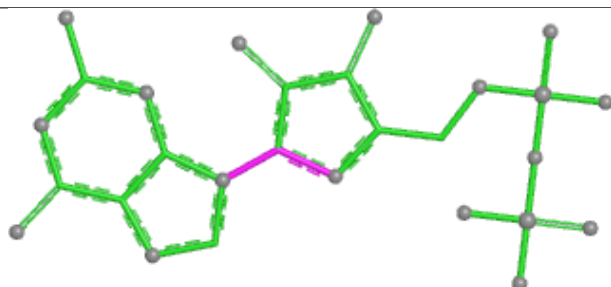


Rings

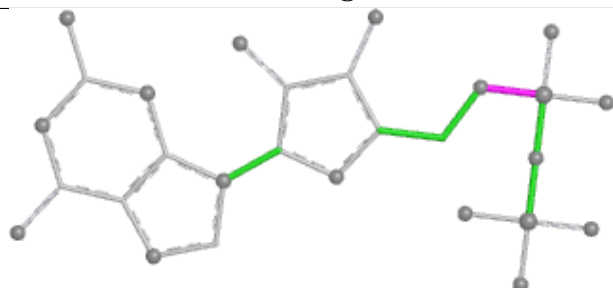
Ligand GDP s 501



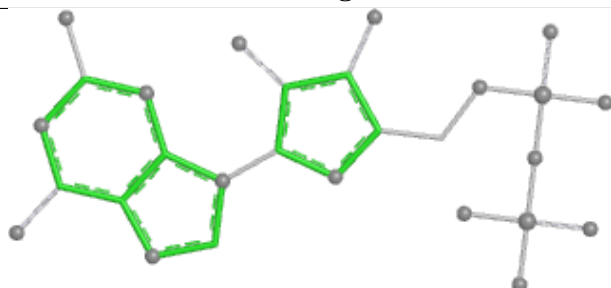
Bond lengths



Bond angles

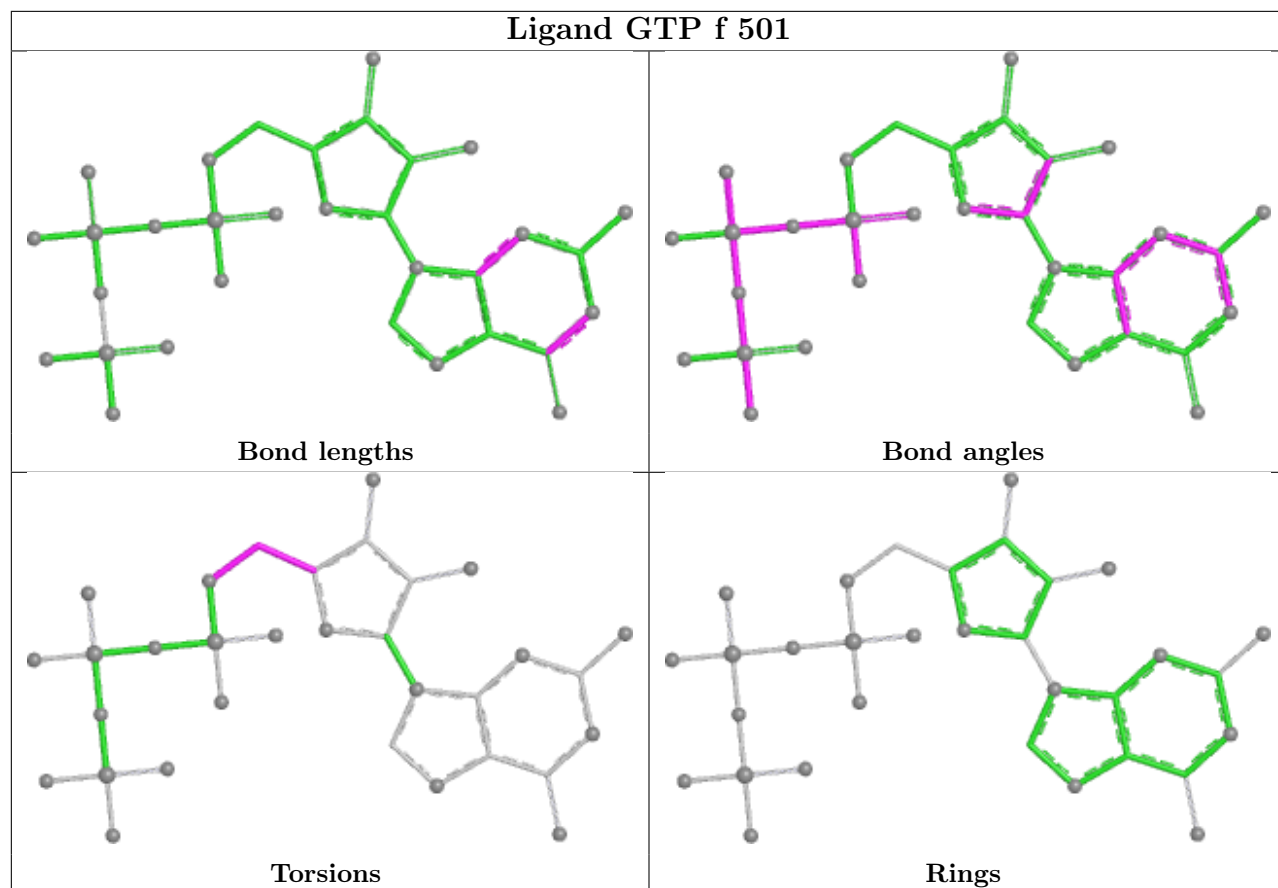


Torsions

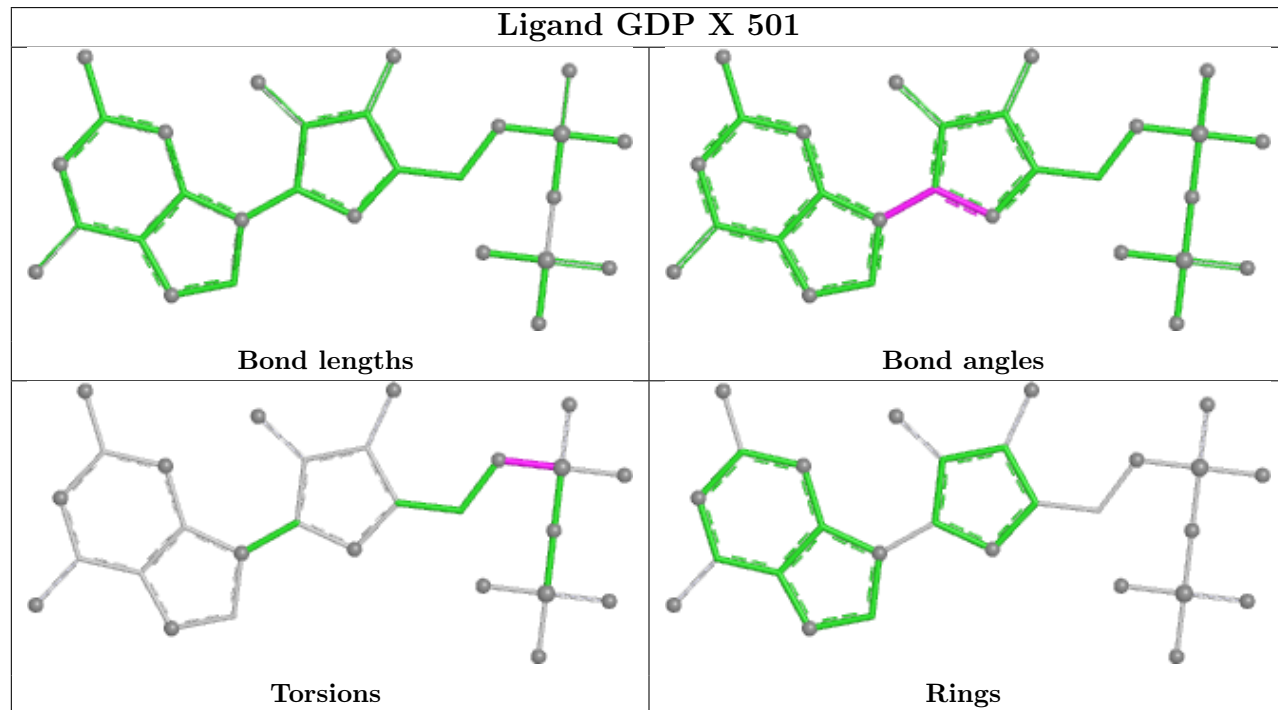


