



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:29 AM UTC

PDB ID : 8IMN / pdb_00008imn
EMDB ID : EMD-35570
Title : Rt1I-Rt1II, Rt2'I-Rt2'II, Rt3I-Rt3II cylinder in cyanobacterial phycobilisome from Anthocerotibacter panamensis (Cluster F)
Authors : Wang, C.H.; Yang, C.H.; Wu, H.Y.; Jiang, H.W.; Ho, M.C.; Ho, M.Y.
Deposited on : 2023-03-07
Resolution : 3.07 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

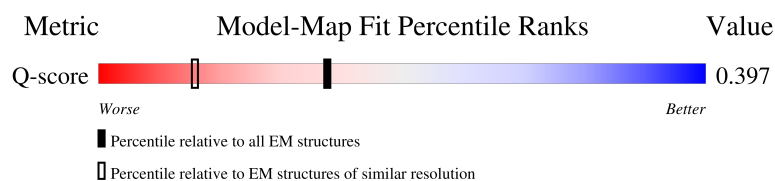
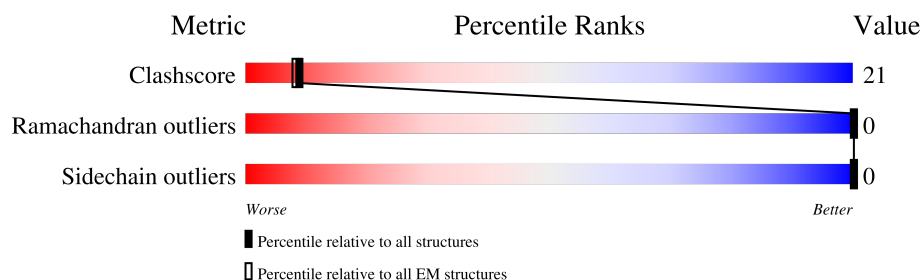
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

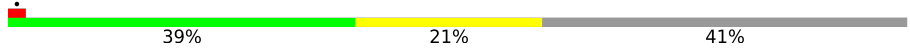
The reported resolution of this entry is 3.07 Å.

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



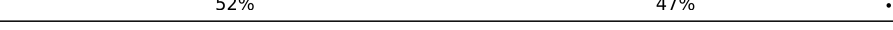
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13977 (2.57 - 3.57)

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	5	1182	
2	A	163	
2	B	163	
2	C	163	

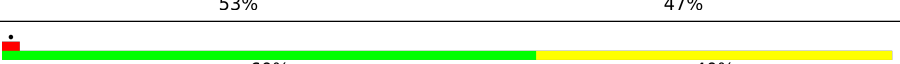
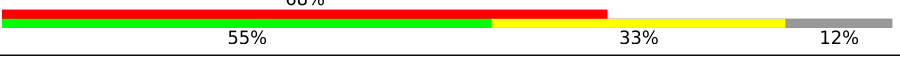
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Mol	Chain	Length	Quality of chain
2	D	163	
2	E	163	
2	F	163	
2	N	163	
2	O	163	
2	P	163	
2	Q	163	
2	R	163	
2	S	163	
2	a	163	
2	b	163	
2	c	163	
2	d	163	
2	e	163	
2	f	163	
3	G	172	
3	H	172	
3	I	172	
3	J	172	
3	K	172	
3	L	172	
3	T	172	
3	U	172	
3	V	172	
3	W	172	

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Mol	Chain	Length	Quality of chain
3	X	172	
3	Y	172	
3	g	172	
3	h	172	
3	i	172	
3	j	172	
3	k	172	
3	l	172	
4	M	78	
4	Z	78	
4	m	78	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 55489 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 CpcN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	702	Total	C	N	O	S	0	0
			5659	3562	995	1093	9		

- Molecule 2 is a protein called CpcA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	B	163	Total	C	N	O	S	0	0
			1262	804	217	239	2		
2	C	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	D	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	E	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	F	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	N	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	O	163	Total	C	N	O	S	0	0
			1262	804	217	239	2		
2	P	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	Q	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	R	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	S	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	a	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	b	163	Total	C	N	O	S	0	0
			1262	804	217	239	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	d	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	e	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	f	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		

- Molecule 3 is a protein called CpcB.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	H	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	I	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	J	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	K	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	L	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	T	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	U	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	V	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	W	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	X	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	Y	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	g	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	h	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	i	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		

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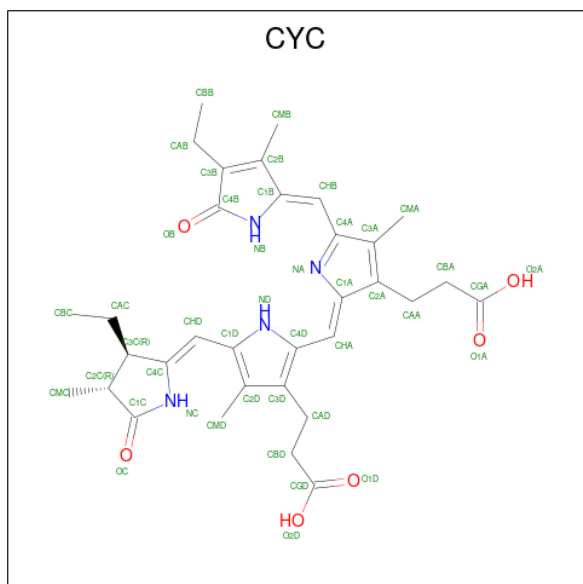
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	j	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	k	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	l	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		

- Molecule 4 is a protein called CpcD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	69	Total	C	N	O	S	0	0
			546	345	101	99	1		
4	Z	69	Total	C	N	O	S	0	0
			546	345	101	99	1		
4	m	69	Total	C	N	O	S	0	0
			546	345	101	99	1		

- Molecule 5 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			43	33	4	6	
5	C	1	Total	C	N	O	0
			43	33	4	6	
5	D	1	Total	C	N	O	0
			43	33	4	6	
5	E	1	Total	C	N	O	0
			43	33	4	6	
5	F	1	Total	C	N	O	0
			43	33	4	6	
5	G	1	Total	C	N	O	0
			43	33	4	6	
5	G	1	Total	C	N	O	0
			43	33	4	6	
5	H	1	Total	C	N	O	0
			43	33	4	6	
5	H	1	Total	C	N	O	0
			43	33	4	6	
5	I	1	Total	C	N	O	0
			43	33	4	6	
5	I	1	Total	C	N	O	0
			43	33	4	6	
5	J	1	Total	C	N	O	0
			43	33	4	6	
5	J	1	Total	C	N	O	0
			43	33	4	6	
5	K	1	Total	C	N	O	0
			43	33	4	6	
5	K	1	Total	C	N	O	0
			43	33	4	6	
5	L	1	Total	C	N	O	0
			43	33	4	6	
5	N	1	Total	C	N	O	0
			43	33	4	6	
5	O	1	Total	C	N	O	0
			43	33	4	6	
5	P	1	Total	C	N	O	0
			43	33	4	6	
5	Q	1	Total	C	N	O	0
			43	33	4	6	
5	R	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
5	S	1	Total 43	C 33	N 4	O 6	0
5	T	1	Total 43	C 33	N 4	O 6	0
5	T	1	Total 43	C 33	N 4	O 6	0
5	U	1	Total 43	C 33	N 4	O 6	0
5	U	1	Total 43	C 33	N 4	O 6	0
5	V	1	Total 43	C 33	N 4	O 6	0
5	V	1	Total 43	C 33	N 4	O 6	0
5	W	1	Total 43	C 33	N 4	O 6	0
5	W	1	Total 43	C 33	N 4	O 6	0
5	X	1	Total 43	C 33	N 4	O 6	0
5	X	1	Total 43	C 33	N 4	O 6	0
5	Y	1	Total 43	C 33	N 4	O 6	0
5	Y	1	Total 43	C 33	N 4	O 6	0
5	a	1	Total 43	C 33	N 4	O 6	0
5	b	1	Total 43	C 33	N 4	O 6	0
5	c	1	Total 43	C 33	N 4	O 6	0
5	d	1	Total 43	C 33	N 4	O 6	0
5	e	1	Total 43	C 33	N 4	O 6	0
5	f	1	Total 43	C 33	N 4	O 6	0
5	g	1	Total 43	C 33	N 4	O 6	0
5	g	1	Total 43	C 33	N 4	O 6	0

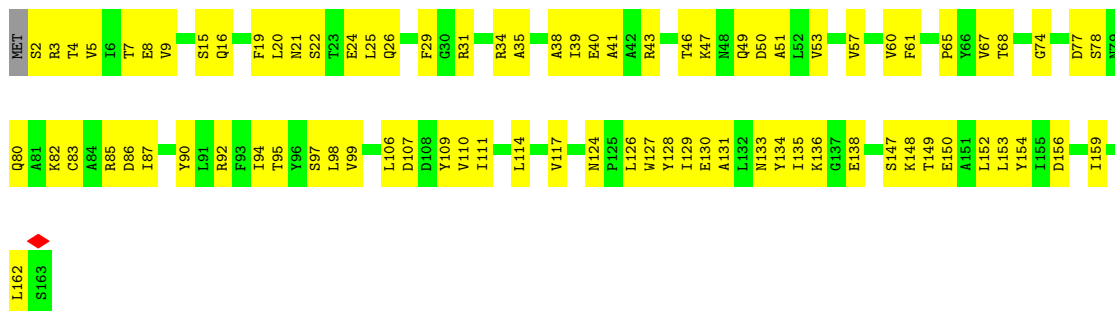
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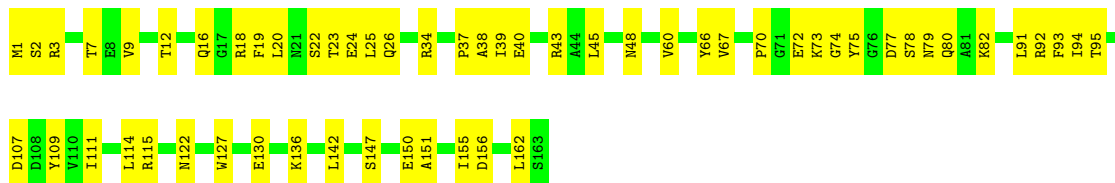
Mol	Chain	Residues	Atoms				AltConf
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			43	33	4	6	
5	h	1	Total	C	N	O	0
			43	33	4	6	
5	i	1	Total	C	N	O	0
			43	33	4	6	
5	i	1	Total	C	N	O	0
			43	33	4	6	
5	j	1	Total	C	N	O	0
			43	33	4	6	
5	j	1	Total	C	N	O	0
			43	33	4	6	
5	k	1	Total	C	N	O	0
			43	33	4	6	
5	k	1	Total	C	N	O	0
			43	33	4	6	
5	l	1	Total	C	N	O	0
			43	33	4	6	

[illegible]

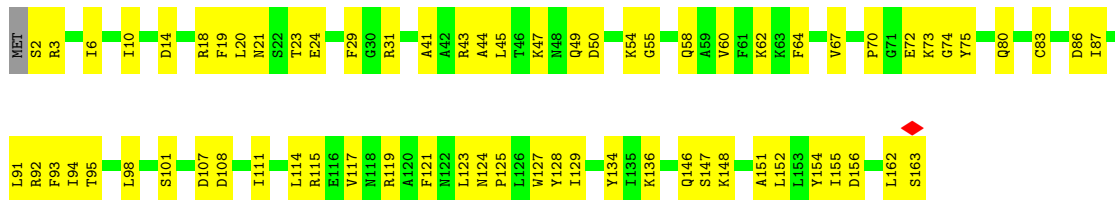
- Molecule 2: CpcA



- Molecule 2: CpcA

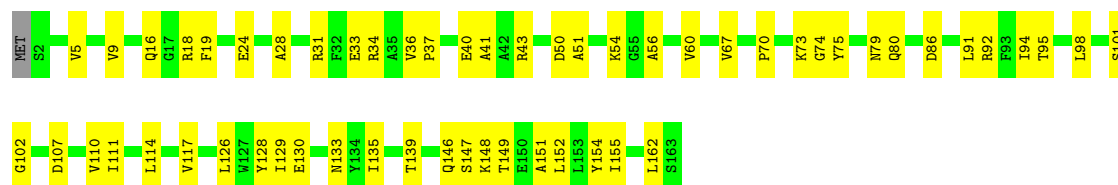


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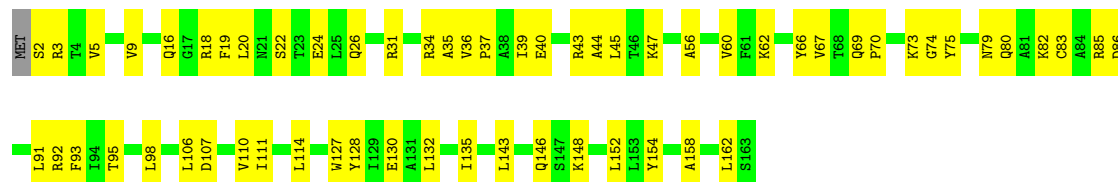
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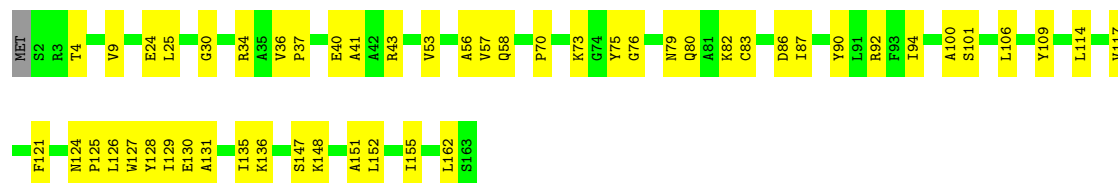
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Chain E: 63% 37%



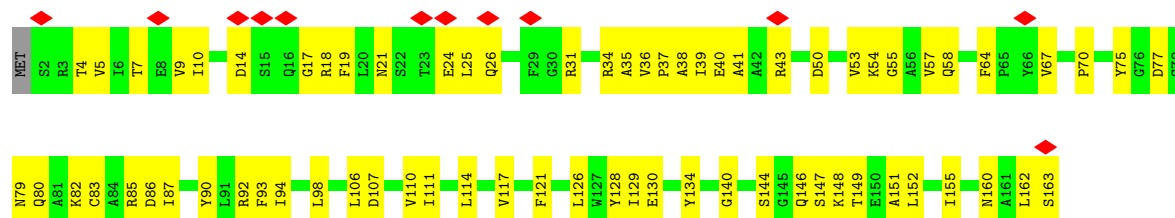
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Chain F: 68% 31%



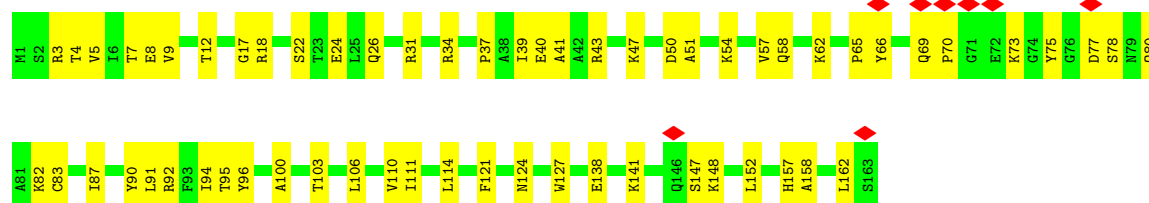
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Chain N: 7% 56% 43%

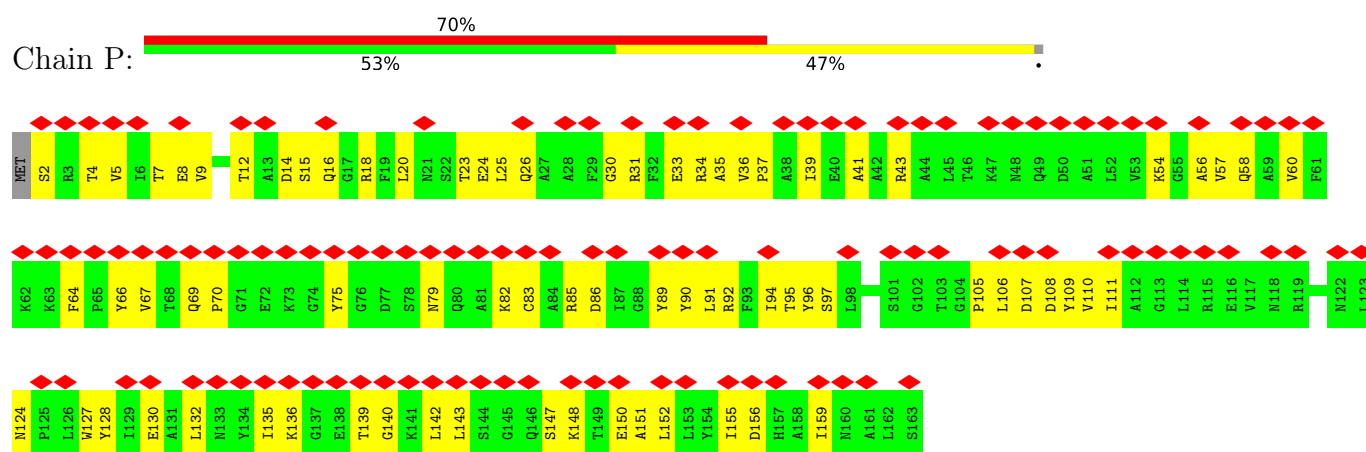


- Molecule 2: CpcA

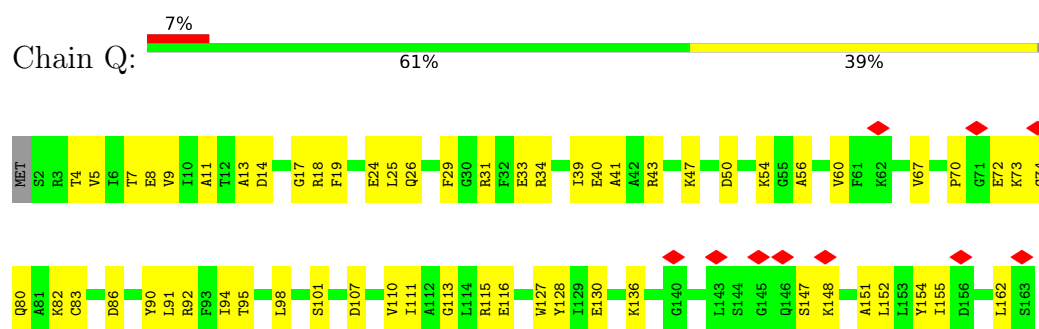
Chain O: 5% 63% 37%



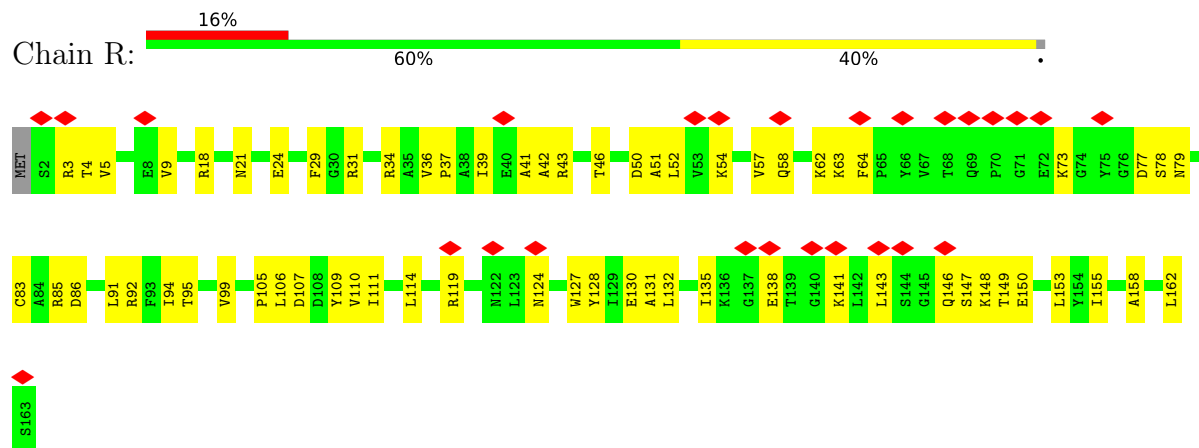
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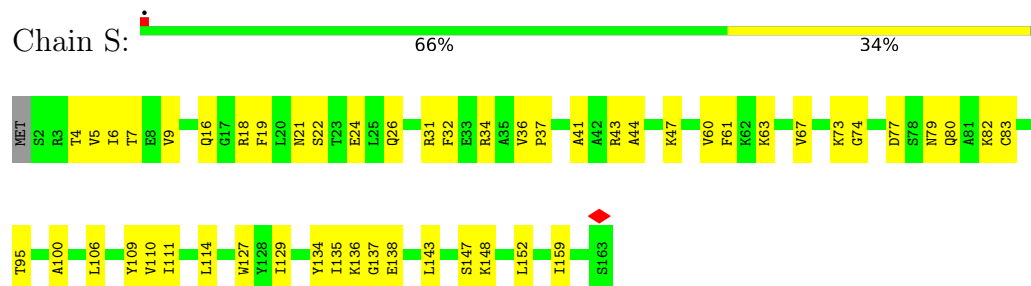
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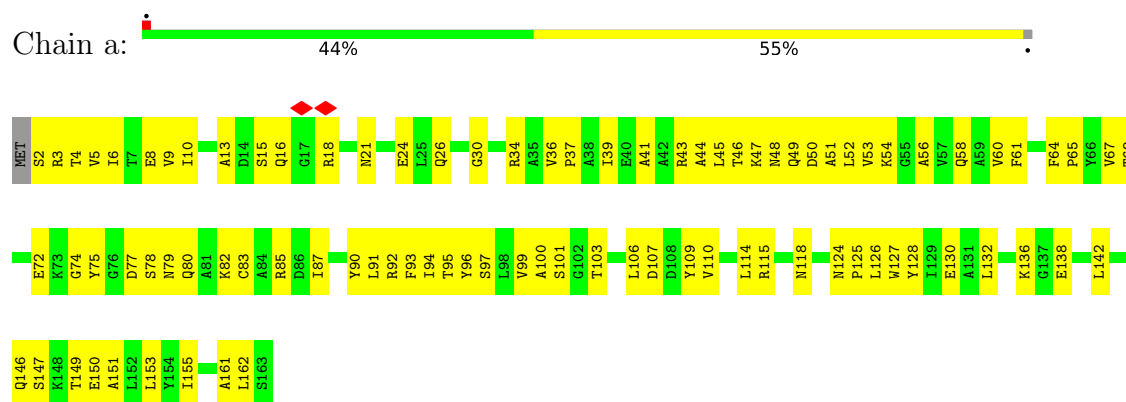
- Molecule 2: CpcA



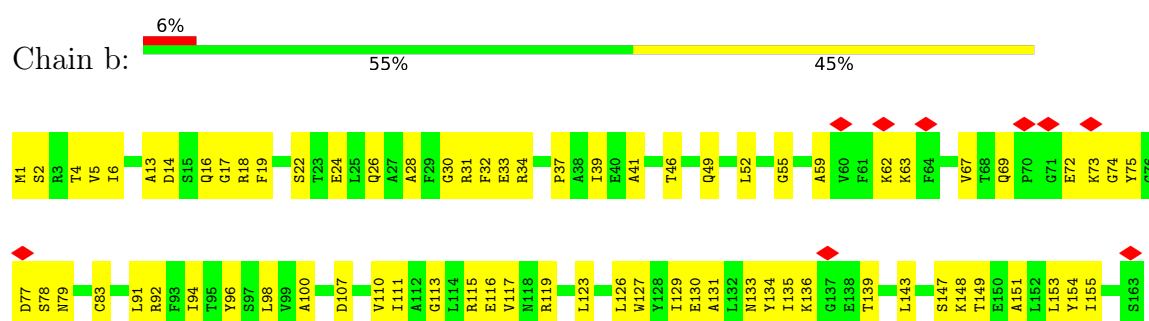
- Molecule 2: CpcA



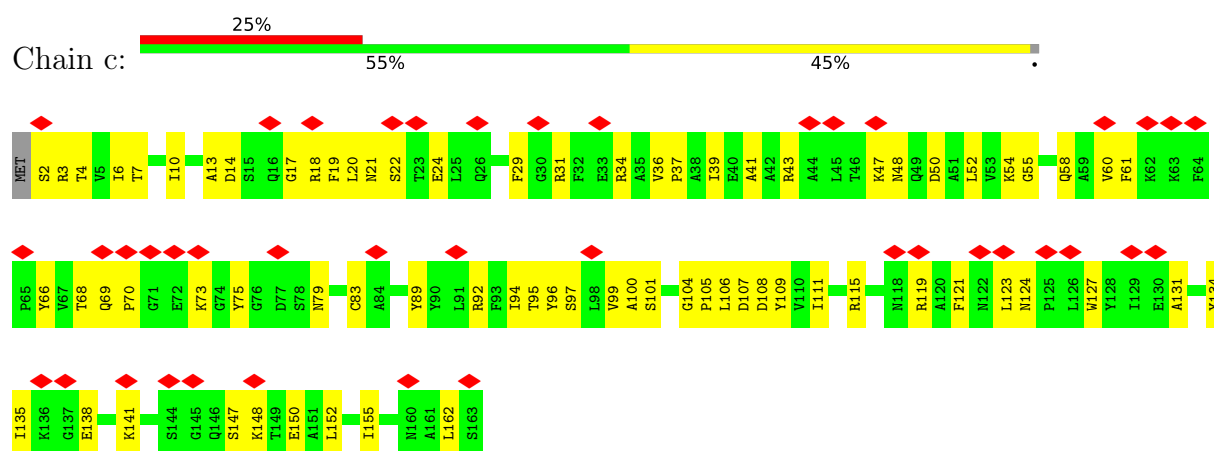
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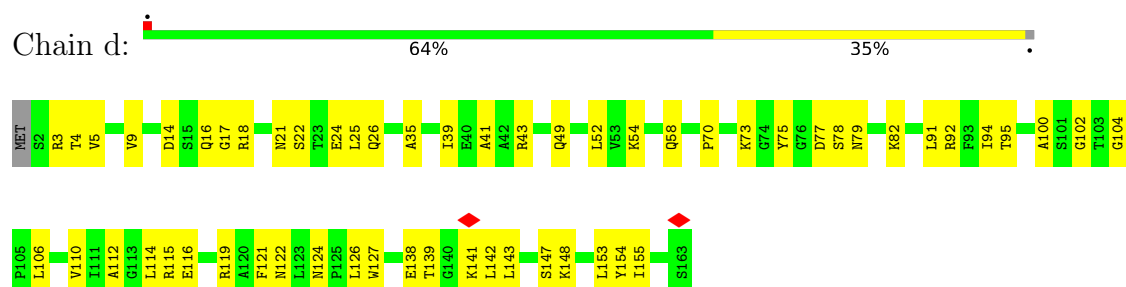
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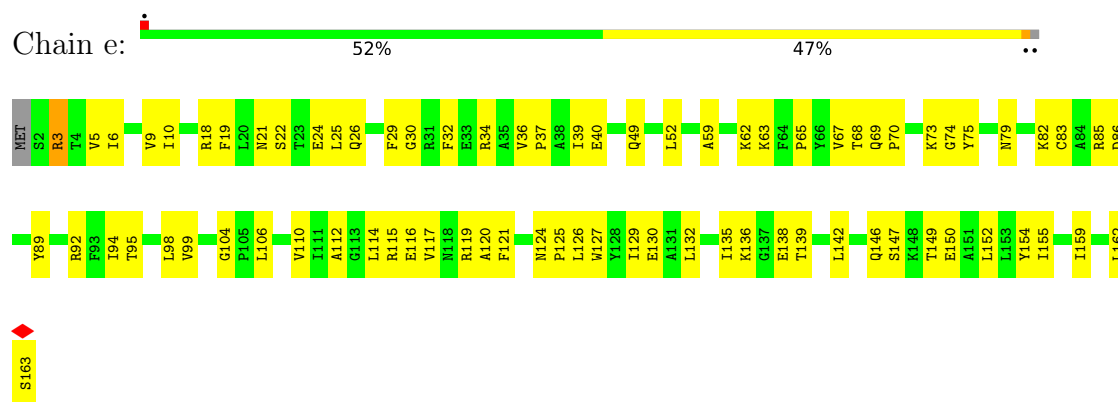
- Molecule 2: CpcA



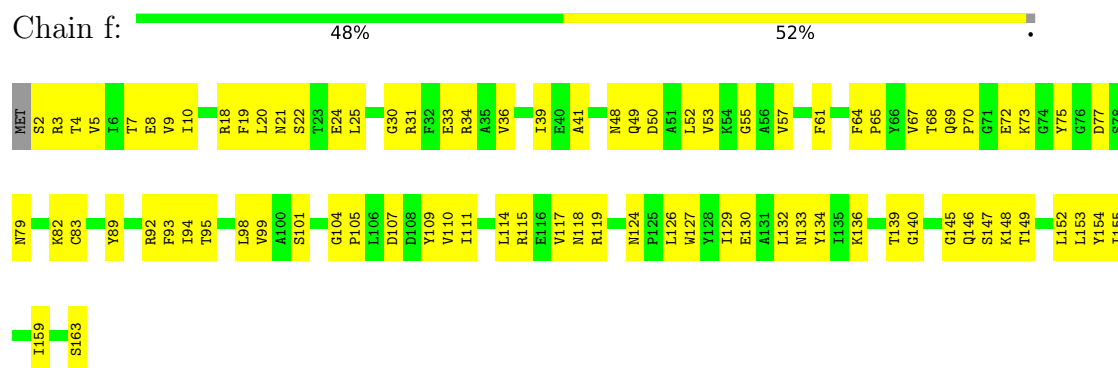
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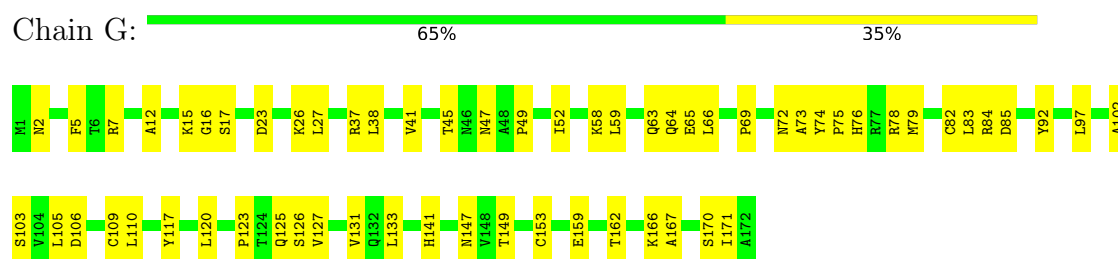
- Molecule 2: CpcA



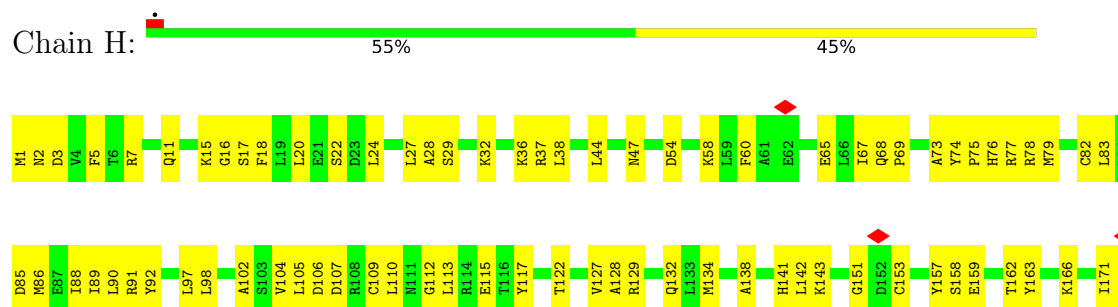
- Molecule 2: CpcA



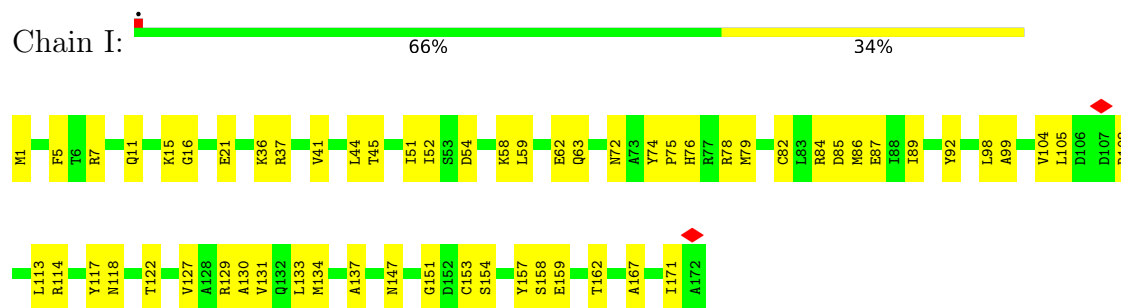
- Molecule 3: CpcB



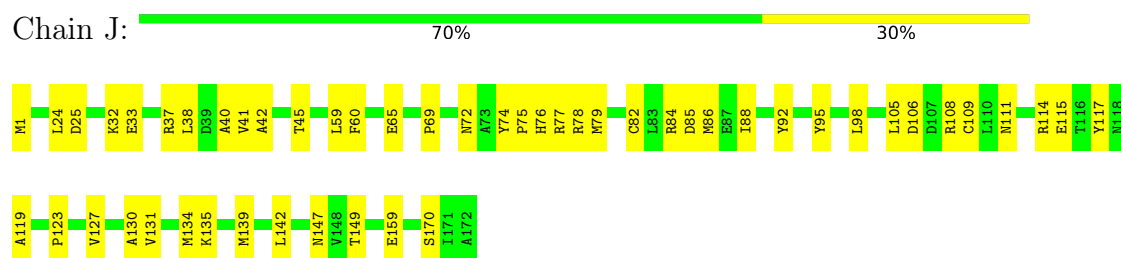
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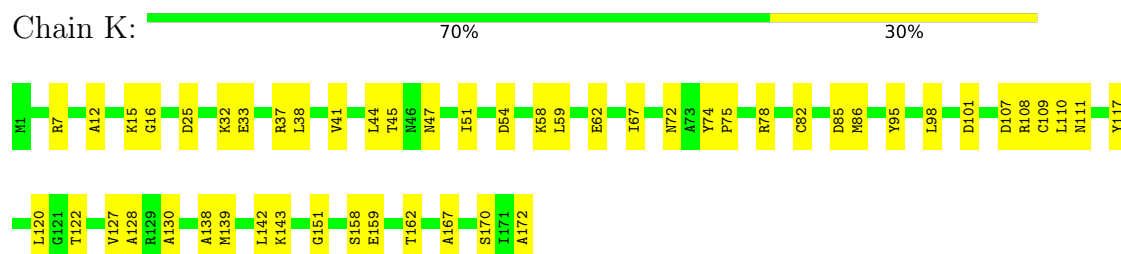
- Molecule 3: CpcB



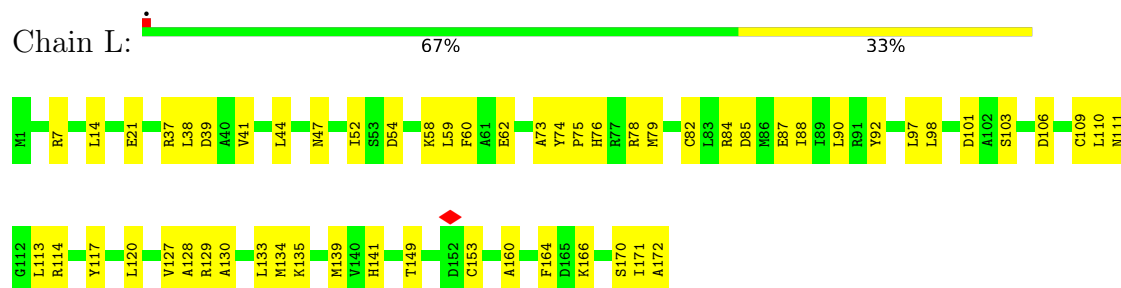
- Molecule 3: CpcB



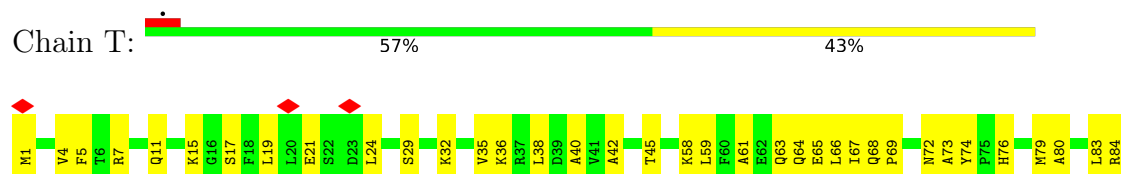
- Molecule 3: CpcB

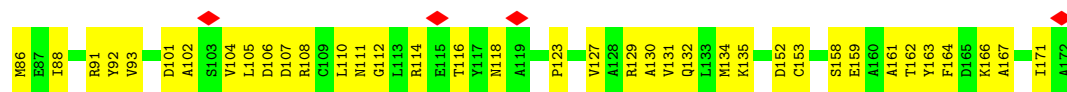


- Molecule 3: CpcB

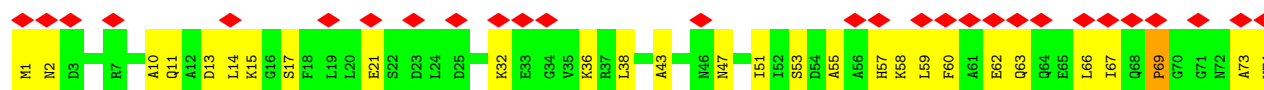


- Molecule 3: CpcB

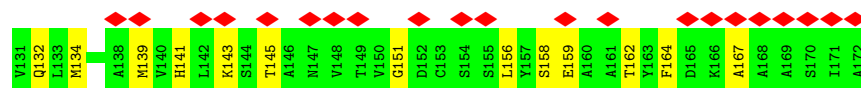
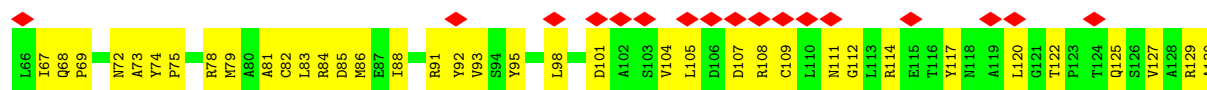
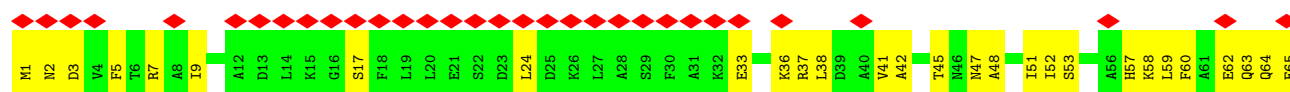
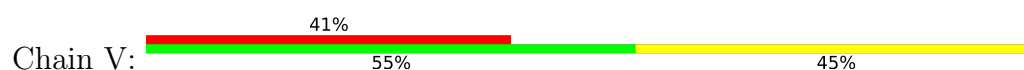




• Molecule 3: CpcB



• Molecule 3: CpcB

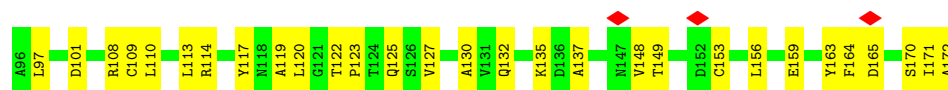


• Molecule 3: CpcB

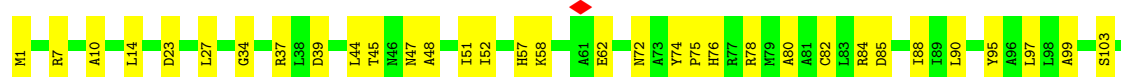


• Molecule 3: CpcB





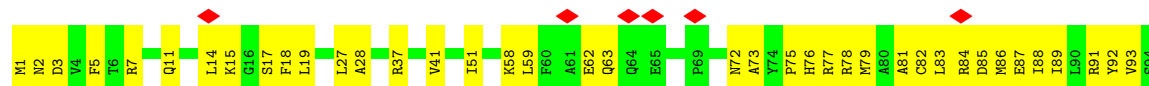
- Molecule 3: CpcB



- Molecule 3: CpcB

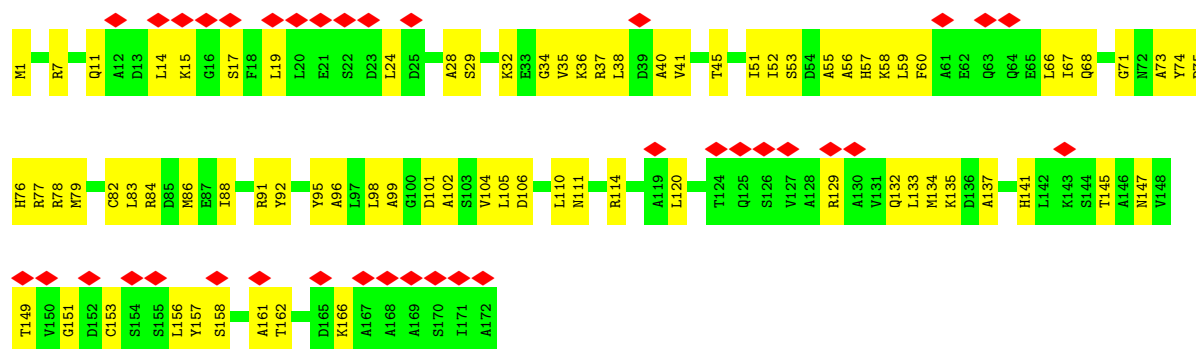


- Molecule 3: CpcB

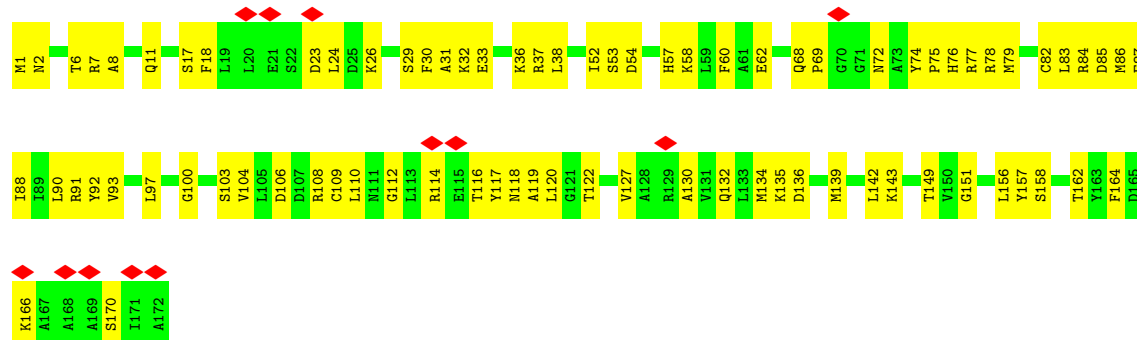


- Molecule 3: CpcB

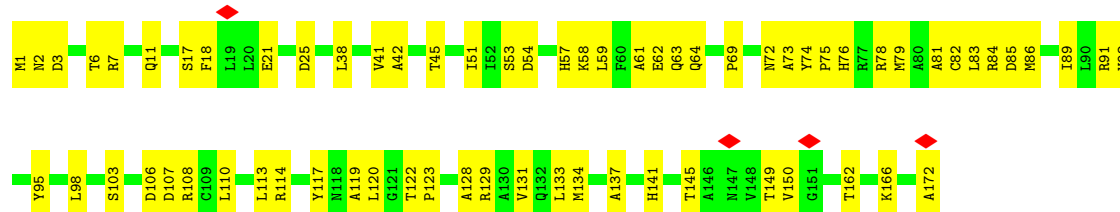




• Molecule 3: CpcB



• Molecule 3: CpcB



• Molecule 3: CpcB

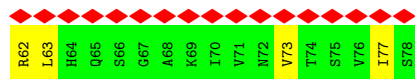
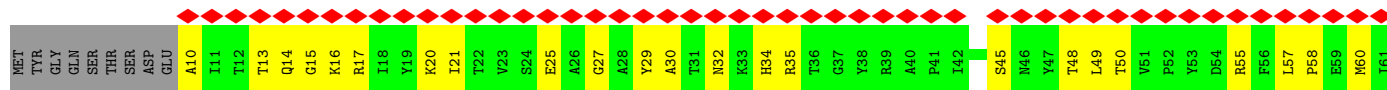
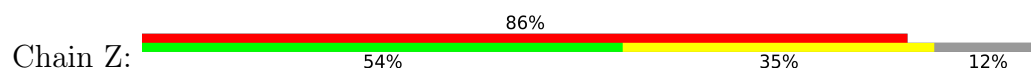




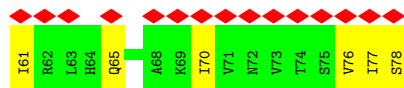
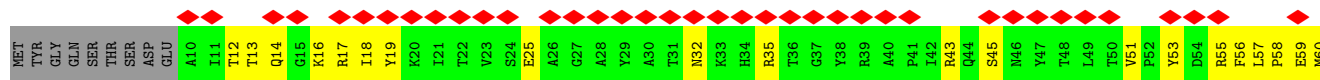
• Molecule 4: CpcD



• Molecule 4: CpcD



• Molecule 4: CpcD



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1109579	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	7.163	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.038	Depositor
Map value standard deviation	0.107	Depositor
Recommended contour level	0.8	Depositor
Map size ($\text{\AA}$)	721.48, 721.48, 721.48	wwPDB
Map dimensions	680, 680, 680	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.061, 1.061, 1.061	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

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	5	0.23	0/5786	0.45	2/7836 (0.0%)
2	A	0.23	0/1277	0.45	0/1729
2	B	0.28	0/1285	0.45	0/1739
2	C	0.21	0/1277	0.45	0/1729
2	D	0.29	0/1277	0.43	0/1729
2	E	0.26	0/1277	0.51	0/1729
2	F	0.30	0/1277	0.45	0/1729
2	N	0.23	0/1277	0.47	0/1729
2	O	0.23	0/1285	0.45	0/1739
2	P	0.17	0/1277	0.42	0/1729
2	Q	0.21	0/1277	0.45	0/1729
2	R	0.20	0/1277	0.45	0/1729
2	S	0.35	0/1277	0.49	2/1729 (0.1%)
2	a	0.19	0/1277	0.48	0/1729
2	b	0.15	0/1285	0.37	0/1739
2	c	0.16	0/1277	0.42	0/1729
2	d	0.15	0/1277	0.36	0/1729
2	e	0.20	0/1277	0.51	0/1729
2	f	0.27	0/1277	0.51	0/1729
3	G	0.20	0/1310	0.46	0/1772
3	H	0.19	0/1310	0.45	0/1772
3	I	0.19	0/1310	0.37	0/1772
3	J	0.29	0/1310	0.44	0/1772
3	K	0.28	0/1310	0.37	0/1772
3	L	0.28	0/1310	0.40	0/1772
3	T	0.20	0/1310	0.46	0/1772
3	U	0.28	1/1310 (0.1%)	0.61	3/1772 (0.2%)
3	V	0.17	0/1310	0.42	0/1772
3	W	0.30	0/1310	0.45	0/1772
3	X	0.22	0/1310	0.40	0/1772
3	Y	0.25	0/1310	0.41	0/1772
3	g	0.17	0/1310	0.43	0/1772

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	h	0.14	0/1310	0.36	0/1772
3	i	0.15	0/1310	0.41	0/1772
3	j	0.19	0/1310	0.45	0/1772
3	k	0.15	0/1310	0.37	0/1772
3	l	0.21	0/1310	0.43	0/1772
4	M	0.13	0/556	0.38	0/753
4	Z	0.15	0/556	0.42	0/753
4	m	0.15	0/556	0.46	0/753
All	All	0.22	1/54044 (0.0%)	0.44	7/73143 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	e	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	69	PRO	CG-CD	-6.27	1.29	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	69	PRO	CA-N-CD	-12.99	93.82	112.00
3	U	69	PRO	N-CD-CG	-9.11	89.53	103.20
2	S	137	GLY	CA-C-N	-5.72	112.02	122.38
2	S	137	GLY	C-N-CA	-5.72	112.02	122.38
3	U	69	PRO	CA-CB-CG	-5.60	93.85	104.50
1	5	355	GLU	CA-C-N	5.11	131.30	121.54
1	5	355	GLU	C-N-CA	5.11	131.30	121.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	e	3	ARG	Peptide

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	5	5659	0	5457	216	0
2	A	1254	0	1254	74	0
2	B	1262	0	1267	48	0
2	C	1254	0	1255	63	0
2	D	1254	0	1255	46	0
2	E	1254	0	1255	63	0
2	F	1254	0	1255	47	0
2	N	1254	0	1253	69	0
2	O	1262	0	1267	48	0
2	P	1254	0	1255	62	0
2	Q	1254	0	1255	68	0
2	R	1254	0	1255	60	0
2	S	1254	0	1255	50	0
2	a	1254	0	1255	87	0
2	b	1262	0	1267	70	0
2	c	1254	0	1255	72	0
2	d	1254	0	1255	54	0
2	e	1254	0	1255	74	0
2	f	1254	0	1255	90	0
3	G	1293	0	1297	51	0
3	H	1293	0	1297	73	0
3	I	1293	0	1297	53	0
3	J	1293	0	1297	54	0
3	K	1293	0	1297	42	0
3	L	1293	0	1297	45	0
3	T	1293	0	1297	60	0
3	U	1293	0	1297	55	0
3	V	1293	0	1297	63	0
3	W	1293	0	1297	54	0
3	X	1293	0	1297	70	0
3	Y	1293	0	1297	47	0
3	g	1293	0	1297	70	0
3	h	1293	0	1297	68	0
3	i	1293	0	1297	75	0
3	j	1293	0	1297	83	0
3	k	1293	0	1297	69	0
3	l	1293	0	1297	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	546	0	563	29	0
4	Z	546	0	563	25	0
4	m	546	0	563	30	0
5	5	86	0	73	19	0
5	A	43	0	38	3	0
5	B	43	0	38	9	0
5	C	43	0	38	7	0
5	D	43	0	38	1	0
5	E	43	0	38	8	0
5	F	43	0	37	6	0
5	G	86	0	76	11	0
5	H	86	0	76	20	0
5	I	86	0	74	12	0
5	J	86	0	76	16	0
5	K	86	0	76	9	0
5	L	43	0	38	5	0
5	N	43	0	38	7	0
5	O	43	0	38	13	0
5	P	43	0	38	4	0
5	Q	43	0	38	10	0
5	R	43	0	38	4	0
5	S	43	0	37	5	0
5	T	86	0	76	9	0
5	U	86	0	76	7	0
5	V	86	0	76	7	0
5	W	86	0	76	11	0
5	X	86	0	76	10	0
5	Y	86	0	76	13	0
5	a	43	0	38	4	0
5	b	43	0	38	2	0
5	c	43	0	38	8	0
5	d	43	0	38	7	0
5	e	43	0	38	4	0
5	f	43	0	38	6	0
5	g	86	0	76	15	0
5	h	86	0	76	13	0
5	i	86	0	76	9	0
5	j	86	0	76	9	0
5	k	86	0	76	13	0
5	l	43	0	38	7	0
All	All	55489	0	55160	2309	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 21.

