



Full wwPDB EM Validation Report ⓘ

Oct 20, 2025 – 02:04 AM JST

PDB ID : 9V7J / pdb_00009v7j
EMDB ID : EMD-64815
Title : Phycobilisome core from *Gloeobacter violaceus* PCC 7421
Authors : Burtseva, A.D.; Baymukhametov, T.N.; Slonimskiy, Y.B.; Popov, V.O.;
Sluchanko, N.N.; Boyko, K.M.
Deposited on : 2025-05-28
Resolution : 2.85 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.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

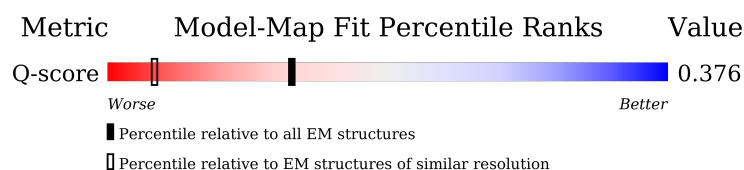
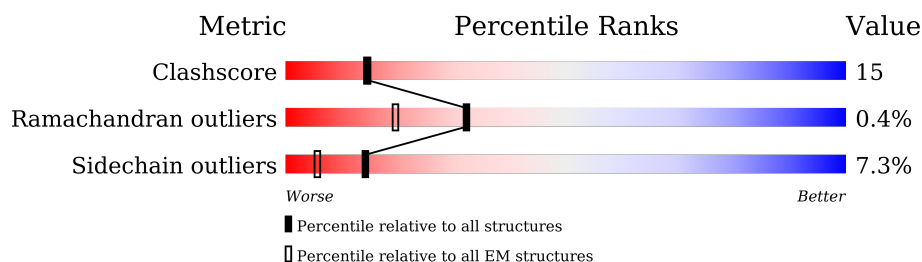
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY





The reported resolution of this entry is 2.85 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	11965 (2.35 - 3.35)

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	1155	
1	C	1155	
2	1	161	
2	3	161	


























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Mol	Chain	Length	Quality of chain
2	5	161	 67% 27% 5% ..
2	7	161	 68% 23% 7% ..
2	9	161	 63% 26% 8% ..
2	AA	161	 70% 23% 5% ..
2	AC	161	 66% 26% 7% ..
2	AE	161	 63% 29% 5% ..
2	AG	161	 61% 29% 7% ..
2	AI	161	 64% 26% 8% ..
2	AK	161	 63% 29% 6% ..
2	AM	161	 70% 24% . ..
2	AO	161	 66% 26% 7% ..
2	AQ	161	 63% 30% 5% ..
2	AS	161	 62% 29% 7% ..
2	AU	161	 63% 27% 8% ..
2	AW	161	 63% 29% 7% ..
2	E	161	 66% 24% 8% ..
2	G	161	 68% 24% 6% ..
2	I	161	 66% 25% 7% ..
2	K	161	 66% 26% 6% ..
2	M	161	 68% 23% 7% ..
2	O	161	 71% 21% 7% .
2	Q	161	 68% 24% 7% ..
2	S	161	 70% 22% 7% .
2	U	161	 66% 24% 9% ..
2	W	161	 68% 24% 6% ..












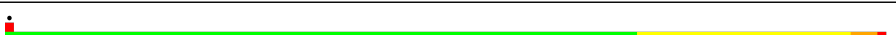

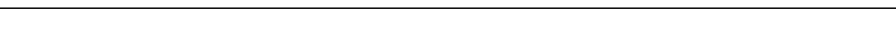
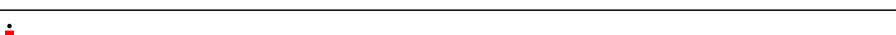
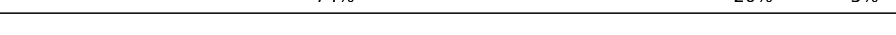

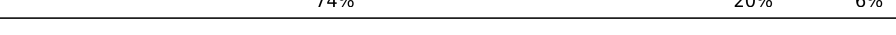







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Mol	Chain	Length	Quality of chain
2	Y	161	
2	a	161	
2	c	161	
2	e	161	
2	g	161	
2	i	161	
2	k	161	
2	m	161	
2	o	161	
2	r	161	
2	t	161	
2	w	161	
2	y	161	
3	0	161	
3	2	161	
3	4	161	
3	6	161	
3	8	161	
3	AB	161	
3	AD	161	
3	AF	161	
3	AH	161	
3	AJ	161	
3	AL	161	
3	AN	161	






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Mol	Chain	Length	Quality of chain
3	AP	161	
3	AR	161	
3	AT	161	
3	AV	161	
3	AX	161	
3	F	161	
3	H	161	
3	J	161	
3	L	161	
3	N	161	
3	P	161	
3	R	161	
3	T	161	
3	V	161	
3	X	161	
3	Z	161	
3	b	161	
3	d	161	
3	f	161	
3	h	161	
3	j	161	
3	l	161	
3	n	161	
3	p	161	
3	q	161	

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Mol	Chain	Length	Quality of chain
3	v	161	
3	x	161	
3	z	161	
4	s	161	
4	u	161	
5	AY	69	
5	AZ	69	
5	Aa	69	
5	Ab	69	
5	Ac	69	
5	Ad	69	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CYC	C	2101	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 123484 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 Phycobiliprotein ApcE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1089	Total	C	N	O	S	0	0
			8678	5505	1533	1621	19		
1	C	1089	Total	C	N	O	S	0	0
			8678	5505	1533	1621	19		

- Molecule 2 is a protein called Allophycocyanin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	O	159	Total	C	N	O	S	0	0
			1213	766	208	234	5		
2	E	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	G	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	I	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	K	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	Q	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	S	159	Total	C	N	O	S	0	0
			1213	766	208	234	5		
2	U	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	W	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	Y	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	a	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	c	159	Total	C	N	O	S	0	0
			1213	766	208	234	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	e	159	Total	C	N	O	S	0	0
			1213	766	208	234	5		
2	g	159	Total	C	N	O	S	0	0
			1213	766	208	234	5		
2	i	158	Total	C	N	O	S	0	0
			1207	763	207	232	5		
2	k	158	Total	C	N	O	S	0	0
			1207	763	207	232	5		
2	m	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	o	159	Total	C	N	O	S	0	0
			1213	766	208	234	5		
2	r	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	t	159	Total	C	N	O	S	0	0
			1213	766	208	234	5		
2	w	159	Total	C	N	O	S	0	0
			1213	766	208	234	5		
2	y	159	Total	C	N	O	S	0	0
			1213	766	208	234	5		
2	1	158	Total	C	N	O	S	0	0
			1207	763	207	232	5		
2	3	159	Total	C	N	O	S	0	0
			1213	766	208	234	5		
2	5	159	Total	C	N	O	S	0	0
			1213	766	208	234	5		
2	7	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	9	158	Total	C	N	O	S	0	0
			1207	763	207	232	5		
2	AA	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	AC	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	AE	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	AG	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	AI	159	Total	C	N	O	S	0	0
			1213	766	208	234	5		
2	AK	159	Total	C	N	O	S	0	0
			1213	766	208	234	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	AM	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	AO	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	AQ	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	AS	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	AU	159	Total	C	N	O	S	0	0
			1213	766	208	234	5		
2	AW	159	Total	C	N	O	S	0	0
			1213	766	208	234	5		

- Molecule 3 is a protein called Allophycocyanin beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	P	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	F	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	H	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	J	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	L	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	R	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	T	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	V	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	X	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	Z	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	b	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	d	158	Total	C	N	O	S	0	0
			1187	753	199	230	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	f	160	Total	C	N	O	S	0	0
			1202	762	201	234	5		
3	h	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	j	158	Total	C	N	O	S	0	0
			1187	753	199	230	5		
3	l	159	Total	C	N	O	S	0	0
			1195	759	200	231	5		
3	n	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	p	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	q	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	v	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	x	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	z	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	2	158	Total	C	N	O	S	0	0
			1187	753	199	230	5		
3	4	158	Total	C	N	O	S	0	0
			1187	753	199	230	5		
3	6	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	8	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	0	159	Total	C	N	O	S	0	0
			1195	759	200	231	5		
3	AB	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	AD	159	Total	C	N	O	S	0	0
			1195	759	200	231	5		
3	AF	160	Total	C	N	O	S	0	0
			1202	762	201	234	5		
3	AH	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	AJ	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	AL	160	Total	C	N	O	S	0	0
			1203	764	201	232	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	AN	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	AP	159	Total	C	N	O	S	0	0
			1195	759	200	231	5		
3	AR	160	Total	C	N	O	S	0	0
			1202	762	201	234	5		
3	AT	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	AV	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	AX	160	Total	C	N	O	S	0	0
			1203	764	201	232	6		

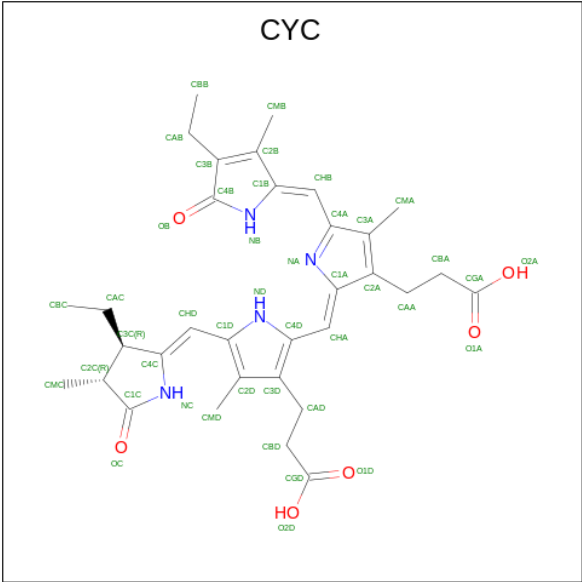
- Molecule 4 is a protein called Phycobilisome core component.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	s	161	Total	C	N	O	S	0	0
			1227	779	206	237	5		
4	u	160	Total	C	N	O	S	0	0
			1217	774	204	234	5		

- Molecule 5 is a protein called Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AY	66	Total	C	N	O	S	0	0
			529	340	96	92	1		
5	AZ	66	Total	C	N	O	S	0	0
			529	340	96	92	1		
5	Aa	66	Total	C	N	O	S	0	0
			529	340	96	92	1		
5	Ab	65	Total	C	N	O	S	0	0
			522	335	95	91	1		
5	Ac	64	Total	C	N	O	S	0	0
			518	333	94	90	1		
5	Ad	66	Total	C	N	O	S	0	0
			529	340	96	92	1		

- Molecule 6 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: C₃₃H₄₀N₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			43	33	4	6	
6	C	1	Total	C	N	O	0
			43	33	4	6	
6	M	1	Total	C	N	O	0
			43	33	4	6	
6	N	1	Total	C	N	O	0
			43	33	4	6	
6	O	1	Total	C	N	O	0
			43	33	4	6	
6	P	1	Total	C	N	O	0
			43	33	4	6	
6	E	1	Total	C	N	O	0
			43	33	4	6	
6	F	1	Total	C	N	O	0
			43	33	4	6	
6	G	1	Total	C	N	O	0
			43	33	4	6	
6	H	1	Total	C	N	O	0
			43	33	4	6	
6	I	1	Total	C	N	O	0
			43	33	4	6	
6	J	1	Total	C	N	O	0
			43	33	4	6	
6	K	1	Total	C	N	O	0
			43	33	4	6	
6	L	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
6	Q	1	Total 43	C 33	N 4	O 6	0
6	R	1	Total 43	C 33	N 4	O 6	0
6	S	1	Total 43	C 33	N 4	O 6	0
6	T	1	Total 43	C 33	N 4	O 6	0
6	U	1	Total 43	C 33	N 4	O 6	0
6	V	1	Total 43	C 33	N 4	O 6	0
6	W	1	Total 43	C 33	N 4	O 6	0
6	X	1	Total 43	C 33	N 4	O 6	0
6	Y	1	Total 43	C 33	N 4	O 6	0
6	Z	1	Total 43	C 33	N 4	O 6	0
6	a	1	Total 43	C 33	N 4	O 6	0
6	b	1	Total 43	C 33	N 4	O 6	0
6	c	1	Total 43	C 33	N 4	O 6	0
6	d	1	Total 43	C 33	N 4	O 6	0
6	e	1	Total 43	C 33	N 4	O 6	0
6	f	1	Total 43	C 33	N 4	O 6	0
6	g	1	Total 43	C 33	N 4	O 6	0
6	h	1	Total 43	C 33	N 4	O 6	0
6	i	1	Total 43	C 33	N 4	O 6	0
6	j	1	Total 43	C 33	N 4	O 6	0
6	k	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
6	l	1	Total 43	C 33	N 4	O 6	0
6	m	1	Total 43	C 33	N 4	O 6	0
6	n	1	Total 43	C 33	N 4	O 6	0
6	o	1	Total 43	C 33	N 4	O 6	0
6	p	1	Total 43	C 33	N 4	O 6	0
6	q	1	Total 43	C 33	N 4	O 6	0
6	r	1	Total 43	C 33	N 4	O 6	0
6	s	1	Total 43	C 33	N 4	O 6	0
6	t	1	Total 43	C 33	N 4	O 6	0
6	u	1	Total 43	C 33	N 4	O 6	0
6	v	1	Total 43	C 33	N 4	O 6	0
6	w	1	Total 43	C 33	N 4	O 6	0
6	x	1	Total 43	C 33	N 4	O 6	0
6	y	1	Total 43	C 33	N 4	O 6	0
6	z	1	Total 43	C 33	N 4	O 6	0
6	1	1	Total 43	C 33	N 4	O 6	0
6	2	1	Total 43	C 33	N 4	O 6	0
6	3	1	Total 43	C 33	N 4	O 6	0
6	4	1	Total 43	C 33	N 4	O 6	0
6	5	1	Total 43	C 33	N 4	O 6	0
6	6	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
6	7	1	Total	C	N	O	0
			43	33	4	6	
6	8	1	Total	C	N	O	0
			43	33	4	6	
6	9	1	Total	C	N	O	0
			43	33	4	6	
6	0	1	Total	C	N	O	0
			43	33	4	6	
6	AA	1	Total	C	N	O	0
			43	33	4	6	
6	AB	1	Total	C	N	O	0
			43	33	4	6	
6	AC	1	Total	C	N	O	0
			43	33	4	6	
6	AD	1	Total	C	N	O	0
			43	33	4	6	
6	AE	1	Total	C	N	O	0
			43	33	4	6	
6	AF	1	Total	C	N	O	0
			43	33	4	6	
6	AG	1	Total	C	N	O	0
			43	33	4	6	
6	AH	1	Total	C	N	O	0
			43	33	4	6	
6	AI	1	Total	C	N	O	0
			43	33	4	6	
6	AJ	1	Total	C	N	O	0
			43	33	4	6	
6	AK	1	Total	C	N	O	0
			43	33	4	6	
6	AL	1	Total	C	N	O	0
			43	33	4	6	
6	AM	1	Total	C	N	O	0
			43	33	4	6	
6	AN	1	Total	C	N	O	0
			43	33	4	6	
6	AO	1	Total	C	N	O	0
			43	33	4	6	
6	AP	1	Total	C	N	O	0
			43	33	4	6	
6	AQ	1	Total	C	N	O	0
			43	33	4	6	

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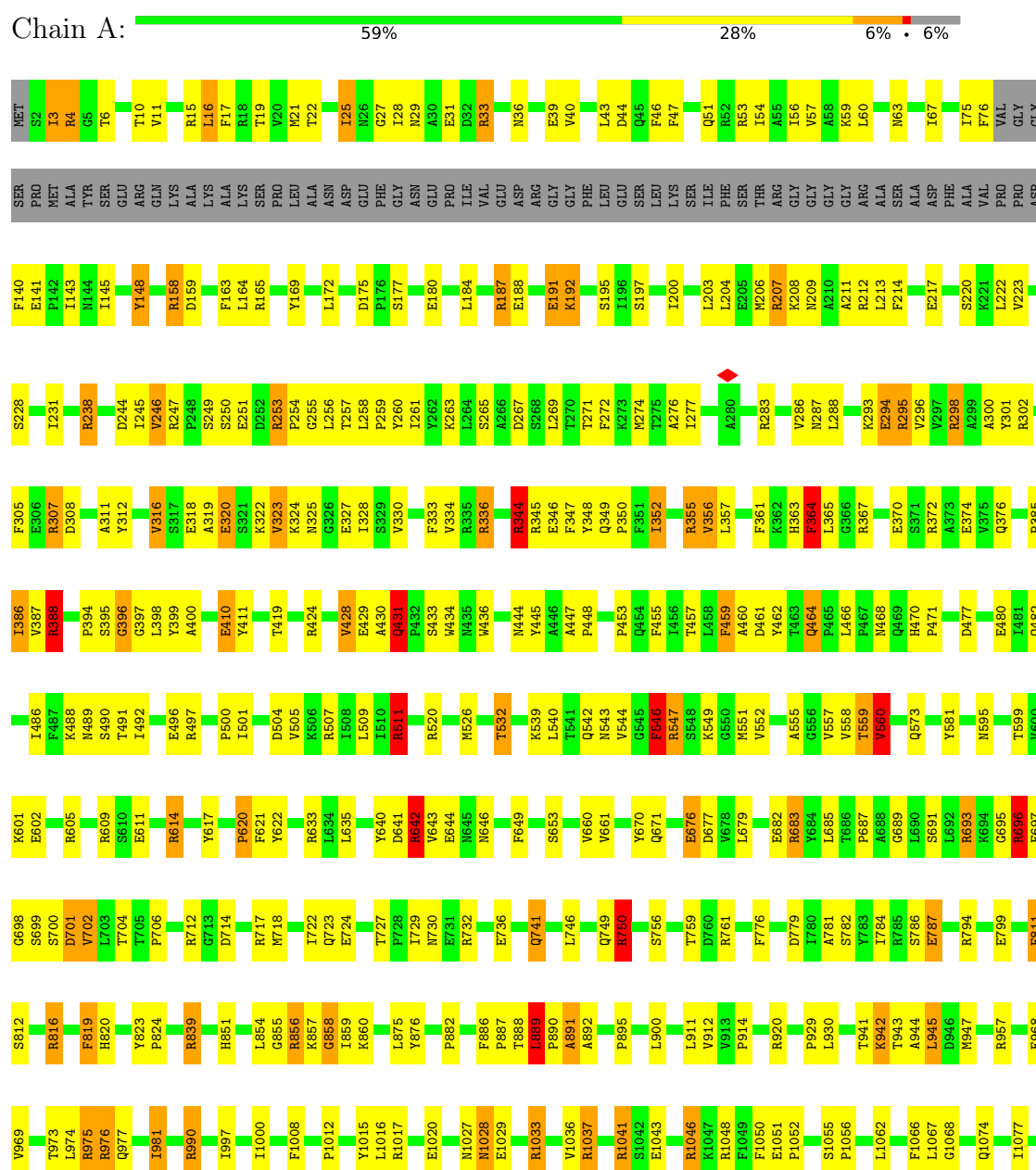
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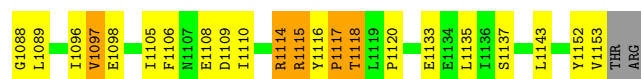
Mol	Chain	Residues	Atoms				AltConf
6	AR	1	Total	C	N	O	0
			43	33	4	6	
6	AS	1	Total	C	N	O	0
			43	33	4	6	
6	AT	1	Total	C	N	O	0
			43	33	4	6	
6	AU	1	Total	C	N	O	0
			43	33	4	6	
6	AV	1	Total	C	N	O	0
			43	33	4	6	
6	AW	1	Total	C	N	O	0
			43	33	4	6	
6	AX	1	Total	C	N	O	0
			43	33	4	6	

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.

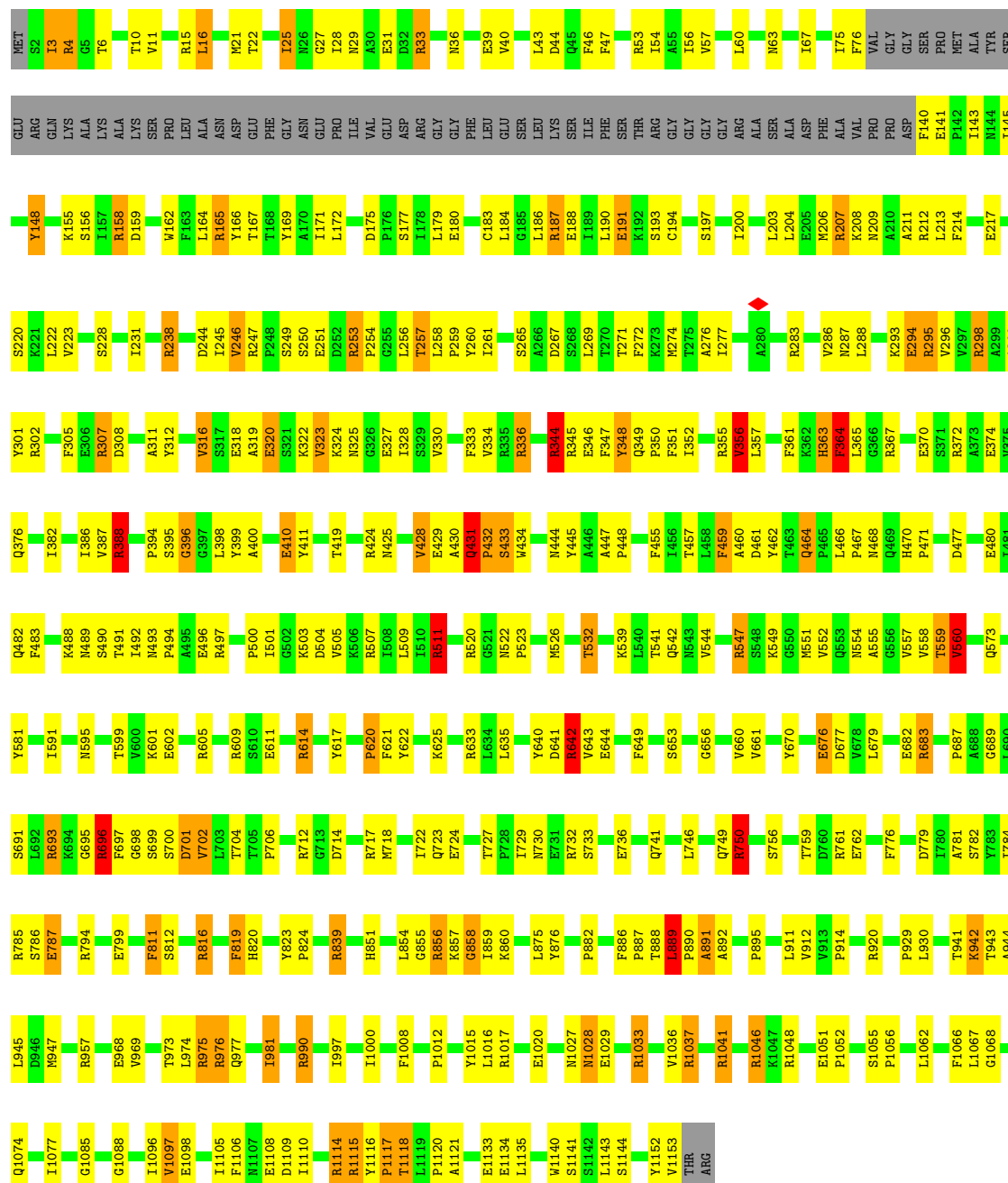
• Molecule 1: Phycobiliprotein ApcE





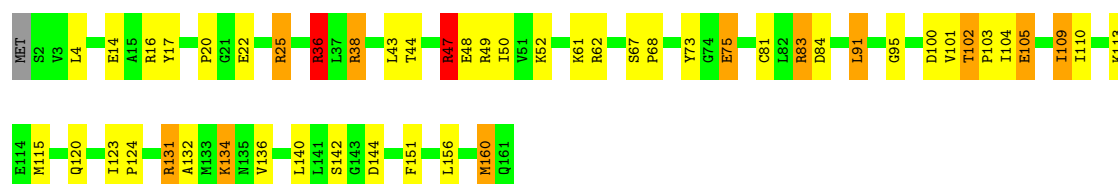
• Molecule 1: Phycobiliprotein ApcE

Chain C: 58% 29% 6% 6%



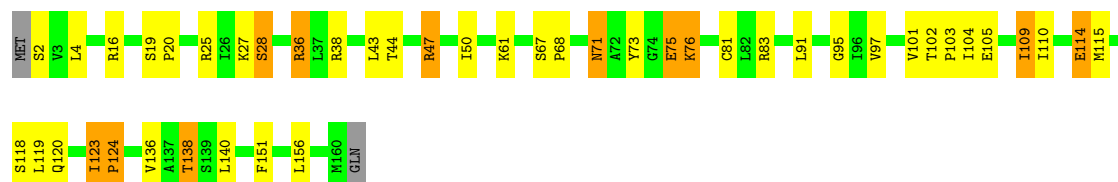
• Molecule 2: Allophycocyanin alpha subunit

Chain M: 68% 23% 7% 2%



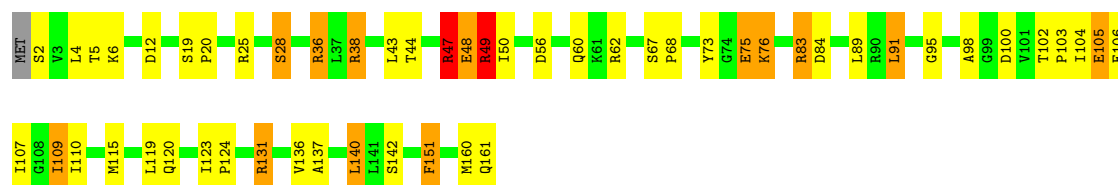
• Molecule 2: Allophycocyanin alpha subunit

Chain O: 71% 21% 7% .



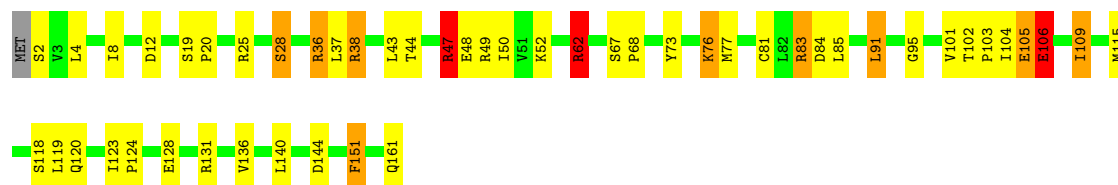
• Molecule 2: Allophycocyanin alpha subunit

Chain E: 66% 24% 8% ..



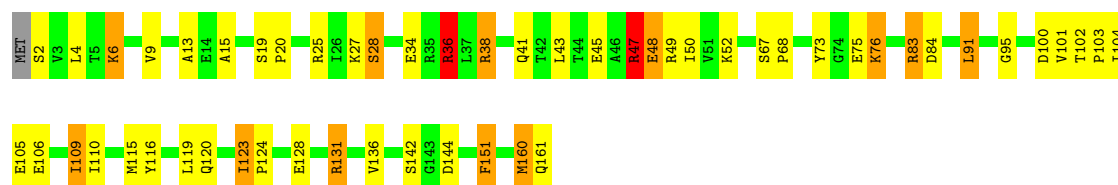
• Molecule 2: Allophycocyanin alpha subunit

Chain G: 68% 24% 6% ..



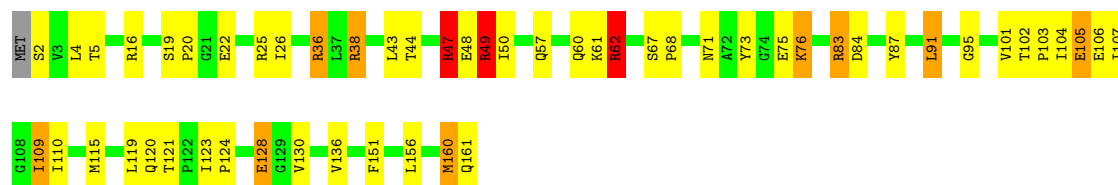
• Molecule 2: Allophycocyanin alpha subunit

Chain I: 66% 25% 7% ..



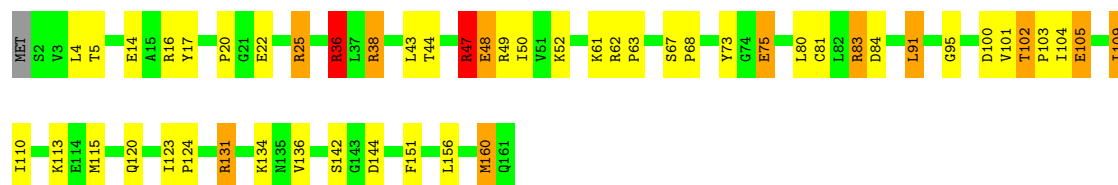
• Molecule 2: Allophycocyanin alpha subunit

Chain K: 66% 26% 6% ..



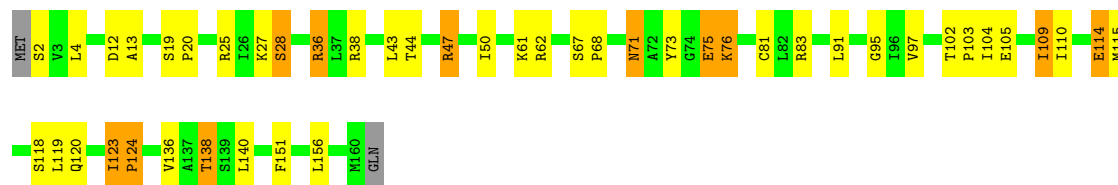
- Molecule 2: Allophycocyanin alpha subunit

Chain Q: 68% 24% 7% ..



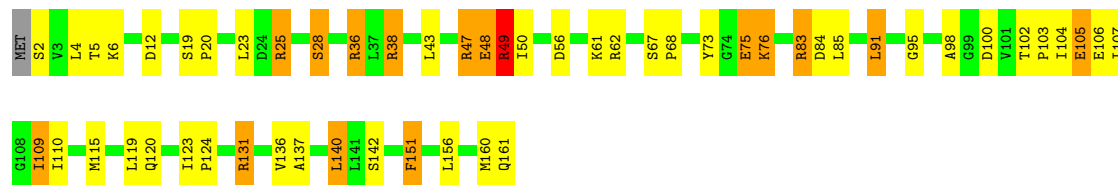
- Molecule 2: Allophycocyanin alpha subunit

Chain S: 70% 22% 7% .



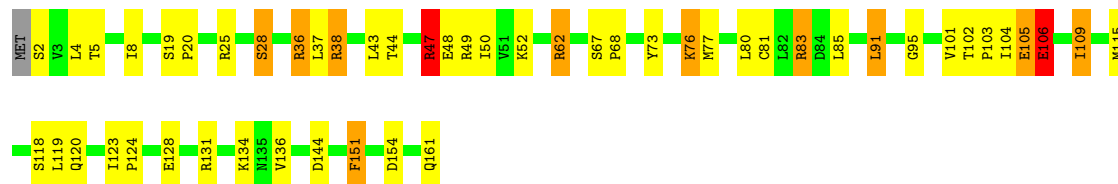
- Molecule 2: Allophycocyanin alpha subunit

Chain U: 66% 24% 9% ..



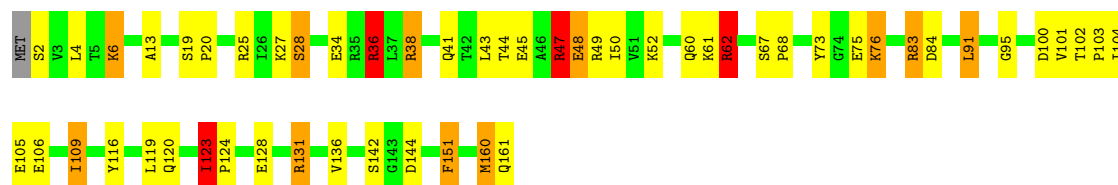
- Molecule 2: Allophycocyanin alpha subunit

Chain W: 68% 24% 6% ..

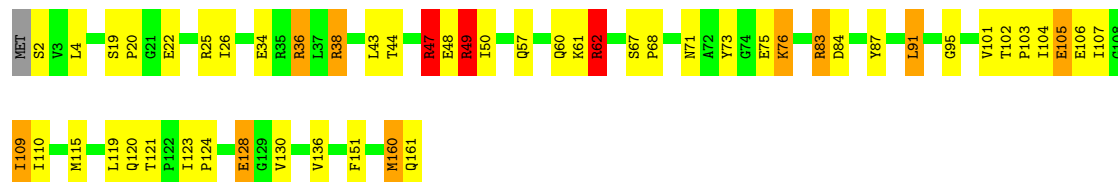


- Molecule 2: Allophycocyanin alpha subunit

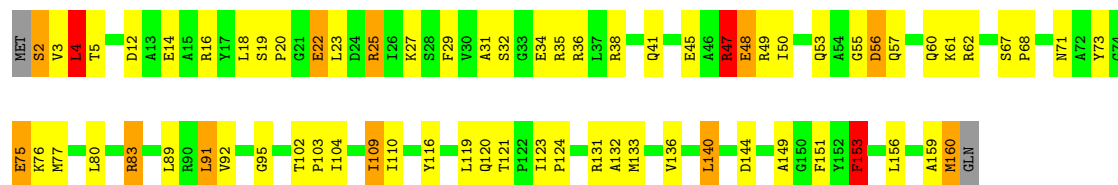
Chain Y: 66% 24% 7% ..



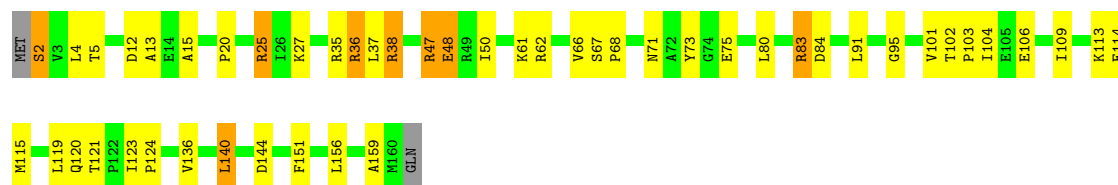
• Molecule 2: Allophycocyanin alpha subunit



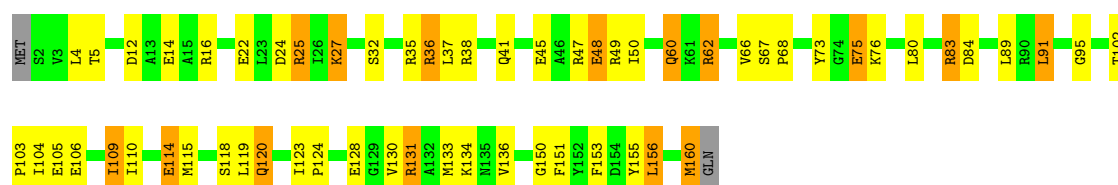
• Molecule 2: Allophycocyanin alpha subunit



• Molecule 2: Allophycocyanin alpha subunit

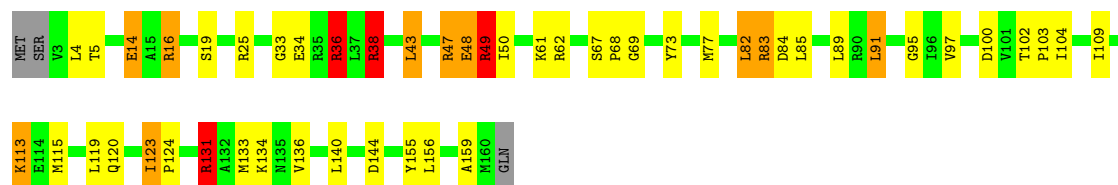


• Molecule 2: Allophycocyanin alpha subunit

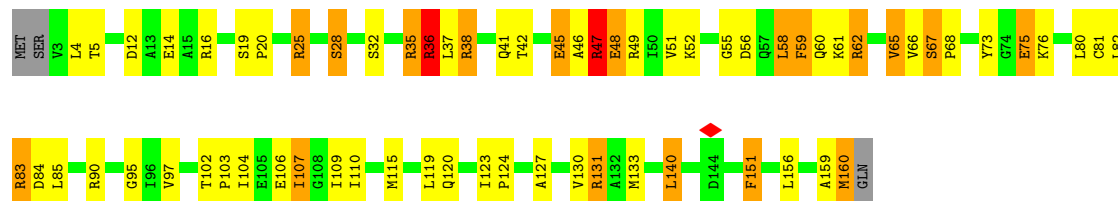


• Molecule 2: Allophycocyanin alpha subunit

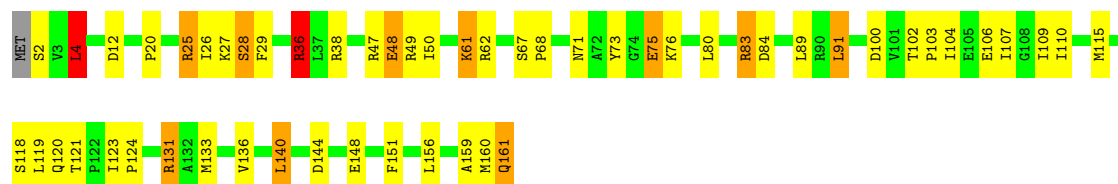




- Molecule 2: Allophycocyanin alpha subunit



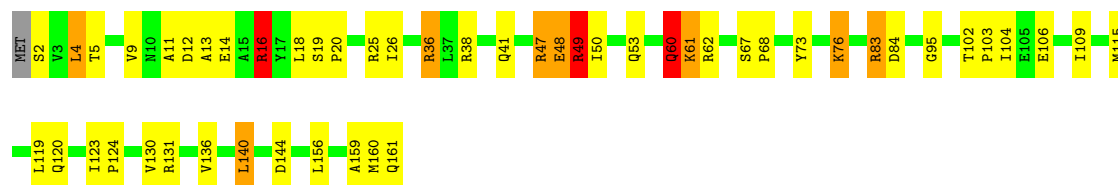
- Molecule 2: Allophycocyanin alpha subunit



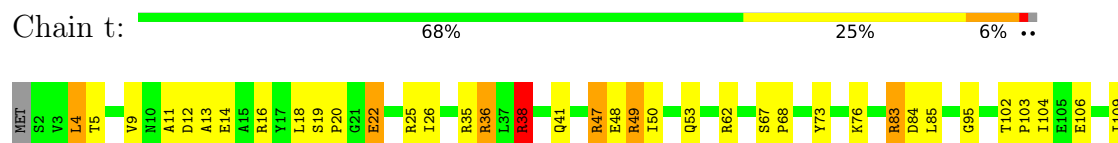
- Molecule 2: Allophycocyanin alpha subunit



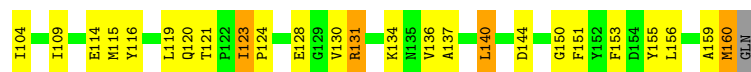
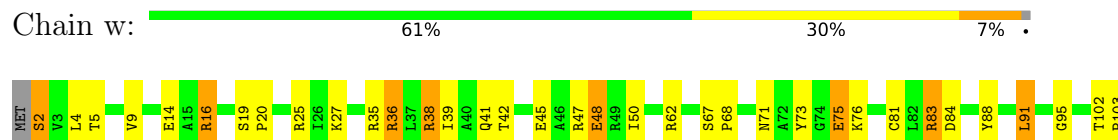
- Molecule 2: Allophycocyanin alpha subunit



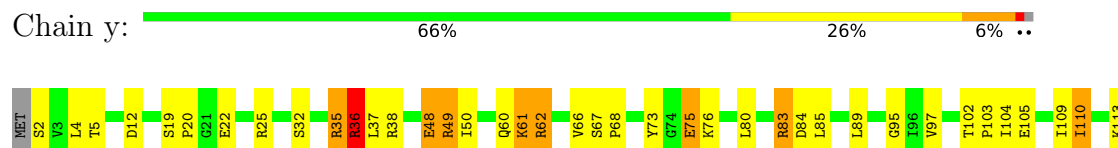
- Molecule 2: Allophycocyanin alpha subunit



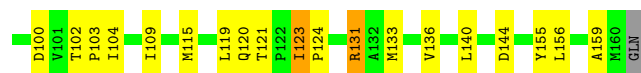
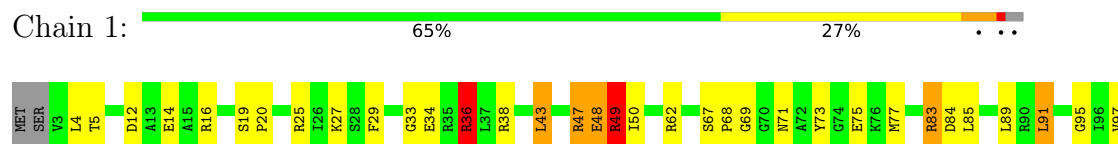
• Molecule 2: Allophycocyanin alpha subunit



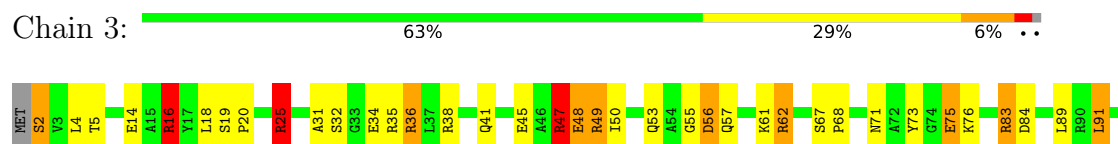
• Molecule 2: Allophycocyanin alpha subunit



• Molecule 2: Allophycocyanin alpha subunit

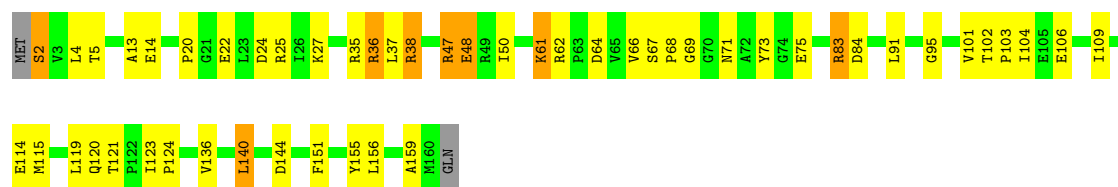


• Molecule 2: Allophycocyanin alpha subunit



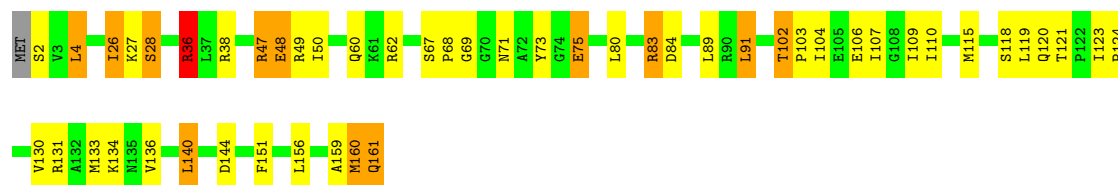
• Molecule 2: Allophycocyanin alpha subunit

Chain 5:  67% 27% 5% •



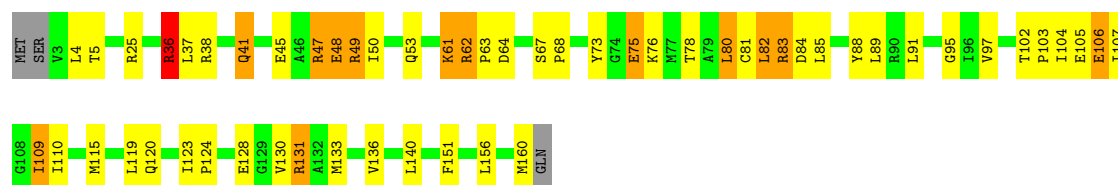
• Molecule 2: Allophycocyanin alpha subunit

Chain 7:  68% 23% 7% ••



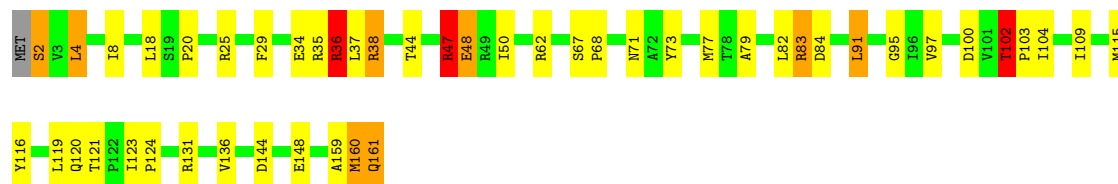
• Molecule 2: Allophycocyanin alpha subunit

Chain 9:  63% 26% 8% ••



• Molecule 2: Allophycocyanin alpha subunit

Chain AA:  70% 23% 5% ••



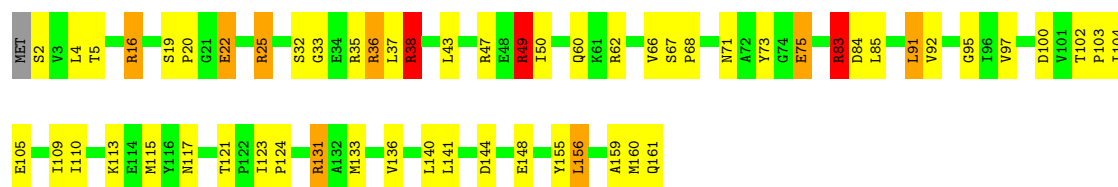
• Molecule 2: Allophycocyanin alpha subunit

Chain AC:  66% 26% 7% ••



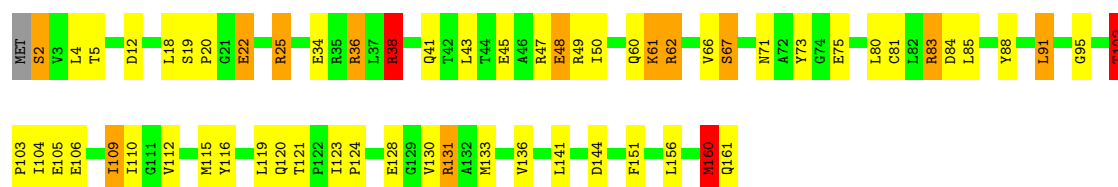
• Molecule 2: Allophycocyanin alpha subunit

Chain AE:  63% 29% 5% ..



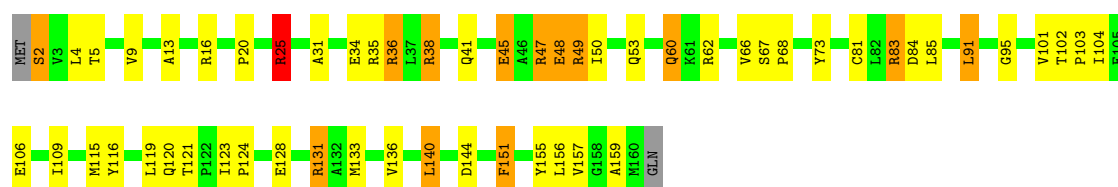
- Molecule 2: Allophycocyanin alpha subunit

Chain AG:  61% 29% 7% ..



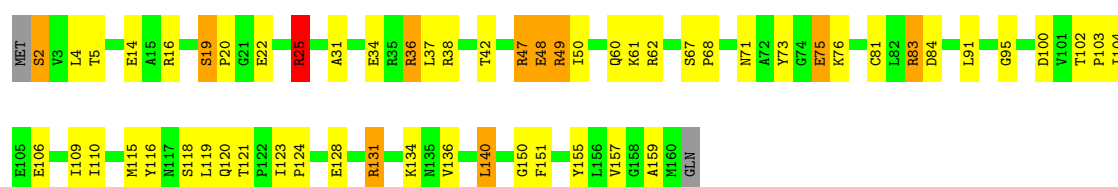
- Molecule 2: Allophycocyanin alpha subunit

Chain AI:  64% 26% 8% ..



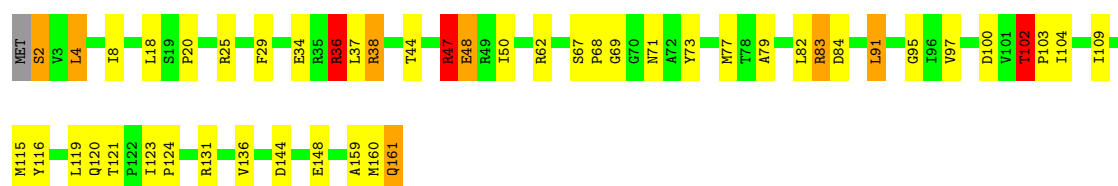
- Molecule 2: Allophycocyanin alpha subunit

Chain AK:  63% 29% 6% ..



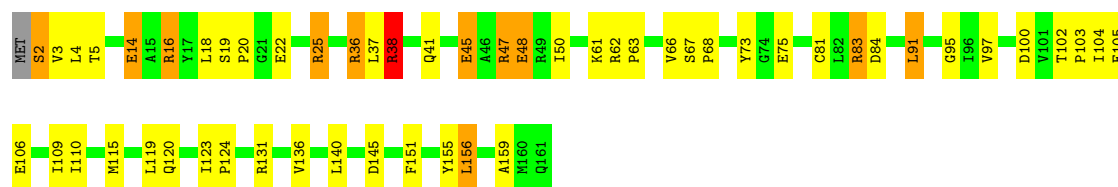
- Molecule 2: Allophycocyanin alpha subunit

Chain AM:  70% 24% ..



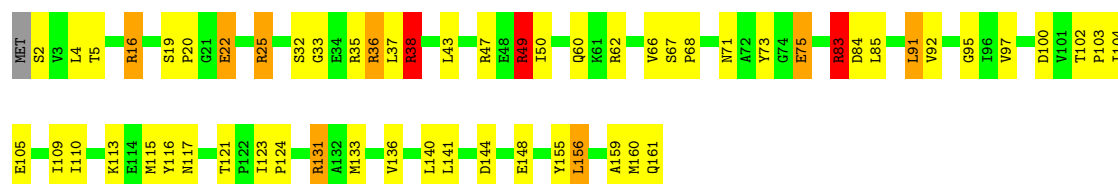
- Molecule 2: Allophycocyanin alpha subunit

Chain AO:  66% 26% 7% ..



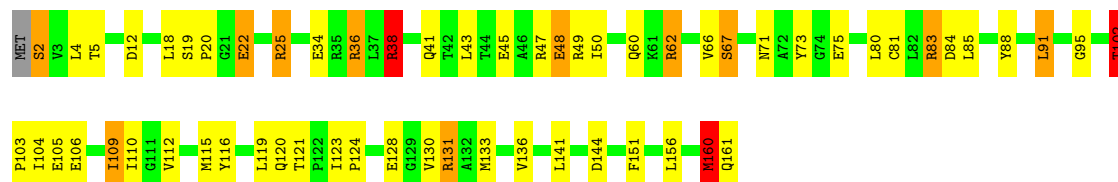
• Molecule 2: Allophycocyanin alpha subunit

Chain AQ:  63% 30% 5% ..



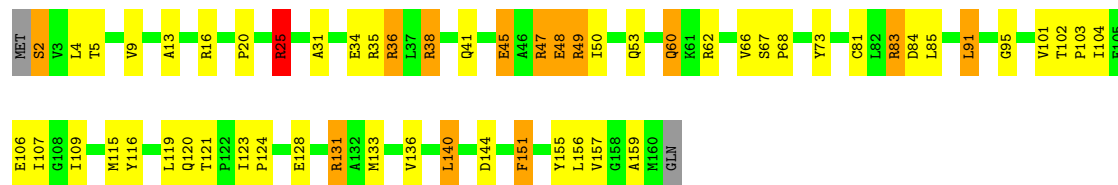
• Molecule 2: Allophycocyanin alpha subunit

Chain AS:  62% 29% 7% ..



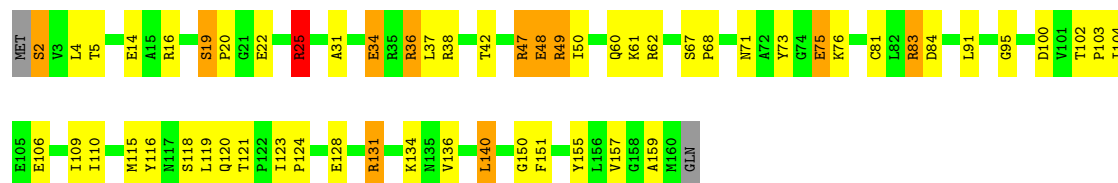
• Molecule 2: Allophycocyanin alpha subunit

Chain AU:  63% 27% 8% ..



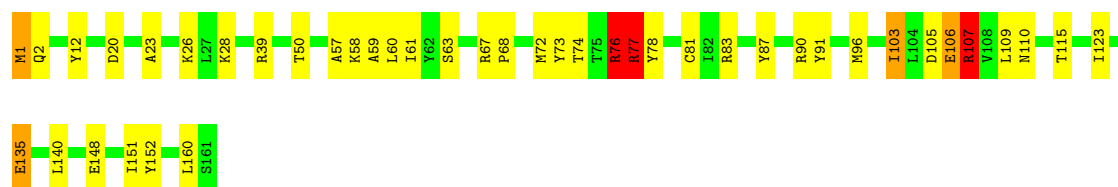
• Molecule 2: Allophycocyanin alpha subunit

Chain AW:  63% 29% 7% ..



• Molecule 3: Allophycocyanin beta subunit

Chain N:  73% 22% ..



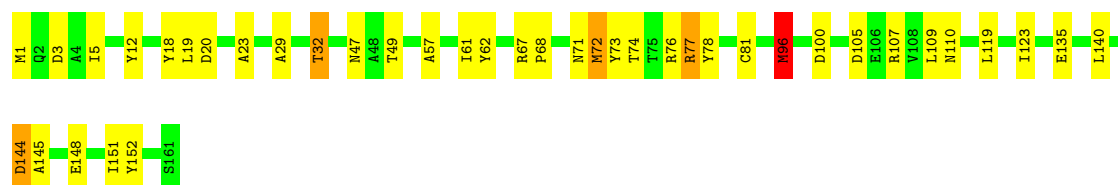
- Molecule 3: Allophycocyanin beta subunit

Chain P:  74% 23% .




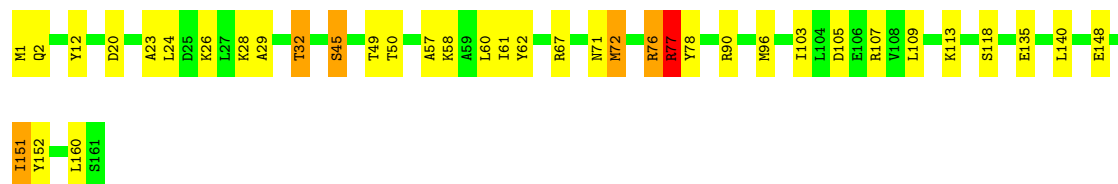
- Molecule 3: Allophycocyanin beta subunit

Chain F:  75% 22% ..



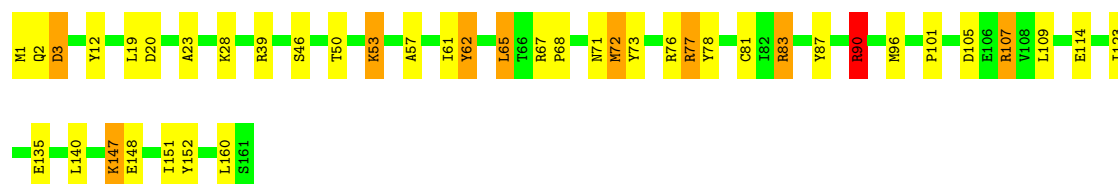
- Molecule 3: Allophycocyanin beta subunit

Chain H:  76% 20% ..



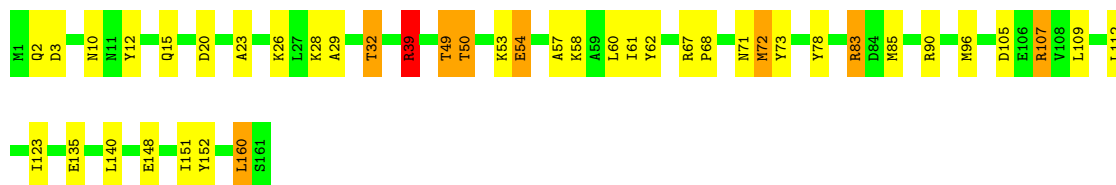
- Molecule 3: Allophycocyanin beta subunit

Chain J:  74% 20% 6% .



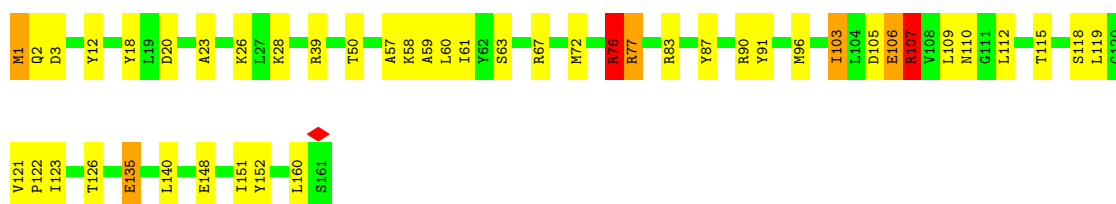
- Molecule 3: Allophycocyanin beta subunit

Chain L:  74% 20% 5% •



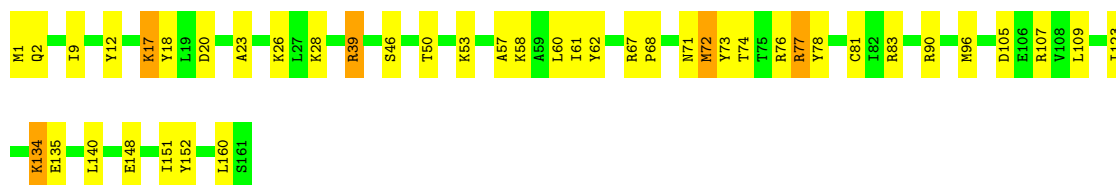
• Molecule 3: Allophycocyanin beta subunit

Chain R:  71% 24% • •




• Molecule 3: Allophycocyanin beta subunit

Chain T:  73% 24% •



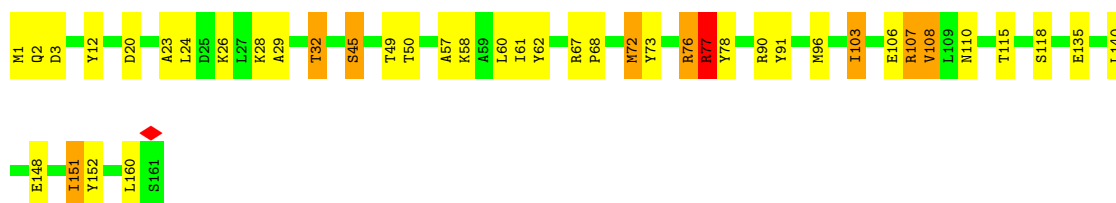
• Molecule 3: Allophycocyanin beta subunit

Chain V:  75% 22% • •



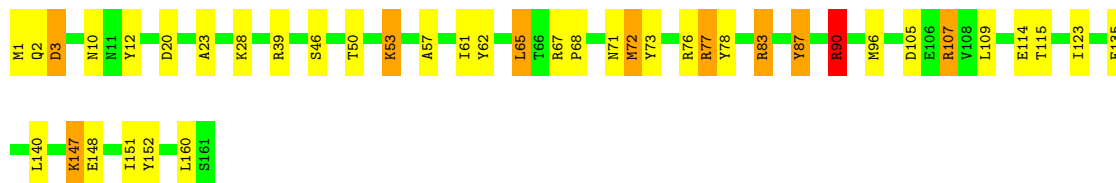
• Molecule 3: Allophycocyanin beta subunit

Chain X:  74% 20% 5% •



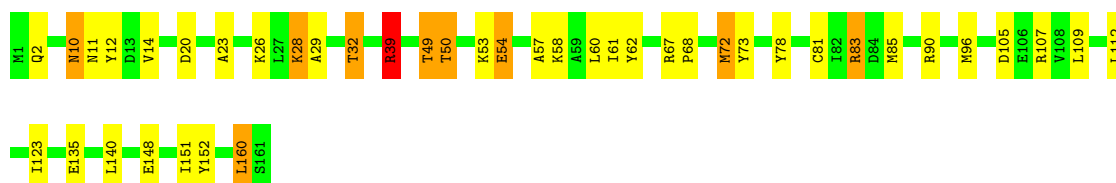
- Molecule 3: Allophycocyanin beta subunit

Chain Z:  75% 19% 6% .



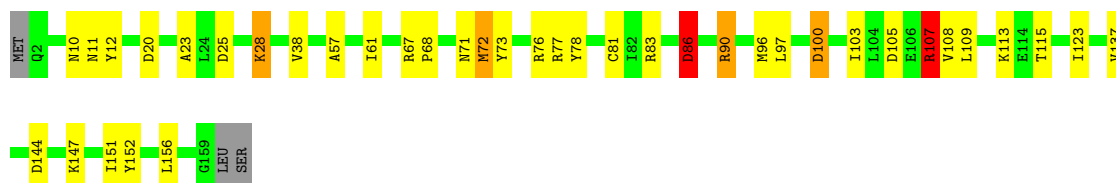
- Molecule 3: Allophycocyanin beta subunit

Chain b:  74% 20% 6% .



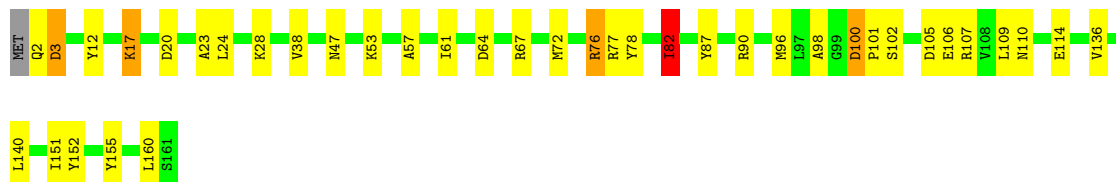
- Molecule 3: Allophycocyanin beta subunit

Chain d:  74% 20% . . .



- Molecule 3: Allophycocyanin beta subunit

Chain f:  75% 21% . . .



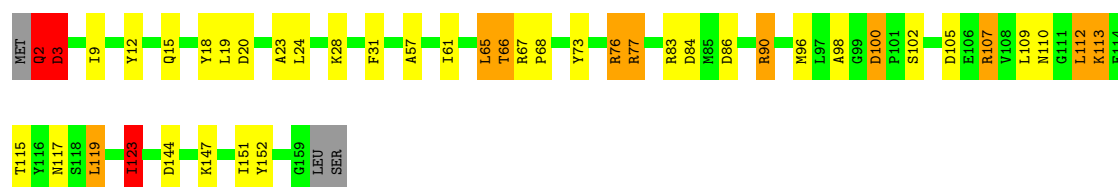
- Molecule 3: Allophycocyanin beta subunit

Chain h:  75% 23% . .



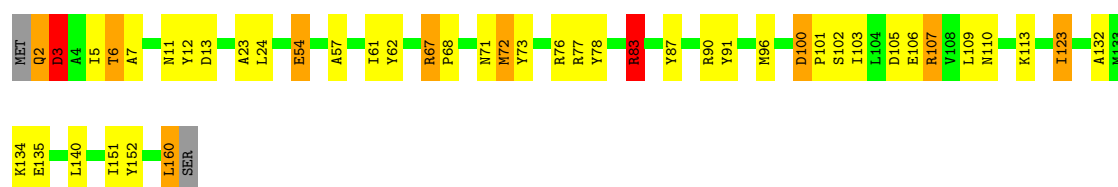
- Molecule 3: Allophycocyanin beta subunit

Chain j:  71% 19% 6% ..




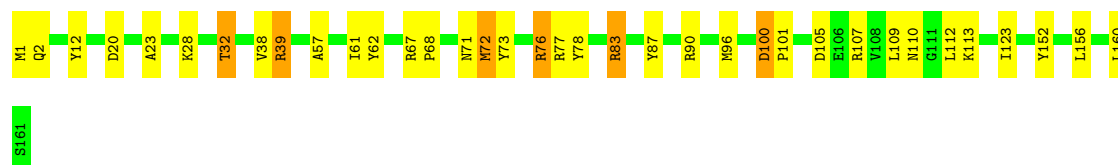
- Molecule 3: Allophycocyanin beta subunit

Chain l:  71% 21% 6% ..




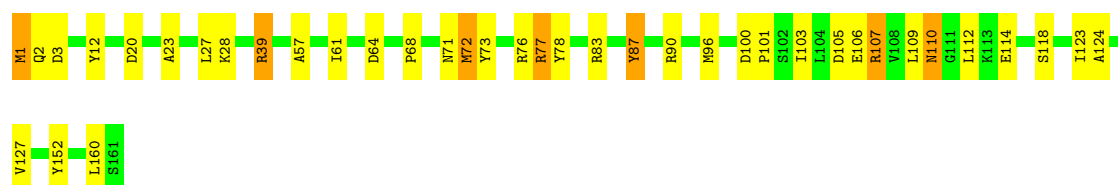
- Molecule 3: Allophycocyanin beta subunit

Chain n:  78% 19% .




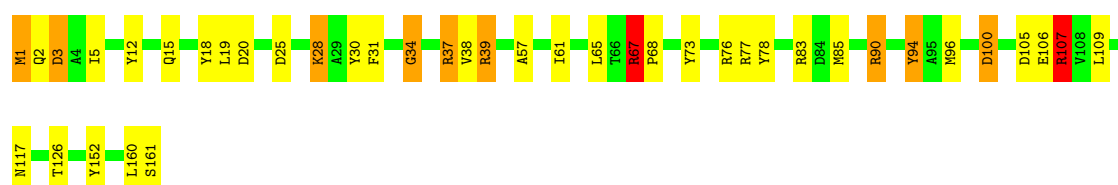
- Molecule 3: Allophycocyanin beta subunit

Chain p:  76% 20% .



- Molecule 3: Allophycocyanin beta subunit

Chain q:  75% 19% 6% .




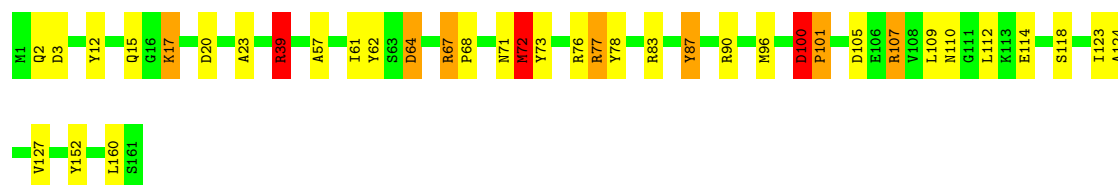
- Molecule 3: Allophycocyanin beta subunit

Chain v:  73% 22% . .



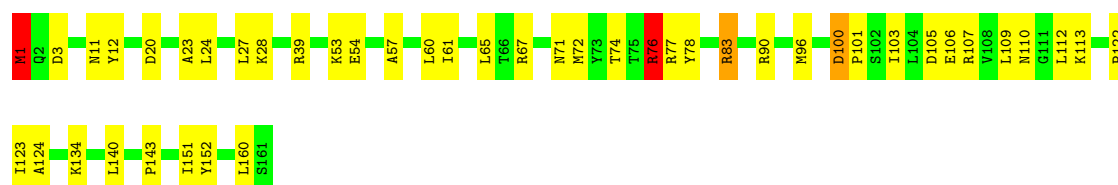
- Molecule 3: Allophycocyanin beta subunit

Chain x:  76% 17% . .



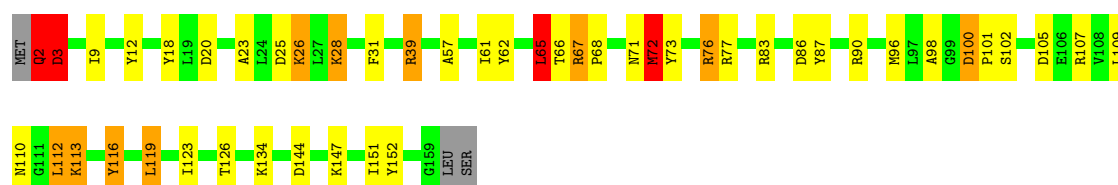
- Molecule 3: Allophycocyanin beta subunit

Chain z:  72% 25% . .



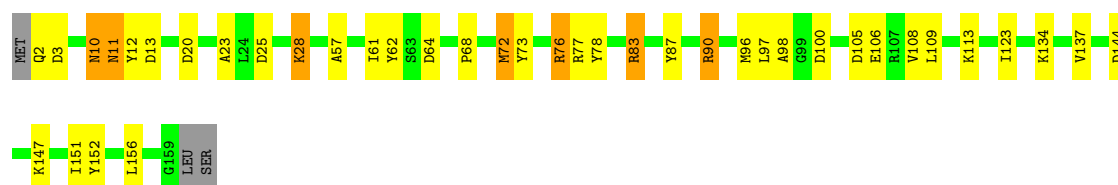
- Molecule 3: Allophycocyanin beta subunit

Chain 2:  68% 21% 6% . .

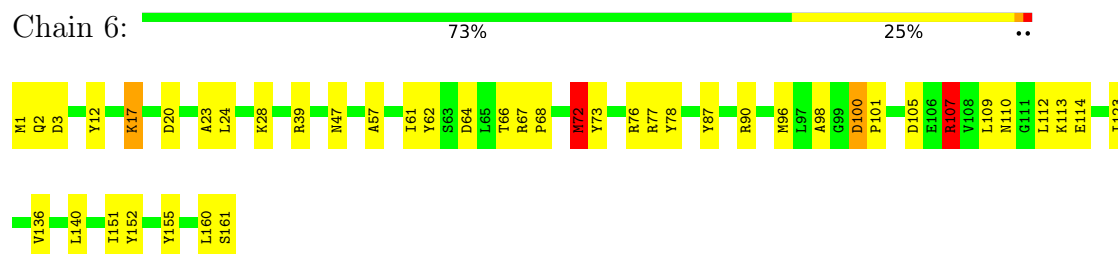


- Molecule 3: Allophycocyanin beta subunit

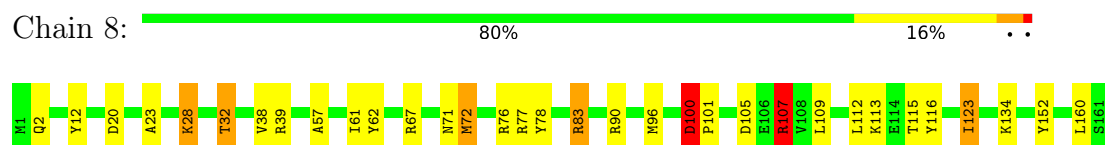
Chain 4:  73% 20% . .



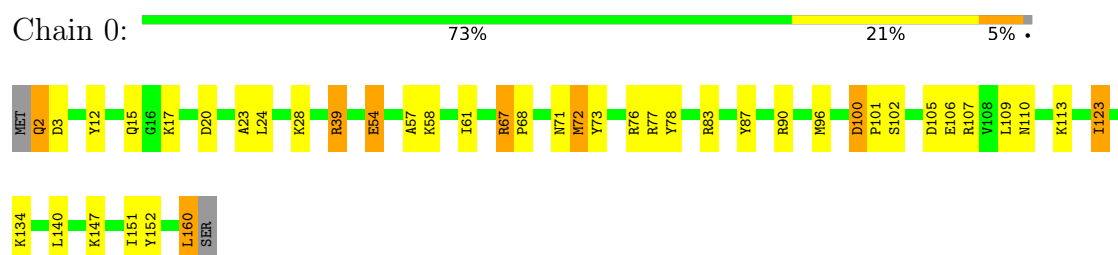
- Molecule 3: Allophycocyanin beta subunit



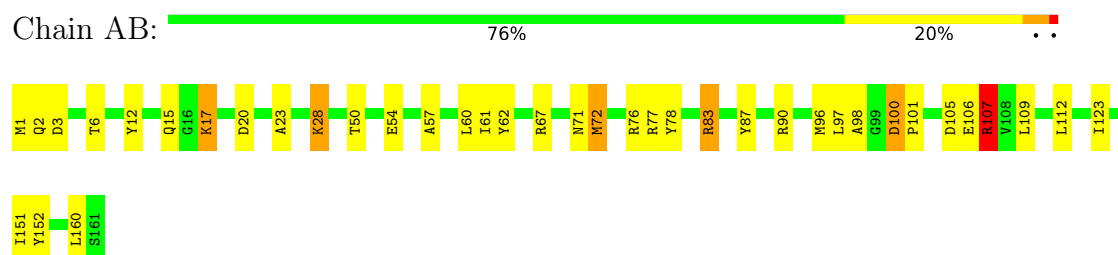
- Molecule 3: Allophycocyanin beta subunit



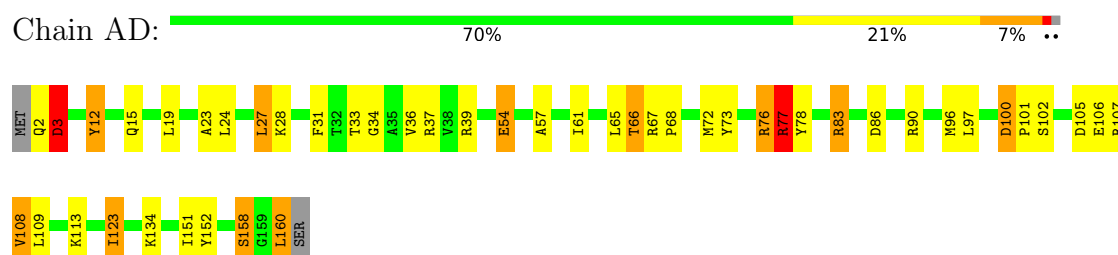
- Molecule 3: Allophycocyanin beta subunit



- Molecule 3: Allophycocyanin beta subunit

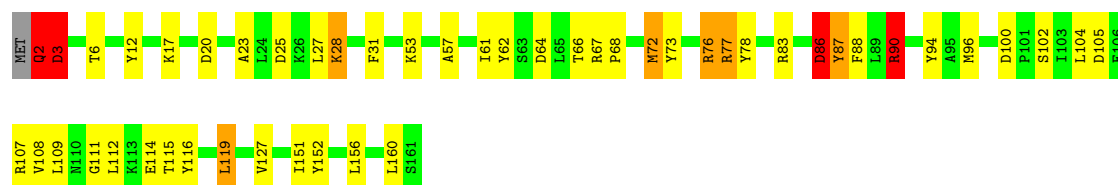


- Molecule 3: Allophycocyanin beta subunit




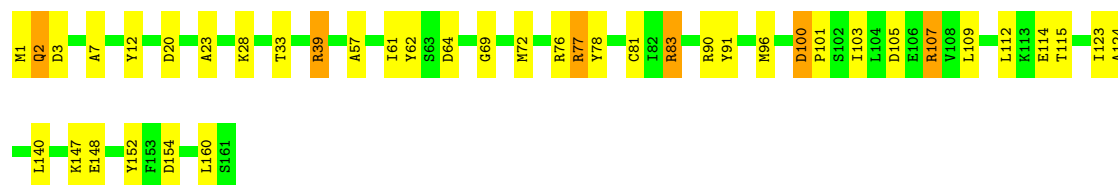
- Molecule 3: Allophycocyanin beta subunit

Chain AF:  69% 24% . .



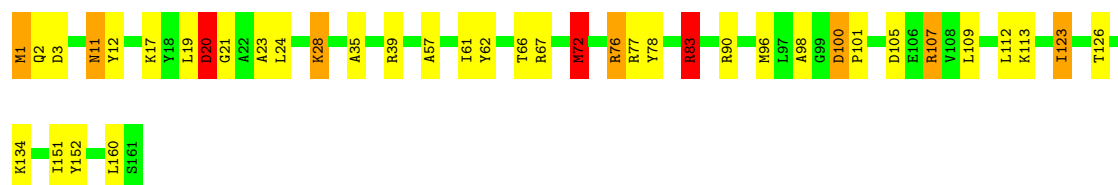
- Molecule 3: Allophycocyanin beta subunit

Chain AH:  75% 22% .



- Molecule 3: Allophycocyanin beta subunit

Chain AJ:  75% 19% . .




- Molecule 3: Allophycocyanin beta subunit

Chain AL:  73% 22% . .



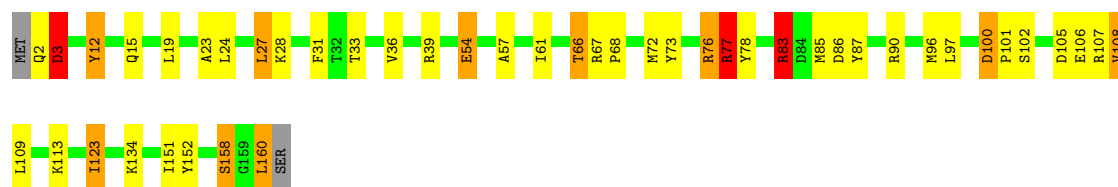
- Molecule 3: Allophycocyanin beta subunit

Chain AN:  74% 22% . .



- Molecule 3: Allophycocyanin beta subunit

Chain AP:  70% 20% 6% ..




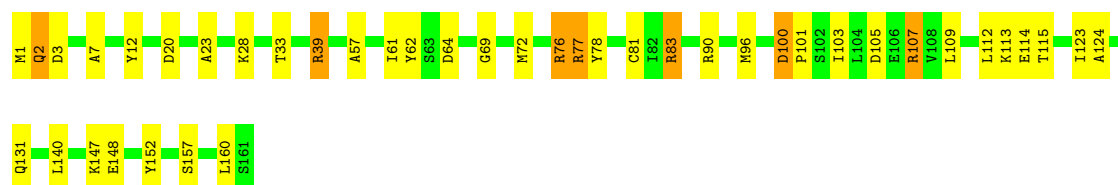
• Molecule 3: Allophycocyanin beta subunit

Chain AR:  69% 25% ..




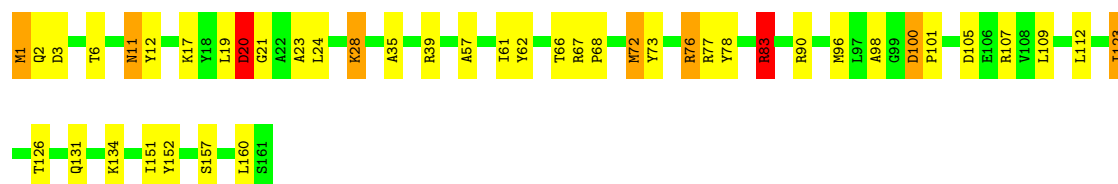
• Molecule 3: Allophycocyanin beta subunit

Chain AT:  74% 22% .



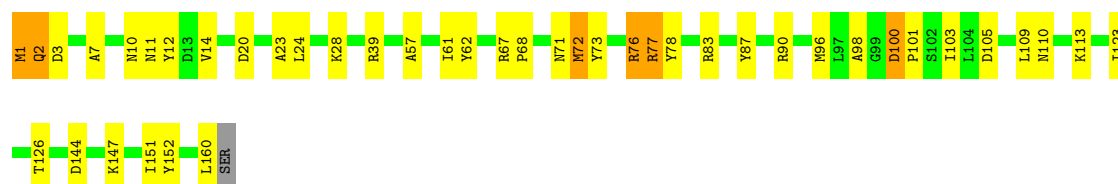
• Molecule 3: Allophycocyanin beta subunit

Chain AV:  73% 22% ..



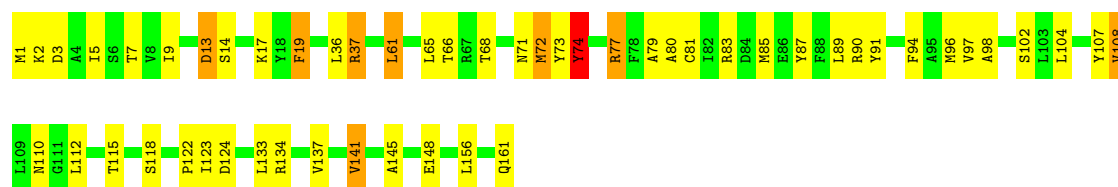
• Molecule 3: Allophycocyanin beta subunit

Chain AX:  73% 23% ..



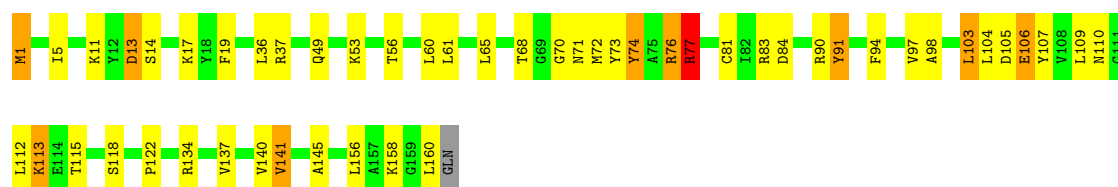
• Molecule 4: Phycobilisome core component

Chain s: 



- Molecule 4: Phycobilisome core component

Chain u: 



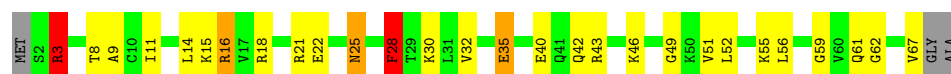
- Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain AY: 



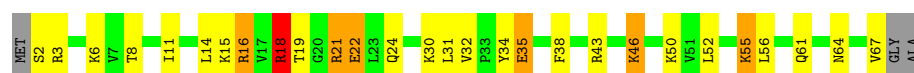
- Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain AZ: 



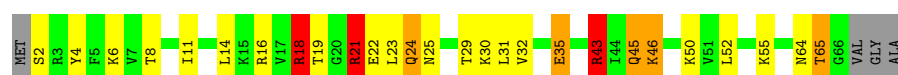
- Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain Aa: 



- Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain Ab: 



- Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain Ac: 



- Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	746972	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	85000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.556	Depositor
Minimum map value	-0.381	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.2	Depositor
Map size (\AA)	840.0, 840.0, 840.0	wwPDB
Map dimensions	672, 672, 672	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.25, 1.25, 1.25	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CYC, MEN

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	0.62	0/8858	1.21	41/11976 (0.3%)
1	C	0.62	0/8858	1.20	38/11976 (0.3%)
2	1	0.69	0/1224	1.30	11/1656 (0.7%)
2	3	0.79	1/1230 (0.1%)	1.38	21/1664 (1.3%)
2	5	0.65	0/1230	1.21	7/1664 (0.4%)
2	7	0.74	0/1240	1.30	12/1676 (0.7%)
2	9	0.75	1/1224 (0.1%)	1.41	15/1656 (0.9%)
2	AA	0.72	2/1240 (0.2%)	1.31	11/1676 (0.7%)
2	AC	0.76	1/1240 (0.1%)	1.45	14/1676 (0.8%)
2	AE	0.83	4/1240 (0.3%)	1.65	25/1676 (1.5%)
2	AG	0.75	2/1240 (0.2%)	1.57	21/1676 (1.3%)
2	AI	0.65	0/1230	1.20	9/1664 (0.5%)
2	AK	0.63	0/1230	1.25	13/1664 (0.8%)
2	AM	0.72	2/1240 (0.2%)	1.31	11/1676 (0.7%)
2	AO	0.76	1/1240 (0.1%)	1.46	15/1676 (0.9%)
2	AQ	0.83	4/1240 (0.3%)	1.65	24/1676 (1.4%)
2	AS	0.75	2/1240 (0.2%)	1.56	21/1676 (1.3%)
2	AU	0.65	0/1230	1.20	8/1664 (0.5%)
2	AW	0.63	0/1230	1.25	14/1664 (0.8%)
2	E	0.69	0/1240	1.29	13/1676 (0.8%)
2	G	0.65	0/1240	1.29	15/1676 (0.9%)
2	I	0.69	0/1240	1.38	14/1676 (0.8%)
2	K	0.65	0/1240	1.30	12/1676 (0.7%)
2	M	0.69	1/1240 (0.1%)	1.41	13/1676 (0.8%)
2	O	0.75	1/1230 (0.1%)	1.39	13/1664 (0.8%)
2	Q	0.69	1/1240 (0.1%)	1.41	13/1676 (0.8%)
2	S	0.76	1/1230 (0.1%)	1.40	14/1664 (0.8%)
2	U	0.68	1/1240 (0.1%)	1.28	13/1676 (0.8%)
2	W	0.65	0/1240	1.29	15/1676 (0.9%)
2	Y	0.69	1/1240 (0.1%)	1.38	14/1676 (0.8%)
2	a	0.64	0/1240	1.30	12/1676 (0.7%)
2	c	0.78	1/1230 (0.1%)	1.40	17/1664 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	e	0.66	0/1230	1.17	4/1664 (0.2%)
2	g	0.78	1/1230 (0.1%)	1.38	19/1664 (1.1%)
2	i	0.67	1/1224 (0.1%)	1.36	13/1656 (0.8%)
2	k	0.85	2/1224 (0.2%)	1.56	20/1656 (1.2%)
2	m	0.72	0/1240	1.39	19/1676 (1.1%)
2	o	0.66	0/1230	1.28	8/1664 (0.5%)
2	r	0.73	0/1240	1.30	10/1676 (0.6%)
2	t	0.70	0/1230	1.46	15/1664 (0.9%)
2	w	0.65	0/1230	1.27	10/1664 (0.6%)
2	y	0.71	1/1230 (0.1%)	1.32	10/1664 (0.6%)
3	0	0.75	0/1203	1.26	7/1630 (0.4%)
3	2	0.90	1/1195 (0.1%)	1.43	19/1619 (1.2%)
3	4	0.70	0/1195	1.28	13/1619 (0.8%)
3	6	0.68	0/1218	1.21	10/1648 (0.6%)
3	8	0.71	1/1218 (0.1%)	1.42	14/1648 (0.8%)
3	AB	0.83	4/1218 (0.3%)	1.30	7/1648 (0.4%)
3	AD	0.74	0/1203	1.32	14/1630 (0.9%)
3	AF	0.79	1/1210 (0.1%)	1.59	19/1638 (1.2%)
3	AH	0.89	1/1218 (0.1%)	1.26	9/1648 (0.5%)
3	AJ	0.66	0/1218	1.22	10/1648 (0.6%)
3	AL	0.63	0/1211	1.15	5/1640 (0.3%)
3	AN	0.83	4/1218 (0.3%)	1.30	7/1648 (0.4%)
3	AP	0.76	0/1203	1.32	14/1630 (0.9%)
3	AR	0.78	1/1210 (0.1%)	1.58	17/1638 (1.0%)
3	AT	0.90	1/1218 (0.1%)	1.26	9/1648 (0.5%)
3	AV	0.67	0/1218	1.22	10/1648 (0.6%)
3	AX	0.63	0/1211	1.14	5/1640 (0.3%)
3	F	0.79	3/1218 (0.2%)	1.25	8/1648 (0.5%)
3	H	0.66	1/1218 (0.1%)	1.16	5/1648 (0.3%)
3	J	0.69	2/1218 (0.2%)	1.41	17/1648 (1.0%)
3	L	0.69	1/1218 (0.1%)	1.27	14/1648 (0.8%)
3	N	0.68	0/1218	1.29	7/1648 (0.4%)
3	P	0.64	1/1218 (0.1%)	1.43	13/1648 (0.8%)
3	R	0.67	0/1218	1.28	7/1648 (0.4%)
3	T	0.64	1/1218 (0.1%)	1.43	14/1648 (0.8%)
3	V	0.79	3/1218 (0.2%)	1.25	8/1648 (0.5%)
3	X	0.69	1/1218 (0.1%)	1.18	8/1648 (0.5%)
3	Z	0.70	2/1218 (0.2%)	1.41	15/1648 (0.9%)
3	b	0.70	1/1218 (0.1%)	1.27	13/1648 (0.8%)
3	d	0.70	1/1195 (0.1%)	1.25	9/1619 (0.6%)
3	f	0.66	0/1210	1.20	4/1638 (0.2%)
3	h	0.82	0/1218	1.48	14/1648 (0.8%)
3	j	0.87	1/1195 (0.1%)	1.35	12/1619 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	l	0.80	1/1203 (0.1%)	1.32	12/1630 (0.7%)
3	n	0.74	0/1218	1.40	10/1648 (0.6%)
3	p	0.81	3/1218 (0.2%)	1.29	13/1648 (0.8%)
3	q	0.89	3/1218 (0.2%)	1.42	15/1648 (0.9%)
3	v	0.89	4/1218 (0.3%)	1.37	11/1648 (0.7%)
3	x	0.73	0/1218	1.30	14/1648 (0.8%)
3	z	0.82	0/1218	1.46	16/1648 (1.0%)
4	s	0.55	0/1246	1.15	1/1682 (0.1%)
4	u	0.55	0/1236	1.25	7/1670 (0.4%)
5	AY	0.51	0/539	1.05	3/725 (0.4%)
5	AZ	0.51	0/539	1.05	3/725 (0.4%)
5	Aa	0.52	0/539	1.07	2/725 (0.3%)
5	Ab	0.51	0/532	1.08	3/715 (0.4%)
5	Ac	0.52	0/528	1.04	0/710
5	Ad	0.52	0/539	1.07	2/725 (0.3%)
All	All	0.71	75/121330 (0.1%)	1.32	1106/164095 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	40
1	C	0	40
2	1	0	8
2	3	0	8
2	5	0	5
2	7	0	7
2	9	0	7
2	AA	0	7
2	AC	0	6
2	AE	0	5
2	AG	0	7
2	AI	0	9
2	AK	0	9
2	AM	0	6
2	AO	0	6
2	AQ	0	5
2	AS	0	7
2	AU	0	9
2	AW	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	6
2	G	0	6
2	I	0	4
2	K	0	6
2	M	0	5
2	O	0	4
2	Q	0	5
2	S	0	4
2	U	0	6
2	W	0	6
2	Y	0	5
2	a	0	5
2	c	0	8
2	e	0	6
2	g	0	9
2	i	0	9
2	k	0	11
2	m	0	7
2	o	0	7
2	r	0	9
2	t	0	8
2	w	0	5
2	y	0	6
3	0	0	6
3	2	0	8
3	4	0	4
3	6	0	5
3	8	0	5
3	AB	0	6
3	AD	0	7
3	AF	0	7
3	AH	0	5
3	AJ	0	6
3	AL	0	6
3	AN	0	6
3	AP	0	7
3	AR	0	7
3	AT	0	6
3	AV	0	5
3	AX	0	6
3	F	0	1
3	H	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	J	0	7
3	L	0	4
3	N	0	3
3	P	0	2
3	R	0	3
3	T	0	2
3	V	0	1
3	X	0	4
3	Z	0	6
3	b	0	4
3	d	0	5
3	f	0	5
3	h	0	4
3	j	0	7
3	l	0	5
3	n	0	5
3	p	0	6
3	q	0	10
3	v	0	9
3	x	0	8
3	z	0	4
4	s	0	4
4	u	0	3
5	AY	0	3
5	AZ	0	3
5	Aa	0	3
5	Ab	0	3
5	Ac	0	5
5	Ad	0	3
All	All	0	584

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	l	83	ARG	NE-CZ	-12.99	1.18	1.33
2	g	62	ARG	CG-CD	-10.83	1.20	1.52
3	2	83	ARG	NE-CZ	-9.64	1.22	1.33
3	j	100	ASP	CG-OD1	-8.95	1.08	1.25
3	p	39	ARG	NE-CZ	-8.51	1.23	1.33
3	Z	3	ASP	CG-OD1	-7.41	1.11	1.25
3	F	145	ALA	CA-CB	-7.40	1.42	1.53
3	J	3	ASP	CG-OD1	-7.37	1.11	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	145	ALA	CA-CB	-7.34	1.42	1.53
3	AN	17	LYS	CB-CG	-7.34	1.30	1.52
3	AB	17	LYS	CB-CG	-7.31	1.30	1.52
2	AM	36	ARG	NE-CZ	-7.02	1.25	1.33
2	AQ	83	ARG	NE-CZ	-6.98	1.25	1.33
2	AE	83	ARG	NE-CZ	-6.97	1.25	1.33
2	AA	36	ARG	NE-CZ	-6.96	1.25	1.33
3	p	100	ASP	CG-OD2	-6.86	1.12	1.25
3	v	5	ILE	CB-CG1	-6.80	1.39	1.53
3	v	20	ASP	CG-OD2	6.40	1.37	1.25
2	3	16	ARG	NE-CZ	-6.40	1.26	1.33
3	q	20	ASP	CG-OD2	6.38	1.37	1.25
2	Q	36	ARG	NE-CZ	-6.35	1.26	1.33
2	i	36	ARG	NE-CZ	6.26	1.40	1.33
2	k	59	PHE	C-O	-6.23	1.16	1.24
2	AE	62	ARG	NE-CZ	6.18	1.39	1.33
2	AQ	62	ARG	NE-CZ	6.15	1.39	1.33
2	M	36	ARG	NE-CZ	-6.08	1.26	1.33
2	9	49	ARG	NE-CZ	5.97	1.39	1.33
3	AF	77	ARG	NE-CZ	-5.74	1.26	1.33
2	c	36	ARG	CZ-NH2	-5.72	1.26	1.33
3	AR	77	ARG	NE-CZ	-5.67	1.26	1.33
3	AN	107	ARG	NE-CZ	5.63	1.39	1.33
3	AB	107	ARG	NE-CZ	5.60	1.39	1.33
3	L	72	MET	CB-CG	-5.58	1.35	1.52
3	AB	72	MET	CB-CG	-5.55	1.35	1.52
3	AN	72	MET	CB-CG	-5.54	1.35	1.52
3	b	72	MET	CB-CG	-5.54	1.35	1.52
2	AC	36	ARG	NE-CZ	5.49	1.39	1.33
3	AN	107	ARG	CG-CD	-5.45	1.36	1.52
3	AB	107	ARG	CG-CD	-5.44	1.36	1.52
2	AA	36	ARG	CG-CD	-5.41	1.36	1.52
3	P	72	MET	CB-CG	-5.41	1.36	1.52
2	AO	36	ARG	NE-CZ	5.41	1.39	1.33
2	k	67	SER	CA-CB	-5.39	1.47	1.53
2	AQ	38	ARG	CZ-NH2	5.39	1.40	1.33
2	AE	38	ARG	CZ-NH2	5.38	1.40	1.33
2	AM	36	ARG	CG-CD	-5.38	1.36	1.52
3	T	72	MET	CB-CG	-5.38	1.36	1.52
3	p	110	ASN	C-O	-5.34	1.17	1.24
3	AT	72	MET	CB-CG	-5.33	1.36	1.52
2	O	38	ARG	CG-CD	-5.32	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	q	37	ARG	NE-CZ	-5.32	1.27	1.33
2	AE	36	ARG	NE-CZ	5.31	1.38	1.33
2	AQ	36	ARG	NE-CZ	5.31	1.38	1.33
2	S	38	ARG	CG-CD	-5.30	1.36	1.52
2	AG	36	ARG	NE-CZ	5.30	1.38	1.33
3	AH	72	MET	CB-CG	-5.30	1.36	1.52
2	AS	36	ARG	NE-CZ	5.30	1.38	1.33
3	F	100	ASP	CG-OD2	-5.28	1.15	1.25
3	v	37	ARG	NE-CZ	-5.26	1.27	1.33
3	H	72	MET	CB-CG	-5.25	1.36	1.52
3	V	100	ASP	CG-OD2	-5.25	1.15	1.25
3	X	72	MET	CB-CG	-5.24	1.36	1.52
3	V	145	ALA	N-CA	-5.21	1.39	1.46
3	Z	2	GLN	C-O	-5.16	1.17	1.23
3	v	100	ASP	CG-OD2	-5.15	1.15	1.25
3	F	145	ALA	N-CA	-5.14	1.39	1.46
2	AG	67	SER	CA-CB	-5.14	1.47	1.53
3	J	2	GLN	C-O	-5.12	1.17	1.23
2	y	48	GLU	CD-OE2	-5.12	1.15	1.25
2	AS	67	SER	CA-CB	-5.11	1.47	1.53
2	Y	123	ILE	CB-CG1	5.10	1.63	1.53
3	q	100	ASP	CG-OD2	-5.09	1.15	1.25
3	8	83	ARG	NE-CZ	-5.06	1.27	1.33
2	U	25	ARG	NE-CZ	-5.03	1.27	1.33
3	d	100	ASP	CG-OD2	-5.01	1.15	1.25