Rings

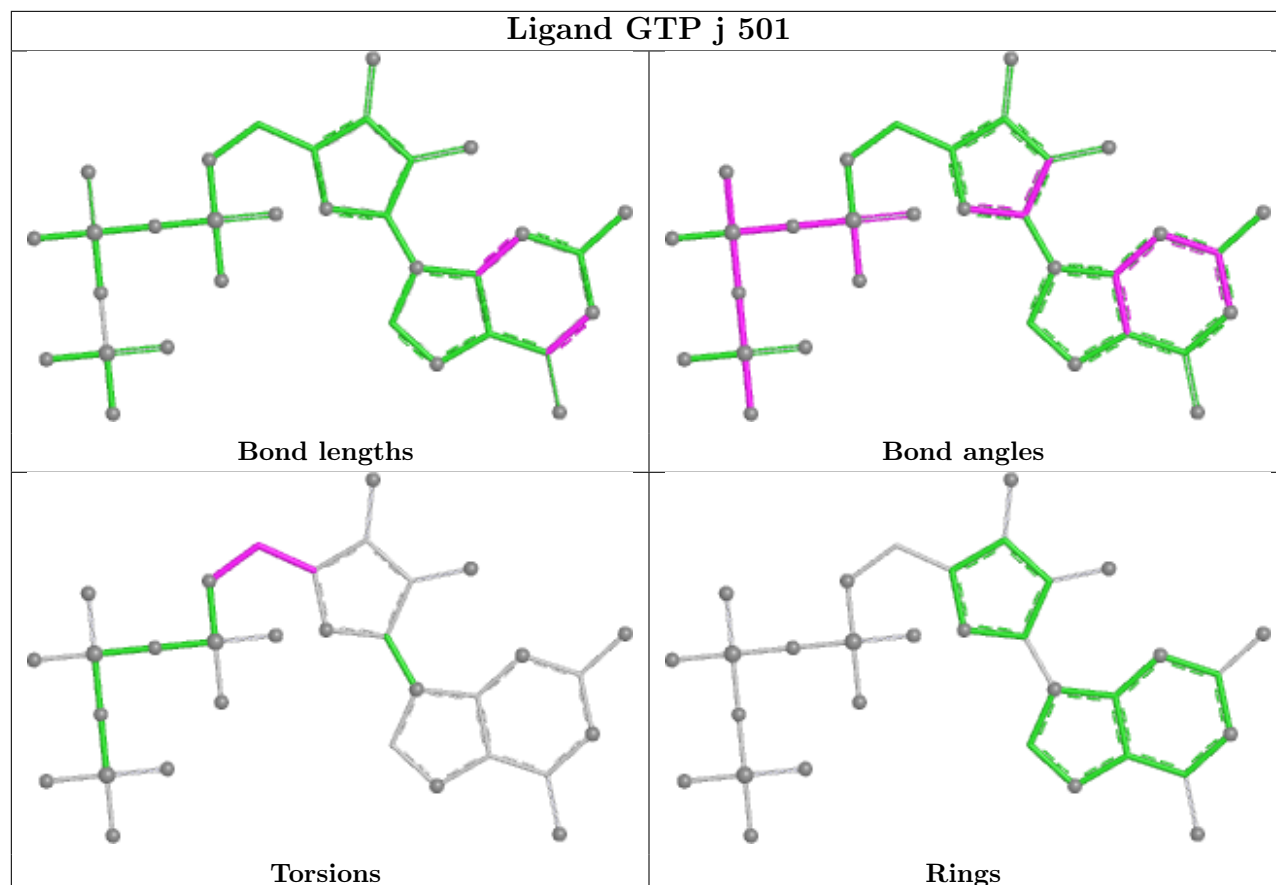
Ligand GTP f 501



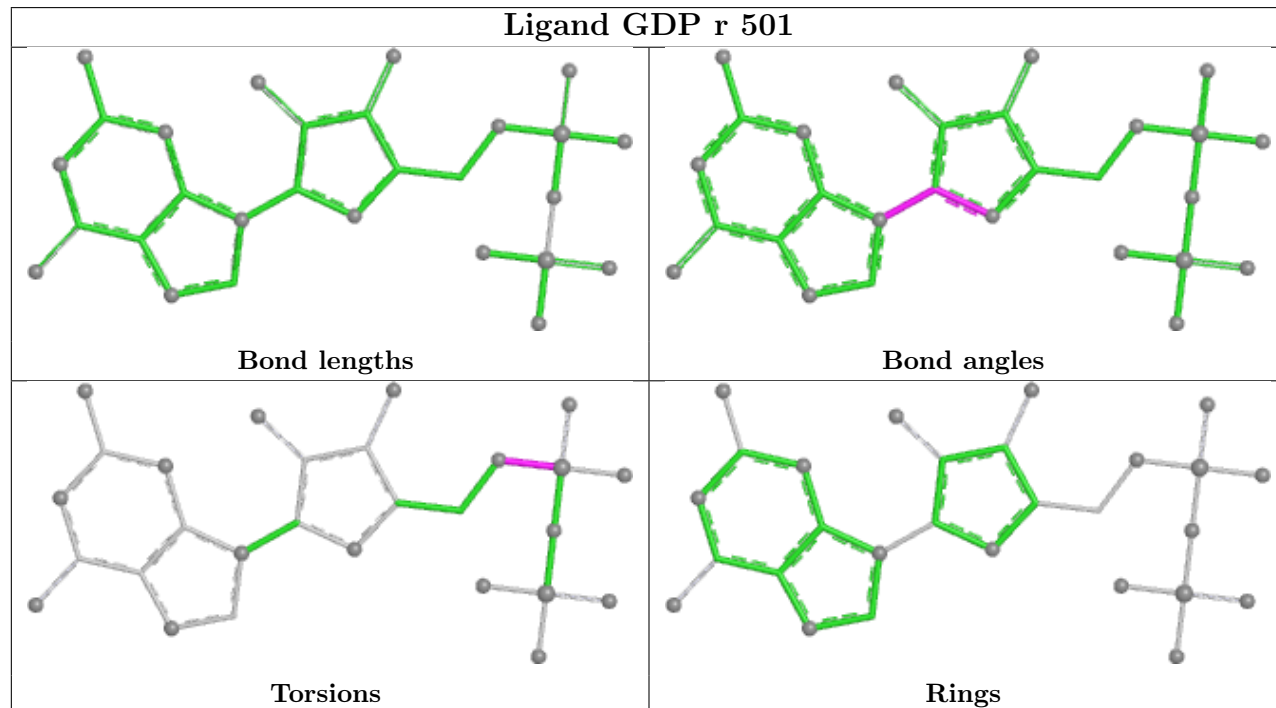
Ligand GDP X 501

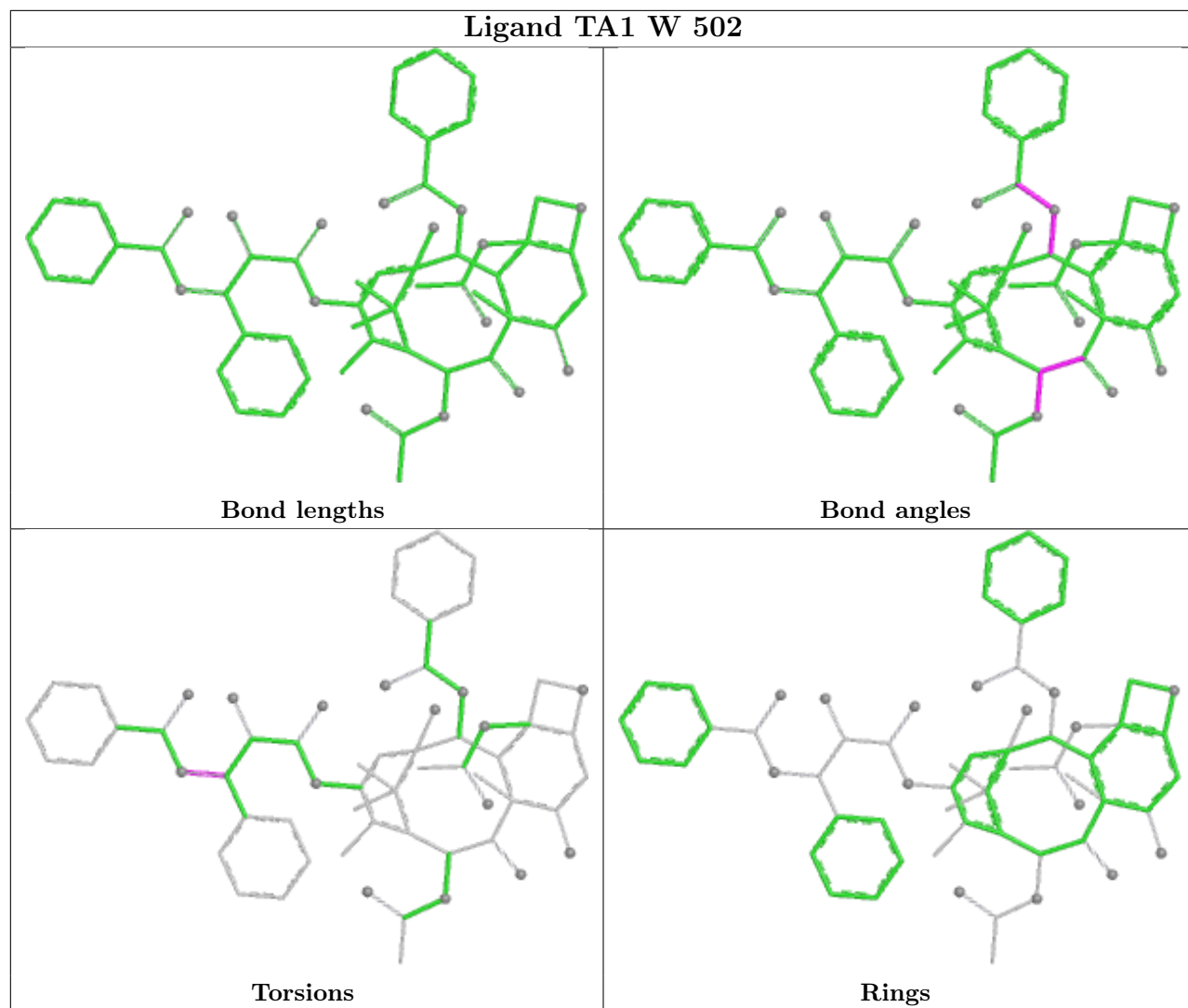


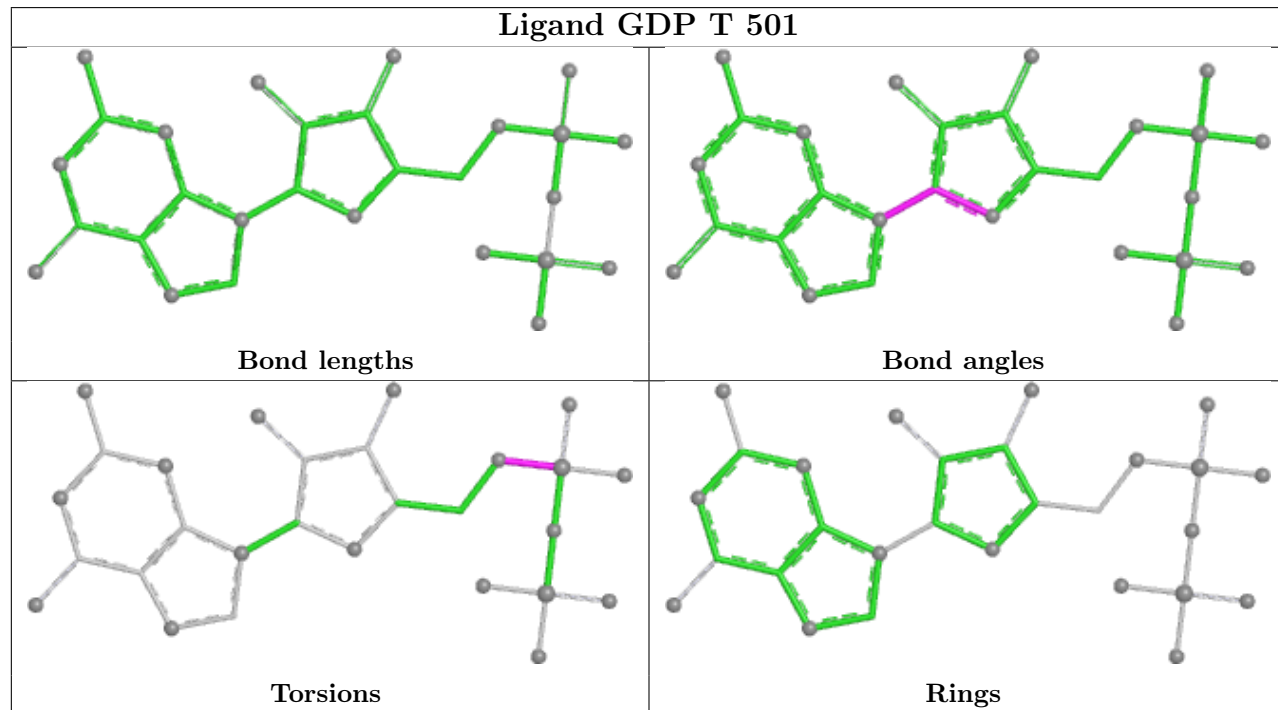
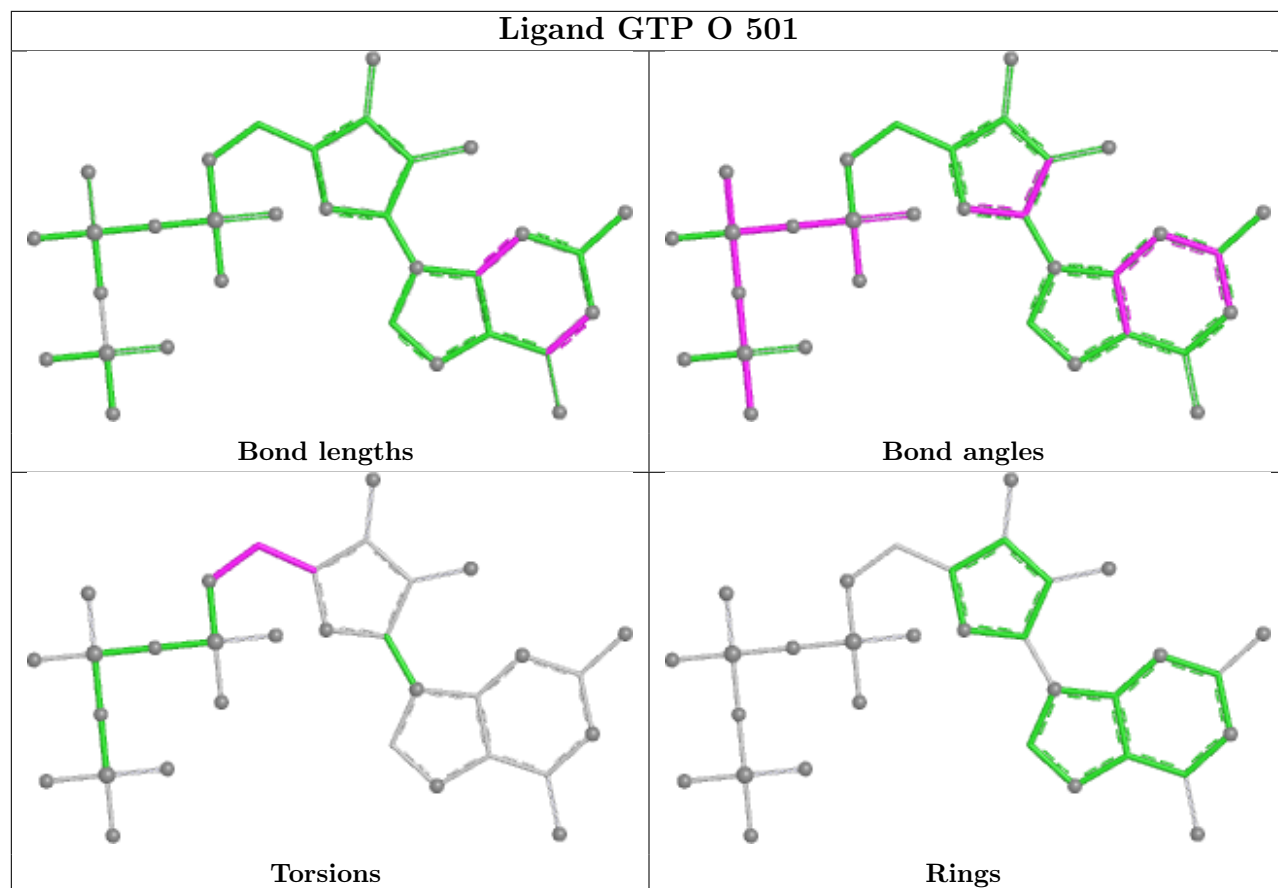
Ligand GTP j 501