All (2309) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:72:ASN:ND2	3:X:122:THR:HA	1.78	0.98
2:a:72:GLU:HB3	2:a:75:TYR:HB2	1.42	0.97
5:O:200:CYC:HMA3	5:O:200:CYC:HB	1.27	0.96
3:h:75:PRO:O	3:h:77:ARG:NH1	2.05	0.90
5:W:200:CYC:HMD1	5:W:200:CYC:HC	1.37	0.88
5:O:200:CYC:HMD1	5:O:200:CYC:HC	1.39	0.88
2:c:3:ARG:HB2	2:c:104:GLY:HA3	1.56	0.87
2:f:79:ASN:HA	2:f:82:LYS:HE2	1.57	0.87
3:U:11:GLN:OE1	3:U:15:LYS:NZ	2.08	0.86
3:G:120:LEU:HD21	5:G:200:CYC:HBD1	1.58	0.86
1:5:436:GLN:HG3	1:5:524:VAL:HG21	1.57	0.85
2:c:115:ARG:HB3	2:c:119:ARG:HH12	1.41	0.84
2:Q:73:LYS:O	2:Q:79:ASN:ND2	2.12	0.83
2:f:107:ASP:HA	2:f:111:ILE:HB	1.61	0.82
3:H:2:ASN:HB2	3:H:7:ARG:HH11	1.43	0.82
1:5:517:THR:O	1:5:521:SER:HB3	1.79	0.82
2:c:115:ARG:HH22	2:c:162:LEU:HA	1.45	0.82
3:g:37:ARG:NH1	3:g:97:LEU:O	2.13	0.81
3:k:7:ARG:HG3	3:k:11:GLN:HE22	1.43	0.81
1:5:353:THR:OG1	2:R:3:ARG:NH1	2.13	0.81
2:R:43:ARG:HH12	3:T:21:GLU:HA	1.46	0.81
2:a:46:THR:HA	2:a:49:GLN:HE21	1.45	0.81
5:5:1201:CYC:HMD1	5:5:1201:CYC:HC	1.45	0.80
3:I:41:VAL:HG11	3:I:98:LEU:HD12	1.63	0.80
3:L:114:ARG:NH1	3:L:171:ILE:O	2.15	0.79
2:f:111:ILE:HA	2:f:114:LEU:HD23	1.64	0.79
1:5:389:ASP:HB3	5:V:200:CYC:HBA2	1.64	0.79
2:N:50:ASP:HB3	2:N:54:LYS:HZ1	1.46	0.79
3:V:41:VAL:HG11	3:V:98:LEU:HD12	1.64	0.79
3:Y:82:CYS:HA	5:Y:200:CYC:HHD	1.65	0.79
1:5:94:THR:O	3:J:78:ARG:NH2	2.16	0.79
2:A:40:GLU:OE2	2:A:147:SER:OG	2.01	0.78
2:c:2:SER:HB2	2:c:105:PRO:HG3	1.63	0.78
2:E:22:SER:O	2:E:26:GLN:HB2	1.82	0.78
3:X:72:ASN:HD21	3:X:122:THR:HA	1.48	0.78
2:a:41:ALA:HB2	2:a:147:SER:HB3	1.63	0.78
2:D:94:ILE:HD13	2:D:155:ILE:HD13	1.64	0.78
2:A:136:LYS:HE3	2:A:152:LEU:HD22	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:575:THR:OG1	2:e:3:ARG:NH1	2.17	0.78
2:f:41:ALA:HB2	2:f:147:SER:HB3	1.66	0.77
3:h:37:ARG:NH1	3:h:97:LEU:O	2.16	0.77
1:5:549:THR:O	3:j:78:ARG:NH2	2.17	0.77
2:A:92:ARG:NH2	3:H:17:SER:O	2.18	0.77
2:b:5:VAL:HB	2:b:31:ARG:HD2	1.65	0.77
3:G:127:VAL:HG22	5:G:200:CYC:H3C	1.66	0.77
2:S:92:ARG:NH2	3:W:74:TYR:OH	2.18	0.77
2:Q:31:ARG:HH12	3:X:5:PHE:HE2	1.31	0.76
4:m:16:LYS:HD2	4:m:17:ARG:HG3	1.67	0.76
3:V:73:ALA:HB1	3:V:79:MET:HB2	1.67	0.76
4:Z:16:LYS:HD2	4:Z:17:ARG:HG3	1.67	0.76
3:i:7:ARG:O	3:i:11:GLN:NE2	2.17	0.76
3:U:66:LEU:HD13	3:U:73:ALA:HB3	1.66	0.76
2:a:13:ALA:O	3:h:91:ARG:NH2	2.17	0.76
2:C:94:ILE:HD13	2:C:155:ILE:HG13	1.68	0.76
3:U:36:LYS:HG3	5:U:201:CYC:HMD3	1.65	0.76
3:i:75:PRO:HD2	3:i:78:ARG:HE	1.51	0.76
5:5:1202:CYC:HAD1	3:l:78:ARG:HG3	1.68	0.76
2:E:92:ARG:NH2	3:I:74:TYR:OH	2.19	0.76
3:l:114:ARG:HD2	3:l:118:ASN:HD21	1.51	0.76
3:W:7:ARG:O	3:W:11:GLN:NE2	2.19	0.75
3:j:132:GLN:HG2	3:j:135:LYS:HE3	1.66	0.75
1:5:328:GLU:O	3:W:78:ARG:NH1	2.19	0.75
2:P:26:GLN:HG3	2:Q:34:ARG:HE	1.52	0.75
2:R:73:LYS:O	2:R:79:ASN:ND2	2.19	0.75
3:T:114:ARG:HH12	3:T:118:ASN:HD21	1.34	0.75
2:E:82:LYS:NZ	5:E:200:CYC:O1A	2.18	0.75
3:K:110:LEU:HD21	3:K:167:ALA:HA	1.67	0.75
1:5:376:GLU:HA	1:5:379:ARG:HG3	1.68	0.75
1:5:419:ARG:HD3	1:5:514:ALA:HA	1.67	0.75
2:N:41:ALA:HB2	2:N:147:SER:HB3	1.67	0.75
2:c:3:ARG:HH21	2:c:7:THR:HG21	1.51	0.75
1:5:637:ALA:O	3:k:108:ARG:NH1	2.20	0.74
3:k:58:LYS:HG3	3:k:133:LEU:HD13	1.70	0.74
2:N:14:ASP:OD1	3:U:108:ARG:NH1	2.21	0.74
2:b:133:ASN:OD1	2:b:136:LYS:NZ	2.19	0.74
5:H:200:CYC:HMA3	5:H:200:CYC:HB	1.50	0.74
4:Z:17:ARG:HA	4:Z:77:ILE:HB	1.67	0.74
1:5:498:ASP:OD2	1:5:515:ARG:NH2	2.20	0.74
1:5:556:ARG:NH1	3:j:118:ASN:O	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:127:VAL:HG22	5:K:200:CYC:H3C	1.69	0.74
2:P:34:ARG:HH22	2:Q:29:PHE:HD1	1.36	0.74
3:j:114:ARG:HH12	3:j:118:ASN:HD21	1.32	0.74
3:g:23:ASP:OD1	3:g:26:LYS:NZ	2.20	0.74
2:E:20:LEU:HB2	3:G:45:THR:HG21	1.69	0.74
3:T:88:ILE:HG21	5:T:200:CYC:HAB2	1.70	0.74
2:b:73:LYS:HE2	5:b:200:CYC:HBD2	1.69	0.74
2:f:92:ARG:NH2	3:l:17:SER:O	2.20	0.74
3:H:38:LEU:HD13	5:H:201:CYC:HBB3	1.70	0.73
2:a:67:VAL:HG22	2:a:72:GLU:HG3	1.70	0.73
4:M:17:ARG:HA	4:M:77:ILE:HB	1.70	0.73
1:5:141:VAL:HG22	1:5:177:ARG:HH12	1.52	0.73
2:C:73:LYS:NZ	2:C:121:PHE:O	2.22	0.73
5:D:200:CYC:OB	3:L:74:TYR:O	2.06	0.73
2:F:92:ARG:NH2	3:J:74:TYR:OH	2.22	0.73
1:5:558:GLN:OE1	3:l:111:ASN:ND2	2.22	0.73
2:B:1:MET:HE3	2:B:3:ARG:HH22	1.53	0.73
3:U:60:PHE:HB3	3:U:67:ILE:HD11	1.68	0.73
2:c:19:PHE:HB3	3:i:45:THR:HG23	1.69	0.73
3:H:102:ALA:O	3:H:166:LYS:NZ	2.22	0.73
2:D:92:ARG:NH2	3:L:74:TYR:OH	2.21	0.73
2:O:83:CYS:HB3	5:O:200:CYC:HAC2	1.69	0.73
2:c:54:LYS:O	2:c:58:GLN:NE2	2.22	0.73
2:f:4:THR:H	2:f:7:THR:HB	1.52	0.73
2:A:153:LEU:HD11	5:J:201:CYC:HAB2	1.71	0.72
2:D:9:VAL:HG13	2:D:24:GLU:HB3	1.70	0.72
2:E:26:GLN:HE21	2:F:34:ARG:NH2	1.87	0.72
2:a:52:LEU:HD11	2:a:138:GLU:HG2	1.70	0.72
1:5:521:SER:HB2	3:X:119:ALA:HB1	1.70	0.72
1:5:456:ASP:OD2	4:Z:55:ARG:NH2	2.22	0.72
2:D:50:ASP:OD1	2:D:51:ALA:N	2.22	0.72
2:O:87:ILE:HD11	5:O:200:CYC:HBC1	1.70	0.72
3:g:149:THR:O	5:g:201:CYC:NC	2.18	0.72
2:C:31:ARG:HE	2:C:101:SER:HB3	1.55	0.72
3:T:61:ALA:O	3:T:64:GLN:NE2	2.22	0.72
3:X:127:VAL:HG22	5:X:200:CYC:H3C	1.70	0.72
3:h:85:ASP:OD2	3:h:117:TYR:OH	2.06	0.72
3:G:75:PRO:HD2	3:G:78:ARG:HD2	1.72	0.72
2:c:3:ARG:HD2	4:m:12:THR:HA	1.72	0.72
1:5:273:ASP:HA	1:5:279:GLN:HB2	1.72	0.72
2:N:10:ILE:O	2:N:14:ASP:HB2	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:7:ARG:NH1	3:Y:103:SER:OG	2.23	0.71
2:f:73:LYS:O	2:f:79:ASN:ND2	2.23	0.71
1:5:230:GLU:OE1	1:5:244:ARG:NH2	2.23	0.71
2:Q:31:ARG:HH22	3:X:5:PHE:HD2	1.39	0.71
3:Y:127:VAL:HG13	5:Y:200:CYC:HBC3	1.72	0.71
2:S:136:LYS:HG3	2:S:152:LEU:HD22	1.71	0.71
3:g:117:TYR:HD2	3:g:171:ILE:HD11	1.55	0.71
2:b:115:ARG:HB3	2:b:119:ARG:HH21	1.56	0.71
2:f:117:VAL:HG11	3:j:76:HIS:HE2	1.55	0.71
1:5:104:ALA:HB1	1:5:107:THR:HG22	1.71	0.71
2:P:26:GLN:OE1	2:Q:34:ARG:NH2	2.22	0.71
2:O:73:LYS:NZ	2:O:121:PHE:O	2.22	0.71
2:b:117:VAL:HG21	3:k:76:HIS:HD1	1.56	0.71
2:c:83:CYS:HA	5:c:200:CYC:HAC2	1.73	0.70
1:5:373:TYR:OH	3:Y:85:ASP:OD1	2.09	0.70
1:5:465:GLN:OE1	4:Z:62:ARG:NH2	2.24	0.70
2:a:10:ILE:HD11	3:h:98:LEU:HD11	1.73	0.70
2:A:82:LYS:HA	2:A:85:ARG:HG2	1.74	0.70
5:B:200:CYC:OB	3:K:74:TYR:O	2.09	0.70
2:O:40:GLU:OE2	2:O:43:ARG:NH1	2.23	0.70
2:a:43:ARG:HG3	2:a:47:LYS:HE3	1.74	0.70
2:B:92:ARG:NH2	3:K:74:TYR:OH	2.25	0.70
2:P:108:ASP:HB2	4:Z:14:GLN:HE22	1.57	0.70
3:U:78:ARG:HB3	5:U:200:CYC:HMD1	1.73	0.70
2:d:54:LYS:O	2:d:58:GLN:NE2	2.24	0.70
5:5:1202:CYC:HBA1	3:l:84:ARG:HH22	1.55	0.70
2:N:19:PHE:HE1	3:U:91:ARG:HG3	1.56	0.70
3:K:72:ASN:ND2	3:K:122:THR:HA	2.06	0.70
3:h:41:VAL:HG11	3:h:98:LEU:HB3	1.72	0.70
3:W:52:ILE:HD13	3:W:87:GLU:HG2	1.74	0.70
2:d:94:ILE:HD13	2:d:155:ILE:HG22	1.73	0.70
3:H:65:GLU:O	3:H:68:GLN:NE2	2.24	0.70
2:c:127:TRP:HB3	5:c:200:CYC:HMC3	1.74	0.70
3:k:72:ASN:HD22	5:k:200:CYC:HMC3	1.56	0.70
2:F:127:TRP:HB3	5:F:200:CYC:HBC3	1.72	0.70
3:I:114:ARG:NH1	3:I:118:ASN:OD1	2.25	0.70
2:N:87:ILE:HD11	5:N:200:CYC:HBC1	1.74	0.69
2:N:9:VAL:HG13	2:N:24:GLU:HB3	1.73	0.69
3:T:4:VAL:HG12	3:T:7:ARG:HH12	1.57	0.69
3:l:71:GLY:O	3:l:78:ARG:NH2	2.24	0.69
3:I:105:LEU:HD21	3:I:167:ALA:HB2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:63:GLN:NE2	3:V:65:GLU:OE1	2.25	0.69
2:A:9:VAL:HG13	2:A:24:GLU:HB2	1.74	0.69
2:C:136:LYS:HD3	2:C:152:LEU:HD13	1.72	0.69
2:Q:43:ARG:NH1	3:X:21:GLU:OE1	2.26	0.69
2:S:41:ALA:HB2	2:S:147:SER:HB3	1.73	0.69
3:j:149:THR:O	5:j:201:CYC:NC	2.26	0.69
3:T:102:ALA:HB1	3:T:166:LYS:HE2	1.74	0.69
3:g:129:ARG:NH1	3:g:132:GLN:OE1	2.24	0.69
1:5:104:ALA:HB1	1:5:107:THR:CG2	2.22	0.69
1:5:366:LYS:NZ	1:5:371:ASN:OD1	2.25	0.69
2:A:67:VAL:HB	2:A:74:GLY:HA3	1.75	0.69
3:L:47:ASN:OD1	3:L:141:HIS:ND1	2.25	0.69
2:a:77:ASP:OD1	2:a:78:SER:N	2.26	0.69
2:f:133:ASN:HA	2:f:136:LYS:HZ2	1.57	0.69
3:H:37:ARG:NH1	3:H:97:LEU:O	2.25	0.69
1:5:373:TYR:HD1	3:Y:84:ARG:HH11	1.41	0.69
2:b:143:LEU:H	2:b:148:LYS:HZ3	1.39	0.69
1:5:571:ARG:HH12	4:m:43:ARG:HB3	1.57	0.68
3:j:82:CYS:HA	5:j:200:CYC:HHD	1.75	0.68
2:e:75:TYR:O	2:e:79:ASN:ND2	2.26	0.68
3:Y:88:ILE:HG21	5:Y:200:CYC:HAB2	1.74	0.68
1:5:621:ARG:NH2	1:5:682:ASP:OD1	2.26	0.68
2:R:41:ALA:HB2	2:R:147:SER:HB2	1.74	0.68
3:X:113:LEU:HD23	3:X:171:ILE:HD11	1.75	0.68
1:5:179:PHE:O	3:K:108:ARG:NH1	2.26	0.68
2:E:83:CYS:SG	5:E:200:CYC:OC	2.52	0.68
3:H:20:LEU:HD23	3:H:22:SER:H	1.58	0.68
2:N:19:PHE:CE1	3:U:91:ARG:HG3	2.29	0.68
2:Q:25:LEU:HG	3:X:38:LEU:HD22	1.74	0.68
2:c:75:TYR:O	2:c:79:ASN:ND2	2.26	0.68
2:D:117:VAL:HG11	3:L:76:HIS:ND1	2.09	0.68
3:i:84:ARG:NH2	5:i:200:CYC:O2A	2.27	0.68
1:5:648:LYS:HB2	1:5:718:LEU:HD21	1.76	0.68
1:5:718:LEU:HD22	1:5:738:LEU:HD11	1.73	0.68
3:I:82:CYS:HA	5:I:200:CYC:HHD	1.74	0.68
2:R:92:ARG:NH2	3:V:74:TYR:OH	2.27	0.68
3:l:59:LEU:HD22	3:l:133:LEU:HD12	1.75	0.68
3:i:52:ILE:HA	3:i:134:MET:HE1	1.76	0.68
3:I:129:ARG:HH22	3:I:133:LEU:HD21	1.57	0.68
2:d:4:THR:HG22	2:d:100:ALA:HB1	1.75	0.68
3:h:137:ALA:O	3:h:141:HIS:ND1	2.19	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:82:LYS:HA	2:e:85:ARG:HG2	1.76	0.67
2:P:43:ARG:HA	2:P:43:ARG:HH21	1.58	0.67
3:X:82:CYS:HA	5:X:200:CYC:HHD	1.76	0.67
2:f:115:ARG:HB3	2:f:119:ARG:HH12	1.59	0.67
2:A:34:ARG:NH2	5:J:201:CYC:OB	2.27	0.67
3:H:11:GLN:HB3	3:H:15:LYS:HZ1	1.59	0.67
3:V:3:ASP:HA	3:V:101:ASP:HB2	1.75	0.67
3:H:60:PHE:HB3	3:H:67:ILE:HD11	1.75	0.67
3:J:86:MET:HE3	3:J:130:ALA:HB1	1.75	0.67
3:V:85:ASP:OD2	3:V:117:TYR:OH	2.12	0.67
2:B:114:LEU:HD21	2:B:162:LEU:HD23	1.76	0.67
2:E:34:ARG:NE	5:L:201:CYC:OB	2.28	0.67
4:M:28:ALA:O	4:M:32:ASN:ND2	2.27	0.67
2:R:43:ARG:HE	3:T:24:LEU:HD13	1.58	0.67
5:A:200:CYC:HBB2	3:G:76:HIS:HB2	1.76	0.67
3:V:37:ARG:NH2	3:V:159:GLU:OE1	2.26	0.67
3:k:7:ARG:O	3:k:11:GLN:NE2	2.28	0.67
2:N:85:ARG:NH1	2:N:86:ASP:OD1	2.28	0.67
2:P:92:ARG:NH1	3:U:74:TYR:OH	2.28	0.67
2:Q:19:PHE:HB3	3:X:45:THR:HG23	1.75	0.67
3:k:61:ALA:O	3:k:64:GLN:NE2	2.26	0.67
1:5:575:THR:H	2:e:3:ARG:HH22	1.42	0.67
2:d:14:ASP:HA	3:k:91:ARG:HH11	1.59	0.67
2:O:83:CYS:SG	5:O:200:CYC:NC	2.67	0.66
3:J:60:PHE:HE2	3:J:79:MET:HE1	1.61	0.66
2:d:75:TYR:O	2:d:79:ASN:ND2	2.28	0.66
2:b:136:LYS:HA	2:b:139:THR:HG22	1.77	0.66
3:l:104:VAL:HG13	3:l:105:LEU:HD12	1.77	0.66
1:5:704:GLN:H	1:5:707:GLN:HG2	1.60	0.66
2:B:107:ASP:HA	2:B:111:ILE:HB	1.77	0.66
3:l:102:ALA:HB1	3:l:166:LYS:HE2	1.76	0.66
1:5:206:ILE:HD11	1:5:287:LEU:HD13	1.77	0.66
3:H:77:ARG:NH1	5:H:200:CYC:O1D	2.28	0.66
3:U:93:VAL:HG11	3:U:164:PHE:CE1	2.31	0.66
2:c:21:ASN:N	2:c:24:GLU:OE1	2.29	0.66
2:e:21:ASN:N	2:e:24:GLU:OE2	2.27	0.66
3:i:96:ALA:HB2	3:i:105:LEU:HB2	1.76	0.66
3:T:104:VAL:O	3:T:108:ARG:NH1	2.29	0.66
2:c:89:TYR:HD1	2:c:92:ARG:HH22	1.43	0.66
3:i:71:GLY:O	3:i:78:ARG:NH2	2.28	0.66
2:A:46:THR:O	2:A:49:GLN:NE2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:74:GLY:O	2:D:80:GLN:NE2	2.28	0.66
5:d:200:CYC:OB	3:l:74:TYR:O	2.13	0.66
1:5:371:ASN:HB2	1:5:503:SER:HB2	1.77	0.65
5:P:200:CYC:HBB2	3:U:76:HIS:HB2	1.78	0.65
3:l:101:ASP:OD1	3:l:102:ALA:N	2.29	0.65
2:F:117:VAL:HG11	3:J:76:HIS:CD2	2.31	0.65
3:J:82:CYS:HA	5:J:200:CYC:HHD	1.78	0.65
3:W:37:ARG:NH1	3:W:159:GLU:OE2	2.23	0.65
2:b:41:ALA:HB2	2:b:147:SER:HB3	1.78	0.65
3:W:52:ILE:HG23	3:W:86:MET:HE2	1.77	0.65
3:W:90:LEU:HB2	3:W:134:MET:HE1	1.79	0.65
3:X:72:ASN:OD1	3:X:72:ASN:O	2.15	0.65
1:5:606:GLU:OE1	1:5:610:ARG:NH2	2.30	0.65
3:H:78:ARG:HG2	5:H:200:CYC:HAD1	1.79	0.65
3:i:84:ARG:HH12	5:i:200:CYC:HB	1.42	0.65
2:R:99:VAL:HG21	3:T:19:LEU:HD21	1.78	0.65
3:i:110:LEU:O	3:i:114:ARG:NH1	2.29	0.65
5:5:1202:CYC:OC	3:l:72:ASN:ND2	2.29	0.65
2:Q:92:ARG:NH1	3:X:16:GLY:O	2.30	0.65
1:5:598:GLU:OE2	2:d:119:ARG:NH2	2.29	0.65
3:h:127:VAL:HG22	5:h:200:CYC:H3C	1.78	0.65
3:k:51:ILE:HG23	3:k:137:ALA:HB3	1.79	0.65
1:5:463:GLU:OE2	1:5:477:ARG:NH2	2.23	0.65
3:W:82:CYS:SG	5:W:200:CYC:HAC2	2.36	0.65
2:D:31:ARG:HE	2:D:101:SER:HB2	1.61	0.65
2:O:43:ARG:O	2:O:47:LYS:HG3	1.97	0.65
3:L:58:LYS:HB2	3:L:133:LEU:HD21	1.78	0.64
2:b:98:LEU:HD23	2:b:154:TYR:HD2	1.62	0.64
2:F:121:PHE:HE2	3:J:79:MET:HE2	1.62	0.64
3:K:37:ARG:NH1	3:K:159:GLU:OE2	2.24	0.64
3:Y:148:VAL:HG21	5:Y:201:CYC:HMC3	1.80	0.64
2:c:29:PHE:HE1	3:i:35:VAL:HG13	1.62	0.64
3:W:5:PHE:HD1	3:W:27:LEU:HD12	1.62	0.64
2:a:18:ARG:O	3:h:91:ARG:NH2	2.28	0.64
3:H:85:ASP:OD2	3:H:117:TYR:OH	2.15	0.64
2:N:7:THR:HG23	3:U:1:MET:HE1	1.79	0.64
2:P:41:ALA:HB2	2:P:147:SER:HB3	1.79	0.64
2:A:21:ASN:N	2:A:24:GLU:OE2	2.29	0.64
3:I:7:ARG:HD2	3:I:11:GLN:HE22	1.63	0.64
2:S:9:VAL:CG1	2:S:24:GLU:HB3	2.28	0.64
4:m:32:ASN:OD1	4:m:35:ARG:NH2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:20:LEU:HB3	2:P:24:GLU:OE2	1.97	0.64
2:P:43:ARG:HA	2:P:43:ARG:NH2	2.13	0.64
2:a:114:LEU:HD21	2:a:162:LEU:HD13	1.80	0.64
2:b:107:ASP:HA	2:b:111:ILE:HB	1.79	0.64
2:F:34:ARG:NH1	2:F:101:SER:OG	2.19	0.64
2:B:43:ARG:NH2	3:J:25:ASP:OD1	2.30	0.63
2:E:114:LEU:HD21	2:E:162:LEU:HD23	1.81	0.63
3:H:44:LEU:HG	3:H:142:LEU:HD11	1.79	0.63
3:J:127:VAL:HG13	5:J:200:CYC:HBC3	1.79	0.63
2:R:43:ARG:NH2	3:T:21:GLU:OE1	2.31	0.63
3:g:132:GLN:NE2	3:g:136:ASP:OD2	2.32	0.63
3:k:129:ARG:HH22	3:k:133:LEU:HD21	1.61	0.63
2:B:18:ARG:NH2	2:B:24:GLU:OE2	2.26	0.63
1:5:244:ARG:O	1:5:249:GLN:NE2	2.31	0.63
1:5:689:CYS:HB3	1:5:699:ARG:CZ	2.29	0.63
2:D:73:LYS:O	2:D:79:ASN:ND2	2.23	0.63
5:F:200:CYC:HBB2	3:J:76:HIS:HB2	1.80	0.63
2:f:155:ILE:O	2:f:159:ILE:HD12	1.97	0.63
2:C:2:SER:N	4:M:13:THR:HG1	1.97	0.63
2:Q:136:LYS:HG3	2:Q:155:ILE:HG21	1.79	0.63
2:f:136:LYS:HA	2:f:139:THR:HG22	1.81	0.63
3:J:131:VAL:HA	3:J:134:MET:HE3	1.81	0.63
3:T:7:ARG:HG2	3:T:11:GLN:HE22	1.63	0.63
2:a:3:ARG:HE	4:m:35:ARG:HH22	1.46	0.63
3:g:39:ASP:HB2	5:g:201:CYC:HAC1	1.81	0.63
3:h:62:GLU:OE2	3:h:129:ARG:NH2	2.31	0.63
3:l:2:ASN:O	3:l:7:ARG:NH1	2.32	0.63
2:F:109:TYR:O	3:J:76:HIS:HB3	1.98	0.63
1:5:519:ARG:HA	1:5:522:ARG:HH12	1.63	0.63
2:B:12:THR:O	2:B:16:GLN:NE2	2.32	0.63
2:f:126:LEU:O	2:f:129:ILE:N	2.31	0.63
3:V:53:SER:O	3:V:57:HIS:ND1	2.30	0.63
3:V:75:PRO:HD2	3:V:78:ARG:HB2	1.79	0.63
1:5:635:ASN:O	3:k:108:ARG:NH2	2.20	0.63
3:I:1:MET:HB2	3:I:104:VAL:HG22	1.81	0.63
2:P:82:LYS:HE2	5:P:200:CYC:HAD2	1.80	0.63
3:U:53:SER:O	3:U:57:HIS:ND1	2.32	0.63
3:X:51:ILE:HG23	3:X:137:ALA:HB3	1.80	0.63
2:B:82:LYS:HZ1	5:B:200:CYC:C4D	2.12	0.62
2:E:40:GLU:HA	2:E:43:ARG:HG2	1.81	0.62
3:T:84:ARG:NH2	3:T:85:ASP:OD1	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:94:ILE:HD13	2:a:106:LEU:HD21	1.80	0.62
2:C:146:GLN:NE2	5:K:201:CYC:O2A	2.32	0.62
2:E:34:ARG:HH22	2:E:146:GLN:HG3	1.64	0.62
2:F:34:ARG:HB2	2:F:34:ARG:CZ	2.28	0.62
2:N:110:VAL:HG23	2:N:111:ILE:HD12	1.81	0.62
2:O:7:THR:HG23	3:W:1:MET:SD	2.39	0.62
2:Q:90:TYR:HE2	2:Q:162:LEU:HD11	1.63	0.62
3:g:37:ARG:NH1	3:g:159:GLU:OE1	2.30	0.62
1:5:571:ARG:HH22	4:m:43:ARG:HA	1.63	0.62
1:5:624:ALA:HB1	1:5:677:ILE:HD13	1.82	0.62
5:G:201:CYC:HMA3	5:G:201:CYC:HB	1.63	0.62
2:S:7:THR:HG23	3:Y:1:MET:HE3	1.81	0.62
1:5:355:GLU:O	1:5:356:GLN:HG3	1.99	0.62
2:A:39:ILE:HD11	3:H:24:LEU:HB3	1.80	0.62
2:R:146:GLN:NE2	5:Y:201:CYC:OB	2.33	0.62
3:V:48:ALA:HA	3:V:51:ILE:HD12	1.81	0.62
1:5:698:PHE:HB3	1:5:715:MET:HE1	1.81	0.62
2:P:139:THR:HA	2:P:142:LEU:HB2	1.82	0.62
2:P:150:GLU:OE2	2:Q:26:GLN:NE2	2.32	0.62
3:V:86:MET:HE3	3:V:130:ALA:HB1	1.81	0.62
2:a:83:CYS:SG	5:a:200:CYC:HAC2	2.40	0.62
2:c:150:GLU:OE1	2:d:26:GLN:NE2	2.32	0.62
2:Q:39:ILE:HD11	3:X:24:LEU:HB3	1.80	0.62
2:f:94:ILE:HD13	2:f:155:ILE:HG22	1.80	0.62
3:Y:131:VAL:HA	3:Y:134:MET:HE3	1.82	0.62
3:J:106:ASP:O	3:J:111:ASN:ND2	2.32	0.62
3:W:130:ALA:O	3:W:134:MET:HG3	2.00	0.62
2:f:75:TYR:O	2:f:79:ASN:ND2	2.33	0.62
4:m:60:MET:HB2	4:m:70:ILE:HD11	1.80	0.62
2:P:16:GLN:HB2	2:P:18:ARG:HG2	1.82	0.62
4:Z:60:MET:HA	4:Z:63:LEU:HG	1.81	0.62
3:h:82:CYS:HA	5:h:200:CYC:HHD	1.82	0.62
3:i:73:ALA:HB1	3:i:79:MET:HB2	1.81	0.62
1:5:140:TYR:O	1:5:177:ARG:NH2	2.32	0.62
2:E:92:ARG:NH1	3:G:16:GLY:O	2.33	0.62
2:a:124:ASN:HB3	2:a:127:TRP:CE2	2.35	0.62
1:5:548:GLN:HB3	3:j:78:ARG:HH12	1.63	0.61
2:O:106:LEU:HD21	2:O:158:ALA:HB2	1.82	0.61
2:e:98:LEU:HD22	2:e:154:TYR:HD2	1.65	0.61
2:A:90:TYR:HE2	2:A:162:LEU:HD21	1.65	0.61
3:H:127:VAL:HA	5:H:200:CYC:HBC3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:60:MET:HE1	4:M:70:ILE:HG21	1.82	0.61
3:U:153:CYS:HB2	3:U:157:TYR:CZ	2.35	0.61
2:b:130:GLU:HA	2:b:133:ASN:HD22	1.65	0.61
2:c:60:VAL:HG11	5:c:200:CYC:HMC2	1.82	0.61
3:i:149:THR:O	5:i:201:CYC:NC	2.30	0.61
3:W:127:VAL:HG22	5:W:200:CYC:H3C	1.81	0.61
3:l:153:CYS:SG	5:l:201:CYC:OC	2.58	0.61
1:5:402:ALA:O	1:5:451:TYR:OH	2.13	0.61
2:R:92:ARG:HH22	3:V:74:TYR:HH	1.47	0.61
2:f:92:ARG:HH22	3:l:17:SER:N	1.98	0.61
2:N:18:ARG:NH2	2:N:19:PHE:O	2.34	0.61
2:O:39:ILE:HG23	3:W:24:LEU:HD22	1.81	0.61
2:Q:92:ARG:NH2	3:Y:74:TYR:OH	2.34	0.61
3:Y:82:CYS:SG	5:Y:200:CYC:HAC2	2.40	0.61
2:a:92:ARG:O	2:a:95:THR:OG1	2.17	0.61
2:c:18:ARG:NH2	2:c:24:GLU:OE2	2.34	0.61
3:g:131:VAL:HA	3:g:134:MET:HE2	1.81	0.61
3:h:131:VAL:HA	3:h:134:MET:HG3	1.82	0.61
2:B:73:LYS:NZ	2:B:122:ASN:O	2.28	0.61
3:J:86:MET:HE2	3:J:134:MET:HE2	1.83	0.61
2:S:73:LYS:O	2:S:79:ASN:ND2	2.32	0.61
2:b:77:ASP:OD1	2:b:78:SER:N	2.34	0.61
2:B:18:ARG:O	3:J:95:TYR:OH	2.18	0.61
2:b:63:LYS:HG2	2:b:130:GLU:HG3	1.83	0.61
3:h:75:PRO:HD2	3:h:78:ARG:HB2	1.83	0.61
3:h:149:THR:O	5:h:201:CYC:NC	2.33	0.61
3:k:3:ASP:N	3:k:6:THR:OG1	2.34	0.61
1:5:634:PHE:O	3:k:108:ARG:NH1	2.34	0.60
2:R:34:ARG:HH22	2:S:26:GLN:HB3	1.66	0.60
2:d:116:GLU:OE1	2:d:116:GLU:N	2.26	0.60
5:O:200:CYC:HMA3	5:O:200:CYC:NB	2.10	0.60
3:X:72:ASN:HD22	3:X:122:THR:HA	1.64	0.60
2:d:41:ALA:HB2	2:d:147:SER:HB3	1.82	0.60
2:f:10:ILE:HD11	3:l:95:TYR:HB3	1.82	0.60
2:f:132:LEU:HB3	2:f:159:ILE:HD11	1.83	0.60
3:i:75:PRO:HB2	3:i:78:ARG:HG3	1.82	0.60
4:M:30:ALA:O	4:M:34:HIS:ND1	2.33	0.60
2:S:82:LYS:HD3	5:S:200:CYC:HHA	1.83	0.60
3:W:82:CYS:HA	5:W:200:CYC:HHD	1.84	0.60
2:Q:115:ARG:HH12	2:R:119:ARG:HH11	1.49	0.60
2:S:60:VAL:HG11	5:S:200:CYC:HBC2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:50:ASP:OD1	2:A:51:ALA:N	2.35	0.60
2:C:49:GLN:OE1	2:C:49:GLN:N	2.29	0.60
2:F:73:LYS:O	2:F:79:ASN:ND2	2.26	0.60
3:U:114:ARG:O	3:U:118:ASN:ND2	2.35	0.60
2:c:83:CYS:SG	5:c:200:CYC:OC	2.58	0.60
2:d:25:LEU:HG	3:k:38:LEU:HD22	1.83	0.60
1:5:417:GLN:OE1	3:X:108:ARG:NH2	2.33	0.60
2:B:73:LYS:O	2:B:79:ASN:ND2	2.30	0.60
3:J:85:ASP:OD2	3:J:117:TYR:OH	2.16	0.60
2:b:75:TYR:O	2:b:79:ASN:ND2	2.34	0.60
2:b:98:LEU:HD21	2:b:151:ALA:HA	1.84	0.60
3:i:59:LEU:HD23	3:i:133:LEU:HD12	1.84	0.60
3:j:82:CYS:SG	5:j:200:CYC:H2C	2.41	0.60
1:5:322:SER:HB2	3:W:68:GLN:HG3	1.84	0.60
2:R:34:ARG:HD2	2:R:146:GLN:HE21	1.67	0.60
3:g:84:ARG:NH1	5:g:200:CYC:HB	2.00	0.60
1:5:655:PRO:O	1:5:714:ARG:NH1	2.33	0.60
5:5:1202:CYC:HBA1	3:l:84:ARG:NH2	2.15	0.60
2:P:90:TYR:O	2:P:94:ILE:HG12	2.02	0.60
2:f:7:THR:HA	2:f:10:ILE:HG22	1.83	0.60
1:5:119:PHE:HZ	1:5:155:LYS:HA	1.67	0.60
2:e:49:GLN:HA	2:e:52:LEU:HD12	1.83	0.60
3:I:154:SER:HA	3:I:157:TYR:HD2	1.66	0.59
2:R:50:ASP:OD1	2:R:51:ALA:N	2.35	0.59
2:f:140:GLY:HA2	2:f:148:LYS:NZ	2.17	0.59
1:5:322:SER:OG	1:5:323:SER:N	2.33	0.59
2:A:16:GLN:O	3:H:91:ARG:NH1	2.34	0.59
2:E:60:VAL:HA	2:E:130:GLU:OE2	2.02	0.59
3:J:78:ARG:HG2	5:J:200:CYC:HAD1	1.83	0.59
2:Q:110:VAL:HA	3:Y:76:HIS:HD2	1.66	0.59
2:e:25:LEU:HD12	3:g:38:LEU:HG	1.83	0.59
3:j:85:ASP:OD2	3:j:117:TYR:OH	2.18	0.59
2:F:136:LYS:HG3	2:F:152:LEU:HD22	1.84	0.59
3:W:5:PHE:CD1	3:W:27:LEU:HD12	2.36	0.59
2:a:39:ILE:HD13	3:h:28:ALA:HB2	1.82	0.59
3:g:135:LYS:NZ	3:g:165:ASP:OD1	2.28	0.59
2:A:110:VAL:HG23	2:A:111:ILE:HD12	1.84	0.59
3:W:110:LEU:HD21	3:W:167:ALA:HA	1.84	0.59
1:5:186:ARG:HH12	1:5:282:ARG:HD2	1.67	0.59
2:P:34:ARG:NH2	2:Q:33:GLU:OE1	2.36	0.59
3:g:84:ARG:NH2	5:g:200:CYC:O1A	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:152:LEU:HD23	2:f:155:ILE:HD11	1.84	0.59
3:L:37:ARG:NH1	3:L:97:LEU:O	2.29	0.59
2:N:34:ARG:NH1	2:N:146:GLN:OE1	2.36	0.59
3:W:32:LYS:NZ	3:W:33:GLU:OE1	2.34	0.59
2:A:41:ALA:HB2	2:A:147:SER:HB3	1.84	0.59
3:L:90:LEU:HD12	3:L:134:MET:HE3	1.84	0.59
2:R:52:LEU:HD21	2:R:138:GLU:CD	2.28	0.59
2:b:16:GLN:OE1	2:b:18:ARG:NE	2.32	0.59
1:5:328:GLU:HG2	3:W:78:ARG:HH12	1.68	0.59
2:B:82:LYS:HZ1	5:B:200:CYC:C3D	2.16	0.59
2:E:98:LEU:HA	2:E:154:TYR:HE2	1.68	0.59
2:N:146:GLN:O	2:N:149:THR:N	2.36	0.59
2:Q:82:LYS:HE3	5:Q:200:CYC:C4D	2.32	0.59
3:X:54:ASP:O	3:X:58:LYS:HG2	2.02	0.59
2:c:36:VAL:HA	2:c:39:ILE:HD12	1.84	0.59
2:E:73:LYS:NZ	5:E:200:CYC:O1D	2.36	0.59
2:E:146:GLN:NE2	5:L:201:CYC:O1A	2.36	0.59
3:J:127:VAL:HG22	5:J:200:CYC:H3C	1.83	0.59
2:f:69:GLN:N	2:f:72:GLU:OE2	2.35	0.59
3:j:72:ASN:HA	3:j:78:ARG:HH11	1.68	0.59
1:5:587:TYR:CE2	1:5:601:ARG:HG2	2.38	0.58
3:G:106:ASP:OD1	3:G:166:LYS:NZ	2.36	0.58
2:P:136:LYS:HB2	2:P:155:ILE:HG21	1.85	0.58
2:b:143:LEU:N	2:b:148:LYS:HZ3	2.01	0.58
2:c:92:ARG:O	2:c:95:THR:OG1	2.19	0.58
2:C:58:GLN:O	2:C:62:LYS:HG2	2.03	0.58
3:V:1:MET:HG2	3:V:2:ASN:N	2.17	0.58
3:l:54:ASP:OD1	3:l:55:ALA:N	2.36	0.58
3:l:59:LEU:HD21	3:l:130:ALA:HA	1.85	0.58
1:5:100:GLU:HB3	1:5:105:LEU:HD12	1.85	0.58
3:J:82:CYS:SG	5:J:200:CYC:HAC2	2.43	0.58
2:N:140:GLY:HA2	2:N:148:LYS:HE2	1.85	0.58
2:R:85:ARG:NH2	2:R:86:ASP:OD1	2.31	0.58
2:S:90:TYR:O	2:S:94:ILE:HG12	2.03	0.58
3:U:75:PRO:HD2	3:U:78:ARG:HD3	1.84	0.58
5:5:1201:CYC:HAB2	3:L:88:ILE:HG21	1.85	0.58
2:b:2:SER:OG	3:j:6:THR:OG1	2.19	0.58
2:f:110:VAL:HA	3:j:76:HIS:ND1	2.17	0.58
3:l:132:GLN:NE2	3:l:136:ASP:OD2	2.37	0.58
3:I:51:ILE:HG23	3:I:137:ALA:HB3	1.85	0.58
2:O:80:GLN:HA	2:O:83:CYS:SG	2.43	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:94:ILE:HD13	2:Q:155:ILE:HD13	1.85	0.58
3:h:73:ALA:HB1	3:h:79:MET:HB3	1.84	0.58
2:A:60:VAL:HG22	2:A:130:GLU:HG3	1.84	0.58
2:C:20:LEU:HD22	3:I:98:LEU:HD13	1.85	0.58
3:L:75:PRO:HD2	3:L:78:ARG:HG2	1.84	0.58
2:e:85:ARG:NH1	2:e:86:ASP:OD1	2.36	0.58
2:e:89:TYR:HD1	2:e:92:ARG:HH12	1.49	0.58
4:m:17:ARG:HA	4:m:77:ILE:HB	1.84	0.58
1:5:561:ALA:O	1:5:565:THR:N	2.32	0.58
3:H:105:LEU:HG	3:H:110:LEU:HD11	1.85	0.58
2:a:15:SER:OG	2:a:16:GLN:OE1	2.22	0.58
3:k:41:VAL:HG11	3:k:98:LEU:HD22	1.84	0.58
2:D:110:VAL:HA	3:L:76:HIS:HD2	1.69	0.58
2:S:127:TRP:HB3	5:S:200:CYC:HBC3	1.86	0.58
3:U:115:GLU:HG2	4:Z:73:VAL:H	1.69	0.58
2:c:39:ILE:HD13	3:i:28:ALA:HB2	1.85	0.58
3:i:88:ILE:HG13	3:i:91:ARG:HH21	1.69	0.58
1:5:599:SER:HB3	2:d:115:ARG:HH12	1.69	0.58
2:A:114:LEU:HA	3:G:76:HIS:CD2	2.39	0.58
3:J:114:ARG:HG2	3:J:114:ARG:HH11	1.69	0.58
2:O:100:ALA:HB2	3:W:9:ILE:HD11	1.86	0.58
3:h:89:ILE:HB	3:h:134:MET:HE1	1.86	0.58
3:l:41:VAL:HG21	3:l:98:LEU:HB2	1.84	0.58
1:5:403:LYS:NZ	1:5:452:ASP:OD1	2.29	0.57
1:5:487:PRO:HG2	3:W:112:GLY:H	1.68	0.57
1:5:598:GLU:HA	1:5:601:ARG:NE	2.19	0.57
3:j:92:TYR:CD2	3:j:109:CYS:HB2	2.39	0.57
3:k:2:ASN:O	3:k:103:SER:OG	2.22	0.57
2:F:152:LEU:HD13	3:G:147:ASN:HD21	1.68	0.57
2:P:30:GLY:O	2:P:34:ARG:HG2	2.04	0.57
2:R:29:PHE:HA	3:T:38:LEU:HD11	1.86	0.57
3:U:82:CYS:HA	5:U:200:CYC:HHD	1.85	0.57
3:g:92:TYR:HB3	3:g:105:LEU:HD13	1.86	0.57
3:l:153:CYS:HB2	3:l:157:TYR:CZ	2.39	0.57
2:B:77:ASP:OD1	2:B:78:SER:N	2.37	0.57
2:C:21:ASN:N	2:C:24:GLU:OE1	2.36	0.57
5:J:200:CYC:HB	5:J:200:CYC:HMA1	1.68	0.57
3:X:82:CYS:SG	5:X:200:CYC:H2C	2.45	0.57
2:c:18:ARG:NH1	2:c:19:PHE:O	2.38	0.57
2:c:41:ALA:HB2	2:c:147:SER:HB3	1.84	0.57
3:g:77:ARG:NH1	3:g:78:ARG:HG3	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:731:ARG:HA	1:5:734:GLN:HG2	1.86	0.57
3:K:32:LYS:NZ	3:K:33:GLU:OE1	2.34	0.57
2:b:39:ILE:HG23	3:j:24:LEU:HD22	1.85	0.57
2:d:35:ALA:O	2:d:39:ILE:N	2.34	0.57
5:5:1202:CYC:H3C	3:l:127:VAL:HG22	1.86	0.57
2:E:43:ARG:HH12	2:E:47:LYS:HE3	1.70	0.57
2:F:121:PHE:CE2	3:J:79:MET:HE2	2.39	0.57
3:T:72:ASN:ND2	3:T:123:PRO:HD2	2.20	0.57
3:g:84:ARG:NH1	3:g:85:ASP:OD1	2.38	0.57
3:l:73:ALA:HA	3:l:78:ARG:HG2	1.86	0.57
3:K:72:ASN:HD21	3:K:122:THR:HA	1.67	0.57
2:P:14:ASP:OD2	3:V:108:ARG:NH2	2.36	0.57
2:S:110:VAL:HG23	2:S:111:ILE:HG13	1.85	0.57
2:a:36:VAL:HB	2:a:37:PRO:HD3	1.87	0.57
2:b:1:MET:N	3:j:2:ASN:OD1	2.31	0.57
2:f:9:VAL:HG13	2:f:24:GLU:HB2	1.86	0.57
3:G:92:TYR:HB3	3:G:105:LEU:HD13	1.85	0.57
3:H:107:ASP:OD1	4:M:69:LYS:NZ	2.31	0.57
2:S:109:TYR:O	3:W:76:HIS:HB3	2.05	0.57
2:c:18:ARG:HH12	2:c:20:LEU:HD23	1.69	0.57
2:e:63:LYS:HB2	2:e:130:GLU:OE1	2.05	0.57
3:l:139:MET:HE1	3:l:157:TYR:HB3	1.87	0.57
1:5:162:ARG:NH1	1:5:227:GLU:OE2	2.37	0.57
2:A:114:LEU:HA	3:G:76:HIS:NE2	2.19	0.57
2:Q:127:TRP:CE3	5:Q:200:CYC:H3C	2.40	0.57
2:e:112:ALA:HB3	3:i:77:ARG:HB3	1.85	0.57
2:f:4:THR:O	2:f:8:GLU:N	2.31	0.57
2:A:77:ASP:OD1	2:A:78:SER:N	2.37	0.57
3:g:1:MET:HB2	3:g:108:ARG:HD2	1.87	0.57
3:h:2:ASN:HB2	3:h:7:ARG:NH1	2.20	0.57
3:l:3:ASP:N	3:l:6:THR:OG1	2.38	0.57
2:O:3:ARG:NH1	2:O:103:THR:OG1	2.37	0.57
2:Q:13:ALA:O	3:X:95:TYR:OH	2.22	0.57
2:R:18:ARG:NH2	2:R:24:GLU:OE1	2.38	0.57
2:a:92:ARG:HG2	3:h:18:PHE:CZ	2.39	0.57
2:D:60:VAL:HA	2:D:130:GLU:OE2	2.05	0.56
2:O:50:ASP:OD1	2:O:51:ALA:N	2.37	0.56
2:P:15:SER:OG	2:P:16:GLN:OE1	2.22	0.56
1:5:591:PHE:HB3	1:5:594:THR:OG1	2.04	0.56
2:F:41:ALA:HB2	2:F:147:SER:HB3	1.86	0.56
2:O:106:LEU:HD23	2:O:157:HIS:HD2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:51:MET:O	1:5:55:MET:HG2	2.05	0.56
5:E:200:CYC:HBB2	3:I:76:HIS:HD2	1.70	0.56
3:H:83:LEU:HA	3:H:86:MET:HE3	1.87	0.56
3:H:92:TYR:HB3	3:H:105:LEU:HD13	1.88	0.56
2:N:114:LEU:HA	3:T:76:HIS:NE2	2.21	0.56
2:S:114:LEU:HD12	3:W:76:HIS:HE1	1.71	0.56
2:a:151:ALA:O	2:a:155:ILE:HG12	2.05	0.56
2:D:43:ARG:NH2	3:K:25:ASP:OD1	2.33	0.56
3:H:113:LEU:HD23	3:H:171:ILE:HG12	1.88	0.56
2:N:92:ARG:NH2	3:U:13:ASP:HA	2.21	0.56
2:Q:83:CYS:HB2	5:Q:200:CYC:NC	2.20	0.56
2:R:9:VAL:HG13	2:R:24:GLU:HB3	1.87	0.56
2:R:63:LYS:HD2	2:R:64:PHE:CE1	2.40	0.56
3:j:132:GLN:NE2	3:j:136:ASP:OD2	2.38	0.56
3:H:109:CYS:HA	4:M:64:HIS:CE1	2.41	0.56
3:H:128:ALA:HB2	3:H:172:ALA:HB3	1.87	0.56
2:d:21:ASN:H	2:d:24:GLU:CD	2.14	0.56
3:g:53:SER:O	3:g:57:HIS:ND1	2.27	0.56
3:l:139:MET:O	3:l:143:LYS:HG2	2.05	0.56
2:E:18:ARG:NH1	2:E:24:GLU:OE2	2.39	0.56
5:O:200:CYC:OB	3:X:74:TYR:O	2.23	0.56
2:Q:18:ARG:O	3:X:95:TYR:OH	2.23	0.56
3:W:85:ASP:OD2	3:W:117:TYR:OH	2.15	0.56
2:b:31:ARG:NH2	2:b:100:ALA:O	2.37	0.56
3:j:139:MET:HA	3:j:142:LEU:HB2	1.87	0.56
3:W:2:ASN:HB2	3:W:7:ARG:NH2	2.21	0.56
3:g:37:ARG:NH2	3:g:159:GLU:OE2	2.39	0.56
2:A:133:ASN:O	2:A:136:LYS:HB2	2.06	0.56
2:N:64:PHE:O	2:N:67:VAL:HG22	2.06	0.56
2:a:5:VAL:HG13	2:a:6:ILE:HD12	1.88	0.56
2:f:124:ASN:HB3	2:f:127:TRP:CD2	2.40	0.56
3:k:145:THR:HG21	3:k:150:VAL:HG22	1.86	0.56
2:A:148:LYS:O	2:A:152:LEU:HG	2.06	0.56
3:K:85:ASP:OD2	3:K:117:TYR:OH	2.13	0.56
3:L:60:PHE:HZ	3:L:82:CYS:HG	1.52	0.56
3:T:63:GLN:OE1	3:T:66:LEU:HG	2.05	0.56
3:i:34:GLY:O	3:i:38:LEU:HG	2.06	0.56
3:i:106:ASP:OD1	3:i:166:LYS:NZ	2.38	0.56
3:k:106:ASP:HA	3:k:110:LEU:HB2	1.88	0.56
2:D:98:LEU:HA	2:D:154:TYR:HE2	1.71	0.56
3:H:151:GLY:HA3	5:H:201:CYC:HMD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:60:VAL:HA	2:Q:130:GLU:OE1	2.06	0.56
3:j:92:TYR:HD2	3:j:109:CYS:HB2	1.71	0.56
1:5:639:GLN:HG2	5:k:200:CYC:HBB2	1.87	0.55
2:C:117:VAL:HG13	3:H:79:MET:HE1	1.89	0.55
2:P:5:VAL:O	2:P:9:VAL:HG23	2.06	0.55
2:P:136:LYS:HG3	2:P:152:LEU:HD22	1.88	0.55
3:Y:39:ASP:OD1	5:Y:201:CYC:HHB	2.04	0.55
3:Y:139:MET:HE3	3:Y:139:MET:HA	1.88	0.55
2:b:83:CYS:SG	5:b:200:CYC:NC	2.79	0.55
3:l:92:TYR:CD2	3:l:109:CYS:HB2	2.41	0.55
1:5:251:GLY:O	3:J:108:ARG:NH1	2.39	0.55
1:5:332:GLN:O	1:5:336:ARG:N	2.39	0.55
1:5:412:LEU:O	3:X:108:ARG:NH1	2.39	0.55
2:E:86:ASP:OD2	2:E:128:TYR:OH	2.22	0.55
2:e:94:ILE:HD12	2:e:155:ILE:HG13	1.88	0.55
3:j:130:ALA:O	3:j:134:MET:HG2	2.06	0.55
1:5:162:ARG:NH2	1:5:237:GLU:OE2	2.37	0.55
1:5:597:MET:HB2	1:5:600:GLU:HG3	1.88	0.55
2:C:55:GLY:HA3	2:C:134:TYR:OH	2.06	0.55
2:C:98:LEU:HA	2:C:154:TYR:HE2	1.69	0.55
2:Q:26:GLN:HG2	5:X:201:CYC:HBB1	1.88	0.55
3:V:93:VAL:HG11	3:V:164:PHE:CE1	2.41	0.55
2:B:18:ARG:NH1	2:B:19:PHE:O	2.39	0.55
2:C:72:GLU:OE1	2:C:74:GLY:N	2.33	0.55
2:E:67:VAL:HG12	2:E:74:GLY:HA3	1.87	0.55
2:O:148:LYS:O	2:O:152:LEU:HG	2.07	0.55
1:5:641:ARG:HD3	1:5:736:ALA:HA	1.88	0.55
2:A:5:VAL:HG22	2:B:23:THR:HG23	1.89	0.55
2:B:39:ILE:HG23	3:J:24:LEU:HD22	1.88	0.55
2:Q:115:ARG:HH12	2:R:119:ARG:NH1	2.05	0.55
3:V:151:GLY:HA3	5:V:201:CYC:HMD2	1.87	0.55
2:c:34:ARG:NH2	5:k:201:CYC:OB	2.38	0.55
3:h:1:MET:HA	3:h:104:VAL:HG12	1.88	0.55
1:5:436:GLN:H	1:5:524:VAL:HG11	1.71	0.55
2:A:7:THR:OG1	3:H:3:ASP:OD2	2.19	0.55
2:D:19:PHE:HB3	3:K:45:THR:HG23	1.89	0.55
2:E:36:VAL:O	2:E:39:ILE:HG12	2.06	0.55
3:J:59:LEU:HD22	3:J:130:ALA:HB2	1.88	0.55
2:P:39:ILE:HG12	3:V:24:LEU:HD11	1.89	0.55
2:f:22:SER:O	2:f:25:LEU:HG	2.06	0.55
2:N:90:TYR:HE2	2:N:162:LEU:HD21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:16:GLN:OE1	2:P:16:GLN:N	2.35	0.55
3:X:85:ASP:OD2	3:X:117:TYR:OH	2.16	0.55
2:a:26:GLN:HB3	2:b:34:ARG:CZ	2.37	0.55
2:d:52:LEU:HD23	2:d:138:GLU:CD	2.32	0.55
1:5:419:ARG:NH1	1:5:504:ASP:OD2	2.26	0.55
2:P:156:ASP:HA	2:P:159:ILE:HG12	1.89	0.55
3:V:38:LEU:HD21	5:V:201:CYC:HAB1	1.88	0.55
3:X:135:LYS:NZ	3:X:165:ASP:OD1	2.38	0.55
2:a:90:TYR:O	2:a:94:ILE:HG12	2.07	0.55
2:f:50:ASP:OD1	2:f:50:ASP:N	2.39	0.55
3:T:107:ASP:OD1	3:T:108:ARG:N	2.40	0.55
3:V:105:LEU:HD21	3:V:167:ALA:HB2	1.88	0.55
2:f:92:ARG:O	2:f:95:THR:OG1	2.24	0.55
3:h:120:LEU:HD22	5:h:200:CYC:HBD1	1.88	0.55
1:5:551:THR:O	1:5:554:GLN:N	2.36	0.55
1:5:743:ALA:HB2	3:k:119:ALA:HB1	1.89	0.55
3:J:75:PRO:HG2	3:J:78:ARG:HE	1.70	0.55
2:c:94:ILE:HG12	2:c:106:LEU:HD11	1.89	0.55
2:f:159:ILE:O	2:f:163:SER:N	2.39	0.55
3:k:82:CYS:HB2	5:k:200:CYC:HC	1.72	0.55
2:A:31:ARG:HH12	2:A:35:ALA:HB2	1.71	0.54
2:B:77:ASP:HA	2:B:80:GLN:NE2	2.22	0.54
3:H:106:ASP:HA	3:H:110:LEU:HD12	1.88	0.54
2:N:90:TYR:HE1	5:N:200:CYC:HMB2	1.72	0.54
3:g:110:LEU:O	3:g:114:ARG:HG2	2.07	0.54
3:i:91:ARG:NH1	3:i:95:TYR:OH	2.37	0.54
3:l:153:CYS:HB3	3:l:156:LEU:HD12	1.89	0.54
1:5:405:GLU:O	1:5:409:SER:OG	2.15	0.54
1:5:740:ASP:OD1	1:5:741:SER:N	2.40	0.54
2:C:19:PHE:HB3	3:I:45:THR:HG23	1.89	0.54
5:G:201:CYC:HB	5:G:201:CYC:CMA	2.20	0.54
3:J:77:ARG:NH1	5:J:200:CYC:O1D	2.40	0.54
2:Q:14:ASP:OD1	3:X:92:TYR:OH	2.17	0.54
2:S:67:VAL:HG12	2:S:74:GLY:HA3	1.89	0.54
1:5:184:GLN:O	1:5:188:ILE:HG12	2.07	0.54
1:5:550:ASN:O	3:j:77:ARG:NH2	2.36	0.54
1:5:660:GLU:HG2	1:5:663:ARG:HH12	1.72	0.54
3:K:7:ARG:NE	3:K:101:ASP:OD2	2.40	0.54
5:O:200:CYC:HMD1	5:O:200:CYC:NC	2.16	0.54
3:X:10:ALA:O	3:X:14:LEU:HG	2.08	0.54
2:e:36:VAL:HA	2:e:39:ILE:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:117:VAL:HG11	3:j:76:HIS:NE2	2.22	0.54
5:5:1202:CYC:HB	3:l:84:ARG:HH12	1.55	0.54
2:C:91:LEU:O	2:C:95:THR:HG23	2.08	0.54
2:N:70:PRO:HG3	2:N:75:TYR:CE1	2.42	0.54
2:O:110:VAL:HG12	2:O:111:ILE:HD13	1.89	0.54
2:Q:127:TRP:HB3	5:Q:200:CYC:HBC3	1.90	0.54
2:a:36:VAL:O	2:a:39:ILE:HG22	2.07	0.54
2:b:6:ILE:HG23	2:b:31:ARG:HD3	1.88	0.54
2:c:79:ASN:HB3	5:c:200:CYC:HMD2	1.89	0.54
3:k:75:PRO:HD2	3:k:78:ARG:HB2	1.88	0.54
1:5:690:PHE:CE1	1:5:696:PRO:HA	2.43	0.54
2:a:2:SER:OG	2:a:3:ARG:NH2	2.41	0.54
2:d:21:ASN:OD1	2:d:22:SER:N	2.32	0.54
2:e:22:SER:HB2	2:e:26:GLN:HE22	1.71	0.54
2:e:117:VAL:HG21	3:i:79:MET:HE1	1.90	0.54
3:h:78:ARG:HB3	5:h:200:CYC:HMD1	1.89	0.54
1:5:559:ALA:HB1	1:5:562:VAL:HB	1.89	0.54
2:C:41:ALA:HB2	2:C:147:SER:HB3	1.89	0.54
3:T:69:PRO:HA	3:T:74:TYR:CG	2.42	0.54
3:U:2:ASN:O	3:U:103:SER:OG	2.23	0.54
3:V:86:MET:HE2	3:V:134:MET:SD	2.48	0.54
2:e:139:THR:HA	2:e:142:LEU:HB2	1.90	0.54
3:i:110:LEU:C	3:i:114:ARG:HH12	2.14	0.54
3:j:23:ASP:HA	3:j:26:LYS:HZ3	1.73	0.54
5:5:1201:CYC:HAA2	3:L:120:LEU:HD11	1.89	0.54
5:Q:200:CYC:CGD	3:Y:57:HIS:HE2	2.21	0.54
2:R:9:VAL:CG1	2:R:24:GLU:HB3	2.37	0.54
3:X:110:LEU:HD23	3:X:170:SER:HB3	1.88	0.54
3:Y:127:VAL:HG22	5:Y:200:CYC:H3C	1.89	0.54
2:b:32:PHE:HD1	3:j:31:ALA:HA	1.71	0.54
3:l:97:LEU:HA	3:l:163:TYR:HE2	1.72	0.54
4:m:14:GLN:HA	4:m:17:ARG:HH12	1.73	0.54
1:5:625:LYS:HE3	1:5:674:GLU:HB3	1.89	0.54
3:I:151:GLY:HA3	5:I:201:CYC:HMD2	1.89	0.54
3:J:114:ARG:NH2	3:J:170:SER:O	2.40	0.54
3:K:151:GLY:HA3	5:K:201:CYC:HMD2	1.89	0.54
3:L:7:ARG:HH11	3:L:103:SER:HB2	1.73	0.54
2:P:85:ARG:NH2	2:P:86:ASP:OD1	2.29	0.54
2:R:64:PHE:HE1	2:R:130:GLU:HG3	1.71	0.54
2:S:18:ARG:HH22	2:S:21:ASN:HB3	1.73	0.54
2:a:128:TYR:O	2:a:132:LEU:HG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:k:73:ALA:O	3:k:79:MET:HB3	2.08	0.54
3:k:110:LEU:C	3:k:114:ARG:HH12	2.15	0.54
1:5:193:LYS:NZ	1:5:271:ASP:OD2	2.34	0.54
2:B:115:ARG:NH2	2:C:119:ARG:HE	2.06	0.54
2:D:92:ARG:NH1	3:K:16:GLY:O	2.40	0.54
2:O:4:THR:O	2:O:8:GLU:N	2.34	0.54
3:V:127:VAL:HG22	5:V:200:CYC:HBC3	1.90	0.54
2:c:73:LYS:HZ3	2:c:127:TRP:HZ3	1.55	0.54
2:D:41:ALA:HB2	2:D:147:SER:HB2	1.89	0.54
2:D:114:LEU:HD21	2:D:162:LEU:HD23	1.90	0.54
3:I:113:LEU:HD23	3:I:171:ILE:HD11	1.89	0.54
2:N:35:ALA:O	2:N:39:ILE:HG13	2.08	0.54
3:V:111:ASN:OD1	3:V:112:GLY:N	2.42	0.54
3:X:11:GLN:O	3:X:15:LYS:HD3	2.08	0.54
3:h:5:PHE:CD1	3:h:27:LEU:HD22	2.43	0.54
3:j:1:MET:HG2	3:j:104:VAL:HA	1.89	0.54
2:E:5:VAL:HB	2:E:31:ARG:HG3	1.89	0.53
2:F:114:LEU:HD21	2:F:162:LEU:HD23	1.90	0.53
3:I:11:GLN:HB3	3:I:15:LYS:NZ	2.23	0.53
2:N:50:ASP:O	2:N:54:LYS:NZ	2.37	0.53
2:N:92:ARG:NH2	3:U:17:SER:O	2.41	0.53
3:U:58:LYS:O	3:U:62:GLU:HG3	2.08	0.53
2:b:18:ARG:NH1	2:b:19:PHE:O	2.41	0.53
2:d:49:GLN:HA	2:d:52:LEU:HD12	1.91	0.53
2:e:159:ILE:O	2:e:163:SER:N	2.36	0.53
2:f:69:GLN:O	2:f:75:TYR:HB2	2.08	0.53
1:5:140:TYR:CE1	3:L:84:ARG:HD2	2.43	0.53
2:C:115:ARG:NH2	2:C:163:SER:O	2.41	0.53
2:D:9:VAL:CG1	2:D:24:GLU:HB3	2.39	0.53
2:F:124:ASN:HD21	2:F:126:LEU:HD12	1.71	0.53
2:N:107:ASP:HA	2:N:111:ILE:HB	1.89	0.53
2:b:73:LYS:HZ2	2:b:123:LEU:HD21	1.71	0.53
2:e:10:ILE:HD13	3:g:104:VAL:HG21	1.90	0.53
2:A:90:TYR:O	2:A:94:ILE:HG12	2.09	0.53
5:R:200:CYC:HMA3	3:V:67:ILE:HD11	1.90	0.53
2:b:139:THR:O	2:b:148:LYS:NZ	2.35	0.53
3:i:1:MET:N	4:m:16:LYS:HG2	2.24	0.53
1:5:332:GLN:HG2	1:5:341:LEU:HD12	1.90	0.53
1:5:524:VAL:HG23	1:5:525:ARG:HG2	1.89	0.53
5:5:1201:CYC:HMD1	5:5:1201:CYC:NC	2.18	0.53
2:D:18:ARG:O	3:K:95:TYR:OH	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:132:GLN:O	3:X:135:LYS:HG2	2.08	0.53
1:5:720:ASP:HB2	1:5:724:THR:HG21	1.89	0.53
3:I:75:PRO:HD2	3:I:78:ARG:HB2	1.90	0.53
3:J:75:PRO:HD2	3:J:78:ARG:HB2	1.90	0.53
3:L:149:THR:O	5:L:201:CYC:NC	2.41	0.53
2:P:75:TYR:O	2:P:79:ASN:ND2	2.41	0.53
3:Y:129:ARG:NH2	3:Y:133:LEU:HD21	2.22	0.53
2:c:97:SER:HA	2:c:105:PRO:HG2	1.90	0.53
3:k:58:LYS:HD2	3:k:133:LEU:HB3	1.90	0.53
3:k:82:CYS:SG	3:k:86:MET:HE1	2.48	0.53
3:l:149:THR:O	5:l:201:CYC:NC	2.30	0.53
3:G:123:PRO:O	3:G:126:SER:OG	2.25	0.53
3:H:73:ALA:O	3:H:79:MET:HB2	2.07	0.53
2:R:43:ARG:HH11	3:T:24:LEU:HB3	1.73	0.53
4:Z:49:LEU:HD12	4:Z:50:THR:H	1.74	0.53
2:e:73:LYS:HG3	5:e:200:CYC:HMD2	1.90	0.53
2:f:98:LEU:HD23	2:f:154:TYR:CD2	2.44	0.53
3:g:91:ARG:HG2	3:g:95:TYR:CZ	2.44	0.53
1:5:707:GLN:O	3:j:108:ARG:NH2	2.42	0.53
2:A:126:LEU:HA	2:A:129:ILE:HG22	1.89	0.53
2:B:40:GLU:OE2	2:B:147:SER:OG	2.20	0.53