All (1106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AQ	38	ARG	NE-CZ-NH2	25.43	142.09	119.20
2	AE	38	ARG	NE-CZ-NH2	25.25	141.93	119.20
2	AS	62	ARG	NE-CZ-NH1	-23.54	97.96	121.50
2	AG	62	ARG	NE-CZ-NH1	-23.50	98.00	121.50
3	AR	90	ARG	NE-CZ-NH2	21.94	138.94	119.20
3	AF	90	ARG	NE-CZ-NH2	21.85	138.87	119.20
3	z	67	ARG	NE-CZ-NH1	-20.16	101.34	121.50
3	h	67	ARG	NE-CZ-NH1	-20.14	101.36	121.50
3	n	67	ARG	NE-CZ-NH1	-19.46	102.04	121.50
3	8	67	ARG	NE-CZ-NH1	-19.43	102.06	121.50
2	t	38	ARG	NE-CZ-NH1	-19.32	102.18	121.50
3	T	67	ARG	NE-CZ-NH1	-19.23	102.28	121.50
3	P	67	ARG	NE-CZ-NH1	-19.07	102.43	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AO	38	ARG	NE-CZ-NH1	-18.70	102.81	121.50
2	AC	38	ARG	NE-CZ-NH1	-18.66	102.84	121.50
2	AQ	38	ARG	NE-CZ-NH1	-18.52	102.98	121.50
2	AE	38	ARG	NE-CZ-NH1	-18.11	103.39	121.50
2	k	38	ARG	NE-CZ-NH1	-17.59	103.91	121.50
2	k	38	ARG	NE-CZ-NH2	17.54	134.99	119.20
3	J	90	ARG	NE-CZ-NH2	16.40	133.96	119.20
3	Z	90	ARG	NE-CZ-NH2	16.36	133.93	119.20
2	t	38	ARG	NE-CZ-NH2	16.23	133.80	119.20
2	AG	38	ARG	NE-CZ-NH2	15.78	133.40	119.20
2	AS	38	ARG	NE-CZ-NH2	15.69	133.32	119.20
2	AO	38	ARG	NE-CZ-NH2	15.43	133.09	119.20
2	AC	38	ARG	NE-CZ-NH2	15.32	132.99	119.20
3	h	67	ARG	CD-NE-CZ	15.26	145.76	124.40
3	z	67	ARG	CD-NE-CZ	15.25	145.75	124.40
3	AN	107	ARG	NE-CZ-NH2	15.22	132.90	119.20
3	AB	107	ARG	NE-CZ-NH2	15.18	132.86	119.20
3	8	67	ARG	CD-NE-CZ	15.03	145.44	124.40
3	n	67	ARG	CD-NE-CZ	15.02	145.42	124.40
3	AF	90	ARG	CD-NE-CZ	14.93	145.29	124.40
3	AR	90	ARG	CD-NE-CZ	14.86	145.21	124.40
3	J	90	ARG	NE-CZ-NH1	-14.79	106.71	121.50
3	Z	90	ARG	NE-CZ-NH1	-14.72	106.78	121.50
3	P	67	ARG	CD-NE-CZ	14.61	144.86	124.40
2	i	38	ARG	NE-CZ-NH2	14.58	132.32	119.20
3	T	67	ARG	CD-NE-CZ	14.53	144.74	124.40
2	M	36	ARG	NE-CZ-NH2	-14.48	106.17	119.20
2	Q	36	ARG	NE-CZ-NH2	-14.48	106.17	119.20
3	T	134	LYS	CD-CE-NZ	14.46	158.17	111.90
3	N	106	GLU	CB-CG-CD	14.45	137.16	112.60
3	P	134	LYS	CD-CE-NZ	14.43	158.09	111.90
2	9	36	ARG	NE-CZ-NH2	-14.40	106.24	119.20
3	R	106	GLU	CB-CG-CD	14.31	136.93	112.60
2	AE	83	ARG	NE-CZ-NH1	-14.21	107.29	121.50
2	AQ	83	ARG	NE-CZ-NH1	-14.15	107.35	121.50
2	Y	36	ARG	NE-CZ-NH2	-14.07	106.53	119.20
3	J	90	ARG	CD-NE-CZ	13.96	143.94	124.40
3	Z	90	ARG	CD-NE-CZ	13.95	143.93	124.40
2	I	36	ARG	NE-CZ-NH2	-13.94	106.65	119.20
3	AJ	20	ASP	CA-CB-CG	13.77	126.37	112.60
3	AV	20	ASP	CA-CB-CG	13.77	126.37	112.60
3	AR	2	GLN	OE1-CD-NE2	13.54	136.14	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AF	2	GLN	OE1-CD-NE2	13.46	136.06	122.60
2	k	36	ARG	NE-CZ-NH2	-13.41	107.13	119.20
3	F	32	THR	CA-CB-OG1	12.98	129.08	109.60
3	V	32	THR	CA-CB-OG1	12.95	129.02	109.60
3	AF	90	ARG	NE-CZ-NH1	-12.86	108.64	121.50
3	AR	90	ARG	NE-CZ-NH1	-12.82	108.68	121.50
3	8	67	ARG	NE-CZ-NH2	12.67	130.60	119.20
3	n	67	ARG	NE-CZ-NH2	12.66	130.60	119.20
3	T	67	ARG	NE-CZ-NH2	12.60	130.54	119.20
3	P	67	ARG	NE-CZ-NH2	12.56	130.50	119.20
3	2	2	GLN	OE1-CD-NE2	12.31	134.91	122.60
3	AF	6	THR	OG1-CB-CG2	-12.12	85.07	109.30
3	AR	6	THR	OG1-CB-CG2	-12.12	85.07	109.30
3	l	6	THR	OG1-CB-CG2	-12.09	85.12	109.30
2	AS	62	ARG	NH1-CZ-NH2	12.07	134.99	119.30
2	AG	62	ARG	NH1-CZ-NH2	12.03	134.94	119.30
2	i	38	ARG	NE-CZ-NH1	-11.92	109.58	121.50
3	z	67	ARG	NE-CZ-NH2	11.88	129.89	119.20
3	h	67	ARG	NE-CZ-NH2	11.86	129.87	119.20
2	AG	38	ARG	NE-CZ-NH1	-11.71	109.79	121.50
2	AS	38	ARG	NE-CZ-NH1	-11.68	109.82	121.50
3	AD	3	ASP	CA-CB-CG	11.63	124.23	112.60
3	AP	3	ASP	CA-CB-CG	11.62	124.22	112.60
3	AF	3	ASP	CA-CB-CG	11.40	124.00	112.60
3	AR	3	ASP	CA-CB-CG	11.38	123.98	112.60
3	2	3	ASP	CA-CB-CG	11.22	123.82	112.60
2	M	36	ARG	NE-CZ-NH1	10.97	132.47	121.50
2	Q	47	ARG	CB-CG-CD	10.93	136.43	111.30
2	Q	36	ARG	NE-CZ-NH1	10.92	132.42	121.50
2	Y	36	ARG	NE-CZ-NH1	10.89	132.39	121.50
2	1	36	ARG	NE-CZ-NH1	10.88	132.38	121.50
2	I	36	ARG	NE-CZ-NH1	10.78	132.28	121.50
2	M	47	ARG	CB-CG-CD	10.74	135.99	111.30
2	S	71	ASN	CA-CB-CG	10.69	123.29	112.60
3	l	83	ARG	NE-CZ-NH1	-10.61	110.89	121.50
3	j	3	ASP	CA-CB-CG	10.60	123.20	112.60
2	O	71	ASN	CA-CB-CG	10.55	123.16	112.60
2	3	16	ARG	CD-NE-CZ	-10.45	109.76	124.40
2	Y	45	GLU	CB-CG-CD	10.40	130.28	112.60
2	S	38	ARG	NE-CZ-NH1	10.34	131.84	121.50
2	I	45	GLU	CB-CG-CD	10.30	130.10	112.60
3	f	82	ILE	CA-CB-CG1	10.29	127.90	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	38	ARG	NE-CZ-NH1	10.23	131.73	121.50
3	l	3	ASP	CA-CB-CG	10.16	122.76	112.60
3	AB	107	ARG	CD-NE-CZ	10.11	138.55	124.40
2	9	36	ARG	NE-CZ-NH1	10.10	131.60	121.50
3	AN	107	ARG	CD-NE-CZ	10.04	138.45	124.40
2	c	4	LEU	CB-CG-CD1	-9.97	80.80	110.70
3	AN	107	ARG	NE-CZ-NH1	-9.96	111.54	121.50
3	2	83	ARG	NE-CZ-NH2	9.93	128.14	119.20
3	AB	107	ARG	NE-CZ-NH1	-9.91	111.58	121.50
3	q	39	ARG	NE-CZ-NH2	9.85	128.06	119.20
3	AP	83	ARG	NE-CZ-NH1	-9.84	111.66	121.50
2	m	48	GLU	CB-CG-CD	9.75	129.18	112.60
2	AS	22	GLU	CA-CB-CG	9.75	133.61	114.10
2	AG	22	GLU	CA-CB-CG	9.75	133.59	114.10
2	i	36	ARG	NE-CZ-NH1	9.72	131.22	121.50
2	AM	36	ARG	CB-CG-CD	9.66	133.53	111.30
2	AA	36	ARG	CB-CG-CD	9.66	133.52	111.30
2	k	36	ARG	NE-CZ-NH1	9.60	131.10	121.50
3	AB	17	LYS	CA-CB-CG	9.56	133.23	114.10
3	AN	17	LYS	CA-CB-CG	9.56	133.23	114.10
3	v	53	LYS	CB-CG-CD	9.45	133.04	111.30
3	V	145	ALA	N-CA-CB	-9.37	96.28	110.33
3	F	145	ALA	N-CA-CB	-9.36	96.29	110.33
1	A	886	PHE	CB-CA-C	-9.35	102.87	111.00
1	C	886	PHE	CB-CA-C	-9.32	102.89	111.00
3	AF	28	LYS	CA-CB-CG	9.31	132.73	114.10
3	AR	28	LYS	CA-CB-CG	9.30	132.69	114.10
3	h	83	ARG	NE-CZ-NH2	9.20	127.48	119.20
1	C	344	ARG	NE-CZ-NH1	-9.18	112.32	121.50
3	z	83	ARG	NE-CZ-NH2	9.17	127.45	119.20
2	m	61	LYS	CB-CG-CD	9.15	132.34	111.30
3	d	86	ASP	CA-CB-CG	9.14	121.74	112.60
1	A	344	ARG	NE-CZ-NH1	-9.08	112.42	121.50
2	o	25	ARG	NE-CZ-NH1	-9.07	112.43	121.50
3	AF	86	ASP	CA-CB-CG	9.00	121.60	112.60
3	J	83	ARG	NE-CZ-NH1	-8.99	112.50	121.50
3	Z	83	ARG	NE-CZ-NH1	-8.98	112.52	121.50
3	AR	86	ASP	CA-CB-CG	8.97	121.58	112.60
3	j	100	ASP	OD1-CG-OD2	-8.96	101.39	122.90
3	x	39	ARG	NE-CZ-NH1	-8.90	112.60	121.50
3	R	110	ASN	OD1-CG-ND2	8.80	131.40	122.60
2	AE	62	ARG	NE-CZ-NH1	8.78	130.28	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	v	107	ARG	NE-CZ-NH1	-8.77	112.73	121.50
2	AE	25	ARG	NE-CZ-NH2	8.75	127.08	119.20
2	AQ	62	ARG	NE-CZ-NH1	8.72	130.22	121.50
2	AS	160	MET	CG-SD-CE	-8.72	81.71	100.90
2	AG	160	MET	CG-SD-CE	-8.72	81.72	100.90
2	AQ	25	ARG	NE-CZ-NH2	8.71	127.04	119.20
2	AE	25	ARG	NE-CZ-NH1	-8.71	112.79	121.50
2	AQ	25	ARG	NE-CZ-NH1	-8.68	112.82	121.50
3	q	107	ARG	NE-CZ-NH1	-8.66	112.84	121.50
2	AO	62	ARG	NE-CZ-NH1	-8.63	112.87	121.50
2	AC	62	ARG	NE-CZ-NH1	-8.63	112.87	121.50
3	N	110	ASN	OD1-CG-ND2	8.60	131.20	122.60
3	j	90	ARG	NE-CZ-NH2	8.54	126.89	119.20
3	x	64	ASP	CA-CB-CG	8.54	121.14	112.60
3	2	83	ARG	NH1-CZ-NH2	-8.51	108.23	119.30
2	g	114	GLU	CB-CG-CD	8.48	127.02	112.60
2	AA	148	GLU	CG-CD-OE2	-8.46	98.93	118.40
2	AM	148	GLU	CG-CD-OE2	-8.45	98.97	118.40
3	4	11	ASN	N-CA-CB	8.44	123.36	110.28
2	O	114	GLU	CB-CG-CD	8.44	126.94	112.60
2	AC	36	ARG	NE-CZ-NH2	8.43	126.79	119.20
2	o	25	ARG	NE-CZ-NH2	8.42	126.78	119.20
2	1	36	ARG	CG-CD-NE	-8.40	93.52	112.00
2	AO	36	ARG	NE-CZ-NH2	8.40	126.76	119.20
2	S	114	GLU	CB-CG-CD	8.38	126.84	112.60
3	2	28	LYS	CA-CB-CG	8.38	130.86	114.10
3	q	67	ARG	NE-CZ-NH1	-8.37	113.13	121.50
2	c	36	ARG	CG-CD-NE	-8.36	93.61	112.00
2	k	151	PHE	CA-CB-CG	8.34	122.14	113.80
3	4	28	LYS	CA-CB-CG	8.33	130.75	114.10
3	d	28	LYS	CA-CB-CG	8.30	130.71	114.10
3	AF	17	LYS	CG-CD-CE	8.23	130.23	111.30
1	A	839	ARG	N-CA-CB	-8.21	98.31	111.62
2	y	38	ARG	NE-CZ-NH1	8.21	129.71	121.50
2	t	38	ARG	CD-NE-CZ	8.21	135.89	124.40
3	AR	17	LYS	CG-CD-CE	8.21	130.17	111.30
1	C	839	ARG	N-CA-CB	-8.20	98.33	111.62
2	a	47	ARG	CB-CG-CD	8.18	130.10	111.30
2	K	47	ARG	CB-CG-CD	8.17	130.10	111.30
3	R	76	ARG	CB-CG-CD	8.17	130.09	111.30
3	P	39	ARG	CB-CG-CD	8.16	130.06	111.30
3	P	67	ARG	CG-CD-NE	8.15	129.94	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	0	39	ARG	CG-CD-NE	8.15	129.93	112.00
3	T	67	ARG	CG-CD-NE	8.14	129.91	112.00
2	g	27	LYS	CA-CB-CG	8.13	130.36	114.10
2	E	47	ARG	CB-CG-CD	8.12	129.98	111.30
2	1	36	ARG	NE-CZ-NH2	-8.11	111.90	119.20
3	T	39	ARG	CB-CG-CD	8.11	129.96	111.30
2	U	47	ARG	CB-CG-CD	8.10	129.94	111.30
2	W	47	ARG	CB-CG-CD	8.09	129.92	111.30
2	g	128	GLU	CG-CD-OE1	-8.09	99.78	118.40
2	9	62	ARG	NE-CZ-NH2	8.09	126.48	119.20
2	m	36	ARG	NE-CZ-NH1	8.09	129.59	121.50
2	G	47	ARG	CB-CG-CD	8.09	129.91	111.30
3	AH	114	GLU	CG-CD-OE1	-8.07	99.83	118.40
2	AQ	131	ARG	NE-CZ-NH1	-8.07	113.43	121.50
3	b	67	ARG	NH1-CZ-NH2	-8.06	108.81	119.30
2	AG	62	ARG	NE-CZ-NH2	8.06	126.45	119.20
3	AT	114	GLU	CG-CD-OE1	-8.04	99.90	118.40
2	AS	62	ARG	NE-CZ-NH2	8.03	126.43	119.20
1	A	620	PRO	N-CA-C	8.02	123.90	114.03
2	AE	131	ARG	NE-CZ-NH1	-8.02	113.48	121.50
3	V	96	MET	CG-SD-CE	-7.97	83.36	100.90
3	F	96	MET	CG-SD-CE	-7.95	83.41	100.90
1	C	620	PRO	N-CA-C	7.95	123.81	114.03
3	2	112	LEU	CD1-CG-CD2	7.93	128.24	110.80
3	L	67	ARG	NH1-CZ-NH2	-7.93	109.00	119.30
3	N	76	ARG	CB-CG-CD	7.92	129.52	111.30
2	AE	36	ARG	NE-CZ-NH2	7.92	126.33	119.20
2	AQ	36	ARG	NE-CZ-NH2	7.91	126.32	119.20
2	g	36	ARG	NE-CZ-NH2	7.87	126.28	119.20
3	V	67	ARG	NH1-CZ-NH2	-7.86	109.08	119.30
2	9	128	GLU	CG-CD-OE1	-7.86	100.33	118.40
3	F	67	ARG	NH1-CZ-NH2	-7.85	109.10	119.30
3	q	20	ASP	CB-CA-C	7.84	125.37	109.76
2	r	61	LYS	CB-CG-CD	7.84	129.32	111.30
2	y	48	GLU	CG-CD-OE2	-7.83	100.38	118.40
2	y	110	ILE	CA-CB-CG1	7.81	123.67	110.40
3	2	119	LEU	CB-CG-CD2	-7.81	87.27	110.70
2	O	75	GLU	CG-CD-OE1	-7.81	100.44	118.40
2	y	36	ARG	NE-CZ-NH2	-7.81	112.17	119.20
3	8	32	THR	CA-CB-OG1	7.80	121.31	109.60
2	Q	14	GLU	CB-CG-CD	7.80	125.86	112.60
2	M	14	GLU	CB-CG-CD	7.80	125.85	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	d	107	ARG	NE-CZ-NH1	-7.79	113.71	121.50
1	A	455	PHE	CA-CB-CG	-7.79	106.01	113.80
3	b	10	ASN	CB-CG-ND2	-7.79	104.72	116.40
2	y	36	ARG	CD-NE-CZ	7.79	135.30	124.40
3	n	32	THR	CA-CB-OG1	7.78	121.27	109.60
2	AG	36	ARG	NE-CZ-NH2	7.77	126.19	119.20
2	W	106	GLU	N-CA-CB	7.76	121.53	110.12
3	6	17	LYS	CG-CD-CE	7.75	129.12	111.30
2	k	110	ILE	CA-CB-CG1	7.75	123.57	110.40
2	w	16	ARG	NH1-CZ-NH2	7.74	129.36	119.30
2	3	25	ARG	NE-CZ-NH2	-7.74	112.24	119.20
2	G	106	GLU	N-CA-CB	7.74	121.49	110.12
3	v	20	ASP	CB-CA-C	7.74	125.15	109.76
2	S	75	GLU	CG-CD-OE1	-7.73	100.61	118.40
2	AS	36	ARG	NE-CZ-NH2	7.72	126.15	119.20
1	C	455	PHE	CA-CB-CG	-7.71	106.09	113.80
2	AE	156	LEU	CB-CG-CD2	7.70	133.79	110.70
2	AQ	156	LEU	CB-CG-CD2	7.69	133.77	110.70
3	f	17	LYS	CG-CD-CE	7.68	128.97	111.30
2	o	36	ARG	NE-CZ-NH2	-7.67	112.30	119.20
2	t	36	ARG	CD-NE-CZ	7.66	135.12	124.40
3	x	17	LYS	CG-CD-CE	7.65	128.90	111.30
2	AG	61	LYS	CB-CG-CD	7.65	128.90	111.30
3	j	100	ASP	CB-CG-OD2	7.64	135.97	118.40
3	L	10	ASN	OD1-CG-ND2	7.62	130.22	122.60
2	O	75	GLU	CG-CD-OE2	7.60	135.87	118.40
1	A	546	PHE	CA-CB-CG	7.58	121.39	113.80
3	l	54	GLU	CB-CG-CD	7.58	125.48	112.60
3	0	54	GLU	CB-CG-CD	7.57	125.47	112.60
3	p	114	GLU	CG-CD-OE1	-7.56	101.02	118.40
2	S	75	GLU	CG-CD-OE2	7.54	135.75	118.40
3	x	114	GLU	CG-CD-OE1	-7.54	101.05	118.40
2	t	38	ARG	CG-CD-NE	-7.53	95.43	112.00
2	7	36	ARG	NE-CZ-NH2	-7.53	112.42	119.20
3	4	64	ASP	CA-CB-CG	7.53	120.13	112.60
2	g	131	ARG	NE-CZ-NH1	-7.53	113.97	121.50
2	Y	144	ASP	CA-CB-CG	7.53	120.13	112.60
4	u	90	ARG	N-CA-CB	7.53	121.15	109.94
2	AA	148	GLU	CG-CD-OE1	7.52	135.70	118.40
2	1	12	ASP	CA-CB-CG	7.49	120.09	112.60
2	9	80	LEU	CB-CG-CD1	7.49	133.17	110.70
2	AM	148	GLU	CG-CD-OE1	7.49	135.62	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	144	ASP	CA-CB-CG	7.47	120.07	112.60
3	L	49	THR	CA-CB-CG2	7.47	123.20	110.50
2	AG	128	GLU	CG-CD-OE2	-7.47	101.23	118.40
3	b	54	GLU	CB-CG-CD	7.46	125.28	112.60
3	b	49	THR	CA-CB-CG2	7.45	123.16	110.50
3	z	39	ARG	CG-CD-NE	7.44	128.37	112.00
2	AO	36	ARG	NE-CZ-NH1	-7.44	114.06	121.50
2	g	114	GLU	CG-CD-OE2	-7.44	101.29	118.40
3	AF	119	LEU	CB-CG-CD1	7.43	132.99	110.70
2	w	36	ARG	NE-CZ-NH1	-7.43	114.07	121.50
2	O	114	GLU	CG-CD-OE2	-7.42	101.34	118.40
3	L	54	GLU	CB-CG-CD	7.41	125.20	112.60
2	AC	36	ARG	NE-CZ-NH1	-7.41	114.09	121.50
2	S	114	GLU	CG-CD-OE2	-7.40	101.37	118.40
2	AE	16	ARG	NE-CZ-NH1	7.40	128.90	121.50
2	w	16	ARG	NE-CZ-NH2	-7.39	112.55	119.20
2	AQ	16	ARG	NE-CZ-NH1	7.39	128.89	121.50
1	C	376	GLN	CB-CA-C	-7.38	97.20	110.70
1	A	776	PHE	N-CA-C	-7.37	100.18	110.35
1	C	776	PHE	N-CA-C	-7.37	100.18	110.35
2	AS	128	GLU	CG-CD-OE2	-7.37	101.46	118.40
1	A	376	GLN	CB-CA-C	-7.37	97.22	110.70
2	K	128	GLU	CG-CD-OE2	7.36	135.33	118.40
3	l	2	GLN	OE1-CD-NE2	7.35	129.95	122.60
2	Y	76	LYS	CA-CB-CG	7.35	128.80	114.10
3	AD	54	GLU	CB-CG-CD	7.34	125.08	112.60
2	1	36	ARG	CB-CG-CD	7.33	128.17	111.30
3	AP	54	GLU	CB-CG-CD	7.33	125.06	112.60
2	I	76	LYS	CA-CB-CG	7.32	128.74	114.10
2	K	128	GLU	CG-CD-OE1	-7.32	101.57	118.40
2	AS	131	ARG	NE-CZ-NH2	-7.31	112.62	119.20
3	h	54	GLU	CB-CG-CD	7.30	125.01	112.60
2	k	65	VAL	CA-CB-CG2	7.28	122.78	110.40
3	h	67	ARG	NH1-CZ-NH2	7.28	128.76	119.30
3	z	67	ARG	NH1-CZ-NH2	7.28	128.76	119.30
2	AG	131	ARG	NE-CZ-NH2	-7.28	112.65	119.20
2	a	128	GLU	CG-CD-OE1	-7.27	101.69	118.40
2	7	36	ARG	NE-CZ-NH1	7.25	128.75	121.50
3	J	65	LEU	CD1-CG-CD2	-7.25	94.85	110.80
2	c	56	ASP	CB-CA-C	-7.24	94.86	109.99
2	a	128	GLU	CG-CD-OE2	7.24	135.04	118.40
2	3	56	ASP	CB-CA-C	-7.23	94.88	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	140	LEU	CB-CG-CD2	-7.22	89.03	110.70
3	2	67	ARG	NE-CZ-NH2	7.22	125.70	119.20
2	E	76	LYS	CA-CB-CG	7.22	128.54	114.10
3	h	39	ARG	CG-CD-NE	7.21	127.86	112.00
1	C	356	VAL	N-CA-CB	7.21	121.39	110.58
1	A	477	ASP	CB-CA-C	-7.19	99.02	109.38
1	C	477	ASP	CB-CA-C	-7.18	99.04	109.38
3	T	77	ARG	CB-CG-CD	7.17	127.80	111.30
2	e	140	LEU	CB-CG-CD2	-7.17	89.20	110.70
2	AM	47	ARG	CB-CG-CD	7.17	127.78	111.30
2	U	76	LYS	CA-CB-CG	7.15	128.40	114.10
2	AA	47	ARG	CB-CG-CD	7.14	127.73	111.30
3	P	77	ARG	CB-CG-CD	7.14	127.72	111.30
3	j	65	LEU	CD1-CG-CD2	-7.12	95.13	110.80
2	9	128	GLU	CG-CD-OE2	7.12	134.77	118.40
2	AG	160	MET	CB-CA-C	-7.11	101.45	112.12
2	AS	160	MET	CB-CA-C	-7.11	101.45	112.12
2	S	138	THR	CA-CB-OG1	7.10	120.25	109.60
2	G	144	ASP	CA-CB-CG	7.10	119.70	112.60
3	q	90	ARG	NE-CZ-NH2	7.08	125.57	119.20
2	I	160	MET	CG-SD-CE	7.07	116.46	100.90
2	W	144	ASP	CA-CB-CG	7.07	119.67	112.60
2	r	144	ASP	CA-CB-CG	7.07	119.67	112.60
3	X	45	SER	CA-CB-OG	7.06	125.21	111.10
2	O	138	THR	CA-CB-OG1	7.05	120.17	109.60
3	H	45	SER	CA-CB-OG	7.05	125.19	111.10
2	5	61	LYS	CB-CG-CD	7.04	127.50	111.30
3	Z	65	LEU	CD1-CG-CD2	-7.04	95.32	110.80
2	o	36	ARG	CD-NE-CZ	7.03	134.24	124.40
3	0	2	GLN	OE1-CD-NE2	7.01	129.61	122.60
2	AQ	100	ASP	CA-CB-CG	7.01	119.61	112.60
1	C	344	ARG	NE-CZ-NH2	7.00	125.50	119.20
2	r	16	ARG	NE-CZ-NH1	-7.00	114.50	121.50
3	AJ	28	LYS	CA-CB-CG	7.00	128.11	114.10
2	7	151	PHE	CA-CB-CG	7.00	120.80	113.80
3	AV	28	LYS	CA-CB-CG	6.99	128.08	114.10
5	AZ	28	PHE	CA-CB-CG	6.99	120.78	113.80
5	AY	28	PHE	CA-CB-CG	6.98	120.78	113.80
2	7	144	ASP	CA-CB-CG	6.96	119.56	112.60
2	AE	100	ASP	CA-CB-CG	6.96	119.56	112.60
3	P	17	LYS	CG-CD-CE	6.96	127.31	111.30
2	w	36	ARG	NE-CZ-NH2	-6.96	112.94	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	t	144	ASP	CA-CB-CG	6.96	119.56	112.60
2	W	76	LYS	CA-CB-CG	6.95	127.99	114.10
2	Q	144	ASP	CA-CB-CG	6.94	119.54	112.60
2	M	144	ASP	CA-CB-CG	6.94	119.54	112.60
2	AG	36	ARG	NE-CZ-NH1	-6.93	114.57	121.50
2	AS	36	ARG	NE-CZ-NH1	-6.93	114.57	121.50
1	A	344	ARG	NE-CZ-NH2	6.93	125.44	119.20
2	c	14	GLU	CG-CD-OE1	6.93	134.34	118.40
2	G	76	LYS	CA-CB-CG	6.93	127.96	114.10
3	T	17	LYS	CG-CD-CE	6.92	127.21	111.30
2	AE	148	GLU	CG-CD-OE2	-6.90	102.53	118.40
2	K	76	LYS	CA-CB-CG	6.90	127.90	114.10
3	z	54	GLU	CG-CD-OE2	-6.90	102.53	118.40
2	r	36	ARG	CD-NE-CZ	6.88	134.03	124.40
2	AQ	148	GLU	CG-CD-OE2	-6.88	102.57	118.40
2	a	76	LYS	CA-CB-CG	6.88	127.86	114.10
3	q	34	GLY	CA-C-O	-6.88	113.67	120.75
2	l	100	ASP	CA-CB-CG	6.88	119.48	112.60
3	AH	77	ARG	CB-CG-CD	6.87	127.09	111.30
1	A	507	ARG	N-CA-CB	6.86	120.05	110.17
1	C	507	ARG	N-CA-CB	6.84	120.03	110.17
2	g	128	GLU	CG-CD-OE2	6.84	134.14	118.40
3	q	39	ARG	NH1-CZ-NH2	-6.84	110.41	119.30
2	AS	128	GLU	CG-CD-OE1	6.84	134.13	118.40
2	o	80	LEU	CB-CG-CD1	6.83	131.20	110.70
3	v	34	GLY	CA-C-O	-6.83	113.71	120.75
2	9	45	GLU	CB-CG-CD	6.83	124.21	112.60
2	AG	128	GLU	CG-CD-OE1	6.82	134.09	118.40
2	m	151	PHE	CA-CB-CG	6.80	120.60	113.80
3	q	28	LYS	CA-CB-CG	6.79	127.68	114.10
3	2	119	LEU	CD1-CG-CD2	-6.78	95.89	110.80
3	X	77	ARG	CB-CG-CD	6.77	126.86	111.30
3	H	77	ARG	CB-CG-CD	6.76	126.86	111.30
2	3	55	GLY	CA-C-N	-6.76	109.32	121.14
2	3	55	GLY	C-N-CA	-6.76	109.32	121.14
2	Y	160	MET	CG-SD-CE	6.75	115.76	100.90
2	y	38	ARG	NE-CZ-NH2	-6.75	113.13	119.20
3	J	77	ARG	CB-CG-CD	6.74	126.80	111.30
3	AP	54	GLU	CG-CD-OE2	-6.74	102.90	118.40
3	X	67	ARG	CD-NE-CZ	6.74	133.83	124.40
3	Z	77	ARG	CB-CG-CD	6.74	126.79	111.30
3	R	77	ARG	CB-CG-CD	6.73	126.78	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	811	PHE	CB-CA-C	-6.73	102.88	111.22
3	b	2	GLN	N-CA-CB	-6.72	99.85	111.55
3	N	77	ARG	CB-CG-CD	6.71	126.74	111.30
3	4	90	ARG	NE-CZ-NH2	-6.71	113.16	119.20
2	G	106	GLU	CA-CB-CG	6.71	127.51	114.10
2	W	106	GLU	CA-CB-CG	6.71	127.51	114.10
3	AD	54	GLU	CG-CD-OE2	-6.70	102.98	118.40
3	h	54	GLU	CG-CD-OE2	-6.68	103.02	118.40
2	c	14	GLU	CG-CD-OE2	-6.68	103.04	118.40
3	6	39	ARG	CB-CG-CD	6.67	126.65	111.30
1	A	811	PHE	CB-CA-C	-6.67	102.95	111.22
2	i	100	ASP	CA-CB-CG	6.66	119.26	112.60
2	AC	62	ARG	NE-CZ-NH2	6.64	125.18	119.20
3	q	2	GLN	N-CA-CB	-6.63	100.01	111.55
3	H	67	ARG	CD-NE-CZ	6.63	133.68	124.40
2	AO	62	ARG	NE-CZ-NH2	6.62	125.16	119.20
2	c	55	GLY	CA-C-N	-6.62	109.56	121.14
2	c	55	GLY	C-N-CA	-6.62	109.56	121.14
3	p	106	GLU	CG-CD-OE1	6.61	133.60	118.40
3	l	54	GLU	CG-CD-OE2	-6.61	103.20	118.40
2	9	151	PHE	CA-CB-CG	6.60	120.40	113.80
3	0	54	GLU	CG-CD-OE2	-6.60	103.22	118.40
2	a	49	ARG	CA-CB-CG	6.60	127.30	114.10
2	Q	75	GLU	CG-CD-OE2	6.59	133.55	118.40
3	q	90	ARG	NH1-CZ-NH2	-6.58	110.75	119.30
2	AW	140	LEU	CB-CG-CD2	-6.57	91.00	110.70
2	m	25	ARG	NE-CZ-NH2	6.56	125.11	119.20
2	AK	140	LEU	CB-CG-CD2	-6.56	91.02	110.70
3	L	20	ASP	CA-CB-CG	6.56	119.16	112.60
2	S	83	ARG	NE-CZ-NH2	6.56	125.10	119.20
3	L	54	GLU	CG-CD-OE2	-6.55	103.33	118.40
2	9	62	ARG	NE-CZ-NH1	-6.55	114.94	121.50
3	v	2	GLN	N-CA-CB	-6.54	100.16	111.55
3	J	114	GLU	CG-CD-OE1	6.54	133.44	118.40
3	b	54	GLU	CG-CD-OE2	-6.54	103.36	118.40
2	K	49	ARG	CA-CB-CG	6.54	127.17	114.10
2	AC	156	LEU	CB-CG-CD2	6.53	130.29	110.70
3	p	39	ARG	NE-CZ-NH2	6.53	125.07	119.20
2	3	131	ARG	CD-NE-CZ	6.52	133.53	124.40
3	AJ	17	LYS	CG-CD-CE	6.52	126.29	111.30
3	AV	17	LYS	CG-CD-CE	6.51	126.28	111.30
3	Z	114	GLU	CG-CD-OE1	6.51	133.37	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9	131	ARG	NE-CZ-NH1	-6.50	115.00	121.50
3	4	113	LYS	CA-CB-CG	6.50	127.10	114.10
2	E	49	ARG	CA-CB-CG	6.50	127.09	114.10
3	AT	77	ARG	CB-CG-CD	6.50	126.24	111.30
2	AK	36	ARG	NE-CZ-NH2	6.50	125.05	119.20
3	b	20	ASP	CA-CB-CG	6.49	119.09	112.60
2	i	82	LEU	CB-CG-CD1	-6.49	91.23	110.70
2	g	120	GLN	OE1-CD-NE2	6.49	129.09	122.60
2	AC	38	ARG	CD-NE-CZ	6.49	133.49	124.40
2	U	49	ARG	CA-CB-CG	6.49	127.07	114.10
3	b	67	ARG	NE-CZ-NH1	6.49	127.99	121.50
2	AW	36	ARG	NE-CZ-NH2	6.49	125.04	119.20
3	AJ	123	ILE	CB-CG1-CD1	6.48	127.41	113.80
3	AV	123	ILE	CB-CG1-CD1	6.48	127.40	113.80
2	M	75	GLU	CG-CD-OE2	6.47	133.29	118.40
2	AA	100	ASP	CA-CB-CG	6.47	119.08	112.60
2	AO	156	LEU	CB-CG-CD2	6.47	130.12	110.70
2	AO	38	ARG	CD-NE-CZ	6.47	133.46	124.40
3	8	2	GLN	N-CA-CB	-6.46	100.32	111.55
3	x	87	TYR	CB-CG-CD1	-6.45	111.12	120.80
3	d	113	LYS	CA-CB-CG	6.45	127.00	114.10
2	i	14	GLU	CG-CD-OE2	-6.44	103.58	118.40
2	AM	100	ASP	CA-CB-CG	6.44	119.04	112.60
3	Z	20	ASP	CA-CB-CG	6.43	119.03	112.60
2	y	48	GLU	CG-CD-OE1	6.42	133.18	118.40
2	g	36	ARG	NE-CZ-NH1	-6.41	115.09	121.50
3	L	67	ARG	NE-CZ-NH1	6.41	127.91	121.50
3	z	83	ARG	NE-CZ-NH1	-6.41	115.09	121.50
4	u	74	TYR	N-CA-CB	6.41	121.32	110.49
3	n	2	GLN	N-CA-CB	-6.40	100.42	111.55
3	J	20	ASP	CA-CB-CG	6.39	118.99	112.60
1	A	889	LEU	N-CA-CB	6.38	121.72	110.37
2	g	60	GLN	CB-CA-C	6.37	121.69	110.85
1	C	889	LEU	N-CA-CB	6.37	121.71	110.37
3	R	2	GLN	N-CA-CB	-6.37	100.47	111.55
3	X	2	GLN	CB-CA-C	6.37	122.68	109.38
3	AT	114	GLU	CB-CG-CD	6.37	123.42	112.60
2	O	36	ARG	NE-CZ-NH2	6.36	124.93	119.20
2	r	49	ARG	NE-CZ-NH2	6.36	124.93	119.20
3	h	83	ARG	CB-CG-CD	6.35	125.90	111.30
3	N	2	GLN	N-CA-CB	-6.35	100.51	111.55
2	t	36	ARG	NE-CZ-NH2	-6.34	113.50	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AO	25	ARG	NE-CZ-NH1	-6.33	115.17	121.50
2	AC	25	ARG	NE-CZ-NH1	-6.33	115.17	121.50
3	b	83	ARG	CG-CD-NE	-6.33	98.08	112.00
2	I	41	GLN	CG-CD-NE2	6.33	125.89	116.40
3	L	83	ARG	CG-CD-NE	-6.33	98.08	112.00
2	O	83	ARG	NE-CZ-NH2	6.32	124.89	119.20
3	AH	114	GLU	CB-CG-CD	6.32	123.35	112.60
2	Y	41	GLN	CG-CD-NE2	6.32	125.88	116.40
2	k	62	ARG	CB-CG-CD	6.32	125.83	111.30
2	w	36	ARG	NH1-CZ-NH2	-6.32	111.09	119.30
3	F	144	ASP	CA-CB-CG	6.31	118.91	112.60
2	S	36	ARG	NE-CZ-NH2	6.31	124.88	119.20
3	j	77	ARG	CB-CG-CD	6.30	125.80	111.30
4	u	106	GLU	CB-CA-C	-6.30	99.97	110.68
2	7	160	MET	CG-SD-CE	-6.30	87.04	100.90
3	b	2	GLN	OE1-CD-NE2	-6.28	116.32	122.60
3	V	144	ASP	CA-CB-CG	6.28	118.88	112.60
2	m	100	ASP	CA-CB-CG	6.27	118.87	112.60
3	L	2	GLN	N-CA-CB	-6.27	99.96	111.37
2	g	25	ARG	NE-CZ-NH1	-6.26	115.23	121.50
2	K	36	ARG	NE-CZ-NH2	6.26	124.83	119.20
2	W	36	ARG	NE-CZ-NH2	6.26	124.83	119.20
2	AO	14	GLU	CG-CD-OE2	-6.25	104.01	118.40
2	I	47	ARG	CB-CG-CD	6.25	125.68	111.30
2	m	131	ARG	NE-CZ-NH1	6.25	127.75	121.50
2	AC	14	GLU	CG-CD-OE2	-6.25	104.02	118.40
3	h	83	ARG	NE-CZ-NH1	-6.25	115.25	121.50
3	l	67	ARG	CG-CD-NE	6.25	125.75	112.00
2	Q	75	GLU	CG-CD-OE1	-6.25	104.03	118.40
2	Y	47	ARG	CB-CG-CD	6.24	125.65	111.30
3	x	123	ILE	CB-CG1-CD1	6.24	126.90	113.80
2	a	36	ARG	NE-CZ-NH2	6.23	124.81	119.20
5	Ab	18	ARG	CG-CD-NE	6.23	125.70	112.00
3	2	67	ARG	NE-CZ-NH1	-6.22	115.28	121.50
2	G	36	ARG	NE-CZ-NH2	6.21	124.79	119.20
3	p	87	TYR	CB-CG-CD1	-6.21	111.48	120.80
2	3	25	ARG	NH1-CZ-NH2	6.20	127.36	119.30
3	n	67	ARG	NH1-CZ-NH2	6.20	127.36	119.30
2	k	14	GLU	CG-CD-OE2	-6.20	104.14	118.40
2	m	61	LYS	CD-CE-NZ	6.20	131.73	111.90
3	p	123	ILE	CB-CG1-CD1	6.19	126.81	113.80
3	l	2	GLN	CG-CD-NE2	-6.19	107.12	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AI	36	ARG	NE-CZ-NH2	6.19	124.77	119.20
3	Z	3	ASP	CA-CB-CG	6.19	118.79	112.60
3	6	107	ARG	NE-CZ-NH2	6.18	124.77	119.20
2	AU	36	ARG	NE-CZ-NH2	6.18	124.77	119.20
3	8	67	ARG	NH1-CZ-NH2	6.18	127.33	119.30
3	L	10	ASN	CB-CG-ND2	-6.17	107.14	116.40
2	m	160	MET	CG-SD-CE	-6.17	87.32	100.90
2	AQ	131	ARG	NE-CZ-NH2	6.17	124.75	119.20
2	U	36	ARG	NE-CZ-NH2	6.16	124.75	119.20
3	H	2	GLN	CB-CA-C	6.16	122.25	109.38
3	z	83	ARG	CB-CG-CD	6.15	125.45	111.30
2	AE	131	ARG	NE-CZ-NH2	6.15	124.73	119.20
2	E	36	ARG	NE-CZ-NH2	6.15	124.73	119.20
2	AQ	49	ARG	NE-CZ-NH2	6.14	124.73	119.20
1	C	642	ARG	N-CA-CB	6.14	119.68	110.22
3	X	108	VAL	N-CA-CB	6.14	121.36	111.23
2	AQ	148	GLU	CG-CD-OE1	6.14	132.53	118.40
3	V	67	ARG	NE-CZ-NH1	6.14	127.64	121.50
2	m	36	ARG	NH1-CZ-NH2	-6.14	111.32	119.30
2	AE	148	GLU	CG-CD-OE1	6.14	132.52	118.40
3	J	3	ASP	CA-CB-CG	6.14	118.74	112.60
2	t	14	GLU	CG-CD-OE2	-6.14	104.29	118.40
2	AK	25	ARG	NE-CZ-NH1	-6.13	115.36	121.50
3	F	67	ARG	NE-CZ-NH1	6.13	127.63	121.50
1	A	364	PHE	N-CA-CB	6.13	120.85	110.49
3	2	65	LEU	CD1-CG-CD2	-6.13	97.32	110.80
3	AF	114	GLU	CG-CD-OE2	-6.12	104.32	118.40
3	J	114	GLU	CG-CD-OE2	-6.12	104.32	118.40
2	AE	49	ARG	NE-CZ-NH2	6.12	124.71	119.20
3	AR	64	ASP	CA-CB-CG	6.12	118.72	112.60
1	C	364	PHE	N-CA-CB	6.11	120.82	110.49
2	M	75	GLU	CG-CD-OE1	-6.11	104.34	118.40
3	Z	114	GLU	CG-CD-OE2	-6.11	104.36	118.40
2	g	14	GLU	CG-CD-OE2	-6.10	104.37	118.40
3	2	72	MET	CB-CG-SD	6.09	130.97	112.70
3	l	83	ARG	NE-CZ-NH2	6.09	124.68	119.20
1	A	356	VAL	N-CA-CB	6.08	119.70	110.58
1	A	693	ARG	CG-CD-NE	6.08	125.38	112.00
2	r	36	ARG	NE-CZ-NH2	-6.07	113.73	119.20
3	8	107	ARG	NE-CZ-NH2	6.07	124.67	119.20
4	s	74	TYR	N-CA-CB	6.07	120.75	110.49
2	k	45	GLU	CG-CD-OE2	-6.06	104.46	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AF	64	ASP	CA-CB-CG	6.06	118.66	112.60
2	7	4	LEU	CB-CG-CD2	-6.06	92.52	110.70
2	g	14	GLU	CG-CD-OE1	6.06	132.33	118.40
2	AW	25	ARG	NE-CZ-NH1	-6.05	115.45	121.50
3	AR	114	GLU	CG-CD-OE2	-6.04	104.50	118.40
5	Ad	3	ARG	CG-CD-NE	6.04	125.30	112.00
3	p	83	ARG	CG-CD-NE	-6.04	98.71	112.00
3	AN	28	LYS	CG-CD-CE	6.03	125.16	111.30
3	v	100	ASP	OD1-CG-OD2	-6.02	108.44	122.90
3	n	28	LYS	CG-CD-CE	6.02	125.14	111.30
3	T	67	ARG	NH1-CZ-NH2	6.01	127.12	119.30
3	AB	28	LYS	CG-CD-CE	6.01	125.13	111.30
2	AW	14	GLU	CG-CD-OE2	-6.01	104.57	118.40
1	C	693	ARG	CG-CD-NE	6.01	125.21	112.00
2	AK	14	GLU	CG-CD-OE2	-6.00	104.59	118.40
2	Q	160	MET	CA-C-O	-6.00	113.86	120.70
2	AE	156	LEU	CD1-CG-CD2	-6.00	97.60	110.80
2	t	14	GLU	CG-CD-OE1	5.99	132.18	118.40
2	AS	22	GLU	CG-CD-OE1	-5.98	104.64	118.40
2	t	22	GLU	CG-CD-OE2	-5.98	104.65	118.40
3	AD	83	ARG	NE-CZ-NH2	5.97	124.58	119.20
2	AG	22	GLU	CG-CD-OE1	-5.97	104.67	118.40
2	I	28	SER	CA-CB-OG	5.97	123.04	111.10
3	8	20	ASP	CA-CB-CG	5.97	118.57	112.60
2	3	131	ARG	CG-CD-NE	5.96	125.12	112.00
5	AZ	3	ARG	CG-CD-NE	5.96	125.12	112.00
1	A	642	ARG	N-CA-CB	5.96	119.40	110.22
2	k	14	GLU	CG-CD-OE1	5.96	132.10	118.40
2	5	14	GLU	CG-CD-OE2	-5.96	104.70	118.40
3	n	20	ASP	CA-CB-CG	5.95	118.55	112.60
2	m	12	ASP	CA-CB-CG	5.94	118.54	112.60
3	AH	20	ASP	CA-CB-CG	5.94	118.54	112.60
2	AQ	156	LEU	CD1-CG-CD2	-5.94	97.73	110.80
2	Y	28	SER	CA-CB-OG	5.94	122.98	111.10
2	W	28	SER	CA-CB-OG	5.93	122.97	111.10
3	0	2	GLN	CG-CD-NE2	-5.93	107.50	116.40
2	U	36	ARG	NE-CZ-NH1	-5.93	115.57	121.50
2	i	14	GLU	CG-CD-OE1	5.92	132.02	118.40
3	AT	39	ARG	CA-CB-CG	5.92	125.94	114.10
3	L	10	ASN	CA-CB-CG	5.92	118.52	112.60
3	P	67	ARG	NH1-CZ-NH2	5.92	126.99	119.30
1	A	682	GLU	CB-CA-C	-5.91	100.89	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	160	MET	CA-C-O	-5.91	113.97	120.70
1	A	819	PHE	CB-CA-C	5.91	120.16	111.65
2	G	28	SER	CA-CB-OG	5.91	122.91	111.10
2	E	36	ARG	NE-CZ-NH1	-5.90	115.60	121.50
3	AP	66	THR	CA-CB-CG2	5.90	120.54	110.50
1	C	819	PHE	CB-CA-C	5.90	120.15	111.65
3	AF	77	ARG	NE-CZ-NH1	-5.90	115.60	121.50
3	AH	39	ARG	CA-CB-CG	5.90	125.90	114.10
2	O	28	SER	CA-CB-OG	5.90	122.89	111.10
3	AT	20	ASP	CA-CB-CG	5.89	118.49	112.60
2	3	36	ARG	NE-CZ-NH2	5.89	124.50	119.20
3	AR	77	ARG	NE-CZ-NH1	-5.89	115.61	121.50
3	AT	2	GLN	CB-CA-C	5.89	121.69	109.38
3	f	20	ASP	CA-CB-CG	5.89	118.49	112.60
3	x	83	ARG	CG-CD-NE	-5.89	99.04	112.00
1	C	507	ARG	CB-CA-C	-5.89	98.70	109.54
2	o	75	GLU	CB-CG-CD	5.89	122.61	112.60
2	S	28	SER	CA-CB-OG	5.88	122.86	111.10
1	A	507	ARG	CB-CA-C	-5.88	98.72	109.54
3	8	123	ILE	CB-CG1-CD1	5.88	126.14	113.80
3	AD	77	ARG	CG-CD-NE	5.88	124.93	112.00
3	AH	2	GLN	CB-CA-C	5.87	121.65	109.38
1	C	682	GLU	CB-CA-C	-5.87	100.97	110.77
2	AC	14	GLU	CG-CD-OE1	5.86	131.88	118.40
2	AS	131	ARG	CD-NE-CZ	5.86	132.61	124.40
3	F	20	ASP	CA-CB-CG	5.85	118.45	112.60
1	A	175	ASP	CA-CB-CG	5.85	118.45	112.60
2	AG	131	ARG	CD-NE-CZ	5.85	132.59	124.40
2	AO	14	GLU	CG-CD-OE1	5.85	131.85	118.40
2	E	28	SER	CA-CB-OG	5.84	122.79	111.10
2	U	28	SER	CA-CB-OG	5.84	122.79	111.10
3	4	77	ARG	NE-CZ-NH1	-5.84	115.66	121.50
2	AE	62	ARG	NH1-CZ-NH2	-5.84	111.70	119.30
3	P	107	ARG	CB-CG-CD	5.84	124.73	111.30
3	x	20	ASP	CA-CB-CG	5.84	118.44	112.60
3	AD	66	THR	CA-CB-CG2	5.83	120.41	110.50
2	O	36	ARG	NE-CZ-NH1	-5.83	115.67	121.50
1	C	175	ASP	CA-CB-CG	5.83	118.43	112.60
2	AQ	62	ARG	NH1-CZ-NH2	-5.83	111.73	119.30
3	6	20	ASP	CA-CB-CG	5.82	118.42	112.60
3	T	107	ARG	CB-CG-CD	5.82	124.68	111.30
3	V	20	ASP	CA-CB-CG	5.82	118.42	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AX	1	MET	CG-SD-CE	-5.82	88.11	100.90
3	AL	1	MET	CG-SD-CE	-5.81	88.12	100.90
2	5	36	ARG	NE-CZ-NH2	5.81	124.43	119.20
2	U	38	ARG	NE-CZ-NH2	-5.80	113.98	119.20
2	U	75	GLU	N-CA-CB	5.80	118.42	110.01
3	n	67	ARG	CG-CD-NE	5.80	124.77	112.00
2	Q	38	ARG	NE-CZ-NH2	-5.79	113.98	119.20
5	AY	3	ARG	CG-CD-NE	5.79	124.75	112.00
2	AK	75	GLU	CB-CG-CD	5.79	122.44	112.60
2	E	75	GLU	N-CA-CB	5.79	118.41	110.01
3	p	20	ASP	CA-CB-CG	5.79	118.39	112.60
3	AD	83	ARG	CG-CD-NE	-5.79	99.26	112.00
3	z	20	ASP	CA-CB-CG	5.78	118.38	112.60
3	P	20	ASP	CA-CB-CG	5.78	118.38	112.60
2	W	36	ARG	NE-CZ-NH1	-5.78	115.72	121.50
2	AW	75	GLU	CB-CG-CD	5.78	122.42	112.60
2	M	38	ARG	NE-CZ-NH2	-5.78	114.00	119.20
3	T	20	ASP	CA-CB-CG	5.78	118.38	112.60
2	w	75	GLU	CB-CG-CD	5.78	122.42	112.60
3	h	20	ASP	CA-CB-CG	5.77	118.37	112.60
3	N	20	ASP	CA-CB-CG	5.77	118.37	112.60
3	8	67	ARG	CG-CD-NE	5.77	124.69	112.00
2	G	36	ARG	NE-CZ-NH1	-5.77	115.73	121.50
2	k	75	GLU	CB-CG-CD	5.77	122.40	112.60
3	AD	158	SER	CA-CB-OG	5.76	122.62	111.10
2	S	36	ARG	NE-CZ-NH1	-5.76	115.74	121.50
1	A	702	VAL	N-CA-C	-5.76	107.52	113.10
4	u	11	LYS	N-CA-CB	5.75	119.20	110.28
2	y	151	PHE	CA-CB-CG	5.75	119.55	113.80
3	AB	20	ASP	CA-CB-CG	5.75	118.35	112.60
3	AN	20	ASP	CA-CB-CG	5.75	118.35	112.60
3	AP	158	SER	CA-CB-OG	5.75	122.59	111.10
2	M	105	GLU	CG-CD-OE2	5.74	131.59	118.40
3	q	65	LEU	CB-CG-CD1	5.73	127.90	110.70
3	6	2	GLN	N-CA-CB	-5.73	101.58	111.55
3	q	67	ARG	CD-NE-CZ	5.72	132.41	124.40
3	x	101	PRO	N-CA-CB	-5.72	97.77	103.20
3	4	90	ARG	NH1-CZ-NH2	5.72	126.73	119.30
3	R	20	ASP	CA-CB-CG	5.72	118.32	112.60
2	Q	105	GLU	CG-CD-OE2	5.71	131.54	118.40
3	Z	83	ARG	CG-CD-NE	-5.71	99.43	112.00
3	AL	20	ASP	CA-CB-CG	5.71	118.31	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	100	ASP	CA-CB-CG	5.71	118.31	112.60
3	J	83	ARG	CG-CD-NE	-5.71	99.45	112.00
3	Z	83	ARG	CA-CB-CG	5.70	125.51	114.10
2	AK	14	GLU	CG-CD-OE1	5.70	131.52	118.40
2	m	148	GLU	CG-CD-OE2	-5.70	105.28	118.40
2	c	75	GLU	CB-CG-CD	5.70	122.28	112.60
2	l	49	ARG	CG-CD-NE	5.70	124.53	112.00
2	AO	16	ARG	NH1-CZ-NH2	-5.69	111.90	119.30
3	H	20	ASP	CA-CB-CG	5.69	118.29	112.60
3	p	39	ARG	NE-CZ-NH1	-5.69	115.81	121.50
2	c	144	ASP	CA-CB-CG	5.69	118.29	112.60
2	AC	16	ARG	NH1-CZ-NH2	-5.69	111.91	119.30
2	e	36	ARG	NE-CZ-NH2	5.68	124.31	119.20
2	3	75	GLU	CB-CG-CD	5.68	122.25	112.60
5	Aa	18	ARG	CG-CD-NE	5.68	124.49	112.00
2	AE	49	ARG	CG-CD-NE	5.67	124.48	112.00
2	k	38	ARG	CD-NE-CZ	5.67	132.34	124.40
2	AW	14	GLU	CG-CD-OE1	5.67	131.44	118.40
3	AP	83	ARG	NH1-CZ-NH2	5.67	126.67	119.30
2	E	38	ARG	NE-CZ-NH2	-5.66	114.10	119.20
2	c	36	ARG	NH1-CZ-NH2	-5.66	111.94	119.30
3	q	100	ASP	OD1-CG-OD2	-5.66	109.31	122.90
3	AX	20	ASP	CA-CB-CG	5.66	118.26	112.60
2	c	109	ILE	CA-CB-CG1	5.66	120.02	110.40
2	AQ	49	ARG	CG-CD-NE	5.66	124.45	112.00
2	g	75	GLU	CB-CG-CD	5.66	122.21	112.60
3	d	20	ASP	CA-CB-CG	5.65	118.25	112.60
2	g	25	ARG	NE-CZ-NH2	5.65	124.29	119.20
2	o	144	ASP	CA-CB-CG	5.65	118.25	112.60
3	4	20	ASP	CA-CB-CG	5.65	118.25	112.60
3	AD	65	LEU	CD1-CG-CD2	-5.65	98.37	110.80
2	AA	160	MET	CG-SD-CE	-5.64	88.48	100.90
4	u	91	TYR	CB-CA-C	5.63	119.72	110.88
2	y	75	GLU	CB-CG-CD	5.63	122.18	112.60
2	9	106	GLU	CB-CG-CD	5.63	122.17	112.60
2	r	76	LYS	CG-CD-CE	-5.63	98.35	111.30
3	x	2	GLN	N-CA-CB	-5.63	101.12	111.37
1	A	819	PHE	CA-CB-CG	-5.63	108.17	113.80
1	C	819	PHE	CA-CB-CG	-5.63	108.17	113.80
3	d	90	ARG	NE-CZ-NH2	-5.63	114.14	119.20
3	X	20	ASP	CA-CB-CG	5.62	118.22	112.60
2	m	4	LEU	CB-CG-CD2	-5.62	93.83	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	k	28	SER	CA-CB-OG	5.62	122.34	111.10
3	AN	83	ARG	NE-CZ-NH1	-5.62	115.88	121.50
3	p	114	GLU	CB-CG-CD	5.62	122.15	112.60
2	c	153	PHE	CB-CG-CD2	-5.62	111.15	120.70
2	m	28	SER	CA-CB-OG	5.61	122.33	111.10
2	i	82	LEU	CB-CG-CD2	5.61	127.53	110.70
2	AE	62	ARG	CD-NE-CZ	-5.61	116.55	124.40
3	N	107	ARG	CG-CD-NE	5.61	124.34	112.00
3	J	83	ARG	CA-CB-CG	5.61	125.31	114.10
2	Q	100	ASP	CA-CB-CG	5.61	118.21	112.60
2	AK	36	ARG	NE-CZ-NH1	-5.61	115.89	121.50
3	2	26	LYS	CD-CE-NZ	-5.61	93.97	111.90
2	Y	38	ARG	NE-CZ-NH2	-5.60	114.16	119.20
2	9	41	GLN	CA-CB-CG	5.60	125.29	114.10
2	r	60	GLN	CA-CB-CG	5.59	125.29	114.10
2	AM	160	MET	CG-SD-CE	-5.59	88.59	100.90
2	AW	36	ARG	NE-CZ-NH1	-5.59	115.91	121.50
3	b	50	THR	CA-CB-CG2	5.59	120.00	110.50
2	I	38	ARG	NE-CZ-NH2	-5.59	114.17	119.20
2	I	131	ARG	CB-CG-CD	5.59	124.15	111.30
2	1	131	ARG	NE-CZ-NH1	-5.59	115.91	121.50
3	h	76	ARG	CD-NE-CZ	5.59	132.22	124.40
3	AP	12	TYR	CB-CG-CD2	-5.59	112.42	120.80
3	AR	90	ARG	NH1-CZ-NH2	-5.59	112.04	119.30
1	A	477	ASP	CA-CB-CG	5.58	118.19	112.60
2	g	151	PHE	CA-CB-CG	5.58	119.38	113.80
3	z	54	GLU	CG-CD-OE1	5.58	131.24	118.40
3	AJ	2	GLN	N-CA-CB	-5.58	101.83	111.55
3	P	2	GLN	N-CA-CB	-5.58	101.98	111.69
3	L	50	THR	CA-CB-CG2	5.58	119.98	110.50
2	AW	14	GLU	CB-CG-CD	5.58	122.08	112.60
3	T	2	GLN	N-CA-CB	-5.58	101.99	111.69
2	m	75	GLU	CB-CG-CD	5.58	122.08	112.60
2	7	28	SER	CA-CB-OG	5.58	122.25	111.10
2	AQ	62	ARG	CD-NE-CZ	-5.57	116.60	124.40
2	t	36	ARG	NH1-CZ-NH2	-5.57	112.06	119.30
3	AV	2	GLN	N-CA-CB	-5.57	101.86	111.55
2	Y	131	ARG	CB-CG-CD	5.56	124.09	111.30
3	AF	20	ASP	CA-CB-CG	5.56	118.16	112.60
3	6	39	ARG	CG-CD-NE	-5.56	99.77	112.00
1	C	912	VAL	N-CA-C	-5.56	105.11	110.72
3	P	77	ARG	CG-CD-NE	5.56	124.22	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	36	ARG	NE-CZ-NH1	-5.56	115.94	121.50
3	v	90	ARG	CA-CB-CG	5.56	125.21	114.10
2	i	61	LYS	CB-CG-CD	5.55	124.07	111.30
3	AR	20	ASP	CA-CB-CG	5.55	118.15	112.60
3	AR	87	TYR	N-CA-CB	5.55	118.06	110.01
1	C	477	ASP	CA-CB-CG	5.55	118.15	112.60
3	R	107	ARG	CG-CD-NE	5.55	124.21	112.00
3	z	76	ARG	CA-CB-CG	5.54	125.19	114.10
3	AJ	123	ILE	CA-CB-CG1	5.54	119.82	110.40
2	AQ	131	ARG	CG-CD-NE	5.54	124.19	112.00
3	AR	6	THR	CA-CB-CG2	5.54	119.92	110.50
3	z	83	ARG	CG-CD-NE	-5.54	99.82	112.00
3	AD	12	TYR	CB-CG-CD2	-5.53	112.50	120.80
2	c	56	ASP	N-CA-CB	5.53	119.42	110.40
2	AK	14	GLU	CB-CG-CD	5.53	122.00	112.60
2	E	105	GLU	CB-CG-CD	5.53	122.00	112.60
2	7	75	GLU	N-CA-CB	5.53	118.03	110.01
2	a	36	ARG	NE-CZ-NH1	-5.53	115.97	121.50
3	AF	87	TYR	N-CA-CB	5.53	118.02	110.01
3	AB	83	ARG	NE-CZ-NH1	-5.52	115.98	121.50
3	AF	6	THR	CA-CB-CG2	5.52	119.89	110.50
2	U	105	GLU	CB-CG-CD	5.52	121.98	112.60
3	2	112	LEU	CB-CG-CD1	-5.52	94.15	110.70
3	AV	123	ILE	CA-CB-CG1	5.52	119.78	110.40
2	AE	131	ARG	CG-CD-NE	5.51	124.13	112.00
3	T	77	ARG	CG-CD-NE	5.51	124.12	112.00
1	A	912	VAL	N-CA-C	-5.51	105.16	110.72
3	2	2	GLN	CB-CG-CD	5.51	121.96	112.60
1	A	385	PRO	N-CA-C	-5.50	102.56	111.19
2	w	151	PHE	CA-CB-CG	5.50	119.30	113.80
3	L	39	ARG	CA-CB-CG	5.50	125.09	114.10
3	AF	90	ARG	NH1-CZ-NH2	-5.50	112.16	119.30
2	k	56	ASP	CA-CB-CG	5.49	118.09	112.60
2	o	151	PHE	CA-CB-CG	5.49	119.29	113.80
2	i	49	ARG	CG-CD-NE	5.49	124.07	112.00
2	3	56	ASP	N-CA-CB	5.48	119.34	110.40
1	A	459	PHE	CA-C-N	-5.48	116.75	126.45
1	A	459	PHE	C-N-CA	-5.48	116.75	126.45
3	J	107	ARG	NE-CZ-NH2	5.48	124.13	119.20
3	2	20	ASP	CA-CB-CG	5.48	118.08	112.60
2	c	77	MET	CG-SD-CE	-5.48	88.85	100.90
2	5	144	ASP	CA-CB-CG	5.48	118.08	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AY	3	ARG	CD-NE-CZ	5.48	132.07	124.40
3	q	90	ARG	CA-CB-CG	5.47	125.04	114.10
2	m	161	GLN	N-CA-CB	-5.47	101.21	110.50
1	A	388	ARG	NE-CZ-NH2	5.46	124.12	119.20
3	j	65	LEU	CB-CG-CD2	5.46	127.09	110.70
2	3	131	ARG	NE-CZ-NH1	-5.46	116.04	121.50
2	K	38	ARG	NE-CZ-NH2	-5.46	114.29	119.20
3	0	20	ASP	CA-CB-CG	5.46	118.06	112.60
2	S	38	ARG	NH1-CZ-NH2	-5.46	112.21	119.30
2	AM	77	MET	CG-SD-CE	5.46	112.90	100.90
3	x	114	GLU	CB-CG-CD	5.45	121.86	112.60
1	C	459	PHE	CA-C-N	-5.44	116.81	126.45
1	C	459	PHE	C-N-CA	-5.44	116.81	126.45
2	AA	77	MET	CG-SD-CE	5.44	112.87	100.90
2	AI	144	ASP	CA-CB-CG	5.44	118.04	112.60
5	AZ	3	ARG	CD-NE-CZ	5.44	132.02	124.40
2	AU	144	ASP	CA-CB-CG	5.44	118.04	112.60
2	7	161	GLN	N-CA-CB	-5.44	101.26	110.50
2	9	75	GLU	N-CA-CB	5.43	117.89	110.01
2	9	41	GLN	CG-CD-NE2	5.43	124.55	116.40
2	AG	144	ASP	CA-CB-CG	5.43	118.03	112.60
2	AS	144	ASP	CA-CB-CG	5.42	118.03	112.60
2	e	144	ASP	CA-CB-CG	5.42	118.02	112.60
2	AA	161	GLN	N-CA-CB	-5.42	101.29	110.50
2	AU	25	ARG	CG-CD-NE	5.42	123.92	112.00
3	v	39	ARG	NH1-CZ-NH2	-5.41	112.26	119.30
2	AI	25	ARG	CG-CD-NE	5.41	123.91	112.00
2	AU	140	LEU	CB-CG-CD2	-5.41	94.46	110.70
2	i	36	ARG	NE-CZ-NH2	-5.41	114.33	119.20
3	AP	77	ARG	CG-CD-NE	5.41	123.90	112.00
1	A	376	GLN	N-CA-CB	5.41	118.26	110.20
2	AE	16	ARG	NH1-CZ-NH2	-5.41	112.27	119.30
3	6	77	ARG	NE-CZ-NH1	-5.41	116.09	121.50
2	t	131	ARG	NE-CZ-NH1	5.40	126.90	121.50
2	AI	140	LEU	CB-CG-CD2	-5.40	94.49	110.70
3	AL	2	GLN	N-CA-CB	-5.40	102.15	111.55
2	AC	45	GLU	CG-CD-OE2	-5.40	105.99	118.40
2	AQ	16	ARG	NH1-CZ-NH2	-5.40	112.28	119.30
3	h	83	ARG	CG-CD-NE	-5.40	100.13	112.00
3	j	20	ASP	CA-CB-CG	5.39	117.99	112.60
3	AV	2	GLN	CB-CA-C	5.39	120.84	109.79
2	AM	161	GLN	N-CA-CB	-5.39	101.34	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AJ	2	GLN	CB-CA-C	5.39	120.83	109.79
1	A	573	GLN	N-CA-CB	5.39	118.63	110.28
1	C	683	ARG	NE-CZ-NH1	-5.39	116.11	121.50
2	M	100	ASP	CA-CB-CG	5.39	117.99	112.60
2	w	131	ARG	NE-CZ-NH1	5.39	126.89	121.50
2	AO	45	GLU	CG-CD-OE2	-5.39	106.01	118.40
2	W	38	ARG	NE-CZ-NH2	-5.38	114.36	119.20
2	3	62	ARG	NE-CZ-NH1	-5.38	116.12	121.50
2	AU	36	ARG	NE-CZ-NH1	-5.38	116.12	121.50
3	T	90	ARG	NE-CZ-NH2	-5.38	114.36	119.20
3	6	66	THR	OG1-CB-CG2	5.38	120.06	109.30
2	g	109	ILE	CG1-CB-CG2	5.38	126.83	110.70
2	k	47	ARG	NE-CZ-NH1	-5.38	116.12	121.50
1	C	573	GLN	N-CA-CB	5.37	118.60	110.28
2	a	38	ARG	NE-CZ-NH2	-5.37	114.37	119.20
3	AP	108	VAL	CG1-CB-CG2	-5.37	98.99	110.80
2	AA	36	ARG	CG-CD-NE	-5.37	100.20	112.00
2	AQ	160	MET	CG-SD-CE	-5.36	89.10	100.90
2	AM	36	ARG	CG-CD-NE	-5.36	100.21	112.00
2	i	144	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	693	ARG	CB-CG-CD	-5.36	98.98	111.30
2	O	38	ARG	NH1-CZ-NH2	-5.36	112.33	119.30
3	b	39	ARG	CA-CB-CG	5.36	124.81	114.10
2	G	38	ARG	NE-CZ-NH2	-5.35	114.38	119.20
3	p	2	GLN	N-CA-CB	-5.35	101.64	111.37
2	AS	151	PHE	CA-CB-CG	5.35	119.15	113.80
2	AI	36	ARG	NE-CZ-NH1	-5.34	116.16	121.50
1	A	683	ARG	NE-CZ-NH1	-5.34	116.16	121.50
3	AX	2	GLN	N-CA-CB	-5.34	102.25	111.55
2	AG	25	ARG	NE-CZ-NH1	-5.34	116.16	121.50
2	AE	144	ASP	CA-CB-CG	5.34	117.94	112.60
3	AP	12	TYR	CB-CG-CD1	5.33	128.80	120.80
2	M	25	ARG	NE-CZ-NH1	5.33	126.83	121.50
2	AG	151	PHE	CA-CB-CG	5.33	119.13	113.80
1	A	1120	PRO	N-CA-C	-5.33	102.91	111.38
2	Y	151	PHE	CA-CB-CG	5.33	119.13	113.80
3	j	66	THR	CA-CB-CG2	5.33	119.56	110.50
1	C	376	GLN	N-CA-CB	5.33	118.13	110.20
2	AQ	144	ASP	CA-CB-CG	5.33	117.93	112.60
2	AE	160	MET	CG-SD-CE	-5.32	89.19	100.90
3	AJ	77	ARG	NE-CZ-NH1	-5.32	116.18	121.50
3	AV	77	ARG	NE-CZ-NH1	-5.32	116.18	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AW	49	ARG	CG-CD-NE	5.32	123.70	112.00
3	l	107	ARG	CA-CB-CG	-5.32	103.47	114.10
2	AS	25	ARG	NE-CZ-NH1	-5.31	116.19	121.50
2	K	105	GLU	CB-CG-CD	5.31	121.63	112.60
2	U	106	GLU	CB-CG-CD	5.31	121.62	112.60
2	AK	49	ARG	CG-CD-NE	5.31	123.68	112.00
3	AD	27	LEU	CB-CG-CD2	-5.31	94.78	110.70
1	C	702	VAL	N-CA-C	-5.31	107.55	112.43
2	E	106	GLU	CB-CG-CD	5.31	121.62	112.60
2	l	144	ASP	CA-CB-CG	5.30	117.90	112.60
3	AD	12	TYR	CB-CG-CD1	5.30	128.76	120.80
3	d	100	ASP	CB-CG-OD2	5.30	130.60	118.40
3	x	2	GLN	CB-CA-C	5.30	120.46	109.38
3	AL	2	GLN	CB-CA-C	5.30	120.66	109.79
3	AP	27	LEU	CB-CG-CD2	-5.30	94.79	110.70
1	C	676	GLU	CB-CA-C	-5.30	104.58	109.83
2	AK	25	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	C	1120	PRO	N-CA-C	-5.30	102.96	111.38
2	k	25	ARG	CG-CD-NE	5.30	123.65	112.00
2	a	105	GLU	CB-CG-CD	5.29	121.60	112.60
2	K	106	GLU	CB-CG-CD	5.29	121.59	112.60
2	a	106	GLU	CB-CG-CD	5.29	121.59	112.60
3	v	3	ASP	CA-CB-CG	5.29	117.89	112.60
3	l	72	MET	CA-CB-CG	5.29	124.67	114.10
2	3	61	LYS	CA-CB-CG	5.29	124.67	114.10
2	AE	75	GLU	N-CA-CB	5.29	117.67	110.01
3	AH	83	ARG	NE-CZ-NH1	-5.28	116.22	121.50
3	J	65	LEU	CB-CG-CD2	5.28	126.54	110.70
2	3	36	ARG	NE-CZ-NH1	-5.28	116.22	121.50
3	4	10	ASN	OD1-CG-ND2	5.28	127.88	122.60
2	AM	144	ASP	CA-CB-CG	5.28	117.88	112.60
3	Z	65	LEU	CB-CG-CD2	5.28	126.53	110.70
2	g	106	GLU	CB-CG-CD	5.28	121.57	112.60
2	m	144	ASP	CA-CB-CG	5.28	117.88	112.60
2	3	106	GLU	CB-CG-CD	5.28	121.57	112.60
3	8	28	LYS	CG-CD-CE	5.28	123.44	111.30
3	AX	2	GLN	CB-CA-C	5.28	120.60	109.79
1	A	388	ARG	CD-NE-CZ	5.27	131.78	124.40
3	AT	83	ARG	NE-CZ-NH1	-5.27	116.23	121.50
3	2	2	GLN	CG-CD-OE1	-5.27	110.26	120.80
3	AJ	83	ARG	NE-CZ-NH1	-5.26	116.24	121.50
2	AK	19	SER	CA-CB-OG	5.26	121.62	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AV	83	ARG	NE-CZ-NH1	-5.26	116.24	121.50
2	7	36	ARG	CD-NE-CZ	5.26	131.76	124.40
2	G	106	GLU	CG-CD-OE1	5.26	130.49	118.40
2	e	106	GLU	CB-CG-CD	5.26	121.53	112.60
2	AW	25	ARG	NE-CZ-NH2	5.25	123.93	119.20
2	5	106	GLU	CB-CG-CD	5.25	121.53	112.60
2	G	128	GLU	CG-CD-OE2	5.25	130.48	118.40
2	I	151	PHE	CA-CB-CG	5.25	119.05	113.80
2	AK	106	GLU	CB-CG-CD	5.25	121.52	112.60
2	AW	106	GLU	CB-CG-CD	5.25	121.52	112.60
1	A	676	GLU	CB-CA-C	-5.24	104.64	109.83
2	3	49	ARG	CG-CD-NE	5.24	123.54	112.00
3	p	101	PRO	N-CA-CB	-5.24	98.22	103.20
2	m	36	ARG	NE-CZ-NH2	-5.24	114.49	119.20
3	n	72	MET	CA-CB-CG	5.24	124.58	114.10
2	AO	106	GLU	CB-CG-CD	5.24	121.51	112.60
2	W	106	GLU	CG-CD-OE1	5.24	130.44	118.40
1	A	388	ARG	NE-CZ-NH1	-5.24	116.27	121.50
1	C	573	GLN	CB-CA-C	-5.24	100.62	110.67
3	L	2	GLN	CB-CA-C	5.23	120.31	109.38
2	AA	144	ASP	CA-CB-CG	5.23	117.83	112.60
3	AD	108	VAL	CG1-CB-CG2	-5.23	99.29	110.80
1	C	363	HIS	CA-CB-CG	5.23	119.03	113.80
2	AI	106	GLU	CB-CG-CD	5.23	121.49	112.60
2	AQ	75	GLU	N-CA-CB	5.23	117.59	110.01
2	W	128	GLU	CG-CD-OE2	5.23	130.43	118.40
2	Q	151	PHE	CA-CB-CG	5.23	119.03	113.80
2	AW	19	SER	CA-CB-OG	5.23	121.55	111.10
2	M	151	PHE	CA-CB-CG	5.22	119.03	113.80
2	AU	106	GLU	CB-CG-CD	5.22	121.48	112.60
3	p	2	GLN	OE1-CD-NE2	-5.22	117.38	122.60
2	g	156	LEU	CB-CG-CD2	-5.22	95.04	110.70
2	Y	6	LYS	CB-CG-CD	5.22	123.31	111.30
2	I	6	LYS	CB-CG-CD	5.21	123.30	111.30
3	b	10	ASN	OD1-CG-ND2	5.21	127.81	122.60
3	2	65	LEU	CB-CG-CD2	5.21	126.33	110.70
2	3	14	GLU	CB-CG-CD	-5.21	103.75	112.60
1	A	573	GLN	CB-CA-C	-5.21	100.67	110.67
3	v	39	ARG	NE-CZ-NH1	5.21	126.71	121.50
2	3	14	GLU	CG-CD-OE1	5.21	130.38	118.40
3	8	83	ARG	CD-NE-CZ	-5.20	117.12	124.40
3	8	72	MET	CA-CB-CG	5.20	124.50	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	697	PHE	CA-CB-CG	-5.20	108.60	113.80
2	U	100	ASP	CA-CB-CG	5.19	117.79	112.60
3	j	90	ARG	NH1-CZ-NH2	-5.19	112.55	119.30
3	AT	76	ARG	CA-CB-CG	5.19	124.48	114.10
3	v	72	MET	CA-CB-CG	5.19	124.47	114.10
2	K	75	GLU	N-CA-CB	5.19	117.53	110.01
2	AS	106	GLU	CB-CG-CD	5.18	121.42	112.60
4	u	113	LYS	N-CA-CB	5.18	118.20	110.22
2	AG	106	GLU	CB-CG-CD	5.18	121.40	112.60
2	AI	151	PHE	CA-CB-CG	5.17	118.97	113.80
2	AU	151	PHE	CA-CB-CG	5.17	118.97	113.80
3	j	112	LEU	CB-CG-CD1	-5.17	95.19	110.70
2	7	134	LYS	CB-CG-CD	5.17	123.19	111.30
2	m	148	GLU	CG-CD-OE1	5.16	130.28	118.40
2	G	128	GLU	CG-CD-OE1	-5.16	106.53	118.40
3	AP	66	THR	OG1-CB-CG2	-5.16	98.98	109.30
2	t	106	GLU	CG-CD-OE1	5.16	130.27	118.40
2	i	131	ARG	NE-CZ-NH2	5.16	123.84	119.20
2	w	144	ASP	CA-CB-CG	5.15	117.75	112.60
2	S	83	ARG	NH1-CZ-NH2	-5.15	112.60	119.30
3	f	3	ASP	CA-CB-CG	5.15	117.75	112.60
3	0	72	MET	CA-CB-CG	5.15	124.40	114.10
2	AU	45	GLU	CG-CD-OE2	-5.15	106.56	118.40
2	AI	45	GLU	CG-CD-OE2	-5.15	106.56	118.40
3	h	113	LYS	CB-CG-CD	5.14	123.12	111.30
3	p	72	MET	CA-CB-CG	5.14	124.38	114.10
3	q	3	ASP	CA-CB-CG	5.14	117.74	112.60
2	AG	102	THR	OG1-CB-CG2	5.14	119.58	109.30
2	AS	102	THR	OG1-CB-CG2	5.14	119.58	109.30
2	G	151	PHE	CA-CB-CG	5.13	118.94	113.80
3	2	26	LYS	CG-CD-CE	5.13	123.11	111.30
3	AX	72	MET	CA-CB-CG	5.13	124.37	114.10
2	a	75	GLU	N-CA-CB	5.13	117.45	110.01
3	x	72	MET	CA-CB-CG	5.13	124.36	114.10
3	4	10	ASN	CB-CG-ND2	-5.13	108.71	116.40
2	O	76	LYS	CB-CG-CD	5.13	123.09	111.30
2	k	106	GLU	CB-CG-CD	5.13	121.32	112.60
2	t	14	GLU	CB-CG-CD	5.13	121.32	112.60
2	w	36	ARG	CD-NE-CZ	5.13	131.58	124.40
2	U	131	ARG	CD-NE-CZ	5.12	131.57	124.40
2	c	56	ASP	CA-C-O	-5.12	112.96	119.31
3	AF	2	GLN	CB-CG-CD	5.12	121.31	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	14	GLU	CG-CD-OE1	5.12	130.18	118.40
2	W	151	PHE	CA-CB-CG	5.12	118.92	113.80
3	8	100	ASP	OD1-CG-OD2	-5.12	110.61	122.90
3	l	6	THR	CA-CB-CG2	5.12	119.20	110.50
2	K	76	LYS	CB-CG-CD	5.11	123.05	111.30
5	Ab	46	LYS	CB-CG-CD	5.11	123.05	111.30
2	1	33	GLY	CA-C-N	5.11	127.43	120.54
2	1	33	GLY	C-N-CA	5.11	127.43	120.54
3	J	72	MET	CA-CB-CG	5.10	124.31	114.10
5	Ad	3	ARG	CD-NE-CZ	5.10	131.55	124.40
3	z	113	LYS	CB-CG-CD	5.10	123.04	111.30
2	W	128	GLU	CG-CD-OE1	-5.10	106.67	118.40
3	6	2	GLN	CB-CA-C	5.10	120.25	109.79
3	AL	72	MET	CA-CB-CG	5.10	124.30	114.10
3	AR	2	GLN	CB-CG-CD	5.10	121.27	112.60
2	r	106	GLU	CG-CD-OE1	5.10	130.13	118.40
5	Ab	43	ARG	NE-CZ-NH1	-5.10	116.40	121.50
1	A	697	PHE	CA-CB-CG	-5.10	108.70	113.80
2	k	14	GLU	CB-CG-CD	5.10	121.26	112.60
3	x	100	ASP	OD1-CG-OD2	-5.10	110.67	122.90
1	A	163	PHE	N-CA-CB	5.09	117.61	110.12
2	E	131	ARG	CD-NE-CZ	5.09	131.53	124.40
2	S	76	LYS	CB-CG-CD	5.09	123.01	111.30
2	W	76	LYS	CB-CG-CD	5.09	123.01	111.30
2	r	49	ARG	CG-CD-NE	5.09	123.20	112.00
2	AE	38	ARG	NH1-CZ-NH2	-5.09	112.68	119.30
2	c	22	GLU	CG-CD-OE1	-5.08	106.71	118.40
3	Z	72	MET	CA-CB-CG	5.08	124.25	114.10
3	AH	83	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	A	727	THR	N-CA-CB	5.07	116.17	110.03
3	J	90	ARG	CG-CD-NE	-5.07	100.84	112.00
4	u	90	ARG	CB-CA-C	-5.07	102.69	110.81
2	E	151	PHE	CA-CB-CG	5.07	118.87	113.80
3	X	2	GLN	CG-CD-OE1	-5.07	110.66	120.80
3	6	72	MET	CA-CB-CG	5.07	124.24	114.10
2	Q	25	ARG	NE-CZ-NH1	5.07	126.57	121.50
3	X	2	GLN	OE1-CD-NE2	5.07	127.67	122.60
3	4	72	MET	CA-CB-CG	5.07	124.23	114.10
3	AJ	72	MET	CA-CB-CG	5.07	124.23	114.10
3	AV	72	MET	CA-CB-CG	5.07	124.23	114.10
1	C	693	ARG	CB-CG-CD	-5.06	99.65	111.30
1	C	727	THR	N-CA-CB	5.06	116.16	110.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	105	GLU	CB-CG-CD	5.06	121.21	112.60
3	4	2	GLN	CB-CA-C	5.06	119.72	110.10
2	a	76	LYS	CB-CG-CD	5.06	122.94	111.30
2	G	76	LYS	CB-CG-CD	5.06	122.94	111.30
2	AA	102	THR	OG1-CB-CG2	-5.05	99.19	109.30
2	AW	100	ASP	CA-CB-CG	5.05	117.65	112.60
2	k	45	GLU	OE1-CD-OE2	5.05	135.01	122.90
2	AM	102	THR	OG1-CB-CG2	-5.05	99.21	109.30
2	AO	100	ASP	CA-CB-CG	5.04	117.64	112.60
2	9	82	LEU	CB-CG-CD1	5.04	125.81	110.70
3	AD	15	GLN	OE1-CD-NE2	-5.04	117.56	122.60
2	AK	100	ASP	CA-CB-CG	5.03	117.63	112.60
3	d	72	MET	CA-CB-CG	5.03	124.16	114.10
2	3	56	ASP	CA-C-O	-5.03	113.07	119.31
3	AP	15	GLN	OE1-CD-NE2	-5.03	117.57	122.60
3	Z	90	ARG	CG-CD-NE	-5.03	100.94	112.00
3	J	101	PRO	N-CA-CB	-5.03	98.43	103.20
2	Y	38	ARG	CA-CB-CG	5.03	124.15	114.10
2	7	102	THR	CA-CB-OG1	-5.03	102.06	109.60
2	AS	22	GLU	CG-CD-OE2	5.03	129.96	118.40
2	G	105	GLU	CB-CG-CD	5.02	121.14	112.60
2	U	151	PHE	CA-CB-CG	5.02	118.82	113.80
1	C	762	GLU	N-CA-CB	5.02	117.97	110.19
2	t	76	LYS	CA-CB-CG	-5.02	104.06	114.10
3	AT	83	ARG	NE-CZ-NH2	5.02	123.72	119.20
2	y	35	ARG	NH1-CZ-NH2	5.02	125.83	119.30
3	AF	115	THR	CA-CB-OG1	-5.02	102.07	109.60
3	d	90	ARG	NH1-CZ-NH2	5.02	125.82	119.30
3	z	1	MET	CG-SD-CE	5.02	111.94	100.90
3	z	67	ARG	CG-CD-NE	5.02	123.04	112.00
2	3	47	ARG	NE-CZ-NH2	5.02	123.72	119.20
3	V	72	MET	CA-CB-CG	5.01	124.13	114.10
2	I	38	ARG	CA-CB-CG	5.01	124.13	114.10
3	F	72	MET	CA-CB-CG	5.01	124.12	114.10
3	4	106	GLU	CG-CD-OE1	5.01	129.92	118.40
2	AI	60	GLN	CA-CB-CG	5.01	124.11	114.10
3	AH	76	ARG	CA-CB-CG	5.00	124.11	114.10
5	Aa	46	LYS	CB-CG-CD	5.00	122.81	111.30
2	c	47	ARG	NE-CZ-NH2	5.00	123.70	119.20
3	j	123	ILE	CA-CB-CG2	5.00	119.01	110.50
1	C	432	PRO	N-CD-CG	-5.00	95.70	103.20
2	AC	100	ASP	CA-CB-CG	5.00	117.60	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AW	34	GLU	CG-CD-OE1	5.00	129.90	118.40

There are no chirality outliers.

All (584) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	0	100	ASP	Sidechain
3	0	107	ARG	Sidechain
3	0	39	ARG	Sidechain
3	0	67	ARG	Sidechain
3	0	76	ARG	Sidechain
3	0	90	ARG	Sidechain
2	1	131	ARG	Sidechain
2	1	25	ARG	Sidechain
2	1	36	ARG	Sidechain
2	1	38	ARG	Sidechain
2	1	47	ARG	Sidechain
2	1	49	ARG	Sidechain
2	1	62	ARG	Sidechain
2	1	83	ARG	Sidechain
3	2	100	ASP	Sidechain
3	2	107	ARG	Sidechain
3	2	116	TYR	Sidechain
3	2	39	ARG	Sidechain
3	2	67	ARG	Sidechain
3	2	76	ARG	Sidechain
3	2	77	ARG	Sidechain
3	2	90	ARG	Sidechain
2	3	16	ARG	Sidechain
2	3	25	ARG	Sidechain
2	3	36	ARG	Sidechain
2	3	38	ARG	Sidechain
2	3	47	ARG	Sidechain
2	3	49	ARG	Sidechain
2	3	62	ARG	Sidechain
2	3	83	ARG	Sidechain
3	4	100	ASP	Sidechain
3	4	76	ARG	Sidechain
3	4	83	ARG	Sidechain
3	4	90	ARG	Sidechain
2	5	36	ARG	Sidechain
2	5	38	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	5	47	ARG	Sidechain
2	5	62	ARG	Sidechain
2	5	83	ARG	Sidechain
3	6	100	ASP	Sidechain
3	6	107	ARG	Sidechain
3	6	67	ARG	Sidechain
3	6	76	ARG	Sidechain
3	6	90	ARG	Sidechain
2	7	131	ARG	Sidechain
2	7	36	ARG	Sidechain
2	7	38	ARG	Sidechain
2	7	47	ARG	Sidechain
2	7	49	ARG	Sidechain
2	7	62	ARG	Sidechain
2	7	83	ARG	Sidechain
3	8	100	ASP	Sidechain
3	8	107	ARG	Sidechain
3	8	76	ARG	Sidechain
3	8	83	ARG	Sidechain
3	8	90	ARG	Sidechain
2	9	131	ARG	Sidechain
2	9	25	ARG	Sidechain
2	9	36	ARG	Sidechain
2	9	38	ARG	Sidechain
2	9	47	ARG	Sidechain
2	9	62	ARG	Sidechain
2	9	83	ARG	Sidechain
1	A	1033	ARG	Sidechain
1	A	1037	ARG	Sidechain
1	A	1041	ARG	Sidechain
1	A	1046	ARG	Sidechain
1	A	1114	ARG	Sidechain
1	A	165	ARG	Sidechain
1	A	187	ARG	Sidechain
1	A	207	ARG	Sidechain
1	A	212	ARG	Sidechain
1	A	238	ARG	Sidechain
1	A	247	ARG	Sidechain
1	A	283	ARG	Sidechain
1	A	295	ARG	Sidechain
1	A	298	ARG	Sidechain
1	A	307	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	33	ARG	Sidechain
1	A	336	ARG	Sidechain
1	A	344	ARG	Sidechain
1	A	355	ARG	Sidechain
1	A	388	ARG	Sidechain
1	A	4	ARG	Sidechain
1	A	511	ARG	Sidechain
1	A	520	ARG	Sidechain
1	A	605	ARG	Sidechain
1	A	609	ARG	Sidechain
1	A	614	ARG	Sidechain
1	A	633	ARG	Sidechain
1	A	642	ARG	Sidechain
1	A	683	ARG	Sidechain
1	A	696	ARG	Sidechain
1	A	750	ARG	Sidechain
1	A	816	ARG	Sidechain
1	A	839	ARG	Sidechain
1	A	856	ARG	Sidechain
1	A	858	GLY	Peptide
1	A	887	PRO	Peptide
1	A	920	ARG	Sidechain
1	A	975	ARG	Sidechain
1	A	976	ARG	Sidechain
1	A	990	ARG	Sidechain
2	AA	131	ARG	Sidechain
2	AA	25	ARG	Sidechain
2	AA	35	ARG	Sidechain
2	AA	36	ARG	Sidechain
2	AA	38	ARG	Sidechain
2	AA	62	ARG	Sidechain
2	AA	83	ARG	Sidechain
3	AB	100	ASP	Sidechain
3	AB	107	ARG	Sidechain
3	AB	67	ARG	Sidechain
3	AB	76	ARG	Sidechain
3	AB	87	TYR	Sidechain
3	AB	90	ARG	Sidechain
2	AC	131	ARG	Sidechain
2	AC	25	ARG	Sidechain
2	AC	36	ARG	Sidechain
2	AC	38	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	AC	47	ARG	Sidechain
2	AC	83	ARG	Sidechain
3	AD	100	ASP	Sidechain
3	AD	107	ARG	Sidechain
3	AD	39	ARG	Sidechain
3	AD	67	ARG	Sidechain
3	AD	76	ARG	Sidechain
3	AD	77	ARG	Sidechain
3	AD	90	ARG	Sidechain
2	AE	36	ARG	Sidechain
2	AE	38	ARG	Sidechain
2	AE	47	ARG	Sidechain
2	AE	49	ARG	Sidechain
2	AE	83	ARG	Sidechain
3	AF	100	ASP	Sidechain
3	AF	107	ARG	Sidechain
3	AF	111	GLY	Mainchain
3	AF	67	ARG	Sidechain
3	AF	76	ARG	Sidechain
3	AF	77	ARG	Sidechain
3	AF	90	ARG	Sidechain
2	AG	131	ARG	Sidechain
2	AG	25	ARG	Sidechain
2	AG	36	ARG	Sidechain
2	AG	38	ARG	Sidechain
2	AG	49	ARG	Sidechain
2	AG	62	ARG	Sidechain
2	AG	83	ARG	Sidechain
3	AH	100	ASP	Sidechain
3	AH	107	ARG	Sidechain
3	AH	39	ARG	Sidechain
3	AH	83	ARG	Sidechain
3	AH	90	ARG	Sidechain
2	AI	131	ARG	Sidechain
2	AI	16	ARG	Sidechain
2	AI	25	ARG	Sidechain
2	AI	36	ARG	Sidechain
2	AI	38	ARG	Sidechain
2	AI	47	ARG	Sidechain
2	AI	49	ARG	Sidechain
2	AI	62	ARG	Sidechain
2	AI	83	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	AJ	100	ASP	Sidechain
3	AJ	107	ARG	Sidechain
3	AJ	67	ARG	Sidechain
3	AJ	76	ARG	Sidechain
3	AJ	83	ARG	Sidechain
3	AJ	90	ARG	Sidechain
2	AK	131	ARG	Sidechain
2	AK	16	ARG	Sidechain
2	AK	25	ARG	Sidechain
2	AK	36	ARG	Sidechain
2	AK	38	ARG	Sidechain
2	AK	47	ARG	Sidechain
2	AK	49	ARG	Sidechain
2	AK	62	ARG	Sidechain
2	AK	83	ARG	Sidechain
3	AL	100	ASP	Sidechain
3	AL	39	ARG	Sidechain
3	AL	67	ARG	Sidechain
3	AL	76	ARG	Sidechain
3	AL	77	ARG	Sidechain
3	AL	90	ARG	Sidechain
2	AM	131	ARG	Sidechain
2	AM	25	ARG	Sidechain
2	AM	36	ARG	Sidechain
2	AM	38	ARG	Sidechain
2	AM	62	ARG	Sidechain
2	AM	83	ARG	Sidechain
3	AN	100	ASP	Sidechain
3	AN	107	ARG	Sidechain
3	AN	67	ARG	Sidechain
3	AN	76	ARG	Sidechain
3	AN	87	TYR	Sidechain
3	AN	90	ARG	Sidechain
2	AO	131	ARG	Sidechain
2	AO	25	ARG	Sidechain
2	AO	36	ARG	Sidechain
2	AO	38	ARG	Sidechain
2	AO	47	ARG	Sidechain
2	AO	83	ARG	Sidechain
3	AP	100	ASP	Sidechain
3	AP	39	ARG	Sidechain
3	AP	67	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	AP	76	ARG	Sidechain
3	AP	77	ARG	Sidechain
3	AP	83	ARG	Sidechain
3	AP	90	ARG	Sidechain
2	AQ	36	ARG	Sidechain
2	AQ	38	ARG	Sidechain
2	AQ	47	ARG	Sidechain
2	AQ	49	ARG	Sidechain
2	AQ	83	ARG	Sidechain
3	AR	100	ASP	Sidechain
3	AR	107	ARG	Sidechain
3	AR	111	GLY	Mainchain
3	AR	67	ARG	Sidechain
3	AR	76	ARG	Sidechain
3	AR	77	ARG	Sidechain
3	AR	90	ARG	Sidechain
2	AS	131	ARG	Sidechain
2	AS	25	ARG	Sidechain
2	AS	36	ARG	Sidechain
2	AS	38	ARG	Sidechain
2	AS	49	ARG	Sidechain
2	AS	62	ARG	Sidechain
2	AS	83	ARG	Sidechain
3	AT	100	ASP	Sidechain
3	AT	107	ARG	Sidechain
3	AT	39	ARG	Sidechain
3	AT	76	ARG	Sidechain
3	AT	83	ARG	Sidechain
3	AT	90	ARG	Sidechain
2	AU	131	ARG	Sidechain
2	AU	16	ARG	Sidechain
2	AU	25	ARG	Sidechain
2	AU	36	ARG	Sidechain
2	AU	38	ARG	Sidechain
2	AU	47	ARG	Sidechain
2	AU	49	ARG	Sidechain
2	AU	62	ARG	Sidechain
2	AU	83	ARG	Sidechain
3	AV	100	ASP	Sidechain
3	AV	67	ARG	Sidechain
3	AV	76	ARG	Sidechain
3	AV	83	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	AV	90	ARG	Sidechain
2	AW	131	ARG	Sidechain
2	AW	16	ARG	Sidechain
2	AW	25	ARG	Sidechain
2	AW	36	ARG	Sidechain
2	AW	38	ARG	Sidechain
2	AW	47	ARG	Sidechain
2	AW	49	ARG	Sidechain
2	AW	62	ARG	Sidechain
2	AW	83	ARG	Sidechain
3	AX	100	ASP	Sidechain
3	AX	39	ARG	Sidechain
3	AX	67	ARG	Sidechain
3	AX	76	ARG	Sidechain
3	AX	77	ARG	Sidechain
3	AX	90	ARG	Sidechain
5	AY	16	ARG	Sidechain
5	AY	3	ARG	Sidechain
5	AY	43	ARG	Sidechain
5	AZ	16	ARG	Sidechain
5	AZ	3	ARG	Sidechain
5	AZ	43	ARG	Sidechain
5	Aa	16	ARG	Sidechain
5	Aa	18	ARG	Sidechain
5	Aa	21	ARG	Sidechain
5	Ab	18	ARG	Sidechain
5	Ab	21	ARG	Sidechain
5	Ab	43	ARG	Sidechain
5	Ac	16	ARG	Sidechain
5	Ac	18	ARG	Sidechain
5	Ac	21	ARG	Sidechain
5	Ac	3	ARG	Sidechain
5	Ac	43	ARG	Sidechain
5	Ad	21	ARG	Sidechain
5	Ad	3	ARG	Sidechain
5	Ad	43	ARG	Sidechain
1	C	1033	ARG	Sidechain
1	C	1037	ARG	Sidechain
1	C	1041	ARG	Sidechain
1	C	1046	ARG	Sidechain
1	C	1114	ARG	Sidechain
1	C	158	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	165	ARG	Sidechain
1	C	187	ARG	Sidechain
1	C	207	ARG	Sidechain
1	C	212	ARG	Sidechain
1	C	238	ARG	Sidechain
1	C	283	ARG	Sidechain
1	C	295	ARG	Sidechain
1	C	298	ARG	Sidechain
1	C	307	ARG	Sidechain
1	C	33	ARG	Sidechain
1	C	336	ARG	Sidechain
1	C	344	ARG	Sidechain
1	C	355	ARG	Sidechain
1	C	388	ARG	Sidechain
1	C	4	ARG	Sidechain
1	C	511	ARG	Sidechain
1	C	520	ARG	Sidechain
1	C	605	ARG	Sidechain
1	C	609	ARG	Sidechain
1	C	614	ARG	Sidechain
1	C	633	ARG	Sidechain
1	C	642	ARG	Sidechain
1	C	683	ARG	Sidechain
1	C	696	ARG	Sidechain
1	C	750	ARG	Sidechain
1	C	816	ARG	Sidechain
1	C	839	ARG	Sidechain
1	C	856	ARG	Sidechain
1	C	858	GLY	Peptide
1	C	887	PRO	Peptide
1	C	920	ARG	Sidechain
1	C	975	ARG	Sidechain
1	C	976	ARG	Sidechain
1	C	990	ARG	Sidechain
2	E	131	ARG	Sidechain
2	E	36	ARG	Sidechain
2	E	38	ARG	Sidechain
2	E	49	ARG	Sidechain
2	E	62	ARG	Sidechain
2	E	83	ARG	Sidechain
3	F	77	ARG	Sidechain
2	G	106	GLU	Sidechain

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Mol	Chain	Res	Type	Group
2	G	25	ARG	Sidechain
2	G	36	ARG	Sidechain
2	G	38	ARG	Sidechain
2	G	62	ARG	Sidechain
2	G	83	ARG	Sidechain
3	H	76	ARG	Sidechain
3	H	77	ARG	Sidechain
3	H	90	ARG	Sidechain
2	I	36	ARG	Sidechain
2	I	38	ARG	Sidechain
2	I	47	ARG	Sidechain
2	I	83	ARG	Sidechain
3	J	39	ARG	Sidechain
3	J	62	TYR	Sidechain
3	J	67	ARG	Sidechain
3	J	76	ARG	Sidechain
3	J	83	ARG	Sidechain
3	J	87	TYR	Sidechain
3	J	90	ARG	Sidechain
2	K	16	ARG	Sidechain
2	K	36	ARG	Sidechain
2	K	38	ARG	Sidechain
2	K	49	ARG	Sidechain
2	K	62	ARG	Sidechain
2	K	83	ARG	Sidechain
3	L	107	ARG	Sidechain
3	L	39	ARG	Sidechain
3	L	83	ARG	Sidechain
3	L	90	ARG	Sidechain
2	M	16	ARG	Sidechain
2	M	36	ARG	Sidechain
2	M	38	ARG	Sidechain
2	M	62	ARG	Sidechain
2	M	83	ARG	Sidechain
3	N	107	ARG	Sidechain
3	N	67	ARG	Sidechain
3	N	76	ARG	Sidechain
2	O	114	GLU	Sidechain
2	O	124	PRO	Mainchain
2	O	16	ARG	Sidechain
2	O	36	ARG	Sidechain
3	P	39	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	P	77	ARG	Sidechain
2	Q	16	ARG	Sidechain
2	Q	36	ARG	Sidechain
2	Q	38	ARG	Sidechain
2	Q	62	ARG	Sidechain
2	Q	83	ARG	Sidechain
3	R	107	ARG	Sidechain
3	R	67	ARG	Sidechain
3	R	76	ARG	Sidechain
2	S	114	GLU	Sidechain
2	S	124	PRO	Mainchain
2	S	36	ARG	Sidechain
2	S	62	ARG	Sidechain
3	T	39	ARG	Sidechain
3	T	77	ARG	Sidechain
2	U	131	ARG	Sidechain
2	U	36	ARG	Sidechain
2	U	38	ARG	Sidechain
2	U	49	ARG	Sidechain
2	U	62	ARG	Sidechain
2	U	83	ARG	Sidechain
3	V	77	ARG	Sidechain
2	W	106	GLU	Sidechain
2	W	25	ARG	Sidechain
2	W	36	ARG	Sidechain
2	W	38	ARG	Sidechain
2	W	62	ARG	Sidechain
2	W	83	ARG	Sidechain
3	X	107	ARG	Sidechain
3	X	76	ARG	Sidechain
3	X	77	ARG	Sidechain
3	X	90	ARG	Sidechain
2	Y	36	ARG	Sidechain
2	Y	38	ARG	Sidechain
2	Y	47	ARG	Sidechain
2	Y	62	ARG	Sidechain
2	Y	83	ARG	Sidechain
3	Z	39	ARG	Sidechain
3	Z	67	ARG	Sidechain
3	Z	76	ARG	Sidechain
3	Z	83	ARG	Sidechain
3	Z	87	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	Z	90	ARG	Sidechain
2	a	36	ARG	Sidechain
2	a	38	ARG	Sidechain
2	a	49	ARG	Sidechain
2	a	62	ARG	Sidechain
2	a	83	ARG	Sidechain
3	b	107	ARG	Sidechain
3	b	39	ARG	Sidechain
3	b	83	ARG	Sidechain
3	b	90	ARG	Sidechain
2	c	131	ARG	Sidechain
2	c	153	PHE	Sidechain
2	c	16	ARG	Sidechain
2	c	25	ARG	Sidechain
2	c	38	ARG	Sidechain
2	c	47	ARG	Sidechain
2	c	62	ARG	Sidechain
2	c	83	ARG	Sidechain
3	d	100	ASP	Sidechain
3	d	107	ARG	Sidechain
3	d	67	ARG	Sidechain
3	d	76	ARG	Sidechain
3	d	90	ARG	Sidechain
2	e	25	ARG	Sidechain
2	e	36	ARG	Sidechain
2	e	38	ARG	Sidechain
2	e	47	ARG	Sidechain
2	e	62	ARG	Sidechain
2	e	83	ARG	Sidechain
3	f	100	ASP	Sidechain
3	f	67	ARG	Sidechain
3	f	76	ARG	Sidechain
3	f	77	ARG	Sidechain
3	f	90	ARG	Sidechain
2	g	114	GLU	Sidechain
2	g	131	ARG	Sidechain
2	g	16	ARG	Sidechain
2	g	25	ARG	Sidechain
2	g	36	ARG	Sidechain
2	g	38	ARG	Sidechain
2	g	49	ARG	Sidechain
2	g	62	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	g	83	ARG	Sidechain
3	h	100	ASP	Sidechain
3	h	76	ARG	Sidechain
3	h	83	ARG	Sidechain
3	h	90	ARG	Sidechain
2	i	131	ARG	Sidechain
2	i	16	ARG	Sidechain
2	i	25	ARG	Sidechain
2	i	36	ARG	Sidechain
2	i	38	ARG	Sidechain
2	i	47	ARG	Sidechain
2	i	49	ARG	Sidechain
2	i	62	ARG	Sidechain
2	i	83	ARG	Sidechain
3	j	100	ASP	Sidechain
3	j	107	ARG	Sidechain
3	j	2	GLN	Sidechain
3	j	67	ARG	Sidechain
3	j	76	ARG	Sidechain
3	j	77	ARG	Sidechain
3	j	90	ARG	Sidechain
2	k	131	ARG	Sidechain
2	k	16	ARG	Sidechain
2	k	25	ARG	Sidechain
2	k	35	ARG	Sidechain
2	k	36	ARG	Sidechain
2	k	38	ARG	Sidechain
2	k	47	ARG	Sidechain
2	k	49	ARG	Sidechain
2	k	62	ARG	Sidechain
2	k	83	ARG	Sidechain
2	k	90	ARG	Sidechain
3	l	100	ASP	Sidechain
3	l	67	ARG	Sidechain
3	l	76	ARG	Sidechain
3	l	83	ARG	Sidechain
3	l	90	ARG	Sidechain
2	m	131	ARG	Sidechain
2	m	25	ARG	Sidechain
2	m	36	ARG	Sidechain
2	m	38	ARG	Sidechain
2	m	47	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	m	62	ARG	Sidechain
2	m	83	ARG	Sidechain
3	n	100	ASP	Sidechain
3	n	39	ARG	Sidechain
3	n	76	ARG	Sidechain
3	n	83	ARG	Sidechain
3	n	90	ARG	Sidechain
2	o	131	ARG	Sidechain
2	o	25	ARG	Sidechain
2	o	36	ARG	Sidechain
2	o	38	ARG	Sidechain
2	o	49	ARG	Sidechain
2	o	62	ARG	Sidechain
2	o	83	ARG	Sidechain
3	p	107	ARG	Sidechain
3	p	39	ARG	Sidechain
3	p	76	ARG	Sidechain
3	p	77	ARG	Sidechain
3	p	87	TYR	Sidechain
3	p	90	ARG	Sidechain
3	q	100	ASP	Sidechain
3	q	107	ARG	Sidechain
3	q	12	TYR	Sidechain
3	q	15	GLN	Sidechain
3	q	39	ARG	Sidechain
3	q	67	ARG	Sidechain
3	q	76	ARG	Sidechain
3	q	77	ARG	Sidechain
3	q	90	ARG	Sidechain
3	q	94	TYR	Sidechain
2	r	131	ARG	Sidechain
2	r	16	ARG	Sidechain
2	r	25	ARG	Sidechain
2	r	36	ARG	Sidechain
2	r	38	ARG	Sidechain
2	r	47	ARG	Sidechain
2	r	49	ARG	Sidechain
2	r	62	ARG	Sidechain
2	r	83	ARG	Sidechain
4	s	134	ARG	Sidechain
4	s	37	ARG	Sidechain
4	s	77	ARG	Sidechain