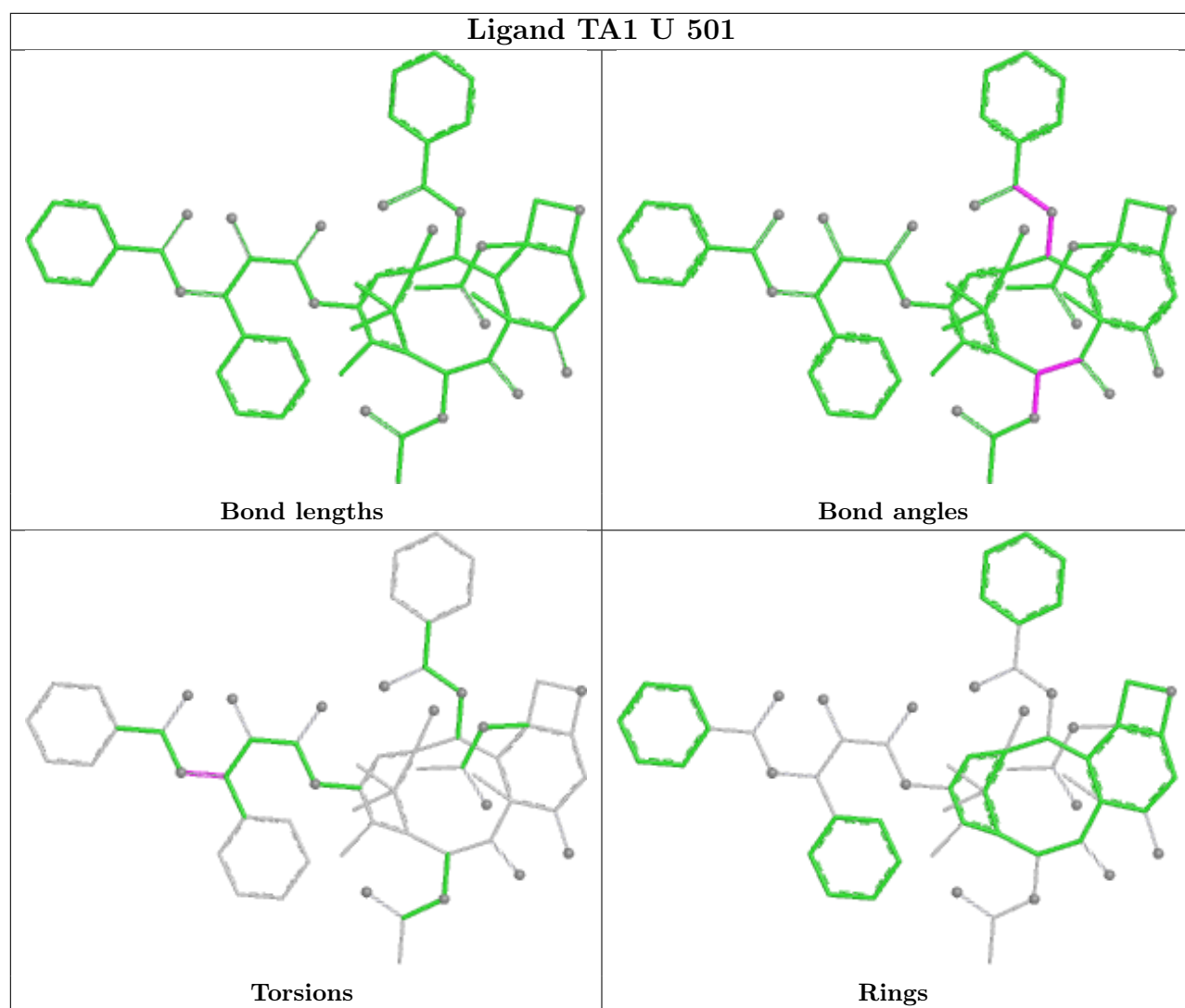


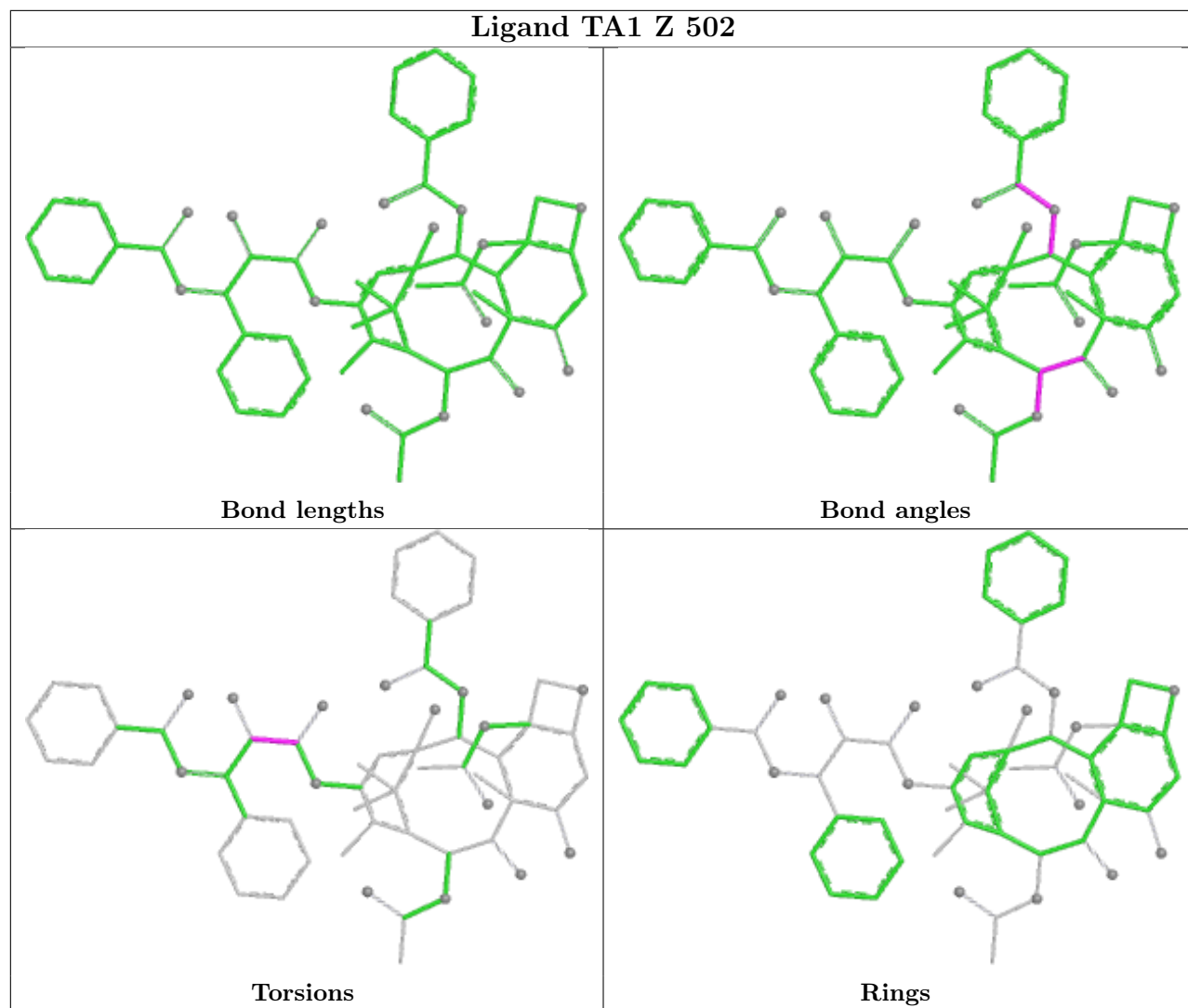
Ligand GDP r 501

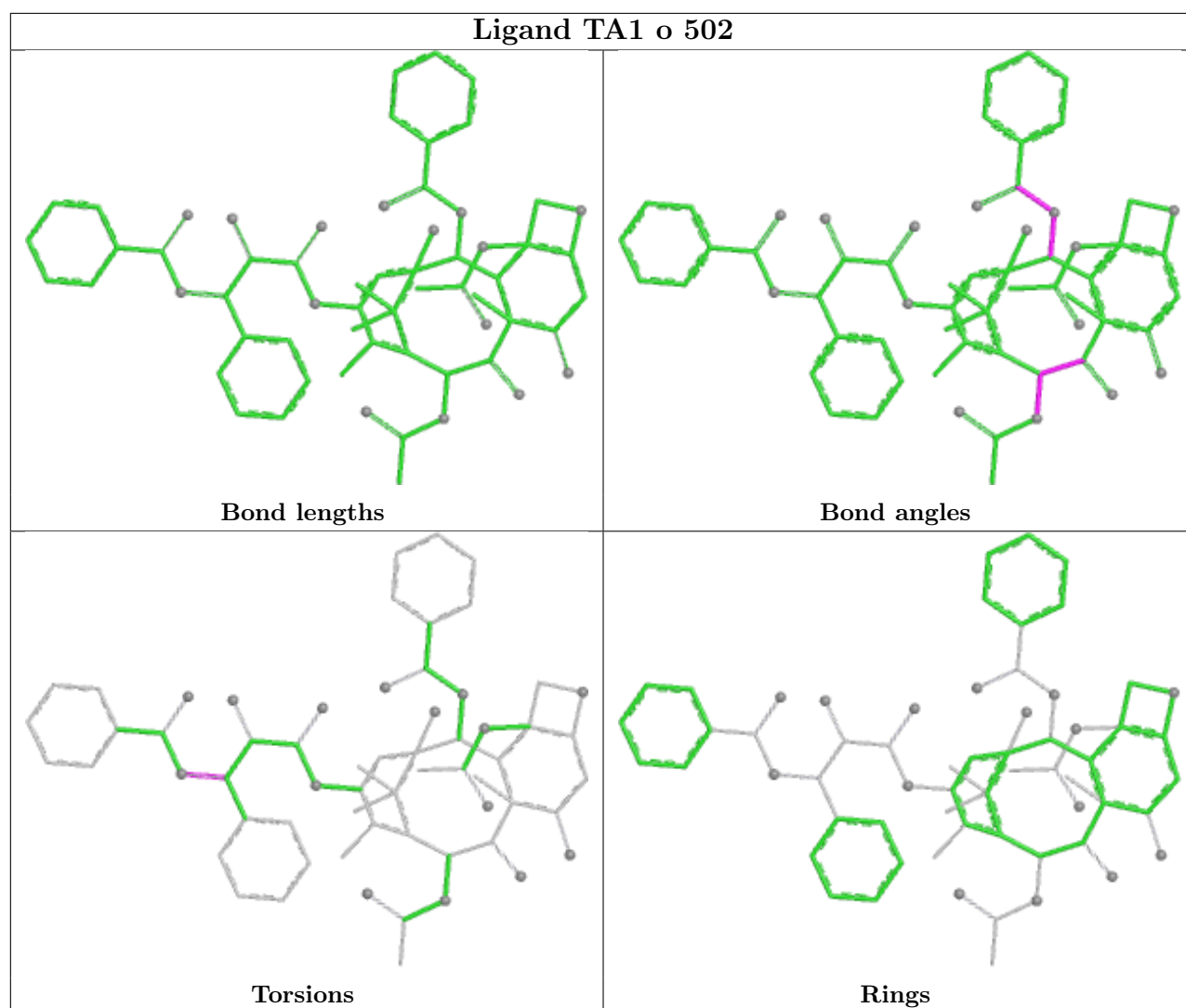




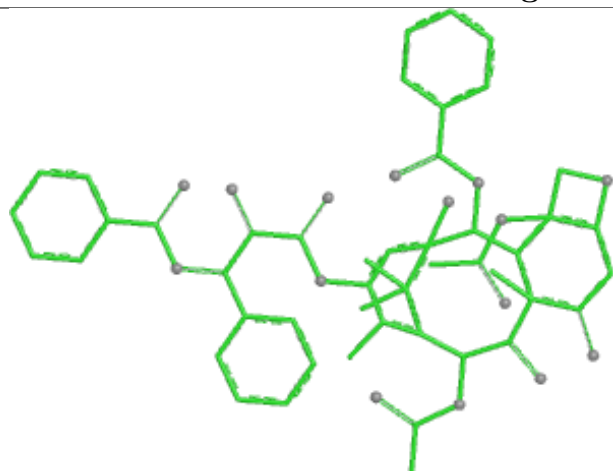




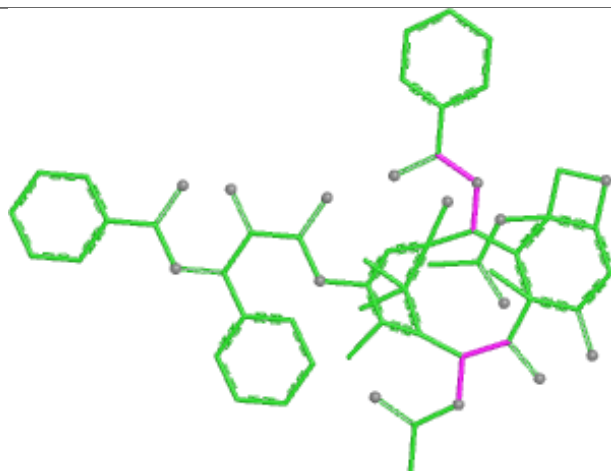




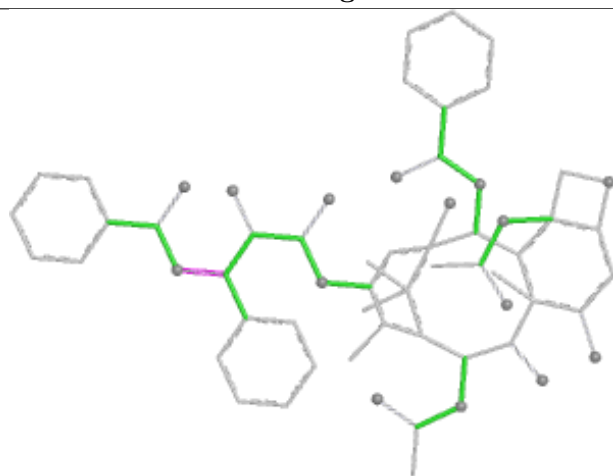
Ligand TA1 b 502



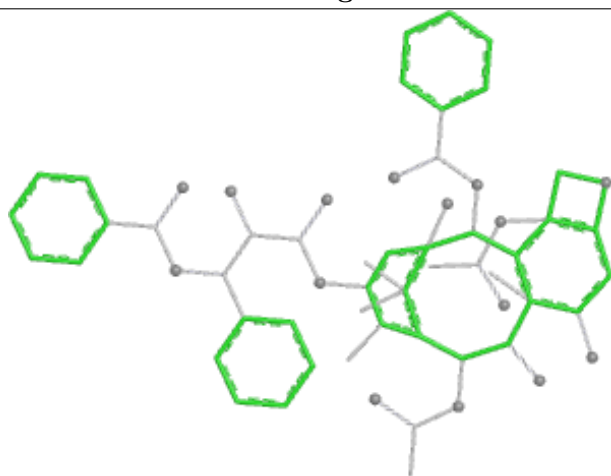
Bond lengths



Bond angles