3:T:92:TYR:HB3	3:T:105:LEU:HD13	1.91	0.53
2:e:59:ALA:HA	2:e:62:LYS:HD2	1.89	0.53
2:E:9:VAL:HG13	2:E:24:GLU:HB2	1.90	0.53
2:E:132:LEU:HD23	2:E:135:ILE:HD12	1.91	0.53
2:F:43:ARG:NH1	3:L:21:GLU:OE1	2.40	0.53
3:H:11:GLN:HB3	3:H:15:LYS:NZ	2.24	0.53
2:P:23:THR:HG23	2:Q:5:VAL:HG22	1.91	0.53
2:P:140:GLY:O	2:P:148:LYS:NZ	2.42	0.53
3:T:135:LYS:HE3	3:T:161:ALA:HA	1.90	0.53
4:Z:57:LEU:HB3	4:Z:58:PRO:HD3	1.91	0.53
2:f:31:ARG:NE	2:f:101:SER:OG	2.42	0.53
3:j:112:GLY:O	3:j:116:THR:OG1	2.18	0.53
3:l:85:ASP:OD2	3:l:117:TYR:OH	2.17	0.53
3:H:82:CYS:HB2	5:H:200:CYC:HC	1.72	0.53
3:I:1:MET:H2	4:M:16:LYS:HD3	1.74	0.53
2:O:57:VAL:HG12	2:O:87:ILE:HD13	1.90	0.53
3:j:151:GLY:N	5:j:201:CYC:OC	2.42	0.53
2:F:76:GLY:O	2:F:80:GLN:HG2	2.09	0.53
3:T:58:LYS:O	3:T:61:ALA:N	2.41	0.53
3:Y:72:ASN:ND2	3:Y:123:PRO:HD2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:82:LYS:HB2	2:a:85:ARG:HE	1.74	0.53
2:d:77:ASP:OD1	2:d:78:SER:N	2.41	0.53
2:d:148:LYS:NZ	3:i:147:ASN:O	2.39	0.53
2:e:146:GLN:O	2:e:149:THR:N	2.41	0.53
3:g:127:VAL:HG22	5:g:200:CYC:HBC3	1.91	0.53
3:h:58:LYS:HE3	3:h:133:LEU:HD22	1.91	0.53
1:5:690:PHE:HB3	1:5:694:THR:HB	1.92	0.52
2:B:1:MET:O	2:B:3:ARG:NH2	2.36	0.52
2:C:64:PHE:O	2:C:67:VAL:HG12	2.09	0.52
5:J:200:CYC:HB	5:J:200:CYC:CMA	2.22	0.52
3:L:41:VAL:HG21	3:L:98:LEU:HB2	1.91	0.52
4:M:60:MET:HE2	4:M:64:HIS:CE1	2.44	0.52
2:N:5:VAL:O	2:N:9:VAL:HG23	2.09	0.52
2:P:97:SER:HB3	2:P:106:LEU:HB2	1.91	0.52
3:i:120:LEU:HD21	5:i:200:CYC:HBD1	1.91	0.52
1:5:349:ARG:HB3	1:5:351:PRO:HD2	1.91	0.52
2:A:83:CYS:HA	5:A:200:CYC:HAC2	1.92	0.52
2:B:48:ASN:HD22	2:B:142:LEU:HD13	1.74	0.52
2:E:2:SER:OG	2:E:3:ARG:N	2.35	0.52
2:N:144:SER:HA	2:N:148:LYS:HD2	1.92	0.52
4:Z:25:GLU:HB3	4:Z:29:TYR:CD2	2.44	0.52
2:a:127:TRP:CE3	5:a:200:CYC:H3C	2.45	0.52
2:a:146:GLN:NE2	2:a:150:GLU:OE1	2.42	0.52
3:g:77:ARG:HH12	3:g:78:ARG:HG3	1.74	0.52
2:B:38:ALA:HA	2:B:150:GLU:OE1	2.08	0.52
2:C:14:ASP:OD2	3:I:108:ARG:NH1	2.41	0.52
3:H:127:VAL:HG22	5:H:200:CYC:H3C	1.91	0.52
3:L:52:ILE:HD11	3:L:87:GLU:HA	1.90	0.52
4:M:72:ASN:OD1	4:M:73:VAL:N	2.43	0.52
2:N:43:ARG:HH22	3:U:21:GLU:HB2	1.74	0.52
3:Y:80:ALA:O	3:Y:84:ARG:HG3	2.10	0.52
2:a:96:TYR:OH	3:h:17:SER:O	2.28	0.52
2:e:116:GLU:OE1	2:e:117:VAL:HG23	2.09	0.52
3:k:2:ASN:HB2	3:k:7:ARG:HH11	1.73	0.52
1:5:572:ALA:O	1:5:574:PHE:HD2	1.93	0.52
1:5:575:THR:H	2:e:3:ARG:NH2	2.06	0.52
2:B:60:VAL:HA	2:B:130:GLU:OE1	2.09	0.52
2:B:127:TRP:CE3	5:B:200:CYC:H3C	2.45	0.52
2:C:64:PHE:CE2	2:C:127:TRP:HD1	2.28	0.52
2:E:106:LEU:HD21	2:E:158:ALA:HB2	1.91	0.52
2:F:90:TYR:O	2:F:94:ILE:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:56:ALA:O	2:P:60:VAL:HG23	2.08	0.52
2:Q:41:ALA:HB2	2:Q:147:SER:HB3	1.92	0.52
2:Q:43:ARG:O	2:Q:47:LYS:HG3	2.10	0.52
2:a:83:CYS:SG	5:a:200:CYC:H2C	2.50	0.52
2:a:124:ASN:HD21	2:a:126:LEU:HD12	1.73	0.52
1:5:581:GLY:HA3	2:f:18:ARG:HH12	1.75	0.52
2:E:114:LEU:HD12	3:I:76:HIS:CE1	2.43	0.52
3:V:7:ARG:HH22	3:V:101:ASP:CG	2.17	0.52
2:d:82:LYS:HD2	5:d:200:CYC:HAD2	1.91	0.52
1:5:656:TYR:O	1:5:714:ARG:NH1	2.39	0.52
2:A:3:ARG:NH1	2:A:8:GLU:OE1	2.42	0.52
2:A:21:ASN:O	2:A:25:LEU:HD23	2.09	0.52
2:F:9:VAL:HG13	2:F:24:GLU:HB3	1.91	0.52
3:K:120:LEU:HD11	5:K:200:CYC:HAA2	1.91	0.52
2:R:50:ASP:HB2	2:R:54:LYS:NZ	2.24	0.52
3:V:114:ARG:HG2	3:V:114:ARG:HH11	1.75	0.52
5:W:200:CYC:HMD1	5:W:200:CYC:NC	2.17	0.52
3:X:7:ARG:HD2	3:X:101:ASP:CG	2.35	0.52
2:f:57:VAL:HG12	2:f:61:PHE:CE2	2.45	0.52
3:g:3:ASP:OD1	3:g:6:THR:N	2.29	0.52
5:C:200:CYC:CGA	3:H:67:ILE:HD13	2.40	0.52
2:E:9:VAL:HG22	2:E:24:GLU:HB2	1.90	0.52
3:V:59:LEU:HD22	3:V:130:ALA:HB2	1.91	0.52
2:b:94:ILE:HD13	2:b:155:ILE:HG22	1.90	0.52
2:d:92:ARG:O	2:d:95:THR:OG1	2.23	0.52
2:f:36:VAL:HA	2:f:39:ILE:HG22	1.90	0.52
3:J:105:LEU:O	3:J:109:CYS:HB3	2.10	0.52
2:a:5:VAL:O	2:a:9:VAL:HG23	2.10	0.52
2:a:146:GLN:O	2:a:149:THR:OG1	2.14	0.52
3:i:134:MET:HA	3:i:134:MET:HE3	1.90	0.52
2:A:148:LYS:HZ1	3:J:147:ASN:HA	1.75	0.52
2:D:36:VAL:HB	2:D:37:PRO:HD3	1.92	0.52
3:K:75:PRO:HD2	3:K:78:ARG:HB2	1.92	0.52
2:N:114:LEU:HA	3:T:76:HIS:CD2	2.44	0.52
2:O:54:LYS:O	2:O:58:GLN:HG2	2.09	0.52
3:V:81:ALA:HA	3:V:84:ARG:HG2	1.92	0.52
3:W:135:LYS:NZ	3:W:165:ASP:OD1	2.35	0.52
3:Y:74:TYR:HB3	3:Y:75:PRO:HD3	1.91	0.52
2:c:10:ILE:HD12	3:i:99:ALA:HB2	1.92	0.52
3:h:7:ARG:NH1	3:h:103:SER:OG	2.43	0.52
3:j:53:SER:O	3:j:57:HIS:ND1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:k:84:ARG:NH2	5:k:200:CYC:O2A	2.42	0.52
2:C:114:LEU:HD21	2:C:162:LEU:HD23	1.91	0.52
3:G:102:ALA:HB1	3:G:166:LYS:HZ3	1.75	0.52
5:W:200:CYC:HB	5:W:200:CYC:CMA	2.23	0.52
3:Y:62:GLU:OE1	3:Y:129:ARG:NH2	2.43	0.52
2:a:136:LYS:HZ1	2:a:155:ILE:HB	1.75	0.52
2:b:13:ALA:O	3:j:91:ARG:NH2	2.42	0.52
2:B:82:LYS:HZ1	5:B:200:CYC:C2D	2.23	0.51
2:Q:17:GLY:O	3:X:91:ARG:NH2	2.43	0.51
2:S:22:SER:O	2:S:26:GLN:HG3	2.10	0.51
2:b:17:GLY:HA2	3:j:91:ARG:HH12	1.75	0.51
2:f:124:ASN:HB3	2:f:127:TRP:CE2	2.45	0.51
3:g:86:MET:HE2	3:g:134:MET:SD	2.50	0.51
3:l:11:GLN:O	3:l:15:LYS:HE2	2.10	0.51
3:G:149:THR:O	5:G:201:CYC:NC	2.42	0.51
2:R:31:ARG:HH22	3:T:5:PHE:HD2	1.58	0.51
3:i:55:ALA:O	3:i:59:LEU:HG	2.09	0.51
3:j:75:PRO:HD2	3:j:78:ARG:HD2	1.92	0.51
3:j:143:LYS:HB3	3:j:157:TYR:HE2	1.76	0.51
3:l:92:TYR:HE2	3:l:108:ARG:HG3	1.75	0.51
2:R:4:THR:HG21	2:R:31:ARG:HH21	1.75	0.51
3:T:1:MET:HA	3:T:104:VAL:HG12	1.91	0.51
4:Z:32:ASN:OD1	4:Z:35:ARG:NH1	2.43	0.51
3:g:78:ARG:HG2	5:g:200:CYC:HAD1	1.92	0.51
3:i:101:ASP:OD1	3:i:102:ALA:N	2.41	0.51
3:j:83:LEU:HA	3:j:86:MET:HE2	1.91	0.51
2:A:3:ARG:HB3	2:A:8:GLU:OE2	2.10	0.51
2:N:36:VAL:HB	2:N:37:PRO:HD3	1.91	0.51
2:N:54:LYS:O	2:N:58:GLN:HG2	2.10	0.51
2:O:9:VAL:HA	2:O:12:THR:HG22	1.93	0.51
3:T:116:THR:HG21	5:T:200:CYC:HMA1	1.92	0.51
3:Y:113:LEU:HD23	3:Y:171:ILE:HG12	1.92	0.51
2:c:39:ILE:HG23	3:i:24:LEU:HB3	1.92	0.51
1:5:689:CYS:HB3	1:5:699:ARG:NH2	2.25	0.51
3:H:143:LYS:HE2	3:H:143:LYS:HA	1.92	0.51
2:a:65:PRO:O	2:a:68:THR:OG1	2.26	0.51
2:c:3:ARG:HE	2:c:7:THR:HG21	1.75	0.51
3:i:153:CYS:HB2	3:i:157:TYR:HE2	1.76	0.51
3:V:129:ARG:O	3:V:132:GLN:HG3	2.10	0.51
2:b:52:LEU:HD13	2:b:91:LEU:HD11	1.92	0.51
2:e:22:SER:HB3	2:f:153:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:114:LEU:O	2:f:118:ASN:ND2	2.43	0.51
3:i:36:LYS:HG2	3:i:156:LEU:HD11	1.92	0.51
2:A:136:LYS:CE	2:A:152:LEU:HD22	2.38	0.51
5:B:200:CYC:HBB2	3:K:75:PRO:HA	1.93	0.51
3:H:47:ASN:OD1	3:H:141:HIS:ND1	2.43	0.51
2:N:121:PHE:CE2	5:N:200:CYC:HAA1	2.46	0.51
2:P:34:ARG:NH2	2:Q:29:PHE:HD1	2.05	0.51
3:T:35:VAL:HG11	5:T:201:CYC:C2A	2.41	0.51
2:c:107:ASP:HA	2:c:111:ILE:HD12	1.93	0.51
2:f:53:VAL:O	2:f:57:VAL:HG23	2.10	0.51
2:f:92:ARG:HA	3:l:18:PHE:CE1	2.46	0.51
2:A:15:SER:HB2	2:A:16:GLN:NE2	2.26	0.51
3:H:143:LYS:HE3	3:H:157:TYR:CE2	2.46	0.51
2:a:51:ALA:HA	2:a:54:LYS:HZ2	1.76	0.51
2:b:72:GLU:CD	2:b:74:GLY:H	2.18	0.51
5:k:200:CYC:HC	5:k:200:CYC:HMD3	1.75	0.51
2:B:70:PRO:HG3	2:B:75:TYR:CE1	2.46	0.51
3:V:47:ASN:OD1	3:V:141:HIS:ND1	2.44	0.51
3:X:72:ASN:HD22	3:X:123:PRO:CD	2.24	0.51
2:b:110:VAL:HA	3:k:76:HIS:HB2	1.92	0.51
2:c:108:ASP:OD1	2:c:109:TYR:N	2.44	0.51
2:c:138:GLU:O	2:c:141:LYS:HG3	2.11	0.51
1:5:598:GLU:HA	1:5:601:ARG:HE	1.76	0.51
2:A:156:ASP:HA	2:A:159:ILE:HB	1.92	0.51
3:G:82:CYS:HA	5:G:200:CYC:HHD	1.93	0.51
3:G:85:ASP:OD2	3:G:117:TYR:OH	2.28	0.51
3:J:84:ARG:O	3:J:88:ILE:HG12	2.11	0.51
2:O:22:SER:O	2:O:26:GLN:HG2	2.11	0.51
2:S:4:THR:HG23	2:S:100:ALA:O	2.11	0.51
2:S:61:PHE:CZ	2:S:80:GLN:HG2	2.46	0.51
3:V:33:GLU:HG2	3:V:36:LYS:HE2	1.93	0.51
3:X:22:SER:O	3:X:26:LYS:HG2	2.11	0.51
2:c:52:LEU:HD21	2:c:138:GLU:HB3	1.93	0.51
2:c:115:ARG:HB3	2:c:119:ARG:NH1	2.20	0.51
2:d:18:ARG:NH2	2:d:24:GLU:OE2	2.44	0.51
2:e:22:SER:O	2:e:25:LEU:N	2.44	0.51
2:e:67:VAL:HG22	2:e:74:GLY:H	1.76	0.51
2:f:10:ILE:HD13	3:l:1:MET:HE1	1.93	0.51
2:f:55:GLY:HA3	2:f:134:TYR:OH	2.11	0.51
3:i:51:ILE:HD11	3:i:141:HIS:HB2	1.93	0.51
3:l:62:GLU:CD	3:l:63:GLN:HG2	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:107:ASP:HA	2:D:111:ILE:HB	1.93	0.50
3:L:39:ASP:OD1	5:L:201:CYC:HHB	2.12	0.50
2:O:5:VAL:HG21	2:O:31:ARG:HB2	1.93	0.50
2:b:1:MET:HA	2:b:1:MET:HE3	1.92	0.50
2:d:3:ARG:H	2:d:104:GLY:HA3	1.76	0.50
2:f:89:TYR:O	2:f:92:ARG:HB3	2.11	0.50
3:l:114:ARG:HD2	3:l:118:ASN:ND2	2.24	0.50
3:H:32:LYS:HE2	3:H:32:LYS:HA	1.94	0.50
2:P:83:CYS:SG	5:P:200:CYC:HAC2	2.50	0.50
3:V:60:PHE:O	3:V:64:GLN:NE2	2.42	0.50
3:W:40:ALA:HB1	3:W:142:LEU:HD11	1.93	0.50
2:a:44:ALA:HA	2:a:47:LYS:HD2	1.93	0.50
1:5:102:ILE:HD11	3:J:119:ALA:HB1	1.93	0.50
2:B:93:PHE:CE1	2:B:109:TYR:HD2	2.29	0.50
2:C:50:ASP:HB3	2:C:54:LYS:HZ1	1.75	0.50
2:E:73:LYS:O	2:E:79:ASN:ND2	2.44	0.50
2:E:83:CYS:HA	5:E:200:CYC:HAC2	1.92	0.50
2:F:151:ALA:O	2:F:155:ILE:HD12	2.12	0.50
3:H:88:ILE:HG21	5:H:200:CYC:HAB1	1.93	0.50
3:L:110:LEU:HD13	3:L:170:SER:HB3	1.93	0.50
2:R:138:GLU:O	2:R:141:LYS:HG2	2.11	0.50
3:U:127:VAL:HG22	5:U:200:CYC:H3C	1.92	0.50
2:c:107:ASP:HA	2:c:111:ILE:HB	1.92	0.50
2:D:151:ALA:O	2:D:155:ILE:HG12	2.11	0.50
2:N:4:THR:H	2:N:7:THR:HB	1.76	0.50
2:Q:50:ASP:HB3	2:Q:54:LYS:HZ1	1.76	0.50
3:X:7:ARG:O	3:X:11:GLN:HG2	2.12	0.50
3:k:149:THR:O	5:k:201:CYC:NC	2.33	0.50
1:5:329:THR:HG21	3:Y:14:LEU:HD21	1.93	0.50
2:A:43:ARG:HG2	2:A:47:LYS:HD2	1.92	0.50
2:P:64:PHE:O	2:P:67:VAL:HG12	2.12	0.50
2:a:4:THR:OG1	3:h:3:ASP:OD2	2.29	0.50
2:b:133:ASN:HA	2:b:136:LYS:NZ	2.27	0.50
3:g:82:CYS:O	3:g:86:MET:HG3	2.12	0.50
3:j:69:PRO:HA	3:j:74:TYR:CG	2.46	0.50
1:5:678:ASP:O	1:5:682:ASP:HB2	2.12	0.50
3:J:40:ALA:HB1	3:J:142:LEU:HD11	1.93	0.50
2:N:50:ASP:HA	2:N:53:VAL:HG12	1.92	0.50
2:N:53:VAL:O	2:N:57:VAL:HG23	2.12	0.50
2:f:49:GLN:HG2	2:f:50:ASP:N	2.27	0.50
3:i:86:MET:HE2	3:i:86:MET:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:72:ASN:HD22	3:J:123:PRO:HD3	1.77	0.50
4:M:10:ALA:HA	4:M:15:GLY:HA3	1.94	0.50
2:N:21:ASN:OD1	2:N:24:GLU:HG2	2.12	0.50
2:P:9:VAL:HG13	2:P:24:GLU:HB2	1.92	0.50
2:P:106:LEU:O	2:P:110:VAL:HG12	2.12	0.50
2:P:124:ASN:HB3	2:P:127:TRP:CE2	2.46	0.50
5:d:200:CYC:HB	5:d:200:CYC:CMA	2.24	0.50
3:g:85:ASP:HA	3:g:88:ILE:HG22	1.93	0.50
2:C:83:CYS:SG	5:C:200:CYC:OC	2.70	0.50
2:O:77:ASP:OD1	2:O:78:SER:N	2.44	0.50
2:P:54:LYS:O	2:P:58:GLN:HG2	2.12	0.50
2:R:107:ASP:HA	2:R:111:ILE:HG12	1.94	0.50
2:S:9:VAL:HG13	2:S:24:GLU:HB3	1.94	0.50
3:T:83:LEU:HA	3:T:86:MET:HG2	1.93	0.50
2:e:70:PRO:HA	2:e:75:TYR:CG	2.47	0.50
2:e:83:CYS:SG	5:e:200:CYC:OC	2.70	0.50
3:i:51:ILE:HG23	3:i:137:ALA:HB3	1.94	0.50
2:D:148:LYS:NZ	3:I:147:ASN:HA	2.26	0.50
2:E:85:ARG:NH2	2:E:86:ASP:OD1	2.45	0.50
5:G:201:CYC:HMA3	5:G:201:CYC:NB	2.27	0.50
2:S:148:LYS:O	2:S:152:LEU:HG	2.12	0.50
2:f:64:PHE:O	2:f:67:VAL:HG22	2.11	0.50
3:h:84:ARG:HA	3:h:87:GLU:HG3	1.94	0.50
5:5:1202:CYC:HHD	3:l:82:CYS:HA	1.93	0.49
3:I:72:ASN:ND2	3:I:122:THR:HA	2.27	0.49
3:K:41:VAL:HG21	3:K:98:LEU:HB2	1.94	0.49
2:N:83:CYS:O	2:N:87:ILE:HG12	2.12	0.49
2:O:82:LYS:HZ2	5:O:200:CYC:C4D	2.25	0.49
2:Q:151:ALA:O	2:Q:155:ILE:HG12	2.12	0.49
5:S:200:CYC:O2D	3:W:57:HIS:NE2	2.34	0.49
2:a:115:ARG:NH2	2:a:161:ALA:O	2.38	0.49
2:c:3:ARG:NH2	2:c:7:THR:HG21	2.22	0.49
2:f:39:ILE:HD13	3:l:28:ALA:HB2	1.93	0.49
3:h:3:ASP:O	3:h:7:ARG:N	2.40	0.49
1:5:230:GLU:O	1:5:234:ASN:ND2	2.43	0.49
1:5:359:GLY:HA3	2:S:16:GLN:HG3	1.94	0.49
1:5:549:THR:HG22	3:l:14:LEU:HD11	1.93	0.49
3:I:1:MET:N	4:M:16:LYS:HD3	2.27	0.49
3:I:92:TYR:OH	3:I:108:ARG:NH2	2.45	0.49
3:K:59:LEU:HD22	3:K:130:ALA:HB2	1.94	0.49
3:L:74:TYR:HB3	3:L:75:PRO:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:86:ASP:HB3	2:N:128:TYR:HE2	1.77	0.49
2:Q:72:GLU:HG3	2:Q:73:LYS:H	1.77	0.49
3:h:51:ILE:HG23	3:h:137:ALA:HB3	1.94	0.49
3:i:99:ALA:HB3	3:i:104:VAL:HG11	1.94	0.49
1:5:183:SER:HB3	3:K:111:ASN:OD1	2.13	0.49
1:5:367:GLN:NE2	1:5:427:LEU:O	2.35	0.49
2:A:4:THR:H	2:A:7:THR:HB	1.76	0.49
2:B:82:LYS:HZ1	5:B:200:CYC:C1D	2.25	0.49
2:D:148:LYS:O	2:D:152:LEU:HD23	2.12	0.49
3:G:75:PRO:CD	3:G:78:ARG:HD2	2.41	0.49
3:L:7:ARG:NH1	3:L:101:ASP:OD2	2.45	0.49
2:P:96:TYR:OH	3:V:17:SER:O	2.30	0.49
3:U:38:LEU:HD23	5:U:201:CYC:OB	2.11	0.49
3:U:139:MET:O	3:U:143:LYS:HG2	2.12	0.49
3:V:92:TYR:HD2	3:V:109:CYS:HB2	1.77	0.49
3:Y:72:ASN:HD21	3:Y:122:THR:HG23	1.77	0.49
2:a:136:LYS:NZ	2:a:155:ILE:HB	2.27	0.49
2:e:124:ASN:HB3	2:e:127:TRP:CD2	2.46	0.49
3:h:79:MET:O	3:h:83:LEU:HG	2.12	0.49
2:A:26:GLN:O	2:A:29:PHE:HB3	2.12	0.49
2:A:61:PHE:CZ	2:A:80:GLN:HG2	2.47	0.49
3:L:135:LYS:HD3	3:L:164:PHE:HB2	1.93	0.49
2:S:9:VAL:HG11	2:S:24:GLU:HB3	1.95	0.49
3:U:93:VAL:HG21	3:U:164:PHE:CE1	2.47	0.49
3:U:149:THR:O	5:U:201:CYC:OC	2.30	0.49
3:X:75:PRO:HD2	3:X:78:ARG:HB2	1.93	0.49
2:c:50:ASP:O	2:c:54:LYS:HG2	2.12	0.49
3:g:10:ALA:O	3:g:14:LEU:HG	2.12	0.49
3:i:153:CYS:HB2	3:i:157:TYR:CE2	2.47	0.49
1:5:460:GLU:O	4:Z:62:ARG:NH1	2.45	0.49
1:5:552:TYR:CE2	1:5:556:ARG:HD2	2.47	0.49
2:C:10:ILE:HD11	3:I:99:ALA:HB2	1.94	0.49
2:F:86:ASP:OD2	2:F:128:TYR:OH	2.28	0.49
3:H:115:GLU:HG2	4:M:73:VAL:HG12	1.94	0.49
2:Q:98:LEU:HA	2:Q:154:TYR:HE2	1.77	0.49
2:R:131:ALA:O	2:R:135:ILE:HG12	2.12	0.49
3:U:128:ALA:HB2	3:U:172:ALA:HB3	1.95	0.49
2:c:4:THR:HG22	2:c:100:ALA:HB1	1.94	0.49
2:c:94:ILE:HD13	2:c:155:ILE:HG22	1.95	0.49
3:h:106:ASP:OD2	3:h:166:LYS:NZ	2.40	0.49
1:5:663:ARG:O	1:5:667:LEU:HG	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:114:LEU:HD12	3:G:76:HIS:NE2	2.28	0.49
2:F:9:VAL:CG1	2:F:24:GLU:HB3	2.42	0.49
3:G:63:GLN:OE1	3:G:65:GLU:HG3	2.12	0.49
5:J:200:CYC:HMA1	5:J:200:CYC:NB	2.27	0.49
3:K:47:ASN:O	3:K:51:ILE:HD12	2.13	0.49
3:T:59:LEU:HD22	3:T:130:ALA:HB2	1.95	0.49
3:X:72:ASN:ND2	3:X:123:PRO:HD2	2.28	0.49
2:b:67:VAL:O	2:b:69:GLN:N	2.45	0.49
3:g:153:CYS:SG	5:g:201:CYC:OC	2.70	0.49
3:k:82:CYS:HB2	5:k:200:CYC:NC	2.28	0.49
3:l:158:SER:O	3:l:162:THR:HG23	2.13	0.49
2:A:98:LEU:HA	2:A:154:TYR:HE2	1.77	0.49
2:B:60:VAL:HG11	5:B:200:CYC:HBC2	1.93	0.49
3:I:36:LYS:HD2	3:I:153:CYS:SG	2.53	0.49
2:a:21:ASN:N	2:a:24:GLU:OE2	2.42	0.49
2:d:24:GLU:OE1	2:d:24:GLU:N	2.36	0.49
3:k:117:TYR:HB3	3:k:122:THR:HB	1.94	0.49
1:5:431:ARG:NH2	1:5:438:GLU:OE1	2.32	0.49
1:5:500:TYR:H	3:Y:111:ASN:HD22	1.61	0.49
2:S:34:ARG:HH22	5:T:201:CYC:HBB2	1.78	0.49
3:V:74:TYR:HB3	3:V:75:PRO:HD3	1.93	0.49
1:5:574:PHE:HE1	1:5:579:PHE:CD1	2.31	0.49
5:5:1202:CYC:HMD3	3:l:82:CYS:HB2	1.95	0.49
2:B:93:PHE:HE1	2:B:109:TYR:HD2	1.61	0.49
2:D:135:ILE:O	2:D:139:THR:HG23	2.13	0.49
3:J:114:ARG:HG2	3:J:114:ARG:NH1	2.27	0.49
2:O:41:ALA:HB2	2:O:147:SER:HB3	1.95	0.49
2:S:19:PHE:HB3	3:Y:45:THR:HG23	1.93	0.49
2:a:127:TRP:O	2:a:130:GLU:HG2	2.13	0.49
5:h:200:CYC:OB	4:m:60:MET:SD	2.71	0.49
3:j:36:LYS:HB3	3:j:156:LEU:HD11	1.95	0.49
3:k:120:LEU:HD22	5:k:200:CYC:HBD1	1.94	0.49
1:5:650:LEU:HD13	1:5:681:LEU:HD11	1.94	0.49
2:D:130:GLU:HA	2:D:133:ASN:HB2	1.95	0.49
2:F:40:GLU:O	2:F:43:ARG:HG2	2.13	0.49
3:K:54:ASP:HB3	3:K:58:LYS:NZ	2.28	0.49
2:P:105:PRO:O	2:P:109:TYR:HB2	2.12	0.49
2:R:86:ASP:OD2	2:R:128:TYR:OH	2.28	0.49
3:W:75:PRO:HD2	3:W:78:ARG:HE	1.77	0.49
3:X:36:LYS:HD2	3:X:153:CYS:SG	2.53	0.49
2:b:113:GLY:O	2:b:117:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:g:201:CYC:HBC2	5:g:201:CYC:H2C	1.73	0.49
3:l:36:LYS:HG2	5:l:201:CYC:C2D	2.43	0.49
3:I:131:VAL:HA	3:I:134:MET:HE2	1.95	0.48
2:N:160:ASN:O	2:N:163:SER:OG	2.28	0.48
2:R:77:ASP:OD1	2:R:78:SER:N	2.46	0.48
3:g:65:GLU:HA	3:g:68:GLN:HG2	1.95	0.48
3:j:82:CYS:SG	3:j:86:MET:HE1	2.53	0.48
3:k:113:LEU:HD13	5:k:200:CYC:C4B	2.43	0.48
3:l:66:LEU:HD13	3:l:72:ASN:HB3	1.93	0.48
1:5:399:ARG:HH21	4:Z:55:ARG:NH1	2.11	0.48
2:B:34:ARG:O	2:B:37:PRO:HD2	2.13	0.48
2:E:107:ASP:HA	2:E:111:ILE:HD13	1.95	0.48
2:F:25:LEU:HD22	3:L:38:LEU:HD22	1.95	0.48
2:N:110:VAL:HG12	5:N:200:CYC:HAB1	1.96	0.48
2:S:6:ILE:HG21	3:Y:99:ALA:HA	1.95	0.48
3:T:86:MET:HB2	3:T:134:MET:HE1	1.94	0.48
3:U:43:ALA:O	3:U:47:ASN:ND2	2.46	0.48
3:U:135:LYS:HA	3:U:164:PHE:CE2	2.48	0.48
3:V:72:ASN:ND2	3:V:122:THR:HA	2.28	0.48
3:W:58:LYS:O	3:W:62:GLU:HG3	2.12	0.48
3:X:127:VAL:HG13	5:X:200:CYC:HBC3	1.94	0.48
3:Y:23:ASP:O	3:Y:27:LEU:HG	2.12	0.48
2:b:110:VAL:HG12	3:k:76:HIS:HD2	1.78	0.48
2:c:43:ARG:HH22	2:c:47:LYS:HB3	1.77	0.48
2:c:47:LYS:NZ	2:c:48:ASN:OD1	2.37	0.48
2:f:19:PHE:HB3	3:l:45:THR:HG23	1.95	0.48
3:h:128:ALA:O	3:h:132:GLN:HG3	2.13	0.48
3:k:129:ARG:O	3:k:133:LEU:HG	2.12	0.48
1:5:90:PRO:HD2	3:J:65:GLU:HG2	1.96	0.48
2:C:14:ASP:CG	3:I:108:ARG:HH22	2.20	0.48
2:E:2:SER:HG	2:E:3:ARG:H	1.59	0.48
2:E:56:ALA:O	2:E:60:VAL:HG23	2.13	0.48
2:R:124:ASN:HB3	2:R:127:TRP:CE2	2.49	0.48
3:U:10:ALA:O	3:U:14:LEU:HG	2.13	0.48
2:e:3:ARG:H	2:e:104:GLY:HA3	1.77	0.48
2:e:65:PRO:O	2:e:68:THR:OG1	2.27	0.48
2:f:146:GLN:HG2	2:f:147:SER:N	2.28	0.48
2:C:14:ASP:OD2	3:I:108:ARG:NH2	2.45	0.48
3:G:105:LEU:HD23	3:G:166:LYS:HZ1	1.78	0.48
5:H:200:CYC:HB	5:H:200:CYC:CMA	2.23	0.48
2:Q:91:LEU:O	2:Q:95:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:g:201:CYC:HB	5:g:201:CYC:CMA	2.26	0.48
3:h:126:SER:HA	3:h:129:ARG:HG2	1.94	0.48
3:j:60:PHE:CE2	3:j:79:MET:HE1	2.48	0.48
3:j:139:MET:HA	3:j:142:LEU:HD12	1.95	0.48
1:5:532:ARG:NE	2:f:77:ASP:OD2	2.44	0.48
2:C:44:ALA:HA	2:C:47:LYS:HD3	1.95	0.48
3:G:110:LEU:HD12	3:G:170:SER:HB3	1.96	0.48
3:J:42:ALA:HA	3:J:45:THR:HG22	1.96	0.48
2:Q:148:LYS:O	2:Q:152:LEU:HD23	2.13	0.48
2:R:83:CYS:SG	5:R:200:CYC:H2C	2.53	0.48
3:Y:85:ASP:OD2	3:Y:117:TYR:OH	2.23	0.48
2:b:32:PHE:CD1	3:j:31:ALA:HA	2.49	0.48
2:b:55:GLY:HA3	2:b:134:TYR:CZ	2.49	0.48
2:d:43:ARG:NH1	3:k:21:GLU:OE1	2.44	0.48
2:f:105:PRO:O	2:f:109:TYR:HD1	1.95	0.48
3:l:51:ILE:HG13	3:l:137:ALA:HB3	1.94	0.48
1:5:102:ILE:HG22	1:5:104:ALA:H	1.78	0.48
2:A:31:ARG:NH1	2:A:35:ALA:HB2	2.29	0.48
3:U:93:VAL:HG11	3:U:164:PHE:HE1	1.79	0.48
3:W:13:ASP:O	3:W:16:GLY:N	2.24	0.48
2:e:29:PHE:O	2:e:32:PHE:N	2.46	0.48
3:g:73:ALA:O	3:g:79:MET:HB3	2.14	0.48
3:i:135:LYS:HE3	3:i:161:ALA:HA	1.95	0.48
1:5:181:LYS:HA	3:K:107:ASP:OD2	2.14	0.48
1:5:597:MET:HG3	2:d:112:ALA:HB1	1.94	0.48
3:T:93:VAL:HG11	3:T:164:PHE:CZ	2.48	0.48
3:V:62:GLU:OE1	3:V:63:GLN:HG2	2.13	0.48
2:d:106:LEU:O	2:d:110:VAL:HG22	2.14	0.48
2:e:124:ASN:HB3	2:e:127:TRP:CE2	2.49	0.48
3:H:5:PHE:HD1	3:H:27:LEU:HD23	1.79	0.48
2:N:148:LYS:HZ3	2:N:152:LEU:HD11	1.78	0.48
4:Z:27:GLY:HA2	4:Z:30:ALA:HB3	1.96	0.48
2:f:130:GLU:HA	2:f:133:ASN:HD22	1.77	0.48
3:h:82:CYS:O	3:h:86:MET:HG2	2.14	0.48
3:i:37:ARG:O	3:i:41:VAL:HG23	2.13	0.48
1:5:255:GLN:O	1:5:259:ARG:HG3	2.14	0.48
2:B:2:SER:O	2:B:7:THR:HG21	2.14	0.48
2:B:25:LEU:HD13	3:J:38:LEU:HD22	1.95	0.48
2:P:26:GLN:HE22	2:Q:31:ARG:HB2	1.79	0.48
2:S:4:THR:HG22	2:S:5:VAL:H	1.78	0.48
3:V:85:ASP:HA	3:V:88:ILE:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:70:PRO:HA	2:c:75:TYR:CD2	2.49	0.48
3:j:135:LYS:HB3	3:j:164:PHE:CD2	2.48	0.48
3:k:75:PRO:HD2	3:k:78:ARG:HD2	1.95	0.48
3:l:154:SER:HA	3:l:157:TYR:CD2	2.49	0.48
1:5:552:TYR:O	1:5:556:ARG:HG2	2.14	0.48
2:C:43:ARG:HE	3:I:21:GLU:CD	2.21	0.48
2:E:127:TRP:CD2	5:E:200:CYC:HMC3	2.49	0.48
3:I:54:ASP:O	3:I:58:LYS:HG2	2.13	0.48
2:N:64:PHE:HE1	2:N:130:GLU:HG3	1.78	0.48
3:U:85:ASP:OD1	3:U:117:TYR:OH	2.32	0.48
3:U:132:GLN:O	3:U:135:LYS:HB3	2.14	0.48
3:W:74:TYR:O	3:W:76:HIS:N	2.46	0.48
2:b:46:THR:HA	2:b:49:GLN:NE2	2.28	0.48
2:b:116:GLU:HA	2:b:119:ARG:HG2	1.95	0.48
3:g:89:ILE:HD12	3:g:131:VAL:HG22	1.96	0.48
3:i:7:ARG:NH2	3:i:101:ASP:OD1	2.46	0.48
3:i:111:ASN:ND2	4:m:76:VAL:O	2.46	0.48
1:5:656:TYR:C	1:5:714:ARG:HH12	2.20	0.47
3:G:72:ASN:OD1	5:G:200:CYC:NC	2.44	0.47
3:G:123:PRO:HB2	3:G:125:GLN:HE22	1.79	0.47
2:P:30:GLY:O	2:P:33:GLU:HG2	2.14	0.47
3:T:127:VAL:HG11	3:T:171:ILE:HG21	1.95	0.47
2:b:131:ALA:O	2:b:135:ILE:HG12	2.14	0.47
2:c:55:GLY:HA3	2:c:134:TYR:CZ	2.48	0.47
1:5:193:LYS:HG3	1:5:243:PHE:HE1	1.79	0.47
1:5:349:ARG:O	1:5:352:PHE:HD1	1.97	0.47
2:C:60:VAL:HG11	5:C:200:CYC:HMC1	1.95	0.47
3:J:92:TYR:CD2	3:J:109:CYS:HB2	2.49	0.47
3:K:110:LEU:HD23	3:K:170:SER:HB3	1.95	0.47
2:Q:136:LYS:HG2	2:Q:152:LEU:HD13	1.95	0.47
4:Z:25:GLU:HG3	4:Z:45:SER:O	2.13	0.47
2:a:36:VAL:O	2:a:39:ILE:N	2.47	0.47
2:e:114:LEU:HD21	2:e:162:LEU:HD23	1.96	0.47
2:e:115:ARG:HH22	2:e:125:PRO:HB3	1.79	0.47
3:j:37:ARG:HD2	3:j:97:LEU:O	2.14	0.47
3:j:68:GLN:HB2	3:j:69:PRO:HD2	1.94	0.47
1:5:310:ARG:HH22	2:S:77:ASP:CG	2.22	0.47
1:5:617:ARG:NH1	1:5:687:GLN:OE1	2.47	0.47
2:C:148:LYS:O	2:C:152:LEU:HD23	2.14	0.47
3:I:85:ASP:O	3:I:89:ILE:HG12	2.15	0.47
2:P:107:ASP:HA	2:P:111:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:106:ASP:HA	3:U:110:LEU:HD13	1.96	0.47
2:a:75:TYR:O	2:a:79:ASN:ND2	2.46	0.47
2:c:18:ARG:O	3:i:95:TYR:OH	2.29	0.47
2:e:114:LEU:HA	3:i:76:HIS:CE1	2.49	0.47
3:h:93:VAL:HG11	3:h:164:PHE:CE1	2.49	0.47
3:i:14:LEU:HD12	3:i:15:LYS:HD3	1.96	0.47
3:l:55:ALA:O	3:l:59:LEU:HD23	2.14	0.47
4:m:25:GLU:HB2	4:m:45:SER:HA	1.96	0.47
4:m:57:LEU:O	4:m:61:ILE:HG12	2.14	0.47
1:5:527:GLN:OE1	1:5:527:GLN:N	2.43	0.47
2:B:45:LEU:HD23	2:B:95:THR:HG22	1.95	0.47
2:F:70:PRO:HA	2:F:75:TYR:CG	2.49	0.47
3:I:52:ILE:HG23	3:I:86:MET:HE2	1.96	0.47
2:N:37:PRO:HA	2:N:40:GLU:CD	2.40	0.47
2:N:55:GLY:HA3	2:N:134:TYR:OH	2.15	0.47
2:Q:107:ASP:HA	2:Q:111:ILE:HB	1.95	0.47
2:b:59:ALA:HA	2:b:62:LYS:HG2	1.97	0.47
2:e:29:PHE:O	2:e:30:GLY:C	2.56	0.47
2:f:31:ARG:HA	2:f:34:ARG:CZ	2.43	0.47
3:h:96:ALA:HB2	3:h:105:LEU:HB2	1.96	0.47
5:h:201:CYC:NC	5:h:201:CYC:HMD3	2.29	0.47
1:5:456:ASP:O	1:5:460:GLU:HG2	2.14	0.47
2:A:53:VAL:HG23	2:A:87:ILE:HB	1.96	0.47
2:C:18:ARG:NH1	2:C:24:GLU:OE2	2.44	0.47
2:E:24:GLU:OE1	2:E:24:GLU:N	2.41	0.47
3:J:41:VAL:HG21	3:J:98:LEU:HB2	1.96	0.47
2:P:132:LEU:HA	2:P:135:ILE:HD12	1.96	0.47
2:R:150:GLU:OE2	5:Y:201:CYC:OB	2.31	0.47
2:a:74:GLY:O	2:a:80:GLN:HG3	2.14	0.47
2:a:94:ILE:HG21	2:a:155:ILE:HD11	1.96	0.47
2:c:31:ARG:HE	2:c:101:SER:HB3	1.79	0.47
2:d:70:PRO:HA	2:d:75:TYR:CG	2.49	0.47
2:e:116:GLU:HA	2:e:119:ARG:CD	2.44	0.47
2:f:30:GLY:O	2:f:33:GLU:HG3	2.15	0.47
3:g:23:ASP:HA	3:g:26:LYS:HD2	1.95	0.47
3:h:112:GLY:HA2	3:h:115:GLU:OE2	2.15	0.47
3:j:127:VAL:HG22	5:j:200:CYC:H3C	1.95	0.47
3:j:158:SER:O	3:j:162:THR:HG23	2.14	0.47
2:A:38:ALA:HA	2:A:150:GLU:OE2	2.14	0.47
2:C:136:LYS:NZ	2:C:156:ASP:HB2	2.30	0.47
2:E:16:GLN:HE22	2:E:18:ARG:HH21	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:60:VAL:HG11	5:E:200:CYC:HMC1	1.96	0.47
5:K:201:CYC:HBC2	5:K:201:CYC:H2C	1.70	0.47
2:N:9:VAL:CG1	2:N:24:GLU:HB3	2.44	0.47
2:N:34:ARG:HA	2:N:34:ARG:HD3	1.69	0.47
2:O:65:PRO:O	2:O:69:GLN:NE2	2.48	0.47
2:Q:98:LEU:HD21	2:Q:151:ALA:HA	1.96	0.47
2:S:21:ASN:OD1	2:S:24:GLU:HG2	2.14	0.47
2:S:91:LEU:HD13	2:S:135:ILE:HD13	1.96	0.47
3:V:91:ARG:HG2	3:V:95:TYR:CE2	2.49	0.47
3:X:72:ASN:HD22	3:X:123:PRO:HD2	1.80	0.47
2:b:98:LEU:HD23	2:b:154:TYR:CD2	2.47	0.47
2:b:151:ALA:O	2:b:155:ILE:HG12	2.14	0.47
3:k:53:SER:O	3:k:57:HIS:ND1	2.29	0.47
1:5:591:PHE:O	1:5:594:THR:N	2.37	0.47
3:I:158:SER:O	3:I:162:THR:HG23	2.14	0.47
3:K:82:CYS:SG	5:K:200:CYC:HAC2	2.55	0.47
3:L:54:ASP:O	3:L:58:LYS:HG2	2.15	0.47
4:M:11:ILE:HG23	4:M:12:THR:HG23	1.97	0.47
2:N:82:LYS:HA	2:N:85:ARG:HG2	1.95	0.47
2:N:148:LYS:NZ	2:N:152:LEU:HD11	2.30	0.47
2:O:17:GLY:HA2	3:W:91:ARG:NH1	2.30	0.47
2:P:89:TYR:HA	2:P:92:ARG:NH2	2.30	0.47
3:U:128:ALA:O	3:U:132:GLN:HG3	2.15	0.47
3:V:108:ARG:HA	3:V:111:ASN:ND2	2.29	0.47
3:W:78:ARG:HB3	5:W:200:CYC:HMD2	1.96	0.47
5:W:201:CYC:HBC2	5:W:201:CYC:H2C	1.73	0.47
2:b:73:LYS:O	2:b:79:ASN:ND2	2.46	0.47
2:e:132:LEU:HA	2:e:135:ILE:HD12	1.97	0.47
3:h:14:LEU:HD12	3:h:15:LYS:HD3	1.97	0.47
3:j:8:ALA:O	3:j:11:GLN:HG2	2.15	0.47
3:j:52:ILE:HG22	3:j:134:MET:HE1	1.97	0.47
3:j:88:ILE:HD12	3:j:91:ARG:HD3	1.97	0.47
1:5:620:ILE:HG22	1:5:681:LEU:HD21	1.97	0.47
2:A:147:SER:O	2:A:150:GLU:HG2	2.15	0.47
3:G:12:ALA:HA	3:G:15:LYS:HE3	1.97	0.47
3:W:7:ARG:NH1	3:W:103:SER:OG	2.48	0.47
2:a:97:SER:OG	2:a:106:LEU:HD23	2.14	0.47
2:C:125:PRO:O	2:C:129:ILE:HD12	2.15	0.47
3:K:58:LYS:O	3:K:62:GLU:HB2	2.15	0.47
3:L:79:MET:O	3:L:82:CYS:HB3	2.14	0.47
3:W:44:LEU:HD22	3:W:90:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:96:TYR:OH	3:i:17:SER:O	2.31	0.47
2:e:121:PHE:CZ	3:i:83:LEU:HD11	2.50	0.47
2:f:82:LYS:HD2	5:f:200:CYC:C4D	2.45	0.47
3:g:8:ALA:HA	3:g:11:GLN:HE21	1.80	0.47
3:j:132:GLN:O	3:j:135:LYS:HG2	2.14	0.47
5:l:201:CYC:NB	5:l:201:CYC:HMA1	2.29	0.47
1:5:119:PHE:CD2	1:5:124:PHE:HB2	2.50	0.47
2:C:124:ASN:HB3	2:C:127:TRP:CE2	2.50	0.47
3:G:37:ARG:NH1	3:G:97:LEU:O	2.41	0.47
2:P:36:VAL:HG23	2:P:37:PRO:HD3	1.96	0.47
2:Q:60:VAL:HG11	5:Q:200:CYC:HBC2	1.97	0.47
2:R:149:THR:O	2:R:153:LEU:HG	2.14	0.47
3:U:105:LEU:HD12	3:U:110:LEU:HD12	1.97	0.47
3:V:48:ALA:O	3:V:52:ILE:HD12	2.15	0.47
2:d:110:VAL:O	2:d:114:LEU:HB3	2.15	0.47
3:k:162:THR:HB	3:k:166:LYS:HZ2	1.79	0.47
2:A:95:THR:O	2:A:99:VAL:HG23	2.16	0.46
2:O:92:ARG:NH1	3:W:16:GLY:O	2.48	0.46
5:W:200:CYC:HHD	5:W:200:CYC:HAC1	1.51	0.46
2:a:4:THR:HG22	2:a:100:ALA:HB1	1.96	0.46
2:b:133:ASN:HA	2:b:136:LYS:HZ3	1.79	0.46
2:c:69:GLN:OE1	2:c:69:GLN:N	2.48	0.46
2:e:147:SER:HA	2:e:150:GLU:OE2	2.13	0.46
2:f:124:ASN:HD21	2:f:126:LEU:HB2	1.79	0.46
3:g:60:PHE:HB3	3:g:67:ILE:HD11	1.97	0.46
1:5:227:GLU:OE1	4:M:55:ARG:NH2	2.48	0.46
1:5:552:TYR:HB3	3:j:78:ARG:HH22	1.80	0.46
1:5:700:GLY:HA3	1:5:715:MET:SD	2.55	0.46
2:C:86:ASP:OD2	2:C:128:TYR:OH	2.27	0.46
3:I:82:CYS:SG	5:I:200:CYC:HAC2	2.54	0.46
2:Q:56:ALA:O	2:Q:60:VAL:HG23	2.15	0.46
2:Q:86:ASP:OD2	2:Q:128:TYR:OH	2.31	0.46
3:W:88:ILE:HG12	3:W:91:ARG:HH21	1.79	0.46
2:b:67:VAL:HG21	2:b:127:TRP:HE1	1.79	0.46
2:d:43:ARG:NH2	3:k:25:ASP:OD1	2.32	0.46
2:e:116:GLU:O	2:e:120:ALA:HB2	2.15	0.46
3:h:11:GLN:O	3:h:14:LEU:HG	2.15	0.46
2:B:77:ASP:HA	2:B:80:GLN:HE22	1.79	0.46
2:C:50:ASP:HB3	2:C:54:LYS:NZ	2.30	0.46
2:D:5:VAL:HB	2:D:31:ARG:HG3	1.97	0.46
3:G:69:PRO:HA	3:G:74:TYR:CG	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:91:LEU:O	2:O:95:THR:HG23	2.15	0.46
3:X:38:LEU:HD23	3:X:38:LEU:HA	1.81	0.46
2:c:124:ASN:HB3	2:c:127:TRP:CD2	2.50	0.46
1:5:95:GLU:OE2	3:J:77:ARG:NH2	2.48	0.46
1:5:186:ARG:NH2	1:5:190:LEU:HD21	2.30	0.46
1:5:423:LEU:HD21	1:5:504:ASP:OD2	2.15	0.46
2:E:26:GLN:HG2	2:F:34:ARG:CZ	2.45	0.46
2:N:19:PHE:CE2	3:U:90:LEU:HD23	2.50	0.46
2:N:26:GLN:HA	5:U:201:CYC:HBB1	1.97	0.46
2:P:86:ASP:OD2	2:P:128:TYR:OH	2.29	0.46
2:c:131:ALA:O	2:c:135:ILE:HG12	2.15	0.46
2:A:107:ASP:HA	2:A:111:ILE:HB	1.97	0.46
2:A:124:ASN:HB3	2:A:127:TRP:CE2	2.51	0.46
2:D:149:THR:HB	5:I:201:CYC:HMB2	1.97	0.46
3:H:44:LEU:HD21	3:H:138:ALA:HB1	1.97	0.46
3:I:117:TYR:HB3	3:I:122:THR:HB	1.98	0.46
2:S:18:ARG:O	3:Y:95:TYR:OH	2.32	0.46
3:U:55:ALA:O	3:U:59:LEU:HB3	2.16	0.46
3:Y:10:ALA:O	3:Y:14:LEU:HD23	2.16	0.46
3:Y:113:LEU:HD12	3:Y:113:LEU:HA	1.74	0.46
2:e:73:LYS:O	2:e:79:ASN:ND2	2.49	0.46
1:5:532:ARG:HA	1:5:535:ARG:HD3	1.96	0.46
1:5:701:PHE:HA	1:5:712:PHE:CE2	2.51	0.46
2:E:62:LYS:HD3	2:E:62:LYS:N	2.31	0.46
3:G:58:LYS:HE3	3:G:133:LEU:HB3	1.98	0.46
3:K:86:MET:HE2	3:K:130:ALA:HB1	1.98	0.46
2:O:96:TYR:CD2	3:W:9:ILE:HG23	2.51	0.46
2:P:4:THR:H	2:P:7:THR:CB	2.28	0.46
2:S:36:VAL:HB	2:S:37:PRO:HD3	1.97	0.46
2:S:129:ILE:HG23	2:S:159:ILE:HG23	1.97	0.46
3:Y:110:LEU:HD13	3:Y:170:SER:OG	2.16	0.46
2:a:50:ASP:HA	2:a:53:VAL:HG22	1.97	0.46
2:c:61:PHE:CD1	2:c:68:THR:HG22	2.50	0.46
3:k:42:ALA:HA	3:k:45:THR:HG22	1.98	0.46
2:D:31:ARG:C	2:D:31:ARG:HD3	2.41	0.46
2:D:146:GLN:HE22	5:I:201:CYC:HMA3	1.81	0.46
2:E:146:GLN:OE1	2:E:146:GLN:HA	2.16	0.46
3:G:105:LEU:HD23	3:G:166:LYS:NZ	2.31	0.46
2:O:4:THR:O	2:O:7:THR:N	2.49	0.46
2:O:70:PRO:HG3	2:O:75:TYR:CE1	2.51	0.46
3:T:7:ARG:NH2	3:T:101:ASP:HB2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:65:GLU:HA	3:T:68:GLN:HG2	1.98	0.46
3:Y:37:ARG:HH12	3:Y:159:GLU:CD	2.24	0.46
2:a:72:GLU:HG2	2:a:74:GLY:H	1.80	0.46
2:e:26:GLN:HG2	2:f:34:ARG:HD2	1.96	0.46
3:g:72:ASN:O	3:g:78:ARG:HD2	2.15	0.46
3:l:151:GLY:HA3	5:l:201:CYC:HMD2	1.96	0.46
2:C:80:GLN:HA	2:C:83:CYS:SG	2.56	0.46
2:E:26:GLN:HG2	2:F:34:ARG:NE	2.31	0.46
2:R:135:ILE:O	2:R:138:GLU:HG3	2.15	0.46
3:T:15:LYS:NZ	3:T:17:SER:HB2	2.31	0.46
3:T:67:ILE:HD12	3:T:67:ILE:H	1.81	0.46
3:U:32:LYS:HD2	3:U:32:LYS:C	2.41	0.46
3:U:84:ARG:O	3:U:88:ILE:HG12	2.16	0.46
2:e:29:PHE:HE2	5:g:201:CYC:C4B	2.28	0.46
2:e:73:LYS:HD2	5:e:200:CYC:HBD2	1.97	0.46
3:i:82:CYS:HB2	5:i:200:CYC:OC	2.15	0.46
5:j:200:CYC:HHD	5:j:200:CYC:HAC1	1.75	0.46
2:N:83:CYS:SG	5:N:200:CYC:H2C	2.56	0.46
2:O:18:ARG:O	3:W:95:TYR:OH	2.34	0.46
2:R:36:VAL:HB	2:R:37:PRO:HD3	1.97	0.46
3:U:106:ASP:OD1	3:U:110:LEU:HD13	2.16	0.46
3:V:120:LEU:HD23	5:V:200:CYC:HBD1	1.98	0.46
2:c:3:ARG:NH1	4:m:13:THR:H	2.13	0.46
3:g:75:PRO:HG2	3:g:78:ARG:HE	1.81	0.46
3:h:72:ASN:HD21	3:h:122:THR:HG23	1.81	0.46
3:j:106:ASP:OD2	3:j:166:LYS:NZ	2.43	0.46
1:5:543:PRO:HA	3:j:68:GLN:OE1	2.15	0.46
1:5:648:LYS:NZ	1:5:726:ASP:OD2	2.49	0.46
2:A:156:ASP:HA	2:A:159:ILE:HD12	1.97	0.46
2:C:93:PHE:HE2	5:C:200:CYC:HBB1	1.80	0.46
3:H:88:ILE:HD13	5:H:200:CYC:HBB3	1.98	0.46
3:W:75:PRO:CD	3:W:78:ARG:HE	2.28	0.46
2:e:92:ARG:O	2:e:95:THR:OG1	2.30	0.46
2:f:20:LEU:HD22	3:l:98:LEU:HD13	1.98	0.46
3:g:3:ASP:H	3:g:6:THR:HG1	1.61	0.46
3:g:110:LEU:HB3	3:g:114:ARG:NH1	2.31	0.46
3:i:29:SER:HA	3:i:32:LYS:HE3	1.98	0.46
3:l:21:GLU:HA	3:l:24:LEU:HD12	1.97	0.46
3:l:51:ILE:HD13	3:l:90:LEU:HD11	1.97	0.46
3:l:86:MET:HA	3:l:89:ILE:HG22	1.98	0.46
1:5:609:LEU:HD13	1:5:619:PHE:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4:THR:O	2:A:8:GLU:HG2	2.17	0.45
2:A:86:ASP:HB3	2:A:128:TYR:HE2	1.81	0.45
5:I:200:CYC:HHD	5:I:200:CYC:HAC1	1.66	0.45
3:K:109:CYS:C	3:K:110:LEU:HD12	2.41	0.45
2:N:148:LYS:O	2:N:152:LEU:HG	2.15	0.45
3:U:55:ALA:HA	3:U:58:LYS:HZ2	1.81	0.45
4:Z:30:ALA:O	4:Z:34:HIS:ND1	2.49	0.45
2:c:109:TYR:HA	3:h:77:ARG:NH1	2.30	0.45
2:e:94:ILE:HG21	2:e:155:ILE:HD11	1.98	0.45
3:i:1:MET:SD	3:i:104:VAL:HG23	2.56	0.45
3:j:110:LEU:HB3	3:j:170:SER:OG	2.17	0.45
4:m:17:ARG:HG2	4:m:78:SER:HB2	1.98	0.45
2:A:83:CYS:SG	5:A:200:CYC:H2C	2.56	0.45
2:B:22:SER:O	2:B:26:GLN:HG2	2.15	0.45
2:F:148:LYS:O	2:F:152:LEU:HG	2.16	0.45
3:G:23:ASP:HA	3:G:26:LYS:HE2	1.97	0.45
2:O:4:THR:H	2:O:7:THR:HB	1.81	0.45
2:O:90:TYR:O	2:O:94:ILE:HG12	2.16	0.45
3:V:125:GLN:OE1	3:V:125:GLN:N	2.47	0.45
3:X:5:PHE:CD1	3:X:27:LEU:HD22	2.51	0.45
3:X:109:CYS:C	3:X:110:LEU:HD12	2.41	0.45
2:b:149:THR:O	2:b:153:LEU:HG	2.15	0.45
2:c:14:ASP:OD1	3:i:92:TYR:OH	2.29	0.45
2:f:2:SER:N	3:l:2:ASN:OD1	2.49	0.45
2:f:126:LEU:O	2:f:127:TRP:C	2.59	0.45
3:j:7:ARG:HA	3:j:7:ARG:HH21	1.82	0.45
3:j:72:ASN:HD22	3:j:122:THR:HA	1.80	0.45
3:l:7:ARG:O	3:l:11:GLN:OE1	2.34	0.45
3:l:47:ASN:OD1	3:l:141:HIS:ND1	2.49	0.45
1:5:417:GLN:O	1:5:421:ILE:HG12	2.15	0.45
1:5:550:ASN:HB2	2:f:109:TYR:CE2	2.51	0.45
2:C:20:LEU:H	2:C:20:LEU:HD12	1.81	0.45
2:C:70:PRO:HG3	2:C:75:TYR:CE1	2.51	0.45
2:O:9:VAL:HB	2:O:24:GLU:HB3	1.97	0.45
4:Z:21:ILE:N	4:Z:49:LEU:O	2.30	0.45
2:d:73:LYS:NZ	2:d:121:PHE:O	2.31	0.45
2:d:91:LEU:O	2:d:95:THR:HG23	2.15	0.45
2:d:124:ASN:HD21	2:d:126:LEU:HD12	1.80	0.45
2:f:83:CYS:SG	5:f:200:CYC:HAC2	2.56	0.45
5:5:1202:CYC:C2A	3:l:84:ARG:HH22	2.28	0.45
2:A:57:VAL:HG22	2:A:83:CYS:SG	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:127:TRP:CD2	5:C:200:CYC:HMC3	2.51	0.45
2:E:66:TYR:HA	2:E:69:GLN:HG2	1.98	0.45
2:Q:50:ASP:HB3	2:Q:54:LYS:NZ	2.32	0.45
3:T:158:SER:O	3:T:162:THR:HG23	2.16	0.45
3:V:139:MET:O	3:V:143:LYS:HG2	2.16	0.45
3:W:90:LEU:HB2	3:W:134:MET:CE	2.46	0.45
3:X:87:GLU:OE1	3:X:91:ARG:HD3	2.17	0.45
3:Y:97:LEU:HA	3:Y:163:TYR:HE2	1.81	0.45
2:a:93:PHE:HA	2:a:96:TYR:HD2	1.81	0.45
2:e:34:ARG:NH1	5:l:201:CYC:OB	2.49	0.45
2:f:3:ARG:NH2	2:f:7:THR:HG22	2.30	0.45
3:g:47:ASN:O	3:g:51:ILE:HG12	2.16	0.45
3:i:75:PRO:HD2	3:i:78:ARG:NE	2.27	0.45
3:j:2:ASN:O	3:j:103:SER:OG	2.30	0.45
3:j:139:MET:O	3:j:143:LYS:HG2	2.16	0.45
3:l:7:ARG:NH1	3:l:101:ASP:HB3	2.32	0.45
4:m:51:VAL:HG11	4:m:59:GLU:HG3	1.98	0.45
1:5:329:THR:HA	3:W:78:ARG:NH2	2.31	0.45
3:K:139:MET:O	3:K:143:LYS:HG3	2.16	0.45
3:U:88:ILE:HD13	3:U:91:ARG:HD3	1.98	0.45
2:a:56:ALA:O	2:a:60:VAL:HG23	2.15	0.45
2:b:41:ALA:HA	2:b:143:LEU:HD22	1.98	0.45
2:b:126:LEU:HA	2:b:129:ILE:HD12	1.98	0.45
2:f:82:LYS:HE3	5:f:200:CYC:C2D	2.47	0.45
3:l:5:PHE:HD1	3:l:27:LEU:HD13	1.81	0.45
1:5:288:VAL:HG13	1:5:289:ARG:HG3	1.98	0.45
1:5:518:ASP:O	1:5:521:SER:OG	2.23	0.45
1:5:574:PHE:HE1	1:5:579:PHE:HD1	1.65	0.45
2:A:65:PRO:O	2:A:68:THR:OG1	2.35	0.45
3:H:82:CYS:SG	3:H:86:MET:HE2	2.56	0.45
3:I:58:LYS:HB2	3:I:133:LEU:HD13	1.99	0.45
3:K:12:ALA:HA	3:K:15:LYS:HD3	1.98	0.45
2:N:17:GLY:O	3:U:91:ARG:HD2	2.16	0.45
2:R:50:ASP:HB2	2:R:54:LYS:HZ3	1.80	0.45
2:R:132:LEU:HD12	2:R:155:ILE:HG23	1.98	0.45
3:X:114:ARG:HH22	3:X:172:ALA:HA	1.81	0.45
2:c:115:ARG:NH1	2:c:162:LEU:O	2.50	0.45
5:j:201:CYC:HBC2	5:j:201:CYC:H2C	1.79	0.45
1:5:92:GLN:HB3	3:L:14:LEU:HD22	1.98	0.45
1:5:418:ASN:O	1:5:422:GLU:HG3	2.17	0.45
5:5:1201:CYC:HMC3	3:L:127:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:97:SER:OG	2:A:106:LEU:HG	2.17	0.45
2:A:131:ALA:O	2:A:135:ILE:HG12	2.16	0.45
5:C:200:CYC:HAB2	3:H:76:HIS:HB2	1.99	0.45
2:R:94:ILE:HD13	2:R:155:ILE:HG12	1.99	0.45
3:Y:62:GLU:CD	3:Y:129:ARG:HH21	2.24	0.45
2:c:73:LYS:HZ3	5:c:200:CYC:HC	1.65	0.45
3:i:41:VAL:HG11	3:i:98:LEU:HB2	1.98	0.45
3:k:145:THR:HG23	5:k:201:CYC:HMC3	1.98	0.45
3:l:72:ASN:ND2	3:l:123:PRO:HD2	2.32	0.45
2:E:36:VAL:O	2:E:39:ILE:N	2.49	0.45
2:E:80:GLN:HA	2:E:83:CYS:SG	2.57	0.45
5:I:201:CYC:HAC1	5:I:201:CYC:HH2	1.63	0.45
2:O:127:TRP:CE3	5:O:200:CYC:H3C	2.52	0.45
3:V:1:MET:HG3	3:V:104:VAL:HG22	1.99	0.45
3:V:37:ARG:HE	3:V:156:LEU:HD21	1.81	0.45
3:g:8:ALA:HA	3:g:11:GLN:NE2	2.32	0.45
3:k:86:MET:HB3	3:k:134:MET:SD	2.56	0.45
1:5:268:ALA:HA	5:5:1201:CYC:HBB3	1.97	0.45
2:D:91:LEU:O	2:D:95:THR:HG23	2.17	0.45
3:H:153:CYS:SG	5:H:201:CYC:HBC2	2.57	0.45
5:H:200:CYC:HBC2	5:H:200:CYC:H2C	1.75	0.45
3:I:82:CYS:SG	5:I:200:CYC:H2C	2.57	0.45
2:P:2:SER:N	4:Z:13:THR:HG1	2.15	0.45
2:P:8:GLU:O	2:P:12:THR:OG1	2.31	0.45
3:T:153:CYS:SG	5:T:201:CYC:HAC2	2.57	0.45
3:X:97:LEU:HA	3:X:163:TYR:HE2	1.81	0.45
2:f:124:ASN:ND2	2:f:126:LEU:HB2	2.31	0.45
5:g:201:CYC:HB	5:g:201:CYC:HMA2	1.82	0.45
1:5:104:ALA:HB1	1:5:107:THR:HG21	1.98	0.45
2:D:70:PRO:HA	2:D:75:TYR:CG	2.52	0.45
3:H:75:PRO:HG2	3:H:78:ARG:HD3	1.98	0.45
3:I:11:GLN:HB3	3:I:15:LYS:HZ3	1.82	0.45
3:T:166:LYS:HG3	3:T:167:ALA:N	2.31	0.45
4:Z:20:LYS:HD2	4:Z:48:THR:HG22	1.99	0.45
2:a:64:PHE:CD2	2:a:127:TRP:HD1	2.35	0.45
2:b:96:TYR:OH	3:j:17:SER:O	2.34	0.45
2:c:6:ILE:HG21	3:i:99:ALA:HA	1.98	0.45
2:d:18:ARG:HH22	2:d:21:ASN:HB2	1.82	0.45
2:d:73:LYS:HE3	2:d:122:ASN:HB2	1.98	0.45
2:d:127:TRP:CD2	5:d:200:CYC:HMC3	2.52	0.45
2:e:135:ILE:HA	2:e:138:GLU:OE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:126:LEU:HA	2:f:129:ILE:HD12	1.99	0.45
3:i:56:ALA:HA	3:i:59:LEU:HG	1.98	0.45
3:l:92:TYR:CE2	3:l:108:ARG:HG3	2.52	0.45
1:5:120:THR:OG1	1:5:121:ASP:N	2.48	0.44