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Mol	Chain	Res	Type	Group
4	s	90	ARG	Sidechain
2	t	16	ARG	Sidechain
2	t	25	ARG	Sidechain
2	t	36	ARG	Sidechain
2	t	38	ARG	Sidechain
2	t	47	ARG	Sidechain
2	t	49	ARG	Sidechain
2	t	62	ARG	Sidechain
2	t	83	ARG	Sidechain
4	u	134	ARG	Sidechain
4	u	76	ARG	Sidechain
4	u	77	ARG	Sidechain
3	v	100	ASP	Sidechain
3	v	107	ARG	Sidechain
3	v	12	TYR	Sidechain
3	v	15	GLN	Sidechain
3	v	67	ARG	Sidechain
3	v	76	ARG	Sidechain
3	v	77	ARG	Sidechain
3	v	90	ARG	Sidechain
3	v	94	TYR	Sidechain
2	w	25	ARG	Sidechain
2	w	36	ARG	Sidechain
2	w	38	ARG	Sidechain
2	w	62	ARG	Sidechain
2	w	83	ARG	Sidechain
3	x	100	ASP	Sidechain
3	x	107	ARG	Sidechain
3	x	39	ARG	Sidechain
3	x	67	ARG	Sidechain
3	x	76	ARG	Sidechain
3	x	77	ARG	Sidechain
3	x	87	TYR	Sidechain
3	x	90	ARG	Sidechain
2	y	131	ARG	Sidechain
2	y	25	ARG	Sidechain
2	y	36	ARG	Sidechain
2	y	49	ARG	Sidechain
2	y	62	ARG	Sidechain
2	y	83	ARG	Sidechain
3	z	100	ASP	Sidechain
3	z	76	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	z	83	ARG	Sidechain
3	z	90	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	8678	0	8690	439	0
1	C	8678	0	8691	474	0
2	1	1207	0	1222	44	0
2	3	1213	0	1227	60	0
2	5	1213	0	1227	59	0
2	7	1223	0	1235	54	0
2	9	1207	0	1222	53	0
2	AA	1223	0	1235	45	0
2	AC	1223	0	1235	55	0
2	AE	1223	0	1235	54	0
2	AG	1223	0	1235	48	0
2	AI	1213	0	1227	65	0
2	AK	1213	0	1227	55	0
2	AM	1223	0	1235	44	0
2	AO	1223	0	1235	55	0
2	AQ	1223	0	1235	53	0
2	AS	1223	0	1235	47	0
2	AU	1213	0	1227	69	0
2	AW	1213	0	1227	55	0
2	E	1223	0	1235	34	0
2	G	1223	0	1235	35	0
2	I	1223	0	1235	40	0
2	K	1223	0	1235	35	0
2	M	1223	0	1235	34	0
2	O	1213	0	1227	25	0
2	Q	1223	0	1235	37	0
2	S	1213	0	1227	25	0
2	U	1223	0	1235	32	0
2	W	1223	0	1235	34	0
2	Y	1223	0	1235	26	0
2	a	1223	0	1235	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	c	1213	0	1227	63	0
2	e	1213	0	1227	52	0
2	g	1213	0	1227	51	0
2	i	1207	0	1222	48	0
2	k	1207	0	1222	62	0
2	m	1223	0	1235	51	0
2	o	1213	0	1227	60	0
2	r	1223	0	1235	44	0
2	t	1213	0	1227	33	0
2	w	1213	0	1227	58	0
2	y	1213	0	1227	55	0
3	0	1195	0	1203	40	0
3	2	1187	0	1192	33	0
3	4	1187	0	1192	30	0
3	6	1210	0	1220	48	0
3	8	1210	0	1220	21	0
3	AB	1210	0	1220	32	0
3	AD	1195	0	1203	41	0
3	AF	1202	0	1208	44	0
3	AH	1210	0	1220	44	0
3	AJ	1210	0	1220	42	0
3	AL	1203	0	1215	41	0
3	AN	1210	0	1220	33	0
3	AP	1195	0	1203	44	0
3	AR	1202	0	1208	41	0
3	AT	1210	0	1220	41	0
3	AV	1210	0	1220	45	0
3	AX	1203	0	1215	47	0
3	F	1210	0	1220	30	0
3	H	1210	0	1220	21	0
3	J	1210	0	1220	17	0
3	L	1210	0	1220	17	0
3	N	1210	0	1220	29	0
3	P	1210	0	1220	21	0
3	R	1210	0	1220	33	0
3	T	1210	0	1220	24	0
3	V	1210	0	1220	32	0
3	X	1210	0	1220	21	0
3	Z	1210	0	1220	24	0
3	b	1210	0	1220	18	0
3	d	1187	0	1192	29	0
3	f	1202	0	1208	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	h	1210	0	1220	38	0
3	j	1187	0	1192	36	0
3	l	1195	0	1203	54	0
3	n	1210	0	1220	29	0
3	p	1210	0	1220	29	0
3	q	1210	0	1220	47	0
3	v	1210	0	1220	51	0
3	x	1210	0	1220	29	0
3	z	1210	0	1220	44	0
4	s	1227	0	1231	51	0
4	u	1217	0	1223	55	0
5	AY	529	0	547	13	0
5	AZ	529	0	547	13	0
5	Aa	529	0	547	22	0
5	Ab	522	0	538	19	0
5	Ac	518	0	535	18	0
5	Ad	529	0	547	24	0
6	0	43	0	37	2	0
6	1	43	0	37	2	0
6	2	43	0	37	1	0
6	3	43	0	37	5	0
6	4	43	0	37	6	0
6	5	43	0	37	8	0
6	6	43	0	37	5	0
6	7	43	0	37	8	0
6	8	43	0	37	1	0
6	9	43	0	37	7	0
6	A	43	0	37	3	0
6	AA	43	0	37	7	0
6	AB	43	0	37	3	0
6	AC	43	0	37	2	0
6	AD	43	0	37	2	0
6	AE	43	0	37	1	0
6	AF	43	0	37	4	0
6	AG	43	0	37	12	0
6	AH	43	0	37	4	0
6	AI	43	0	37	1	0
6	AJ	43	0	37	3	0
6	AK	43	0	37	11	0
6	AL	43	0	37	3	0
6	AM	43	0	37	7	0
6	AN	43	0	37	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AO	43	0	37	2	0
6	AP	43	0	37	4	0
6	AQ	43	0	37	1	0
6	AR	43	0	37	1	0
6	AS	43	0	37	13	0
6	AT	43	0	37	4	0
6	AU	43	0	37	1	0
6	AV	43	0	37	3	0
6	AW	43	0	37	11	0
6	AX	43	0	37	4	0
6	C	43	0	38	33	0
6	E	43	0	37	8	0
6	F	43	0	37	9	0
6	G	43	0	37	5	0
6	H	43	0	37	5	0
6	I	43	0	37	3	0
6	J	43	0	37	2	0
6	K	43	0	37	3	0
6	L	43	0	37	2	0
6	M	43	0	37	6	0
6	N	43	0	37	7	0
6	O	43	0	37	3	0
6	P	43	0	37	3	0
6	Q	43	0	37	10	0
6	R	43	0	37	13	0
6	S	43	0	37	3	0
6	T	43	0	37	5	0
6	U	43	0	37	7	0
6	V	43	0	37	8	0
6	W	43	0	37	5	0
6	X	43	0	37	8	0
6	Y	43	0	37	3	0
6	Z	43	0	37	3	0
6	a	43	0	37	4	0
6	b	43	0	37	2	0
6	c	43	0	37	6	0
6	d	43	0	37	5	0
6	e	43	0	37	10	0
6	f	43	0	37	3	0
6	g	43	0	37	6	0
6	h	43	0	37	1	0
6	i	43	0	37	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	j	43	0	37	2	0
6	k	43	0	37	5	0
6	l	43	0	37	1	0
6	m	43	0	37	9	0
6	n	43	0	37	4	0
6	o	43	0	37	3	0
6	p	43	0	37	3	0
6	q	43	0	37	2	0
6	r	43	0	37	4	0
6	s	43	0	38	12	0
6	t	43	0	37	4	0
6	u	43	0	38	14	0
6	v	43	0	37	1	0
6	w	43	0	37	1	0
6	x	43	0	37	3	0
6	y	43	0	37	9	0
6	z	43	0	37	2	0
All	All	123484	0	124009	3743	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 (3743) 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:AU:116:TYR:CD1	2:AU:121:THR:HG21	1.66	1.30
2:AI:116:TYR:CD1	2:AI:121:THR:HG21	1.67	1.29
3:v:161:SER:OXT	3:6:101:PRO:HG3	1.31	1.28
3:f:101:PRO:HG3	3:q:161:SER:OXT	1.33	1.24
3:l:103:ILE:HD11	3:l:107:ARG:NH2	1.55	1.21
2:r:49:ARG:NH2	2:r:140:LEU:HD21	1.58	1.19
2:AC:37:LEU:HD11	3:AD:27:LEU:HD11	1.24	1.16
2:3:89:LEU:HB2	2:3:133:MET:HE1	1.17	1.15
4:s:81:CYS:CB	6:s:201:CYC:HAC1	1.77	1.15
2:c:89:LEU:HB2	2:c:133:MET:HE1	1.16	1.14
1:C:352:ILE:HG22	3:p:107:ARG:O	1.47	1.13
3:x:64:ASP:OD1	3:z:124:ALA:HB3	1.46	1.12
2:9:89:LEU:HB2	2:9:133:MET:HE1	1.15	1.12
1:C:976:ARG:O	1:C:977:GLN:HG2	1.50	1.11
1:A:319:ALA:O	1:A:320:GLU:HG2	1.50	1.11
4:s:81:CYS:HB3	6:s:201:CYC:HAC1	1.12	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:v:3:ASP:OD1	3:v:5:ILE:HG13	1.50	1.10
2:7:89:LEU:HB2	2:7:133:MET:HE1	1.15	1.10
1:A:976:ARG:O	1:A:977:GLN:HG2	1.50	1.10
2:AO:37:LEU:HD11	3:AP:27:LEU:HD11	1.24	1.10
1:C:511:ARG:HE	1:C:526:MET:HE1	1.08	1.09
1:C:319:ALA:O	1:C:320:GLU:HG2	1.50	1.09
2:g:89:LEU:HB2	2:g:133:MET:HE1	1.16	1.08
2:y:89:LEU:HB2	2:y:133:MET:HE1	1.15	1.08
2:m:89:LEU:HB2	2:m:133:MET:HE1	1.15	1.08
1:A:511:ARG:HE	1:A:526:MET:HE1	1.08	1.07
2:AG:112:VAL:HG21	2:AG:160:MET:HE1	1.32	1.07
2:i:4:LEU:HD11	3:j:3:ASP:HB2	1.36	1.06
2:AS:112:VAL:HG21	2:AS:160:MET:HE1	1.32	1.06
4:s:81:CYS:HB3	6:s:201:CYC:CAC	1.87	1.05
2:AE:4:LEU:HD11	3:AF:3:ASP:HB2	1.39	1.05
2:AQ:4:LEU:HD11	3:AR:3:ASP:HB2	1.39	1.04
2:i:14:GLU:HG2	2:i:16:ARG:HD3	1.37	1.03
2:y:102:THR:CG2	2:y:103:PRO:HD3	1.90	1.02
2:AI:116:TYR:CD1	2:AI:121:THR:CG2	2.43	1.02
2:Y:34:GLU:OE2	3:Z:28:LYS:HG3	1.60	1.01
1:C:733:SER:HB2	3:AH:154:ASP:OD2	1.59	1.01
3:AP:33:THR:O	3:AP:36:VAL:HG12	1.61	1.01
1:C:346:GLU:OE1	1:C:347:PHE:CD1	2.14	1.01
2:I:34:GLU:OE2	3:J:28:LYS:HG3	1.61	1.01
3:Z:61:ILE:HG13	3:Z:62:TYR:CD2	1.96	1.01
3:AD:33:THR:O	3:AD:36:VAL:HG12	1.61	1.00
3:AD:100:ASP:OD1	3:AD:101:PRO:HD2	1.61	1.00
3:AN:100:ASP:OD1	3:AN:101:PRO:HD2	1.61	1.00
3:AP:100:ASP:OD1	3:AP:101:PRO:HD2	1.61	1.00
3:h:14:VAL:HG21	4:s:161:GLN:HG2	1.43	1.00
2:AU:116:TYR:CD1	2:AU:121:THR:CG2	2.43	1.00
3:6:100:ASP:OD1	3:6:101:PRO:HD2	1.62	1.00
3:AT:100:ASP:OD1	3:AT:101:PRO:HD2	1.61	1.00
3:h:100:ASP:OD1	3:h:101:PRO:HD2	1.62	1.00
3:AH:100:ASP:OD1	3:AH:101:PRO:HD2	1.61	0.99
3:2:100:ASP:OD1	3:2:101:PRO:HD2	1.62	0.99
1:C:40:VAL:HG13	3:q:38:VAL:HG13	1.42	0.99
3:l:100:ASP:OD1	3:l:101:PRO:HD2	1.62	0.99
3:AB:100:ASP:OD1	3:AB:101:PRO:HD2	1.61	0.99
3:z:100:ASP:OD1	3:z:101:PRO:HD2	1.62	0.99
3:AJ:100:ASP:OD1	3:AJ:101:PRO:HD2	1.63	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:100:ASP:OD1	3:0:101:PRO:HD2	1.62	0.99
1:C:40:VAL:HG13	3:q:38:VAL:CG1	1.92	0.99
3:f:100:ASP:OD1	3:f:101:PRO:HD2	1.62	0.99
2:1:4:LEU:HD11	3:2:3:ASP:HB2	1.42	0.99
1:A:1046:ARG:HG2	1:A:1089:LEU:HD23	1.43	0.98
2:m:140:LEU:HD23	3:AH:140:LEU:CD2	1.94	0.98
3:AX:100:ASP:OD1	3:AX:101:PRO:HD2	1.63	0.98
3:x:100:ASP:OD1	3:x:101:PRO:HD2	1.64	0.98
2:AI:131:ARG:HH21	2:AI:157:VAL:HG11	1.28	0.98
1:A:40:VAL:HG13	3:v:38:VAL:HG13	1.43	0.97
2:AW:131:ARG:HH21	2:AW:157:VAL:HG11	1.29	0.97
3:n:100:ASP:OD1	3:n:101:PRO:HD2	1.63	0.97
1:A:40:VAL:HG13	3:v:38:VAL:CG1	1.94	0.97
2:7:140:LEU:HD23	3:AT:140:LEU:CD2	1.94	0.97
3:8:100:ASP:OD1	3:8:101:PRO:HD2	1.63	0.97
2:AU:60:GLN:HA	2:AU:60:GLN:HE21	1.28	0.97
3:j:19:LEU:HD13	3:j:24:LEU:HD21	1.44	0.96
5:Ab:24:GLN:OE1	5:Ab:24:GLN:N	1.97	0.96
3:AL:100:ASP:OD1	3:AL:101:PRO:HD2	1.63	0.96
3:AV:100:ASP:OD1	3:AV:101:PRO:HD2	1.63	0.96
2:AW:4:LEU:HD11	3:AX:3:ASP:HB3	1.48	0.96
2:3:4:LEU:HD11	3:4:3:ASP:CB	1.96	0.96
2:AC:37:LEU:CD1	3:AD:27:LEU:HD11	1.96	0.95
6:5:201:CYC:O1D	3:8:62:TYR:OH	1.84	0.95
2:AK:131:ARG:HH21	2:AK:157:VAL:HG11	1.30	0.95
2:AO:37:LEU:CD1	3:AP:27:LEU:HD11	1.96	0.94
2:y:102:THR:HG23	2:y:103:PRO:HD3	1.49	0.94
3:q:25:ASP:HA	3:q:28:LYS:HG2	1.50	0.94
2:AU:131:ARG:HH21	2:AU:157:VAL:HG11	1.28	0.94
1:A:444:ASN:OD1	1:A:445:TYR:N	2.00	0.94
2:AK:4:LEU:HD11	3:AL:3:ASP:HB3	1.48	0.94
2:Y:151:PHE:HB3	2:a:20:PRO:HB3	1.49	0.94
1:A:546:PHE:CZ	3:0:110:ASN:ND2	2.35	0.94
2:9:37:LEU:HD22	3:0:24:LEU:HD22	1.49	0.94
2:m:140:LEU:CD2	3:AH:140:LEU:CD2	2.46	0.94
2:7:140:LEU:CD2	3:AT:140:LEU:CD2	2.46	0.94
2:e:4:LEU:HD11	3:f:3:ASP:CB	1.97	0.94
1:C:444:ASN:OD1	1:C:445:TYR:N	2.00	0.93
2:AO:37:LEU:HD11	3:AP:27:LEU:CD1	1.98	0.93
2:AC:37:LEU:HD11	3:AD:27:LEU:CD1	1.98	0.93
3:AP:24:LEU:O	3:AP:27:LEU:HG	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:29:PHE:HE1	2:1:36:ARG:HH22	0.95	0.93
2:AC:37:LEU:HD22	3:AD:24:LEU:HD22	1.48	0.92
1:C:851:HIS:CE1	3:AV:83:ARG:HH12	1.86	0.92
1:A:851:HIS:CE1	3:AJ:83:ARG:HH12	1.86	0.92
3:2:25:ASP:HA	3:2:28:LYS:HG2	1.50	0.92
3:AF:25:ASP:HA	3:AF:28:LYS:HG2	1.51	0.92
3:AR:25:ASP:HA	3:AR:28:LYS:HG2	1.51	0.92
2:AK:4:LEU:HD11	3:AL:3:ASP:CB	2.00	0.92
2:AO:37:LEU:HD22	3:AP:24:LEU:HD22	1.48	0.92
1:C:1153:VAL:HG11	3:N:59:ALA:O	1.68	0.92
2:r:49:ARG:HH21	2:r:140:LEU:HD21	1.30	0.92
3:F:49:THR:HG21	2:G:161:GLN:HG2	1.52	0.92
3:V:49:THR:HG21	2:W:161:GLN:HG2	1.51	0.92
2:AI:20:PRO:HB3	2:AK:151:PHE:HB3	1.50	0.92
3:AD:24:LEU:O	3:AD:27:LEU:HG	1.68	0.92
1:C:1143:LEU:HD11	2:I:103:PRO:HA	1.52	0.91
3:Z:61:ILE:HG13	3:Z:62:TYR:HD2	1.31	0.91
1:A:1118:THR:HG23	6:X:201:CYC:HMA2	1.48	0.91
2:3:4:LEU:HD11	3:4:3:ASP:HB3	1.51	0.91
3:d:25:ASP:HA	3:d:28:LYS:HG2	1.50	0.91
2:AW:4:LEU:HD11	3:AX:3:ASP:CB	2.00	0.91
2:I:151:PHE:HB3	2:K:20:PRO:HB3	1.49	0.91
1:C:733:SER:CB	3:AH:154:ASP:OD2	2.18	0.91
1:C:532:THR:HG21	2:m:102:THR:HG23	1.51	0.90
2:AU:20:PRO:HB3	2:AW:151:PHE:HB3	1.50	0.90
2:U:20:PRO:HG2	2:W:101:VAL:HG13	1.52	0.90
3:4:25:ASP:HA	3:4:28:LYS:HG2	1.51	0.90
2:AC:14:GLU:OE1	2:AC:16:ARG:HD3	1.71	0.90
1:C:156:SER:CB	6:C:2101:CYC:H3C	2.01	0.90
3:l:103:ILE:HD11	3:l:107:ARG:HH22	1.27	0.90
6:U:201:CYC:HB	6:U:201:CYC:HMA1	1.35	0.90
2:k:42:THR:HG22	2:k:140:LEU:HD21	1.52	0.90
1:C:4:ARG:HD3	1:C:464:GLN:O	1.71	0.90
1:C:483:PHE:CZ	3:n:83:ARG:NH1	2.41	0.89
2:AI:4:LEU:HD11	3:AJ:3:ASP:HB3	1.53	0.89
2:3:151:PHE:HB3	2:5:20:PRO:HB3	1.52	0.89
2:E:20:PRO:HG2	2:G:101:VAL:HG13	1.51	0.89
2:AU:4:LEU:HD11	3:AV:3:ASP:HB3	1.53	0.89
1:A:4:ARG:HD3	1:A:464:GLN:O	1.71	0.89
1:C:1143:LEU:CD1	2:I:103:PRO:HA	2.02	0.89
1:A:496:GLU:HG2	3:6:114:GLU:HG3	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:20:PRO:HG2	2:5:101:VAL:HG13	1.55	0.89
1:C:496:GLU:HG2	3:f:114:GLU:HG3	1.55	0.88
2:AO:14:GLU:OE1	2:AO:16:ARG:HD3	1.71	0.88
2:AO:104:ILE:HG21	2:AO:156:LEU:HD11	1.55	0.88
5:Ab:24:GLN:H	5:Ab:24:GLN:CD	1.80	0.88
1:A:974:LEU:HD13	3:R:1:MET:H1	1.37	0.88
1:C:164:LEU:HB3	3:q:18:TYR:OH	1.74	0.88
1:A:875:LEU:HD11	1:A:876:TYR:CE2	2.09	0.88
2:7:140:LEU:HD23	3:AT:140:LEU:HD22	1.55	0.88
2:AU:4:LEU:HD11	3:AV:3:ASP:CB	2.03	0.88
2:m:140:LEU:HD23	3:AH:140:LEU:HD22	1.56	0.87
2:r:49:ARG:NH2	2:r:140:LEU:CD2	2.36	0.87
2:w:4:LEU:HD11	3:x:3:ASP:CB	2.03	0.87
2:AI:4:LEU:HD11	3:AJ:3:ASP:CB	2.04	0.87
1:C:194:CYS:SG	6:C:2101:CYC:C4C	2.63	0.86
2:c:20:PRO:HG2	2:e:101:VAL:HG13	1.55	0.86
2:g:130:VAL:HG11	2:g:156:LEU:HD22	1.56	0.86
2:AC:104:ILE:HG21	2:AC:156:LEU:HD11	1.55	0.86
2:AC:102:THR:HG23	2:AC:103:PRO:HD3	1.58	0.86
1:A:532:THR:HG21	2:7:102:THR:HG23	1.57	0.86
2:o:4:LEU:HD11	3:p:3:ASP:CB	2.06	0.86
6:n:201:CYC:HB	6:n:201:CYC:HMA1	1.41	0.86
1:C:875:LEU:HD11	1:C:876:TYR:CE2	2.09	0.86
4:u:81:CYS:SG	6:u:201:CYC:C4C	2.64	0.86
2:AE:22:GLU:O	2:AE:25:ARG:HG2	1.76	0.86
2:AQ:43:LEU:HD11	2:AQ:141:LEU:HD11	1.58	0.86
2:AE:43:LEU:HD11	2:AE:141:LEU:HD11	1.58	0.85
1:C:511:ARG:NE	1:C:526:MET:HE1	1.92	0.85
2:AO:102:THR:HG23	2:AO:103:PRO:HD3	1.58	0.85
2:AQ:22:GLU:O	2:AQ:25:ARG:HG2	1.76	0.85
6:6:201:CYC:HB	6:6:201:CYC:HMA1	1.40	0.85
1:C:344:ARG:NH1	2:o:9:VAL:CG1	2.40	0.84
6:f:201:CYC:HB	6:f:201:CYC:HMA1	1.43	0.84
2:t:47:ARG:HG2	2:t:48:GLU:OE2	1.77	0.84
1:C:194:CYS:SG	6:C:2101:CYC:CHD	2.66	0.84
1:A:496:GLU:CD	3:6:114:GLU:HG2	2.01	0.84
2:g:102:THR:HG23	2:g:103:PRO:HD3	1.57	0.84
2:AI:47:ARG:HG2	2:AI:48:GLU:OE2	1.78	0.83
2:AW:47:ARG:HG2	2:AW:48:GLU:OE2	1.78	0.83
1:A:428:VAL:HB	1:A:429:GLU:OE1	1.78	0.83
6:F:201:CYC:HMA3	6:F:201:CYC:HB	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AO:47:ARG:HG2	2:AO:48:GLU:OE2	1.78	0.83
2:k:4:LEU:HD21	3:l:3:ASP:OD1	1.79	0.83
2:O:81:CYS:HA	6:O:201:CYC:HHD	1.60	0.83
2:5:47:ARG:HG2	2:5:48:GLU:OE2	1.78	0.83
2:AU:47:ARG:HG2	2:AU:48:GLU:OE2	1.78	0.83
2:i:73:TYR:O	2:i:77:MET:SD	2.37	0.83
1:A:257:THR:O	4:u:83:ARG:HD2	1.78	0.83
2:o:47:ARG:HG2	2:o:48:GLU:OE2	1.79	0.83
2:7:47:ARG:HG2	2:7:48:GLU:OE2	1.78	0.83
2:AG:47:ARG:HG2	2:AG:48:GLU:OE2	1.79	0.83
2:r:47:ARG:HG2	2:r:48:GLU:OE2	1.78	0.83
2:c:47:ARG:HG2	2:c:48:GLU:OE2	1.79	0.83
2:7:89:LEU:HB2	2:7:133:MET:CE	2.06	0.83
1:A:546:PHE:CE2	3:0:110:ASN:ND2	2.47	0.83
1:C:496:GLU:CD	3:f:114:GLU:HG2	2.03	0.83
1:A:1118:THR:CG2	6:X:201:CYC:HMA2	2.09	0.82
1:C:698:GLY:HA3	3:p:127:VAL:CG1	2.09	0.82
2:3:47:ARG:HG2	2:3:48:GLU:OE2	1.78	0.82
1:C:249:SER:HB3	1:C:253:ARG:HG3	1.61	0.82
2:1:29:PHE:CE1	2:1:36:ARG:NH2	2.46	0.82
3:N:91:TYR:HD2	3:N:103:ILE:HD11	1.44	0.82
2:1:47:ARG:HG2	2:1:48:GLU:OE2	1.79	0.82
1:A:698:GLY:HA3	3:x:127:VAL:CG1	2.08	0.82
2:k:37:LEU:HD22	3:l:24:LEU:HD22	1.61	0.82
1:A:249:SER:HB3	1:A:253:ARG:HG3	1.61	0.82
2:c:22:GLU:O	2:c:25:ARG:HG2	1.80	0.82
1:A:344:ARG:NH1	2:w:9:VAL:CG1	2.43	0.82
1:A:511:ARG:NE	1:A:526:MET:HE1	1.92	0.82
2:g:105:GLU:HG3	2:g:109:ILE:HD11	1.61	0.82
1:A:480:GLU:OE1	1:A:689:GLY:HA3	1.80	0.82
1:C:480:GLU:OE1	1:C:689:GLY:HA3	1.80	0.82
3:R:91:TYR:HD2	3:R:103:ILE:HD11	1.43	0.82
2:e:47:ARG:HG2	2:e:48:GLU:OE2	1.78	0.82
2:3:20:PRO:HG2	2:5:101:VAL:CG1	2.10	0.81
1:C:186:LEU:HD21	6:C:2101:CYC:C2B	2.10	0.81
2:i:47:ARG:HG2	2:i:48:GLU:OE2	1.79	0.81
2:k:12:ASP:OD2	3:l:107:ARG:CZ	2.27	0.81
1:A:352:ILE:HG21	3:x:110:ASN:O	1.80	0.81
1:C:851:HIS:HE1	3:AV:83:ARG:HH12	1.28	0.81
2:1:73:TYR:O	2:1:77:MET:SD	2.38	0.81
2:AQ:35:ARG:O	2:AQ:38:ARG:HG2	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AK:47:ARG:HG2	2:AK:48:GLU:OE2	1.78	0.81
6:U:201:CYC:HMA1	6:U:201:CYC:NB	1.95	0.81
6:X:201:CYC:NC	6:X:201:CYC:HMD1	1.94	0.81
2:c:20:PRO:HG2	2:e:101:VAL:CG1	2.09	0.81
3:AN:12:TYR:CD2	3:AN:17:LYS:HG3	2.16	0.81
2:AS:47:ARG:HG2	2:AS:48:GLU:OE2	1.79	0.81
1:C:193:SER:HB3	6:C:2101:CYC:HBD2	1.61	0.81
2:AE:49:ARG:NH1	2:AE:140:LEU:HD21	1.96	0.81
2:AC:47:ARG:HG2	2:AC:48:GLU:OE2	1.78	0.81
1:A:254:PRO:HD3	4:u:107:TYR:CE1	2.16	0.80
2:k:47:ARG:HG2	2:k:48:GLU:OE2	1.80	0.80
2:9:47:ARG:HG2	2:9:48:GLU:OE2	1.81	0.80
2:AQ:49:ARG:NH1	2:AQ:140:LEU:HD21	1.96	0.80
2:AE:35:ARG:O	2:AE:38:ARG:HG2	1.81	0.80
2:AU:60:GLN:HA	2:AU:60:GLN:NE2	1.95	0.80
2:AC:4:LEU:HD11	3:AD:3:ASP:HB2	1.63	0.80
1:A:851:HIS:HE1	3:AJ:83:ARG:HH12	1.28	0.80
1:C:352:ILE:CG2	3:p:107:ARG:O	2.29	0.80
6:V:201:CYC:HMA3	6:V:201:CYC:HB	1.46	0.80
2:AM:4:LEU:HD21	3:AN:98:ALA:HA	1.63	0.80
1:C:779:ASP:OD2	6:AN:201:CYC:HMA2	1.81	0.80
3:j:151:ILE:HD11	3:j:152:TYR:CE2	2.17	0.79
6:9:201:CYC:HB	6:9:201:CYC:HMA1	1.45	0.79
3:AB:12:TYR:CD2	3:AB:17:LYS:HG3	2.16	0.79
3:AD:27:LEU:HD12	3:AD:28:LYS:N	1.97	0.79
2:9:89:LEU:HB2	2:9:133:MET:CE	2.08	0.79
3:v:25:ASP:HA	3:v:28:LYS:HE2	1.65	0.79
2:I:6:LYS:O	2:I:9:VAL:HG22	1.82	0.79
2:AO:4:LEU:HD11	3:AP:3:ASP:HB2	1.63	0.79
1:A:779:ASP:OD2	6:AB:201:CYC:HMA2	1.82	0.79
1:C:702:VAL:HG11	1:C:712:ARG:CZ	2.13	0.79
2:e:4:LEU:HD11	3:f:3:ASP:HB2	1.64	0.79
1:C:483:PHE:CE1	3:n:87:TYR:CE2	2.71	0.79
3:l:151:ILE:HD11	3:l:152:TYR:CE2	2.18	0.79
3:AP:151:ILE:HD11	3:AP:152:TYR:CE2	2.18	0.79
1:A:698:GLY:HA3	3:x:127:VAL:HG12	1.64	0.79
2:i:14:GLU:HG2	2:i:16:ARG:CD	2.11	0.79
2:5:4:LEU:HD11	3:6:3:ASP:CB	2.12	0.79
3:AP:27:LEU:HD12	3:AP:28:LYS:N	1.97	0.79
3:AR:151:ILE:HD11	3:AR:152:TYR:CE2	2.18	0.79
1:A:164:LEU:HB3	3:v:18:TYR:OH	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:483:PHE:CE2	3:n:83:ARG:NH1	2.51	0.79
3:AD:151:ILE:HD11	3:AD:152:TYR:CE2	2.18	0.79
1:C:483:PHE:CE1	3:n:87:TYR:HE2	2.01	0.79
2:AA:4:LEU:HD21	3:AB:98:ALA:HA	1.63	0.79
2:k:107:ILE:HD12	3:l:13:ASP:OD2	1.83	0.78
3:l:91:TYR:HE2	3:l:107:ARG:HE	1.31	0.78
2:w:4:LEU:HD11	3:x:3:ASP:HB2	1.63	0.78
2:y:4:LEU:HD11	3:z:3:ASP:CB	2.13	0.78
1:C:31:GLU:HG3	1:C:33:ARG:CZ	2.14	0.78
1:C:344:ARG:NH1	2:o:9:VAL:HG12	1.99	0.78
2:o:4:LEU:HD11	3:p:3:ASP:HB2	1.65	0.78
3:2:151:ILE:HD11	3:2:152:TYR:CE2	2.18	0.78
1:A:265:SER:OG	4:u:76:ARG:HD3	1.84	0.78
1:C:698:GLY:HA3	3:p:127:VAL:HG12	1.65	0.78
2:Q:81:CYS:HA	6:Q:201:CYC:HHD	1.64	0.78
3:h:151:ILE:HD11	3:h:152:TYR:CE2	2.19	0.78
2:g:4:LEU:HD11	3:h:3:ASP:CB	2.14	0.78
1:A:700:SER:O	1:A:701:ASP:HB3	1.83	0.77
2:m:89:LEU:HB2	2:m:133:MET:CE	2.07	0.77
2:5:22:GLU:O	2:5:25:ARG:HG2	1.83	0.77
2:AM:29:PHE:HD1	2:AM:36:ARG:HH12	1.32	0.77
6:AS:201:CYC:HB	6:AS:201:CYC:HMA1	1.48	0.77
2:c:151:PHE:HB3	2:e:20:PRO:HB3	1.66	0.77
3:h:124:ALA:HB3	3:p:64:ASP:OD1	1.83	0.77
3:z:151:ILE:HD11	3:z:152:TYR:CE2	2.19	0.77
3:6:151:ILE:HD11	3:6:152:TYR:CE2	2.20	0.77
3:0:151:ILE:HD11	3:0:152:TYR:CE2	2.19	0.77
4:u:60:LEU:HB3	4:u:72:MET:HE3	1.67	0.77
6:9:201:CYC:HMA1	6:9:201:CYC:NB	1.99	0.77
1:A:974:LEU:HD13	3:R:1:MET:N	1.98	0.77
2:c:71:ASN:OD1	2:c:121:THR:HA	1.84	0.77
3:f:151:ILE:HD11	3:f:152:TYR:CE2	2.20	0.77
1:A:31:GLU:HG3	1:A:33:ARG:CZ	2.14	0.77
1:C:1118:THR:HG23	6:H:201:CYC:HMA2	1.65	0.77
3:AF:151:ILE:HD11	3:AF:152:TYR:CE2	2.18	0.77
2:w:156:LEU:HD11	2:w:160:MET:HE1	1.66	0.77
3:AL:151:ILE:HD11	3:AL:152:TYR:CE2	2.20	0.77
3:R:87:TYR:CE1	3:R:91:TYR:HE1	2.03	0.77
1:A:344:ARG:NH1	2:w:9:VAL:HG12	1.99	0.77
2:y:102:THR:HG22	2:y:103:PRO:HD3	1.67	0.77
3:AL:2:GLN:HE21	3:AL:7:ALA:HA	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AN:151:ILE:HD11	3:AN:152:TYR:CE2	2.20	0.77
1:A:254:PRO:HD3	4:u:107:TYR:CD1	2.20	0.77
1:A:702:VAL:HG11	1:A:712:ARG:CZ	2.13	0.77
1:A:459:PHE:O	1:A:460:ALA:HB3	1.84	0.77
1:C:700:SER:O	1:C:701:ASP:HB3	1.83	0.76
1:C:1118:THR:CG2	6:H:201:CYC:HMA2	2.15	0.76
2:g:37:LEU:HD22	3:h:24:LEU:HD22	1.67	0.76
2:c:89:LEU:HB2	2:c:133:MET:CE	2.08	0.76
3:AX:2:GLN:HE21	3:AX:7:ALA:HA	1.49	0.76
2:k:75:GLU:HG2	2:k:76:LYS:N	2.00	0.76
2:y:75:GLU:HG2	2:y:76:LYS:N	2.01	0.76
1:A:257:THR:O	4:u:83:ARG:CD	2.33	0.76
3:AJ:151:ILE:HD11	3:AJ:152:TYR:CE2	2.19	0.76
3:AV:151:ILE:HD11	3:AV:152:TYR:CE2	2.20	0.76
3:AX:151:ILE:HD11	3:AX:152:TYR:CE2	2.20	0.76
2:AQ:4:LEU:HD11	3:AR:3:ASP:CB	2.15	0.76
1:C:459:PHE:O	1:C:460:ALA:HB3	1.84	0.76
3:AF:53:LYS:HD3	2:AK:118:SER:O	1.85	0.76
6:AG:201:CYC:HB	6:AG:201:CYC:HMA1	1.48	0.76
3:AV:123:ILE:HG23	3:AV:160:LEU:HG	1.68	0.76
2:o:97:VAL:HG11	3:p:27:LEU:HD13	1.67	0.76
3:AR:53:LYS:HD3	2:AW:118:SER:O	1.85	0.76
1:C:63:ASN:HB2	1:C:213:LEU:HD21	1.69	0.75
2:AW:75:GLU:HG2	2:AW:76:LYS:N	2.00	0.75
1:C:288:LEU:HB2	1:C:293:LYS:HB2	1.67	0.75
2:c:75:GLU:HG2	2:c:76:LYS:N	2.01	0.75
2:w:75:GLU:HG2	2:w:76:LYS:N	2.01	0.75
1:A:288:LEU:HB2	1:A:293:LYS:HB2	1.67	0.75
1:A:539:LYS:NZ	5:Aa:24:GLN:HE21	1.82	0.75
3:d:151:ILE:HD11	3:d:152:TYR:CE2	2.21	0.75
3:AB:151:ILE:HD11	3:AB:152:TYR:CE2	2.20	0.75
3:AJ:123:ILE:HG23	3:AJ:160:LEU:HG	1.68	0.75
3:AR:87:TYR:CE2	5:Ad:38:PHE:CZ	2.75	0.75
1:A:254:PRO:HB2	4:u:91:TYR:OH	1.86	0.75
3:N:87:TYR:CE1	3:N:91:TYR:HE1	2.04	0.75
2:E:56:ASP:CB	2:5:75:GLU:OE1	2.34	0.75
2:m:75:GLU:HG2	2:m:76:LYS:N	2.02	0.75
3:4:151:ILE:HD11	3:4:152:TYR:CE2	2.21	0.75
2:AK:75:GLU:HG2	2:AK:76:LYS:N	2.00	0.75
1:A:10:THR:O	4:u:118:SER:HB2	1.86	0.75
2:5:4:LEU:HD11	3:6:3:ASP:HB3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:68:PRO:HG2	2:9:61:LYS:HE2	1.67	0.74
2:i:14:GLU:CG	2:i:16:ARG:HD3	2.15	0.74
1:A:706:PRO:HG3	3:z:65:LEU:HD12	1.70	0.74
2:y:89:LEU:HB2	2:y:133:MET:CE	2.07	0.74
2:3:89:LEU:HB2	2:3:133:MET:CE	2.08	0.74
2:AM:29:PHE:CD1	2:AM:36:ARG:NH1	2.55	0.74
6:c:201:CYC:HMA3	6:c:201:CYC:HB	1.52	0.74
2:k:32:SER:O	2:k:35:ARG:HG2	1.87	0.74
1:A:63:ASN:HB2	1:A:213:LEU:HD21	1.69	0.74
6:A:2101:CYC:HB	6:A:2101:CYC:HMA1	1.51	0.74
3:AX:14:VAL:HG13	5:Ad:64:ASN:HD21	1.50	0.74
1:C:156:SER:HB3	6:C:2101:CYC:H3C	1.69	0.74
3:R:115:THR:HG21	6:R:201:CYC:HMA3	1.69	0.74
2:g:75:GLU:HG2	2:g:76:LYS:N	2.01	0.74
2:3:75:GLU:HG2	2:3:76:LYS:N	2.01	0.74
2:AE:4:LEU:HD11	3:AF:3:ASP:CB	2.16	0.74
2:AE:104:ILE:HG21	2:AE:156:LEU:HD11	1.68	0.74
1:A:975:ARG:HD3	1:A:1116:TYR:CE2	2.23	0.74
2:r:14:GLU:HB3	2:r:16:ARG:HD3	1.69	0.74
3:h:50:THR:HG22	3:h:54:GLU:CD	2.12	0.74
1:A:3:ILE:HG21	4:u:110:ASN:HA	1.68	0.74
1:C:47:PHE:HE2	3:q:38:VAL:HG23	1.52	0.74
2:o:75:GLU:HG2	2:o:76:LYS:N	2.01	0.74
3:AF:87:TYR:CE2	5:Ac:38:PHE:CZ	2.75	0.74
2:g:89:LEU:HB2	2:g:133:MET:CE	2.08	0.73
6:3:201:CYC:HB	6:3:201:CYC:CMA	2.01	0.73
3:AX:110:ASN:ND2	5:Ad:57:PHE:CD1	2.56	0.73
1:A:19:THR:HG21	3:v:5:ILE:HD11	1.70	0.73
1:A:496:GLU:HG2	3:6:114:GLU:CG	2.18	0.73
2:y:37:LEU:HD22	3:z:24:LEU:HD22	1.70	0.73
6:3:201:CYC:HB	6:3:201:CYC:HMA3	1.51	0.73
1:A:47:PHE:HE2	3:v:38:VAL:HG23	1.51	0.73
1:C:975:ARG:HD3	1:C:1116:TYR:CE2	2.23	0.73
6:k:201:CYC:HMA1	6:k:201:CYC:HB	1.53	0.73
2:AS:43:LEU:HD11	2:AS:141:LEU:HD11	1.69	0.73
1:A:875:LEU:HD11	1:A:876:TYR:CZ	2.24	0.73
1:C:316:VAL:HB	1:C:319:ALA:HB3	1.71	0.73
2:AG:43:LEU:HD11	2:AG:141:LEU:HD11	1.69	0.73
2:AI:131:ARG:NH2	2:AI:157:VAL:HG11	2.02	0.73
2:AQ:104:ILE:HG21	2:AQ:156:LEU:HD11	1.68	0.72
2:AW:131:ARG:NH2	2:AW:157:VAL:HG11	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:LEU:HD23	1:C:207:ARG:NH2	2.04	0.72
6:s:201:CYC:HMD1	6:s:201:CYC:HC	1.53	0.72
3:2:119:LEU:HD21	5:Aa:34:TYR:OH	1.87	0.72
2:E:20:PRO:HG2	2:G:101:VAL:CG1	2.18	0.72
2:S:81:CYS:HA	6:S:201:CYC:HHD	1.72	0.72
2:AG:80:LEU:HD13	6:AG:201:CYC:HAD2	1.71	0.72
1:A:316:VAL:HB	1:A:319:ALA:HB3	1.71	0.72
6:C:2101:CYC:HB	6:C:2101:CYC:HMA1	1.53	0.72
2:U:20:PRO:HG2	2:W:101:VAL:CG1	2.19	0.72
1:C:706:PRO:HG3	3:h:65:LEU:HD12	1.70	0.72
1:C:875:LEU:HD11	1:C:876:TYR:CZ	2.24	0.72
2:U:161:GLN:HG2	3:X:49:THR:HG21	1.71	0.72
1:A:204:LEU:HD23	1:A:207:ARG:NH2	2.05	0.72
2:w:156:LEU:CD1	2:w:160:MET:HE1	2.19	0.72
2:AA:29:PHE:HD1	2:AA:36:ARG:HH12	1.32	0.72
3:AL:151:ILE:HD11	3:AL:152:TYR:CZ	2.25	0.72
2:AQ:35:ARG:O	2:AQ:38:ARG:CG	2.38	0.72
3:AX:151:ILE:HD11	3:AX:152:TYR:CZ	2.25	0.72
3:F:78:TYR:CD2	2:K:115:MET:HG3	2.24	0.72
1:C:496:GLU:HG2	3:f:114:GLU:CG	2.19	0.72
1:C:702:VAL:HG11	1:C:712:ARG:NH1	2.05	0.72
2:AS:80:LEU:HD13	6:AS:201:CYC:HAD2	1.72	0.72
2:c:12:ASP:OD2	3:d:107:ARG:NH1	2.22	0.72
3:f:151:ILE:HD11	3:f:152:TYR:CZ	2.25	0.72
4:u:81:CYS:HB3	6:u:201:CYC:CBC	2.20	0.72
3:AH:1:MET:HG2	3:AH:103:ILE:HD12	1.72	0.72
1:A:702:VAL:HG11	1:A:712:ARG:NH1	2.05	0.71
1:C:1140:TRP:HZ2	2:I:110:ILE:HD12	1.55	0.71
3:4:151:ILE:HD11	3:4:152:TYR:CZ	2.25	0.71
2:AA:29:PHE:CD1	2:AA:36:ARG:NH1	2.55	0.71
3:AN:151:ILE:HD11	3:AN:152:TYR:CZ	2.25	0.71
2:AU:131:ARG:NH2	2:AU:157:VAL:HG11	2.02	0.71
1:A:11:VAL:HG11	3:6:161:SER:HB2	1.70	0.71
1:C:10:THR:O	4:s:118:SER:HB2	1.89	0.71
1:A:54:ILE:HD13	3:v:28:LYS:HG2	1.70	0.71
1:C:695:GLY:O	1:C:696:ARG:C	2.34	0.71
3:AF:119:LEU:HD11	5:Ac:5:PHE:HZ	1.56	0.71
2:AS:4:LEU:HD11	3:AT:3:ASP:CB	2.20	0.71
1:C:25:ILE:HG21	3:q:1:MET:HE3	1.71	0.71
2:i:49:ARG:NH1	2:i:140:LEU:HD21	2.05	0.71
2:k:109:ILE:HD11	2:k:156:LEU:HD12	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:151:ILE:HD11	3:2:152:TYR:CZ	2.26	0.71
3:AP:27:LEU:HD12	3:AP:27:LEU:C	2.16	0.71
3:AR:160:LEU:C	3:AR:160:LEU:HD23	2.16	0.71
1:C:1121:ALA:CB	3:H:107:ARG:O	2.38	0.71
3:V:78:TYR:CD2	2:a:115:MET:HG3	2.24	0.71
6:k:201:CYC:HMA1	6:k:201:CYC:NB	2.06	0.71
2:r:60:GLN:HE22	2:7:69:GLY:CA	2.04	0.71
3:AB:151:ILE:HD11	3:AB:152:TYR:CZ	2.25	0.71
3:6:151:ILE:HD11	3:6:152:TYR:CZ	2.25	0.71
2:7:4:LEU:CD1	2:7:26:ILE:HD13	2.20	0.71
2:AC:102:THR:CG2	2:AC:103:PRO:HD3	2.20	0.71
3:AP:151:ILE:HD11	3:AP:152:TYR:CZ	2.26	0.71
2:9:49:ARG:HH21	2:9:140:LEU:HD21	1.55	0.71
3:AD:27:LEU:HD12	3:AD:27:LEU:C	2.16	0.71
3:AJ:151:ILE:HD11	3:AJ:152:TYR:CZ	2.25	0.71
3:d:151:ILE:HD11	3:d:152:TYR:CZ	2.25	0.71
3:AD:151:ILE:HD11	3:AD:152:TYR:CZ	2.26	0.71
1:A:36:ASN:HD21	1:A:39:GLU:HG2	1.56	0.70
1:C:36:ASN:HD21	1:C:39:GLU:HG2	1.56	0.70
3:z:151:ILE:HD11	3:z:152:TYR:CZ	2.26	0.70
2:AG:4:LEU:HD11	3:AH:3:ASP:CB	2.20	0.70
6:AG:201:CYC:HMA1	6:AG:201:CYC:NB	2.06	0.70
3:j:151:ILE:HD11	3:j:152:TYR:CZ	2.26	0.70
3:0:151:ILE:HD11	3:0:152:TYR:CZ	2.26	0.70
3:l:151:ILE:HD11	3:l:152:TYR:CZ	2.26	0.70
3:AF:160:LEU:HD23	3:AF:160:LEU:C	2.16	0.70
3:AV:151:ILE:HD11	3:AV:152:TYR:CZ	2.25	0.70
2:G:83:ARG:NH1	6:G:201:CYC:O1A	2.24	0.70
2:Q:81:CYS:HA	6:Q:201:CYC:CHD	2.21	0.70
3:h:151:ILE:HD11	3:h:152:TYR:CZ	2.26	0.70
2:t:49:ARG:NH1	2:t:140:LEU:HD21	2.06	0.70
2:AE:35:ARG:O	2:AE:38:ARG:CG	2.38	0.70
2:e:83:ARG:NH1	6:e:201:CYC:O1A	2.21	0.70
1:C:194:CYS:HB3	6:C:2101:CYC:HAC2	1.72	0.70
3:AT:1:MET:HG2	3:AT:103:ILE:HD12	1.72	0.70
1:C:649:PHE:CZ	3:f:87:TYR:CE2	2.80	0.70
1:C:816:ARG:HH12	2:AU:9:VAL:HG12	1.56	0.70
2:r:60:GLN:NE2	2:7:69:GLY:HA3	2.06	0.70
2:AO:102:THR:CG2	2:AO:103:PRO:HD3	2.20	0.70
3:AR:151:ILE:HD11	3:AR:152:TYR:CZ	2.26	0.70
1:A:557:VAL:O	2:9:106:GLU:HG3	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:ARG:HH12	2:AI:9:VAL:HG12	1.56	0.70
1:C:346:GLU:OE1	1:C:347:PHE:CE1	2.45	0.70
2:E:161:GLN:HG2	3:H:49:THR:HG21	1.73	0.70
2:c:116:TYR:CD1	2:c:121:THR:OG1	2.44	0.70
2:g:102:THR:CG2	2:g:103:PRO:HD3	2.21	0.70
4:u:81:CYS:HB3	6:u:201:CYC:HBC2	1.74	0.70
1:A:372:ARG:NH1	6:x:201:CYC:O1A	2.25	0.70
1:C:875:LEU:HD12	1:C:876:TYR:N	2.07	0.70
3:h:50:THR:HG22	3:h:54:GLU:OE1	1.91	0.70
2:k:58:LEU:C	2:k:58:LEU:HD12	2.16	0.70
1:A:319:ALA:O	1:A:320:GLU:CG	2.37	0.69
1:C:541:THR:O	5:Ab:24:GLN:HG3	1.91	0.69
2:r:16:ARG:HH12	2:r:19:SER:HB2	1.56	0.69
2:AK:131:ARG:NH2	2:AK:157:VAL:HG11	2.03	0.69
3:AN:106:GLU:CD	3:AN:107:ARG:HH21	2.00	0.69
2:9:49:ARG:HH21	2:9:140:LEU:CD2	2.05	0.69
3:AF:151:ILE:HD11	3:AF:152:TYR:CZ	2.26	0.69
3:AX:14:VAL:CG1	5:Ad:64:ASN:HD21	2.06	0.69
1:A:642:ARG:NH2	6:6:201:CYC:O1A	2.25	0.69
1:A:976:ARG:O	1:A:977:GLN:CG	2.37	0.69
2:m:4:LEU:CD1	2:m:29:PHE:CE2	2.76	0.69
2:AG:19:SER:OG	2:AG:20:PRO:HD2	1.92	0.69
3:h:14:VAL:HG21	4:s:161:GLN:CG	2.19	0.69
3:v:161:SER:O	3:6:155:TYR:CE1	2.45	0.69
6:AS:201:CYC:HMA1	6:AS:201:CYC:NB	2.07	0.69
2:AU:116:TYR:HD1	2:AU:121:THR:HG21	1.51	0.69
1:A:649:PHE:CZ	3:6:87:TYR:CE2	2.80	0.69
1:A:695:GLY:O	1:A:696:ARG:C	2.34	0.69
3:AL:2:GLN:HE21	3:AL:7:ALA:CA	2.06	0.69
3:AL:10:ASN:OD1	3:AL:11:ASN:N	2.26	0.69
1:A:25:ILE:HG21	3:v:1:MET:HE3	1.74	0.69
3:AB:106:GLU:CD	3:AB:107:ARG:HH21	2.00	0.69
3:AR:87:TYR:CE2	5:Ad:38:PHE:HZ	2.09	0.69
3:AX:10:ASN:OD1	3:AX:11:ASN:N	2.26	0.69
1:A:851:HIS:CE1	3:AJ:83:ARG:NH1	2.61	0.69
4:u:97:VAL:O	4:u:98:ALA:HB3	1.94	0.69
1:C:186:LEU:HD11	6:C:2101:CYC:C4A	2.24	0.68
2:c:2:SER:O	2:c:5:THR:HG22	1.93	0.68
2:c:49:ARG:NH1	2:c:140:LEU:HD21	2.08	0.68
1:A:875:LEU:HD12	1:A:876:TYR:N	2.07	0.68
1:A:1046:ARG:HG2	1:A:1089:LEU:CD2	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:42:THR:CG2	2:k:140:LEU:HD21	2.22	0.68
2:m:140:LEU:HD22	3:AH:140:LEU:HD23	1.75	0.68
2:g:32:SER:O	2:g:35:ARG:HG2	1.93	0.68
2:o:123:ILE:CD1	2:o:124:PRO:HD3	2.24	0.68
2:r:49:ARG:HH21	2:r:140:LEU:CD2	2.02	0.68
6:AG:201:CYC:CGD	3:AJ:62:TYR:HH	2.06	0.68
4:s:81:CYS:CA	6:s:201:CYC:HAC1	2.23	0.68
2:3:19:SER:OG	2:3:20:PRO:HD2	1.93	0.68
2:AS:19:SER:OG	2:AS:20:PRO:HD2	1.92	0.68
1:C:3:ILE:HG21	4:s:110:ASN:HA	1.75	0.68
1:C:344:ARG:O	1:C:345:ARG:HG2	1.93	0.68
3:J:71:MEN:HE21	6:J:201:CYC:HBD2	1.75	0.68
3:AH:2:GLN:HE21	3:AH:7:ALA:CB	2.06	0.68
1:A:823:TYR:O	3:AJ:107:ARG:NH1	2.27	0.68
1:C:695:GLY:O	1:C:698:GLY:N	2.24	0.68
3:L:112:LEU:HD23	3:L:160:LEU:HD21	1.76	0.68
2:W:80:LEU:HD11	3:Z:62:TYR:HE1	1.58	0.68
4:s:97:VAL:O	4:s:98:ALA:HB3	1.93	0.68
3:v:161:SER:C	3:6:101:PRO:HG3	2.17	0.68
3:AL:87:TYR:CG	6:AL:201:CYC:HBB3	2.29	0.68
1:C:1143:LEU:HD12	2:I:106:GLU:HB2	1.75	0.68
6:n:201:CYC:HMA1	6:n:201:CYC:NB	2.09	0.68
2:AU:60:GLN:NE2	2:AU:60:GLN:CA	2.54	0.68
2:o:19:SER:OG	2:o:20:PRO:HD2	1.93	0.68
2:9:123:ILE:N	2:9:124:PRO:HD2	2.09	0.68
3:AH:124:ALA:HB3	3:AT:124:ALA:HB3	1.75	0.68
1:A:40:VAL:CG1	3:v:38:VAL:CG1	2.71	0.67
6:X:201:CYC:HMD1	6:X:201:CYC:HC	1.59	0.67
2:i:4:LEU:HD11	3:j:3:ASP:CB	2.21	0.67
1:A:344:ARG:O	1:A:345:ARG:HG2	1.94	0.67
2:Q:101:VAL:CG1	2:S:20:PRO:HG2	2.24	0.67
3:AX:2:GLN:HE21	3:AX:7:ALA:CA	2.05	0.67
1:C:40:VAL:CG1	3:q:38:VAL:CG1	2.70	0.67
1:C:186:LEU:HD11	6:C:2101:CYC:CHB	2.24	0.67
3:b:112:LEU:HD23	3:b:160:LEU:HD21	1.76	0.67
2:c:19:SER:OG	2:c:20:PRO:HD2	1.94	0.67
2:AC:2:SER:O	2:AC:5:THR:HG22	1.95	0.67
3:AT:2:GLN:HE21	3:AT:7:ALA:CB	2.06	0.67
3:AX:14:VAL:CG1	5:Ad:64:ASN:ND2	2.58	0.67
1:C:54:ILE:HD11	3:q:31:PHE:CE1	2.30	0.67
3:T:83:ARG:HH22	6:T:201:CYC:C1A	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:12:ASP:OD2	3:f:107:ARG:NH1	2.28	0.67
2:k:19:SER:OG	2:k:20:PRO:HD2	1.93	0.67
2:AQ:32:SER:O	2:AQ:35:ARG:HG2	1.94	0.67
1:C:274:MET:HE2	1:C:296:VAL:HG21	1.77	0.67
2:AO:2:SER:O	2:AO:5:THR:HG22	1.95	0.67
1:A:722:ILE:HD11	2:AA:82:LEU:HD12	1.76	0.67
1:C:722:ILE:HD11	2:AM:82:LEU:HD12	1.76	0.67
2:g:47:ARG:HG2	2:g:48:GLU:OE1	1.95	0.67
2:1:27:LYS:HE2	3:2:39:ARG:HH12	1.57	0.67
2:AE:32:SER:O	2:AE:35:ARG:HG2	1.94	0.67
2:AG:2:SER:O	2:AG:5:THR:HG22	1.95	0.67
2:AM:4:LEU:CD2	3:AN:98:ALA:HA	2.25	0.67
1:C:851:HIS:CE1	3:AV:83:ARG:NH1	2.61	0.67
2:w:47:ARG:HG2	2:w:48:GLU:OE1	1.95	0.67
2:y:123:ILE:N	2:y:124:PRO:HD2	2.10	0.67
2:1:29:PHE:HE1	2:1:36:ARG:NH2	1.80	0.67
1:C:875:LEU:HD12	1:C:875:LEU:C	2.20	0.67
2:K:83:ARG:NH1	6:K:201:CYC:O1A	2.26	0.67
2:o:123:ILE:N	2:o:124:PRO:HD2	2.09	0.67
2:AS:2:SER:O	2:AS:5:THR:HG22	1.94	0.67
6:F:201:CYC:HBB2	5:AZ:42:GLN:NE2	2.09	0.67
2:e:2:SER:O	2:e:5:THR:HG22	1.95	0.66
3:l:3:ASP:OD2	3:l:5:ILE:HB	1.95	0.66
4:u:49:GLN:O	4:u:53:LYS:HG2	1.94	0.66
2:w:2:SER:O	2:w:5:THR:HG22	1.95	0.66
6:x:201:CYC:HB	6:x:201:CYC:HMA1	1.58	0.66
3:AH:2:GLN:HE21	3:AH:7:ALA:HA	1.60	0.66
2:AI:41:GLN:OE1	3:AJ:24:LEU:HD11	1.95	0.66
2:AC:16:ARG:HH12	2:AC:19:SER:HB2	1.61	0.66
3:AF:87:TYR:CE2	5:Ac:38:PHE:HZ	2.12	0.66
3:F:49:THR:CG2	2:G:161:GLN:HG2	2.26	0.66
2:S:47:ARG:HD3	3:T:18:TYR:CE1	2.30	0.66
2:g:102:THR:HG23	2:g:103:PRO:CD	2.25	0.66
3:l:91:TYR:HE2	3:l:107:ARG:NE	1.92	0.66
2:1:49:ARG:NH1	2:1:140:LEU:HD21	2.10	0.66
1:A:274:MET:HE2	1:A:296:VAL:HG21	1.77	0.66
2:Q:123:ILE:N	2:Q:124:PRO:HD2	2.10	0.66
2:AO:16:ARG:HH12	2:AO:19:SER:HB2	1.61	0.66
1:A:263:LYS:HE2	1:A:428:VAL:HG12	1.76	0.66
2:r:60:GLN:HE22	2:7:69:GLY:C	2.04	0.66
3:v:161:SER:OXT	3:6:101:PRO:CG	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:201:CYC:HMA3	6:3:201:CYC:NB	2.11	0.66
3:AT:2:GLN:HE21	3:AT:7:ALA:HA	1.60	0.66
1:A:249:SER:CB	1:A:253:ARG:HG3	2.26	0.66
1:A:875:LEU:HD12	1:A:875:LEU:C	2.20	0.66
1:C:1033:ARG:HD3	1:C:1108:GLU:OE2	1.96	0.66
2:M:101:VAL:CG1	2:O:20:PRO:HG2	2.26	0.66
2:M:123:ILE:N	2:M:124:PRO:HD2	2.10	0.66
2:c:123:ILE:N	2:c:124:PRO:HD2	2.10	0.66
2:g:89:LEU:CB	2:g:133:MET:HE1	2.10	0.66
2:AU:41:GLN:OE1	3:AV:24:LEU:HD11	1.95	0.66
1:A:15:ARG:HH12	1:A:22:THR:HG21	1.61	0.66
1:A:200:ILE:HG23	1:A:231:ILE:HD11	1.77	0.66
2:o:34:GLU:OE1	3:p:28:LYS:HG3	1.96	0.66
2:9:49:ARG:HG2	2:9:53:GLN:OE1	1.96	0.66
3:AF:104:LEU:O	3:AF:108:VAL:HG12	1.96	0.66
3:AX:87:TYR:CG	6:AX:201:CYC:HBB3	2.31	0.66
1:A:942:LYS:HG2	1:A:943:THR:HG23	1.77	0.66
1:C:1015:TYR:CD1	1:C:1016:LEU:HD22	2.31	0.66
2:Q:83:ARG:NH1	6:Q:201:CYC:O1A	2.21	0.66
3:f:155:TYR:CE1	3:q:161:SER:O	2.49	0.66
2:o:2:SER:O	2:o:5:THR:HG22	1.96	0.66
2:1:16:ARG:HH12	2:1:19:SER:HB2	1.60	0.66
2:m:4:LEU:CD1	2:m:29:PHE:CD2	2.79	0.66
3:2:110:ASN:HD21	5:Aa:50:LYS:HA	1.61	0.66
2:7:140:LEU:HD22	3:AT:140:LEU:HD23	1.76	0.66
2:AI:116:TYR:CG	2:AI:121:THR:CG2	2.79	0.66
1:A:1015:TYR:CE1	1:A:1016:LEU:CD2	2.79	0.66
1:C:148:TYR:OH	6:C:2101:CYC:HAC1	1.96	0.66
1:C:249:SER:CB	1:C:253:ARG:HG3	2.26	0.66
3:d:11:ASN:OD1	3:d:12:TYR:HD1	1.79	0.66
1:A:1033:ARG:HD3	1:A:1108:GLU:OE2	1.96	0.65
1:C:976:ARG:O	1:C:977:GLN:CG	2.37	0.65
6:R:201:CYC:HB	6:R:201:CYC:CMA	2.09	0.65
4:s:68:THR:HG22	4:s:73:TYR:CE2	2.32	0.65
1:A:1015:TYR:CD1	1:A:1016:LEU:HD22	2.31	0.65
1:C:193:SER:HB3	6:C:2101:CYC:CBD	2.26	0.65
2:AO:102:THR:HG23	2:AO:103:PRO:CD	2.25	0.65
2:k:42:THR:HG22	2:k:140:LEU:CD2	2.26	0.65
2:AA:4:LEU:CD2	3:AB:98:ALA:HA	2.25	0.65
3:z:1:MET:HB3	3:z:106:GLU:OE2	1.97	0.65
1:A:698:GLY:CA	3:x:127:VAL:HG11	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AP:201:CYC:NC	6:AP:201:CYC:HMD1	2.11	0.65
2:AW:5:THR:HG23	3:AX:1:MET:SD	2.37	0.65
1:A:254:PRO:HB3	2:t:12:ASP:OD2	1.97	0.65
1:A:990:ARG:HG2	2:S:110:ILE:HD12	1.79	0.65
1:C:942:LYS:HG2	1:C:943:THR:HG23	1.77	0.65
6:A:2101:CYC:HMA1	6:A:2101:CYC:NB	2.11	0.65
1:C:194:CYS:SG	6:C:2101:CYC:CAC	2.85	0.65
1:C:1015:TYR:CE1	1:C:1016:LEU:CD2	2.79	0.65
2:AC:102:THR:HG23	2:AC:103:PRO:CD	2.25	0.65
1:A:824:PRO:HB3	3:AJ:107:ARG:O	1.97	0.65
6:d:201:CYC:HHA	6:d:201:CYC:HBA2	1.79	0.65
2:r:60:GLN:HE22	2:7:69:GLY:HA3	1.61	0.65
3:AR:104:LEU:O	3:AR:108:VAL:HG12	1.96	0.65
6:AW:201:CYC:CMA	6:AW:201:CYC:HB	2.10	0.65
3:Z:71:MEN:HE21	6:Z:201:CYC:HBD2	1.78	0.65
6:AK:201:CYC:HB	6:AK:201:CYC:CMA	2.10	0.65
1:C:430:ALA:O	1:C:431:GLN:HB2	1.97	0.65
3:T:76:ARG:HB2	2:U:110:ILE:HG13	1.78	0.65
2:o:32:SER:O	2:o:35:ARG:HG2	1.97	0.65
2:1:4:LEU:HD11	3:2:3:ASP:CB	2.24	0.65
1:C:190:LEU:HA	1:C:193:SER:OG	1.98	0.64
1:C:386:ILE:HG22	1:C:395:SER:O	1.97	0.64
6:V:201:CYC:HB	6:V:201:CYC:CMA	2.10	0.64
2:k:12:ASP:OD2	3:l:107:ARG:NE	2.30	0.64
2:y:32:SER:O	2:y:35:ARG:HG2	1.98	0.64
1:C:824:PRO:HB3	3:AV:107:ARG:O	1.97	0.64
2:3:32:SER:O	2:3:35:ARG:HG2	1.97	0.64
3:0:83:ARG:HD2	5:Aa:18:ARG:O	1.97	0.64
1:A:581:TYR:HB3	2:5:114:GLU:OE2	1.97	0.64
3:AD:24:LEU:HA	3:AD:27:LEU:HG	1.80	0.64
6:AS:201:CYC:CGD	3:AV:62:TYR:HH	2.10	0.64
1:C:457:THR:O	1:C:461:ASP:HB2	1.97	0.64
4:u:71:ASN:O	4:u:77:ARG:HB3	1.97	0.64
2:AC:102:THR:CG2	2:AC:103:PRO:CD	2.76	0.64
3:AH:2:GLN:HE21	3:AH:7:ALA:CA	2.11	0.64
2:AO:102:THR:CG2	2:AO:103:PRO:CD	2.76	0.64
1:A:344:ARG:CZ	2:w:9:VAL:CG1	2.75	0.64
1:C:698:GLY:CA	3:p:127:VAL:CG1	2.76	0.64
2:O:47:ARG:HD3	3:P:18:TYR:CE1	2.32	0.64
3:b:10:ASN:OD1	3:b:11:ASN:N	2.31	0.64
2:r:130:VAL:HG21	2:r:160:MET:HE1	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AX:14:VAL:HG12	5:Ad:64:ASN:ND2	2.12	0.64
1:A:191:GLU:HG3	1:A:192:LYS:H	1.61	0.64
1:C:307:ARG:HH22	1:C:346:GLU:HG3	1.62	0.64
1:C:559:THR:O	1:C:560:VAL:HG22	1.98	0.64
3:V:49:THR:CG2	2:W:161:GLN:HG2	2.26	0.64
2:AA:29:PHE:CE1	2:AA:36:ARG:NH2	2.65	0.64
2:AK:5:THR:HG23	3:AL:1:MET:SD	2.37	0.64
1:A:698:GLY:CA	3:x:127:VAL:CG1	2.75	0.64
1:A:816:ARG:HH12	2:AI:9:VAL:CG1	2.11	0.64
1:C:483:PHE:HE1	3:n:87:TYR:CE2	2.16	0.64
1:A:254:PRO:CB	4:u:91:TYR:OH	2.45	0.64
3:AD:24:LEU:C	3:AD:27:LEU:HG	2.23	0.64
2:AU:116:TYR:CG	2:AU:121:THR:CG2	2.79	0.64
1:A:346:GLU:OE1	1:A:347:PHE:CD1	2.51	0.64
4:u:36:LEU:C	4:u:36:LEU:HD12	2.23	0.64
2:7:4:LEU:HD12	2:7:26:ILE:HD13	1.79	0.64
3:f:64:ASP:OD2	4:s:122:PRO:HB3	1.99	0.63
2:5:83:ARG:NH1	6:5:201:CYC:O1A	2.25	0.63
2:AM:29:PHE:CE1	2:AM:36:ARG:NH2	2.65	0.63
1:A:54:ILE:HD11	3:v:31:PHE:CE1	2.33	0.63
1:C:15:ARG:HH12	1:C:22:THR:HG21	1.61	0.63
1:C:698:GLY:CA	3:p:127:VAL:HG11	2.27	0.63
2:g:102:THR:CG2	2:g:103:PRO:CD	2.76	0.63
4:s:36:LEU:C	4:s:36:LEU:HD12	2.24	0.63
3:x:64:ASP:OD2	3:z:122:PRO:HB2	1.98	0.63
1:A:559:THR:O	1:A:560:VAL:HG22	1.98	0.63
2:c:32:SER:O	2:c:35:ARG:HG2	1.98	0.63
3:f:101:PRO:HG3	3:q:161:SER:C	2.21	0.63
3:l:103:ILE:CD1	3:l:107:ARG:NH2	2.49	0.63
2:9:89:LEU:CB	2:9:133:MET:HE1	2.10	0.63
3:AP:24:LEU:C	3:AP:27:LEU:HG	2.23	0.63
1:A:457:THR:O	1:A:461:ASP:HB2	1.97	0.63
6:I:201:CYC:HMA3	6:I:201:CYC:HB	1.63	0.63
1:A:47:PHE:HE2	3:v:38:VAL:CG2	2.11	0.63
3:v:112:LEU:HD23	3:v:160:LEU:HD21	1.81	0.63
2:AI:116:TYR:HD1	2:AI:121:THR:HG21	1.51	0.63
3:AP:24:LEU:HA	3:AP:27:LEU:HG	1.80	0.63
1:A:547:ARG:HG2	3:0:106:GLU:HA	1.80	0.63
1:C:254:PRO:HB3	2:r:12:ASP:OD2	1.99	0.63
1:C:344:ARG:CZ	2:o:9:VAL:CG1	2.76	0.63
3:j:110:ASN:HD21	5:Ab:50:LYS:HA	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:z:53:LYS:HE3	2:7:118:SER:O	1.98	0.63
1:C:1140:TRP:CZ2	2:I:110:ILE:HD12	2.34	0.63
1:C:1153:VAL:HG13	3:N:63:SER:HB2	1.79	0.63
2:AC:14:GLU:OE1	2:AC:16:ARG:CD	2.46	0.63
3:AT:2:GLN:HE21	3:AT:7:ALA:CA	2.11	0.63
1:A:15:ARG:NH1	1:A:22:THR:HG21	2.14	0.63
1:C:700:SER:O	1:C:701:ASP:CB	2.47	0.63
1:A:706:PRO:HG3	3:z:65:LEU:CD1	2.29	0.63
3:AR:88:PHE:HB3	3:AR:156:LEU:HD21	1.79	0.63
3:AX:2:GLN:NE2	3:AX:7:ALA:HA	2.14	0.63
1:C:466:LEU:C	1:C:466:LEU:HD12	2.24	0.62
1:C:820:HIS:HD2	1:C:859:ILE:HD12	1.64	0.62
2:i:131:ARG:HH21	2:i:134:LYS:HE2	1.64	0.62
1:A:256:LEU:N	1:A:256:LEU:HD12	2.15	0.62
1:C:581:TYR:HB3	2:e:114:GLU:OE2	1.98	0.62
2:c:89:LEU:CB	2:c:133:MET:HE1	2.10	0.62
2:m:140:LEU:HD22	3:AH:140:LEU:CD2	2.29	0.62
2:AW:4:LEU:HD13	3:AX:98:ALA:HA	1.82	0.62
1:C:547:ARG:HG2	3:l:106:GLU:HA	1.80	0.62
1:C:816:ARG:HH12	2:AU:9:VAL:CG1	2.11	0.62
3:AL:10:ASN:HA	5:Ac:64:ASN:HD21	1.65	0.62
6:c:201:CYC:HB	6:c:201:CYC:CMA	2.12	0.62
3:2:76:ARG:HB2	2:3:110:ILE:HG13	1.80	0.62
3:AF:88:PHE:HB3	3:AF:156:LEU:HD21	1.79	0.62
6:AN:201:CYC:CMD	6:AN:201:CYC:HC	2.12	0.62
1:A:466:LEU:C	1:A:466:LEU:HD12	2.24	0.62
2:AA:4:LEU:HD21	3:AB:98:ALA:CA	2.30	0.62
2:t:4:LEU:HD23	2:t:26:ILE:HG23	1.80	0.62
4:u:81:CYS:HA	6:u:201:CYC:HAC2	1.82	0.62
1:C:194:CYS:SG	6:C:2101:CYC:HAC1	2.39	0.62
1:C:509:LEU:HD12	1:C:640:TYR:CE1	2.34	0.62
2:E:20:PRO:CG	2:G:101:VAL:CG1	2.77	0.62
2:k:55:GLY:O	2:k:58:LEU:HG	1.98	0.62
2:AK:4:LEU:HD13	3:AL:98:ALA:HA	1.82	0.62
3:AR:87:TYR:HE2	5:Ad:38:PHE:CZ	2.18	0.62
1:A:54:ILE:HD13	3:v:28:LYS:CG	2.29	0.62
1:A:509:LEU:HD12	1:A:640:TYR:CE1	2.34	0.62
1:A:895:PRO:HG3	3:AH:115:THR:OG1	2.00	0.62
1:C:823:TYR:O	3:AV:107:ARG:NH1	2.31	0.62
2:U:20:PRO:CG	2:W:101:VAL:CG1	2.78	0.62
1:A:700:SER:O	1:A:701:ASP:CB	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:HIS:HD2	1:A:859:ILE:HD12	1.64	0.62
1:C:319:ALA:O	1:C:320:GLU:CG	2.37	0.62
1:C:875:LEU:HD11	1:C:876:TYR:CD2	2.34	0.62
3:V:76:ARG:HB2	2:a:110:ILE:HG13	1.82	0.62
6:V:201:CYC:HBB2	5:AY:42:GLN:NE2	2.15	0.62
6:s:201:CYC:HMD1	6:s:201:CYC:NC	2.14	0.62
3:O:87:TYR:HE1	5:Aa:19:THR:O	1.83	0.62
1:A:695:GLY:O	1:A:698:GLY:N	2.24	0.62
1:C:344:ARG:HH12	2:o:9:VAL:CG1	2.13	0.62
3:T:81:CYS:HA	6:T:201:CYC:CHD	2.29	0.62
1:A:367:ARG:HH21	1:A:370:GLU:HG2	1.65	0.61
2:M:81:CYS:HA	6:M:201:CYC:HHD	1.81	0.61
3:AF:87:TYR:HD1	3:AF:90:ARG:HH21	1.48	0.61
2:AG:112:VAL:CG2	2:AG:160:MET:HE1	2.19	0.61
1:A:1143:LEU:HD12	2:Y:106:GLU:HB2	1.83	0.61
3:h:50:THR:HG22	3:h:54:GLU:OE2	1.99	0.61
3:AL:2:GLN:NE2	3:AL:7:ALA:HA	2.14	0.61
1:A:370:GLU:N	1:A:374:GLU:OE2	2.31	0.61
1:A:1043:GLU:HA	1:A:1046:ARG:HE	1.65	0.61
1:C:367:ARG:HH21	1:C:370:GLU:HG2	1.65	0.61
2:c:149:ALA:O	2:c:153:PHE:HD2	1.82	0.61
2:e:4:LEU:HD11	3:f:3:ASP:HB3	1.81	0.61
2:k:156:LEU:HG	2:k:160:MET:HE3	1.81	0.61
2:y:89:LEU:CB	2:y:133:MET:HE1	2.10	0.61
3:z:1:MET:CA	3:z:106:GLU:OE2	2.49	0.61
1:C:706:PRO:HG3	3:h:65:LEU:CD1	2.29	0.61
1:A:875:LEU:HD11	1:A:876:TYR:CD2	2.34	0.61
2:c:109:ILE:HD11	2:c:156:LEU:HD23	1.81	0.61
2:1:34:GLU:OE2	3:2:31:PHE:HB3	1.99	0.61
6:AB:201:CYC:HC	6:AB:201:CYC:CMD	2.13	0.61
1:C:433:SER:HA	4:s:115:THR:HG21	1.83	0.61
2:AM:4:LEU:HD21	3:AN:98:ALA:CA	2.30	0.61
3:AR:87:TYR:HD1	3:AR:90:ARG:HH21	1.48	0.61
1:C:1088:GLY:HA2	2:I:13:ALA:O	2.01	0.61
1:A:1152:TYR:OH	2:AO:63:PRO:HG3	2.00	0.61
1:C:47:PHE:HE2	3:q:38:VAL:CG2	2.12	0.61
6:F:201:CYC:HB	6:F:201:CYC:CMA	2.11	0.61
6:U:201:CYC:CMD	6:U:201:CYC:HC	2.13	0.61
2:a:83:ARG:NH1	6:a:201:CYC:O1A	2.33	0.61
2:k:4:LEU:HD11	3:l:3:ASP:HB2	1.81	0.61
6:p:201:CYC:HB	6:p:201:CYC:HMA1	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ALA:O	1:A:431:GLN:HB2	2.01	0.61
1:C:11:VAL:O	1:C:11:VAL:HG13	2.01	0.61
3:T:74:THR:HG22	2:U:107:ILE:HG23	1.83	0.61
2:i:89:LEU:HB3	3:j:18:TYR:OH	2.01	0.61
2:r:60:GLN:CD	2:7:69:GLY:HA3	2.26	0.61
1:A:11:VAL:O	1:A:11:VAL:HG13	2.00	0.61
1:A:76:PHE:HB3	1:A:145:ILE:HG13	1.83	0.61
3:AX:1:MET:HG2	3:AX:103:ILE:HD12	1.83	0.61
1:C:15:ARG:NH1	1:C:22:THR:HG21	2.14	0.60
1:C:895:PRO:HG3	3:AT:115:THR:OG1	2.00	0.60
3:F:29:ALA:O	3:F:32:THR:CG2	2.49	0.60
4:u:72:MET:HE2	6:u:201:CYC:H2C	1.83	0.60
2:w:81:CYS:HA	6:w:201:CYC:HHD	1.82	0.60
2:o:123:ILE:HG13	2:o:124:PRO:HD3	1.82	0.60
2:AG:2:SER:OG	2:AG:4:LEU:HG	2.01	0.60
2:AI:131:ARG:HH21	2:AI:157:VAL:CG1	2.09	0.60
1:C:325:ASN:HB2	1:C:327:GLU:OE1	2.01	0.60
3:F:81:CYS:HA	6:F:201:CYC:HHD	1.82	0.60
2:G:12:ASP:OD2	3:H:107:ARG:NH1	2.33	0.60
6:5:201:CYC:HMA3	6:5:201:CYC:HB	1.66	0.60
2:AK:2:SER:OG	2:AK:4:LEU:HG	2.02	0.60
1:C:344:ARG:HA	1:C:347:PHE:O	2.01	0.60
3:d:10:ASN:ND2	5:Ab:65:THR:HB	2.17	0.60
2:y:37:LEU:HD23	2:y:97:VAL:HG22	1.83	0.60
6:AK:201:CYC:CMD	6:AK:201:CYC:HC	2.14	0.60
2:AS:112:VAL:CG2	2:AS:160:MET:HE1	2.19	0.60
5:Ab:23:LEU:N	5:Ab:24:GLN:OE1	2.34	0.60
1:C:718:MET:HE1	2:AM:79:ALA:HB2	1.84	0.60
2:M:68:PRO:HD3	2:9:61:LYS:HD2	1.84	0.60
4:u:36:LEU:HD12	4:u:37:ARG:N	2.15	0.60
1:A:386:ILE:HG13	1:A:395:SER:HB3	1.82	0.60
1:C:350:PRO:HG2	1:C:351:PHE:CE2	2.37	0.60
1:C:1067:LEU:HD11	1:C:1096:ILE:HG23	1.83	0.60
3:q:25:ASP:CA	3:q:28:LYS:HG2	2.30	0.60
3:2:25:ASP:CA	3:2:28:LYS:HG2	2.29	0.60
2:3:83:ARG:NH1	6:3:201:CYC:O1A	2.22	0.60
6:6:201:CYC:HMA1	6:6:201:CYC:NB	2.16	0.60
6:AW:201:CYC:HC	6:AW:201:CYC:CMD	2.15	0.60
1:C:214:PHE:CE2	1:C:223:VAL:HG21	2.37	0.60
1:C:649:PHE:CZ	3:f:87:TYR:HE2	2.20	0.60
4:s:36:LEU:HD12	4:s:37:ARG:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AA:37:LEU:HD23	2:AA:97:VAL:HG22	1.83	0.60
2:AO:14:GLU:OE1	2:AO:16:ARG:CD	2.46	0.60
2:AU:2:SER:OG	2:AU:4:LEU:HG	2.02	0.60
1:C:166:TYR:HD1	6:C:2101:CYC:HBB1	1.66	0.60
3:F:76:ARG:HB2	2:K:110:ILE:HG13	1.83	0.60
3:AF:25:ASP:CA	3:AF:28:LYS:HG2	2.30	0.60
6:AW:201:CYC:NB	6:AW:201:CYC:HMA3	2.16	0.60
1:A:172:LEU:HD11	3:v:19:LEU:HD22	1.83	0.60
1:A:363:HIS:O	1:A:364:PHE:CG	2.55	0.60
1:A:1067:LEU:HD11	1:A:1096:ILE:HG23	1.83	0.60
1:C:761:ARG:NH1	2:AO:105:GLU:OE2	2.34	0.60
3:F:71:MEN:O	3:F:77:ARG:HD3	2.01	0.60
2:e:80:LEU:CD1	6:e:201:CYC:HAD2	2.32	0.60
6:m:201:CYC:CMD	6:m:201:CYC:HC	2.15	0.60
2:AC:37:LEU:HD23	2:AC:97:VAL:HG22	1.84	0.60
6:AK:201:CYC:NB	6:AK:201:CYC:HMA3	2.16	0.60
2:AW:131:ARG:HH21	2:AW:157:VAL:CG1	2.10	0.60
3:AX:71:MEN:O	3:AX:77:ARG:HD3	2.02	0.60
1:A:1046:ARG:CG	1:A:1089:LEU:HD23	2.24	0.59
1:C:172:LEU:CD1	3:q:19:LEU:HD22	2.32	0.59
3:P:76:ARG:HB2	2:E:110:ILE:HG13	1.83	0.59
2:U:12:ASP:OD2	3:V:107:ARG:NH1	2.34	0.59
2:o:2:SER:OG	2:o:4:LEU:HG	2.02	0.59
2:3:2:SER:OG	2:3:4:LEU:HG	2.02	0.59
3:0:140:LEU:CD2	2:AQ:140:LEU:CD2	2.80	0.59
2:AO:38:ARG:NH2	2:AO:145:ASP:OD2	2.35	0.59
3:AX:2:GLN:HE21	3:AX:7:ALA:CB	2.14	0.59
1:A:228:SER:O	1:A:231:ILE:HG22	2.02	0.59
1:C:363:HIS:O	1:C:364:PHE:CG	2.55	0.59
1:C:430:ALA:O	6:s:201:CYC:O2A	2.20	0.59
3:X:29:ALA:O	3:X:32:THR:HG23	2.03	0.59
3:AL:1:MET:HG2	3:AL:103:ILE:HD12	1.83	0.59
1:A:214:PHE:CE2	1:A:223:VAL:HG21	2.37	0.59
1:A:325:ASN:HB2	1:A:327:GLU:OE1	2.01	0.59
1:A:394:PRO:HB2	1:A:399:TYR:CE2	2.37	0.59
1:C:76:PHE:HB3	1:C:145:ILE:HG13	1.84	0.59
1:C:254:PRO:HB2	4:s:91:TYR:OH	2.01	0.59
1:C:1152:TYR:OH	2:AC:63:PRO:HG3	2.01	0.59
3:V:29:ALA:O	3:V:32:THR:CG2	2.50	0.59
6:Y:201:CYC:HMA3	6:Y:201:CYC:HB	1.66	0.59
3:AL:2:GLN:HE21	3:AL:7:ALA:CB	2.14	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:ILE:HD13	1:C:222:LEU:HD21	1.85	0.59
1:C:228:SER:O	1:C:231:ILE:HG22	2.02	0.59
1:C:398:LEU:HD12	1:C:398:LEU:C	2.27	0.59
3:h:112:LEU:HD23	3:h:160:LEU:HD21	1.84	0.59
2:y:2:SER:OG	2:y:4:LEU:HG	2.02	0.59
1:A:398:LEU:C	1:A:398:LEU:HD12	2.27	0.59
3:f:53:LYS:CD	2:g:120:GLN:OE1	2.51	0.59
2:5:2:SER:OG	2:5:4:LEU:HG	2.02	0.59
1:A:261:ILE:CD1	4:u:76:ARG:HA	2.33	0.59
1:A:307:ARG:HH22	1:A:346:GLU:HG3	1.67	0.59
1:C:370:GLU:N	1:C:374:GLU:OE2	2.31	0.59
3:l:91:TYR:HE2	3:l:107:ARG:NH2	2.00	0.59
3:q:67:ARG:HG3	3:q:68:PRO:HD2	1.83	0.59
2:r:4:LEU:HD23	2:r:26:ILE:HG23	1.84	0.59
2:w:2:SER:OG	2:w:4:LEU:HG	2.02	0.59
3:AN:78:TYR:CD2	2:AU:115:MET:HG3	2.37	0.59
2:AO:37:LEU:HD23	2:AO:97:VAL:HG22	1.84	0.59
1:A:352:ILE:HB	3:x:107:ARG:O	2.02	0.59
3:X:29:ALA:O	3:X:32:THR:CG2	2.51	0.59
2:e:2:SER:OG	2:e:4:LEU:HG	2.02	0.59
3:h:53:LYS:HE3	2:m:118:SER:O	2.01	0.59
2:m:140:LEU:CD2	3:AH:140:LEU:HD21	2.32	0.59
2:9:4:LEU:HD11	3:0:3:ASP:HB3	1.84	0.59
3:0:15:GLN:NE2	3:0:17:LYS:HD3	2.18	0.59
2:AS:2:SER:OG	2:AS:4:LEU:HG	2.01	0.59
1:C:347:PHE:O	1:C:348:TYR:HB3	2.01	0.59
1:C:394:PRO:HB2	1:C:399:TYR:CE2	2.37	0.59
1:C:459:PHE:O	1:C:460:ALA:CB	2.50	0.59
3:V:71:MEN:O	3:V:77:ARG:HD3	2.01	0.59
2:3:20:PRO:CG	2:5:101:VAL:CG1	2.81	0.59
1:A:293:LYS:O	1:A:294:GLU:HB3	2.02	0.59
1:A:1008:PHE:CZ	3:R:83:ARG:NH1	2.70	0.59
1:C:890:PRO:O	1:C:891:ALA:HB2	2.02	0.59
6:AK:201:CYC:HB	6:AK:201:CYC:HMA3	1.68	0.59
3:AL:71:MEN:O	3:AL:77:ARG:HD3	2.02	0.59
3:AR:25:ASP:CA	3:AR:28:LYS:HG2	2.30	0.59
1:A:11:VAL:HG11	3:6:161:SER:CB	2.33	0.59
1:A:56:ILE:HD13	1:A:222:LEU:HD21	1.85	0.59
2:M:68:PRO:CD	2:9:61:LYS:HD2	2.33	0.59
3:l:132:ALA:O	3:l:135:GLU:HG2	2.03	0.59
3:AT:2:GLN:HE21	3:AT:7:ALA:HB2	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AC:201:CYC:HB	6:AC:201:CYC:HMA3	1.68	0.58
1:A:855:GLY:O	1:A:856:ARG:HG2	2.03	0.58
3:R:115:THR:HG21	6:R:201:CYC:CMA	2.33	0.58
3:8:71:MEN:O	3:8:77:ARG:HD3	2.03	0.58
6:AN:201:CYC:HC	6:AN:201:CYC:HMD3	1.68	0.58
1:A:890:PRO:O	1:A:891:ALA:HB2	2.02	0.58
1:C:888:THR:O	1:C:889:LEU:HB2	2.03	0.58
1:C:974:LEU:HD13	3:N:1:MET:H1	1.68	0.58
2:o:37:LEU:HD23	2:o:97:VAL:HG22	1.85	0.58
2:9:83:ARG:NH1	6:9:201:CYC:O1A	2.29	0.58
3:AB:78:TYR:CD2	2:AI:115:MET:HG3	2.37	0.58
2:AM:37:LEU:HD23	2:AM:97:VAL:HG22	1.83	0.58
2:AW:2:SER:OG	2:AW:4:LEU:HG	2.02	0.58
2:E:151:PHE:HB3	2:G:20:PRO:HB3	1.85	0.58
2:G:115:MET:HG3	3:J:78:TYR:CD2	2.39	0.58
3:H:29:ALA:O	3:H:32:THR:HG23	2.03	0.58
2:c:109:ILE:O	2:c:109:ILE:HG22	2.02	0.58
2:g:156:LEU:HD23	2:g:156:LEU:C	2.27	0.58
2:m:4:LEU:HD13	2:m:29:PHE:CE2	2.38	0.58
3:z:112:LEU:HD23	3:z:160:LEU:HD21	1.84	0.58
6:7:201:CYC:HC	6:7:201:CYC:CMD	2.16	0.58
2:AI:2:SER:OG	2:AI:4:LEU:HG	2.02	0.58
3:AJ:126:THR:HB	3:AJ:160:LEU:HD21	1.86	0.58
3:AT:112:LEU:HD23	3:AT:160:LEU:HD21	1.85	0.58
1:A:718:MET:HE1	2:AA:79:ALA:HB2	1.84	0.58
2:k:48:GLU:O	2:k:51:VAL:HG12	2.03	0.58
4:u:122:PRO:HB3	3:6:64:ASP:OD2	2.04	0.58
2:AC:38:ARG:NH2	2:AC:145:ASP:OD2	2.35	0.58
1:A:255:GLY:C	1:A:256:LEU:HD12	2.28	0.58
1:A:276:ALA:HA	1:A:286:VAL:HG22	1.86	0.58
1:C:293:LYS:O	1:C:294:GLU:HB3	2.02	0.58
2:c:109:ILE:HG23	2:c:159:ALA:HB1	1.86	0.58
2:AE:37:LEU:HD23	2:AE:97:VAL:HG22	1.86	0.58
3:AH:2:GLN:HE21	3:AH:7:ALA:HB2	1.68	0.58
5:Ad:3:ARG:HG2	5:Ad:59:GLY:HA3	1.85	0.58
2:y:102:THR:HG23	2:y:103:PRO:CD	2.28	0.58
2:1:29:PHE:CD1	2:1:36:ARG:NH2	2.71	0.58
3:2:105:ASP:HA	3:2:109:LEU:HB2	1.84	0.58
2:AA:4:LEU:HD23	2:AA:8:ILE:HD12	1.86	0.58
2:AI:131:ARG:NH2	2:AI:157:VAL:CG1	2.66	0.58
1:C:3:ILE:HG22	4:s:110:ASN:OD1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:76:ARG:HB3	2:m:110:ILE:HG13	1.86	0.58
3:n:71:MEN:O	3:n:77:ARG:HD3	2.04	0.58
2:1:89:LEU:HB3	3:2:18:TYR:OH	2.03	0.58
3:4:105:ASP:HA	3:4:109:LEU:HB2	1.86	0.58
3:AH:112:LEU:HD23	3:AH:160:LEU:HD21	1.86	0.58
1:A:172:LEU:CD1	3:v:19:LEU:HD22	2.33	0.58
3:H:29:ALA:O	3:H:32:THR:CG2	2.51	0.58
3:q:67:ARG:CG	3:q:68:PRO:HD2	2.33	0.58
3:q:126:THR:HB	3:q:160:LEU:HD21	1.86	0.58
3:AB:71:MEN:O	3:AB:77:ARG:HD3	2.04	0.58
6:AH:201:CYC:HB	6:AH:201:CYC:HMA1	1.69	0.58
1:A:31:GLU:OE1	1:A:295:ARG:HD2	2.04	0.58
6:AB:201:CYC:HC	6:AB:201:CYC:HMD3	1.68	0.58
6:AW:201:CYC:HB	6:AW:201:CYC:HMA3	1.68	0.58
1:A:3:ILE:HG22	4:u:110:ASN:OD1	2.04	0.57
1:C:287:ASN:O	1:C:287:ASN:OD1	2.22	0.57
2:M:68:PRO:HG2	2:9:61:LYS:CE	2.34	0.57
2:W:115:MET:HG3	3:Z:78:TYR:CD2	2.39	0.57
2:c:20:PRO:CG	2:e:101:VAL:CG1	2.80	0.57
3:d:105:ASP:HA	3:d:109:LEU:HB2	1.86	0.57
2:g:118:SER:O	2:g:120:GLN:NE2	2.37	0.57
2:m:27:LYS:HZ1	3:n:39:ARG:HH12	1.52	0.57
3:AJ:11:ASN:C	3:AJ:11:ASN:OD1	2.46	0.57
3:AL:110:ASN:ND2	5:Ac:57:PHE:CD1	2.71	0.57
2:AU:131:ARG:NH2	2:AU:157:VAL:CG1	2.66	0.57
1:A:344:ARG:HA	1:A:347:PHE:O	2.04	0.57
1:A:888:THR:O	1:A:889:LEU:HB2	2.03	0.57
1:C:855:GLY:O	1:C:856:ARG:HG2	2.03	0.57
2:c:92:VAL:HG11	2:c:153:PHE:CZ	2.39	0.57
3:f:53:LYS:HD3	2:g:120:GLN:OE1	2.04	0.57
3:f:136:VAL:O	3:f:140:LEU:HD13	2.04	0.57
3:AL:2:GLN:NE2	3:AL:10:ASN:HD21	2.02	0.57
1:C:820:HIS:CD2	1:C:859:ILE:HD12	2.39	0.57
2:S:47:ARG:HD3	3:T:18:TYR:CZ	2.39	0.57
2:AK:5:THR:OG1	3:AL:3:ASP:OD2	2.22	0.57
3:AV:126:THR:HB	3:AV:160:LEU:HD21	1.86	0.57
2:AW:131:ARG:NH2	2:AW:157:VAL:CG1	2.67	0.57
3:P:74:THR:HG22	2:E:107:ILE:HG23	1.85	0.57
3:l:87:TYR:HE1	5:Ab:19:THR:O	1.86	0.57
4:u:105:ASP:OD1	4:u:106:GLU:N	2.37	0.57
2:y:131:ARG:HB2	2:y:131:ARG:HH11	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:y:201:CYC:O2D	3:6:62:TYR:OH	2.22	0.57
1:A:254:PRO:O	1:A:256:LEU:CD1	2.51	0.57
2:M:68:PRO:CG	2:9:61:LYS:HD2	2.33	0.57
2:c:83:ARG:NH2	6:c:201:CYC:O1A	2.37	0.57
2:k:107:ILE:CD1	3:l:13:ASP:OD2	2.51	0.57
2:m:27:LYS:CE	3:n:39:ARG:NH1	2.68	0.57
2:o:85:LEU:HD22	2:o:133:MET:HE2	1.87	0.57
2:3:16:ARG:NH2	2:5:155:TYR:CE1	2.73	0.57
2:AK:131:ARG:NH2	2:AK:157:VAL:CG1	2.67	0.57
3:AV:11:ASN:C	3:AV:11:ASN:OD1	2.46	0.57
1:C:889:LEU:CB	1:C:890:PRO:HD3	2.35	0.57
1:C:1140:TRP:CZ2	2:I:110:ILE:CD1	2.88	0.57
3:V:81:CYS:HA	6:V:201:CYC:HHD	1.87	0.57
2:m:4:LEU:HD13	2:m:29:PHE:HE2	1.69	0.57
2:9:37:LEU:HD22	3:0:24:LEU:CD2	2.31	0.57
1:A:53:ARG:HA	1:A:56:ILE:HD12	1.87	0.57
1:A:244:ASP:HB3	1:A:258:LEU:O	2.04	0.57
1:A:820:HIS:CD2	1:A:859:ILE:HD12	2.39	0.57
1:C:1121:ALA:HB2	3:H:107:ARG:O	2.03	0.57
6:R:201:CYC:HB	6:R:201:CYC:HMA2	1.69	0.57
3:d:25:ASP:CA	3:d:28:LYS:HG2	2.29	0.57
2:m:48:GLU:HG2	2:m:49:ARG:N	2.19	0.57
2:AA:29:PHE:CE1	2:AA:36:ARG:NH1	2.73	0.57
1:C:172:LEU:HD11	3:q:19:LEU:HD22	1.85	0.57
2:AM:115:MET:HG3	3:AT:78:TYR:CD2	2.40	0.57
1:A:649:PHE:CZ	3:6:87:TYR:HE2	2.20	0.57
1:C:276:ALA:HA	1:C:286:VAL:HG22	1.86	0.57
3:l:2:GLN:N	3:l:102:SER:HG	2.02	0.57
3:l:140:LEU:CD2	2:AE:140:LEU:CD2	2.83	0.57
6:AR:201:CYC:HB	6:AR:201:CYC:CMA	2.17	0.57
6:AT:201:CYC:HMA1	6:AT:201:CYC:HB	1.69	0.57
1:A:274:MET:HE2	1:A:296:VAL:CG2	2.35	0.57
1:C:702:VAL:O	1:C:702:VAL:HG12	2.04	0.57
6:c:201:CYC:HMA3	6:c:201:CYC:NB	2.18	0.57
4:u:72:MET:HE1	6:u:201:CYC:HBC2	1.86	0.57
3:6:136:VAL:O	3:6:140:LEU:HD13	2.04	0.57
2:AQ:37:LEU:HD23	2:AQ:97:VAL:HG22	1.85	0.57
5:AY:3:ARG:HG2	5:AY:59:GLY:HA3	1.86	0.57
1:A:345:ARG:HA	1:A:349:GLN:HB3	1.86	0.56
1:C:1109:ASP:CG	5:AZ:25:ASN:OD1	2.48	0.56
2:y:80:LEU:HD13	6:y:201:CYC:HAD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AR:107:ARG:HA	5:Ad:45:GLN:HG2	1.86	0.56
3:AX:2:GLN:NE2	3:AX:10:ASN:HD21	2.02	0.56
1:A:702:VAL:O	1:A:702:VAL:HG12	2.05	0.56
1:C:532:THR:CG2	2:m:102:THR:HG23	2.28	0.56
2:o:123:ILE:HG13	2:o:124:PRO:CD	2.35	0.56
2:9:37:LEU:HD23	2:9:97:VAL:HG22	1.86	0.56
2:AA:115:MET:HG3	3:AH:78:TYR:CD2	2.40	0.56
2:AM:4:LEU:HD23	2:AM:8:ILE:HD12	1.86	0.56
2:AM:29:PHE:HD1	2:AM:36:ARG:NH1	2.00	0.56
1:A:429:GLU:O	1:A:430:ALA:HB3	2.05	0.56
1:A:601:LYS:HE2	1:A:670:TYR:CE1	2.40	0.56
1:C:169:TYR:HE1	3:q:19:LEU:CD1	2.19	0.56
1:C:601:LYS:HE2	1:C:670:TYR:CE1	2.40	0.56
2:O:47:ARG:HD3	3:P:18:TYR:CZ	2.40	0.56
2:Q:101:VAL:HG13	2:S:20:PRO:HG2	1.87	0.56
3:l:71:MEN:O	3:l:77:ARG:HD3	2.04	0.56
6:5:201:CYC:HB	6:5:201:CYC:CMA	2.19	0.56
2:7:140:LEU:CD2	3:AT:140:LEU:HD21	2.32	0.56
2:9:4:LEU:HD11	3:0:3:ASP:CB	2.36	0.56
2:AO:4:LEU:HD12	2:AO:5:THR:N	2.20	0.56
1:A:344:ARG:HH12	2:w:9:VAL:CG1	2.15	0.56
1:C:244:ASP:HB3	1:C:258:LEU:O	2.06	0.56
4:s:80:ALA:O	4:s:83:ARG:HG3	2.05	0.56
2:y:5:THR:OG1	3:z:3:ASP:OD2	2.22	0.56
3:AF:87:TYR:HE2	5:Ac:38:PHE:CZ	2.20	0.56
3:AV:24:LEU:O	3:AV:28:LYS:HG3	2.06	0.56
1:A:246:VAL:HG23	1:A:256:LEU:O	2.05	0.56
1:A:646:ASN:HB2	6:6:201:CYC:O2A	2.05	0.56
1:A:889:LEU:CB	1:A:890:PRO:HD3	2.35	0.56
1:C:274:MET:HE2	1:C:296:VAL:CG2	2.35	0.56
1:C:320:GLU:O	1:C:324:LYS:HG2	2.06	0.56
2:U:20:PRO:HB3	2:W:151:PHE:HB3	1.88	0.56
3:p:71:MEN:O	3:p:77:ARG:HD3	2.05	0.56
3:4:83:ARG:NH2	6:4:201:CYC:O1A	2.39	0.56
3:0:67:ARG:HG3	3:0:68:PRO:HD2	1.87	0.56
3:AN:71:MEN:O	3:AN:77:ARG:HD3	2.04	0.56
1:A:287:ASN:OD1	1:A:287:ASN:O	2.22	0.56
3:N:87:TYR:CE1	3:N:91:TYR:CE1	2.91	0.56
2:O:115:MET:HG3	3:L:78:TYR:CD2	2.41	0.56
2:g:4:LEU:HD11	3:h:3:ASP:HB3	1.86	0.56
2:7:4:LEU:HD13	2:7:26:ILE:HD13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AH:2:GLN:NE2	3:AH:7:ALA:HA	2.21	0.56
6:AO:201:CYC:HMA3	6:AO:201:CYC:HB	1.70	0.56
2:AW:134:LYS:HE2	2:AW:150:GLY:HA2	1.87	0.56
1:A:640:TYR:N	1:A:644:GLU:OE2	2.35	0.56
1:C:190:LEU:O	1:C:191:GLU:HG2	2.05	0.56
1:C:1033:ARG:HH11	1:C:1097:VAL:HG12	1.71	0.56
2:W:37:LEU:HD22	3:X:24:LEU:HD22	1.87	0.56
4:s:89:LEU:HD13	4:s:133:LEU:HD22	1.87	0.56
3:AL:105:ASP:HA	3:AL:109:LEU:HB2	1.88	0.56
3:AX:105:ASP:HA	3:AX:109:LEU:HB2	1.88	0.56
5:AZ:3:ARG:HG2	5:AZ:59:GLY:HA3	1.87	0.56
1:A:320:GLU:O	1:A:324:LYS:HG2	2.06	0.56
1:C:31:GLU:OE1	1:C:295:ARG:HD2	2.04	0.56
2:U:151:PHE:HB3	2:W:20:PRO:HB3	1.87	0.56
2:m:27:LYS:HE2	3:n:39:ARG:NH1	2.20	0.56
4:u:81:CYS:SG	6:u:201:CYC:NC	2.78	0.56
2:3:4:LEU:HD13	3:4:98:ALA:HA	1.87	0.56
2:3:16:ARG:NH2	2:5:155:TYR:HE1	2.04	0.56
3:4:78:TYR:CD2	2:9:115:MET:HG3	2.41	0.56
2:AI:4:LEU:HD13	3:AJ:98:ALA:HA	1.88	0.56
2:AK:134:LYS:HE2	2:AK:150:GLY:HA2	1.87	0.56
1:C:429:GLU:O	1:C:430:ALA:HB3	2.06	0.56
2:W:119:LEU:O	3:Z:53:LYS:NZ	2.38	0.56
3:4:25:ASP:CA	3:4:28:LYS:HG2	2.29	0.56
1:A:819:PHE:O	1:A:823:TYR:HD2	1.89	0.56
1:C:1117:PRO:O	1:C:1118:THR:CB	2.54	0.56
3:l:91:TYR:HE2	3:l:107:ARG:HH21	1.54	0.56
3:x:71:MEN:O	3:x:77:ARG:HD3	2.05	0.56
2:AG:34:GLU:OE2	2:AG:38:ARG:NH1	2.39	0.56
3:AJ:24:LEU:O	3:AJ:28:LYS:HG3	2.06	0.56
3:V:29:ALA:O	3:V:32:THR:HG23	2.06	0.55
2:g:105:GLU:HA	2:g:109:ILE:HG12	1.88	0.55
2:i:131:ARG:NH2	2:i:134:LYS:CE	2.69	0.55
2:y:61:LYS:HG3	2:y:62:ARG:HG2	1.87	0.55
2:AI:85:LEU:HD22	2:AI:133:MET:HE2	1.87	0.55
2:AU:4:LEU:HD13	3:AV:98:ALA:HA	1.88	0.55
1:A:396:GLY:O	1:A:399:TYR:HB2	2.06	0.55
1:C:3:ILE:CG2	4:s:110:ASN:OD1	2.54	0.55
1:C:396:GLY:O	1:C:399:TYR:HB2	2.06	0.55
2:G:37:LEU:HD22	3:H:24:LEU:HD22	1.88	0.55
3:j:105:ASP:HA	3:j:109:LEU:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:y:4:LEU:HD11	3:z:3:ASP:HB3	1.88	0.55
3:AD:76:ARG:HB2	2:AE:110:ILE:HG13	1.88	0.55
1:A:249:SER:HB2	1:A:253:ARG:O	2.06	0.55
1:A:1033:ARG:HH11	1:A:1097:VAL:HG12	1.71	0.55
2:E:20:PRO:HB3	2:G:151:PHE:HB3	1.88	0.55
2:I:34:GLU:OE2	3:J:28:LYS:CG	2.45	0.55
3:J:147:LYS:HZ1	3:J:151:ILE:CG2	2.19	0.55
2:3:4:LEU:HD11	3:4:3:ASP:HB2	1.85	0.55
3:O:87:TYR:CE1	5:Aa:19:THR:O	2.59	0.55
2:AC:4:LEU:HD12	2:AC:5:THR:N	2.20	0.55
3:AP:78:TYR:CD2	2:AQ:115:MET:HG3	2.42	0.55
1:A:911:LEU:HD13	1:A:914:PRO:HA	1.89	0.55
1:C:617:TYR:O	1:C:621:PHE:HD2	1.90	0.55
2:O:118:SER:O	3:L:53:LYS:HE3	2.06	0.55
3:F:29:ALA:O	3:F:32:THR:HG23	2.06	0.55
2:AG:66:VAL:HG22	2:AG:73:TYR:HD1	1.71	0.55
1:A:191:GLU:HG3	1:A:192:LYS:N	2.21	0.55
1:A:532:THR:CG2	2:7:102:THR:HG23	2.34	0.55
2:i:131:ARG:HH21	2:i:134:LYS:CE	2.18	0.55
2:w:134:LYS:HE2	2:w:150:GLY:HA2	1.88	0.55
3:4:13:ASP:HB3	5:Aa:64:ASN:ND2	2.20	0.55
3:AJ:76:ARG:NH1	6:AJ:201:CYC:O2D	2.38	0.55
1:A:489:ASN:HD22	1:A:492:ILE:HG23	1.72	0.55
1:A:875:LEU:CD1	1:A:876:TYR:CE1	2.90	0.55
1:A:1117:PRO:O	1:A:1118:THR:CB	2.54	0.55
1:C:204:LEU:O	1:C:208:LYS:HG2	2.06	0.55
1:C:222:LEU:HD12	1:C:223:VAL:N	2.22	0.55
1:C:911:LEU:HD13	1:C:914:PRO:HA	1.89	0.55
1:C:1143:LEU:HD13	2:I:103:PRO:HA	1.88	0.55
2:M:81:CYS:HA	6:M:201:CYC:CHD	2.36	0.55
3:f:76:ARG:HD3	2:g:110:ILE:HD12	1.88	0.55
2:k:58:LEU:HD12	2:k:59:PHE:N	2.22	0.55
2:AU:131:ARG:HH21	2:AU:157:VAL:CG1	2.09	0.55
1:A:204:LEU:O	1:A:208:LYS:HG2	2.07	0.55
1:A:1027:ASN:HB3	1:A:1029:GLU:HG3	1.88	0.55
1:C:4:ARG:CD	1:C:464:GLN:O	2.50	0.55
1:C:496:GLU:CD	3:f:114:GLU:CG	2.79	0.55
2:E:12:ASP:OD2	3:F:107:ARG:NH1	2.39	0.55
6:E:201:CYC:CMA	6:E:201:CYC:HB	2.20	0.55
6:g:201:CYC:HC	6:g:201:CYC:CMD	2.20	0.55
2:o:123:ILE:CG1	2:o:124:PRO:HD3	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:78:THR:O	2:9:82:LEU:HD13	2.07	0.55
2:AS:66:VAL:HG22	2:AS:73:TYR:HD1	1.71	0.55
1:C:819:PHE:O	1:C:823:TYR:HD2	1.89	0.55
2:W:77:MET:HE1	3:Z:62:TYR:OH	2.07	0.55
3:2:119:LEU:O	5:Aa:61:GLN:HG3	2.07	0.55
3:AT:2:GLN:NE2	3:AT:7:ALA:HA	2.21	0.55
2:AW:5:THR:OG1	3:AX:3:ASP:OD2	2.22	0.55
6:Y:201:CYC:HB	6:Y:201:CYC:CMA	2.19	0.55
2:t:49:ARG:NH2	2:t:53:GLN:HE22	2.05	0.55
2:3:151:PHE:CE1	2:5:24:ASP:OD1	2.59	0.55
1:A:1088:GLY:HA2	2:Y:13:ALA:O	2.07	0.55
1:C:489:ASN:HD22	1:C:492:ILE:HG23	1.72	0.55
2:G:119:LEU:O	3:J:53:LYS:NZ	2.40	0.55
2:I:20:PRO:HG2	2:K:101:VAL:CG1	2.37	0.55
4:u:65:LEU:C	4:u:72:MET:HB2	2.31	0.55
6:AM:201:CYC:HC	6:AM:201:CYC:CMD	2.20	0.55
2:AO:81:CYS:HA	6:AO:201:CYC:HHD	1.89	0.55
2:AS:34:GLU:OE2	2:AS:38:ARG:NH1	2.39	0.55
2:AU:85:LEU:HD22	2:AU:133:MET:HE2	1.87	0.55
1:A:44:ASP:HA	1:A:47:PHE:CD2	2.42	0.54
2:M:20:PRO:HB3	2:O:151:PHE:HB3	1.88	0.54
6:Y:201:CYC:HMA3	6:Y:201:CYC:NB	2.22	0.54
3:0:140:LEU:CD2	2:AQ:140:LEU:HD23	2.35	0.54
2:AG:85:LEU:HD22	2:AG:133:MET:HE2	1.88	0.54
2:AI:116:TYR:HD1	2:AI:121:THR:CG2	2.13	0.54
1:A:1153:VAL:HG11	3:R:59:ALA:O	2.06	0.54
1:C:53:ARG:HA	1:C:56:ILE:HD12	1.88	0.54
1:C:249:SER:HB2	1:C:253:ARG:O	2.06	0.54
6:N:201:CYC:HB	6:N:201:CYC:CMA	2.20	0.54
2:S:12:ASP:OD1	2:S:13:ALA:N	2.40	0.54
2:k:58:LEU:HD11	2:k:59:PHE:CD1	2.42	0.54
3:0:2:GLN:N	3:0:102:SER:HG	2.04	0.54
2:AI:41:GLN:OE1	3:AJ:24:LEU:CD1	2.55	0.54
2:AU:41:GLN:OE1	3:AV:24:LEU:CD1	2.55	0.54
1:C:166:TYR:CD1	6:C:2101:CYC:HBB1	2.41	0.54
1:C:875:LEU:CD1	1:C:876:TYR:CE1	2.90	0.54
2:c:110:ILE:HG13	3:j:76:ARG:HB2	1.88	0.54
2:o:5:THR:HB	3:p:3:ASP:OD2	2.07	0.54
2:AC:81:CYS:HA	6:AC:201:CYC:HHD	1.90	0.54
3:AD:78:TYR:CD2	2:AE:115:MET:HG3	2.42	0.54
2:AO:18:LEU:HD22	3:AP:97:LEU:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AT:81:CYS:HA	6:AT:201:CYC:HHD	1.89	0.54
1:A:3:ILE:CG2	4:u:110:ASN:OD1	2.55	0.54
1:A:4:ARG:CD	1:A:464:GLN:O	2.50	0.54
1:A:386:ILE:HG22	1:A:397:GLY:N	2.23	0.54
2:t:67:SER:O	2:t:73:TYR:HB2	2.08	0.54
2:1:69:GLY:HA3	2:AQ:60:GLN:HG2	1.89	0.54
3:AP:83:ARG:HH22	6:AP:201:CYC:C4A	2.20	0.54
1:C:254:PRO:HD3	4:s:107:TYR:CD2	2.42	0.54
1:C:258:LEU:HD13	1:C:430:ALA:HA	1.88	0.54
6:E:201:CYC:CMD	6:E:201:CYC:HC	2.19	0.54
3:R:121:VAL:HG13	6:R:201:CYC:NC	2.22	0.54
2:AM:29:PHE:CE1	2:AM:36:ARG:NH1	2.73	0.54
5:Ab:6:LYS:HD2	5:Ab:29:THR:HG22	1.89	0.54
1:A:249:SER:CB	1:A:253:ARG:O	2.55	0.54
1:C:249:SER:CB	1:C:253:ARG:O	2.55	0.54
3:l:140:LEU:CD2	2:AE:140:LEU:HD23	2.38	0.54
3:q:25:ASP:HA	3:q:28:LYS:HE2	1.90	0.54
3:AX:110:ASN:ND2	5:Ad:57:PHE:CE1	2.76	0.54
1:A:222:LEU:HD12	1:A:223:VAL:N	2.22	0.54
1:A:347:PHE:O	1:A:348:TYR:HB3	2.08	0.54
1:A:1066:PHE:O	1:A:1067:LEU:HB2	2.08	0.54
1:C:875:LEU:CD1	1:C:876:TYR:CD1	2.91	0.54
1:C:1027:ASN:HB3	1:C:1029:GLU:HG3	1.89	0.54
3:F:119:LEU:HD22	6:F:201:CYC:HBD1	1.89	0.54
2:Y:34:GLU:OE2	3:Z:28:LYS:CG	2.44	0.54
2:c:71:ASN:OD1	2:c:121:THR:CA	2.56	0.54
2:g:105:GLU:HG3	2:g:109:ILE:CD1	2.37	0.54
3:l:87:TYR:CE1	5:Ab:19:THR:O	2.61	0.54
4:s:96:MET:HE1	4:s:148:GLU:HB2	1.89	0.54
4:u:105:ASP:HA	4:u:109:LEU:HB2	1.89	0.54
5:Ab:21:ARG:NH1	5:Ab:23:LEU:HB3	2.23	0.54
1:A:4:ARG:HD2	1:A:462:TYR:O	2.08	0.54
1:A:244:ASP:HB2	1:A:260:TYR:HA	1.90	0.54
1:A:617:TYR:O	1:A:621:PHE:HD2	1.90	0.54
1:C:44:ASP:HA	1:C:47:PHE:CD2	2.42	0.54
3:b:105:ASP:HA	3:b:109:LEU:HB2	1.89	0.54
2:m:140:LEU:CD2	3:AH:140:LEU:HD23	2.29	0.54
6:AA:201:CYC:HC	6:AA:201:CYC:CMD	2.20	0.54
6:AF:201:CYC:CMA	6:AF:201:CYC:HB	2.20	0.54
1:C:1008:PHE:CE2	3:N:83:ARG:NH1	2.76	0.54
1:C:1152:TYR:CE1	2:AI:68:PRO:HG2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:201:CYC:HB	6:I:201:CYC:CMA	2.20	0.54
2:S:115:MET:HG3	3:b:78:TYR:CD2	2.42	0.54
2:i:109:ILE:HG23	2:i:159:ALA:HB1	1.90	0.54
2:k:151:PHE:CE2	2:m:20:PRO:HB3	2.43	0.54
4:u:81:CYS:CA	6:u:201:CYC:HAC2	2.37	0.54
2:1:119:LEU:O	2:1:120:GLN:HB3	2.08	0.54
2:3:89:LEU:CB	2:3:133:MET:HE1	2.11	0.54
1:A:307:ARG:HH21	1:A:307:ARG:HG2	1.73	0.54
1:A:875:LEU:CD1	1:A:876:TYR:CD1	2.91	0.54
1:C:1036:VAL:HG13	1:C:1066:PHE:HE1	1.73	0.54
2:r:67:SER:O	2:r:73:TYR:HB2	2.08	0.54
2:3:109:ILE:O	2:3:109:ILE:HG22	2.08	0.54
3:AP:24:LEU:CA	3:AP:27:LEU:HG	2.38	0.54
1:C:1066:PHE:O	1:C:1067:LEU:HB2	2.08	0.53
2:c:3:VAL:HG11	2:c:29:PHE:CD2	2.43	0.53
2:o:123:ILE:HD12	2:o:124:PRO:HD3	1.89	0.53
2:w:14:GLU:HB3	2:w:16:ARG:HD3	1.90	0.53
2:AA:29:PHE:HD1	2:AA:36:ARG:NH1	2.00	0.53
2:AQ:4:LEU:HD11	3:AR:3:ASP:CG	2.33	0.53
6:I:201:CYC:HMA3	6:I:201:CYC:NB	2.24	0.53
3:h:71:MEN:O	3:h:77:ARG:HD3	2.09	0.53
2:r:60:GLN:OE1	2:7:69:GLY:HA3	2.08	0.53
4:s:66:THR:HG22	4:s:72:MET:HE2	1.90	0.53
2:1:115:MET:HG3	3:0:78:TYR:CD2	2.44	0.53
3:AP:76:ARG:HB2	2:AQ:110:ILE:HG13	1.90	0.53
2:AS:85:LEU:HD22	2:AS:133:MET:HE2	1.89	0.53
1:A:496:GLU:CG	3:6:114:GLU:CG	2.87	0.53
1:C:386:ILE:HG23	2:o:14:GLU:O	2.09	0.53
1:C:1152:TYR:CD1	2:AI:68:PRO:HG2	2.43	0.53
3:R:87:TYR:CE1	3:R:91:TYR:CE1	2.91	0.53
2:U:105:GLU:HA	2:U:109:ILE:HG12	1.90	0.53
2:c:61:LYS:NZ	2:c:132:ALA:HB2	2.24	0.53
3:f:105:ASP:HA	3:f:109:LEU:HB2	1.91	0.53
4:s:97:VAL:O	4:s:98:ALA:CB	2.56	0.53
3:AD:24:LEU:CA	3:AD:27:LEU:HG	2.38	0.53
1:C:141:GLU:OE1	1:C:143:ILE:HG23	2.09	0.53
1:C:209:ASN:O	1:C:213:LEU:HD13	2.09	0.53
2:S:118:SER:O	3:b:53:LYS:HE3	2.08	0.53
3:n:105:ASP:HA	3:n:109:LEU:HB2	1.90	0.53
2:y:4:LEU:HD12	2:y:5:THR:N	2.24	0.53
3:z:71:MEN:O	3:z:77:ARG:HD3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AE:4:LEU:HD11	3:AF:3:ASP:CG	2.33	0.53
3:AV:105:ASP:HA	3:AV:109:LEU:HB2	1.91	0.53
1:A:930:LEU:HD13	3:AH:148:GLU:HB2	1.91	0.53
1:C:4:ARG:HG3	1:C:4:ARG:HH11	1.73	0.53
1:C:357:LEU:C	1:C:357:LEU:HD12	2.33	0.53
2:Y:20:PRO:HG2	2:a:101:VAL:CG1	2.38	0.53
2:Y:27:LYS:HE3	2:a:151:PHE:CE1	2.44	0.53
2:i:85:LEU:HD22	2:i:133:MET:HE2	1.90	0.53
1:A:3:ILE:CG2	4:u:110:ASN:HA	2.37	0.53
1:A:4:ARG:HH11	1:A:4:ARG:HG3	1.73	0.53
1:A:36:ASN:ND2	1:A:39:GLU:HG2	2.23	0.53
1:A:794:ARG:HD2	1:A:799:GLU:CD	2.34	0.53
3:v:3:ASP:OD1	3:v:5:ILE:CG1	2.40	0.53
6:7:201:CYC:HBC2	6:7:201:CYC:HMC1	1.90	0.53
3:0:113:LYS:HD2	3:0:123:ILE:HD13	1.91	0.53
3:AF:78:TYR:CD2	2:AK:115:MET:HG3	2.43	0.53
2:AK:131:ARG:HH21	2:AK:157:VAL:CG1	2.10	0.53
3:AN:50:THR:HG22	3:AN:54:GLU:OE1	2.09	0.53
1:A:141:GLU:OE1	1:A:143:ILE:HG23	2.09	0.53
1:A:693:ARG:HH11	1:A:693:ARG:CG	2.22	0.53
1:C:1008:PHE:CZ	3:N:83:ARG:NH1	2.76	0.53
2:k:37:LEU:HD23	2:k:97:VAL:HG22	1.89	0.53
2:t:49:ARG:HH21	2:t:53:GLN:HE22	1.56	0.53
2:1:85:LEU:HD22	2:1:133:MET:HE2	1.91	0.53
2:1:120:GLN:O	2:1:120:GLN:HG2	2.09	0.53
2:AA:36:ARG:NH2	2:AA:97:VAL:O	2.41	0.53
3:AN:112:LEU:HD23	3:AN:160:LEU:HD21	1.90	0.53
3:AR:78:TYR:CD2	2:AW:115:MET:HG3	2.43	0.53
1:A:347:PHE:HE2	1:A:448:PRO:HB3	1.74	0.53
1:C:547:ARG:HD3	3:l:110:ASN:HB2	1.91	0.53
3:R:87:TYR:CZ	3:R:91:TYR:CE1	2.97	0.53
2:W:105:GLU:HA	2:W:109:ILE:HG12	1.91	0.53
3:Z:105:ASP:HA	3:Z:109:LEU:HB2	1.90	0.53
2:a:105:GLU:HA	2:a:109:ILE:HG12	1.91	0.53
2:c:20:PRO:CG	2:e:101:VAL:HG11	2.38	0.53
3:h:60:LEU:HB3	3:h:72:MET:HE1	1.90	0.53
2:k:4:LEU:HD12	2:k:5:THR:N	2.24	0.53
3:z:60:LEU:HB3	3:z:72:MET:HE1	1.91	0.53
3:z:76:ARG:HB3	2:7:110:ILE:HG13	1.91	0.53
2:1:109:ILE:HG23	2:1:159:ALA:HB1	1.89	0.53
3:4:11:ASN:OD1	3:4:12:TYR:HD1	1.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:115:MET:HG3	3:8:78:TYR:CD2	2.44	0.53
2:AC:18:LEU:HD22	3:AD:97:LEU:HD13	1.91	0.53
3:AD:12:TYR:CD2	3:AD:19:LEU:HD23	2.44	0.53
2:AE:109:ILE:HG23	2:AE:159:ALA:HB1	1.91	0.53
2:AG:4:LEU:HD12	2:AG:5:THR:N	2.24	0.53
3:AH:81:CYS:HA	6:AH:201:CYC:HHD	1.89	0.53
1:A:298:ARG:HG3	1:A:302:ARG:NH1	2.24	0.53
1:A:1036:VAL:HG13	1:A:1066:PHE:HE1	1.73	0.53
1:C:36:ASN:ND2	1:C:39:GLU:HG2	2.23	0.53
3:f:101:PRO:CG	3:q:161:SER:OXT	2.28	0.53
2:w:109:ILE:HG23	2:w:159:ALA:HB1	1.91	0.53
6:y:201:CYC:HC	6:y:201:CYC:CMD	2.22	0.53
3:AV:76:ARG:NH1	6:AV:201:CYC:O2D	2.38	0.53
1:A:54:ILE:HD11	3:v:31:PHE:CD1	2.43	0.53
1:C:200:ILE:HA	1:C:231:ILE:CD1	2.39	0.53
2:G:77:MET:HE1	3:J:62:TYR:OH	2.09	0.53
2:Q:20:PRO:HB3	2:S:151:PHE:HB3	1.90	0.53
2:e:115:MET:HG3	3:n:78:TYR:CD2	2.44	0.53
2:o:71:ASN:HD22	2:o:122:PRO:HD3	1.74	0.53
3:AB:112:LEU:HD23	3:AB:160:LEU:HD21	1.90	0.53
5:Ac:25:ASN:OD1	5:Ac:25:ASN:N	2.37	0.53
1:C:4:ARG:HD2	1:C:462:TYR:O	2.08	0.52
1:C:156:SER:O	6:C:2101:CYC:HMC3	2.10	0.52
1:C:347:PHE:O	1:C:348:TYR:CB	2.57	0.52
1:C:539:LYS:NZ	5:Ab:24:GLN:HE21	2.07	0.52
6:a:201:CYC:HB	6:a:201:CYC:CMA	2.22	0.52
2:c:109:ILE:CG2	2:c:159:ALA:HB1	2.38	0.52
2:o:109:ILE:HG23	2:o:159:ALA:HB1	1.91	0.52
3:v:83:ARG:HH22	6:v:201:CYC:C1A	2.22	0.52
2:3:20:PRO:CG	2:5:101:VAL:HG11	2.39	0.52
2:7:67:SER:O	2:7:73:TYR:HB2	2.09	0.52
3:0:140:LEU:HD21	2:AQ:140:LEU:CD2	2.39	0.52
2:AG:12:ASP:OD2	3:AH:107:ARG:NH1	2.39	0.52
2:AS:67:SER:O	2:AS:73:TYR:HB2	2.09	0.52
1:A:269:LEU:HD23	1:A:428:VAL:HG11	1.91	0.52
1:A:386:ILE:HG22	1:A:397:GLY:H	1.74	0.52
1:A:539:LYS:NZ	5:Aa:24:GLN:NE2	2.54	0.52
1:C:67:ILE:HD11	1:C:213:LEU:CD2	2.39	0.52
1:C:693:ARG:HH11	1:C:693:ARG:CG	2.21	0.52
3:P:105:ASP:HA	3:P:109:LEU:HB2	1.91	0.52
3:T:105:ASP:HA	3:T:109:LEU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:201:CYC:HMA3	6:V:201:CYC:NB	2.20	0.52
2:e:4:LEU:HD12	2:e:5:THR:N	2.24	0.52
2:3:4:LEU:HD12	2:3:5:THR:N	2.24	0.52
2:5:4:LEU:HD12	2:5:5:THR:N	2.25	0.52
3:8:105:ASP:HA	3:8:109:LEU:HB2	1.90	0.52
2:AA:67:SER:O	2:AA:73:TYR:HB2	2.08	0.52
2:AS:4:LEU:HD11	3:AT:3:ASP:HB2	1.91	0.52
2:AW:4:LEU:HD12	2:AW:5:THR:N	2.24	0.52
1:A:889:LEU:HB3	1:A:890:PRO:HD3	1.91	0.52
1:C:930:LEU:HD13	3:AT:148:GLU:HB2	1.90	0.52
1:C:990:ARG:HG2	2:O:110:ILE:HD12	1.90	0.52
2:Y:20:PRO:HG2	2:a:101:VAL:HG11	1.91	0.52
2:i:115:MET:HG3	3:l:78:TYR:CD2	2.44	0.52
3:x:105:ASP:HA	3:x:109:LEU:HB2	1.91	0.52
3:z:78:TYR:CD2	2:7:115:MET:HG3	2.44	0.52
2:AG:43:LEU:HD11	2:AG:141:LEU:CD1	2.38	0.52
2:AM:36:ARG:NH2	2:AM:97:VAL:O	2.41	0.52
2:AM:67:SER:O	2:AM:73:TYR:HB2	2.08	0.52
1:A:981:ILE:HG23	1:A:1110:ILE:HG23	1.91	0.52
1:C:228:SER:HA	1:C:231:ILE:HG22	1.91	0.52
1:C:246:VAL:HG23	1:C:256:LEU:O	2.08	0.52
1:C:349:GLN:O	3:p:107:ARG:NE	2.30	0.52
1:C:794:ARG:HD2	1:C:799:GLU:CD	2.34	0.52
1:C:1152:TYR:CE2	2:AI:68:PRO:HD2	2.44	0.52
3:H:105:ASP:HA	3:H:109:LEU:HB2	1.91	0.52
2:I:20:PRO:HG2	2:K:101:VAL:HG11	1.90	0.52
2:c:12:ASP:OD2	3:d:107:ARG:CZ	2.57	0.52
6:g:201:CYC:HB	6:g:201:CYC:CMA	2.23	0.52
2:9:105:GLU:HG3	2:9:109:ILE:HD11	1.92	0.52
2:AE:4:LEU:HD12	2:AE:5:THR:N	2.25	0.52
2:AI:4:LEU:HD12	2:AI:5:THR:N	2.25	0.52
6:AS:201:CYC:O2A	3:AV:62:TYR:N	2.30	0.52
1:C:169:TYR:CE1	3:q:19:LEU:CD1	2.92	0.52
2:E:56:ASP:HB3	2:5:75:GLU:OE1	2.10	0.52
3:L:105:ASP:HA	3:L:109:LEU:HB2	1.89	0.52
2:W:80:LEU:HD11	3:Z:62:TYR:CE1	2.43	0.52
3:h:78:TYR:CD2	2:m:115:MET:HG3	2.44	0.52
2:o:4:LEU:HD12	2:o:5:THR:N	2.25	0.52
3:p:112:LEU:HD23	3:p:160:LEU:HD21	1.90	0.52
3:AJ:35:ALA:HB1	3:AJ:39:ARG:HH21	1.75	0.52
3:AP:12:TYR:CD2	3:AP:19:LEU:HD23	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AS:4:LEU:HD12	2:AS:5:THR:N	2.24	0.52
1:A:621:PHE:O	3:6:107:ARG:NH2	2.41	0.52
1:A:1037:ARG:O	1:A:1041:ARG:HG2	2.10	0.52
2:O:105:GLU:HA	2:O:109:ILE:HG12	1.91	0.52
2:i:4:LEU:HD12	2:i:5:THR:N	2.25	0.52
2:i:113:LYS:HE2	2:i:123:ILE:HG21	1.92	0.52
3:p:105:ASP:HA	3:p:109:LEU:HB2	1.91	0.52
2:AU:116:TYR:HD1	2:AU:121:THR:CG2	2.13	0.52
1:A:67:ILE:HD11	1:A:213:LEU:CD2	2.39	0.52
1:C:244:ASP:HB2	1:C:260:TYR:HA	1.91	0.52
1:C:298:ARG:HG3	1:C:302:ARG:NH1	2.24	0.52
1:C:892:ALA:O	1:C:895:PRO:HD2	2.10	0.52
2:I:27:LYS:HE3	2:K:151:PHE:CE1	2.45	0.52
2:i:38:ARG:HH12	3:j:28:LYS:HE3	1.75	0.52
6:m:201:CYC:HBC2	6:m:201:CYC:HMC1	1.91	0.52
2:3:53:GLN:O	2:3:56:ASP:OD1	2.28	0.52
2:AC:109:ILE:HG23	2:AC:159:ALA:HB1	1.91	0.52
2:AU:4:LEU:HD12	2:AU:5:THR:N	2.24	0.52
1:A:496:GLU:CD	3:6:114:GLU:CG	2.79	0.52
1:A:875:LEU:HD12	1:A:876:TYR:CG	2.45	0.52
1:A:892:ALA:O	1:A:895:PRO:HD2	2.10	0.52
3:J:105:ASP:HA	3:J:109:LEU:HB2	1.90	0.52
2:a:34:GLU:OE1	3:b:28:LYS:NZ	2.31	0.52
2:c:3:VAL:HG13	2:c:4:LEU:N	2.24	0.52
3:f:76:ARG:HD3	2:g:110:ILE:CD1	2.39	0.52
3:l:91:TYR:HE2	3:l:107:ARG:CZ	2.22	0.52
4:u:81:CYS:SG	6:u:201:CYC:C3C	2.97	0.52
2:w:4:LEU:HD12	2:w:5:THR:N	2.25	0.52
2:w:5:THR:HB	3:x:3:ASP:OD2	2.09	0.52
2:y:12:ASP:OD2	3:z:107:ARG:NH1	2.43	0.52
2:y:102:THR:CG2	2:y:103:PRO:CD	2.77	0.52
2:1:4:LEU:HD12	2:1:5:THR:N	2.25	0.52
3:AB:50:THR:HG22	3:AB:54:GLU:OE1	2.09	0.52
3:AH:105:ASP:HA	3:AH:109:LEU:HB2	1.91	0.52
2:AK:4:LEU:HD12	2:AK:5:THR:N	2.25	0.52
2:AS:102:THR:N	2:AS:103:PRO:HD2	2.25	0.52
1:A:274:MET:HG3	1:A:286:VAL:HG11	1.92	0.52
1:C:256:LEU:HD21	6:s:201:CYC:OB	2.10	0.52
1:C:489:ASN:ND2	1:C:492:ILE:HG23	2.25	0.52
1:C:889:LEU:HB3	1:C:890:PRO:HD3	1.91	0.52
1:C:1037:ARG:O	1:C:1041:ARG:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:87:TYR:CZ	3:N:91:TYR:CE1	2.98	0.52
3:P:83:ARG:HH22	6:P:201:CYC:C1A	2.23	0.52
3:j:19:LEU:CD1	3:j:24:LEU:HD21	2.29	0.52
3:6:112:LEU:HD23	3:6:160:LEU:HD21	1.91	0.52
2:7:89:LEU:CB	2:7:133:MET:HE1	2.10	0.52
3:0:12:TYR:CZ	3:0:23:ALA:HB2	2.45	0.52
3:0:83:ARG:NH2	6:0:201:CYC:O2A	2.42	0.52
3:AB:2:GLN:HG3	3:AB:100:ASP:OD2	2.10	0.52
2:AG:4:LEU:HD11	3:AH:3:ASP:HB2	1.92	0.52
2:AG:67:SER:O	2:AG:73:TYR:HB2	2.09	0.52
3:AJ:105:ASP:HA	3:AJ:109:LEU:HB2	1.91	0.52
2:AS:66:VAL:CG2	2:AS:73:TYR:HD1	2.23	0.52
1:A:209:ASN:O	1:A:213:LEU:HD13	2.09	0.52
2:I:105:GLU:HA	2:I:109:ILE:HG12	1.92	0.52
2:k:109:ILE:CG2	2:k:159:ALA:HB1	2.39	0.52
2:3:89:LEU:HD22	2:3:133:MET:CE	2.40	0.52
3:AF:105:ASP:HA	3:AF:109:LEU:HB2	1.92	0.52
5:Ad:6:LYS:HB3	5:Ad:55:LYS:HG2	1.92	0.52
1:C:345:ARG:HA	1:C:349:GLN:HB3	1.91	0.51
2:G:105:GLU:HA	2:G:109:ILE:HG12	1.91	0.51
2:K:105:GLU:HA	2:K:109:ILE:HG12	1.91	0.51
2:Y:67:SER:O	2:Y:73:TYR:HB2	2.11	0.51
2:c:56:ASP:OD1	2:c:57:GLN:N	2.43	0.51
6:e:201:CYC:HBD2	6:e:201:CYC:HHA	1.91	0.51
2:m:67:SER:O	2:m:73:TYR:HB2	2.09	0.51
1:A:1152:TYR:CE2	2:AU:68:PRO:HD2	2.45	0.51
1:C:186:LEU:HD21	6:C:2101:CYC:CMB	2.40	0.51
2:M:101:VAL:HG13	2:O:20:PRO:HG2	1.91	0.51
3:R:122:PRO:HD2	6:R:201:CYC:OC	2.09	0.51
2:S:105:GLU:HA	2:S:109:ILE:HG12	1.91	0.51
4:s:2:LYS:HE2	4:s:7:THR:HG22	1.93	0.51
4:s:141:VAL:HG13	4:s:145:ALA:HB3	1.91	0.51
6:2:201:CYC:HMA3	6:2:201:CYC:HB	1.75	0.51
3:6:105:ASP:HA	3:6:109:LEU:HB2	1.91	0.51
2:9:4:LEU:HD12	2:9:5:THR:N	2.25	0.51
2:9:61:LYS:HB3	2:9:61:LYS:NZ	2.24	0.51
2:AQ:109:ILE:HG23	2:AQ:159:ALA:HB1	1.91	0.51
1:C:981:ILE:HG23	1:C:1110:ILE:HG23	1.92	0.51
2:E:105:GLU:HA	2:E:109:ILE:HG12	1.90	0.51
2:S:97:VAL:HG23	3:T:9:ILE:HD11	1.92	0.51
3:d:78:TYR:CD2	2:k:115:MET:HG3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:4:LEU:HD12	2:g:5:THR:N	2.24	0.51
1:C:54:ILE:HD11	3:q:31:PHE:CD1	2.46	0.51
1:C:274:MET:HG3	1:C:286:VAL:HG11	1.92	0.51
1:C:640:TYR:N	1:C:644:GLU:OE2	2.35	0.51
2:Q:83:ARG:HH22	6:Q:201:CYC:C1A	2.23	0.51
2:e:67:SER:O	2:e:73:TYR:HB2	2.10	0.51
3:j:113:LYS:HD2	3:j:117:ASN:HD21	1.75	0.51
6:7:201:CYC:HC	6:7:201:CYC:HMD2	1.75	0.51
2:AG:102:THR:N	2:AG:103:PRO:HD2	2.25	0.51
2:AM:34:GLU:OE2	2:AM:38:ARG:NH1	2.44	0.51
1:A:430:ALA:O	6:u:201:CYC:HBA2	2.10	0.51
1:A:547:ARG:CG	3:0:106:GLU:HA	2.40	0.51
1:C:856:ARG:O	1:C:857:LYS:HG2	2.11	0.51
3:l:105:ASP:HA	3:l:109:LEU:HB2	1.92	0.51
3:v:105:ASP:HA	3:v:109:LEU:HB2	1.92	0.51
2:1:67:SER:O	2:1:73:TYR:HB2	2.11	0.51
2:3:109:ILE:HG23	2:3:159:ALA:HB1	1.93	0.51
2:7:27:LYS:NZ	3:8:39:ARG:HH22	2.09	0.51
2:9:67:SER:O	2:9:73:TYR:HB2	2.11	0.51
2:AA:34:GLU:OE2	2:AA:38:ARG:NH1	2.44	0.51
3:AJ:20:ASP:OD1	3:AJ:21:GLY:N	2.44	0.51
2:AQ:109:ILE:HG12	2:AQ:159:ALA:CB	2.40	0.51
3:AT:105:ASP:HA	3:AT:109:LEU:HB2	1.91	0.51
1:A:249:SER:O	2:t:13:ALA:HB1	2.11	0.51
1:A:505:VAL:HG13	3:z:110:ASN:ND2	2.24	0.51
1:A:1152:TYR:CE1	2:AU:68:PRO:HG2	2.45	0.51
1:C:22:THR:HG23	3:q:3:ASP:OD2	2.11	0.51
1:C:162:TRP:HZ2	4:s:73:TYR:CE2	2.29	0.51
1:C:549:LYS:HE2	1:C:555:ALA:HB2	1.93	0.51
2:Q:68:PRO:HD3	2:k:61:LYS:HE2	1.93	0.51
2:c:53:GLN:O	2:c:56:ASP:OD1	2.28	0.51
3:f:76:ARG:HB2	2:g:110:ILE:HG13	1.91	0.51
6:f:201:CYC:HMA1	6:f:201:CYC:NB	2.20	0.51
6:g:201:CYC:HC	6:g:201:CYC:HMD2	1.75	0.51
3:l:12:TYR:CZ	3:l:23:ALA:HB2	2.45	0.51
3:q:105:ASP:HA	3:q:109:LEU:HB2	1.91	0.51
2:w:39:ILE:O	2:w:42:THR:OG1	2.29	0.51
6:y:201:CYC:HB	6:y:201:CYC:CMA	2.23	0.51
2:5:109:ILE:CG2	2:5:159:ALA:HB1	2.41	0.51
1:C:200:ILE:HG23	1:C:231:ILE:HD11	1.92	0.51
1:C:269:LEU:HD23	1:C:428:VAL:HG11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:123:ILE:N	2:O:124:PRO:CD	2.74	0.51
6:F:201:CYC:HMA3	6:F:201:CYC:NB	2.18	0.51
2:Q:105:GLU:HA	2:Q:109:ILE:HG12	1.92	0.51
2:e:80:LEU:HD13	6:e:201:CYC:HAD2	1.93	0.51
4:s:77:ARG:HD2	6:s:201:CYC:O2D	2.11	0.51
2:3:56:ASP:OD1	2:3:57:GLN:N	2.44	0.51
2:AA:18:LEU:HD22	3:AB:97:LEU:HD13	1.92	0.51
2:AQ:19:SER:OG	2:AQ:20:PRO:HD2	2.11	0.51
3:AR:66:THR:CG2	6:AW:201:CYC:HMA2	2.41	0.51
1:A:1143:LEU:CD2	3:Z:10:ASN:OD1	2.58	0.51
1:C:156:SER:CA	6:C:2101:CYC:H3C	2.41	0.51
2:O:97:VAL:HG23	3:P:9:ILE:HD11	1.93	0.51
2:K:47:ARG:HD2	2:K:48:GLU:HG3	1.93	0.51
2:K:67:SER:O	2:K:73:TYR:HB2	2.11	0.51
2:U:56:ASP:OD2	2:e:75:GLU:CD	2.53	0.51
2:a:47:ARG:HD2	2:a:48:GLU:HG3	1.93	0.51
3:d:10:ASN:HD21	5:Ab:65:THR:HB	1.75	0.51
2:AE:109:ILE:HG12	2:AE:159:ALA:CB	2.40	0.51
3:AN:2:GLN:HG3	3:AN:100:ASP:OD2	2.10	0.51
2:AO:109:ILE:HG23	2:AO:159:ALA:HB1	1.91	0.51
2:AQ:4:LEU:HD12	2:AQ:5:THR:N	2.25	0.51
1:A:496:GLU:OE1	1:A:496:GLU:HA	2.11	0.51
1:C:875:LEU:HD12	1:C:876:TYR:CG	2.45	0.51
2:e:37:LEU:HD22	3:f:24:LEU:HD22	1.93	0.51
3:n:12:TYR:CZ	3:n:23:ALA:HB2	2.46	0.51
3:8:12:TYR:CZ	3:8:23:ALA:HB2	2.46	0.51
2:AG:66:VAL:CG2	2:AG:73:TYR:HD1	2.23	0.51
2:AI:67:SER:O	2:AI:73:TYR:HB2	2.11	0.51
1:A:433:SER:HA	4:u:115:THR:HG21	1.93	0.51
1:A:1067:LEU:CD1	1:A:1096:ILE:HG23	2.41	0.51
1:C:505:VAL:HG13	3:h:110:ASN:ND2	2.26	0.51
1:C:811:PHE:HA	1:C:860:LYS:HD2	1.93	0.51
1:C:1067:LEU:CD1	1:C:1096:ILE:HG23	2.41	0.51
3:N:12:TYR:CZ	3:N:23:ALA:HB2	2.46	0.51
2:S:19:SER:OG	2:S:20:PRO:HD2	2.11	0.51
2:a:67:SER:O	2:a:73:TYR:HB2	2.11	0.51
3:l:140:LEU:HD21	2:AE:140:LEU:CD2	2.41	0.51
2:r:19:SER:OG	2:r:20:PRO:HD2	2.11	0.51
2:w:19:SER:OG	2:w:20:PRO:HD2	2.11	0.51
3:z:74:THR:HG22	2:7:107:ILE:HG23	1.92	0.51
2:9:49:ARG:HG2	2:9:53:GLN:CD	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AA:201:CYC:HC	6:AA:201:CYC:HMD2	1.75	0.51
2:AS:105:GLU:HA	2:AS:109:ILE:HG12	1.93	0.51
2:AU:67:SER:O	2:AU:73:TYR:HB2	2.11	0.51
1:A:228:SER:HA	1:A:231:ILE:HG22	1.92	0.50
1:A:549:LYS:HE2	1:A:555:ALA:HB2	1.93	0.50
1:A:1137:SER:HB2	3:R:118:SER:CB	2.41	0.50
1:C:25:ILE:HG21	3:q:1:MET:CE	2.40	0.50
1:C:496:GLU:CG	3:f:114:GLU:CG	2.87	0.50
3:l:132:ALA:O	3:l:135:GLU:CG	2.60	0.50
2:t:19:SER:OG	2:t:20:PRO:HD2	2.12	0.50
3:x:112:LEU:HD23	3:x:160:LEU:HD21	1.92	0.50
3:z:1:MET:CB	3:z:106:GLU:OE2	2.59	0.50
6:1:201:CYC:HMA3	6:1:201:CYC:HB	1.76	0.50
3:AF:66:THR:CG2	6:AK:201:CYC:HMA2	2.41	0.50
3:AH:100:ASP:OD1	3:AH:101:PRO:CD	2.49	0.50
2:AI:49:ARG:HH11	2:AI:53:GLN:NE2	2.08	0.50
3:AL:87:TYR:CD2	6:AL:201:CYC:HBB3	2.45	0.50
3:AP:105:ASP:HA	3:AP:109:LEU:HB2	1.92	0.50
3:AR:105:ASP:HA	3:AR:109:LEU:HB2	1.92	0.50
3:AV:35:ALA:HB1	3:AV:39:ARG:HH21	1.75	0.50
1:A:761:ARG:O	1:A:761:ARG:HG2	2.12	0.50
1:C:1144:SER:OG	3:N:74:THR:HG21	2.11	0.50
2:U:67:SER:O	2:U:73:TYR:HB2	2.11	0.50
2:e:5:THR:HB	3:f:3:ASP:OD2	2.12	0.50
2:y:48:GLU:HG2	2:y:49:ARG:N	2.26	0.50
2:y:97:VAL:HG11	3:z:27:LEU:HD13	1.93	0.50
2:3:109:ILE:CG2	2:3:159:ALA:HB1	2.41	0.50
6:5:201:CYC:HMA3	6:5:201:CYC:NB	2.25	0.50
3:AD:105:ASP:HA	3:AD:109:LEU:HB2	1.92	0.50
2:AE:67:SER:O	2:AE:73:TYR:HB2	2.11	0.50
2:AI:101:VAL:CG1	2:AK:20:PRO:HG2	2.41	0.50
2:AS:66:VAL:HG22	2:AS:73:TYR:CD1	2.46	0.50
1:A:489:ASN:ND2	1:A:492:ILE:HG23	2.25	0.50
1:A:875:LEU:CD1	1:A:876:TYR:CZ	2.94	0.50
1:A:1118:THR:HG21	6:X:201:CYC:HBA1	1.93	0.50
1:C:188:GLU:HG3	1:C:238:ARG:HG2	1.93	0.50
1:C:322:LYS:CB	1:C:328:ILE:HG12	2.41	0.50
1:C:496:GLU:OE1	1:C:496:GLU:HA	2.11	0.50
2:M:105:GLU:HA	2:M:109:ILE:HG12	1.92	0.50
3:P:12:TYR:CZ	3:P:23:ALA:HB2	2.46	0.50
2:g:67:SER:O	2:g:73:TYR:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:w:67:SER:O	2:w:73:TYR:HB2	2.11	0.50
2:9:105:GLU:HA	2:9:109:ILE:HG12	1.92	0.50
2:AU:49:ARG:HH11	2:AU:53:GLN:NE2	2.09	0.50
1:A:322:LYS:CB	1:A:328:ILE:HG12	2.41	0.50
1:A:1152:TYR:CD1	2:AU:68:PRO:HG2	2.46	0.50
2:E:67:SER:O	2:E:73:TYR:HB2	2.11	0.50
2:G:67:SER:O	2:G:73:TYR:HB2	2.11	0.50
3:V:119:LEU:HD22	6:V:201:CYC:HBD1	1.92	0.50
3:f:47:ASN:ND2	3:f:140:LEU:HD23	2.27	0.50
6:m:201:CYC:HC	6:m:201:CYC:HMD2	1.75	0.50
4:u:81:CYS:CB	6:u:201:CYC:HAC2	2.41	0.50
2:1:14:GLU:HB3	2:1:16:ARG:HD3	1.94	0.50
2:5:67:SER:O	2:5:73:TYR:HB2	2.11	0.50
2:AE:19:SER:OG	2:AE:20:PRO:HD2	2.11	0.50
3:AN:105:ASP:HA	3:AN:109:LEU:HB2	1.92	0.50
2:AO:67:SER:O	2:AO:73:TYR:HB2	2.11	0.50
3:AP:123:ILE:HG23	3:AP:160:LEU:HD13	1.93	0.50
1:A:254:PRO:HG3	4:u:107:TYR:CD1	2.47	0.50
1:C:6:THR:HG23	1:C:500:PRO:HD3	1.93	0.50
1:C:344:ARG:CZ	2:o:9:VAL:HG13	2.40	0.50
1:C:433:SER:HB2	4:s:115:THR:HG21	1.93	0.50
2:M:67:SER:O	2:M:73:TYR:HB2	2.11	0.50
3:H:12:TYR:CZ	3:H:23:ALA:HB2	2.47	0.50
2:Q:67:SER:O	2:Q:73:TYR:HB2	2.11	0.50
3:b:12:TYR:CZ	3:b:23:ALA:HB2	2.47	0.50
2:e:109:ILE:CG2	2:e:159:ALA:HB1	2.41	0.50
3:v:112:LEU:CD2	3:v:160:LEU:HD21	2.42	0.50
2:7:27:LYS:HZ2	3:8:39:ARG:NH2	2.09	0.50
3:AT:12:TYR:CZ	3:AT:23:ALA:HB2	2.47	0.50
1:A:344:ARG:CZ	2:w:9:VAL:HG13	2.41	0.50
1:C:1143:LEU:HD12	2:I:106:GLU:OE1	2.12	0.50
3:F:105:ASP:HA	3:F:109:LEU:HB2	1.94	0.50
3:R:105:ASP:HA	3:R:109:LEU:HB2	1.93	0.50
2:S:67:SER:O	2:S:73:TYR:HB2	2.11	0.50
2:Y:105:GLU:HA	2:Y:109:ILE:HG12	1.92	0.50
3:j:12:TYR:CZ	3:j:23:ALA:HB2	2.47	0.50
2:k:156:LEU:CD1	2:k:160:MET:HE3	2.41	0.50
3:l:2:GLN:HG3	3:l:100:ASP:OD2	2.12	0.50
2:o:80:LEU:HD22	6:o:201:CYC:HAD2	1.92	0.50
2:w:102:THR:N	2:w:103:PRO:HD2	2.27	0.50
2:w:128:GLU:OE2	2:w:131:ARG:NH1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:47:ASN:ND2	3:6:140:LEU:HD23	2.27	0.50
3:0:105:ASP:HA	3:0:109:LEU:HB2	1.93	0.50
3:AB:105:ASP:HA	3:AB:109:LEU:HB2	1.92	0.50
2:AE:102:THR:N	2:AE:103:PRO:HD2	2.27	0.50
2:AG:105:GLU:HA	2:AG:109:ILE:HG12	1.94	0.50
2:AI:109:ILE:CG2	2:AI:159:ALA:HB1	2.41	0.50
6:AM:201:CYC:HC	6:AM:201:CYC:HMD2	1.75	0.50
3:AN:12:TYR:CZ	3:AN:23:ALA:HB2	2.47	0.50
3:AV:20:ASP:OD1	3:AV:21:GLY:N	2.44	0.50
2:AW:67:SER:O	2:AW:73:TYR:HB2	2.12	0.50
2:AW:109:ILE:HG23	2:AW:159:ALA:HB1	1.93	0.50
1:A:169:TYR:HE1	3:v:19:LEU:CD1	2.25	0.50
1:A:595:ASN:OD1	6:4:201:CYC:HBA1	2.11	0.50
1:A:811:PHE:HA	1:A:860:LYS:HD2	1.93	0.50
6:E:201:CYC:NB	6:E:201:CYC:HMA3	2.27	0.50
2:I:67:SER:O	2:I:73:TYR:HB2	2.11	0.50
3:J:12:TYR:CZ	3:J:23:ALA:HB2	2.47	0.50
3:V:12:TYR:CZ	3:V:23:ALA:HB2	2.47	0.50
2:W:47:ARG:HD2	2:W:48:GLU:HG3	1.94	0.50
2:k:127:ALA:HB1	2:k:131:ARG:HH11	1.77	0.50
2:m:4:LEU:HD11	2:m:29:PHE:CD2	2.46	0.50
2:o:67:SER:O	2:o:73:TYR:HB2	2.11	0.50
2:y:4:LEU:HD11	3:z:3:ASP:CG	2.36	0.50
2:y:19:SER:OG	2:y:20:PRO:HD2	2.12	0.50
3:z:12:TYR:CZ	3:z:23:ALA:HB2	2.46	0.50
2:AG:66:VAL:HG22	2:AG:73:TYR:CD1	2.47	0.50
6:AG:201:CYC:O2A	3:AJ:62:TYR:N	2.29	0.50
2:AK:109:ILE:HG23	2:AK:159:ALA:HB1	1.92	0.50
2:AO:115:MET:HG3	3:AX:78:TYR:CD2	2.46	0.50
5:Aa:6:LYS:HB3	5:Aa:55:LYS:HG2	1.92	0.50
1:A:974:LEU:CD1	3:R:1:MET:H1	2.18	0.50
1:C:200:ILE:HG12	1:C:231:ILE:HD11	1.92	0.50
1:C:622:TYR:CD1	3:f:110:ASN:O	2.65	0.50
6:N:201:CYC:HB	6:N:201:CYC:HMA2	1.77	0.50
3:T:12:TYR:CZ	3:T:23:ALA:HB2	2.46	0.50
3:V:105:ASP:HA	3:V:109:LEU:HB2	1.94	0.50
3:f:78:TYR:CD2	2:g:115:MET:HG3	2.47	0.50
3:h:12:TYR:CZ	3:h:23:ALA:HB2	2.46	0.50
2:t:109:ILE:CG2	2:t:159:ALA:HB1	2.41	0.50
4:u:141:VAL:HG13	4:u:145:ALA:HB3	1.94	0.50
3:2:12:TYR:CZ	3:2:23:ALA:HB2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:67:SER:O	2:3:73:TYR:HB2	2.12	0.50
2:AC:67:SER:O	2:AC:73:TYR:HB2	2.11	0.50
3:AL:12:TYR:CZ	3:AL:23:ALA:HB2	2.47	0.50
2:AQ:67:SER:O	2:AQ:73:TYR:HB2	2.11	0.50
3:N:76:ARG:HB2	2:I:110:ILE:HG13	1.93	0.50
3:N:105:ASP:HA	3:N:109:LEU:HB2	1.93	0.50
3:X:12:TYR:CZ	3:X:23:ALA:HB2	2.47	0.50
3:Z:12:TYR:CZ	3:Z:23:ALA:HB2	2.47	0.50
2:a:102:THR:N	2:a:103:PRO:HD2	2.27	0.50
3:d:10:ASN:HA	5:Ab:64:ASN:HD21	1.77	0.50
2:i:67:SER:O	2:i:73:TYR:HB2	2.11	0.50
3:x:12:TYR:CZ	3:x:23:ALA:HB2	2.47	0.50
2:1:19:SER:OG	2:1:20:PRO:HD2	2.12	0.50
3:4:12:TYR:CZ	3:4:23:ALA:HB2	2.47	0.50
2:7:27:LYS:HZ2	3:8:39:ARG:HH22	1.60	0.50
3:0:140:LEU:CD2	2:AQ:140:LEU:HD22	2.41	0.50
2:AC:115:MET:HG3	3:AL:78:TYR:CD2	2.47	0.50
1:A:47:PHE:CE2	3:v:38:VAL:HG23	2.40	0.49
1:A:856:ARG:O	1:A:857:LYS:HG2	2.11	0.49
1:C:653:SER:HB3	3:f:87:TYR:OH	2.12	0.49
2:O:19:SER:OG	2:O:20:PRO:HD2	2.11	0.49
3:L:85:MET:HG2	6:L:201:CYC:HBC1	1.93	0.49
2:Q:68:PRO:CD	2:k:61:LYS:HG2	2.41	0.49
3:X:106:GLU:O	3:X:110:ASN:ND2	2.44	0.49
3:Z:148:GLU:O	3:Z:151:ILE:HG12	2.12	0.49
2:c:102:THR:N	2:c:103:PRO:HD2	2.27	0.49
2:i:34:GLU:OE2	3:j:31:PHE:HB3	2.11	0.49
2:k:67:SER:O	2:k:73:TYR:HB2	2.12	0.49
2:AC:102:THR:N	2:AC:103:PRO:HD2	2.27	0.49
3:AJ:12:TYR:CZ	3:AJ:23:ALA:HB2	2.47	0.49
2:AS:43:LEU:HD11	2:AS:141:LEU:CD1	2.38	0.49
2:AU:5:THR:OG1	3:AV:3:ASP:OD2	2.30	0.49
1:A:601:LYS:HE2	1:A:670:TYR:CD1	2.48	0.49
1:C:293:LYS:O	1:C:294:GLU:CB	2.60	0.49
1:C:1118:THR:HG21	6:H:201:CYC:HBA1	1.94	0.49
3:R:12:TYR:CZ	3:R:23:ALA:HB2	2.46	0.49
2:k:102:THR:N	2:k:103:PRO:HD2	2.26	0.49
4:s:71:ASN:HB3	6:s:201:CYC:OC	2.12	0.49
4:u:97:VAL:O	4:u:98:ALA:CB	2.56	0.49
2:1:102:THR:N	2:1:103:PRO:HD2	2.27	0.49
3:AF:87:TYR:CZ	5:Ac:38:PHE:HZ	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AJ:112:LEU:HD11	6:AJ:201:CYC:HMB3	1.94	0.49
2:AQ:109:ILE:CG2	2:AQ:159:ALA:HB1	2.42	0.49
3:AX:12:TYR:CZ	3:AX:23:ALA:HB2	2.47	0.49
1:A:312:TYR:C	2:w:114:GLU:OE2	2.55	0.49
1:A:1068:GLY:O	1:A:1114:ARG:O	2.31	0.49
1:C:625:LYS:HE3	3:f:110:ASN:HD21	1.78	0.49
1:C:679:LEU:C	1:C:679:LEU:HD12	2.38	0.49
1:C:1068:GLY:O	1:C:1114:ARG:O	2.31	0.49
2:O:102:THR:N	2:O:103:PRO:HD2	2.27	0.49
3:F:47:ASN:OD1	2:G:131:ARG:NH2	2.45	0.49
6:U:201:CYC:HC	6:U:201:CYC:HMD2	1.77	0.49
2:W:67:SER:O	2:W:73:TYR:HB2	2.11	0.49
2:g:102:THR:N	2:g:103:PRO:HD2	2.27	0.49
3:j:19:LEU:HD13	3:j:24:LEU:CD2	2.30	0.49
3:p:12:TYR:CZ	3:p:23:ALA:HB2	2.47	0.49
2:7:109:ILE:HG23	2:7:159:ALA:HB1	1.94	0.49
2:AE:85:LEU:HD22	2:AE:133:MET:HE2	1.94	0.49
2:AE:109:ILE:CG2	2:AE:159:ALA:HB1	2.42	0.49
2:AG:81:CYS:HA	6:AG:201:CYC:HHD	1.95	0.49
2:AM:18:LEU:HD22	3:AN:97:LEU:HD13	1.93	0.49
3:AR:12:TYR:CZ	3:AR:23:ALA:HB2	2.47	0.49
2:AU:109:ILE:CG2	2:AU:159:ALA:HB1	2.41	0.49
1:A:679:LEU:HD12	1:A:679:LEU:C	2.38	0.49
2:O:67:SER:O	2:O:73:TYR:HB2	2.11	0.49
3:F:148:GLU:O	3:F:151:ILE:HG12	2.13	0.49
2:S:123:ILE:N	2:S:124:PRO:CD	2.74	0.49
2:c:3:VAL:HG11	2:c:29:PHE:CG	2.47	0.49
3:d:12:TYR:CZ	3:d:23:ALA:HB2	2.47	0.49
2:g:109:ILE:CD1	2:g:155:TYR:OH	2.60	0.49
2:r:41:GLN:HE22	3:z:143:PRO:HG3	1.77	0.49
2:r:109:ILE:CG2	2:r:159:ALA:HB1	2.43	0.49
4:s:74:TYR:HD2	4:s:77:ARG:HG3	1.77	0.49
2:y:67:SER:O	2:y:73:TYR:HB2	2.11	0.49
3:6:12:TYR:CZ	3:6:23:ALA:HB2	2.47	0.49
3:AD:2:GLN:HG3	3:AD:100:ASP:OD2	2.12	0.49
2:AK:67:SER:O	2:AK:73:TYR:HB2	2.12	0.49
2:AO:102:THR:N	2:AO:103:PRO:HD2	2.27	0.49
1:A:256:LEU:N	1:A:256:LEU:CD1	2.76	0.49
3:L:12:TYR:CZ	3:L:23:ALA:HB2	2.47	0.49
3:L:148:GLU:O	3:L:151:ILE:HG12	2.13	0.49
2:c:71:ASN:OD1	2:c:120:GLN:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AI:109:ILE:O	2:AI:109:ILE:HG22	2.12	0.49
2:AU:101:VAL:CG1	2:AW:20:PRO:HG2	2.41	0.49
3:AV:112:LEU:HD11	6:AV:201:CYC:HMB3	1.94	0.49
1:C:159:ASP:OD2	6:C:2101:CYC:NC	2.45	0.49
1:C:258:LEU:HB2	1:C:430:ALA:HB2	1.94	0.49
1:C:312:TYR:C	2:o:114:GLU:OE2	2.56	0.49
3:T:148:GLU:O	3:T:151:ILE:HG12	2.13	0.49
2:c:67:SER:O	2:c:73:TYR:HB2	2.12	0.49
2:i:102:THR:N	2:i:103:PRO:HD2	2.27	0.49
3:j:151:ILE:CD1	3:j:152:TYR:CE2	2.95	0.49
2:o:102:THR:N	2:o:103:PRO:HD2	2.27	0.49
4:u:81:CYS:SG	6:u:201:CYC:C2C	3.01	0.49
2:w:123:ILE:N	2:w:124:PRO:CD	2.76	0.49
3:8:112:LEU:HD23	3:8:160:LEU:HD21	1.94	0.49
3:AB:12:TYR:CZ	3:AB:23:ALA:HB2	2.47	0.49
3:AH:12:TYR:CZ	3:AH:23:ALA:HB2	2.47	0.49
2:AQ:102:THR:N	2:AQ:103:PRO:HD2	2.27	0.49
2:AW:109:ILE:CG2	2:AW:159:ALA:HB1	2.43	0.49
1:A:6:THR:HG23	1:A:500:PRO:HD3	1.94	0.49
1:A:344:ARG:O	1:A:345:ARG:CG	2.60	0.49
1:A:386:ILE:HG21	1:A:395:SER:O	2.12	0.49
1:C:344:ARG:O	1:C:345:ARG:CG	2.60	0.49
1:C:346:GLU:OE2	1:C:347:PHE:CZ	2.65	0.49
1:C:875:LEU:CD1	1:C:876:TYR:CZ	2.94	0.49
1:C:1141:SER:HB2	2:I:106:GLU:HG2	1.95	0.49
2:M:83:ARG:NH1	6:M:201:CYC:O1A	2.31	0.49
2:E:102:THR:N	2:E:103:PRO:HD2	2.28	0.49
2:K:61:LYS:HD3	2:K:128:GLU:HG3	1.95	0.49
2:Q:83:ARG:NH2	6:Q:201:CYC:NA	2.60	0.49
3:V:77:ARG:NH2	5:AY:62:GLY:HA2	2.27	0.49
2:W:83:ARG:NH1	6:W:201:CYC:O1A	2.46	0.49
2:c:89:LEU:HD22	2:c:133:MET:CE	2.42	0.49
3:h:74:THR:HG22	2:m:107:ILE:HG23	1.93	0.49
2:k:107:ILE:HD12	3:l:13:ASP:CG	2.37	0.49
3:n:100:ASP:OD1	3:n:101:PRO:CD	2.51	0.49
2:o:109:ILE:CG2	2:o:159:ALA:HB1	2.43	0.49
6:p:201:CYC:HMA1	6:p:201:CYC:NB	2.27	0.49
2:t:102:THR:N	2:t:103:PRO:HD2	2.28	0.49
4:u:56:THR:HG22	4:u:60:LEU:HD12	1.94	0.49
2:y:109:ILE:CG2	2:y:159:ALA:HB1	2.41	0.49
2:y:115:MET:HG3	3:6:78:TYR:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AS:12:ASP:OD2	3:AT:107:ARG:NH1	2.39	0.49
1:A:254:PRO:CD	4:u:107:TYR:CD1	2.95	0.49
2:I:123:ILE:N	2:I:124:PRO:CD	2.76	0.49
6:V:201:CYC:OB	5:AY:42:GLN:NE2	2.45	0.49
3:f:12:TYR:CZ	3:f:23:ALA:HB2	2.47	0.49
2:g:80:LEU:HD13	6:g:201:CYC:HAD2	1.95	0.49
3:j:107:ARG:HA	5:Ab:45:GLN:HG2	1.94	0.49
2:o:71:ASN:ND2	2:o:122:PRO:HD3	2.28	0.49
2:r:102:THR:N	2:r:103:PRO:HD2	2.27	0.49
4:s:104:LEU:HD13	4:s:156:LEU:HG	1.94	0.49
6:1:201:CYC:HB	6:1:201:CYC:CMA	2.26	0.49
3:4:10:ASN:HA	5:Aa:64:ASN:HD21	1.78	0.49
3:4:83:ARG:NH2	6:4:201:CYC:CGA	2.76	0.49
3:0:67:ARG:CG	3:0:68:PRO:HD2	2.43	0.49
3:AD:123:ILE:HG23	3:AD:160:LEU:HD13	1.94	0.49
3:AF:12:TYR:CZ	3:AF:23:ALA:HB2	2.47	0.49
2:AU:109:ILE:HG23	2:AU:159:ALA:HB1	1.94	0.49
1:A:1015:TYR:CE1	1:A:1016:LEU:HD22	2.47	0.49
1:C:21:MET:HE2	3:q:30:TYR:OH	2.13	0.49
1:C:761:ARG:O	1:C:761:ARG:HG2	2.11	0.49
3:b:148:GLU:O	3:b:151:ILE:HG12	2.13	0.49
2:e:4:LEU:HD13	3:f:98:ALA:HA	1.94	0.49
2:e:80:LEU:HD12	6:e:201:CYC:HAD2	1.95	0.49
2:r:123:ILE:N	2:r:124:PRO:CD	2.76	0.49
2:w:16:ARG:HH12	2:w:19:SER:HB2	1.77	0.49
2:AG:112:VAL:HG11	2:AG:160:MET:HE1	1.95	0.49
6:AS:201:CYC:HMA3	3:AV:66:THR:CG2	2.43	0.49
1:A:21:MET:HE2	3:v:30:TYR:OH	2.12	0.49
1:C:625:LYS:HE3	3:f:110:ASN:ND2	2.27	0.49
1:C:1141:SER:OG	3:N:76:ARG:CZ	2.61	0.49
3:N:58:LYS:NZ	3:N:135:GLU:OE2	2.42	0.49
3:N:148:GLU:O	3:N:151:ILE:HG12	2.13	0.49
3:P:148:GLU:O	3:P:151:ILE:HG12	2.13	0.49
2:G:123:ILE:N	2:G:124:PRO:CD	2.76	0.49
3:V:47:ASN:OD1	2:W:131:ARG:NH2	2.46	0.49
2:g:24:ASP:HA	2:g:27:LYS:HG2	1.95	0.49
2:y:109:ILE:HG23	2:y:159:ALA:HB1	1.95	0.49
2:AA:102:THR:N	2:AA:103:PRO:HD2	2.28	0.49
2:AA:109:ILE:HG23	2:AA:159:ALA:HB1	1.93	0.49
6:AG:201:CYC:HMA3	3:AJ:66:THR:CG2	2.42	0.49
2:AI:109:ILE:HG23	2:AI:159:ALA:HB1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AK:102:THR:N	2:AK:103:PRO:HD2	2.28	0.49
3:AP:2:GLN:HG3	3:AP:100:ASP:OD2	2.13	0.49
1:A:293:LYS:O	1:A:294:GLU:CB	2.61	0.48
1:A:543:ASN:OD1	1:A:546:PHE:HB3	2.12	0.48
1:A:1135:LEU:HD22	6:R:201:CYC:OB	2.12	0.48
1:A:1153:VAL:HG13	3:R:63:SER:HB2	1.94	0.48
2:U:123:ILE:N	2:U:124:PRO:CD	2.76	0.48
2:W:102:THR:N	2:W:103:PRO:HD2	2.27	0.48
2:e:102:THR:N	2:e:103:PRO:HD2	2.28	0.48
2:w:27:LYS:NZ	3:x:39:ARG:HH22	2.10	0.48
2:9:102:THR:N	2:9:103:PRO:HD2	2.26	0.48
2:AC:109:ILE:CG2	2:AC:159:ALA:HB1	2.42	0.48
2:AM:109:ILE:HG23	2:AM:159:ALA:HB1	1.93	0.48