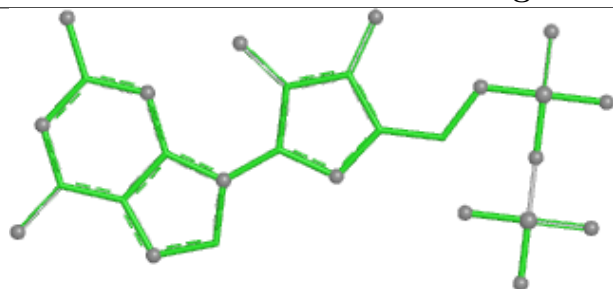


Torsions

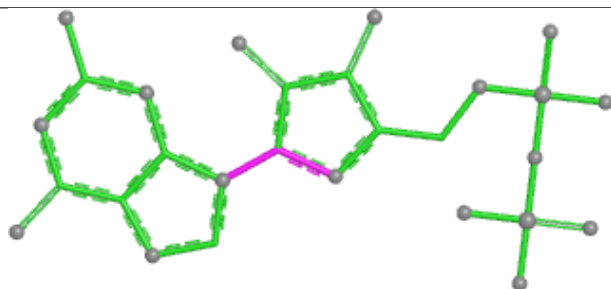


Rings

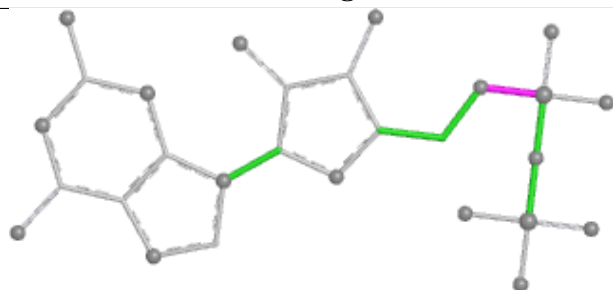
Ligand GDP F 502



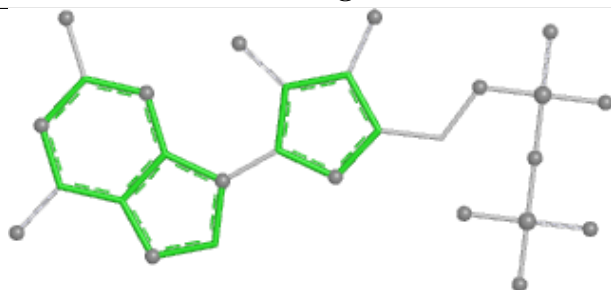
Bond lengths



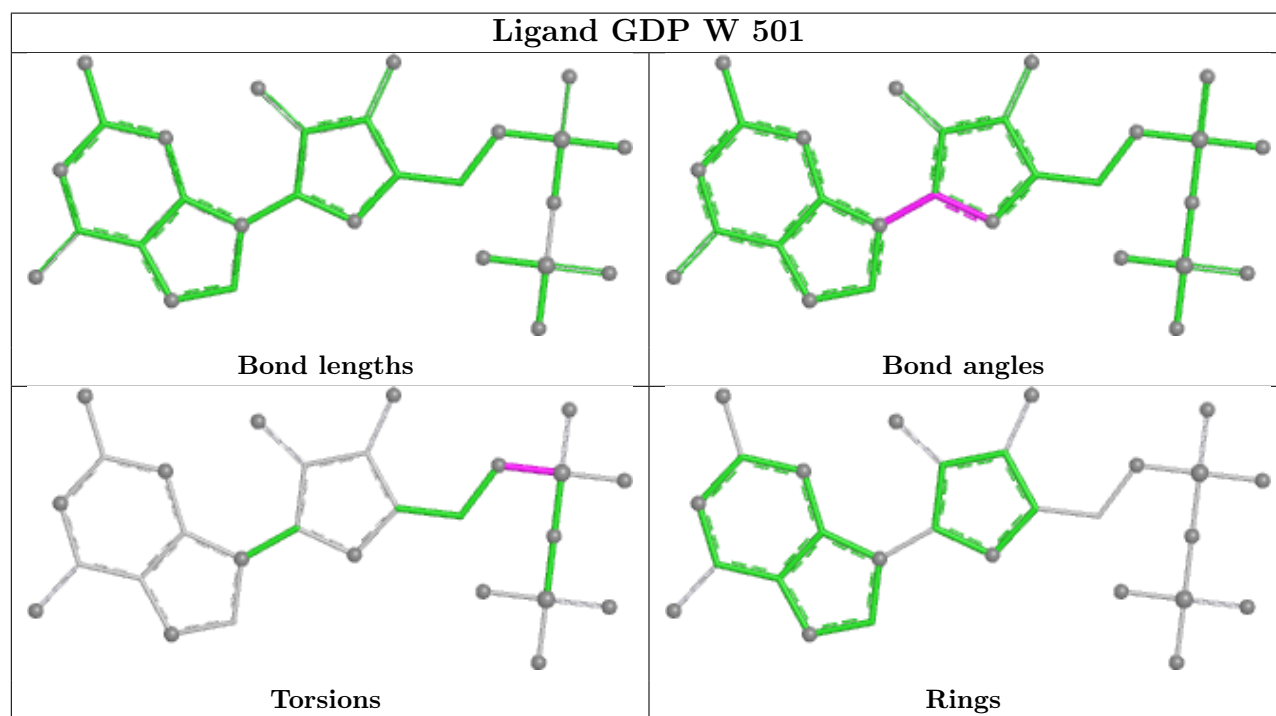
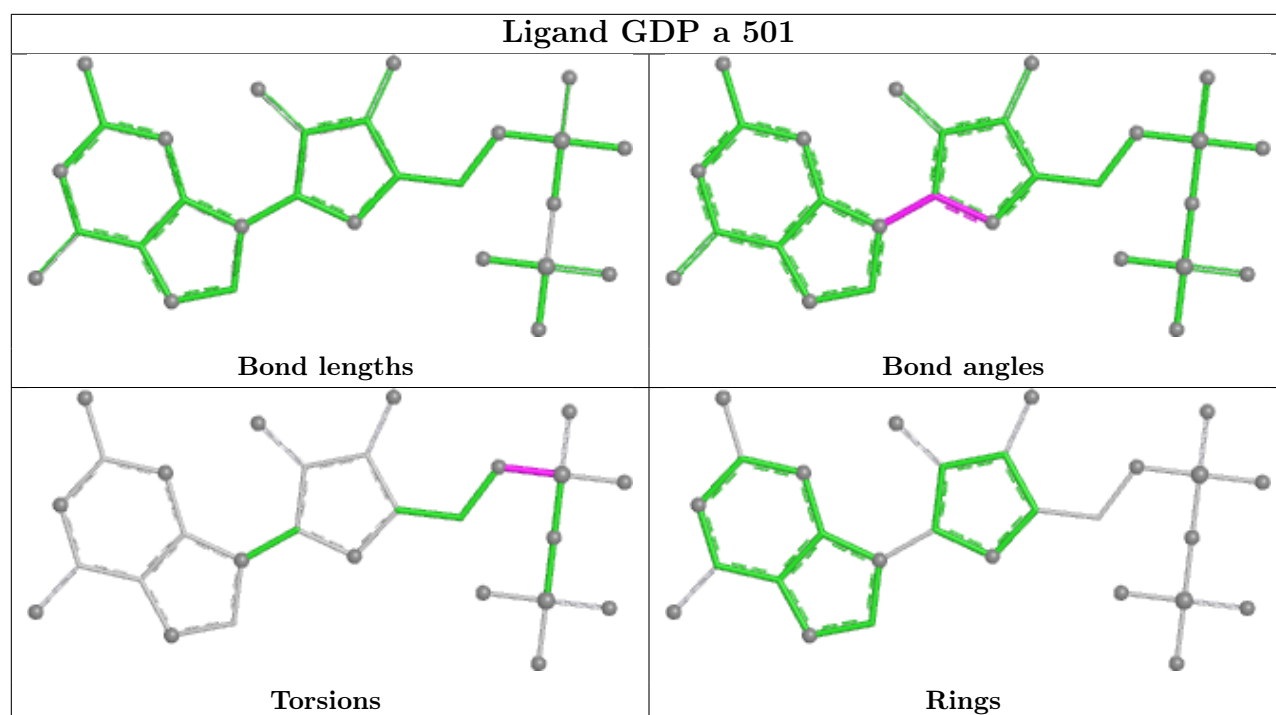
Bond angles

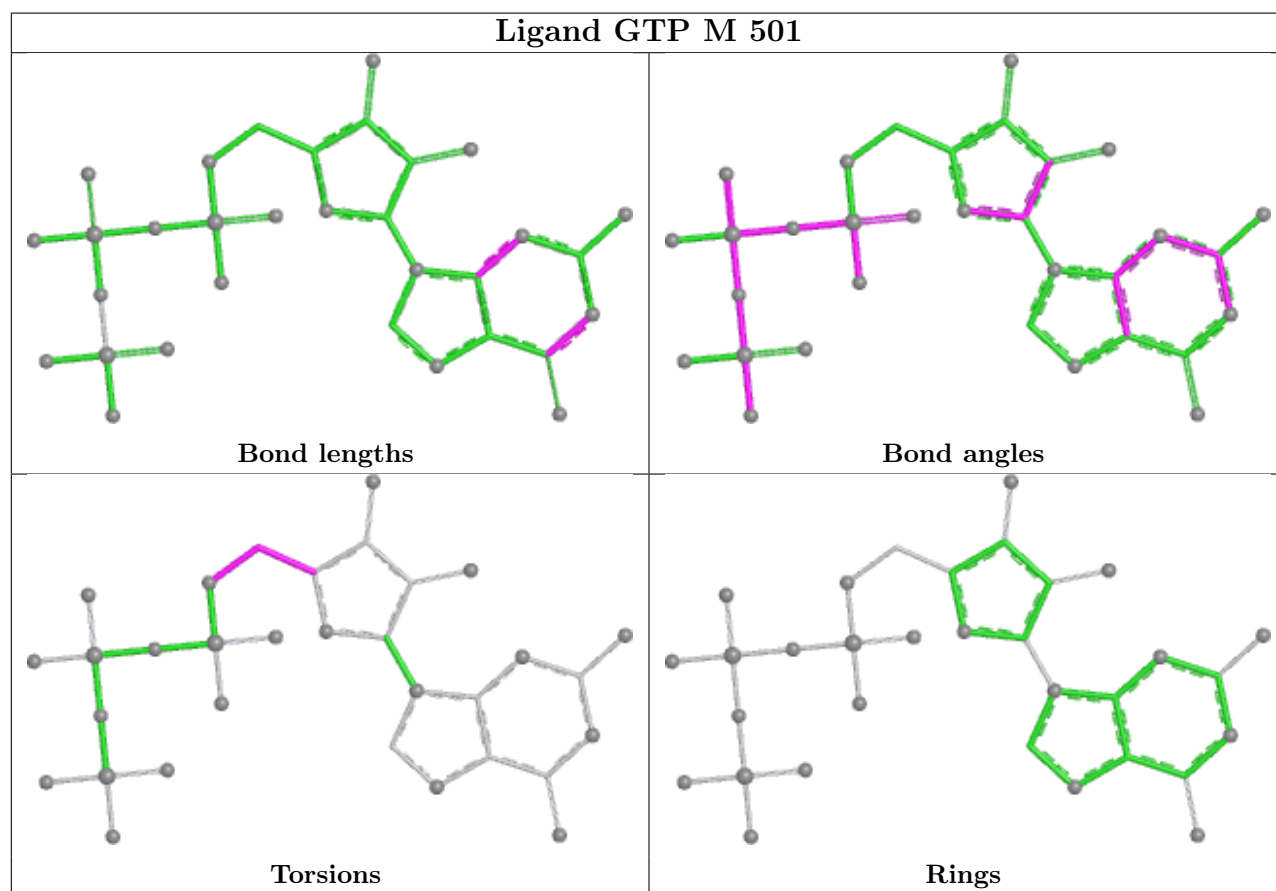
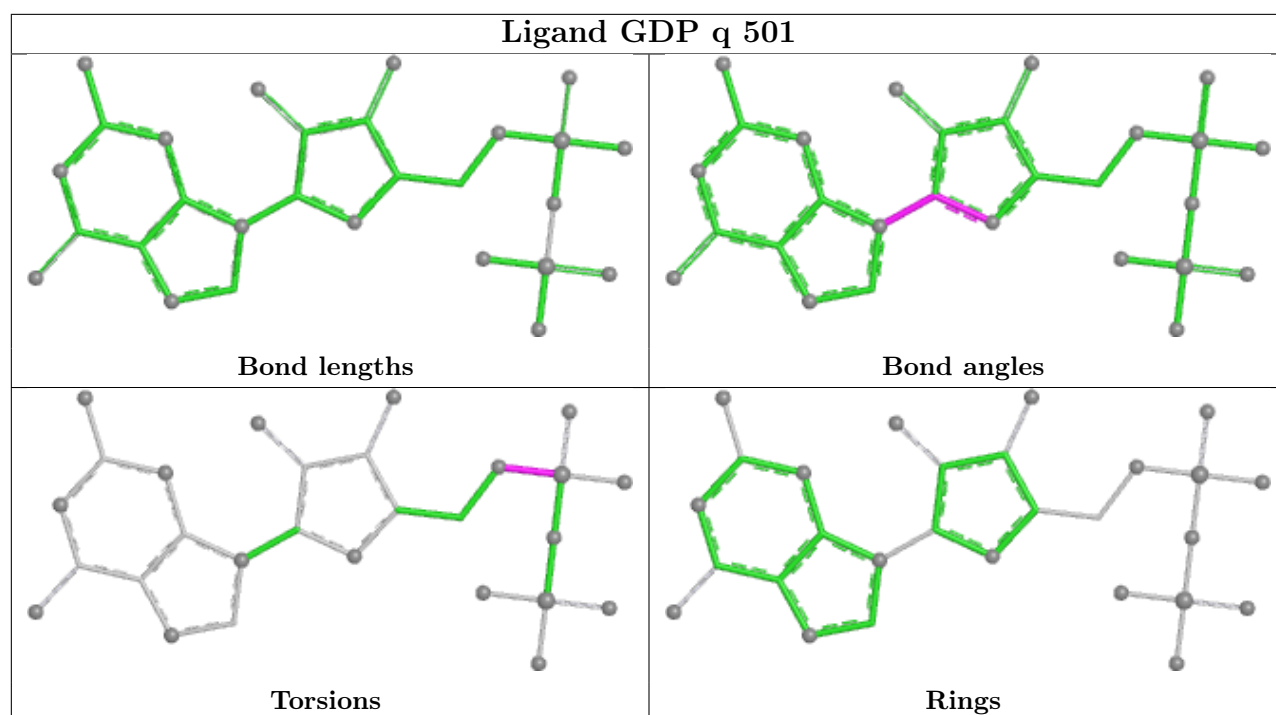