1:5:690:PHE:HE1	1:5:697:PHE:H	1.65	0.44
2:B:94:ILE:HD13	2:B:155:ILE:HG12	1.99	0.44
2:F:73:LYS:HD2	5:F:200:CYC:HMD3	1.99	0.44
3:L:128:ALA:HB2	3:L:172:ALA:HB2	2.00	0.44
2:Q:77:ASP:HA	2:Q:80:GLN:NE2	2.32	0.44
3:Y:48:ALA:O	3:Y:52:ILE:HD12	2.16	0.44
2:d:21:ASN:N	2:d:24:GLU:OE2	2.50	0.44
2:e:10:ILE:HD11	3:g:99:ALA:HB2	2.00	0.44
2:f:140:GLY:HA2	2:f:148:LYS:HZ3	1.82	0.44
4:m:13:THR:O	4:m:16:LYS:HG3	2.17	0.44
3:G:92:TYR:HE2	3:G:109:CYS:HG	1.64	0.44
3:I:59:LEU:HD22	3:I:130:ALA:HB2	1.98	0.44
2:P:26:GLN:CG	2:Q:34:ARG:HE	2.24	0.44
2:S:94:ILE:HD13	2:S:106:LEU:HD21	1.99	0.44
3:T:36:LYS:HZ1	3:T:152:ASP:C	2.25	0.44
3:X:85:ASP:O	3:X:89:ILE:HG12	2.18	0.44
2:f:70:PRO:HA	2:f:75:TYR:CG	2.52	0.44
3:j:54:ASP:HB2	3:j:58:LYS:NZ	2.33	0.44
1:5:425:HIS:CD2	1:5:458:TYR:HE2	2.35	0.44
2:E:75:TYR:O	2:E:79:ASN:ND2	2.50	0.44
2:N:5:VAL:HG11	2:N:31:ARG:HB2	2.00	0.44
2:N:151:ALA:O	2:N:155:ILE:HG12	2.18	0.44
2:Q:94:ILE:HG21	2:Q:155:ILE:HD13	2.00	0.44
2:R:34:ARG:HH12	2:S:26:GLN:HG2	1.83	0.44
5:Y:201:CYC:HBC2	5:Y:201:CYC:H2C	1.73	0.44
2:c:3:ARG:HG2	2:c:3:ARG:HH11	1.82	0.44
2:d:73:LYS:O	2:d:79:ASN:ND2	2.48	0.44
3:h:82:CYS:HA	5:h:200:CYC:HAC1	1.99	0.44
3:i:58:LYS:HA	3:i:58:LYS:HD3	1.78	0.44
3:i:60:PHE:HD1	3:i:66:LEU:HD11	1.82	0.44
3:i:133:LEU:HD23	3:i:133:LEU:HA	1.76	0.44
3:j:78:ARG:HB3	5:j:200:CYC:HMD1	1.99	0.44
3:j:84:ARG:O	3:j:87:GLU:HG3	2.18	0.44
2:A:20:LEU:HD13	3:H:98:LEU:HD22	1.98	0.44
3:H:79:MET:O	3:H:83:LEU:HG	2.18	0.44
3:I:37:ARG:HH12	3:I:159:GLU:CD	2.25	0.44
5:J:201:CYC:HBC2	5:J:201:CYC:H2C	1.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:201:CYC:CMA	5:K:201:CYC:HB	2.30	0.44
3:L:113:LEU:HD23	3:L:171:ILE:HG12	1.99	0.44
2:P:24:GLU:OE2	2:P:25:LEU:HG	2.17	0.44
3:T:35:VAL:HA	3:T:38:LEU:HD12	1.98	0.44
3:Y:58:LYS:HB2	3:Y:133:LEU:HD13	2.00	0.44
2:a:48:ASN:HD22	2:a:142:LEU:HD13	1.83	0.44
3:g:79:MET:O	3:g:83:LEU:HG	2.16	0.44
3:h:77:ARG:HH21	4:m:14:GLN:HG2	1.81	0.44
1:5:550:ASN:OD1	3:j:77:ARG:NH1	2.49	0.44
2:B:66:TYR:O	2:B:72:GLU:HG3	2.16	0.44
2:C:41:ALA:O	2:C:45:LEU:HG	2.18	0.44
2:E:45:LEU:HD12	2:E:91:LEU:HD11	2.00	0.44
5:G:201:CYC:HHD	5:G:201:CYC:HAC1	1.54	0.44
3:H:29:SER:O	3:H:32:LYS:N	2.50	0.44
3:I:84:ARG:O	3:I:87:GLU:HG3	2.18	0.44
3:J:82:CYS:SG	5:J:200:CYC:H2C	2.58	0.44
4:M:19:TYR:HE2	4:M:53:TYR:HD2	1.66	0.44
2:P:91:LEU:O	2:P:95:THR:HG23	2.18	0.44
2:a:118:ASN:ND2	2:a:125:PRO:HG3	2.31	0.44
2:b:28:ALA:HB3	3:j:38:LEU:HD21	1.99	0.44
2:b:92:ARG:HA	3:j:18:PHE:CE1	2.53	0.44
2:e:26:GLN:HE21	5:g:201:CYC:HBB1	1.82	0.44
2:f:133:ASN:HA	2:f:136:LYS:HG2	1.99	0.44
3:k:54:ASP:O	3:k:58:LYS:HG2	2.18	0.44
1:5:558:GLN:HG2	1:5:720:ASP:C	2.43	0.44
1:5:570:LEU:HD21	1:5:582:ALA:HB1	1.98	0.44
2:F:58:GLN:OE1	2:F:58:GLN:HA	2.17	0.44
3:G:63:GLN:OE1	3:G:64:GLN:N	2.49	0.44
5:I:200:CYC:NC	5:I:200:CYC:HMD1	2.32	0.44
2:R:42:ALA:O	2:R:46:THR:HG22	2.17	0.44
3:T:127:VAL:O	3:T:131:VAL:HG23	2.16	0.44
3:T:159:GLU:HG2	3:T:163:TYR:CE2	2.51	0.44
4:Z:13:THR:HG23	4:Z:16:LYS:HE3	1.98	0.44
2:b:92:ARG:HG2	3:j:18:PHE:CZ	2.52	0.44
2:d:5:VAL:O	2:d:9:VAL:HG23	2.17	0.44
2:f:130:GLU:HA	2:f:133:ASN:ND2	2.33	0.44
1:5:232:LEU:HD13	4:M:62:ARG:NH1	2.32	0.44
2:F:36:VAL:HB	2:F:37:PRO:HD3	2.00	0.44
3:G:159:GLU:O	3:G:162:THR:HG22	2.18	0.44
3:I:78:ARG:O	5:I:200:CYC:HMD2	2.17	0.44
3:J:135:LYS:O	3:J:139:MET:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:62:GLU:OE2	3:L:129:ARG:NH2	2.42	0.44
3:L:153:CYS:SG	5:L:201:CYC:HAC2	2.58	0.44
2:N:10:ILE:HD11	3:U:99:ALA:HB2	1.99	0.44
2:O:83:CYS:O	2:O:87:ILE:HD12	2.17	0.44
3:U:135:LYS:HG3	3:U:164:PHE:HD2	1.83	0.44
3:V:36:LYS:HD3	5:V:201:CYC:HMD3	1.99	0.44
3:X:74:TYR:HB3	3:X:75:PRO:HD3	1.98	0.44
2:e:37:PRO:HA	2:e:40:GLU:OE2	2.17	0.44
2:f:3:ARG:O	2:f:104:GLY:HA3	2.16	0.44
3:j:54:ASP:HA	3:j:57:HIS:HD1	1.82	0.44
3:j:79:MET:HE3	3:j:83:LEU:HD21	2.00	0.44
1:5:544:SER:HB3	3:j:68:GLN:NE2	2.32	0.44
2:A:83:CYS:O	2:A:87:ILE:HG12	2.18	0.44
2:A:134:TYR:O	2:A:138:GLU:HG2	2.18	0.44
2:B:20:LEU:HD13	3:J:98:LEU:HD22	2.00	0.44
3:L:41:VAL:HG23	3:L:97:LEU:HD22	1.99	0.44
2:Q:67:VAL:HG12	2:Q:74:GLY:HA3	1.99	0.44
2:Q:136:LYS:HG2	2:Q:152:LEU:CD1	2.48	0.44
5:R:200:CYC:OB	3:V:74:TYR:O	2.36	0.44
3:V:42:ALA:HA	3:V:45:THR:HG22	2.00	0.44
3:X:37:ARG:HH22	3:X:159:GLU:CD	2.25	0.44
4:Z:32:ASN:HA	4:Z:35:ARG:HG2	1.99	0.44
2:a:43:ARG:O	2:a:47:LYS:HG3	2.18	0.44
2:c:148:LYS:HG2	2:c:152:LEU:HD23	2.00	0.44
3:g:127:VAL:O	3:g:131:VAL:HG23	2.17	0.44
3:h:81:ALA:O	3:h:84:ARG:HG3	2.18	0.44
3:i:60:PHE:CD1	3:i:66:LEU:HD11	2.53	0.44
3:G:47:ASN:OD1	3:G:141:HIS:ND1	2.51	0.44
3:H:85:ASP:O	3:H:89:ILE:HG12	2.18	0.44
2:R:91:LEU:O	2:R:95:THR:HG23	2.18	0.44
3:V:158:SER:O	3:V:162:THR:HG23	2.18	0.44
3:W:7:ARG:NH2	3:W:103:SER:OG	2.51	0.44
4:Z:10:ALA:HA	4:Z:15:GLY:HA3	2.00	0.44
2:d:138:GLU:O	2:d:141:LYS:HG2	2.18	0.44
2:f:79:ASN:O	2:f:82:LYS:HG2	2.18	0.44
3:g:1:MET:HB2	3:g:108:ARG:HH11	1.83	0.44
3:g:97:LEU:HA	3:g:163:TYR:HE2	1.83	0.44
3:h:72:ASN:ND2	5:h:200:CYC:OC	2.51	0.44
3:l:159:GLU:O	3:l:162:THR:OG1	2.29	0.44
1:5:571:ARG:HH22	4:m:43:ARG:CA	2.31	0.43
2:A:86:ASP:O	2:A:90:TYR:HD1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:67:VAL:HG12	2:D:74:GLY:HA3	2.00	0.43
2:F:34:ARG:NH2	2:F:34:ARG:HB2	2.33	0.43
3:G:84:ARG:NH2	5:G:200:CYC:O1A	2.43	0.43
3:L:59:LEU:HD22	3:L:130:ALA:HB2	1.99	0.43
4:M:32:ASN:O	4:M:36:THR:HG23	2.19	0.43
2:N:94:ILE:HD13	2:N:106:LEU:HD11	2.00	0.43
2:P:143:LEU:HD22	2:P:147:SER:HB3	1.99	0.43
2:Q:110:VAL:HA	3:Y:76:HIS:CD2	2.49	0.43
3:T:72:ASN:HD22	3:T:123:PRO:HD2	1.83	0.43
5:d:200:CYC:HB	5:d:200:CYC:HMA2	1.83	0.43
2:e:5:VAL:O	2:e:9:VAL:HG23	2.18	0.43
2:f:3:ARG:NH2	2:f:8:GLU:HA	2.32	0.43
3:k:92:TYR:HD1	3:k:95:TYR:HD2	1.65	0.43
3:l:47:ASN:O	3:l:51:ILE:HG22	2.18	0.43
3:l:125:GLN:H	3:l:125:GLN:CD	2.23	0.43
1:5:527:GLN:H	1:5:527:GLN:CD	2.26	0.43
1:5:579:PHE:O	1:5:583:LEU:HD23	2.17	0.43
2:F:83:CYS:O	2:F:87:ILE:HG12	2.17	0.43
2:F:130:GLU:OE1	2:F:130:GLU:HA	2.17	0.43
3:H:69:PRO:HA	3:H:74:TYR:CG	2.53	0.43
3:H:75:PRO:HD2	3:H:78:ARG:HD3	2.00	0.43
3:H:82:CYS:SG	5:H:200:CYC:HAC2	2.58	0.43
2:P:151:ALA:O	2:P:155:ILE:HG12	2.18	0.43
2:Q:83:CYS:SG	5:Q:200:CYC:HAC2	2.57	0.43
2:S:32:PHE:CD2	3:Y:34:GLY:HA3	2.53	0.43
3:T:84:ARG:O	3:T:88:ILE:HG12	2.18	0.43
3:W:82:CYS:SG	5:W:200:CYC:H2C	2.57	0.43
2:d:18:ARG:NH2	2:d:21:ASN:HB2	2.33	0.43
3:i:151:GLY:HA3	5:i:201:CYC:HMD2	2.00	0.43
3:i:158:SER:O	3:i:162:THR:HG23	2.17	0.43
3:j:60:PHE:HE2	3:j:79:MET:HE1	1.83	0.43
3:k:128:ALA:HB2	3:k:172:ALA:HB3	2.00	0.43
4:m:19:TYR:HE2	4:m:53:TYR:HD1	1.66	0.43
2:C:121:PHE:HB3	2:C:123:LEU:HD13	2.00	0.43
2:F:30:GLY:O	2:F:34:ARG:HG3	2.18	0.43
3:L:106:ASP:OD1	3:L:166:LYS:NZ	2.50	0.43
2:N:5:VAL:HB	2:N:31:ARG:HG3	1.99	0.43
2:P:70:PRO:HA	2:P:75:TYR:CD2	2.53	0.43
2:S:91:LEU:O	2:S:95:THR:HG23	2.18	0.43
3:V:92:TYR:CD2	3:V:109:CYS:HB2	2.53	0.43
3:X:93:VAL:HG11	3:X:164:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:114:ARG:NH2	3:X:172:ALA:HA	2.34	0.43
2:a:34:ARG:HH11	2:a:146:GLN:NE2	2.16	0.43
3:i:40:ALA:HA	5:i:201:CYC:HBC1	2.00	0.43
3:G:153:CYS:SG	5:G:201:CYC:H2C	2.59	0.43
2:P:54:LYS:HA	2:P:57:VAL:HG22	1.99	0.43
2:b:24:GLU:OE1	2:b:24:GLU:N	2.35	0.43
2:e:37:PRO:HA	2:e:40:GLU:CD	2.42	0.43
3:h:129:ARG:HA	3:h:132:GLN:CD	2.43	0.43
3:j:30:PHE:HZ	3:j:100:GLY:HA3	1.82	0.43
3:j:72:ASN:ND2	3:j:122:THR:OG1	2.51	0.43
2:A:117:VAL:HG13	3:G:79:MET:HE1	2.01	0.43
2:B:7:THR:HG23	3:J:1:MET:SD	2.59	0.43
2:F:106:LEU:HD23	2:F:106:LEU:HA	1.89	0.43
5:H:200:CYC:HAA1	4:M:56:PHE:HD2	1.83	0.43
3:T:29:SER:O	3:T:32:LYS:HG3	2.18	0.43
2:a:30:GLY:O	2:a:34:ARG:HG2	2.18	0.43
2:a:146:GLN:O	2:a:149:THR:N	2.52	0.43
5:c:200:CYC:HAB2	3:h:76:HIS:HB2	1.99	0.43
2:d:17:GLY:HA2	3:k:91:ARG:HH12	1.83	0.43
2:e:21:ASN:O	2:e:25:LEU:HD23	2.18	0.43
3:k:72:ASN:O	3:k:78:ARG:HD3	2.18	0.43
1:5:492:GLY:O	1:5:496:LEU:HG	2.18	0.43
1:5:661:ILE:HG13	1:5:742:LEU:HD13	1.99	0.43
2:C:107:ASP:HA	2:C:111:ILE:HB	2.00	0.43
3:G:2:ASN:N	3:G:103:SER:OG	2.51	0.43
3:J:37:ARG:NH1	3:J:159:GLU:OE1	2.28	0.43
3:K:158:SER:O	3:K:162:THR:HG23	2.18	0.43
3:L:97:LEU:HD12	3:L:160:ALA:HB2	2.00	0.43
2:N:38:ALA:HB1	2:N:98:LEU:O	2.19	0.43
2:O:62:LYS:HE2	2:O:62:LYS:HB3	1.80	0.43
5:Q:200:CYC:HB	5:Q:200:CYC:CMA	2.32	0.43
2:R:63:LYS:O	2:R:63:LYS:HD3	2.18	0.43
3:T:42:ALA:HA	3:T:45:THR:HG22	2.00	0.43
3:U:58:LYS:HD2	3:U:133:LEU:HD12	2.00	0.43
3:W:112:GLY:HA2	3:W:115:GLU:OE1	2.18	0.43
2:a:109:TYR:O	3:g:76:HIS:HB3	2.17	0.43
2:b:18:ARG:NH2	2:b:24:GLU:OE2	2.31	0.43
2:e:116:GLU:HA	2:e:119:ARG:NE	2.33	0.43
5:k:200:CYC:HBC2	5:k:200:CYC:H2C	1.69	0.43
1:5:556:ARG:NE	3:j:119:ALA:O	2.51	0.43
5:5:1202:CYC:CHD	3:l:82:CYS:HA	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:LYS:HD2	2:B:156:ASP:OD1	2.18	0.43
2:D:37:PRO:HA	2:D:40:GLU:CD	2.43	0.43
2:E:152:LEU:HD23	2:E:152:LEU:HA	1.87	0.43
3:K:128:ALA:HB2	3:K:172:ALA:HB2	2.00	0.43
4:M:55:ARG:C	4:M:58:PRO:HD2	2.44	0.43
2:R:110:VAL:HG12	2:R:111:ILE:HD13	1.99	0.43
2:b:4:THR:OG1	2:b:100:ALA:O	2.33	0.43
2:d:102:GLY:N	2:d:154:TYR:OH	2.51	0.43
5:d:200:CYC:OC	5:d:200:CYC:HMD1	2.18	0.43
5:f:200:CYC:HBA2	5:f:200:CYC:HAD2	2.01	0.43
3:h:77:ARG:HH21	4:m:14:GLN:CD	2.26	0.43
3:i:36:LYS:HG3	5:i:201:CYC:HMD3	2.00	0.43
5:B:200:CYC:HBA2	3:K:67:ILE:HD12	1.99	0.43
2:F:43:ARG:HH12	3:L:21:GLU:CD	2.26	0.43
3:H:17:SER:OG	3:H:18:PHE:N	2.51	0.43
3:H:105:LEU:HB3	3:H:166:LYS:NZ	2.33	0.43
3:J:92:TYR:CG	3:J:109:CYS:HB2	2.53	0.43
2:O:82:LYS:HZ2	5:O:200:CYC:C3D	2.32	0.43
3:T:66:LEU:HD22	3:T:72:ASN:OD1	2.19	0.43
2:d:17:GLY:HA2	3:k:91:ARG:NH1	2.34	0.43
2:f:9:VAL:CG1	2:f:24:GLU:HB2	2.49	0.43
2:f:92:ARG:HH12	3:l:16:GLY:HA2	1.84	0.43
3:h:108:ARG:NE	3:h:108:ARG:HA	2.33	0.43
1:5:687:GLN:HE22	1:5:692:GLU:CD	2.27	0.43
1:5:730:ASP:HA	3:l:119:ALA:HB1	2.01	0.43
2:A:2:SER:O	2:A:7:THR:HG21	2.19	0.43
3:I:114:ARG:HG3	3:I:171:ILE:HA	1.99	0.43
3:I:129:ARG:O	3:I:133:LEU:HG	2.19	0.43
4:M:61:ILE:O	4:M:65:GLN:HG2	2.18	0.43
2:O:138:GLU:OE1	2:O:141:LYS:NZ	2.52	0.43
2:R:114:LEU:HD21	2:R:162:LEU:HD23	2.01	0.43
2:S:4:THR:HG22	2:S:5:VAL:N	2.34	0.43
3:T:106:ASP:HA	3:T:110:LEU:HD22	2.00	0.43
3:W:91:ARG:HG2	3:W:95:TYR:CE2	2.54	0.43
3:Y:44:LEU:HD22	3:Y:90:LEU:HD11	2.01	0.43
2:a:153:LEU:HD22	2:b:22:SER:HB3	2.00	0.43
2:c:121:PHE:HB2	2:c:123:LEU:HD13	2.01	0.43
3:i:41:VAL:HG11	3:i:98:LEU:HD12	2.01	0.43
1:5:156:ASP:HB2	5:I:200:CYC:HAA1	2.00	0.43
1:5:554:GLN:HB3	1:5:560:ASN:HA	2.01	0.43
5:5:1202:CYC:HMB1	3:l:113:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:9:VAL:HG12	2:A:20:LEU:HD22	2.01	0.43
2:A:19:PHE:CE2	3:H:90:LEU:HD22	2.54	0.43
2:B:67:VAL:HG12	2:B:74:GLY:HA3	2.01	0.43
2:C:6:ILE:O	2:C:10:ILE:HG13	2.18	0.43
2:C:83:CYS:O	2:C:87:ILE:HG12	2.19	0.43
2:D:37:PRO:HA	2:D:40:GLU:OE2	2.19	0.43
2:D:126:LEU:HD23	2:D:129:ILE:HD12	2.00	0.43
2:F:53:VAL:O	2:F:57:VAL:HG23	2.18	0.43
3:G:59:LEU:HD21	3:G:66:LEU:HD12	1.99	0.43
3:G:73:ALA:O	3:G:79:MET:HB2	2.19	0.43
3:H:122:THR:HG23	5:H:200:CYC:HMC3	2.01	0.43
2:Q:72:GLU:HG3	2:Q:73:LYS:N	2.33	0.43
3:T:73:ALA:O	3:T:79:MET:HB2	2.19	0.43
2:f:93:PHE:HD2	2:f:110:VAL:HG13	1.83	0.43
3:h:91:ARG:HG2	3:h:95:TYR:CZ	2.54	0.43
4:m:51:VAL:HG21	4:m:59:GLU:HG3	1.99	0.43
1:5:116:ARG:O	1:5:119:PHE:HD1	2.01	0.42
1:5:706:GLY:C	3:j:108:ARG:HH12	2.27	0.42
2:A:98:LEU:HA	2:A:154:TYR:CE2	2.53	0.42
2:D:50:ASP:O	2:D:54:LYS:HG3	2.19	0.42
3:G:79:MET:HE3	3:G:79:MET:HB3	1.77	0.42
3:G:127:VAL:O	3:G:131:VAL:HG23	2.19	0.42
2:N:25:LEU:O	3:U:38:LEU:HD21	2.19	0.42
2:N:117:VAL:HG23	3:T:80:ALA:HB2	2.00	0.42
2:O:34:ARG:O	2:O:37:PRO:HD2	2.19	0.42
2:S:18:ARG:HH22	2:S:21:ASN:CG	2.27	0.42
3:T:65:GLU:OE1	3:T:66:LEU:HD23	2.19	0.42
2:d:124:ASN:HB3	2:d:127:TRP:CE2	2.53	0.42
2:f:21:ASN:N	2:f:24:GLU:OE2	2.42	0.42
2:f:49:GLN:HA	2:f:52:LEU:HD12	2.01	0.42
3:g:145:THR:O	3:g:145:THR:HG22	2.19	0.42
5:h:200:CYC:CMA	5:h:200:CYC:HB	2.32	0.42
3:l:86:MET:HB3	3:l:134:MET:HE3	2.00	0.42
2:C:107:ASP:HA	2:C:111:ILE:HD12	2.00	0.42
5:H:200:CYC:HAA1	4:M:56:PHE:CD2	2.54	0.42
3:L:73:ALA:HA	3:L:78:ARG:HG3	2.01	0.42
2:Q:39:ILE:HD11	3:X:24:LEU:HD22	2.01	0.42
3:T:111:ASN:OD1	3:T:112:GLY:N	2.50	0.42
2:a:74:GLY:O	2:a:79:ASN:HB2	2.18	0.42
2:a:110:VAL:HG12	5:a:200:CYC:HAB2	2.02	0.42
2:a:125:PRO:HA	2:a:128:TYR:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:37:PRO:O	2:b:147:SER:OG	2.30	0.42
3:h:145:THR:HG22	3:h:145:THR:O	2.19	0.42
3:j:29:SER:O	3:j:32:LYS:HG3	2.18	0.42
3:k:62:GLU:HG3	3:k:63:GLN:OE1	2.18	0.42
3:k:129:ARG:HA	3:k:129:ARG:HH11	1.84	0.42
3:l:44:LEU:HD23	3:l:44:LEU:HA	1.85	0.42
3:l:80:ALA:O	3:l:83:LEU:HG	2.19	0.42
3:l:133:LEU:HD23	3:l:133:LEU:HA	1.87	0.42
3:l:154:SER:HA	3:l:157:TYR:HD2	1.84	0.42
1:5:425:HIS:HD2	1:5:429:LEU:HD12	1.83	0.42
1:5:518:ASP:OD1	1:5:519:ARG:N	2.52	0.42
2:D:34:ARG:O	2:D:37:PRO:HD2	2.19	0.42
2:E:18:ARG:HD2	2:E:19:PHE:O	2.20	0.42
3:K:44:LEU:HD23	3:K:44:LEU:HA	1.86	0.42
3:L:90:LEU:HB2	3:L:134:MET:HE1	1.99	0.42
2:R:21:ASN:OD1	2:R:24:GLU:HG3	2.18	0.42
2:R:34:ARG:O	2:R:37:PRO:HD2	2.19	0.42
2:S:83:CYS:SG	5:S:200:CYC:HAC2	2.59	0.42
3:T:79:MET:HB3	3:T:79:MET:HE3	1.57	0.42
2:a:3:ARG:NE	4:m:35:ARG:HH12	2.17	0.42
3:g:168:ALA:HA	3:g:171:ILE:HG22	2.01	0.42
3:h:135:LYS:HE2	3:h:135:LYS:HB3	1.73	0.42
2:A:92:ARG:HH22	3:H:16:GLY:C	2.28	0.42
2:E:43:ARG:HG3	2:E:44:ALA:N	2.33	0.42
3:H:54:ASP:O	3:H:58:LYS:HG3	2.19	0.42
3:H:112:GLY:HA3	4:M:70:ILE:HD11	2.01	0.42
3:H:159:GLU:HG2	3:H:163:TYR:CE2	2.55	0.42
3:I:62:GLU:HG2	3:I:63:GLN:HG3	2.01	0.42
3:J:33:GLU:N	3:J:33:GLU:OE2	2.52	0.42
3:J:149:THR:O	5:J:201:CYC:NC	2.52	0.42
3:K:72:ASN:O	3:K:78:ARG:HD3	2.20	0.42
3:U:47:ASN:O	3:U:51:ILE:HG13	2.20	0.42
3:k:131:VAL:HA	3:k:134:MET:HE3	2.01	0.42
1:5:531:ASP:O	1:5:535:ARG:HG3	2.19	0.42
1:5:587:TYR:HE2	1:5:601:ARG:HG2	1.84	0.42
1:5:593:ASN:HB2	1:5:724:THR:O	2.19	0.42
2:E:93:PHE:HD2	2:E:110:VAL:HG23	1.85	0.42
2:F:82:LYS:HD3	5:F:200:CYC:CHA	2.50	0.42
3:K:138:ALA:O	3:K:142:LEU:HG	2.19	0.42
2:R:58:GLN:HB3	2:R:62:LYS:HE3	2.02	0.42
3:T:129:ARG:HA	3:T:132:GLN:OE1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:82:CYS:SG	5:X:200:CYC:HAC2	2.59	0.42
2:a:6:ILE:HD12	2:a:6:ILE:H	1.85	0.42
2:a:26:GLN:OE1	2:b:34:ARG:NE	2.53	0.42
2:b:30:GLY:O	2:b:33:GLU:HG2	2.19	0.42
2:d:14:ASP:OD2	3:k:108:ARG:HD2	2.20	0.42
2:e:125:PRO:O	2:e:129:ILE:HG12	2.20	0.42
3:g:110:LEU:HB3	3:g:114:ARG:HH12	1.83	0.42
3:l:51:ILE:HG13	3:l:137:ALA:CB	2.50	0.42
3:l:153:CYS:SG	5:l:201:CYC:HMD3	2.59	0.42
1:5:576:GLU:OE2	1:5:610:ARG:NH1	2.53	0.42
2:N:75:TYR:O	2:N:79:ASN:ND2	2.52	0.42
3:W:106:ASP:OD2	3:W:166:LYS:HD3	2.20	0.42
3:X:3:ASP:O	3:X:7:ARG:HG3	2.20	0.42
3:g:91:ARG:O	3:g:94:SER:OG	2.26	0.42
1:5:704:GLN:HB2	1:5:707:GLN:HB3	2.02	0.42
2:C:3:ARG:HH12	2:D:16:GLN:HE22	1.67	0.42
2:C:54:LYS:HE2	2:C:54:LYS:HB2	1.81	0.42
2:D:146:GLN:O	2:D:149:THR:OG1	2.33	0.42
2:E:34:ARG:O	2:E:37:PRO:HD2	2.19	0.42
2:E:143:LEU:HB2	2:E:148:LYS:HG2	2.02	0.42
2:P:66:TYR:O	2:P:69:GLN:HG2	2.20	0.42
5:Q:200:CYC:HB	5:Q:200:CYC:HMA2	1.84	0.42
3:U:1:MET:SD	3:U:104:VAL:HG12	2.60	0.42
3:U:62:GLU:OE1	3:U:63:GLN:HG2	2.19	0.42
3:Y:72:ASN:O	3:Y:78:ARG:HD2	2.19	0.42
2:c:66:TYR:HA	2:c:69:GLN:HE22	1.84	0.42
2:c:99:VAL:HG11	3:i:19:LEU:HD13	2.02	0.42
2:d:16:GLN:HB2	2:d:18:ARG:HG2	2.01	0.42
2:d:143:LEU:HD23	2:d:143:LEU:HA	1.91	0.42
2:e:106:LEU:O	2:e:110:VAL:HG12	2.20	0.42
2:e:132:LEU:O	2:e:136:LYS:HG2	2.18	0.42
1:5:379:ARG:HG2	1:5:379:ARG:HH11	1.84	0.42
2:C:29:PHE:HE2	2:D:33:GLU:OE2	2.03	0.42
2:E:37:PRO:HA	2:E:40:GLU:OE2	2.20	0.42
2:E:98:LEU:HA	2:E:154:TYR:CE2	2.53	0.42
2:F:82:LYS:HD3	5:F:200:CYC:HHA	2.02	0.42
3:G:15:LYS:NZ	3:G:17:SER:HB2	2.35	0.42
4:M:60:MET:HE3	4:M:60:MET:HA	2.00	0.42
2:R:5:VAL:O	2:R:9:VAL:HG23	2.20	0.42
3:V:92:TYR:OH	3:V:108:ARG:NH1	2.48	0.42
3:X:23:ASP:O	3:X:27:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:15:SER:HA	4:m:65:GLN:HE21	1.84	0.42
2:a:118:ASN:HD22	2:a:125:PRO:HG3	1.85	0.42
2:e:18:ARG:NH1	2:e:19:PHE:O	2.51	0.42
2:e:83:CYS:HA	5:e:200:CYC:HHD	2.02	0.42
2:e:99:VAL:HG21	3:g:19:LEU:HD13	2.01	0.42
2:f:5:VAL:HG11	2:f:34:ARG:HH12	1.85	0.42
2:f:48:ASN:O	2:f:52:LEU:HG	2.20	0.42
3:h:11:GLN:HB3	3:h:15:LYS:NZ	2.35	0.42
3:i:145:THR:O	3:i:145:THR:HG22	2.20	0.42
3:j:30:PHE:CZ	3:j:100:GLY:HA3	2.55	0.42
3:k:69:PRO:HA	3:k:74:TYR:CG	2.55	0.42
1:5:360:ALA:O	1:5:364:ILE:HG13	2.19	0.42
1:5:369:PHE:O	1:5:372:THR:OG1	2.30	0.42
1:5:400:LEU:O	1:5:404:THR:HG23	2.20	0.42
1:5:419:ARG:NE	1:5:513:VAL:O	2.43	0.42
1:5:531:ASP:HA	1:5:534:GLU:OE1	2.19	0.42
1:5:556:ARG:HE	3:j:119:ALA:C	2.28	0.42
2:B:91:LEU:O	2:B:95:THR:HG23	2.20	0.42
2:C:92:ARG:NE	3:I:16:GLY:O	2.53	0.42
3:L:85:ASP:OD2	3:L:117:TYR:OH	2.25	0.42
2:N:146:GLN:NE2	2:N:149:THR:HB	2.35	0.42
2:Q:11:ALA:HB2	3:X:1:MET:HE1	2.02	0.42
3:X:72:ASN:HD21	3:X:122:THR:CA	2.26	0.42
3:X:120:LEU:HD13	5:X:200:CYC:HHA	2.02	0.42
3:X:125:GLN:NE2	3:j:62:GLU:HA	2.35	0.42
2:a:97:SER:O	2:a:101:SER:N	2.53	0.42
2:e:85:ARG:HG3	2:e:86:ASP:N	2.34	0.42
2:f:70:PRO:HD3	2:f:75:TYR:CE1	2.54	0.42
3:j:90:LEU:HA	3:j:93:VAL:HG12	2.01	0.42
4:m:19:TYR:CE2	4:m:53:TYR:HD1	2.37	0.42
1:5:520:LEU:O	1:5:520:LEU:HD23	2.20	0.42
1:5:576:GLU:HG3	2:e:112:ALA:HA	2.01	0.42
2:A:38:ALA:HB1	2:A:98:LEU:O	2.20	0.42
2:E:36:VAL:HA	2:E:39:ILE:HG12	2.02	0.42
5:E:200:CYC:HAC2	5:E:200:CYC:HHD	1.85	0.42
4:M:69:LYS:HA	4:M:69:LYS:HD3	1.85	0.42
2:P:5:VAL:HB	2:P:31:ARG:HG3	2.01	0.42
2:Q:4:THR:H	2:Q:7:THR:HB	1.83	0.42
2:R:57:VAL:HG12	2:R:83:CYS:SG	2.60	0.42
3:V:145:THR:O	3:V:145:THR:HG22	2.20	0.42
3:X:113:LEU:HD12	3:X:113:LEU:HA	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:13:ALA:O	2:c:17:GLY:N	2.53	0.42
2:d:124:ASN:HB3	2:d:127:TRP:CD2	2.55	0.42
2:e:85:ARG:CZ	3:i:67:ILE:HD12	2.50	0.42
2:f:99:VAL:HG21	3:l:19:LEU:HD12	2.00	0.42
3:k:79:MET:O	3:k:83:LEU:HG	2.20	0.42
4:m:32:ASN:HA	4:m:35:ARG:HE	1.85	0.42
1:5:267:TRP:H	3:L:111:ASN:ND2	2.18	0.41
1:5:684:GLU:O	1:5:688:GLU:HG3	2.20	0.41
2:A:149:THR:O	2:A:153:LEU:HG	2.20	0.41
2:C:64:PHE:CD2	2:C:127:TRP:HD1	2.37	0.41
2:E:148:LYS:NZ	2:E:148:LYS:HB3	2.35	0.41
2:F:83:CYS:SG	5:F:200:CYC:HAC2	2.59	0.41
3:G:38:LEU:HD23	3:G:38:LEU:HA	1.88	0.41
2:R:83:CYS:SG	5:R:200:CYC:HAC2	2.60	0.41
3:V:107:ASP:HB3	4:Z:77:ILE:HD13	2.02	0.41
3:W:23:ASP:O	3:W:27:LEU:HD23	2.19	0.41
3:X:79:MET:HE2	3:X:79:MET:HB2	1.94	0.41
3:Y:82:CYS:SG	5:Y:200:CYC:H2C	2.60	0.41
2:a:34:ARG:HH21	2:b:26:GLN:HA	1.84	0.41
2:c:107:ASP:O	2:c:111:ILE:HB	2.20	0.41
2:e:135:ILE:HA	2:e:138:GLU:CD	2.45	0.41
3:g:105:LEU:HD23	3:g:166:LYS:NZ	2.35	0.41
3:g:145:THR:HG21	3:g:150:VAL:HG22	2.02	0.41
2:C:67:VAL:O	2:C:74:GLY:HA3	2.20	0.41
2:C:151:ALA:O	2:C:152:LEU:C	2.63	0.41
2:D:28:ALA:HB3	3:K:38:LEU:HD21	2.02	0.41
3:H:97:LEU:HA	3:H:163:TYR:HE2	1.85	0.41
3:I:127:VAL:HB	3:I:171:ILE:HG21	2.03	0.41
3:J:74:TYR:O	3:J:76:HIS:N	2.52	0.41
2:Q:34:ARG:NH1	2:Q:101:SER:OG	2.52	0.41
2:a:58:GLN:HA	2:a:61:PHE:CD2	2.55	0.41
5:c:200:CYC:HAC2	5:c:200:CYC:HH2	1.93	0.41
2:d:92:ARG:HD2	3:k:17:SER:C	2.45	0.41
2:e:39:ILE:HD13	3:g:28:ALA:HB2	2.01	0.41
2:f:95:THR:O	2:f:99:VAL:HG23	2.20	0.41
2:f:148:LYS:NZ	3:g:147:ASN:HD21	2.17	0.41
3:h:82:CYS:SG	5:h:200:CYC:H2C	2.60	0.41
3:k:85:ASP:O	3:k:89:ILE:HG13	2.19	0.41
4:m:19:TYR:HB2	4:m:56:PHE:CE1	2.55	0.41
1:5:247:LYS:HA	5:J:200:CYC:HBA2	2.01	0.41
1:5:436:GLN:HG2	1:5:520:LEU:CD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:56:ALA:O	2:D:60:VAL:HG23	2.20	0.41
3:H:29:SER:HA	3:H:32:LYS:HG2	2.02	0.41
3:H:112:GLY:HA2	3:H:115:GLU:OE2	2.19	0.41
5:J:200:CYC:NC	5:J:200:CYC:HMD1	2.36	0.41
2:N:128:TYR:CZ	5:N:200:CYC:HAC1	2.55	0.41
2:Q:9:VAL:HG13	2:Q:24:GLU:HG2	2.02	0.41
2:R:36:VAL:O	2:R:39:ILE:N	2.52	0.41
2:R:105:PRO:O	2:R:109:TYR:HB2	2.20	0.41
2:S:134:TYR:O	2:S:138:GLU:OE1	2.39	0.41
2:a:67:VAL:O	2:a:72:GLU:HB2	2.19	0.41
2:f:79:ASN:HA	2:f:82:LYS:HG2	2.02	0.41
2:f:82:LYS:HD2	5:f:200:CYC:C3D	2.50	0.41
3:g:3:ASP:OD1	3:g:6:THR:HG23	2.21	0.41
3:h:85:ASP:HA	3:h:88:ILE:HG22	2.02	0.41
5:h:200:CYC:HHD	5:h:200:CYC:HAC1	1.69	0.41
5:h:200:CYC:HB	5:h:200:CYC:HMA2	1.86	0.41
3:l:7:ARG:HH22	3:l:103:SER:HB2	1.85	0.41
3:l:110:LEU:HB3	3:l:170:SER:OG	2.20	0.41
1:5:415:THR:O	3:X:108:ARG:HD2	2.20	0.41
2:D:86:ASP:OD2	2:D:128:TYR:OH	2.31	0.41
2:E:37:PRO:HA	2:E:40:GLU:CD	2.46	0.41
3:G:166:LYS:HB3	3:G:166:LYS:HE3	1.89	0.41
3:H:1:MET:HG2	3:H:104:VAL:HG22	2.01	0.41
3:H:36:LYS:HG2	5:H:201:CYC:CMD	2.51	0.41
3:L:92:TYR:CG	3:L:109:CYS:HB2	2.55	0.41
2:P:35:ALA:O	2:P:39:ILE:HG13	2.20	0.41
3:V:79:MET:O	3:V:83:LEU:HG	2.20	0.41
2:a:103:THR:OG1	2:a:107:ASP:OD2	2.31	0.41
2:f:65:PRO:O	2:f:68:THR:OG1	2.39	0.41
3:g:82:CYS:SG	5:g:200:CYC:H2C	2.59	0.41
3:g:158:SER:O	3:g:162:THR:HG23	2.20	0.41
3:h:59:LEU:HD12	3:h:63:GLN:OE1	2.20	0.41
3:k:85:ASP:OD2	3:k:117:TYR:OH	2.25	0.41
5:k:201:CYC:HBC2	5:k:201:CYC:H2C	1.84	0.41
1:5:274:ARG:HD2	5:5:1201:CYC:O1D	2.20	0.41
1:5:419:ARG:NH2	1:5:504:ASP:OD1	2.54	0.41
1:5:507:ARG:HH11	5:Y:200:CYC:CAD	2.33	0.41
1:5:533:ILE:O	1:5:537:LEU:HD23	2.21	0.41
2:C:108:ASP:HB2	4:M:14:GLN:NE2	2.36	0.41
2:F:131:ALA:O	2:F:135:ILE:HG12	2.21	0.41
4:M:17:ARG:H	4:M:77:ILE:HD12	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:26:GLN:CD	2:O:34:ARG:HH12	2.28	0.41
2:N:93:PHE:HE2	5:N:200:CYC:HBB1	1.85	0.41
2:O:31:ARG:NH2	3:W:5:PHE:CD2	2.89	0.41
2:P:128:TYR:CE1	5:P:200:CYC:HAC1	2.56	0.41
3:X:69:PRO:HA	3:X:74:TYR:CG	2.56	0.41
3:X:148:VAL:HG21	5:X:201:CYC:H3C	2.03	0.41
3:g:7:ARG:CZ	3:g:7:ARG:HB3	2.51	0.41
3:g:62:GLU:HG2	3:g:63:GLN:OE1	2.20	0.41
1:5:500:TYR:H	3:Y:111:ASN:ND2	2.18	0.41
1:5:732:GLY:HA3	1:5:737:ARG:HH21	1.86	0.41
2:A:2:SER:O	2:A:3:ARG:HD2	2.19	0.41
2:A:26:GLN:HG3	2:B:34:ARG:CZ	2.51	0.41
3:G:5:PHE:CD1	3:G:27:LEU:HD13	2.55	0.41
3:G:79:MET:O	3:G:83:LEU:HG	2.21	0.41
3:H:158:SER:O	3:H:162:THR:HG23	2.21	0.41
2:O:127:TRP:CD2	5:O:200:CYC:HMC3	2.56	0.41
2:Q:5:VAL:O	2:Q:9:VAL:HG23	2.20	0.41
3:T:40:ALA:HB2	5:T:201:CYC:HBC1	2.03	0.41
3:V:125:GLN:O	3:V:129:ARG:HG2	2.20	0.41
3:W:135:LYS:O	3:W:139:MET:HG2	2.21	0.41
2:a:114:LEU:HD21	2:a:162:LEU:HA	2.01	0.41
2:a:147:SER:HA	2:a:150:GLU:CD	2.46	0.41
3:g:41:VAL:O	3:g:45:THR:HG23	2.20	0.41
3:h:106:ASP:HA	3:h:110:LEU:HD12	2.01	0.41
3:h:114:ARG:NH2	3:h:170:SER:OG	2.53	0.41
3:j:114:ARG:HH12	3:j:118:ASN:ND2	2.08	0.41
3:k:91:ARG:HG2	3:k:95:TYR:CE2	2.56	0.41
3:k:137:ALA:O	3:k:141:HIS:ND1	2.41	0.41
3:l:104:VAL:O	3:l:108:ARG:HG2	2.21	0.41
1:5:185:ASN:O	1:5:189:GLU:HG3	2.21	0.41
2:B:9:VAL:HB	2:B:24:GLU:HB3	2.03	0.41
2:C:23:THR:HG22	2:D:102:GLY:HA2	2.02	0.41
2:D:98:LEU:HA	2:D:154:TYR:CE2	2.52	0.41
2:E:93:PHE:CD2	2:E:110:VAL:HG23	2.55	0.41
3:G:167:ALA:O	3:G:171:ILE:HG12	2.20	0.41
3:H:86:MET:O	3:H:134:MET:HE1	2.21	0.41
3:I:79:MET:HE2	3:I:79:MET:HB2	1.88	0.41
2:N:126:LEU:HD23	2:N:129:ILE:HD12	2.03	0.41
2:R:106:LEU:HD21	2:R:158:ALA:HB2	2.01	0.41
2:R:143:LEU:C	2:R:148:LYS:HB2	2.45	0.41
3:V:156:LEU:HD23	3:V:156:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:36:LYS:HG2	3:X:156:LEU:CD1	2.51	0.41
2:b:129:ILE:O	2:b:133:ASN:ND2	2.54	0.41
2:c:3:ARG:CZ	2:c:3:ARG:HA	2.51	0.41
2:c:109:TYR:O	3:h:77:ARG:NH1	2.54	0.41
2:d:92:ARG:HG3	3:k:18:PHE:CG	2.56	0.41
2:d:139:THR:HA	2:d:142:LEU:HB2	2.03	0.41
3:g:82:CYS:HA	5:g:200:CYC:HHD	2.03	0.41
3:h:75:PRO:C	3:h:77:ARG:H	2.28	0.41
3:k:72:ASN:ND2	3:k:123:PRO:HD2	2.35	0.41
3:l:22:SER:O	3:l:26:LYS:HG2	2.20	0.41
3:l:114:ARG:HH11	3:l:118:ASN:ND2	2.19	0.41
1:5:67:LEU:O	1:5:71:ARG:HG3	2.21	0.41
1:5:198:ARG:HD2	1:5:201:TYR:CZ	2.56	0.41
1:5:507:ARG:NH1	5:Y:200:CYC:O1D	2.52	0.41
2:C:54:LYS:O	2:C:58:GLN:HG2	2.21	0.41
3:G:41:VAL:O	3:G:45:THR:HG23	2.20	0.41
3:H:7:ARG:O	3:H:11:GLN:OE1	2.39	0.41
3:H:109:CYS:SG	5:H:200:CYC:HAB2	2.61	0.41
3:I:44:LEU:HD12	3:I:44:LEU:HA	1.81	0.41
2:O:114:LEU:HD21	2:O:162:LEU:HD23	2.03	0.41
2:P:108:ASP:HB2	4:Z:14:GLN:NE2	2.30	0.41
2:S:18:ARG:NH2	2:S:21:ASN:HB3	2.36	0.41
3:V:86:MET:CE	3:V:130:ALA:HB1	2.50	0.41
2:a:50:ASP:O	2:a:54:LYS:HG2	2.21	0.41
2:b:117:VAL:HG22	3:k:79:MET:SD	2.61	0.41
3:h:7:ARG:HG3	3:h:11:GLN:NE2	2.35	0.41
3:h:113:LEU:HD11	3:h:117:TYR:CZ	2.55	0.41
3:i:114:ARG:H	3:i:114:ARG:HG2	1.74	0.41
3:k:54:ASP:C	3:k:58:LYS:HZ2	2.29	0.41
3:k:59:LEU:HG	3:k:63:GLN:OE1	2.20	0.41
3:k:81:ALA:O	3:k:84:ARG:HG3	2.20	0.41
1:5:320:LEU:HD23	1:5:320:LEU:HA	1.90	0.41
1:5:341:LEU:HD21	1:5:479:PHE:HB2	2.03	0.41
1:5:630:LYS:HA	1:5:634:PHE:HB3	2.03	0.41
5:5:1202:CYC:H2C	3:l:82:CYS:SG	2.61	0.41
2:A:3:ARG:HD3	4:M:35:ARG:HH22	1.86	0.41
2:A:109:TYR:O	3:G:76:HIS:HB3	2.21	0.41
2:B:150:GLU:HG3	2:B:151:ALA:N	2.35	0.41
2:C:18:ARG:HH12	2:C:24:GLU:CD	2.29	0.41
2:E:35:ALA:O	2:E:39:ILE:HG23	2.21	0.41
2:E:91:LEU:O	2:E:95:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:148:LYS:HB2	2:F:148:LYS:HE2	1.86	0.41
3:G:2:ASN:HB3	3:G:7:ARG:HH11	1.86	0.41
3:H:163:TYR:O	3:H:166:LYS:HG2	2.21	0.41
5:H:201:CYC:HBC3	5:H:201:CYC:H2C	1.85	0.41
3:J:69:PRO:HA	3:J:74:TYR:CG	2.55	0.41
3:J:115:GLU:OE1	3:J:115:GLU:N	2.51	0.41
3:K:54:ASP:HB3	3:K:58:LYS:HZ3	1.86	0.41
3:K:74:TYR:HB3	3:K:75:PRO:HD3	2.02	0.41
3:L:139:MET:HE1	3:L:160:ALA:HB3	2.03	0.41
2:P:127:TRP:O	2:P:130:GLU:HG3	2.21	0.41
2:Q:40:GLU:HA	2:Q:40:GLU:OE2	2.20	0.41
2:Q:67:VAL:HG11	5:Q:200:CYC:HMC2	2.02	0.41
2:S:18:ARG:HH22	2:S:21:ASN:ND2	2.19	0.41
2:S:61:PHE:HZ	2:S:80:GLN:HG2	1.83	0.41
3:T:35:VAL:HG11	5:T:201:CYC:C3A	2.51	0.41
3:T:114:ARG:HH12	3:T:118:ASN:ND2	2.10	0.41
5:T:201:CYC:HAC1	5:T:201:CYC:HHD	1.72	0.41
3:U:69:PRO:HD3	3:U:74:TYR:CE1	2.56	0.41
3:V:5:PHE:O	3:V:9:ILE:HG12	2.21	0.41
3:V:65:GLU:HA	3:V:68:GLN:NE2	2.36	0.41
3:V:69:PRO:HA	3:V:74:TYR:CD2	2.56	0.41
3:W:79:MET:O	3:W:83:LEU:HG	2.20	0.41
3:X:36:LYS:HG2	3:X:156:LEU:HD11	2.01	0.41
3:Y:47:ASN:O	3:Y:51:ILE:HG13	2.21	0.41
2:a:5:VAL:HA	2:a:8:GLU:OE2	2.20	0.41
2:a:91:LEU:HD12	2:a:91:LEU:HA	1.85	0.41
2:b:34:ARG:O	2:b:37:PRO:HD2	2.21	0.41
2:b:148:LYS:HB2	2:b:148:LYS:HE2	1.87	0.41
2:d:39:ILE:HG23	2:d:43:ARG:HE	1.85	0.41
5:d:200:CYC:HBA1	3:l:67:ILE:HD12	2.03	0.41
2:e:136:LYS:HE3	2:e:152:LEU:HD23	2.03	0.41
2:f:145:GLY:O	2:f:149:THR:N	2.38	0.41
3:g:30:PHE:HE1	3:g:37:ARG:NH2	2.19	0.41
3:g:114:ARG:NH2	3:g:171:ILE:HA	2.35	0.41
3:g:135:LYS:HE3	3:g:161:ALA:HA	2.03	0.41
5:g:201:CYC:HAC2	5:g:201:CYC:HHD	1.62	0.41
3:h:88:ILE:HG13	3:h:92:TYR:CZ	2.55	0.41
3:i:91:ARG:HG2	3:i:95:TYR:CZ	2.56	0.41
3:i:132:GLN:NE2	3:i:133:LEU:HG	2.36	0.41
3:j:120:LEU:HD22	5:j:200:CYC:HBD1	2.02	0.41
3:k:89:ILE:HG21	3:k:131:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:l:69:PRO:HA	3:l:74:TYR:CD2	2.55	0.41
4:m:55:ARG:C	4:m:58:PRO:HD2	2.46	0.41
1:5:570:LEU:HD21	1:5:582:ALA:CB	2.51	0.41
2:A:22:SER:O	2:A:26:GLN:HG2	2.20	0.41
2:C:114:LEU:HA	3:H:76:HIS:NE2	2.36	0.41
2:C:123:LEU:HD11	5:C:200:CYC:HBD2	2.02	0.41
2:F:125:PRO:O	2:F:129:ILE:HG13	2.21	0.41
3:I:84:ARG:NH1	5:I:200:CYC:O1A	2.49	0.41
2:S:43:ARG:HG2	2:S:47:LYS:HE3	2.03	0.41
2:S:44:ALA:HB3	2:S:143:LEU:HD21	2.03	0.41
3:W:113:LEU:HA	3:W:113:LEU:HD12	1.81	0.41
3:X:3:ASP:OD1	3:X:3:ASP:N	2.53	0.41
2:a:99:VAL:HG21	3:h:19:LEU:HD12	2.03	0.41
2:d:148:LYS:HE3	2:d:148:LYS:HB3	1.80	0.41
2:e:69:GLN:O	2:e:75:TYR:HB2	2.21	0.41
5:f:200:CYC:HAD2	5:f:200:CYC:CGA	2.51	0.41
3:i:53:SER:O	3:i:57:HIS:ND1	2.48	0.41
3:i:68:GLN:O	3:i:74:TYR:HB2	2.21	0.41
3:j:156:LEU:HD23	3:j:156:LEU:HA	1.95	0.41
1:5:406:ALA:O	1:5:410:ARG:HG3	2.21	0.40
1:5:456:ASP:OD2	4:Z:55:ARG:HD3	2.20	0.40
1:5:627:ASP:OD1	1:5:628:THR:N	2.54	0.40
1:5:639:GLN:HA	1:5:642:PHE:HB3	2.02	0.40
1:5:644:GLU:HB3	1:5:738:LEU:HD12	2.02	0.40
2:B:1:MET:C	2:B:3:ARG:HH21	2.25	0.40
2:E:9:VAL:HG13	2:E:24:GLU:HG3	2.03	0.40
2:F:4:THR:HG22	2:F:100:ALA:HB1	2.03	0.40
2:F:56:ALA:HB2	2:F:135:ILE:HD11	2.03	0.40
3:G:49:PRO:HA	3:G:52:ILE:HG12	2.02	0.40
5:K:200:CYC:NB	5:K:200:CYC:HMA1	2.36	0.40
2:Q:73:LYS:HG3	2:Q:127:TRP:HH2	1.86	0.40
2:b:14:ASP:HA	3:j:91:ARG:NH2	2.36	0.40
2:c:10:ILE:HG21	3:i:104:VAL:HG21	2.03	0.40
2:c:22:SER:OG	2:d:153:LEU:HD22	2.20	0.40
2:c:43:ARG:NH2	2:c:47:LYS:HB3	2.36	0.40
3:g:58:LYS:HB2	3:g:133:LEU:HD13	2.03	0.40
3:j:33:GLU:HA	3:j:36:LYS:HE2	2.02	0.40
3:k:92:TYR:CZ	3:k:108:ARG:HB3	2.56	0.40
2:E:26:GLN:HE21	2:F:34:ARG:CZ	2.33	0.40
3:K:82:CYS:SG	5:K:200:CYC:H2C	2.61	0.40
2:Q:113:GLY:HA2	2:Q:116:GLU:OE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:34:ARG:HH22	2:S:26:GLN:CB	2.33	0.40
2:S:5:VAL:HB	2:S:31:ARG:HG3	2.03	0.40
3:X:59:LEU:HD22	3:X:130:ALA:HB2	2.03	0.40
3:Y:72:ASN:HD22	3:Y:123:PRO:HD2	1.86	0.40
2:a:48:ASN:HB3	2:a:52:LEU:HD23	2.03	0.40
2:a:64:PHE:CE2	2:a:127:TRP:HD1	2.40	0.40
2:c:36:VAL:HG23	2:c:37:PRO:HD3	2.04	0.40
3:g:101:ASP:OD1	3:g:102:ALA:N	2.53	0.40
2:A:39:ILE:HG21	3:H:28:ALA:HB2	2.03	0.40
2:B:1:MET:HE3	2:B:3:ARG:NH2	2.28	0.40
2:C:31:ARG:NH1	3:I:5:PHE:CE2	2.89	0.40
2:N:14:ASP:OD1	3:U:91:ARG:NH2	2.55	0.40
2:O:66:TYR:HA	2:O:69:GLN:NE2	2.36	0.40
2:O:124:ASN:HB3	2:O:127:TRP:CE2	2.56	0.40
2:R:18:ARG:O	3:T:91:ARG:HD2	2.21	0.40
2:R:58:GLN:O	2:R:62:LYS:HG2	2.22	0.40
2:S:18:ARG:HH22	2:S:21:ASN:CB	2.34	0.40
3:V:82:CYS:HB2	5:V:200:CYC:HC	1.87	0.40
5:W:200:CYC:HB	5:W:200:CYC:HMA2	1.85	0.40
2:e:124:ASN:ND2	2:e:126:LEU:HB2	2.36	0.40
3:l:135:LYS:NZ	3:l:136:ASP:OD1	2.42	0.40
1:5:79:LEU:O	1:5:83:LYS:HG2	2.22	0.40
1:5:730:ASP:C	1:5:732:GLY:H	2.29	0.40
2:D:60:VAL:HG22	2:D:130:GLU:OE2	2.22	0.40
3:I:74:TYR:HB3	3:I:75:PRO:HD3	2.02	0.40
3:J:86:MET:CE	3:J:130:ALA:HB1	2.48	0.40
5:O:200:CYC:HAC1	5:O:200:CYC:HHD	1.81	0.40
2:Q:8:GLU:HA	2:Q:8:GLU:OE2	2.21	0.40
2:Q:70:PRO:HA	2:Q:75:TYR:CG	2.56	0.40
3:T:36:LYS:HG3	5:T:201:CYC:HMD3	2.02	0.40
3:W:65:GLU:HA	3:W:68:GLN:HE21	1.87	0.40
3:X:39:ASP:HB3	5:X:201:CYC:HAC2	2.03	0.40
3:X:149:THR:O	5:X:201:CYC:NC	2.49	0.40
2:a:87:ILE:HA	2:a:90:TYR:CD2	2.56	0.40
2:e:6:ILE:O	2:e:10:ILE:HG13	2.22	0.40
2:e:136:LYS:CE	2:e:152:LEU:HA	2.51	0.40
2:f:64:PHE:CE2	2:f:127:TRP:HD1	2.40	0.40
3:h:130:ALA:O	3:h:134:MET:HG3	2.21	0.40
3:i:11:GLN:O	3:i:15:LYS:HE2	2.21	0.40
3:i:78:ARG:O	5:i:200:CYC:HMD3	2.21	0.40
3:i:129:ARG:O	3:i:132:GLN:NE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:k:1:MET:HG2	3:k:107:ASP:OD2	2.22	0.40
2:E:70:PRO:HA	2:E:75:TYR:CG	2.57	0.40
3:H:129:ARG:HA	3:H:132:GLN:OE1	2.21	0.40
3:J:32:LYS:HE3	3:J:33:GLU:OE2	2.22	0.40
3:L:44:LEU:HA	3:L:44:LEU:HD23	1.81	0.40
4:M:18:ILE:HG13	4:M:76:VAL:HB	2.02	0.40
2:N:77:ASP:HA	2:N:80:GLN:HG2	2.03	0.40
2:S:63:LYS:O	2:S:63:LYS:HG3	2.21	0.40
3:V:58:LYS:HB2	3:V:58:LYS:HE2	1.91	0.40
3:V:83:LEU:HA	3:V:86:MET:HG3	2.03	0.40
3:Y:159:GLU:O	3:Y:162:THR:OG1	2.34	0.40
2:a:45:LEU:HD21	2:a:91:LEU:HG	2.04	0.40
2:a:74:GLY:HA2	2:a:79:ASN:HB3	2.03	0.40
3:h:106:ASP:CG	3:h:166:LYS:HZ3	2.27	0.40
3:h:166:LYS:HB3	3:h:166:LYS:HE2	1.76	0.40
4:m:18:ILE:HG23	4:m:51:VAL:C	2.46	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	5	700/1182 (59%)	665 (95%)	35 (5%)	0	100	100
2	A	160/163 (98%)	155 (97%)	5 (3%)	0	100	100
2	B	161/163 (99%)	154 (96%)	7 (4%)	0	100	100
2	C	160/163 (98%)	155 (97%)	5 (3%)	0	100	100
2	D	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	E	160/163 (98%)	153 (96%)	7 (4%)	0	100	100
2	F	160/163 (98%)	156 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	O	161/163 (99%)	158 (98%)	3 (2%)	0	100	100
2	P	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	Q	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	R	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
2	S	160/163 (98%)	155 (97%)	5 (3%)	0	100	100
2	a	160/163 (98%)	152 (95%)	8 (5%)	0	100	100
2	b	161/163 (99%)	157 (98%)	4 (2%)	0	100	100
2	c	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	d	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	e	160/163 (98%)	154 (96%)	6 (4%)	0	100	100
2	f	160/163 (98%)	153 (96%)	7 (4%)	0	100	100
3	G	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
3	H	170/172 (99%)	164 (96%)	6 (4%)	0	100	100
3	I	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
3	J	170/172 (99%)	160 (94%)	10 (6%)	0	100	100
3	K	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	L	170/172 (99%)	162 (95%)	8 (5%)	0	100	100
3	T	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
3	U	170/172 (99%)	167 (98%)	3 (2%)	0	100	100
3	V	170/172 (99%)	169 (99%)	1 (1%)	0	100	100
3	W	170/172 (99%)	161 (95%)	9 (5%)	0	100	100
3	X	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	Y	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
3	g	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
3	h	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
3	i	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	j	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
3	k	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	l	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
4	M	67/78 (86%)	62 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Z	67/78 (86%)	62 (92%)	5 (8%)	0	100	100
4	m	67/78 (86%)	65 (97%)	2 (3%)	0	100	100
All	All	6844/7446 (92%)	6630 (97%)	214 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5	594/1003 (59%)	594 (100%)	0	100	100
2	A	128/129 (99%)	128 (100%)	0	100	100
2	B	129/129 (100%)	129 (100%)	0	100	100
2	C	128/129 (99%)	128 (100%)	0	100	100
2	D	128/129 (99%)	128 (100%)	0	100	100
2	E	128/129 (99%)	128 (100%)	0	100	100
2	F	128/129 (99%)	128 (100%)	0	100	100
2	N	128/129 (99%)	128 (100%)	0	100	100
2	O	129/129 (100%)	129 (100%)	0	100	100
2	P	128/129 (99%)	128 (100%)	0	100	100
2	Q	128/129 (99%)	128 (100%)	0	100	100
2	R	128/129 (99%)	128 (100%)	0	100	100
2	S	128/129 (99%)	128 (100%)	0	100	100
2	a	128/129 (99%)	128 (100%)	0	100	100
2	b	129/129 (100%)	129 (100%)	0	100	100
2	c	128/129 (99%)	128 (100%)	0	100	100
2	d	128/129 (99%)	128 (100%)	0	100	100
2	e	128/129 (99%)	128 (100%)	0	100	100
2	f	128/129 (99%)	128 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	133/133 (100%)	133 (100%)	0	100	100
3	H	133/133 (100%)	133 (100%)	0	100	100
3	I	133/133 (100%)	133 (100%)	0	100	100
3	J	133/133 (100%)	133 (100%)	0	100	100
3	K	133/133 (100%)	133 (100%)	0	100	100
3	L	133/133 (100%)	133 (100%)	0	100	100
3	T	133/133 (100%)	133 (100%)	0	100	100
3	U	133/133 (100%)	133 (100%)	0	100	100
3	V	133/133 (100%)	133 (100%)	0	100	100
3	W	133/133 (100%)	133 (100%)	0	100	100
3	X	133/133 (100%)	133 (100%)	0	100	100
3	Y	133/133 (100%)	133 (100%)	0	100	100
3	g	133/133 (100%)	133 (100%)	0	100	100
3	h	133/133 (100%)	133 (100%)	0	100	100
3	i	133/133 (100%)	133 (100%)	0	100	100
3	j	133/133 (100%)	133 (100%)	0	100	100
3	k	133/133 (100%)	133 (100%)	0	100	100
3	l	133/133 (100%)	133 (100%)	0	100	100
4	M	59/67 (88%)	59 (100%)	0	100	100
4	Z	59/67 (88%)	59 (100%)	0	100	100
4	m	59/67 (88%)	59 (100%)	0	100	100
All	All	5472/5920 (92%)	5472 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	5	425	HIS
2	A	157	HIS
2	B	48	ASN
2	B	157	HIS
2	C	48	ASN
2	D	26	GLN