3:AV:12:TYR:CZ	3:AV:23:ALA:HB2	2.47	0.48
1:C:254:PRO:HG3	4:s:107:TYR:CG	2.47	0.48
3:F:12:TYR:CZ	3:F:23:ALA:HB2	2.47	0.48
2:G:102:THR:N	2:G:103:PRO:HD2	2.27	0.48
2:K:102:THR:N	2:K:103:PRO:HD2	2.27	0.48
6:K:201:CYC:CMA	6:K:201:CYC:HB	2.26	0.48
2:W:123:ILE:N	2:W:124:PRO:CD	2.76	0.48
6:e:201:CYC:HB	6:e:201:CYC:CMA	2.26	0.48
2:1:123:ILE:N	2:1:124:PRO:CD	2.77	0.48
2:3:109:ILE:HD11	2:3:156:LEU:CD2	2.43	0.48
6:5:201:CYC:HBC2	6:5:201:CYC:HMC1	1.93	0.48
2:9:80:LEU:HD23	6:9:201:CYC:HAD2	1.95	0.48
2:AC:14:GLU:HB3	2:AC:16:ARG:HD2	1.95	0.48
2:AK:109:ILE:HD13	2:AK:155:TYR:HE2	1.78	0.48
2:AQ:85:LEU:HD22	2:AQ:133:MET:HE2	1.94	0.48
3:AT:100:ASP:OD1	3:AT:101:PRO:CD	2.49	0.48
2:AU:5:THR:HG23	3:AV:1:MET:SD	2.53	0.48
1:C:307:ARG:HG2	1:C:307:ARG:HH21	1.78	0.48
2:M:102:THR:N	2:M:103:PRO:HD2	2.28	0.48
3:F:29:ALA:O	3:F:32:THR:HG22	2.13	0.48
2:I:102:THR:N	2:I:103:PRO:HD2	2.28	0.48
3:R:112:LEU:CD1	6:R:201:CYC:HMB3	2.42	0.48
3:X:115:THR:HG21	6:X:201:CYC:HMA3	1.96	0.48
2:Y:123:ILE:N	2:Y:124:PRO:CD	2.76	0.48
2:g:119:LEU:O	2:g:120:GLN:HB2	2.12	0.48
3:h:143:PRO:HG3	2:t:41:GLN:HE22	1.77	0.48
3:l:123:ILE:HG23	3:l:160:LEU:HD13	1.94	0.48
4:u:83:ARG:NH1	4:u:84:ASP:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AF:116:TYR:HE2	3:AF:160:LEU:HD11	1.79	0.48
2:AO:109:ILE:CG2	2:AO:159:ALA:HB1	2.42	0.48
2:AU:109:ILE:HG22	2:AU:109:ILE:O	2.12	0.48
1:C:254:PRO:HD3	4:s:107:TYR:CE2	2.48	0.48
1:C:1036:VAL:HG13	1:C:1066:PHE:CE1	2.48	0.48
6:C:2101:CYC:HMA1	6:C:2101:CYC:NB	2.24	0.48
2:G:47:ARG:HD2	2:G:48:GLU:HG3	1.94	0.48
2:I:116:TYR:HB2	2:I:123:ILE:HD11	1.95	0.48
6:R:201:CYC:CMA	6:R:201:CYC:NB	2.76	0.48
3:V:148:GLU:O	3:V:151:ILE:HG12	2.12	0.48
2:g:130:VAL:HG21	2:g:156:LEU:CD2	2.43	0.48
2:o:123:ILE:N	2:o:124:PRO:CD	2.76	0.48
2:t:4:LEU:CD2	2:t:26:ILE:HG23	2.43	0.48
4:u:1:MET:SD	4:u:103:LEU:HA	2.53	0.48
2:5:4:LEU:HD13	3:6:98:ALA:HA	1.95	0.48
2:5:102:THR:N	2:5:103:PRO:HD2	2.28	0.48
3:6:57:ALA:HA	3:6:61:ILE:HG12	1.96	0.48
2:7:4:LEU:HD12	2:7:26:ILE:CD1	2.43	0.48
2:AI:102:THR:N	2:AI:103:PRO:HD2	2.28	0.48
2:AK:109:ILE:CG2	2:AK:159:ALA:HB1	2.43	0.48
2:AU:109:ILE:CG2	2:AU:109:ILE:O	2.62	0.48
2:AW:81:CYS:HA	6:AW:201:CYC:HHD	1.96	0.48
1:A:539:LYS:HZ1	5:Aa:24:GLN:HE21	1.60	0.48
1:A:1133:GLU:O	1:A:1135:LEU:N	2.44	0.48
1:C:372:ARG:NH1	6:p:201:CYC:O1A	2.46	0.48
2:M:131:ARG:HH22	3:P:46:SER:HB2	1.78	0.48
2:E:5:THR:OG1	3:F:3:ASP:OD2	2.30	0.48
3:F:77:ARG:NH2	5:AZ:62:GLY:HA2	2.28	0.48
2:K:123:ILE:N	2:K:124:PRO:CD	2.76	0.48
2:e:109:ILE:HG23	2:e:159:ALA:HB1	1.96	0.48
2:g:5:THR:OG1	3:h:3:ASP:OD2	2.29	0.48
2:m:123:ILE:N	2:m:124:PRO:CD	2.76	0.48
3:v:78:TYR:CD2	2:w:115:MET:HG3	2.49	0.48
2:5:37:LEU:HD22	3:6:24:LEU:HD22	1.96	0.48
2:7:60:GLN:OE1	2:AM:69:GLY:HA3	2.13	0.48
6:7:201:CYC:HB	6:7:201:CYC:CMA	2.26	0.48
2:AQ:33:GLY:HA3	3:AR:31:PHE:CZ	2.48	0.48
2:AU:102:THR:N	2:AU:103:PRO:HD2	2.28	0.48
1:A:732:ARG:NE	3:AH:69:GLY:HA3	2.28	0.48
1:C:3:ILE:CG2	4:s:110:ASN:HA	2.42	0.48
1:C:21:MET:HG3	3:q:5:ILE:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:SER:HB2	6:C:2101:CYC:H3C	1.89	0.48
1:C:601:LYS:HE2	1:C:670:TYR:CD1	2.48	0.48
2:M:123:ILE:N	2:M:124:PRO:CD	2.76	0.48
2:E:123:ILE:N	2:E:124:PRO:CD	2.76	0.48
2:Q:17:TYR:CE2	3:R:90:ARG:HA	2.48	0.48
2:Q:102:THR:N	2:Q:103:PRO:HD2	2.28	0.48
2:S:102:THR:N	2:S:103:PRO:HD2	2.27	0.48
3:X:72:MET:HE2	6:X:201:CYC:H2C	1.95	0.48
2:a:123:ILE:N	2:a:124:PRO:CD	2.76	0.48
2:k:123:ILE:N	2:k:124:PRO:CD	2.77	0.48
6:m:201:CYC:HMA3	6:m:201:CYC:HB	1.78	0.48
2:t:128:GLU:OE2	2:t:131:ARG:NH1	2.46	0.48
3:z:103:ILE:HA	3:z:106:GLU:HG2	1.95	0.48
6:7:201:CYC:HB	6:7:201:CYC:HMA3	1.78	0.48
2:AE:33:GLY:HA3	3:AF:31:PHE:CZ	2.49	0.48
2:AI:5:THR:HG23	3:AJ:1:MET:SD	2.54	0.48
1:A:551:MET:HG3	1:A:552:VAL:HG12	1.96	0.48
1:C:641:ASP:OD1	1:C:643:VAL:HB	2.14	0.48
1:C:974:LEU:HD13	3:N:1:MET:N	2.27	0.48
3:T:60:LEU:HB3	3:T:72:MET:HE1	1.96	0.48
3:V:29:ALA:O	3:V:32:THR:HG22	2.13	0.48
2:e:4:LEU:HD11	3:f:3:ASP:CG	2.37	0.48
2:AA:4:LEU:HD22	3:AB:3:ASP:HB2	1.96	0.48
2:AE:43:LEU:HD11	2:AE:141:LEU:CD1	2.35	0.48
2:AW:102:THR:N	2:AW:103:PRO:HD2	2.28	0.48
1:A:29:ASN:OD1	3:v:94:TYR:CE2	2.66	0.48
1:A:1143:LEU:HD22	3:Z:10:ASN:OD1	2.14	0.48
1:C:162:TRP:CZ3	6:C:2101:CYC:C1B	2.97	0.48
1:C:254:PRO:HG3	4:s:107:TYR:HB3	1.94	0.48
1:C:732:ARG:NE	3:AT:69:GLY:HA3	2.29	0.48
6:E:201:CYC:HC	6:E:201:CYC:HMD2	1.78	0.48
2:c:109:ILE:HD12	2:c:159:ALA:CB	2.44	0.48
2:c:123:ILE:N	2:c:124:PRO:CD	2.77	0.48
1:A:622:TYR:CD1	3:6:110:ASN:O	2.67	0.48
1:A:718:MET:CE	2:AA:79:ALA:HB2	2.44	0.48
1:C:258:LEU:HD12	1:C:259:PRO:HD2	1.94	0.48
1:C:733:SER:OG	3:AH:154:ASP:OD2	2.32	0.48
2:Q:131:ARG:HH22	3:T:46:SER:HB2	1.79	0.48
3:R:148:GLU:O	3:R:151:ILE:HG12	2.13	0.48
2:Y:102:THR:N	2:Y:103:PRO:HD2	2.28	0.48
3:h:105:ASP:HA	3:h:109:LEU:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:66:VAL:HG23	2:k:73:TYR:HA	1.96	0.48
3:q:85:MET:HG2	6:q:201:CYC:HBC1	1.96	0.48
3:x:57:ALA:HA	3:x:61:ILE:HG12	1.96	0.48
6:x:201:CYC:HMA1	6:x:201:CYC:NB	2.27	0.48
3:z:105:ASP:HA	3:z:109:LEU:HB2	1.95	0.48
2:3:109:ILE:O	2:3:109:ILE:CG2	2.61	0.48
2:5:123:ILE:N	2:5:124:PRO:CD	2.77	0.48
2:7:71:ASN:ND2	2:7:121:THR:OG1	2.47	0.48
3:AD:24:LEU:O	3:AD:27:LEU:CG	2.51	0.48
2:AK:123:ILE:N	2:AK:124:PRO:CD	2.77	0.48
6:AK:201:CYC:HC	6:AK:201:CYC:HMD2	1.78	0.48
2:AM:20:PRO:HB3	2:AO:151:PHE:CZ	2.49	0.48
2:AM:102:THR:N	2:AM:103:PRO:HD2	2.28	0.48
2:AO:14:GLU:HB3	2:AO:16:ARG:HD2	1.95	0.48
3:AP:87:TYR:CE1	5:Ad:19:THR:O	2.66	0.48
2:AQ:43:LEU:HD11	2:AQ:141:LEU:CD1	2.35	0.48
2:AS:81:CYS:HA	6:AS:201:CYC:HHD	1.96	0.48
1:A:25:ILE:HG21	3:v:1:MET:CE	2.43	0.48
1:C:166:TYR:CD1	6:C:2101:CYC:CBB	2.96	0.48
1:C:701:ASP:OD1	1:C:701:ASP:C	2.57	0.48
3:P:60:LEU:HB3	3:P:72:MET:HE1	1.96	0.48
3:J:148:GLU:O	3:J:151:ILE:HG12	2.12	0.48
2:U:102:THR:N	2:U:103:PRO:HD2	2.28	0.48
2:W:105:GLU:HG3	2:W:109:ILE:CG1	2.44	0.48
2:Y:6:LYS:HE2	2:Y:100:ASP:OD2	2.14	0.48
2:c:109:ILE:O	2:c:109:ILE:CG2	2.61	0.48
3:l:140:LEU:CD2	2:AE:140:LEU:HD22	2.44	0.48
2:m:109:ILE:HG23	2:m:159:ALA:HB1	1.94	0.48
2:7:123:ILE:N	2:7:124:PRO:CD	2.76	0.48
3:0:134:LYS:HB3	3:0:134:LYS:HE3	1.78	0.48
2:AE:35:ARG:O	2:AE:38:ARG:HG3	2.13	0.48
2:AI:25:ARG:NH2	2:AK:25:ARG:NH2	2.62	0.48
3:AJ:35:ALA:HB1	3:AJ:39:ARG:NH2	2.29	0.48
3:AX:2:GLN:HE21	3:AX:7:ALA:HB2	1.79	0.48
5:AZ:9:ALA:HB3	5:AZ:28:PHE:HE2	1.79	0.48
1:A:27:GLY:O	1:A:31:GLU:HG2	2.14	0.47
1:A:470:HIS:CG	1:A:471:PRO:HD2	2.49	0.47
1:C:749:GLN:O	1:C:750:ARG:O	2.32	0.47
3:Z:115:THR:HG21	6:Z:201:CYC:HMA2	1.96	0.47
2:i:97:VAL:HG23	3:j:9:ILE:HD11	1.95	0.47
2:o:2:SER:HG	2:o:4:LEU:HG	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:76:LYS:O	2:9:80:LEU:HD13	2.13	0.47
2:AS:115:MET:HG3	3:AV:78:TYR:CD2	2.49	0.47
3:AV:35:ALA:HB1	3:AV:39:ARG:NH2	2.29	0.47
2:AW:109:ILE:HD13	2:AW:155:TYR:HE2	1.78	0.47
1:A:611:GLU:HA	1:A:614:ARG:HH11	1.79	0.47
1:C:27:GLY:O	1:C:31:GLU:HG2	2.14	0.47
3:d:115:THR:HG21	6:d:201:CYC:HMA2	1.96	0.47
3:f:2:GLN:N	3:f:102:SER:HG	2.11	0.47
3:v:24:LEU:O	3:v:28:LYS:HG3	2.14	0.47
3:2:66:THR:CG2	6:3:201:CYC:HMA2	2.45	0.47
2:3:123:ILE:N	2:3:124:PRO:CD	2.78	0.47
2:AG:115:MET:HG3	3:AJ:78:TYR:CD2	2.49	0.47
2:AM:29:PHE:CE1	2:AM:36:ARG:CZ	2.97	0.47
2:AS:112:VAL:HG11	2:AS:160:MET:HE1	1.95	0.47
2:AU:25:ARG:NH2	2:AW:25:ARG:NH2	2.62	0.47
1:A:386:ILE:HG23	2:w:14:GLU:O	2.14	0.47
1:A:491:THR:CB	3:v:117:ASN:HD22	2.27	0.47
1:A:547:ARG:HD3	3:0:110:ASN:HB2	1.96	0.47
1:A:741:GLN:OE1	3:AH:77:ARG:CZ	2.62	0.47
1:A:749:GLN:O	1:A:750:ARG:O	2.32	0.47
1:C:29:ASN:OD1	3:q:94:TYR:CE2	2.67	0.47
2:I:6:LYS:HE2	2:I:100:ASP:OD2	2.14	0.47
2:K:130:VAL:HG21	2:K:160:MET:HE1	1.97	0.47
4:s:85:MET:HG2	6:s:201:CYC:HBC1	1.95	0.47
2:5:109:ILE:O	2:5:109:ILE:HG22	2.14	0.47
2:AA:71:ASN:ND2	2:AA:121:THR:OG1	2.48	0.47
6:AG:201:CYC:HB	6:AG:201:CYC:CMA	2.24	0.47
2:AM:123:ILE:N	2:AM:124:PRO:CD	2.77	0.47
3:AP:12:TYR:CZ	3:AP:23:ALA:HB2	2.50	0.47
2:AW:123:ILE:N	2:AW:124:PRO:CD	2.77	0.47
1:A:3:ILE:CD1	1:A:6:THR:HG22	2.45	0.47
1:A:641:ASP:OD1	1:A:643:VAL:HB	2.14	0.47
1:A:858:GLY:HA2	2:AI:13:ALA:O	2.14	0.47
1:A:875:LEU:CD1	1:A:876:TYR:CD2	2.98	0.47
1:A:1043:GLU:HA	1:A:1046:ARG:NE	2.28	0.47
1:C:1153:VAL:HG13	3:N:63:SER:CB	2.45	0.47
3:P:71:MEN:HE21	6:P:201:CYC:HBD2	1.97	0.47
2:G:105:GLU:HG3	2:G:109:ILE:CG1	2.44	0.47
2:i:4:LEU:HD13	3:j:98:ALA:HA	1.95	0.47
2:m:71:ASN:ND2	2:m:121:THR:OG1	2.47	0.47
6:m:201:CYC:HB	6:m:201:CYC:CMA	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:r:109:ILE:HG23	2:r:159:ALA:HB1	1.96	0.47
3:2:151:ILE:CD1	3:2:152:TYR:CE2	2.95	0.47
2:5:109:ILE:HG23	2:5:159:ALA:HB1	1.96	0.47
2:AA:29:PHE:CE1	2:AA:36:ARG:CZ	2.97	0.47
3:AF:83:ARG:O	3:AF:86:ASP:OD1	2.33	0.47
3:AL:2:GLN:HE21	3:AL:7:ALA:HB2	1.79	0.47
3:AR:87:TYR:CZ	5:Ad:38:PHE:HZ	2.32	0.47
3:AR:116:TYR:HE2	3:AR:160:LEU:HD11	1.79	0.47
1:C:162:TRP:CG	6:C:2101:CYC:HBB2	2.50	0.47
2:M:61:LYS:NZ	2:M:132:ALA:HB2	2.29	0.47
2:Q:63:PRO:HB2	2:k:60:GLN:HG2	1.95	0.47
2:g:4:LEU:HD11	3:h:3:ASP:CG	2.40	0.47
2:t:109:ILE:HG22	2:t:109:ILE:O	2.13	0.47
2:AA:109:ILE:O	2:AA:109:ILE:CG2	2.63	0.47
2:AC:19:SER:OG	2:AC:20:PRO:HD2	2.14	0.47
2:AC:123:ILE:N	2:AC:124:PRO:CD	2.77	0.47
2:AI:123:ILE:N	2:AI:124:PRO:CD	2.78	0.47
2:AM:109:ILE:O	2:AM:109:ILE:CG2	2.63	0.47
3:AR:83:ARG:O	3:AR:86:ASP:OD1	2.32	0.47
1:C:166:TYR:HB3	1:C:179:LEU:HD23	1.97	0.47
2:E:50:ILE:HA	2:E:136:VAL:HG11	1.97	0.47
2:m:27:LYS:CE	3:n:39:ARG:CZ	2.92	0.47
4:s:13:ASP:OD1	4:s:14:SER:N	2.48	0.47
2:t:35:ARG:HG3	2:t:38:ARG:NH2	2.29	0.47
3:6:96:MET:HA	3:6:152:TYR:CE1	2.50	0.47
2:AS:80:LEU:HD13	6:AS:201:CYC:CAD	2.43	0.47
2:AU:123:ILE:N	2:AU:124:PRO:CD	2.78	0.47
5:Ad:28:PHE:HE1	5:Ad:30:LYS:HZ2	1.63	0.47
1:A:15:ARG:HG3	1:A:267:ASP:OD2	2.15	0.47
1:A:781:ALA:HA	1:A:784:ILE:HD12	1.97	0.47
1:C:3:ILE:CD1	1:C:6:THR:HG22	2.44	0.47
1:C:718:MET:CE	2:AM:79:ALA:HB2	2.44	0.47
2:E:89:LEU:HB3	3:F:18:TYR:OH	2.15	0.47
3:F:81:CYS:HA	6:F:201:CYC:CHD	2.45	0.47
2:K:119:LEU:O	2:K:120:GLN:HB2	2.15	0.47
2:Q:115:MET:HG3	3:X:78:TYR:CD2	2.50	0.47
2:Q:123:ILE:N	2:Q:124:PRO:CD	2.76	0.47
2:U:91:LEU:HB3	2:U:104:ILE:HG23	1.97	0.47
3:V:96:MET:HA	3:V:152:TYR:CE1	2.50	0.47
2:Y:27:LYS:HE3	2:a:151:PHE:HE1	1.80	0.47
2:a:91:LEU:HB3	2:a:104:ILE:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:85:MET:HG2	6:b:201:CYC:HBC1	1.96	0.47
2:c:27:LYS:HG3	3:d:38:VAL:HG11	1.96	0.47
2:c:71:ASN:OD1	2:c:120:GLN:C	2.58	0.47
3:f:96:MET:HA	3:f:152:TYR:CE1	2.50	0.47
2:g:89:LEU:HD22	2:g:133:MET:CE	2.45	0.47
2:i:91:LEU:HB3	2:i:104:ILE:HG23	1.97	0.47
2:i:123:ILE:N	2:i:124:PRO:CD	2.77	0.47
2:m:109:ILE:CG2	2:m:159:ALA:HB1	2.45	0.47
6:m:201:CYC:HBD2	6:m:201:CYC:HHA	1.96	0.47
2:r:5:THR:OG1	4:s:3:ASP:OD2	2.26	0.47
2:t:109:ILE:CG2	2:t:109:ILE:O	2.62	0.47
4:u:13:ASP:OD1	4:u:14:SER:N	2.48	0.47
3:v:161:SER:O	3:6:155:TYR:HE1	1.96	0.47
2:w:4:LEU:HD11	3:x:3:ASP:CG	2.39	0.47
2:1:91:LEU:HB3	2:1:104:ILE:HG23	1.97	0.47
3:2:87:TYR:CE2	5:Aa:38:PHE:CZ	3.03	0.47
2:7:89:LEU:HD22	2:7:133:MET:CE	2.45	0.47
2:7:109:ILE:CG2	2:7:109:ILE:O	2.63	0.47
6:8:201:CYC:CMA	6:8:201:CYC:HB	2.28	0.47
2:AE:123:ILE:N	2:AE:124:PRO:CD	2.77	0.47
2:AG:81:CYS:HA	6:AG:201:CYC:CHD	2.45	0.47
2:AG:123:ILE:N	2:AG:124:PRO:CD	2.78	0.47
2:AI:109:ILE:CG2	2:AI:109:ILE:O	2.62	0.47
2:AM:4:LEU:HD22	3:AN:3:ASP:HB2	1.96	0.47
2:AM:4:LEU:HD11	3:AN:97:LEU:O	2.15	0.47
2:AM:71:ASN:ND2	2:AM:121:THR:OG1	2.48	0.47
3:AN:60:LEU:HB3	3:AN:72:MET:HE1	1.96	0.47
2:AO:123:ILE:N	2:AO:124:PRO:CD	2.77	0.47
2:AQ:109:ILE:CG2	2:AQ:109:ILE:O	2.63	0.47
2:AS:123:ILE:N	2:AS:124:PRO:CD	2.78	0.47
2:AU:116:TYR:CE1	2:AU:121:THR:HG21	2.38	0.47
6:AW:201:CYC:HC	6:AW:201:CYC:HMD2	1.78	0.47
1:A:459:PHE:O	1:A:460:ALA:CB	2.50	0.47
1:A:539:LYS:HZ2	5:Aa:24:GLN:NE2	2.12	0.47
1:C:15:ARG:HG3	1:C:267:ASP:OD2	2.15	0.47
3:V:81:CYS:HA	6:V:201:CYC:CHD	2.45	0.47
2:a:119:LEU:O	2:a:120:GLN:HB2	2.15	0.47
3:f:57:ALA:HA	3:f:61:ILE:HG12	1.97	0.47
2:g:91:LEU:HB3	2:g:104:ILE:HG23	1.97	0.47
2:w:109:ILE:CG2	2:w:159:ALA:HB1	2.45	0.47
3:4:108:VAL:HG21	3:4:156:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AA:119:LEU:O	2:AA:120:GLN:HB2	2.15	0.47
2:AA:123:ILE:N	2:AA:124:PRO:CD	2.77	0.47
3:AB:60:LEU:HB3	3:AB:72:MET:HE1	1.96	0.47
3:AV:96:MET:HA	3:AV:152:TYR:CE1	2.50	0.47
3:AX:96:MET:HA	3:AX:152:TYR:CE1	2.50	0.47
1:A:505:VAL:HG13	3:z:110:ASN:HD22	1.80	0.47
1:C:470:HIS:CG	1:C:471:PRO:HD2	2.49	0.47
1:C:714:ASP:OD2	1:C:717:ARG:NH2	2.47	0.47
1:C:781:ALA:HA	1:C:784:ILE:HD12	1.97	0.47
1:C:858:GLY:HA2	2:AU:13:ALA:O	2.14	0.47
6:E:201:CYC:HB	6:E:201:CYC:HMA3	1.80	0.47
2:G:62:ARG:HE	2:G:62:ARG:HB3	1.61	0.47
2:K:156:LEU:HD23	2:K:156:LEU:HA	1.79	0.47
3:d:96:MET:HA	3:d:152:TYR:CE1	2.50	0.47
2:e:109:ILE:CG2	2:e:109:ILE:O	2.63	0.47
2:g:134:LYS:HE2	2:g:150:GLY:HA2	1.96	0.47
2:k:52:LYS:O	2:k:52:LYS:NZ	2.47	0.47
3:n:57:ALA:HA	3:n:61:ILE:HG12	1.97	0.47
2:o:115:MET:HG3	3:q:78:TYR:CD2	2.50	0.47
2:3:91:LEU:HB3	2:3:104:ILE:HG23	1.97	0.47
3:0:2:GLN:HG3	3:0:100:ASP:OD2	2.15	0.47
2:AA:50:ILE:HA	2:AA:136:VAL:HG11	1.97	0.47
2:AC:91:LEU:HB3	2:AC:104:ILE:HG23	1.97	0.47
2:AE:109:ILE:CG2	2:AE:109:ILE:O	2.63	0.47
2:AG:83:ARG:HH22	6:AG:201:CYC:C1A	2.27	0.47
2:AI:156:LEU:HA	2:AI:156:LEU:HD23	1.81	0.47
2:AO:91:LEU:HB3	2:AO:104:ILE:HG23	1.97	0.47
2:AQ:97:VAL:HG11	3:AR:27:LEU:HD13	1.97	0.47
2:AW:119:LEU:O	2:AW:120:GLN:HB2	2.15	0.47
1:C:611:GLU:HA	1:C:614:ARG:HH11	1.79	0.47
3:N:96:MET:HA	3:N:152:TYR:CE1	2.50	0.47
2:I:91:LEU:HB3	2:I:104:ILE:HG23	1.97	0.47
2:S:50:ILE:HA	2:S:136:VAL:HG11	1.97	0.47
3:T:78:TYR:CD2	2:U:115:MET:HG3	2.51	0.47
2:a:130:VAL:HG21	2:a:160:MET:HE1	1.97	0.47
2:c:160:MET:HE3	2:c:160:MET:HB2	1.79	0.47
3:l:132:ALA:HA	3:l:135:GLU:HG2	1.97	0.47
2:t:109:ILE:HG23	2:t:159:ALA:HB1	1.97	0.47
4:u:104:LEU:HD13	4:u:156:LEU:HG	1.97	0.47
2:7:119:LEU:O	2:7:120:GLN:HB2	2.15	0.47
6:AS:201:CYC:HB	6:AS:201:CYC:CMA	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AW:109:ILE:CG2	2:AW:109:ILE:O	2.62	0.47
1:C:396:GLY:HA2	1:C:400:ALA:HB2	1.96	0.46
2:M:91:LEU:HB3	2:M:104:ILE:HG23	1.97	0.46
2:E:56:ASP:CG	2:5:75:GLU:OE1	2.58	0.46
2:Y:116:TYR:HB2	2:Y:123:ILE:HD11	1.95	0.46
2:c:20:PRO:HB3	2:e:151:PHE:HB3	1.96	0.46
3:h:50:THR:CG2	3:h:54:GLU:OE2	2.62	0.46
3:j:96:MET:HA	3:j:152:TYR:CE1	2.50	0.46
2:k:109:ILE:O	2:k:109:ILE:HG22	2.15	0.46
2:o:91:LEU:HB3	2:o:104:ILE:HG23	1.97	0.46
2:r:140:LEU:CD2	3:z:140:LEU:HD21	2.45	0.46
2:t:119:LEU:O	2:t:120:GLN:HB2	2.15	0.46
3:2:96:MET:HA	3:2:152:TYR:CE1	2.50	0.46
2:5:5:THR:OG1	3:6:3:ASP:OD2	2.29	0.46
2:AA:20:PRO:HB3	2:AC:151:PHE:CZ	2.49	0.46
2:AE:43:LEU:CD1	2:AE:141:LEU:HD11	2.39	0.46
2:AI:91:LEU:HB3	2:AI:104:ILE:HG23	1.97	0.46
2:AK:109:ILE:CG2	2:AK:109:ILE:O	2.62	0.46
6:AK:201:CYC:CMA	6:AK:201:CYC:NB	2.77	0.46
2:AS:83:ARG:HH22	6:AS:201:CYC:C1A	2.28	0.46
1:C:1144:SER:O	3:N:77:ARG:NH2	2.30	0.46
2:E:56:ASP:HB2	2:5:75:GLU:OE1	2.12	0.46
2:K:71:ASN:ND2	2:K:121:THR:OG1	2.48	0.46
2:a:71:ASN:ND2	2:a:121:THR:OG1	2.48	0.46
2:c:149:ALA:O	2:c:153:PHE:CD2	2.67	0.46
2:i:109:ILE:O	2:i:109:ILE:CG2	2.64	0.46
6:r:201:CYC:HB	6:r:201:CYC:CMA	2.28	0.46
2:t:50:ILE:HA	2:t:136:VAL:HG11	1.97	0.46
2:t:123:ILE:N	2:t:124:PRO:CD	2.77	0.46
6:t:201:CYC:HB	6:t:201:CYC:CMA	2.29	0.46
2:3:102:THR:N	2:3:103:PRO:HD2	2.28	0.46
3:6:47:ASN:HD22	3:6:140:LEU:HD23	1.80	0.46
2:9:123:ILE:N	2:9:124:PRO:CD	2.77	0.46
2:AE:91:LEU:HB3	2:AE:104:ILE:HG23	1.97	0.46
2:AM:119:LEU:O	2:AM:120:GLN:HB2	2.15	0.46
2:AU:128:GLU:OE1	2:AU:131:ARG:NH1	2.49	0.46
5:Ad:13:SER:OG	5:Ad:16:ARG:NH1	2.48	0.46
1:A:67:ILE:HG22	1:A:206:MET:HG2	1.98	0.46
1:A:491:THR:HB	3:v:117:ASN:HD22	1.80	0.46
1:A:547:ARG:HD2	3:0:110:ASN:ND2	2.31	0.46
1:A:581:TYR:CB	2:5:114:GLU:OE2	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:ASP:C	1:A:701:ASP:OD1	2.57	0.46
1:C:396:GLY:CA	1:C:400:ALA:HB2	2.45	0.46
1:C:491:THR:CB	3:q:117:ASN:HD22	2.28	0.46
2:M:115:MET:HG3	3:H:78:TYR:CD2	2.50	0.46
2:O:50:ILE:HA	2:O:136:VAL:HG11	1.97	0.46
2:K:91:LEU:HB3	2:K:104:ILE:HG23	1.97	0.46
2:Q:50:ILE:HA	2:Q:136:VAL:HG11	1.98	0.46
2:S:12:ASP:OD1	2:S:12:ASP:C	2.58	0.46
3:h:100:ASP:OD1	3:h:101:PRO:CD	2.50	0.46
2:r:119:LEU:O	2:r:120:GLN:HB2	2.16	0.46
2:w:109:ILE:CG2	2:w:109:ILE:O	2.64	0.46
3:4:83:ARG:HH21	6:4:201:CYC:CGA	2.28	0.46
3:4:96:MET:HA	3:4:152:TYR:CE1	2.51	0.46
2:AI:116:TYR:CE1	2:AI:121:THR:HG21	2.38	0.46
3:AN:96:MET:HA	3:AN:152:TYR:CE1	2.51	0.46
2:AQ:123:ILE:N	2:AQ:124:PRO:CD	2.77	0.46
2:AW:109:ILE:O	2:AW:109:ILE:HG22	2.15	0.46
1:A:253:ARG:NH2	1:A:410:GLU:OE2	2.48	0.46
1:A:323:VAL:HG12	1:A:328:ILE:CD1	2.45	0.46
1:C:253:ARG:NH2	1:C:410:GLU:OE2	2.48	0.46
1:C:620:PRO:HG2	1:C:621:PHE:CD2	2.51	0.46
3:H:96:MET:HA	3:H:152:TYR:CE1	2.50	0.46
2:K:50:ILE:HA	2:K:136:VAL:HG11	1.98	0.46
2:a:61:LYS:HD3	2:a:128:GLU:HG3	1.96	0.46
2:i:119:LEU:O	2:i:120:GLN:HB2	2.16	0.46
2:i:156:LEU:HD23	2:i:156:LEU:HA	1.81	0.46
3:l:151:ILE:CD1	3:l:152:TYR:CE2	2.96	0.46
2:o:4:LEU:HD11	3:p:3:ASP:CG	2.40	0.46
2:r:109:ILE:CG2	2:r:109:ILE:O	2.64	0.46
2:1:71:ASN:ND2	2:1:121:THR:OG1	2.49	0.46
2:3:20:PRO:HB3	2:5:151:PHE:HB3	1.98	0.46
2:5:109:ILE:CG2	2:5:109:ILE:O	2.63	0.46
2:7:102:THR:N	2:7:103:PRO:HD2	2.30	0.46
2:7:140:LEU:CD2	3:AT:140:LEU:HD23	2.29	0.46
2:AA:109:ILE:CG2	2:AA:159:ALA:HB1	2.45	0.46
3:AD:2:GLN:N	3:AD:102:SER:HG	2.13	0.46
3:AL:2:GLN:NE2	3:AL:10:ASN:ND2	2.64	0.46
2:AM:50:ILE:HA	2:AM:136:VAL:HG11	1.96	0.46
1:C:311:ALA:C	2:o:114:GLU:OE2	2.58	0.46
1:C:346:GLU:OE1	1:C:347:PHE:CG	2.65	0.46
1:C:551:MET:HG3	1:C:552:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:614:ARG:HH21	2:e:13:ALA:CB	2.29	0.46
1:C:968:GLU:HG2	1:C:973:THR:HG23	1.98	0.46
3:P:78:TYR:CD2	2:E:115:MET:HG3	2.50	0.46
2:E:119:LEU:O	2:E:120:GLN:HB2	2.16	0.46
2:G:119:LEU:O	2:G:120:GLN:HB2	2.16	0.46
2:Q:91:LEU:HB3	2:Q:104:ILE:HG23	1.97	0.46
2:U:50:ILE:HA	2:U:136:VAL:HG11	1.97	0.46
2:c:49:ARG:NH2	2:c:53:GLN:NE2	2.62	0.46
2:e:109:ILE:O	2:e:109:ILE:HG22	2.15	0.46
2:e:123:ILE:N	2:e:124:PRO:CD	2.77	0.46
2:m:109:ILE:CG2	2:m:109:ILE:O	2.63	0.46
3:x:96:MET:HA	3:x:152:TYR:CE1	2.50	0.46
2:7:109:ILE:CG2	2:7:159:ALA:HB1	2.45	0.46
2:AM:109:ILE:CG2	2:AM:159:ALA:HB1	2.45	0.46
2:AO:19:SER:OG	2:AO:20:PRO:HD2	2.14	0.46
3:AP:27:LEU:HD13	3:AP:31:PHE:HE1	1.80	0.46
2:AW:2:SER:HG	2:AW:4:LEU:HG	1.81	0.46
5:AY:9:ALA:HB3	5:AY:28:PHE:HE2	1.79	0.46
1:A:482:GLN:NE2	3:8:107:ARG:HB3	2.31	0.46
1:A:875:LEU:CD1	1:A:876:TYR:CG	2.99	0.46
1:A:1137:SER:HB2	3:R:118:SER:OG	2.15	0.46
1:C:875:LEU:CD1	1:C:876:TYR:CD2	2.98	0.46
2:M:110:ILE:HG13	3:H:76:ARG:HB2	1.98	0.46
2:E:105:GLU:HG3	2:E:109:ILE:CG1	2.46	0.46
3:F:74:THR:HG22	2:K:107:ILE:HG23	1.98	0.46
2:I:50:ILE:HA	2:I:136:VAL:HG11	1.98	0.46
2:Q:44:THR:HG23	3:R:18:TYR:CD2	2.50	0.46
2:g:123:ILE:N	2:g:124:PRO:CD	2.79	0.46
3:j:113:LYS:HE3	3:j:113:LYS:HB3	1.78	0.46
2:m:50:ILE:HA	2:m:136:VAL:HG11	1.98	0.46
2:y:123:ILE:N	2:y:124:PRO:CD	2.78	0.46
2:3:16:ARG:CZ	2:5:155:TYR:HE1	2.29	0.46
2:3:71:ASN:ND2	2:3:121:THR:OG1	2.49	0.46
2:AI:128:GLU:OE1	2:AI:131:ARG:NH1	2.49	0.46
3:AJ:96:MET:HA	3:AJ:152:TYR:CE1	2.50	0.46
2:AK:119:LEU:O	2:AK:120:GLN:HB2	2.15	0.46
3:AP:151:ILE:CD1	3:AP:152:TYR:CE2	2.96	0.46
1:A:1036:VAL:HG13	1:A:1066:PHE:CE1	2.48	0.46
1:C:322:LYS:HB2	1:C:328:ILE:HG12	1.98	0.46
3:n:96:MET:HA	3:n:152:TYR:CE1	2.51	0.46
2:o:97:VAL:CG1	3:p:27:LEU:HD13	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:w:2:SER:HG	2:w:4:LEU:HG	1.80	0.46
2:y:4:LEU:HD11	3:z:3:ASP:HB2	1.95	0.46
3:2:100:ASP:OD1	3:2:101:PRO:CD	2.50	0.46
2:5:50:ILE:HA	2:5:136:VAL:HG11	1.98	0.46
2:7:50:ILE:HA	2:7:136:VAL:HG11	1.98	0.46
3:8:57:ALA:HA	3:8:61:ILE:HG12	1.97	0.46
2:AK:109:ILE:O	2:AK:109:ILE:HG22	2.15	0.46
3:AL:57:ALA:HA	3:AL:61:ILE:HG12	1.98	0.46
2:AS:112:VAL:HG21	2:AS:160:MET:CE	2.24	0.46
5:Ab:31:LEU:HD23	5:Ab:31:LEU:HA	1.80	0.46
1:A:1066:PHE:O	1:A:1067:LEU:CB	2.64	0.46
1:C:166:TYR:CE1	6:C:2101:CYC:CBB	2.99	0.46
1:C:614:ARG:HH21	2:e:13:ALA:HB1	1.81	0.46
1:C:1015:TYR:CE1	1:C:1016:LEU:HD22	2.47	0.46
3:P:96:MET:HA	3:P:152:TYR:CE1	2.51	0.46
2:I:119:LEU:O	2:I:120:GLN:HB2	2.15	0.46
2:K:105:GLU:HG3	2:K:109:ILE:CG1	2.46	0.46
2:U:156:LEU:HD23	2:U:156:LEU:HA	1.80	0.46
2:W:119:LEU:O	2:W:120:GLN:HB2	2.16	0.46
3:b:96:MET:HA	3:b:152:TYR:CE1	2.51	0.46
2:e:50:ILE:HA	2:e:136:VAL:HG11	1.98	0.46
3:f:100:ASP:OD1	3:f:101:PRO:CD	2.50	0.46
2:k:109:ILE:CG2	2:k:109:ILE:O	2.63	0.46
3:8:96:MET:HA	3:8:152:TYR:CE1	2.51	0.46
3:AB:96:MET:HA	3:AB:152:TYR:CE1	2.51	0.46
2:AC:4:LEU:HD11	3:AD:3:ASP:CB	2.42	0.46
2:AC:110:ILE:HG13	3:AL:76:ARG:HB2	1.98	0.46
3:AL:96:MET:HA	3:AL:152:TYR:CE1	2.50	0.46
2:AU:140:LEU:C	2:AU:140:LEU:HD12	2.41	0.46
3:AV:57:ALA:HA	3:AV:61:ILE:HG12	1.97	0.46
3:AX:14:VAL:HG12	5:Ad:64:ASN:HD22	1.81	0.46
1:C:156:SER:HA	6:C:2101:CYC:H3C	1.96	0.46
1:C:165:ARG:NH2	1:C:169:TYR:OH	2.49	0.46
1:C:247:ARG:HH11	1:C:256:LEU:HD12	1.81	0.46
3:T:71:MEN:HE21	6:T:201:CYC:HBD2	1.98	0.46
2:c:23:LEU:HB3	2:e:151:PHE:HE2	1.80	0.46
2:e:119:LEU:O	2:e:120:GLN:HB2	2.16	0.46
3:f:47:ASN:HD22	3:f:140:LEU:HD23	1.80	0.46
6:h:201:CYC:C2A	6:h:201:CYC:O1A	2.64	0.46
2:m:89:LEU:HD22	2:m:133:MET:CE	2.46	0.46
2:1:109:ILE:HD13	2:1:155:TYR:HE2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:109:ILE:CG2	2:1:159:ALA:HB1	2.46	0.46
6:6:201:CYC:HB	6:6:201:CYC:CMA	2.18	0.46
3:0:140:LEU:HD21	2:AQ:140:LEU:HD23	1.98	0.46
2:AG:50:ILE:HA	2:AG:136:VAL:HG11	1.98	0.46
2:AG:71:ASN:ND2	2:AG:121:THR:OG1	2.49	0.46
2:AI:5:THR:OG1	3:AJ:3:ASP:OD2	2.29	0.46
2:AQ:83:ARG:NH2	2:AQ:84:ASP:OD1	2.49	0.46
5:Aa:18:ARG:HD3	5:Aa:22:GLU:CD	2.41	0.46
1:A:496:GLU:CG	3:6:114:GLU:HG2	2.46	0.46
1:A:702:VAL:O	1:A:702:VAL:CG1	2.64	0.46
1:A:1114:ARG:O	1:A:1115:ARG:C	2.59	0.46
1:C:67:ILE:HG22	1:C:206:MET:HG2	1.98	0.46
1:C:158:ARG:NH2	6:C:2101:CYC:O2A	2.49	0.46
1:C:166:TYR:CE1	6:C:2101:CYC:HBB2	2.50	0.46
1:C:300:ALA:O	1:C:301:TYR:C	2.59	0.46
1:C:434:TRP:HA	4:s:110:ASN:O	2.16	0.46
1:C:444:ASN:OD1	1:C:444:ASN:C	2.58	0.46
1:C:875:LEU:CD1	1:C:876:TYR:CG	2.99	0.46
3:F:57:ALA:HA	3:F:61:ILE:HG12	1.98	0.46
2:G:91:LEU:HB3	2:G:104:ILE:HG23	1.97	0.46
3:R:58:LYS:NZ	3:R:135:GLU:OE2	2.42	0.46
3:X:96:MET:HA	3:X:152:TYR:CE1	2.50	0.46
3:b:81:CYS:HA	6:b:201:CYC:CHD	2.46	0.46
3:d:83:ARG:O	3:d:86:ASP:OD1	2.33	0.46
2:o:119:LEU:O	2:o:120:GLN:HB2	2.16	0.46
3:p:96:MET:HA	3:p:152:TYR:CE1	2.51	0.46
2:r:50:ILE:HA	2:r:136:VAL:HG11	1.97	0.46
2:w:91:LEU:HB3	2:w:104:ILE:HG23	1.97	0.46
2:w:109:ILE:HD13	2:w:155:TYR:HE2	1.81	0.46
2:y:89:LEU:HD22	2:y:133:MET:CE	2.46	0.46
2:AI:50:ILE:HA	2:AI:136:VAL:HG11	1.98	0.46
3:AP:2:GLN:N	3:AP:102:SER:HG	2.14	0.46
2:AQ:35:ARG:O	2:AQ:38:ARG:HG3	2.13	0.46
3:AR:96:MET:HA	3:AR:152:TYR:CE1	2.51	0.46
2:AW:116:TYR:HB2	2:AW:123:ILE:HD11	1.98	0.46
3:AX:2:GLN:HE22	3:AX:10:ASN:HD21	1.64	0.46
3:AX:126:THR:HG23	6:AX:201:CYC:HBC3	1.99	0.46
1:A:47:PHE:CE2	3:v:38:VAL:CG2	2.96	0.45
1:A:388:ARG:HA	1:A:388:ARG:HD2	1.48	0.45
1:A:620:PRO:HG2	1:A:621:PHE:CD2	2.51	0.45
1:A:1033:ARG:HH11	1:A:1097:VAL:CG1	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1055:SER:HB3	1:A:1056:PRO:HD3	1.98	0.45
1:C:1033:ARG:HH11	1:C:1097:VAL:CG1	2.28	0.45
1:C:1062:LEU:HB3	1:C:1096:ILE:CD1	2.46	0.45
2:M:160:MET:HE3	2:M:160:MET:HB2	1.90	0.45
2:E:91:LEU:HB3	2:E:104:ILE:HG23	1.97	0.45
2:Q:160:MET:HE3	2:Q:160:MET:HB2	1.90	0.45
2:S:156:LEU:HA	2:S:156:LEU:HD23	1.78	0.45
3:Z:96:MET:HA	3:Z:152:TYR:CE1	2.51	0.45
2:w:119:LEU:O	2:w:120:GLN:HB2	2.16	0.45
2:y:109:ILE:HG12	2:y:159:ALA:CB	2.46	0.45
3:z:151:ILE:CD1	3:z:152:TYR:CE2	2.97	0.45
3:AD:12:TYR:CZ	3:AD:23:ALA:HB2	2.50	0.45
3:AD:27:LEU:HD13	3:AD:31:PHE:HE1	1.80	0.45
3:AD:96:MET:HA	3:AD:152:TYR:CE1	2.51	0.45
2:AE:43:LEU:CD1	2:AE:141:LEU:HD21	2.46	0.45
6:AM:201:CYC:HMA3	6:AM:201:CYC:HB	1.81	0.45
2:AQ:71:ASN:ND2	2:AQ:121:THR:OG1	2.49	0.45
1:A:436:TRP:CG	4:u:115:THR:HG22	2.51	0.45
1:C:1015:TYR:CE1	1:C:1016:LEU:HD21	2.51	0.45
1:C:1133:GLU:O	1:C:1135:LEU:N	2.44	0.45
6:M:201:CYC:HMA3	6:M:201:CYC:HB	1.80	0.45
3:N:60:LEU:HB3	3:N:72:MET:HE1	1.98	0.45
2:S:97:VAL:CG2	3:T:9:ILE:HD11	2.46	0.45
2:a:62:ARG:HE	2:a:62:ARG:HB3	1.61	0.45
2:i:109:ILE:CG2	2:i:159:ALA:HB1	2.46	0.45
2:i:109:ILE:HD13	2:i:155:TYR:HE2	1.81	0.45
2:k:12:ASP:OD2	3:l:107:ARG:NH1	2.49	0.45
2:k:119:LEU:O	2:k:120:GLN:HB2	2.16	0.45
4:s:72:MET:HE3	4:s:72:MET:HB3	1.77	0.45
2:w:75:GLU:HG2	2:w:76:LYS:H	1.80	0.45
2:w:88:TYR:HB3	2:w:156:LEU:HD21	1.97	0.45
2:y:48:GLU:HG2	2:y:49:ARG:H	1.80	0.45
2:1:109:ILE:CG2	2:1:109:ILE:O	2.64	0.45
2:3:2:SER:HG	2:3:4:LEU:HG	1.80	0.45
6:5:201:CYC:HC	6:5:201:CYC:CMD	2.29	0.45
3:8:100:ASP:OD1	3:8:101:PRO:CD	2.51	0.45
2:AG:119:LEU:O	2:AG:120:GLN:HB2	2.16	0.45
3:AN:100:ASP:OD1	3:AN:101:PRO:CD	2.49	0.45
2:AQ:109:ILE:O	2:AQ:109:ILE:HG22	2.16	0.45
3:AR:88:PHE:HB3	3:AR:156:LEU:CD2	2.44	0.45
2:AU:50:ILE:HA	2:AU:136:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AU:95:GLY:HA3	2:AU:104:ILE:HD11	1.99	0.45
2:AW:71:ASN:ND2	2:AW:121:THR:OG1	2.49	0.45
3:AX:2:GLN:NE2	3:AX:10:ASN:ND2	2.63	0.45
5:Ad:11:ILE:HG12	5:Ad:49:GLY:HA3	1.98	0.45
1:A:322:LYS:HZ3	1:A:336:ARG:HH12	1.65	0.45
1:C:186:LEU:O	1:C:190:LEU:HG	2.15	0.45
1:C:388:ARG:HA	1:C:388:ARG:HD2	1.47	0.45
6:M:201:CYC:HBC2	6:M:201:CYC:HMC1	1.98	0.45
2:E:98:ALA:HA	3:F:5:ILE:HG21	1.97	0.45
3:F:96:MET:HA	3:F:152:TYR:CE1	2.50	0.45
3:H:60:LEU:HB3	3:H:72:MET:HE1	1.98	0.45
3:R:60:LEU:HB3	3:R:72:MET:HE1	1.99	0.45
3:T:96:MET:HA	3:T:152:TYR:CE1	2.51	0.45
2:U:119:LEU:O	2:U:120:GLN:HB2	2.15	0.45
2:c:91:LEU:HB3	2:c:104:ILE:HG23	1.98	0.45
2:c:95:GLY:HA3	2:c:104:ILE:HD11	1.98	0.45
2:c:119:LEU:O	2:c:120:GLN:HB2	2.16	0.45
6:e:201:CYC:HB	6:e:201:CYC:HMA3	1.81	0.45
2:i:38:ARG:HH22	3:j:28:LYS:CE	2.29	0.45
2:k:66:VAL:O	2:k:66:VAL:HG13	2.16	0.45
3:l:96:MET:HA	3:l:152:TYR:CE1	2.51	0.45
3:q:83:ARG:HH22	6:q:201:CYC:C1A	2.30	0.45
4:s:65:LEU:HB3	4:s:72:MET:HG3	1.99	0.45
2:5:95:GLY:HA3	2:5:104:ILE:HD11	1.98	0.45
3:0:96:MET:HA	3:0:152:TYR:CE1	2.51	0.45
2:AC:109:ILE:CG2	2:AC:109:ILE:O	2.64	0.45
2:AE:83:ARG:NH2	2:AE:84:ASP:OD1	2.49	0.45
2:AE:97:VAL:HG11	3:AF:27:LEU:HD13	1.97	0.45
3:AF:88:PHE:HB3	3:AF:156:LEU:CD2	2.44	0.45
2:AK:140:LEU:C	2:AK:140:LEU:HD12	2.41	0.45
2:AQ:50:ILE:HA	2:AQ:136:VAL:HG11	1.99	0.45
2:AS:119:LEU:O	2:AS:120:GLN:HB2	2.17	0.45
1:A:16:LEU:O	1:A:265:SER:HB3	2.17	0.45
1:A:1015:TYR:CE1	1:A:1016:LEU:HD21	2.51	0.45
1:A:1062:LEU:HB3	1:A:1096:ILE:CD1	2.47	0.45
1:C:194:CYS:SG	6:C:2101:CYC:C1D	3.05	0.45
1:C:782:SER:OG	3:AN:83:ARG:HD3	2.17	0.45
2:M:50:ILE:HA	2:M:136:VAL:HG11	1.98	0.45
2:G:50:ILE:HA	2:G:136:VAL:HG11	1.98	0.45
2:Q:110:ILE:HG13	3:X:76:ARG:HB2	1.97	0.45
3:R:96:MET:HA	3:R:152:TYR:CE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:126:THR:OG1	6:R:201:CYC:HMC3	2.17	0.45
2:U:105:GLU:HG3	2:U:109:ILE:CG1	2.46	0.45
2:Y:91:LEU:HB3	2:Y:104:ILE:HG23	1.97	0.45
2:Y:119:LEU:O	2:Y:120:GLN:HB2	2.15	0.45
2:a:50:ILE:HA	2:a:136:VAL:HG11	1.98	0.45
2:e:140:LEU:C	2:e:140:LEU:HD12	2.42	0.45
3:f:155:TYR:HE1	3:q:161:SER:O	1.99	0.45
2:i:14:GLU:HB3	2:i:16:ARG:HG2	1.98	0.45
3:l:100:ASP:OD1	3:l:101:PRO:CD	2.50	0.45
2:m:102:THR:N	2:m:103:PRO:HD2	2.31	0.45
2:o:109:ILE:HD13	2:o:155:TYR:HE2	1.82	0.45
2:r:11:ALA:HB2	2:r:18:LEU:HD23	1.97	0.45
3:z:96:MET:HA	3:z:152:TYR:CE1	2.52	0.45
2:1:50:ILE:HA	2:1:136:VAL:HG11	1.99	0.45
2:3:95:GLY:HA3	2:3:104:ILE:HD11	1.98	0.45
3:4:57:ALA:HA	3:4:61:ILE:HG12	1.98	0.45
2:AG:91:LEU:HB3	2:AG:104:ILE:HG23	1.97	0.45
2:AI:95:GLY:HA3	2:AI:104:ILE:HD11	1.99	0.45
2:AK:95:GLY:HA3	2:AK:104:ILE:HD11	1.99	0.45
2:AM:91:LEU:HB3	2:AM:104:ILE:HG23	1.99	0.45
3:AP:96:MET:HA	3:AP:152:TYR:CE1	2.51	0.45
2:AU:151:PHE:HB3	2:AW:20:PRO:HB3	1.99	0.45
1:A:169:TYR:CE1	3:v:19:LEU:CD1	2.99	0.45
1:A:200:ILE:HG12	1:A:231:ILE:HD11	1.98	0.45
1:C:47:PHE:CE2	3:q:38:VAL:CG2	2.98	0.45
1:C:197:SER:HA	1:C:200:ILE:HD12	1.98	0.45
2:G:81:CYS:HA	6:G:201:CYC:HHD	1.98	0.45
3:H:148:GLU:O	3:H:151:ILE:HG12	2.17	0.45
3:J:96:MET:HA	3:J:152:TYR:CE1	2.51	0.45
6:U:201:CYC:HB	6:U:201:CYC:CMA	2.18	0.45
2:a:57:GLN:HB3	2:a:61:LYS:HE3	1.98	0.45
3:l:57:ALA:HA	3:l:61:ILE:HG12	1.99	0.45
2:o:81:CYS:HA	6:o:201:CYC:HHD	1.99	0.45
2:y:62:ARG:HH22	2:y:124:PRO:HB2	1.81	0.45
2:3:50:ILE:HA	2:3:136:VAL:HG11	1.98	0.45
2:AA:4:LEU:HD11	3:AB:97:LEU:O	2.16	0.45
6:AA:201:CYC:HMA3	6:AA:201:CYC:HB	1.81	0.45
3:AD:83:ARG:HD2	5:Ac:18:ARG:O	2.15	0.45
2:AE:50:ILE:HA	2:AE:136:VAL:HG11	1.99	0.45
2:AS:130:VAL:CG1	2:AS:156:LEU:HD23	2.47	0.45
1:A:148:TYR:HD2	1:A:148:TYR:HA	1.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:968:GLU:HG2	1:A:973:THR:HG23	1.98	0.45
1:C:254:PRO:HB3	2:r:12:ASP:CG	2.41	0.45
1:C:482:GLN:CD	3:n:107:ARG:HH21	2.25	0.45
1:C:759:THR:O	3:AP:106:GLU:OE2	2.35	0.45
3:L:60:LEU:HB3	3:L:72:MET:HE1	1.99	0.45
6:Q:201:CYC:HBC2	6:Q:201:CYC:HMC1	1.98	0.45
2:S:119:LEU:O	2:S:120:GLN:HB2	2.17	0.45
2:a:95:GLY:HA3	2:a:104:ILE:HD11	1.99	0.45
6:a:201:CYC:NB	6:a:201:CYC:HMA3	2.31	0.45
3:b:60:LEU:HB3	3:b:72:MET:HE1	1.98	0.45
2:c:116:TYR:HD1	2:c:121:THR:OG1	1.99	0.45
2:g:4:LEU:HD11	3:h:3:ASP:HB2	1.98	0.45
2:i:33:GLY:HA3	3:j:31:PHE:CZ	2.52	0.45
3:q:67:ARG:CG	3:q:68:PRO:CD	2.93	0.45
2:w:83:ARG:NH2	2:w:84:ASP:OD1	2.50	0.45
2:3:140:LEU:HD12	2:3:140:LEU:C	2.42	0.45
2:7:27:LYS:HG3	3:8:38:VAL:HG11	1.99	0.45
2:AC:140:LEU:C	2:AC:140:LEU:HD12	2.41	0.45
2:AK:2:SER:HG	2:AK:4:LEU:HG	1.80	0.45
3:AN:78:TYR:CE2	2:AU:115:MET:HG3	2.52	0.45
2:AO:109:ILE:CG2	2:AO:109:ILE:O	2.64	0.45
2:AO:140:LEU:HD12	2:AO:140:LEU:C	2.41	0.45
6:AS:201:CYC:CGD	3:AV:62:TYR:OH	2.65	0.45
2:AU:91:LEU:HB3	2:AU:104:ILE:HG23	1.97	0.45
2:AW:83:ARG:NH2	2:AW:84:ASP:OD1	2.50	0.45
1:A:782:SER:OG	3:AB:83:ARG:HD3	2.17	0.45
1:C:204:LEU:HD23	1:C:207:ARG:HH21	1.78	0.45
1:C:323:VAL:HG12	1:C:328:ILE:CD1	2.45	0.45
2:O:97:VAL:CG2	3:P:9:ILE:HD11	2.47	0.45
3:P:134:LYS:HB3	3:P:134:LYS:HE3	1.65	0.45
2:E:20:PRO:CG	2:G:101:VAL:HG13	2.32	0.45
3:J:57:ALA:HA	3:J:61:ILE:HG12	1.99	0.45
2:W:91:LEU:HB3	2:W:104:ILE:HG23	1.97	0.45
3:X:91:TYR:HD2	3:X:103:ILE:HD11	1.81	0.45
2:m:83:ARG:NH2	2:m:84:ASP:OD1	2.50	0.45
2:5:71:ASN:ND2	2:5:121:THR:OG1	2.50	0.45
3:AF:96:MET:HA	3:AF:152:TYR:CE1	2.51	0.45
2:AG:83:ARG:NH2	2:AG:84:ASP:OD1	2.50	0.45
2:AK:50:ILE:HA	2:AK:136:VAL:HG11	1.98	0.45
6:AM:201:CYC:HMC1	6:AM:201:CYC:HBC2	1.99	0.45
3:AP:24:LEU:O	3:AP:27:LEU:CG	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AQ:91:LEU:HB3	2:AQ:104:ILE:HG23	1.97	0.45
2:AS:81:CYS:HA	6:AS:201:CYC:CHD	2.46	0.45
2:AW:140:LEU:C	2:AW:140:LEU:HD12	2.41	0.45
1:A:396:GLY:CA	1:A:400:ALA:HB2	2.47	0.45
1:A:930:LEU:HB3	3:AH:33:THR:CG2	2.47	0.45
1:C:298:ARG:HG3	1:C:302:ARG:HH11	1.81	0.45
1:C:352:ILE:HG21	3:p:110:ASN:O	2.16	0.45
2:E:83:ARG:NH2	2:E:84:ASP:OD1	2.50	0.45
2:W:83:ARG:HH22	6:W:201:CYC:C1A	2.29	0.45
2:W:95:GLY:HA3	2:W:104:ILE:HD11	1.98	0.45
2:c:12:ASP:OD2	3:d:107:ARG:NH2	2.50	0.45
2:c:25:ARG:HD2	2:e:25:ARG:HD3	1.98	0.45
2:g:50:ILE:HA	2:g:136:VAL:HG11	1.98	0.45
3:h:96:MET:HA	3:h:152:TYR:CE1	2.52	0.45
2:i:36:ARG:HG2	2:i:36:ARG:HH11	1.82	0.45
2:m:91:LEU:HB3	2:m:104:ILE:HG23	1.99	0.45
3:q:57:ALA:HA	3:q:61:ILE:HG12	1.98	0.45
2:r:4:LEU:CD2	2:r:26:ILE:HG23	2.47	0.45
2:r:83:ARG:NH2	2:r:84:ASP:OD1	2.50	0.45
2:y:2:SER:HG	2:y:4:LEU:HG	1.81	0.45
2:3:119:LEU:O	2:3:120:GLN:HB2	2.17	0.45
6:9:201:CYC:HB	6:9:201:CYC:CMA	2.21	0.45
2:AE:71:ASN:ND2	2:AE:121:THR:OG1	2.49	0.45
3:AR:57:ALA:HA	3:AR:61:ILE:HG12	1.99	0.45
2:AS:71:ASN:ND2	2:AS:121:THR:OG1	2.49	0.45
2:AS:91:LEU:HB3	2:AS:104:ILE:HG23	1.97	0.45
3:AX:87:TYR:CD2	6:AX:201:CYC:HBB3	2.51	0.45
1:A:300:ALA:O	1:A:301:TYR:C	2.59	0.45
1:A:395:SER:O	1:A:396:GLY:C	2.60	0.45
1:C:47:PHE:CE2	3:q:38:VAL:HG23	2.41	0.45
1:C:288:LEU:HD13	1:C:293:LYS:CG	2.47	0.45
1:C:1074:GLN:HA	1:C:1077:ILE:HD12	1.98	0.45
1:C:1121:ALA:HB1	3:H:107:ARG:O	2.13	0.45
2:M:101:VAL:HG11	2:O:20:PRO:HG2	1.99	0.45
3:F:78:TYR:CE2	2:K:115:MET:HG3	2.52	0.45
3:R:57:ALA:HA	3:R:61:ILE:HG12	1.98	0.45
2:a:105:GLU:HG3	2:a:109:ILE:CG1	2.46	0.45
3:d:71:MEN:O	3:d:77:ARG:HD3	2.16	0.45
2:k:58:LEU:CD1	2:k:59:PHE:CD1	2.99	0.45
2:o:109:ILE:CG2	2:o:109:ILE:O	2.64	0.45
2:o:123:ILE:HD12	2:o:124:PRO:CD	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:q:96:MET:HA	3:q:152:TYR:CE1	2.52	0.45
4:u:81:CYS:SG	6:u:201:CYC:C1C	3.05	0.45
2:y:109:ILE:CG2	2:y:109:ILE:O	2.64	0.45
3:z:134:LYS:HB3	3:z:134:LYS:HE3	1.79	0.45
3:2:144:ASP:O	3:2:147:LYS:HG2	2.17	0.45
2:5:119:LEU:O	2:5:120:GLN:HB2	2.16	0.45
2:AI:151:PHE:HB3	2:AK:20:PRO:HB3	1.99	0.45
2:AK:128:GLU:OE1	2:AK:131:ARG:NH1	2.50	0.45
2:AM:4:LEU:CD2	2:AM:8:ILE:HD12	2.47	0.45
2:AO:119:LEU:O	2:AO:120:GLN:HB2	2.17	0.45
2:AW:50:ILE:HA	2:AW:136:VAL:HG11	1.98	0.45
3:AX:57:ALA:HA	3:AX:61:ILE:HG12	1.98	0.45
5:Ac:9:ALA:HB3	5:Ac:28:PHE:CE2	2.52	0.45
1:C:67:ILE:HD11	1:C:213:LEU:HD21	1.99	0.45
2:M:17:TYR:CE2	3:N:90:ARG:HA	2.51	0.45
3:P:81:CYS:HA	6:P:201:CYC:CHD	2.46	0.45
6:H:201:CYC:HBD1	6:H:201:CYC:HHA	1.99	0.45
2:W:50:ILE:HA	2:W:136:VAL:HG11	1.98	0.45
3:X:60:LEU:HB3	3:X:72:MET:HE1	1.99	0.45
2:Y:50:ILE:HA	2:Y:136:VAL:HG11	1.98	0.45
3:b:57:ALA:HA	3:b:61:ILE:HG12	1.99	0.45
2:c:50:ILE:HA	2:c:136:VAL:HG11	1.99	0.45
2:i:16:ARG:HH12	2:i:19:SER:HB3	1.82	0.45
6:i:201:CYC:HB	6:i:201:CYC:CMA	2.30	0.45
3:j:144:ASP:O	3:j:147:LYS:HG2	2.17	0.45
2:w:71:ASN:ND2	2:w:121:THR:OG1	2.50	0.45
3:AB:112:LEU:CD2	3:AB:160:LEU:HD21	2.47	0.45
3:AD:57:ALA:HA	3:AD:61:ILE:HG12	1.99	0.45
3:AJ:57:ALA:HA	3:AJ:61:ILE:HG12	1.97	0.45
2:AO:109:ILE:HD13	2:AO:155:TYR:HE2	1.82	0.45
2:AQ:43:LEU:CD1	2:AQ:141:LEU:HD21	2.47	0.45
3:AR:62:TYR:HH	6:AW:201:CYC:CGD	2.29	0.45
3:AR:151:ILE:CD1	3:AR:152:TYR:CE2	2.95	0.45
2:AS:83:ARG:NH2	2:AS:84:ASP:OD1	2.50	0.45
1:C:1055:SER:HB3	1:C:1056:PRO:HD3	1.98	0.44
3:N:57:ALA:HA	3:N:61:ILE:HG12	1.99	0.44
6:O:201:CYC:HB	6:O:201:CYC:CMA	2.30	0.44
2:G:83:ARG:NH2	2:G:84:ASP:OD1	2.50	0.44
2:I:83:ARG:NH2	2:I:84:ASP:OD1	2.50	0.44
2:Q:5:THR:OG1	3:R:3:ASP:OD2	2.34	0.44
2:i:69:GLY:HA3	2:AE:60:GLN:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:119:LEU:O	2:m:120:GLN:HB2	2.17	0.44
2:t:83:ARG:NH2	2:t:84:ASP:OD1	2.51	0.44
4:u:73:TYR:OH	3:v:13:ASP:OD1	2.28	0.44
2:y:119:LEU:O	2:y:120:GLN:HB2	2.16	0.44
3:4:87:TYR:CD2	6:4:201:CYC:HBB3	2.52	0.44
2:9:119:LEU:O	2:9:120:GLN:HB2	2.16	0.44
3:AB:78:TYR:CE2	2:AI:115:MET:HG3	2.51	0.44
2:AI:140:LEU:C	2:AI:140:LEU:HD12	2.41	0.44
2:AK:81:CYS:HA	6:AK:201:CYC:HHD	1.98	0.44
2:AO:50:ILE:HA	2:AO:136:VAL:HG11	2.00	0.44
3:AP:57:ALA:HA	3:AP:61:ILE:HG12	1.99	0.44
2:AS:50:ILE:HA	2:AS:136:VAL:HG11	1.98	0.44
3:AV:134:LYS:HB3	3:AV:134:LYS:HE3	1.83	0.44
2:AW:95:GLY:HA3	2:AW:104:ILE:HD11	1.99	0.44
2:AW:128:GLU:OE1	2:AW:131:ARG:NH1	2.50	0.44
1:A:322:LYS:HB2	1:A:328:ILE:HG12	1.98	0.44
1:A:601:LYS:HB2	1:A:676:GLU:HA	1.98	0.44
1:A:653:SER:HB3	3:6:87:TYR:OH	2.17	0.44
1:A:1109:ASP:CG	5:AY:25:ASN:OD1	2.60	0.44
1:A:1115:ARG:O	1:A:1115:ARG:HG3	2.17	0.44
1:C:395:SER:O	1:C:396:GLY:C	2.60	0.44
1:C:693:ARG:HH11	1:C:693:ARG:HG3	1.82	0.44
1:C:1066:PHE:O	1:C:1067:LEU:CB	2.64	0.44
1:C:1114:ARG:O	1:C:1115:ARG:C	2.59	0.44
3:P:53:LYS:NZ	2:E:120:GLN:HG3	2.33	0.44
3:L:96:MET:HA	3:L:152:TYR:CE1	2.51	0.44
2:i:50:ILE:HA	2:i:136:VAL:HG11	1.99	0.44
6:k:201:CYC:HB	6:k:201:CYC:CMA	2.26	0.44
2:o:109:ILE:HG12	2:o:159:ALA:CB	2.47	0.44
2:w:50:ILE:HA	2:w:136:VAL:HG11	1.98	0.44
2:3:50:ILE:HD11	2:3:140:LEU:HD21	1.99	0.44
2:3:83:ARG:NH2	2:3:84:ASP:OD1	2.51	0.44
2:9:83:ARG:NH2	2:9:84:ASP:OD1	2.51	0.44
2:9:130:VAL:CG1	2:9:156:LEU:HD23	2.47	0.44
3:0:123:ILE:HG23	3:0:160:LEU:HD13	1.99	0.44
2:AE:109:ILE:O	2:AE:109:ILE:HG22	2.16	0.44
2:AK:22:GLU:O	2:AK:25:ARG:HG2	2.17	0.44
2:AK:109:ILE:HG12	2:AK:159:ALA:CB	2.47	0.44
3:AP:85:MET:HG2	6:AP:201:CYC:HBC1	2.00	0.44
2:AW:22:GLU:O	2:AW:25:ARG:HG2	2.17	0.44
2:AW:109:ILE:HG12	2:AW:159:ALA:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ARG:HD3	1:A:453:PRO:HA	1.99	0.44
1:A:539:LYS:CE	5:Aa:24:GLN:HE21	2.30	0.44
2:G:95:GLY:HA3	2:G:104:ILE:HD11	1.98	0.44
3:L:57:ALA:HA	3:L:61:ILE:HG12	1.99	0.44
3:X:148:GLU:O	3:X:151:ILE:HG12	2.17	0.44
3:Z:57:ALA:HA	3:Z:61:ILE:HG12	1.99	0.44
2:c:80:LEU:HD13	6:c:201:CYC:HAD2	1.99	0.44
2:e:71:ASN:ND2	2:e:121:THR:OG1	2.50	0.44
2:e:83:ARG:NH2	2:e:84:ASP:OD1	2.51	0.44
2:g:83:ARG:NH2	2:g:84:ASP:OD1	2.50	0.44
3:v:96:MET:HA	3:v:152:TYR:CE1	2.52	0.44
6:y:201:CYC:HB	6:y:201:CYC:HMA3	1.82	0.44
2:1:83:ARG:NH2	2:1:84:ASP:OD1	2.51	0.44
3:6:72:MET:HB3	3:6:72:MET:HE2	1.80	0.44
2:7:36:ARG:HG2	2:7:36:ARG:HH11	1.83	0.44
2:9:89:LEU:HD22	2:9:133:MET:CE	2.48	0.44
2:AC:14:GLU:CD	2:AC:16:ARG:HD3	2.42	0.44
3:AD:100:ASP:OD1	3:AD:101:PRO:CD	2.49	0.44
2:AK:116:TYR:HB2	2:AK:123:ILE:HD11	1.98	0.44
3:AL:113:LYS:HB3	3:AL:113:LYS:HE3	1.84	0.44
2:AO:110:ILE:HG13	3:AX:76:ARG:HB2	2.00	0.44
5:Aa:35:GLU:CD	5:Aa:35:GLU:H	2.26	0.44
1:A:298:ARG:HG3	1:A:302:ARG:HH11	1.81	0.44
1:C:177:SER:HA	1:C:180:GLU:HB2	1.99	0.44
1:C:322:LYS:HZ3	1:C:336:ARG:HH12	1.65	0.44
1:C:581:TYR:CB	2:e:114:GLU:OE2	2.64	0.44
3:H:57:ALA:HA	3:H:61:ILE:HG12	1.99	0.44
2:g:66:VAL:HG13	2:g:66:VAL:O	2.18	0.44
2:k:12:ASP:CG	3:l:107:ARG:CZ	2.91	0.44
3:p:160:LEU:HD23	3:p:160:LEU:HA	1.90	0.44
3:q:5:ILE:HD11	3:q:31:PHE:HE2	1.81	0.44
2:r:49:ARG:HH11	2:r:53:GLN:NE2	2.15	0.44
3:x:64:ASP:OD1	3:z:124:ALA:CB	2.39	0.44
2:y:109:ILE:HD11	2:y:156:LEU:HD23	1.99	0.44
3:2:134:LYS:HB3	3:2:134:LYS:HE3	1.83	0.44
3:4:144:ASP:O	3:4:147:LYS:HG2	2.18	0.44
6:5:201:CYC:HC	6:5:201:CYC:HMD2	1.83	0.44
2:AA:4:LEU:CD2	2:AA:8:ILE:HD12	2.47	0.44
2:AA:91:LEU:HB3	2:AA:104:ILE:HG23	1.99	0.44
2:AA:109:ILE:O	2:AA:109:ILE:HG22	2.18	0.44
2:AC:18:LEU:HD22	3:AD:97:LEU:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AF:57:ALA:HA	3:AF:61:ILE:HG12	1.99	0.44
3:AH:81:CYS:HA	6:AH:201:CYC:CHD	2.47	0.44
3:AN:12:TYR:HA	3:AN:15:GLN:HE21	1.83	0.44
3:AR:76:ARG:HB2	2:AW:110:ILE:HG13	1.99	0.44
5:Ab:35:GLU:CD	5:Ab:35:GLU:H	2.25	0.44
1:A:177:SER:HA	1:A:180:GLU:HB2	2.00	0.44
1:A:256:LEU:HD11	1:A:434:TRP:HH2	1.82	0.44
1:A:722:ILE:HD11	2:AA:82:LEU:CD1	2.47	0.44
1:A:759:THR:O	3:AD:106:GLU:OE2	2.35	0.44
1:C:251:GLU:HA	2:r:9:VAL:HG13	1.99	0.44
1:C:505:VAL:HG13	3:h:110:ASN:HD22	1.82	0.44
1:C:702:VAL:O	1:C:702:VAL:CG1	2.64	0.44
1:C:930:LEU:HB3	3:AT:33:THR:CG2	2.46	0.44
2:K:95:GLY:HA3	2:K:104:ILE:HD11	1.99	0.44
2:W:118:SER:O	3:Z:53:LYS:HE3	2.18	0.44
2:Y:62:ARG:HE	2:Y:62:ARG:HB3	1.61	0.44
3:h:57:ALA:HA	3:h:61:ILE:HG12	1.99	0.44
2:o:50:ILE:HA	2:o:136:VAL:HG11	1.99	0.44
2:o:160:MET:HB2	2:o:160:MET:HE3	1.72	0.44
2:3:151:PHE:CD1	2:5:24:ASP:OD1	2.70	0.44
3:6:100:ASP:OD1	3:6:101:PRO:CD	2.50	0.44
6:7:201:CYC:HMA3	6:7:201:CYC:NB	2.33	0.44
6:7:201:CYC:HBD2	6:7:201:CYC:HHA	1.98	0.44
2:AC:109:ILE:HD13	2:AC:155:TYR:HE2	1.82	0.44
6:AG:201:CYC:CGD	3:AJ:62:TYR:OH	2.65	0.44
2:AI:119:LEU:O	2:AI:120:GLN:HB2	2.17	0.44
3:AP:100:ASP:OD1	3:AP:101:PRO:CD	2.50	0.44
2:AS:18:LEU:HD23	2:AS:22:GLU:HG2	1.98	0.44
1:A:271:THR:HG23	1:A:419:THR:HG23	2.00	0.44
1:A:347:PHE:O	1:A:348:TYR:CB	2.63	0.44
1:A:693:ARG:HH11	1:A:693:ARG:HG3	1.82	0.44
1:A:1050:PHE:CZ	3:Z:107:ARG:NH2	2.85	0.44
1:C:31:GLU:HG3	1:C:33:ARG:NH2	2.32	0.44
1:C:31:GLU:HG3	1:C:33:ARG:NH1	2.32	0.44
6:F:201:CYC:OB	5:AZ:42:GLN:NE2	2.51	0.44
2:K:62:ARG:HE	2:K:62:ARG:HB3	1.62	0.44
3:T:57:ALA:HA	3:T:61:ILE:HG12	2.00	0.44
2:U:95:GLY:HA3	2:U:104:ILE:HD11	2.00	0.44
3:V:57:ALA:HA	3:V:61:ILE:HG12	1.98	0.44
3:V:74:THR:HG22	2:a:107:ILE:HG23	1.98	0.44
3:h:24:LEU:O	3:h:28:LYS:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:68:PRO:HA	2:k:73:TYR:CD2	2.52	0.44
2:k:83:ARG:NH2	2:k:84:ASP:OD1	2.50	0.44
2:k:95:GLY:HA3	2:k:104:ILE:HD11	2.00	0.44
6:t:201:CYC:HB	6:t:201:CYC:HMA3	1.82	0.44
6:u:201:CYC:HB	6:u:201:CYC:CMA	2.31	0.44
3:z:1:MET:N	3:z:106:GLU:OE2	2.50	0.44
2:1:14:GLU:OE1	2:1:16:ARG:NE	2.50	0.44
3:2:65:LEU:HB3	3:2:72:MET:HG2	2.00	0.44
3:2:113:LYS:HE3	3:2:113:LYS:HB3	1.73	0.44
2:7:140:LEU:HD23	3:AT:140:LEU:HD21	1.93	0.44
2:AC:50:ILE:HA	2:AC:136:VAL:HG11	2.00	0.44
2:AC:119:LEU:O	2:AC:120:GLN:HB2	2.17	0.44
2:AI:66:VAL:O	2:AI:66:VAL:HG13	2.18	0.44
2:AI:101:VAL:HG11	2:AK:20:PRO:HG2	1.99	0.44
2:AO:4:LEU:HD11	3:AP:3:ASP:CB	2.42	0.44
3:AT:81:CYS:HA	6:AT:201:CYC:CHD	2.47	0.44
3:AX:113:LYS:HE3	3:AX:113:LYS:HB3	1.84	0.44
1:A:22:THR:HG23	3:v:3:ASP:OD2	2.18	0.44
1:A:504:ASP:OD1	1:A:504:ASP:N	2.51	0.44
1:A:891:ALA:HB2	3:AH:107:ARG:O	2.18	0.44
1:A:945:LEU:HD22	1:A:945:LEU:HA	1.92	0.44
1:C:334:VAL:HG21	1:C:411:TYR:OH	2.17	0.44
1:C:749:GLN:O	1:C:750:ARG:C	2.61	0.44
1:C:1115:ARG:HG3	1:C:1115:ARG:O	2.17	0.44
3:P:57:ALA:HA	3:P:61:ILE:HG12	2.00	0.44
6:Q:201:CYC:HMA3	6:Q:201:CYC:HB	1.83	0.44
2:m:27:LYS:HG3	3:n:38:VAL:HG11	2.00	0.44
4:s:83:ARG:NH2	4:s:87:TYR:HE2	2.16	0.44
3:z:57:ALA:HA	3:z:61:ILE:HG12	1.99	0.44
2:5:140:LEU:C	2:5:140:LEU:HD12	2.42	0.44
3:AB:12:TYR:HA	3:AB:15:GLN:HE21	1.83	0.44
3:AB:15:GLN:HB3	3:AB:17:LYS:HE3	1.99	0.44
3:AB:100:ASP:OD1	3:AB:101:PRO:CD	2.49	0.44
2:AC:83:ARG:NH2	2:AC:84:ASP:OD1	2.51	0.44
2:AG:112:VAL:HG11	2:AG:160:MET:CE	2.48	0.44
2:AG:130:VAL:CG1	2:AG:156:LEU:HD23	2.47	0.44
2:AO:18:LEU:HD22	3:AP:97:LEU:CD1	2.47	0.44
3:AR:87:TYR:CD1	3:AR:90:ARG:NH2	2.86	0.44
3:AR:127:VAL:HG23	3:AR:160:LEU:HD22	1.99	0.44
2:AS:66:VAL:HG13	2:AS:66:VAL:O	2.18	0.44
2:AU:2:SER:HG	2:AU:4:LEU:HG	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AU:119:LEU:O	2:AU:120:GLN:HB2	2.17	0.44
1:A:31:GLU:HG3	1:A:33:ARG:NH2	2.32	0.44
1:A:148:TYR:OH	6:A:2101:CYC:HAC1	2.17	0.44
1:A:274:MET:HE1	1:A:323:VAL:HG23	1.99	0.44
1:A:1074:GLN:HA	1:A:1077:ILE:HD12	1.98	0.44
6:N:201:CYC:CMA	6:N:201:CYC:NB	2.81	0.44
2:O:119:LEU:O	2:O:120:GLN:HB2	2.17	0.44
2:Q:83:ARG:NH2	2:Q:84:ASP:OD1	2.51	0.44
3:b:10:ASN:OD1	3:b:10:ASN:C	2.61	0.44
2:y:83:ARG:NH2	2:y:84:ASP:OD1	2.51	0.44
2:y:95:GLY:HA3	2:y:104:ILE:HD11	2.00	0.44
2:5:64:ASP:HB2	2:9:64:ASP:HB2	2.00	0.44
2:9:50:ILE:HA	2:9:136:VAL:HG11	1.99	0.44
2:AG:18:LEU:HD23	2:AG:22:GLU:HG2	1.98	0.44
2:AG:43:LEU:CD1	2:AG:141:LEU:HD21	2.48	0.44
1:A:43:LEU:O	1:A:46:PHE:HB3	2.18	0.44
1:A:539:LYS:HZ2	5:Aa:24:GLN:HE21	1.63	0.44
1:A:889:LEU:HA	1:A:889:LEU:HD13	1.56	0.44
1:C:271:THR:HG23	1:C:419:THR:HG23	2.00	0.44
1:C:483:PHE:CZ	3:n:87:TYR:HE2	2.35	0.44
1:C:997:ILE:HA	1:C:1000:ILE:HD12	2.00	0.44
1:C:1152:TYR:CG	2:AI:68:PRO:HG2	2.53	0.44
2:I:6:LYS:O	2:I:9:VAL:CG2	2.61	0.44
2:I:101:VAL:HG13	2:K:20:PRO:HG2	1.99	0.44
2:Q:95:GLY:HA3	2:Q:104:ILE:HD11	2.00	0.44
3:R:87:TYR:CD1	3:R:91:TYR:HE1	2.35	0.44
2:U:83:ARG:NH2	2:U:84:ASP:OD1	2.50	0.44
2:c:68:PRO:HA	2:c:73:TYR:CD2	2.53	0.44
2:e:66:VAL:HG13	2:e:66:VAL:O	2.18	0.44
3:h:112:LEU:CD2	3:h:160:LEU:HD21	2.48	0.44
2:w:68:PRO:HA	2:w:73:TYR:CD2	2.53	0.44
2:y:50:ILE:HA	2:y:136:VAL:HG11	1.98	0.44
3:z:100:ASP:OD1	3:z:101:PRO:CD	2.50	0.44
2:AG:80:LEU:HD13	6:AG:201:CYC:CAD	2.42	0.44
2:AK:71:ASN:ND2	2:AK:121:THR:OG1	2.49	0.44
3:AL:126:THR:HG23	6:AL:201:CYC:HBC3	1.99	0.44
3:AN:15:GLN:HB3	3:AN:17:LYS:HE3	1.99	0.44
2:AO:83:ARG:NH2	2:AO:84:ASP:OD1	2.51	0.44
2:AQ:95:GLY:HA3	2:AQ:104:ILE:HD11	2.00	0.44
3:AT:112:LEU:CD2	3:AT:160:LEU:HD21	2.47	0.44
6:AW:201:CYC:CMA	6:AW:201:CYC:NB	2.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Aa:31:LEU:HD23	5:Aa:31:LEU:HA	1.91	0.44
1:A:1105:ILE:HG13	1:A:1106:PHE:CD2	2.53	0.43
1:C:504:ASP:OD1	1:C:504:ASP:N	2.52	0.43
1:C:730:ASN:OD1	3:AT:64:ASP:OD2	2.35	0.43
2:E:95:GLY:HA3	2:E:104:ILE:HD11	2.00	0.43
2:I:95:GLY:HA3	2:I:104:ILE:HD11	2.00	0.43
2:K:5:THR:OG1	3:L:3:ASP:OD2	2.31	0.43
2:K:57:GLN:HB3	2:K:61:LYS:HE3	1.99	0.43
2:Q:52:LYS:HA	2:Q:52:LYS:HD2	1.81	0.43
2:Q:110:ILE:HD12	3:X:76:ARG:HD3	1.99	0.43
3:V:68:PRO:HD3	2:a:87:TYR:OH	2.18	0.43
2:Y:83:ARG:NH2	2:Y:84:ASP:OD1	2.50	0.43
2:a:68:PRO:HA	2:a:73:TYR:CD2	2.53	0.43
2:a:83:ARG:NH2	2:a:84:ASP:OD1	2.51	0.43
2:c:80:LEU:CD1	6:c:201:CYC:HAD2	2.48	0.43
2:i:4:LEU:HD21	3:j:3:ASP:OD1	2.18	0.43
2:i:97:VAL:CG2	3:j:9:ILE:HD11	2.47	0.43
3:j:24:LEU:O	3:j:28:LYS:HG3	2.18	0.43
3:j:110:ASN:O	5:Ab:45:GLN:NE2	2.51	0.43
4:u:94:PHE:O	4:u:97:VAL:O	2.36	0.43
2:w:109:ILE:HG12	2:w:159:ALA:CB	2.47	0.43
2:y:66:VAL:O	2:y:66:VAL:HG13	2.18	0.43
2:y:105:GLU:HA	2:y:109:ILE:HD13	1.99	0.43
3:z:112:LEU:CD2	3:z:160:LEU:HD21	2.48	0.43
2:1:4:LEU:HD13	3:2:98:ALA:HA	2.00	0.43
2:5:83:ARG:NH2	2:5:84:ASP:OD1	2.51	0.43
2:7:68:PRO:HA	2:7:73:TYR:CD2	2.53	0.43
2:AC:4:LEU:HD12	2:AC:4:LEU:C	2.43	0.43
3:AD:151:ILE:CD1	3:AD:152:TYR:CE2	2.96	0.43
2:AK:83:ARG:NH2	2:AK:84:ASP:OD1	2.50	0.43
3:AL:24:LEU:O	3:AL:28:LYS:HG3	2.18	0.43
2:AM:109:ILE:O	2:AM:109:ILE:HG22	2.18	0.43
2:AO:4:LEU:HD12	2:AO:4:LEU:C	2.43	0.43
3:AP:24:LEU:O	3:AP:28:LYS:HG3	2.18	0.43
2:AU:68:PRO:HA	2:AU:73:TYR:CD2	2.53	0.43
2:AU:155:TYR:HB2	2:AW:20:PRO:HG3	2.00	0.43
2:AW:68:PRO:HA	2:AW:73:TYR:CD2	2.54	0.43
3:AX:24:LEU:O	3:AX:28:LYS:HG3	2.18	0.43
3:AX:144:ASP:O	3:AX:147:LYS:HG2	2.18	0.43
5:Ac:35:GLU:H	5:Ac:35:GLU:CD	2.25	0.43
1:A:197:SER:HA	1:A:200:ILE:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:PHE:C	1:C:307:ARG:H	2.26	0.43
1:C:351:PHE:HB2	1:C:356:VAL:HG12	2.00	0.43
1:C:532:THR:OG1	2:m:106:GLU:OE2	2.36	0.43
1:C:656:GLY:CA	2:e:15:ALA:HB2	2.48	0.43
1:C:1105:ILE:HG13	1:C:1106:PHE:CD2	2.53	0.43
2:S:95:GLY:HA3	2:S:104:ILE:HD11	2.00	0.43
6:S:201:CYC:CMA	6:S:201:CYC:HB	2.31	0.43
2:W:68:PRO:HA	2:W:73:TYR:CD2	2.53	0.43
3:d:144:ASP:O	3:d:147:LYS:HG2	2.18	0.43
2:e:95:GLY:HA3	2:e:104:ILE:HD11	1.98	0.43
3:6:160:LEU:HD23	3:6:160:LEU:HA	1.88	0.43
2:7:83:ARG:NH2	2:7:84:ASP:OD1	2.50	0.43
2:9:61:LYS:NZ	2:9:61:LYS:CB	2.81	0.43
3:AB:57:ALA:HA	3:AB:61:ILE:HG12	2.00	0.43
2:AE:4:LEU:HD12	2:AE:4:LEU:C	2.44	0.43
2:AE:66:VAL:HG13	2:AE:66:VAL:O	2.18	0.43
2:AE:85:LEU:HD23	2:AE:85:LEU:HA	1.89	0.43
2:AE:95:GLY:HA3	2:AE:104:ILE:HD11	2.00	0.43
3:AF:76:ARG:HB2	2:AK:110:ILE:HG13	1.99	0.43
3:AH:96:MET:HA	3:AH:152:TYR:CE1	2.53	0.43
3:AN:112:LEU:CD2	3:AN:160:LEU:HD21	2.47	0.43
2:AU:109:ILE:HD11	2:AU:156:LEU:CD2	2.49	0.43
1:A:67:ILE:HD11	1:A:213:LEU:HD21	1.99	0.43
1:A:204:LEU:HD23	1:A:207:ARG:HH21	1.78	0.43
1:A:749:GLN:O	1:A:750:ARG:C	2.61	0.43
1:A:1143:LEU:HD11	2:Y:103:PRO:HA	2.00	0.43
1:C:54:ILE:CD1	3:q:31:PHE:CE1	3.01	0.43
1:C:547:ARG:CG	3:l:106:GLU:HA	2.46	0.43
1:C:601:LYS:HB2	1:C:676:GLU:HA	1.99	0.43
1:C:1085:GLY:O	2:I:15:ALA:HB1	2.18	0.43
2:M:95:GLY:HA3	2:M:104:ILE:HD11	2.00	0.43
2:U:98:ALA:HA	3:V:5:ILE:HG21	2.01	0.43
3:X:57:ALA:HA	3:X:61:ILE:HG12	2.00	0.43
3:j:2:GLN:N	3:j:102:SER:HG	2.15	0.43
3:2:57:ALA:HA	3:2:61:ILE:HG12	2.00	0.43
3:6:24:LEU:O	3:6:28:LYS:HG3	2.19	0.43
2:AE:35:ARG:C	2:AE:38:ARG:HG2	2.43	0.43
3:AF:119:LEU:HD11	5:Ac:5:PHE:CZ	2.44	0.43
2:AI:68:PRO:HA	2:AI:73:TYR:CD2	2.53	0.43
2:AI:116:TYR:CB	2:AI:121:THR:CG2	2.96	0.43
2:AM:20:PRO:HB3	2:AO:151:PHE:HZ	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AR:160:LEU:HD23	3:AR:160:LEU:O	2.18	0.43
1:A:288:LEU:HD13	1:A:293:LYS:HG3	2.00	0.43
1:A:614:ARG:HH21	2:5:13:ALA:CB	2.31	0.43
1:C:274:MET:HE1	1:C:323:VAL:HG23	1.99	0.43
1:C:503:LYS:HA	1:C:642:ARG:HB2	2.01	0.43
1:C:756:SER:HA	5:Ad:24:GLN:HE21	1.83	0.43
2:M:83:ARG:NH2	2:M:84:ASP:OD1	2.51	0.43
2:K:83:ARG:NH2	2:K:84:ASP:OD1	2.51	0.43
3:T:53:LYS:NZ	2:U:120:GLN:HG3	2.34	0.43
3:Z:46:SER:O	2:a:161:GLN:NE2	2.51	0.43
3:Z:147:LYS:HZ1	3:Z:151:ILE:CG2	2.32	0.43
3:d:108:VAL:HG21	3:d:156:LEU:HD21	2.01	0.43
2:k:156:LEU:CG	2:k:160:MET:HE3	2.47	0.43
2:o:123:ILE:HD12	2:o:124:PRO:N	2.33	0.43
3:0:151:ILE:CD1	3:0:152:TYR:CE2	2.96	0.43
2:AC:66:VAL:O	2:AC:66:VAL:HG13	2.18	0.43
3:AF:151:ILE:CD1	3:AF:152:TYR:CE2	2.95	0.43
3:AL:110:ASN:ND2	5:Ac:57:PHE:CE1	2.86	0.43
2:AM:83:ARG:NH2	2:AM:84:ASP:OD1	2.50	0.43
2:AO:37:LEU:HD21	3:AP:27:LEU:CD2	2.48	0.43
2:AQ:105:GLU:HA	2:AQ:109:ILE:HD13	2.01	0.43
2:AS:34:GLU:OE1	3:AT:28:LYS:HG2	2.18	0.43
3:AT:96:MET:HA	3:AT:152:TYR:CE1	2.53	0.43
2:AU:83:ARG:NH2	2:AU:84:ASP:OD1	2.51	0.43
2:AU:116:TYR:HB3	2:AU:121:THR:CG2	2.48	0.43
3:AX:83:ARG:NH2	6:AX:201:CYC:O2A	2.51	0.43
5:AZ:3:ARG:HB3	5:AZ:56:LEU:HD11	2.01	0.43
1:A:288:LEU:HD13	1:A:293:LYS:CG	2.47	0.43
1:A:305:PHE:C	1:A:307:ARG:H	2.26	0.43
1:A:349:GLN:N	1:A:350:PRO:HD2	2.34	0.43
1:A:614:ARG:HH21	2:5:13:ALA:HB1	1.84	0.43
1:A:997:ILE:HA	1:A:1000:ILE:HD12	2.00	0.43
1:C:16:LEU:O	1:C:265:SER:HB3	2.18	0.43
2:E:68:PRO:HA	2:E:73:TYR:CD2	2.54	0.43
2:Y:95:GLY:HA3	2:Y:104:ILE:HD11	2.00	0.43
3:d:57:ALA:HA	3:d:61:ILE:HG12	2.00	0.43
2:k:130:VAL:CG1	2:k:156:LEU:HD23	2.48	0.43
2:r:109:ILE:O	2:r:109:ILE:HG22	2.17	0.43
3:x:72:MET:HB3	3:x:72:MET:HE2	1.85	0.43
6:y:201:CYC:HC	6:y:201:CYC:HMD2	1.84	0.43
2:1:97:VAL:HG23	3:2:9:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:109:ILE:HG12	2:1:159:ALA:CB	2.49	0.43
3:0:24:LEU:O	3:0:28:LYS:HG3	2.18	0.43
2:AA:20:PRO:HB3	2:AC:151:PHE:HZ	1.84	0.43
2:AC:85:LEU:HD23	2:AC:85:LEU:HA	1.90	0.43
2:AC:109:ILE:HG12	2:AC:159:ALA:CB	2.49	0.43
2:AG:34:GLU:OE1	3:AH:28:LYS:HG2	2.18	0.43
2:AK:68:PRO:HA	2:AK:73:TYR:CD2	2.54	0.43
2:AO:14:GLU:CD	2:AO:16:ARG:HD3	2.42	0.43
2:AO:66:VAL:O	2:AO:66:VAL:HG13	2.18	0.43
2:AQ:68:PRO:HA	2:AQ:73:TYR:CD2	2.53	0.43
3:AT:2:GLN:NE2	3:AT:7:ALA:CB	2.80	0.43
5:AZ:35:GLU:CD	5:AZ:35:GLU:H	2.26	0.43
1:A:31:GLU:HG3	1:A:33:ARG:NH1	2.32	0.43
1:A:311:ALA:C	2:w:114:GLU:OE2	2.62	0.43
1:A:334:VAL:HG21	1:A:411:TYR:OH	2.17	0.43
1:A:756:SER:HB2	5:Ac:21:ARG:HD3	2.01	0.43
1:C:1135:LEU:HD22	6:N:201:CYC:OB	2.19	0.43
2:I:68:PRO:HA	2:I:73:TYR:CD2	2.53	0.43
2:Y:68:PRO:HA	2:Y:73:TYR:CD2	2.53	0.43
2:e:156:LEU:HD23	2:e:156:LEU:HA	1.80	0.43
2:g:68:PRO:HA	2:g:73:TYR:CD2	2.53	0.43
2:i:68:PRO:HA	2:i:73:TYR:CD2	2.53	0.43
2:y:109:ILE:O	2:y:109:ILE:HG22	2.17	0.43
3:z:24:LEU:O	3:z:28:LYS:HG3	2.18	0.43
2:1:109:ILE:HD11	2:1:156:LEU:HD23	2.01	0.43
3:4:151:ILE:CD1	3:4:152:TYR:CE2	2.98	0.43
3:6:113:LYS:HE3	3:6:113:LYS:HB3	1.82	0.43
3:8:109:LEU:HD23	3:8:109:LEU:HA	1.89	0.43
2:AA:68:PRO:HA	2:AA:73:TYR:CD2	2.53	0.43
3:AF:112:LEU:CD1	6:AF:201:CYC:HMB2	2.49	0.43
3:AL:2:GLN:NE2	3:AL:7:ALA:CB	2.82	0.43
3:AL:2:GLN:HE22	3:AL:10:ASN:HD21	1.64	0.43
2:AM:68:PRO:HA	2:AM:73:TYR:CD2	2.53	0.43
2:AO:95:GLY:HA3	2:AO:104:ILE:HD11	2.01	0.43
2:AQ:66:VAL:O	2:AQ:66:VAL:HG13	2.18	0.43
1:A:714:ASP:OD2	1:A:717:ARG:NH2	2.48	0.43
1:A:761:ARG:HD2	2:AC:110:ILE:CD1	2.49	0.43
1:C:249:SER:O	2:r:13:ALA:HB1	2.18	0.43
6:C:2101:CYC:CMB	6:C:2101:CYC:HBB3	2.49	0.43
2:M:68:PRO:HA	2:M:73:TYR:CD2	2.53	0.43
3:H:113:LYS:HE3	3:H:113:LYS:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:20:PRO:CG	2:W:101:VAL:HG11	2.49	0.43
3:j:57:ALA:HA	3:j:61:ILE:HG12	2.00	0.43
2:5:66:VAL:O	2:5:66:VAL:HG13	2.18	0.43
2:7:91:LEU:HB3	2:7:104:ILE:HG23	1.99	0.43
2:9:95:GLY:HA3	2:9:104:ILE:HD11	2.00	0.43
3:0:57:ALA:HA	3:0:61:ILE:HG12	1.99	0.43
3:0:71:MEN:O	3:0:77:ARG:HD3	2.19	0.43
2:AA:83:ARG:NH2	2:AA:84:ASP:OD1	2.50	0.43
6:AF:201:CYC:HB	6:AF:201:CYC:HMA2	1.83	0.43
2:AG:88:TYR:HB3	2:AG:156:LEU:HD21	1.99	0.43
2:AI:155:TYR:HB2	2:AK:20:PRO:HG3	2.00	0.43
3:AJ:126:THR:HG23	6:AJ:201:CYC:HBC3	2.01	0.43
2:AQ:4:LEU:HD12	2:AQ:4:LEU:C	2.44	0.43
1:A:468:ASN:OD1	1:A:687:PRO:HD2	2.19	0.43
1:C:155:LYS:HB3	1:C:158:ARG:HH11	1.84	0.43
1:C:349:GLN:N	1:C:350:PRO:HD2	2.33	0.43
2:c:18:LEU:HD22	3:d:97:LEU:HD13	2.00	0.43
2:m:68:PRO:HA	2:m:73:TYR:CD2	2.53	0.43
2:o:68:PRO:HA	2:o:73:TYR:CD2	2.53	0.43
2:w:116:TYR:HB2	2:w:123:ILE:HD11	2.01	0.43
2:y:68:PRO:HA	2:y:73:TYR:CD2	2.54	0.43
3:4:134:LYS:HB3	3:4:134:LYS:HE3	1.82	0.43
3:8:134:LYS:HB3	3:8:134:LYS:HE3	1.83	0.43
2:9:68:PRO:HA	2:9:73:TYR:CD2	2.53	0.43
2:AC:95:GLY:HA3	2:AC:104:ILE:HD11	2.01	0.43
2:AE:68:PRO:HA	2:AE:73:TYR:CD2	2.53	0.43
2:AG:95:GLY:HA3	2:AG:104:ILE:HD11	2.01	0.43
3:AL:144:ASP:O	3:AL:147:LYS:HG2	2.18	0.43
2:AO:68:PRO:HA	2:AO:73:TYR:CD2	2.54	0.43
2:AO:109:ILE:HG12	2:AO:159:ALA:CB	2.49	0.43
2:AQ:43:LEU:CD1	2:AQ:141:LEU:HD11	2.39	0.43
2:AU:101:VAL:HG11	2:AW:20:PRO:HG2	2.00	0.43
5:AY:3:ARG:HB3	5:AY:56:LEU:HD11	2.00	0.43
1:A:258:LEU:HD12	1:A:259:PRO:HD2	1.99	0.43
1:C:246:VAL:HB	1:C:257:THR:HB	2.01	0.43
1:C:269:LEU:HD12	1:C:269:LEU:O	2.19	0.43
1:C:288:LEU:HD13	1:C:293:LYS:HG3	2.00	0.43
2:E:20:PRO:CG	2:G:101:VAL:HG11	2.48	0.43
2:K:68:PRO:HA	2:K:73:TYR:CD2	2.53	0.43
2:U:137:ALA:HA	2:U:140:LEU:HD12	2.01	0.43
3:V:78:TYR:CE2	2:a:115:MET:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:68:PRO:HA	2:e:73:TYR:CD2	2.54	0.43
2:i:109:ILE:HD11	2:i:156:LEU:HD23	2.01	0.43
2:m:109:ILE:HD13	2:m:109:ILE:HA	1.84	0.43
2:AC:68:PRO:HA	2:AC:73:TYR:CD2	2.54	0.43
2:AE:105:GLU:HA	2:AE:109:ILE:HD13	2.01	0.43
3:AF:160:LEU:HD23	3:AF:160:LEU:O	2.17	0.43
3:AR:88:PHE:CB	3:AR:156:LEU:HD21	2.48	0.43
2:AU:81:CYS:HA	6:AU:201:CYC:HHD	2.01	0.43
2:AU:116:TYR:CB	2:AU:121:THR:CG2	2.96	0.43
1:C:43:LEU:O	1:C:46:PHE:HB3	2.18	0.43
1:C:891:ALA:HB2	3:AT:107:ARG:O	2.18	0.43
2:O:68:PRO:HA	2:O:73:TYR:CD2	2.54	0.43
2:G:68:PRO:HA	2:G:73:TYR:CD2	2.53	0.43
2:G:85:LEU:HD23	2:G:85:LEU:HA	1.92	0.43
2:I:27:LYS:HE3	2:K:151:PHE:HE1	1.80	0.43
3:R:112:LEU:HD11	6:R:201:CYC:HMB3	2.00	0.43
2:S:68:PRO:HA	2:S:73:TYR:CD2	2.54	0.43
3:T:76:ARG:HD3	2:U:110:ILE:HD12	2.00	0.43
2:g:12:ASP:OD2	3:h:107:ARG:NH1	2.52	0.43
2:i:83:ARG:NH2	2:i:84:ASP:OD1	2.51	0.43
2:i:109:ILE:HG12	2:i:159:ALA:CB	2.49	0.43
2:m:109:ILE:O	2:m:109:ILE:HG22	2.18	0.43
2:o:123:ILE:CG1	2:o:124:PRO:CD	2.97	0.43
2:w:95:GLY:HA3	2:w:104:ILE:HD11	2.00	0.43
2:w:130:VAL:CG1	2:w:156:LEU:HD23	2.47	0.43
2:1:68:PRO:HA	2:1:73:TYR:CD2	2.53	0.43
3:6:112:LEU:CD2	3:6:160:LEU:HD21	2.48	0.43
2:9:105:GLU:HG3	2:9:109:ILE:CG1	2.48	0.43
2:AC:37:LEU:HD21	3:AD:27:LEU:CD2	2.49	0.43
3:AF:127:VAL:HG23	3:AF:160:LEU:HD22	1.99	0.43
2:AG:66:VAL:O	2:AG:66:VAL:HG13	2.18	0.43
2:AI:81:CYS:HA	6:AI:201:CYC:HHD	2.01	0.43
2:AI:83:ARG:NH2	2:AI:84:ASP:OD1	2.51	0.43
2:AU:66:VAL:O	2:AU:66:VAL:HG13	2.18	0.43
3:AV:109:LEU:HD23	3:AV:109:LEU:HA	1.90	0.43
1:A:28:ILE:HG23	1:A:33:ARG:O	2.19	0.42
1:A:323:VAL:HG11	1:A:333:PHE:HB2	2.01	0.42
1:A:447:ALA:N	1:A:448:PRO:CD	2.82	0.42
1:A:699:SER:HB2	3:x:124:ALA:HB1	2.00	0.42
1:C:28:ILE:HG23	1:C:33:ARG:O	2.19	0.42
1:C:194:CYS:CB	6:C:2101:CYC:HAC2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:501:ILE:O	1:C:642:ARG:HD2	2.19	0.42
3:H:71:MEN:HD2	6:H:201:CYC:HMD2	1.84	0.42
3:f:82:ILE:HG21	3:f:82:ILE:HD13	1.79	0.42
2:m:156:LEU:HD23	2:m:156:LEU:HA	1.82	0.42
2:o:83:ARG:NH2	2:o:84:ASP:OD1	2.51	0.42
4:s:94:PHE:O	4:s:97:VAL:O	2.37	0.42
2:3:68:PRO:HA	2:3:73:TYR:CD2	2.54	0.42
3:AH:112:LEU:CD2	3:AH:160:LEU:HD21	2.47	0.42
2:AI:109:ILE:HD11	2:AI:156:LEU:CD2	2.49	0.42
2:AS:88:TYR:HB3	2:AS:156:LEU:HD21	1.99	0.42
2:AW:81:CYS:HA	6:AW:201:CYC:CHD	2.49	0.42
5:Ab:24:GLN:N	5:Ab:24:GLN:CD	2.52	0.42
1:A:211:ALA:HA	1:A:220:SER:HB2	2.01	0.42
1:C:1033:ARG:NH2	5:AZ:40:GLU:OE2	2.52	0.42
6:G:201:CYC:HMA3	6:G:201:CYC:HB	1.84	0.42
2:o:95:GLY:HA3	2:o:104:ILE:HD11	2.01	0.42
3:2:2:GLN:N	3:2:102:SER:HG	2.17	0.42
2:3:5:THR:OG1	3:4:3:ASP:OD2	2.27	0.42
2:5:69:GLY:HA3	2:9:63:PRO:HD2	2.01	0.42
2:9:81:CYS:HA	6:9:201:CYC:CHD	2.49	0.42
6:0:201:CYC:NB	6:0:201:CYC:HMA1	2.34	0.42
6:AA:201:CYC:HBC2	6:AA:201:CYC:HMC1	2.00	0.42
3:AD:134:LYS:HB3	3:AD:134:LYS:HE3	1.80	0.42
6:AE:201:CYC:HB	6:AE:201:CYC:CMA	2.32	0.42
2:AI:116:TYR:HB3	2:AI:121:THR:CG2	2.48	0.42
2:AK:75:GLU:HG2	2:AK:76:LYS:H	1.79	0.42
2:AM:2:SER:HB3	3:AN:6:THR:HG23	2.01	0.42
5:Ad:35:GLU:H	5:Ad:35:GLU:CD	2.25	0.42
1:A:396:GLY:HA2	1:A:400:ALA:HB2	2.00	0.42
1:A:542:GLN:O	1:A:542:GLN:NE2	2.53	0.42
1:A:671:GLN:HB2	5:Aa:43:ARG:HH21	1.83	0.42
1:C:156:SER:HA	6:C:2101:CYC:C3C	2.50	0.42
1:C:929:PRO:HG2	3:AT:147:LYS:HG3	2.01	0.42
1:C:1016:LEU:HD11	1:C:1048:ARG:NE	2.35	0.42
3:N:115:THR:HG21	6:N:201:CYC:HMA3	2.00	0.42
3:F:110:ASN:HD21	5:AZ:51:VAL:H	1.66	0.42
6:G:201:CYC:HB	6:G:201:CYC:CMA	2.32	0.42
3:L:71:MEN:HE21	6:L:201:CYC:HBD2	2.01	0.42
2:Q:68:PRO:HA	2:Q:73:TYR:CD2	2.54	0.42
6:U:201:CYC:HMD3	6:U:201:CYC:NC	2.34	0.42
6:l:201:CYC:NB	6:l:201:CYC:HMA1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:s:61:LEU:HD23	4:s:72:MET:HE1	2.01	0.42
2:t:35:ARG:HG3	2:t:38:ARG:HH22	1.83	0.42
2:t:49:ARG:NH2	2:t:53:GLN:NE2	2.67	0.42
2:y:105:GLU:HA	2:y:109:ILE:CD1	2.49	0.42
2:5:68:PRO:HA	2:5:73:TYR:CD2	2.54	0.42
2:5:156:LEU:HD23	2:5:156:LEU:HA	1.80	0.42
2:7:109:ILE:O	2:7:109:ILE:HG22	2.18	0.42
2:AA:2:SER:HB3	3:AB:6:THR:HG23	2.02	0.42
2:AA:4:LEU:HD22	3:AB:3:ASP:CB	2.49	0.42
3:AD:24:LEU:O	3:AD:28:LYS:HG3	2.18	0.42
2:AG:110:ILE:HG13	3:AJ:76:ARG:HB2	2.01	0.42
3:AP:134:LYS:HE3	3:AP:134:LYS:HB3	1.80	0.42
1:A:269:LEU:HD12	1:A:269:LEU:O	2.18	0.42
1:A:732:ARG:HE	3:AH:69:GLY:HA3	1.84	0.42
1:A:1008:PHE:CD1	1:A:1008:PHE:C	2.97	0.42
1:A:1135:LEU:HD13	6:R:201:CYC:C4B	2.50	0.42
1:C:40:VAL:HG13	3:q:38:VAL:HG12	1.90	0.42
1:C:361:PHE:O	1:C:365:LEU:O	2.37	0.42
1:C:522:ASN:HA	1:C:523:PRO:HD2	1.86	0.42
1:C:732:ARG:HE	3:AT:69:GLY:HA3	1.84	0.42
1:C:1051:GLU:N	1:C:1052:PRO:HD2	2.34	0.42
2:E:137:ALA:HA	2:E:140:LEU:HD12	2.01	0.42
3:F:68:PRO:HD3	2:K:87:TYR:OH	2.19	0.42
6:y:201:CYC:HMA3	6:y:201:CYC:NB	2.35	0.42
2:3:4:LEU:HD12	2:3:4:LEU:C	2.45	0.42
3:8:28:LYS:HE2	3:8:28:LYS:HB2	1.84	0.42
2:AK:31:ALA:O	2:AK:34:GLU:OE1	2.38	0.42
6:AM:201:CYC:CMD	6:AM:201:CYC:NC	2.82	0.42
2:AO:41:GLN:HG3	2:AO:45:GLU:OE2	2.20	0.42
2:AS:43:LEU:CD1	2:AS:141:LEU:HD21	2.48	0.42
2:AS:110:ILE:HG13	3:AV:76:ARG:HB2	2.01	0.42
2:AU:4:LEU:HD12	2:AU:4:LEU:C	2.45	0.42
3:AX:10:ASN:OD1	3:AX:10:ASN:C	2.63	0.42
1:A:1027:ASN:O	1:A:1028:ASN:HB3	2.20	0.42
1:C:761:ARG:HD2	2:AO:110:ILE:CD1	2.49	0.42
1:C:820:HIS:CE1	3:AV:107:ARG:NH2	2.88	0.42
1:C:1140:TRP:CH2	2:I:110:ILE:CD1	3.02	0.42
6:S:201:CYC:HB	6:S:201:CYC:HMA3	1.85	0.42
2:U:68:PRO:HA	2:U:73:TYR:CD2	2.54	0.42
6:U:201:CYC:CMD	6:U:201:CYC:NC	2.81	0.42
2:i:43:LEU:HA	2:i:43:LEU:HD12	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:l:91:TYR:CE2	3:l:107:ARG:NE	2.66	0.42
3:l:134:LYS:HB3	3:l:134:LYS:HE3	1.79	0.42
3:l:140:LEU:HD21	2:AE:140:LEU:HD23	2.01	0.42
2:m:80:LEU:HD13	6:m:201:CYC:HAD2	2.01	0.42
2:o:62:ARG:HH22	2:o:124:PRO:HB2	1.83	0.42
2:t:109:ILE:CD1	2:t:160:MET:CE	2.98	0.42
2:3:25:ARG:HD3	2:5:25:ARG:HD2	2.01	0.42
2:5:2:SER:HG	2:5:4:LEU:HG	1.83	0.42
2:AG:116:TYR:HB2	2:AG:123:ILE:HD11	2.02	0.42
2:AI:41:GLN:HG3	2:AI:45:GLU:OE2	2.20	0.42
3:AJ:134:LYS:HB3	3:AJ:134:LYS:HE3	1.83	0.42
3:AP:106:GLU:CD	3:AP:107:ARG:HH11	2.27	0.42
2:AS:4:LEU:HD12	2:AS:4:LEU:C	2.45	0.42
2:AS:112:VAL:HG11	2:AS:160:MET:CE	2.48	0.42
2:AW:31:ALA:O	2:AW:34:GLU:OE1	2.38	0.42
2:AW:75:GLU:HG2	2:AW:76:LYS:H	1.79	0.42
5:Ac:18:ARG:HG3	5:Ac:22:GLU:OE2	2.19	0.42
1:A:51:GLN:HE22	3:v:28:LYS:HB3	1.85	0.42
1:A:272:PHE:HD1	1:A:295:ARG:NH1	2.18	0.42
1:A:532:THR:OG1	2:7:106:GLU:OE2	2.37	0.42
1:A:1152:TYR:CZ	2:AU:68:PRO:HG2	2.55	0.42
1:C:272:PHE:HD1	1:C:295:ARG:NH1	2.18	0.42
1:C:491:THR:HB	3:q:117:ASN:HD22	1.83	0.42
1:C:1143:LEU:CD1	2:I:106:GLU:OE1	2.67	0.42
2:O:156:LEU:HD23	2:O:156:LEU:HA	1.78	0.42
3:F:76:ARG:HD3	2:K:110:ILE:CD1	2.49	0.42
6:K:201:CYC:NB	6:K:201:CYC:HMA3	2.35	0.42
3:T:81:CYS:HA	6:T:201:CYC:HHD	2.00	0.42
3:V:77:ARG:HH22	5:AY:62:GLY:C	2.28	0.42
2:c:156:LEU:HD23	2:c:156:LEU:HA	1.81	0.42
2:e:2:SER:HG	2:e:4:LEU:HG	1.83	0.42
2:g:4:LEU:HD12	2:g:4:LEU:C	2.45	0.42
2:k:58:LEU:HD11	2:k:59:PHE:CE1	2.55	0.42
2:k:81:CYS:HA	6:k:201:CYC:CHD	2.50	0.42
2:r:49:ARG:CZ	2:r:140:LEU:HD21	2.41	0.42
2:r:95:GLY:HA3	2:r:104:ILE:HD11	2.01	0.42
2:1:4:LEU:HD12	2:1:4:LEU:C	2.45	0.42
2:1:156:LEU:HD23	2:1:156:LEU:HA	1.80	0.42
2:3:75:GLU:HG2	2:3:76:LYS:H	1.80	0.42
2:9:48:GLU:H	2:9:48:GLU:CD	2.28	0.42
6:AA:201:CYC:CMD	6:AA:201:CYC:NC	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AB:109:LEU:HD23	3:AB:109:LEU:HA	1.91	0.42
2:AI:35:ARG:HA	2:AI:38:ARG:HH21	1.84	0.42
3:AN:57:ALA:HA	3:AN:61:ILE:HG12	2.00	0.42
3:AX:2:GLN:NE2	3:AX:7:ALA:CB	2.82	0.42
5:AY:35:GLU:CD	5:AY:35:GLU:H	2.26	0.42
1:A:251:GLU:HA	2:t:9:VAL:HG13	2.01	0.42
1:A:876:TYR:CD1	1:A:882:PRO:HA	2.55	0.42
1:A:1051:GLU:N	1:A:1052:PRO:HD2	2.34	0.42
1:A:1137:SER:HB2	3:R:118:SER:HB2	2.00	0.42
1:C:211:ALA:HA	1:C:220:SER:HB2	2.01	0.42
1:C:468:ASN:OD1	1:C:687:PRO:HD2	2.19	0.42
1:C:557:VAL:HG22	2:k:103:PRO:HA	2.00	0.42
1:C:595:ASN:ND2	6:d:201:CYC:HMA3	2.35	0.42
1:C:699:SER:HB2	3:p:124:ALA:HB1	2.00	0.42
1:C:875:LEU:HD12	1:C:876:TYR:CD1	2.55	0.42
2:O:95:GLY:HA3	2:O:104:ILE:HD11	2.00	0.42
3:l:7:ALA:O	3:l:11:ASN:OD1	2.37	0.42
2:w:35:ARG:HA	2:w:38:ARG:HH21	1.85	0.42
2:y:80:LEU:CD1	6:y:201:CYC:HAD2	2.49	0.42
3:6:151:ILE:CD1	3:6:152:TYR:CE2	2.97	0.42
2:7:156:LEU:HD23	2:7:156:LEU:HA	1.82	0.42
2:9:61:LYS:HB3	2:9:61:LYS:HZ2	1.84	0.42
2:AE:83:ARG:HE	2:AE:83:ARG:HB3	1.71	0.42
6:AQ:201:CYC:CMA	6:AQ:201:CYC:HB	2.32	0.42
2:AS:116:TYR:HB2	2:AS:123:ILE:HD11	2.02	0.42
6:AT:201:CYC:HMA1	6:AT:201:CYC:NB	2.34	0.42
1:A:287:ASN:O	1:A:288:LEU:HG	2.19	0.42
1:A:599:THR:HG22	1:A:602:GLU:HG2	2.01	0.42
1:C:67:ILE:HD11	1:C:213:LEU:HD22	2.02	0.42
1:C:203:LEU:CD2	1:C:231:ILE:HB	2.50	0.42
1:C:447:ALA:N	1:C:448:PRO:CD	2.83	0.42
3:N:81:CYS:HA	6:N:201:CYC:CHD	2.49	0.42
2:E:48:GLU:H	2:E:48:GLU:CD	2.27	0.42
3:T:83:ARG:NH1	6:T:201:CYC:O2A	2.52	0.42
3:X:29:ALA:O	3:X:32:THR:HG22	2.19	0.42
2:c:31:ALA:O	2:c:34:GLU:OE1	2.38	0.42
3:h:151:ILE:CD1	3:h:152:TYR:CE2	2.97	0.42
2:i:48:GLU:CD	2:i:48:GLU:H	2.28	0.42
2:i:131:ARG:NH2	2:i:134:LYS:HE3	2.35	0.42
2:m:48:GLU:HG2	2:m:49:ARG:H	1.85	0.42
6:m:201:CYC:HMA3	6:m:201:CYC:NB	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:t:201:CYC:HMA3	6:t:201:CYC:NB	2.35	0.42
3:v:57:ALA:HA	3:v:61:ILE:HG12	2.00	0.42
3:z:1:MET:HA	3:z:106:GLU:OE2	2.18	0.42
2:1:95:GLY:HA3	2:1:104:ILE:HD11	2.01	0.42
3:AV:19:LEU:HD23	3:AV:19:LEU:HA	1.94	0.42
1:A:3:ILE:H	1:A:3:ILE:HG13	1.62	0.42
1:A:40:VAL:HG13	3:v:38:VAL:HG12	1.93	0.42
1:A:544:VAL:HG22	1:A:560:VAL:HG23	2.01	0.42
1:A:900:LEU:HD23	1:A:900:LEU:HA	1.85	0.42
1:C:542:GLN:O	1:C:542:GLN:NE2	2.53	0.42
1:C:876:TYR:CD1	1:C:882:PRO:HA	2.54	0.42
2:M:156:LEU:HD23	2:M:156:LEU:HA	1.79	0.42
6:O:201:CYC:HB	6:O:201:CYC:HMA3	1.84	0.42
3:J:19:LEU:HD23	3:J:19:LEU:HA	1.95	0.42
3:L:29:ALA:O	3:L:32:THR:HG22	2.20	0.42
2:e:4:LEU:HD12	2:e:4:LEU:C	2.45	0.42
3:f:24:LEU:O	3:f:28:LYS:HG3	2.18	0.42
3:j:19:LEU:HD12	3:j:19:LEU:O	2.20	0.42
3:j:123:ILE:H	3:j:123:ILE:HG13	1.71	0.42
3:l:3:ASP:HB3	3:l:6:THR:HG23	2.01	0.42
3:n:156:LEU:O	3:n:160:LEU:HD13	2.20	0.42
2:t:48:GLU:H	2:t:48:GLU:CD	2.28	0.42
4:u:68:THR:HA	4:u:73:TYR:CG	2.55	0.42
3:v:160:LEU:HD23	3:v:160:LEU:HA	1.87	0.42
2:3:151:PHE:HE1	2:5:24:ASP:OD1	2.01	0.42
2:3:156:LEU:HD23	2:3:156:LEU:HA	1.79	0.42
3:8:113:LYS:HB3	3:8:113:LYS:HE3	1.83	0.42
6:AD:201:CYC:OB	5:Ac:21:ARG:HB2	2.20	0.42
3:AF:78:TYR:CE2	2:AK:115:MET:HG3	2.55	0.42
2:AK:42:THR:HG22	2:AK:140:LEU:HD13	2.02	0.42
2:AQ:92:VAL:HG23	2:AQ:156:LEU:HD22	2.02	0.42
2:AS:95:GLY:HA3	2:AS:104:ILE:HD11	2.01	0.42
3:AV:126:THR:HG23	6:AV:201:CYC:HBC3	2.01	0.42
3:AX:100:ASP:OD1	3:AX:101:PRO:CD	2.50	0.42
1:A:54:ILE:HG21	3:v:28:LYS:CG	2.50	0.42
1:A:158:ARG:NH1	1:A:159:ASP:OD1	2.52	0.42
1:A:361:PHE:O	1:A:365:LEU:O	2.37	0.42
1:A:730:ASN:OD1	3:AH:64:ASP:OD2	2.37	0.42
1:C:165:ARG:HA	3:q:18:TYR:CE2	2.55	0.42
1:C:323:VAL:HG11	1:C:333:PHE:HB2	2.01	0.42
1:C:890:PRO:O	1:C:891:ALA:CB	2.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:131:ARG:HH21	2:M:134:LYS:HZ2	1.67	0.42
6:F:201:CYC:HBB2	5:AZ:42:GLN:HE22	1.81	0.42
2:g:95:GLY:HA3	2:g:104:ILE:HD11	2.00	0.42
2:g:130:VAL:HG21	2:g:156:LEU:HD22	2.01	0.42
2:i:95:GLY:HA3	2:i:104:ILE:HD11	2.01	0.42
3:j:84:ASP:CG	6:j:201:CYC:HB	2.26	0.42
3:l:83:ARG:HH11	3:l:87:TYR:HE2	1.67	0.42
2:o:35:ARG:HA	2:o:38:ARG:HH21	1.85	0.42
3:v:106:GLU:OE2	3:v:107:ARG:NH1	2.53	0.42
2:y:109:ILE:HD13	2:y:155:TYR:HE2	1.85	0.42
2:5:91:LEU:HB3	2:5:104:ILE:HG23	2.02	0.42
3:8:116:TYR:HD2	3:8:123:ILE:HD13	1.85	0.42
6:AA:201:CYC:HB	6:AA:201:CYC:CMA	2.33	0.42
2:AC:48:GLU:CD	2:AC:48:GLU:H	2.28	0.42
2:AI:31:ALA:O	2:AI:34:GLU:OE1	2.38	0.42
3:AJ:113:LYS:HB3	3:AJ:113:LYS:HE3	1.81	0.42
2:AK:4:LEU:HD12	2:AK:4:LEU:C	2.45	0.42
2:AU:109:ILE:HD11	2:AU:156:LEU:HD22	2.02	0.42
2:AW:4:LEU:HD12	2:AW:4:LEU:C	2.45	0.42
5:AY:11:ILE:HG12	5:AY:49:GLY:HA3	2.02	0.42
5:AY:61:GLN:H	5:AY:61:GLN:CD	2.25	0.42
1:A:28:ILE:HG21	3:v:94:TYR:CE1	2.56	0.41
1:A:67:ILE:HD11	1:A:213:LEU:HD22	2.02	0.41
1:A:203:LEU:CD2	1:A:231:ILE:HB	2.50	0.41
1:C:591:ILE:HD11	3:d:83:ARG:NH1	2.35	0.41
2:M:20:PRO:HG2	2:O:101:VAL:HG13	2.02	0.41
2:Q:44:THR:O	2:Q:47:ARG:HB3	2.20	0.41
2:Y:44:THR:O	2:Y:47:ARG:HB3	2.21	0.41
2:e:91:LEU:HB3	2:e:104:ILE:HG23	2.02	0.41
2:m:89:LEU:CB	2:m:133:MET:HE1	2.10	0.41
2:r:68:PRO:HA	2:r:73:TYR:CD2	2.55	0.41
2:r:156:LEU:HD23	2:r:156:LEU:HA	1.81	0.41
4:s:36:LEU:C	4:s:36:LEU:CD1	2.93	0.41
2:t:68:PRO:HA	2:t:73:TYR:CD2	2.55	0.41
2:t:109:ILE:HD11	2:t:156:LEU:CD2	2.50	0.41
2:9:4:LEU:HD12	2:9:4:LEU:C	2.45	0.41
3:AB:151:ILE:CD1	3:AB:152:TYR:CE2	2.97	0.41
2:AC:37:LEU:CD2	3:AD:27:LEU:HD21	2.50	0.41
3:AF:119:LEU:O	5:Ac:61:GLN:HB2	2.20	0.41
3:AJ:151:ILE:CD1	3:AJ:152:TYR:CE2	2.97	0.41
6:AM:201:CYC:HB	6:AM:201:CYC:CMA	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AO:37:LEU:CD2	3:AP:27:LEU:HD21	2.50	0.41
2:AO:48:GLU:CD	2:AO:48:GLU:H	2.28	0.41
6:AP:201:CYC:HMA3	5:Ad:23:LEU:HD23	2.02	0.41
3:AR:154:ASP:O	3:AR:157:SER:OG	2.36	0.41
2:AU:41:GLN:HG3	2:AU:45:GLU:OE2	2.20	0.41
2:AW:48:GLU:CD	2:AW:48:GLU:H	2.28	0.41
1:A:59:LYS:HB2	1:A:214:PHE:HE1	1.85	0.41
1:A:889:LEU:O	1:A:890:PRO:C	2.64	0.41
1:C:3:ILE:H	1:C:3:ILE:HG13	1.62	0.41
1:C:344:ARG:HH12	2:o:9:VAL:HG11	1.83	0.41
1:C:554:ASN:HA	3:d:77:ARG:HH12	1.85	0.41
1:C:599:THR:HG22	1:C:602:GLU:HG2	2.01	0.41
1:C:670:TYR:CD1	1:C:670:TYR:C	2.98	0.41
1:C:696:ARG:H	1:C:696:ARG:HG2	1.47	0.41
1:C:761:ARG:HD2	2:AO:110:ILE:HD12	2.01	0.41
2:Q:80:LEU:HD13	6:Q:201:CYC:HAD2	2.02	0.41
3:R:119:LEU:HD11	6:R:201:CYC:C2A	2.50	0.41
3:V:110:ASN:HD21	5:AY:51:VAL:H	1.68	0.41
6:W:201:CYC:HB	6:W:201:CYC:CMA	2.33	0.41
3:j:115:THR:HG22	3:j:119:LEU:HD22	2.03	0.41
3:n:113:LYS:HE3	3:n:113:LYS:HB3	1.83	0.41
2:7:80:LEU:HD13	6:7:201:CYC:HAD2	2.01	0.41
2:9:88:TYR:HB3	2:9:156:LEU:HD21	2.02	0.41
2:AA:95:GLY:HA3	2:AA:104:ILE:HD11	2.02	0.41
3:AF:2:GLN:N	3:AF:102:SER:HG	2.19	0.41
2:AK:37:LEU:HD22	3:AL:24:LEU:HD22	2.03	0.41
3:AR:78:TYR:CE2	2:AW:115:MET:HG3	2.55	0.41
2:AS:48:GLU:CD	2:AS:48:GLU:H	2.28	0.41
1:A:11:VAL:CG1	3:6:161:SER:HB2	2.45	0.41
1:A:620:PRO:HG2	1:A:621:PHE:CE2	2.55	0.41
1:A:929:PRO:HG2	3:AH:147:LYS:HG3	2.01	0.41
1:C:180:GLU:O	1:C:183:CYS:SG	2.70	0.41
1:C:287:ASN:O	1:C:288:LEU:HG	2.19	0.41
1:C:1152:TYR:CZ	2:AI:68:PRO:HG2	2.55	0.41
3:P:113:LYS:HE3	3:P:113:LYS:HB3	1.87	0.41
3:F:19:LEU:HD23	3:F:19:LEU:HA	1.96	0.41
2:Q:80:LEU:CD1	6:Q:201:CYC:HAD2	2.50	0.41
3:V:160:LEU:HD23	3:V:160:LEU:HA	1.96	0.41
2:W:134:LYS:NZ	2:W:154:ASP:OD1	2.51	0.41
2:e:27:LYS:HG3	3:f:38:VAL:HG11	2.03	0.41
2:i:4:LEU:HD12	2:i:4:LEU:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:4:LEU:HD12	2:k:4:LEU:C	2.45	0.41
6:m:201:CYC:CMD	6:m:201:CYC:NC	2.82	0.41
3:n:76:ARG:NH1	6:n:201:CYC:O2D	2.52	0.41
2:3:48:GLU:CD	2:3:48:GLU:H	2.28	0.41
2:AC:109:ILE:O	2:AC:109:ILE:HG22	2.20	0.41
2:AE:109:ILE:HD13	2:AE:155:TYR:HE2	1.86	0.41
3:AF:87:TYR:CD1	3:AF:90:ARG:NH2	2.86	0.41
2:AM:4:LEU:HD22	3:AN:3:ASP:CB	2.49	0.41
2:AM:48:GLU:H	2:AM:48:GLU:CD	2.28	0.41
2:AW:22:GLU:O	2:AW:25:ARG:CG	2.69	0.41
2:AW:42:THR:HG22	2:AW:140:LEU:HD13	2.02	0.41
5:AZ:11:ILE:HG12	5:AZ:49:GLY:HA3	2.01	0.41
1:A:820:HIS:CE1	3:AJ:107:ARG:NH2	2.88	0.41
1:A:1016:LEU:HD11	1:A:1048:ARG:NE	2.34	0.41
1:C:622:TYR:HD1	3:f:107:ARG:O	2.03	0.41
2:M:52:LYS:HD2	2:M:52:LYS:HA	1.81	0.41
2:O:118:SER:O	3:L:53:LYS:CE	2.68	0.41
3:H:29:ALA:O	3:H:32:THR:HG22	2.19	0.41
2:Q:156:LEU:HD23	2:Q:156:LEU:HA	1.79	0.41
2:U:5:THR:OG1	3:V:3:ASP:OD2	2.30	0.41
3:d:81:CYS:HA	6:d:201:CYC:HHD	2.03	0.41
6:i:201:CYC:HC	6:i:201:CYC:HMD2	1.86	0.41
2:k:75:GLU:HG2	2:k:76:LYS:H	1.80	0.41
3:l:113:LYS:HE3	3:l:113:LYS:HB3	1.86	0.41
2:m:36:ARG:HG2	2:m:36:ARG:HH11	1.85	0.41
3:p:57:ALA:HA	3:p:61:ILE:HG12	2.03	0.41
3:p:78:TYR:CD2	2:r:115:MET:HG3	2.56	0.41
2:r:48:GLU:CD	2:r:48:GLU:H	2.28	0.41
2:t:95:GLY:HA3	2:t:104:ILE:HD11	2.02	0.41
4:u:83:ARG:HH11	4:u:83:ARG:HG2	1.85	0.41
4:u:112:LEU:HD23	4:u:160:LEU:HG	2.02	0.41
2:y:4:LEU:HD12	2:y:4:LEU:C	2.44	0.41
2:1:48:GLU:CD	2:1:48:GLU:H	2.28	0.41
2:5:35:ARG:HA	2:5:38:ARG:HH21	1.85	0.41
2:AA:48:GLU:CD	2:AA:48:GLU:H	2.28	0.41
2:AA:160:MET:HB2	2:AA:160:MET:HE3	1.76	0.41
2:AG:48:GLU:CD	2:AG:48:GLU:H	2.28	0.41
2:AM:116:TYR:HB2	2:AM:123:ILE:HD11	2.02	0.41
2:AU:35:ARG:HA	2:AU:38:ARG:HH21	1.84	0.41
3:AX:10:ASN:HB3	5:Ad:65:THR:OG1	2.20	0.41
5:AZ:61:GLN:H	5:AZ:61:GLN:CD	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:PHE:O	1:A:411:TYR:CE1	2.73	0.41
1:A:540:LEU:HD12	1:A:540:LEU:HA	1.88	0.41
1:A:685:LEU:C	1:A:685:LEU:HD12	2.45	0.41
1:A:736:GLU:CD	1:A:736:GLU:H	2.28	0.41
1:A:1012:PRO:HB2	1:A:1017:ARG:HG2	2.02	0.41
1:C:722:ILE:HD11	2:AM:82:LEU:CD1	2.46	0.41
2:G:44:THR:O	2:G:47:ARG:HB3	2.21	0.41
2:I:48:GLU:CD	2:I:48:GLU:H	2.28	0.41
2:Q:48:GLU:H	2:Q:48:GLU:CD	2.29	0.41
3:V:61:ILE:HG13	3:V:62:TYR:CD1	2.56	0.41
3:X:115:THR:HG21	6:X:201:CYC:CMA	2.50	0.41
6:e:201:CYC:HC	6:e:201:CYC:HMD2	1.86	0.41
6:n:201:CYC:HB	6:n:201:CYC:CMA	2.23	0.41
3:p:1:MET:HG2	3:p:103:ILE:HD12	2.02	0.41
3:p:1:MET:HB3	3:p:107:ARG:HH22	1.86	0.41
6:r:201:CYC:HB	6:r:201:CYC:HMA3	1.84	0.41
6:r:201:CYC:HC	6:r:201:CYC:CMD	2.34	0.41
4:s:104:LEU:HA	4:s:108:VAL:HG23	2.02	0.41
4:u:156:LEU:O	4:u:160:LEU:HD13	2.21	0.41
2:w:4:LEU:HD11	3:x:3:ASP:HB3	1.98	0.41
3:x:15:GLN:HE21	3:x:15:GLN:HB2	1.71	0.41
2:y:75:GLU:HG2	2:y:76:LYS:H	1.80	0.41
2:3:18:LEU:HD22	3:4:97:LEU:HD13	2.03	0.41
2:5:4:LEU:HD12	2:5:4:LEU:C	2.45	0.41
2:9:85:LEU:HD23	2:9:85:LEU:HA	1.95	0.41
2:AE:16:ARG:O	3:AF:94:TYR:OH	2.33	0.41
2:AE:92:VAL:HG23	2:AE:156:LEU:HD22	2.02	0.41
2:AG:4:LEU:HD12	2:AG:4:LEU:C	2.44	0.41
2:AI:116:TYR:CB	2:AI:121:THR:HG22	2.51	0.41
2:AK:2:SER:HB3	3:AL:6:THR:HG23	2.03	0.41
2:AQ:113:LYS:HG2	2:AQ:117:ASN:HD21	1.86	0.41
1:A:347:PHE:CE2	1:A:448:PRO:HB3	2.55	0.41
1:C:445:TYR:O	1:C:448:PRO:HD2	2.20	0.41
1:C:693:ARG:HG2	3:n:110:ASN:ND2	2.36	0.41
1:C:1141:SER:CB	2:I:106:GLU:HG2	2.50	0.41
2:M:110:ILE:HD12	3:H:76:ARG:HD3	2.03	0.41
6:E:201:CYC:CMD	6:E:201:CYC:NC	2.83	0.41
2:G:48:GLU:H	2:G:48:GLU:CD	2.28	0.41
2:K:44:THR:O	2:K:47:ARG:HB3	2.21	0.41
2:K:48:GLU:CD	2:K:48:GLU:H	2.28	0.41
2:U:85:LEU:HD23	2:U:85:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:44:THR:O	2:a:47:ARG:HB3	2.21	0.41
2:e:35:ARG:HA	2:e:38:ARG:HH21	1.85	0.41
2:g:134:LYS:HD2	2:g:153:PHE:HB3	2.02	0.41
3:q:68:PRO:HA	3:q:73:TYR:CG	2.56	0.41
2:y:116:TYR:HB2	2:y:123:ILE:HD11	2.03	0.41
2:3:89:LEU:HD22	2:3:133:MET:HE3	2.02	0.41
2:3:137:ALA:O	2:3:140:LEU:HG	2.20	0.41
2:7:48:GLU:H	2:7:48:GLU:CD	2.29	0.41
3:AF:68:PRO:HA	3:AF:73:TYR:CG	2.56	0.41
2:AI:109:ILE:HD11	2:AI:156:LEU:HD22	2.01	0.41
3:AJ:100:ASP:OD1	3:AJ:101:PRO:CD	2.50	0.41
2:AK:81:CYS:HA	6:AK:201:CYC:CHD	2.50	0.41
3:AN:61:ILE:HG13	3:AN:62:TYR:CD1	2.56	0.41
1:A:696:ARG:H	1:A:696:ARG:HG2	1.47	0.41
1:C:364:PHE:O	1:C:411:TYR:CE1	2.73	0.41
1:C:736:GLU:CD	1:C:736:GLU:H	2.28	0.41
1:C:1117:PRO:C	1:C:1118:THR:HG1	2.28	0.41
2:M:44:THR:O	2:M:47:ARG:HB3	2.20	0.41
3:N:68:PRO:HA	3:N:73:TYR:CG	2.56	0.41
2:O:44:THR:O	2:O:47:ARG:HB3	2.20	0.41
2:G:83:ARG:HH22	6:G:201:CYC:C1A	2.33	0.41
3:T:68:PRO:HA	3:T:73:TYR:CG	2.56	0.41
2:W:44:THR:O	2:W:47:ARG:HB3	2.21	0.41
2:W:81:CYS:HA	6:W:201:CYC:HHD	2.03	0.41
6:e:201:CYC:HC	6:e:201:CYC:CMD	2.33	0.41
3:f:140:LEU:N	3:f:140:LEU:HD12	2.36	0.41
2:k:48:GLU:CD	2:k:48:GLU:H	2.27	0.41
2:t:11:ALA:HB2	2:t:18:LEU:HD23	2.01	0.41
2:w:137:ALA:O	2:w:140:LEU:HG	2.21	0.41
2:3:25:ARG:HD3	2:5:25:ARG:CD	2.51	0.41
2:7:109:ILE:HD13	2:7:109:ILE:HA	1.84	0.41
2:AK:22:GLU:O	2:AK:25:ARG:CG	2.69	0.41
3:AL:100:ASP:OD1	3:AL:101:PRO:CD	2.50	0.41
2:AU:116:TYR:CB	2:AU:121:THR:HG22	2.51	0.41
2:AW:37:LEU:HD22	3:AX:24:LEU:HD22	2.02	0.41
1:A:28:ILE:CG2	3:v:94:TYR:CE1	3.04	0.41
1:C:162:TRP:CZ2	4:s:73:TYR:HE2	2.38	0.41
1:C:167:THR:O	1:C:171:ILE:HG13	2.21	0.41
1:C:424:ARG:HH11	1:C:424:ARG:HG3	1.86	0.41
1:C:482:GLN:NE2	3:n:107:ARG:HB3	2.36	0.41
1:C:1027:ASN:O	1:C:1028:ASN:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:46:SER:O	2:K:161:GLN:NE2	2.52	0.41
3:L:68:PRO:HA	3:L:73:TYR:CG	2.56	0.41
2:Q:101:VAL:HG11	2:S:20:PRO:HG2	2.00	0.41
2:U:48:GLU:H	2:U:48:GLU:CD	2.27	0.41
2:W:85:LEU:HD23	2:W:85:LEU:HA	1.92	0.41
3:d:68:PRO:HA	3:d:73:TYR:CG	2.56	0.41
6:j:201:CYC:HMA3	6:j:201:CYC:HBA1	2.03	0.41
2:m:27:LYS:HE3	3:n:39:ARG:CZ	2.51	0.41
6:t:201:CYC:HC	6:t:201:CYC:CMD	2.34	0.41
4:u:65:LEU:HA	4:u:70:GLY:HA3	2.03	0.41
2:w:4:LEU:HD12	2:w:4:LEU:C	2.45	0.41
2:w:14:GLU:CD	2:w:16:ARG:HE	2.29	0.41
2:w:134:LYS:HE2	2:w:150:GLY:CA	2.51	0.41
3:2:116:TYR:HE2	3:2:126:THR:HG21	1.85	0.41
3:4:61:ILE:HG13	3:4:62:TYR:CD1	2.56	0.41
2:5:109:ILE:HD11	2:5:156:LEU:HD22	2.03	0.41
6:AA:201:CYC:HBA1	3:AH:62:TYR:CD2	2.56	0.41
3:AF:62:TYR:OH	6:AK:201:CYC:O1D	2.35	0.41
3:AL:68:PRO:HA	3:AL:73:TYR:CG	2.56	0.41
3:AN:151:ILE:CD1	3:AN:152:TYR:CE2	2.97	0.41
3:AP:27:LEU:CD1	3:AP:27:LEU:C	2.92	0.41
3:AR:68:PRO:HA	3:AR:73:TYR:CG	2.56	0.41
3:AV:151:ILE:CD1	3:AV:152:TYR:CE2	2.97	0.41
2:AW:91:LEU:HB3	2:AW:104:ILE:HG23	2.02	0.41
5:Ad:30:LYS:HE3	5:Ad:40:GLU:HG2	2.02	0.41
1:A:54:ILE:CD1	3:v:31:PHE:CD1	3.03	0.41
1:A:67:ILE:HG12	1:A:209:ASN:HB3	2.03	0.41
1:A:188:GLU:HG3	1:A:238:ARG:HG2	2.02	0.41
1:A:434:TRP:HA	4:u:110:ASN:O	2.21	0.41
1:A:677:ASP:OD2	1:A:677:ASP:N	2.54	0.41
1:C:411:TYR:CD2	1:C:411:TYR:C	2.99	0.41
1:C:493:ASN:HA	1:C:494:PRO:HD3	1.95	0.41
1:C:620:PRO:HG2	1:C:621:PHE:CE2	2.55	0.41
6:M:201:CYC:HB	6:M:201:CYC:CMA	2.34	0.41
3:N:81:CYS:HB2	6:N:201:CYC:HMD3	2.03	0.41
6:E:201:CYC:HMB3	6:E:201:CYC:HHB	1.98	0.41
3:F:68:PRO:HA	3:F:73:TYR:CG	2.56	0.41
3:J:81:CYS:HA	6:J:201:CYC:CHD	2.50	0.41
3:L:61:ILE:HG13	3:L:62:TYR:CD1	2.55	0.41
3:V:68:PRO:HA	3:V:73:TYR:CG	2.56	0.41
3:V:109:LEU:HD23	3:V:109:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:48:GLU:CD	2:Y:48:GLU:H	2.28	0.41
2:Y:101:VAL:HG13	2:a:20:PRO:HG2	2.01	0.41
6:a:201:CYC:CMA	6:a:201:CYC:NB	2.84	0.41
3:b:29:ALA:O	3:b:32:THR:HG22	2.20	0.41
3:b:61:ILE:HG13	3:b:62:TYR:CD1	2.55	0.41
6:e:201:CYC:HMA3	6:e:201:CYC:NB	2.35	0.41
3:h:19:LEU:HD23	3:h:19:LEU:HA	1.97	0.41
2:k:41:GLN:HG3	2:k:45:GLU:OE2	2.21	0.41
2:k:46:ALA:HB2	2:k:140:LEU:HD11	2.02	0.41
2:k:80:LEU:HD13	6:k:201:CYC:HAD2	2.01	0.41
2:k:85:LEU:HD23	2:k:85:LEU:HA	1.90	0.41
2:k:156:LEU:CD1	2:k:160:MET:CE	2.99	0.41
3:n:68:PRO:HA	3:n:73:TYR:CG	2.56	0.41
6:r:201:CYC:HMA3	6:r:201:CYC:NB	2.36	0.41
4:s:9:ILE:HG12	4:s:19:PHE:CZ	2.56	0.41
4:s:112:LEU:HD11	6:s:201:CYC:HMB3	2.02	0.41
2:w:50:ILE:HD11	2:w:140:LEU:HD21	2.03	0.41
3:x:68:PRO:HA	3:x:73:TYR:CG	2.56	0.41
6:z:201:CYC:HHA	6:z:201:CYC:HAA2	1.84	0.41
3:2:68:PRO:HA	3:2:73:TYR:CG	2.56	0.41
2:3:31:ALA:O	2:3:34:GLU:OE1	2.39	0.41
2:5:48:GLU:CD	2:5:48:GLU:H	2.28	0.41
2:5:109:ILE:HD11	2:5:156:LEU:CD2	2.51	0.41
3:6:68:PRO:HA	3:6:73:TYR:CG	2.56	0.41
2:7:160:MET:HE3	2:7:160:MET:HB2	1.73	0.41
2:AC:41:GLN:HG3	2:AC:45:GLU:OE2	2.20	0.41
3:AD:68:PRO:HA	3:AD:73:TYR:CG	2.56	0.41
3:AF:72:MET:HB3	3:AF:72:MET:HE2	1.89	0.41
3:AF:119:LEU:HD23	6:AF:201:CYC:HBD1	2.01	0.41
2:AG:12:ASP:OD1	3:AH:91:TYR:OH	2.27	0.41
6:AH:201:CYC:HMA1	6:AH:201:CYC:NB	2.33	0.41
2:AI:4:LEU:HD12	2:AI:4:LEU:C	2.45	0.41
2:AK:91:LEU:HB3	2:AK:104:ILE:HG23	2.02	0.41
6:AM:201:CYC:HBA1	3:AT:62:TYR:CD2	2.56	0.41
3:AN:68:PRO:HA	3:AN:73:TYR:CG	2.56	0.41
2:AQ:43:LEU:HD12	2:AQ:141:LEU:HD21	2.03	0.41
2:AQ:105:GLU:HA	2:AQ:109:ILE:CD1	2.51	0.41
3:AR:2:GLN:N	3:AR:102:SER:HG	2.19	0.41
3:AR:15:GLN:HE21	3:AR:15:GLN:HB2	1.71	0.41
3:AT:113:LYS:HB3	3:AT:113:LYS:HE3	1.90	0.41
2:AU:31:ALA:O	2:AU:34:GLU:OE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AW:83:ARG:HH22	6:AW:201:CYC:C1A	2.34	0.41
1:A:228:SER:C	1:A:231:ILE:HG22	2.46	0.41
1:A:670:TYR:CD1	1:A:670:TYR:C	2.98	0.41
3:N:87:TYR:CD1	3:N:91:TYR:HE1	2.36	0.41
3:X:61:ILE:HG13	3:X:62:TYR:CD1	2.56	0.41
3:j:68:PRO:HA	3:j:73:TYR:CG	2.56	0.41
2:k:109:ILE:HG23	2:k:159:ALA:HB1	2.01	0.41
2:r:14:GLU:OE1	2:r:16:ARG:NE	2.53	0.41
2:t:115:MET:HG3	3:x:78:TYR:CD2	2.56	0.41
4:u:158:LYS:HE2	3:z:11:ASN:HB2	2.03	0.41
2:AA:109:ILE:HD13	2:AA:109:ILE:HA	1.86	0.41
3:AB:61:ILE:HG13	3:AB:62:TYR:CD1	2.56	0.41
2:AG:4:LEU:HD11	3:AH:3:ASP:CG	2.46	0.41
2:AG:41:GLN:HG3	2:AG:45:GLU:OE2	2.21	0.41
3:AL:10:ASN:OD1	3:AL:10:ASN:C	2.63	0.41
2:AM:95:GLY:HA3	2:AM:104:ILE:HD11	2.02	0.41
2:AQ:109:ILE:HD13	2:AQ:155:TYR:HE2	1.85	0.41
2:AQ:116:TYR:HB2	2:AQ:123:ILE:HD11	2.03	0.41
3:AT:57:ALA:HA	3:AT:61:ILE:HG12	2.03	0.41
1:A:444:ASN:OD1	1:A:444:ASN:C	2.58	0.40
1:A:445:TYR:O	1:A:448:PRO:HD2	2.20	0.40
1:A:557:VAL:HG22	2:9:103:PRO:HA	2.03	0.40
1:A:1117:PRO:C	1:A:1118:THR:HG1	2.28	0.40
1:C:67:ILE:HG12	1:C:209:ASN:HB3	2.03	0.40
1:C:318:GLU:HG3	1:C:322:LYS:HE3	2.03	0.40
1:C:541:THR:O	5:Ab:24:GLN:CG	2.63	0.40
1:C:677:ASP:OD2	1:C:677:ASP:N	2.54	0.40
2:E:44:THR:O	2:E:47:ARG:HB3	2.21	0.40
2:G:118:SER:O	3:J:53:LYS:HE3	2.20	0.40
3:T:61:ILE:HG13	3:T:62:TYR:CD1	2.57	0.40
2:U:23:LEU:HD22	3:V:38:VAL:HG13	2.03	0.40
6:W:201:CYC:HB	6:W:201:CYC:HMA3	1.85	0.40
3:f:78:TYR:O	3:f:82:ILE:HG13	2.20	0.40
2:g:41:GLN:HG3	2:g:45:GLU:OE2	2.21	0.40
3:j:15:GLN:HE21	3:j:15:GLN:HB2	1.71	0.40
3:l:61:ILE:HG13	3:l:62:TYR:CD1	2.56	0.40
3:l:68:PRO:HA	3:l:73:TYR:CG	2.56	0.40
3:n:112:LEU:HD23	3:n:160:LEU:HD11	2.03	0.40
2:o:4:LEU:HD12	2:o:4:LEU:C	2.45	0.40
2:t:85:LEU:HD23	2:t:85:LEU:HA	1.89	0.40
3:v:61:ILE:HG13	3:v:62:TYR:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:w:14:GLU:OE1	2:w:16:ARG:NE	2.53	0.40
2:w:41:GLN:HG3	2:w:45:GLU:OE2	2.22	0.40
2:w:134:LYS:HD2	2:w:153:PHE:HB3	2.03	0.40
2:1:43:LEU:HD12	2:1:43:LEU:HA	1.80	0.40
3:4:76:ARG:HB2	2:9:110:ILE:HG13	2.03	0.40
2:AA:44:THR:O	2:AA:47:ARG:HB3	2.20	0.40
3:AD:113:LYS:HE3	3:AD:113:LYS:HB3	1.91	0.40
6:AD:201:CYC:HMA1	5:Ac:26:THR:HG21	2.03	0.40
2:AE:105:GLU:HA	2:AE:109:ILE:CD1	2.51	0.40
3:AF:62:TYR:HH	6:AK:201:CYC:CGD	2.31	0.40
3:AV:68:PRO:HA	3:AV:73:TYR:CG	2.56	0.40
5:Aa:18:ARG:NH2	5:Aa:22:GLU:HB3	2.36	0.40
1:A:271:THR:CG2	1:A:419:THR:HG23	2.52	0.40
1:A:486:ILE:CD1	3:8:115:THR:HG23	2.51	0.40
1:A:698:GLY:N	3:x:127:VAL:HG11	2.35	0.40
1:C:298:ARG:HD2	1:C:308:ASP:OD2	2.21	0.40
1:C:496:GLU:OE2	3:f:114:GLU:HB3	2.20	0.40
1:C:544:VAL:HG22	1:C:560:VAL:HG23	2.01	0.40
1:C:649:PHE:CZ	6:f:201:CYC:NB	2.90	0.40
2:S:44:THR:O	2:S:47:ARG:HB3	2.20	0.40
3:Z:68:PRO:HA	3:Z:73:TYR:CG	2.56	0.40
3:b:14:VAL:HG13	5:AY:64:ASN:HD21	1.86	0.40
3:d:151:ILE:CD1	3:d:152:TYR:CE2	2.98	0.40
6:g:201:CYC:NB	6:g:201:CYC:HMA3	2.36	0.40
3:p:68:PRO:HA	3:p:73:TYR:CG	2.56	0.40
2:r:41:GLN:NE2	3:z:143:PRO:HG3	2.36	0.40
4:s:19:PHE:HD1	4:s:19:PHE:HA	1.75	0.40
3:0:113:LYS:HD2	3:0:123:ILE:CD1	2.51	0.40
1:A:318:GLU:CG	1:A:322:LYS:HE3	2.52	0.40
1:A:712:ARG:HH12	3:x:62:TYR:HB2	1.86	0.40
1:A:875:LEU:HD12	1:A:876:TYR:CD1	2.55	0.40
1:C:1117:PRO:C	1:C:1118:THR:OG1	2.63	0.40
3:N:78:TYR:CD2	2:I:115:MET:HG3	2.56	0.40
3:P:68:PRO:HA	3:P:73:TYR:CG	2.56	0.40
3:F:61:ILE:HG13	3:F:62:TYR:CD1	2.56	0.40
3:b:68:PRO:HA	3:b:73:TYR:CG	2.56	0.40
3:d:108:VAL:HG12	6:d:201:CYC:HAB1	2.02	0.40
3:f:151:ILE:CD1	3:f:152:TYR:CE2	2.97	0.40
6:i:201:CYC:HC	6:i:201:CYC:CMD	2.35	0.40
2:m:75:GLU:HG2	2:m:76:LYS:H	1.82	0.40
3:n:61:ILE:HG13	3:n:62:TYR:CD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:o:71:ASN:ND2	2:o:121:THR:HA	2.36	0.40
2:o:97:VAL:HG11	3:p:27:LEU:CD1	2.44	0.40
3:q:34:GLY:HA2	3:q:37:ARG:HD2	2.04	0.40
2:y:85:LEU:HD23	2:y:85:LEU:HA	1.96	0.40
3:2:61:ILE:HG13	3:2:62:TYR:CD1	2.57	0.40
6:4:201:CYC:O2A	6:4:201:CYC:C2A	2.69	0.40
2:7:130:VAL:HG21	2:7:160:MET:HE1	2.04	0.40
2:AE:43:LEU:HD12	2:AE:141:LEU:HD21	2.03	0.40
2:AE:113:LYS:HG2	2:AE:117:ASN:HD21	1.86	0.40
3:AH:57:ALA:HA	3:AH:61:ILE:HG12	2.03	0.40
3:AP:68:PRO:HA	3:AP:73:TYR:CG	2.56	0.40
3:AP:113:LYS:HE3	3:AP:113:LYS:HB3	1.88	0.40
3:AT:131:GLN:NE2	3:AT:157:SER:OG	2.54	0.40
3:AV:100:ASP:OD1	3:AV:101:PRO:CD	2.50	0.40
1:A:57:VAL:HG21	1:A:172:LEU:HG	2.03	0.40
1:A:298:ARG:HD2	1:A:308:ASP:OD2	2.21	0.40
1:A:424:ARG:HH11	1:A:424:ARG:HG3	1.86	0.40
1:A:501:ILE:O	1:A:642:ARG:HD2	2.21	0.40
1:C:466:LEU:HB2	1:C:467:PRO:HD2	2.03	0.40
1:C:785:ARG:HD3	1:C:785:ARG:HA	1.96	0.40
1:C:876:TYR:CE1	1:C:882:PRO:HA	2.57	0.40
1:C:889:LEU:HB3	1:C:890:PRO:CD	2.52	0.40
1:C:1012:PRO:HB2	1:C:1017:ARG:HG2	2.02	0.40
2:I:6:LYS:C	2:I:9:VAL:HG22	2.45	0.40
3:L:15:GLN:HE21	3:L:15:GLN:HB2	1.71	0.40
6:Q:201:CYC:HB	6:Q:201:CYC:CMA	2.35	0.40
3:V:19:LEU:HD23	3:V:19:LEU:HA	1.96	0.40
3:Z:87:TYR:CG	6:Z:201:CYC:HBB3	2.57	0.40
6:g:201:CYC:CMD	6:g:201:CYC:NC	2.84	0.40
2:1:34:GLU:OE2	3:2:31:PHE:CB	2.68	0.40
2:3:41:GLN:HG3	2:3:45:GLU:OE2	2.21	0.40
3:4:25:ASP:O	3:4:28:LYS:HG2	2.21	0.40
2:5:4:LEU:HD11	3:6:3:ASP:CG	2.46	0.40
2:9:80:LEU:CD2	6:9:201:CYC:HAD2	2.51	0.40
2:AC:137:ALA:O	2:AC:140:LEU:HG	2.21	0.40
3:AJ:72:MET:HE2	3:AJ:72:MET:HB3	1.83	0.40
2:AQ:16:ARG:O	3:AR:94:TYR:OH	2.33	0.40
2:AQ:35:ARG:C	2:AQ:38:ARG:HG2	2.43	0.40
6:AS:201:CYC:O1D	3:AV:62:TYR:OH	2.36	0.40
2:AU:2:SER:HB3	3:AV:6:THR:HG23	2.04	0.40
3:AX:61:ILE:HG13	3:AX:62:TYR:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AX:68:PRO:HA	3:AX:73:TYR:CG	2.56	0.40
1:A:17:PHE:HE2	3:v:6:THR:HG22	1.87	0.40
1:A:164:LEU:HD12	1:A:164:LEU:HA	1.94	0.40
1:A:819:PHE:O	1:A:820:HIS:C	2.65	0.40
1:C:57:VAL:HG21	1:C:172:LEU:HG	2.02	0.40
1:C:261:ILE:HD11	4:s:79:ALA:CB	2.52	0.40
6:E:201:CYC:CMA	6:E:201:CYC:NB	2.84	0.40
3:H:61:ILE:HG13	3:H:62:TYR:CD1	2.56	0.40
3:J:68:PRO:HA	3:J:73:TYR:CG	2.56	0.40
2:Q:47:ARG:HG3	3:R:18:TYR:CZ	2.56	0.40
3:T:134:LYS:HB3	3:T:134:LYS:HE3	1.65	0.40
2:W:5:THR:OG1	3:X:3:ASP:OD2	2.39	0.40
3:X:68:PRO:HA	3:X:73:TYR:CG	2.56	0.40
2:c:41:GLN:HG3	2:c:45:GLU:OE2	2.21	0.40
2:g:156:LEU:HD21	2:g:160:MET:HE1	2.03	0.40
6:i:201:CYC:CMD	6:i:201:CYC:NC	2.84	0.40
2:k:156:LEU:HG	2:k:160:MET:CE	2.51	0.40
6:o:201:CYC:HB	6:o:201:CYC:CMA	2.34	0.40
3:q:106:GLU:OE2	3:q:107:ARG:NH1	2.54	0.40
2:y:83:ARG:HH22	6:y:201:CYC:C1A	2.34	0.40
6:z:201:CYC:O1A	6:z:201:CYC:C2A	2.68	0.40
3:4:68:PRO:HA	3:4:73:TYR:CG	2.56	0.40
3:6:140:LEU:HD12	3:6:140:LEU:N	2.36	0.40
2:9:91:LEU:HD21	2:9:107:ILE:HG21	2.04	0.40
3:0:68:PRO:HA	3:0:73:TYR:CG	2.56	0.40
2:AA:116:TYR:HB2	2:AA:123:ILE:HD11	2.02	0.40
3:AD:34:GLY:HA2	3:AD:37:ARG:HD2	2.04	0.40
3:AJ:19:LEU:HD23	3:AJ:19:LEU:HA	1.94	0.40
2:AK:48:GLU:CD	2:AK:48:GLU:H	2.28	0.40
3:AL:61:ILE:HG13	3:AL:62:TYR:CD1	2.57	0.40
2:AM:44:THR:O	2:AM:47:ARG:HB3	2.21	0.40
3:AN:74:THR:HG22	2:AU:107:ILE:HG23	2.03	0.40
2:AO:109:ILE:O	2:AO:109:ILE:HG22	2.21	0.40
2:AS:41:GLN:HG3	2:AS:45:GLU:OE2	2.22	0.40
3:AV:131:GLN:NE2	3:AV:157:SER:OG	2.55	0.40
3:AX:10:ASN:HB2	5:Ad:64:ASN:OD1	2.21	0.40
5:Aa:3:ARG:HB3	5:Aa:56:LEU:HD11	2.02	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	1085/1155 (94%)	1016 (94%)	46 (4%)	23 (2%)	5	13
1	C	1085/1155 (94%)	1017 (94%)	42 (4%)	26 (2%)	5	11
2	1	156/161 (97%)	153 (98%)	3 (2%)	0	100	100
2	3	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
2	5	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
2	7	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	9	156/161 (97%)	153 (98%)	3 (2%)	0	100	100
2	AA	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	AC	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	22	40
2	AE	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	AG	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	AI	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
2	AK	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
2	AM	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	AO	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	22	40
2	AQ	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	AS	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	AU	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
2	AW	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
2	E	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	G	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	I	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	K	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	M	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	O	157/161 (98%)	154 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Q	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	S	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
2	U	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	W	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	Y	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	a	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	c	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
2	e	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
2	g	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
2	i	156/161 (97%)	153 (98%)	3 (2%)	0	100	100
2	k	156/161 (97%)	153 (98%)	3 (2%)	0	100	100
2	m	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	o	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
2	r	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	t	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
2	w	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
2	y	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
3	0	156/161 (97%)	153 (98%)	3 (2%)	0	100	100
3	2	155/161 (96%)	151 (97%)	4 (3%)	0	100	100
3	4	155/161 (96%)	152 (98%)	3 (2%)	0	100	100
3	6	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	8	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	AB	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	AD	156/161 (97%)	152 (97%)	4 (3%)	0	100	100
3	AF	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
3	AH	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	AJ	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	AL	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
3	AN	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	AP	156/161 (97%)	152 (97%)	4 (3%)	0	100	100
3	AR	157/161 (98%)	153 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AT	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	AV	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	AX	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
3	F	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
3	H	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	J	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	L	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
3	N	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	P	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
3	R	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	T	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
3	V	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
3	X	158/161 (98%)	155 (98%)	2 (1%)	1 (1%)	22	40
3	Z	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	b	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
3	d	155/161 (96%)	152 (98%)	3 (2%)	0	100	100
3	f	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
3	h	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	j	155/161 (96%)	151 (97%)	4 (3%)	0	100	100
3	l	156/161 (97%)	153 (98%)	3 (2%)	0	100	100
3	n	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	p	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
3	q	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	v	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
3	x	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
3	z	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
4	s	159/161 (99%)	153 (96%)	4 (2%)	2 (1%)	10	22
4	u	158/161 (98%)	153 (97%)	4 (2%)	1 (1%)	22	40
5	AY	64/69 (93%)	63 (98%)	1 (2%)	0	100	100
5	AZ	64/69 (93%)	63 (98%)	1 (2%)	0	100	100
5	Aa	64/69 (93%)	63 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Ab	63/69 (91%)	62 (98%)	1 (2%)	0	100	100
5	Ac	62/69 (90%)	62 (100%)	0	0	100	100
5	Ad	64/69 (93%)	64 (100%)	0	0	100	100
All	All	15460/15926 (97%)	15054 (97%)	351 (2%)	55 (0%)	32	49