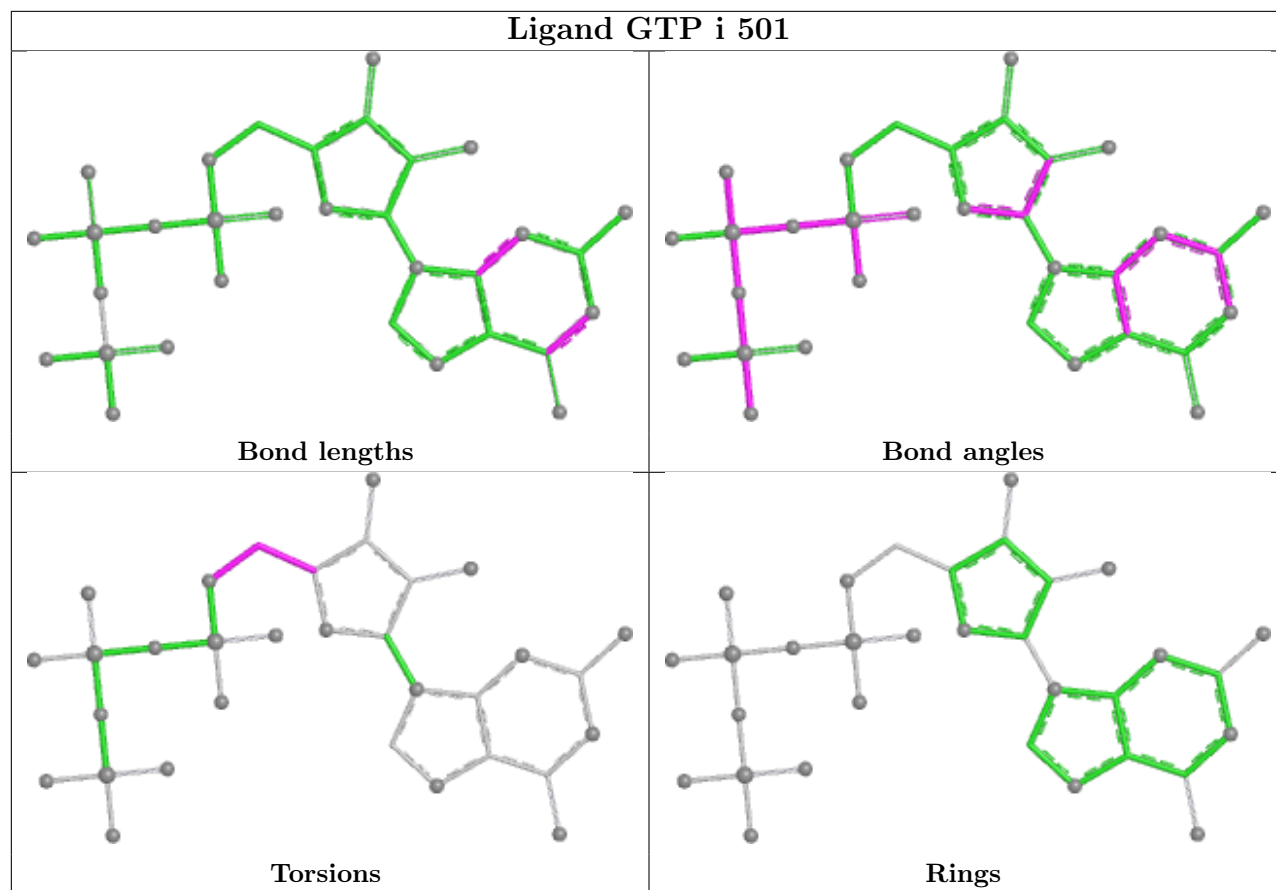
Torsions



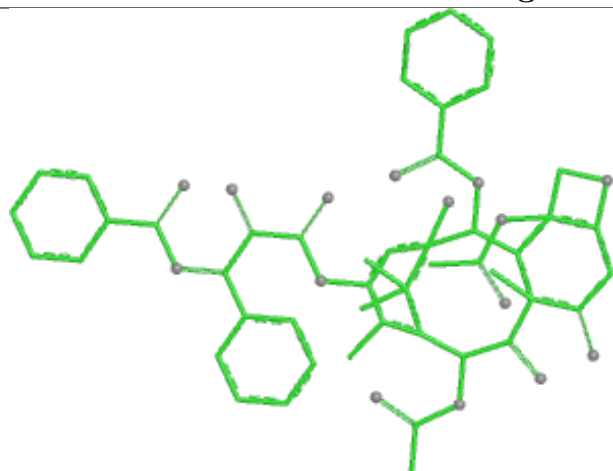
Rings



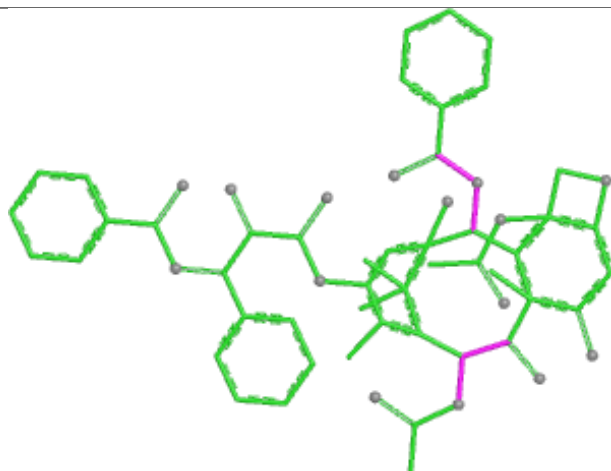




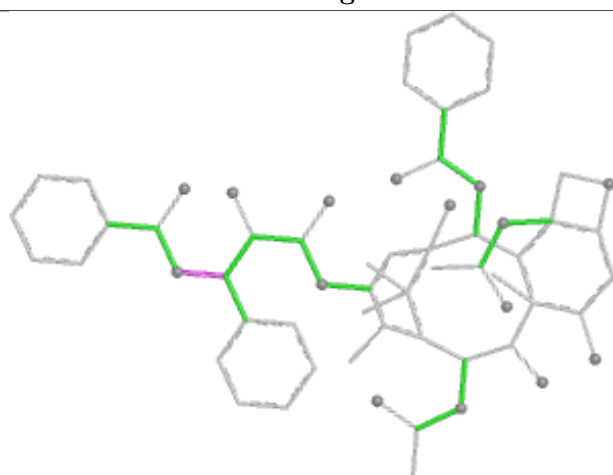
Ligand TA1 R 502



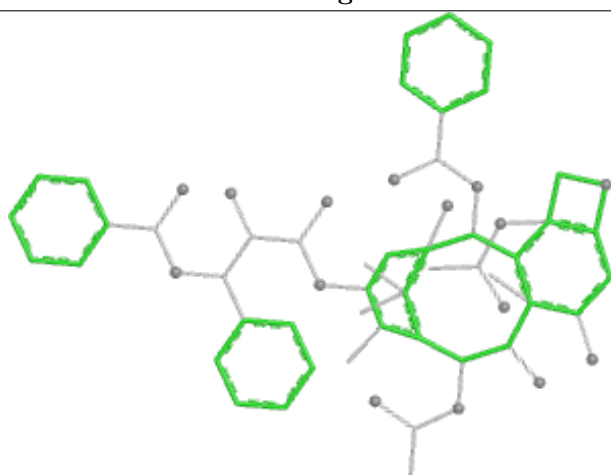
Bond lengths



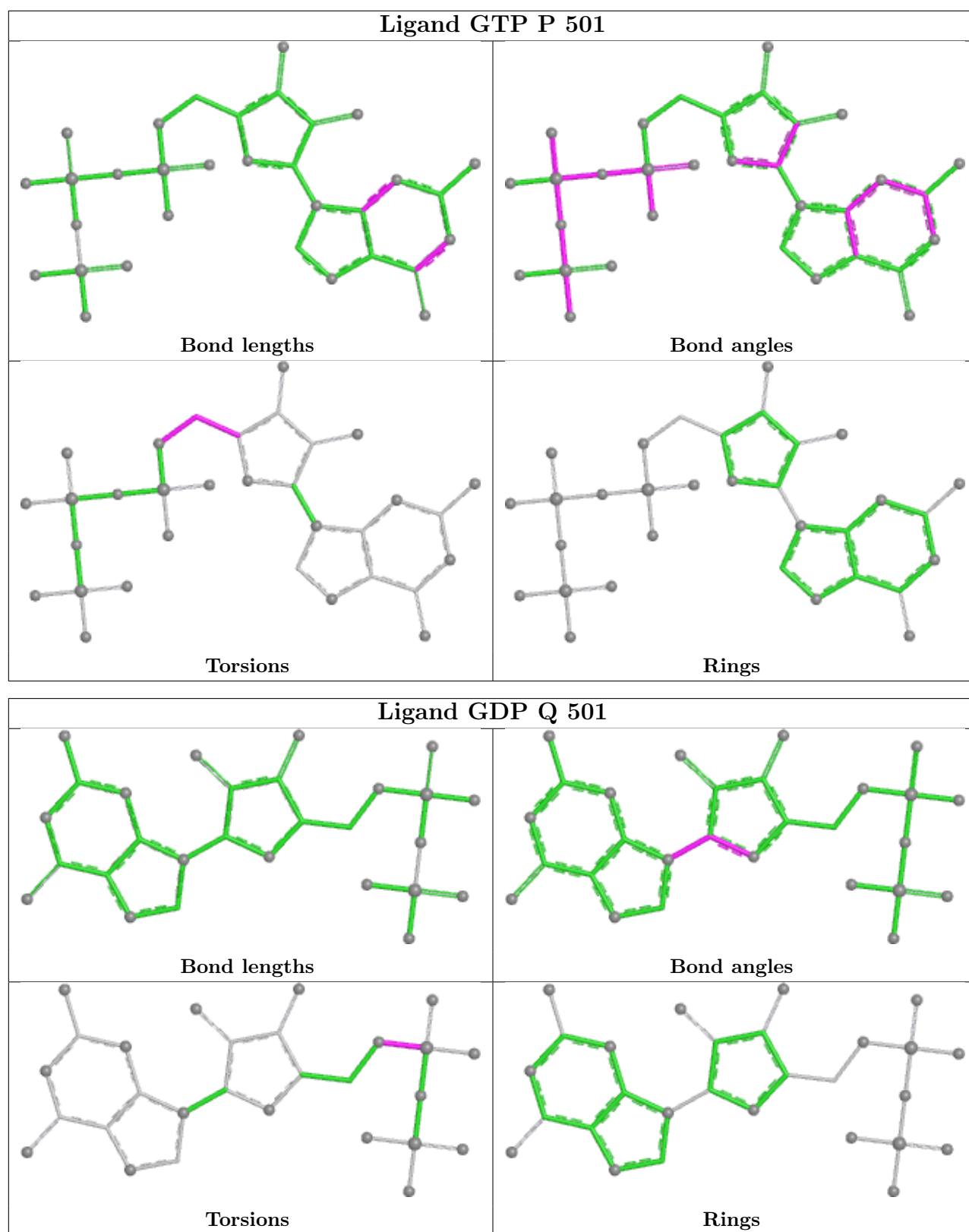
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

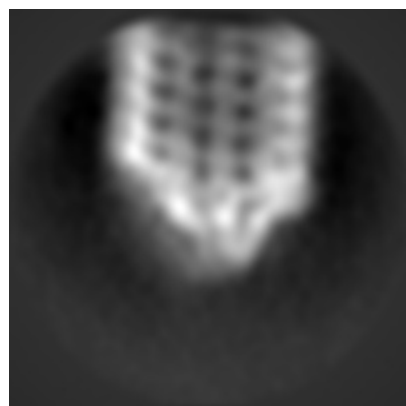
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19862. These allow visual inspection of the internal detail of the map and identification of artifacts.