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Mol	Chain	Res	Type
2	D	48	ASN
2	E	26	GLN
2	E	79	ASN
2	F	48	ASN
3	G	68	GLN
3	G	111	ASN
3	I	63	GLN
3	J	47	ASN
3	J	111	ASN
3	K	132	GLN
2	O	48	ASN
2	Q	48	ASN
2	R	48	ASN
2	R	69	GLN
2	R	146	GLN
3	U	118	ASN
3	V	63	GLN
3	W	11	GLN
3	W	68	GLN
3	W	76	HIS
3	X	72	ASN
3	X	147	ASN
3	Y	47	ASN
3	Y	72	ASN
2	a	49	GLN
2	a	118	ASN
2	a	146	GLN
2	b	49	GLN
2	b	79	ASN
2	c	58	GLN
2	c	160	ASN
2	d	58	GLN
2	f	26	GLN
2	f	157	HIS
2	f	160	ASN
3	g	11	GLN
3	g	46	ASN
3	h	72	ASN
3	i	11	GLN
3	i	64	GLN
3	i	132	GLN
3	j	72	ASN

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Mol	Chain	Res	Type
3	k	11	GLN
3	k	72	ASN
3	l	68	GLN
3	l	72	ASN
3	l	118	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

54 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	$\# Z > 2$
5	CYC	k	200	-	46,46,46	5.29	26 (56%)	63,67,67	4.02	16 (25%)
5	CYC	U	200	-	46,46,46	5.33	25 (54%)	63,67,67	3.97	17 (26%)
5	CYC	I	200	-	46,46,46	5.26	26 (56%)	63,67,67	3.92	13 (20%)
5	CYC	T	201	-	46,46,46	5.27	26 (56%)	63,67,67	4.06	15 (23%)
5	CYC	D	200	-	46,46,46	5.20	27 (58%)	63,67,67	4.27	18 (28%)
5	CYC	c	200	-	46,46,46	5.35	26 (56%)	63,67,67	4.02	16 (25%)
5	CYC	j	200	-	46,46,46	5.27	26 (56%)	63,67,67	4.06	17 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CYC	W	200	-	46,46,46	5.22	25 (54%)	63,67,67	3.99	18 (28%)
5	CYC	V	201	-	46,46,46	5.29	25 (54%)	63,67,67	4.20	11 (17%)
5	CYC	k	201	-	46,46,46	5.34	25 (54%)	63,67,67	3.98	15 (23%)
5	CYC	Y	201	-	46,46,46	5.29	26 (56%)	63,67,67	4.07	15 (23%)
5	CYC	A	200	-	46,46,46	5.25	26 (56%)	63,67,67	4.25	15 (23%)
5	CYC	I	201	-	46,46,46	5.23	25 (54%)	63,67,67	4.28	16 (25%)
5	CYC	l	201	-	46,46,46	5.33	26 (56%)	63,67,67	4.07	15 (23%)
5	CYC	Q	200	-	46,46,46	5.31	27 (58%)	63,67,67	4.15	15 (23%)
5	CYC	R	200	-	46,46,46	5.36	25 (54%)	63,67,67	4.03	14 (22%)
5	CYC	V	200	-	46,46,46	5.30	26 (56%)	63,67,67	4.09	13 (20%)
5	CYC	E	200	-	46,46,46	5.27	26 (56%)	63,67,67	3.95	18 (28%)
5	CYC	i	200	-	46,46,46	5.34	25 (54%)	63,67,67	3.99	14 (22%)
5	CYC	5	1202	-	46,46,46	5.29	26 (56%)	63,67,67	4.02	13 (20%)
5	CYC	i	201	-	46,46,46	5.33	25 (54%)	63,67,67	4.13	12 (19%)
5	CYC	f	200	-	46,46,46	5.28	26 (56%)	63,67,67	4.28	13 (20%)
5	CYC	5	1201	-	46,46,46	5.23	26 (56%)	63,67,67	3.92	16 (25%)
5	CYC	W	201	-	46,46,46	5.24	26 (56%)	63,67,67	4.07	13 (20%)
5	CYC	j	201	-	46,46,46	5.27	26 (56%)	63,67,67	4.20	13 (20%)
5	CYC	O	200	-	46,46,46	5.29	26 (56%)	63,67,67	4.26	17 (26%)
5	CYC	G	201	-	46,46,46	5.32	26 (56%)	63,67,67	3.98	14 (22%)
5	CYC	g	200	-	46,46,46	5.35	25 (54%)	63,67,67	3.89	15 (23%)
5	CYC	d	200	-	46,46,46	5.34	25 (54%)	63,67,67	3.81	13 (20%)
5	CYC	S	200	-	46,46,46	5.22	26 (56%)	63,67,67	4.29	14 (22%)
5	CYC	B	200	-	46,46,46	5.31	26 (56%)	63,67,67	4.15	16 (25%)
5	CYC	X	201	-	46,46,46	5.30	26 (56%)	63,67,67	4.03	14 (22%)
5	CYC	L	201	-	46,46,46	5.26	26 (56%)	63,67,67	4.01	18 (28%)
5	CYC	K	201	-	46,46,46	5.22	26 (56%)	63,67,67	4.17	17 (26%)
5	CYC	J	200	-	46,46,46	5.27	26 (56%)	63,67,67	4.08	16 (25%)
5	CYC	H	201	-	46,46,46	5.31	26 (56%)	63,67,67	4.16	13 (20%)
5	CYC	F	200	-	46,46,46	5.21	27 (58%)	63,67,67	3.94	14 (22%)
5	CYC	K	200	-	46,46,46	5.25	25 (54%)	63,67,67	4.07	16 (25%)
5	CYC	b	200	-	46,46,46	5.33	26 (56%)	63,67,67	4.13	14 (22%)
5	CYC	G	200	-	46,46,46	5.30	26 (56%)	63,67,67	3.88	14 (22%)
5	CYC	e	200	-	46,46,46	5.32	26 (56%)	63,67,67	4.06	13 (20%)
5	CYC	U	201	-	46,46,46	5.30	26 (56%)	63,67,67	4.12	14 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CYC	T	200	-	46,46,46	5.33	26 (56%)	63,67,67	3.88	14 (22%)
5	CYC	X	200	-	46,46,46	5.29	25 (54%)	63,67,67	4.10	15 (23%)
5	CYC	a	200	-	46,46,46	5.34	26 (56%)	63,67,67	4.19	17 (26%)
5	CYC	g	201	-	46,46,46	5.28	26 (56%)	63,67,67	3.99	13 (20%)
5	CYC	Y	200	-	46,46,46	5.22	26 (56%)	63,67,67	4.03	16 (25%)
5	CYC	C	200	-	46,46,46	5.28	25 (54%)	63,67,67	3.92	14 (22%)
5	CYC	H	200	-	46,46,46	5.30	26 (56%)	63,67,67	4.11	19 (30%)
5	CYC	N	200	-	46,46,46	5.26	26 (56%)	63,67,67	4.16	19 (30%)
5	CYC	P	200	-	46,46,46	5.35	24 (52%)	63,67,67	3.86	15 (23%)
5	CYC	h	201	-	46,46,46	5.32	26 (56%)	63,67,67	4.09	14 (22%)
5	CYC	h	200	-	46,46,46	5.32	26 (56%)	63,67,67	3.97	17 (26%)
5	CYC	J	201	-	46,46,46	5.25	26 (56%)	63,67,67	4.18	14 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CYC	k	200	-	-	14/26/74/74	0/4/4/4
5	CYC	U	200	-	-	6/26/74/74	0/4/4/4
5	CYC	I	200	-	-	11/26/74/74	0/4/4/4
5	CYC	T	201	-	-	12/26/74/74	0/4/4/4
5	CYC	D	200	-	-	14/26/74/74	0/4/4/4
5	CYC	c	200	-	-	16/26/74/74	0/4/4/4
5	CYC	j	200	-	-	10/26/74/74	0/4/4/4
5	CYC	W	200	-	-	13/26/74/74	0/4/4/4
5	CYC	V	201	-	-	12/26/74/74	0/4/4/4
5	CYC	k	201	-	-	7/26/74/74	0/4/4/4
5	CYC	Y	201	-	-	19/26/74/74	0/4/4/4
5	CYC	A	200	-	-	18/26/74/74	0/4/4/4
5	CYC	I	201	-	-	10/26/74/74	0/4/4/4
5	CYC	l	201	-	-	15/26/74/74	0/4/4/4
5	CYC	Q	200	-	-	13/26/74/74	0/4/4/4
5	CYC	R	200	-	-	14/26/74/74	0/4/4/4
5	CYC	V	200	-	-	11/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CYC	E	200	-	-	14/26/74/74	0/4/4/4
5	CYC	i	200	-	-	14/26/74/74	0/4/4/4
5	CYC	5	1202	-	-	11/26/74/74	0/4/4/4
5	CYC	i	201	-	-	16/26/74/74	0/4/4/4
5	CYC	f	200	-	-	16/26/74/74	0/4/4/4
5	CYC	5	1201	-	-	8/26/74/74	0/4/4/4
5	CYC	W	201	-	-	10/26/74/74	0/4/4/4
5	CYC	j	201	-	-	9/26/74/74	0/4/4/4
5	CYC	O	200	-	-	16/26/74/74	0/4/4/4
5	CYC	G	201	-	-	15/26/74/74	0/4/4/4
5	CYC	g	200	-	-	7/26/74/74	0/4/4/4
5	CYC	d	200	-	-	16/26/74/74	0/4/4/4
5	CYC	S	200	-	-	16/26/74/74	0/4/4/4
5	CYC	B	200	-	-	18/26/74/74	0/4/4/4
5	CYC	X	201	-	-	13/26/74/74	0/4/4/4
5	CYC	L	201	-	-	14/26/74/74	0/4/4/4
5	CYC	K	201	-	-	14/26/74/74	0/4/4/4
5	CYC	J	200	-	-	8/26/74/74	0/4/4/4
5	CYC	H	201	-	-	16/26/74/74	0/4/4/4
5	CYC	F	200	-	-	14/26/74/74	0/4/4/4
5	CYC	K	200	-	-	11/26/74/74	0/4/4/4
5	CYC	b	200	-	-	11/26/74/74	0/4/4/4
5	CYC	G	200	-	-	11/26/74/74	0/4/4/4
5	CYC	e	200	-	-	17/26/74/74	0/4/4/4
5	CYC	U	201	-	-	17/26/74/74	0/4/4/4
5	CYC	T	200	-	-	8/26/74/74	0/4/4/4
5	CYC	X	200	-	-	13/26/74/74	0/4/4/4
5	CYC	a	200	-	-	21/26/74/74	0/4/4/4
5	CYC	g	201	-	-	15/26/74/74	0/4/4/4
5	CYC	Y	200	-	-	10/26/74/74	0/4/4/4
5	CYC	C	200	-	-	16/26/74/74	0/4/4/4
5	CYC	H	200	-	-	13/26/74/74	0/4/4/4
5	CYC	N	200	-	-	12/26/74/74	0/4/4/4
5	CYC	P	200	-	-	12/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CYC	h	201	-	-	13/26/74/74	0/4/4/4
5	CYC	h	200	-	-	12/26/74/74	0/4/4/4
5	CYC	J	201	-	-	18/26/74/74	0/4/4/4