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	GLU
1	A	364	PHE
1	A	560	VAL
1	A	701	ASP
1	A	750	ARG
1	A	889	LEU
1	A	891	ALA
1	A	1115	ARG
1	C	191	GLU
1	C	364	PHE
1	C	560	VAL
1	C	701	ASP
1	C	750	ARG
1	C	889	LEU
1	C	891	ALA
1	C	1115	ARG
3	X	108	VAL
1	A	320	GLU
1	A	558	VAL
1	A	1118	THR
1	C	320	GLU
1	C	558	VAL
1	A	786	SER
1	A	1028	ASN
1	A	1117	PRO
1	C	786	SER
1	C	1028	ASN
1	C	1117	PRO
1	C	1118	THR
1	A	184	LEU
1	A	250	SER
1	A	294	GLU
1	A	431	GLN

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Mol	Chain	Res	Type
1	A	559	THR
1	A	787	GLU
1	A	944	ALA
1	C	184	LEU
1	C	250	SER
1	C	294	GLU
1	C	348	TYR
1	C	559	THR
1	C	787	GLU
1	C	944	ALA
4	s	74	TYR
4	u	74	TYR
2	AC	3	VAL
2	AO	3	VAL
1	A	253	ARG
1	A	396	GLY
1	C	253	ARG
1	C	431	GLN
1	C	1134	GLU
4	s	102	SER
1	C	396	GLY
1	C	432	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	927/977 (95%)	866 (93%)	61 (7%)	14	28
1	C	927/977 (95%)	868 (94%)	59 (6%)	14	29
2	1	125/128 (98%)	120 (96%)	5 (4%)	27	51
2	3	126/128 (98%)	122 (97%)	4 (3%)	34	60
2	5	126/128 (98%)	122 (97%)	4 (3%)	34	60
2	7	127/128 (99%)	119 (94%)	8 (6%)	15	30
2	9	125/128 (98%)	118 (94%)	7 (6%)	17	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AA	127/128 (99%)	120 (94%)	7 (6%)	18	37
2	AC	127/128 (99%)	121 (95%)	6 (5%)	22	44
2	AE	127/128 (99%)	120 (94%)	7 (6%)	18	37
2	AG	127/128 (99%)	117 (92%)	10 (8%)	10	21
2	AI	126/128 (98%)	121 (96%)	5 (4%)	27	51
2	AK	126/128 (98%)	120 (95%)	6 (5%)	21	42
2	AM	127/128 (99%)	120 (94%)	7 (6%)	18	37
2	AO	127/128 (99%)	121 (95%)	6 (5%)	22	44
2	AQ	127/128 (99%)	120 (94%)	7 (6%)	18	37
2	AS	127/128 (99%)	118 (93%)	9 (7%)	12	26
2	AU	126/128 (98%)	121 (96%)	5 (4%)	27	51
2	AW	126/128 (98%)	120 (95%)	6 (5%)	21	42
2	E	127/128 (99%)	109 (86%)	18 (14%)	2	4
2	G	127/128 (99%)	112 (88%)	15 (12%)	4	8
2	I	127/128 (99%)	106 (84%)	21 (16%)	2	3
2	K	127/128 (99%)	112 (88%)	15 (12%)	4	8
2	M	127/128 (99%)	109 (86%)	18 (14%)	2	4
2	O	126/128 (98%)	110 (87%)	16 (13%)	3	6
2	Q	127/128 (99%)	109 (86%)	18 (14%)	2	4
2	S	126/128 (98%)	110 (87%)	16 (13%)	3	6
2	U	127/128 (99%)	109 (86%)	18 (14%)	2	4
2	W	127/128 (99%)	113 (89%)	14 (11%)	5	9
2	Y	127/128 (99%)	103 (81%)	24 (19%)	1	1
2	a	127/128 (99%)	112 (88%)	15 (12%)	4	8
2	c	126/128 (98%)	119 (94%)	7 (6%)	17	35
2	e	126/128 (98%)	122 (97%)	4 (3%)	34	60
2	g	126/128 (98%)	121 (96%)	5 (4%)	27	51
2	i	125/128 (98%)	119 (95%)	6 (5%)	21	42
2	k	125/128 (98%)	115 (92%)	10 (8%)	10	20
2	m	127/128 (99%)	119 (94%)	8 (6%)	15	30
2	o	126/128 (98%)	120 (95%)	6 (5%)	21	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	r	127/128 (99%)	119 (94%)	8 (6%)	15	30
2	t	126/128 (98%)	121 (96%)	5 (4%)	27	51
2	w	126/128 (98%)	120 (95%)	6 (5%)	21	42
2	y	126/128 (98%)	120 (95%)	6 (5%)	21	42
3	0	119/121 (98%)	113 (95%)	6 (5%)	20	40
3	2	118/121 (98%)	109 (92%)	9 (8%)	11	23
3	4	118/121 (98%)	115 (98%)	3 (2%)	42	68
3	6	121/121 (100%)	117 (97%)	4 (3%)	33	59
3	8	121/121 (100%)	119 (98%)	2 (2%)	56	78
3	AB	121/121 (100%)	118 (98%)	3 (2%)	42	68
3	AD	119/121 (98%)	109 (92%)	10 (8%)	9	19
3	AF	120/121 (99%)	115 (96%)	5 (4%)	25	48
3	AH	121/121 (100%)	120 (99%)	1 (1%)	79	90
3	AJ	121/121 (100%)	117 (97%)	4 (3%)	33	59
3	AL	120/121 (99%)	117 (98%)	3 (2%)	42	68
3	AN	121/121 (100%)	118 (98%)	3 (2%)	42	68
3	AP	119/121 (98%)	109 (92%)	10 (8%)	9	19
3	AR	120/121 (99%)	115 (96%)	5 (4%)	25	48
3	AT	121/121 (100%)	119 (98%)	2 (2%)	56	78
3	AV	121/121 (100%)	117 (97%)	4 (3%)	33	59
3	AX	120/121 (99%)	117 (98%)	3 (2%)	42	68
3	F	121/121 (100%)	114 (94%)	7 (6%)	17	34
3	H	121/121 (100%)	107 (88%)	14 (12%)	4	8
3	J	121/121 (100%)	107 (88%)	14 (12%)	4	8
3	L	121/121 (100%)	108 (89%)	13 (11%)	5	10
3	N	121/121 (100%)	107 (88%)	14 (12%)	4	8
3	P	121/121 (100%)	111 (92%)	10 (8%)	9	19
3	R	121/121 (100%)	107 (88%)	14 (12%)	4	8
3	T	121/121 (100%)	111 (92%)	10 (8%)	9	19
3	V	121/121 (100%)	114 (94%)	7 (6%)	17	34
3	X	121/121 (100%)	106 (88%)	15 (12%)	4	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Z	121/121 (100%)	107 (88%)	14 (12%)	4	8
3	b	121/121 (100%)	109 (90%)	12 (10%)	6	12
3	d	118/121 (98%)	113 (96%)	5 (4%)	25	48
3	f	120/121 (99%)	115 (96%)	5 (4%)	25	48
3	h	121/121 (100%)	118 (98%)	3 (2%)	42	68
3	j	118/121 (98%)	108 (92%)	10 (8%)	8	18
3	l	119/121 (98%)	114 (96%)	5 (4%)	25	48
3	n	121/121 (100%)	117 (97%)	4 (3%)	33	59
3	p	121/121 (100%)	118 (98%)	3 (2%)	42	68
3	q	121/121 (100%)	120 (99%)	1 (1%)	79	90
3	v	121/121 (100%)	119 (98%)	2 (2%)	56	78
3	x	121/121 (100%)	117 (97%)	4 (3%)	33	59
3	z	121/121 (100%)	118 (98%)	3 (2%)	42	68
4	s	123/123 (100%)	111 (90%)	12 (10%)	6	13
4	u	122/123 (99%)	110 (90%)	12 (10%)	6	13
5	AY	57/58 (98%)	41 (72%)	16 (28%)	0	0
5	AZ	57/58 (98%)	41 (72%)	16 (28%)	0	0
5	Aa	57/58 (98%)	41 (72%)	16 (28%)	0	0
5	Ab	56/58 (97%)	36 (64%)	20 (36%)	0	0
5	Ac	56/58 (97%)	39 (70%)	17 (30%)	0	0
5	Ad	57/58 (98%)	41 (72%)	16 (28%)	0	0
All	All	12311/12508 (98%)	11412 (93%)	899 (7%)	14	24

All (899) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	16	LEU
1	A	25	ILE
1	A	60	LEU
1	A	75	ILE
1	A	140	PHE
1	A	148	TYR
1	A	158	ARG
1	A	187	ARG

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Mol	Chain	Res	Type
1	A	192	LYS
1	A	195	SER
1	A	217	GLU
1	A	245	ILE
1	A	246	VAL
1	A	277	ILE
1	A	316	VAL
1	A	323	VAL
1	A	330	VAL
1	A	352	ILE
1	A	356	VAL
1	A	357	LEU
1	A	386	ILE
1	A	387	VAL
1	A	388	ARG
1	A	410	GLU
1	A	428	VAL
1	A	431	GLN
1	A	464	GLN
1	A	488	LYS
1	A	490	SER
1	A	497	ARG
1	A	511	ARG
1	A	532	THR
1	A	546	PHE
1	A	547	ARG
1	A	560	VAL
1	A	635	LEU
1	A	660	VAL
1	A	661	VAL
1	A	691	SER
1	A	696	ARG
1	A	704	THR
1	A	723	GLN
1	A	724	GLU
1	A	729	ILE
1	A	741	GLN
1	A	746	LEU
1	A	787	GLU
1	A	812	SER
1	A	854	LEU
1	A	889	LEU

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Mol	Chain	Res	Type
1	A	941	THR
1	A	942	LYS
1	A	945	LEU
1	A	947	MET
1	A	957	ARG
1	A	969	VAL
1	A	981	ILE
1	A	1020	GLU
1	A	1097	VAL
1	A	1098	GLU
1	C	3	ILE
1	C	16	LEU
1	C	25	ILE
1	C	60	LEU
1	C	75	ILE
1	C	140	PHE
1	C	148	TYR
1	C	187	ARG
1	C	217	GLU
1	C	245	ILE
1	C	246	VAL
1	C	257	THR
1	C	277	ILE
1	C	316	VAL
1	C	323	VAL
1	C	330	VAL
1	C	356	VAL
1	C	382	ILE
1	C	387	VAL
1	C	388	ARG
1	C	410	GLU
1	C	425	ASN
1	C	428	VAL
1	C	431	GLN
1	C	433	SER
1	C	464	GLN
1	C	488	LYS
1	C	490	SER
1	C	497	ARG
1	C	511	ARG
1	C	532	THR
1	C	547	ARG

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Mol	Chain	Res	Type
1	C	560	VAL
1	C	635	LEU
1	C	660	VAL
1	C	661	VAL
1	C	691	SER
1	C	696	ARG
1	C	704	THR
1	C	723	GLN
1	C	724	GLU
1	C	729	ILE
1	C	741	GLN
1	C	746	LEU
1	C	787	GLU
1	C	812	SER
1	C	854	LEU
1	C	889	LEU
1	C	941	THR
1	C	942	LYS
1	C	945	LEU
1	C	947	MET
1	C	957	ARG
1	C	969	VAL
1	C	981	ILE
1	C	1020	GLU
1	C	1046	ARG
1	C	1097	VAL
1	C	1098	GLU
2	M	4	LEU
2	M	22	GLU
2	M	25	ARG
2	M	36	ARG
2	M	43	LEU
2	M	47	ARG
2	M	48	GLU
2	M	49	ARG
2	M	75	GLU
2	M	91	LEU
2	M	102	THR
2	M	109	ILE
2	M	113	LYS
2	M	120	GLN
2	M	131	ARG

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Mol	Chain	Res	Type
2	M	134	LYS
2	M	140	LEU
2	M	142	SER
3	N	1	MET
3	N	26	LYS
3	N	28	LYS
3	N	39	ARG
3	N	50	THR
3	N	76	ARG
3	N	77	ARG
3	N	103	ILE
3	N	106	GLU
3	N	107	ARG
3	N	123	ILE
3	N	135	GLU
3	N	140	LEU
3	N	160	LEU
2	O	2	SER
2	O	4	LEU
2	O	25	ARG
2	O	27	LYS
2	O	28	SER
2	O	43	LEU
2	O	47	ARG
2	O	61	LYS
2	O	71	ASN
2	O	75	GLU
2	O	76	LYS
2	O	91	LEU
2	O	109	ILE
2	O	123	ILE
2	O	138	THR
2	O	140	LEU
3	P	1	MET
3	P	17	LYS
3	P	26	LYS
3	P	28	LYS
3	P	50	THR
3	P	58	LYS
3	P	123	ILE
3	P	135	GLU
3	P	140	LEU

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Mol	Chain	Res	Type
3	P	160	LEU
2	E	2	SER
2	E	4	LEU
2	E	6	LYS
2	E	19	SER
2	E	25	ARG
2	E	28	SER
2	E	43	LEU
2	E	47	ARG
2	E	48	GLU
2	E	49	ARG
2	E	60	GLN
2	E	75	GLU
2	E	76	LYS
2	E	91	LEU
2	E	109	ILE
2	E	140	LEU
2	E	142	SER
2	E	160	MET
3	F	1	MET
3	F	72	MET
3	F	96	MET
3	F	123	ILE
3	F	135	GLU
3	F	140	LEU
3	F	144	ASP
2	G	2	SER
2	G	4	LEU
2	G	8	ILE
2	G	19	SER
2	G	28	SER
2	G	43	LEU
2	G	47	ARG
2	G	49	ARG
2	G	52	LYS
2	G	62	ARG
2	G	76	LYS
2	G	91	LEU
2	G	106	GLU
2	G	109	ILE
2	G	140	LEU
3	H	1	MET

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Mol	Chain	Res	Type
3	H	26	LYS
3	H	28	LYS
3	H	32	THR
3	H	45	SER
3	H	50	THR
3	H	58	LYS
3	H	77	ARG
3	H	103	ILE
3	H	118	SER
3	H	135	GLU
3	H	140	LEU
3	H	151	ILE
3	H	160	LEU
2	I	2	SER
2	I	4	LEU
2	I	19	SER
2	I	25	ARG
2	I	28	SER
2	I	36	ARG
2	I	43	LEU
2	I	47	ARG
2	I	48	GLU
2	I	49	ARG
2	I	52	LYS
2	I	75	GLU
2	I	76	LYS
2	I	91	LEU
2	I	109	ILE
2	I	123	ILE
2	I	128	GLU
2	I	131	ARG
2	I	142	SER
2	I	160	MET
2	I	161	GLN
3	J	1	MET
3	J	3	ASP
3	J	50	THR
3	J	53	LYS
3	J	65	LEU
3	J	72	MET
3	J	77	ARG
3	J	90	ARG

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Mol	Chain	Res	Type
3	J	107	ARG
3	J	123	ILE
3	J	135	GLU
3	J	140	LEU
3	J	147	LYS
3	J	160	LEU
2	K	2	SER
2	K	4	LEU
2	K	19	SER
2	K	22	GLU
2	K	25	ARG
2	K	26	ILE
2	K	43	LEU
2	K	47	ARG
2	K	49	ARG
2	K	60	GLN
2	K	62	ARG
2	K	76	LYS
2	K	91	LEU
2	K	109	ILE
2	K	160	MET
3	L	26	LYS
3	L	28	LYS
3	L	32	THR
3	L	39	ARG
3	L	49	THR
3	L	50	THR
3	L	54	GLU
3	L	58	LYS
3	L	107	ARG
3	L	123	ILE
3	L	135	GLU
3	L	140	LEU
3	L	160	LEU
2	Q	4	LEU
2	Q	22	GLU
2	Q	25	ARG
2	Q	36	ARG
2	Q	43	LEU
2	Q	47	ARG
2	Q	48	GLU
2	Q	49	ARG

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Mol	Chain	Res	Type
2	Q	61	LYS
2	Q	75	GLU
2	Q	91	LEU
2	Q	102	THR
2	Q	109	ILE
2	Q	113	LYS
2	Q	120	GLN
2	Q	131	ARG
2	Q	134	LYS
2	Q	142	SER
3	R	1	MET
3	R	26	LYS
3	R	28	LYS
3	R	39	ARG
3	R	50	THR
3	R	76	ARG
3	R	77	ARG
3	R	103	ILE
3	R	106	GLU
3	R	107	ARG
3	R	123	ILE
3	R	135	GLU
3	R	140	LEU
3	R	160	LEU
2	S	2	SER
2	S	4	LEU
2	S	25	ARG
2	S	27	LYS
2	S	28	SER
2	S	43	LEU
2	S	47	ARG
2	S	61	LYS
2	S	71	ASN
2	S	75	GLU
2	S	76	LYS
2	S	91	LEU
2	S	109	ILE
2	S	123	ILE
2	S	138	THR
2	S	140	LEU
3	T	1	MET
3	T	17	LYS

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Mol	Chain	Res	Type
3	T	26	LYS
3	T	28	LYS
3	T	50	THR
3	T	58	LYS
3	T	123	ILE
3	T	135	GLU
3	T	140	LEU
3	T	160	LEU
2	U	2	SER
2	U	4	LEU
2	U	6	LYS
2	U	19	SER
2	U	25	ARG
2	U	28	SER
2	U	43	LEU
2	U	47	ARG
2	U	48	GLU
2	U	49	ARG
2	U	61	LYS
2	U	75	GLU
2	U	76	LYS
2	U	91	LEU
2	U	109	ILE
2	U	140	LEU
2	U	142	SER
2	U	160	MET
3	V	1	MET
3	V	72	MET
3	V	96	MET
3	V	123	ILE
3	V	135	GLU
3	V	140	LEU
3	V	144	ASP
2	W	2	SER
2	W	4	LEU
2	W	8	ILE
2	W	19	SER
2	W	28	SER
2	W	43	LEU
2	W	47	ARG
2	W	49	ARG
2	W	52	LYS

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Mol	Chain	Res	Type
2	W	62	ARG
2	W	76	LYS
2	W	91	LEU
2	W	106	GLU
2	W	109	ILE
3	X	1	MET
3	X	26	LYS
3	X	28	LYS
3	X	32	THR
3	X	45	SER
3	X	50	THR
3	X	58	LYS
3	X	77	ARG
3	X	103	ILE
3	X	107	ARG
3	X	118	SER
3	X	135	GLU
3	X	140	LEU
3	X	151	ILE
3	X	160	LEU
2	Y	2	SER
2	Y	4	LEU
2	Y	19	SER
2	Y	25	ARG
2	Y	28	SER
2	Y	36	ARG
2	Y	43	LEU
2	Y	47	ARG
2	Y	48	GLU
2	Y	49	ARG
2	Y	52	LYS
2	Y	60	GLN
2	Y	61	LYS
2	Y	62	ARG
2	Y	75	GLU
2	Y	76	LYS
2	Y	91	LEU
2	Y	109	ILE
2	Y	123	ILE
2	Y	128	GLU
2	Y	131	ARG
2	Y	142	SER

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Mol	Chain	Res	Type
2	Y	160	MET
2	Y	161	GLN
3	Z	1	MET
3	Z	3	ASP
3	Z	50	THR
3	Z	53	LYS
3	Z	65	LEU
3	Z	72	MET
3	Z	77	ARG
3	Z	90	ARG
3	Z	107	ARG
3	Z	123	ILE
3	Z	135	GLU
3	Z	140	LEU
3	Z	147	LYS
3	Z	160	LEU
2	a	2	SER
2	a	4	LEU
2	a	19	SER
2	a	22	GLU
2	a	25	ARG
2	a	26	ILE
2	a	43	LEU
2	a	47	ARG
2	a	49	ARG
2	a	60	GLN
2	a	62	ARG
2	a	76	LYS
2	a	91	LEU
2	a	109	ILE
2	a	160	MET
3	b	26	LYS
3	b	28	LYS
3	b	32	THR
3	b	39	ARG
3	b	49	THR
3	b	50	THR
3	b	54	GLU
3	b	58	LYS
3	b	123	ILE
3	b	135	GLU
3	b	140	LEU

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Mol	Chain	Res	Type
3	b	160	LEU
2	c	2	SER
2	c	4	LEU
2	c	48	GLU
2	c	60	GLN
2	c	91	LEU
2	c	140	LEU
2	c	160	MET
3	d	72	MET
3	d	86	ASP
3	d	103	ILE
3	d	123	ILE
3	d	137	VAL
2	e	2	SER
2	e	48	GLU
2	e	61	LYS
2	e	113	LYS
3	f	17	LYS
3	f	72	MET
3	f	82	ILE
3	f	106	GLU
3	f	160	LEU
2	g	22	GLU
2	g	48	GLU
2	g	60	GLN
2	g	91	LEU
2	g	160	MET
3	h	1	MET
3	h	54	GLU
3	h	123	ILE
2	i	43	LEU
2	i	48	GLU
2	i	82	LEU
2	i	91	LEU
2	i	113	LYS
2	i	123	ILE
3	j	2	GLN
3	j	3	ASP
3	j	65	LEU
3	j	66	THR
3	j	83	ARG
3	j	86	ASP

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Mol	Chain	Res	Type
3	j	112	LEU
3	j	113	LYS
3	j	119	LEU
3	j	123	ILE
2	k	28	SER
2	k	36	ARG
2	k	48	GLU
2	k	58	LEU
2	k	65	VAL
2	k	82	LEU
2	k	107	ILE
2	k	133	MET
2	k	140	LEU
2	k	160	MET
3	l	3	ASP
3	l	54	GLU
3	l	72	MET
3	l	123	ILE
3	l	160	LEU
2	m	2	SER
2	m	4	LEU
2	m	26	ILE
2	m	28	SER
2	m	61	LYS
2	m	91	LEU
2	m	140	LEU
2	m	161	GLN
3	n	1	MET
3	n	32	THR
3	n	72	MET
3	n	123	ILE
2	o	2	SER
2	o	36	ARG
2	o	48	GLU
2	o	60	GLN
2	o	91	LEU
2	o	102	THR
3	p	1	MET
3	p	72	MET
3	p	118	SER
3	q	1	MET
2	r	2	SER

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Mol	Chain	Res	Type
2	r	4	LEU
2	r	48	GLU
2	r	60	GLN
2	r	61	LYS
2	r	76	LYS
2	r	140	LEU
2	r	161	GLN
4	s	1	MET
4	s	5	ILE
4	s	13	ASP
4	s	17	LYS
4	s	19	PHE
4	s	61	LEU
4	s	72	MET
4	s	108	VAL
4	s	123	ILE
4	s	124	ASP
4	s	137	VAL
4	s	141	VAL
2	t	4	LEU
2	t	5	THR
2	t	22	GLU
2	t	140	LEU
2	t	160	MET
4	u	1	MET
4	u	5	ILE
4	u	13	ASP
4	u	17	LYS
4	u	19	PHE
4	u	61	LEU
4	u	77	ARG
4	u	103	LEU
4	u	113	LYS
4	u	137	VAL
4	u	140	VAL
4	u	141	VAL
3	v	1	MET
3	v	72	MET
2	w	2	SER
2	w	48	GLU
2	w	91	LEU
2	w	123	ILE

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Mol	Chain	Res	Type
2	w	140	LEU
2	w	160	MET
3	x	17	LYS
3	x	67	ARG
3	x	72	MET
3	x	118	SER
2	y	22	GLU
2	y	36	ARG
2	y	60	GLN
2	y	61	LYS
2	y	110	ILE
2	y	113	LYS
3	z	1	MET
3	z	76	ARG
3	z	123	ILE
2	1	43	LEU
2	1	48	GLU
2	1	75	GLU
2	1	91	LEU
2	1	123	ILE
3	2	2	GLN
3	2	3	ASP
3	2	26	LYS
3	2	65	LEU
3	2	72	MET
3	2	86	ASP
3	2	112	LEU
3	2	113	LYS
3	2	123	ILE
2	3	2	SER
2	3	48	GLU
2	3	91	LEU
2	3	100	ASP
3	4	72	MET
3	4	123	ILE
3	4	137	VAL
2	5	2	SER
2	5	27	LYS
2	5	48	GLU
2	5	61	LYS
3	6	1	MET
3	6	17	LYS

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Mol	Chain	Res	Type
3	6	72	MET
3	6	123	ILE
2	7	2	SER
2	7	26	ILE
2	7	28	SER
2	7	48	GLU
2	7	75	GLU
2	7	91	LEU
2	7	140	LEU
2	7	161	GLN
3	8	32	THR
3	8	72	MET
2	9	36	ARG
2	9	41	GLN
2	9	48	GLU
2	9	61	LYS
2	9	75	GLU
2	9	109	ILE
2	9	160	MET
3	0	54	GLU
3	0	58	LYS
3	0	72	MET
3	0	123	ILE
3	0	147	LYS
3	0	160	LEU
2	AA	2	SER
2	AA	4	LEU
2	AA	47	ARG
2	AA	48	GLU
2	AA	91	LEU
2	AA	102	THR
2	AA	161	GLN
3	AB	1	MET
3	AB	28	LYS
3	AB	123	ILE
2	AC	2	SER
2	AC	22	GLU
2	AC	48	GLU
2	AC	61	LYS
2	AC	75	GLU
2	AC	91	LEU
3	AD	3	ASP

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Mol	Chain	Res	Type
3	AD	54	GLU
3	AD	66	THR
3	AD	72	MET
3	AD	77	ARG
3	AD	86	ASP
3	AD	108	VAL
3	AD	123	ILE
3	AD	158	SER
3	AD	160	LEU
2	AE	2	SER
2	AE	22	GLU
2	AE	75	GLU
2	AE	83	ARG
2	AE	91	LEU
2	AE	131	ARG
2	AE	161	GLN
3	AF	2	GLN
3	AF	3	ASP
3	AF	72	MET
3	AF	86	ASP
3	AF	90	ARG
2	AG	2	SER
2	AG	48	GLU
2	AG	60	GLN
2	AG	61	LYS
2	AG	75	GLU
2	AG	91	LEU
2	AG	102	THR
2	AG	109	ILE
2	AG	160	MET
2	AG	161	GLN
3	AH	123	ILE
2	AI	2	SER
2	AI	25	ARG
2	AI	48	GLU
2	AI	60	GLN
2	AI	91	LEU
3	AJ	1	MET
3	AJ	11	ASN
3	AJ	20	ASP
3	AJ	72	MET
2	AK	2	SER

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Mol	Chain	Res	Type
2	AK	19	SER
2	AK	25	ARG
2	AK	48	GLU
2	AK	60	GLN
2	AK	61	LYS
3	AL	72	MET
3	AL	123	ILE
3	AL	160	LEU
2	AM	2	SER
2	AM	4	LEU
2	AM	47	ARG
2	AM	48	GLU
2	AM	91	LEU
2	AM	102	THR
2	AM	161	GLN
3	AN	1	MET
3	AN	28	LYS
3	AN	123	ILE
2	AO	2	SER
2	AO	22	GLU
2	AO	48	GLU
2	AO	61	LYS
2	AO	75	GLU
2	AO	91	LEU
3	AP	3	ASP
3	AP	54	GLU
3	AP	66	THR
3	AP	72	MET
3	AP	77	ARG
3	AP	86	ASP
3	AP	108	VAL
3	AP	123	ILE
3	AP	158	SER
3	AP	160	LEU
2	AQ	2	SER
2	AQ	22	GLU
2	AQ	75	GLU
2	AQ	83	ARG
2	AQ	91	LEU
2	AQ	131	ARG
2	AQ	161	GLN
3	AR	2	GLN

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Mol	Chain	Res	Type
3	AR	3	ASP
3	AR	72	MET
3	AR	86	ASP
3	AR	90	ARG
2	AS	2	SER
2	AS	48	GLU
2	AS	60	GLN
2	AS	75	GLU
2	AS	91	LEU
2	AS	102	THR
2	AS	109	ILE
2	AS	160	MET
2	AS	161	GLN
3	AT	77	ARG
3	AT	123	ILE
2	AU	2	SER
2	AU	25	ARG
2	AU	48	GLU
2	AU	60	GLN
2	AU	91	LEU
3	AV	1	MET
3	AV	11	ASN
3	AV	20	ASP
3	AV	72	MET
2	AW	2	SER
2	AW	19	SER
2	AW	25	ARG
2	AW	48	GLU
2	AW	60	GLN
2	AW	61	LYS
3	AX	72	MET
3	AX	123	ILE
3	AX	160	LEU
5	AY	8	THR
5	AY	14	LEU
5	AY	15	LYS
5	AY	16	ARG
5	AY	18	ARG
5	AY	21	ARG
5	AY	22	GLU
5	AY	25	ASN
5	AY	28	PHE

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Mol	Chain	Res	Type
5	AY	30	LYS
5	AY	32	VAL
5	AY	35	GLU
5	AY	46	LYS
5	AY	52	LEU
5	AY	55	LYS
5	AY	67	VAL
5	AZ	8	THR
5	AZ	14	LEU
5	AZ	15	LYS
5	AZ	16	ARG
5	AZ	18	ARG
5	AZ	21	ARG
5	AZ	22	GLU
5	AZ	25	ASN
5	AZ	28	PHE
5	AZ	30	LYS
5	AZ	32	VAL
5	AZ	35	GLU
5	AZ	46	LYS
5	AZ	52	LEU
5	AZ	55	LYS
5	AZ	67	VAL
5	Aa	2	SER
5	Aa	8	THR
5	Aa	11	ILE
5	Aa	14	LEU
5	Aa	15	LYS
5	Aa	16	ARG
5	Aa	18	ARG
5	Aa	21	ARG
5	Aa	22	GLU
5	Aa	30	LYS
5	Aa	32	VAL
5	Aa	35	GLU
5	Aa	46	LYS
5	Aa	52	LEU
5	Aa	55	LYS
5	Aa	67	VAL
5	Ab	2	SER
5	Ab	4	TYR
5	Ab	8	THR

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Mol	Chain	Res	Type
5	Ab	11	ILE
5	Ab	14	LEU
5	Ab	16	ARG
5	Ab	18	ARG
5	Ab	21	ARG
5	Ab	22	GLU
5	Ab	24	GLN
5	Ab	25	ASN
5	Ab	30	LYS
5	Ab	32	VAL
5	Ab	35	GLU
5	Ab	43	ARG
5	Ab	45	GLN
5	Ab	46	LYS
5	Ab	52	LEU
5	Ab	55	LYS
5	Ab	65	THR
5	Ac	8	THR
5	Ac	14	LEU
5	Ac	15	LYS
5	Ac	16	ARG
5	Ac	18	ARG
5	Ac	21	ARG
5	Ac	22	GLU
5	Ac	23	LEU
5	Ac	24	GLN
5	Ac	25	ASN
5	Ac	27	PHE
5	Ac	30	LYS
5	Ac	32	VAL
5	Ac	35	GLU
5	Ac	42	GLN
5	Ac	52	LEU
5	Ac	55	LYS
5	Ad	8	THR
5	Ad	14	LEU
5	Ad	15	LYS
5	Ad	16	ARG
5	Ad	18	ARG
5	Ad	21	ARG
5	Ad	22	GLU
5	Ad	23	LEU

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Mol	Chain	Res	Type
5	Ad	25	ASN
5	Ad	32	VAL
5	Ad	35	GLU
5	Ad	45	GLN
5	Ad	52	LEU
5	Ad	55	LYS
5	Ad	61	GLN
5	Ad	67	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (223) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	287	ASN
1	A	376	GLN
1	A	482	GLN
1	A	489	ASN
1	A	573	GLN
1	A	579	GLN
1	A	749	GLN
1	A	820	HIS
1	A	851	HIS
1	A	939	GLN
1	A	1065	HIS
1	A	1107	ASN
1	C	287	ASN
1	C	376	GLN
1	C	425	ASN
1	C	482	GLN
1	C	489	ASN
1	C	573	GLN
1	C	579	GLN
1	C	749	GLN
1	C	820	HIS
1	C	851	HIS
1	C	939	GLN
1	C	980	HIS
1	C	1065	HIS
1	C	1107	ASN
1	C	1131	ASN
2	M	57	GLN
2	M	60	GLN

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Mol	Chain	Res	Type
2	M	120	GLN
3	N	11	ASN
3	N	15	GLN
3	N	47	ASN
3	N	110	ASN
3	N	131	GLN
3	P	11	ASN
3	P	15	GLN
3	P	47	ASN
3	P	131	GLN
3	F	11	ASN
3	F	131	GLN
2	G	60	GLN
2	G	120	GLN
3	H	11	ASN
3	H	15	GLN
3	H	47	ASN
2	I	41	GLN
3	J	11	ASN
3	J	15	GLN
3	J	47	ASN
3	J	131	GLN
2	K	71	ASN
3	L	11	ASN
3	L	15	GLN
3	L	47	ASN
3	L	131	GLN
2	Q	57	GLN
2	Q	120	GLN
3	R	11	ASN
3	R	15	GLN
3	R	47	ASN
3	R	131	GLN
2	S	41	GLN
3	T	11	ASN
3	T	15	GLN
3	T	47	ASN
3	T	131	GLN
3	V	11	ASN
2	W	120	GLN
3	X	11	ASN
3	X	15	GLN

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Mol	Chain	Res	Type
3	X	47	ASN
2	Y	41	GLN
3	Z	11	ASN
3	Z	15	GLN
3	Z	47	ASN
3	Z	131	GLN
2	a	71	ASN
3	b	11	ASN
3	b	15	GLN
3	b	47	ASN
3	b	131	GLN
2	c	53	GLN
2	c	57	GLN
3	d	10	ASN
3	d	47	ASN
2	e	71	ASN
3	f	11	ASN
3	f	15	GLN
3	f	47	ASN
3	f	110	ASN
3	h	11	ASN
3	h	15	GLN
3	h	47	ASN
2	i	41	GLN
2	i	71	ASN
3	j	15	GLN
3	j	47	ASN
3	j	117	ASN
2	k	53	GLN
3	l	15	GLN
3	l	47	ASN
3	l	131	GLN
2	m	41	GLN
2	m	71	ASN
3	n	11	ASN
3	n	15	GLN
3	n	47	ASN
2	o	57	GLN
2	o	71	ASN
3	p	11	ASN
3	p	15	GLN
3	p	47	ASN

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Mol	Chain	Res	Type
3	p	110	ASN
3	q	47	ASN
3	q	117	ASN
2	r	41	GLN
2	r	53	GLN
2	r	60	GLN
4	s	26	GLN
4	s	155	HIS
4	s	161	GLN
2	t	41	GLN
2	t	53	GLN
4	u	26	GLN
3	v	47	ASN
3	v	117	ASN
2	w	71	ASN
3	x	11	ASN
3	x	15	GLN
3	x	47	ASN
3	z	11	ASN
3	z	15	GLN
3	z	47	ASN
3	z	131	GLN
2	1	41	GLN
2	1	71	ASN
3	2	10	ASN
3	2	15	GLN
3	2	47	ASN
3	2	131	GLN
2	3	71	ASN
3	4	15	GLN
3	4	47	ASN
3	4	131	GLN
2	5	71	ASN
3	6	11	ASN
3	6	15	GLN
3	6	47	ASN
3	6	131	GLN
2	7	41	GLN
2	7	71	ASN
3	8	15	GLN
3	8	47	ASN
3	8	131	GLN

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Mol	Chain	Res	Type
3	0	11	ASN
3	0	15	GLN
3	0	47	ASN
3	0	110	ASN
3	0	131	GLN
2	AA	71	ASN
3	AB	15	GLN
3	AB	47	ASN
2	AC	71	ASN
3	AD	10	ASN
3	AD	11	ASN
3	AD	47	ASN
2	AE	71	ASN
3	AF	10	ASN
3	AF	15	GLN
3	AF	47	ASN
2	AG	41	GLN
2	AG	71	ASN
2	AG	161	GLN
3	AH	2	GLN
3	AH	11	ASN
3	AH	15	GLN
3	AH	47	ASN
3	AJ	47	ASN
3	AJ	131	GLN
2	AK	71	ASN
3	AL	2	GLN
3	AL	11	ASN
3	AL	15	GLN
3	AL	47	ASN
2	AM	41	GLN
2	AM	71	ASN
3	AN	15	GLN
3	AN	47	ASN
2	AO	71	ASN
3	AP	11	ASN
3	AP	47	ASN
2	AQ	71	ASN
3	AR	15	GLN
3	AR	47	ASN
2	AS	71	ASN
2	AS	161	GLN

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Mol	Chain	Res	Type
3	AT	2	GLN
3	AT	11	ASN
3	AT	15	GLN
3	AT	47	ASN
2	AU	60	GLN
3	AV	47	ASN
3	AV	131	GLN
2	AW	71	ASN
3	AX	2	GLN
3	AX	11	ASN
3	AX	15	GLN
3	AX	47	ASN
5	AY	41	GLN
5	AY	42	GLN
5	AZ	41	GLN
5	AZ	42	GLN
5	AZ	64	ASN
5	Aa	24	GLN
5	Aa	36	ASN
5	Aa	61	GLN
5	Ab	41	GLN
5	Ab	45	GLN
5	Ad	42	GLN
5	Ad	45	GLN
5	Ad	61	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

40 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MEN	l	71	3	7,8,9	0.55	0	6,9,11	0.50	0
3	MEN	0	71	3	7,8,9	0.57	0	6,9,11	0.46	0
3	MEN	H	71	3	7,8,9	0.47	0	6,9,11	0.79	0
3	MEN	p	71	3	7,8,9	0.68	0	6,9,11	0.77	0
3	MEN	V	71	3	7,8,9	0.60	0	6,9,11	0.42	0
3	MEN	AT	71	3	7,8,9	0.52	0	6,9,11	0.74	0
3	MEN	h	71	3	7,8,9	0.75	0	6,9,11	0.90	0
3	MEN	J	71	3	7,8,9	0.50	0	6,9,11	0.49	0
3	MEN	AN	71	3	7,8,9	0.53	0	6,9,11	0.58	0
3	MEN	X	71	3	7,8,9	0.48	0	6,9,11	0.75	0
3	MEN	N	71	3	7,8,9	0.48	0	6,9,11	0.59	0
3	MEN	6	71	3	7,8,9	0.69	0	6,9,11	0.78	0
3	MEN	d	71	3	7,8,9	0.65	0	6,9,11	0.58	0
3	MEN	AX	71	3	7,8,9	0.48	0	6,9,11	0.52	0
3	MEN	n	71	3	7,8,9	0.52	0	6,9,11	0.66	0
3	MEN	b	71	3	7,8,9	0.47	0	6,9,11	0.52	0
3	MEN	AV	71	3	7,8,9	0.55	0	6,9,11	0.72	0
3	MEN	4	71	3	7,8,9	0.51	0	6,9,11	0.63	0
3	MEN	T	71	3	7,8,9	0.49	0	6,9,11	0.59	0
3	MEN	v	71	3	7,8,9	0.76	0	6,9,11	0.72	0
3	MEN	8	71	3	7,8,9	0.54	0	6,9,11	0.68	0
3	MEN	x	71	3	7,8,9	0.68	0	6,9,11	0.79	0
3	MEN	q	71	3	7,8,9	0.75	0	6,9,11	0.85	0
3	MEN	AH	71	3	7,8,9	0.54	0	6,9,11	0.75	0
3	MEN	j	71	3	7,8,9	0.95	0	6,9,11	0.79	0
3	MEN	AB	71	3	7,8,9	0.52	0	6,9,11	0.57	0
3	MEN	F	71	3	7,8,9	0.61	0	6,9,11	0.41	0
3	MEN	AD	71	3	7,8,9	0.56	0	6,9,11	0.58	0
3	MEN	f	71	3	7,8,9	0.48	0	6,9,11	0.32	0
3	MEN	2	71	3	7,8,9	1.02	0	6,9,11	1.82	1 (16%)
3	MEN	R	71	3	7,8,9	0.49	0	6,9,11	0.71	0
3	MEN	AR	71	3	7,8,9	0.46	0	6,9,11	0.59	0
3	MEN	AP	71	3	7,8,9	0.52	0	6,9,11	0.52	0
3	MEN	L	71	3	7,8,9	0.48	0	6,9,11	0.53	0
3	MEN	z	71	3	7,8,9	0.75	0	6,9,11	0.87	0
3	MEN	AF	71	3	7,8,9	0.48	0	6,9,11	0.58	0
3	MEN	P	71	3	7,8,9	0.49	0	6,9,11	0.53	0
3	MEN	Z	71	3	7,8,9	0.51	0	6,9,11	0.44	0
3	MEN	AJ	71	3	7,8,9	0.56	0	6,9,11	0.72	0
3	MEN	AL	71	3	7,8,9	0.48	0	6,9,11	0.52	0

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
3	MEN	l	71	3	-	5/7/8/10	-
3	MEN	0	71	3	-	5/7/8/10	-
3	MEN	H	71	3	-	6/7/8/10	-
3	MEN	p	71	3	-	4/7/8/10	-
3	MEN	V	71	3	-	3/7/8/10	-
3	MEN	AT	71	3	-	3/7/8/10	-
3	MEN	h	71	3	-	3/7/8/10	-
3	MEN	J	71	3	-	5/7/8/10	-
3	MEN	AN	71	3	-	5/7/8/10	-
3	MEN	X	71	3	-	6/7/8/10	-
3	MEN	N	71	3	-	5/7/8/10	-
3	MEN	6	71	3	-	4/7/8/10	-
3	MEN	d	71	3	-	5/7/8/10	-
3	MEN	AX	71	3	-	4/7/8/10	-
3	MEN	n	71	3	-	5/7/8/10	-
3	MEN	b	71	3	-	5/7/8/10	-
3	MEN	AV	71	3	-	4/7/8/10	-
3	MEN	4	71	3	-	5/7/8/10	-
3	MEN	T	71	3	-	5/7/8/10	-
3	MEN	v	71	3	-	5/7/8/10	-
3	MEN	8	71	3	-	5/7/8/10	-
3	MEN	x	71	3	-	4/7/8/10	-
3	MEN	q	71	3	-	5/7/8/10	-
3	MEN	AH	71	3	-	3/7/8/10	-
3	MEN	j	71	3	-	4/7/8/10	-
3	MEN	AB	71	3	-	5/7/8/10	-
3	MEN	F	71	3	-	3/7/8/10	-
3	MEN	AD	71	3	-	5/7/8/10	-
3	MEN	f	71	3	-	5/7/8/10	-
3	MEN	2	71	3	-	4/7/8/10	-
3	MEN	R	71	3	-	5/7/8/10	-
3	MEN	AR	71	3	-	4/7/8/10	-
3	MEN	AP	71	3	-	5/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MEN	L	71	3	-	4/7/8/10	-
3	MEN	z	71	3	-	3/7/8/10	-
3	MEN	AF	71	3	-	4/7/8/10	-
3	MEN	P	71	3	-	4/7/8/10	-
3	MEN	Z	71	3	-	5/7/8/10	-
3	MEN	AJ	71	3	-	4/7/8/10	-
3	MEN	AL	71	3	-	4/7/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	71	MEN	OD1-CG-CB	4.04	127.41	121.50

There are no chirality outliers.

All (177) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	N	71	MEN	C-CA-CB-CG
3	N	71	MEN	CB-CG-ND2-CE2
3	P	71	MEN	C-CA-CB-CG
3	P	71	MEN	CB-CG-ND2-CE2
3	F	71	MEN	O-C-CA-CB
3	H	71	MEN	C-CA-CB-CG
3	H	71	MEN	CB-CG-ND2-CE2
3	J	71	MEN	O-C-CA-CB
3	J	71	MEN	C-CA-CB-CG
3	J	71	MEN	CB-CG-ND2-CE2
3	J	71	MEN	OD1-CG-ND2-CE2
3	L	71	MEN	C-CA-CB-CG
3	L	71	MEN	CB-CG-ND2-CE2
3	R	71	MEN	C-CA-CB-CG
3	R	71	MEN	CB-CG-ND2-CE2
3	T	71	MEN	C-CA-CB-CG
3	T	71	MEN	CB-CG-ND2-CE2
3	V	71	MEN	O-C-CA-CB
3	X	71	MEN	C-CA-CB-CG
3	X	71	MEN	CB-CG-ND2-CE2
3	Z	71	MEN	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
3	Z	71	MEN	C-CA-CB-CG
3	Z	71	MEN	CB-CG-ND2-CE2
3	Z	71	MEN	OD1-CG-ND2-CE2
3	b	71	MEN	C-CA-CB-CG
3	b	71	MEN	CB-CG-ND2-CE2
3	d	71	MEN	O-C-CA-CB
3	f	71	MEN	O-C-CA-CB
3	f	71	MEN	CB-CG-ND2-CE2
3	j	71	MEN	CB-CG-ND2-CE2
3	l	71	MEN	O-C-CA-CB
3	n	71	MEN	O-C-CA-CB
3	p	71	MEN	O-C-CA-CB
3	q	71	MEN	O-C-CA-CB
3	v	71	MEN	O-C-CA-CB
3	x	71	MEN	O-C-CA-CB
3	2	71	MEN	CB-CG-ND2-CE2
3	4	71	MEN	O-C-CA-CB
3	6	71	MEN	O-C-CA-CB
3	8	71	MEN	O-C-CA-CB
3	0	71	MEN	O-C-CA-CB
3	AB	71	MEN	O-C-CA-CB
3	AD	71	MEN	O-C-CA-CB
3	AF	71	MEN	O-C-CA-CB
3	AJ	71	MEN	O-C-CA-CB
3	AL	71	MEN	O-C-CA-CB
3	AN	71	MEN	O-C-CA-CB
3	AP	71	MEN	O-C-CA-CB
3	AR	71	MEN	O-C-CA-CB
3	AV	71	MEN	O-C-CA-CB
3	AX	71	MEN	O-C-CA-CB
3	P	71	MEN	OD1-CG-ND2-CE2
3	H	71	MEN	OD1-CG-ND2-CE2
3	L	71	MEN	OD1-CG-ND2-CE2
3	T	71	MEN	OD1-CG-ND2-CE2
3	X	71	MEN	OD1-CG-ND2-CE2
3	f	71	MEN	OD1-CG-ND2-CE2
3	h	71	MEN	OD1-CG-ND2-CE2
3	j	71	MEN	OD1-CG-ND2-CE2
3	l	71	MEN	OD1-CG-ND2-CE2
3	z	71	MEN	OD1-CG-ND2-CE2
3	6	71	MEN	OD1-CG-ND2-CE2
3	0	71	MEN	OD1-CG-ND2-CE2

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Mol	Chain	Res	Type	Atoms
3	AH	71	MEN	OD1-CG-ND2-CE2
3	AL	71	MEN	OD1-CG-ND2-CE2
3	AT	71	MEN	OD1-CG-ND2-CE2
3	AX	71	MEN	OD1-CG-ND2-CE2
3	N	71	MEN	N-CA-CB-CG
3	P	71	MEN	N-CA-CB-CG
3	J	71	MEN	N-CA-CB-CG
3	L	71	MEN	N-CA-CB-CG
3	R	71	MEN	N-CA-CB-CG
3	T	71	MEN	N-CA-CB-CG
3	X	71	MEN	N-CA-CB-CG
3	Z	71	MEN	N-CA-CB-CG
3	b	71	MEN	N-CA-CB-CG
3	d	71	MEN	CB-CG-ND2-CE2
3	q	71	MEN	CB-CG-ND2-CE2
3	v	71	MEN	CB-CG-ND2-CE2
3	4	71	MEN	CB-CG-ND2-CE2
3	6	71	MEN	CB-CG-ND2-CE2
3	AB	71	MEN	CB-CG-ND2-CE2
3	AD	71	MEN	CB-CG-ND2-CE2
3	AF	71	MEN	CB-CG-ND2-CE2
3	AJ	71	MEN	CB-CG-ND2-CE2
3	AN	71	MEN	CB-CG-ND2-CE2
3	AP	71	MEN	CB-CG-ND2-CE2
3	AR	71	MEN	CB-CG-ND2-CE2
3	AV	71	MEN	CB-CG-ND2-CE2
3	N	71	MEN	OD1-CG-ND2-CE2
3	R	71	MEN	OD1-CG-ND2-CE2
3	b	71	MEN	OD1-CG-ND2-CE2
3	d	71	MEN	OD1-CG-ND2-CE2
3	n	71	MEN	OD1-CG-ND2-CE2
3	p	71	MEN	OD1-CG-ND2-CE2
3	q	71	MEN	OD1-CG-ND2-CE2
3	v	71	MEN	OD1-CG-ND2-CE2
3	x	71	MEN	OD1-CG-ND2-CE2
3	2	71	MEN	OD1-CG-ND2-CE2
3	4	71	MEN	OD1-CG-ND2-CE2
3	8	71	MEN	OD1-CG-ND2-CE2
3	AB	71	MEN	OD1-CG-ND2-CE2
3	AD	71	MEN	OD1-CG-ND2-CE2
3	AF	71	MEN	OD1-CG-ND2-CE2
3	AJ	71	MEN	OD1-CG-ND2-CE2

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Mol	Chain	Res	Type	Atoms
3	AN	71	MEN	OD1-CG-ND2-CE2
3	AP	71	MEN	OD1-CG-ND2-CE2
3	AR	71	MEN	OD1-CG-ND2-CE2
3	AV	71	MEN	OD1-CG-ND2-CE2
3	f	71	MEN	CA-CB-CG-OD1
3	F	71	MEN	OD1-CG-ND2-CE2
3	V	71	MEN	OD1-CG-ND2-CE2
3	H	71	MEN	N-CA-CB-CG
3	F	71	MEN	CA-CB-CG-OD1
3	H	71	MEN	CA-CB-CG-OD1
3	V	71	MEN	CA-CB-CG-OD1
3	X	71	MEN	CA-CB-CG-OD1
3	q	71	MEN	CA-CB-CG-OD1
3	h	71	MEN	CB-CG-ND2-CE2
3	l	71	MEN	CB-CG-ND2-CE2
3	n	71	MEN	CB-CG-ND2-CE2
3	z	71	MEN	CB-CG-ND2-CE2
3	8	71	MEN	CB-CG-ND2-CE2
3	0	71	MEN	CB-CG-ND2-CE2
3	AH	71	MEN	CB-CG-ND2-CE2
3	AL	71	MEN	CB-CG-ND2-CE2
3	AT	71	MEN	CB-CG-ND2-CE2
3	AX	71	MEN	CB-CG-ND2-CE2
3	d	71	MEN	CA-CB-CG-OD1
3	p	71	MEN	CA-CB-CG-OD1
3	v	71	MEN	CA-CB-CG-OD1
3	x	71	MEN	CA-CB-CG-OD1
3	H	71	MEN	CA-CB-CG-ND2
3	X	71	MEN	CA-CB-CG-ND2
3	f	71	MEN	CA-CB-CG-ND2
3	h	71	MEN	CA-CB-CG-OD1
3	l	71	MEN	CA-CB-CG-OD1
3	n	71	MEN	CA-CB-CG-OD1
3	z	71	MEN	CA-CB-CG-OD1
3	4	71	MEN	CA-CB-CG-OD1
3	8	71	MEN	CA-CB-CG-OD1
3	0	71	MEN	CA-CB-CG-OD1
3	AB	71	MEN	CA-CB-CG-OD1
3	AF	71	MEN	CA-CB-CG-OD1
3	AH	71	MEN	CA-CB-CG-OD1
3	AN	71	MEN	CA-CB-CG-OD1
3	AR	71	MEN	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
3	AT	71	MEN	CA-CB-CG-OD1
3	p	71	MEN	CB-CG-ND2-CE2
3	x	71	MEN	CB-CG-ND2-CE2
3	6	71	MEN	CA-CB-CG-OD1
3	AD	71	MEN	CA-CB-CG-OD1
3	AJ	71	MEN	CA-CB-CG-OD1
3	AL	71	MEN	CA-CB-CG-OD1
3	AP	71	MEN	CA-CB-CG-OD1
3	AV	71	MEN	CA-CB-CG-OD1
3	AX	71	MEN	CA-CB-CG-OD1
3	2	71	MEN	CA-CB-CG-OD1
3	q	71	MEN	CA-CB-CG-ND2
3	R	71	MEN	CA-CB-CG-OD1
3	T	71	MEN	CA-CB-CG-OD1
3	b	71	MEN	CA-CB-CG-OD1
3	j	71	MEN	CA-CB-CG-OD1
3	N	71	MEN	CA-CB-CG-ND2
3	d	71	MEN	CA-CB-CG-ND2
3	j	71	MEN	CA-CB-CG-ND2
3	l	71	MEN	CA-CB-CG-ND2
3	n	71	MEN	CA-CB-CG-ND2
3	v	71	MEN	CA-CB-CG-ND2
3	2	71	MEN	CA-CB-CG-ND2
3	4	71	MEN	CA-CB-CG-ND2
3	8	71	MEN	CA-CB-CG-ND2
3	0	71	MEN	CA-CB-CG-ND2
3	AB	71	MEN	CA-CB-CG-ND2
3	AD	71	MEN	CA-CB-CG-ND2
3	AN	71	MEN	CA-CB-CG-ND2
3	AP	71	MEN	CA-CB-CG-ND2

There are no ring outliers.

21 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	l	71	MEN	1	0
3	0	71	MEN	1	0
3	H	71	MEN	1	0
3	p	71	MEN	1	0
3	V	71	MEN	1	0
3	h	71	MEN	1	0
3	J	71	MEN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AN	71	MEN	1	0
3	d	71	MEN	1	0
3	AX	71	MEN	1	0
3	n	71	MEN	1	0
3	T	71	MEN	1	0
3	8	71	MEN	1	0
3	x	71	MEN	1	0
3	AB	71	MEN	1	0
3	F	71	MEN	1	0
3	L	71	MEN	1	0
3	z	71	MEN	1	0
3	P	71	MEN	1	0
3	Z	71	MEN	1	0
3	AL	71	MEN	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

84 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	CYC	A	2101	1	42,46,46	1.21	2 (4%)	50,67,67	1.21	4 (8%)
6	CYC	4	201	3	42,46,46	0.97	1 (2%)	50,67,67	1.07	2 (4%)
6	CYC	l	201	3	42,46,46	0.93	1 (2%)	50,67,67	1.31	3 (6%)
6	CYC	0	201	3	42,46,46	0.94	1 (2%)	50,67,67	1.26	3 (6%)
6	CYC	M	201	2	42,46,46	0.96	1 (2%)	50,67,67	1.36	6 (12%)
6	CYC	a	201	2	42,46,46	1.14	1 (2%)	50,67,67	1.21	3 (6%)
6	CYC	h	201	3	42,46,46	1.34	5 (11%)	50,67,67	1.46	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CYC	5	201	2	42,46,46	0.96	2 (4%)	50,67,67	1.32	3 (6%)
6	CYC	AD	201	3	42,46,46	0.92	1 (2%)	50,67,67	1.14	3 (6%)
6	CYC	AS	201	2	42,46,46	1.14	1 (2%)	50,67,67	1.24	4 (8%)
6	CYC	AX	201	3	42,46,46	1.06	2 (4%)	50,67,67	1.03	2 (4%)
6	CYC	z	201	3	42,46,46	1.35	4 (9%)	50,67,67	1.47	9 (18%)
6	CYC	6	201	3	42,46,46	0.94	1 (2%)	50,67,67	1.49	9 (18%)
6	CYC	AN	201	3	42,46,46	1.12	4 (9%)	50,67,67	1.34	7 (14%)
6	CYC	8	201	3	42,46,46	1.14	5 (11%)	50,67,67	1.48	8 (16%)
6	CYC	R	201	3	42,46,46	0.92	1 (2%)	50,67,67	1.36	2 (4%)
6	CYC	e	201	2	42,46,46	1.10	2 (4%)	50,67,67	1.30	5 (10%)
6	CYC	AC	201	2	42,46,46	0.99	1 (2%)	50,67,67	1.25	6 (12%)
6	CYC	C	2101	-	42,46,46	1.26	2 (4%)	50,67,67	1.45	9 (18%)
6	CYC	L	201	3	42,46,46	0.93	1 (2%)	50,67,67	1.25	5 (10%)
6	CYC	c	201	2	42,46,46	0.88	1 (2%)	50,67,67	1.32	5 (10%)
6	CYC	AP	201	3	42,46,46	0.94	1 (2%)	50,67,67	1.17	4 (8%)
6	CYC	Y	201	2	42,46,46	1.04	1 (2%)	50,67,67	1.31	5 (10%)
6	CYC	AL	201	3	42,46,46	1.05	2 (4%)	50,67,67	1.06	2 (4%)
6	CYC	Z	201	3	42,46,46	1.03	2 (4%)	50,67,67	1.11	3 (6%)
6	CYC	AO	201	2	42,46,46	1.00	1 (2%)	50,67,67	1.24	6 (12%)
6	CYC	t	201	2	42,46,46	1.14	4 (9%)	50,67,67	1.44	8 (16%)
6	CYC	G	201	2	42,46,46	1.16	2 (4%)	50,67,67	1.28	6 (12%)
6	CYC	b	201	3	42,46,46	0.93	1 (2%)	50,67,67	1.27	5 (10%)
6	CYC	2	201	3	42,46,46	1.17	2 (4%)	50,67,67	1.26	6 (12%)
6	CYC	S	201	2	42,46,46	0.95	1 (2%)	50,67,67	1.23	5 (10%)
6	CYC	w	201	2	42,46,46	1.05	1 (2%)	50,67,67	1.14	4 (8%)
6	CYC	J	201	3	42,46,46	0.99	1 (2%)	50,67,67	1.11	3 (6%)
6	CYC	AJ	201	3	42,46,46	1.04	2 (4%)	50,67,67	1.39	6 (12%)
6	CYC	k	201	2	42,46,46	0.97	1 (2%)	50,67,67	1.27	5 (10%)
6	CYC	u	201	-	42,46,46	1.04	2 (4%)	50,67,67	1.14	6 (12%)
6	CYC	g	201	2	42,46,46	1.20	1 (2%)	50,67,67	1.13	5 (10%)
6	CYC	W	201	2	42,46,46	1.16	2 (4%)	50,67,67	1.28	6 (12%)
6	CYC	U	201	2	42,46,46	1.06	1 (2%)	50,67,67	1.32	6 (12%)
6	CYC	j	201	3	42,46,46	1.29	2 (4%)	50,67,67	1.05	2 (4%)
6	CYC	AR	201	3	42,46,46	0.96	1 (2%)	50,67,67	1.21	3 (6%)
6	CYC	o	201	2	42,46,46	0.94	1 (2%)	50,67,67	1.22	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CYC	O	201	2	42,46,46	0.98	1 (2%)	50,67,67	1.25	5 (10%)
6	CYC	AU	201	2	42,46,46	0.98	1 (2%)	50,67,67	1.16	4 (8%)
6	CYC	K	201	2	42,46,46	1.12	1 (2%)	50,67,67	1.21	3 (6%)
6	CYC	9	201	2	42,46,46	0.92	1 (2%)	50,67,67	1.29	6 (12%)
6	CYC	AW	201	2	42,46,46	1.00	1 (2%)	50,67,67	1.22	4 (8%)
6	CYC	1	201	2	42,46,46	0.86	1 (2%)	50,67,67	1.25	4 (8%)
6	CYC	d	201	3	42,46,46	1.05	1 (2%)	50,67,67	1.05	2 (4%)
6	CYC	AF	201	3	42,46,46	0.97	1 (2%)	50,67,67	1.21	3 (6%)
6	CYC	n	201	3	42,46,46	1.15	4 (9%)	50,67,67	1.38	7 (14%)
6	CYC	x	201	3	42,46,46	1.09	2 (4%)	50,67,67	1.13	4 (8%)
6	CYC	AI	201	2	42,46,46	0.99	1 (2%)	50,67,67	1.17	5 (10%)
6	CYC	AB	201	3	42,46,46	1.11	4 (9%)	50,67,67	1.34	7 (14%)
6	CYC	y	201	2	42,46,46	1.09	1 (2%)	50,67,67	1.13	4 (8%)
6	CYC	AM	201	2	42,46,46	1.15	4 (9%)	50,67,67	1.50	9 (18%)
6	CYC	AQ	201	2	42,46,46	0.88	1 (2%)	50,67,67	1.16	3 (6%)
6	CYC	i	201	2	42,46,46	0.79	0	50,67,67	1.32	4 (8%)
6	CYC	s	201	-	42,46,46	1.11	1 (2%)	50,67,67	1.30	5 (10%)
6	CYC	AE	201	2	42,46,46	0.87	1 (2%)	50,67,67	1.16	3 (6%)
6	CYC	N	201	3	42,46,46	0.93	1 (2%)	50,67,67	1.31	2 (4%)
6	CYC	P	201	3	42,46,46	0.92	1 (2%)	50,67,67	1.28	4 (8%)
6	CYC	I	201	2	42,46,46	1.00	1 (2%)	50,67,67	1.32	4 (8%)
6	CYC	AT	201	3	42,46,46	1.11	6 (14%)	50,67,67	1.48	8 (16%)
6	CYC	T	201	3	42,46,46	0.93	1 (2%)	50,67,67	1.28	5 (10%)
6	CYC	AV	201	3	42,46,46	1.05	2 (4%)	50,67,67	1.38	5 (10%)
6	CYC	3	201	2	42,46,46	0.88	1 (2%)	50,67,67	1.22	5 (10%)
6	CYC	Q	201	2	42,46,46	1.08	1 (2%)	50,67,67	1.34	4 (8%)
6	CYC	q	201	3	42,46,46	1.09	2 (4%)	50,67,67	1.11	3 (6%)
6	CYC	AG	201	2	42,46,46	1.14	1 (2%)	50,67,67	1.23	4 (8%)
6	CYC	r	201	2	42,46,46	1.13	4 (9%)	50,67,67	1.46	10 (20%)
6	CYC	p	201	3	42,46,46	1.09	2 (4%)	50,67,67	1.13	4 (8%)
6	CYC	f	201	3	42,46,46	0.88	1 (2%)	50,67,67	1.51	7 (14%)
6	CYC	E	201	2	42,46,46	1.12	1 (2%)	50,67,67	1.32	6 (12%)
6	CYC	H	201	3	42,46,46	1.04	2 (4%)	50,67,67	1.35	6 (12%)
6	CYC	F	201	3	42,46,46	1.18	1 (2%)	50,67,67	1.21	4 (8%)
6	CYC	X	201	3	42,46,46	1.03	2 (4%)	50,67,67	1.40	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CYC	7	201	2	42,46,46	1.38	6 (14%)	50,67,67	1.55	12 (24%)
6	CYC	V	201	3	42,46,46	1.17	1 (2%)	50,67,67	1.20	4 (8%)
6	CYC	AK	201	2	42,46,46	0.99	1 (2%)	50,67,67	1.21	4 (8%)
6	CYC	m	201	2	42,46,46	1.35	6 (14%)	50,67,67	1.55	12 (24%)
6	CYC	v	201	3	42,46,46	1.08	2 (4%)	50,67,67	1.10	3 (6%)
6	CYC	AH	201	3	42,46,46	1.12	5 (11%)	50,67,67	1.47	8 (16%)
6	CYC	AA	201	2	42,46,46	1.15	4 (9%)	50,67,67	1.50	9 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CYC	A	2101	1	-	16/25/74/74	0/4/4/4
6	CYC	4	201	3	-	5/25/74/74	0/4/4/4
6	CYC	l	201	3	-	9/25/74/74	0/4/4/4
6	CYC	0	201	3	-	8/25/74/74	0/4/4/4
6	CYC	M	201	2	-	8/25/74/74	0/4/4/4
6	CYC	a	201	2	-	6/25/74/74	0/4/4/4
6	CYC	h	201	3	-	9/25/74/74	0/4/4/4
6	CYC	5	201	2	-	11/25/74/74	0/4/4/4
6	CYC	AD	201	3	-	7/25/74/74	0/4/4/4
6	CYC	AS	201	2	-	7/25/74/74	0/4/4/4
6	CYC	AX	201	3	-	7/25/74/74	0/4/4/4
6	CYC	z	201	3	-	9/25/74/74	0/4/4/4
6	CYC	6	201	3	-	7/25/74/74	0/4/4/4
6	CYC	AN	201	3	-	8/25/74/74	0/4/4/4
6	CYC	8	201	3	-	7/25/74/74	0/4/4/4
6	CYC	R	201	3	-	7/25/74/74	0/4/4/4
6	CYC	e	201	2	-	13/25/74/74	0/4/4/4
6	CYC	AC	201	2	-	8/25/74/74	0/4/4/4
6	CYC	C	2101	-	-	11/25/74/74	0/4/4/4
6	CYC	L	201	3	-	11/25/74/74	0/4/4/4
6	CYC	c	201	2	-	8/25/74/74	0/4/4/4
6	CYC	AP	201	3	-	11/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CYC	Y	201	2	-	10/25/74/74	0/4/4/4
6	CYC	AL	201	3	-	6/25/74/74	0/4/4/4
6	CYC	Z	201	3	-	8/25/74/74	0/4/4/4
6	CYC	AO	201	2	-	8/25/74/74	0/4/4/4
6	CYC	t	201	2	-	12/25/74/74	0/4/4/4
6	CYC	G	201	2	-	7/25/74/74	0/4/4/4
6	CYC	b	201	3	-	11/25/74/74	0/4/4/4
6	CYC	2	201	3	-	5/25/74/74	0/4/4/4
6	CYC	S	201	2	-	8/25/74/74	0/4/4/4
6	CYC	w	201	2	-	8/25/74/74	0/4/4/4
6	CYC	J	201	3	-	8/25/74/74	0/4/4/4
6	CYC	AJ	201	3	-	6/25/74/74	0/4/4/4
6	CYC	k	201	2	-	8/25/74/74	0/4/4/4
6	CYC	u	201	-	-	14/25/74/74	0/4/4/4
6	CYC	g	201	2	-	9/25/74/74	0/4/4/4
6	CYC	W	201	2	-	6/25/74/74	0/4/4/4
6	CYC	U	201	2	-	5/25/74/74	0/4/4/4
6	CYC	j	201	3	-	7/25/74/74	0/4/4/4
6	CYC	AR	201	3	-	7/25/74/74	0/4/4/4
6	CYC	o	201	2	-	4/25/74/74	0/4/4/4
6	CYC	O	201	2	-	8/25/74/74	0/4/4/4
6	CYC	AU	201	2	-	8/25/74/74	0/4/4/4
6	CYC	K	201	2	-	6/25/74/74	0/4/4/4
6	CYC	9	201	2	-	7/25/74/74	0/4/4/4
6	CYC	AW	201	2	-	7/25/74/74	0/4/4/4
6	CYC	1	201	2	-	11/25/74/74	0/4/4/4
6	CYC	d	201	3	-	8/25/74/74	0/4/4/4
6	CYC	AF	201	3	-	7/25/74/74	0/4/4/4
6	CYC	n	201	3	-	9/25/74/74	0/4/4/4
6	CYC	x	201	3	-	8/25/74/74	0/4/4/4
6	CYC	AI	201	2	-	8/25/74/74	0/4/4/4
6	CYC	AB	201	3	-	8/25/74/74	0/4/4/4
6	CYC	y	201	2	-	10/25/74/74	0/4/4/4
6	CYC	AM	201	2	-	11/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CYC	AQ	201	2	-	4/25/74/74	0/4/4/4
6	CYC	i	201	2	-	10/25/74/74	0/4/4/4
6	CYC	s	201	-	-	13/25/74/74	0/4/4/4
6	CYC	AE	201	2	-	4/25/74/74	0/4/4/4
6	CYC	N	201	3	-	9/25/74/74	0/4/4/4
6	CYC	P	201	3	-	10/25/74/74	0/4/4/4
6	CYC	I	201	2	-	10/25/74/74	0/4/4/4
6	CYC	AT	201	3	-	6/25/74/74	0/4/4/4
6	CYC	T	201	3	-	10/25/74/74	0/4/4/4
6	CYC	AV	201	3	-	6/25/74/74	0/4/4/4
6	CYC	3	201	2	-	7/25/74/74	0/4/4/4
6	CYC	Q	201	2	-	9/25/74/74	0/4/4/4
6	CYC	q	201	3	-	11/25/74/74	0/4/4/4
6	CYC	AG	201	2	-	7/25/74/74	0/4/4/4
6	CYC	r	201	2	-	12/25/74/74	0/4/4/4
6	CYC	p	201	3	-	8/25/74/74	0/4/4/4
6	CYC	f	201	3	-	9/25/74/74	0/4/4/4
6	CYC	E	201	2	-	5/25/74/74	0/4/4/4
6	CYC	H	201	3	-	9/25/74/74	0/4/4/4
6	CYC	F	201	3	-	7/25/74/74	0/4/4/4
6	CYC	X	201	3	-	6/25/74/74	0/4/4/4
6	CYC	7	201	2	-	11/25/74/74	0/4/4/4
6	CYC	V	201	3	-	7/25/74/74	0/4/4/4
6	CYC	AK	201	2	-	7/25/74/74	0/4/4/4
6	CYC	m	201	2	-	11/25/74/74	0/4/4/4
6	CYC	v	201	3	-	11/25/74/74	0/4/4/4
6	CYC	AH	201	3	-	6/25/74/74	0/4/4/4
6	CYC	AA	201	2	-	11/25/74/74	0/4/4/4

All (154) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	j	201	CYC	CHA-C1A	6.35	1.40	1.35
6	F	201	CYC	CHA-C1A	6.29	1.40	1.35
6	V	201	CYC	CHA-C1A	6.18	1.40	1.35
6	g	201	CYC	CHA-C1A	6.09	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	2101	CYC	CHA-C1A	6.06	1.40	1.35
6	AG	201	CYC	CHA-C1A	6.00	1.40	1.35
6	AS	201	CYC	CHA-C1A	5.94	1.40	1.35
6	A	2101	CYC	CHA-C1A	5.92	1.40	1.35
6	G	201	CYC	CHA-C1A	5.36	1.39	1.35
6	a	201	CYC	CHA-C1A	5.35	1.39	1.35
6	y	201	CYC	CHA-C1A	5.32	1.39	1.35
6	W	201	CYC	CHA-C1A	5.29	1.39	1.35
6	2	201	CYC	CHA-C1A	5.29	1.39	1.35
6	Q	201	CYC	CHA-C1A	5.21	1.39	1.35
6	K	201	CYC	CHA-C1A	5.20	1.39	1.35
6	w	201	CYC	CHA-C1A	5.05	1.39	1.35
6	E	201	CYC	CHA-C1A	4.89	1.39	1.35
6	d	201	CYC	CHA-C1A	4.88	1.39	1.35
6	s	201	CYC	CHA-C1A	4.81	1.39	1.35
6	q	201	CYC	CHA-C1A	4.78	1.39	1.35
6	v	201	CYC	CHA-C1A	4.65	1.39	1.35
6	u	201	CYC	CHA-C1A	4.57	1.38	1.35
6	Y	201	CYC	CHA-C1A	4.47	1.38	1.35
6	AO	201	CYC	CHA-C1A	4.45	1.38	1.35
6	AC	201	CYC	CHA-C1A	4.43	1.38	1.35
6	AI	201	CYC	CHA-C1A	4.39	1.38	1.35
6	H	201	CYC	CHA-C1A	4.36	1.38	1.35
6	U	201	CYC	CHA-C1A	4.36	1.38	1.35
6	Z	201	CYC	CHA-C1A	4.34	1.38	1.35
6	AU	201	CYC	CHA-C1A	4.32	1.38	1.35
6	x	201	CYC	CHA-C1A	4.28	1.38	1.35
6	e	201	CYC	CHA-C1A	4.25	1.38	1.35
6	AW	201	CYC	CHA-C1A	4.22	1.38	1.35
6	AX	201	CYC	CHA-C1A	4.20	1.38	1.35
6	X	201	CYC	CHA-C1A	4.19	1.38	1.35
6	M	201	CYC	CHA-C1A	4.12	1.38	1.35
6	p	201	CYC	CHA-C1A	4.12	1.38	1.35
6	AL	201	CYC	CHA-C1A	4.11	1.38	1.35
6	AK	201	CYC	CHA-C1A	4.10	1.38	1.35
6	AF	201	CYC	CHA-C1A	4.08	1.38	1.35
6	I	201	CYC	CHA-C1A	4.05	1.38	1.35
6	4	201	CYC	CHA-C1A	4.05	1.38	1.35
6	AR	201	CYC	CHA-C1A	3.98	1.38	1.35
6	k	201	CYC	CHA-C1A	3.96	1.38	1.35
6	J	201	CYC	CHA-C1A	3.92	1.38	1.35
6	O	201	CYC	CHA-C1A	3.82	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	o	201	CYC	CHA-C1A	3.81	1.38	1.35
6	7	201	CYC	CHA-C1A	3.77	1.38	1.35
6	7	201	CYC	C1B-C2B	-3.76	1.38	1.45
6	m	201	CYC	C1B-C2B	-3.67	1.38	1.45
6	S	201	CYC	CHA-C1A	3.62	1.38	1.35
6	N	201	CYC	CHA-C1A	3.56	1.38	1.35
6	m	201	CYC	CHA-C1A	3.50	1.38	1.35
6	0	201	CYC	CHA-C1A	3.48	1.38	1.35
6	1	201	CYC	CHA-C1A	3.47	1.38	1.35
6	R	201	CYC	CHA-C1A	3.46	1.38	1.35
6	h	201	CYC	C1B-C2B	-3.44	1.38	1.45
6	3	201	CYC	CHA-C1A	3.38	1.37	1.35
6	z	201	CYC	C1B-C2B	-3.37	1.39	1.45
6	AP	201	CYC	CHA-C1A	3.35	1.37	1.35
6	L	201	CYC	CHA-C1A	3.34	1.37	1.35
6	9	201	CYC	CHA-C1A	3.30	1.37	1.35
6	c	201	CYC	CHA-C1A	3.25	1.37	1.35
6	l	201	CYC	CHA-C1A	3.22	1.37	1.35
6	AA	201	CYC	C1B-C2B	-3.20	1.39	1.45
6	AM	201	CYC	C1B-C2B	-3.20	1.39	1.45
6	b	201	CYC	CHA-C1A	3.15	1.37	1.35
6	n	201	CYC	C1B-C2B	-3.15	1.39	1.45
6	AV	201	CYC	C1B-C2B	-3.13	1.39	1.45
6	AJ	201	CYC	C1B-C2B	-3.13	1.39	1.45
6	h	201	CYC	C2C-C1C	-3.10	1.49	1.52
6	z	201	CYC	C2C-C1C	-3.10	1.49	1.52
6	T	201	CYC	CHA-C1A	3.09	1.37	1.35
6	AD	201	CYC	CHA-C1A	3.04	1.37	1.35
6	AQ	201	CYC	CHA-C1A	3.01	1.37	1.35
6	P	201	CYC	CHA-C1A	2.91	1.37	1.35
6	AE	201	CYC	CHA-C1A	2.89	1.37	1.35
6	r	201	CYC	C1B-C2B	-2.88	1.39	1.45
6	z	201	CYC	CHB-C4A	-2.85	1.33	1.40
6	AB	201	CYC	CHB-C4A	-2.81	1.33	1.40
6	AN	201	CYC	CHB-C4A	-2.81	1.33	1.40
6	t	201	CYC	C1B-C2B	-2.81	1.40	1.45
6	8	201	CYC	C1B-C2B	-2.80	1.40	1.45
6	AH	201	CYC	C2C-C1C	-2.80	1.49	1.52
6	AN	201	CYC	C1B-C2B	-2.80	1.40	1.45
6	AB	201	CYC	C1B-C2B	-2.79	1.40	1.45
6	h	201	CYC	CHB-C4A	-2.73	1.34	1.40
6	t	201	CYC	C2C-C1C	-2.73	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	AA	201	CYC	CHA-C1A	2.71	1.37	1.35
6	z	201	CYC	O2A-CGA	-2.71	1.21	1.30
6	7	201	CYC	C2C-C1C	-2.70	1.49	1.52
6	AN	201	CYC	CHA-C1A	2.69	1.37	1.35
6	h	201	CYC	O2A-CGA	-2.67	1.21	1.30
6	r	201	CYC	C2C-C1C	-2.66	1.49	1.52
6	AT	201	CYC	C2C-C1C	-2.63	1.49	1.52
6	m	201	CYC	C2C-C1C	-2.63	1.49	1.52
6	AM	201	CYC	CHA-C1A	2.63	1.37	1.35
6	AM	201	CYC	C2C-C1C	-2.59	1.49	1.52
6	p	201	CYC	C1B-C2B	-2.58	1.40	1.45
6	n	201	CYC	CHB-C4A	-2.57	1.34	1.40
6	AM	201	CYC	O2A-CGA	-2.55	1.22	1.30
6	AB	201	CYC	CHA-C1A	2.55	1.37	1.35
6	AA	201	CYC	O2A-CGA	-2.54	1.22	1.30
6	AA	201	CYC	C2C-C1C	-2.51	1.49	1.52
6	m	201	CYC	O2A-CGA	-2.49	1.22	1.30
6	n	201	CYC	C2C-C1C	-2.48	1.49	1.52
6	t	201	CYC	O2A-CGA	-2.47	1.22	1.30
6	8	201	CYC	C2C-C1C	-2.46	1.49	1.52
6	8	201	CYC	CHB-C4A	-2.44	1.34	1.40
6	r	201	CYC	O2A-CGA	-2.42	1.22	1.30
6	AV	201	CYC	CHB-C4A	-2.42	1.34	1.40
6	AJ	201	CYC	CHB-C4A	-2.39	1.34	1.40
6	7	201	CYC	O2A-CGA	-2.38	1.22	1.30
6	r	201	CYC	O2D-CGD	-2.37	1.22	1.30
6	AT	201	CYC	C1B-C2B	-2.34	1.40	1.45
6	AH	201	CYC	C1C-NC	-2.32	1.34	1.37
6	AT	201	CYC	C1C-NC	-2.31	1.34	1.37
6	AH	201	CYC	C1B-C2B	-2.30	1.41	1.45
6	6	201	CYC	O2A-CGA	-2.29	1.23	1.30
6	W	201	CYC	C1B-NB	2.28	1.41	1.37
6	e	201	CYC	C1B-C2B	-2.24	1.41	1.45
6	j	201	CYC	CHB-C1B	-2.24	1.32	1.38
6	t	201	CYC	O2D-CGD	-2.23	1.23	1.30
6	G	201	CYC	C1B-NB	2.21	1.41	1.37
6	x	201	CYC	C1B-C2B	-2.21	1.41	1.45
6	2	201	CYC	C1B-C2B	-2.18	1.41	1.45
6	X	201	CYC	C1B-C2B	-2.17	1.41	1.45
6	5	201	CYC	C1B-C2B	-2.15	1.41	1.45
6	AH	201	CYC	CHA-C1A	2.15	1.36	1.35
6	AH	201	CYC	OC-C1C	-2.14	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	AT	201	CYC	OC-C1C	-2.13	1.19	1.23
6	7	201	CYC	CHB-C1B	-2.13	1.32	1.38
6	7	201	CYC	C1B-NB	-2.13	1.34	1.37
6	H	201	CYC	C1B-C2B	-2.11	1.41	1.45
6	8	201	CYC	CHA-C1A	2.10	1.36	1.35
6	AL	201	CYC	C1B-C2B	-2.09	1.41	1.45
6	Z	201	CYC	C1B-C2B	-2.08	1.41	1.45
6	C	2101	CYC	CHD-C4C	2.08	1.43	1.38
6	AX	201	CYC	C1B-C2B	-2.08	1.41	1.45
6	AN	201	CYC	O2A-CGA	-2.08	1.23	1.30
6	AB	201	CYC	O2A-CGA	-2.07	1.23	1.30
6	m	201	CYC	C1B-NB	-2.07	1.34	1.37
6	n	201	CYC	CHB-C1B	-2.07	1.33	1.38
6	A	2101	CYC	C1B-C2B	-2.07	1.41	1.45
6	q	201	CYC	C1B-C2B	-2.06	1.41	1.45
6	m	201	CYC	CHB-C1B	-2.05	1.33	1.38
6	8	201	CYC	CHB-C1B	-2.04	1.33	1.38
6	v	201	CYC	C1B-C2B	-2.03	1.41	1.45
6	AT	201	CYC	CHA-C1A	2.03	1.36	1.35
6	h	201	CYC	O2D-CGD	-2.03	1.23	1.30
6	u	201	CYC	C1B-C2B	-2.03	1.41	1.45
6	f	201	CYC	O2A-CGA	-2.03	1.23	1.30
6	5	201	CYC	C2C-C1C	-2.02	1.50	1.52
6	AT	201	CYC	O2A-CGA	-2.00	1.24	1.30

All (426) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	201	CYC	CMB-C2B-C1B	6.17	131.87	124.17
6	6	201	CYC	CMB-C2B-C1B	5.58	131.13	124.17
6	AT	201	CYC	CMB-C2B-C1B	5.09	130.52	124.17
6	AH	201	CYC	CMB-C2B-C1B	5.08	130.51	124.17
6	Q	201	CYC	CMB-C2B-C1B	4.88	130.26	124.17
6	l	201	CYC	CMB-C2B-C1B	4.80	130.16	124.17
6	8	201	CYC	CMB-C2B-C1B	4.77	130.13	124.17
6	M	201	CYC	CMB-C2B-C1B	4.75	130.10	124.17
6	R	201	CYC	CMB-C2B-C1B	4.72	130.06	124.17
6	0	201	CYC	CMB-C2B-C1B	4.61	129.92	124.17
6	T	201	CYC	CHA-C1A-NA	-4.60	122.45	128.83
6	P	201	CYC	CHA-C1A-NA	-4.57	122.48	128.83
6	N	201	CYC	CMB-C2B-C1B	4.54	129.84	124.17
6	AG	201	CYC	CMB-C2B-C1B	4.53	129.83	124.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	5	201	CYC	CMB-C2B-C1B	4.52	129.81	124.17
6	AS	201	CYC	CMB-C2B-C1B	4.51	129.79	124.17
6	Y	201	CYC	CHB-C1B-C2B	-4.36	118.31	126.95
6	I	201	CYC	CHB-C1B-C2B	-4.25	118.54	126.95
6	n	201	CYC	CMB-C2B-C1B	4.22	129.43	124.17
6	b	201	CYC	CHA-C1A-NA	-4.16	123.05	128.83
6	i	201	CYC	CMB-C2B-C1B	4.16	129.36	124.17
6	X	201	CYC	CBD-CAD-C3D	4.15	119.70	112.62
6	J	201	CYC	CHA-C1A-NA	-4.11	123.12	128.83
6	l	201	CYC	CHA-C1A-NA	-4.09	123.15	128.83
6	R	201	CYC	CHA-C1A-NA	-4.07	123.17	128.83
6	N	201	CYC	CHA-C1A-NA	-4.07	123.19	128.83
6	j	201	CYC	CMB-C2B-C1B	4.05	129.23	124.17
6	Z	201	CYC	CHA-C1A-NA	-4.04	123.22	128.83
6	L	201	CYC	CHA-C1A-NA	-4.04	123.22	128.83
6	AF	201	CYC	CHA-C1A-NA	-4.03	123.24	128.83
6	0	201	CYC	CHA-C1A-NA	-4.02	123.25	128.83
6	AR	201	CYC	CHA-C1A-NA	-4.01	123.27	128.83
6	AV	201	CYC	CHA-C1A-NA	-3.99	123.29	128.83
6	AJ	201	CYC	CHA-C1A-NA	-3.98	123.30	128.83
6	e	201	CYC	CBD-CAD-C3D	3.96	119.38	112.62
6	P	201	CYC	CMB-C2B-C1B	3.96	129.11	124.17
6	T	201	CYC	CMB-C2B-C1B	3.95	129.10	124.17
6	H	201	CYC	CBD-CAD-C3D	3.94	119.35	112.62
6	o	201	CYC	CMB-C2B-C1B	3.94	129.08	124.17
6	E	201	CYC	CHB-C1B-C2B	-3.92	119.18	126.95
6	G	201	CYC	CHB-C1B-C2B	-3.92	119.18	126.95
6	2	201	CYC	CHB-C1B-C2B	-3.91	119.19	126.95
6	8	201	CYC	CHA-C1A-NA	-3.91	123.40	128.83
6	U	201	CYC	CHB-C1B-C2B	-3.87	119.29	126.95
6	K	201	CYC	CHA-C1A-NA	-3.84	123.50	128.83
6	H	201	CYC	CHA-C1A-NA	-3.84	123.50	128.83
6	X	201	CYC	CHA-C1A-NA	-3.81	123.53	128.83
6	F	201	CYC	CMB-C2B-C1B	3.80	128.92	124.17
6	3	201	CYC	CHA-C1A-NA	-3.80	123.56	128.83
6	W	201	CYC	CHB-C1B-C2B	-3.80	119.43	126.95
6	a	201	CYC	CHA-C1A-NA	-3.78	123.58	128.83
6	V	201	CYC	CMB-C2B-C1B	3.77	128.88	124.17
6	3	201	CYC	CMB-C2B-C1B	3.74	128.84	124.17
6	AP	201	CYC	CMB-C2B-C1B	3.72	128.81	124.17
6	AR	201	CYC	CMB-C2B-C1B	3.72	128.81	124.17
6	1	201	CYC	CMB-C2B-C1B	3.71	128.80	124.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	AF	201	CYC	CMB-C2B-C1B	3.71	128.80	124.17
6	c	201	CYC	CHA-C1A-NA	-3.70	123.70	128.83
6	c	201	CYC	CMB-C2B-C1B	3.66	128.74	124.17
6	i	201	CYC	CHA-C1A-NA	-3.65	123.76	128.83
6	o	201	CYC	CHA-C1A-NA	-3.64	123.78	128.83
6	E	201	CYC	CHA-C1A-NA	-3.63	123.79	128.83
6	AN	201	CYC	CHB-C1B-C2B	-3.62	119.78	126.95
6	z	201	CYC	OC-C1C-C2C	-3.62	123.30	126.17
6	AK	201	CYC	CMB-C2B-C1B	3.61	128.68	124.17
6	z	201	CYC	CMB-C2B-C1B	3.61	128.67	124.17
6	AW	201	CYC	CMB-C2B-C1B	3.60	128.67	124.17
6	U	201	CYC	CHA-C1A-NA	-3.58	123.86	128.83
6	AB	201	CYC	CHB-C1B-C2B	-3.58	119.86	126.95
6	AL	201	CYC	CHA-C1A-NA	-3.55	123.90	128.83
6	AE	201	CYC	CHA-C1A-NA	-3.55	123.90	128.83
6	AQ	201	CYC	CHA-C1A-NA	-3.55	123.91	128.83
6	h	201	CYC	OC-C1C-C2C	-3.54	123.36	126.17
6	m	201	CYC	CMA-C3A-C4A	3.54	130.51	125.06
6	AO	201	CYC	C1B-CHB-C4A	3.53	136.72	128.08
6	4	201	CYC	CMB-C2B-C1B	3.53	128.57	124.17
6	AD	201	CYC	CMB-C2B-C1B	3.52	128.56	124.17
6	AC	201	CYC	C1B-CHB-C4A	3.52	136.68	128.08
6	AN	201	CYC	CHA-C1A-NA	-3.51	123.95	128.83
6	e	201	CYC	CMB-C2B-C1B	3.50	128.54	124.17
6	h	201	CYC	CMB-C2B-C1B	3.50	128.53	124.17
6	AB	201	CYC	CHA-C1A-NA	-3.49	123.99	128.83
6	r	201	CYC	CMA-C3A-C4A	3.46	130.38	125.06
6	7	201	CYC	CMA-C3A-C4A	3.44	130.36	125.06
6	M	201	CYC	CHA-C1A-NA	-3.44	124.06	128.83
6	f	201	CYC	CHA-C1A-NA	-3.43	124.06	128.83
6	k	201	CYC	CHA-C1A-NA	-3.42	124.08	128.83
6	Q	201	CYC	CHA-C1A-NA	-3.42	124.08	128.83
6	C	2101	CYC	C1B-CHB-C4A	3.41	136.41	128.08
6	s	201	CYC	CHA-C1A-NA	-3.41	124.10	128.83
6	d	201	CYC	CHA-C1A-NA	-3.41	124.10	128.83
6	x	201	CYC	CMB-C2B-C1B	3.40	128.41	124.17
6	C	2101	CYC	CHB-C1B-C2B	-3.37	120.27	126.95
6	I	201	CYC	CHA-C1A-NA	-3.35	124.18	128.83
6	W	201	CYC	CHA-C1A-NA	-3.35	124.18	128.83
6	AN	201	CYC	CMB-C2B-C1B	3.35	128.34	124.17
6	AB	201	CYC	CMB-C2B-C1B	3.34	128.33	124.17
6	t	201	CYC	CMA-C3A-C4A	3.33	130.19	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	t	201	CYC	CMB-C2B-C1B	3.33	128.32	124.17
6	9	201	CYC	CHA-C1A-NA	-3.32	124.22	128.83
6	AJ	201	CYC	CMB-C2B-C1B	3.30	128.29	124.17
6	AV	201	CYC	CMB-C2B-C1B	3.28	128.26	124.17
6	V	201	CYC	CHA-C1A-NA	-3.28	124.28	128.83
6	AW	201	CYC	CHA-C1A-NA	-3.26	124.30	128.83
6	5	201	CYC	CHA-C1A-NA	-3.25	124.32	128.83
6	G	201	CYC	CHA-C1A-NA	-3.24	124.33	128.83
6	q	201	CYC	CHA-C1A-NA	-3.23	124.35	128.83
6	v	201	CYC	CHA-C1A-NA	-3.23	124.35	128.83
6	AK	201	CYC	CHA-C1A-NA	-3.22	124.36	128.83
6	9	201	CYC	CMB-C2B-C1B	3.21	128.18	124.17
6	2	201	CYC	CHA-C1A-NA	-3.21	124.38	128.83
6	AM	201	CYC	C1B-CHB-C4A	3.20	135.91	128.08
6	s	201	CYC	CMB-C2B-C1B	3.20	128.16	124.17
6	F	201	CYC	CHA-C1A-NA	-3.19	124.39	128.83
6	M	201	CYC	CHB-C1B-C2B	-3.19	120.64	126.95
6	AA	201	CYC	CMA-C3A-C4A	3.18	129.96	125.06
6	r	201	CYC	CMB-C2B-C1B	3.17	128.13	124.17
6	AA	201	CYC	C1B-CHB-C4A	3.17	135.82	128.08
6	AM	201	CYC	CMB-C2B-C1B	3.16	128.11	124.17
6	n	201	CYC	CHA-C1A-NA	-3.16	124.44	128.83
6	AA	201	CYC	CMB-C2B-C1B	3.16	128.11	124.17
6	p	201	CYC	CMB-C2B-C1B	3.14	128.09	124.17
6	Y	201	CYC	CHA-C1A-NA	-3.14	124.47	128.83
6	AC	201	CYC	CHB-C1B-C2B	-3.14	120.73	126.95
6	7	201	CYC	CMB-C2B-C1B	3.14	128.08	124.17
6	AM	201	CYC	CMA-C3A-C4A	3.14	129.90	125.06
6	AX	201	CYC	CHA-C1A-NA	-3.13	124.48	128.83
6	A	2101	CYC	CHB-C1B-C2B	-3.13	120.75	126.95
6	k	201	CYC	CMB-C2B-C1B	3.12	128.06	124.17
6	X	201	CYC	CHB-C1B-C2B	-3.12	120.77	126.95
6	AL	201	CYC	CMB-C2B-C1B	3.12	128.06	124.17
6	AI	201	CYC	C1B-CHB-C4A	3.11	135.67	128.08
6	H	201	CYC	CHB-C1B-C2B	-3.09	120.83	126.95
6	7	201	CYC	CBD-CAD-C3D	3.09	117.89	112.62
6	AD	201	CYC	CHA-C1A-NA	-3.08	124.55	128.83
6	AU	201	CYC	C1B-CHB-C4A	3.08	135.61	128.08
6	AO	201	CYC	CHB-C1B-C2B	-3.07	120.86	126.95
6	AX	201	CYC	CMB-C2B-C1B	3.05	127.98	124.17
6	m	201	CYC	CMB-C2B-C1B	3.05	127.97	124.17
6	O	201	CYC	CHB-C1B-C2B	-3.05	120.91	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	201	CYC	CMB-C2B-C1B	3.05	127.97	124.17
6	a	201	CYC	CMB-C2B-C1B	3.04	127.96	124.17
6	AA	201	CYC	CHA-C1A-NA	-3.03	124.62	128.83
6	m	201	CYC	CBD-CAD-C3D	3.03	117.80	112.62
6	AM	201	CYC	CHA-C1A-NA	-3.02	124.64	128.83
6	A	2101	CYC	C4D-CHA-C1A	3.01	132.41	128.81
6	e	201	CYC	CHA-C1A-NA	-3.01	124.65	128.83
6	Q	201	CYC	CHB-C1B-C2B	-2.99	121.02	126.95
6	w	201	CYC	C1B-CHB-C4A	2.99	135.38	128.08
6	c	201	CYC	CHB-C1B-C2B	-2.99	121.03	126.95
6	S	201	CYC	CHB-C1B-C2B	-2.98	121.04	126.95
6	AO	201	CYC	CMB-C2B-C1B	2.98	127.89	124.17
6	AH	201	CYC	C1B-CHB-C4A	2.98	135.36	128.08
6	AC	201	CYC	CMB-C2B-C1B	2.97	127.88	124.17
6	k	201	CYC	CHB-C1B-C2B	-2.97	121.06	126.95
6	l	201	CYC	CHB-C1B-C2B	-2.96	121.09	126.95
6	AT	201	CYC	C1B-CHB-C4A	2.96	135.30	128.08
6	J	201	CYC	CMB-C2B-C1B	2.95	127.85	124.17
6	I	201	CYC	CHB-C1B-NB	2.95	132.39	126.06
6	Y	201	CYC	CHB-C1B-NB	2.95	132.39	126.06
6	d	201	CYC	CMB-C2B-C1B	2.95	127.84	124.17
6	AP	201	CYC	CHA-C1A-NA	-2.94	124.74	128.83
6	6	201	CYC	CHA-C1A-NA	-2.94	124.75	128.83
6	AP	201	CYC	CHB-C1B-C2B	-2.93	121.14	126.95
6	f	201	CYC	C1B-CHB-C4A	2.93	135.23	128.08
6	g	201	CYC	CHA-C1A-NA	-2.93	124.77	128.83
6	AU	201	CYC	CHB-C1B-C2B	-2.93	121.15	126.95
6	l	201	CYC	C1B-CHB-C4A	2.92	135.22	128.08
6	AI	201	CYC	CHB-C1B-C2B	-2.92	121.16	126.95
6	s	201	CYC	CAC-C3C-C4C	2.92	120.17	112.67
6	AJ	201	CYC	CHB-C1B-C2B	-2.89	121.22	126.95
6	M	201	CYC	C1B-CHB-C4A	2.89	135.14	128.08
6	AV	201	CYC	CHB-C1B-C2B	-2.88	121.25	126.95
6	AE	201	CYC	CMB-C2B-C1B	2.88	127.76	124.17
6	AD	201	CYC	CHB-C1B-C2B	-2.87	121.27	126.95
6	Z	201	CYC	CMB-C2B-C1B	2.87	127.74	124.17
6	r	201	CYC	OC-C1C-C2C	-2.85	123.90	126.17
6	9	201	CYC	CHB-C1B-C2B	-2.85	121.30	126.95
6	AQ	201	CYC	CMB-C2B-C1B	2.85	127.72	124.17
6	H	201	CYC	CMB-C2B-C1B	2.85	127.72	124.17
6	O	201	CYC	C4D-CHA-C1A	2.85	132.21	128.81
6	C	2101	CYC	CHA-C1A-NA	-2.84	124.89	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	w	201	CYC	CHB-C1B-C2B	-2.84	121.33	126.95
6	t	201	CYC	OC-C1C-C2C	-2.84	123.92	126.17
6	E	201	CYC	CMB-C2B-C1B	2.83	127.71	124.17
6	w	201	CYC	CMB-C2B-C1B	2.83	127.70	124.17
6	q	201	CYC	CMB-C2B-C1B	2.83	127.70	124.17
6	AU	201	CYC	CHA-C1A-NA	-2.82	124.92	128.83
6	L	201	CYC	CBD-CAD-C3D	2.81	117.42	112.62
6	I	201	CYC	C1B-CHB-C4A	2.81	134.95	128.08
6	AC	201	CYC	CHA-C1A-NA	-2.81	124.93	128.83
6	4	201	CYC	CHA-C1A-NA	-2.81	124.93	128.83
6	AI	201	CYC	CHA-C1A-NA	-2.79	124.95	128.83
6	6	201	CYC	C1B-CHB-C4A	2.79	134.90	128.08
6	X	201	CYC	CMB-C2B-C1B	2.78	127.64	124.17
6	C	2101	CYC	C2C-C3C-C4C	2.78	105.50	101.34
6	h	201	CYC	CHD-C4C-NC	2.77	128.50	125.20
6	u	201	CYC	CHD-C4C-NC	2.77	128.50	125.20
6	AO	201	CYC	CHA-C1A-NA	-2.77	124.98	128.83
6	t	201	CYC	C1B-CHB-C4A	2.76	134.83	128.08
6	w	201	CYC	CHA-C1A-NA	-2.75	125.01	128.83
6	z	201	CYC	C2C-C1C-NC	2.75	110.64	108.27
6	l	201	CYC	CHA-C1A-NA	-2.75	125.01	128.83
6	c	201	CYC	C1B-CHB-C4A	2.74	134.78	128.08
6	h	201	CYC	C2C-C1C-NC	2.74	110.64	108.27
6	y	201	CYC	CHB-C1B-C2B	-2.74	121.52	126.95
6	G	201	CYC	CHB-C1B-NB	2.74	131.94	126.06
6	6	201	CYC	CMA-C3A-C4A	2.74	129.28	125.06
6	z	201	CYC	CHD-C4C-NC	2.74	128.46	125.20
6	8	201	CYC	OC-C1C-C2C	-2.73	124.00	126.17
6	AH	201	CYC	CHB-C1B-C2B	-2.73	121.55	126.95
6	x	201	CYC	CHA-C1A-NA	-2.72	125.05	128.83
6	b	201	CYC	CMB-C2B-C1B	2.72	127.57	124.17
6	i	201	CYC	CHB-C1B-C2B	-2.72	121.56	126.95
6	AT	201	CYC	CMA-C3A-C4A	2.72	129.25	125.06
6	p	201	CYC	CHA-C1A-NA	-2.71	125.06	128.83
6	AT	201	CYC	CHB-C1B-C2B	-2.71	121.59	126.95
6	W	201	CYC	CMB-C2B-C1B	2.70	127.54	124.17
6	b	201	CYC	CBD-CAD-C3D	2.70	117.23	112.62
6	G	201	CYC	CMB-C2B-C1B	2.70	127.54	124.17
6	v	201	CYC	CMB-C2B-C1B	2.69	127.53	124.17
6	8	201	CYC	C2C-C1C-NC	2.69	110.59	108.27
6	AH	201	CYC	CMA-C3A-C4A	2.68	129.19	125.06
6	Q	201	CYC	C1B-CHB-C4A	2.68	134.62	128.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	a	201	CYC	CHB-C1B-C2B	-2.67	121.66	126.95
6	AI	201	CYC	CMB-C2B-C1B	2.66	127.49	124.17
6	m	201	CYC	C1B-CHB-C4A	2.66	134.57	128.08
6	C	2101	CYC	CMA-C3A-C4A	2.66	129.15	125.06
6	AS	201	CYC	C1B-CHB-C4A	2.65	134.56	128.08
6	n	201	CYC	OC-C1C-C2C	-2.65	124.06	126.17
6	AG	201	CYC	C1B-CHB-C4A	2.65	134.56	128.08
6	S	201	CYC	C4D-CHA-C1A	2.65	131.97	128.81
6	K	201	CYC	CHB-C1B-C2B	-2.63	121.74	126.95
6	r	201	CYC	C1B-CHB-C4A	2.62	134.49	128.08
6	t	201	CYC	CHD-C4C-NC	2.62	128.32	125.20
6	m	201	CYC	CAC-C3C-C4C	2.62	119.40	112.67
6	AU	201	CYC	CMB-C2B-C1B	2.62	127.44	124.17
6	v	201	CYC	CHB-C1B-C2B	-2.61	121.77	126.95
6	Y	201	CYC	C1B-CHB-C4A	2.61	134.47	128.08
6	7	201	CYC	CAC-C3C-C4C	2.61	119.38	112.67
6	AW	201	CYC	CHB-C1B-C2B	-2.61	121.78	126.95
6	n	201	CYC	C2C-C1C-NC	2.60	110.52	108.27
6	W	201	CYC	CHB-C1B-NB	2.60	131.63	126.06
6	U	201	CYC	C1B-CHB-C4A	2.59	134.42	128.08
6	AK	201	CYC	CHB-C1B-C2B	-2.59	121.81	126.95
6	7	201	CYC	CAB-C3B-C2B	2.59	131.96	127.53
6	2	201	CYC	CHB-C1B-NB	2.57	131.58	126.06
6	AA	201	CYC	C2C-C1C-NC	2.57	110.49	108.27
6	AQ	201	CYC	CHB-C1B-C2B	-2.56	121.87	126.95
6	U	201	CYC	CHB-C1B-NB	2.56	131.56	126.06
6	m	201	CYC	CAB-C3B-C2B	2.56	131.91	127.53
6	E	201	CYC	C1B-CHB-C4A	2.56	134.34	128.08
6	AE	201	CYC	CHB-C1B-C2B	-2.56	121.88	126.95
6	7	201	CYC	C1B-CHB-C4A	2.55	134.32	128.08
6	t	201	CYC	CHA-C1A-NA	-2.55	125.29	128.83
6	g	201	CYC	CHB-C1B-C2B	-2.55	121.90	126.95
6	L	201	CYC	CMB-C2B-C1B	2.54	127.34	124.17
6	E	201	CYC	CHB-C1B-NB	2.54	131.51	126.06
6	f	201	CYC	C2C-C3C-C4C	2.52	105.11	101.34
6	AM	201	CYC	C2C-C1C-NC	2.51	110.44	108.27
6	t	201	CYC	CHB-C1B-C2B	-2.51	121.97	126.95
6	AS	201	CYC	CHB-C1B-C2B	-2.51	121.98	126.95
6	S	201	CYC	CHD-C4C-NC	2.51	128.19	125.20
6	O	201	CYC	CHD-C4C-NC	2.51	128.19	125.20
6	p	201	CYC	C1B-CHB-C4A	2.50	134.19	128.08
6	5	201	CYC	CMA-C3A-C4A	2.50	128.91	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2	201	CYC	C1B-CHB-C4A	2.50	134.18	128.08
6	AG	201	CYC	CHB-C1B-C2B	-2.49	122.02	126.95
6	C	2101	CYC	CHB-C1B-NB	2.48	131.37	126.06
6	t	201	CYC	C2C-C1C-NC	2.47	110.40	108.27
6	e	201	CYC	CMA-C3A-C4A	2.47	128.86	125.06
6	G	201	CYC	C1B-CHB-C4A	2.47	134.10	128.08
6	s	201	CYC	OC-C1C-C2C	-2.47	124.21	126.17
6	S	201	CYC	CMB-C2B-C1B	2.46	127.24	124.17
6	O	201	CYC	CMB-C2B-C1B	2.45	127.23	124.17
6	U	201	CYC	CMB-C2B-C1B	2.44	127.22	124.17
6	r	201	CYC	CHB-C1B-C2B	-2.44	122.11	126.95
6	O	201	CYC	CMA-C3A-C4A	2.44	128.81	125.06
6	F	201	CYC	C1B-CHB-C4A	2.43	134.03	128.08
6	AA	201	CYC	C2C-C3C-C4C	2.43	104.98	101.34
6	AM	201	CYC	C2C-C3C-C4C	2.43	104.98	101.34
6	AM	201	CYC	CAC-C3C-C2C	-2.43	108.19	114.26
6	S	201	CYC	CMA-C3A-C4A	2.43	128.80	125.06
6	f	201	CYC	CMB-C2B-C3B	-2.42	119.56	126.12
6	r	201	CYC	CHA-C1A-NA	-2.41	125.48	128.83
6	q	201	CYC	CHB-C1B-C2B	-2.41	122.17	126.95
6	W	201	CYC	C1B-CHB-C4A	2.39	133.92	128.08
6	AA	201	CYC	CAC-C3C-C2C	-2.39	108.29	114.26
6	C	2101	CYC	CMB-C2B-C1B	2.39	127.15	124.17
6	x	201	CYC	C1B-CHB-C4A	2.39	133.91	128.08
6	r	201	CYC	C2C-C1C-NC	2.38	110.33	108.27
6	AR	201	CYC	CMA-C3A-C4A	2.38	128.73	125.06
6	k	201	CYC	C1B-CHB-C4A	2.38	133.89	128.08
6	F	201	CYC	CMA-C3A-C4A	2.37	128.72	125.06
6	f	201	CYC	CMA-C3A-C4A	2.37	128.72	125.06
6	AB	201	CYC	CHD-C4C-NC	2.36	128.01	125.20
6	g	201	CYC	CMB-C2B-C1B	2.36	127.11	124.17
6	9	201	CYC	CMA-C3A-C4A	2.36	128.70	125.06
6	p	201	CYC	CHB-C1B-C2B	-2.36	122.28	126.95
6	2	201	CYC	CMA-C3A-C4A	2.35	128.68	125.06
6	7	201	CYC	CHD-C4C-NC	2.35	127.99	125.20
6	b	201	CYC	CHB-C1B-C2B	-2.34	122.31	126.95
6	A	2101	CYC	CMA-C3A-C4A	2.34	128.67	125.06
6	7	201	CYC	CHA-C1A-NA	-2.34	125.59	128.83
6	m	201	CYC	CHD-C4C-NC	2.33	127.98	125.20
6	y	201	CYC	CHD-C4C-NC	2.33	127.98	125.20
6	AJ	201	CYC	C2C-C3C-C4C	2.33	104.83	101.34
6	u	201	CYC	OC-C1C-C2C	-2.32	124.33	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	m	201	CYC	CHA-C1A-NA	-2.32	125.61	128.83
6	AF	201	CYC	CMA-C3A-C4A	2.32	128.64	125.06
6	AV	201	CYC	C2C-C3C-C4C	2.31	104.80	101.34
6	AN	201	CYC	CHD-C4C-NC	2.31	127.95	125.20
6	V	201	CYC	CMA-C3A-C4A	2.31	128.62	125.06
6	m	201	CYC	CAC-C3C-C2C	-2.30	108.51	114.26
6	8	201	CYC	CHB-C1B-C2B	-2.30	122.39	126.95
6	s	201	CYC	CHB-C1B-C2B	-2.30	122.39	126.95
6	b	201	CYC	C4D-CHA-C1A	-2.29	126.07	128.81
6	L	201	CYC	CHB-C1B-C2B	-2.29	122.41	126.95
6	m	201	CYC	OC-C1C-C2C	-2.29	124.36	126.17
6	i	201	CYC	C1B-CHB-C4A	2.28	133.66	128.08
6	X	201	CYC	C2C-C3C-C4C	2.28	104.76	101.34
6	n	201	CYC	CAC-C3C-C4C	2.28	118.54	112.67
6	7	201	CYC	CAC-C3C-C2C	-2.28	108.57	114.26
6	6	201	CYC	C2C-C3C-C4C	2.28	104.75	101.34
6	V	201	CYC	C1B-CHB-C4A	2.27	133.63	128.08
6	AV	201	CYC	CHD-C4C-NC	2.27	127.90	125.20
6	AT	201	CYC	C2C-C3C-C4C	2.26	104.73	101.34
6	AB	201	CYC	CBD-CAD-C3D	-2.25	108.78	112.62
6	g	201	CYC	CHD-C4C-NC	2.25	127.88	125.20
6	7	201	CYC	OC-C1C-C2C	-2.25	124.39	126.17
6	n	201	CYC	CHB-C1B-C2B	-2.25	122.50	126.95
6	y	201	CYC	CHA-C1A-NA	-2.25	125.71	128.83
6	x	201	CYC	CHB-C1B-C2B	-2.24	122.50	126.95
6	AJ	201	CYC	CHD-C4C-NC	2.24	127.87	125.20
6	X	201	CYC	C4D-CHA-C1A	-2.24	126.13	128.81
6	h	201	CYC	CBA-CAA-C2A	2.24	118.85	112.63
6	A	2101	CYC	CMB-C2B-C1B	2.24	126.96	124.17
6	9	201	CYC	C1B-CHB-C4A	2.24	133.54	128.08
6	AH	201	CYC	C2C-C3C-C4C	2.23	104.68	101.34
6	r	201	CYC	CHD-C4C-NC	2.23	127.86	125.20
6	C	2101	CYC	CAC-C3C-C4C	2.23	118.40	112.67
6	l	201	CYC	CHB-C1B-C2B	-2.22	122.56	126.95
6	u	201	CYC	CMA-C3A-C4A	2.21	128.47	125.06
6	T	201	CYC	C2C-C3C-C4C	2.21	104.65	101.34
6	AA	201	CYC	CHB-C1B-C2B	-2.21	122.57	126.95
6	u	201	CYC	CHA-C1A-NA	-2.21	125.77	128.83
6	AN	201	CYC	CBD-CAD-C3D	-2.21	108.86	112.62
6	AM	201	CYC	CHB-C1B-C2B	-2.20	122.58	126.95
6	L	201	CYC	C4D-CHA-C1A	-2.20	126.18	128.81
6	2	201	CYC	CMB-C2B-C1B	2.20	126.91	124.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	2101	CYC	CBD-CAD-C3D	2.19	116.36	112.62
6	H	201	CYC	C2C-C3C-C4C	2.19	104.62	101.34
6	m	201	CYC	C2C-C3C-C4C	2.19	104.61	101.34
6	7	201	CYC	C2C-C3C-C4C	2.18	104.60	101.34
6	y	201	CYC	C1B-CHB-C4A	2.18	133.41	128.08
6	AN	201	CYC	CHB-C1B-NB	2.17	130.71	126.06
6	3	201	CYC	CMA-C3A-C4A	2.16	128.39	125.06
6	8	201	CYC	CAC-C3C-C4C	2.15	118.19	112.67
6	AB	201	CYC	CHB-C1B-NB	2.15	130.66	126.06
6	AK	201	CYC	C1B-CHB-C4A	2.14	133.30	128.08
6	T	201	CYC	C4D-CHA-C1A	-2.13	126.27	128.81
6	AW	201	CYC	C1B-CHB-C4A	2.12	133.27	128.08
6	7	201	CYC	C2C-C1C-NC	2.12	110.10	108.27
6	z	201	CYC	CHB-C1B-C2B	-2.12	122.75	126.95
6	c	201	CYC	CMA-C3A-C4A	2.12	128.32	125.06
6	6	201	CYC	CMB-C2B-C3B	-2.12	120.37	126.12
6	J	201	CYC	C4D-CHA-C1A	-2.12	126.28	128.81
6	m	201	CYC	C2C-C1C-NC	2.11	110.09	108.27
6	Z	201	CYC	C4D-CHA-C1A	-2.11	126.28	128.81
6	P	201	CYC	C2C-C3C-C4C	2.10	104.48	101.34
6	u	201	CYC	CMB-C2B-C1B	2.10	126.78	124.17
6	AC	201	CYC	CHB-C1B-NB	2.09	130.56	126.06
6	AT	201	CYC	CHA-C1A-NA	-2.09	125.92	128.83
6	j	201	CYC	CHA-C1A-NA	-2.09	125.92	128.83
6	3	201	CYC	C1B-CHB-C4A	2.09	133.18	128.08
6	AC	201	CYC	CMA-C3A-C4A	2.09	128.28	125.06
6	AH	201	CYC	CHA-C1A-NA	-2.08	125.94	128.83
6	k	201	CYC	C2C-C3C-C4C	2.08	104.45	101.34
6	G	201	CYC	CMA-C3A-C4A	2.07	128.26	125.06
6	W	201	CYC	CMA-C3A-C4A	2.07	128.26	125.06
6	AS	201	CYC	CHA-C1A-NA	-2.07	125.95	128.83
6	AG	201	CYC	CHA-C1A-NA	-2.07	125.95	128.83
6	6	201	CYC	CHB-C1B-C2B	-2.07	122.85	126.95
6	P	201	CYC	C4D-CHA-C1A	-2.06	126.35	128.81
6	AT	201	CYC	CAB-C3B-C2B	2.06	131.05	127.53
6	AO	201	CYC	CMA-C3A-C4A	2.06	128.23	125.06
6	E	201	CYC	C2C-C3C-C4C	2.06	104.42	101.34
6	AA	201	CYC	CHB-C4A-C3A	2.05	130.17	124.90
6	8	201	CYC	C2C-C3C-C4C	2.05	104.41	101.34
6	h	201	CYC	C2C-C3C-C4C	2.04	104.40	101.34
6	AM	201	CYC	CHB-C4A-C3A	2.04	130.16	124.90
6	e	201	CYC	C1B-CHB-C4A	2.04	133.07	128.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	r	201	CYC	CBD-CAD-C3D	2.04	116.10	112.62
6	h	201	CYC	CHB-C1B-C2B	-2.04	122.91	126.95
6	0	201	CYC	CHB-C1B-C2B	-2.04	122.91	126.95
6	9	201	CYC	C2C-C3C-C4C	2.04	104.39	101.34
6	8	201	CYC	C1B-CHB-C4A	2.04	133.05	128.08
6	g	201	CYC	C1B-CHB-C4A	2.03	133.05	128.08
6	z	201	CYC	CAC-C3C-C4C	2.03	117.89	112.67
6	f	201	CYC	CHB-C4A-NA	-2.03	120.68	124.93
6	z	201	CYC	CBA-CAA-C2A	2.03	118.28	112.63
6	AH	201	CYC	OC-C1C-C2C	-2.03	124.56	126.17
6	AN	201	CYC	C2C-C3C-C4C	2.03	104.38	101.34
6	M	201	CYC	CHB-C1B-NB	2.03	130.42	126.06
6	h	201	CYC	CAC-C3C-C4C	2.03	117.89	112.67
6	AB	201	CYC	C2C-C3C-C4C	2.03	104.38	101.34
6	AH	201	CYC	CAB-C3B-C2B	2.03	131.00	127.53
6	AT	201	CYC	OC-C1C-C2C	-2.03	124.56	126.17
6	AI	201	CYC	CMA-C3A-C4A	2.03	128.19	125.06
6	AJ	201	CYC	CAC-C3C-C4C	2.03	117.88	112.67
6	3	201	CYC	CHB-C1B-C2B	-2.03	122.93	126.95
6	U	201	CYC	C2C-C3C-C4C	2.02	104.37	101.34
6	r	201	CYC	C2C-C3C-C4C	2.02	104.37	101.34
6	z	201	CYC	C1B-CHB-C4A	2.02	133.02	128.08
6	6	201	CYC	C2C-C1C-NC	2.02	110.02	108.27
6	AO	201	CYC	CHB-C1B-NB	2.02	130.40	126.06
6	6	201	CYC	CHB-C4A-NA	-2.02	120.71	124.93
6	X	201	CYC	CHB-C1B-NB	2.02	130.39	126.06
6	Y	201	CYC	CMA-C3A-C4A	2.01	128.17	125.06
6	AP	201	CYC	CHB-C1B-NB	2.01	130.38	126.06
6	H	201	CYC	C4D-CHA-C1A	-2.01	126.41	128.81
6	T	201	CYC	CHB-C1B-C2B	-2.01	122.97	126.95
6	u	201	CYC	C2C-C1C-NC	2.01	110.00	108.27
6	n	201	CYC	C2C-C3C-C4C	2.00	104.34	101.34
6	M	201	CYC	CMA-C3A-C4A	2.00	128.15	125.06
6	z	201	CYC	C2C-C3C-C4C	2.00	104.34	101.34

There are no chirality outliers.