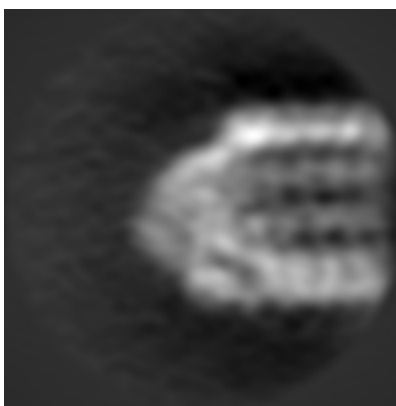
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

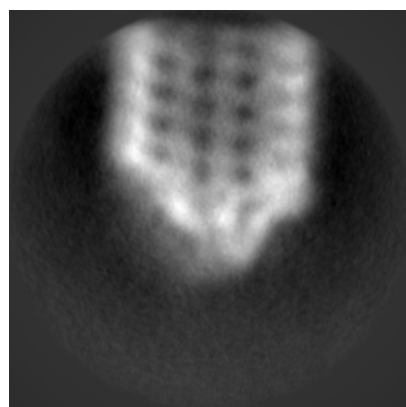


Y

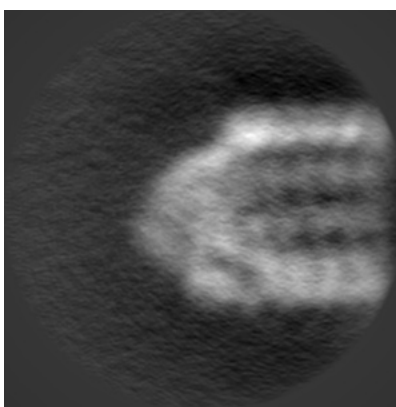


Z

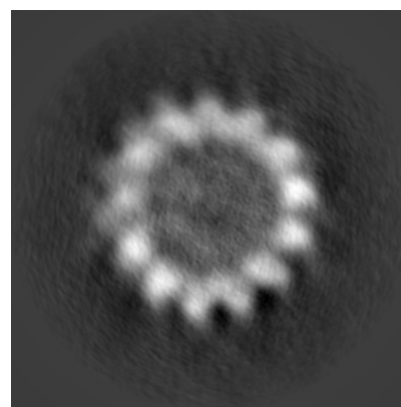
6.1.2 Raw map



X



Y

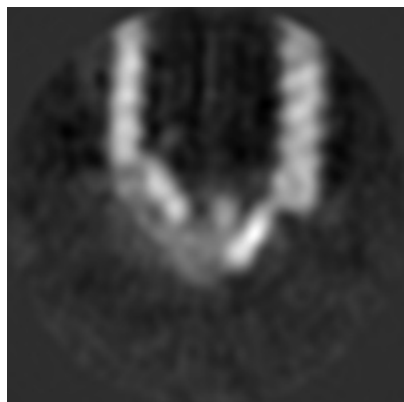


Z

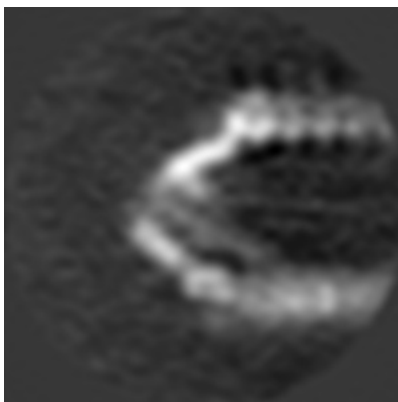
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 128

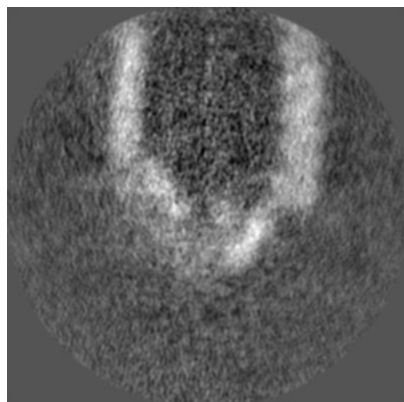


Y Index: 128

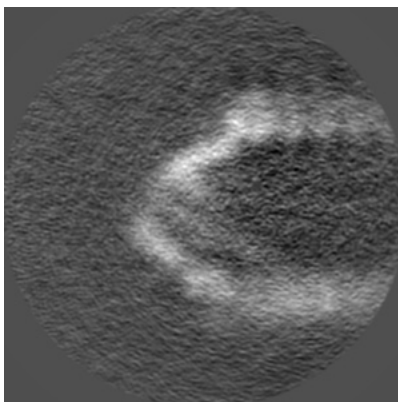


Z Index: 128

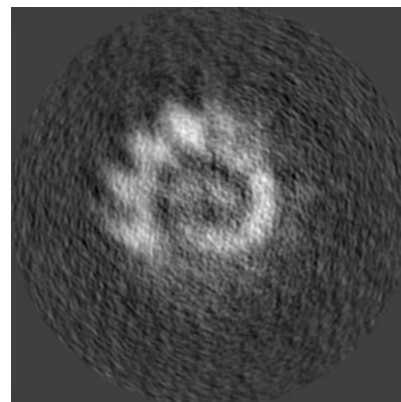
6.2.2 Raw map



X Index: 128



Y Index: 128

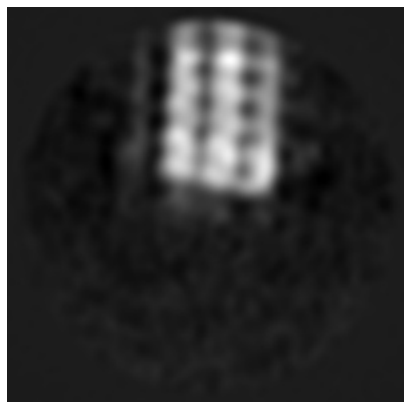


Z Index: 128

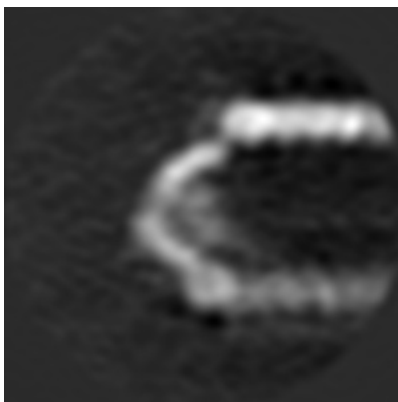
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 179

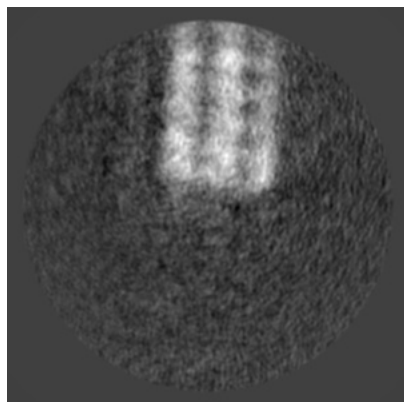


Y Index: 140

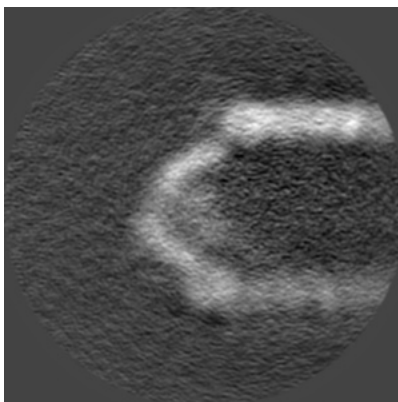


Z Index: 162

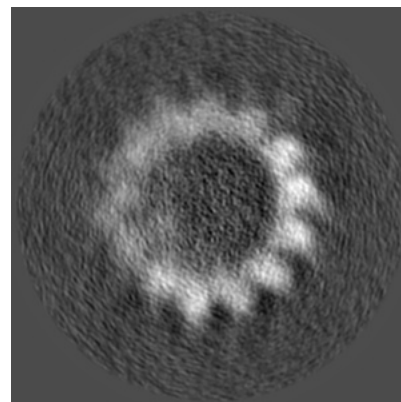
6.3.2 Raw map



X Index: 180



Y Index: 140

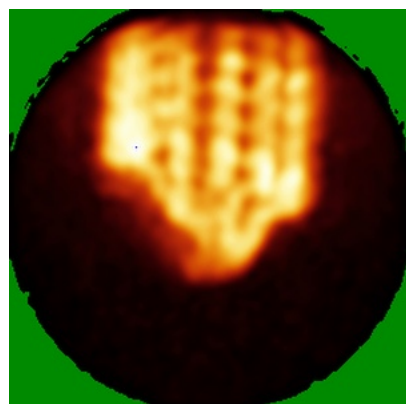


Z Index: 162

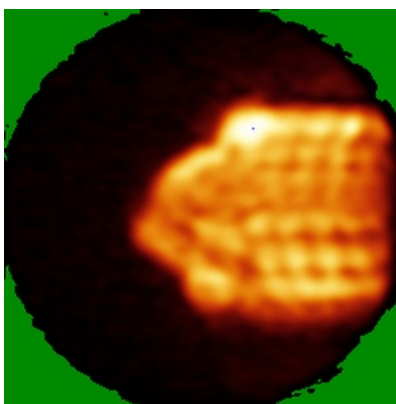
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

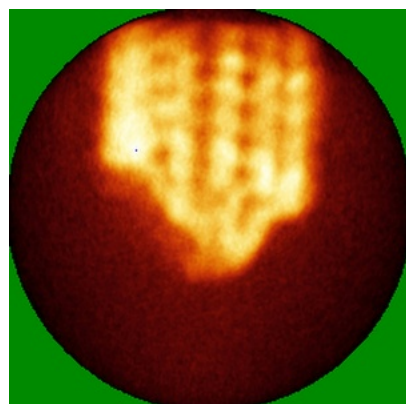


Y

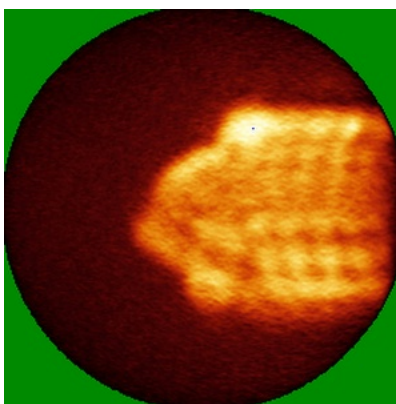


Z

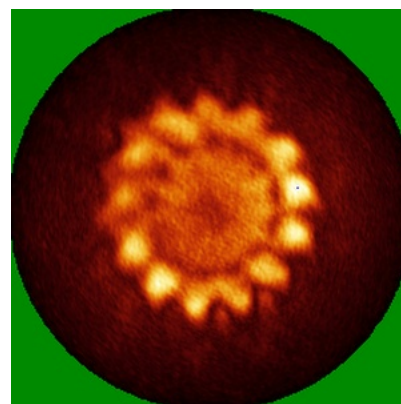
6.4.2 Raw map



X



Y

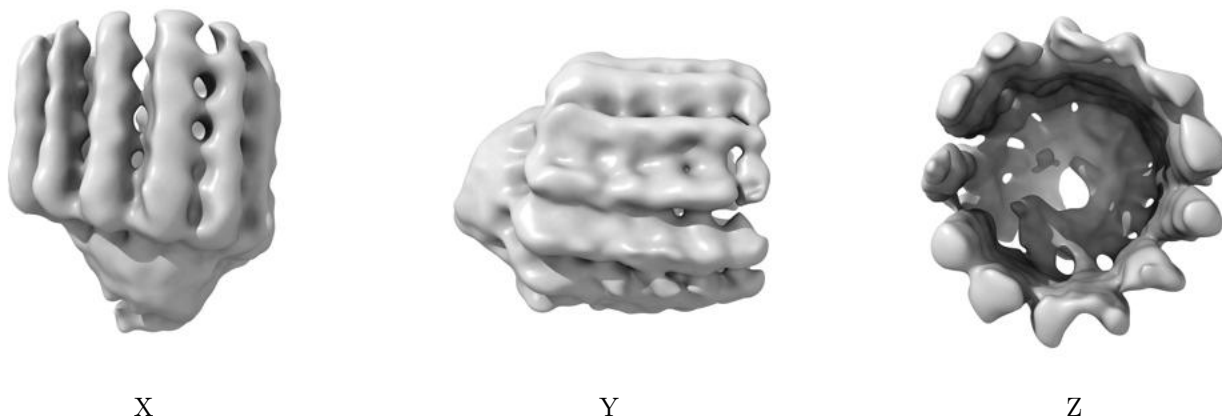


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0157. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