All (1392) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	c	200	CYC	C2C-C1C	13.78	1.64	1.52
5	a	200	CYC	C2C-C1C	13.68	1.64	1.52
5	f	200	CYC	C2C-C1C	13.62	1.64	1.52
5	R	200	CYC	C2C-C1C	13.61	1.64	1.52
5	b	200	CYC	C2C-C1C	13.55	1.64	1.52
5	H	201	CYC	C2C-C1C	13.52	1.64	1.52
5	i	201	CYC	C2C-C1C	13.48	1.64	1.52
5	h	201	CYC	C2C-C1C	13.46	1.64	1.52
5	k	201	CYC	C2C-C1C	13.45	1.64	1.52
5	h	200	CYC	C2C-C1C	13.33	1.64	1.52
5	Q	200	CYC	C2C-C1C	13.32	1.64	1.52
5	g	200	CYC	C2C-C1C	13.29	1.63	1.52
5	k	200	CYC	C2C-C1C	13.28	1.63	1.52
5	P	200	CYC	C2C-C1C	13.23	1.63	1.52
5	V	201	CYC	C2C-C1C	13.21	1.63	1.52
5	e	200	CYC	C2C-C1C	13.20	1.63	1.52
5	B	200	CYC	C2C-C1C	13.19	1.63	1.52
5	C	200	CYC	C2C-C1C	13.17	1.63	1.52
5	i	200	CYC	C2C-C1C	13.17	1.63	1.52
5	l	201	CYC	C2C-C1C	13.15	1.63	1.52
5	Y	201	CYC	C2C-C1C	13.12	1.63	1.52
5	g	201	CYC	C2C-C1C	13.03	1.63	1.52
5	X	201	CYC	C2C-C1C	12.99	1.63	1.52
5	d	200	CYC	C2C-C1C	12.96	1.63	1.52
5	U	200	CYC	C2C-C1C	12.96	1.63	1.52
5	H	200	CYC	C2C-C1C	12.96	1.63	1.52
5	T	201	CYC	C2C-C1C	12.92	1.63	1.52
5	j	200	CYC	C2C-C1C	12.92	1.63	1.52
5	j	201	CYC	C2C-C1C	12.86	1.63	1.52
5	J	201	CYC	C2C-C1C	12.83	1.63	1.52
5	V	200	CYC	C2C-C1C	12.83	1.63	1.52
5	S	200	CYC	C2C-C1C	12.80	1.63	1.52
5	G	201	CYC	C2C-C1C	12.78	1.63	1.52
5	E	200	CYC	C2C-C1C	12.76	1.63	1.52
5	T	200	CYC	C2C-C1C	12.71	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	200	CYC	C2C-C1C	12.70	1.63	1.52
5	I	200	CYC	C2C-C1C	12.65	1.63	1.52
5	G	200	CYC	C2C-C1C	12.64	1.63	1.52
5	5	1202	CYC	C2C-C1C	12.64	1.63	1.52
5	L	201	CYC	C2C-C1C	12.63	1.63	1.52
5	5	1201	CYC	C2C-C1C	12.56	1.63	1.52
5	N	200	CYC	C2C-C1C	12.52	1.63	1.52
5	F	200	CYC	C2C-C1C	12.52	1.63	1.52
5	U	201	CYC	C2C-C1C	12.51	1.63	1.52
5	O	200	CYC	C2C-C1C	12.47	1.63	1.52
5	X	200	CYC	C2C-C1C	12.46	1.63	1.52
5	K	200	CYC	C2C-C1C	12.34	1.63	1.52
5	J	200	CYC	C2C-C1C	12.34	1.63	1.52
5	W	201	CYC	C2C-C1C	12.25	1.63	1.52
5	I	201	CYC	C2C-C1C	12.14	1.62	1.52
5	d	200	CYC	C1C-NC	12.12	1.53	1.37
5	g	200	CYC	C1C-NC	12.04	1.53	1.37
5	e	200	CYC	C1C-NC	12.04	1.53	1.37
5	H	201	CYC	C1C-NC	12.03	1.53	1.37
5	a	200	CYC	C1C-NC	12.03	1.53	1.37
5	K	201	CYC	C2C-C1C	11.99	1.62	1.52
5	X	201	CYC	C1C-NC	11.98	1.53	1.37
5	U	200	CYC	C1C-NC	11.98	1.53	1.37
5	R	200	CYC	C1C-NC	11.97	1.53	1.37
5	D	200	CYC	C2C-C1C	11.96	1.62	1.52
5	i	200	CYC	C1C-NC	11.96	1.53	1.37
5	i	201	CYC	C1C-NC	11.92	1.53	1.37
5	l	201	CYC	C1C-NC	11.91	1.53	1.37
5	c	200	CYC	C1C-NC	11.91	1.53	1.37
5	P	200	CYC	C1C-NC	11.90	1.53	1.37
5	U	201	CYC	C1C-NC	11.87	1.53	1.37
5	h	200	CYC	C1C-NC	11.87	1.53	1.37
5	k	201	CYC	C1C-NC	11.86	1.53	1.37
5	j	200	CYC	C1C-NC	11.84	1.53	1.37
5	G	200	CYC	C1C-NC	11.83	1.53	1.37
5	I	200	CYC	C1C-NC	11.82	1.53	1.37
5	b	200	CYC	C1C-NC	11.81	1.53	1.37
5	X	200	CYC	C1C-NC	11.81	1.53	1.37
5	5	1202	CYC	C1C-NC	11.80	1.53	1.37
5	h	201	CYC	C1C-NC	11.80	1.53	1.37
5	g	201	CYC	C1C-NC	11.79	1.53	1.37
5	Y	200	CYC	C2C-C1C	11.77	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	201	CYC	C1C-NC	11.76	1.53	1.37
5	T	200	CYC	C1C-NC	11.75	1.53	1.37
5	J	200	CYC	C1C-NC	11.74	1.53	1.37
5	W	201	CYC	C1C-NC	11.73	1.53	1.37
5	T	201	CYC	C1C-NC	11.70	1.53	1.37
5	C	200	CYC	C1C-NC	11.69	1.53	1.37
5	V	201	CYC	C1C-NC	11.64	1.53	1.37
5	j	201	CYC	C1C-NC	11.63	1.53	1.37
5	H	200	CYC	C1C-NC	11.61	1.53	1.37
5	5	1201	CYC	C1C-NC	11.60	1.53	1.37
5	k	200	CYC	C1C-NC	11.60	1.52	1.37
5	K	200	CYC	C1C-NC	11.54	1.52	1.37
5	V	200	CYC	C1C-NC	11.54	1.52	1.37
5	f	200	CYC	C1C-NC	11.53	1.52	1.37
5	E	200	CYC	C1C-NC	11.53	1.52	1.37
5	Y	201	CYC	C1C-NC	11.53	1.52	1.37
5	Y	200	CYC	C1C-NC	11.51	1.52	1.37
5	L	201	CYC	C1C-NC	11.50	1.52	1.37
5	K	201	CYC	C1C-NC	11.48	1.52	1.37
5	B	200	CYC	C1C-NC	11.47	1.52	1.37
5	W	200	CYC	C2C-C1C	11.46	1.62	1.52
5	V	201	CYC	OB-C4B	11.45	1.45	1.23
5	F	200	CYC	C1C-NC	11.44	1.52	1.37
5	V	200	CYC	OB-C4B	11.43	1.45	1.23
5	c	200	CYC	OB-C4B	11.43	1.45	1.23
5	J	200	CYC	OB-C4B	11.43	1.45	1.23
5	k	200	CYC	OB-C4B	11.43	1.45	1.23
5	g	201	CYC	OB-C4B	11.42	1.45	1.23
5	P	200	CYC	OB-C4B	11.42	1.45	1.23
5	H	200	CYC	OB-C4B	11.41	1.45	1.23
5	X	200	CYC	OB-C4B	11.41	1.45	1.23
5	i	200	CYC	OB-C4B	11.41	1.45	1.23
5	R	200	CYC	OB-C4B	11.40	1.45	1.23
5	b	200	CYC	OB-C4B	11.40	1.45	1.23
5	5	1202	CYC	OB-C4B	11.39	1.45	1.23
5	h	201	CYC	OB-C4B	11.39	1.45	1.23
5	T	200	CYC	OB-C4B	11.38	1.45	1.23
5	h	200	CYC	OB-C4B	11.38	1.45	1.23
5	e	200	CYC	OB-C4B	11.38	1.45	1.23
5	J	201	CYC	C1C-NC	11.37	1.52	1.37
5	N	200	CYC	OB-C4B	11.36	1.45	1.23
5	l	201	CYC	OB-C4B	11.35	1.45	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	g	200	CYC	OB-C4B	11.35	1.45	1.23
5	G	200	CYC	OB-C4B	11.35	1.45	1.23
5	H	201	CYC	OB-C4B	11.35	1.45	1.23
5	a	200	CYC	OB-C4B	11.34	1.45	1.23
5	Q	200	CYC	OB-C4B	11.34	1.45	1.23
5	i	201	CYC	OB-C4B	11.34	1.45	1.23
5	k	201	CYC	OB-C4B	11.33	1.45	1.23
5	E	200	CYC	OB-C4B	11.33	1.45	1.23
5	Q	200	CYC	C1C-NC	11.33	1.52	1.37
5	Y	201	CYC	OB-C4B	11.33	1.45	1.23
5	Y	200	CYC	OB-C4B	11.32	1.45	1.23
5	C	200	CYC	OB-C4B	11.32	1.45	1.23
5	U	200	CYC	OB-C4B	11.32	1.45	1.23
5	j	200	CYC	OB-C4B	11.31	1.45	1.23
5	O	200	CYC	OB-C4B	11.31	1.45	1.23
5	I	200	CYC	OB-C4B	11.30	1.45	1.23
5	F	200	CYC	OB-C4B	11.30	1.45	1.23
5	A	200	CYC	OB-C4B	11.29	1.45	1.23
5	K	201	CYC	OB-C4B	11.29	1.45	1.23
5	T	201	CYC	OB-C4B	11.27	1.45	1.23
5	K	200	CYC	OB-C4B	11.27	1.44	1.23
5	j	201	CYC	OB-C4B	11.27	1.44	1.23
5	I	201	CYC	OB-C4B	11.26	1.44	1.23
5	d	200	CYC	OB-C4B	11.26	1.44	1.23
5	5	1201	CYC	OB-C4B	11.25	1.44	1.23
5	A	200	CYC	C1C-NC	11.25	1.52	1.37
5	U	201	CYC	OB-C4B	11.24	1.44	1.23
5	O	200	CYC	C1C-NC	11.24	1.52	1.37
5	W	201	CYC	OB-C4B	11.24	1.44	1.23
5	S	200	CYC	C1C-NC	11.23	1.52	1.37
5	W	200	CYC	OB-C4B	11.23	1.44	1.23
5	f	200	CYC	OB-C4B	11.23	1.44	1.23
5	N	200	CYC	C1C-NC	11.22	1.52	1.37
5	I	201	CYC	C1C-NC	11.21	1.52	1.37
5	X	201	CYC	OB-C4B	11.20	1.44	1.23
5	G	201	CYC	OB-C4B	11.19	1.44	1.23
5	B	200	CYC	OB-C4B	11.18	1.44	1.23
5	D	200	CYC	OB-C4B	11.18	1.44	1.23
5	J	201	CYC	OB-C4B	11.16	1.44	1.23
5	S	200	CYC	OB-C4B	11.14	1.44	1.23
5	L	201	CYC	OB-C4B	11.09	1.44	1.23
5	W	200	CYC	C1C-NC	11.08	1.52	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	200	CYC	C1C-NC	11.05	1.52	1.37
5	Y	200	CYC	C2C-C3C	-10.66	1.25	1.54
5	j	200	CYC	C2C-C3C	-10.48	1.26	1.54
5	J	200	CYC	C2C-C3C	-10.44	1.26	1.54
5	W	200	CYC	C2C-C3C	-10.44	1.26	1.54
5	I	200	CYC	C2C-C3C	-10.43	1.26	1.54
5	5	1201	CYC	C2C-C3C	-10.43	1.26	1.54
5	K	200	CYC	C2C-C3C	-10.37	1.26	1.54
5	U	201	CYC	C2C-C3C	-10.36	1.26	1.54
5	F	200	CYC	C2C-C3C	-10.36	1.26	1.54
5	X	200	CYC	C2C-C3C	-10.32	1.26	1.54
5	W	201	CYC	C2C-C3C	-10.30	1.26	1.54
5	K	201	CYC	C2C-C3C	-10.30	1.26	1.54
5	G	201	CYC	C2C-C3C	-10.28	1.26	1.54
5	S	200	CYC	C2C-C3C	-10.27	1.26	1.54
5	5	1202	CYC	C2C-C3C	-10.26	1.26	1.54
5	a	200	CYC	C2C-C3C	-10.24	1.26	1.54
5	I	201	CYC	C2C-C3C	-10.23	1.26	1.54
5	D	200	CYC	C2C-C3C	-10.22	1.26	1.54
5	d	200	CYC	C2C-C3C	-10.21	1.26	1.54
5	H	201	CYC	C2C-C3C	-10.20	1.26	1.54
5	N	200	CYC	C2C-C3C	-10.20	1.26	1.54
5	X	201	CYC	C2C-C3C	-10.18	1.26	1.54
5	U	200	CYC	C2C-C3C	-10.18	1.26	1.54
5	G	200	CYC	C2C-C3C	-10.18	1.26	1.54
5	J	201	CYC	C2C-C3C	-10.18	1.26	1.54
5	A	200	CYC	C2C-C3C	-10.17	1.27	1.54
5	H	200	CYC	C2C-C3C	-10.17	1.27	1.54
5	k	200	CYC	C2C-C3C	-10.17	1.27	1.54
5	l	201	CYC	C2C-C3C	-10.16	1.27	1.54
5	j	201	CYC	C2C-C3C	-10.16	1.27	1.54
5	Q	200	CYC	C2C-C3C	-10.16	1.27	1.54
5	h	200	CYC	C2C-C3C	-10.15	1.27	1.54
5	T	200	CYC	CHA-C1A	10.15	1.57	1.38
5	f	200	CYC	C2C-C3C	-10.15	1.27	1.54
5	e	200	CYC	C2C-C3C	-10.13	1.27	1.54
5	i	201	CYC	C2C-C3C	-10.11	1.27	1.54
5	T	200	CYC	C2C-C3C	-10.11	1.27	1.54
5	Y	201	CYC	C2C-C3C	-10.10	1.27	1.54
5	L	201	CYC	C2C-C3C	-10.10	1.27	1.54
5	B	200	CYC	C2C-C3C	-10.10	1.27	1.54
5	C	200	CYC	C2C-C3C	-10.10	1.27	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	T	201	CYC	C2C-C3C	-10.09	1.27	1.54
5	h	201	CYC	C2C-C3C	-10.09	1.27	1.54
5	R	200	CYC	C2C-C3C	-10.09	1.27	1.54
5	l	201	CYC	CHB-C4A	10.08	1.64	1.40
5	c	200	CYC	C2C-C3C	-10.07	1.27	1.54
5	V	201	CYC	C2C-C3C	-10.07	1.27	1.54
5	i	200	CYC	C2C-C3C	-10.06	1.27	1.54
5	g	200	CYC	C2C-C3C	-10.05	1.27	1.54
5	b	200	CYC	C2C-C3C	-10.04	1.27	1.54
5	k	201	CYC	C2C-C3C	-10.04	1.27	1.54
5	V	200	CYC	C2C-C3C	-10.03	1.27	1.54
5	g	201	CYC	C2C-C3C	-10.02	1.27	1.54
5	E	200	CYC	C2C-C3C	-10.00	1.27	1.54
5	G	201	CYC	CHB-C4A	10.00	1.63	1.40
5	g	200	CYC	CHA-C1A	9.99	1.57	1.38
5	V	200	CYC	CHA-C1A	9.99	1.57	1.38
5	O	200	CYC	C2C-C3C	-9.97	1.27	1.54
5	i	201	CYC	CHA-C1A	9.96	1.57	1.38
5	O	200	CYC	CHB-C4A	9.95	1.63	1.40
5	i	200	CYC	CHB-C4A	9.95	1.63	1.40
5	O	200	CYC	CHA-C1A	9.95	1.57	1.38
5	i	200	CYC	CHA-C1A	9.92	1.57	1.38
5	P	200	CYC	C2C-C3C	-9.91	1.27	1.54
5	S	200	CYC	CHA-C1A	9.91	1.57	1.38
5	X	200	CYC	CHB-C4A	9.90	1.63	1.40
5	B	200	CYC	CHA-C1A	9.90	1.57	1.38
5	l	201	CYC	CHA-C1A	9.89	1.57	1.38
5	G	200	CYC	CHA-C1A	9.89	1.57	1.38
5	k	201	CYC	CHA-C1A	9.89	1.57	1.38
5	c	200	CYC	CHA-C1A	9.87	1.57	1.38
5	G	201	CYC	CHA-C1A	9.85	1.57	1.38
5	U	200	CYC	CHB-C4A	9.83	1.63	1.40
5	a	200	CYC	CHA-C1A	9.83	1.57	1.38
5	e	200	CYC	CHA-C1A	9.83	1.57	1.38
5	K	200	CYC	CHB-C4A	9.83	1.63	1.40
5	T	200	CYC	CHB-C4A	9.82	1.63	1.40
5	Y	200	CYC	CHA-C1A	9.81	1.57	1.38
5	j	201	CYC	CHA-C1A	9.81	1.57	1.38
5	H	200	CYC	CHB-C4A	9.81	1.63	1.40
5	K	201	CYC	CHB-C4A	9.81	1.63	1.40
5	X	201	CYC	CHA-C1A	9.79	1.57	1.38
5	b	200	CYC	CHA-C1A	9.79	1.57	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	200	CYC	CHA-C1A	9.78	1.57	1.38
5	h	200	CYC	CHA-C1A	9.77	1.57	1.38
5	L	201	CYC	CHA-C1A	9.76	1.57	1.38
5	V	201	CYC	CHA-C1A	9.76	1.57	1.38
5	P	200	CYC	CHA-C1A	9.75	1.57	1.38
5	G	200	CYC	CHB-C4A	9.75	1.63	1.40
5	a	200	CYC	CHB-C4A	9.75	1.63	1.40
5	J	200	CYC	CHB-C4A	9.75	1.63	1.40
5	W	200	CYC	CHB-C4A	9.75	1.63	1.40
5	U	201	CYC	CHA-C1A	9.74	1.57	1.38
5	Q	200	CYC	CHA-C1A	9.72	1.57	1.38
5	R	200	CYC	CHB-C4A	9.72	1.63	1.40
5	W	201	CYC	CHA-C1A	9.72	1.57	1.38
5	Y	201	CYC	CHA-C1A	9.72	1.57	1.38
5	X	200	CYC	CHA-C1A	9.72	1.57	1.38
5	N	200	CYC	CHB-C4A	9.71	1.63	1.40
5	5	1202	CYC	CHA-C1A	9.71	1.57	1.38
5	d	200	CYC	CHB-C4A	9.71	1.63	1.40
5	Y	200	CYC	CHB-C4A	9.71	1.63	1.40
5	H	200	CYC	CHA-C1A	9.71	1.57	1.38
5	W	200	CYC	CHA-C1A	9.70	1.57	1.38
5	B	200	CYC	CHB-C4A	9.68	1.63	1.40
5	d	200	CYC	CHA-C1A	9.68	1.57	1.38
5	I	201	CYC	CHA-C1A	9.67	1.57	1.38
5	j	200	CYC	CHA-C1A	9.65	1.56	1.38
5	h	201	CYC	CHA-C1A	9.65	1.56	1.38
5	W	201	CYC	CHB-C4A	9.65	1.63	1.40
5	T	201	CYC	CHA-C1A	9.64	1.56	1.38
5	h	200	CYC	CHB-C4A	9.64	1.63	1.40
5	K	200	CYC	CHA-C1A	9.64	1.56	1.38
5	k	200	CYC	CHA-C1A	9.64	1.56	1.38
5	Y	201	CYC	CHB-C4A	9.64	1.63	1.40
5	i	201	CYC	CHB-C4A	9.63	1.62	1.40
5	g	200	CYC	CHB-C4A	9.63	1.62	1.40
5	R	200	CYC	CHA-C1A	9.61	1.56	1.38
5	5	1202	CYC	CHB-C4A	9.61	1.62	1.40
5	J	200	CYC	CHA-C1A	9.59	1.56	1.38
5	b	200	CYC	CHB-C4A	9.57	1.62	1.40
5	E	200	CYC	CHB-C4A	9.57	1.62	1.40
5	I	200	CYC	CHA-C1A	9.56	1.56	1.38
5	A	200	CYC	CHB-C4A	9.56	1.62	1.40
5	H	201	CYC	CHA-C1A	9.55	1.56	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	200	CYC	CHB-C4A	9.55	1.62	1.40
5	B	200	CYC	CHA-C4D	9.54	1.62	1.40
5	I	201	CYC	CHB-C4A	9.54	1.62	1.40
5	D	200	CYC	CHB-C4A	9.54	1.62	1.40
5	J	201	CYC	CHA-C1A	9.53	1.56	1.38
5	k	201	CYC	CHB-C4A	9.52	1.62	1.40
5	N	200	CYC	CHA-C1A	9.52	1.56	1.38
5	E	200	CYC	CHA-C1A	9.51	1.56	1.38
5	j	200	CYC	CHB-C4A	9.51	1.62	1.40
5	T	201	CYC	CHB-C4A	9.51	1.62	1.40
5	e	200	CYC	CHB-C4A	9.51	1.62	1.40
5	L	201	CYC	CHB-C4A	9.51	1.62	1.40
5	A	200	CYC	CHA-C1A	9.51	1.56	1.38
5	K	201	CYC	CHA-C1A	9.50	1.56	1.38
5	c	200	CYC	CHB-C4A	9.50	1.62	1.40
5	P	200	CYC	CHA-C4D	9.49	1.61	1.40
5	g	201	CYC	CHA-C1A	9.49	1.56	1.38
5	g	201	CYC	CHB-C4A	9.48	1.62	1.40
5	P	200	CYC	CHB-C4A	9.47	1.62	1.40
5	T	200	CYC	CHA-C4D	9.46	1.61	1.40
5	f	200	CYC	CHA-C1A	9.45	1.56	1.38
5	X	201	CYC	CHB-C4A	9.45	1.62	1.40
5	5	1201	CYC	CHB-C4A	9.44	1.62	1.40
5	5	1201	CYC	CHA-C1A	9.44	1.56	1.38
5	S	200	CYC	CHA-C4D	9.43	1.61	1.40
5	j	201	CYC	CHB-C4A	9.42	1.62	1.40
5	C	200	CYC	CHA-C1A	9.42	1.56	1.38
5	D	200	CYC	CHA-C1A	9.41	1.56	1.38
5	P	200	CYC	CHD-C4C	9.41	1.52	1.36
5	J	201	CYC	CHB-C4A	9.41	1.62	1.40
5	V	200	CYC	CHB-C4A	9.41	1.62	1.40
5	F	200	CYC	CHA-C1A	9.40	1.56	1.38
5	G	200	CYC	CHA-C4D	9.39	1.61	1.40
5	U	201	CYC	CHA-C4D	9.39	1.61	1.40
5	F	200	CYC	CHB-C4A	9.39	1.62	1.40
5	U	201	CYC	CHB-C4A	9.37	1.62	1.40
5	C	200	CYC	CHB-C4A	9.36	1.62	1.40
5	S	200	CYC	CHB-C4A	9.36	1.62	1.40
5	k	200	CYC	CHB-C4A	9.35	1.62	1.40
5	i	201	CYC	CHA-C4D	9.35	1.61	1.40
5	k	201	CYC	CHA-C4D	9.34	1.61	1.40
5	b	200	CYC	CHA-C4D	9.34	1.61	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	200	CYC	CHA-C4D	9.33	1.61	1.40
5	V	200	CYC	CHA-C4D	9.33	1.61	1.40
5	V	201	CYC	CHA-C4D	9.33	1.61	1.40
5	U	201	CYC	CHD-C4C	9.32	1.51	1.36
5	c	200	CYC	CHA-C4D	9.32	1.61	1.40
5	R	200	CYC	CHA-C4D	9.31	1.61	1.40
5	g	200	CYC	CHA-C4D	9.30	1.61	1.40
5	V	201	CYC	CHB-C4A	9.30	1.62	1.40
5	G	201	CYC	CHA-C4D	9.28	1.61	1.40
5	j	201	CYC	CHA-C4D	9.28	1.61	1.40
5	a	200	CYC	CHA-C4D	9.28	1.61	1.40
5	i	200	CYC	CHA-C4D	9.27	1.61	1.40
5	h	201	CYC	CHB-C4A	9.27	1.62	1.40
5	Y	200	CYC	CHA-C4D	9.26	1.61	1.40
5	e	200	CYC	CHA-C4D	9.26	1.61	1.40
5	W	200	CYC	CHA-C4D	9.25	1.61	1.40
5	I	200	CYC	CHB-C4A	9.25	1.62	1.40
5	F	200	CYC	CHA-C4D	9.25	1.61	1.40
5	I	201	CYC	CHA-C4D	9.25	1.61	1.40
5	U	200	CYC	CHA-C4D	9.25	1.61	1.40
5	O	200	CYC	CHA-C4D	9.23	1.61	1.40
5	d	200	CYC	CHD-C4C	9.22	1.51	1.36
5	N	200	CYC	CHA-C4D	9.22	1.61	1.40
5	X	201	CYC	CHA-C4D	9.22	1.61	1.40
5	E	200	CYC	CHA-C4D	9.21	1.61	1.40
5	5	1202	CYC	CHA-C4D	9.20	1.61	1.40
5	J	201	CYC	CHA-C4D	9.20	1.61	1.40
5	H	200	CYC	CHA-C4D	9.19	1.61	1.40
5	R	200	CYC	CHD-C4C	9.19	1.51	1.36
5	i	200	CYC	CHD-C4C	9.17	1.51	1.36
5	L	201	CYC	CHA-C4D	9.17	1.61	1.40
5	O	200	CYC	CHD-C4C	9.15	1.51	1.36
5	H	201	CYC	CHA-C4D	9.15	1.61	1.40
5	Y	201	CYC	CHA-C4D	9.15	1.61	1.40
5	I	200	CYC	CHA-C4D	9.14	1.61	1.40
5	H	201	CYC	CHB-C4A	9.14	1.61	1.40
5	P	200	CYC	C3C-C4C	9.14	1.70	1.50
5	f	200	CYC	CHB-C4A	9.14	1.61	1.40
5	V	200	CYC	CHD-C1D	9.14	1.61	1.40
5	h	200	CYC	CHA-C4D	9.13	1.61	1.40
5	j	200	CYC	CHA-C4D	9.13	1.61	1.40
5	g	201	CYC	CHA-C4D	9.13	1.61	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	200	CYC	CHD-C4C	9.13	1.51	1.36
5	K	200	CYC	CHA-C4D	9.12	1.61	1.40
5	g	200	CYC	C3C-C4C	9.11	1.70	1.50
5	b	200	CYC	CHD-C4C	9.11	1.51	1.36
5	I	201	CYC	C3C-C4C	9.11	1.70	1.50
5	h	201	CYC	CHD-C4C	9.11	1.51	1.36
5	k	200	CYC	CHD-C4C	9.11	1.51	1.36
5	d	200	CYC	CHA-C4D	9.10	1.61	1.40
5	W	201	CYC	CHA-C4D	9.09	1.61	1.40
5	h	201	CYC	CHA-C4D	9.09	1.61	1.40
5	k	201	CYC	CHD-C4C	9.09	1.51	1.36
5	X	200	CYC	CHA-C4D	9.09	1.61	1.40
5	T	200	CYC	C3C-C4C	9.09	1.69	1.50
5	J	200	CYC	CHA-C4D	9.08	1.61	1.40
5	k	201	CYC	C3C-C4C	9.08	1.69	1.50
5	C	200	CYC	CHA-C4D	9.07	1.60	1.40
5	h	201	CYC	CHD-C1D	9.07	1.60	1.40
5	k	200	CYC	CHA-C4D	9.07	1.60	1.40
5	d	200	CYC	C3C-C4C	9.07	1.69	1.50
5	l	201	CYC	CHA-C4D	9.05	1.60	1.40
5	e	200	CYC	CHD-C4C	9.05	1.51	1.36
5	P	200	CYC	CHD-C1D	9.05	1.60	1.40
5	g	200	CYC	CHD-C4C	9.04	1.51	1.36
5	W	200	CYC	CHD-C4C	9.04	1.51	1.36
5	D	200	CYC	CHA-C4D	9.03	1.60	1.40
5	U	201	CYC	C3C-C4C	9.02	1.69	1.50
5	V	200	CYC	CHD-C4C	9.02	1.51	1.36
5	U	201	CYC	CHD-C1D	9.02	1.60	1.40
5	A	200	CYC	CHA-C4D	9.01	1.60	1.40
5	j	201	CYC	C3C-C4C	9.00	1.69	1.50
5	X	201	CYC	C3C-C4C	9.00	1.69	1.50
5	I	201	CYC	CHD-C4C	9.00	1.51	1.36
5	E	200	CYC	CHD-C4C	9.00	1.51	1.36
5	T	201	CYC	CHA-C4D	9.00	1.60	1.40
5	f	200	CYC	CHA-C4D	8.99	1.60	1.40
5	W	200	CYC	C3C-C4C	8.99	1.69	1.50
5	O	200	CYC	C3C-C4C	8.99	1.69	1.50
5	K	201	CYC	CHA-C4D	8.98	1.60	1.40
5	Q	200	CYC	CHD-C1D	8.98	1.60	1.40
5	H	200	CYC	CHD-C4C	8.98	1.51	1.36
5	i	200	CYC	C3C-C4C	8.98	1.69	1.50
5	N	200	CYC	CHD-C4C	8.98	1.51	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	201	CYC	C3C-C4C	8.98	1.69	1.50
5	i	201	CYC	CHD-C4C	8.97	1.51	1.36
5	T	201	CYC	C3C-C4C	8.97	1.69	1.50
5	H	201	CYC	CHD-C4C	8.97	1.51	1.36
5	G	200	CYC	C3C-C4C	8.96	1.69	1.50
5	G	201	CYC	C3C-C4C	8.96	1.69	1.50
5	U	200	CYC	C3C-C4C	8.96	1.69	1.50
5	R	200	CYC	C3C-C4C	8.96	1.69	1.50
5	C	200	CYC	C3C-C4C	8.96	1.69	1.50
5	V	201	CYC	C3C-C4C	8.95	1.69	1.50
5	5	1202	CYC	C3C-C4C	8.95	1.69	1.50
5	h	200	CYC	CHD-C4C	8.95	1.51	1.36
5	k	200	CYC	CHD-C1D	8.94	1.60	1.40
5	L	201	CYC	CHD-C4C	8.93	1.51	1.36
5	i	201	CYC	C3C-C4C	8.93	1.69	1.50
5	I	200	CYC	CHD-C4C	8.92	1.51	1.36
5	N	200	CYC	C3C-C4C	8.92	1.69	1.50
5	c	200	CYC	CHD-C4C	8.92	1.51	1.36
5	C	200	CYC	CHD-C4C	8.92	1.51	1.36
5	A	200	CYC	CHD-C4C	8.91	1.51	1.36
5	X	200	CYC	C3C-C4C	8.90	1.69	1.50
5	H	201	CYC	CHD-C1D	8.90	1.60	1.40
5	b	200	CYC	CHD-C1D	8.88	1.60	1.40
5	H	200	CYC	CHD-C1D	8.88	1.60	1.40
5	B	200	CYC	CHD-C1D	8.88	1.60	1.40
5	E	200	CYC	C3C-C4C	8.88	1.69	1.50
5	5	1201	CYC	CHD-C4C	8.87	1.51	1.36
5	X	200	CYC	CHD-C4C	8.87	1.51	1.36
5	l	201	CYC	C3C-C4C	8.87	1.69	1.50
5	5	1202	CYC	CHD-C4C	8.86	1.51	1.36
5	B	200	CYC	CHD-C4C	8.86	1.51	1.36
5	Q	200	CYC	CHD-C4C	8.86	1.51	1.36
5	l	201	CYC	CHD-C4C	8.86	1.51	1.36
5	W	201	CYC	C3C-C4C	8.86	1.69	1.50
5	Y	201	CYC	C3C-C4C	8.85	1.69	1.50
5	A	200	CYC	CHD-C1D	8.85	1.60	1.40
5	D	200	CYC	CHD-C1D	8.85	1.60	1.40
5	g	201	CYC	C3C-C4C	8.84	1.69	1.50
5	T	201	CYC	CHD-C4C	8.84	1.51	1.36
5	f	200	CYC	CHD-C4C	8.84	1.51	1.36
5	f	200	CYC	C3C-C4C	8.83	1.69	1.50
5	V	201	CYC	CHD-C4C	8.83	1.51	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	201	CYC	C3C-C4C	8.83	1.69	1.50
5	g	201	CYC	CHD-C4C	8.83	1.51	1.36
5	V	200	CYC	C3C-C4C	8.83	1.69	1.50
5	K	200	CYC	C3C-C4C	8.82	1.69	1.50
5	X	201	CYC	CHD-C4C	8.82	1.51	1.36
5	K	201	CYC	C3C-C4C	8.82	1.69	1.50
5	C	200	CYC	CHD-C1D	8.81	1.60	1.40
5	W	200	CYC	CHD-C1D	8.81	1.60	1.40
5	J	201	CYC	CHD-C4C	8.81	1.51	1.36
5	T	200	CYC	CHD-C4C	8.81	1.51	1.36
5	e	200	CYC	C3C-C4C	8.81	1.69	1.50
5	h	200	CYC	C3C-C4C	8.81	1.69	1.50
5	Y	201	CYC	CHD-C4C	8.80	1.51	1.36
5	5	1201	CYC	CHA-C4D	8.80	1.60	1.40
5	c	200	CYC	C3C-C4C	8.80	1.69	1.50
5	D	200	CYC	C3C-C4C	8.79	1.69	1.50
5	G	201	CYC	CHD-C4C	8.79	1.51	1.36
5	G	200	CYC	CHD-C4C	8.79	1.51	1.36
5	K	200	CYC	CHD-C4C	8.78	1.51	1.36
5	h	201	CYC	C3C-C4C	8.78	1.69	1.50
5	A	200	CYC	C3C-C4C	8.78	1.69	1.50
5	b	200	CYC	C3C-C4C	8.77	1.69	1.50
5	O	200	CYC	CHD-C1D	8.77	1.60	1.40
5	I	201	CYC	CHD-C1D	8.76	1.60	1.40
5	N	200	CYC	CHD-C1D	8.76	1.60	1.40
5	d	200	CYC	CHD-C1D	8.76	1.60	1.40
5	T	200	CYC	CHD-C1D	8.75	1.60	1.40
5	g	200	CYC	CHD-C1D	8.75	1.60	1.40
5	E	200	CYC	CHD-C1D	8.75	1.60	1.40
5	B	200	CYC	C3C-C4C	8.74	1.69	1.50
5	J	200	CYC	C3C-C4C	8.73	1.69	1.50
5	a	200	CYC	CHD-C4C	8.73	1.50	1.36
5	k	200	CYC	C3C-C4C	8.71	1.69	1.50
5	D	200	CYC	CHD-C4C	8.71	1.50	1.36
5	W	201	CYC	CHD-C4C	8.69	1.50	1.36
5	i	200	CYC	CHD-C1D	8.69	1.60	1.40
5	J	200	CYC	CHD-C4C	8.69	1.50	1.36
5	j	200	CYC	C3C-C4C	8.69	1.69	1.50
5	U	200	CYC	CHD-C1D	8.68	1.60	1.40
5	j	201	CYC	CHD-C4C	8.66	1.50	1.36
5	h	200	CYC	CHD-C1D	8.66	1.60	1.40
5	I	200	CYC	C3C-C4C	8.66	1.69	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	200	CYC	CHD-C1D	8.65	1.60	1.40
5	Q	200	CYC	C3C-C4C	8.65	1.69	1.50
5	K	201	CYC	CHD-C4C	8.65	1.50	1.36
5	G	200	CYC	CHD-C1D	8.65	1.60	1.40
5	V	201	CYC	CHD-C1D	8.64	1.59	1.40
5	Y	200	CYC	C3C-C4C	8.64	1.69	1.50
5	g	201	CYC	CHD-C1D	8.63	1.59	1.40
5	I	200	CYC	CHD-C1D	8.62	1.59	1.40
5	X	201	CYC	CHD-C1D	8.62	1.59	1.40
5	k	201	CYC	CHD-C1D	8.62	1.59	1.40
5	R	200	CYC	CHD-C1D	8.60	1.59	1.40
5	5	1202	CYC	CHD-C1D	8.59	1.59	1.40
5	j	200	CYC	CHD-C4C	8.59	1.50	1.36
5	S	200	CYC	C3C-C4C	8.59	1.68	1.50
5	i	201	CYC	CHD-C1D	8.58	1.59	1.40
5	Y	200	CYC	CHD-C4C	8.58	1.50	1.36
5	F	200	CYC	C3C-C4C	8.57	1.68	1.50
5	H	201	CYC	C3C-C4C	8.57	1.68	1.50
5	c	200	CYC	CHD-C1D	8.54	1.59	1.40
5	K	200	CYC	CHD-C1D	8.54	1.59	1.40
5	j	201	CYC	CHD-C1D	8.53	1.59	1.40
5	f	200	CYC	CHD-C1D	8.53	1.59	1.40
5	j	200	CYC	CHD-C1D	8.53	1.59	1.40
5	l	201	CYC	CHD-C1D	8.51	1.59	1.40
5	T	201	CYC	CHD-C1D	8.50	1.59	1.40
5	Y	200	CYC	CHD-C1D	8.50	1.59	1.40
5	K	201	CYC	CHD-C1D	8.49	1.59	1.40
5	Y	201	CYC	CHD-C1D	8.49	1.59	1.40
5	L	201	CYC	CHD-C1D	8.48	1.59	1.40
5	G	201	CYC	CHD-C1D	8.47	1.59	1.40
5	J	200	CYC	CHD-C1D	8.46	1.59	1.40
5	H	200	CYC	C3C-C4C	8.46	1.68	1.50
5	X	200	CYC	CHD-C1D	8.43	1.59	1.40
5	J	201	CYC	CHD-C1D	8.43	1.59	1.40
5	a	200	CYC	C3C-C4C	8.42	1.68	1.50
5	W	201	CYC	CHD-C1D	8.40	1.59	1.40
5	a	200	CYC	CHD-C1D	8.37	1.59	1.40
5	F	200	CYC	CHD-C4C	8.33	1.50	1.36
5	5	1201	CYC	C3C-C4C	8.29	1.68	1.50
5	F	200	CYC	CHD-C1D	8.28	1.59	1.40
5	5	1201	CYC	CHD-C1D	8.15	1.58	1.40
5	S	200	CYC	CHD-C1D	8.12	1.58	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	200	CYC	CHD-C4C	8.07	1.49	1.36
5	L	201	CYC	C4B-C3B	-6.51	1.36	1.48
5	G	201	CYC	C4B-C3B	-6.42	1.36	1.48
5	K	201	CYC	C4B-C3B	-6.41	1.36	1.48
5	5	1201	CYC	C4B-C3B	-6.35	1.36	1.48
5	W	200	CYC	C4B-C3B	-6.34	1.36	1.48
5	l	201	CYC	CHB-C1B	6.34	1.53	1.37
5	J	200	CYC	C4B-C3B	-6.32	1.36	1.48
5	Y	200	CYC	C4B-C3B	-6.32	1.36	1.48
5	E	200	CYC	C4B-C3B	-6.32	1.36	1.48
5	K	200	CYC	C4B-C3B	-6.31	1.36	1.48
5	X	200	CYC	C4B-C3B	-6.31	1.36	1.48
5	U	200	CYC	CHB-C1B	6.30	1.53	1.37
5	U	200	CYC	C4B-C3B	-6.28	1.36	1.48
5	j	200	CYC	C4B-C3B	-6.28	1.36	1.48
5	H	200	CYC	CHB-C1B	6.27	1.52	1.37
5	X	200	CYC	CHB-C1B	6.27	1.52	1.37
5	D	200	CYC	C4B-C3B	-6.26	1.36	1.48
5	J	201	CYC	C4B-C3B	-6.24	1.36	1.48
5	H	200	CYC	C4B-C3B	-6.23	1.36	1.48
5	B	200	CYC	C4B-C3B	-6.21	1.36	1.48
5	G	201	CYC	CHB-C1B	6.21	1.52	1.37
5	i	200	CYC	CHB-C1B	6.21	1.52	1.37
5	W	201	CYC	C4B-C3B	-6.19	1.36	1.48
5	T	200	CYC	C4B-C3B	-6.19	1.36	1.48
5	5	1202	CYC	C4B-C3B	-6.18	1.36	1.48
5	T	200	CYC	CHB-C1B	6.17	1.52	1.37
5	I	201	CYC	C4B-C3B	-6.15	1.36	1.48
5	G	200	CYC	CHB-C1B	6.14	1.52	1.37
5	d	200	CYC	C4B-C3B	-6.14	1.36	1.48
5	I	200	CYC	C4B-C3B	-6.14	1.36	1.48
5	G	200	CYC	C4B-C3B	-6.14	1.36	1.48
5	Q	200	CYC	CHB-C1B	6.13	1.52	1.37
5	a	200	CYC	C4B-C3B	-6.13	1.36	1.48
5	h	200	CYC	CHB-C1B	6.12	1.52	1.37
5	T	201	CYC	C4B-C3B	-6.12	1.36	1.48
5	R	200	CYC	C4B-C3B	-6.12	1.36	1.48
5	K	200	CYC	CHB-C1B	6.11	1.52	1.37
5	g	201	CYC	C4B-C3B	-6.11	1.37	1.48
5	O	200	CYC	CHB-C1B	6.10	1.52	1.37
5	E	200	CYC	CHB-C1B	6.10	1.52	1.37
5	d	200	CYC	CHB-C1B	6.10	1.52	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	k	201	CYC	CHB-C1B	6.10	1.52	1.37
5	h	200	CYC	C4B-C3B	-6.09	1.37	1.48
5	J	200	CYC	CHB-C1B	6.09	1.52	1.37
5	K	201	CYC	CHB-C1B	6.09	1.52	1.37
5	X	201	CYC	C4B-C3B	-6.08	1.37	1.48
5	N	200	CYC	CHB-C1B	6.08	1.52	1.37
5	j	200	CYC	CHB-C1B	6.08	1.52	1.37
5	Y	201	CYC	C4B-C3B	-6.08	1.37	1.48
5	X	201	CYC	CHB-C1B	6.08	1.52	1.37
5	5	1202	CYC	CHB-C1B	6.07	1.52	1.37
5	P	200	CYC	CHB-C1B	6.06	1.52	1.37
5	k	201	CYC	C4B-C3B	-6.06	1.37	1.48
5	f	200	CYC	C4B-C3B	-6.05	1.37	1.48
5	g	200	CYC	CHB-C1B	6.05	1.52	1.37
5	b	200	CYC	CHB-C1B	6.04	1.52	1.37
5	A	200	CYC	CHB-C1B	6.03	1.52	1.37
5	W	200	CYC	CHB-C1B	6.03	1.52	1.37
5	Q	200	CYC	C4B-C3B	-6.02	1.37	1.48
5	T	201	CYC	CHB-C1B	6.02	1.52	1.37
5	i	201	CYC	CHB-C1B	6.02	1.52	1.37
5	k	200	CYC	C4B-C3B	-6.02	1.37	1.48
5	g	201	CYC	CHB-C1B	6.02	1.52	1.37
5	c	200	CYC	CHB-C1B	6.01	1.52	1.37
5	I	201	CYC	CHB-C1B	6.01	1.52	1.37
5	a	200	CYC	CHB-C1B	6.01	1.52	1.37
5	e	200	CYC	C4B-C3B	-6.00	1.37	1.48
5	Y	200	CYC	CHB-C1B	6.00	1.52	1.37
5	V	200	CYC	CHB-C1B	6.00	1.52	1.37
5	j	201	CYC	C4B-C3B	-6.00	1.37	1.48
5	e	200	CYC	CHB-C1B	5.99	1.52	1.37
5	L	201	CYC	CHB-C1B	5.99	1.52	1.37
5	i	200	CYC	C4B-C3B	-5.99	1.37	1.48
5	O	200	CYC	C4B-C3B	-5.98	1.37	1.48
5	A	200	CYC	C4B-C3B	-5.97	1.37	1.48
5	I	200	CYC	CHB-C1B	5.96	1.52	1.37
5	g	200	CYC	C4B-C3B	-5.96	1.37	1.48
5	R	200	CYC	CHB-C1B	5.95	1.52	1.37
5	h	201	CYC	C4B-C3B	-5.95	1.37	1.48
5	V	200	CYC	C4B-C3B	-5.95	1.37	1.48
5	C	200	CYC	C4B-C3B	-5.95	1.37	1.48
5	S	200	CYC	CHB-C1B	5.94	1.52	1.37
5	5	1201	CYC	CHB-C1B	5.94	1.52	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	200	CYC	C4B-C3B	-5.94	1.37	1.48
5	B	200	CYC	CHB-C1B	5.94	1.52	1.37
5	P	200	CYC	C4B-C3B	-5.94	1.37	1.48
5	c	200	CYC	C4B-C3B	-5.92	1.37	1.48
5	V	201	CYC	CHB-C1B	5.92	1.52	1.37
5	b	200	CYC	C4B-C3B	-5.92	1.37	1.48
5	Y	201	CYC	CHB-C1B	5.90	1.52	1.37
5	F	200	CYC	CHB-C1B	5.90	1.52	1.37
5	h	201	CYC	CHB-C1B	5.89	1.52	1.37
5	V	201	CYC	C4B-C3B	-5.89	1.37	1.48
5	C	200	CYC	CHB-C1B	5.87	1.51	1.37
5	i	201	CYC	C4B-C3B	-5.87	1.37	1.48
5	U	201	CYC	C4B-C3B	-5.86	1.37	1.48
5	W	201	CYC	CHB-C1B	5.82	1.51	1.37
5	k	200	CYC	CHB-C1B	5.81	1.51	1.37
5	l	201	CYC	C4B-C3B	-5.80	1.37	1.48
5	j	201	CYC	CHB-C1B	5.79	1.51	1.37
5	H	201	CYC	C4B-C3B	-5.79	1.37	1.48
5	J	201	CYC	CHB-C1B	5.79	1.51	1.37
5	D	200	CYC	CHB-C1B	5.78	1.51	1.37
5	F	200	CYC	C4B-C3B	-5.78	1.37	1.48
5	f	200	CYC	CHB-C1B	5.75	1.51	1.37
5	S	200	CYC	C4B-C3B	-5.72	1.37	1.48
5	U	201	CYC	CHB-C1B	5.71	1.51	1.37
5	H	201	CYC	CHB-C1B	5.52	1.51	1.37
5	5	1201	CYC	C1A-C2A	-5.28	1.37	1.45
5	D	200	CYC	C1A-C2A	-5.00	1.37	1.45
5	A	200	CYC	C1A-C2A	-4.97	1.38	1.45
5	S	200	CYC	C1B-C2B	-4.91	1.36	1.45
5	F	200	CYC	C1A-C2A	-4.86	1.38	1.45
5	J	200	CYC	C1A-C2A	-4.85	1.38	1.45
5	F	200	CYC	C1B-C2B	-4.82	1.36	1.45
5	D	200	CYC	C1B-C2B	-4.82	1.36	1.45
5	E	200	CYC	C1A-C2A	-4.82	1.38	1.45
5	J	201	CYC	C1B-C2B	-4.71	1.36	1.45
5	N	200	CYC	C1A-C2A	-4.69	1.38	1.45
5	Y	201	CYC	C1B-C2B	-4.67	1.36	1.45
5	5	1201	CYC	C1B-C2B	-4.67	1.36	1.45
5	Q	200	CYC	C1A-C2A	-4.61	1.38	1.45
5	C	200	CYC	C1B-C2B	-4.61	1.36	1.45
5	K	201	CYC	C1A-C2A	-4.59	1.38	1.45
5	W	201	CYC	C1B-C2B	-4.58	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	X	200	CYC	C1A-C2A	-4.58	1.38	1.45
5	S	200	CYC	C1A-C2A	-4.58	1.38	1.45
5	Q	200	CYC	C1B-C2B	-4.58	1.36	1.45
5	N	200	CYC	C1B-C2B	-4.57	1.36	1.45
5	W	200	CYC	C1A-C2A	-4.57	1.38	1.45
5	l	201	CYC	C1A-C2A	-4.57	1.38	1.45
5	U	200	CYC	C1A-C2A	-4.56	1.38	1.45
5	k	200	CYC	C1B-C2B	-4.55	1.37	1.45
5	H	200	CYC	C1A-C2A	-4.55	1.38	1.45
5	Y	201	CYC	C1A-C2A	-4.55	1.38	1.45
5	j	200	CYC	C1A-C2A	-4.54	1.38	1.45
5	G	201	CYC	C1A-C2A	-4.54	1.38	1.45
5	d	200	CYC	C1A-C2A	-4.53	1.38	1.45
5	f	200	CYC	C1B-C2B	-4.51	1.37	1.45
5	E	200	CYC	C1B-C2B	-4.50	1.37	1.45
5	A	200	CYC	C1B-C2B	-4.49	1.37	1.45
5	C	200	CYC	C1A-C2A	-4.49	1.38	1.45
5	h	200	CYC	C1A-C2A	-4.47	1.38	1.45
5	Y	200	CYC	C1A-C2A	-4.46	1.38	1.45
5	J	201	CYC	C1A-C2A	-4.46	1.38	1.45
5	B	200	CYC	C1B-C2B	-4.45	1.37	1.45
5	J	200	CYC	C1B-C2B	-4.45	1.37	1.45
5	K	200	CYC	C1A-C2A	-4.44	1.38	1.45
5	G	200	CYC	C1A-C2A	-4.43	1.38	1.45
5	H	201	CYC	C1B-C2B	-4.42	1.37	1.45
5	W	201	CYC	C1A-C2A	-4.41	1.38	1.45
5	X	200	CYC	C1B-C2B	-4.39	1.37	1.45
5	V	201	CYC	C1B-C2B	-4.39	1.37	1.45
5	R	200	CYC	C1B-C2B	-4.39	1.37	1.45
5	a	200	CYC	C1B-C2B	-4.38	1.37	1.45
5	Y	200	CYC	C1B-C2B	-4.37	1.37	1.45
5	T	200	CYC	C1A-C2A	-4.36	1.38	1.45
5	h	201	CYC	C1B-C2B	-4.35	1.37	1.45
5	K	200	CYC	C1B-C2B	-4.35	1.37	1.45
5	I	200	CYC	C1A-C2A	-4.34	1.38	1.45
5	L	201	CYC	C1B-C2B	-4.34	1.37	1.45
5	c	200	CYC	C1A-C2A	-4.33	1.39	1.45
5	K	201	CYC	C1B-C2B	-4.33	1.37	1.45
5	5	1202	CYC	CBA-CGA	4.33	1.60	1.50
5	j	201	CYC	C1B-C2B	-4.33	1.37	1.45
5	f	200	CYC	C1A-C2A	-4.32	1.39	1.45
5	g	201	CYC	C1A-C2A	-4.31	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	200	CYC	C1B-C2B	-4.30	1.37	1.45
5	I	201	CYC	C1A-C2A	-4.30	1.39	1.45
5	I	200	CYC	C1B-C2B	-4.29	1.37	1.45
5	P	200	CYC	C1B-C2B	-4.29	1.37	1.45
5	V	200	CYC	C1A-C2A	-4.29	1.39	1.45
5	a	200	CYC	C1A-C2A	-4.28	1.39	1.45
5	D	200	CYC	C1B-NB	-4.28	1.30	1.37
5	c	200	CYC	C1B-C2B	-4.28	1.37	1.45
5	G	200	CYC	C1B-C2B	-4.27	1.37	1.45
5	X	201	CYC	C1B-C2B	-4.27	1.37	1.45
5	R	200	CYC	C1A-C2A	-4.26	1.39	1.45
5	g	200	CYC	C1A-C2A	-4.26	1.39	1.45
5	W	200	CYC	C1B-NB	-4.25	1.30	1.37
5	j	201	CYC	C1A-C2A	-4.25	1.39	1.45
5	i	200	CYC	C1A-C2A	-4.25	1.39	1.45
5	O	200	CYC	C1B-NB	-4.25	1.30	1.37
5	W	200	CYC	C1B-C2B	-4.24	1.37	1.45
5	O	200	CYC	C1A-C2A	-4.24	1.39	1.45
5	H	201	CYC	C1A-C2A	-4.24	1.39	1.45
5	L	201	CYC	C1A-C2A	-4.24	1.39	1.45
5	V	200	CYC	C1B-C2B	-4.23	1.37	1.45
5	O	200	CYC	C1B-C2B	-4.23	1.37	1.45
5	k	201	CYC	C1B-C2B	-4.22	1.37	1.45
5	T	201	CYC	C1A-C2A	-4.22	1.39	1.45
5	X	201	CYC	C1A-C2A	-4.22	1.39	1.45
5	U	201	CYC	C1B-C2B	-4.21	1.37	1.45
5	b	200	CYC	C1A-C2A	-4.20	1.39	1.45
5	T	201	CYC	C1B-C2B	-4.20	1.37	1.45
5	i	201	CYC	C1B-C2B	-4.20	1.37	1.45
5	5	1202	CYC	C1B-C2B	-4.19	1.37	1.45
5	B	200	CYC	C1A-C2A	-4.19	1.39	1.45
5	j	200	CYC	C1B-C2B	-4.19	1.37	1.45
5	h	200	CYC	C1B-C2B	-4.19	1.37	1.45
5	b	200	CYC	C1B-C2B	-4.19	1.37	1.45
5	5	1202	CYC	C1A-C2A	-4.18	1.39	1.45
5	d	200	CYC	C1B-C2B	-4.18	1.37	1.45
5	G	201	CYC	C1B-C2B	-4.17	1.37	1.45
5	I	201	CYC	C1B-C2B	-4.17	1.37	1.45
5	J	200	CYC	C1B-NB	-4.16	1.30	1.37
5	S	200	CYC	C1B-NB	-4.15	1.30	1.37
5	g	201	CYC	C1B-C2B	-4.15	1.37	1.45
5	T	200	CYC	C1B-C2B	-4.13	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	g	200	CYC	C1B-C2B	-4.13	1.37	1.45
5	H	200	CYC	C1B-C2B	-4.12	1.37	1.45
5	i	200	CYC	C1B-C2B	-4.10	1.37	1.45
5	F	200	CYC	C1B-NB	-4.09	1.30	1.37
5	B	200	CYC	C1B-NB	-4.08	1.30	1.37
5	P	200	CYC	C1A-C2A	-4.08	1.39	1.45
5	K	200	CYC	C1B-NB	-4.08	1.30	1.37
5	U	200	CYC	C1B-C2B	-4.07	1.37	1.45
5	N	200	CYC	C1B-NB	-4.07	1.30	1.37
5	k	201	CYC	C1A-C2A	-4.06	1.39	1.45
5	h	201	CYC	C1A-C2A	-4.06	1.39	1.45
5	H	201	CYC	C1B-NB	-4.06	1.30	1.37
5	K	201	CYC	C1B-NB	-4.05	1.30	1.37
5	J	201	CYC	C1B-NB	-4.05	1.30	1.37
5	Y	200	CYC	C1B-NB	-4.05	1.30	1.37
5	G	201	CYC	C1B-NB	-4.04	1.30	1.37
5	5	1201	CYC	C1B-NB	-4.04	1.30	1.37
5	U	201	CYC	CBA-CGA	4.03	1.59	1.50
5	l	201	CYC	C1B-C2B	-4.00	1.37	1.45
5	U	201	CYC	C1A-C2A	-4.00	1.39	1.45
5	U	200	CYC	CBA-CGA	4.00	1.59	1.50
5	T	201	CYC	C1B-NB	-3.99	1.31	1.37
5	A	200	CYC	CBA-CGA	3.99	1.59	1.50
5	i	201	CYC	C1A-C2A	-3.99	1.39	1.45
5	k	200	CYC	C1A-C2A	-3.98	1.39	1.45
5	V	201	CYC	C1A-C2A	-3.98	1.39	1.45
5	h	200	CYC	CBA-CGA	3.98	1.59	1.50
5	R	200	CYC	CBA-CGA	3.97	1.59	1.50
5	V	201	CYC	CBA-CGA	3.97	1.59	1.50
5	N	200	CYC	CBA-CGA	3.97	1.59	1.50
5	U	201	CYC	C1B-NB	-3.96	1.31	1.37
5	c	200	CYC	CBA-CGA	3.95	1.59	1.50
5	g	201	CYC	C1B-NB	-3.95	1.31	1.37
5	d	200	CYC	C1B-NB	-3.95	1.31	1.37
5	h	201	CYC	CBA-CGA	3.95	1.59	1.50
5	W	201	CYC	CBA-CGA	3.95	1.59	1.50
5	e	200	CYC	CBA-CGA	3.94	1.59	1.50
5	I	201	CYC	C1B-NB	-3.94	1.31	1.37
5	f	200	CYC	C1B-NB	-3.94	1.31	1.37
5	a	200	CYC	CBA-CGA	3.94	1.59	1.50
5	E	200	CYC	C1B-NB	-3.94	1.31	1.37
5	j	201	CYC	CBA-CGA	3.93	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	201	CYC	CBA-CGA	3.93	1.59	1.50
5	O	200	CYC	CBA-CGA	3.93	1.59	1.50
5	J	201	CYC	CBA-CGA	3.92	1.59	1.50
5	Q	200	CYC	C1B-NB	-3.92	1.31	1.37
5	e	200	CYC	C1A-C2A	-3.92	1.39	1.45
5	Y	201	CYC	CBA-CGA	3.92	1.59	1.50
5	R	200	CYC	CMC-C2C	3.92	1.61	1.53
5	b	200	CYC	CBA-CGA	3.91	1.59	1.50
5	l	201	CYC	CBA-CGA	3.91	1.59	1.50
5	B	200	CYC	CBA-CGA	3.91	1.59	1.50
5	H	200	CYC	C1B-NB	-3.91	1.31	1.37
5	R	200	CYC	C1B-NB	-3.91	1.31	1.37
5	I	201	CYC	CBA-CGA	3.90	1.59	1.50
5	L	201	CYC	C1B-NB	-3.90	1.31	1.37
5	f	200	CYC	CBA-CGA	3.90	1.59	1.50
5	i	201	CYC	CBA-CGA	3.90	1.59	1.50
5	Y	201	CYC	C1B-NB	-3.90	1.31	1.37
5	P	200	CYC	CBA-CGA	3.89	1.59	1.50
5	W	201	CYC	C1B-NB	-3.89	1.31	1.37
5	g	200	CYC	C1B-NB	-3.89	1.31	1.37
5	X	201	CYC	CBA-CGA	3.89	1.59	1.50
5	g	200	CYC	CMC-C2C	3.88	1.61	1.53
5	K	201	CYC	CBA-CGA	3.88	1.59	1.50
5	G	201	CYC	CBA-CGA	3.88	1.59	1.50
5	G	200	CYC	C1B-NB	-3.88	1.31	1.37
5	X	200	CYC	C1B-NB	-3.88	1.31	1.37
5	T	201	CYC	CBA-CGA	3.87	1.59	1.50
5	T	200	CYC	C1B-NB	-3.87	1.31	1.37
5	j	201	CYC	C1B-NB	-3.86	1.31	1.37
5	P	200	CYC	CMC-C2C	3.86	1.61	1.53
5	l	201	CYC	C1B-NB	-3.86	1.31	1.37
5	g	200	CYC	CBA-CGA	3.86	1.59	1.50
5	d	200	CYC	CBA-CGA	3.85	1.59	1.50
5	I	200	CYC	C1B-NB	-3.85	1.31	1.37
5	j	200	CYC	CBA-CGA	3.85	1.59	1.50
5	H	201	CYC	CBA-CGA	3.85	1.59	1.50
5	T	200	CYC	CBA-CGA	3.85	1.59	1.50
5	k	200	CYC	C1B-NB	-3.84	1.31	1.37
5	g	201	CYC	CBA-CGA	3.84	1.59	1.50
5	k	201	CYC	CBA-CGA	3.84	1.59	1.50
5	G	200	CYC	CBA-CGA	3.84	1.59	1.50
5	H	200	CYC	CBA-CGA	3.83	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	200	CYC	C1B-NB	-3.83	1.31	1.37
5	i	200	CYC	CBA-CGA	3.83	1.59	1.50
5	d	200	CYC	CMC-C2C	3.82	1.61	1.53
5	k	200	CYC	CBA-CGA	3.81	1.59	1.50
5	e	200	CYC	CMC-C2C	3.81	1.61	1.53
5	c	200	CYC	CMC-C2C	3.81	1.61	1.53
5	V	201	CYC	C1B-NB	-3.80	1.31	1.37
5	U	200	CYC	CMC-C2C	3.80	1.61	1.53
5	j	201	CYC	CMC-C2C	3.79	1.61	1.53
5	a	200	CYC	CMC-C2C	3.79	1.61	1.53
5	I	200	CYC	CBA-CGA	3.79	1.59	1.50
5	C	200	CYC	CBA-CGA	3.79	1.59	1.50
5	k	201	CYC	CMC-C2C	3.79	1.61	1.53
5	5	1202	CYC	C1B-NB	-3.79	1.31	1.37
5	C	200	CYC	C1B-NB	-3.79	1.31	1.37
5	g	201	CYC	CMC-C2C	3.79	1.61	1.53
5	j	200	CYC	C1B-NB	-3.78	1.31	1.37
5	X	201	CYC	C1B-NB	-3.78	1.31	1.37
5	T	201	CYC	CMC-C2C	3.78	1.61	1.53
5	J	200	CYC	CBA-CGA	3.77	1.59	1.50
5	V	201	CYC	CMC-C2C	3.77	1.61	1.53
5	X	201	CYC	CMC-C2C	3.77	1.61	1.53
5	V	200	CYC	CMC-C2C	3.76	1.61	1.53
5	5	1202	CYC	CMC-C2C	3.76	1.61	1.53
5	V	200	CYC	C1B-NB	-3.76	1.31	1.37
5	i	200	CYC	CMC-C2C	3.76	1.61	1.53
5	i	201	CYC	C1B-NB	-3.76	1.31	1.37
5	h	201	CYC	C1B-NB	-3.75	1.31	1.37
5	h	200	CYC	C1B-NB	-3.75	1.31	1.37
5	f	200	CYC	CMC-C2C	3.75	1.61	1.53
5	i	201	CYC	CMC-C2C	3.75	1.61	1.53
5	H	201	CYC	CMC-C2C	3.75	1.61	1.53
5	a	200	CYC	C1B-NB	-3.75	1.31	1.37
5	L	201	CYC	CMC-C2C	3.74	1.61	1.53
5	X	200	CYC	CMC-C2C	3.73	1.61	1.53
5	k	201	CYC	C1B-NB	-3.73	1.31	1.37
5	5	1201	CYC	CBA-CGA	3.73	1.59	1.50
5	h	200	CYC	CMC-C2C	3.73	1.61	1.53
5	T	200	CYC	CMC-C2C	3.73	1.61	1.53
5	W	200	CYC	CBA-CGA	3.72	1.59	1.50
5	P	200	CYC	C1B-NB	-3.72	1.31	1.37
5	D	200	CYC	CBA-CGA	3.72	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	V	200	CYC	CBA-CGA	3.72	1.59	1.50
5	U	201	CYC	CMC-C2C	3.72	1.61	1.53
5	O	200	CYC	CMC-C2C	3.71	1.61	1.53
5	e	200	CYC	C1B-NB	-3.71	1.31	1.37
5	h	201	CYC	CMC-C2C	3.71	1.61	1.53
5	b	200	CYC	C1B-NB	-3.69	1.31	1.37
5	G	201	CYC	CMC-C2C	3.69	1.61	1.53
5	U	200	CYC	C1B-NB	-3.69	1.31	1.37
5	E	200	CYC	CBA-CGA	3.69	1.59	1.50
5	c	200	CYC	C1B-NB	-3.68	1.31	1.37
5	5	1201	CYC	CMC-C2C	3.68	1.61	1.53
5	Y	201	CYC	CMC-C2C	3.67	1.61	1.53
5	H	200	CYC	CMC-C2C	3.67	1.60	1.53
5	Y	200	CYC	CBA-CGA	3.66	1.59	1.50
5	Q	200	CYC	CBA-CGA	3.66	1.59	1.50
5	l	201	CYC	CMC-C2C	3.66	1.60	1.53
5	i	200	CYC	C1B-NB	-3.65	1.31	1.37
5	K	200	CYC	CMC-C2C	3.64	1.60	1.53
5	E	200	CYC	CMC-C2C	3.64	1.60	1.53
5	G	200	CYC	CMC-C2C	3.64	1.60	1.53
5	X	200	CYC	CBA-CGA	3.64	1.59	1.50
5	J	201	CYC	CMC-C2C	3.64	1.60	1.53
5	F	200	CYC	CMC-C2C	3.64	1.60	1.53
5	B	200	CYC	CMC-C2C	3.64	1.60	1.53
5	k	200	CYC	CMC-C2C	3.64	1.60	1.53
5	I	201	CYC	CMC-C2C	3.63	1.60	1.53
5	S	200	CYC	CMC-C2C	3.63	1.60	1.53
5	K	200	CYC	CBA-CGA	3.63	1.59	1.50
5	b	200	CYC	CMC-C2C	3.63	1.60	1.53
5	j	200	CYC	CMC-C2C	3.61	1.60	1.53
5	D	200	CYC	CMC-C2C	3.61	1.60	1.53
5	F	200	CYC	CBA-CGA	3.61	1.58	1.50
5	N	200	CYC	CMC-C2C	3.60	1.60	1.53
5	W	200	CYC	CMC-C2C	3.59	1.60	1.53
5	I	200	CYC	CMC-C2C	3.59	1.60	1.53
5	C	200	CYC	CMC-C2C	3.59	1.60	1.53
5	A	200	CYC	CMC-C2C	3.58	1.60	1.53
5	S	200	CYC	CBA-CGA	3.56	1.58	1.50
5	Q	200	CYC	CMC-C2C	3.55	1.60	1.53
5	W	201	CYC	CMC-C2C	3.55	1.60	1.53
5	K	201	CYC	CMC-C2C	3.53	1.60	1.53
5	J	200	CYC	CMC-C2C	3.53	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Y	200	CYC	CMC-C2C	3.42	1.60	1.53
5	l	201	CYC	CAB-C3B	3.20	1.59	1.51
5	Q	200	CYC	CMD-C2D	3.17	1.57	1.50
5	H	201	CYC	CMD-C2D	3.11	1.57	1.50
5	H	200	CYC	CMD-C2D	3.09	1.57	1.50
5	S	200	CYC	CAB-C3B	3.08	1.59	1.51
5	J	201	CYC	C1A-NA	-3.08	1.32	1.38
5	V	200	CYC	CAB-C3B	3.07	1.58	1.51
5	V	201	CYC	C4A-C3A	-3.07	1.39	1.45
5	P	200	CYC	CAB-C3B	3.07	1.58	1.51
5	i	200	CYC	CAB-C3B	3.06	1.58	1.51
5	H	201	CYC	C4A-C3A	-3.06	1.39	1.45
5	B	200	CYC	CMD-C2D	3.05	1.57	1.50
5	X	200	CYC	CAB-C3B	3.05	1.58	1.51
5	f	200	CYC	C4A-C3A	-3.03	1.39	1.45
5	c	200	CYC	CAB-C3B	3.03	1.58	1.51
5	T	200	CYC	CAB-C3B	3.03	1.58	1.51
5	g	200	CYC	CAB-C3B	3.03	1.58	1.51
5	j	201	CYC	CMD-C2D	3.02	1.57	1.50
5	F	200	CYC	CAB-C3B	3.02	1.58	1.51
5	Y	201	CYC	CAB-C3B	3.02	1.58	1.51
5	X	201	CYC	CAB-C3B	3.01	1.58	1.51
5	S	200	CYC	CMD-C2D	3.01	1.56	1.50
5	U	200	CYC	CAB-C3B	3.01	1.58	1.51
5	O	200	CYC	CAB-C3B	3.00	1.58	1.51
5	S	200	CYC	C4A-C3A	-2.99	1.39	1.45
5	i	201	CYC	CAB-C3B	2.99	1.58	1.51
5	N	200	CYC	CAB-C3B	2.99	1.58	1.51
5	b	200	CYC	CAB-C3B	2.99	1.58	1.51
5	j	201	CYC	CAB-C3B	2.99	1.58	1.51
5	V	200	CYC	CMD-C2D	2.99	1.56	1.50
5	d	200	CYC	CAB-C3B	2.99	1.58	1.51
5	D	200	CYC	C1A-NA	-2.99	1.32	1.38
5	G	200	CYC	CAB-C3B	2.98	1.58	1.51
5	S	200	CYC	C1D-ND	-2.98	1.32	1.37
5	W	200	CYC	C1A-NA	-2.98	1.32	1.38
5	H	200	CYC	CAB-C3B	2.98	1.58	1.51
5	J	201	CYC	CMD-C2D	2.97	1.56	1.50
5	K	201	CYC	C1A-NA	-2.97	1.32	1.38
5	X	201	CYC	CMD-C2D	2.97	1.56	1.50
5	e	200	CYC	CAB-C3B	2.96	1.58	1.51
5	b	200	CYC	CMD-C2D	2.96	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	i	201	CYC	CMD-C2D	2.96	1.56	1.50
5	h	200	CYC	CAB-C3B	2.96	1.58	1.51
5	A	200	CYC	CAB-C3B	2.96	1.58	1.51
5	V	201	CYC	CMD-C2D	2.96	1.56	1.50
5	F	200	CYC	C1A-NA	-2.96	1.32	1.38
5	J	200	CYC	CAB-C3B	2.96	1.58	1.51
5	I	201	CYC	CAB-C3B	2.96	1.58	1.51
5	D	200	CYC	CMD-C2D	2.95	1.56	1.50
5	E	200	CYC	CMD-C2D	2.95	1.56	1.50
5	h	201	CYC	CAB-C3B	2.95	1.58	1.51
5	V	201	CYC	CAB-C3B	2.95	1.58	1.51
5	U	201	CYC	CMD-C2D	2.95	1.56	1.50
5	X	201	CYC	CAC-C3C	2.94	1.59	1.54
5	B	200	CYC	CAB-C3B	2.94	1.58	1.51
5	C	200	CYC	C4A-C3A	-2.93	1.39	1.45
5	I	200	CYC	C1A-NA	-2.93	1.32	1.38
5	a	200	CYC	C1D-ND	-2.93	1.32	1.37
5	J	200	CYC	C1A-NA	-2.93	1.32	1.38
5	k	200	CYC	CAB-C3B	2.93	1.58	1.51
5	c	200	CYC	CMD-C2D	2.93	1.56	1.50
5	g	201	CYC	C1A-NA	-2.93	1.32	1.38
5	Y	200	CYC	CAB-C3B	2.93	1.58	1.51
5	L	201	CYC	CMD-C2D	2.92	1.56	1.50
5	C	200	CYC	CMD-C2D	2.92	1.56	1.50
5	W	200	CYC	CAB-C3B	2.92	1.58	1.51
5	U	201	CYC	CAB-C3B	2.91	1.58	1.51
5	R	200	CYC	C1A-NA	-2.91	1.32	1.38
5	k	201	CYC	CMD-C2D	2.91	1.56	1.50
5	C	200	CYC	CAB-C3B	2.91	1.58	1.51
5	k	201	CYC	CAB-C3B	2.91	1.58	1.51
5	5	1201	CYC	C1D-ND	-2.91	1.32	1.37
5	G	201	CYC	CAB-C3B	2.91	1.58	1.51
5	I	200	CYC	CAB-C3B	2.90	1.58	1.51
5	K	200	CYC	CAB-C3B	2.90	1.58	1.51
5	W	201	CYC	C1A-NA	-2.90	1.32	1.38
5	V	200	CYC	C4A-C3A	-2.89	1.39	1.45
5	f	200	CYC	CMD-C2D	2.89	1.56	1.50
5	O	200	CYC	C1A-NA	-2.89	1.32	1.38
5	K	200	CYC	C1A-NA	-2.89	1.32	1.38
5	L	201	CYC	CAB-C3B	2.88	1.58	1.51
5	Q	200	CYC	CAB-C3B	2.88	1.58	1.51
5	f	200	CYC	CAB-C3B	2.88	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	200	CYC	CMD-C2D	2.88	1.56	1.50
5	G	200	CYC	CMD-C2D	2.88	1.56	1.50
5	X	201	CYC	C4A-C3A	-2.88	1.39	1.45
5	R	200	CYC	CAB-C3B	2.87	1.58	1.51
5	j	200	CYC	CAB-C3B	2.87	1.58	1.51
5	Y	200	CYC	CMD-C2D	2.87	1.56	1.50
5	T	201	CYC	CAB-C3B	2.87	1.58	1.51
5	a	200	CYC	CAB-C3B	2.87	1.58	1.51
5	g	201	CYC	CAB-C3B	2.86	1.58	1.51
5	I	200	CYC	CMD-C2D	2.86	1.56	1.50
5	h	201	CYC	CMD-C2D	2.86	1.56	1.50
5	A	200	CYC	C4A-C3A	-2.86	1.39	1.45
5	O	200	CYC	CMD-C2D	2.86	1.56	1.50
5	I	200	CYC	C4A-C3A	-2.86	1.39	1.45
5	5	1201	CYC	C4D-ND	-2.85	1.32	1.37
5	B	200	CYC	C1A-NA	-2.85	1.32	1.38
5	A	200	CYC	CMD-C2D	2.85	1.56	1.50
5	5	1201	CYC	CAB-C3B	2.85	1.58	1.51
5	5	1202	CYC	CAB-C3B	2.85	1.58	1.51
5	U	201	CYC	C4A-C3A	-2.84	1.39	1.45
5	Y	201	CYC	C1A-NA	-2.84	1.32	1.38
5	H	201	CYC	CAB-C3B	2.84	1.58	1.51
5	I	201	CYC	CMD-C2D	2.83	1.56	1.50
5	g	201	CYC	CMD-C2D	2.83	1.56	1.50
5	c	200	CYC	CAC-C3C	2.83	1.59	1.54
5	h	201	CYC	C4A-C3A	-2.83	1.39	1.45
5	l	201	CYC	CMD-C2D	2.82	1.56	1.50
5	k	201	CYC	CAC-C3C	2.82	1.59	1.54
5	N	200	CYC	C1A-NA	-2.82	1.32	1.38
5	G	201	CYC	CMD-C2D	2.81	1.56	1.50
5	T	201	CYC	CMD-C2D	2.81	1.56	1.50
5	Y	201	CYC	CMD-C2D	2.81	1.56	1.50
5	C	200	CYC	C1A-NA	-2.81	1.32	1.38
5	T	201	CYC	C1A-NA	-2.80	1.32	1.38
5	e	200	CYC	CMD-C2D	2.80	1.56	1.50
5	T	200	CYC	CMD-C2D	2.80	1.56	1.50
5	D	200	CYC	CAB-C3B	2.79	1.58	1.51
5	a	200	CYC	CMD-C2D	2.79	1.56	1.50
5	F	200	CYC	C4A-C3A	-2.79	1.39	1.45
5	5	1201	CYC	C1A-NA	-2.79	1.32	1.38
5	X	200	CYC	C1A-NA	-2.79	1.32	1.38
5	d	200	CYC	CMD-C2D	2.79	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	W	200	CYC	CMD-C2D	2.78	1.56	1.50
5	k	200	CYC	CMD-C2D	2.78	1.56	1.50
5	K	201	CYC	CAB-C3B	2.78	1.58	1.51
5	K	201	CYC	CMD-C2D	2.78	1.56	1.50
5	E	200	CYC	C1A-NA	-2.78	1.32	1.38
5	L	201	CYC	CAC-C3C	2.77	1.59	1.54
5	L	201	CYC	C1A-NA	-2.77	1.32	1.38
5	Q	200	CYC	C1A-NA	-2.77	1.32	1.38
5	W	201	CYC	CMD-C2D	2.77	1.56	1.50
5	H	201	CYC	CAC-C3C	2.76	1.59	1.54
5	a	200	CYC	C1A-NA	-2.76	1.32	1.38
5	g	201	CYC	CAC-C3C	2.76	1.59	1.54
5	g	200	CYC	CMD-C2D	2.75	1.56	1.50
5	W	201	CYC	C1D-ND	-2.75	1.33	1.37
5	G	201	CYC	C1A-NA	-2.75	1.32	1.38
5	I	201	CYC	C4A-C3A	-2.75	1.39	1.45
5	Y	201	CYC	CAC-C3C	2.74	1.59	1.54
5	c	200	CYC	C4A-C3A	-2.74	1.39	1.45
5	F	200	CYC	CAC-C3C	2.74	1.59	1.54
5	E	200	CYC	CAB-C3B	2.74	1.58	1.51
5	e	200	CYC	C4A-C3A	-2.74	1.39	1.45
5	U	201	CYC	CAC-C3C	2.74	1.59	1.54
5	W	200	CYC	C4B-NB	-2.74	1.31	1.38
5	L	201	CYC	C1D-ND	-2.74	1.33	1.37
5	f	200	CYC	C1A-NA	-2.74	1.32	1.38
5	H	200	CYC	C1A-NA	-2.74	1.32	1.38
5	T	200	CYC	CAC-C3C	2.73	1.59	1.54
5	f	200	CYC	C1D-ND	-2.73	1.33	1.37
5	J	201	CYC	CAB-C3B	2.72	1.58	1.51
5	b	200	CYC	CAC-C3C	2.72	1.59	1.54
5	P	200	CYC	C4A-C3A	-2.72	1.39	1.45
5	S	200	CYC	C1A-NA	-2.72	1.32	1.38
5	W	201	CYC	CAB-C3B	2.72	1.58	1.51
5	h	200	CYC	CMD-C2D	2.71	1.56	1.50
5	F	200	CYC	C1D-ND	-2.71	1.33	1.37
5	j	200	CYC	C4A-C3A	-2.71	1.40	1.45
5	j	201	CYC	C1D-ND	-2.71	1.33	1.37
5	G	200	CYC	C1A-NA	-2.71	1.32	1.38
5	k	200	CYC	C1A-NA	-2.70	1.32	1.38
5	E	200	CYC	C4A-C3A	-2.70	1.40	1.45
5	c	200	CYC	C1D-ND	-2.70	1.33	1.37
5	g	200	CYC	CAC-C3C	2.70	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	j	201	CYC	C1A-NA	-2.69	1.32	1.38
5	N	200	CYC	CMD-C2D	2.69	1.56	1.50
5	l	201	CYC	C1D-ND	-2.69	1.33	1.37
5	d	200	CYC	C1A-NA	-2.69	1.32	1.38
5	5	1202	CYC	CMD-C2D	2.69	1.56	1.50
5	h	201	CYC	C1A-NA	-2.68	1.32	1.38
5	V	201	CYC	C1A-NA	-2.68	1.32	1.38
5	I	201	CYC	C1A-NA	-2.68	1.32	1.38
5	Y	201	CYC	C4A-C3A	-2.68	1.40	1.45
5	G	200	CYC	CAC-C3C	2.67	1.59	1.54
5	k	201	CYC	C4A-C3A	-2.67	1.40	1.45
5	P	200	CYC	CAC-C3C	2.67	1.59	1.54
5	b	200	CYC	C4A-C3A	-2.67	1.40	1.45
5	D	200	CYC	C4B-NB	-2.66	1.31	1.38
5	T	201	CYC	CAC-C3C	2.66	1.59	1.54
5	d	200	CYC	CAC-C3C	2.66	1.59	1.54
5	Y	201	CYC	C1D-ND	-2.66	1.33	1.37
5	K	200	CYC	CMD-C2D	2.66	1.56	1.50
5	A	200	CYC	C1A-NA	-2.66	1.32	1.38
5	H	200	CYC	CAC-C3C	2.66	1.59	1.54
5	X	200	CYC	CMD-C2D	2.66	1.56	1.50
5	j	201	CYC	CAC-C3C	2.65	1.59	1.54
5	G	201	CYC	C1D-ND	-2.65	1.33	1.37
5	V	200	CYC	CAC-C3C	2.65	1.59	1.54
5	i	201	CYC	C4A-C3A	-2.65	1.40	1.45
5	j	200	CYC	CMD-C2D	2.65	1.56	1.50
5	O	200	CYC	C4B-NB	-2.64	1.31	1.38
5	j	200	CYC	C1A-NA	-2.64	1.33	1.38
5	R	200	CYC	CMD-C2D	2.64	1.56	1.50
5	J	200	CYC	CMD-C2D	2.64	1.56	1.50
5	J	201	CYC	C1D-ND	-2.64	1.33	1.37
5	k	200	CYC	C4A-C3A	-2.64	1.40	1.45
5	j	201	CYC	C4A-C3A	-2.64	1.40	1.45
5	g	201	CYC	C1D-ND	-2.64	1.33	1.37
5	g	200	CYC	C4A-C3A	-2.63	1.40	1.45
5	F	200	CYC	CMD-C2D	2.63	1.56	1.50
5	S	200	CYC	C4B-NB	-2.63	1.31	1.38
5	h	200	CYC	C1A-NA	-2.63	1.33	1.38
5	5	1201	CYC	C4A-C3A	-2.63	1.40	1.45
5	J	201	CYC	C4A-C3A	-2.63	1.40	1.45
5	X	200	CYC	CAC-C3C	2.62	1.59	1.54
5	H	201	CYC	C4B-NB	-2.62	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	i	200	CYC	C1A-NA	-2.62	1.33	1.38
5	H	201	CYC	C1A-NA	-2.62	1.33	1.38
5	U	201	CYC	C1A-NA	-2.62	1.33	1.38
5	a	200	CYC	CAC-C3C	2.62	1.59	1.54
5	5	1202	CYC	C1A-NA	-2.61	1.33	1.38
5	i	200	CYC	C1D-ND	-2.61	1.33	1.37
5	E	200	CYC	C4B-NB	-2.61	1.32	1.38
5	B	200	CYC	C4B-NB	-2.61	1.32	1.38
5	U	200	CYC	CMD-C2D	2.61	1.56	1.50
5	Y	200	CYC	C1A-NA	-2.61	1.33	1.38
5	G	200	CYC	C4A-C3A	-2.61	1.40	1.45
5	e	200	CYC	C1A-NA	-2.61	1.33	1.38
5	V	201	CYC	CAC-C3C	2.61	1.59	1.54
5	e	200	CYC	CAC-C3C	2.61	1.59	1.54
5	O	200	CYC	C1D-ND	-2.60	1.33	1.37
5	l	201	CYC	CAC-C3C	2.60	1.59	1.54
5	h	201	CYC	CAC-C3C	2.60	1.59	1.54
5	V	200	CYC	C1A-NA	-2.60	1.33	1.38
5	K	201	CYC	CAC-C3C	2.60	1.59	1.54
5	T	201	CYC	C1D-ND	-2.60	1.33	1.37
5	X	200	CYC	C4A-C3A	-2.59	1.40	1.45
5	T	200	CYC	C1A-NA	-2.59	1.33	1.38
5	5	1201	CYC	C4B-NB	-2.59	1.32	1.38
5	i	200	CYC	CMD-C2D	2.59	1.56	1.50
5	U	201	CYC	C4B-NB	-2.58	1.32	1.38
5	k	201	CYC	C1A-NA	-2.58	1.33	1.38
5	J	200	CYC	CAC-C3C	2.58	1.58	1.54
5	R	200	CYC	CAC-C3C	2.58	1.58	1.54
5	l	201	CYC	C1A-NA	-2.57	1.33	1.38
5	i	201	CYC	C1A-NA	-2.57	1.33	1.38
5	K	201	CYC	C1D-ND	-2.57	1.33	1.37
5	X	201	CYC	C1A-NA	-2.57	1.33	1.38
5	k	200	CYC	CAC-C3C	2.57	1.58	1.54
5	U	200	CYC	C1A-NA	-2.57	1.33	1.38
5	5	1202	CYC	C1D-ND	-2.57	1.33	1.37
5	c	200	CYC	C1A-NA	-2.56	1.33	1.38
5	L	201	CYC	C4A-C3A	-2.56	1.40	1.45
5	W	200	CYC	CAC-C3C	2.55	1.58	1.54
5	b	200	CYC	C1A-NA	-2.55	1.33	1.38
5	g	201	CYC	C4B-NB	-2.55	1.32	1.38
5	K	201	CYC	C4B-NB	-2.55	1.32	1.38
5	5	1202	CYC	C4A-C3A	-2.55	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	200	CYC	C1A-NA	-2.55	1.33	1.38
5	X	200	CYC	C1D-ND	-2.54	1.33	1.37
5	G	201	CYC	CAC-C3C	2.54	1.58	1.54
5	T	200	CYC	C1D-ND	-2.53	1.33	1.37
5	N	200	CYC	C4B-NB	-2.53	1.32	1.38
5	Q	200	CYC	C4B-NB	-2.53	1.32	1.38
5	I	201	CYC	CAC-C3C	2.52	1.58	1.54
5	f	200	CYC	CAC-C3C	2.52	1.58	1.54
5	R	200	CYC	C1D-ND	-2.52	1.33	1.37
5	I	201	CYC	C4B-NB	-2.52	1.32	1.38
5	G	201	CYC	C4B-NB	-2.52	1.32	1.38
5	i	201	CYC	CAC-C3C	2.52	1.58	1.54
5	F	200	CYC	C4B-NB	-2.52	1.32	1.38
5	h	200	CYC	CAC-C3C	2.52	1.58	1.54
5	O	200	CYC	CAC-C3C	2.51	1.58	1.54
5	B	200	CYC	C1D-ND	-2.51	1.33	1.37
5	H	200	CYC	C4B-NB	-2.51	1.32	1.38
5	G	200	CYC	C4B-NB	-2.51	1.32	1.38
5	K	200	CYC	CAC-C3C	2.51	1.58	1.54
5	W	201	CYC	C4B-NB	-2.50	1.32	1.38
5	T	200	CYC	C4B-NB	-2.50	1.32	1.38
5	Y	200	CYC	C4A-C3A	-2.50	1.40	1.45
5	J	200	CYC	C4B-NB	-2.50	1.32	1.38
5	Q	200	CYC	CAC-C3C	2.50	1.58	1.54
5	T	201	CYC	C4A-C3A	-2.50	1.40	1.45
5	W	201	CYC	CAC-C3C	2.50	1.58	1.54
5	f	200	CYC	C4B-NB	-2.49	1.32	1.38
5	E	200	CYC	CAC-C3C	2.49	1.58	1.54
5	C	200	CYC	C1D-ND	-2.49	1.33	1.37
5	5	1202	CYC	CAC-C3C	2.49	1.58	1.54
5	K	200	CYC	C4B-NB	-2.49	1.32	1.38
5	I	200	CYC	C1D-ND	-2.49	1.33	1.37
5	C	200	CYC	CAC-C3C	2.48	1.58	1.54
5	I	200	CYC	CAC-C3C	2.48	1.58	1.54
5	W	200	CYC	C4A-C3A	-2.48	1.40	1.45
5	J	200	CYC	C1D-ND	-2.48	1.33	1.37
5	D	200	CYC	C4A-C3A	-2.47	1.40	1.45
5	d	200	CYC	C4A-C3A	-2.47	1.40	1.45
5	R	200	CYC	C4B-NB	-2.47	1.32	1.38
5	B	200	CYC	CAC-C3C	2.47	1.58	1.54
5	5	1201	CYC	CMD-C2D	2.47	1.55	1.50
5	Y	200	CYC	C4B-NB	-2.47	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	200	CYC	C4D-ND	-2.46	1.33	1.37
5	C	200	CYC	C4B-NB	-2.46	1.32	1.38
5	T	201	CYC	C4B-NB	-2.45	1.32	1.38
5	A	200	CYC	C1D-ND	-2.45	1.33	1.37
5	V	201	CYC	C4B-NB	-2.45	1.32	1.38
5	A	200	CYC	C4B-NB	-2.45	1.32	1.38
5	Q	200	CYC	C4A-C3A	-2.45	1.40	1.45
5	U	200	CYC	C4B-NB	-2.45	1.32	1.38
5	h	201	CYC	C4B-NB	-2.45	1.32	1.38
5	U	200	CYC	CAC-C3C	2.45	1.58	1.54
5	J	201	CYC	CAC-C3C	2.45	1.58	1.54
5	g	200	CYC	C1A-NA	-2.45	1.33	1.38
5	V	200	CYC	C1D-ND	-2.44	1.33	1.37
5	Y	201	CYC	C4D-ND	-2.44	1.33	1.37
5	j	200	CYC	C1D-ND	-2.44	1.33	1.37
5	S	200	CYC	CAC-C3C	2.44	1.58	1.54
5	d	200	CYC	C4B-NB	-2.44	1.32	1.38
5	K	200	CYC	C4A-C3A	-2.44	1.40	1.45
5	i	201	CYC	C1D-ND	-2.43	1.33	1.37
5	T	200	CYC	C4A-C3A	-2.43	1.40	1.45
5	B	200	CYC	C4A-C3A	-2.43	1.40	1.45
5	j	200	CYC	CAC-C3C	2.42	1.58	1.54
5	N	200	CYC	CAC-C3C	2.42	1.58	1.54
5	g	201	CYC	C4A-C3A	-2.42	1.40	1.45
5	5	1202	CYC	C4B-NB	-2.41	1.32	1.38
5	g	200	CYC	CMA-C3A	2.41	1.55	1.50
5	h	200	CYC	C4B-NB	-2.41	1.32	1.38
5	h	200	CYC	C4A-C3A	-2.41	1.40	1.45
5	U	200	CYC	C4A-C3A	-2.41	1.40	1.45
5	a	200	CYC	CMA-C3A	2.41	1.55	1.50
5	J	201	CYC	C4B-NB	-2.41	1.32	1.38
5	X	201	CYC	C4B-NB	-2.40	1.32	1.38
5	l	201	CYC	C4B-NB	-2.40	1.32	1.38
5	j	201	CYC	C4B-NB	-2.39	1.32	1.38
5	Y	200	CYC	CAC-C3C	2.39	1.58	1.54
5	l	201	CYC	C4D-ND	-2.39	1.33	1.37
5	j	200	CYC	C4B-NB	-2.39	1.32	1.38
5	N	200	CYC	C4A-C3A	-2.39	1.40	1.45
5	a	200	CYC	C4B-NB	-2.39	1.32	1.38
5	g	200	CYC	C4B-NB	-2.38	1.32	1.38
5	A	200	CYC	CAC-C3C	2.38	1.58	1.54
5	L	201	CYC	C4B-NB	-2.38	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	h	200	CYC	C1D-ND	-2.38	1.33	1.37
5	e	200	CYC	C1D-ND	-2.38	1.33	1.37
5	k	201	CYC	C4B-NB	-2.37	1.32	1.38
5	V	200	CYC	C4D-ND	-2.37	1.33	1.37
5	I	200	CYC	C4B-NB	-2.36	1.32	1.38
5	V	200	CYC	C4B-NB	-2.36	1.32	1.38
5	i	201	CYC	C4B-NB	-2.36	1.32	1.38
5	c	200	CYC	C4B-NB	-2.35	1.32	1.38
5	X	200	CYC	C4B-NB	-2.35	1.32	1.38
5	h	201	CYC	C1D-ND	-2.35	1.33	1.37
5	D	200	CYC	C4D-ND	-2.35	1.33	1.37
5	d	200	CYC	C1D-ND	-2.35	1.33	1.37
5	O	200	CYC	C4D-ND	-2.35	1.33	1.37
5	G	200	CYC	C1D-ND	-2.35	1.33	1.37
5	k	201	CYC	C1D-ND	-2.35	1.33	1.37
5	V	201	CYC	C1D-ND	-2.35	1.33	1.37
5	E	200	CYC	C1D-ND	-2.35	1.33	1.37
5	R	200	CYC	C4A-C3A	-2.34	1.40	1.45
5	5	1202	CYC	CMA-C3A	2.34	1.55	1.50
5	Y	201	CYC	C4B-NB	-2.34	1.32	1.38
5	b	200	CYC	C4B-NB	-2.34	1.32	1.38
5	i	200	CYC	C4B-NB	-2.34	1.32	1.38
5	Q	200	CYC	C1D-ND	-2.33	1.33	1.37
5	K	200	CYC	C1D-ND	-2.33	1.33	1.37
5	W	201	CYC	C4A-C3A	-2.33	1.40	1.45
5	U	201	CYC	C1D-ND	-2.33	1.33	1.37
5	X	201	CYC	C1D-ND	-2.33	1.33	1.37
5	5	1201	CYC	C4C-NC	-2.32	1.32	1.37
5	J	200	CYC	C4A-C3A	-2.32	1.40	1.45
5	J	200	CYC	C4D-ND	-2.31	1.33	1.37
5	f	200	CYC	C4D-ND	-2.31	1.33	1.37
5	b	200	CYC	C1D-ND	-2.31	1.33	1.37
5	L	201	CYC	C4D-ND	-2.31	1.33	1.37
5	i	200	CYC	CAC-C3C	2.31	1.58	1.54
5	W	200	CYC	C4D-ND	-2.30	1.33	1.37
5	D	200	CYC	C1D-ND	-2.30	1.33	1.37
5	D	200	CYC	CAC-C3C	2.30	1.58	1.54
5	H	201	CYC	C1D-ND	-2.29	1.33	1.37
5	P	200	CYC	CMA-C3A	2.29	1.55	1.50
5	W	201	CYC	CMA-C3A	2.29	1.55	1.50
5	b	200	CYC	CMA-C3A	2.29	1.55	1.50
5	P	200	CYC	C4B-NB	-2.29	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	201	CYC	CMA-C3A	2.28	1.55	1.50
5	i	200	CYC	C4A-C3A	-2.27	1.40	1.45
5	W	201	CYC	C4D-ND	-2.27	1.33	1.37
5	g	201	CYC	CMA-C3A	2.27	1.55	1.50
5	e	200	CYC	C4B-NB	-2.27	1.32	1.38
5	O	200	CYC	CMA-C3A	2.27	1.55	1.50
5	k	201	CYC	CMA-C3A	2.27	1.55	1.50
5	G	201	CYC	C4D-ND	-2.26	1.34	1.37
5	T	200	CYC	CMA-C3A	2.26	1.55	1.50
5	h	200	CYC	CMA-C3A	2.26	1.55	1.50
5	k	200	CYC	C4B-NB	-2.26	1.32	1.38
5	i	200	CYC	CMA-C3A	2.26	1.55	1.50
5	F	200	CYC	C4D-ND	-2.26	1.34	1.37
5	K	201	CYC	C4A-C3A	-2.26	1.40	1.45
5	W	200	CYC	C1D-ND	-2.26	1.34	1.37
5	H	200	CYC	C4D-ND	-2.25	1.34	1.37
5	a	200	CYC	C4A-C3A	-2.25	1.40	1.45
5	Y	200	CYC	C1D-ND	-2.25	1.34	1.37
5	Q	200	CYC	CMA-C3A	2.25	1.55	1.50
5	k	200	CYC	CMA-C3A	2.25	1.55	1.50
5	K	201	CYC	C4D-ND	-2.24	1.34	1.37
5	Y	200	CYC	C4D-ND	-2.24	1.34	1.37
5	U	200	CYC	CMA-C3A	2.24	1.55	1.50
5	H	200	CYC	C4A-C3A	-2.24	1.41	1.45
5	C	200	CYC	C4D-ND	-2.24	1.34	1.37
5	g	200	CYC	C1D-ND	-2.24	1.34	1.37
5	G	200	CYC	CMA-C3A	2.24	1.55	1.50
5	K	200	CYC	C4D-ND	-2.23	1.34	1.37
5	X	200	CYC	C4D-ND	-2.23	1.34	1.37
5	k	200	CYC	C1D-ND	-2.23	1.34	1.37
5	V	200	CYC	CMA-C3A	2.23	1.55	1.50
5	j	201	CYC	CMA-C3A	2.23	1.55	1.50
5	h	201	CYC	CMA-C3A	2.22	1.55	1.50
5	f	200	CYC	CMA-C3A	2.22	1.55	1.50
5	e	200	CYC	CMA-C3A	2.22	1.55	1.50
5	Q	200	CYC	C4D-ND	-2.22	1.34	1.37
5	U	200	CYC	C1D-ND	-2.22	1.34	1.37
5	l	201	CYC	C4A-C3A	-2.21	1.41	1.45
5	X	201	CYC	CMA-C3A	2.21	1.55	1.50
5	c	200	CYC	CMA-C3A	2.21	1.55	1.50
5	T	201	CYC	CMA-C3A	2.21	1.55	1.50
5	i	201	CYC	CMA-C3A	2.21	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	200	CYC	CMA-C3A	2.20	1.55	1.50
5	g	201	CYC	C4D-ND	-2.20	1.34	1.37
5	T	200	CYC	C4D-ND	-2.20	1.34	1.37
5	N	200	CYC	C1D-ND	-2.20	1.34	1.37
5	a	200	CYC	C4D-ND	-2.20	1.34	1.37
5	j	200	CYC	CMA-C3A	2.19	1.55	1.50
5	A	200	CYC	C4D-ND	-2.18	1.34	1.37
5	G	201	CYC	CMA-C3A	2.17	1.55	1.50
5	H	200	CYC	C1D-ND	-2.17	1.34	1.37
5	N	200	CYC	C4C-NC	-2.17	1.33	1.37
5	J	201	CYC	C4D-ND	-2.17	1.34	1.37
5	B	200	CYC	C4D-ND	-2.16	1.34	1.37
5	I	200	CYC	CMA-C3A	2.16	1.55	1.50
5	X	201	CYC	C4D-ND	-2.16	1.34	1.37
5	I	200	CYC	C4D-ND	-2.16	1.34	1.37
5	T	201	CYC	C4D-ND	-2.15	1.34	1.37
5	j	200	CYC	C4D-ND	-2.15	1.34	1.37
5	L	201	CYC	CMA-C3A	2.15	1.55	1.50
5	j	201	CYC	C4D-ND	-2.14	1.34	1.37
5	U	201	CYC	C4D-ND	-2.14	1.34	1.37
5	E	200	CYC	C4D-ND	-2.14	1.34	1.37
5	l	201	CYC	CMA-C3A	2.13	1.55	1.50
5	R	200	CYC	CMA-C3A	2.13	1.55	1.50
5	N	200	CYC	CMA-C3A	2.13	1.55	1.50
5	5	1202	CYC	C4D-ND	-2.12	1.34	1.37
5	H	200	CYC	CMA-C3A	2.12	1.55	1.50
5	D	200	CYC	C4C-NC	-2.11	1.33	1.37
5	H	201	CYC	C4D-ND	-2.11	1.34	1.37
5	G	201	CYC	C4A-C3A	-2.11	1.41	1.45
5	H	201	CYC	CMA-C3A	2.11	1.55	1.50
5	h	201	CYC	C4D-ND	-2.10	1.34	1.37
5	O	200	CYC	C4A-C3A	-2.09	1.41	1.45
5	V	201	CYC	CMA-C3A	2.09	1.55	1.50
5	G	200	CYC	C4D-ND	-2.09	1.34	1.37
5	I	201	CYC	C1D-ND	-2.08	1.34	1.37
5	Y	201	CYC	CMA-C3A	2.08	1.55	1.50
5	E	200	CYC	CMA-C3A	2.08	1.55	1.50
5	e	200	CYC	C4D-ND	-2.07	1.34	1.37
5	5	1201	CYC	CMA-C3A	2.07	1.55	1.50
5	k	200	CYC	C4D-ND	-2.07	1.34	1.37
5	S	200	CYC	C4C-NC	-2.07	1.33	1.37
5	K	201	CYC	CMA-C3A	2.07	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	200	CYC	CMA-C3A	2.07	1.55	1.50
5	F	200	CYC	CMA-C3A	2.06	1.55	1.50
5	J	201	CYC	CMA-C3A	2.05	1.55	1.50
5	F	200	CYC	C4C-NC	-2.05	1.33	1.37
5	d	200	CYC	CMA-C3A	2.05	1.55	1.50
5	D	200	CYC	CMA-C3A	2.04	1.55	1.50
5	A	200	CYC	C4C-NC	-2.04	1.33	1.37
5	Y	200	CYC	CMA-C3A	2.04	1.55	1.50
5	c	200	CYC	C4D-ND	-2.04	1.34	1.37
5	I	201	CYC	CMA-C3A	2.03	1.54	1.50
5	Q	200	CYC	C4C-NC	-2.01	1.33	1.37
5	h	200	CYC	C4D-ND	-2.01	1.34	1.37
5	b	200	CYC	C4D-ND	-2.00	1.34	1.37