All (702) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2101	CYC	NA-C4A-CHB-C1B
6	A	2101	CYC	C3A-C4A-CHB-C1B
6	A	2101	CYC	C2B-C1B-CHB-C4A

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Mol	Chain	Res	Type	Atoms
6	A	2101	CYC	C2C-C3C-CAC-CBC
6	A	2101	CYC	NC-C4C-CHD-C1D
6	A	2101	CYC	ND-C1D-CHD-C4C
6	A	2101	CYC	C2D-C1D-CHD-C4C
6	A	2101	CYC	C2D-C3D-CAD-CBD
6	A	2101	CYC	C4D-C3D-CAD-CBD
6	A	2101	CYC	C3D-CAD-CBD-CGD
6	C	2101	CYC	C4B-C3B-CAB-CBB
6	C	2101	CYC	ND-C1D-CHD-C4C
6	C	2101	CYC	C2D-C1D-CHD-C4C
6	M	201	CYC	NA-C4A-CHB-C1B
6	M	201	CYC	C3A-C4A-CHB-C1B
6	M	201	CYC	C2D-C3D-CAD-CBD
6	M	201	CYC	C4D-C3D-CAD-CBD
6	N	201	CYC	NA-C4A-CHB-C1B
6	N	201	CYC	C2B-C3B-CAB-CBB
6	O	201	CYC	NA-C4A-CHB-C1B
6	O	201	CYC	C3A-C4A-CHB-C1B
6	P	201	CYC	NA-C4A-CHB-C1B
6	P	201	CYC	C3A-C4A-CHB-C1B
6	P	201	CYC	ND-C1D-CHD-C4C
6	P	201	CYC	C2D-C1D-CHD-C4C
6	E	201	CYC	ND-C1D-CHD-C4C
6	E	201	CYC	C2D-C1D-CHD-C4C
6	G	201	CYC	NA-C4A-CHB-C1B
6	G	201	CYC	C3A-C4A-CHB-C1B
6	H	201	CYC	NA-C4A-CHB-C1B
6	H	201	CYC	C3A-C4A-CHB-C1B
6	H	201	CYC	ND-C1D-CHD-C4C
6	H	201	CYC	C2D-C1D-CHD-C4C
6	H	201	CYC	C2D-C3D-CAD-CBD
6	H	201	CYC	C4D-C3D-CAD-CBD
6	I	201	CYC	ND-C1D-CHD-C4C
6	J	201	CYC	NA-C4A-CHB-C1B
6	J	201	CYC	C3A-C4A-CHB-C1B
6	K	201	CYC	C4C-C3C-CAC-CBC
6	L	201	CYC	NA-C4A-CHB-C1B
6	L	201	CYC	C3A-C4A-CHB-C1B
6	L	201	CYC	ND-C1D-CHD-C4C
6	L	201	CYC	C2D-C1D-CHD-C4C
6	Q	201	CYC	NA-C4A-CHB-C1B
6	Q	201	CYC	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
6	Q	201	CYC	C2D-C3D-CAD-CBD
6	Q	201	CYC	C4D-C3D-CAD-CBD
6	R	201	CYC	C4B-C3B-CAB-CBB
6	S	201	CYC	NA-C4A-CHB-C1B
6	S	201	CYC	C3A-C4A-CHB-C1B
6	T	201	CYC	NA-C4A-CHB-C1B
6	T	201	CYC	C3A-C4A-CHB-C1B
6	T	201	CYC	ND-C1D-CHD-C4C
6	T	201	CYC	C2D-C1D-CHD-C4C
6	U	201	CYC	ND-C1D-CHD-C4C
6	U	201	CYC	C2D-C1D-CHD-C4C
6	W	201	CYC	NA-C4A-CHB-C1B
6	W	201	CYC	C3A-C4A-CHB-C1B
6	W	201	CYC	ND-C1D-CHD-C4C
6	X	201	CYC	NA-C4A-CHB-C1B
6	X	201	CYC	C3A-C4A-CHB-C1B
6	X	201	CYC	ND-C1D-CHD-C4C
6	X	201	CYC	C2D-C1D-CHD-C4C
6	X	201	CYC	C2D-C3D-CAD-CBD
6	Y	201	CYC	ND-C1D-CHD-C4C
6	Z	201	CYC	NA-C4A-CHB-C1B
6	Z	201	CYC	C3A-C4A-CHB-C1B
6	a	201	CYC	C4C-C3C-CAC-CBC
6	b	201	CYC	NA-C4A-CHB-C1B
6	b	201	CYC	C3A-C4A-CHB-C1B
6	b	201	CYC	C2A-CAA-CBA-CGA
6	b	201	CYC	ND-C1D-CHD-C4C
6	b	201	CYC	C2D-C1D-CHD-C4C
6	c	201	CYC	ND-C1D-CHD-C4C
6	c	201	CYC	C2D-C1D-CHD-C4C
6	d	201	CYC	NA-C4A-CHB-C1B
6	d	201	CYC	C3A-C4A-CHB-C1B
6	e	201	CYC	NA-C4A-CHB-C1B
6	e	201	CYC	C3A-C4A-CHB-C1B
6	e	201	CYC	ND-C1D-CHD-C4C
6	e	201	CYC	C2D-C1D-CHD-C4C
6	e	201	CYC	C2D-C3D-CAD-CBD
6	e	201	CYC	C4D-C3D-CAD-CBD
6	f	201	CYC	NA-C4A-CHB-C1B
6	f	201	CYC	C3A-C4A-CHB-C1B
6	f	201	CYC	ND-C1D-CHD-C4C
6	f	201	CYC	C2D-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
6	g	201	CYC	NA-C4A-CHB-C1B
6	g	201	CYC	C3A-C4A-CHB-C1B
6	g	201	CYC	ND-C1D-CHD-C4C
6	g	201	CYC	C2D-C1D-CHD-C4C
6	h	201	CYC	C1A-C2A-CAA-CBA
6	h	201	CYC	NA-C4A-CHB-C1B
6	h	201	CYC	C3A-C4A-CHB-C1B
6	h	201	CYC	ND-C1D-CHD-C4C
6	h	201	CYC	C2D-C1D-CHD-C4C
6	i	201	CYC	ND-C1D-CHD-C4C
6	i	201	CYC	C2D-C1D-CHD-C4C
6	j	201	CYC	NA-C4A-CHB-C1B
6	j	201	CYC	C3A-C4A-CHB-C1B
6	j	201	CYC	C2B-C1B-CHB-C4A
6	j	201	CYC	ND-C1D-CHD-C4C
6	k	201	CYC	C4C-C3C-CAC-CBC
6	k	201	CYC	ND-C1D-CHD-C4C
6	l	201	CYC	NA-C4A-CHB-C1B
6	l	201	CYC	C3A-C4A-CHB-C1B
6	l	201	CYC	ND-C1D-CHD-C4C
6	m	201	CYC	C3A-C4A-CHB-C1B
6	m	201	CYC	ND-C1D-CHD-C4C
6	m	201	CYC	C2D-C1D-CHD-C4C
6	m	201	CYC	C2D-C3D-CAD-CBD
6	m	201	CYC	C4D-C3D-CAD-CBD
6	n	201	CYC	NA-C4A-CHB-C1B
6	n	201	CYC	C3A-C4A-CHB-C1B
6	n	201	CYC	ND-C1D-CHD-C4C
6	n	201	CYC	C2D-C1D-CHD-C4C
6	o	201	CYC	NA-C4A-CHB-C1B
6	o	201	CYC	C3A-C4A-CHB-C1B
6	p	201	CYC	NA-C4A-CHB-C1B
6	p	201	CYC	C3A-C4A-CHB-C1B
6	p	201	CYC	C2A-CAA-CBA-CGA
6	p	201	CYC	NB-C1B-CHB-C4A
6	p	201	CYC	C2B-C1B-CHB-C4A
6	p	201	CYC	ND-C1D-CHD-C4C
6	q	201	CYC	NA-C4A-CHB-C1B
6	q	201	CYC	C3A-C4A-CHB-C1B
6	r	201	CYC	ND-C1D-CHD-C4C
6	r	201	CYC	C2D-C1D-CHD-C4C
6	r	201	CYC	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
6	r	201	CYC	C4D-C3D-CAD-CBD
6	r	201	CYC	C3D-CAD-CBD-CGD
6	s	201	CYC	NA-C4A-CHB-C1B
6	s	201	CYC	C3A-C4A-CHB-C1B
6	s	201	CYC	C4B-C3B-CAB-CBB
6	s	201	CYC	C4C-C3C-CAC-CBC
6	s	201	CYC	ND-C1D-CHD-C4C
6	s	201	CYC	C2D-C1D-CHD-C4C
6	t	201	CYC	ND-C1D-CHD-C4C
6	t	201	CYC	C2D-C1D-CHD-C4C
6	t	201	CYC	C2D-C3D-CAD-CBD
6	t	201	CYC	C4D-C3D-CAD-CBD
6	u	201	CYC	NA-C4A-CHB-C1B
6	u	201	CYC	C3A-C4A-CHB-C1B
6	u	201	CYC	C4B-C3B-CAB-CBB
6	u	201	CYC	C2C-C3C-CAC-CBC
6	u	201	CYC	C4C-C3C-CAC-CBC
6	u	201	CYC	ND-C1D-CHD-C4C
6	u	201	CYC	C2D-C1D-CHD-C4C
6	u	201	CYC	C3D-CAD-CBD-CGD
6	v	201	CYC	NA-C4A-CHB-C1B
6	v	201	CYC	C3A-C4A-CHB-C1B
6	v	201	CYC	ND-C1D-CHD-C4C
6	w	201	CYC	NA-C4A-CHB-C1B
6	w	201	CYC	C3A-C4A-CHB-C1B
6	w	201	CYC	C4C-C3C-CAC-CBC
6	w	201	CYC	C3D-CAD-CBD-CGD
6	x	201	CYC	NA-C4A-CHB-C1B
6	x	201	CYC	C3A-C4A-CHB-C1B
6	x	201	CYC	NB-C1B-CHB-C4A
6	x	201	CYC	C2B-C1B-CHB-C4A
6	x	201	CYC	ND-C1D-CHD-C4C
6	y	201	CYC	NA-C4A-CHB-C1B
6	y	201	CYC	C3A-C4A-CHB-C1B
6	y	201	CYC	ND-C1D-CHD-C4C
6	y	201	CYC	C2D-C1D-CHD-C4C
6	z	201	CYC	C1A-C2A-CAA-CBA
6	z	201	CYC	NA-C4A-CHB-C1B
6	z	201	CYC	C3A-C4A-CHB-C1B
6	z	201	CYC	ND-C1D-CHD-C4C
6	z	201	CYC	C2D-C1D-CHD-C4C
6	1	201	CYC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
6	1	201	CYC	ND-C1D-CHD-C4C
6	1	201	CYC	C2D-C1D-CHD-C4C
6	2	201	CYC	NA-C4A-CHB-C1B
6	2	201	CYC	C3A-C4A-CHB-C1B
6	2	201	CYC	C2B-C1B-CHB-C4A
6	3	201	CYC	ND-C1D-CHD-C4C
6	3	201	CYC	C3D-CAD-CBD-CGD
6	4	201	CYC	NA-C4A-CHB-C1B
6	4	201	CYC	C3A-C4A-CHB-C1B
6	5	201	CYC	NA-C4A-CHB-C1B
6	5	201	CYC	C3A-C4A-CHB-C1B
6	5	201	CYC	ND-C1D-CHD-C4C
6	5	201	CYC	C2D-C1D-CHD-C4C
6	6	201	CYC	NA-C4A-CHB-C1B
6	6	201	CYC	ND-C1D-CHD-C4C
6	6	201	CYC	C2D-C1D-CHD-C4C
6	7	201	CYC	C3A-C4A-CHB-C1B
6	7	201	CYC	ND-C1D-CHD-C4C
6	7	201	CYC	C2D-C1D-CHD-C4C
6	7	201	CYC	C2D-C3D-CAD-CBD
6	7	201	CYC	C4D-C3D-CAD-CBD
6	8	201	CYC	NA-C4A-CHB-C1B
6	8	201	CYC	C3A-C4A-CHB-C1B
6	8	201	CYC	ND-C1D-CHD-C4C
6	8	201	CYC	C2D-C1D-CHD-C4C
6	9	201	CYC	C4C-C3C-CAC-CBC
6	9	201	CYC	ND-C1D-CHD-C4C
6	0	201	CYC	NA-C4A-CHB-C1B
6	0	201	CYC	C3A-C4A-CHB-C1B
6	AA	201	CYC	ND-C1D-CHD-C4C
6	AA	201	CYC	C2D-C1D-CHD-C4C
6	AA	201	CYC	C2D-C3D-CAD-CBD
6	AA	201	CYC	C4D-C3D-CAD-CBD
6	AA	201	CYC	C3D-CAD-CBD-CGD
6	AB	201	CYC	NA-C4A-CHB-C1B
6	AB	201	CYC	C3A-C4A-CHB-C1B
6	AB	201	CYC	ND-C1D-CHD-C4C
6	AB	201	CYC	C2D-C1D-CHD-C4C
6	AC	201	CYC	NA-C4A-CHB-C1B
6	AC	201	CYC	C3A-C4A-CHB-C1B
6	AC	201	CYC	C4C-C3C-CAC-CBC
6	AC	201	CYC	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
6	AD	201	CYC	NA-C4A-CHB-C1B
6	AD	201	CYC	C3A-C4A-CHB-C1B
6	AD	201	CYC	ND-C1D-CHD-C4C
6	AE	201	CYC	ND-C1D-CHD-C4C
6	AE	201	CYC	C3D-CAD-CBD-CGD
6	AF	201	CYC	NA-C4A-CHB-C1B
6	AF	201	CYC	C3A-C4A-CHB-C1B
6	AF	201	CYC	C2A-CAA-CBA-CGA
6	AF	201	CYC	ND-C1D-CHD-C4C
6	AF	201	CYC	C2D-C1D-CHD-C4C
6	AH	201	CYC	NA-C4A-CHB-C1B
6	AH	201	CYC	C3A-C4A-CHB-C1B
6	AI	201	CYC	NA-C4A-CHB-C1B
6	AI	201	CYC	C3A-C4A-CHB-C1B
6	AI	201	CYC	C4C-C3C-CAC-CBC
6	AI	201	CYC	C3D-CAD-CBD-CGD
6	AJ	201	CYC	NA-C4A-CHB-C1B
6	AJ	201	CYC	C3A-C4A-CHB-C1B
6	AJ	201	CYC	ND-C1D-CHD-C4C
6	AJ	201	CYC	C2D-C1D-CHD-C4C
6	AK	201	CYC	ND-C1D-CHD-C4C
6	AK	201	CYC	C2D-C1D-CHD-C4C
6	AL	201	CYC	NA-C4A-CHB-C1B
6	AL	201	CYC	C3A-C4A-CHB-C1B
6	AL	201	CYC	C4C-C3C-CAC-CBC
6	AM	201	CYC	ND-C1D-CHD-C4C
6	AM	201	CYC	C2D-C1D-CHD-C4C
6	AM	201	CYC	C2D-C3D-CAD-CBD
6	AM	201	CYC	C4D-C3D-CAD-CBD
6	AM	201	CYC	C3D-CAD-CBD-CGD
6	AN	201	CYC	NA-C4A-CHB-C1B
6	AN	201	CYC	C3A-C4A-CHB-C1B
6	AN	201	CYC	ND-C1D-CHD-C4C
6	AN	201	CYC	C2D-C1D-CHD-C4C
6	AO	201	CYC	NA-C4A-CHB-C1B
6	AO	201	CYC	C3A-C4A-CHB-C1B
6	AO	201	CYC	C4C-C3C-CAC-CBC
6	AO	201	CYC	C3D-CAD-CBD-CGD
6	AP	201	CYC	NA-C4A-CHB-C1B
6	AP	201	CYC	C3A-C4A-CHB-C1B
6	AP	201	CYC	ND-C1D-CHD-C4C
6	AP	201	CYC	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
6	AQ	201	CYC	ND-C1D-CHD-C4C
6	AQ	201	CYC	C3D-CAD-CBD-CGD
6	AR	201	CYC	NA-C4A-CHB-C1B
6	AR	201	CYC	C3A-C4A-CHB-C1B
6	AR	201	CYC	C2A-CAA-CBA-CGA
6	AR	201	CYC	ND-C1D-CHD-C4C
6	AR	201	CYC	C2D-C1D-CHD-C4C
6	AT	201	CYC	NA-C4A-CHB-C1B
6	AT	201	CYC	C3A-C4A-CHB-C1B
6	AU	201	CYC	NA-C4A-CHB-C1B
6	AU	201	CYC	C3A-C4A-CHB-C1B
6	AU	201	CYC	C4C-C3C-CAC-CBC
6	AU	201	CYC	C3D-CAD-CBD-CGD
6	AV	201	CYC	NA-C4A-CHB-C1B
6	AV	201	CYC	C3A-C4A-CHB-C1B
6	AV	201	CYC	ND-C1D-CHD-C4C
6	AV	201	CYC	C2D-C1D-CHD-C4C
6	AW	201	CYC	ND-C1D-CHD-C4C
6	AW	201	CYC	C2D-C1D-CHD-C4C
6	AX	201	CYC	NA-C4A-CHB-C1B
6	AX	201	CYC	C3A-C4A-CHB-C1B
6	R	201	CYC	C2B-C3B-CAB-CBB
6	s	201	CYC	C2B-C3B-CAB-CBB
6	AP	201	CYC	C2B-C3B-CAB-CBB
6	d	201	CYC	C2B-C3B-CAB-CBB
6	u	201	CYC	C2B-C3B-CAB-CBB
6	A	2101	CYC	NB-C1B-CHB-C4A
6	2	201	CYC	NB-C1B-CHB-C4A
6	y	201	CYC	C2B-C3B-CAB-CBB
6	J	201	CYC	C2B-C3B-CAB-CBB
6	q	201	CYC	C2B-C3B-CAB-CBB
6	A	2101	CYC	C2A-CAA-CBA-CGA
6	P	201	CYC	C2A-CAA-CBA-CGA
6	J	201	CYC	C2A-CAA-CBA-CGA
6	R	201	CYC	C2A-CAA-CBA-CGA
6	T	201	CYC	C2A-CAA-CBA-CGA
6	l	201	CYC	C2A-CAA-CBA-CGA
6	m	201	CYC	NA-C4A-CHB-C1B
6	s	201	CYC	C2A-CAA-CBA-CGA
6	u	201	CYC	C2A-CAA-CBA-CGA
6	x	201	CYC	C2A-CAA-CBA-CGA
6	z	201	CYC	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
6	7	201	CYC	NA-C4A-CHB-C1B
6	AE	201	CYC	NA-C4A-CHB-C1B
6	AQ	201	CYC	NA-C4A-CHB-C1B
6	C	2101	CYC	C3A-C4A-CHB-C1B
6	r	201	CYC	C3A-C4A-CHB-C1B
6	t	201	CYC	C3A-C4A-CHB-C1B
6	j	201	CYC	NB-C1B-CHB-C4A
6	Z	201	CYC	C2B-C3B-CAB-CBB
6	C	2101	CYC	C2B-C3B-CAB-CBB
6	Q	201	CYC	C2B-C3B-CAB-CBB
6	v	201	CYC	C2B-C3B-CAB-CBB
6	M	201	CYC	C3D-CAD-CBD-CGD
6	O	201	CYC	C3D-CAD-CBD-CGD
6	K	201	CYC	C3D-CAD-CBD-CGD
6	Q	201	CYC	C3D-CAD-CBD-CGD
6	S	201	CYC	C3D-CAD-CBD-CGD
6	a	201	CYC	C3D-CAD-CBD-CGD
6	c	201	CYC	C3D-CAD-CBD-CGD
6	m	201	CYC	C3D-CAD-CBD-CGD
6	t	201	CYC	C3D-CAD-CBD-CGD
6	9	201	CYC	C3D-CAD-CBD-CGD
6	AG	201	CYC	C3D-CAD-CBD-CGD
6	AS	201	CYC	C3D-CAD-CBD-CGD
6	N	201	CYC	C4B-C3B-CAB-CBB
6	y	201	CYC	C4B-C3B-CAB-CBB
6	AP	201	CYC	C4B-C3B-CAB-CBB
6	g	201	CYC	C2B-C3B-CAB-CBB
6	q	201	CYC	NB-C1B-CHB-C4A
6	N	201	CYC	C2A-CAA-CBA-CGA
6	h	201	CYC	C2A-CAA-CBA-CGA
6	q	201	CYC	C2A-CAA-CBA-CGA
6	4	201	CYC	C2A-CAA-CBA-CGA
6	0	201	CYC	C2A-CAA-CBA-CGA
6	AL	201	CYC	C2A-CAA-CBA-CGA
6	x	201	CYC	C2B-C3B-CAB-CBB
6	1	201	CYC	C2B-C3B-CAB-CBB
6	f	201	CYC	NB-C1B-CHB-C4A
6	d	201	CYC	C3A-C2A-CAA-CBA
6	C	2101	CYC	NA-C4A-CHB-C1B
6	E	201	CYC	NA-C4A-CHB-C1B
6	F	201	CYC	NA-C4A-CHB-C1B
6	I	201	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
6	K	201	CYC	NA-C4A-CHB-C1B
6	R	201	CYC	NA-C4A-CHB-C1B
6	U	201	CYC	NA-C4A-CHB-C1B
6	V	201	CYC	NA-C4A-CHB-C1B
6	Y	201	CYC	NA-C4A-CHB-C1B
6	a	201	CYC	NA-C4A-CHB-C1B
6	c	201	CYC	NA-C4A-CHB-C1B
6	i	201	CYC	NA-C4A-CHB-C1B
6	k	201	CYC	NA-C4A-CHB-C1B
6	r	201	CYC	NA-C4A-CHB-C1B
6	t	201	CYC	NA-C4A-CHB-C1B
6	1	201	CYC	NA-C4A-CHB-C1B
6	3	201	CYC	NA-C4A-CHB-C1B
6	9	201	CYC	NA-C4A-CHB-C1B
6	AA	201	CYC	NA-C4A-CHB-C1B
6	AG	201	CYC	NA-C4A-CHB-C1B
6	AG	201	CYC	C2A-CAA-CBA-CGA
6	AK	201	CYC	NA-C4A-CHB-C1B
6	AM	201	CYC	NA-C4A-CHB-C1B
6	AS	201	CYC	NA-C4A-CHB-C1B
6	AS	201	CYC	C2A-CAA-CBA-CGA
6	AW	201	CYC	NA-C4A-CHB-C1B
6	N	201	CYC	C3A-C4A-CHB-C1B
6	E	201	CYC	C3A-C4A-CHB-C1B
6	F	201	CYC	C3A-C4A-CHB-C1B
6	I	201	CYC	C3A-C4A-CHB-C1B
6	K	201	CYC	C3A-C4A-CHB-C1B
6	R	201	CYC	C3A-C4A-CHB-C1B
6	U	201	CYC	C3A-C4A-CHB-C1B
6	V	201	CYC	C3A-C4A-CHB-C1B
6	Y	201	CYC	C3A-C4A-CHB-C1B
6	a	201	CYC	C3A-C4A-CHB-C1B
6	c	201	CYC	C3A-C4A-CHB-C1B
6	i	201	CYC	C3A-C4A-CHB-C1B
6	k	201	CYC	C3A-C4A-CHB-C1B
6	1	201	CYC	C3A-C4A-CHB-C1B
6	3	201	CYC	C3A-C4A-CHB-C1B
6	6	201	CYC	C3A-C4A-CHB-C1B
6	9	201	CYC	C3A-C4A-CHB-C1B
6	AA	201	CYC	C3A-C4A-CHB-C1B
6	AE	201	CYC	C3A-C4A-CHB-C1B
6	AG	201	CYC	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
6	AK	201	CYC	C3A-C4A-CHB-C1B
6	AM	201	CYC	C3A-C4A-CHB-C1B
6	AQ	201	CYC	C3A-C4A-CHB-C1B
6	AS	201	CYC	C3A-C4A-CHB-C1B
6	AW	201	CYC	C3A-C4A-CHB-C1B
6	E	201	CYC	C3D-CAD-CBD-CGD
6	k	201	CYC	C3D-CAD-CBD-CGD
6	7	201	CYC	C3D-CAD-CBD-CGD
6	AK	201	CYC	C3D-CAD-CBD-CGD
6	AW	201	CYC	C3D-CAD-CBD-CGD
6	AD	201	CYC	C2B-C3B-CAB-CBB
6	I	201	CYC	C2B-C3B-CAB-CBB
6	T	201	CYC	C2B-C3B-CAB-CBB
6	Y	201	CYC	C2B-C3B-CAB-CBB
6	L	201	CYC	C2A-CAA-CBA-CGA
6	Z	201	CYC	C2A-CAA-CBA-CGA
6	M	201	CYC	C2B-C3B-CAB-CBB
6	d	201	CYC	C1A-C2A-CAA-CBA
6	5	201	CYC	C2B-C3B-CAB-CBB
6	6	201	CYC	NB-C1B-CHB-C4A
6	I	201	CYC	C3D-CAD-CBD-CGD
6	Y	201	CYC	C3D-CAD-CBD-CGD
6	g	201	CYC	C3D-CAD-CBD-CGD
6	s	201	CYC	C2C-C3C-CAC-CBC
6	AI	201	CYC	C2C-C3C-CAC-CBC
6	AU	201	CYC	C2C-C3C-CAC-CBC
6	d	201	CYC	C4B-C3B-CAB-CBB
6	j	201	CYC	C1A-C2A-CAA-CBA
6	AP	201	CYC	NB-C1B-CHB-C4A
6	z	201	CYC	C3A-C2A-CAA-CBA
6	AN	201	CYC	C2B-C3B-CAB-CBB
6	AB	201	CYC	C2B-C3B-CAB-CBB
6	b	201	CYC	C2B-C3B-CAB-CBB
6	n	201	CYC	NB-C1B-CHB-C4A
6	U	201	CYC	C3D-CAD-CBD-CGD
6	v	201	CYC	C2A-CAA-CBA-CGA
6	1	201	CYC	C2A-CAA-CBA-CGA
6	5	201	CYC	C4B-C3B-CAB-CBB
6	n	201	CYC	C1A-C2A-CAA-CBA
6	L	201	CYC	C2B-C3B-CAB-CBB
6	W	201	CYC	C2B-C3B-CAB-CBB
6	P	201	CYC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
6	AU	201	CYC	C2B-C3B-CAB-CBB
6	AI	201	CYC	C2B-C3B-CAB-CBB
6	H	201	CYC	C4C-C3C-CAC-CBC
6	I	201	CYC	C4C-C3C-CAC-CBC
6	L	201	CYC	C4C-C3C-CAC-CBC
6	c	201	CYC	C4C-C3C-CAC-CBC
6	i	201	CYC	C4C-C3C-CAC-CBC
6	AD	201	CYC	C4C-C3C-CAC-CBC
6	AP	201	CYC	C4C-C3C-CAC-CBC
6	AX	201	CYC	C4C-C3C-CAC-CBC
6	e	201	CYC	C2B-C3B-CAB-CBB
6	v	201	CYC	NB-C1B-CHB-C4A
6	AT	201	CYC	NB-C1B-CHB-C4A
6	AO	201	CYC	C2B-C3B-CAB-CBB
6	g	201	CYC	C4B-C3B-CAB-CBB
6	q	201	CYC	C4B-C3B-CAB-CBB
6	G	201	CYC	C2B-C3B-CAB-CBB
6	2	201	CYC	C2B-C3B-CAB-CBB
6	h	201	CYC	C3A-C2A-CAA-CBA
6	j	201	CYC	C3A-C2A-CAA-CBA
6	AH	201	CYC	C2B-C3B-CAB-CBB
6	AC	201	CYC	C2B-C3B-CAB-CBB
6	AT	201	CYC	C2B-C3B-CAB-CBB
6	AC	201	CYC	NB-C1B-CHB-C4A
6	AH	201	CYC	NB-C1B-CHB-C4A
6	AO	201	CYC	NB-C1B-CHB-C4A
6	w	201	CYC	C2B-C3B-CAB-CBB
6	q	201	CYC	C2B-C1B-CHB-C4A
6	k	201	CYC	C2A-CAA-CBA-CGA
6	p	201	CYC	C2B-C3B-CAB-CBB
6	Q	201	CYC	C4B-C3B-CAB-CBB
6	e	201	CYC	C4B-C3B-CAB-CBB
6	v	201	CYC	C4B-C3B-CAB-CBB
6	C	2101	CYC	CAD-CBD-CGD-O1D
6	L	201	CYC	CAD-CBD-CGD-O2D
6	4	201	CYC	CAA-CBA-CGA-O1A
6	AD	201	CYC	CAD-CBD-CGD-O1D
6	O	201	CYC	CAD-CBD-CGD-O1D
6	R	201	CYC	CAD-CBD-CGD-O1D
6	r	201	CYC	CAA-CBA-CGA-O2A
6	s	201	CYC	CAD-CBD-CGD-O1D
6	G	201	CYC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
6	T	201	CYC	CAD-CBD-CGD-O1D
6	f	201	CYC	CAA-CBA-CGA-O2A
6	0	201	CYC	CAA-CBA-CGA-O2A
6	AR	201	CYC	CAA-CBA-CGA-O2A
6	AS	201	CYC	C2B-C3B-CAB-CBB
6	a	201	CYC	CAA-CBA-CGA-O2A
6	e	201	CYC	CAD-CBD-CGD-O1D
6	u	201	CYC	CAA-CBA-CGA-O1A
6	AG	201	CYC	C2B-C3B-CAB-CBB
6	f	201	CYC	CAA-CBA-CGA-O1A
6	m	201	CYC	CAD-CBD-CGD-O1D
6	r	201	CYC	CAD-CBD-CGD-O1D
6	r	201	CYC	CAD-CBD-CGD-O2D
6	1	201	CYC	CAA-CBA-CGA-O2A
6	7	201	CYC	CAD-CBD-CGD-O1D
6	AC	201	CYC	CAA-CBA-CGA-O2A
6	K	201	CYC	CAA-CBA-CGA-O2A
6	b	201	CYC	CAD-CBD-CGD-O1D
6	h	201	CYC	CAD-CBD-CGD-O1D
6	AF	201	CYC	CAA-CBA-CGA-O1A
6	AF	201	CYC	CAA-CBA-CGA-O2A
6	AL	201	CYC	CAA-CBA-CGA-O1A
6	AO	201	CYC	CAA-CBA-CGA-O2A
6	H	201	CYC	C1A-C2A-CAA-CBA
6	l	201	CYC	C3D-CAD-CBD-CGD
6	q	201	CYC	CAD-CBD-CGD-O1D
6	0	201	CYC	CAA-CBA-CGA-O1A
6	P	201	CYC	CAA-CBA-CGA-O1A
6	K	201	CYC	CAA-CBA-CGA-O1A
6	Q	201	CYC	CAA-CBA-CGA-O1A
6	l	201	CYC	CAD-CBD-CGD-O1D
6	m	201	CYC	CAA-CBA-CGA-O1A
6	m	201	CYC	CAA-CBA-CGA-O2A
6	7	201	CYC	CAA-CBA-CGA-O1A
6	Q	201	CYC	CAA-CBA-CGA-O2A
6	S	201	CYC	CAD-CBD-CGD-O1D
6	W	201	CYC	CAA-CBA-CGA-O2A
6	0	201	CYC	CAD-CBD-CGD-O1D
6	L	201	CYC	CAD-CBD-CGD-O1D
6	W	201	CYC	CAA-CBA-CGA-O1A
6	m	201	CYC	CAD-CBD-CGD-O2D
6	z	201	CYC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
6	7	201	CYC	CAA-CBA-CGA-O2A
6	AO	201	CYC	CAA-CBA-CGA-O1A
6	AR	201	CYC	CAA-CBA-CGA-O1A
6	AU	201	CYC	CAA-CBA-CGA-O1A
6	5	201	CYC	NB-C1B-CHB-C4A
6	C	2101	CYC	CAA-CBA-CGA-O1A
6	G	201	CYC	CAA-CBA-CGA-O1A
6	R	201	CYC	CAD-CBD-CGD-O2D
6	S	201	CYC	CAD-CBD-CGD-O2D
6	a	201	CYC	CAA-CBA-CGA-O1A
6	1	201	CYC	CAA-CBA-CGA-O1A
6	b	201	CYC	CAD-CBD-CGD-O2D
6	d	201	CYC	CAD-CBD-CGD-O1D
6	u	201	CYC	CAA-CBA-CGA-O2A
6	3	201	CYC	CAA-CBA-CGA-O1A
6	7	201	CYC	CAD-CBD-CGD-O2D
6	9	201	CYC	CAA-CBA-CGA-O1A
6	AC	201	CYC	CAA-CBA-CGA-O1A
6	P	201	CYC	CAA-CBA-CGA-O2A
6	T	201	CYC	CAA-CBA-CGA-O1A
6	T	201	CYC	CAA-CBA-CGA-O2A
6	e	201	CYC	CAD-CBD-CGD-O2D
6	l	201	CYC	CAA-CBA-CGA-O1A
6	q	201	CYC	CAD-CBD-CGD-O2D
6	s	201	CYC	CAA-CBA-CGA-O2A
6	P	201	CYC	CAD-CBD-CGD-O1D
6	L	201	CYC	CAA-CBA-CGA-O1A
6	v	201	CYC	CAD-CBD-CGD-O1D
6	y	201	CYC	CAD-CBD-CGD-O2D
6	AI	201	CYC	CAA-CBA-CGA-O1A
6	C	2101	CYC	CAA-CBA-CGA-O2A
6	P	201	CYC	CAD-CBD-CGD-O2D
6	l	201	CYC	CAA-CBA-CGA-O2A
6	r	201	CYC	CAA-CBA-CGA-O1A
6	v	201	CYC	CAD-CBD-CGD-O2D
6	y	201	CYC	CAD-CBD-CGD-O1D
6	AM	201	CYC	CAA-CBA-CGA-O1A
6	AM	201	CYC	CAA-CBA-CGA-O2A
6	AU	201	CYC	CAA-CBA-CGA-O2A
6	n	201	CYC	C2B-C1B-CHB-C4A
6	V	201	CYC	CAA-CBA-CGA-O2A
6	s	201	CYC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
6	z	201	CYC	CAD-CBD-CGD-O1D
6	4	201	CYC	CAA-CBA-CGA-O2A
6	5	201	CYC	CAA-CBA-CGA-O1A
6	5	201	CYC	CAA-CBA-CGA-O2A
6	0	201	CYC	CAD-CBD-CGD-O2D
6	V	201	CYC	CAA-CBA-CGA-O1A
6	l	201	CYC	CAD-CBD-CGD-O2D
6	s	201	CYC	CAD-CBD-CGD-O2D
6	t	201	CYC	CAD-CBD-CGD-O1D
6	C	2101	CYC	CAD-CBD-CGD-O2D
6	w	201	CYC	CAA-CBA-CGA-O1A
6	AA	201	CYC	CAA-CBA-CGA-O1A
6	AA	201	CYC	CAA-CBA-CGA-O2A
6	AD	201	CYC	CAD-CBD-CGD-O2D
6	AG	201	CYC	CAA-CBA-CGA-O2A
6	AS	201	CYC	CAA-CBA-CGA-O2A
6	O	201	CYC	CAD-CBD-CGD-O2D
6	T	201	CYC	CAD-CBD-CGD-O2D
6	AL	201	CYC	CAA-CBA-CGA-O2A
6	w	201	CYC	CAA-CBA-CGA-O2A
6	3	201	CYC	CAA-CBA-CGA-O2A
6	6	201	CYC	CAA-CBA-CGA-O2A
6	w	201	CYC	C2C-C3C-CAC-CBC
6	AP	201	CYC	C2B-C1B-CHB-C4A
6	M	201	CYC	CAA-CBA-CGA-O1A
6	F	201	CYC	CAA-CBA-CGA-O2A
6	b	201	CYC	CAA-CBA-CGA-O2A
6	c	201	CYC	CAA-CBA-CGA-O2A
6	h	201	CYC	CAD-CBD-CGD-O2D
6	AP	201	CYC	CAD-CBD-CGD-O1D
6	L	201	CYC	CAA-CBA-CGA-O2A
6	AI	201	CYC	CAA-CBA-CGA-O2A
6	A	2101	CYC	CAA-CBA-CGA-O2A
6	M	201	CYC	CAA-CBA-CGA-O2A
6	b	201	CYC	CAA-CBA-CGA-O1A
6	t	201	CYC	CAA-CBA-CGA-O1A
6	9	201	CYC	CAA-CBA-CGA-O2A
6	AJ	201	CYC	CAA-CBA-CGA-O2A
6	N	201	CYC	CAD-CBD-CGD-O1D
6	6	201	CYC	CAA-CBA-CGA-O1A
6	AG	201	CYC	CAA-CBA-CGA-O1A
6	Y	201	CYC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
6	b	201	CYC	C4C-C3C-CAC-CBC
6	3	201	CYC	C4C-C3C-CAC-CBC
6	AB	201	CYC	C2A-CAA-CBA-CGA
6	O	201	CYC	CAA-CBA-CGA-O2A
6	AB	201	CYC	CAA-CBA-CGA-O2A
6	AS	201	CYC	CAA-CBA-CGA-O1A
6	AV	201	CYC	CAA-CBA-CGA-O2A
6	A	2101	CYC	CAA-CBA-CGA-O1A
6	I	201	CYC	CAD-CBD-CGD-O2D
6	i	201	CYC	CAA-CBA-CGA-O2A
6	o	201	CYC	CAA-CBA-CGA-O2A
6	q	201	CYC	CAA-CBA-CGA-O2A
6	F	201	CYC	CAD-CBD-CGD-O2D
6	I	201	CYC	CAA-CBA-CGA-O2A
6	J	201	CYC	CAA-CBA-CGA-O2A
6	Y	201	CYC	CAD-CBD-CGD-O2D
6	c	201	CYC	CAA-CBA-CGA-O1A
6	t	201	CYC	CAD-CBD-CGD-O2D
6	O	201	CYC	CAA-CBA-CGA-O1A
6	F	201	CYC	CAA-CBA-CGA-O1A
6	AN	201	CYC	CAA-CBA-CGA-O2A
6	Y	201	CYC	CAA-CBA-CGA-O2A
6	d	201	CYC	CAD-CBD-CGD-O2D
6	8	201	CYC	CAD-CBD-CGD-O1D
6	AX	201	CYC	CAA-CBA-CGA-O1A
6	e	201	CYC	CAA-CBA-CGA-O1A
6	AA	201	CYC	CAD-CBD-CGD-O1D
6	AM	201	CYC	CAD-CBD-CGD-O1D
6	q	201	CYC	CAA-CBA-CGA-O1A
6	5	201	CYC	CAD-CBD-CGD-O2D
6	AX	201	CYC	CAA-CBA-CGA-O2A
6	f	201	CYC	C2B-C1B-CHB-C4A
6	I	201	CYC	CAA-CBA-CGA-O1A
6	V	201	CYC	CAD-CBD-CGD-O2D
6	Y	201	CYC	CAA-CBA-CGA-O1A
6	e	201	CYC	CAA-CBA-CGA-O2A
6	k	201	CYC	CAA-CBA-CGA-O2A
6	u	201	CYC	CAD-CBD-CGD-O2D
6	AW	201	CYC	CAA-CBA-CGA-O2A
6	r	201	CYC	C2B-C3B-CAB-CBB
6	AN	201	CYC	C2A-CAA-CBA-CGA
6	t	201	CYC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
6	J	201	CYC	CAD-CBD-CGD-O1D
6	Y	201	CYC	CAD-CBD-CGD-O1D
6	i	201	CYC	CAA-CBA-CGA-O1A
6	v	201	CYC	CAA-CBA-CGA-O2A
6	F	201	CYC	CAD-CBD-CGD-O1D
6	5	201	CYC	CAD-CBD-CGD-O1D
6	AK	201	CYC	CAA-CBA-CGA-O2A
6	J	201	CYC	CAA-CBA-CGA-O1A
6	i	201	CYC	CAD-CBD-CGD-O2D
6	I	201	CYC	CAD-CBD-CGD-O1D
6	S	201	CYC	CAA-CBA-CGA-O2A
6	k	201	CYC	CAA-CBA-CGA-O1A
6	o	201	CYC	CAA-CBA-CGA-O1A
6	AA	201	CYC	CAD-CBD-CGD-O2D
6	AN	201	CYC	CAA-CBA-CGA-O1A
6	G	201	CYC	CAD-CBD-CGD-O2D
6	Z	201	CYC	CAA-CBA-CGA-O2A
6	Z	201	CYC	CAD-CBD-CGD-O1D
6	u	201	CYC	CAD-CBD-CGD-O1D
6	AM	201	CYC	CAD-CBD-CGD-O2D
6	X	201	CYC	NB-C1B-CHB-C4A
6	8	201	CYC	NB-C1B-CHB-C4A
6	S	201	CYC	CAA-CBA-CGA-O1A
6	i	201	CYC	CAD-CBD-CGD-O1D
6	n	201	CYC	CAD-CBD-CGD-O1D
6	AB	201	CYC	CAA-CBA-CGA-O1A
6	t	201	CYC	C2B-C3B-CAB-CBB
6	AH	201	CYC	CAD-CBD-CGD-O2D
6	AJ	201	CYC	CAA-CBA-CGA-O1A
6	J	201	CYC	CAD-CBD-CGD-O2D
6	V	201	CYC	CAD-CBD-CGD-O1D
6	Z	201	CYC	CAA-CBA-CGA-O1A
6	v	201	CYC	CAA-CBA-CGA-O1A
6	AV	201	CYC	CAA-CBA-CGA-O1A
6	G	201	CYC	CAD-CBD-CGD-O1D
6	y	201	CYC	CAA-CBA-CGA-O2A
6	8	201	CYC	CAD-CBD-CGD-O2D
6	AW	201	CYC	CAA-CBA-CGA-O1A
6	AT	201	CYC	CAD-CBD-CGD-O2D
6	AP	201	CYC	CAD-CBD-CGD-O2D
6	AK	201	CYC	CAA-CBA-CGA-O1A
6	1	201	CYC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
6	C	2101	CYC	C2A-CAA-CBA-CGA
6	g	201	CYC	C2A-CAA-CBA-CGA
6	i	201	CYC	C2A-CAA-CBA-CGA
6	F	201	CYC	NB-C1B-CHB-C4A
6	AH	201	CYC	CAD-CBD-CGD-O1D
6	N	201	CYC	CAA-CBA-CGA-O2A
6	N	201	CYC	CAD-CBD-CGD-O2D
6	V	201	CYC	NB-C1B-CHB-C4A
6	e	201	CYC	NB-C1B-CHB-C4A
6	Z	201	CYC	CAD-CBD-CGD-O2D
6	AT	201	CYC	CAD-CBD-CGD-O1D
6	A	2101	CYC	CAD-CBD-CGD-O2D
6	N	201	CYC	CAA-CBA-CGA-O1A
6	l	201	CYC	CAD-CBD-CGD-O1D
6	A	2101	CYC	CAD-CBD-CGD-O1D
6	f	201	CYC	CAD-CBD-CGD-O2D
6	g	201	CYC	CAA-CBA-CGA-O2A
6	n	201	CYC	CAD-CBD-CGD-O2D
6	y	201	CYC	CAA-CBA-CGA-O1A
6	H	201	CYC	NB-C1B-CHB-C4A
6	S	201	CYC	NB-C1B-CHB-C4A
6	O	201	CYC	NC-C4C-CHD-C1D
6	AX	201	CYC	CAD-CBD-CGD-O1D
6	0	201	CYC	C3D-CAD-CBD-CGD
6	x	201	CYC	CAD-CBD-CGD-O2D
6	AX	201	CYC	CAD-CBD-CGD-O2D
6	p	201	CYC	CAD-CBD-CGD-O1D

There are no ring outliers.

84 monomers are involved in 429 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2101	CYC	3	0
6	4	201	CYC	6	0
6	l	201	CYC	1	0
6	0	201	CYC	2	0
6	M	201	CYC	6	0
6	a	201	CYC	4	0
6	h	201	CYC	1	0
6	5	201	CYC	8	0
6	AD	201	CYC	2	0
6	AS	201	CYC	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	AX	201	CYC	4	0
6	z	201	CYC	2	0
6	6	201	CYC	5	0
6	AN	201	CYC	3	0
6	8	201	CYC	1	0
6	R	201	CYC	13	0
6	e	201	CYC	10	0
6	AC	201	CYC	2	0
6	C	2101	CYC	33	0
6	L	201	CYC	2	0
6	c	201	CYC	6	0
6	AP	201	CYC	4	0
6	Y	201	CYC	3	0
6	AL	201	CYC	3	0
6	Z	201	CYC	3	0
6	AO	201	CYC	2	0
6	t	201	CYC	4	0
6	G	201	CYC	5	0
6	b	201	CYC	2	0
6	2	201	CYC	1	0
6	S	201	CYC	3	0
6	w	201	CYC	1	0
6	J	201	CYC	2	0
6	AJ	201	CYC	3	0
6	k	201	CYC	5	0
6	u	201	CYC	14	0
6	g	201	CYC	6	0
6	W	201	CYC	5	0
6	U	201	CYC	7	0
6	j	201	CYC	2	0
6	AR	201	CYC	1	0
6	o	201	CYC	3	0
6	O	201	CYC	3	0
6	AU	201	CYC	1	0
6	K	201	CYC	3	0
6	9	201	CYC	7	0
6	AW	201	CYC	11	0
6	1	201	CYC	2	0
6	d	201	CYC	5	0
6	AF	201	CYC	4	0
6	n	201	CYC	4	0
6	x	201	CYC	3	0

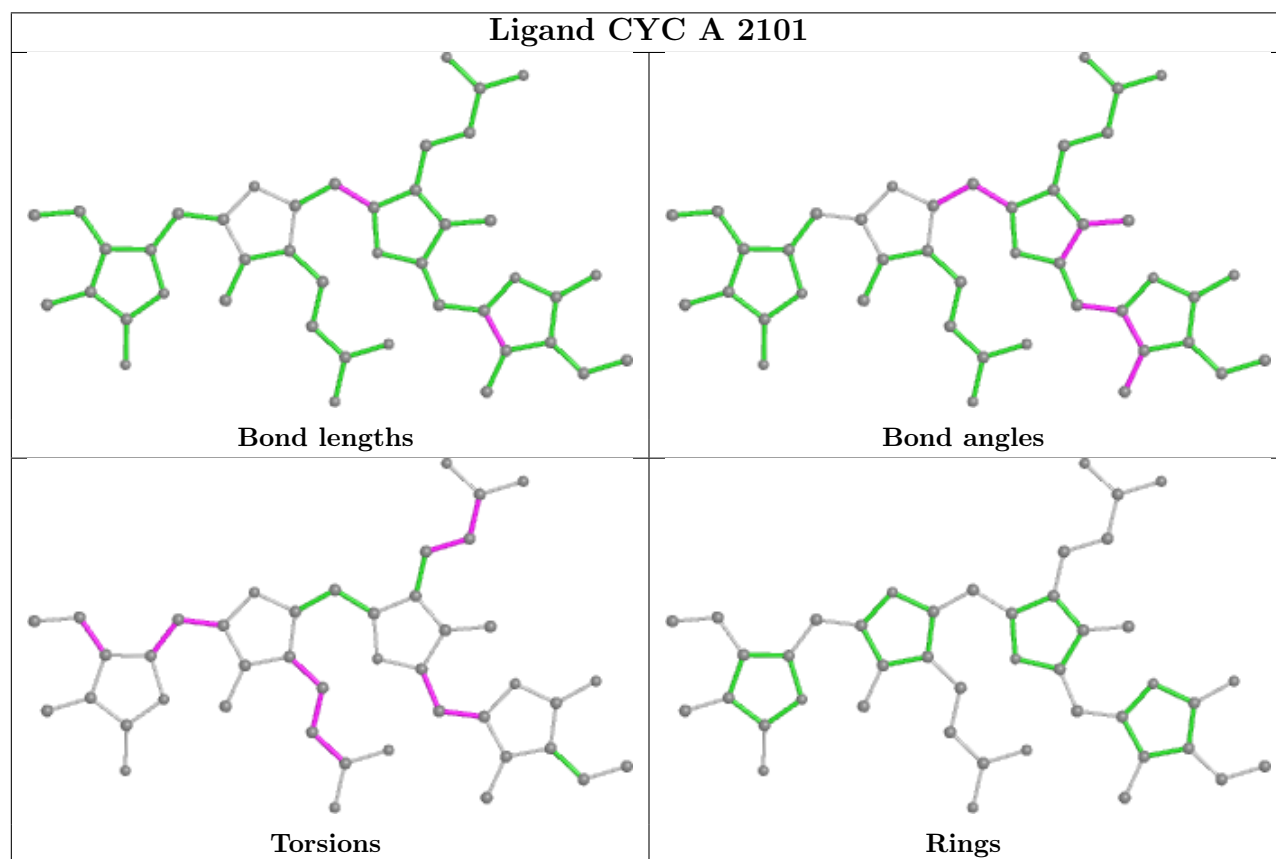
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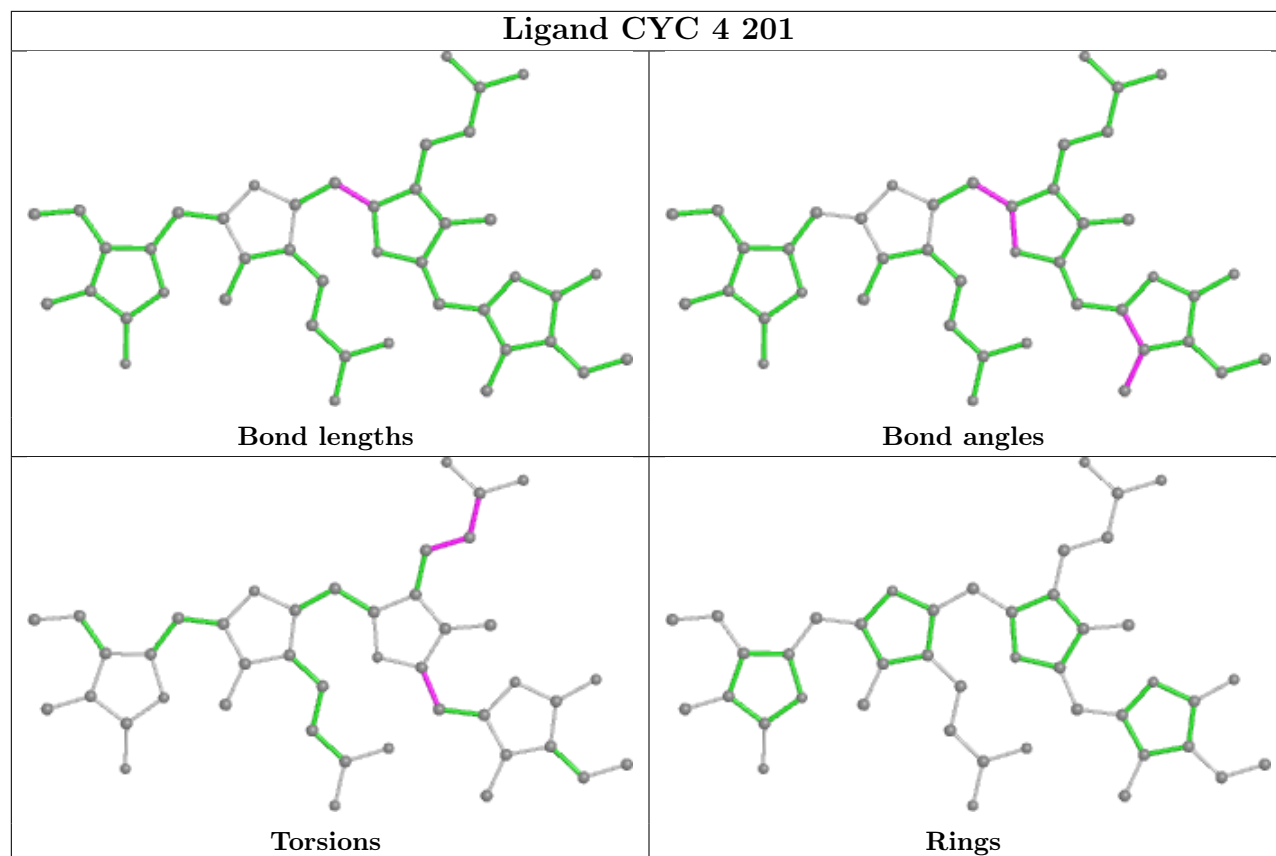
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	AI	201	CYC	1	0
6	AB	201	CYC	3	0
6	y	201	CYC	9	0
6	AM	201	CYC	7	0
6	AQ	201	CYC	1	0
6	i	201	CYC	4	0
6	s	201	CYC	12	0
6	AE	201	CYC	1	0
6	N	201	CYC	7	0
6	P	201	CYC	3	0
6	I	201	CYC	3	0
6	AT	201	CYC	4	0
6	T	201	CYC	5	0
6	AV	201	CYC	3	0
6	3	201	CYC	5	0
6	Q	201	CYC	10	0
6	q	201	CYC	2	0
6	AG	201	CYC	12	0
6	r	201	CYC	4	0
6	p	201	CYC	3	0
6	f	201	CYC	3	0
6	E	201	CYC	8	0
6	H	201	CYC	5	0
6	F	201	CYC	9	0
6	X	201	CYC	8	0
6	7	201	CYC	8	0
6	V	201	CYC	8	0
6	AK	201	CYC	11	0
6	m	201	CYC	9	0
6	v	201	CYC	1	0
6	AH	201	CYC	4	0
6	AA	201	CYC	7	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.

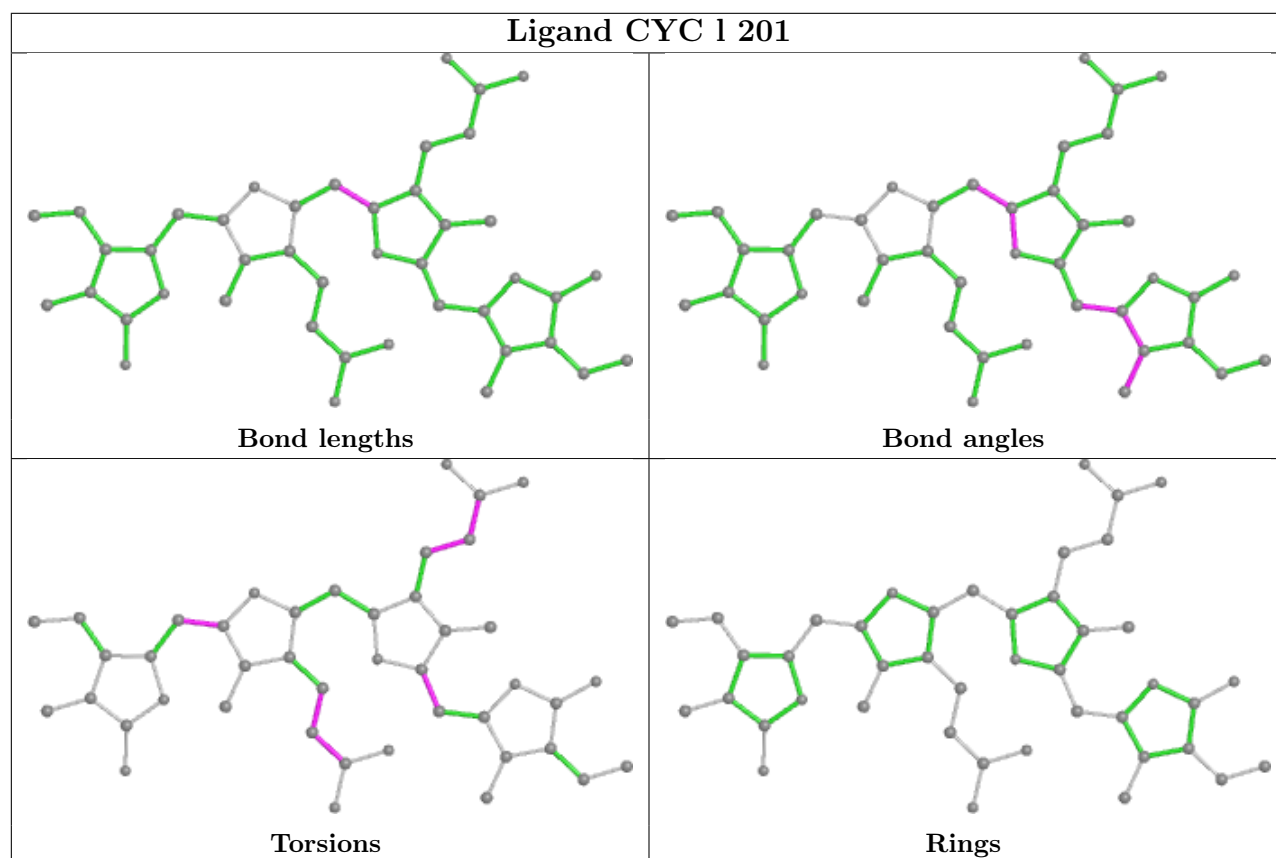
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



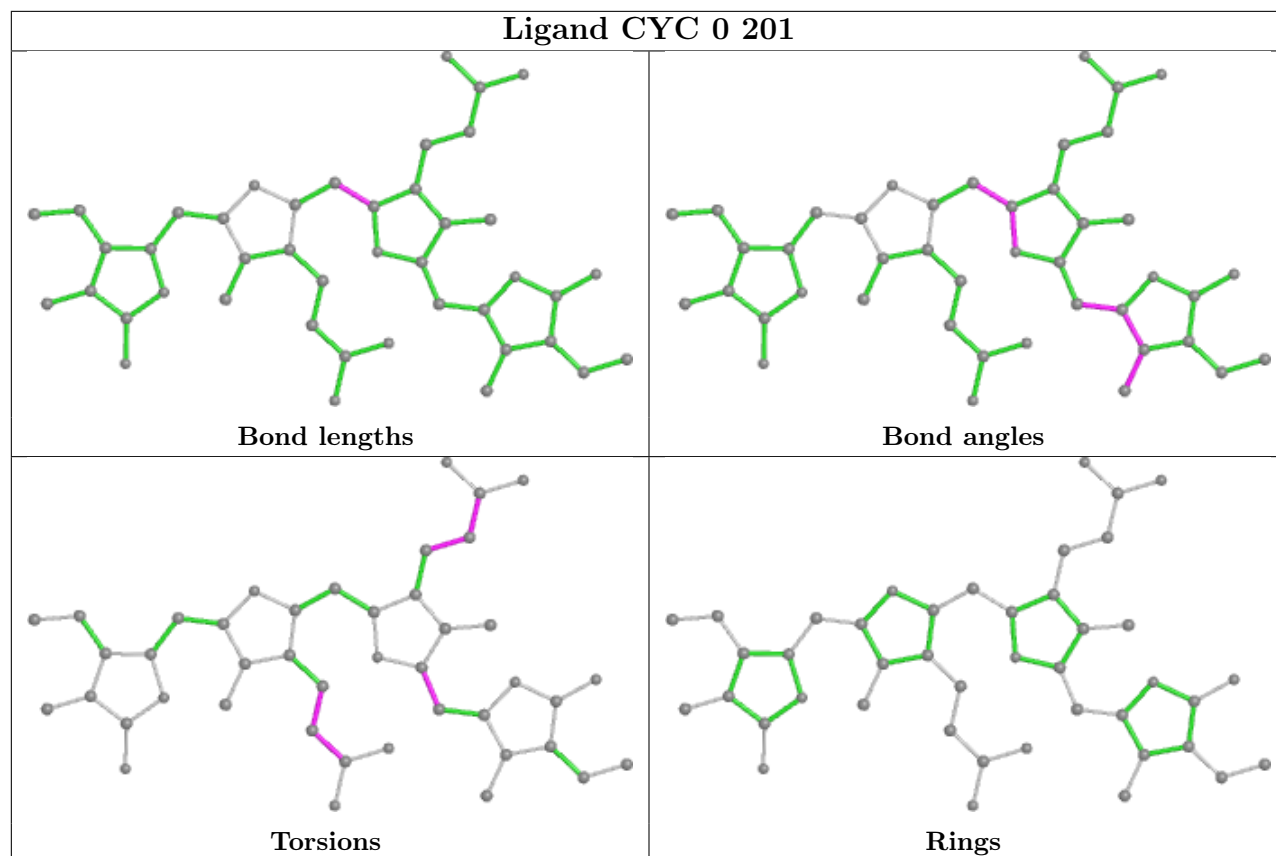
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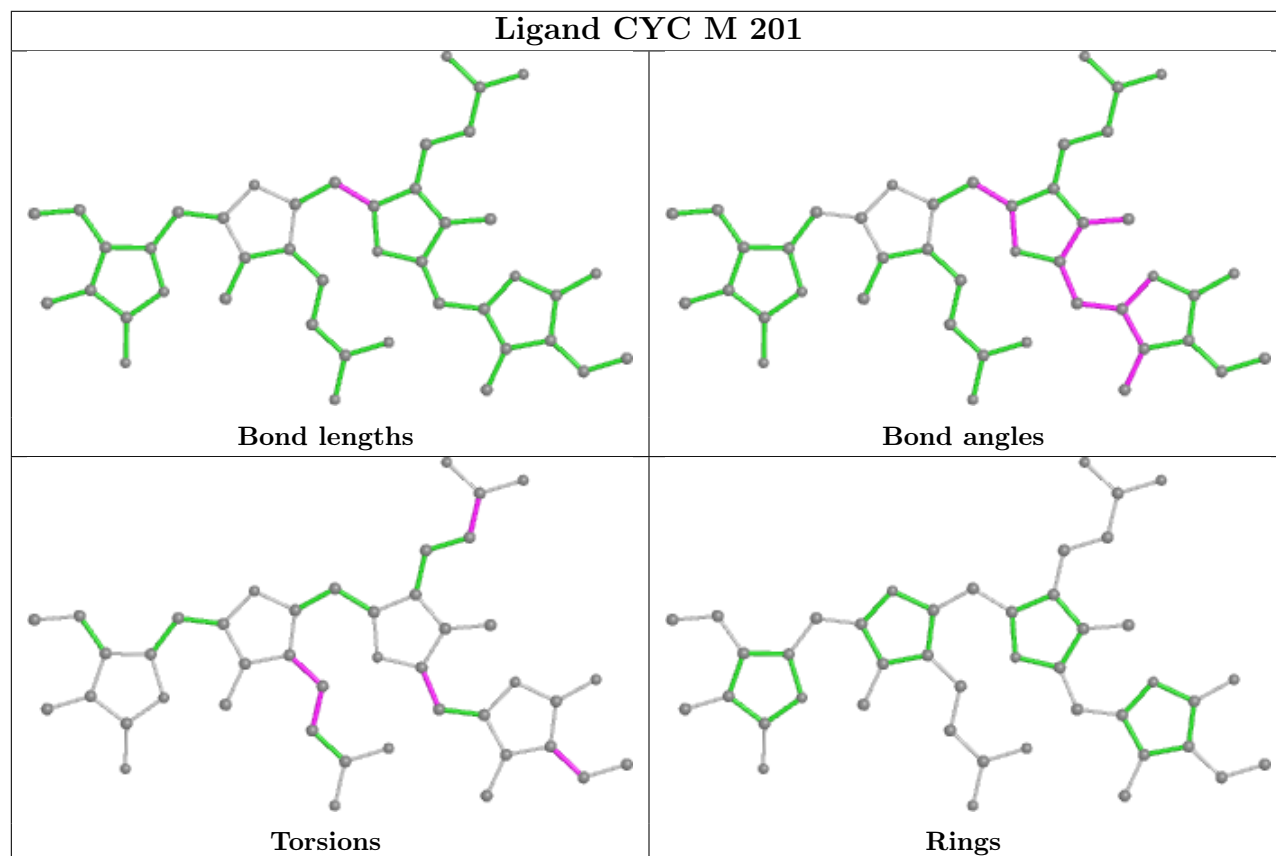
Ligand CYC 1 201



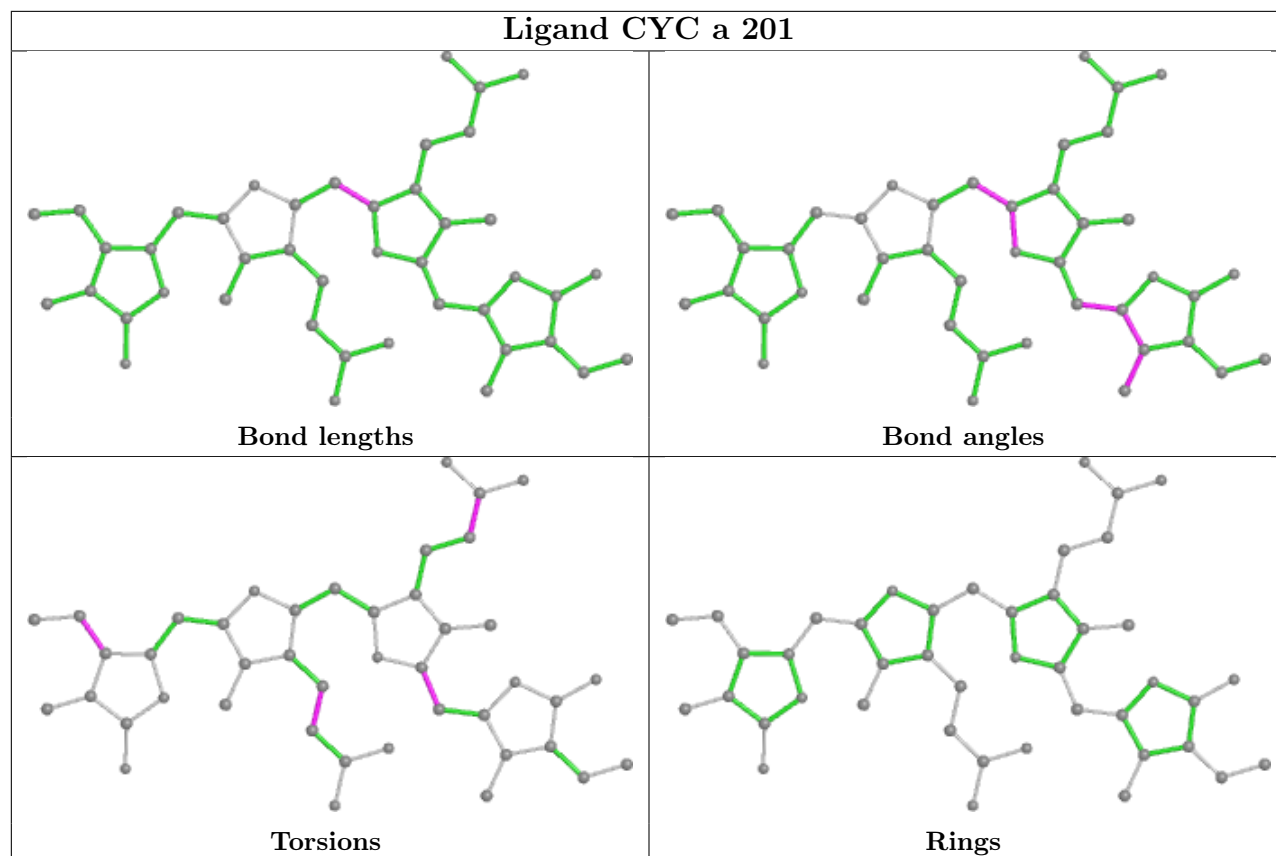
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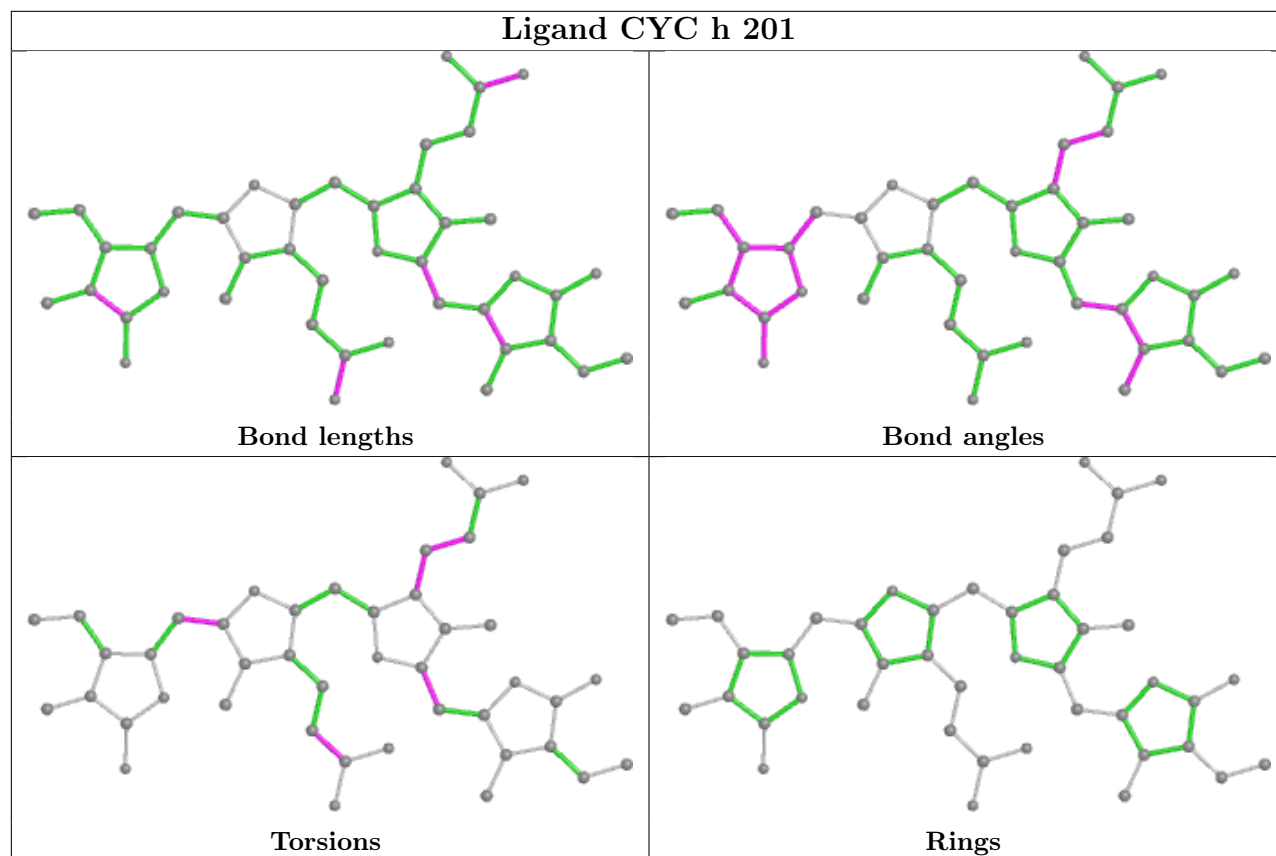
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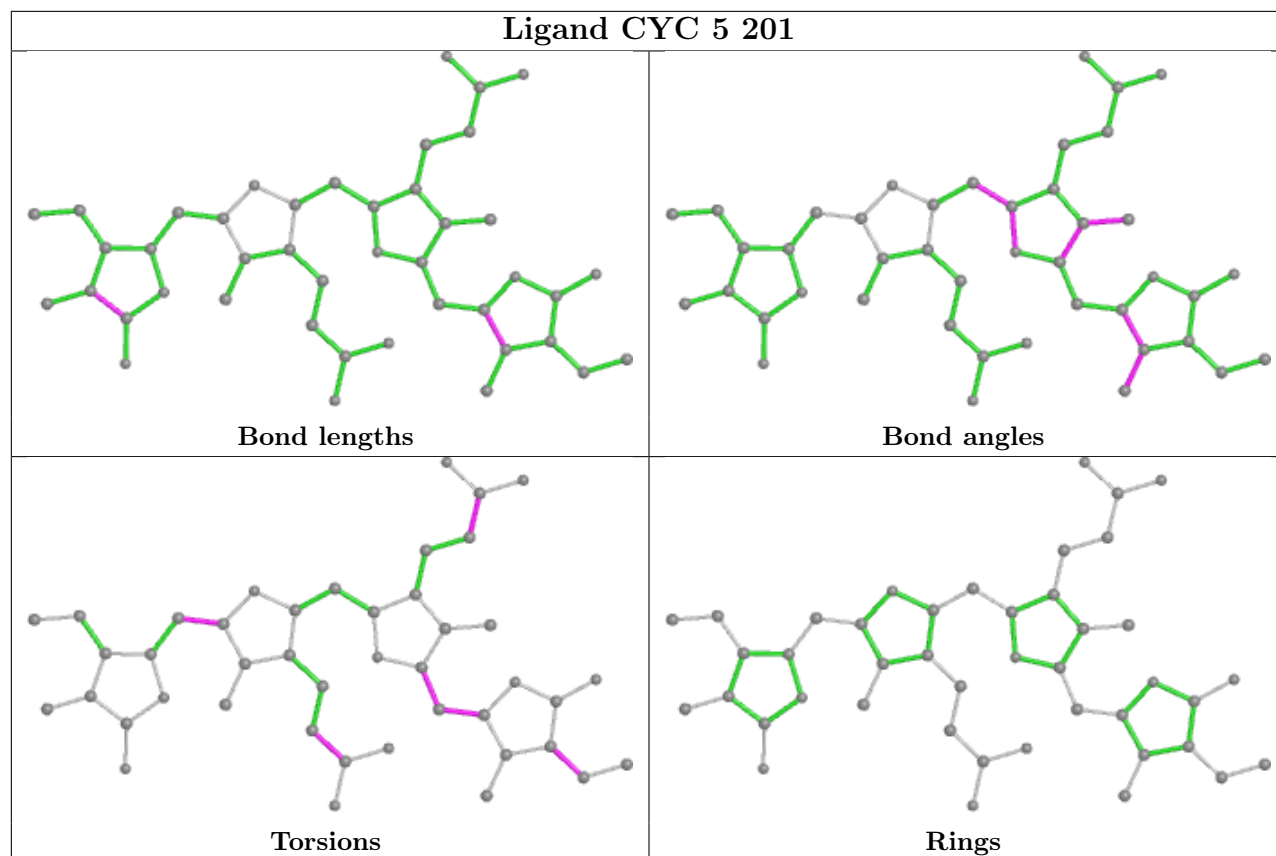
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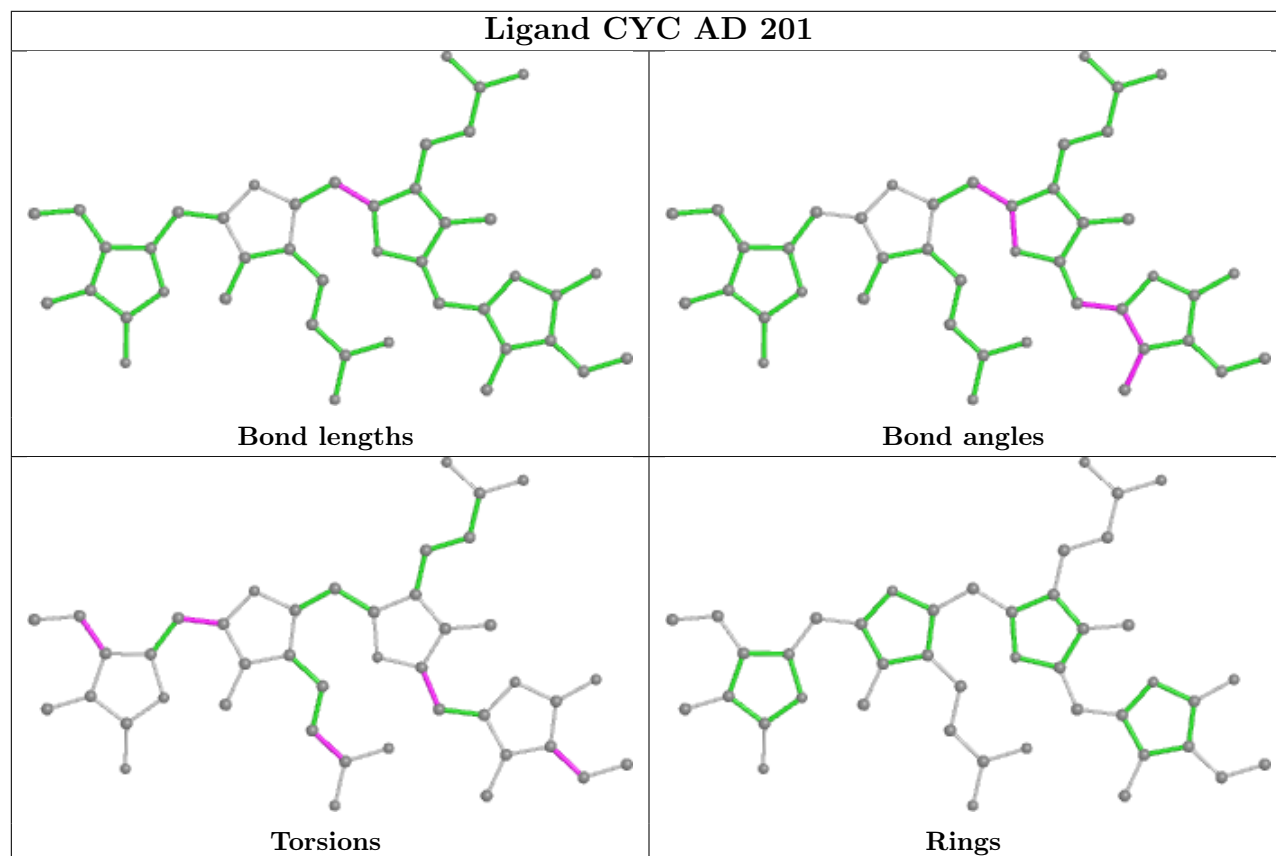
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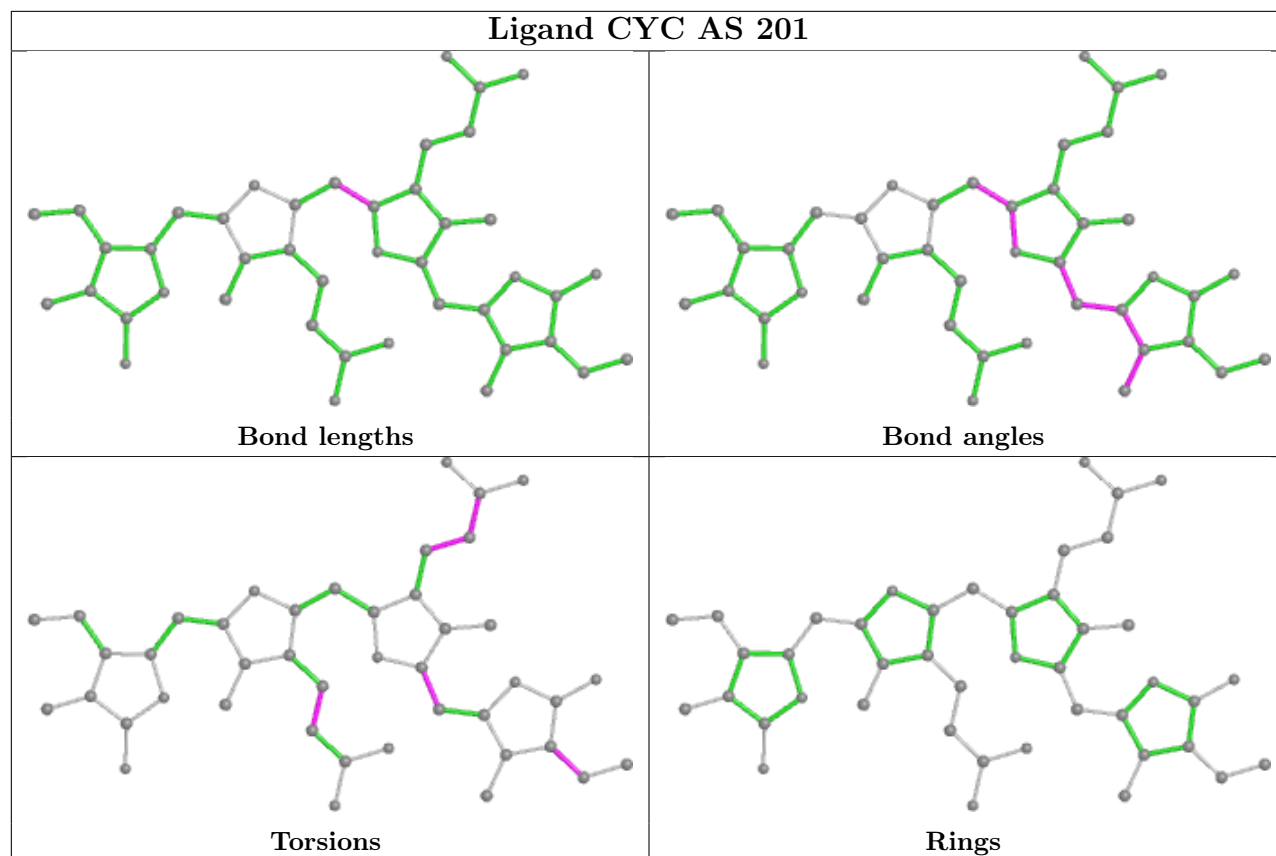
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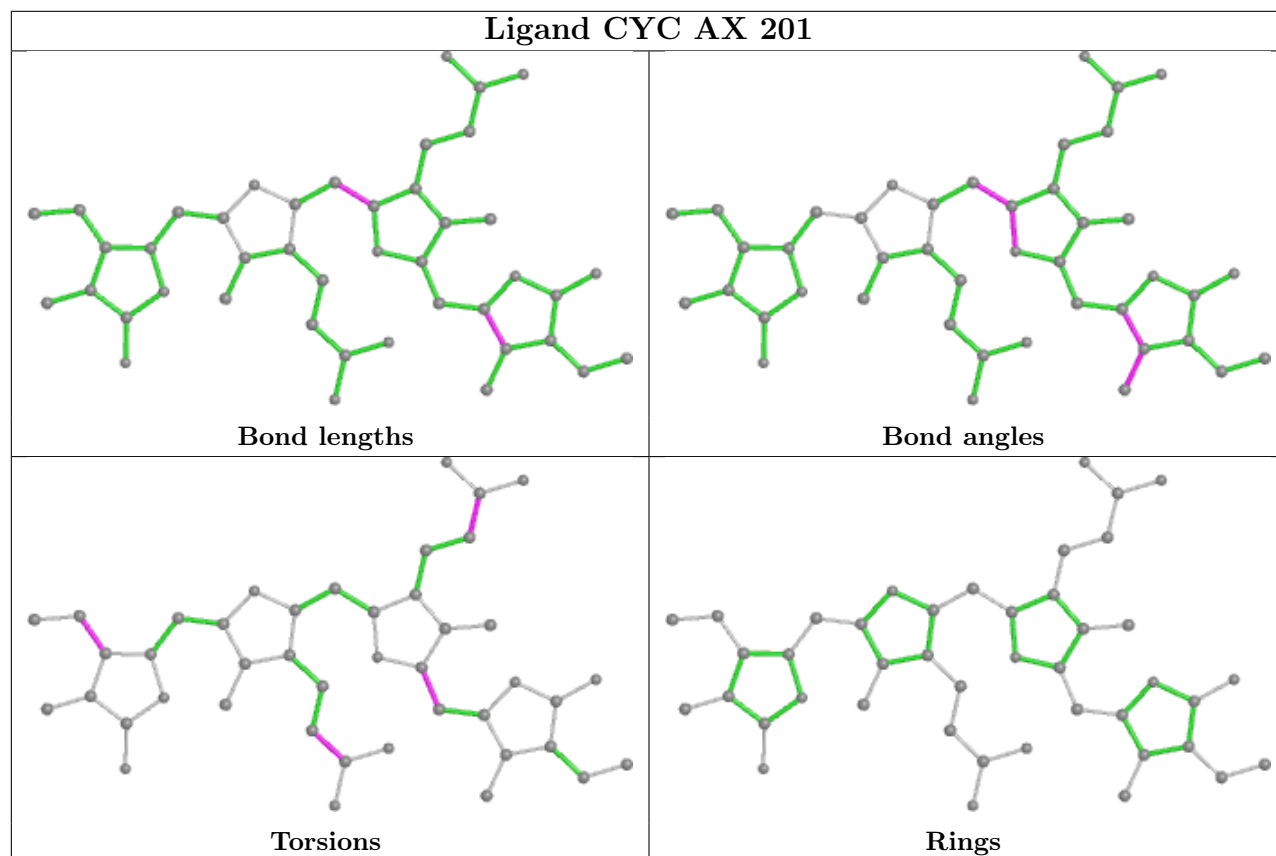
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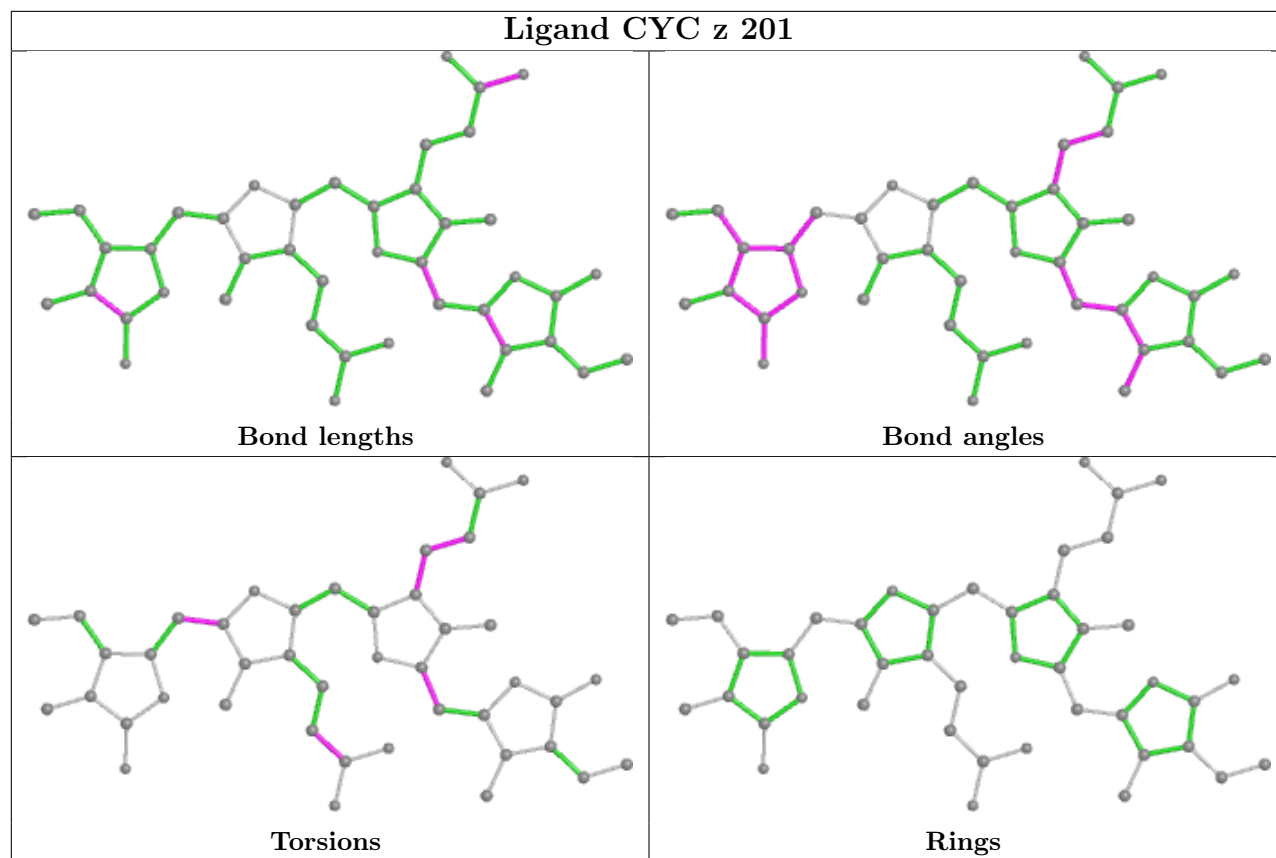
Ligand CYC AS 201



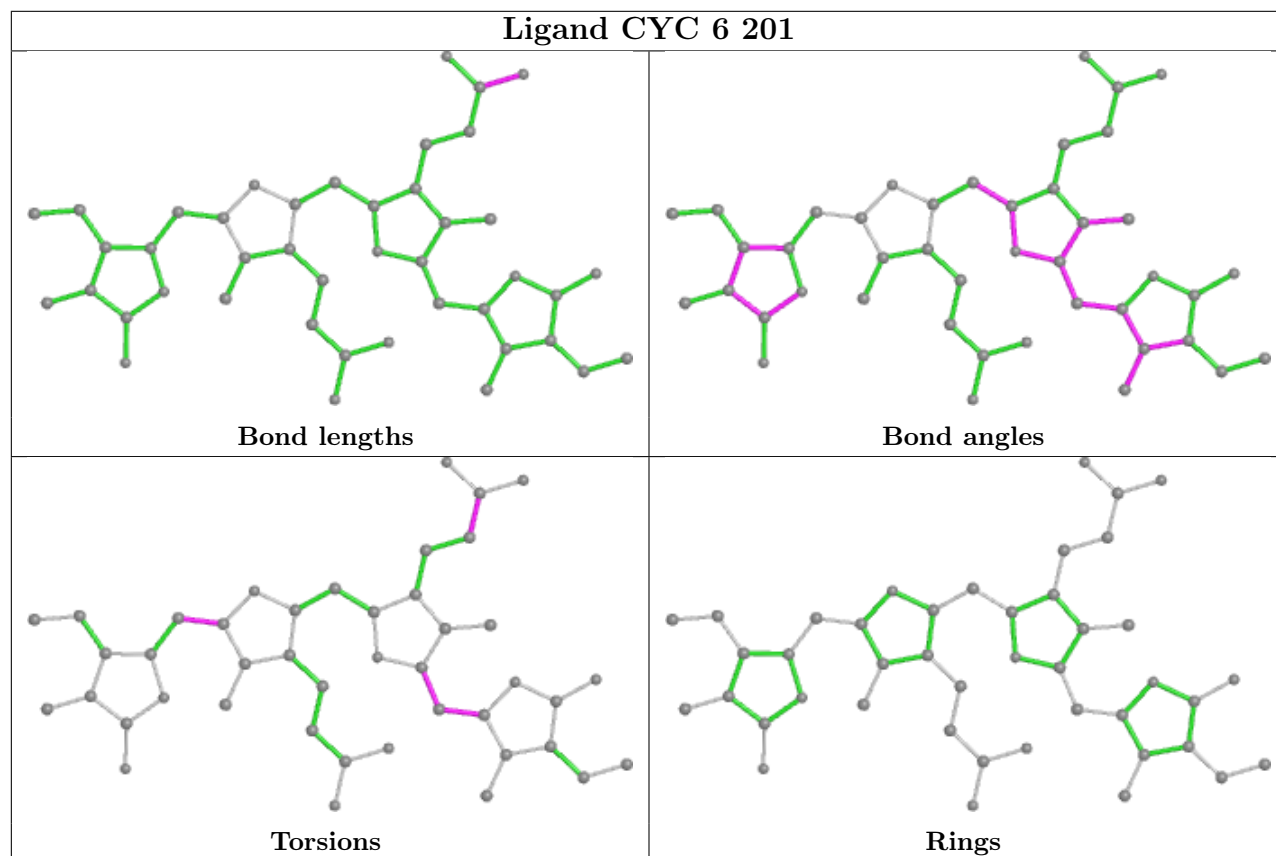
Ligand CYC AX 201



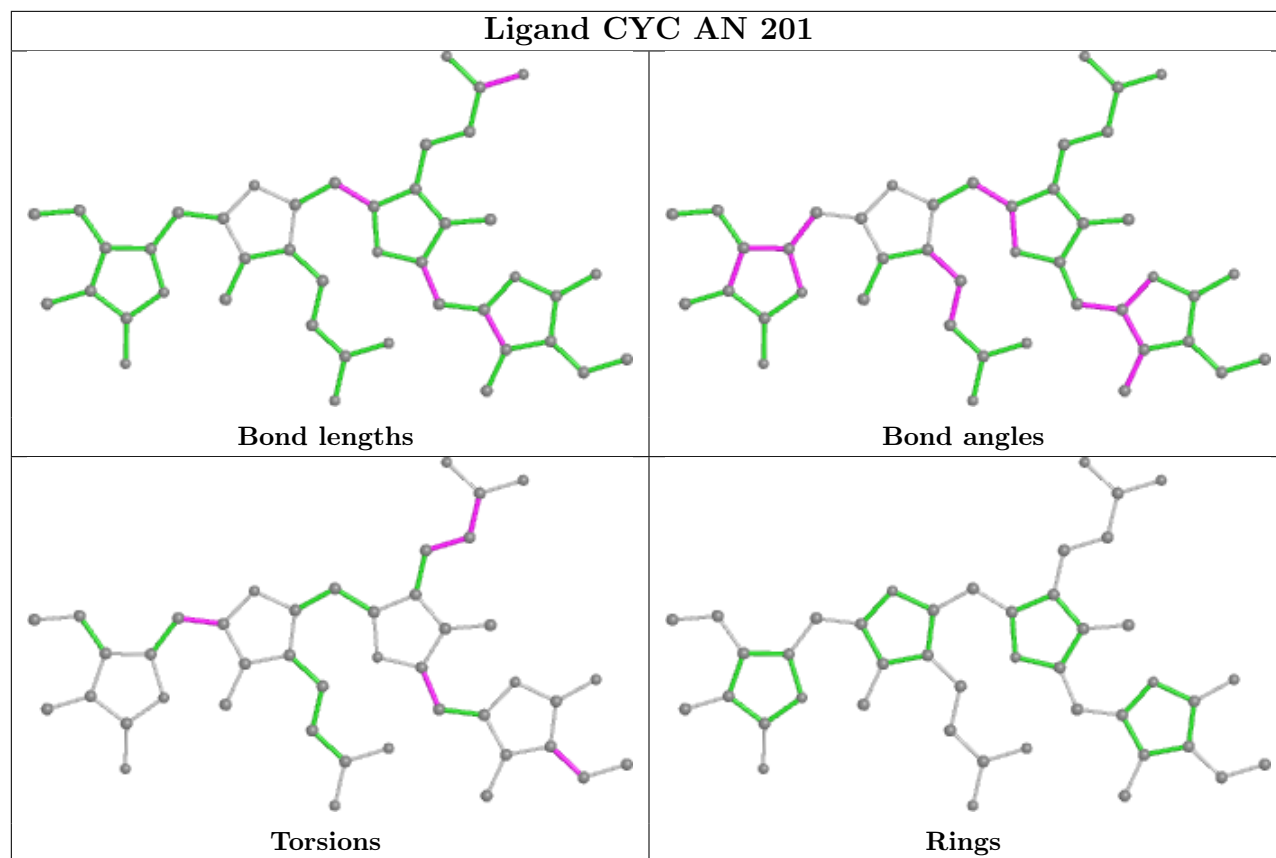
Ligand CYC z 201



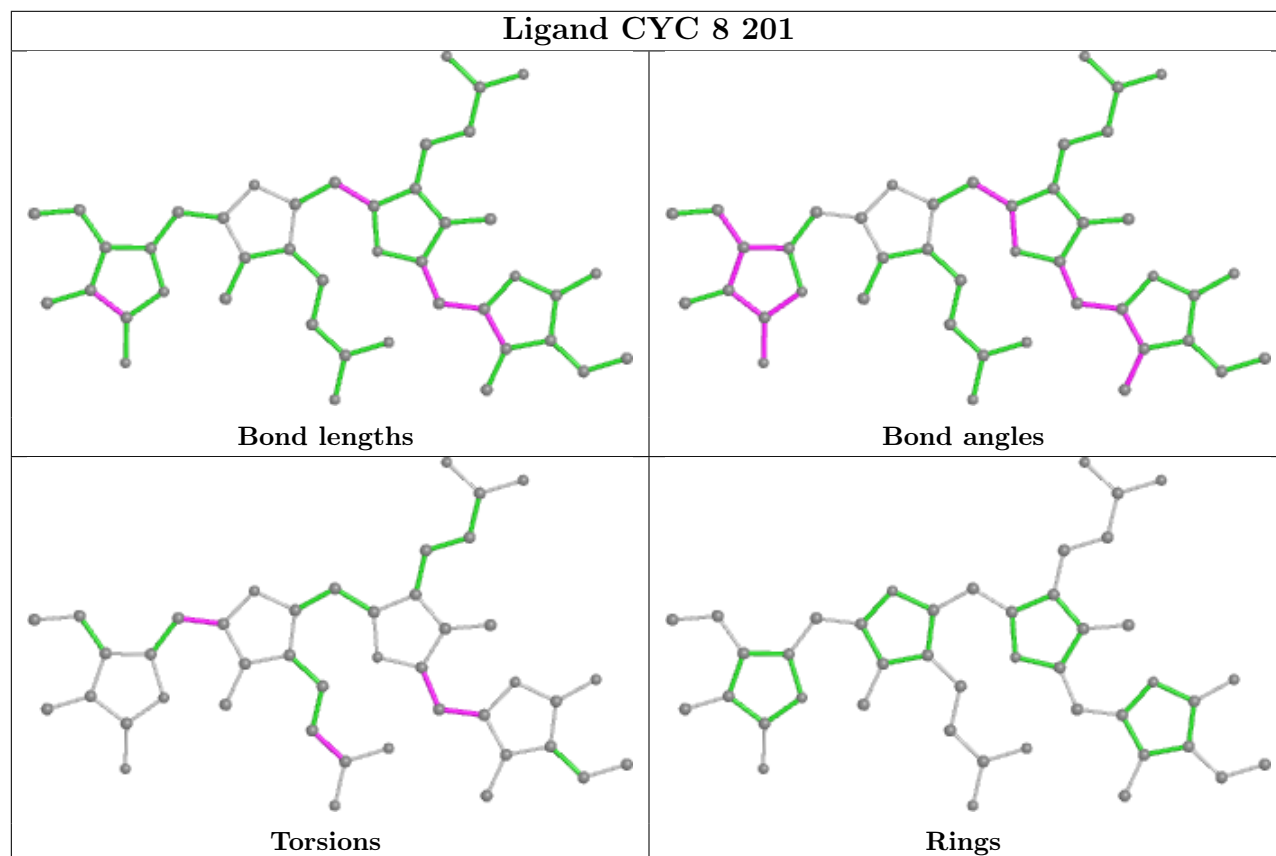
Ligand CYC 6 201

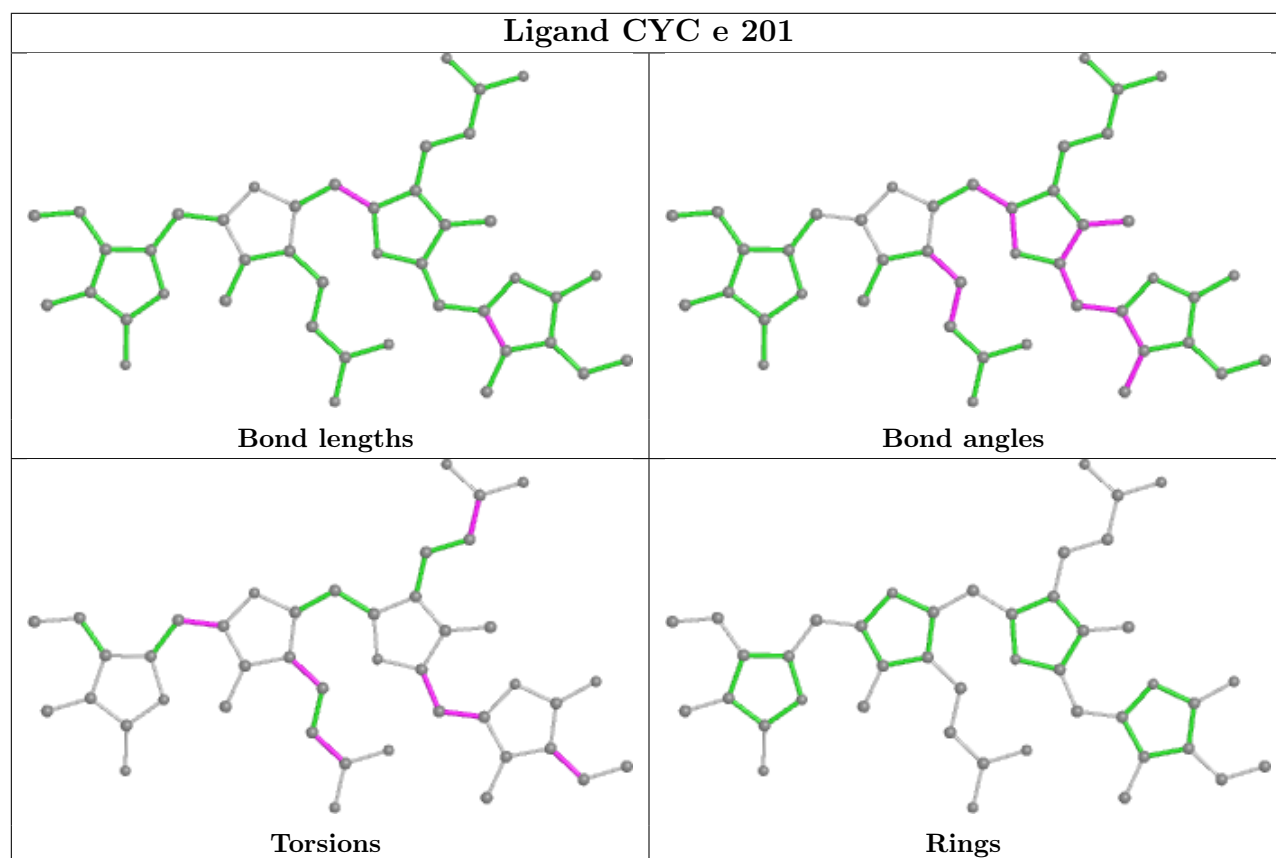
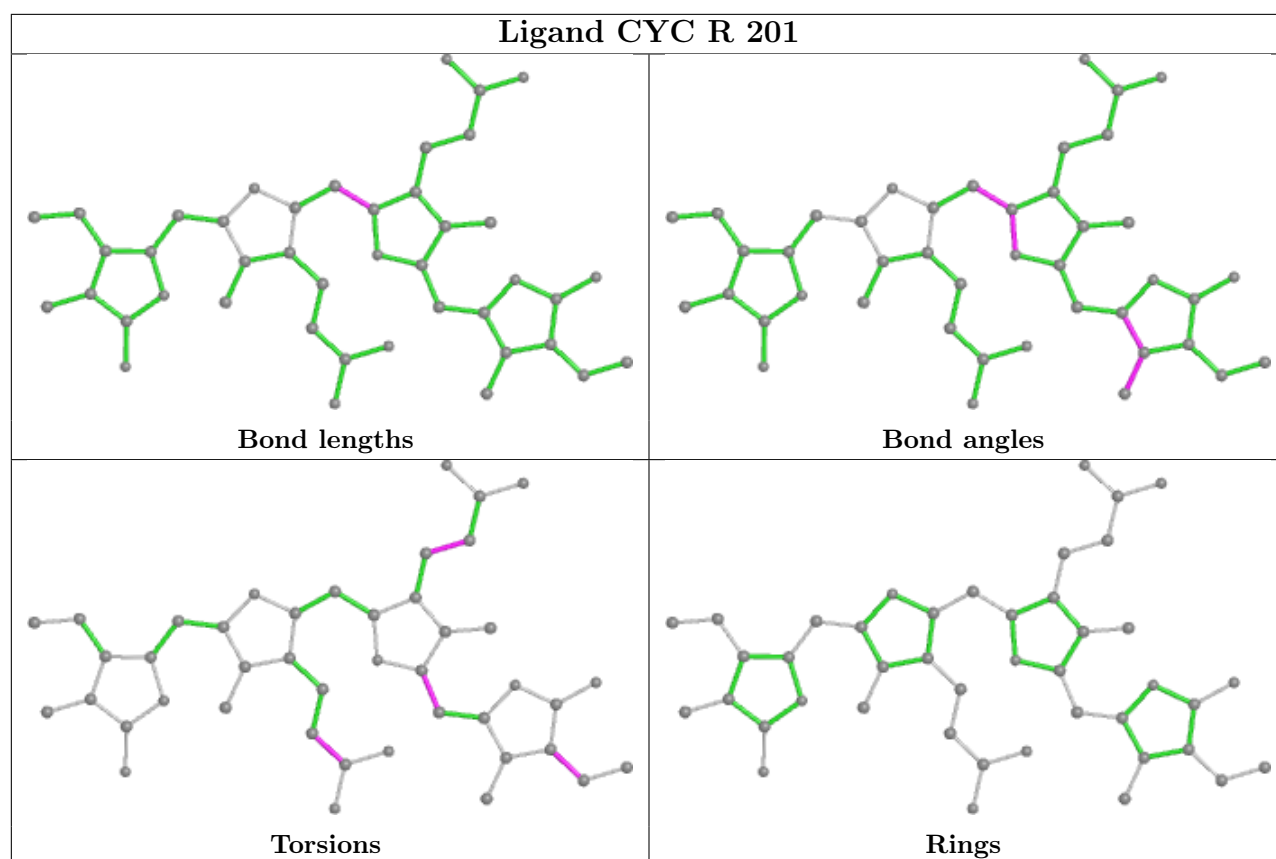