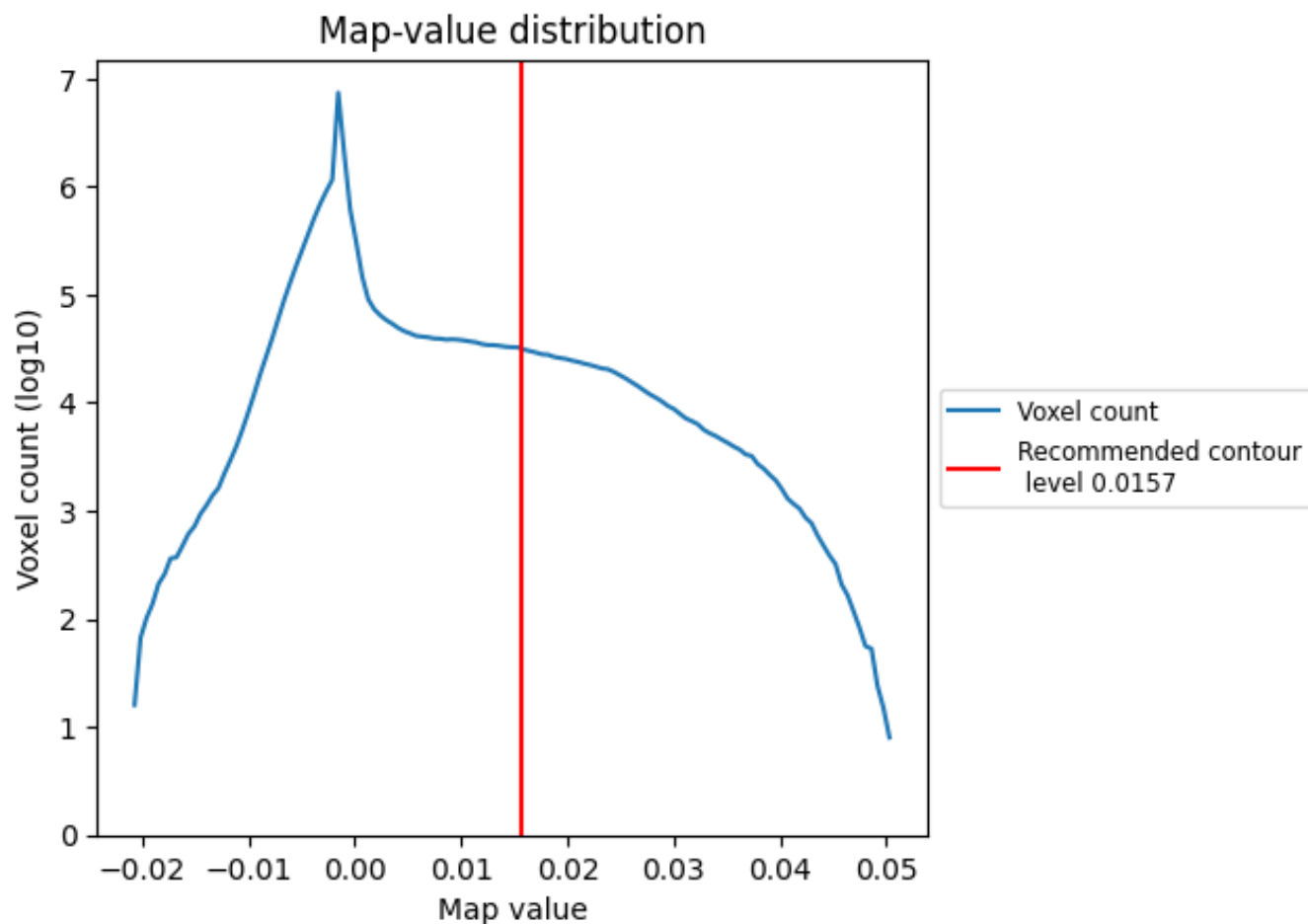
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

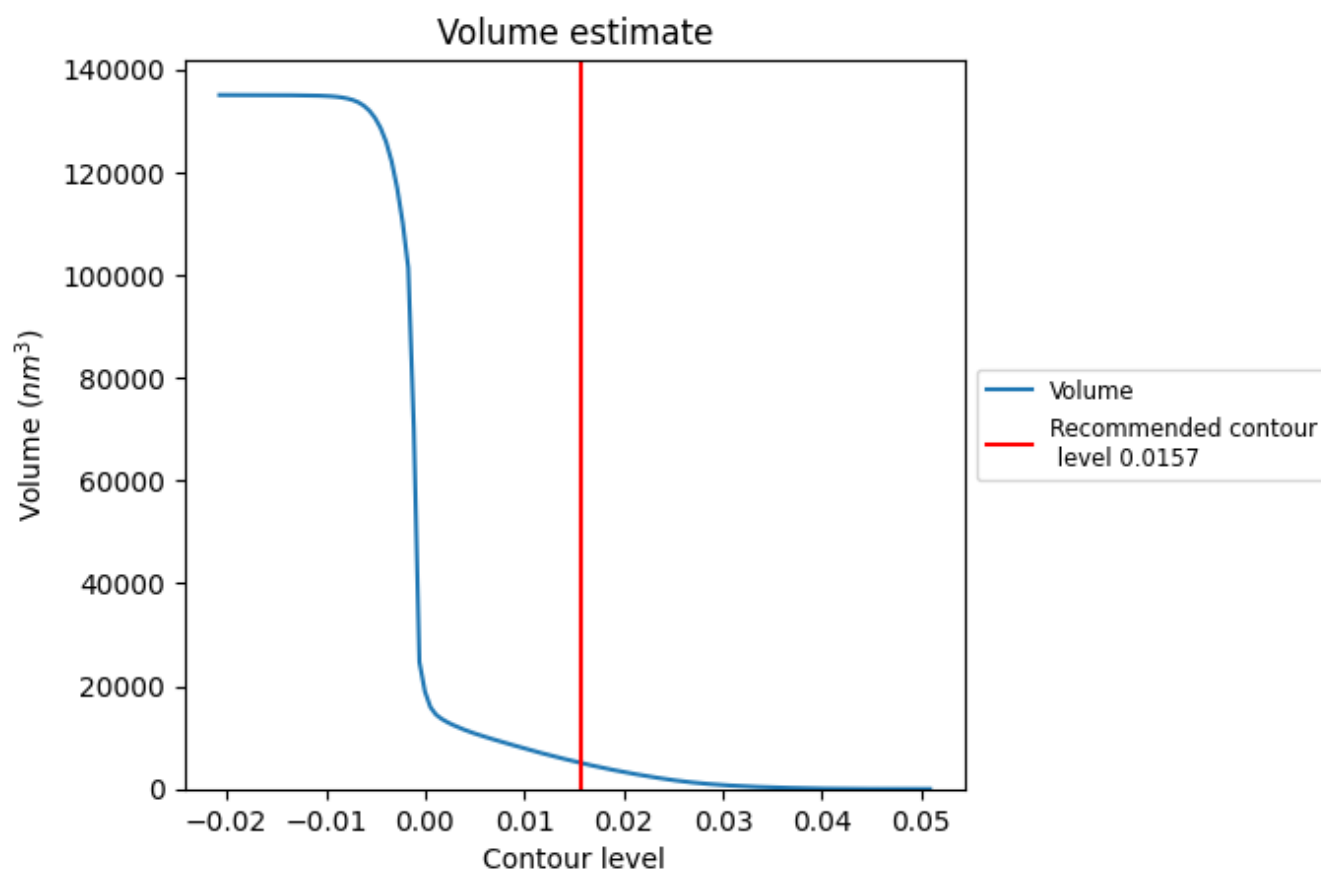
This section contains the results of statistical analysis of the map.

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.

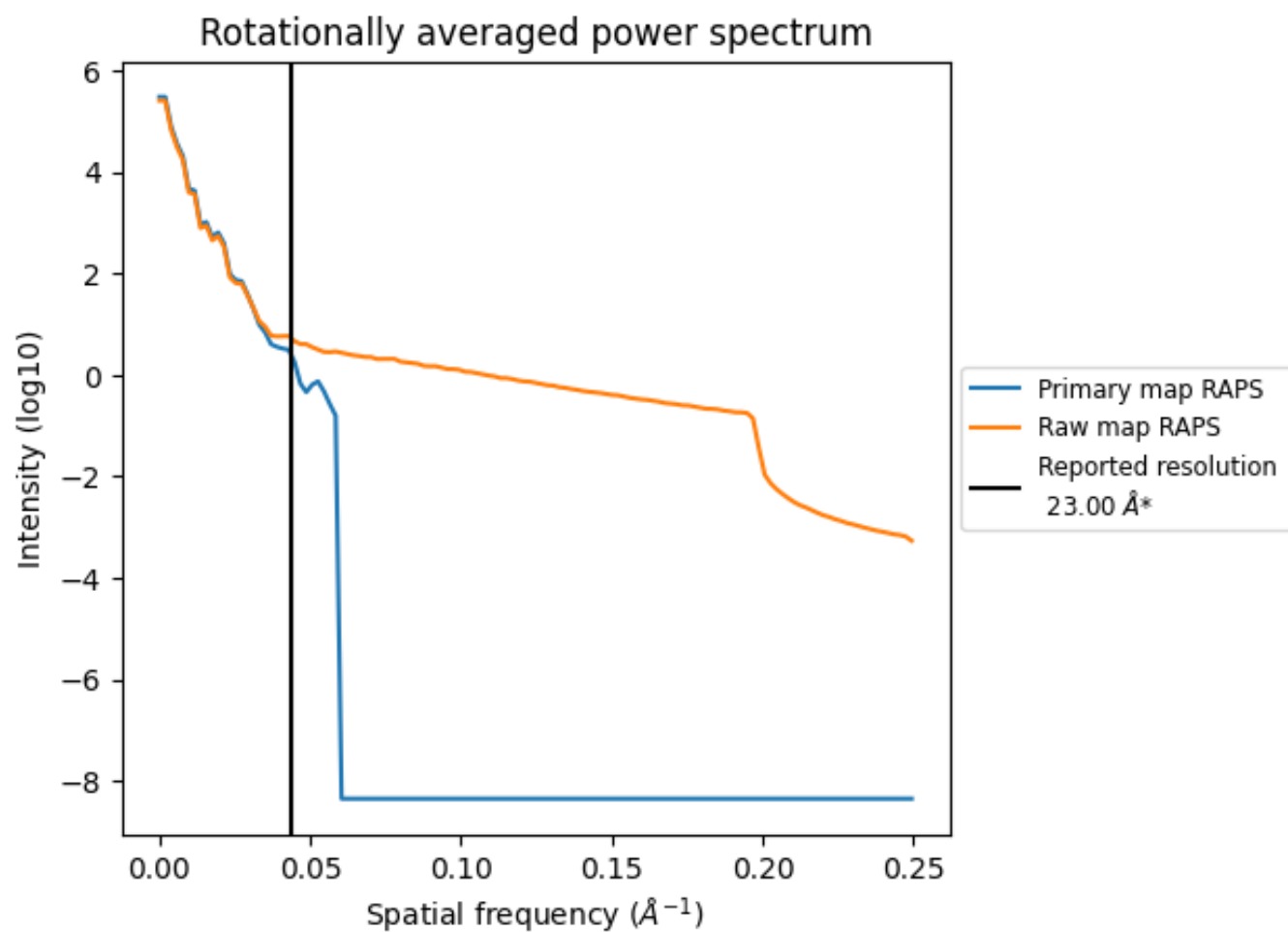
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5060 nm^3 ; this corresponds to an approximate mass of 4571 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 ⓘ