All (810) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	X	200	CYC	OC-C1C-C2C	-22.17	108.55	126.17
5	J	200	CYC	OC-C1C-C2C	-22.07	108.62	126.17
5	K	200	CYC	OC-C1C-C2C	-21.85	108.80	126.17
5	I	201	CYC	OC-C1C-C2C	-21.84	108.81	126.17
5	e	200	CYC	OC-C1C-C2C	-21.31	109.23	126.17
5	W	200	CYC	OC-C1C-C2C	-21.30	109.24	126.17
5	Y	200	CYC	OC-C1C-C2C	-21.14	109.36	126.17
5	K	201	CYC	OC-C1C-C2C	-21.12	109.38	126.17
5	j	200	CYC	OC-C1C-C2C	-20.98	109.49	126.17
5	l	201	CYC	OC-C1C-C2C	-20.97	109.50	126.17
5	G	200	CYC	OC-C1C-C2C	-20.93	109.53	126.17
5	5	1202	CYC	OC-C1C-C2C	-20.88	109.57	126.17
5	J	201	CYC	OC-C1C-C2C	-20.86	109.59	126.17
5	H	200	CYC	OC-C1C-C2C	-20.75	109.67	126.17
5	I	200	CYC	OC-C1C-C2C	-20.75	109.67	126.17
5	5	1201	CYC	OC-C1C-C2C	-20.75	109.67	126.17
5	U	200	CYC	OC-C1C-C2C	-20.60	109.80	126.17
5	X	201	CYC	OC-C1C-C2C	-20.56	109.82	126.17
5	H	201	CYC	OC-C1C-C2C	-20.56	109.82	126.17
5	W	201	CYC	OC-C1C-C2C	-20.56	109.83	126.17
5	T	201	CYC	OC-C1C-C2C	-20.52	109.86	126.17
5	T	200	CYC	OC-C1C-C2C	-20.51	109.86	126.17
5	V	200	CYC	OC-C1C-C2C	-20.51	109.87	126.17
5	Q	200	CYC	OC-C1C-C2C	-20.36	109.98	126.17
5	U	201	CYC	OC-C1C-C2C	-20.34	110.00	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	b	200	CYC	OC-C1C-C2C	-20.28	110.05	126.17
5	f	200	CYC	OC-C1C-C2C	-20.26	110.06	126.17
5	g	200	CYC	OC-C1C-C2C	-20.26	110.06	126.17
5	k	201	CYC	OC-C1C-C2C	-20.24	110.08	126.17
5	F	200	CYC	OC-C1C-C2C	-20.24	110.08	126.17
5	P	200	CYC	OC-C1C-C2C	-20.23	110.09	126.17
5	j	201	CYC	OC-C1C-C2C	-20.22	110.10	126.17
5	Y	201	CYC	OC-C1C-C2C	-20.17	110.14	126.17
5	D	200	CYC	OC-C1C-C2C	-20.16	110.14	126.17
5	i	201	CYC	OC-C1C-C2C	-20.16	110.14	126.17
5	O	200	CYC	OC-C1C-C2C	-20.07	110.22	126.17
5	V	201	CYC	OC-C1C-C2C	-20.06	110.22	126.17
5	a	200	CYC	OC-C1C-C2C	-20.03	110.25	126.17
5	h	200	CYC	OC-C1C-C2C	-20.01	110.27	126.17
5	C	200	CYC	OC-C1C-C2C	-19.89	110.36	126.17
5	k	200	CYC	OC-C1C-C2C	-19.87	110.38	126.17
5	g	201	CYC	OC-C1C-C2C	-19.78	110.44	126.17
5	S	200	CYC	OC-C1C-C2C	-19.76	110.46	126.17
5	h	201	CYC	OC-C1C-C2C	-19.75	110.47	126.17
5	L	201	CYC	OC-C1C-C2C	-19.75	110.47	126.17
5	E	200	CYC	OC-C1C-C2C	-19.70	110.51	126.17
5	A	200	CYC	OC-C1C-C2C	-19.66	110.54	126.17
5	d	200	CYC	OC-C1C-C2C	-19.59	110.59	126.17
5	N	200	CYC	OC-C1C-C2C	-19.56	110.62	126.17
5	c	200	CYC	OC-C1C-C2C	-19.55	110.63	126.17
5	R	200	CYC	OC-C1C-C2C	-19.52	110.65	126.17
5	B	200	CYC	OC-C1C-C2C	-19.38	110.76	126.17
5	i	200	CYC	OC-C1C-C2C	-19.13	110.97	126.17
5	G	201	CYC	OC-C1C-C2C	-18.89	111.15	126.17
5	Y	200	CYC	OC-C1C-NC	-13.42	109.11	124.93
5	A	200	CYC	CHD-C4C-NC	-13.42	108.88	125.63
5	O	200	CYC	CHD-C4C-NC	-13.41	108.89	125.63
5	U	201	CYC	CHD-C4C-NC	-13.34	108.97	125.63
5	S	200	CYC	CHD-C4C-NC	-13.28	109.05	125.63
5	K	200	CYC	OC-C1C-NC	-13.27	109.28	124.93
5	S	200	CYC	OC-C1C-NC	-13.24	109.32	124.93
5	H	200	CYC	CHD-C4C-NC	-13.18	109.18	125.63
5	H	200	CYC	OC-C1C-NC	-13.17	109.41	124.93
5	j	201	CYC	CHD-C4C-NC	-13.15	109.21	125.63
5	f	200	CYC	OC-C1C-NC	-13.11	109.48	124.93
5	J	201	CYC	OC-C1C-NC	-13.01	109.59	124.93
5	B	200	CYC	CHD-C4C-NC	-12.99	109.42	125.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	200	CYC	OC-C1C-NC	-12.98	109.63	124.93
5	k	200	CYC	CHD-C4C-NC	-12.95	109.47	125.63
5	J	200	CYC	OC-C1C-NC	-12.93	109.69	124.93
5	a	200	CYC	CHD-C4C-NC	-12.91	109.52	125.63
5	5	1202	CYC	OC-C1C-NC	-12.86	109.77	124.93
5	b	200	CYC	CHD-C4C-NC	-12.81	109.64	125.63
5	I	201	CYC	OC-C1C-NC	-12.80	109.83	124.93
5	j	200	CYC	OC-C1C-NC	-12.79	109.86	124.93
5	V	200	CYC	CHD-C4C-NC	-12.77	109.69	125.63
5	D	200	CYC	CHD-C4C-NC	-12.77	109.69	125.63
5	h	201	CYC	CHD-C4C-NC	-12.75	109.71	125.63
5	V	201	CYC	CHD-C4C-NC	-12.75	109.72	125.63
5	k	200	CYC	OC-C1C-NC	-12.71	109.94	124.93
5	F	200	CYC	OC-C1C-NC	-12.71	109.95	124.93
5	Q	200	CYC	CHD-C4C-NC	-12.69	109.79	125.63
5	b	200	CYC	OC-C1C-NC	-12.68	109.98	124.93
5	H	201	CYC	OC-C1C-NC	-12.59	110.08	124.93
5	h	200	CYC	OC-C1C-NC	-12.59	110.09	124.93
5	a	200	CYC	OC-C1C-NC	-12.59	110.09	124.93
5	c	200	CYC	CHD-C4C-NC	-12.58	109.93	125.63
5	U	201	CYC	OC-C1C-NC	-12.57	110.11	124.93
5	V	200	CYC	OC-C1C-NC	-12.51	110.18	124.93
5	I	200	CYC	OC-C1C-NC	-12.48	110.22	124.93
5	h	201	CYC	OC-C1C-NC	-12.44	110.27	124.93
5	D	200	CYC	OC-C1C-NC	-12.41	110.30	124.93
5	l	201	CYC	CHD-C4C-NC	-12.41	110.14	125.63
5	K	201	CYC	OC-C1C-NC	-12.38	110.34	124.93
5	G	201	CYC	OC-C1C-NC	-12.37	110.35	124.93
5	i	201	CYC	CHD-C4C-NC	-12.36	110.21	125.63
5	G	201	CYC	CHD-C4C-NC	-12.35	110.21	125.63
5	A	200	CYC	OC-C1C-NC	-12.35	110.37	124.93
5	X	200	CYC	OC-C1C-NC	-12.34	110.38	124.93
5	f	200	CYC	CHD-C4C-NC	-12.32	110.25	125.63
5	K	201	CYC	CHD-C4C-NC	-12.29	110.29	125.63
5	O	200	CYC	OC-C1C-NC	-12.27	110.47	124.93
5	i	201	CYC	OC-C1C-NC	-12.25	110.49	124.93
5	W	201	CYC	CHD-C4C-NC	-12.25	110.34	125.63
5	N	200	CYC	OC-C1C-NC	-12.22	110.53	124.93
5	k	201	CYC	OC-C1C-NC	-12.22	110.53	124.93
5	g	201	CYC	CHD-C4C-NC	-12.17	110.44	125.63
5	L	201	CYC	OC-C1C-NC	-12.15	110.61	124.93
5	X	201	CYC	CHD-C4C-NC	-12.14	110.48	125.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	T	200	CYC	OC-C1C-NC	-12.14	110.62	124.93
5	W	201	CYC	OC-C1C-NC	-12.12	110.64	124.93
5	T	201	CYC	OC-C1C-NC	-12.10	110.67	124.93
5	X	201	CYC	OC-C1C-NC	-12.09	110.67	124.93
5	j	201	CYC	OC-C1C-NC	-12.09	110.68	124.93
5	Y	200	CYC	CHD-C4C-NC	-12.09	110.54	125.63
5	N	200	CYC	CHD-C4C-NC	-12.08	110.55	125.63
5	U	200	CYC	CHD-C4C-NC	-12.06	110.58	125.63
5	V	201	CYC	OC-C1C-NC	-12.06	110.72	124.93
5	W	200	CYC	OC-C1C-NC	-12.05	110.73	124.93
5	c	200	CYC	OC-C1C-NC	-12.04	110.74	124.93
5	L	201	CYC	CHD-C4C-NC	-12.03	110.61	125.63
5	j	200	CYC	CHD-C4C-NC	-12.00	110.64	125.63
5	G	200	CYC	OC-C1C-NC	-11.99	110.80	124.93
5	T	201	CYC	CHD-C4C-NC	-11.97	110.69	125.63
5	e	200	CYC	CHD-C4C-NC	-11.95	110.71	125.63
5	Y	201	CYC	CHD-C4C-NC	-11.94	110.73	125.63
5	i	200	CYC	CHD-C4C-NC	-11.93	110.74	125.63
5	k	201	CYC	CHD-C4C-NC	-11.92	110.75	125.63
5	B	200	CYC	OC-C1C-NC	-11.90	110.91	124.93
5	J	201	CYC	CHD-C4C-NC	-11.89	110.78	125.63
5	S	200	CYC	C1D-CHD-C4C	-11.80	107.62	127.76
5	C	200	CYC	CHD-C4C-NC	-11.78	110.92	125.63
5	R	200	CYC	CHD-C4C-NC	-11.78	110.93	125.63
5	J	200	CYC	CHD-C4C-NC	-11.76	110.95	125.63
5	X	200	CYC	CHD-C4C-NC	-11.76	110.95	125.63
5	d	200	CYC	CHD-C4C-NC	-11.72	111.00	125.63
5	l	201	CYC	OC-C1C-NC	-11.72	111.12	124.93
5	5	1201	CYC	OC-C1C-NC	-11.70	111.13	124.93
5	P	200	CYC	OC-C1C-NC	-11.69	111.15	124.93
5	R	200	CYC	OC-C1C-NC	-11.66	111.18	124.93
5	E	200	CYC	CHD-C4C-NC	-11.65	111.09	125.63
5	h	200	CYC	CHD-C4C-NC	-11.64	111.10	125.63
5	Y	201	CYC	OC-C1C-NC	-11.63	111.21	124.93
5	H	201	CYC	CHD-C4C-NC	-11.63	111.12	125.63
5	g	201	CYC	OC-C1C-NC	-11.60	111.25	124.93
5	i	200	CYC	C1D-CHD-C4C	-11.59	107.98	127.76
5	I	201	CYC	CHD-C4C-NC	-11.54	111.23	125.63
5	g	200	CYC	OC-C1C-NC	-11.53	111.34	124.93
5	C	200	CYC	OC-C1C-NC	-11.52	111.36	124.93
5	e	200	CYC	OC-C1C-NC	-11.46	111.42	124.93
5	5	1202	CYC	CHD-C4C-NC	-11.45	111.34	125.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	i	200	CYC	OC-C1C-NC	-11.44	111.45	124.93
5	U	200	CYC	OC-C1C-NC	-11.44	111.45	124.93
5	E	200	CYC	OC-C1C-NC	-11.43	111.46	124.93
5	a	200	CYC	C1D-CHD-C4C	-11.36	108.37	127.76
5	d	200	CYC	OC-C1C-NC	-11.31	111.59	124.93
5	J	201	CYC	C1D-CHD-C4C	-11.25	108.56	127.76
5	F	200	CYC	CHD-C4C-NC	-11.24	111.60	125.63
5	I	200	CYC	CHD-C4C-NC	-11.23	111.61	125.63
5	i	201	CYC	C1D-CHD-C4C	-11.21	108.63	127.76
5	R	200	CYC	C1D-CHD-C4C	-11.08	108.85	127.76
5	g	200	CYC	CHD-C4C-NC	-11.05	111.83	125.63
5	W	200	CYC	CHD-C4C-NC	-11.04	111.85	125.63
5	T	200	CYC	CHD-C4C-NC	-11.01	111.89	125.63
5	K	200	CYC	CHD-C4C-NC	-10.99	111.91	125.63
5	G	200	CYC	CHD-C4C-NC	-10.84	112.10	125.63
5	P	200	CYC	CHD-C4C-NC	-10.73	112.23	125.63
5	j	201	CYC	C1D-CHD-C4C	-10.44	109.94	127.76
5	U	200	CYC	C1D-CHD-C4C	-10.01	110.68	127.76
5	V	201	CYC	C1D-CHD-C4C	-9.99	110.70	127.76
5	D	200	CYC	C2C-C1C-NC	-9.71	100.20	108.29
5	Y	201	CYC	C1D-CHD-C4C	-9.69	111.21	127.76
5	I	201	CYC	C1D-CHD-C4C	-9.68	111.24	127.76
5	X	201	CYC	C1D-CHD-C4C	-9.59	111.39	127.76
5	A	200	CYC	C1D-CHD-C4C	-9.54	111.48	127.76
5	k	201	CYC	C1D-CHD-C4C	-9.47	111.60	127.76
5	G	201	CYC	C1D-CHD-C4C	-9.45	111.64	127.76
5	H	201	CYC	C1B-CHB-C4A	-9.41	104.95	128.06
5	b	200	CYC	C1D-CHD-C4C	-9.39	111.74	127.76
5	O	200	CYC	C1D-CHD-C4C	-9.37	111.76	127.76
5	f	200	CYC	C1B-CHB-C4A	-9.31	105.19	128.06
5	B	200	CYC	C1C-NC-C4C	-9.26	101.80	113.41
5	f	200	CYC	C1D-CHD-C4C	-9.20	112.06	127.76
5	e	200	CYC	C1D-CHD-C4C	-9.19	112.08	127.76
5	j	200	CYC	C1D-CHD-C4C	-9.17	112.10	127.76
5	N	200	CYC	C1C-NC-C4C	-9.09	102.01	113.41
5	l	201	CYC	C1D-CHD-C4C	-9.09	112.25	127.76
5	X	200	CYC	C1D-CHD-C4C	-9.07	112.29	127.76
5	K	201	CYC	C1D-CHD-C4C	-9.06	112.30	127.76
5	A	200	CYC	C1C-NC-C4C	-9.05	102.06	113.41
5	5	1201	CYC	CHD-C4C-NC	-9.01	114.39	125.63
5	T	201	CYC	C1D-CHD-C4C	-8.95	112.48	127.76
5	c	200	CYC	C1D-CHD-C4C	-8.93	112.51	127.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	U	201	CYC	C1B-CHB-C4A	-8.86	106.30	128.06
5	Q	200	CYC	C1C-NC-C4C	-8.76	102.42	113.41
5	g	201	CYC	C4D-CHA-C1A	-8.72	109.18	128.22
5	D	200	CYC	C1C-NC-C4C	-8.67	102.53	113.41
5	E	200	CYC	C1D-CHD-C4C	-8.55	113.17	127.76
5	Y	201	CYC	C1C-NC-C4C	-8.53	102.71	113.41
5	R	200	CYC	C4D-CHA-C1A	-8.41	109.85	128.22
5	N	200	CYC	C2C-C1C-NC	-8.37	101.32	108.29
5	I	201	CYC	C1C-NC-C4C	-8.36	102.92	113.41
5	W	201	CYC	C1D-CHD-C4C	-8.35	113.50	127.76
5	5	1201	CYC	C1C-NC-C4C	-8.32	102.98	113.41
5	h	200	CYC	C1D-CHD-C4C	-8.31	113.58	127.76
5	d	200	CYC	C1D-CHD-C4C	-8.29	113.61	127.76
5	V	201	CYC	C1B-CHB-C4A	-8.21	107.89	128.06
5	h	201	CYC	C1B-CHB-C4A	-8.20	107.92	128.06
5	h	201	CYC	C4D-CHA-C1A	-8.19	110.34	128.22
5	N	200	CYC	C1D-CHD-C4C	-8.17	113.81	127.76
5	V	201	CYC	C1C-NC-C4C	-8.10	103.24	113.41
5	H	201	CYC	C1C-NC-C4C	-8.07	103.29	113.41
5	L	201	CYC	C1D-CHD-C4C	-8.04	114.03	127.76
5	c	200	CYC	C1B-CHB-C4A	-8.01	108.39	128.06
5	A	200	CYC	C2C-C1C-NC	-7.95	101.67	108.29
5	g	201	CYC	C1D-CHD-C4C	-7.94	114.20	127.76
5	5	1202	CYC	C1D-CHD-C4C	-7.83	114.40	127.76
5	f	200	CYC	C1C-NC-C4C	-7.81	103.61	113.41
5	L	201	CYC	C4D-CHA-C1A	-7.76	111.28	128.22
5	Q	200	CYC	C1D-CHD-C4C	-7.73	114.57	127.76
5	W	200	CYC	C2C-C1C-NC	-7.72	101.86	108.29
5	J	200	CYC	C1D-CHD-C4C	-7.68	114.66	127.76
5	Y	200	CYC	C1D-CHD-C4C	-7.65	114.71	127.76
5	H	201	CYC	C1D-CHD-C4C	-7.60	114.79	127.76
5	H	200	CYC	C1D-CHD-C4C	-7.59	114.80	127.76
5	J	201	CYC	C4D-CHA-C1A	-7.58	111.66	128.22
5	B	200	CYC	C4D-CHA-C1A	-7.55	111.73	128.22
5	a	200	CYC	C4D-CHA-C1A	-7.54	111.75	128.22
5	V	200	CYC	C1C-NC-C4C	-7.54	103.95	113.41
5	O	200	CYC	C2C-C1C-NC	-7.54	102.01	108.29
5	k	200	CYC	C1D-CHD-C4C	-7.54	114.90	127.76
5	I	200	CYC	C1D-CHD-C4C	-7.51	114.94	127.76
5	S	200	CYC	C1C-NC-C4C	-7.50	104.00	113.41
5	a	200	CYC	C1C-NC-C4C	-7.49	104.02	113.41
5	b	200	CYC	C1C-NC-C4C	-7.47	104.04	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	f	200	CYC	C4D-CHA-C1A	-7.46	111.92	128.22
5	P	200	CYC	C1D-CHD-C4C	-7.42	115.09	127.76
5	g	200	CYC	C1B-CHB-C4A	-7.40	109.88	128.06
5	X	201	CYC	C1B-CHB-C4A	-7.39	109.90	128.06
5	O	200	CYC	C1C-NC-C4C	-7.35	104.19	113.41
5	j	201	CYC	C1C-NC-C4C	-7.31	104.24	113.41
5	B	200	CYC	C1D-CHD-C4C	-7.29	115.31	127.76
5	j	201	CYC	C4D-CHA-C1A	-7.28	112.32	128.22
5	V	200	CYC	C1B-CHB-C4A	-7.23	110.30	128.06
5	C	200	CYC	C1D-CHD-C4C	-7.23	115.42	127.76
5	D	200	CYC	C1D-CHD-C4C	-7.19	115.49	127.76
5	g	200	CYC	C1D-CHD-C4C	-7.17	115.53	127.76
5	T	201	CYC	C4D-CHA-C1A	-7.16	112.59	128.22
5	W	201	CYC	C4D-CHA-C1A	-7.10	112.71	128.22
5	F	200	CYC	C1D-CHD-C4C	-7.08	115.67	127.76
5	K	200	CYC	C1D-CHD-C4C	-7.07	115.69	127.76
5	T	200	CYC	C1D-CHD-C4C	-7.04	115.75	127.76
5	I	201	CYC	C2C-C1C-NC	-7.03	102.44	108.29
5	O	200	CYC	C4D-CHA-C1A	-7.03	112.88	128.22
5	U	201	CYC	C4D-CHA-C1A	-6.93	113.09	128.22
5	i	201	CYC	C4D-CHA-C1A	-6.89	113.17	128.22
5	C	200	CYC	C1B-CHB-C4A	-6.88	111.16	128.06
5	G	201	CYC	C4D-CHA-C1A	-6.85	113.25	128.22
5	P	200	CYC	C1B-CHB-C4A	-6.85	111.24	128.06
5	U	201	CYC	C1D-CHD-C4C	-6.84	116.08	127.76
5	b	200	CYC	C1B-CHB-C4A	-6.83	111.29	128.06
5	L	201	CYC	C1C-NC-C4C	-6.76	104.93	113.41
5	h	201	CYC	C1C-NC-C4C	-6.74	104.95	113.41
5	K	201	CYC	C4D-CHA-C1A	-6.70	113.59	128.22
5	i	201	CYC	C1B-CHB-C4A	-6.69	111.62	128.06
5	c	200	CYC	C1C-NC-C4C	-6.68	105.03	113.41
5	5	1202	CYC	C1B-CHB-C4A	-6.67	111.67	128.06
5	e	200	CYC	C1B-CHB-C4A	-6.65	111.72	128.06
5	K	201	CYC	C1C-NC-C4C	-6.63	105.09	113.41
5	d	200	CYC	C4D-CHA-C1A	-6.62	113.77	128.22
5	T	201	CYC	C1C-NC-C4C	-6.61	105.12	113.41
5	i	200	CYC	C1C-NC-C4C	-6.59	105.15	113.41
5	j	200	CYC	C1B-CHB-C4A	-6.57	111.92	128.06
5	V	201	CYC	C4D-CHA-C1A	-6.57	113.88	128.22
5	G	200	CYC	C1D-CHD-C4C	-6.57	116.55	127.76
5	h	200	CYC	C1C-NC-C4C	-6.54	105.20	113.41
5	h	201	CYC	C1D-CHD-C4C	-6.49	116.68	127.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	200	CYC	C1C-NC-C4C	-6.49	105.27	113.41
5	e	200	CYC	C4D-CHA-C1A	-6.43	114.17	128.22
5	H	201	CYC	C4D-CHA-C1A	-6.42	114.20	128.22
5	c	200	CYC	C4D-CHA-C1A	-6.41	114.22	128.22
5	W	200	CYC	C1C-NC-C4C	-6.41	105.37	113.41
5	j	201	CYC	C2C-C1C-NC	-6.38	102.97	108.29
5	B	200	CYC	C2C-C1C-NC	-6.37	102.98	108.29
5	C	200	CYC	C4D-CHA-C1A	-6.32	114.42	128.22
5	E	200	CYC	C1B-CHB-C4A	-6.30	112.58	128.06
5	G	201	CYC	C1C-NC-C4C	-6.27	105.55	113.41
5	Y	201	CYC	C4D-CHA-C1A	-6.23	114.62	128.22
5	K	201	CYC	C2C-C1C-NC	-6.21	103.11	108.29
5	R	200	CYC	C1C-NC-C4C	-6.21	105.62	113.41
5	k	200	CYC	C1C-NC-C4C	-6.18	105.65	113.41
5	P	200	CYC	C1C-NC-C4C	-6.18	105.66	113.41
5	Y	201	CYC	C2C-C1C-NC	-6.15	103.17	108.29
5	C	200	CYC	C1C-NC-C4C	-6.12	105.73	113.41
5	S	200	CYC	CAB-C3B-C4B	6.11	130.81	121.37
5	S	200	CYC	C1B-CHB-C4A	-6.10	113.09	128.06
5	E	200	CYC	C1C-NC-C4C	-6.07	105.79	113.41
5	W	201	CYC	C2C-C1C-NC	-6.07	103.23	108.29
5	i	201	CYC	C1C-NC-C4C	-6.05	105.82	113.41
5	g	201	CYC	C1C-NC-C4C	-6.04	105.83	113.41
5	V	201	CYC	C2C-C1C-NC	-6.00	103.29	108.29
5	e	200	CYC	C1C-NC-C4C	-5.98	105.91	113.41
5	g	200	CYC	C1C-NC-C4C	-5.97	105.91	113.41
5	T	200	CYC	C1C-NC-C4C	-5.95	105.94	113.41
5	5	1202	CYC	C4D-CHA-C1A	-5.95	115.22	128.22
5	F	200	CYC	C4D-CHA-C1A	-5.95	115.23	128.22
5	W	201	CYC	C1C-NC-C4C	-5.94	105.96	113.41
5	I	200	CYC	C4D-CHA-C1A	-5.93	115.27	128.22
5	b	200	CYC	C4D-CHA-C1A	-5.88	115.37	128.22
5	5	1201	CYC	C4D-CHA-C1A	-5.87	115.41	128.22
5	G	201	CYC	C2C-C1C-NC	-5.85	103.42	108.29
5	k	201	CYC	C1C-NC-C4C	-5.83	106.09	113.41
5	G	200	CYC	C1C-NC-C4C	-5.83	106.10	113.41
5	Y	200	CYC	C1C-NC-C4C	-5.81	106.12	113.41
5	A	200	CYC	C1B-CHB-C4A	-5.79	113.85	128.06
5	F	200	CYC	C1B-CHB-C4A	-5.77	113.89	128.06
5	j	201	CYC	C1B-CHB-C4A	-5.76	113.90	128.06
5	I	200	CYC	C1B-CHB-C4A	-5.76	113.90	128.06
5	I	201	CYC	C1B-CHB-C4A	-5.76	113.91	128.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	l	201	CYC	C4D-CHA-C1A	-5.76	115.64	128.22
5	X	200	CYC	C4D-CHA-C1A	-5.73	115.72	128.22
5	X	201	CYC	C4D-CHA-C1A	-5.70	115.78	128.22
5	k	200	CYC	C1B-CHB-C4A	-5.69	114.08	128.06
5	k	201	CYC	C4D-CHA-C1A	-5.69	115.80	128.22
5	V	200	CYC	C1D-CHD-C4C	-5.65	118.12	127.76
5	i	200	CYC	C4D-CHA-C1A	-5.62	115.95	128.22
5	k	200	CYC	C4D-CHA-C1A	-5.60	116.00	128.22
5	l	201	CYC	C1C-NC-C4C	-5.59	106.39	113.41
5	J	200	CYC	C1C-NC-C4C	-5.57	106.42	113.41
5	F	200	CYC	C1C-NC-C4C	-5.56	106.44	113.41
5	V	200	CYC	C4D-CHA-C1A	-5.55	116.10	128.22
5	Q	200	CYC	C4D-CHA-C1A	-5.51	116.20	128.22
5	j	200	CYC	C4D-CHA-C1A	-5.50	116.22	128.22
5	5	1201	CYC	C2C-C1C-NC	-5.48	103.72	108.29
5	f	200	CYC	C2C-C1C-NC	-5.45	103.75	108.29
5	5	1201	CYC	C1B-CHB-C4A	-5.45	114.68	128.06
5	h	200	CYC	C4D-CHA-C1A	-5.42	116.39	128.22
5	D	200	CYC	C1B-CHB-C4A	-5.42	114.76	128.06
5	F	200	CYC	CAB-C3B-C4B	5.39	129.71	121.37
5	d	200	CYC	C1C-NC-C4C	-5.38	106.66	113.41
5	S	200	CYC	C2C-C1C-NC	-5.38	103.81	108.29
5	J	201	CYC	C1C-NC-C4C	-5.36	106.69	113.41
5	k	201	CYC	C1B-CHB-C4A	-5.34	114.94	128.06
5	K	200	CYC	C1C-NC-C4C	-5.33	106.72	113.41
5	K	200	CYC	C2C-C3C-C4C	5.33	109.32	101.34
5	I	200	CYC	C1C-NC-C4C	-5.32	106.73	113.41
5	j	200	CYC	C1C-NC-C4C	-5.32	106.73	113.41
5	L	201	CYC	C2C-C1C-NC	-5.31	103.87	108.29
5	5	1202	CYC	C1C-NC-C4C	-5.30	106.76	113.41
5	U	201	CYC	C1C-NC-C4C	-5.30	106.76	113.41
5	X	200	CYC	C1C-NC-C4C	-5.28	106.78	113.41
5	l	201	CYC	CAB-C3B-C4B	5.26	129.51	121.37
5	T	200	CYC	C2C-C3C-C4C	5.24	109.19	101.34
5	E	200	CYC	C2C-C1C-NC	-5.24	103.93	108.29
5	S	200	CYC	C4D-CHA-C1A	-5.23	116.79	128.22
5	5	1202	CYC	C2C-C3C-C4C	5.20	109.14	101.34
5	g	201	CYC	C1B-CHB-C4A	-5.19	115.32	128.06
5	Q	200	CYC	CMD-C2D-C1D	5.18	133.16	125.62
5	T	200	CYC	C4D-CHA-C1A	-5.18	116.92	128.22
5	G	200	CYC	C1B-CHB-C4A	-5.16	115.39	128.06
5	D	200	CYC	C4D-CHA-C1A	-5.12	117.04	128.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	V	200	CYC	C2C-C1C-NC	-5.12	104.03	108.29
5	U	200	CYC	C4D-CHA-C1A	-5.10	117.09	128.22
5	G	200	CYC	C4D-CHA-C1A	-5.10	117.09	128.22
5	G	200	CYC	C2C-C3C-C4C	5.08	108.95	101.34
5	X	201	CYC	C1C-NC-C4C	-5.04	107.08	113.41
5	K	200	CYC	C4D-CHA-C1A	-5.02	117.25	128.22
5	5	1201	CYC	C2C-C3C-C4C	4.99	108.81	101.34
5	i	200	CYC	C2C-C3C-C4C	4.96	108.76	101.34
5	g	200	CYC	C4D-CHA-C1A	-4.91	117.49	128.22
5	i	201	CYC	C2C-C3C-C4C	4.91	108.69	101.34
5	Y	200	CYC	C1B-CHB-C4A	-4.89	116.05	128.06
5	J	200	CYC	C4D-CHA-C1A	-4.89	117.55	128.22
5	l	201	CYC	C2C-C3C-C4C	4.89	108.66	101.34
5	A	200	CYC	C4D-CHA-C1A	-4.87	117.59	128.22
5	g	201	CYC	C2C-C3C-C4C	4.85	108.60	101.34
5	a	200	CYC	C1B-CHB-C4A	-4.84	116.18	128.06
5	k	201	CYC	C2C-C3C-C4C	4.83	108.57	101.34
5	g	200	CYC	C2C-C3C-C4C	4.80	108.53	101.34
5	h	200	CYC	C1B-CHB-C4A	-4.77	116.33	128.06
5	T	201	CYC	C2C-C3C-C4C	4.75	108.45	101.34
5	U	200	CYC	C1B-CHB-C4A	-4.74	116.42	128.06
5	U	200	CYC	C1C-NC-C4C	-4.73	107.48	113.41
5	J	201	CYC	C2C-C3C-C4C	4.72	108.42	101.34
5	U	200	CYC	C2C-C3C-C4C	4.72	108.41	101.34
5	J	201	CYC	CAB-C3B-C4B	4.72	128.67	121.37
5	g	201	CYC	C2C-C1C-NC	-4.71	104.37	108.29
5	E	200	CYC	C4D-CHA-C1A	-4.69	117.97	128.22
5	P	200	CYC	C2C-C3C-C4C	4.65	108.30	101.34
5	Q	200	CYC	C1B-CHB-C4A	-4.62	116.72	128.06
5	h	200	CYC	C2C-C3C-C4C	4.61	108.24	101.34
5	H	200	CYC	C4D-CHA-C1A	-4.59	118.19	128.22
5	X	200	CYC	C2C-C3C-C4C	4.58	108.20	101.34
5	I	201	CYC	C4D-CHA-C1A	-4.58	118.22	128.22
5	T	201	CYC	C1B-CHB-C4A	-4.58	116.81	128.06
5	E	200	CYC	C2C-C3C-C4C	4.55	108.15	101.34
5	h	201	CYC	C2C-C1C-NC	-4.55	104.50	108.29
5	N	200	CYC	CAB-C3B-C4B	4.55	128.40	121.37
5	Q	200	CYC	C2C-C1C-NC	-4.53	104.51	108.29
5	i	200	CYC	C2C-C1C-NC	-4.53	104.52	108.29
5	T	200	CYC	C1B-CHB-C4A	-4.48	117.06	128.06
5	N	200	CYC	C4D-CHA-C1A	-4.48	118.44	128.22
5	O	200	CYC	C2C-C3C-C4C	4.47	108.04	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	200	CYC	C2C-C1C-NC	-4.42	104.61	108.29
5	C	200	CYC	C2C-C3C-C4C	4.39	107.91	101.34
5	f	200	CYC	C2C-C3C-C4C	4.37	107.88	101.34
5	V	201	CYC	C2C-C3C-C4C	4.34	107.84	101.34
5	T	201	CYC	C2C-C1C-NC	-4.34	104.67	108.29
5	W	200	CYC	C4D-CHA-C1A	-4.33	118.78	128.22
5	U	201	CYC	CAB-C3B-C4B	4.30	128.03	121.37
5	F	200	CYC	C2C-C3C-C4C	4.30	107.78	101.34
5	W	201	CYC	C1B-CHB-C4A	-4.26	117.59	128.06
5	d	200	CYC	C2C-C1C-NC	-4.25	104.75	108.29
5	S	200	CYC	C2C-C3C-C4C	4.25	107.71	101.34
5	N	200	CYC	C1B-CHB-C4A	-4.24	117.64	128.06
5	D	200	CYC	CAB-C3B-C4B	4.23	127.92	121.37
5	N	200	CYC	C2C-C3C-C4C	4.23	107.67	101.34
5	N	200	CYC	C3C-C4C-NC	-4.22	102.51	107.94
5	W	200	CYC	C2C-C3C-C4C	4.21	107.64	101.34
5	D	200	CYC	C2C-C3C-C4C	4.19	107.61	101.34
5	R	200	CYC	C2C-C3C-C4C	4.16	107.57	101.34
5	H	201	CYC	CMD-C2D-C1D	4.16	131.66	125.62
5	K	201	CYC	C2C-C3C-C4C	4.16	107.56	101.34
5	B	200	CYC	CMD-C2D-C1D	4.16	131.66	125.62
5	A	200	CYC	C2C-C3C-C4C	4.15	107.56	101.34
5	Q	200	CYC	CAB-C3B-C4B	4.15	127.79	121.37
5	U	201	CYC	C2C-C1C-NC	-4.12	104.86	108.29
5	l	201	CYC	CMA-C3A-C4A	4.12	131.49	125.10
5	K	200	CYC	CMA-C3A-C4A	4.12	131.49	125.10
5	L	201	CYC	C2C-C3C-C4C	4.11	107.49	101.34
5	O	200	CYC	CAB-C3B-C4B	4.11	127.72	121.37
5	V	200	CYC	C2C-C3C-C4C	4.09	107.47	101.34
5	k	200	CYC	C2C-C1C-NC	-4.09	104.88	108.29
5	O	200	CYC	CMA-C3A-C4A	4.09	131.45	125.10
5	C	200	CYC	CAB-C3B-C4B	4.08	127.68	121.37
5	Y	201	CYC	C2C-C3C-C4C	4.06	107.42	101.34
5	b	200	CYC	C2C-C1C-NC	-4.05	104.91	108.29
5	h	200	CYC	C2C-C1C-NC	-4.04	104.92	108.29
5	A	200	CYC	CAB-C3B-C4B	4.02	127.59	121.37
5	B	200	CYC	C2C-C3C-C4C	4.02	107.36	101.34
5	5	1201	CYC	CMA-C3A-C4A	4.01	131.32	125.10
5	H	200	CYC	CMD-C2D-C1D	4.00	131.44	125.62
5	J	200	CYC	CMA-C3A-C4A	3.99	131.29	125.10
5	I	200	CYC	C2C-C1C-NC	-3.98	104.97	108.29
5	d	200	CYC	C1B-CHB-C4A	-3.98	118.29	128.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	W	201	CYC	C2C-C3C-C4C	3.98	107.29	101.34
5	H	201	CYC	C2C-C1C-NC	-3.96	104.99	108.29
5	H	201	CYC	CAB-C3B-C4B	3.96	127.49	121.37
5	P	200	CYC	CAB-C3B-C4B	3.94	127.46	121.37
5	j	201	CYC	C2C-C3C-C4C	3.91	107.19	101.34
5	W	200	CYC	C1B-CHB-C4A	-3.88	118.53	128.06
5	P	200	CYC	C2C-C1C-NC	-3.87	105.06	108.29
5	B	200	CYC	CAB-C3B-C4B	3.87	127.35	121.37
5	I	201	CYC	C2C-C3C-C4C	3.86	107.12	101.34
5	X	201	CYC	C2C-C3C-C4C	3.86	107.12	101.34
5	h	201	CYC	C3C-C4C-NC	-3.85	102.98	107.94
5	R	200	CYC	CAB-C3B-C4B	3.84	127.30	121.37
5	W	201	CYC	CAB-C3B-C4B	3.83	127.30	121.37
5	G	201	CYC	CMA-C3A-C4A	3.83	131.04	125.10
5	H	200	CYC	CMA-C3A-C4A	3.82	131.03	125.10
5	h	201	CYC	CAB-C3B-C4B	3.81	127.26	121.37
5	K	201	CYC	CMA-C3A-C4A	3.80	131.01	125.10
5	Y	200	CYC	C2C-C1C-NC	-3.80	105.12	108.29
5	b	200	CYC	CAB-C3B-C4B	3.80	127.25	121.37
5	T	201	CYC	CAB-C3B-C4B	3.79	127.23	121.37
5	i	201	CYC	CAB-C3B-C4B	3.75	127.17	121.37
5	i	200	CYC	CAB-C3B-C4B	3.74	127.15	121.37
5	f	200	CYC	CAB-C3B-C4B	3.73	127.14	121.37
5	D	200	CYC	CMD-C2D-C1D	3.73	131.04	125.62
5	W	200	CYC	CMA-C3A-C4A	3.73	130.89	125.10
5	P	200	CYC	C4D-CHA-C1A	-3.72	120.10	128.22
5	H	200	CYC	C2C-C1C-NC	-3.71	105.20	108.29
5	k	200	CYC	CAB-C3B-C4B	3.69	127.08	121.37
5	X	201	CYC	CAB-C3B-C4B	3.69	127.08	121.37
5	G	201	CYC	C2C-C3C-C4C	3.67	106.84	101.34
5	V	200	CYC	CMD-C2D-C1D	3.65	130.93	125.62
5	I	201	CYC	CAB-C3B-C4B	3.65	127.01	121.37
5	j	200	CYC	C2C-C3C-C4C	3.65	106.80	101.34
5	a	200	CYC	C2C-C1C-NC	-3.64	105.26	108.29
5	E	200	CYC	CAB-C3B-C4B	3.63	126.99	121.37
5	c	200	CYC	CAB-C3B-C4B	3.63	126.98	121.37
5	G	200	CYC	CAB-C3B-C4B	3.63	126.98	121.37
5	V	201	CYC	CAB-C3B-C4B	3.62	126.97	121.37
5	5	1201	CYC	C3C-C4C-NC	-3.61	103.29	107.94
5	e	200	CYC	C2C-C3C-C4C	3.61	106.74	101.34
5	J	200	CYC	CAB-C3B-C4B	3.61	126.95	121.37
5	W	200	CYC	C1D-CHD-C4C	-3.60	121.61	127.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	k	200	CYC	CMD-C2D-C1D	3.59	130.84	125.62
5	G	201	CYC	CAB-C3B-C4B	3.59	126.92	121.37
5	5	1202	CYC	CAB-C3B-C4B	3.58	126.91	121.37
5	j	201	CYC	CAB-C3B-C4B	3.58	126.90	121.37
5	W	200	CYC	CAB-C3B-C4B	3.56	126.88	121.37
5	D	200	CYC	C3C-C4C-NC	-3.56	103.36	107.94
5	L	201	CYC	CAB-C3B-C4B	3.56	126.87	121.37
5	K	200	CYC	CAB-C3B-C4B	3.56	126.87	121.37
5	V	200	CYC	CAB-C3B-C4B	3.55	126.87	121.37
5	H	201	CYC	C3C-C4C-NC	-3.55	103.37	107.94
5	D	200	CYC	CMA-C3A-C4A	3.55	130.62	125.10
5	i	200	CYC	C1B-CHB-C4A	-3.54	119.36	128.06
5	e	200	CYC	CAB-C3B-C4B	3.54	126.84	121.37
5	g	200	CYC	CAB-C3B-C4B	3.53	126.83	121.37
5	Y	201	CYC	CAB-C3B-C4B	3.53	126.82	121.37
5	J	200	CYC	C2C-C3C-C4C	3.52	106.61	101.34
5	k	201	CYC	CAB-C3B-C4B	3.52	126.81	121.37
5	H	200	CYC	C2C-C3C-C4C	3.51	106.60	101.34
5	h	201	CYC	CMD-C2D-C1D	3.49	130.69	125.62
5	R	200	CYC	C2C-C1C-NC	-3.46	105.41	108.29
5	X	200	CYC	CAB-C3B-C4B	3.45	126.71	121.37
5	O	200	CYC	CMD-C2D-C1D	3.45	130.63	125.62
5	U	201	CYC	CMD-C2D-C1D	3.45	130.63	125.62
5	N	200	CYC	CMD-C2D-C1D	3.44	130.62	125.62
5	W	201	CYC	CMA-C3A-C4A	3.44	130.44	125.10
5	g	200	CYC	C2C-C1C-NC	-3.43	105.44	108.29
5	i	201	CYC	C2C-C1C-NC	-3.41	105.44	108.29
5	G	201	CYC	CHB-C4A-C3A	3.41	133.63	124.87
5	O	200	CYC	CHB-C4A-C3A	3.41	133.62	124.87
5	L	201	CYC	OB-C4B-C3B	-3.39	124.47	128.03
5	l	201	CYC	C2C-C1C-NC	-3.38	105.47	108.29
5	I	200	CYC	CAB-C3B-C4B	3.36	126.57	121.37
5	X	200	CYC	CMA-C3A-C4A	3.36	130.31	125.10
5	H	200	CYC	CAB-C3B-C4B	3.29	126.46	121.37
5	a	200	CYC	CAB-C3B-C4B	3.29	126.45	121.37
5	R	200	CYC	C1B-CHB-C4A	-3.29	119.99	128.06
5	d	200	CYC	CAB-C3B-C4B	3.28	126.45	121.37
5	B	200	CYC	C1B-CHB-C4A	-3.28	120.00	128.06
5	h	200	CYC	CAB-C3B-C4B	3.25	126.40	121.37
5	h	200	CYC	CMA-C3A-C4A	3.25	130.15	125.10
5	A	200	CYC	C3C-C4C-NC	-3.25	103.76	107.94
5	k	200	CYC	C2C-C3C-C4C	3.24	106.19	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	200	CYC	CMD-C2D-C1D	3.23	130.32	125.62
5	Y	200	CYC	C4D-CHA-C1A	-3.23	121.16	128.22
5	Y	200	CYC	CMA-C3A-C4A	3.23	130.12	125.10
5	h	201	CYC	C2C-C3C-C4C	3.23	106.17	101.34
5	T	200	CYC	CAB-C3B-C4B	3.22	126.36	121.37
5	J	200	CYC	CHB-C4A-C3A	3.22	133.15	124.87
5	K	201	CYC	CAB-C3B-C4B	3.21	126.34	121.37
5	j	200	CYC	CAB-C3B-C4B	3.21	126.33	121.37
5	5	1201	CYC	CMD-C2D-C1D	3.18	130.25	125.62
5	e	200	CYC	C2C-C1C-NC	-3.18	105.64	108.29
5	G	201	CYC	C1A-NA-C4A	3.18	112.35	106.52
5	O	200	CYC	C1A-NA-C4A	3.16	112.32	106.52
5	Y	201	CYC	C1B-CHB-C4A	-3.16	120.29	128.06
5	I	201	CYC	CHA-C4D-C3D	-3.14	120.46	127.22
5	N	200	CYC	CMA-C3A-C4A	3.12	129.94	125.10
5	i	200	CYC	CMA-C3A-C4A	3.12	129.94	125.10
5	Q	200	CYC	C2C-C3C-C4C	3.11	105.99	101.34
5	K	200	CYC	CHB-C4A-C3A	3.08	132.78	124.87
5	V	200	CYC	C3C-C4C-NC	-3.07	103.98	107.94
5	E	200	CYC	CMA-C3A-C4A	3.05	129.84	125.10
5	c	200	CYC	C2C-C3C-C4C	3.05	105.90	101.34
5	B	200	CYC	CMA-C3A-C4A	3.04	129.82	125.10
5	g	201	CYC	CMA-C3A-C4A	3.04	129.82	125.10
5	g	201	CYC	CAB-C3B-C4B	3.03	126.06	121.37
5	Y	200	CYC	CHA-C4D-C3D	-3.03	120.71	127.22
5	U	201	CYC	CMB-C2B-C1B	3.01	127.82	124.16
5	A	200	CYC	CMD-C2D-C1D	3.01	130.00	125.62
5	C	200	CYC	CMD-C2D-C1D	3.01	130.00	125.62
5	U	200	CYC	CMA-C3A-C4A	3.00	129.76	125.10
5	T	200	CYC	C2C-C1C-NC	-2.99	105.80	108.29
5	T	200	CYC	CMA-C3A-C4A	2.98	129.73	125.10
5	G	200	CYC	C2C-C1C-NC	-2.98	105.81	108.29
5	a	200	CYC	CMA-C3A-C4A	2.98	129.72	125.10
5	l	201	CYC	CMB-C2B-C1B	2.96	127.76	124.16
5	K	200	CYC	C1A-NA-C4A	2.96	111.95	106.52
5	c	200	CYC	C2C-C1C-NC	-2.95	105.83	108.29
5	H	200	CYC	CHA-C4D-C3D	-2.95	120.89	127.22
5	k	201	CYC	C2C-C1C-NC	-2.94	105.84	108.29
5	k	200	CYC	C3C-C4C-NC	-2.93	104.17	107.94
5	D	200	CYC	CHA-C4D-C3D	-2.93	120.93	127.22
5	X	200	CYC	C1A-NA-C4A	2.92	111.88	106.52
5	B	200	CYC	C1A-NA-C4A	2.92	111.87	106.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	201	CYC	C1B-CHB-C4A	-2.92	120.89	128.06
5	5	1201	CYC	C1D-CHD-C4C	-2.91	122.80	127.76
5	T	200	CYC	C1A-NA-C4A	2.90	111.84	106.52
5	K	201	CYC	CHB-C4A-C3A	2.89	132.31	124.87
5	j	200	CYC	C2C-C1C-NC	-2.89	105.88	108.29
5	5	1201	CYC	CAB-C3B-C4B	2.88	125.82	121.37
5	Y	200	CYC	CHA-C1A-NA	2.87	130.63	124.60
5	B	200	CYC	CAD-C3D-C4D	2.87	130.33	125.77
5	K	201	CYC	C1B-CHB-C4A	-2.87	121.01	128.06
5	i	200	CYC	C1A-NA-C4A	2.86	111.77	106.52
5	U	201	CYC	C2C-C3C-C4C	2.86	105.62	101.34
5	F	200	CYC	CMC-C2C-C1C	-2.86	106.25	112.40
5	5	1201	CYC	CHA-C1A-NA	2.85	130.58	124.60
5	Y	200	CYC	CAB-C3B-C4B	2.85	125.77	121.37
5	K	201	CYC	C1A-NA-C4A	2.85	111.74	106.52
5	O	200	CYC	C3C-C4C-NC	-2.84	104.28	107.94
5	R	200	CYC	CMA-C3A-C4A	2.83	129.50	125.10
5	l	201	CYC	C1A-NA-C4A	2.83	111.71	106.52
5	5	1201	CYC	CAC-C3C-C4C	-2.83	105.40	112.67
5	W	201	CYC	C1A-NA-C4A	2.82	111.70	106.52
5	a	200	CYC	C1A-NA-C4A	2.82	111.70	106.52
5	J	201	CYC	C2C-C1C-NC	-2.82	105.94	108.29
5	W	200	CYC	C1A-NA-C4A	2.82	111.69	106.52
5	N	200	CYC	CHA-C4D-C3D	-2.82	121.16	127.22
5	l	201	CYC	C1B-CHB-C4A	-2.82	121.14	128.06
5	d	200	CYC	C2C-C3C-C4C	2.81	105.55	101.34
5	R	200	CYC	C1A-NA-C4A	2.81	111.67	106.52
5	L	201	CYC	CMA-C3A-C4A	2.80	129.45	125.10
5	L	201	CYC	C1A-NA-C4A	2.80	111.66	106.52
5	W	200	CYC	CMD-C2D-C1D	2.80	129.69	125.62
5	E	200	CYC	CHA-C4D-C3D	-2.80	121.20	127.22
5	Q	200	CYC	CMA-C3A-C4A	2.79	129.43	125.10
5	J	201	CYC	C1A-NA-C4A	2.76	111.59	106.52
5	J	200	CYC	C1A-NA-C4A	2.75	111.57	106.52
5	F	200	CYC	C2C-C1C-NC	-2.75	106.00	108.29
5	J	200	CYC	CHA-C4D-C3D	-2.74	121.33	127.22
5	X	201	CYC	C2C-C1C-NC	-2.73	106.01	108.29
5	T	201	CYC	CMA-C3A-C4A	2.73	129.34	125.10
5	g	200	CYC	CMB-C2B-C1B	2.72	127.47	124.16
5	W	200	CYC	CHA-C4D-C3D	-2.72	121.38	127.22
5	Y	201	CYC	C1A-NA-C4A	2.71	111.50	106.52
5	U	200	CYC	CAB-C3B-C4B	2.71	125.56	121.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	201	CYC	CMB-C2B-C1B	2.69	127.43	124.16
5	j	200	CYC	CMB-C2B-C1B	2.68	127.42	124.16
5	H	200	CYC	CHB-C4A-C3A	2.68	131.75	124.87
5	J	201	CYC	CMA-C3A-C4A	2.68	129.26	125.10
5	H	200	CYC	C3C-C4C-NC	-2.68	104.50	107.94
5	5	1202	CYC	CMB-C2B-C1B	2.68	127.41	124.16
5	U	200	CYC	OB-C4B-C3B	-2.67	125.23	128.03
5	U	200	CYC	CHA-C4D-C3D	-2.64	121.54	127.22
5	X	200	CYC	CHB-C4A-C3A	2.64	131.66	124.87
5	d	200	CYC	CMA-C3A-C4A	2.64	129.20	125.10
5	L	201	CYC	CMB-C2B-C1B	2.64	127.36	124.16
5	A	200	CYC	CHA-C1A-NA	2.63	130.12	124.60
5	b	200	CYC	C2C-C3C-C4C	2.63	105.28	101.34
5	H	200	CYC	C1A-NA-C4A	2.63	111.34	106.52
5	R	200	CYC	CHB-C4A-C3A	2.63	131.62	124.87
5	g	201	CYC	C1A-NA-C4A	2.63	111.34	106.52
5	d	200	CYC	C1A-NA-C4A	2.63	111.33	106.52
5	l	201	CYC	CHB-C4A-C3A	2.62	131.61	124.87
5	j	201	CYC	C1A-NA-C4A	2.62	111.33	106.52
5	H	200	CYC	C1B-CHB-C4A	-2.62	121.63	128.06
5	G	200	CYC	C1A-NA-C4A	2.62	111.32	106.52
5	S	200	CYC	CAC-C3C-C4C	-2.61	105.97	112.67
5	B	200	CYC	C3C-C4C-NC	-2.61	104.58	107.94
5	b	200	CYC	C3C-C4C-NC	-2.60	104.60	107.94
5	T	201	CYC	C1A-NA-C4A	2.59	111.26	106.52
5	b	200	CYC	CMD-C2D-C1D	2.58	129.37	125.62
5	k	200	CYC	CHA-C4D-C3D	-2.56	121.71	127.22
5	L	201	CYC	CHB-C4A-C3A	2.56	131.46	124.87
5	5	1202	CYC	O2A-CGA-CBA	2.55	122.07	114.00
5	B	200	CYC	CHB-C4A-C3A	2.55	131.43	124.87
5	j	200	CYC	OB-C4B-C3B	-2.55	125.35	128.03
5	C	200	CYC	C3C-C4C-NC	-2.55	104.66	107.94
5	I	200	CYC	C2C-C3C-C4C	2.55	105.15	101.34
5	X	201	CYC	OB-C4B-C3B	-2.54	125.36	128.03
5	i	201	CYC	C1A-NA-C4A	2.53	111.17	106.52
5	J	201	CYC	CHB-C1B-C2B	-2.53	121.93	126.97
5	F	200	CYC	CAC-C3C-C4C	-2.51	106.23	112.67
5	W	201	CYC	CHB-C4A-C3A	2.50	131.31	124.87
5	a	200	CYC	C3C-C4C-NC	-2.50	104.72	107.94
5	e	200	CYC	C1A-NA-C4A	2.50	111.11	106.52
5	I	201	CYC	CMB-C2B-C1B	2.50	127.19	124.16
5	Y	201	CYC	CMA-C3A-C4A	2.49	128.97	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	X	201	CYC	CMB-C2B-C1B	2.49	127.18	124.16
5	U	200	CYC	C1A-NA-C4A	2.48	111.07	106.52
5	F	200	CYC	CMA-C3A-C4A	2.48	128.95	125.10
5	J	200	CYC	C2C-C1C-NC	-2.48	106.22	108.29
5	J	201	CYC	CHB-C4A-C3A	2.46	131.19	124.87
5	E	200	CYC	CMB-C2B-C1B	2.45	127.14	124.16
5	N	200	CYC	C1A-NA-C4A	2.44	110.99	106.52
5	k	201	CYC	C1A-NA-C4A	2.43	110.98	106.52
5	h	200	CYC	C3C-C4C-NC	-2.43	104.81	107.94
5	E	200	CYC	C3C-C4C-NC	-2.42	104.82	107.94
5	T	201	CYC	CMB-C2B-C1B	2.42	127.11	124.16
5	c	200	CYC	C1A-NA-C4A	2.42	110.96	106.52
5	K	200	CYC	CHA-C4D-C3D	-2.41	122.03	127.22
5	a	200	CYC	CAD-C3D-C4D	2.41	129.60	125.77
5	W	200	CYC	CHB-C4A-C3A	2.41	131.06	124.87
5	I	200	CYC	CHA-C4D-C3D	-2.41	122.04	127.22
5	P	200	CYC	CHA-C4D-C3D	-2.41	122.04	127.22
5	G	200	CYC	CMA-C3A-C4A	2.40	128.82	125.10
5	I	201	CYC	C1A-NA-C4A	2.39	110.91	106.52
5	h	200	CYC	C1A-NA-C4A	2.39	110.91	106.52
5	j	200	CYC	CHA-C4D-C3D	-2.39	122.08	127.22
5	Y	200	CYC	C1A-NA-C4A	2.39	110.90	106.52
5	H	201	CYC	CHA-C4D-C3D	-2.39	122.09	127.22
5	D	200	CYC	C1A-NA-C4A	2.38	110.88	106.52
5	g	200	CYC	CHA-C4D-C3D	-2.38	122.11	127.22
5	k	201	CYC	CMB-C2B-C1B	2.38	127.05	124.16
5	h	200	CYC	CHA-C4D-C3D	-2.37	122.12	127.22
5	E	200	CYC	CMC-C2C-C1C	-2.37	107.29	112.40
5	S	200	CYC	C1A-NA-C4A	2.37	110.87	106.52
5	V	200	CYC	C1A-NA-C4A	2.37	110.87	106.52
5	O	200	CYC	CHB-C4A-NA	-2.37	119.84	124.95
5	Y	200	CYC	CHA-C4D-ND	2.36	130.62	125.29
5	g	200	CYC	CHA-C1A-NA	2.36	129.55	124.60
5	Q	200	CYC	CMD-C2D-C3D	-2.36	120.62	125.62
5	k	200	CYC	C1A-NA-C4A	2.36	110.84	106.52
5	j	200	CYC	CMA-C3A-C4A	2.35	128.75	125.10
5	k	201	CYC	OB-C4B-C3B	-2.35	125.56	128.03
5	c	200	CYC	CAD-C3D-C4D	2.35	129.49	125.77
5	L	201	CYC	CMC-C2C-C1C	-2.34	107.35	112.40
5	g	200	CYC	C1A-NA-C4A	2.34	110.82	106.52
5	G	201	CYC	CHB-C4A-NA	-2.34	119.90	124.95
5	K	200	CYC	C1B-CHB-C4A	-2.34	122.32	128.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	1202	CYC	C1A-NA-C4A	2.33	110.80	106.52
5	Y	201	CYC	OB-C4B-C3B	-2.33	125.58	128.03
5	i	201	CYC	CMB-C2B-C1B	2.33	126.99	124.16
5	b	200	CYC	C1A-NA-C4A	2.33	110.79	106.52
5	I	200	CYC	C1A-NA-C4A	2.32	110.78	106.52
5	b	200	CYC	CMB-C2B-C1B	2.32	126.98	124.16
5	O	200	CYC	C1B-CHB-C4A	-2.32	122.37	128.06
5	i	200	CYC	CHB-C4A-C3A	2.32	130.82	124.87
5	E	200	CYC	C1A-NA-C4A	2.31	110.76	106.52
5	J	200	CYC	CHB-C4A-NA	-2.31	119.97	124.95
5	j	201	CYC	OB-C4B-C3B	-2.30	125.61	128.03
5	T	200	CYC	CMB-C2B-C1B	2.30	126.95	124.16
5	N	200	CYC	CHA-C1A-NA	2.30	129.42	124.60
5	h	201	CYC	C1A-NA-C4A	2.29	110.72	106.52
5	g	201	CYC	CMB-C2B-C1B	2.29	126.94	124.16
5	a	200	CYC	CHB-C4A-C3A	2.29	130.75	124.87
5	E	200	CYC	CHA-C1A-NA	2.28	129.39	124.60
5	T	201	CYC	OB-C4B-C3B	-2.28	125.64	128.03
5	V	201	CYC	C1A-NA-C4A	2.28	110.70	106.52
5	X	200	CYC	OB-C4B-C3B	-2.28	125.64	128.03
5	Q	200	CYC	C1A-NA-C4A	2.27	110.69	106.52
5	L	201	CYC	C1B-CHB-C4A	-2.27	122.48	128.06
5	P	200	CYC	CHA-C1A-NA	2.27	129.37	124.60
5	F	200	CYC	C1A-NA-C4A	2.26	110.67	106.52
5	O	200	CYC	CMC-C2C-C1C	-2.26	107.53	112.40
5	l	201	CYC	CHA-C1A-NA	2.26	129.34	124.60
5	I	201	CYC	CMA-C3A-C4A	2.26	128.60	125.10
5	i	200	CYC	CMB-C2B-C1B	2.25	126.90	124.16
5	I	201	CYC	CHA-C4D-ND	2.25	130.38	125.29
5	k	200	CYC	OB-C4B-C3B	-2.25	125.67	128.03
5	K	201	CYC	CHA-C4D-C3D	-2.24	122.40	127.22
5	I	200	CYC	OB-C4B-C3B	-2.24	125.68	128.03
5	U	200	CYC	CHA-C1A-NA	2.23	129.28	124.60
5	e	200	CYC	CMD-C2D-C1D	2.23	128.85	125.62
5	N	200	CYC	O2A-CGA-CBA	2.22	121.02	114.00
5	j	201	CYC	CMA-C3A-C4A	2.22	128.55	125.10
5	H	200	CYC	CHA-C4D-ND	2.22	130.30	125.29
5	X	200	CYC	C1B-CHB-C4A	-2.22	122.61	128.06
5	H	200	CYC	CHA-C1A-NA	2.21	129.25	124.60
5	e	200	CYC	OB-C4B-C3B	-2.21	125.71	128.03
5	d	200	CYC	CHA-C4D-C3D	-2.20	122.48	127.22
5	Y	201	CYC	CHB-C4A-C3A	2.20	130.53	124.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	201	CYC	CMB-C2B-C1B	2.20	126.83	124.16
5	W	200	CYC	CHA-C4D-ND	2.20	130.26	125.29
5	j	200	CYC	C1A-NA-C4A	2.20	110.55	106.52
5	U	200	CYC	C2C-C1C-NC	-2.19	106.46	108.29
5	L	201	CYC	CHB-C1B-C2B	-2.19	122.60	126.97
5	f	200	CYC	CMB-C2B-C1B	2.19	126.82	124.16
5	Y	200	CYC	C2C-C3C-C4C	2.19	104.62	101.34
5	P	200	CYC	C1A-NA-C4A	2.18	110.52	106.52
5	T	200	CYC	CHA-C1A-NA	2.17	129.15	124.60
5	G	200	CYC	CHA-C4D-C3D	-2.17	122.56	127.22
5	H	200	CYC	CMB-C2B-C1B	2.17	126.80	124.16
5	U	201	CYC	C1A-NA-C4A	2.16	110.49	106.52
5	5	1201	CYC	C1A-NA-C4A	2.16	110.47	106.52
5	J	200	CYC	CHA-C1A-NA	2.15	129.12	124.60
5	h	201	CYC	CMB-C2B-C1B	2.15	126.77	124.16
5	h	200	CYC	CHA-C1A-NA	2.15	129.10	124.60
5	P	200	CYC	CMD-C2D-C1D	2.14	128.74	125.62
5	X	201	CYC	C1A-NA-C4A	2.14	110.45	106.52
5	A	200	CYC	C1A-NA-C4A	2.14	110.44	106.52
5	A	200	CYC	O2A-CGA-CBA	2.14	120.76	114.00
5	K	201	CYC	OB-C4B-C3B	-2.14	125.79	128.03
5	C	200	CYC	C1A-NA-C4A	2.13	110.43	106.52
5	j	200	CYC	CHA-C1A-NA	2.13	129.07	124.60
5	h	200	CYC	CMD-C2D-C1D	2.13	128.71	125.62
5	Q	200	CYC	CHA-C4D-C3D	-2.12	122.66	127.22
5	I	201	CYC	OB-C4B-C3B	-2.12	125.81	128.03
5	K	200	CYC	CAA-C2A-C1A	2.11	128.73	125.02
5	c	200	CYC	CAC-C3C-C4C	-2.11	107.25	112.67
5	a	200	CYC	OB-C4B-C3B	-2.11	125.82	128.03
5	c	200	CYC	CMB-C2B-C1B	2.11	126.72	124.16
5	X	201	CYC	CHA-C4D-C3D	-2.10	122.70	127.22
5	S	200	CYC	CAB-C3B-C2B	-2.10	123.70	127.56
5	X	200	CYC	CHA-C4D-C3D	-2.10	122.70	127.22
5	K	200	CYC	C2C-C1C-NC	-2.10	106.54	108.29
5	5	1202	CYC	C2C-C1C-NC	-2.10	106.54	108.29
5	S	200	CYC	CMA-C3A-C4A	2.10	128.35	125.10
5	Y	201	CYC	CHB-C1B-C2B	-2.10	122.79	126.97
5	R	200	CYC	CMB-C2B-C1B	2.09	126.71	124.16
5	W	200	CYC	CMB-C2B-C1B	2.08	126.69	124.16
5	f	200	CYC	C4D-C3D-C2D	-2.08	105.20	107.62
5	f	200	CYC	CBD-CAD-C3D	2.07	118.27	112.53
5	C	200	CYC	CMB-C2B-C1B	2.07	126.68	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	a	200	CYC	O2A-CGA-CBA	2.07	120.54	114.00
5	k	201	CYC	CMA-C3A-C4A	2.07	128.31	125.10
5	D	200	CYC	CHA-C4D-ND	2.06	129.96	125.29
5	N	200	CYC	CHA-C4D-ND	2.06	129.96	125.29
5	j	200	CYC	O2A-CGA-CBA	2.06	120.51	114.00
5	k	200	CYC	CMA-C3A-C4A	2.06	128.30	125.10
5	N	200	CYC	CHB-C4A-C3A	2.05	130.14	124.87
5	X	200	CYC	CHB-C1B-C2B	-2.05	122.88	126.97
5	D	200	CYC	CHA-C1A-NA	2.05	128.90	124.60
5	J	200	CYC	CMC-C2C-C1C	-2.05	107.99	112.40
5	K	201	CYC	CMB-C2B-C1B	2.04	126.64	124.16
5	Y	200	CYC	OB-C4B-C3B	-2.04	125.89	128.03
5	c	200	CYC	C4D-C3D-C2D	-2.03	105.26	107.62
5	P	200	CYC	OB-C4B-C3B	-2.03	125.90	128.03
5	T	201	CYC	CHA-C4D-C3D	-2.03	122.86	127.22
5	K	200	CYC	O2A-CGA-CBA	2.03	120.40	114.00
5	U	201	CYC	O2A-CGA-CBA	2.02	120.39	114.00
5	k	201	CYC	CHA-C4D-C3D	-2.02	122.88	127.22
5	L	201	CYC	C3B-C4B-NB	2.02	108.37	106.77
5	G	200	CYC	CMB-C2B-C1B	2.02	126.61	124.16
5	U	200	CYC	CMC-C2C-C1C	-2.01	108.06	112.40
5	h	200	CYC	O2A-CGA-CBA	2.01	120.36	114.00
5	W	200	CYC	O2A-CGA-CBA	2.01	120.36	114.00
5	a	200	CYC	O2D-CGD-CBD	2.01	120.35	114.00
5	U	200	CYC	CMB-C2B-C1B	2.01	126.60	124.16
5	g	200	CYC	CMA-C3A-C4A	2.01	128.22	125.10
5	D	200	CYC	O2A-CGA-CBA	2.01	120.34	114.00
5	K	201	CYC	O2A-CGA-CBA	2.00	120.32	114.00
5	c	200	CYC	O2A-CGA-CBA	2.00	120.32	114.00