Ligand CYC AN 201

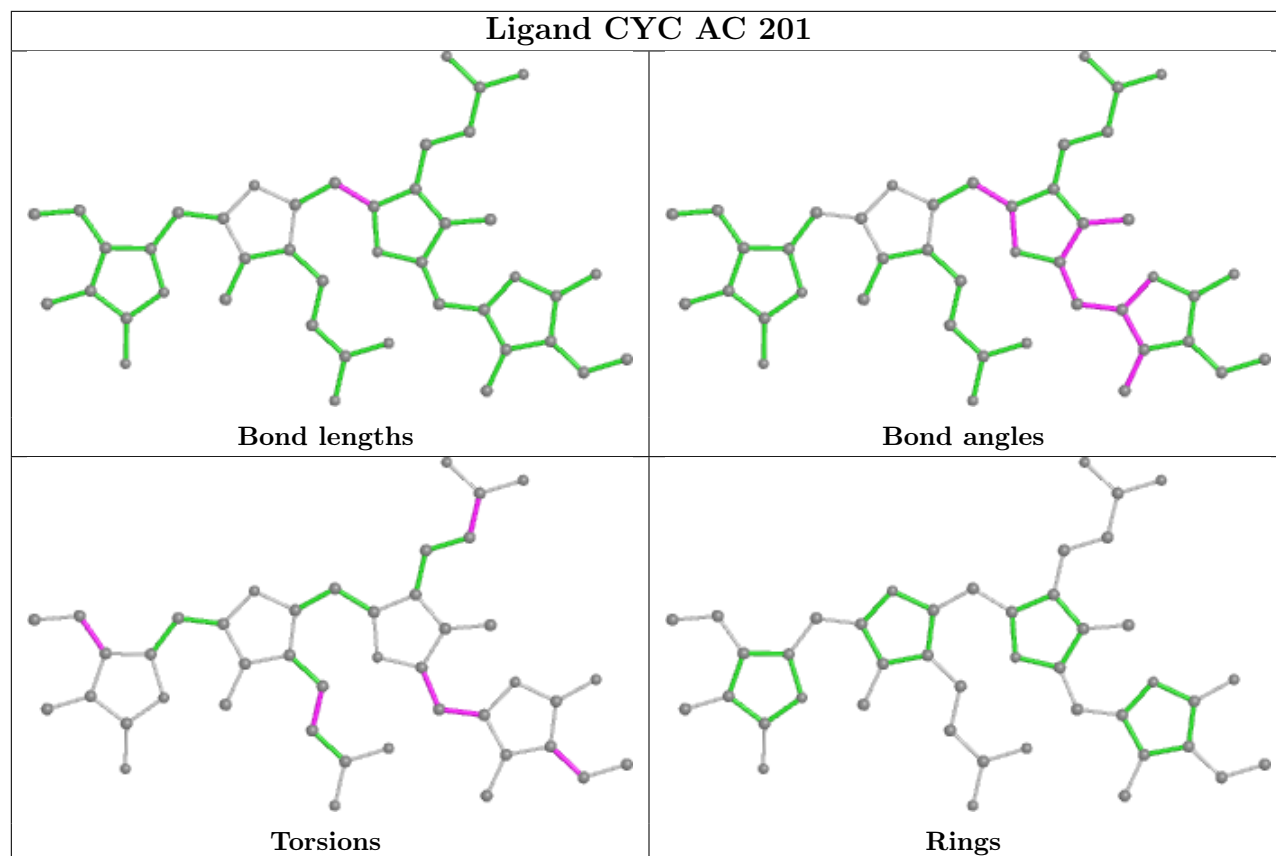


Ligand CYC 8 201

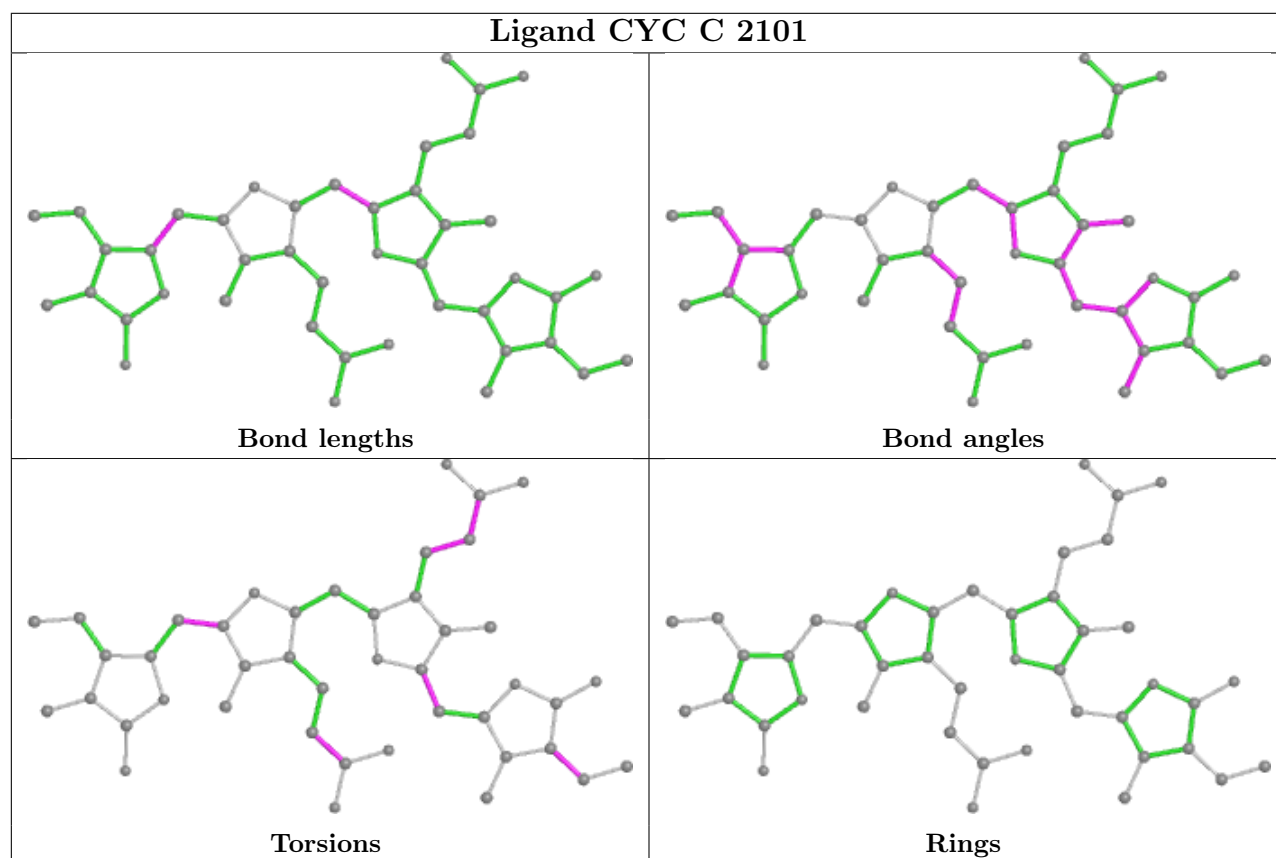




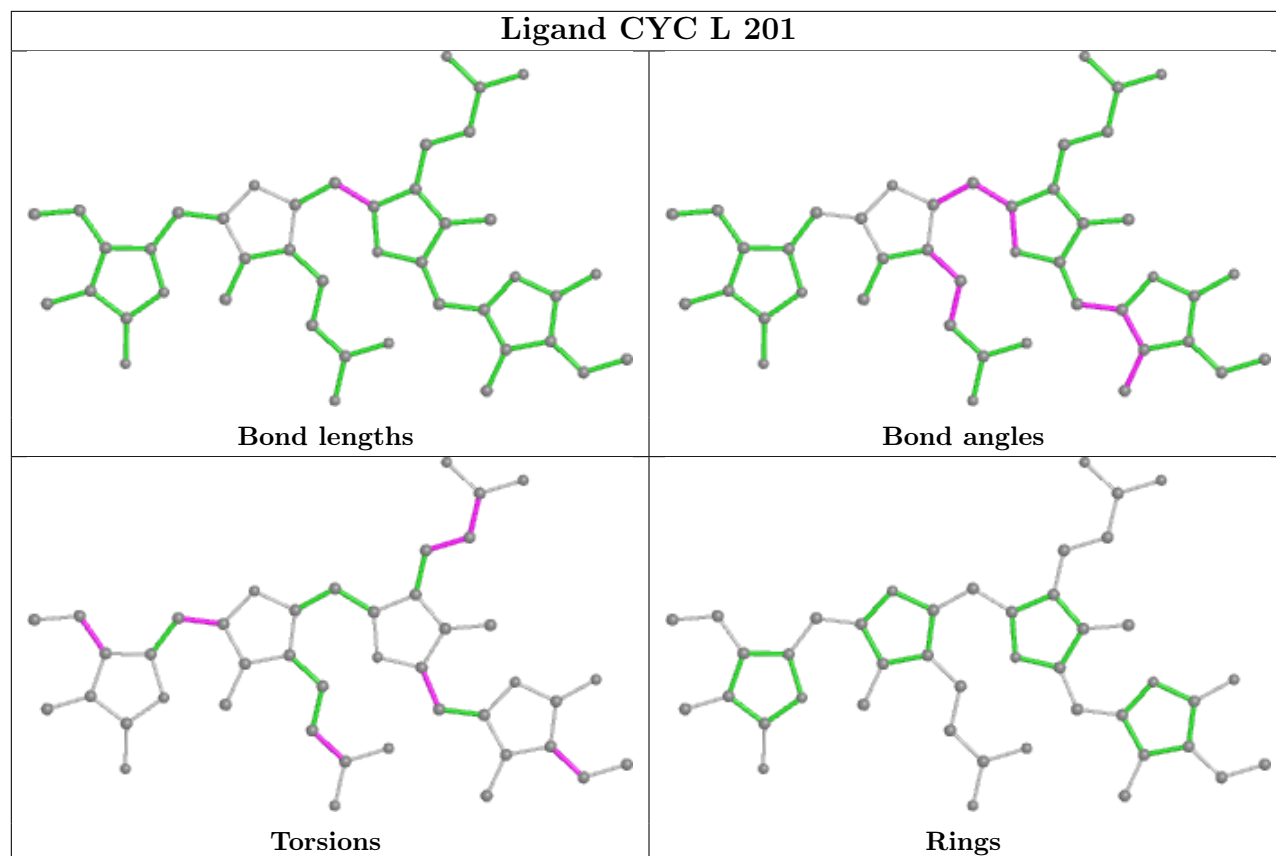
Ligand CYC AC 201



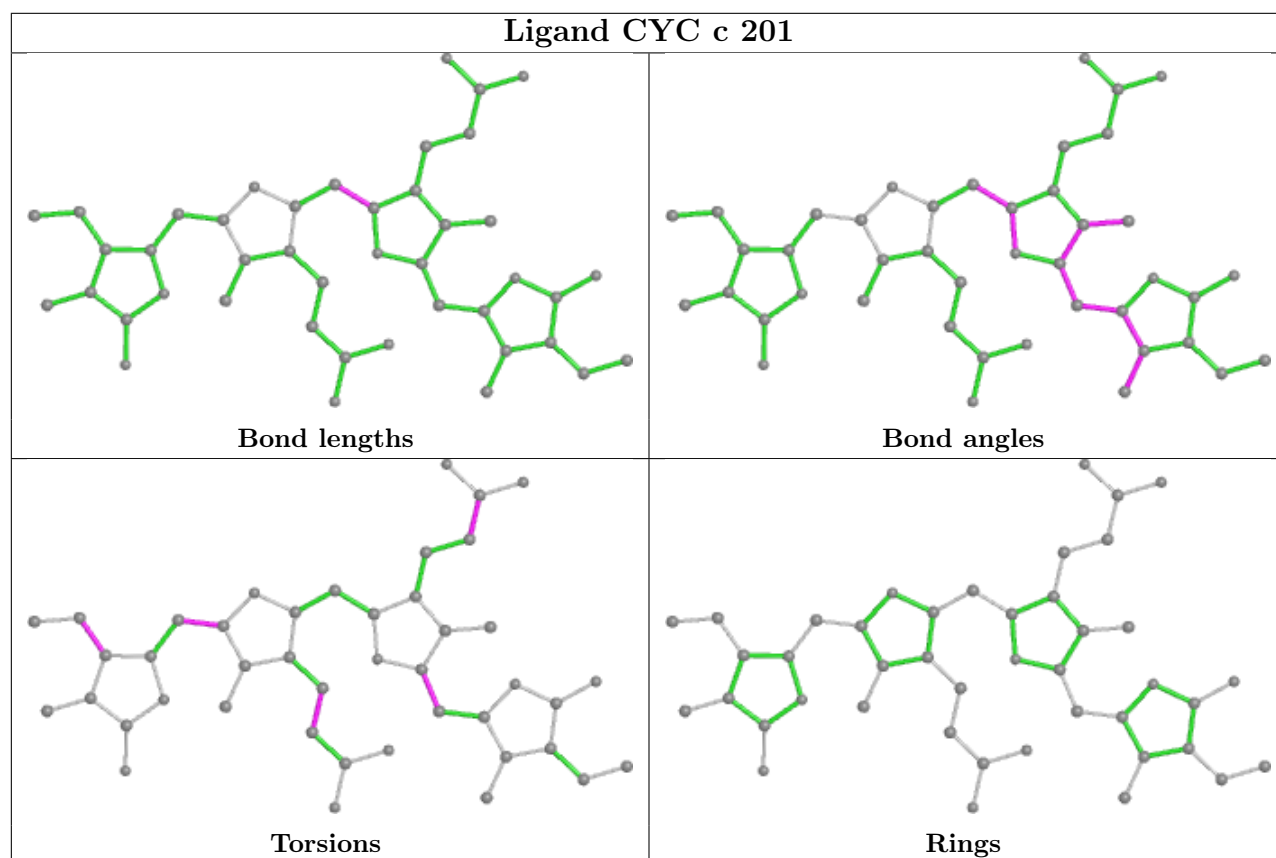
Ligand CYC C 2101



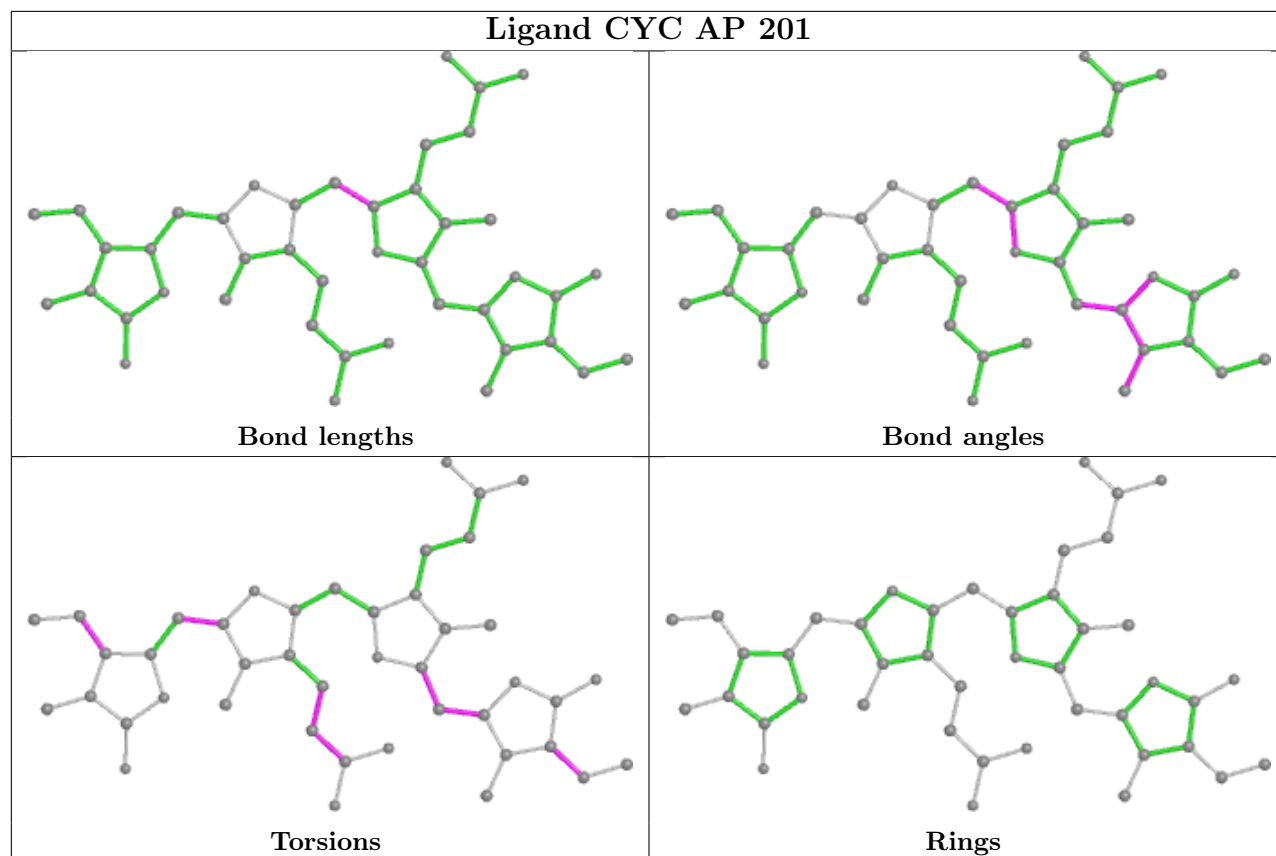
Ligand CYC L 201



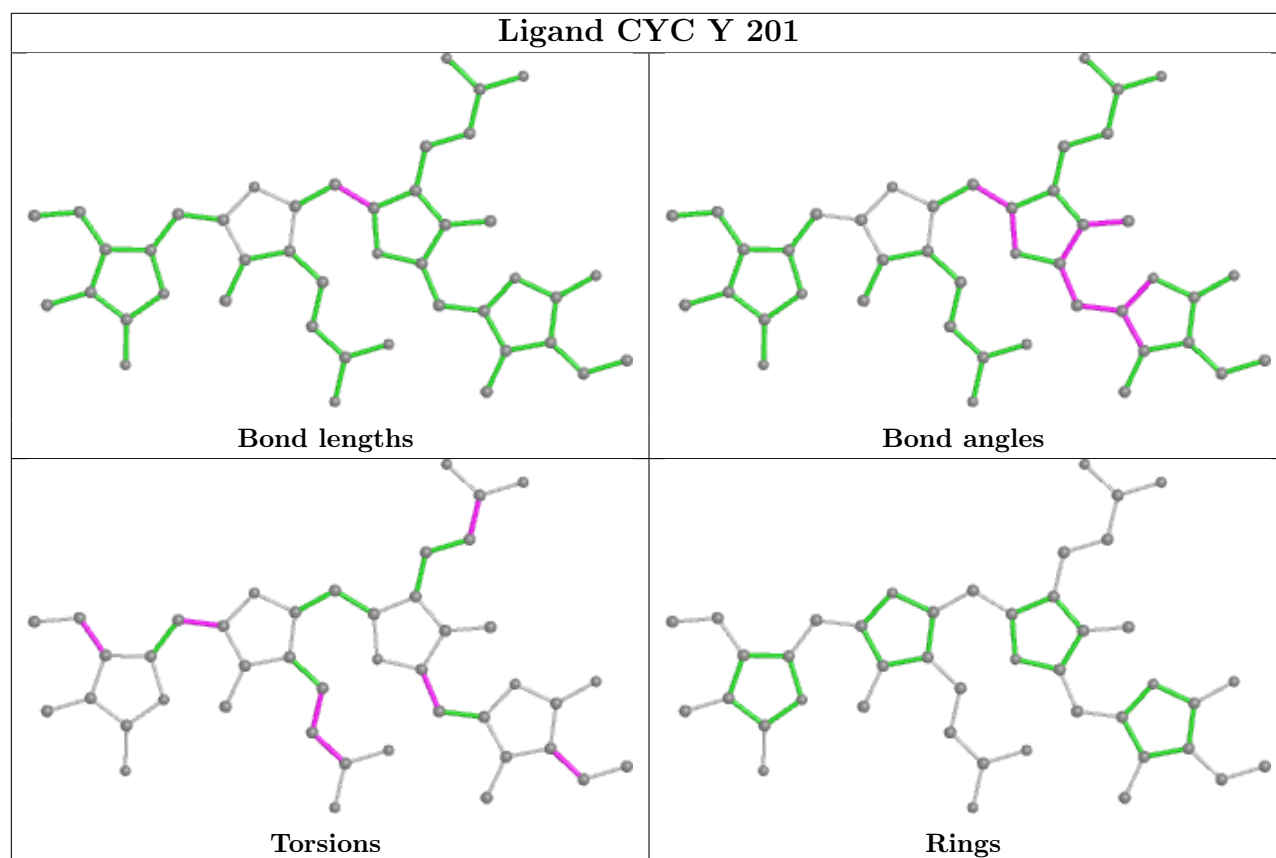
Ligand CYC c 201



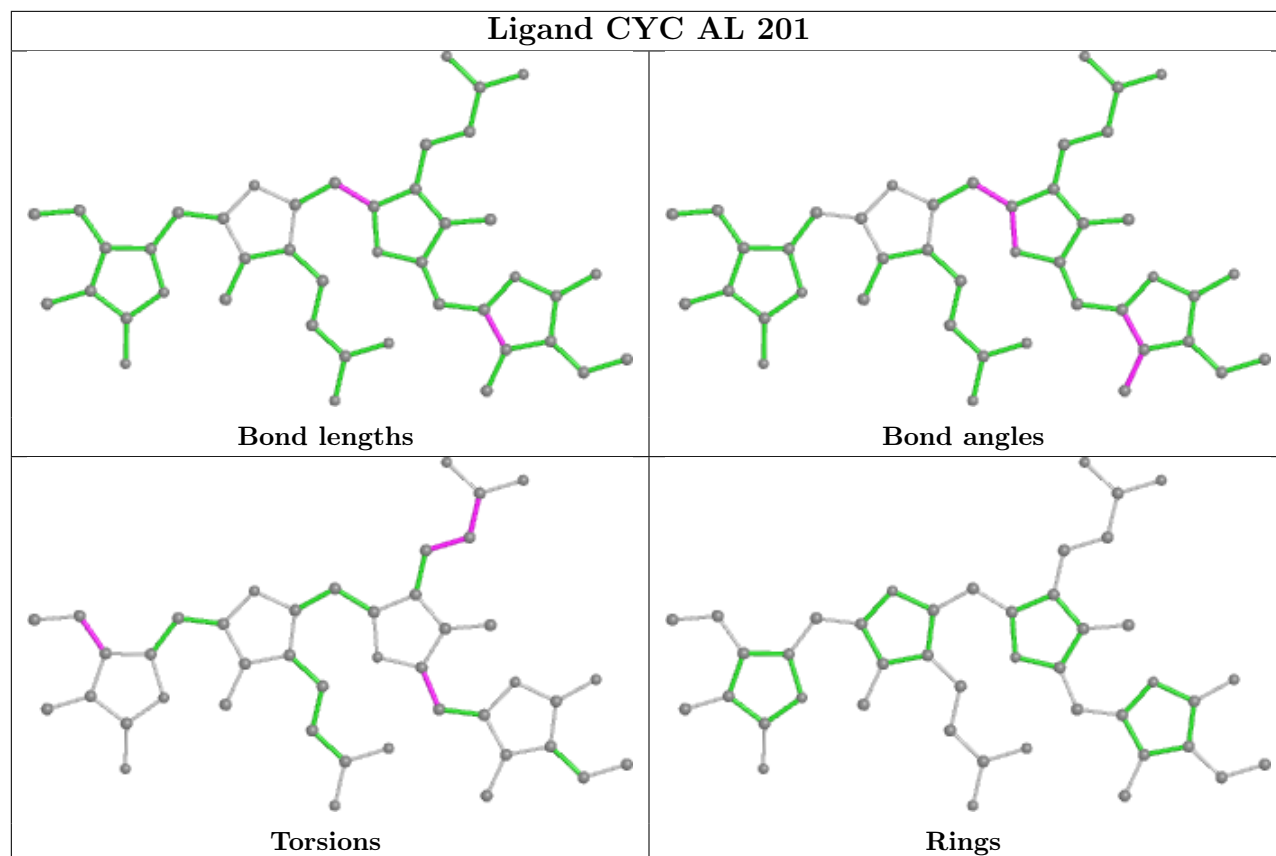
Ligand CYC AP 201



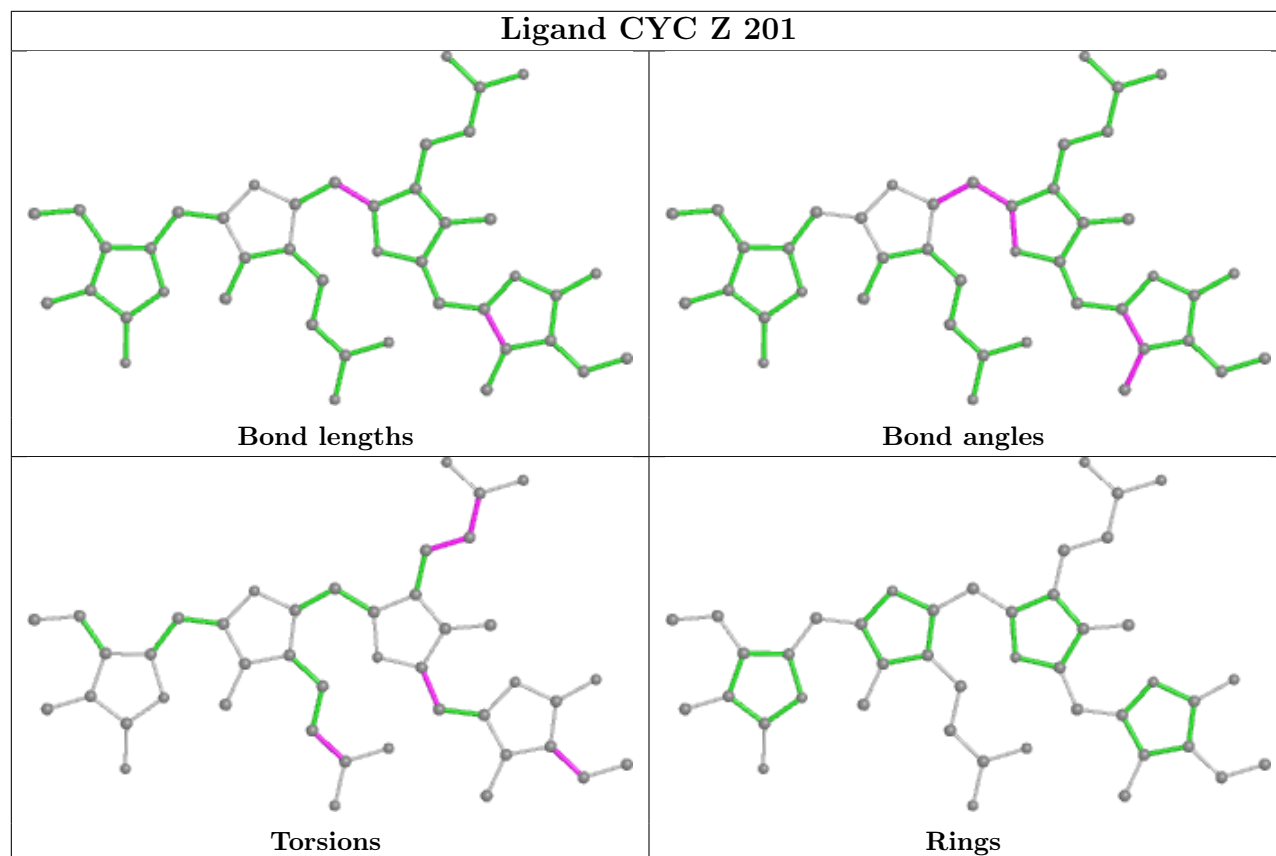
Ligand CYC Y 201



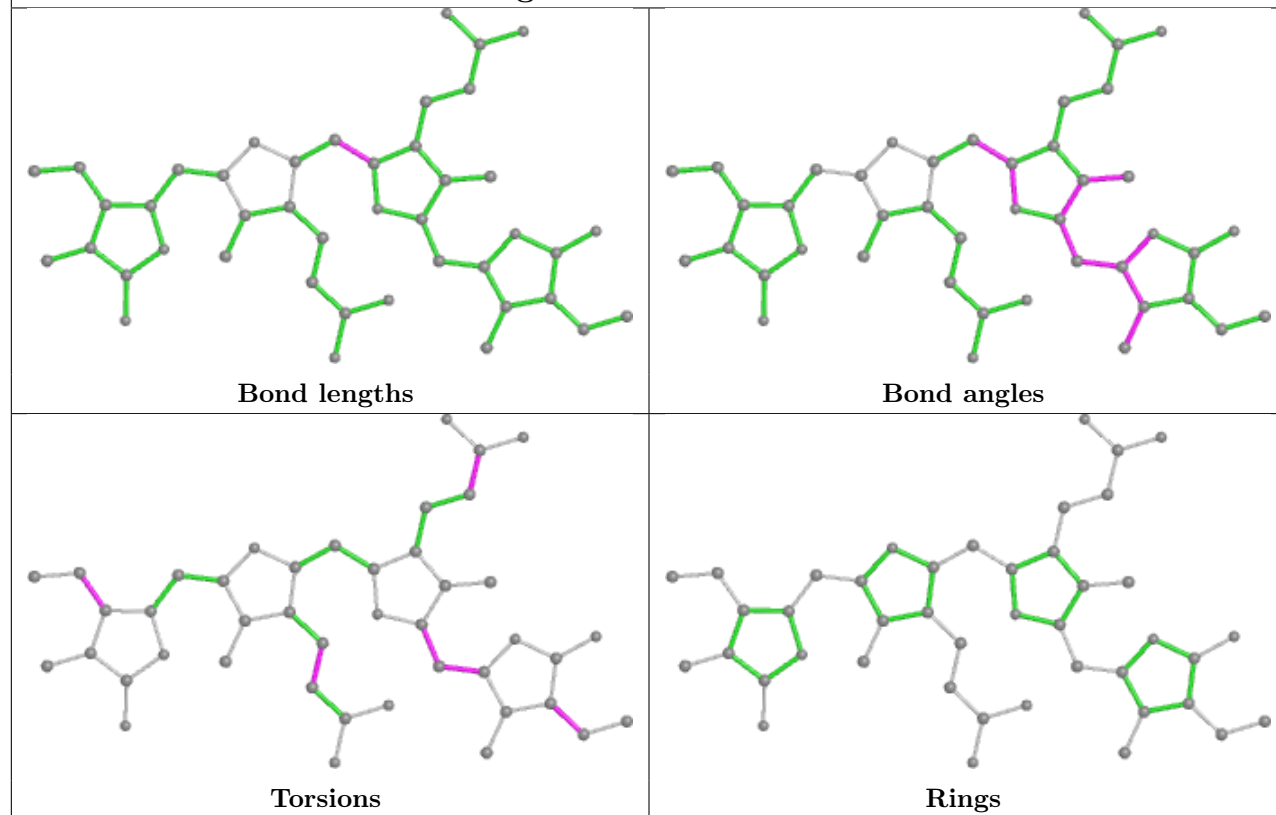
Ligand CYC AL 201



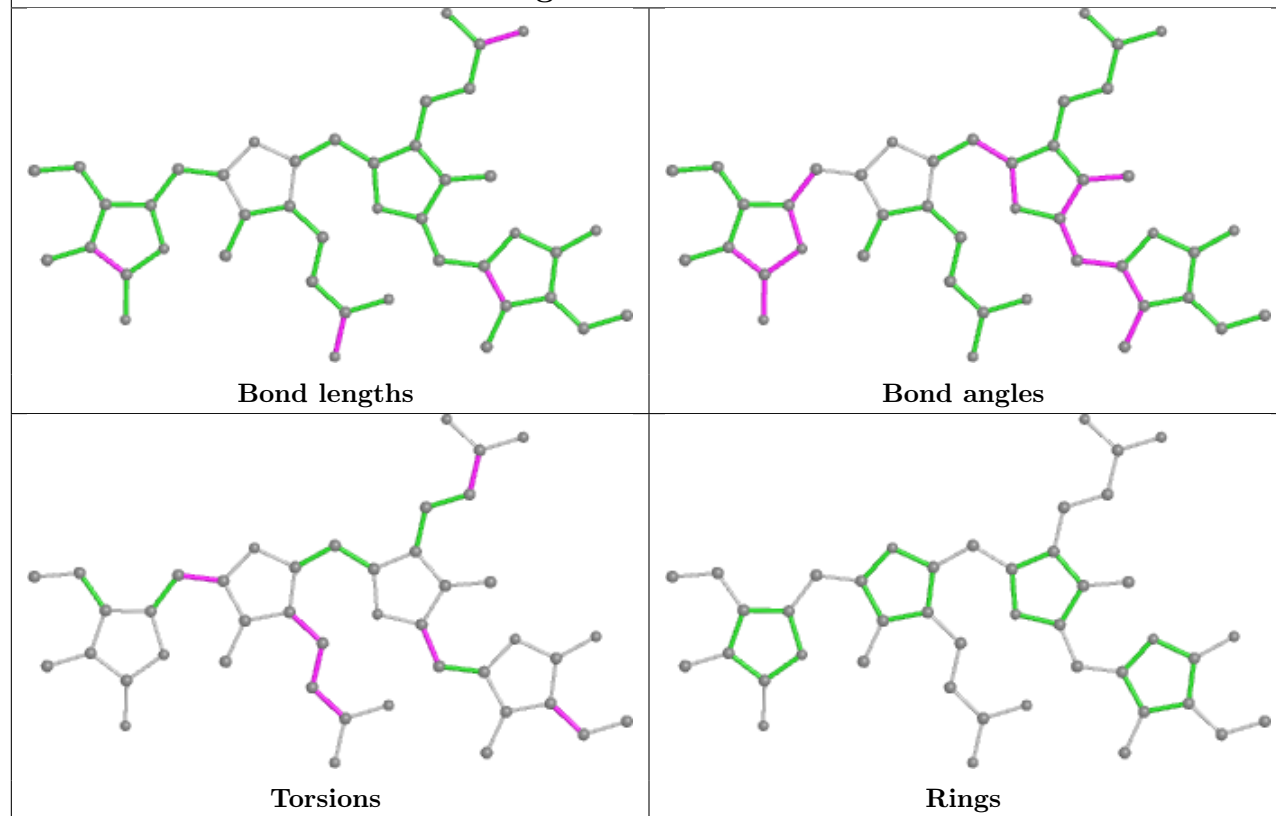
Ligand CYC Z 201

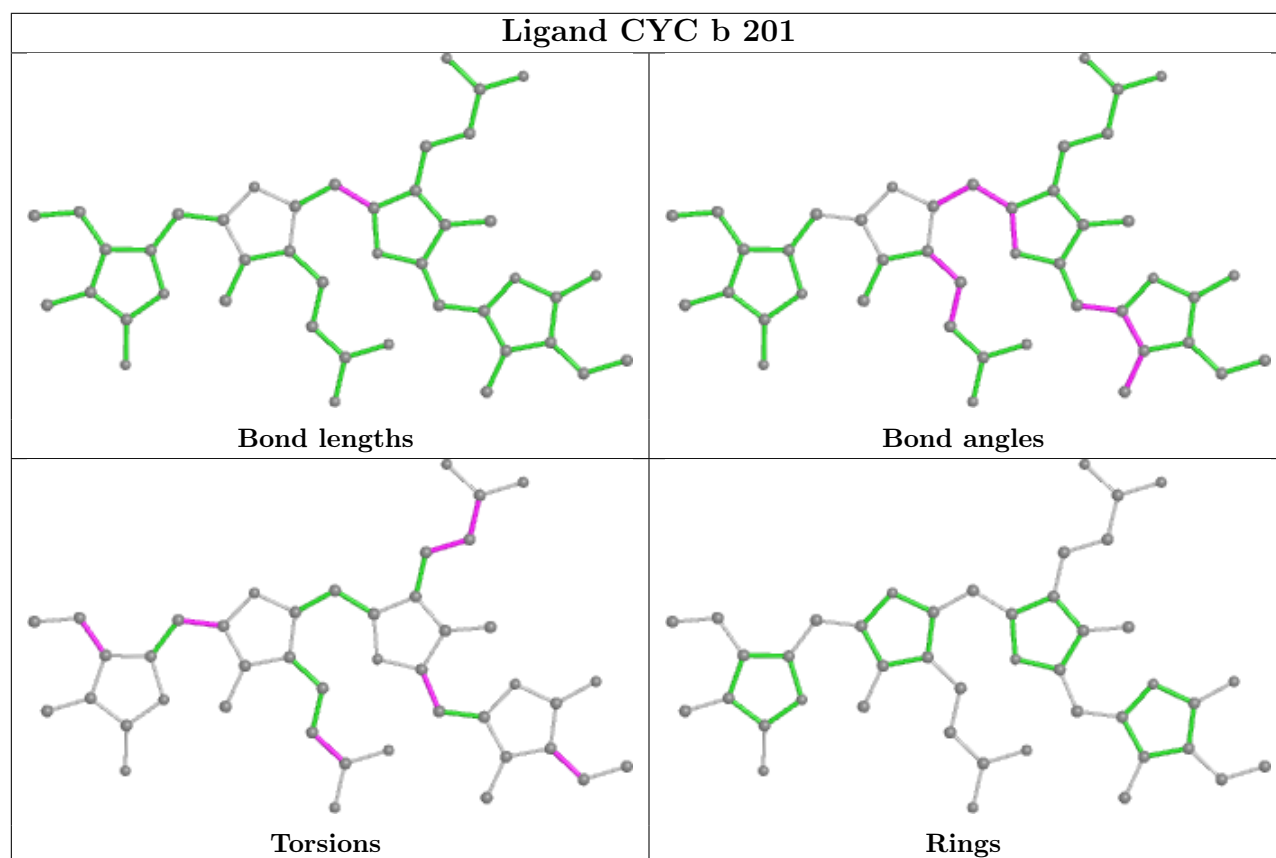
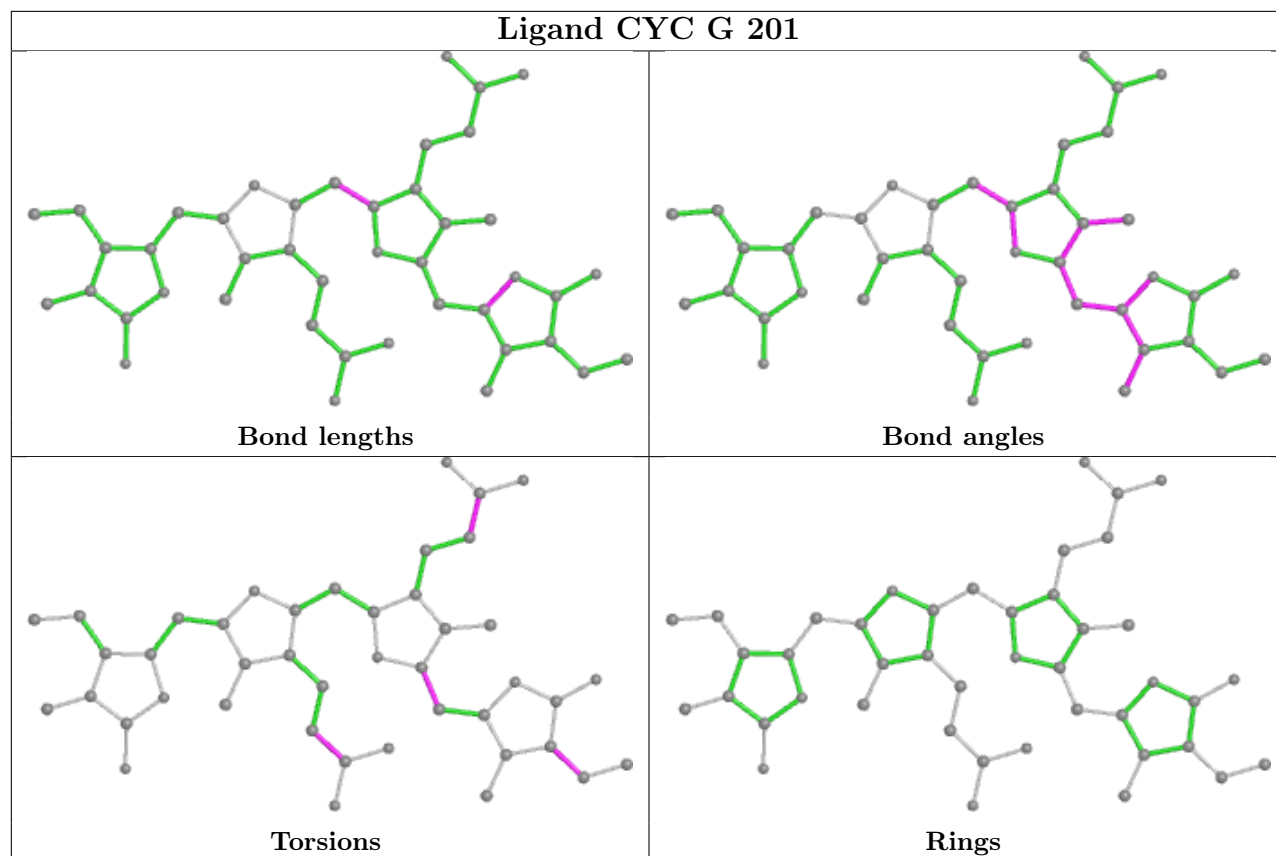


Ligand CYC AO 201

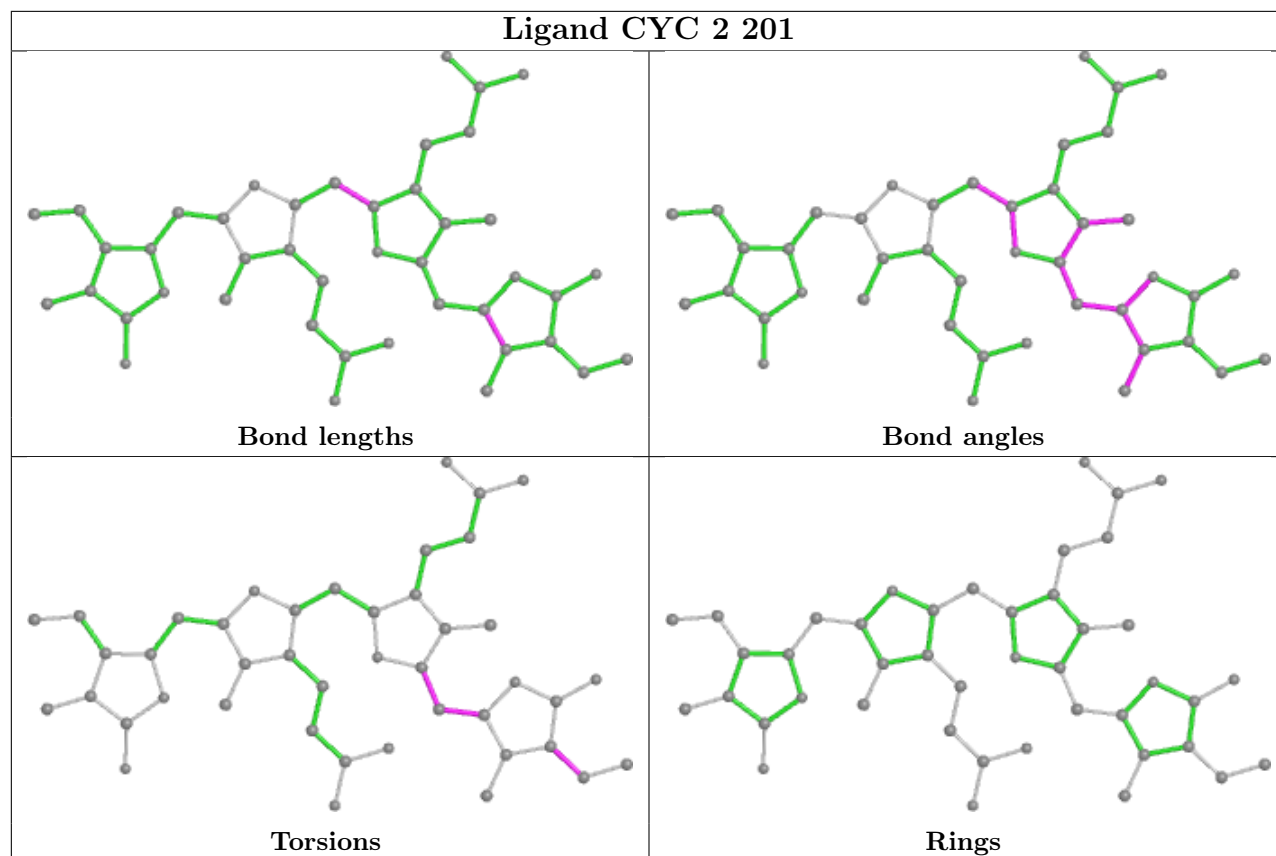


Ligand CYC t 201

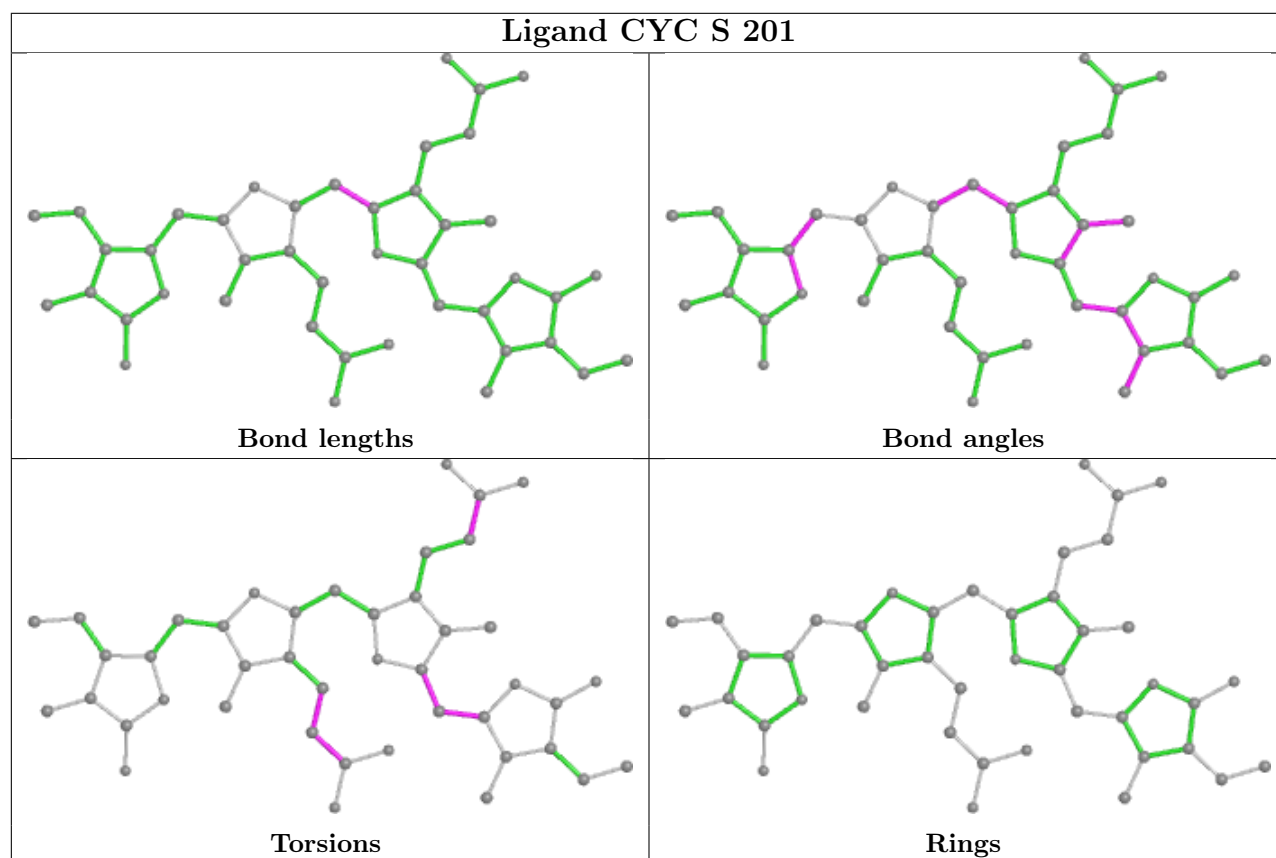


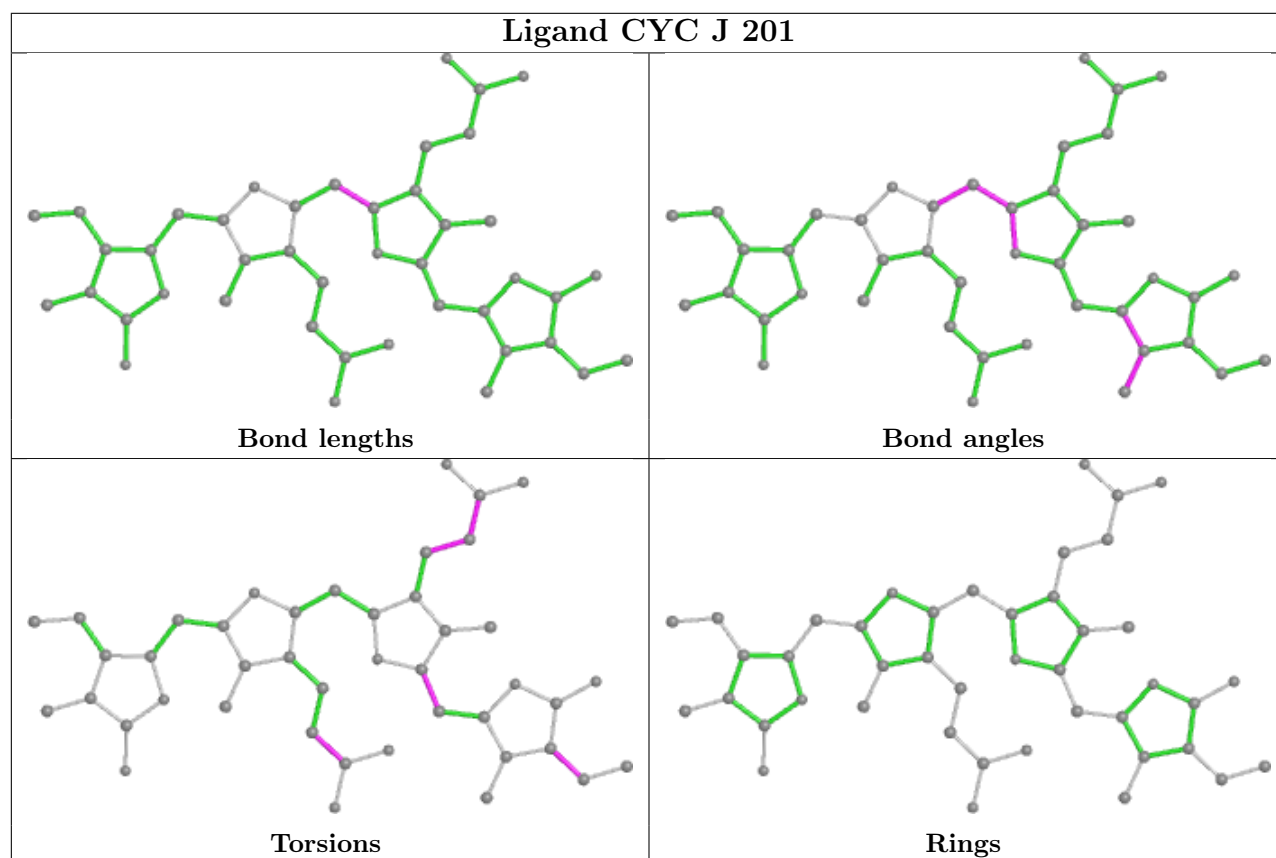
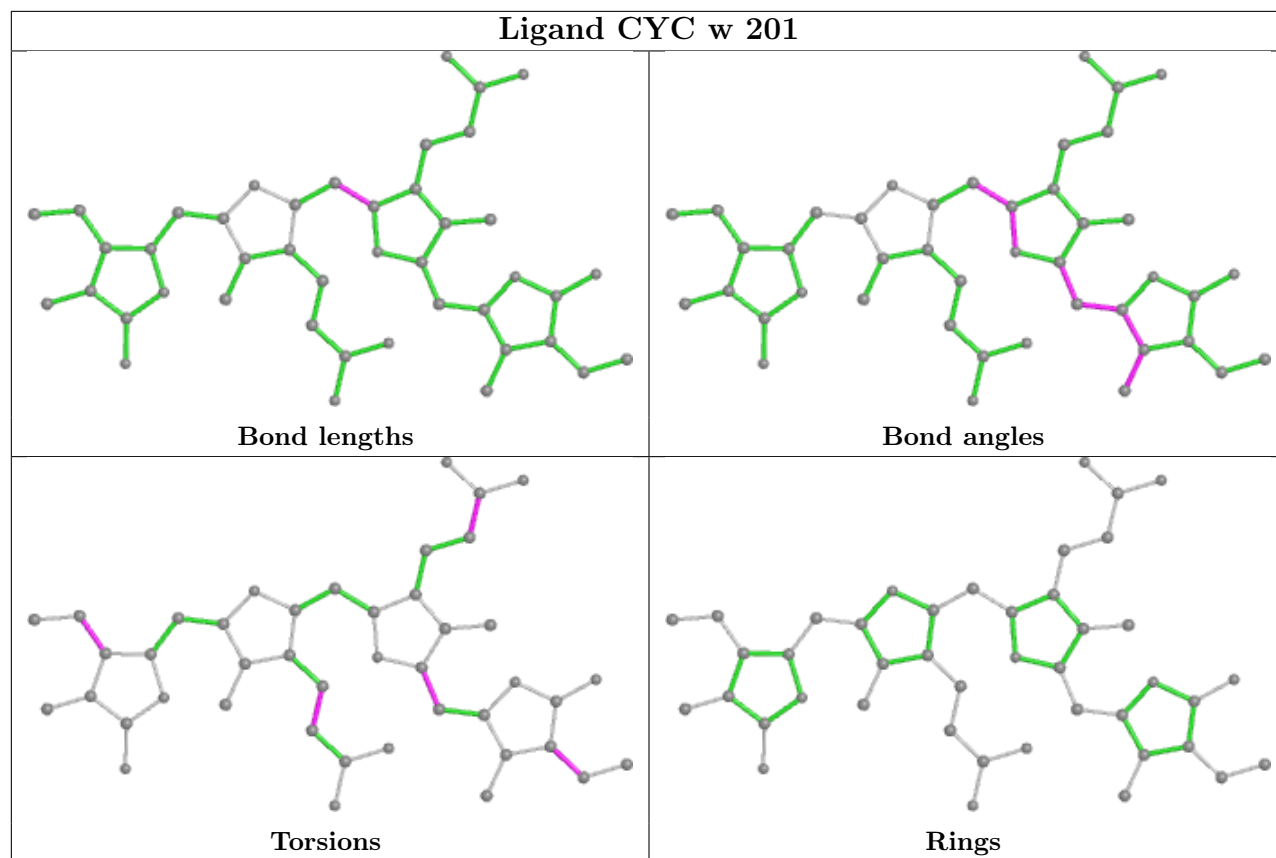


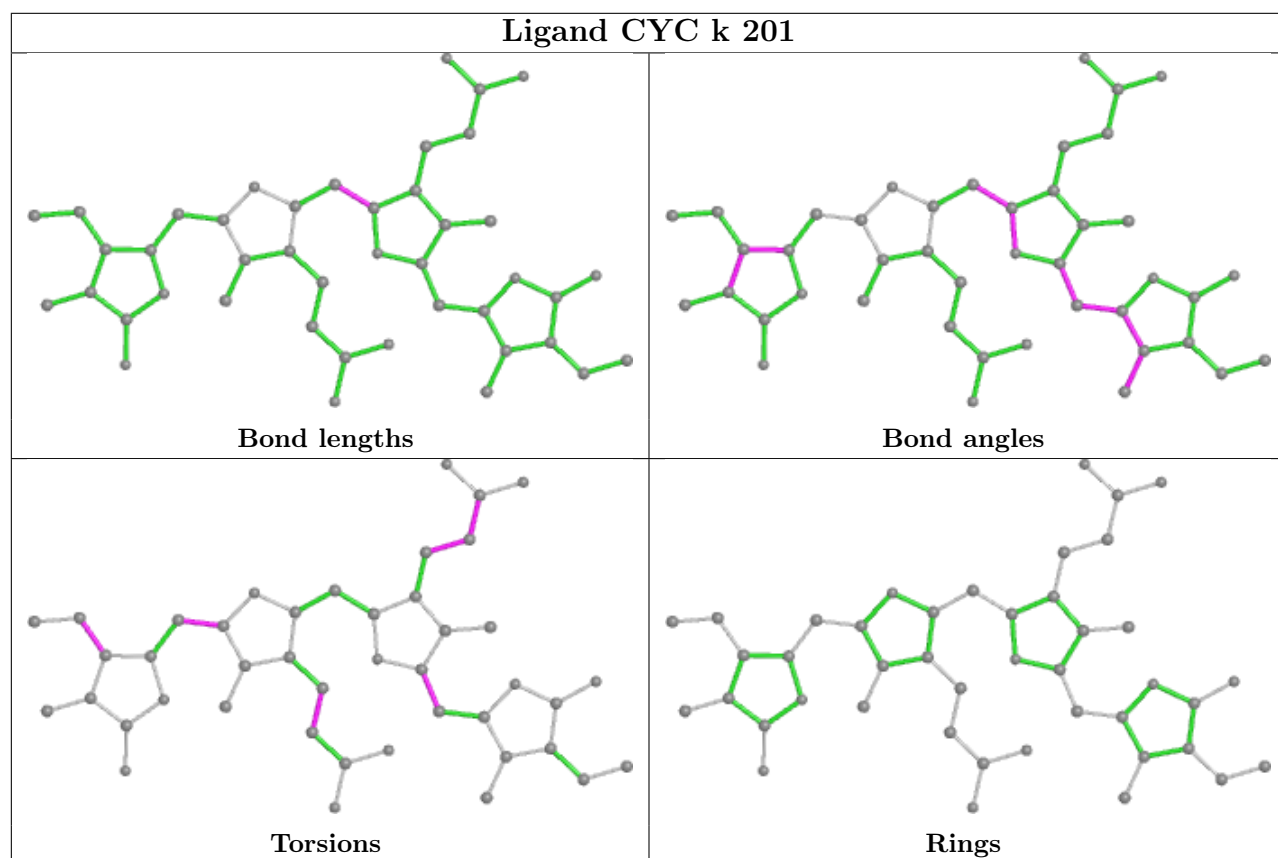
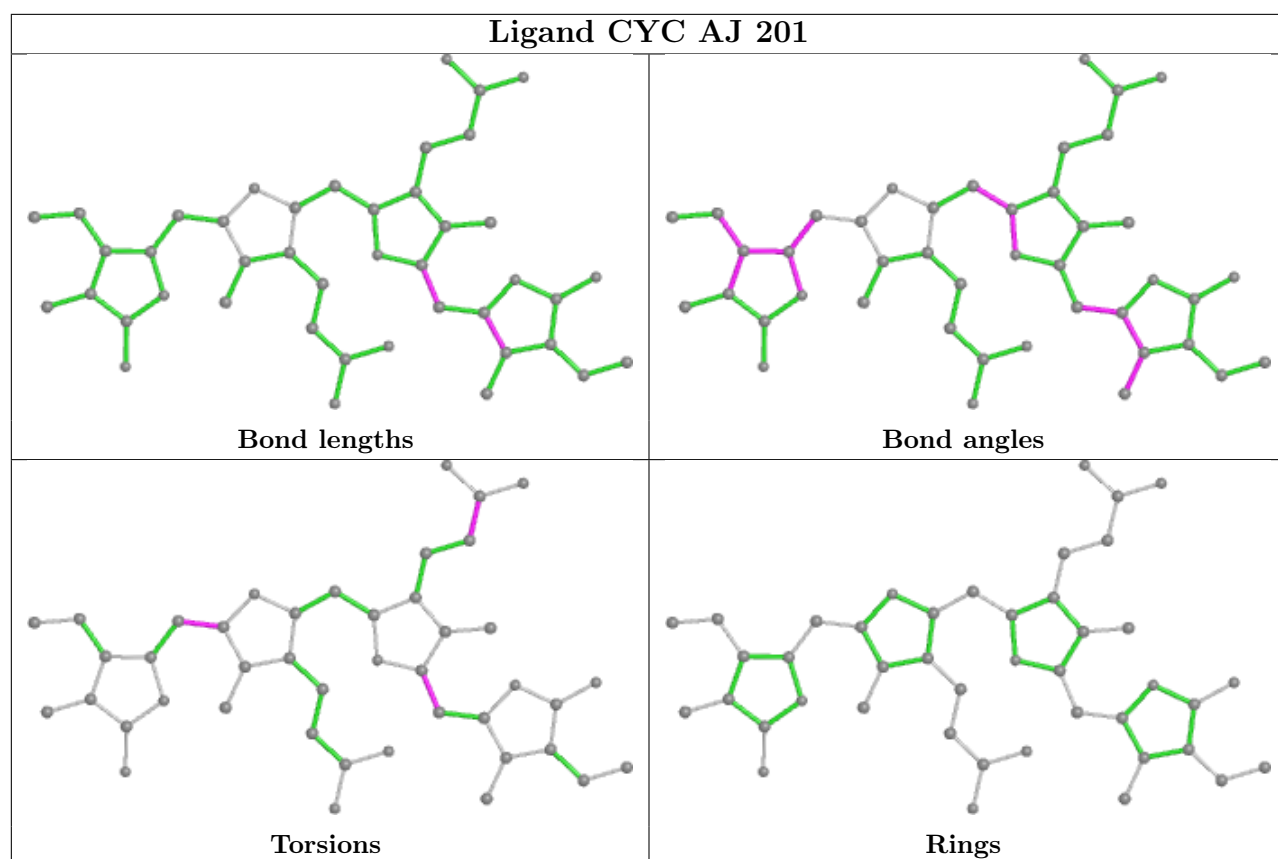
Ligand CYC 2 201



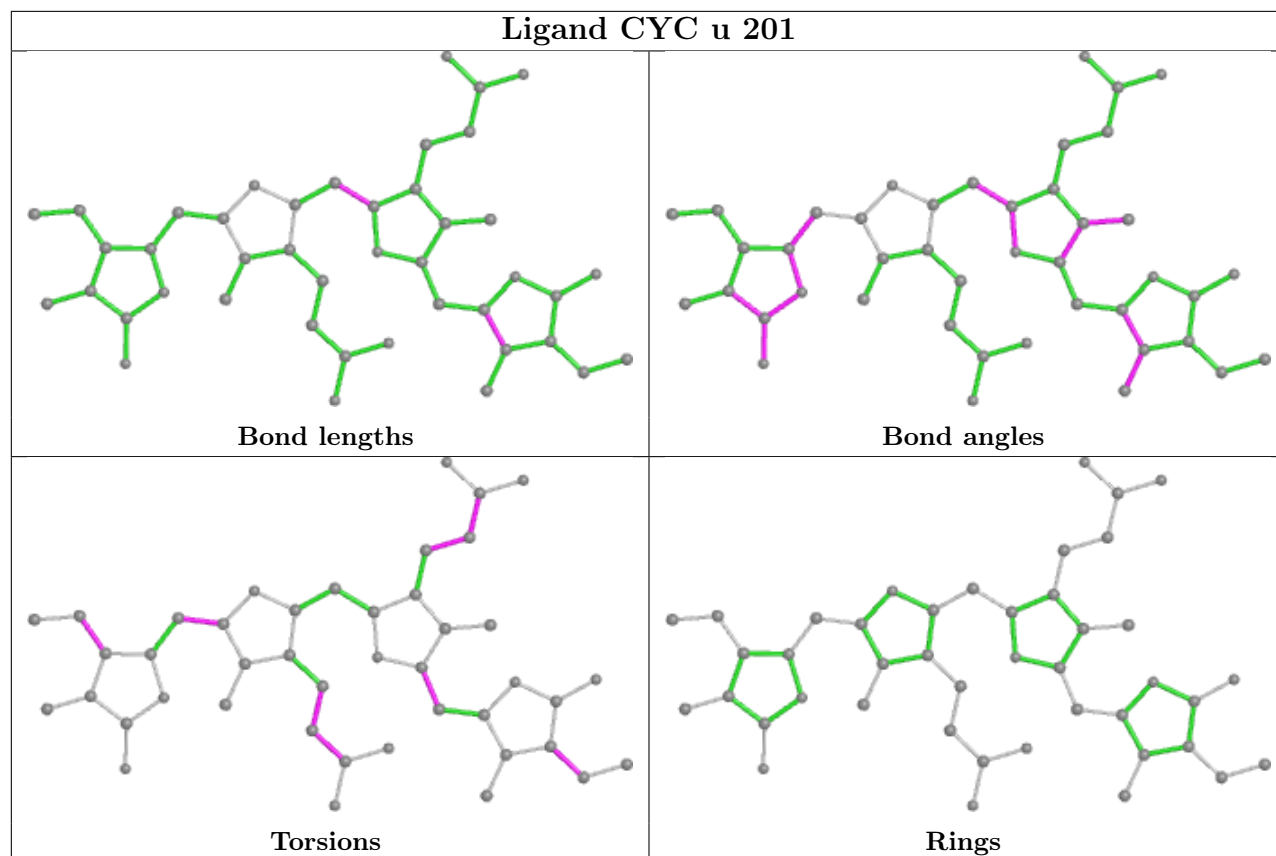
Ligand CYC S 201



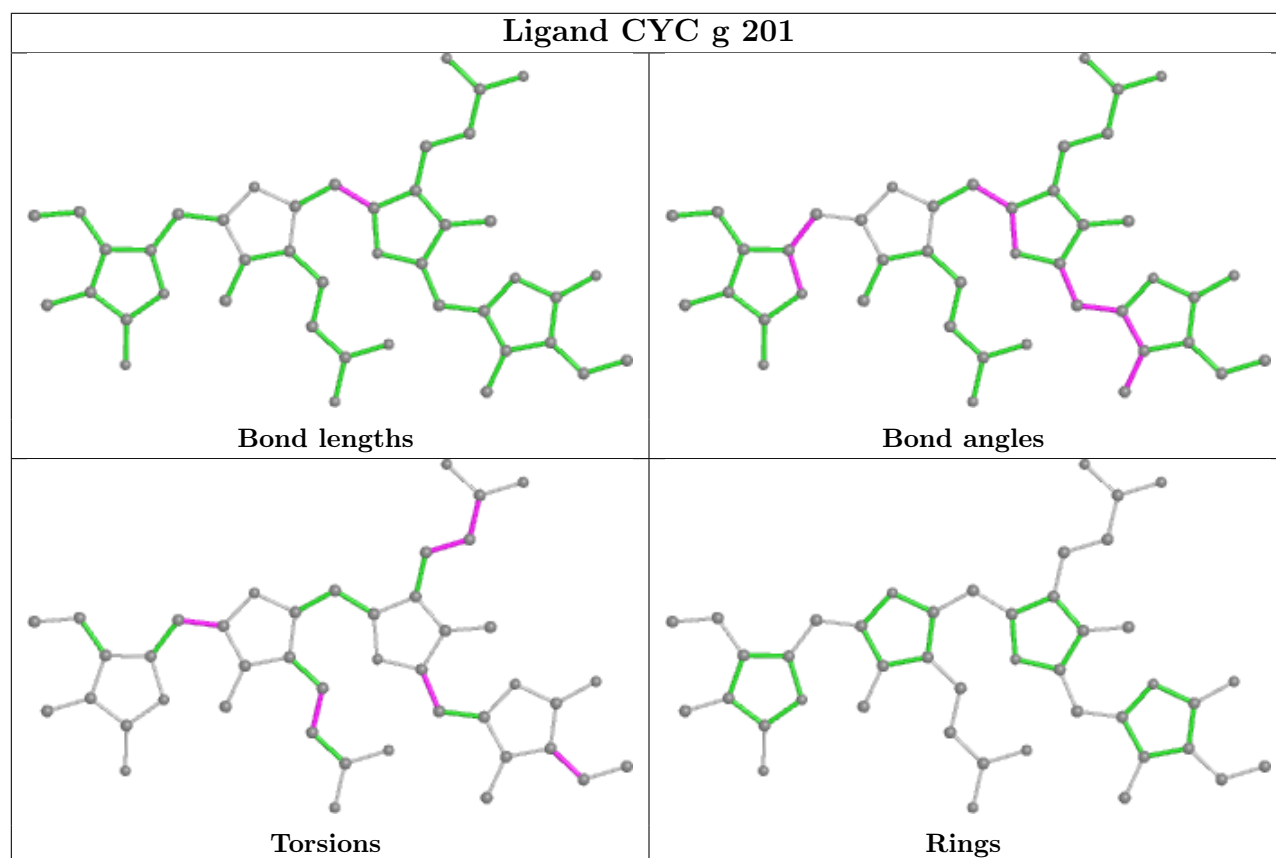


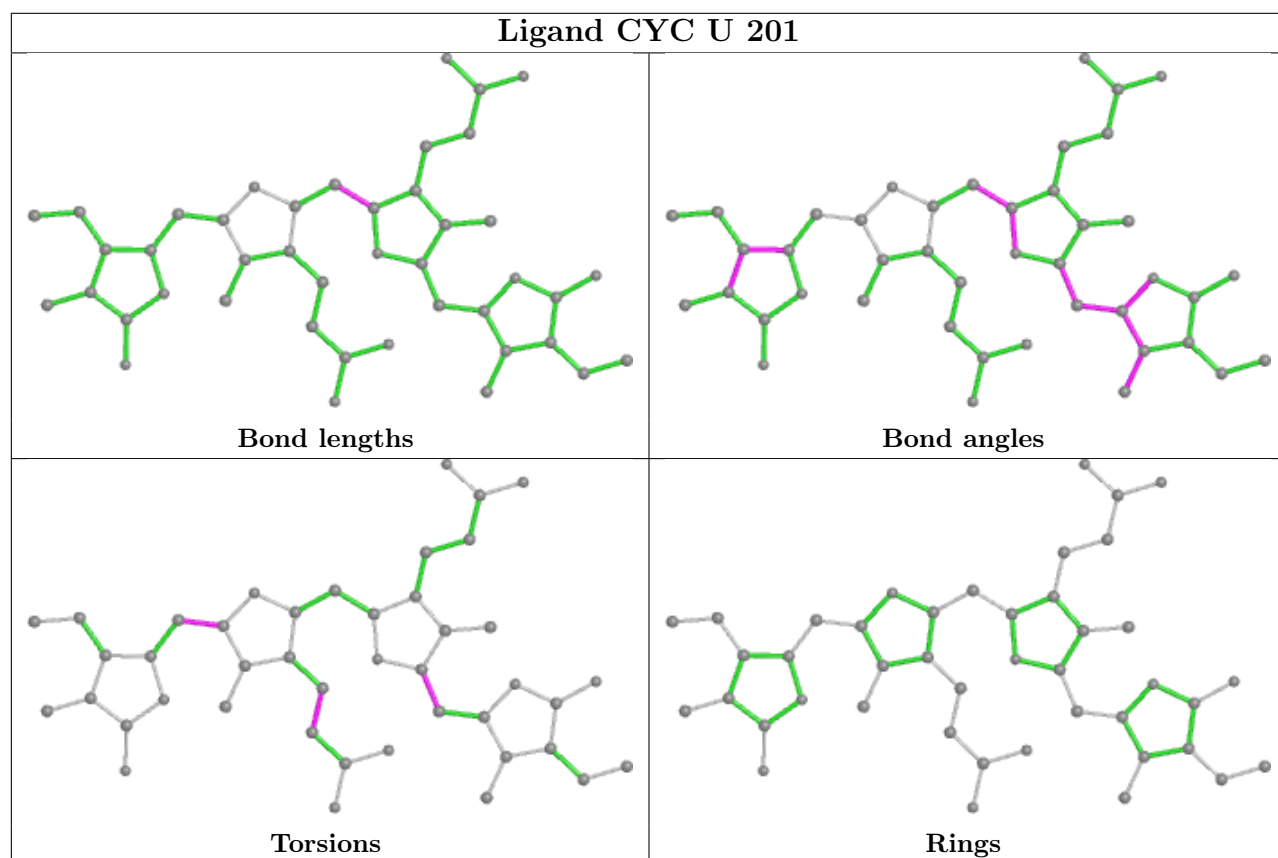
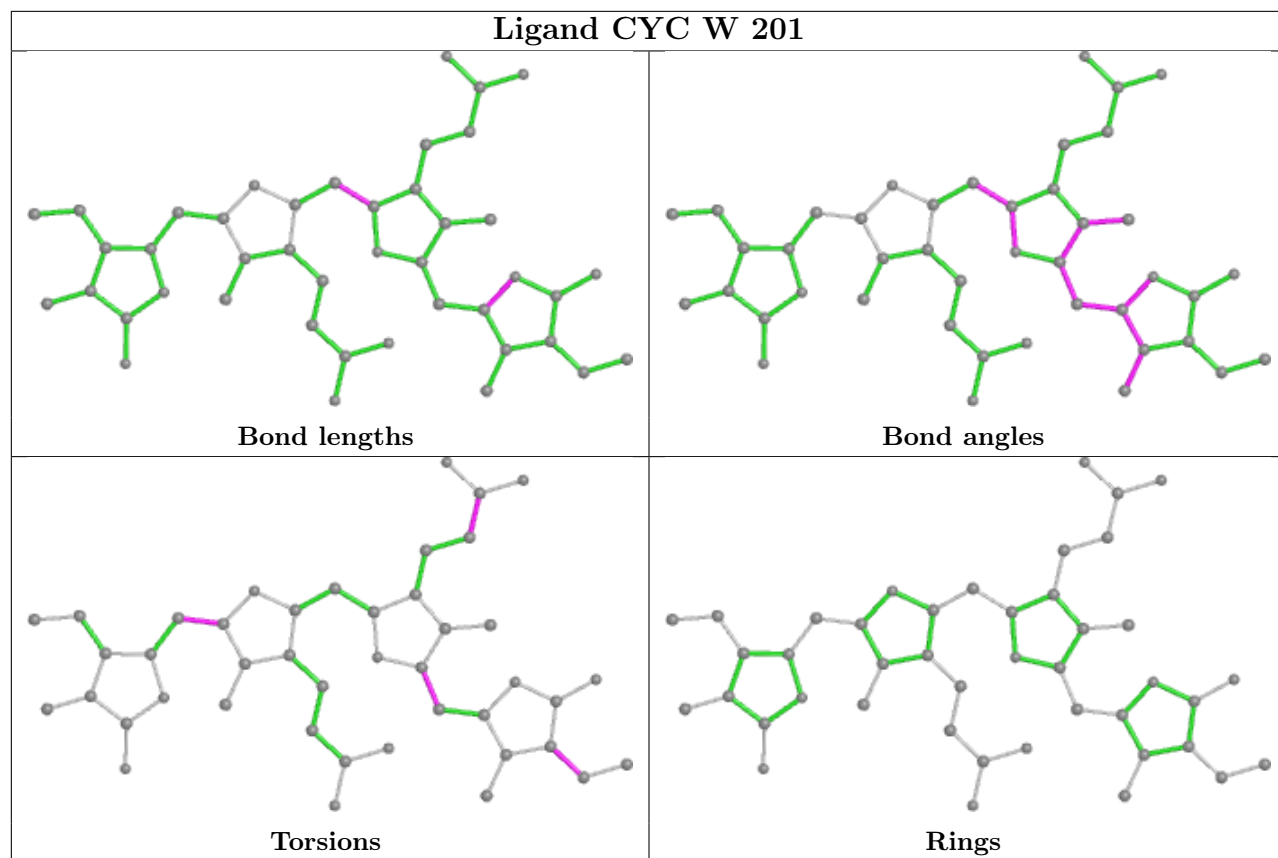


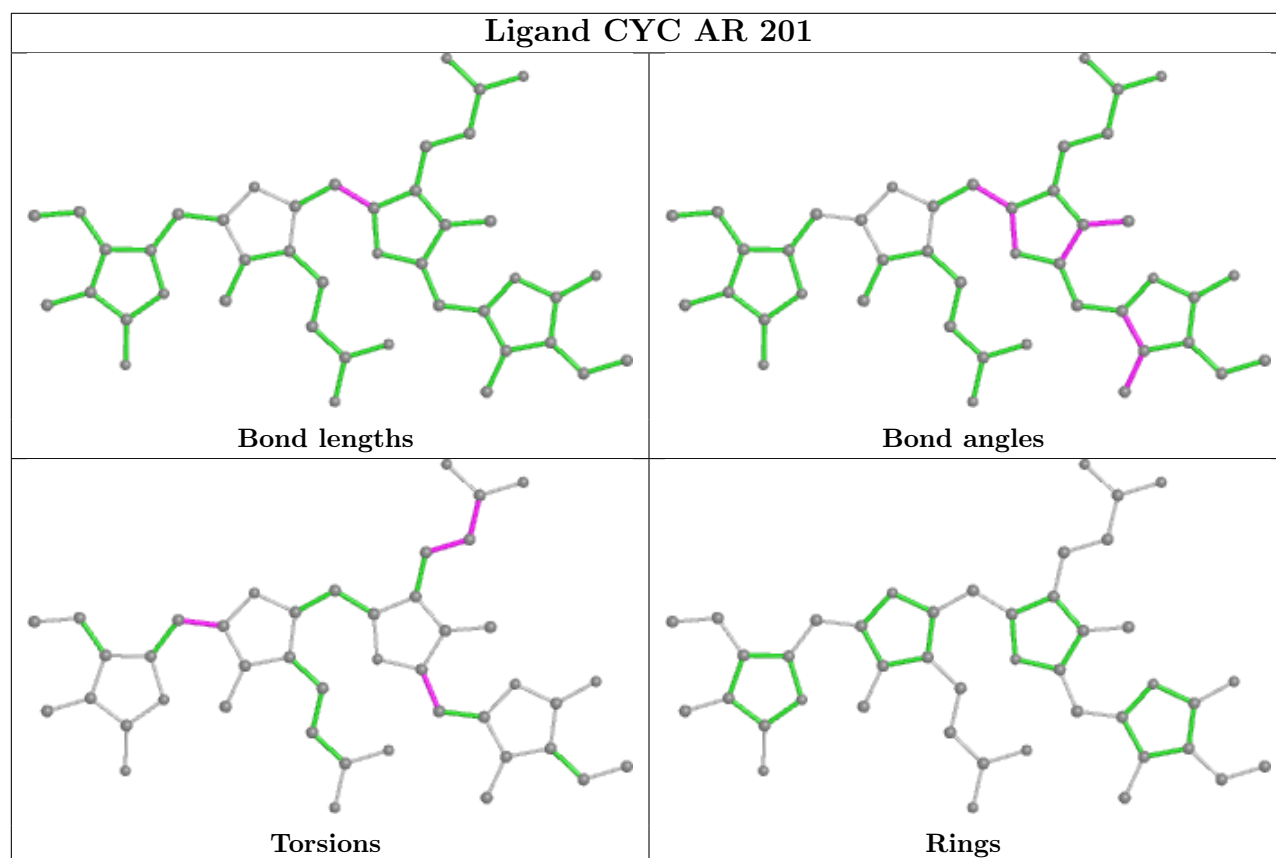
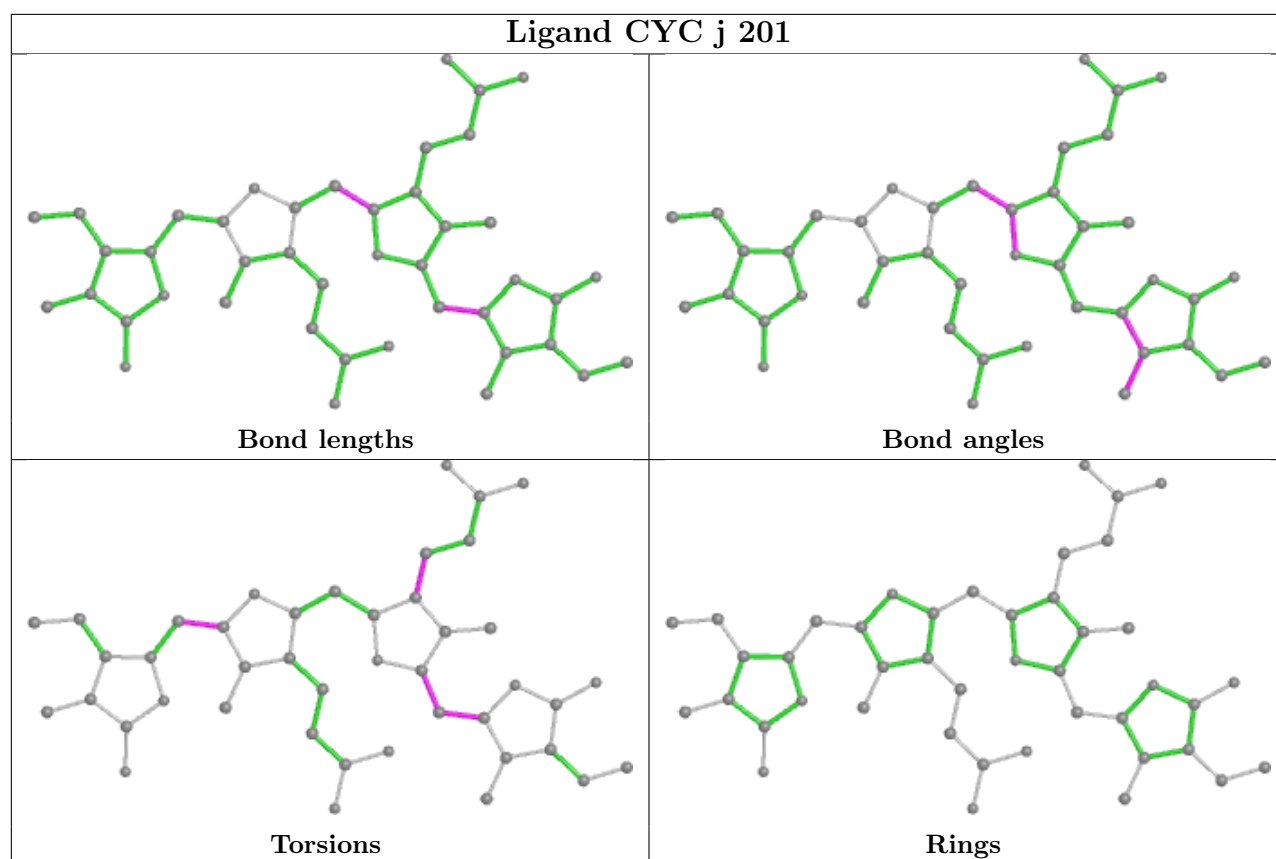
Ligand CYC u 201

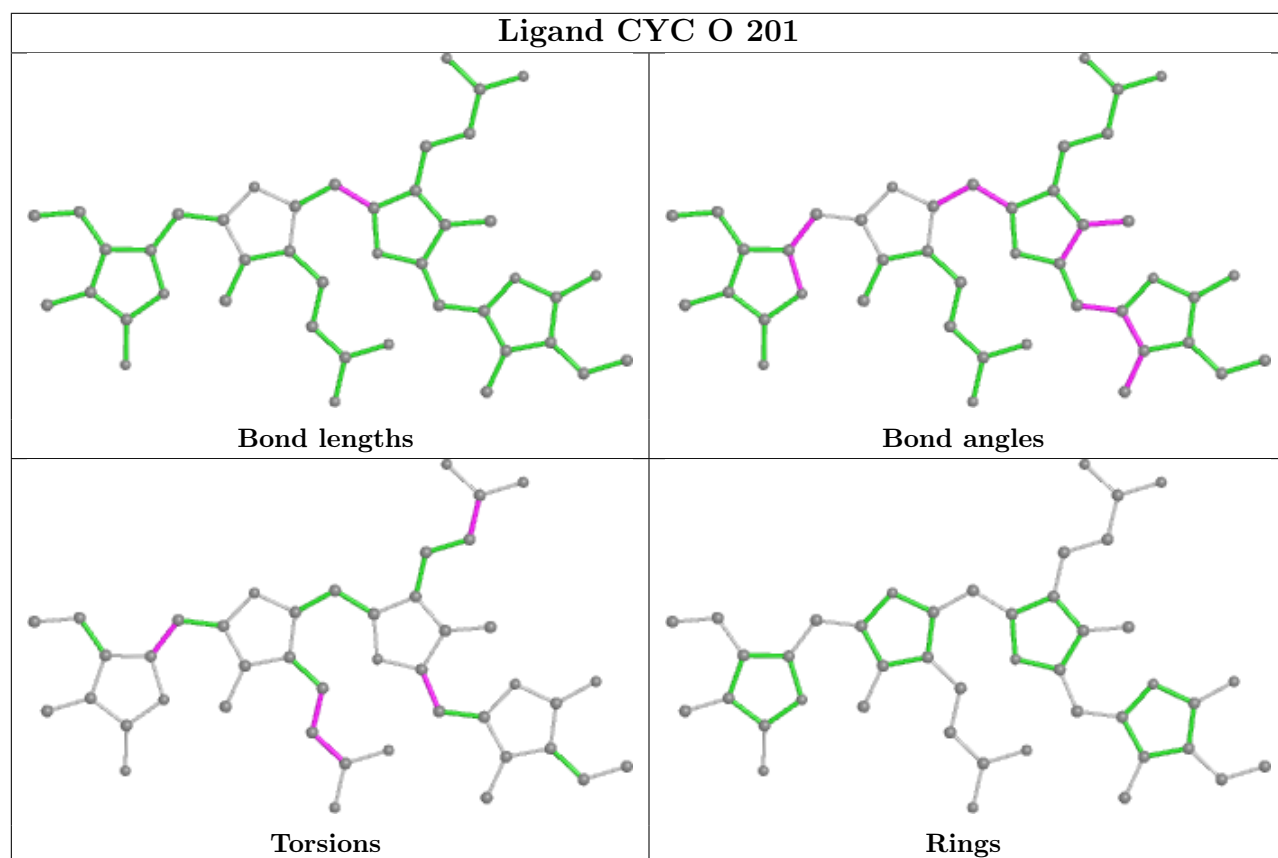
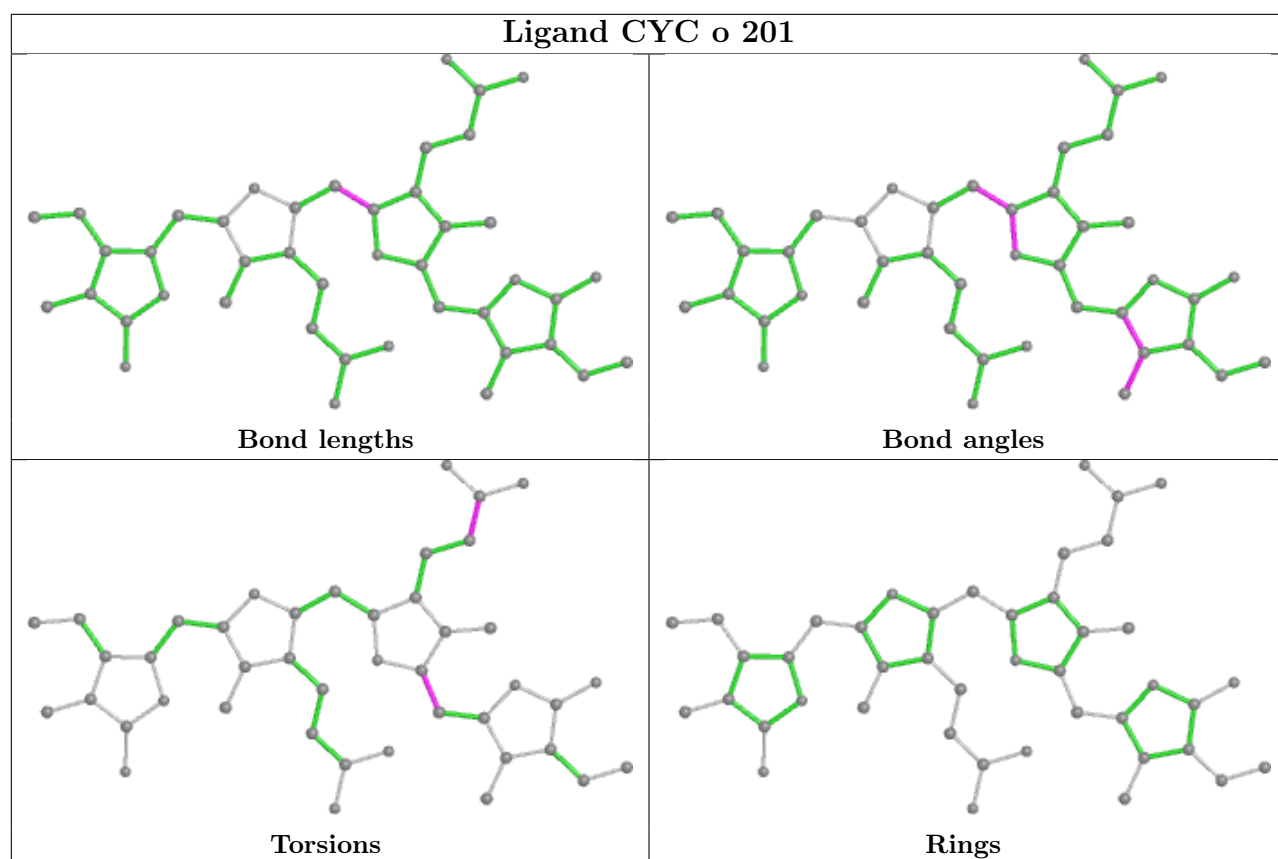


Ligand CYC g 201

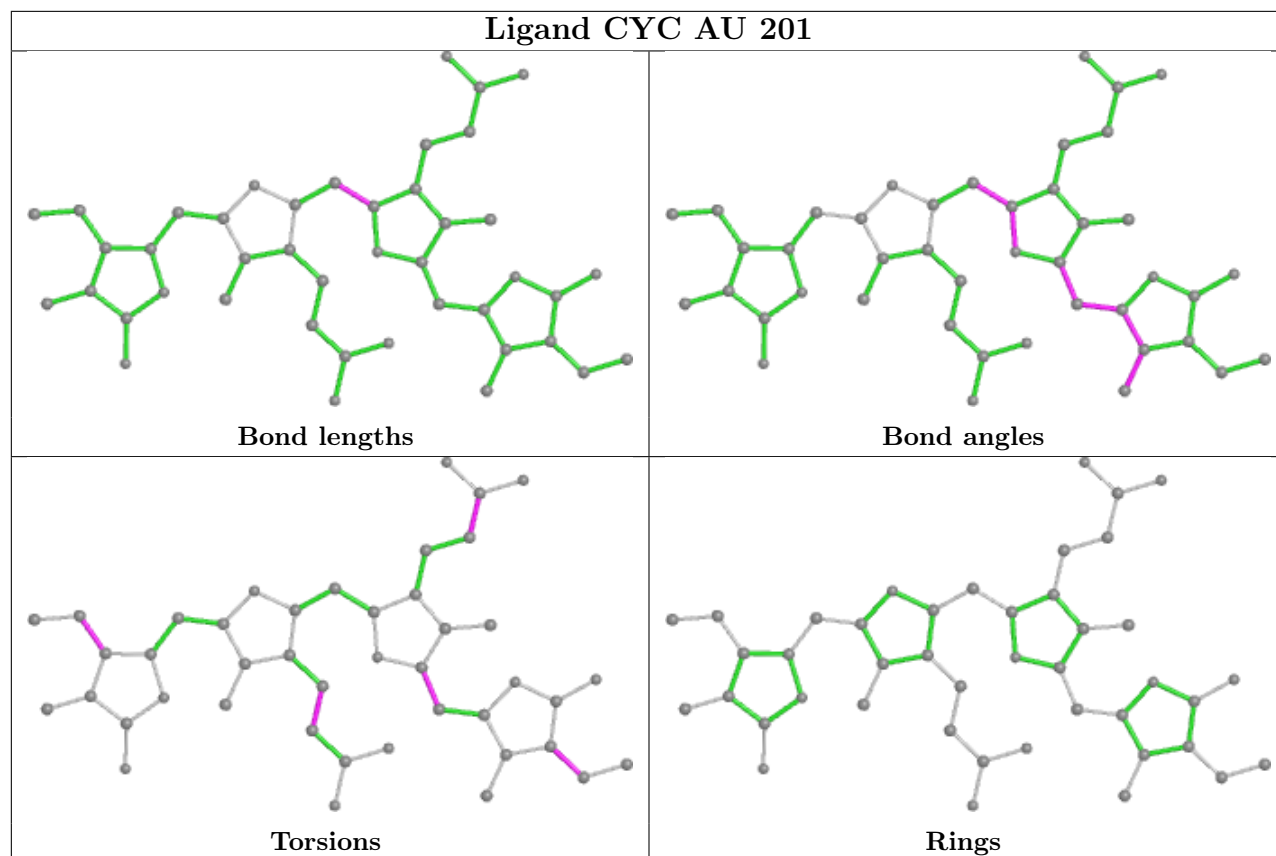




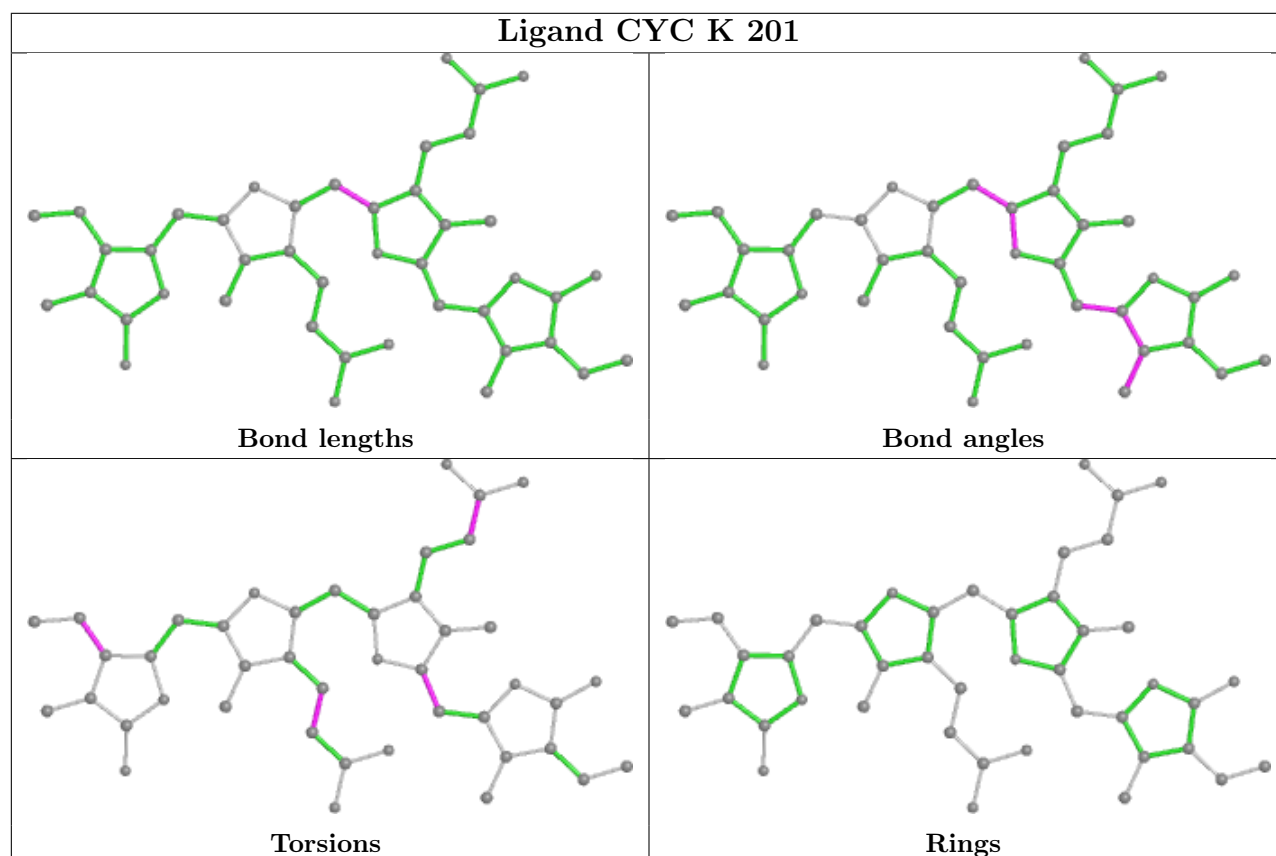




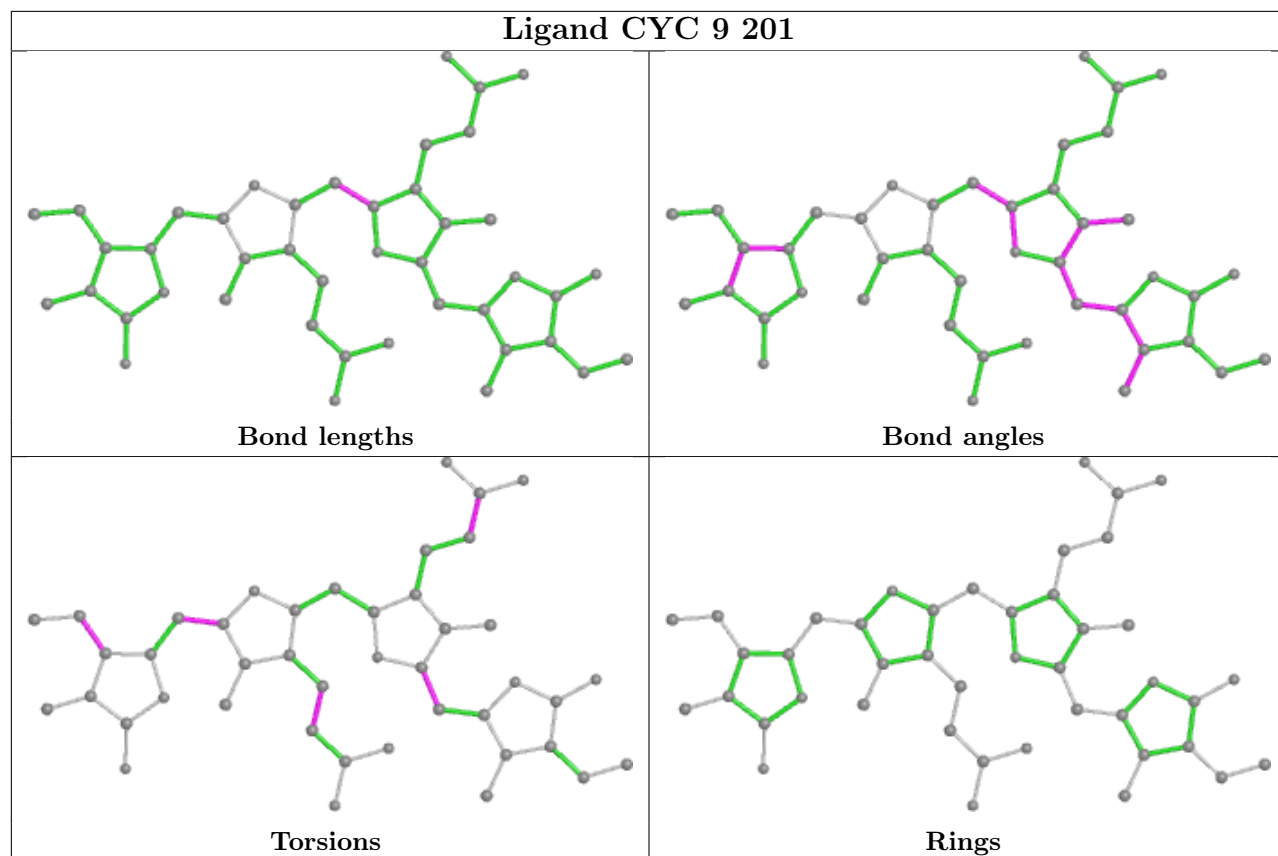
Ligand CYC AU 201



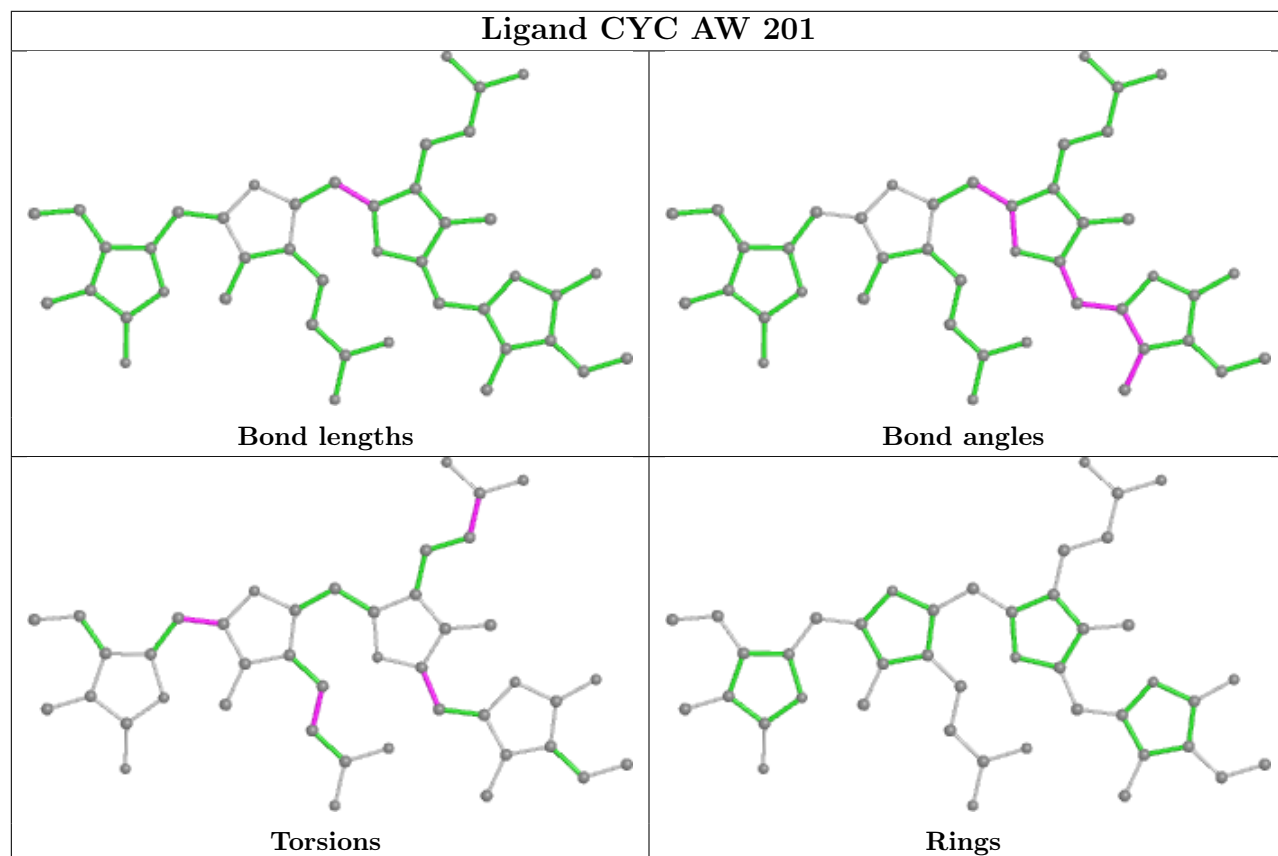
Ligand CYC K 201



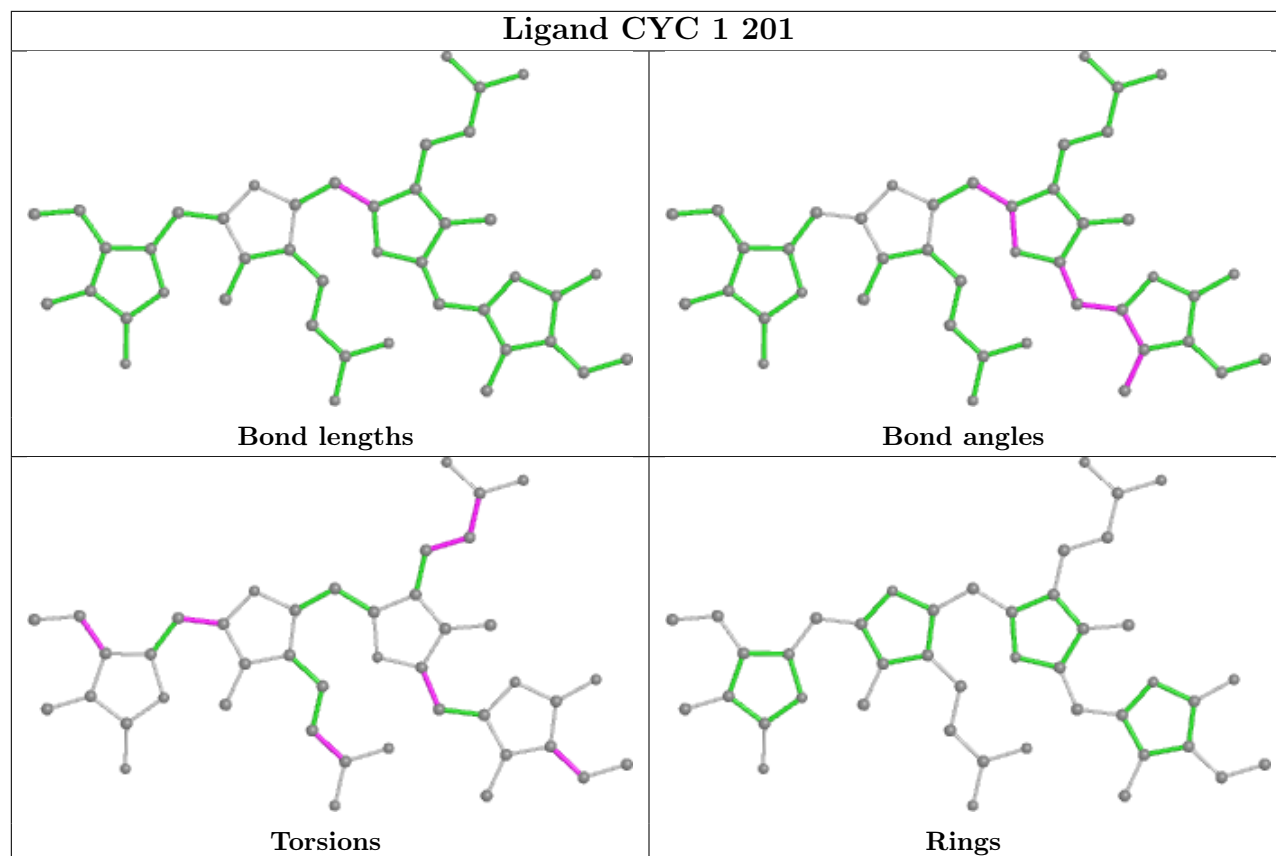
Ligand CYC 9 201



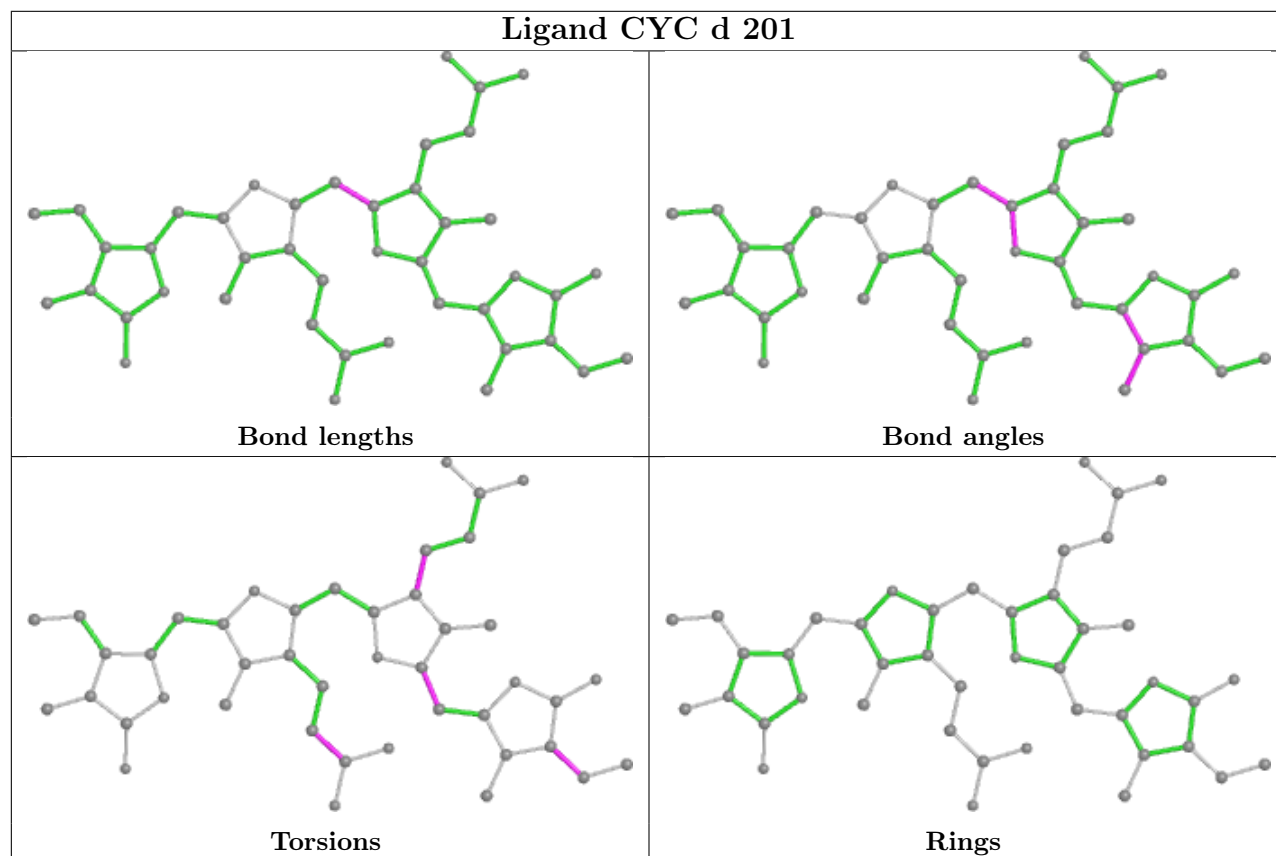
Ligand CYC AW 201



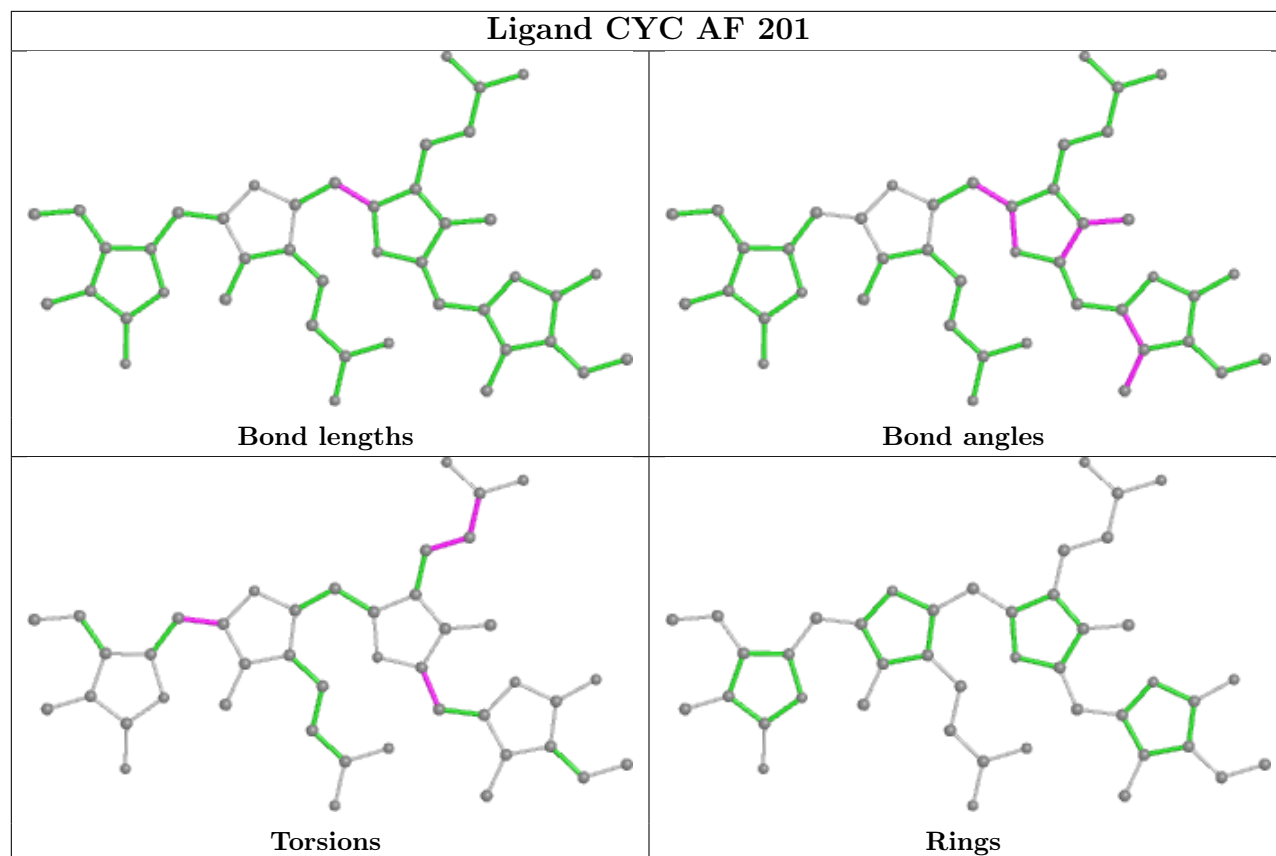
Ligand CYC 1 201



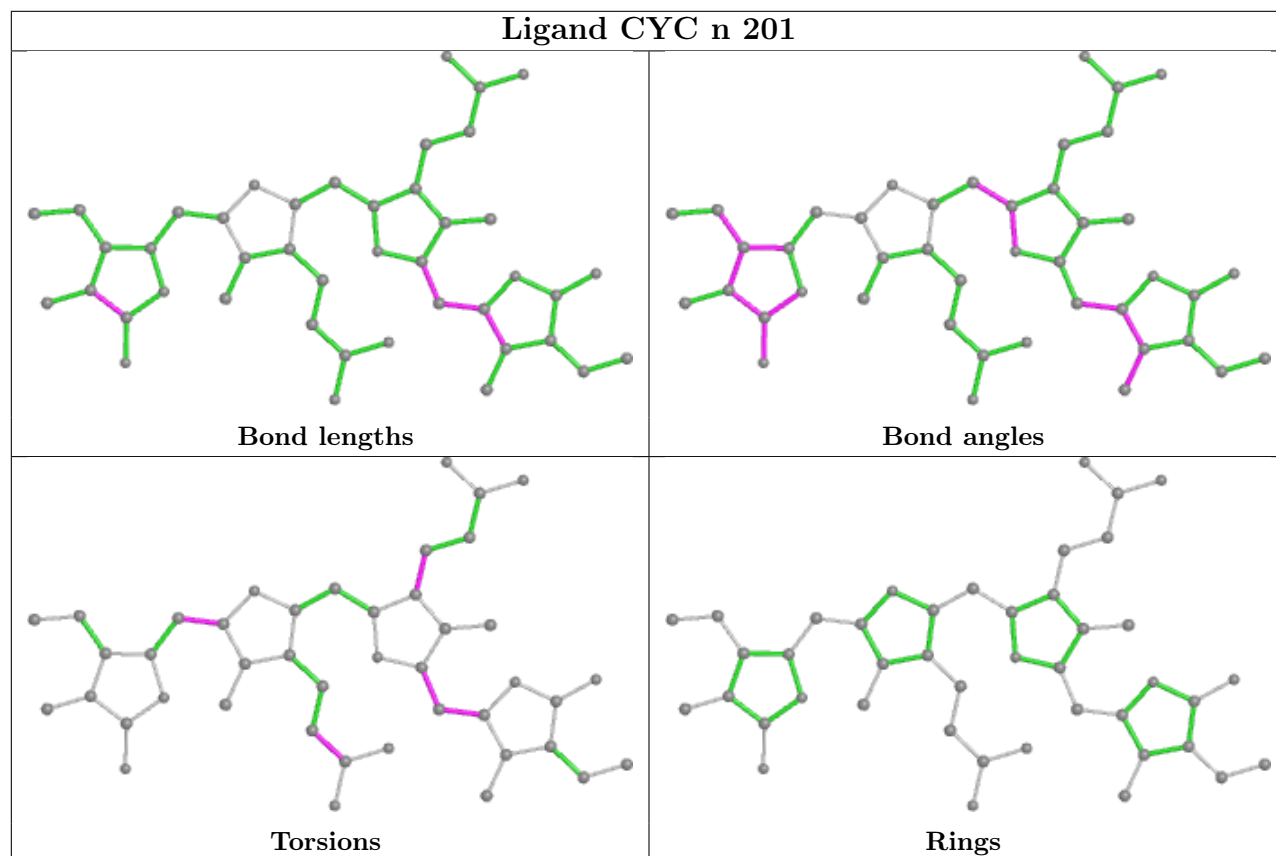
Ligand CYC d 201

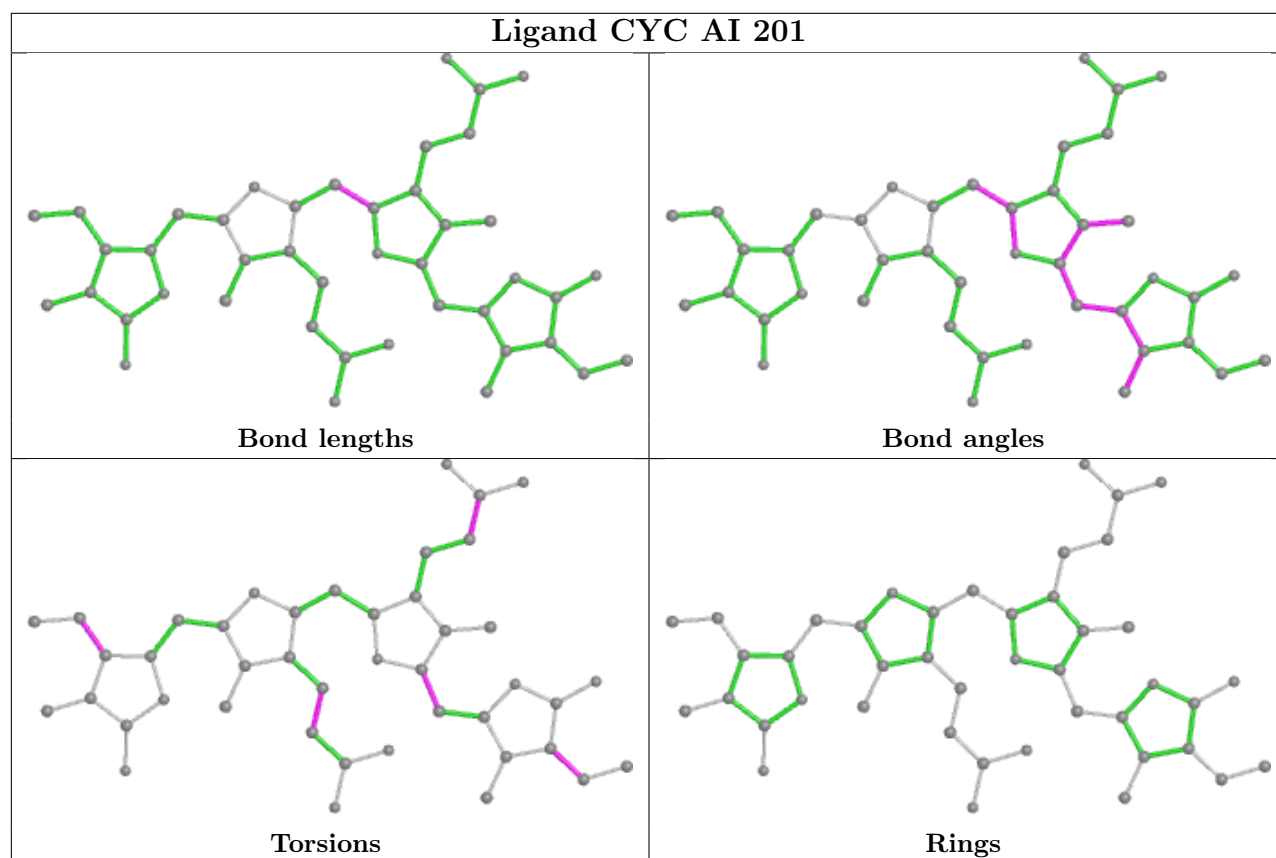
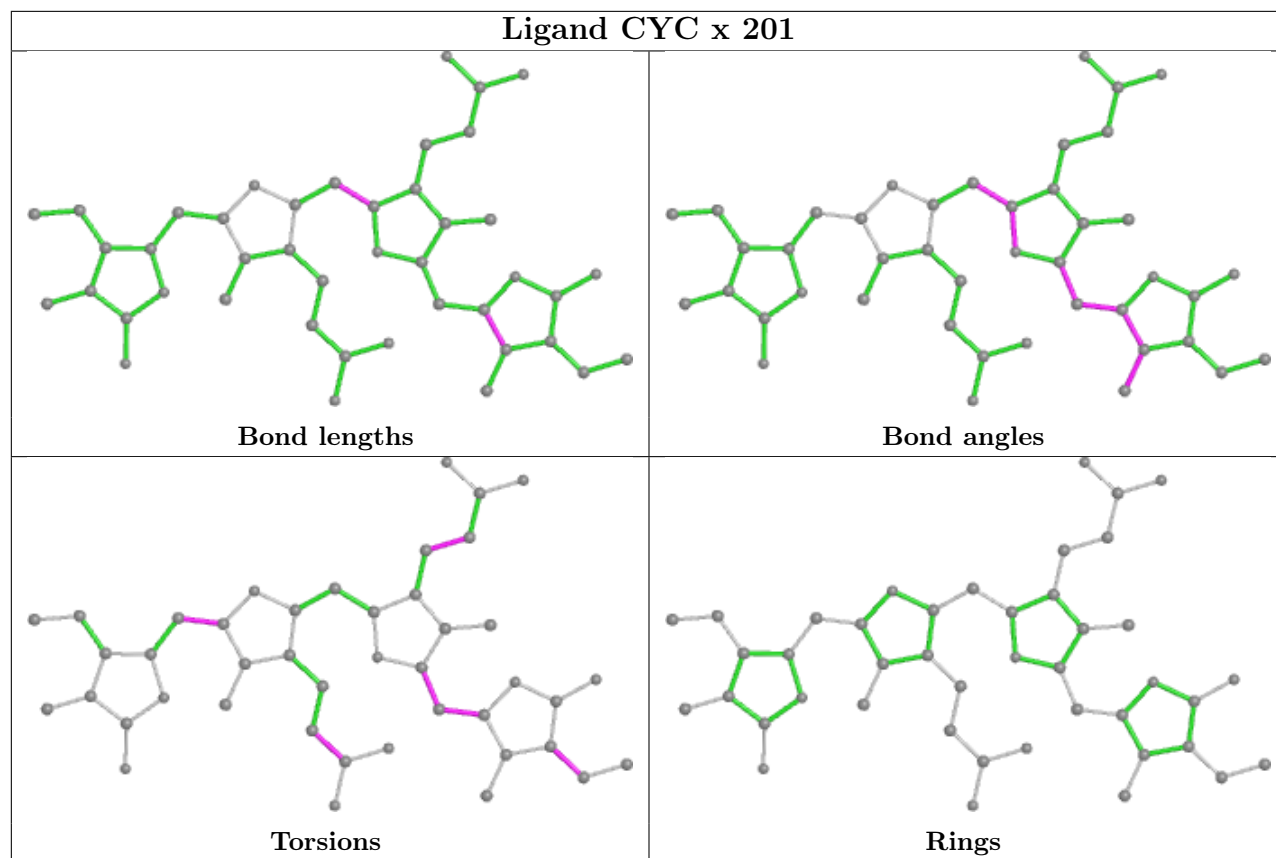


Ligand CYC AF 201

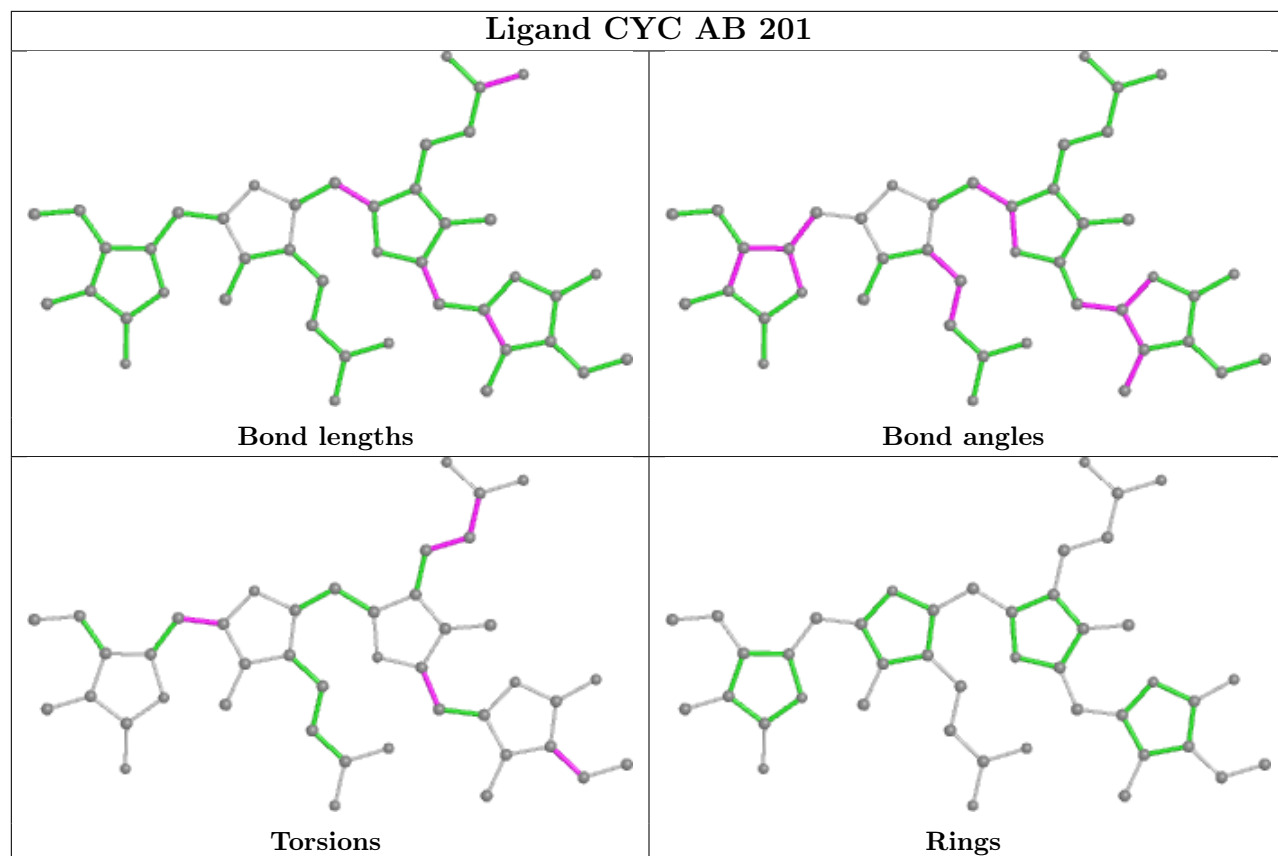


Ligand CYC n 201

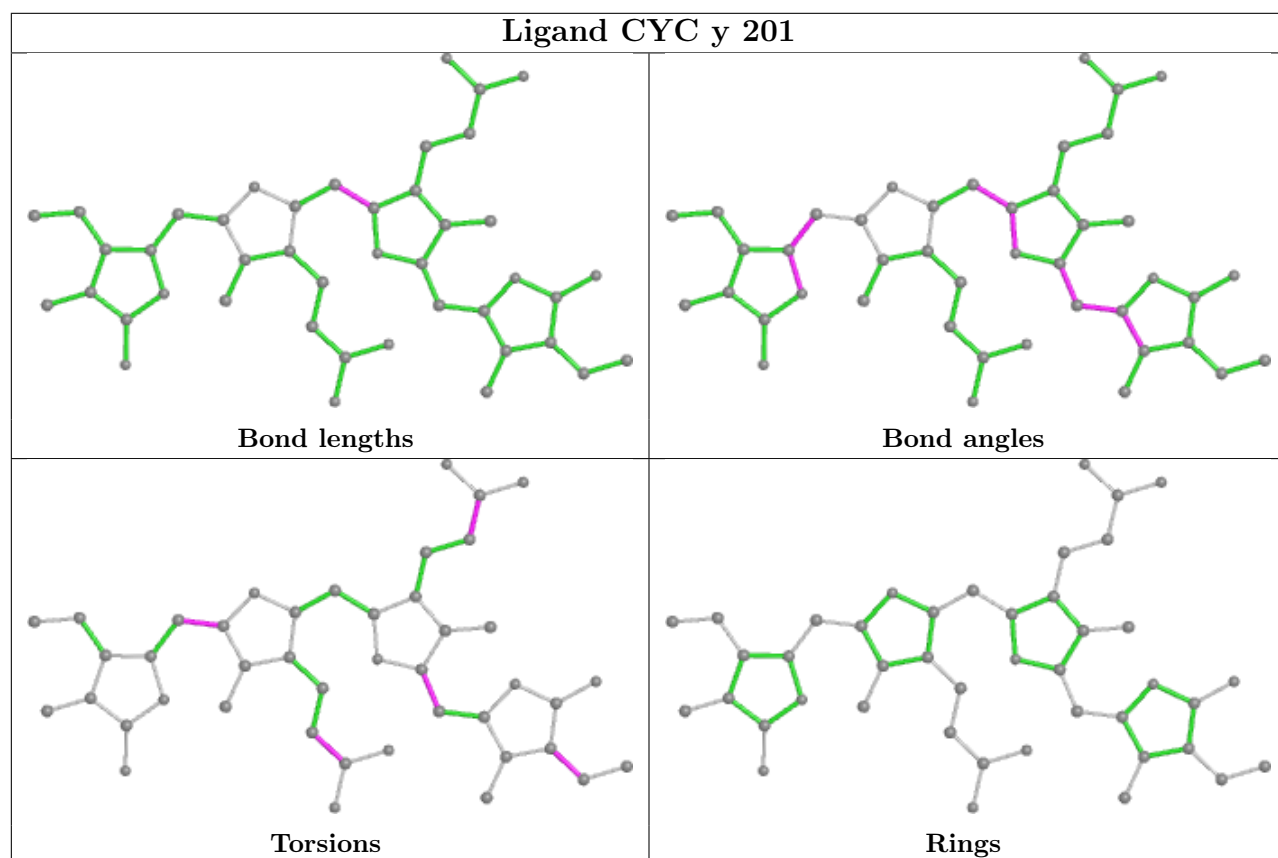




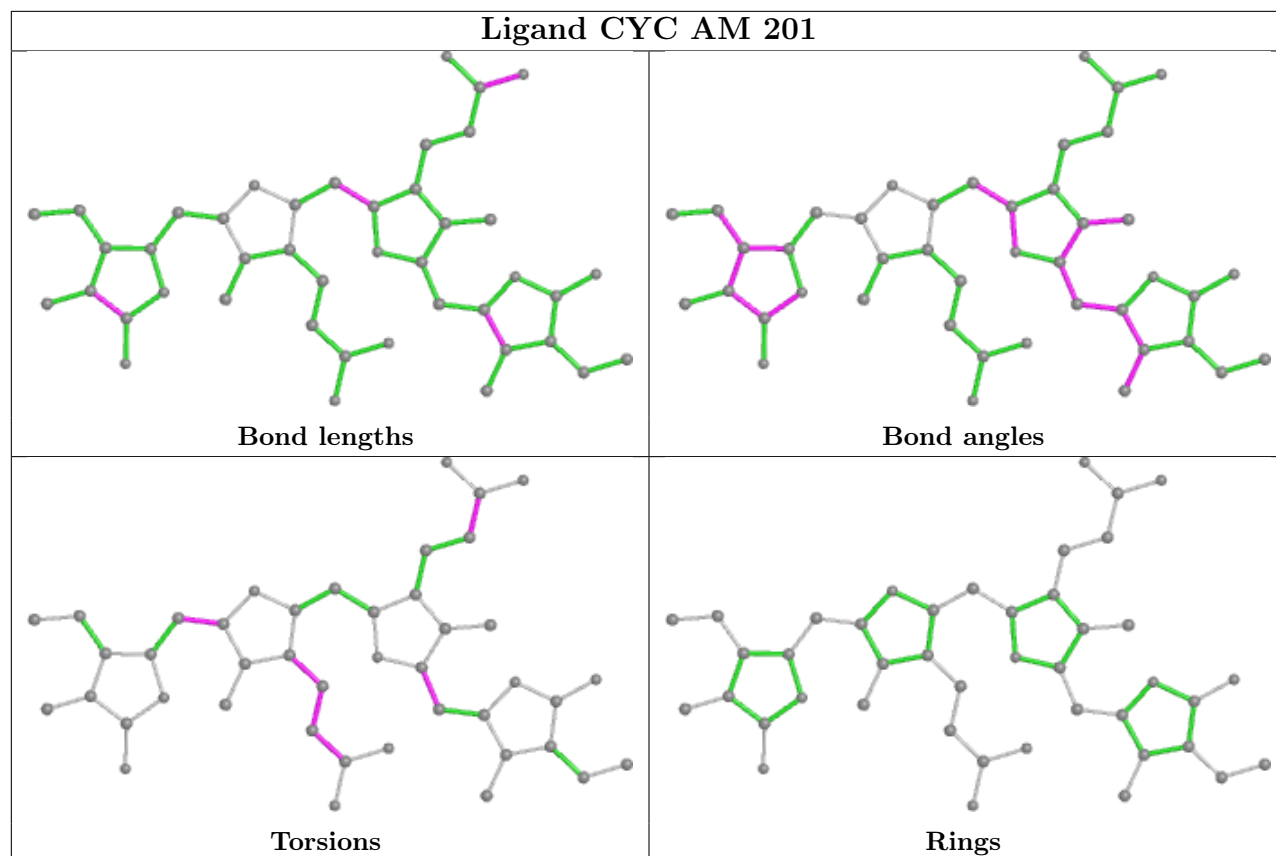
Ligand CYC AB 201



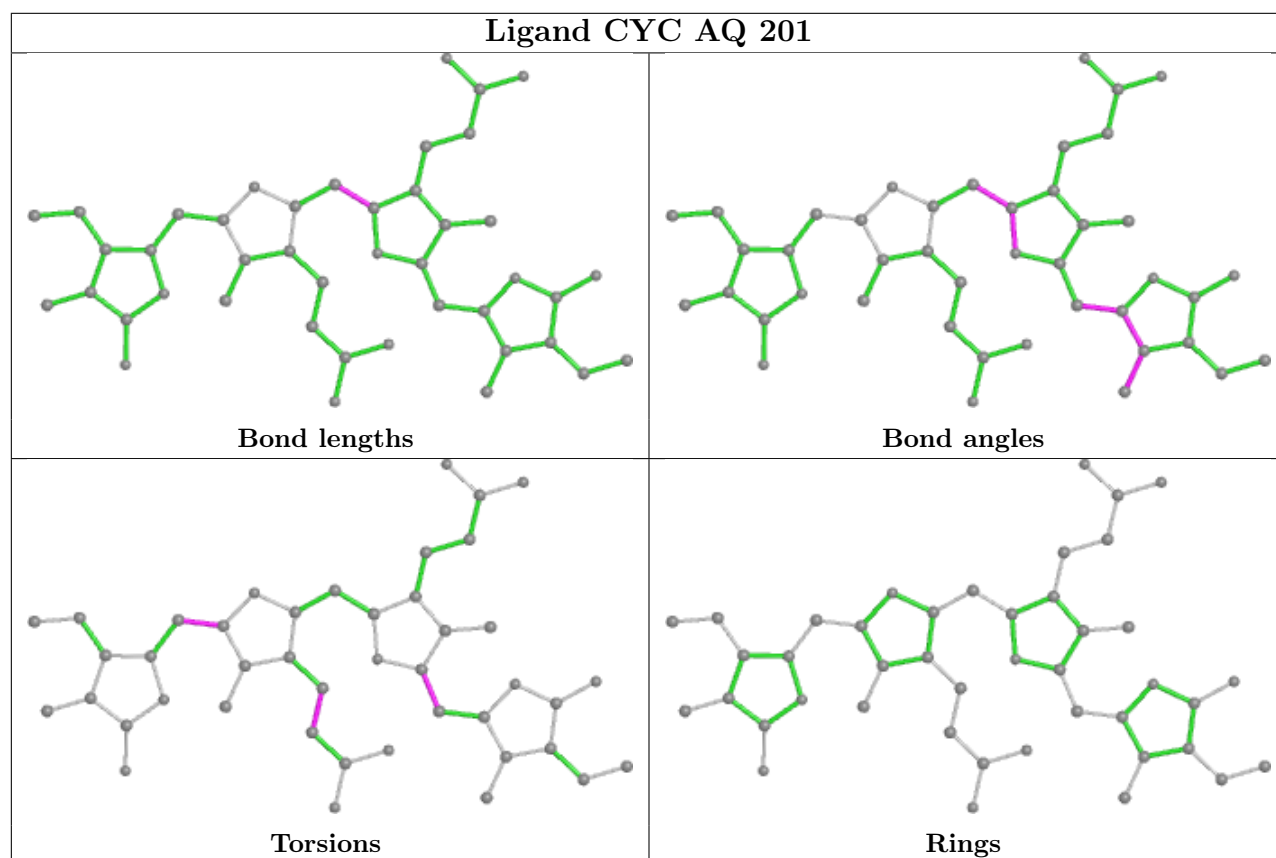
Ligand CYC y 201

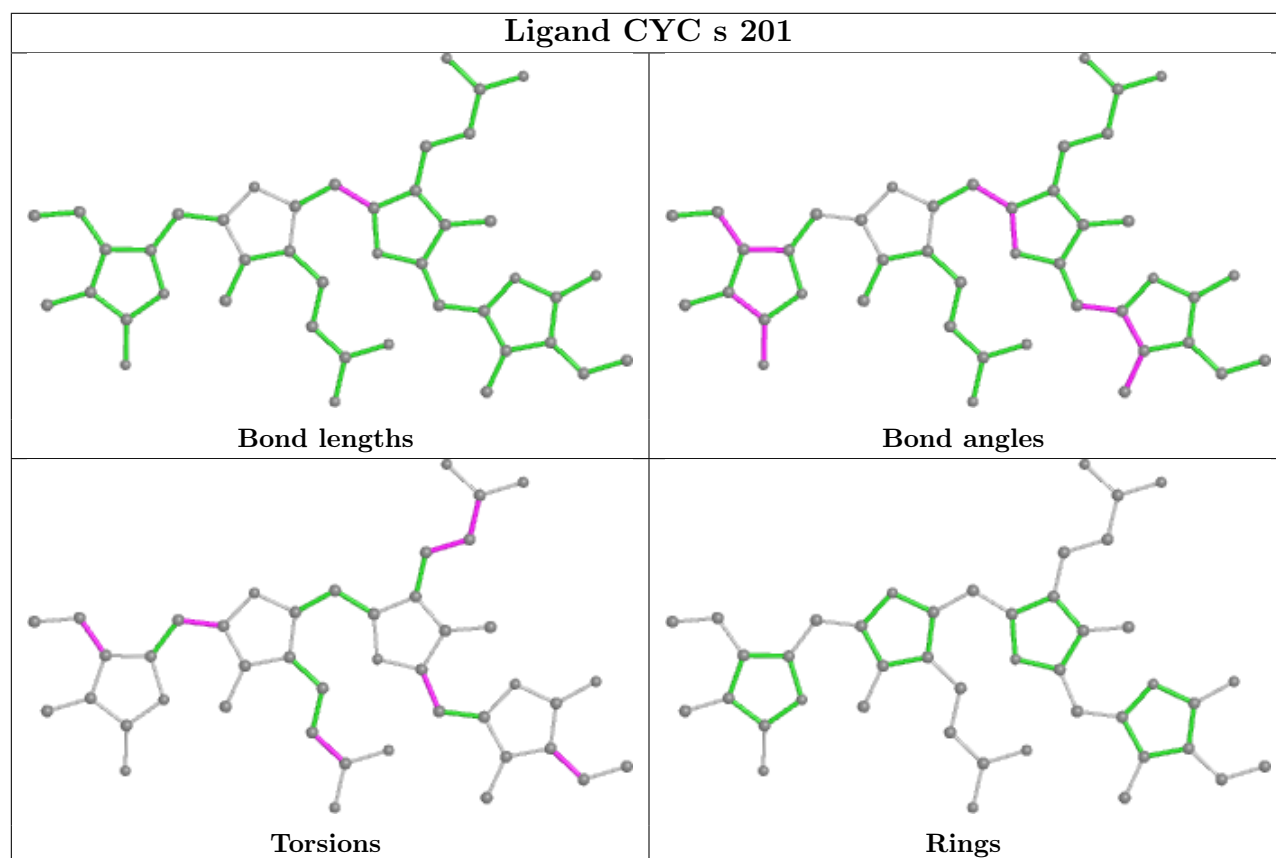
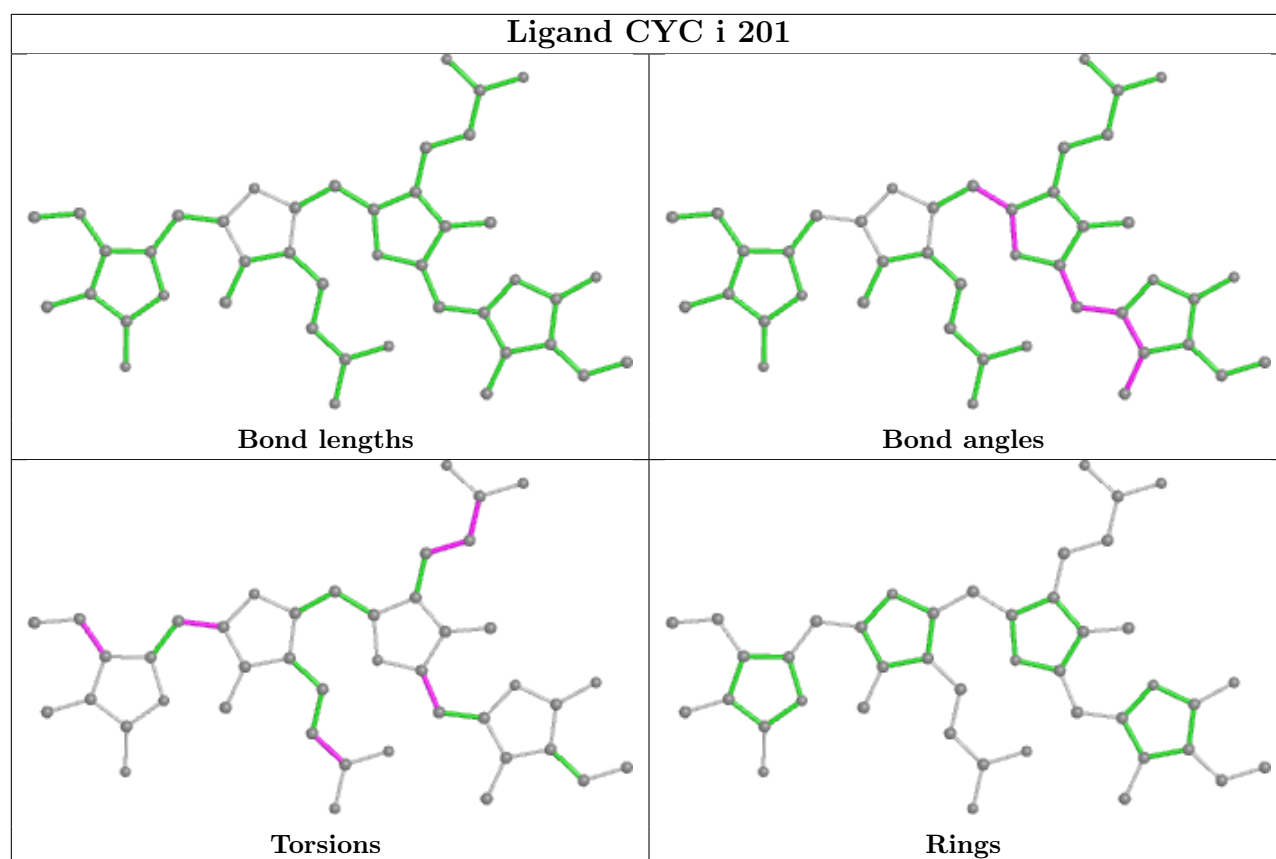