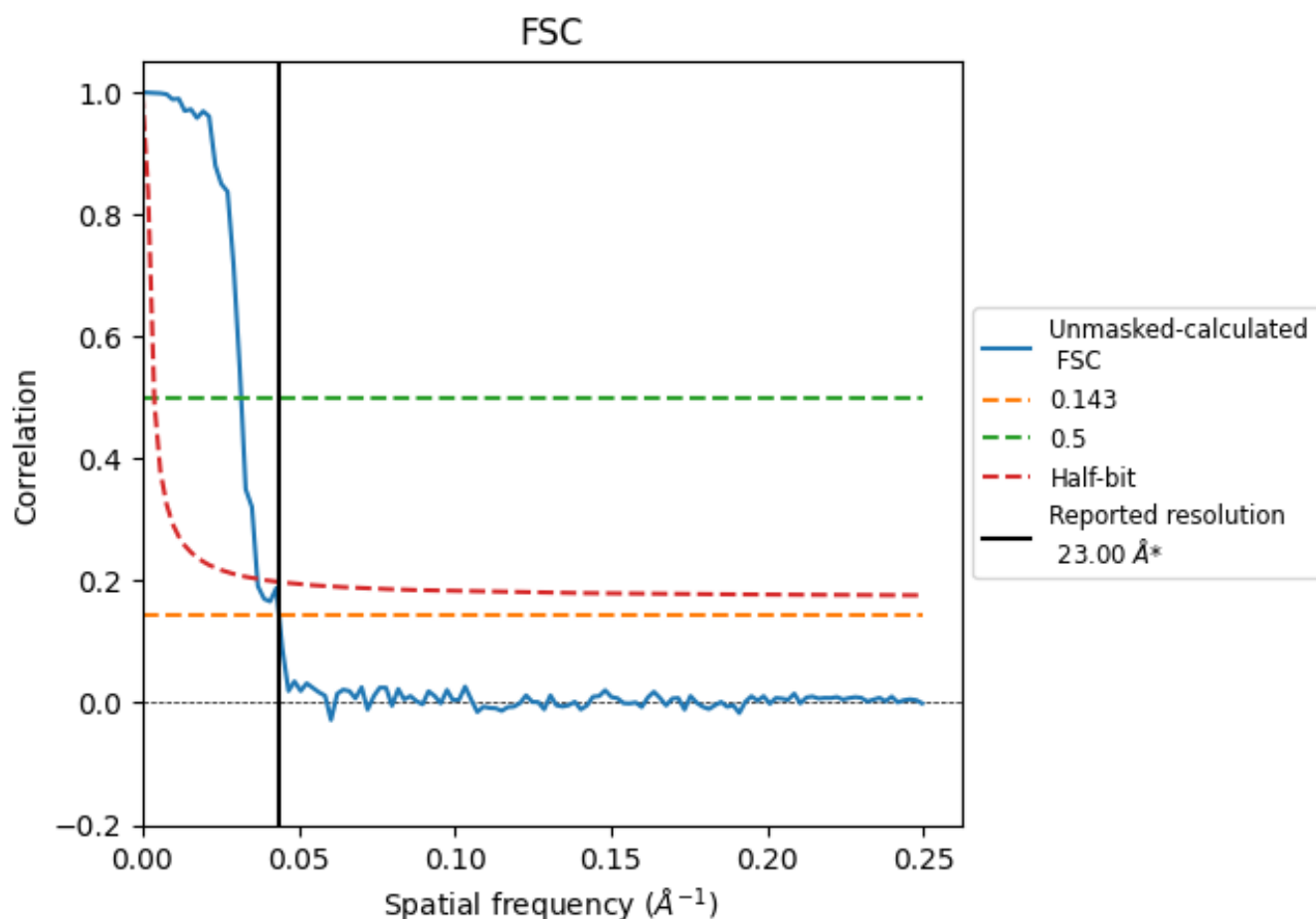


*Reported resolution corresponds to spatial frequency of $0.043 \text{ \AA}^{-1}$

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 0.043 Å⁻¹

8.2 Resolution estimates [i](#)

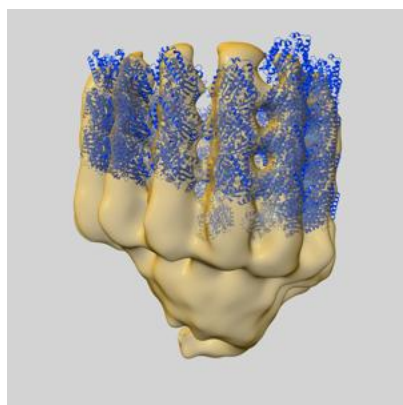
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	23.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	22.83	31.55	27.10

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

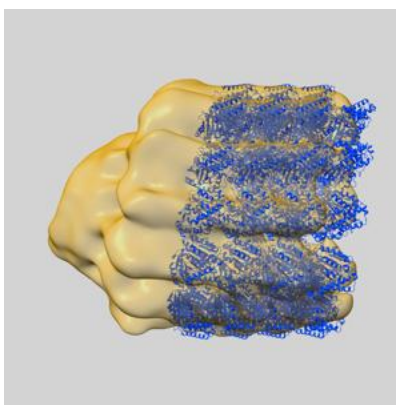
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19862 and PDB model 9EOK. Per-residue inclusion information can be found in section [3](#) on page [13](#).

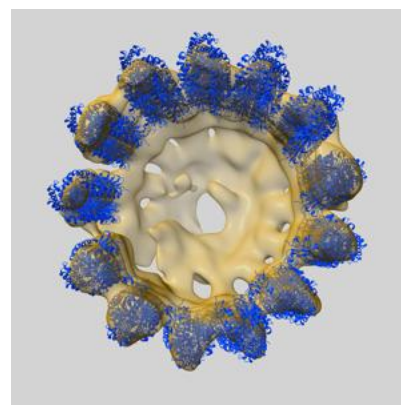
9.1 Map-model overlay [i](#)



X



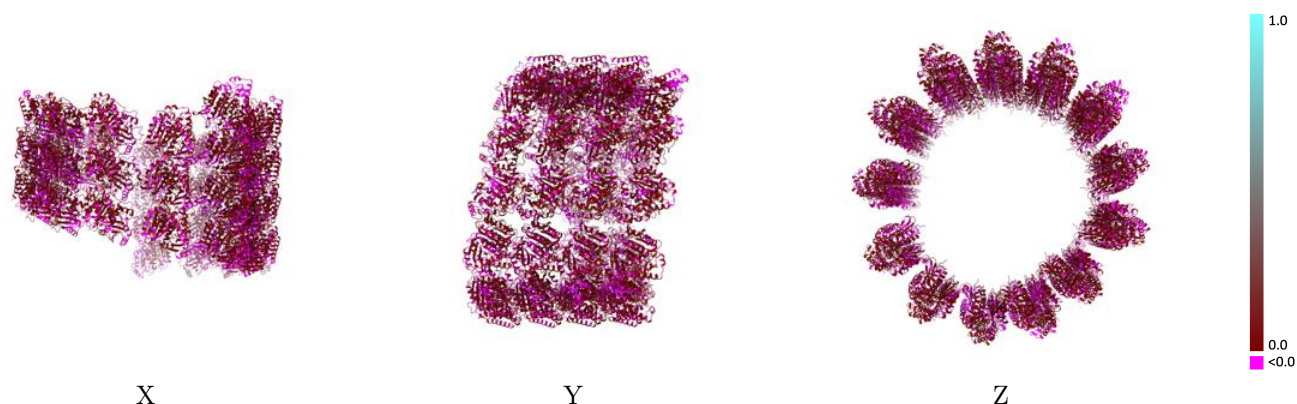
Y



Z

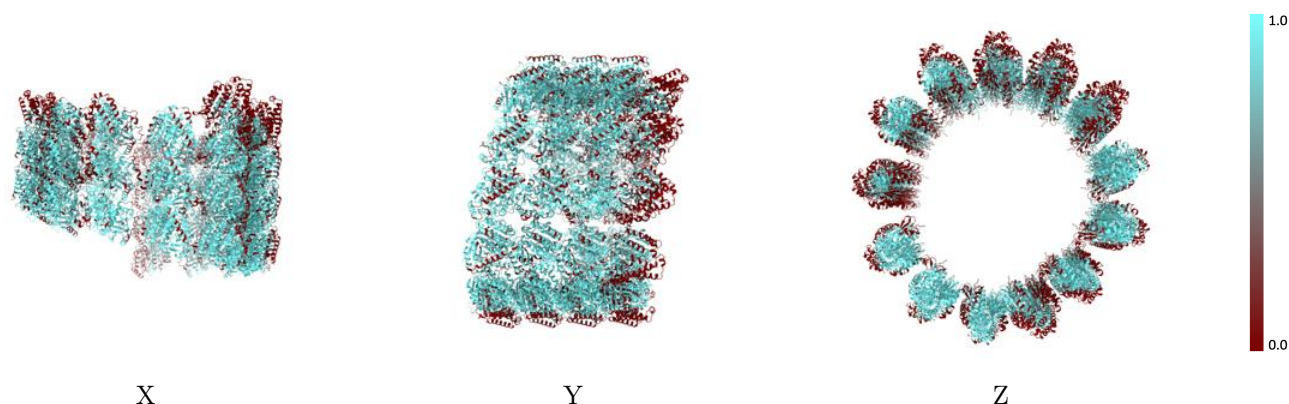
The images above show the 3D surface view of the map at the recommended contour level 0.0157 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



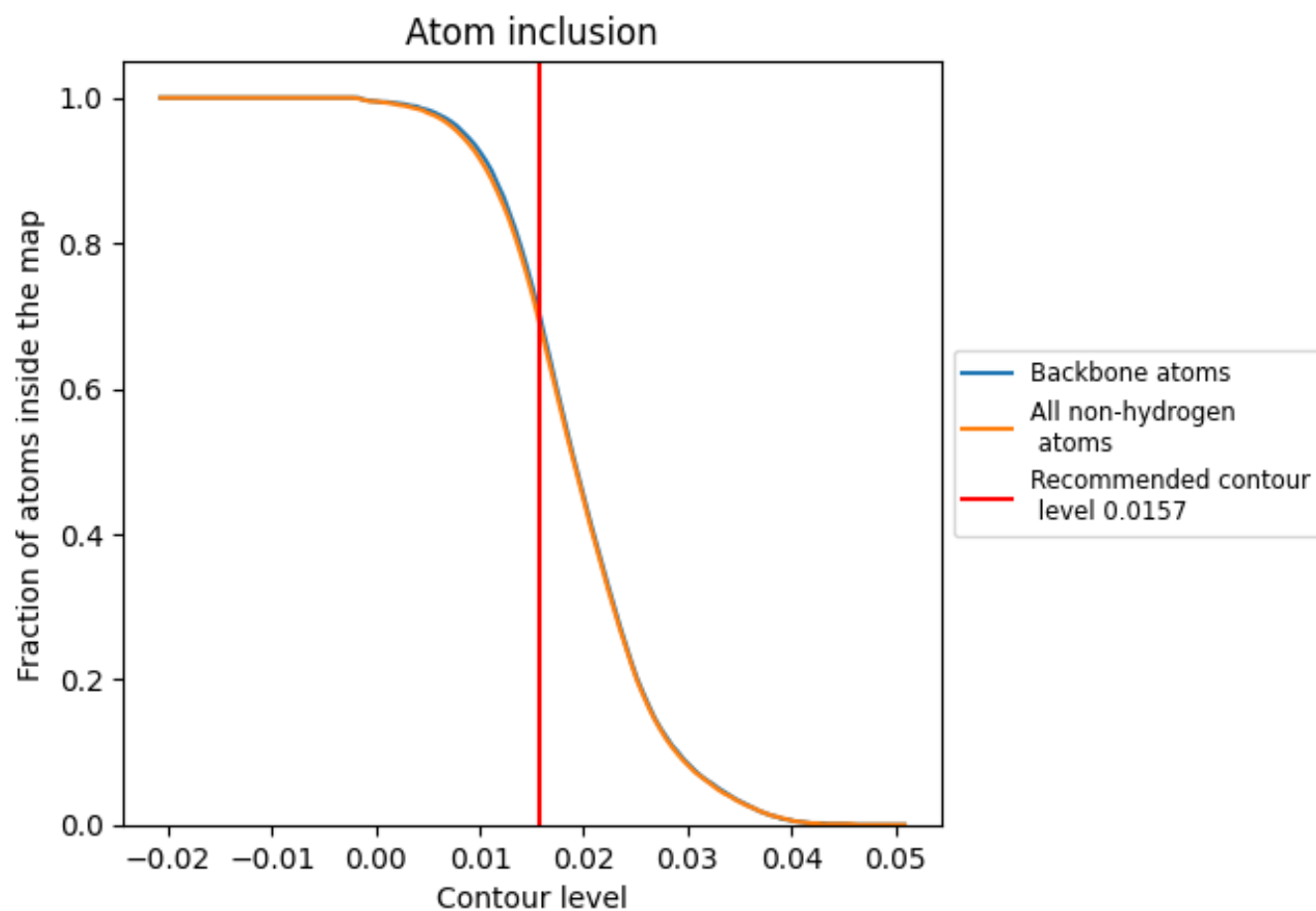
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0157).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 69% 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 (0.0157) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6930	 0.0360
A	 0.3640	 0.0190
B	 0.5850	 0.0330
C	 0.7340	 0.0330
D	 0.7730	 0.0370
E	 0.5630	 0.0340
F	 0.2140	 0.0230
G	 0.7930	 0.0360
H	 0.7940	 0.0400
I	 0.8330	 0.0360
J	 0.8780	 0.0360
K	 0.8300	 0.0370
L	 0.7820	 0.0370
M	 0.8120	 0.0390
N	 0.8360	 0.0330
O	 0.9170	 0.0360
P	 0.8570	 0.0350
Q	 0.7610	 0.0350
R	 0.8070	 0.0400
S	 0.7990	 0.0390
T	 0.8330	 0.0460
U	 0.8250	 0.0410
V	 0.8720	 0.0380
W	 0.7940	 0.0370
X	 0.7390	 0.0390
Y	 0.7500	 0.0360
Z	 0.7530	 0.0350
a	 0.8550	 0.0410
b	 0.6820	 0.0350
c	 0.7650	 0.0320
d	 0.7850	 0.0440
e	 0.7930	 0.0400
f	 0.7600	 0.0400
g	 0.7620	 0.0390
h	 0.8250	 0.0330



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Chain	Atom inclusion	Q-score
i	 0.6170	 0.0360
j	 0.5830	 0.0400
k	 0.3460	 0.0250
o	 0.5250	 0.0260
p	 0.4760	 0.0380
q	 0.2780	 0.0390
r	 0.2480	 0.0290
s	 0.3130	 0.0250