Ligand CYC AM 201

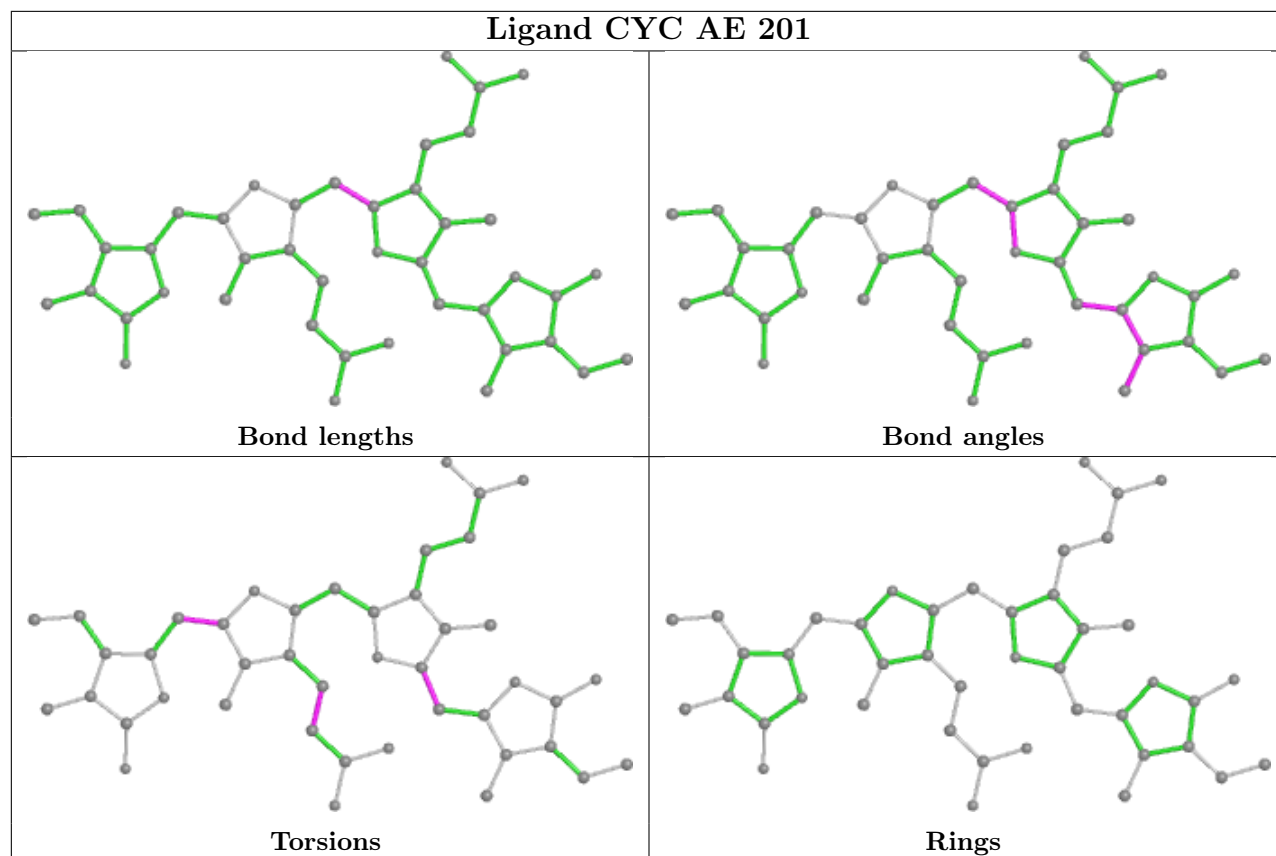


Ligand CYC AQ 201

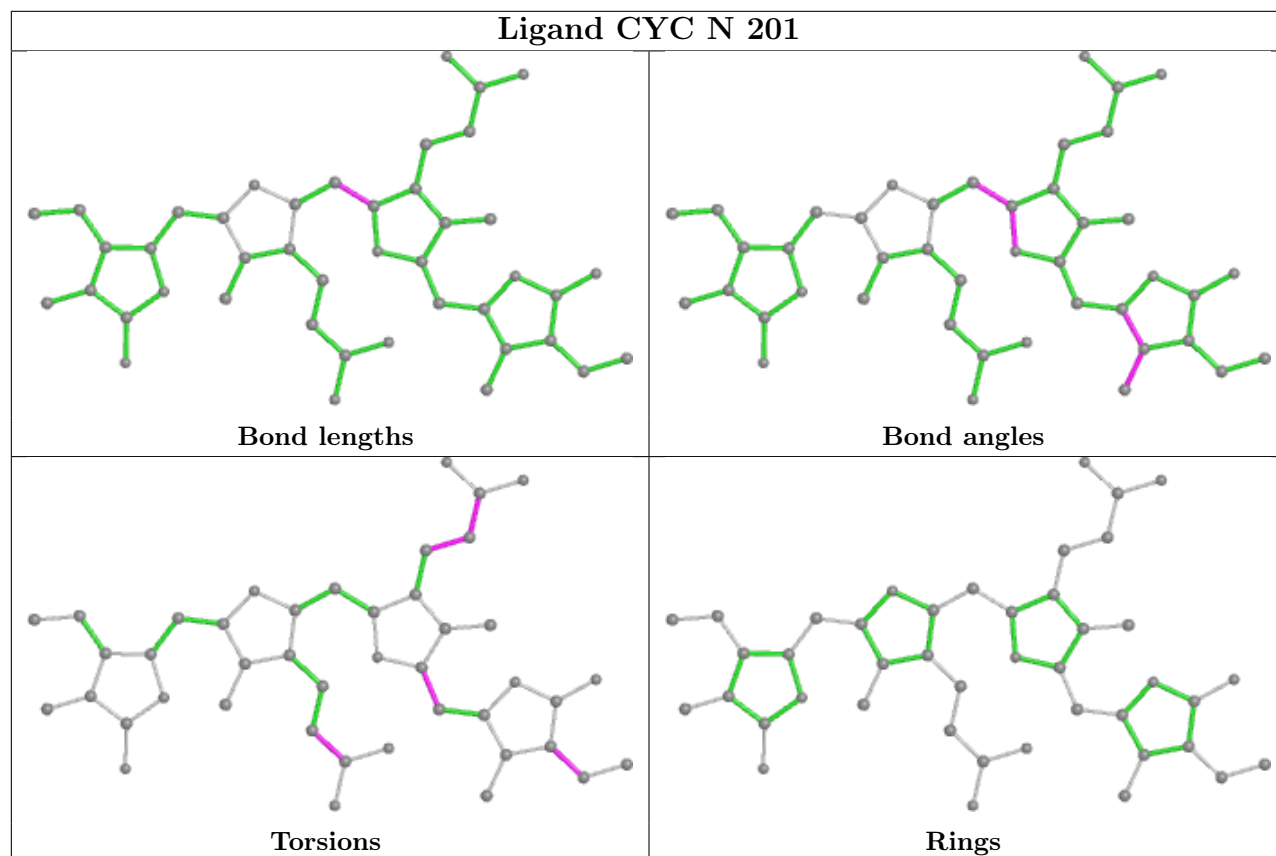




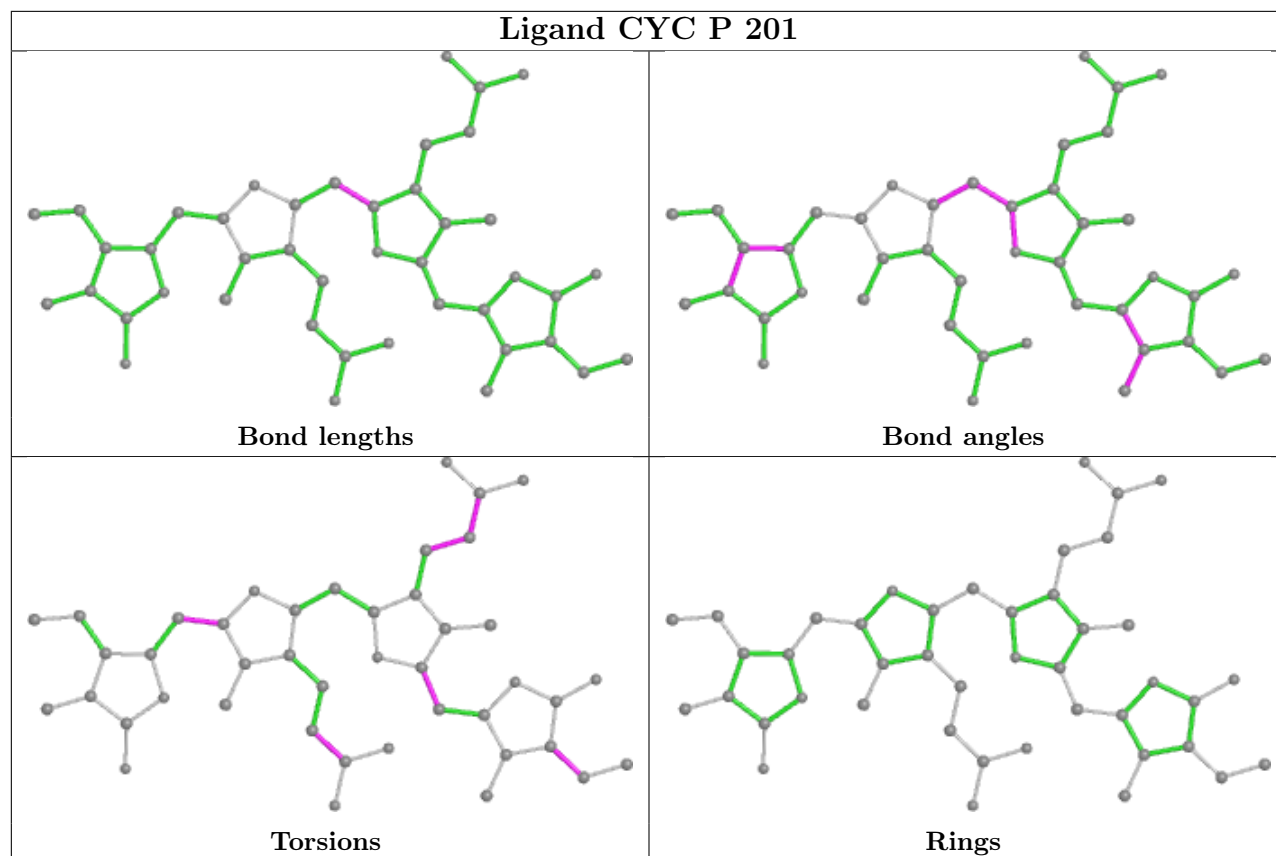
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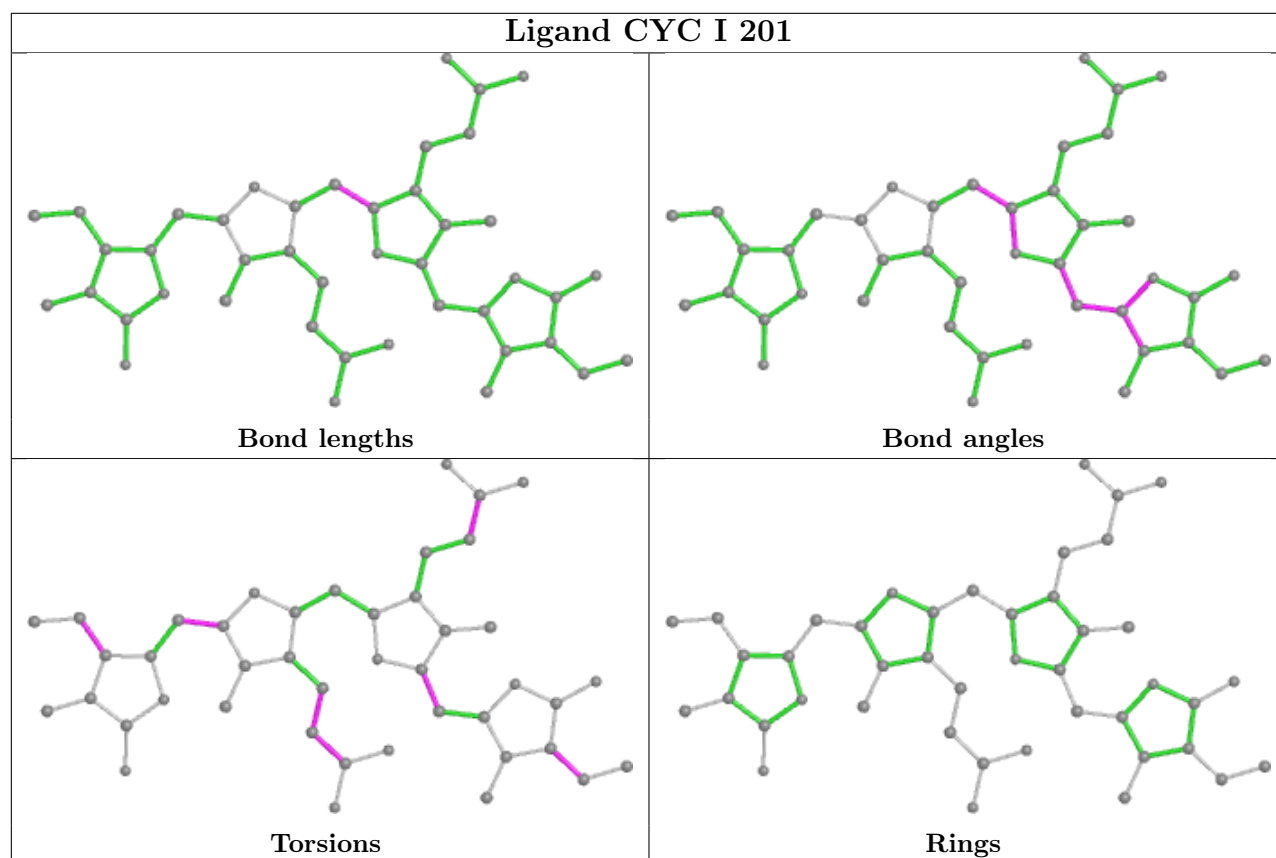
Ligand CYC N 201



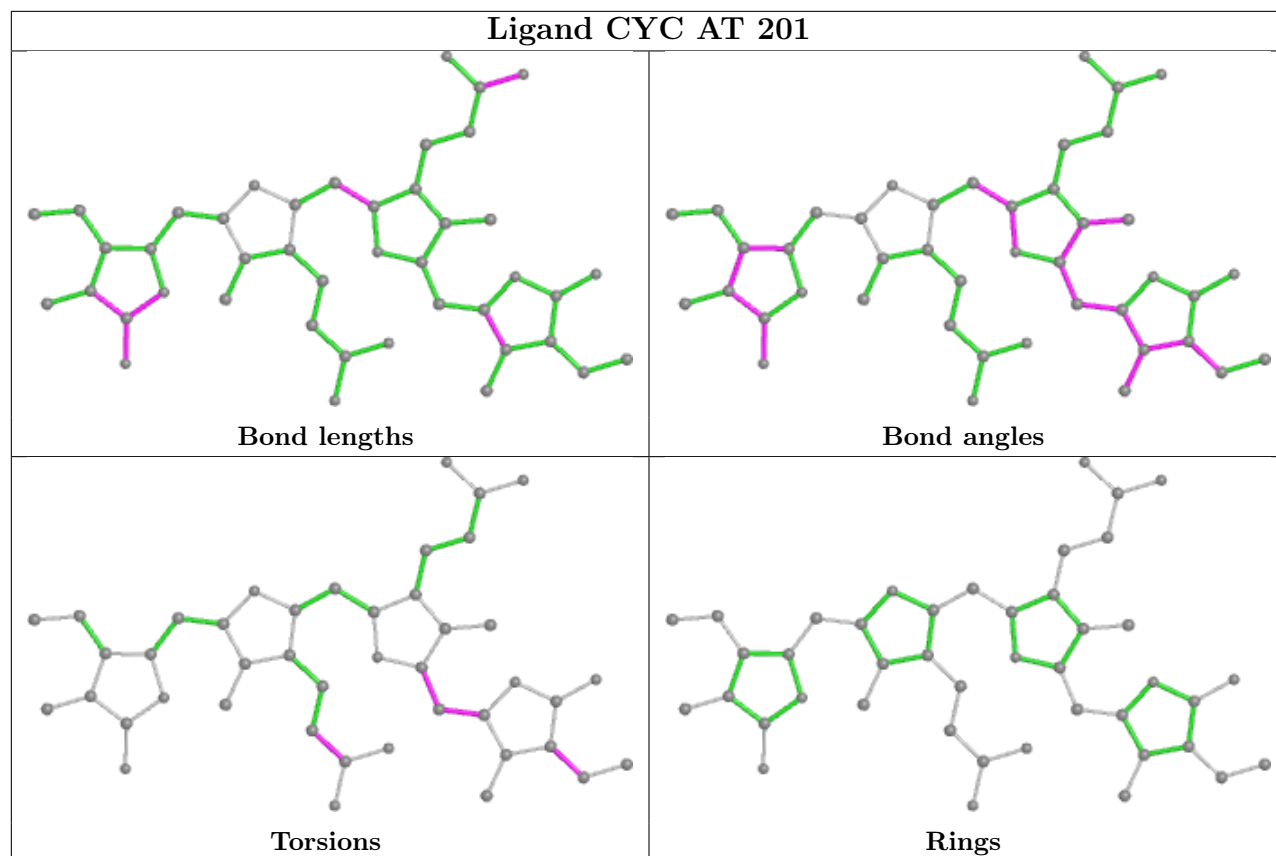
Ligand CYC P 201



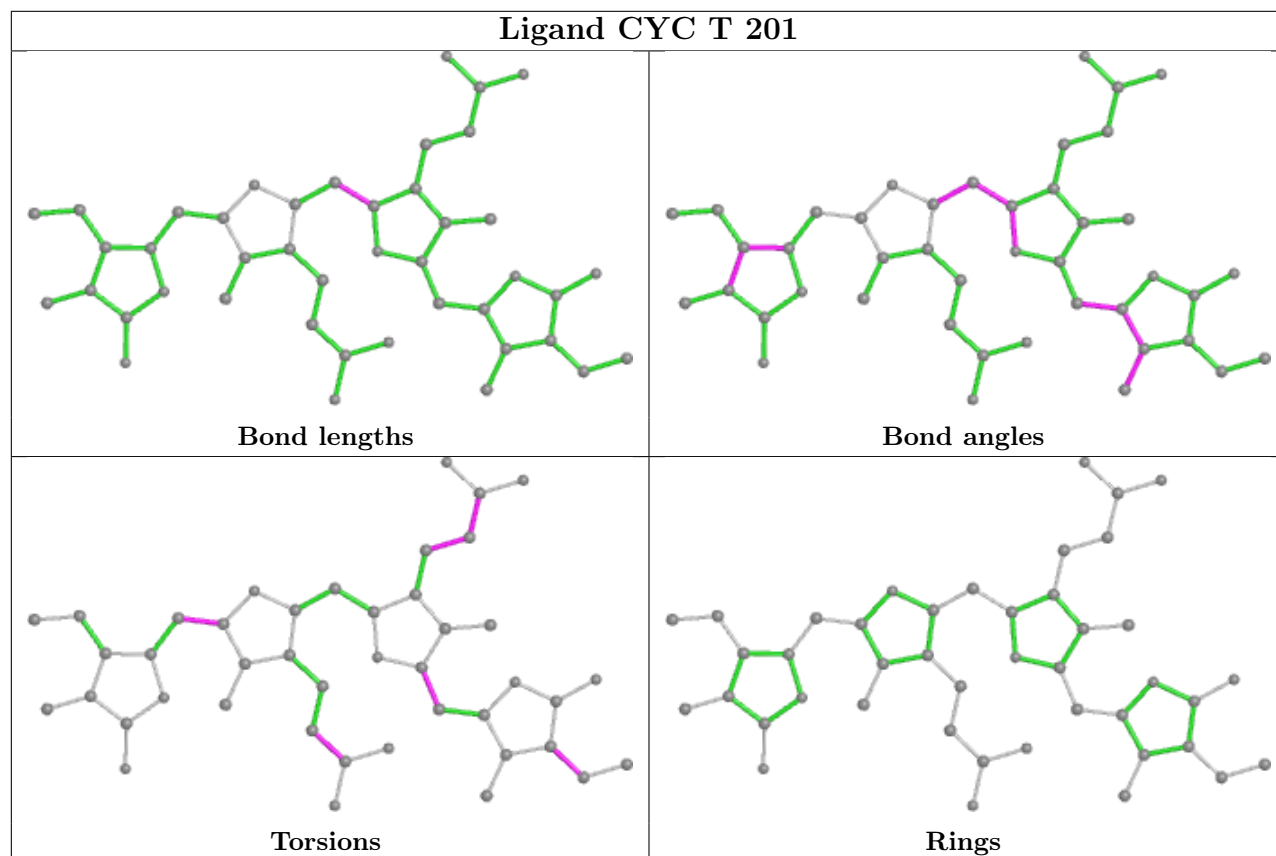
Ligand CYC I 201



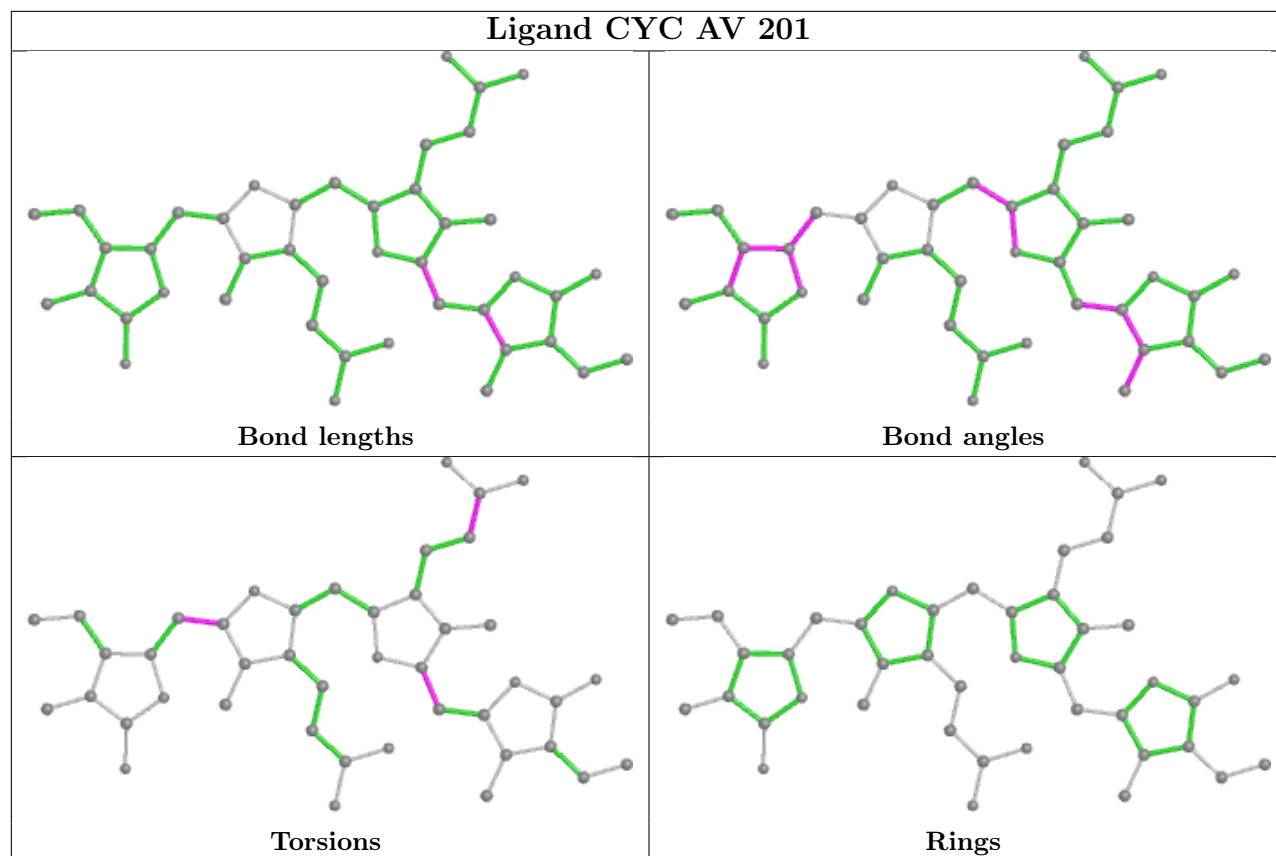
Ligand CYC AT 201



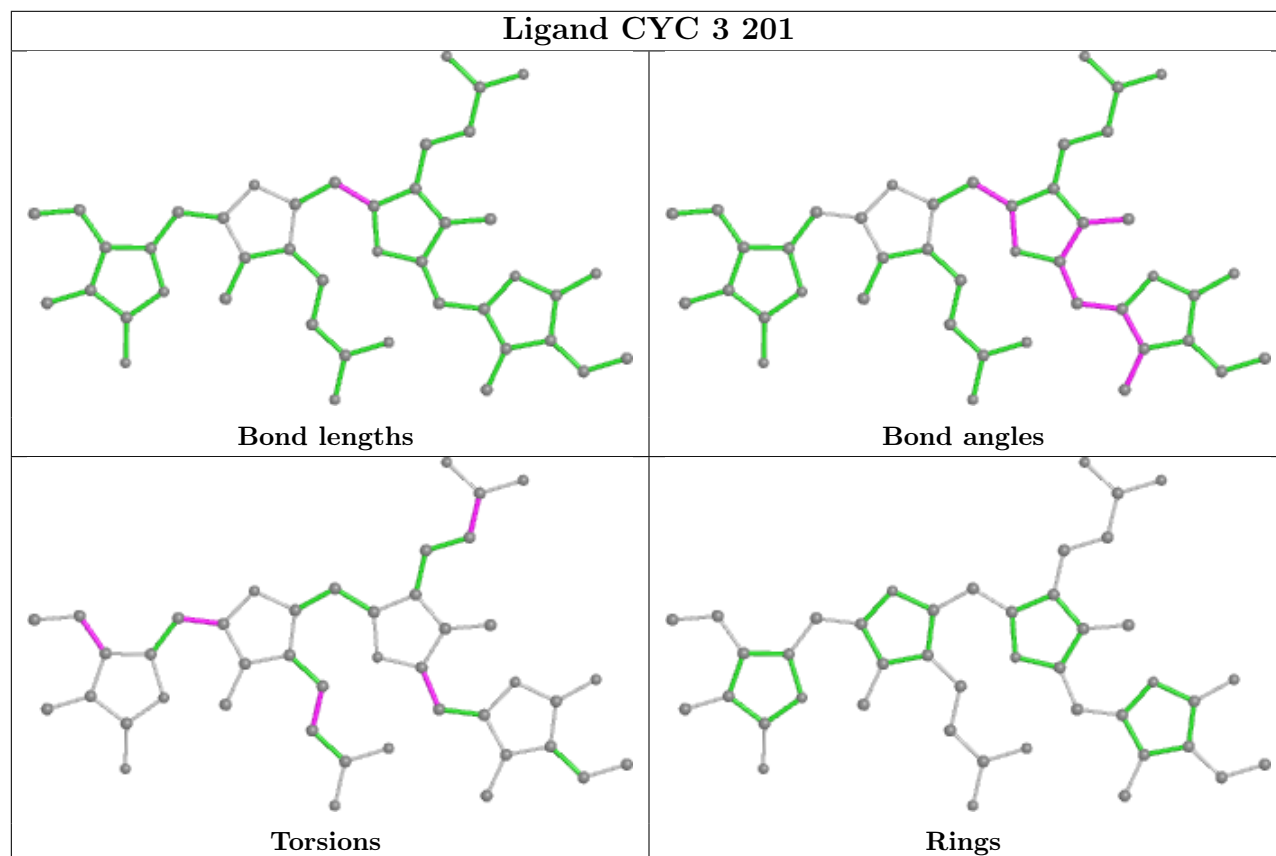
Ligand CYC T 201

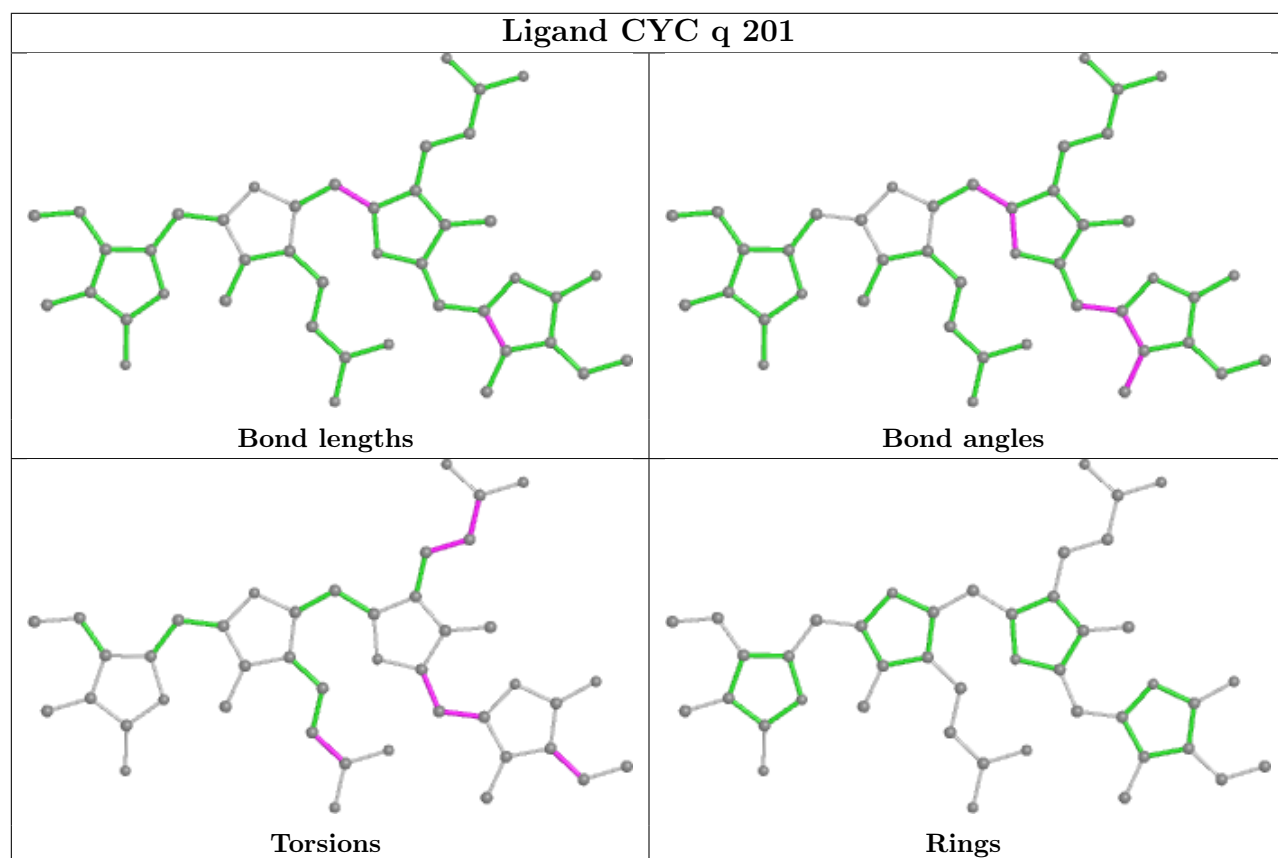
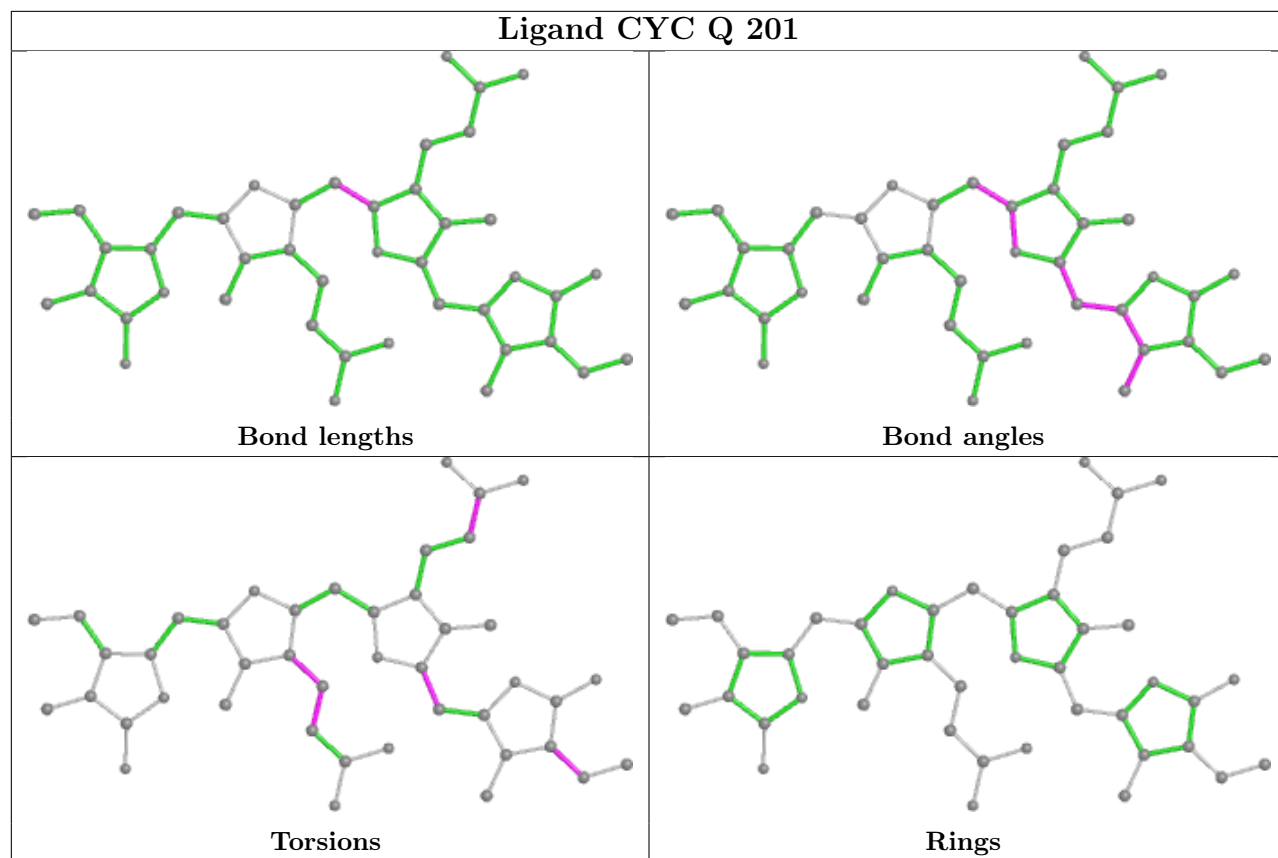


Ligand CYC AV 201

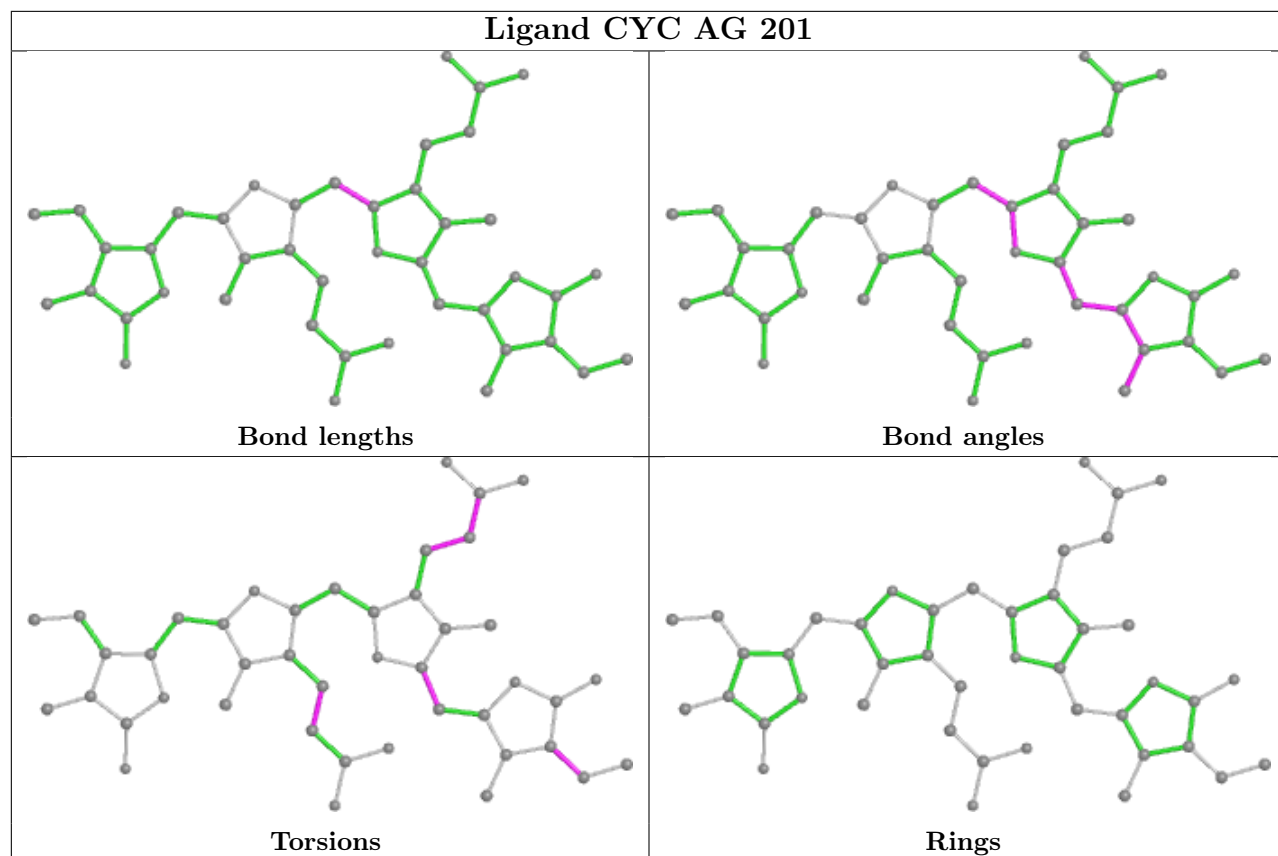


Ligand CYC 3 201

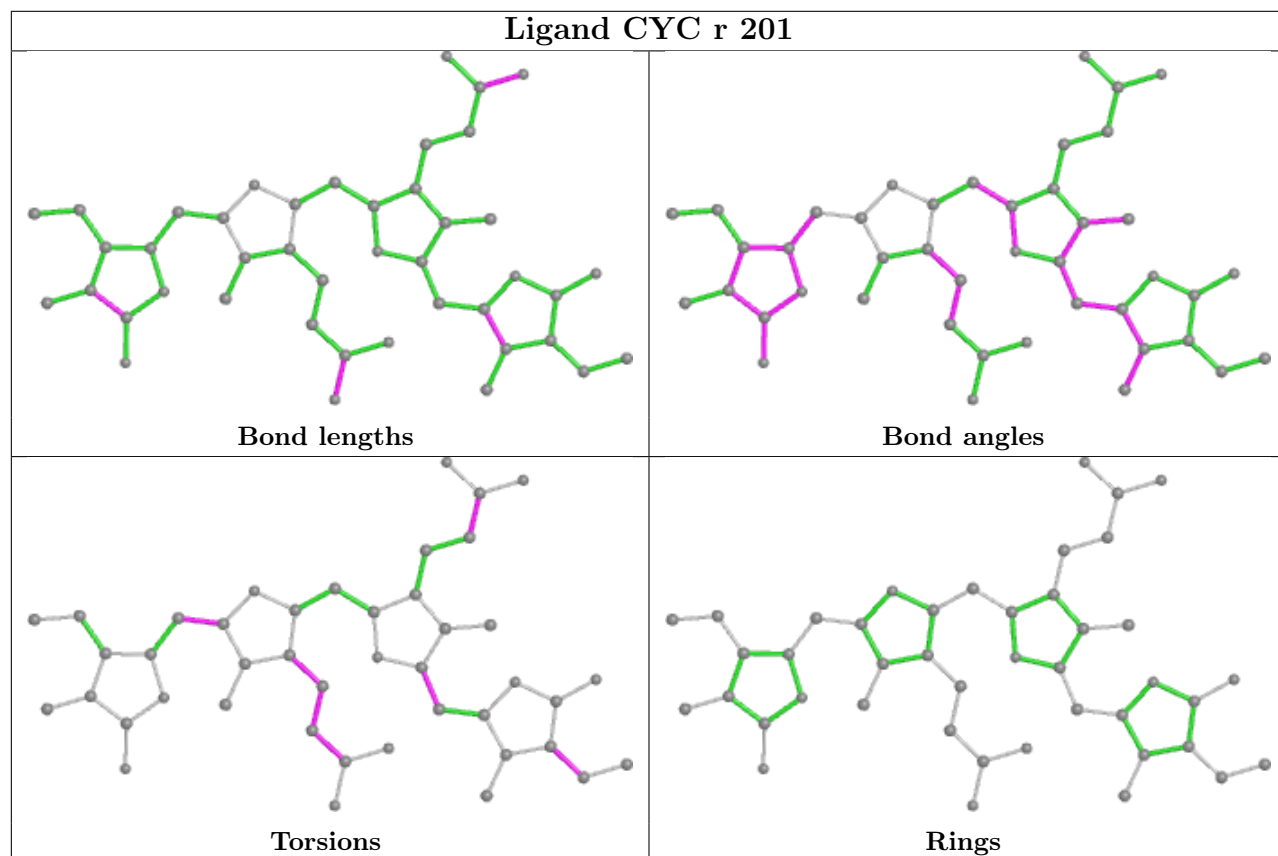




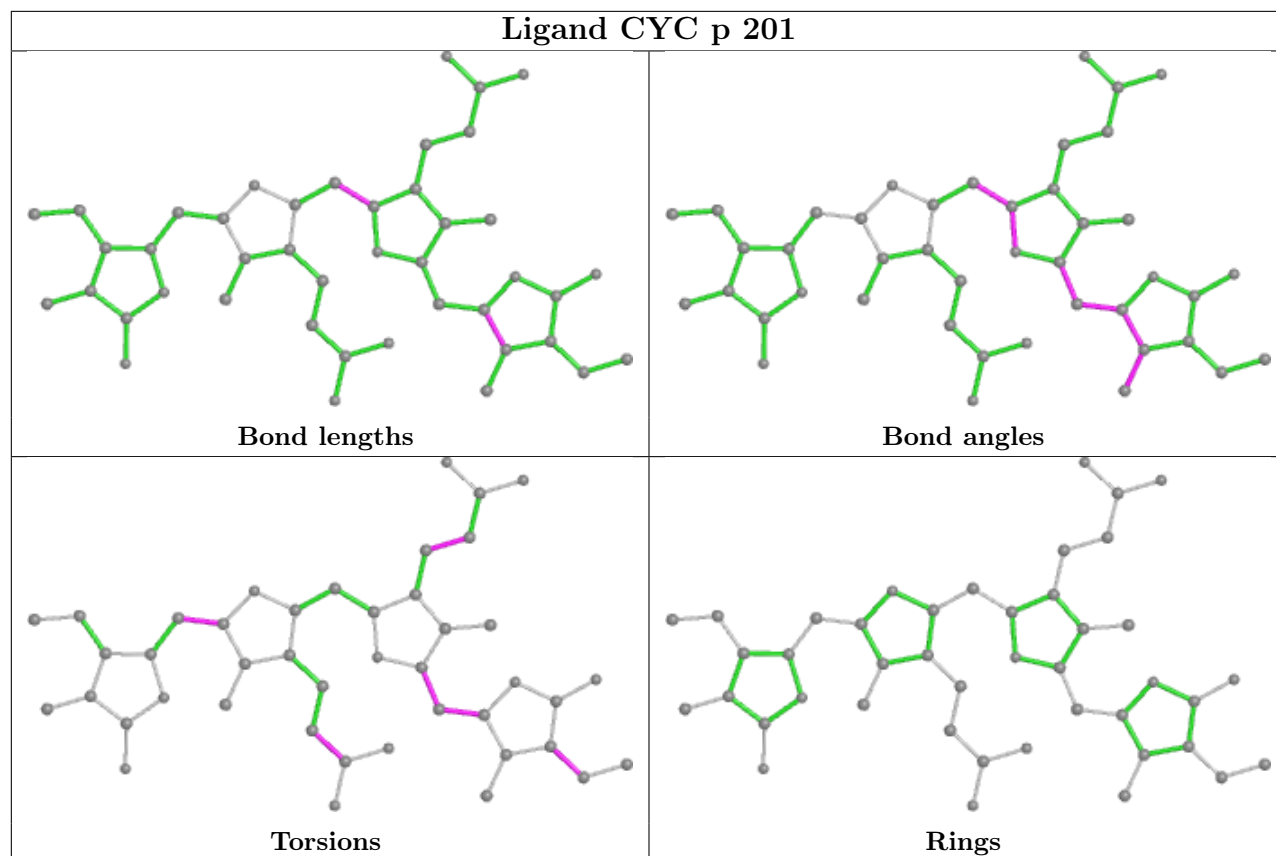
Ligand CYC AG 201



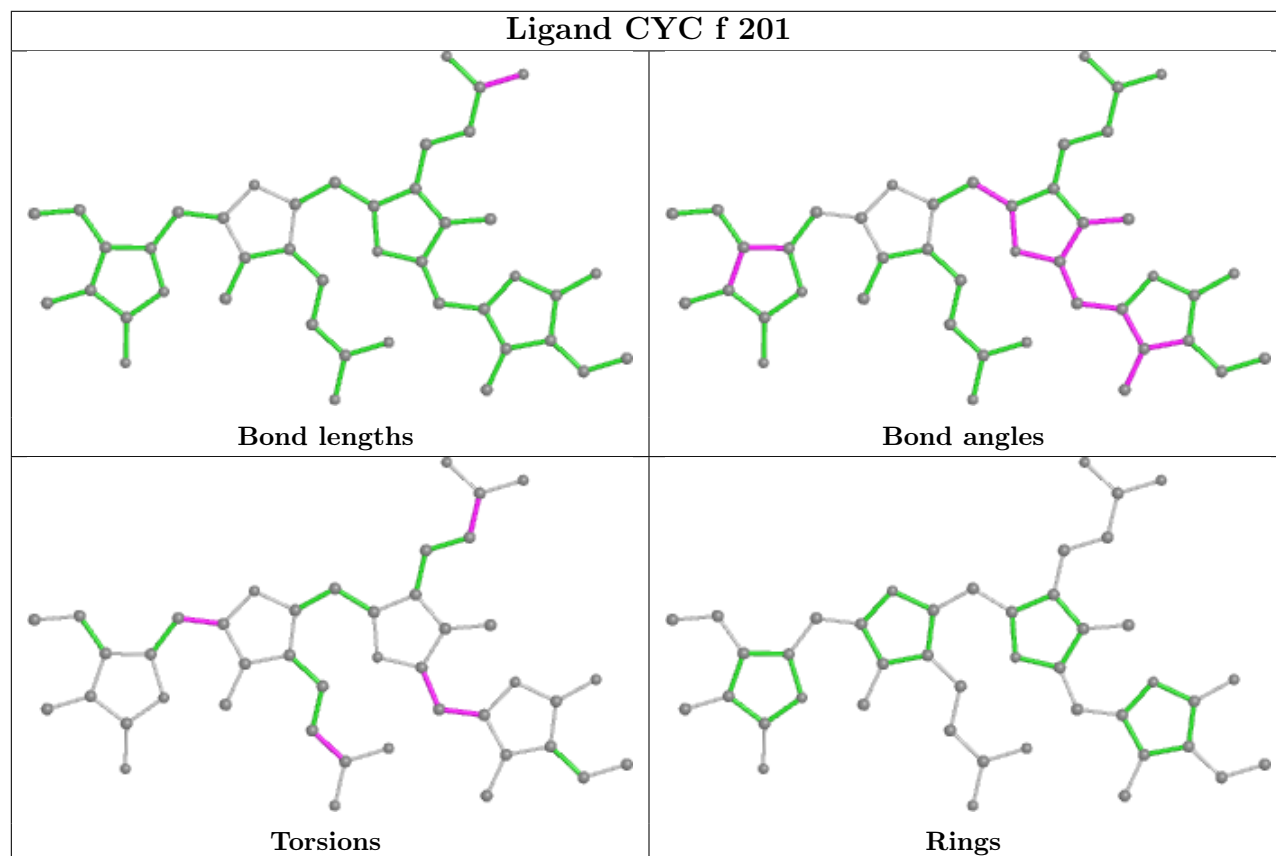
Ligand CYC r 201



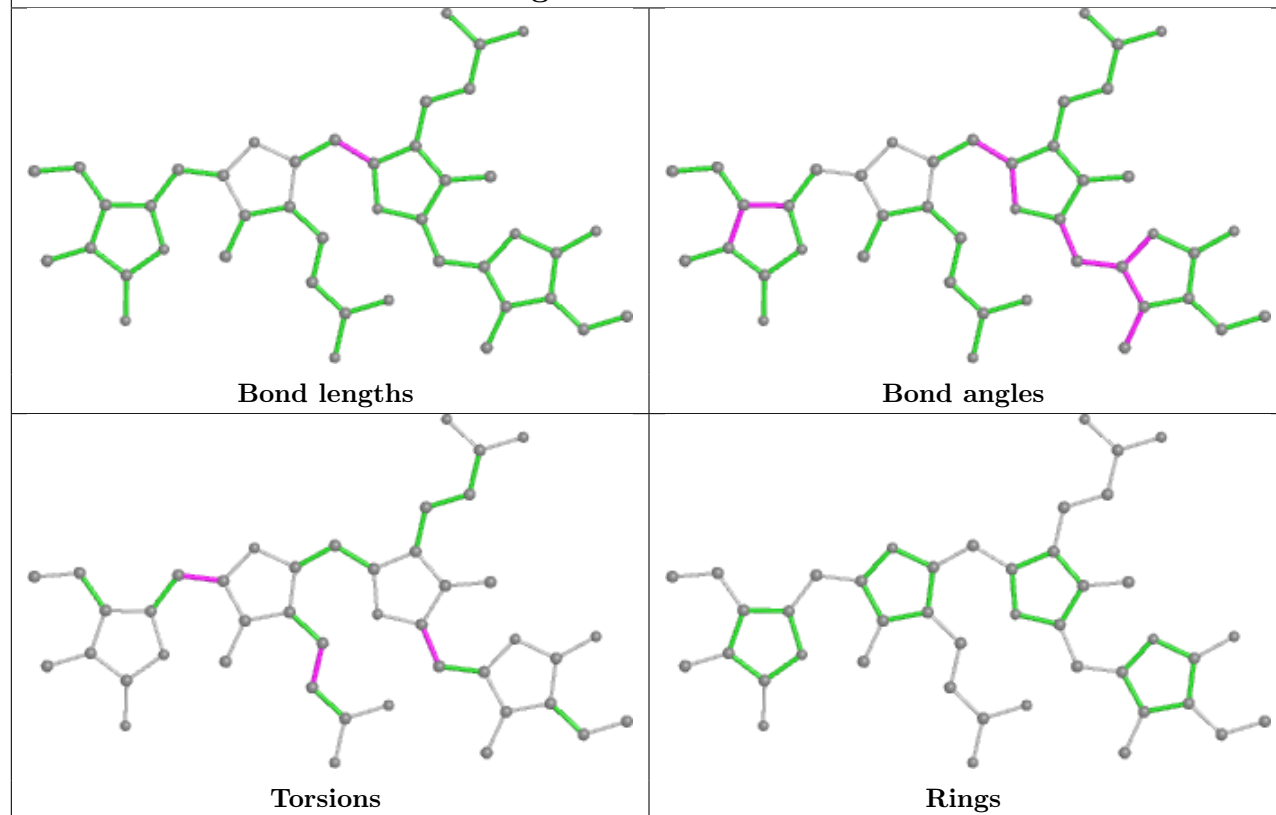
Ligand CYC p 201



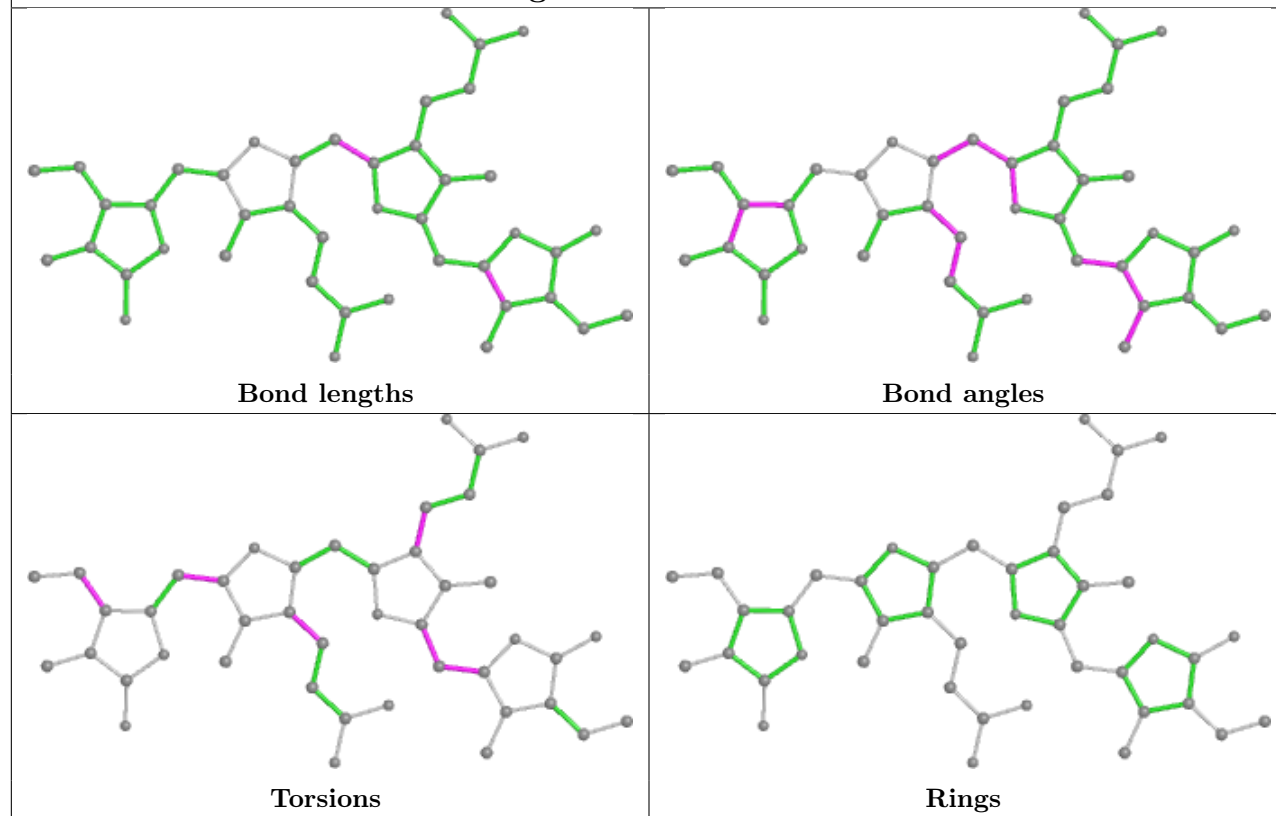
Ligand CYC f 201



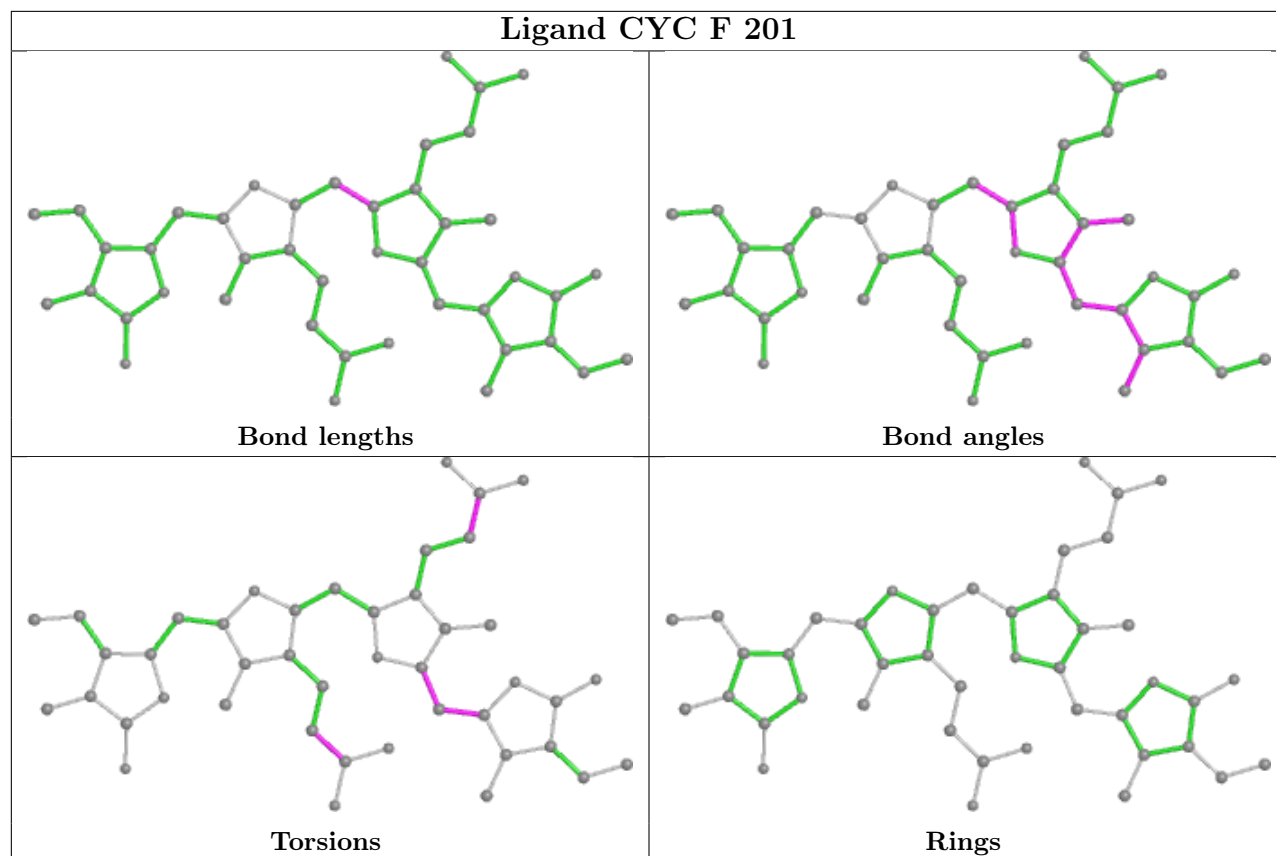
Ligand CYC E 201



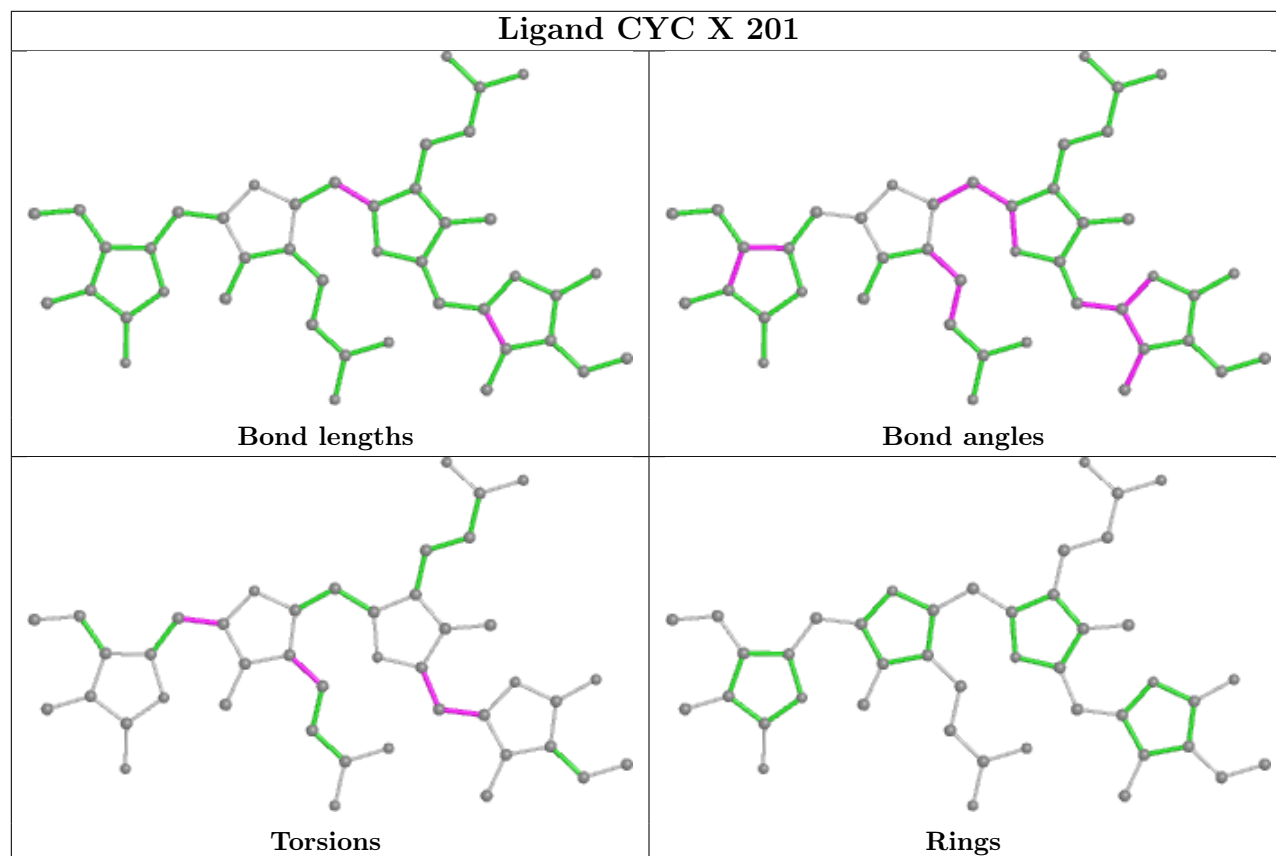
Ligand CYC H 201



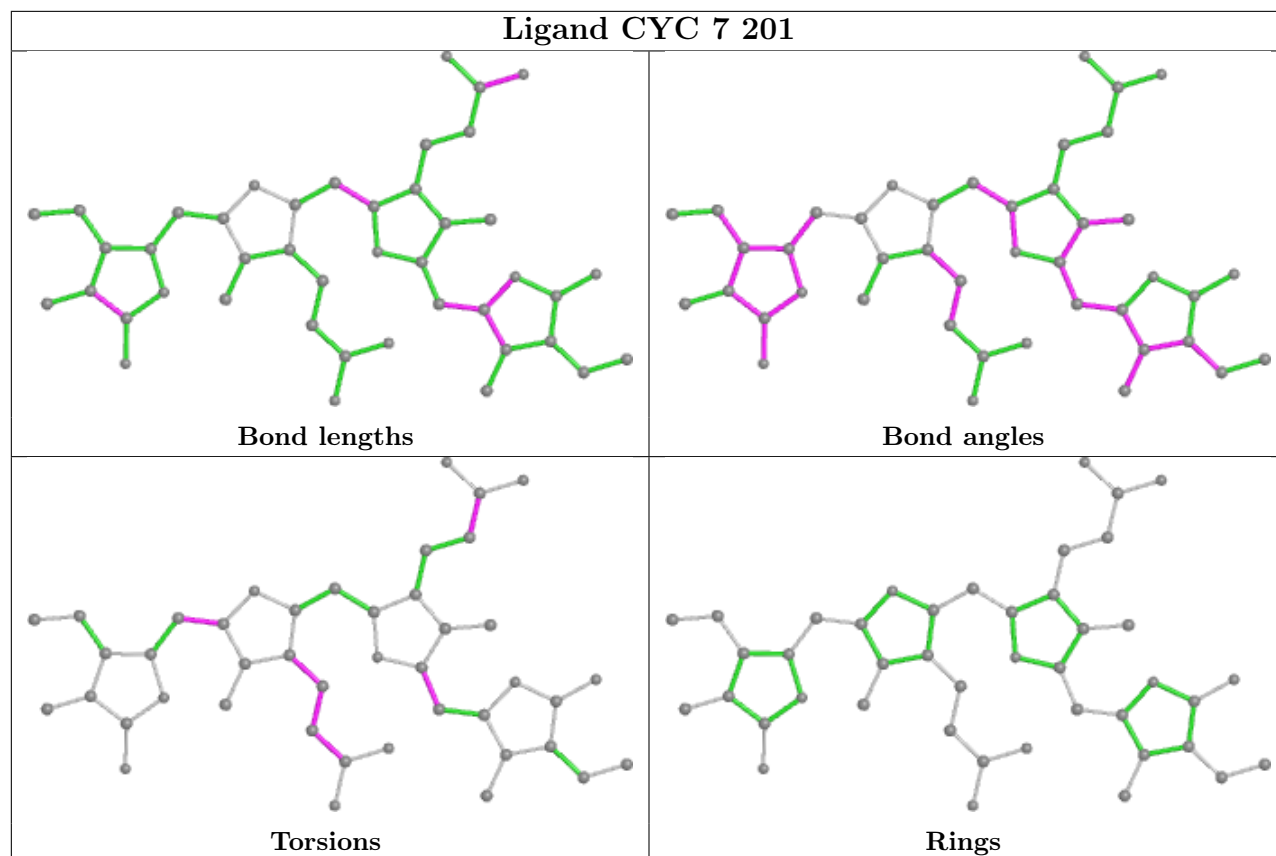
Ligand CYC F 201



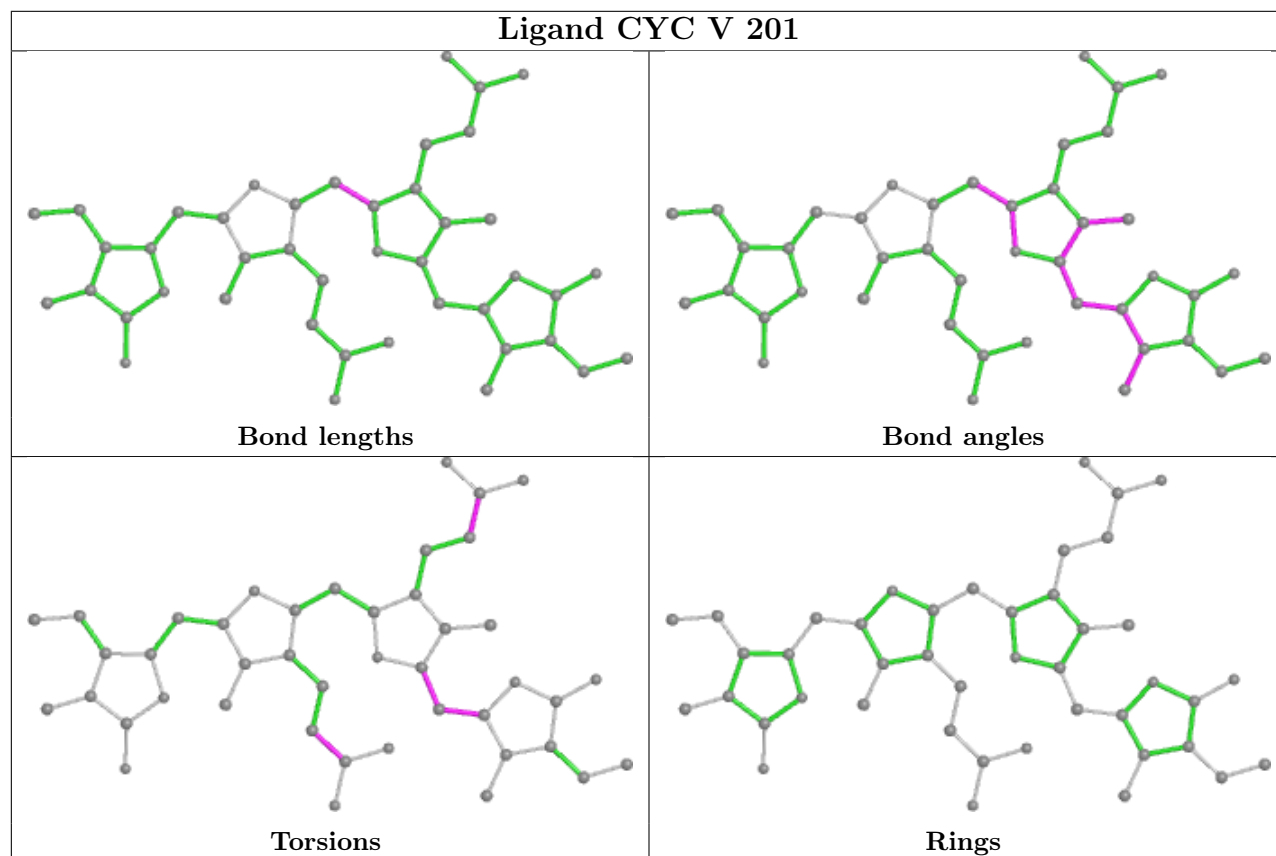
Ligand CYC X 201



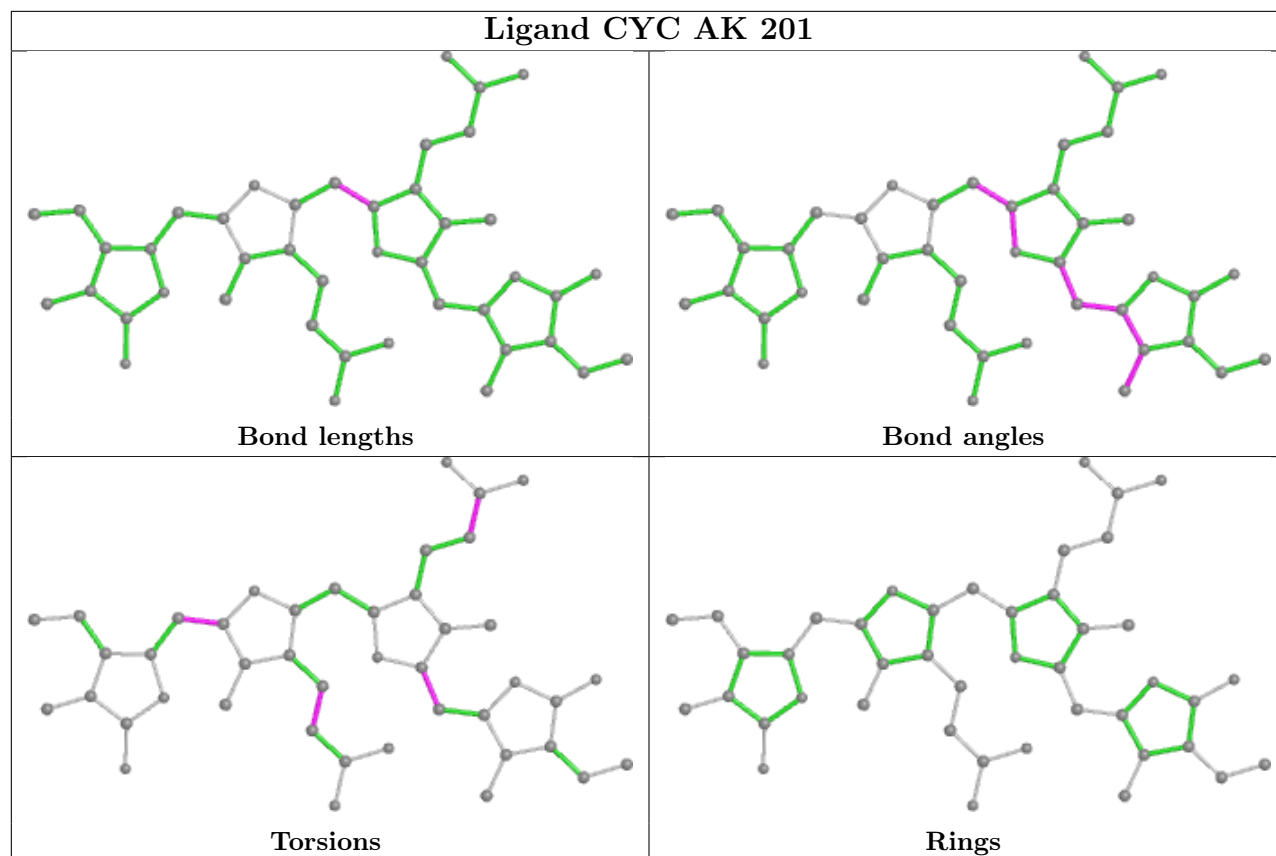
Ligand CYC 7 201



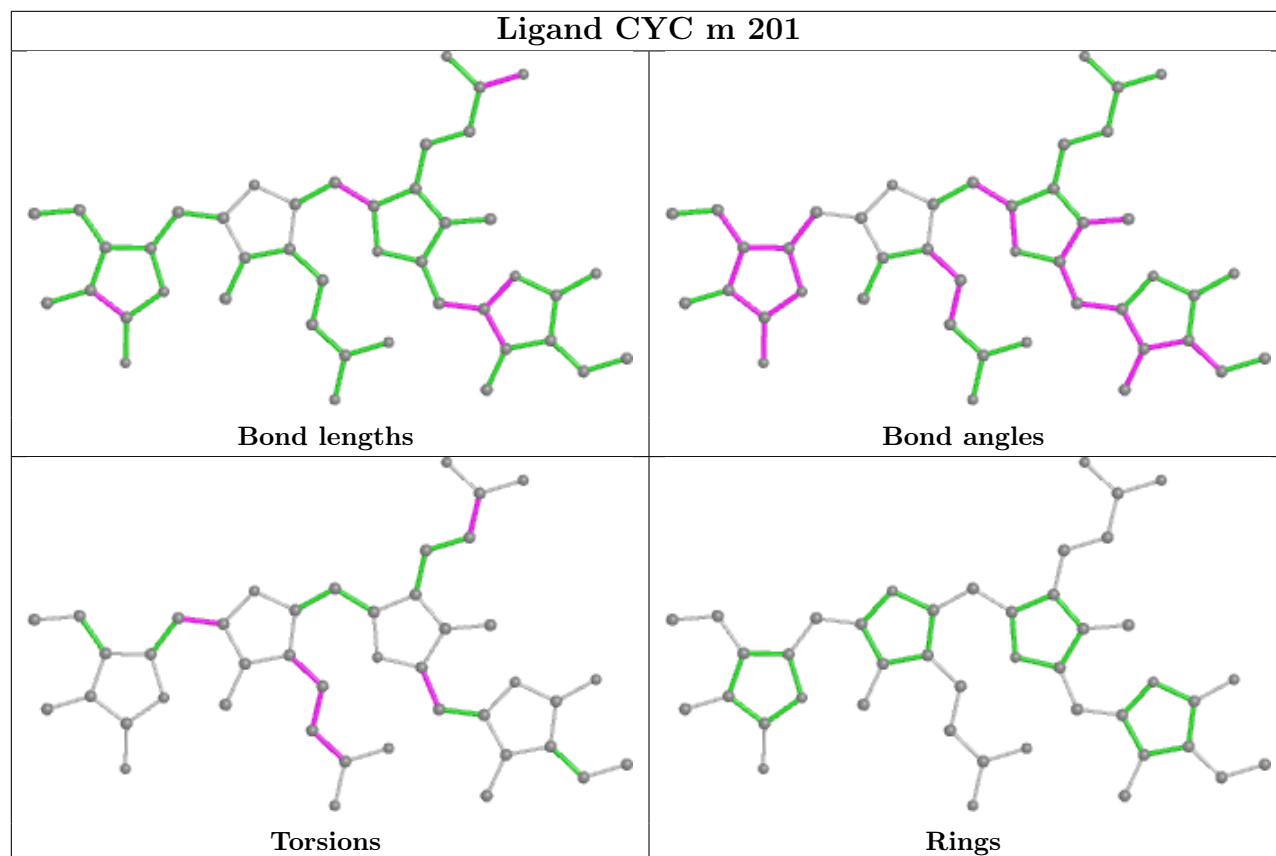
Ligand CYC V 201

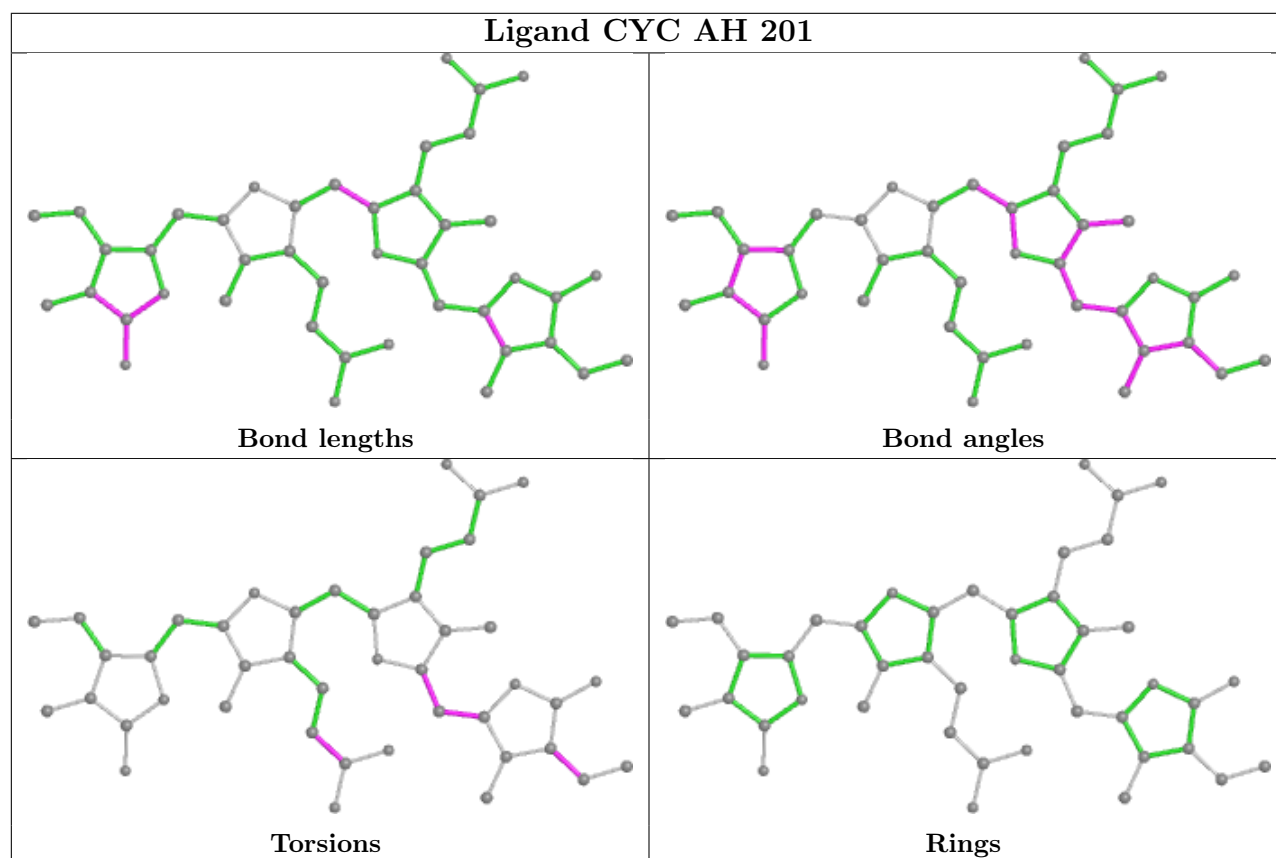
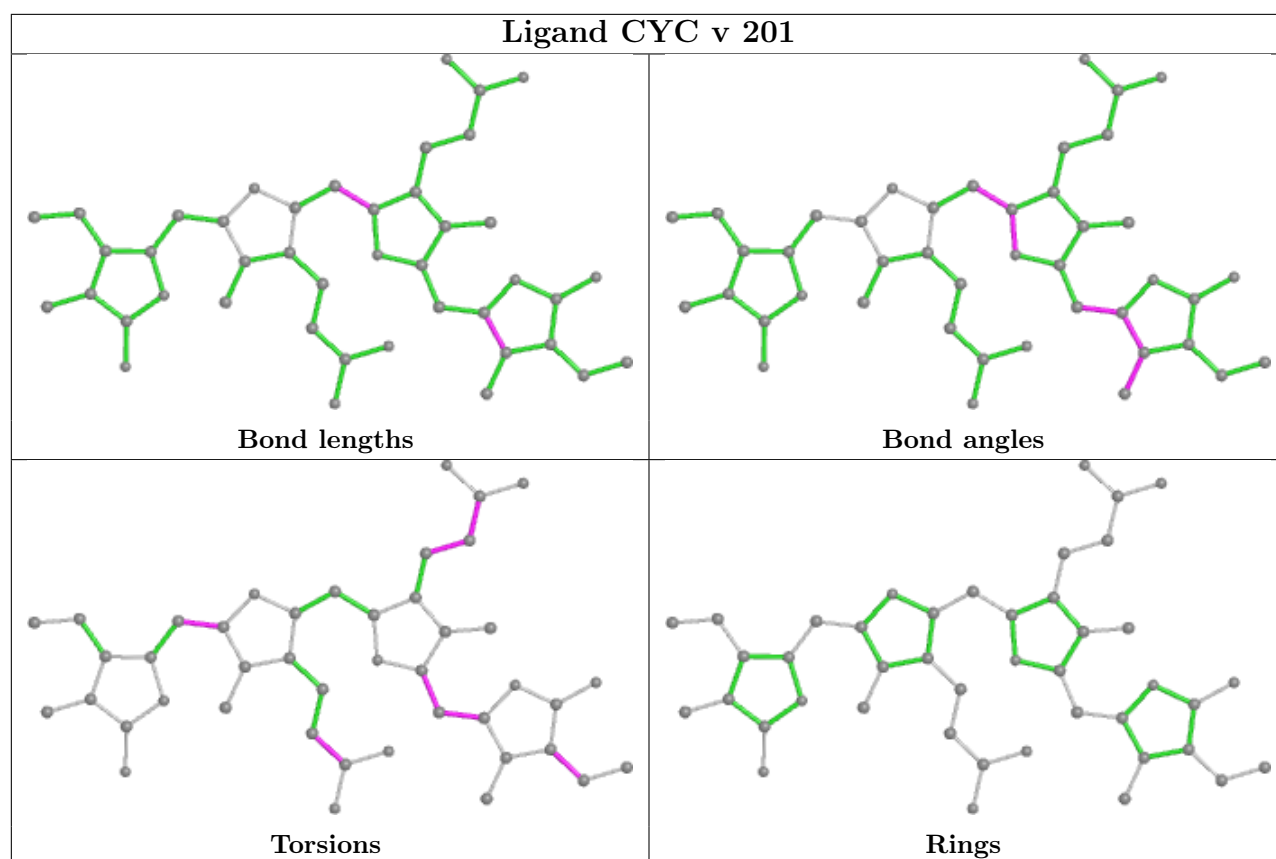


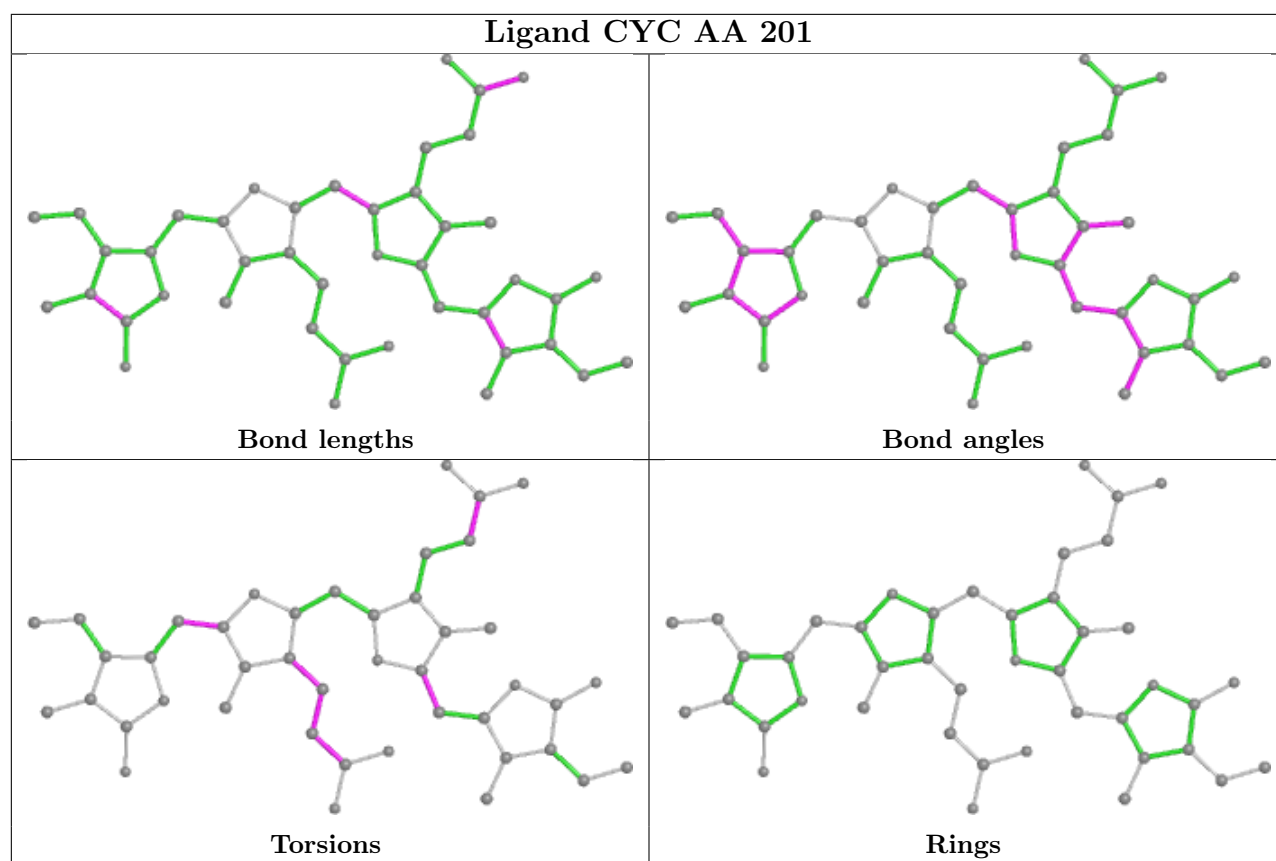
Ligand CYC AK 201



Ligand CYC m 201







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

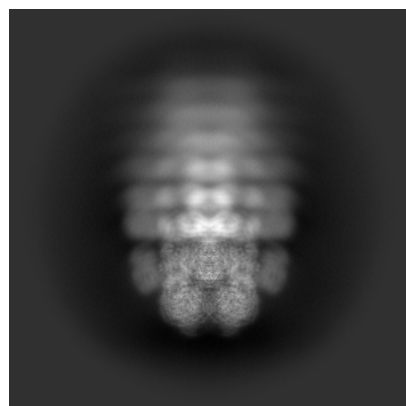
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64815. These allow visual inspection of the internal detail of the map and identification of artifacts.

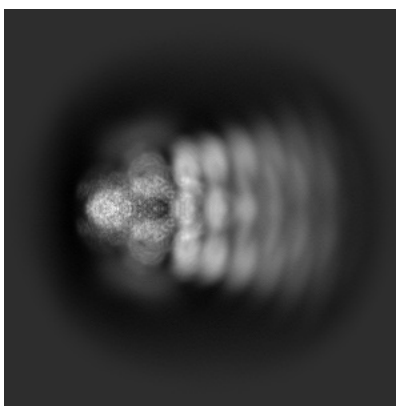
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

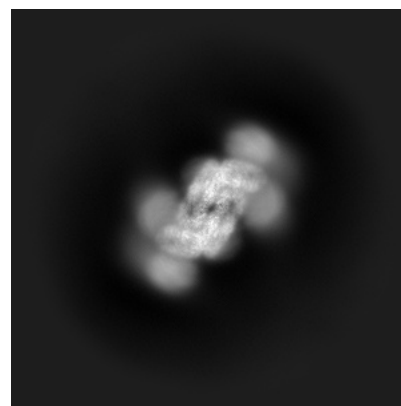
6.1.1 Primary map



X

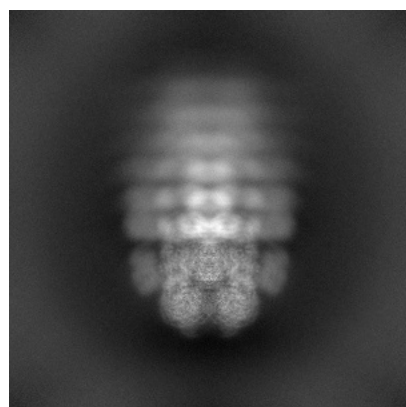


Y

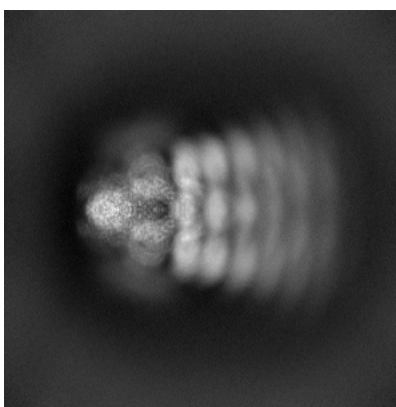


Z

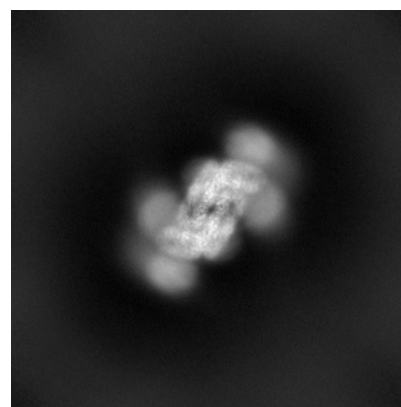
6.1.2 Raw map



X



Y

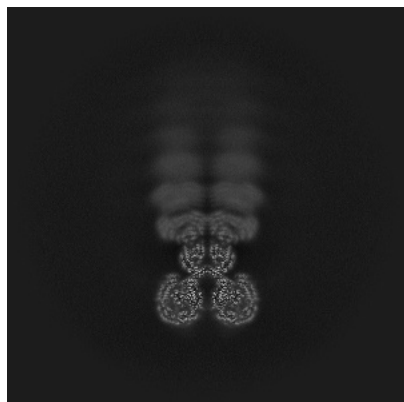


Z

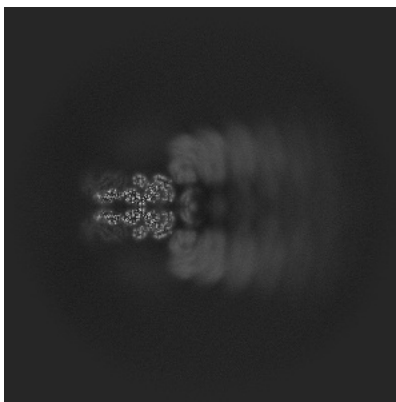
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

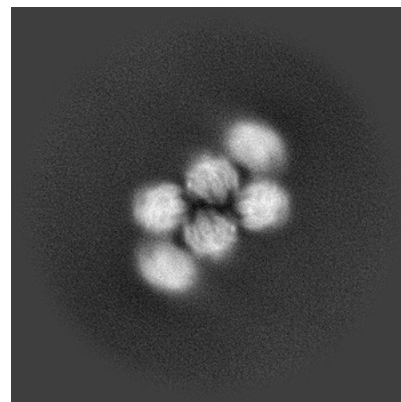
6.2.1 Primary map



X Index: 336

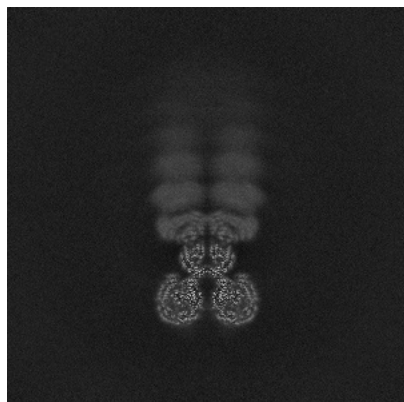


Y Index: 336

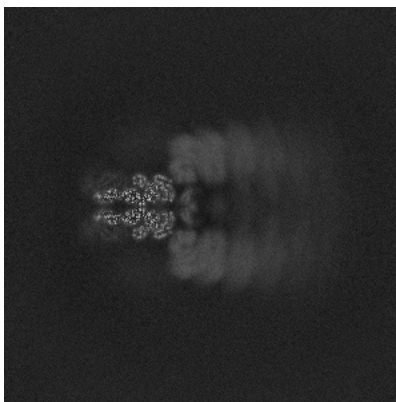


Z Index: 336

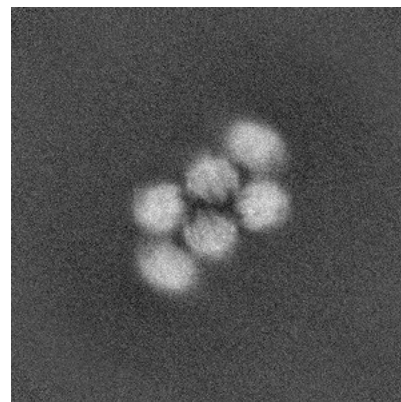
6.2.2 Raw map



X Index: 336



Y Index: 336

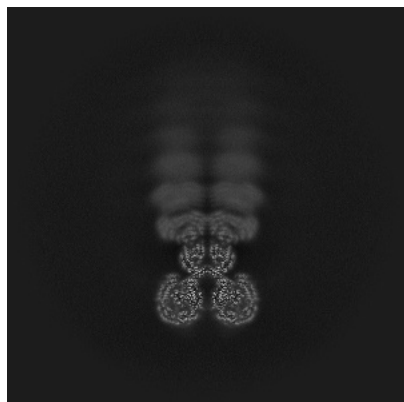


Z Index: 336

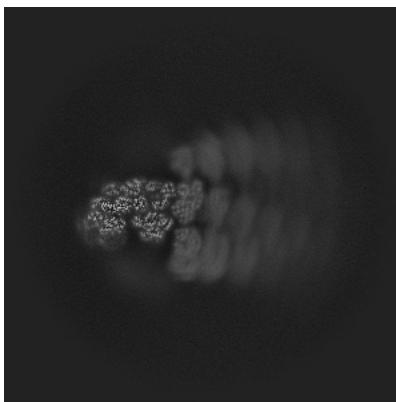
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

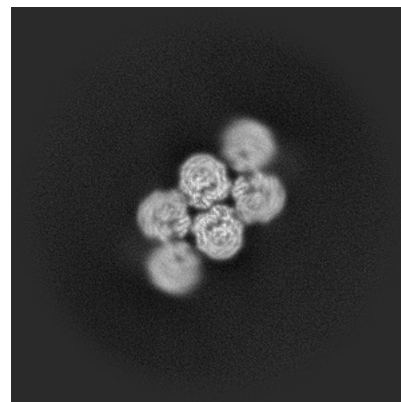
6.3.1 Primary map



X Index: 336

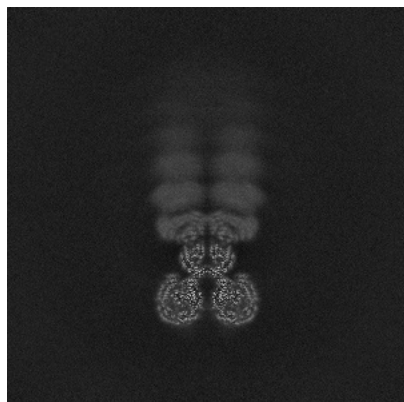


Y Index: 316

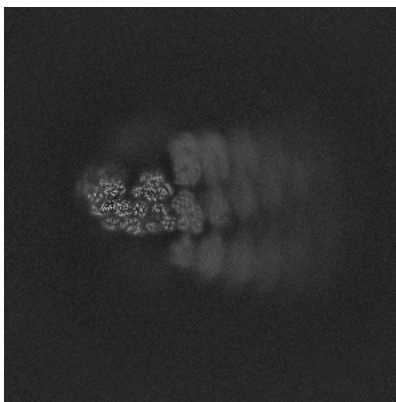


Z Index: 307

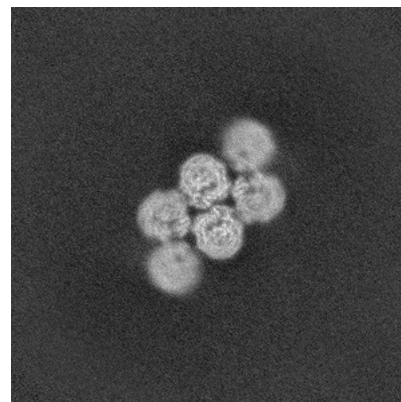
6.3.2 Raw map



X Index: 336



Y Index: 356

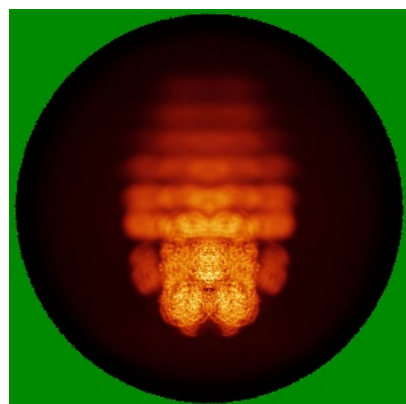


Z Index: 307

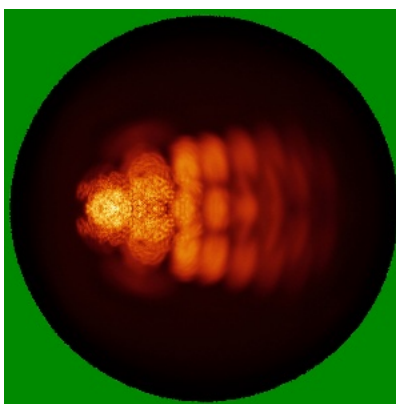
The images above show the largest variance slices of the map in three orthogonal directions.

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

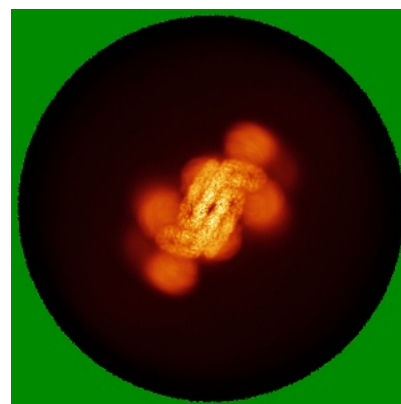
6.4.1 Primary map



X

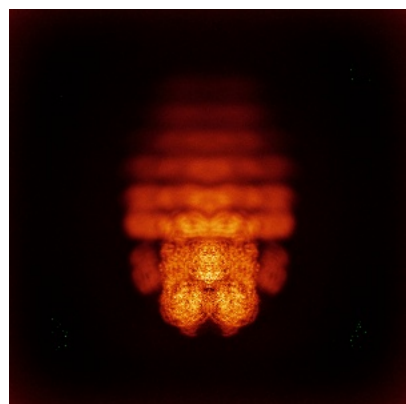


Y

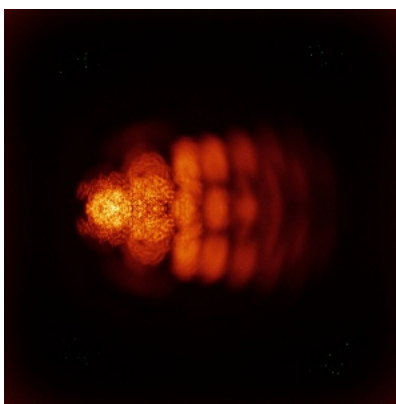


Z

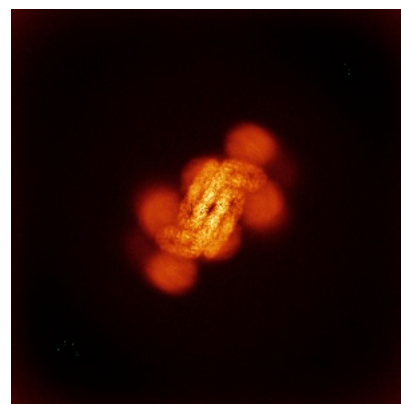
6.4.2 Raw map



X



Y



Z

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

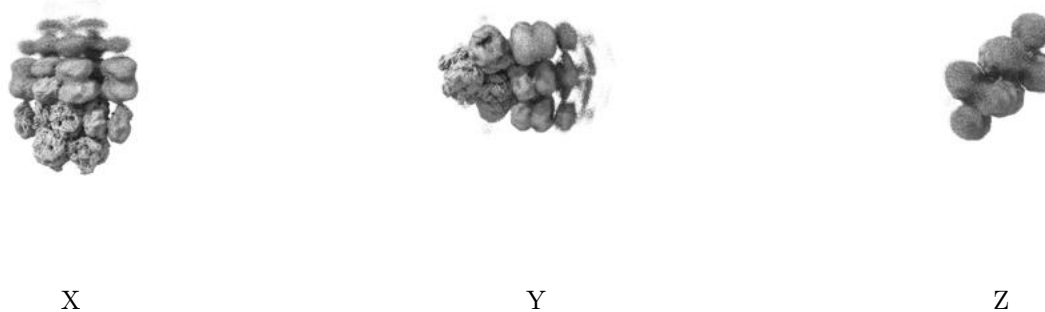
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

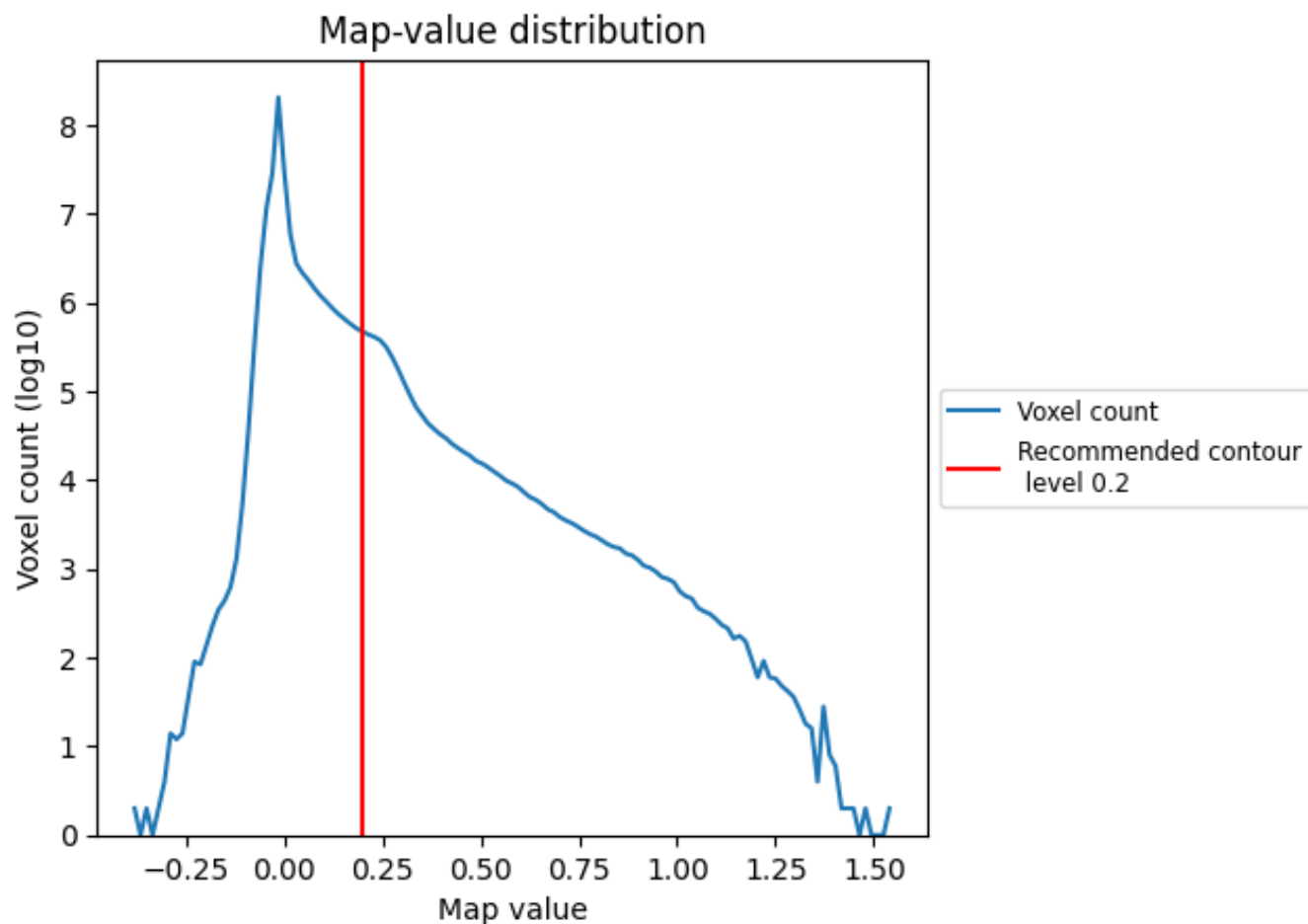
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

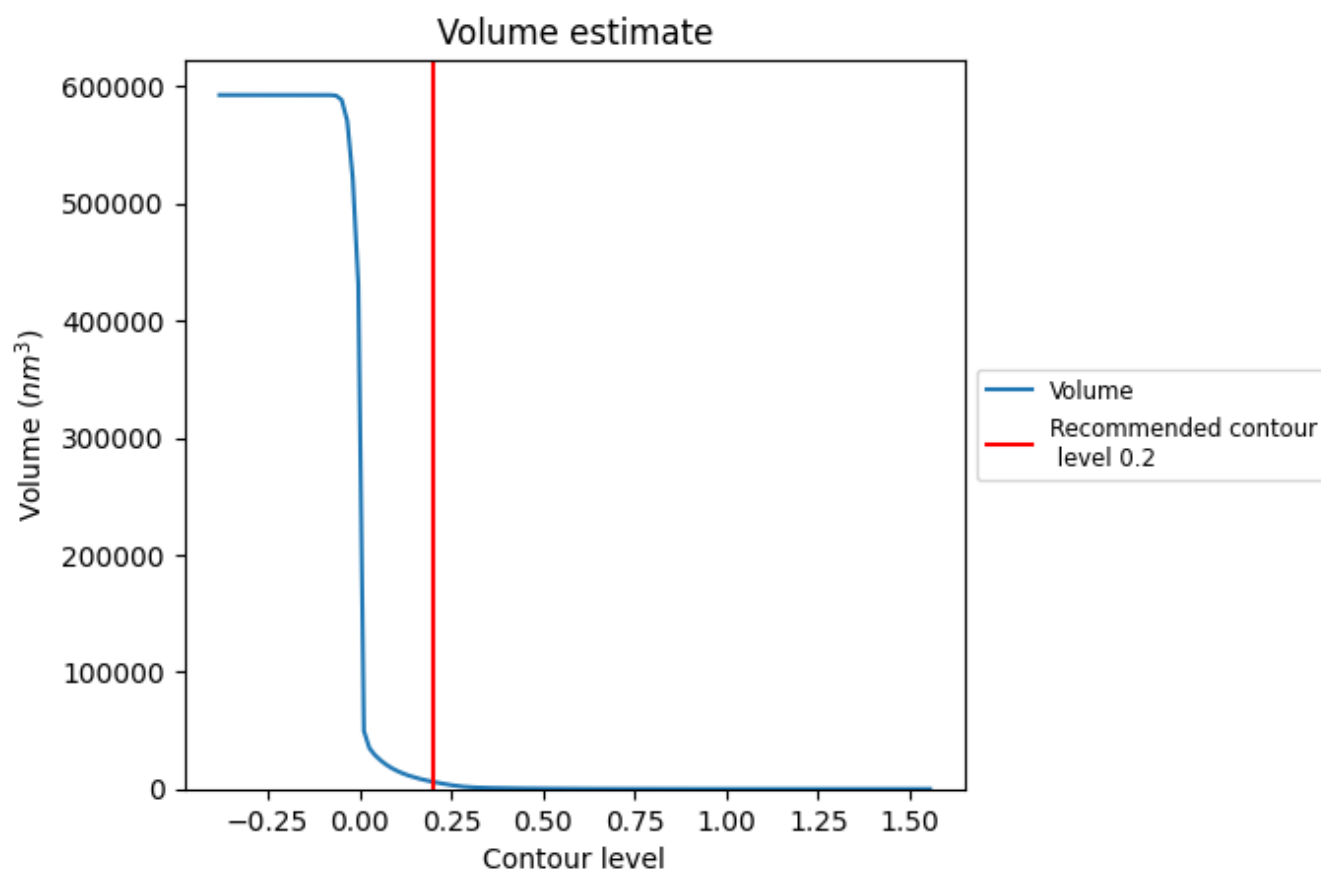
This section contains the results of statistical analysis of the map.

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.

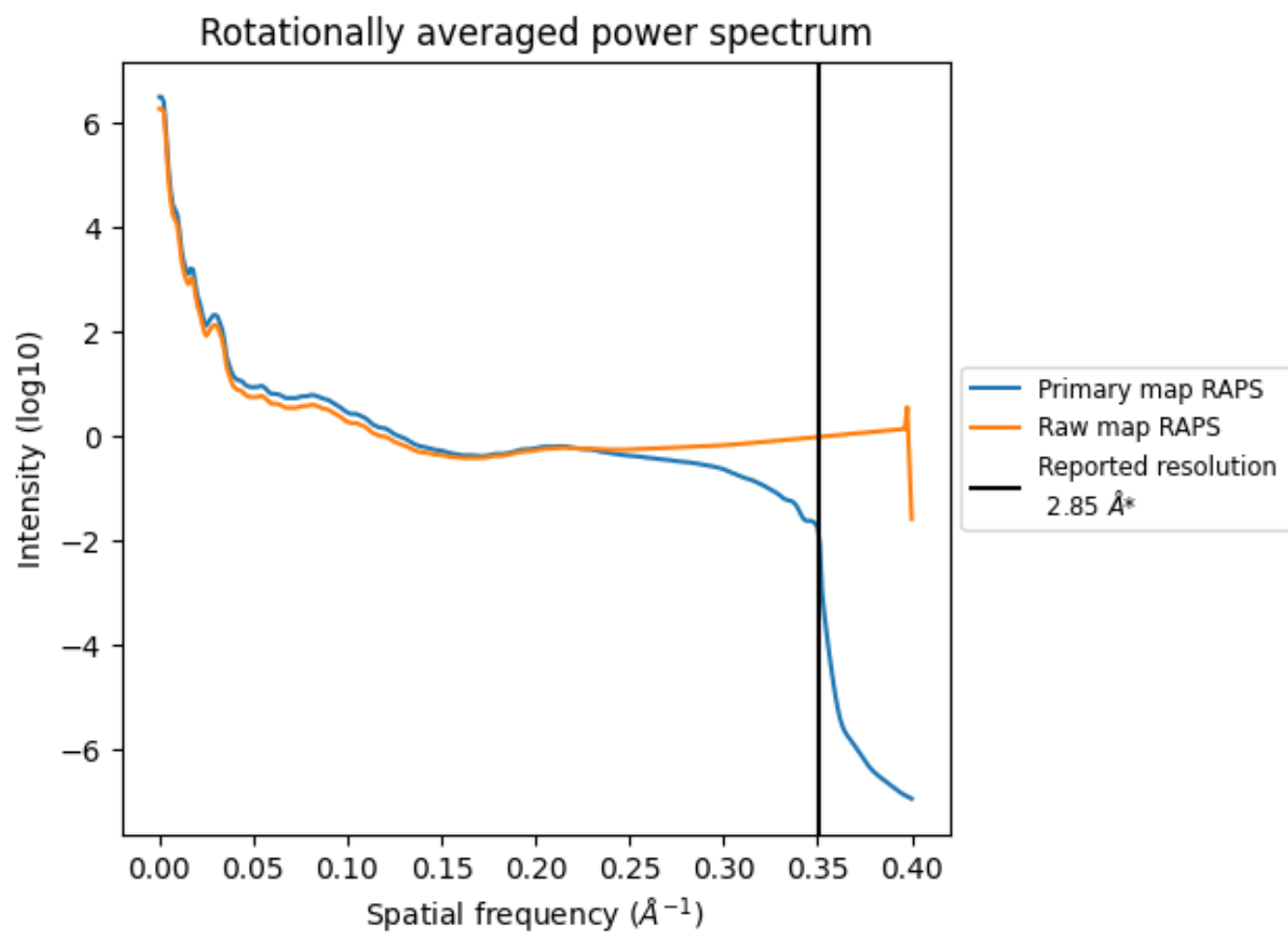
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6137 nm^3 ; this corresponds to an approximate mass of 5544 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 ⓘ

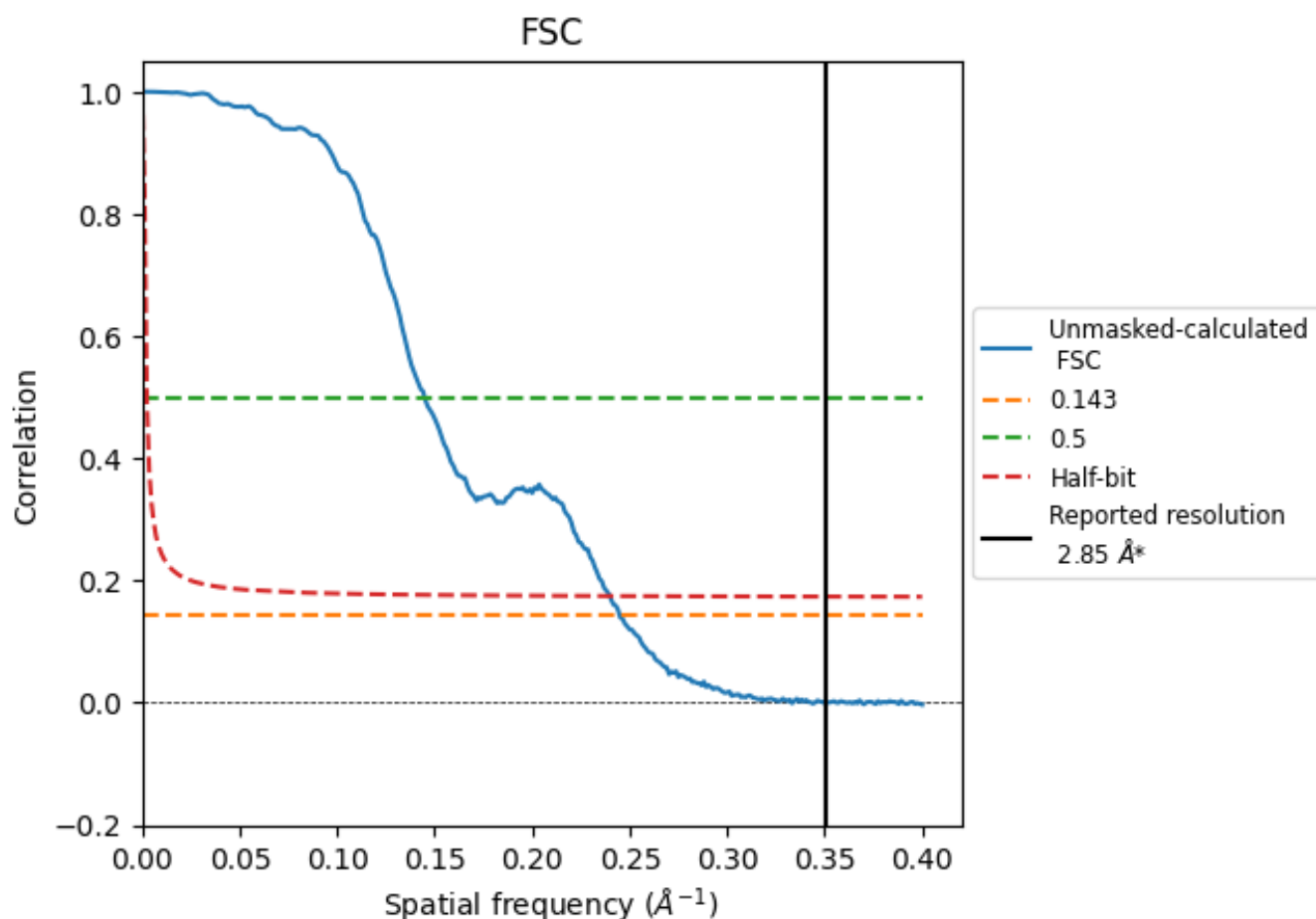


*Reported resolution corresponds to spatial frequency of 0.351 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.351 \AA^{-1}

8.2 Resolution estimates [i](#)

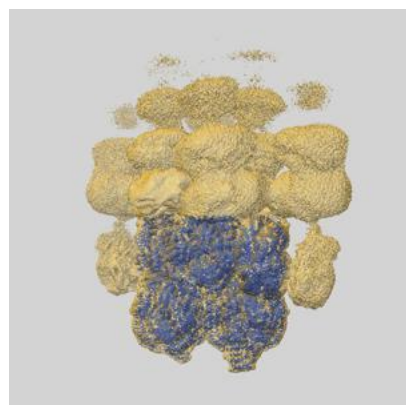
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.08	6.90	4.17

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.08 differs from the reported value 2.85 by more than 10 %

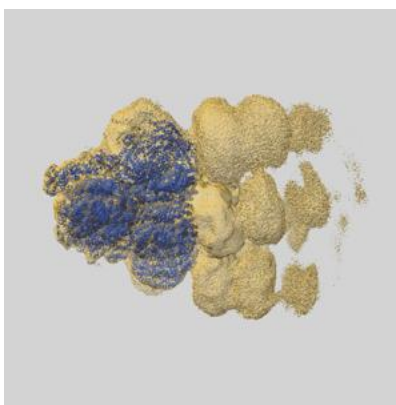
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-64815 and PDB model 9V7J. Per-residue inclusion information can be found in section [3](#) on page [17](#).

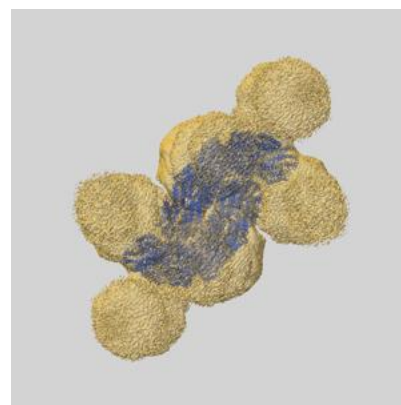
9.1 Map-model overlay [i](#)



X



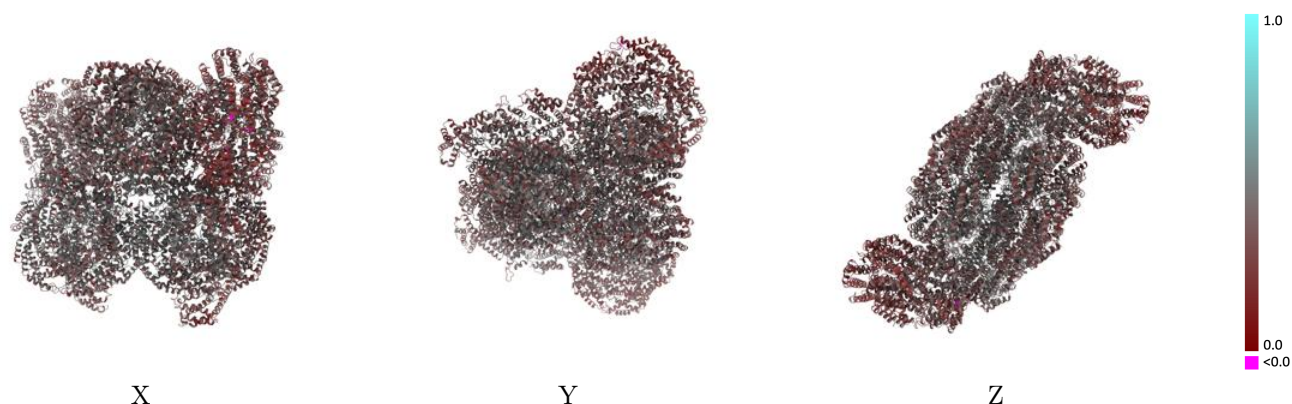
Y



Z

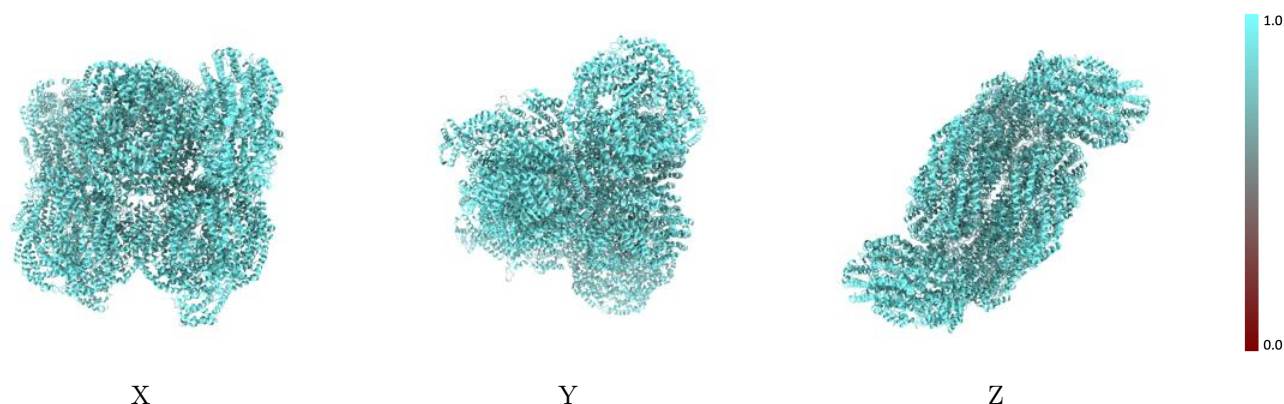
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



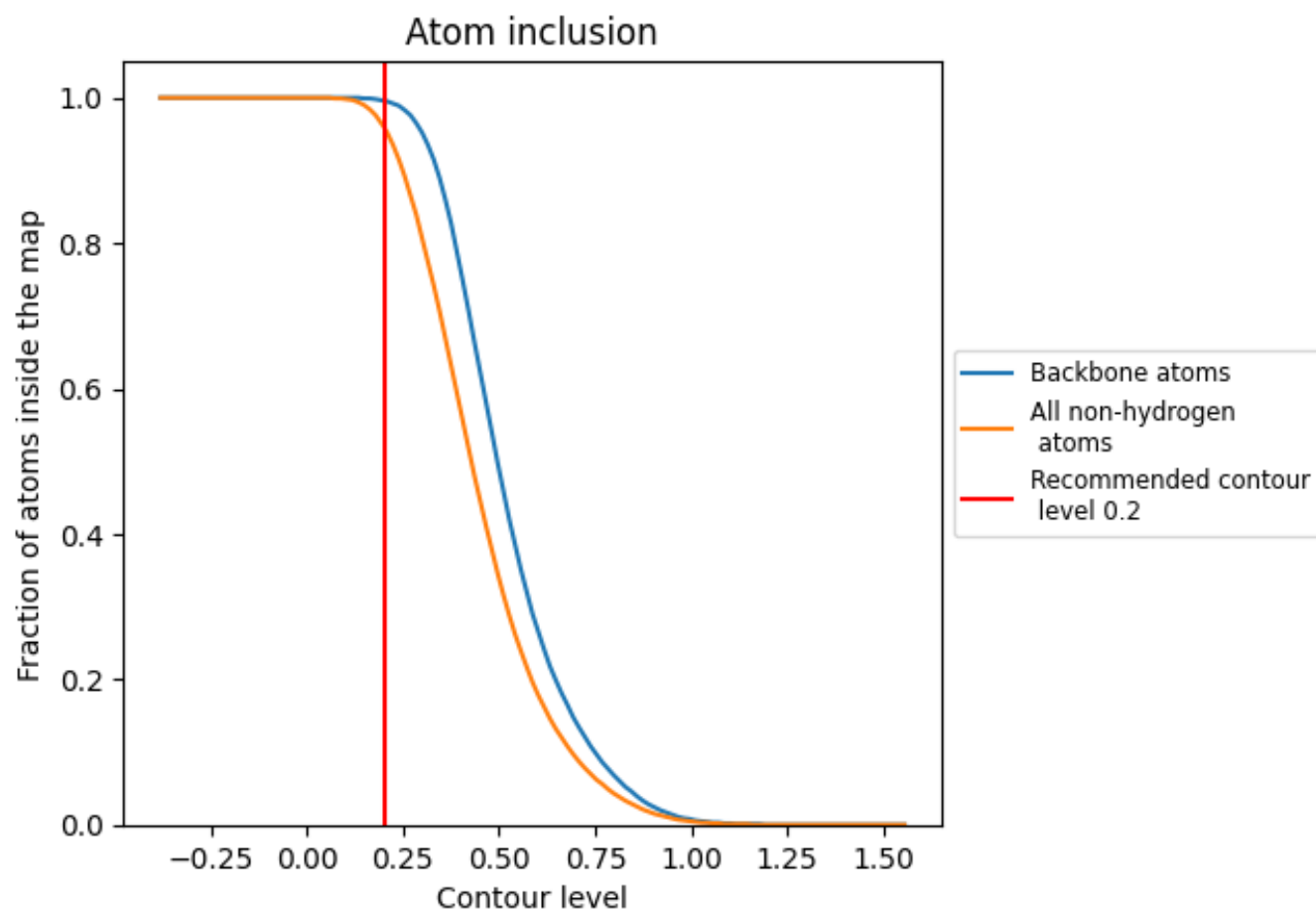
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9600	 0.3760
0	 0.9740	 0.3860
1	 0.9550	 0.3720
2	 0.9810	 0.3800
3	 0.9780	 0.4030
4	 0.9800	 0.3880
5	 0.9880	 0.4310
6	 0.9940	 0.4490
7	 0.9530	 0.4270
8	 0.9660	 0.4680
9	 0.9280	 0.4050
A	 0.9620	 0.4140
AA	 0.9590	 0.4480
AB	 0.9520	 0.4410
AC	 0.9380	 0.3750
AD	 0.9720	 0.3660
AE	 0.9560	 0.3680
AF	 0.9630	 0.3560
AG	 0.9280	 0.3580
AH	 0.9620	 0.4350
AI	 0.9470	 0.3900
AJ	 0.9330	 0.3880
AK	 0.9170	 0.3340
AL	 0.9540	 0.3880
AM	 0.9600	 0.4220
AN	 0.9390	 0.4140
AO	 0.9290	 0.3440
AP	 0.9630	 0.3450
AQ	 0.9450	 0.3740
AR	 0.9560	 0.3650
AS	 0.9310	 0.3680
AT	 0.9620	 0.4600
AU	 0.9190	 0.3490
AV	 0.9380	 0.4000
AW	 0.9340	 0.3640































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Chain	Atom inclusion	Q-score
AX	 0.9390	 0.3580
AY	 0.9850	 0.3500
AZ	 0.9830	 0.3190
Aa	 0.9590	 0.4100
Ab	 0.9750	 0.3750
Ac	 0.8910	 0.3650
Ad	 0.8800	 0.3390
C	 0.9610	 0.3940
E	 0.9890	 0.3420
F	 0.9860	 0.2820
G	 0.9730	 0.2440
H	 0.9540	 0.3200
I	 0.9600	 0.2930
J	 0.9480	 0.2580
K	 0.9710	 0.2310
L	 0.9760	 0.2740
M	 0.9530	 0.3620
N	 0.9250	 0.3500
O	 0.9490	 0.3010
P	 0.9800	 0.3520
Q	 0.9480	 0.3800
R	 0.9240	 0.4000
S	 0.9360	 0.3100
T	 0.9710	 0.3730
U	 0.9800	 0.3720
V	 0.9910	 0.2960
W	 0.9810	 0.2550
X	 0.9530	 0.3520
Y	 0.9660	 0.3250
Z	 0.9460	 0.2900
a	 0.9720	 0.2440
b	 0.9800	 0.3000
c	 0.9800	 0.3640
d	 0.9780	 0.3660
e	 0.9780	 0.3730
f	 0.9860	 0.4090
g	 0.9830	 0.3930
h	 0.9800	 0.4500
i	 0.9620	 0.3810
j	 0.9770	 0.3810
k	 0.9150	 0.3740
l	 0.9640	 0.3770

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Chain	Atom inclusion	Q-score
m	 0.9650	 0.4410
n	 0.9430	 0.4230
o	 0.9610	 0.3260
p	 0.9560	 0.4240
q	 0.9670	 0.3880
r	 0.9660	 0.4330
s	 0.9690	 0.4130
t	 0.9710	 0.4310
u	 0.9680	 0.4100
v	 0.9660	 0.4010
w	 0.9830	 0.3940
x	 0.9590	 0.4550
y	 0.9860	 0.3990
z	 0.9810	 0.4540