There are no chirality outliers.

All (710) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	5	1201	CYC	NA-C4A-CHB-C1B
5	5	1201	CYC	C3A-C4A-CHB-C1B
5	5	1201	CYC	C4C-C3C-CAC-CBC
5	5	1201	CYC	NC-C4C-CHD-C1D
5	5	1201	CYC	C3C-C4C-CHD-C1D
5	5	1202	CYC	NA-C4A-CHB-C1B
5	5	1202	CYC	C3A-C4A-CHB-C1B
5	5	1202	CYC	NC-C4C-CHD-C1D

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Mol	Chain	Res	Type	Atoms
5	A	200	CYC	NA-C4A-CHB-C1B
5	A	200	CYC	C3A-C4A-CHB-C1B
5	A	200	CYC	NC-C4C-CHD-C1D
5	A	200	CYC	C3C-C4C-CHD-C1D
5	B	200	CYC	NA-C1A-CHA-C4D
5	B	200	CYC	C2A-C1A-CHA-C4D
5	B	200	CYC	ND-C4D-CHA-C1A
5	B	200	CYC	C3D-C4D-CHA-C1A
5	B	200	CYC	NA-C4A-CHB-C1B
5	B	200	CYC	C3A-C4A-CHB-C1B
5	B	200	CYC	NC-C4C-CHD-C1D
5	B	200	CYC	C3C-C4C-CHD-C1D
5	B	200	CYC	C4D-C3D-CAD-CBD
5	C	200	CYC	NA-C1A-CHA-C4D
5	C	200	CYC	C2A-C1A-CHA-C4D
5	C	200	CYC	ND-C4D-CHA-C1A
5	C	200	CYC	C3D-C4D-CHA-C1A
5	C	200	CYC	NA-C4A-CHB-C1B
5	C	200	CYC	C3A-C4A-CHB-C1B
5	C	200	CYC	C4C-C3C-CAC-CBC
5	C	200	CYC	NC-C4C-CHD-C1D
5	D	200	CYC	NA-C4A-CHB-C1B
5	D	200	CYC	C3A-C4A-CHB-C1B
5	D	200	CYC	NC-C4C-CHD-C1D
5	E	200	CYC	NA-C4A-CHB-C1B
5	E	200	CYC	C3A-C4A-CHB-C1B
5	E	200	CYC	C2A-CAA-CBA-CGA
5	E	200	CYC	NC-C4C-CHD-C1D
5	F	200	CYC	NA-C4A-CHB-C1B
5	F	200	CYC	C3A-C4A-CHB-C1B
5	F	200	CYC	C2B-C3B-CAB-CBB
5	F	200	CYC	NC-C4C-CHD-C1D
5	G	200	CYC	NA-C4A-CHB-C1B
5	G	200	CYC	C3A-C4A-CHB-C1B
5	G	200	CYC	NC-C4C-CHD-C1D
5	G	201	CYC	NA-C4A-CHB-C1B
5	G	201	CYC	C3A-C4A-CHB-C1B
5	G	201	CYC	C2C-C3C-CAC-CBC
5	G	201	CYC	C4C-C3C-CAC-CBC
5	G	201	CYC	NC-C4C-CHD-C1D
5	G	201	CYC	C3C-C4C-CHD-C1D
5	G	201	CYC	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
5	G	201	CYC	C2D-C1D-CHD-C4C
5	H	200	CYC	NA-C4A-CHB-C1B
5	H	200	CYC	C2C-C3C-CAC-CBC
5	H	200	CYC	C4C-C3C-CAC-CBC
5	H	200	CYC	NC-C4C-CHD-C1D
5	H	200	CYC	C3C-C4C-CHD-C1D
5	H	201	CYC	NA-C4A-CHB-C1B
5	H	201	CYC	C3A-C4A-CHB-C1B
5	H	201	CYC	C2C-C3C-CAC-CBC
5	H	201	CYC	NC-C4C-CHD-C1D
5	I	200	CYC	NA-C4A-CHB-C1B
5	I	200	CYC	C3A-C4A-CHB-C1B
5	I	200	CYC	C4C-C3C-CAC-CBC
5	I	200	CYC	NC-C4C-CHD-C1D
5	I	201	CYC	NA-C4A-CHB-C1B
5	I	201	CYC	C3A-C4A-CHB-C1B
5	I	201	CYC	C2C-C3C-CAC-CBC
5	I	201	CYC	C4C-C3C-CAC-CBC
5	I	201	CYC	NC-C4C-CHD-C1D
5	J	200	CYC	NA-C4A-CHB-C1B
5	J	200	CYC	C3A-C4A-CHB-C1B
5	J	200	CYC	C2C-C3C-CAC-CBC
5	J	200	CYC	C4C-C3C-CAC-CBC
5	J	200	CYC	NC-C4C-CHD-C1D
5	J	201	CYC	ND-C4D-CHA-C1A
5	J	201	CYC	C3D-C4D-CHA-C1A
5	J	201	CYC	NA-C4A-CHB-C1B
5	J	201	CYC	C3A-C4A-CHB-C1B
5	J	201	CYC	C2C-C3C-CAC-CBC
5	J	201	CYC	NC-C4C-CHD-C1D
5	J	201	CYC	ND-C1D-CHD-C4C
5	J	201	CYC	C2D-C1D-CHD-C4C
5	K	200	CYC	C3A-C4A-CHB-C1B
5	K	200	CYC	C2A-CAA-CBA-CGA
5	K	200	CYC	NC-C4C-CHD-C1D
5	K	201	CYC	NA-C4A-CHB-C1B
5	K	201	CYC	C2C-C3C-CAC-CBC
5	K	201	CYC	NC-C4C-CHD-C1D
5	K	201	CYC	C2D-C1D-CHD-C4C
5	L	201	CYC	NA-C4A-CHB-C1B
5	L	201	CYC	NC-C4C-CHD-C1D
5	L	201	CYC	C3C-C4C-CHD-C1D

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Mol	Chain	Res	Type	Atoms
5	N	200	CYC	NA-C4A-CHB-C1B
5	N	200	CYC	C3A-C4A-CHB-C1B
5	N	200	CYC	NC-C4C-CHD-C1D
5	O	200	CYC	NA-C1A-CHA-C4D
5	O	200	CYC	C2A-C1A-CHA-C4D
5	O	200	CYC	ND-C4D-CHA-C1A
5	O	200	CYC	C3D-C4D-CHA-C1A
5	O	200	CYC	NC-C4C-CHD-C1D
5	P	200	CYC	NA-C4A-CHB-C1B
5	P	200	CYC	C3A-C4A-CHB-C1B
5	P	200	CYC	NC-C4C-CHD-C1D
5	Q	200	CYC	NA-C4A-CHB-C1B
5	Q	200	CYC	C3A-C4A-CHB-C1B
5	Q	200	CYC	NC-C4C-CHD-C1D
5	Q	200	CYC	C3C-C4C-CHD-C1D
5	Q	200	CYC	ND-C1D-CHD-C4C
5	Q	200	CYC	C2D-C1D-CHD-C4C
5	R	200	CYC	NA-C1A-CHA-C4D
5	R	200	CYC	C2A-C1A-CHA-C4D
5	R	200	CYC	ND-C4D-CHA-C1A
5	R	200	CYC	C3D-C4D-CHA-C1A
5	R	200	CYC	NA-C4A-CHB-C1B
5	R	200	CYC	NC-C4C-CHD-C1D
5	R	200	CYC	ND-C1D-CHD-C4C
5	R	200	CYC	C2D-C1D-CHD-C4C
5	S	200	CYC	NA-C1A-CHA-C4D
5	S	200	CYC	C2A-C1A-CHA-C4D
5	S	200	CYC	NA-C4A-CHB-C1B
5	S	200	CYC	C3A-C4A-CHB-C1B
5	S	200	CYC	C2B-C3B-CAB-CBB
5	S	200	CYC	C4B-C3B-CAB-CBB
5	S	200	CYC	NC-C4C-CHD-C1D
5	S	200	CYC	ND-C1D-CHD-C4C
5	S	200	CYC	C2D-C1D-CHD-C4C
5	T	200	CYC	NA-C4A-CHB-C1B
5	T	200	CYC	C3A-C4A-CHB-C1B
5	T	200	CYC	NC-C4C-CHD-C1D
5	T	201	CYC	NA-C1A-CHA-C4D
5	T	201	CYC	NA-C4A-CHB-C1B
5	T	201	CYC	C3A-C4A-CHB-C1B
5	T	201	CYC	NC-C4C-CHD-C1D
5	U	200	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
5	U	200	CYC	C3A-C4A-CHB-C1B
5	U	200	CYC	NC-C4C-CHD-C1D
5	U	201	CYC	NA-C4A-CHB-C1B
5	U	201	CYC	C3A-C4A-CHB-C1B
5	U	201	CYC	C2C-C3C-CAC-CBC
5	U	201	CYC	C4C-C3C-CAC-CBC
5	U	201	CYC	NC-C4C-CHD-C1D
5	U	201	CYC	C3C-C4C-CHD-C1D
5	V	200	CYC	NA-C1A-CHA-C4D
5	V	200	CYC	C2A-C1A-CHA-C4D
5	V	200	CYC	NA-C4A-CHB-C1B
5	V	200	CYC	C3A-C4A-CHB-C1B
5	V	200	CYC	NC-C4C-CHD-C1D
5	V	201	CYC	NA-C4A-CHB-C1B
5	V	201	CYC	C3A-C4A-CHB-C1B
5	V	201	CYC	NC-C4C-CHD-C1D
5	V	201	CYC	C3C-C4C-CHD-C1D
5	W	200	CYC	NA-C4A-CHB-C1B
5	W	200	CYC	C3A-C4A-CHB-C1B
5	W	200	CYC	C2C-C3C-CAC-CBC
5	W	200	CYC	C4C-C3C-CAC-CBC
5	W	200	CYC	NC-C4C-CHD-C1D
5	W	201	CYC	NC-C4C-CHD-C1D
5	W	201	CYC	C3D-CAD-CBD-CGD
5	X	200	CYC	C4C-C3C-CAC-CBC
5	X	200	CYC	NC-C4C-CHD-C1D
5	X	200	CYC	C2D-C1D-CHD-C4C
5	X	201	CYC	NA-C4A-CHB-C1B
5	X	201	CYC	C3A-C4A-CHB-C1B
5	X	201	CYC	C2C-C3C-CAC-CBC
5	X	201	CYC	C4C-C3C-CAC-CBC
5	X	201	CYC	NC-C4C-CHD-C1D
5	X	201	CYC	ND-C1D-CHD-C4C
5	X	201	CYC	C2D-C1D-CHD-C4C
5	Y	200	CYC	NA-C4A-CHB-C1B
5	Y	200	CYC	C3A-C4A-CHB-C1B
5	Y	200	CYC	C2C-C3C-CAC-CBC
5	Y	200	CYC	C4C-C3C-CAC-CBC
5	Y	200	CYC	NC-C4C-CHD-C1D
5	Y	201	CYC	NA-C1A-CHA-C4D
5	Y	201	CYC	C2A-C1A-CHA-C4D
5	Y	201	CYC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
5	Y	201	CYC	C4C-C3C-CAC-CBC
5	Y	201	CYC	NC-C4C-CHD-C1D
5	Y	201	CYC	ND-C1D-CHD-C4C
5	Y	201	CYC	C2D-C1D-CHD-C4C
5	a	200	CYC	C2B-C1B-CHB-C4A
5	a	200	CYC	C2C-C3C-CAC-CBC
5	a	200	CYC	C4C-C3C-CAC-CBC
5	a	200	CYC	NC-C4C-CHD-C1D
5	a	200	CYC	ND-C1D-CHD-C4C
5	a	200	CYC	C2D-C1D-CHD-C4C
5	a	200	CYC	C4D-C3D-CAD-CBD
5	b	200	CYC	NA-C4A-CHB-C1B
5	b	200	CYC	C3A-C4A-CHB-C1B
5	b	200	CYC	C2C-C3C-CAC-CBC
5	b	200	CYC	C4C-C3C-CAC-CBC
5	b	200	CYC	NC-C4C-CHD-C1D
5	b	200	CYC	C3C-C4C-CHD-C1D
5	c	200	CYC	NA-C4A-CHB-C1B
5	c	200	CYC	C3A-C4A-CHB-C1B
5	c	200	CYC	NC-C4C-CHD-C1D
5	c	200	CYC	C3C-C4C-CHD-C1D
5	c	200	CYC	ND-C1D-CHD-C4C
5	c	200	CYC	C2D-C1D-CHD-C4C
5	c	200	CYC	C4D-C3D-CAD-CBD
5	d	200	CYC	NA-C4A-CHB-C1B
5	d	200	CYC	C3A-C4A-CHB-C1B
5	d	200	CYC	C2C-C3C-CAC-CBC
5	d	200	CYC	C4C-C3C-CAC-CBC
5	d	200	CYC	NC-C4C-CHD-C1D
5	d	200	CYC	C3C-C4C-CHD-C1D
5	e	200	CYC	NA-C1A-CHA-C4D
5	e	200	CYC	C2A-C1A-CHA-C4D
5	e	200	CYC	NA-C4A-CHB-C1B
5	e	200	CYC	C3A-C4A-CHB-C1B
5	e	200	CYC	C2B-C1B-CHB-C4A
5	e	200	CYC	C2C-C3C-CAC-CBC
5	e	200	CYC	C4C-C3C-CAC-CBC
5	e	200	CYC	NC-C4C-CHD-C1D
5	f	200	CYC	NA-C1A-CHA-C4D
5	f	200	CYC	C2A-C1A-CHA-C4D
5	f	200	CYC	ND-C4D-CHA-C1A
5	f	200	CYC	C3D-C4D-CHA-C1A

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Mol	Chain	Res	Type	Atoms
5	f	200	CYC	NA-C4A-CHB-C1B
5	f	200	CYC	C3A-C4A-CHB-C1B
5	f	200	CYC	C4C-C3C-CAC-CBC
5	f	200	CYC	NC-C4C-CHD-C1D
5	f	200	CYC	ND-C1D-CHD-C4C
5	f	200	CYC	C2D-C1D-CHD-C4C
5	f	200	CYC	C2D-C3D-CAD-CBD
5	f	200	CYC	C4D-C3D-CAD-CBD
5	g	200	CYC	NA-C4A-CHB-C1B
5	g	200	CYC	C3A-C4A-CHB-C1B
5	g	200	CYC	NB-C1B-CHB-C4A
5	g	200	CYC	C2B-C1B-CHB-C4A
5	g	200	CYC	NC-C4C-CHD-C1D
5	g	201	CYC	NA-C1A-CHA-C4D
5	g	201	CYC	C2A-C1A-CHA-C4D
5	g	201	CYC	ND-C4D-CHA-C1A
5	g	201	CYC	C3D-C4D-CHA-C1A
5	g	201	CYC	NA-C4A-CHB-C1B
5	g	201	CYC	C3A-C4A-CHB-C1B
5	g	201	CYC	C2C-C3C-CAC-CBC
5	g	201	CYC	NC-C4C-CHD-C1D
5	h	200	CYC	NA-C4A-CHB-C1B
5	h	200	CYC	C3A-C4A-CHB-C1B
5	h	200	CYC	C2C-C3C-CAC-CBC
5	h	200	CYC	C4C-C3C-CAC-CBC
5	h	200	CYC	NC-C4C-CHD-C1D
5	h	201	CYC	NA-C1A-CHA-C4D
5	h	201	CYC	C2A-C1A-CHA-C4D
5	h	201	CYC	NA-C4A-CHB-C1B
5	h	201	CYC	NC-C4C-CHD-C1D
5	i	200	CYC	NA-C1A-CHA-C4D
5	i	200	CYC	C2A-C1A-CHA-C4D
5	i	200	CYC	ND-C4D-CHA-C1A
5	i	200	CYC	C3D-C4D-CHA-C1A
5	i	200	CYC	C3A-C4A-CHB-C1B
5	i	200	CYC	NB-C1B-CHB-C4A
5	i	200	CYC	C2B-C1B-CHB-C4A
5	i	200	CYC	NC-C4C-CHD-C1D
5	i	200	CYC	ND-C1D-CHD-C4C
5	i	201	CYC	NA-C4A-CHB-C1B
5	i	201	CYC	C3A-C4A-CHB-C1B
5	i	201	CYC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
5	i	201	CYC	NC-C4C-CHD-C1D
5	i	201	CYC	ND-C1D-CHD-C4C
5	i	201	CYC	C2D-C1D-CHD-C4C
5	j	200	CYC	NA-C4A-CHB-C1B
5	j	200	CYC	C3A-C4A-CHB-C1B
5	j	200	CYC	C4C-C3C-CAC-CBC
5	j	200	CYC	NC-C4C-CHD-C1D
5	j	201	CYC	NA-C4A-CHB-C1B
5	j	201	CYC	C3A-C4A-CHB-C1B
5	j	201	CYC	NC-C4C-CHD-C1D
5	j	201	CYC	ND-C1D-CHD-C4C
5	j	201	CYC	C2D-C1D-CHD-C4C
5	j	201	CYC	C3D-CAD-CBD-CGD
5	k	200	CYC	NA-C4A-CHB-C1B
5	k	200	CYC	C3A-C4A-CHB-C1B
5	k	200	CYC	C2C-C3C-CAC-CBC
5	k	200	CYC	NC-C4C-CHD-C1D
5	k	200	CYC	C3C-C4C-CHD-C1D
5	k	201	CYC	NA-C4A-CHB-C1B
5	k	201	CYC	C3A-C4A-CHB-C1B
5	k	201	CYC	NC-C4C-CHD-C1D
5	k	201	CYC	ND-C1D-CHD-C4C
5	k	201	CYC	C2D-C1D-CHD-C4C
5	l	201	CYC	C2B-C1B-CHB-C4A
5	l	201	CYC	C2B-C3B-CAB-CBB
5	l	201	CYC	C4B-C3B-CAB-CBB
5	l	201	CYC	C2C-C3C-CAC-CBC
5	l	201	CYC	C4C-C3C-CAC-CBC
5	l	201	CYC	NC-C4C-CHD-C1D
5	l	201	CYC	ND-C1D-CHD-C4C
5	l	201	CYC	C2D-C1D-CHD-C4C
5	J	201	CYC	C2B-C3B-CAB-CBB
5	N	200	CYC	C2B-C3B-CAB-CBB
5	O	200	CYC	C2B-C3B-CAB-CBB
5	H	201	CYC	C2B-C3B-CAB-CBB
5	W	200	CYC	C2B-C3B-CAB-CBB
5	B	200	CYC	ND-C1D-CHD-C4C
5	C	200	CYC	ND-C1D-CHD-C4C
5	H	200	CYC	ND-C1D-CHD-C4C
5	H	201	CYC	ND-C1D-CHD-C4C
5	I	201	CYC	ND-C1D-CHD-C4C
5	K	201	CYC	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
5	L	201	CYC	ND-C1D-CHD-C4C
5	N	200	CYC	ND-C1D-CHD-C4C
5	O	200	CYC	ND-C1D-CHD-C4C
5	T	201	CYC	ND-C1D-CHD-C4C
5	U	200	CYC	ND-C1D-CHD-C4C
5	U	201	CYC	ND-C1D-CHD-C4C
5	V	201	CYC	ND-C1D-CHD-C4C
5	W	201	CYC	ND-C1D-CHD-C4C
5	X	200	CYC	ND-C1D-CHD-C4C
5	F	200	CYC	C2D-C1D-CHD-C4C
5	H	200	CYC	C2D-C1D-CHD-C4C
5	I	201	CYC	C2D-C1D-CHD-C4C
5	J	200	CYC	C2D-C1D-CHD-C4C
5	L	201	CYC	C2D-C1D-CHD-C4C
5	T	201	CYC	C2D-C1D-CHD-C4C
5	U	200	CYC	C2D-C1D-CHD-C4C
5	U	201	CYC	C2D-C1D-CHD-C4C
5	V	201	CYC	C2D-C1D-CHD-C4C
5	W	201	CYC	C2D-C1D-CHD-C4C
5	h	201	CYC	C2D-C1D-CHD-C4C
5	i	200	CYC	C2D-C1D-CHD-C4C
5	j	200	CYC	C2D-C1D-CHD-C4C
5	e	200	CYC	NB-C1B-CHB-C4A
5	F	200	CYC	NA-C1A-CHA-C4D
5	J	201	CYC	NA-C1A-CHA-C4D
5	L	201	CYC	NA-C1A-CHA-C4D
5	U	201	CYC	NA-C1A-CHA-C4D
5	G	200	CYC	C2B-C3B-CAB-CBB
5	5	1202	CYC	C3D-CAD-CBD-CGD
5	B	200	CYC	C2A-CAA-CBA-CGA
5	L	201	CYC	C3D-CAD-CBD-CGD
5	T	200	CYC	C2A-CAA-CBA-CGA
5	X	201	CYC	C2A-CAA-CBA-CGA
5	X	201	CYC	C3D-CAD-CBD-CGD
5	Y	200	CYC	C2A-CAA-CBA-CGA
5	a	200	CYC	C2A-CAA-CBA-CGA
5	a	200	CYC	C3D-CAD-CBD-CGD
5	c	200	CYC	C2A-CAA-CBA-CGA
5	f	200	CYC	C3D-CAD-CBD-CGD
5	h	201	CYC	C3D-CAD-CBD-CGD
5	j	200	CYC	C2A-CAA-CBA-CGA
5	l	201	CYC	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
5	A	200	CYC	C2B-C3B-CAB-CBB
5	H	200	CYC	C3A-C4A-CHB-C1B
5	K	201	CYC	C3A-C4A-CHB-C1B
5	R	200	CYC	C3A-C4A-CHB-C1B
5	h	201	CYC	C3A-C4A-CHB-C1B
5	5	1201	CYC	ND-C1D-CHD-C4C
5	5	1202	CYC	ND-C1D-CHD-C4C
5	A	200	CYC	ND-C1D-CHD-C4C
5	D	200	CYC	ND-C1D-CHD-C4C
5	E	200	CYC	ND-C1D-CHD-C4C
5	F	200	CYC	ND-C1D-CHD-C4C
5	G	200	CYC	ND-C1D-CHD-C4C
5	I	200	CYC	ND-C1D-CHD-C4C
5	J	200	CYC	ND-C1D-CHD-C4C
5	K	200	CYC	ND-C1D-CHD-C4C
5	P	200	CYC	ND-C1D-CHD-C4C
5	T	200	CYC	ND-C1D-CHD-C4C
5	W	200	CYC	ND-C1D-CHD-C4C
5	Y	200	CYC	ND-C1D-CHD-C4C
5	Y	201	CYC	ND-C4D-CHA-C1A
5	b	200	CYC	ND-C1D-CHD-C4C
5	d	200	CYC	ND-C1D-CHD-C4C
5	e	200	CYC	ND-C1D-CHD-C4C
5	g	200	CYC	ND-C1D-CHD-C4C
5	g	201	CYC	ND-C1D-CHD-C4C
5	h	200	CYC	ND-C1D-CHD-C4C
5	h	201	CYC	ND-C1D-CHD-C4C
5	j	200	CYC	ND-C1D-CHD-C4C
5	k	200	CYC	ND-C1D-CHD-C4C
5	5	1201	CYC	C2D-C1D-CHD-C4C
5	5	1202	CYC	C2D-C1D-CHD-C4C
5	A	200	CYC	C2D-C1D-CHD-C4C
5	B	200	CYC	C2D-C1D-CHD-C4C
5	D	200	CYC	C2D-C1D-CHD-C4C
5	G	200	CYC	C2D-C1D-CHD-C4C
5	H	201	CYC	C2D-C1D-CHD-C4C
5	I	200	CYC	C2D-C1D-CHD-C4C
5	K	200	CYC	C2D-C1D-CHD-C4C
5	N	200	CYC	C2D-C1D-CHD-C4C
5	O	200	CYC	C2D-C1D-CHD-C4C
5	P	200	CYC	C2D-C1D-CHD-C4C
5	T	200	CYC	C2D-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
5	W	200	CYC	C2D-C1D-CHD-C4C
5	Y	200	CYC	C2D-C1D-CHD-C4C
5	b	200	CYC	C2D-C1D-CHD-C4C
5	d	200	CYC	C2D-C1D-CHD-C4C
5	e	200	CYC	C2D-C1D-CHD-C4C
5	g	200	CYC	C2D-C1D-CHD-C4C
5	g	201	CYC	C2D-C1D-CHD-C4C
5	h	200	CYC	C2D-C1D-CHD-C4C
5	k	200	CYC	C2D-C1D-CHD-C4C
5	W	201	CYC	NB-C1B-CHB-C4A
5	a	200	CYC	NB-C1B-CHB-C4A
5	l	201	CYC	NB-C1B-CHB-C4A
5	W	201	CYC	C2B-C1B-CHB-C4A
5	V	200	CYC	ND-C1D-CHD-C4C
5	C	200	CYC	C2D-C1D-CHD-C4C
5	E	200	CYC	C2D-C1D-CHD-C4C
5	V	200	CYC	C2D-C1D-CHD-C4C
5	Y	201	CYC	C3D-C4D-CHA-C1A
5	h	200	CYC	C2B-C3B-CAB-CBB
5	F	200	CYC	C4B-C3B-CAB-CBB
5	J	201	CYC	C4B-C3B-CAB-CBB
5	N	200	CYC	C4B-C3B-CAB-CBB
5	O	200	CYC	C4B-C3B-CAB-CBB
5	B	200	CYC	C2B-C3B-CAB-CBB
5	H	200	CYC	C2B-C1B-CHB-C4A
5	K	200	CYC	NA-C4A-CHB-C1B
5	A	200	CYC	C2A-CAA-CBA-CGA
5	A	200	CYC	C3D-CAD-CBD-CGD
5	G	200	CYC	C3D-CAD-CBD-CGD
5	I	200	CYC	C2A-CAA-CBA-CGA
5	J	201	CYC	C2A-CAA-CBA-CGA
5	R	200	CYC	C3D-CAD-CBD-CGD
5	S	200	CYC	C2A-CAA-CBA-CGA
5	X	200	CYC	C2A-CAA-CBA-CGA
5	f	200	CYC	C2A-CAA-CBA-CGA
5	h	201	CYC	C2A-CAA-CBA-CGA
5	k	201	CYC	C3D-CAD-CBD-CGD
5	c	200	CYC	C2B-C3B-CAB-CBB
5	O	200	CYC	C3A-C4A-CHB-C1B
5	U	201	CYC	ND-C4D-CHA-C1A
5	D	200	CYC	C2B-C3B-CAB-CBB
5	H	200	CYC	NB-C1B-CHB-C4A

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Mol	Chain	Res	Type	Atoms
5	Y	201	CYC	NB-C1B-CHB-C4A
5	i	201	CYC	NB-C1B-CHB-C4A
5	d	200	CYC	NA-C1A-CHA-C4D
5	a	200	CYC	C2D-C3D-CAD-CBD
5	c	200	CYC	C2D-C3D-CAD-CBD
5	T	201	CYC	C2A-C1A-CHA-C4D
5	U	201	CYC	C2A-C1A-CHA-C4D
5	C	200	CYC	C2B-C3B-CAB-CBB
5	P	200	CYC	C2B-C3B-CAB-CBB
5	O	200	CYC	NA-C4A-CHB-C1B
5	W	201	CYC	NA-C4A-CHB-C1B
5	X	200	CYC	NA-C4A-CHB-C1B
5	Y	201	CYC	NA-C4A-CHB-C1B
5	a	200	CYC	NA-C4A-CHB-C1B
5	i	200	CYC	NA-C4A-CHB-C1B
5	l	201	CYC	NA-C4A-CHB-C1B
5	C	200	CYC	C3D-CAD-CBD-CGD
5	Q	200	CYC	C3D-CAD-CBD-CGD
5	e	200	CYC	C2A-CAA-CBA-CGA
5	V	200	CYC	NB-C1B-CHB-C4A
5	L	201	CYC	C3A-C4A-CHB-C1B
5	W	201	CYC	C3A-C4A-CHB-C1B
5	X	200	CYC	C3A-C4A-CHB-C1B
5	Y	201	CYC	C3A-C4A-CHB-C1B
5	a	200	CYC	C3A-C4A-CHB-C1B
5	l	201	CYC	C3A-C4A-CHB-C1B
5	J	200	CYC	C2B-C3B-CAB-CBB
5	Y	201	CYC	C2B-C1B-CHB-C4A
5	i	201	CYC	C2B-C1B-CHB-C4A
5	a	200	CYC	NA-C1A-CHA-C4D
5	L	201	CYC	C2B-C3B-CAB-CBB
5	a	200	CYC	C2B-C3B-CAB-CBB
5	H	201	CYC	C4B-C3B-CAB-CBB
5	W	200	CYC	C4B-C3B-CAB-CBB
5	F	200	CYC	C2A-C1A-CHA-C4D
5	J	201	CYC	C2A-C1A-CHA-C4D
5	L	201	CYC	C2A-C1A-CHA-C4D
5	B	200	CYC	C2D-C3D-CAD-CBD
5	L	201	CYC	ND-C4D-CHA-C1A
5	V	200	CYC	C2B-C1B-CHB-C4A
5	J	201	CYC	C3D-CAD-CBD-CGD
5	N	200	CYC	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
5	P	200	CYC	C2A-CAA-CBA-CGA
5	T	201	CYC	C3D-CAD-CBD-CGD
5	b	200	CYC	C2A-CAA-CBA-CGA
5	h	200	CYC	C2A-CAA-CBA-CGA
5	U	201	CYC	C3D-C4D-CHA-C1A
5	S	200	CYC	C2D-C3D-CAD-CBD
5	S	200	CYC	ND-C4D-CHA-C1A
5	X	201	CYC	NB-C1B-CHB-C4A
5	W	200	CYC	NA-C1A-CHA-C4D
5	L	201	CYC	C3D-C4D-CHA-C1A
5	5	1201	CYC	C2C-C3C-CAC-CBC
5	I	200	CYC	C2C-C3C-CAC-CBC
5	i	201	CYC	C2C-C3C-CAC-CBC
5	j	200	CYC	C2C-C3C-CAC-CBC
5	A	200	CYC	ND-C4D-CHA-C1A
5	S	200	CYC	C3D-C4D-CHA-C1A
5	G	201	CYC	ND-C4D-CHA-C1A
5	k	200	CYC	ND-C4D-CHA-C1A
5	H	200	CYC	C2B-C3B-CAB-CBB
5	G	201	CYC	C3D-C4D-CHA-C1A
5	d	200	CYC	C2A-C1A-CHA-C4D
5	D	200	CYC	NA-C1A-CHA-C4D
5	G	201	CYC	NA-C1A-CHA-C4D
5	F	200	CYC	C2A-CAA-CBA-CGA
5	U	201	CYC	C2A-CAA-CBA-CGA
5	i	200	CYC	C2A-CAA-CBA-CGA
5	i	201	CYC	C3D-CAD-CBD-CGD
5	k	200	CYC	C2A-CAA-CBA-CGA
5	G	200	CYC	C4B-C3B-CAB-CBB
5	a	200	CYC	C2A-C1A-CHA-C4D
5	K	200	CYC	NB-C1B-CHB-C4A
5	E	200	CYC	NA-C1A-CHA-C4D
5	X	201	CYC	C2B-C1B-CHB-C4A
5	k	200	CYC	C3D-C4D-CHA-C1A
5	d	200	CYC	NB-C1B-CHB-C4A
5	G	201	CYC	C2A-C1A-CHA-C4D
5	W	200	CYC	C2A-C1A-CHA-C4D
5	H	201	CYC	NA-C1A-CHA-C4D
5	U	200	CYC	C4C-C3C-CAC-CBC
5	k	200	CYC	C4C-C3C-CAC-CBC
5	a	200	CYC	ND-C4D-CHA-C1A
5	P	200	CYC	C4D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
5	S	200	CYC	C4D-C3D-CAD-CBD
5	A	200	CYC	C4B-C3B-CAB-CBB
5	Y	201	CYC	C4B-C3B-CAB-CBB
5	A	200	CYC	C3D-C4D-CHA-C1A
5	a	200	CYC	C3D-C4D-CHA-C1A
5	V	201	CYC	C3D-CAD-CBD-CGD
5	X	200	CYC	NB-C1B-CHB-C4A
5	I	201	CYC	C3D-CAD-CBD-CGD
5	B	200	CYC	C4B-C3B-CAB-CBB
5	h	200	CYC	C4B-C3B-CAB-CBB
5	D	200	CYC	C2A-C1A-CHA-C4D
5	X	200	CYC	C2C-C3C-CAC-CBC
5	i	201	CYC	NA-C1A-CHA-C4D
5	B	200	CYC	C3D-CAD-CBD-CGD
5	C	200	CYC	C2A-CAA-CBA-CGA
5	E	200	CYC	C2A-C1A-CHA-C4D
5	H	201	CYC	C2A-C1A-CHA-C4D
5	Y	201	CYC	C2B-C3B-CAB-CBB
5	g	201	CYC	NB-C1B-CHB-C4A
5	E	200	CYC	ND-C4D-CHA-C1A
5	h	201	CYC	ND-C4D-CHA-C1A
5	c	200	CYC	C4B-C3B-CAB-CBB
5	H	201	CYC	C2A-CAA-CBA-CGA
5	X	200	CYC	ND-C4D-CHA-C1A
5	5	1202	CYC	CAA-CBA-CGA-O2A
5	V	201	CYC	C2B-C3B-CAB-CBB
5	K	200	CYC	C3D-CAD-CBD-CGD
5	K	201	CYC	NA-C1A-CHA-C4D
5	c	200	CYC	NA-C1A-CHA-C4D
5	W	200	CYC	CAA-CBA-CGA-O1A
5	c	200	CYC	CAD-CBD-CGD-O1D
5	i	201	CYC	CAA-CBA-CGA-O1A
5	A	200	CYC	CAA-CBA-CGA-O2A
5	C	200	CYC	CAA-CBA-CGA-O2A
5	J	201	CYC	CAD-CBD-CGD-O2D
5	S	200	CYC	CAA-CBA-CGA-O1A
5	a	200	CYC	CAA-CBA-CGA-O2A
5	j	200	CYC	CAA-CBA-CGA-O1A
5	l	201	CYC	CAA-CBA-CGA-O2A
5	5	1202	CYC	C2A-CAA-CBA-CGA
5	A	200	CYC	CAA-CBA-CGA-O1A
5	L	201	CYC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
5	Y	200	CYC	CAA-CBA-CGA-O1A
5	Y	201	CYC	CAA-CBA-CGA-O2A
5	d	200	CYC	CAD-CBD-CGD-O1D
5	D	200	CYC	CAA-CBA-CGA-O1A
5	P	200	CYC	CAA-CBA-CGA-O2A
5	c	200	CYC	CAA-CBA-CGA-O2A
5	g	201	CYC	CAD-CBD-CGD-O1D
5	H	201	CYC	CAD-CBD-CGD-O1D
5	N	200	CYC	CAA-CBA-CGA-O1A
5	i	201	CYC	CAD-CBD-CGD-O2D
5	D	200	CYC	CAA-CBA-CGA-O2A
5	Q	200	CYC	CAA-CBA-CGA-O2A
5	Y	201	CYC	CAA-CBA-CGA-O1A
5	a	200	CYC	CAA-CBA-CGA-O1A
5	c	200	CYC	CAD-CBD-CGD-O2D
5	F	200	CYC	CAA-CBA-CGA-O1A
5	G	201	CYC	CAD-CBD-CGD-O2D
5	I	200	CYC	CAA-CBA-CGA-O1A
5	K	201	CYC	CAA-CBA-CGA-O1A
5	N	200	CYC	CAA-CBA-CGA-O2A
5	i	201	CYC	CAA-CBA-CGA-O2A
5	G	200	CYC	CAA-CBA-CGA-O1A
5	I	201	CYC	CAA-CBA-CGA-O1A
5	Q	200	CYC	CAA-CBA-CGA-O1A
5	b	200	CYC	CAD-CBD-CGD-O1D
5	d	200	CYC	CAD-CBD-CGD-O2D
5	e	200	CYC	CAD-CBD-CGD-O2D
5	G	200	CYC	CAA-CBA-CGA-O2A
5	V	201	CYC	CAA-CBA-CGA-O2A
5	H	201	CYC	CAD-CBD-CGD-O2D
5	L	201	CYC	CAA-CBA-CGA-O2A
5	T	201	CYC	CAA-CBA-CGA-O2A
5	U	201	CYC	CAA-CBA-CGA-O2A
5	V	201	CYC	CAD-CBD-CGD-O1D
5	Y	200	CYC	CAA-CBA-CGA-O2A
5	i	200	CYC	CAA-CBA-CGA-O1A
5	j	200	CYC	CAA-CBA-CGA-O2A
5	O	200	CYC	C2A-CAA-CBA-CGA
5	g	201	CYC	C2A-CAA-CBA-CGA
5	T	201	CYC	CAA-CBA-CGA-O1A
5	W	200	CYC	CAA-CBA-CGA-O2A
5	W	201	CYC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
5	J	201	CYC	CAA-CBA-CGA-O2A
5	e	200	CYC	CAA-CBA-CGA-O1A
5	i	200	CYC	CAA-CBA-CGA-O2A
5	J	201	CYC	CAA-CBA-CGA-O1A
5	h	200	CYC	CAA-CBA-CGA-O2A
5	d	200	CYC	C2B-C1B-CHB-C4A
5	A	200	CYC	CAD-CBD-CGD-O1D
5	K	201	CYC	CAA-CBA-CGA-O2A
5	J	201	CYC	CAD-CBD-CGD-O1D
5	U	201	CYC	CAA-CBA-CGA-O1A
5	V	200	CYC	CAA-CBA-CGA-O2A
5	g	201	CYC	CAD-CBD-CGD-O2D
5	C	200	CYC	CAA-CBA-CGA-O1A
5	T	200	CYC	CAA-CBA-CGA-O2A
5	e	200	CYC	CAD-CBD-CGD-O1D
5	h	200	CYC	CAA-CBA-CGA-O1A
5	I	200	CYC	C2B-C3B-CAB-CBB
5	G	201	CYC	CAD-CBD-CGD-O1D
5	V	201	CYC	CAA-CBA-CGA-O1A
5	k	201	CYC	NB-C1B-CHB-C4A
5	O	200	CYC	CAA-CBA-CGA-O2A
5	O	200	CYC	CAD-CBD-CGD-O1D
5	b	200	CYC	CAD-CBD-CGD-O2D
5	K	201	CYC	C2A-CAA-CBA-CGA
5	k	200	CYC	C3D-CAD-CBD-CGD
5	i	201	CYC	C2A-C1A-CHA-C4D
5	R	200	CYC	CAA-CBA-CGA-O1A
5	S	200	CYC	CAA-CBA-CGA-O2A
5	W	201	CYC	CAD-CBD-CGD-O2D
5	e	200	CYC	CAA-CBA-CGA-O2A
5	H	201	CYC	C4C-C3C-CAC-CBC
5	I	201	CYC	CAA-CBA-CGA-O2A
5	P	200	CYC	CAA-CBA-CGA-O1A
5	c	200	CYC	CAA-CBA-CGA-O1A
5	d	200	CYC	CAA-CBA-CGA-O1A
5	i	201	CYC	CAD-CBD-CGD-O1D
5	F	200	CYC	CAD-CBD-CGD-O2D
5	d	200	CYC	CAA-CBA-CGA-O2A
5	l	201	CYC	CAA-CBA-CGA-O1A
5	5	1202	CYC	CAA-CBA-CGA-O1A
5	I	200	CYC	CAA-CBA-CGA-O2A
5	Q	200	CYC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
5	T	201	CYC	CAD-CBD-CGD-O2D
5	X	201	CYC	CAD-CBD-CGD-O1D
5	X	201	CYC	CAD-CBD-CGD-O2D
5	h	201	CYC	C3D-C4D-CHA-C1A
5	A	200	CYC	CAD-CBD-CGD-O2D
5	V	201	CYC	CAD-CBD-CGD-O2D
5	j	201	CYC	CAD-CBD-CGD-O1D
5	j	201	CYC	CAD-CBD-CGD-O2D
5	F	200	CYC	CAA-CBA-CGA-O2A
5	T	200	CYC	CAA-CBA-CGA-O1A
5	A	200	CYC	C4D-C3D-CAD-CBD
5	5	1202	CYC	CAD-CBD-CGD-O2D
5	V	200	CYC	CAA-CBA-CGA-O1A
5	h	201	CYC	CAD-CBD-CGD-O1D
5	E	200	CYC	CAA-CBA-CGA-O1A
5	F	200	CYC	CAD-CBD-CGD-O1D
5	O	200	CYC	CAA-CBA-CGA-O1A
5	T	201	CYC	CAD-CBD-CGD-O1D
5	Q	200	CYC	C3A-C2A-CAA-CBA
5	Q	200	CYC	C1A-C2A-CAA-CBA
5	k	200	CYC	C1A-C2A-CAA-CBA
5	X	200	CYC	CAA-CBA-CGA-O2A
5	K	200	CYC	C2B-C1B-CHB-C4A
5	K	201	CYC	CAD-CBD-CGD-O2D
5	l	201	CYC	NA-C1A-CHA-C4D
5	Q	200	CYC	CAD-CBD-CGD-O1D
5	K	201	CYC	CAD-CBD-CGD-O1D
5	X	200	CYC	CAA-CBA-CGA-O1A
5	k	200	CYC	C3A-C2A-CAA-CBA
5	j	201	CYC	C2A-CAA-CBA-CGA
5	E	200	CYC	CAD-CBD-CGD-O1D
5	5	1202	CYC	CAD-CBD-CGD-O1D
5	O	200	CYC	CAD-CBD-CGD-O2D
5	g	201	CYC	C2B-C1B-CHB-C4A
5	C	200	CYC	C4B-C3B-CAB-CBB
5	D	200	CYC	C4B-C3B-CAB-CBB
5	K	201	CYC	C2A-C1A-CHA-C4D
5	Y	201	CYC	C3D-CAD-CBD-CGD
5	R	200	CYC	CAA-CBA-CGA-O2A
5	B	200	CYC	CAD-CBD-CGD-O2D
5	H	200	CYC	CAA-CBA-CGA-O2A
5	E	200	CYC	C3D-C4D-CHA-C1A

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Mol	Chain	Res	Type	Atoms
5	P	200	CYC	C2D-C3D-CAD-CBD
5	f	200	CYC	CAA-CBA-CGA-O2A
5	U	201	CYC	CAD-CBD-CGD-O1D
5	D	200	CYC	CAD-CBD-CGD-O2D
5	D	200	CYC	CAD-CBD-CGD-O1D
5	E	200	CYC	CAA-CBA-CGA-O2A
5	U	201	CYC	CAD-CBD-CGD-O2D
5	h	201	CYC	CAD-CBD-CGD-O2D
5	H	201	CYC	CAA-CBA-CGA-O1A
5	A	200	CYC	C2D-C3D-CAD-CBD
5	P	200	CYC	C4B-C3B-CAB-CBB
5	H	200	CYC	CAA-CBA-CGA-O1A
5	G	200	CYC	NA-C1A-CHA-C4D
5	f	200	CYC	CAA-CBA-CGA-O1A
5	X	200	CYC	C3D-C4D-CHA-C1A
5	D	200	CYC	C2A-CAA-CBA-CGA
5	N	200	CYC	C3D-CAD-CBD-CGD
5	E	200	CYC	CAD-CBD-CGD-O2D
5	B	200	CYC	CAD-CBD-CGD-O1D
5	e	200	CYC	C2B-C3B-CAB-CBB
5	K	200	CYC	CAA-CBA-CGA-O2A
5	N	200	CYC	CAD-CBD-CGD-O2D
5	H	201	CYC	CAA-CBA-CGA-O2A
5	R	200	CYC	CAD-CBD-CGD-O2D
5	G	201	CYC	C2B-C3B-CAB-CBB
5	Y	201	CYC	C2A-CAA-CBA-CGA
5	K	200	CYC	CAA-CBA-CGA-O1A
5	a	200	CYC	C4B-C3B-CAB-CBB
5	K	201	CYC	C2B-C3B-CAB-CBB
5	R	200	CYC	CAD-CBD-CGD-O1D

There are no ring outliers.

54 monomers are involved in 323 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	k	200	CYC	9	0
5	U	200	CYC	3	0
5	I	200	CYC	8	0
5	T	201	CYC	7	0
5	D	200	CYC	1	0
5	c	200	CYC	8	0
5	j	200	CYC	6	0

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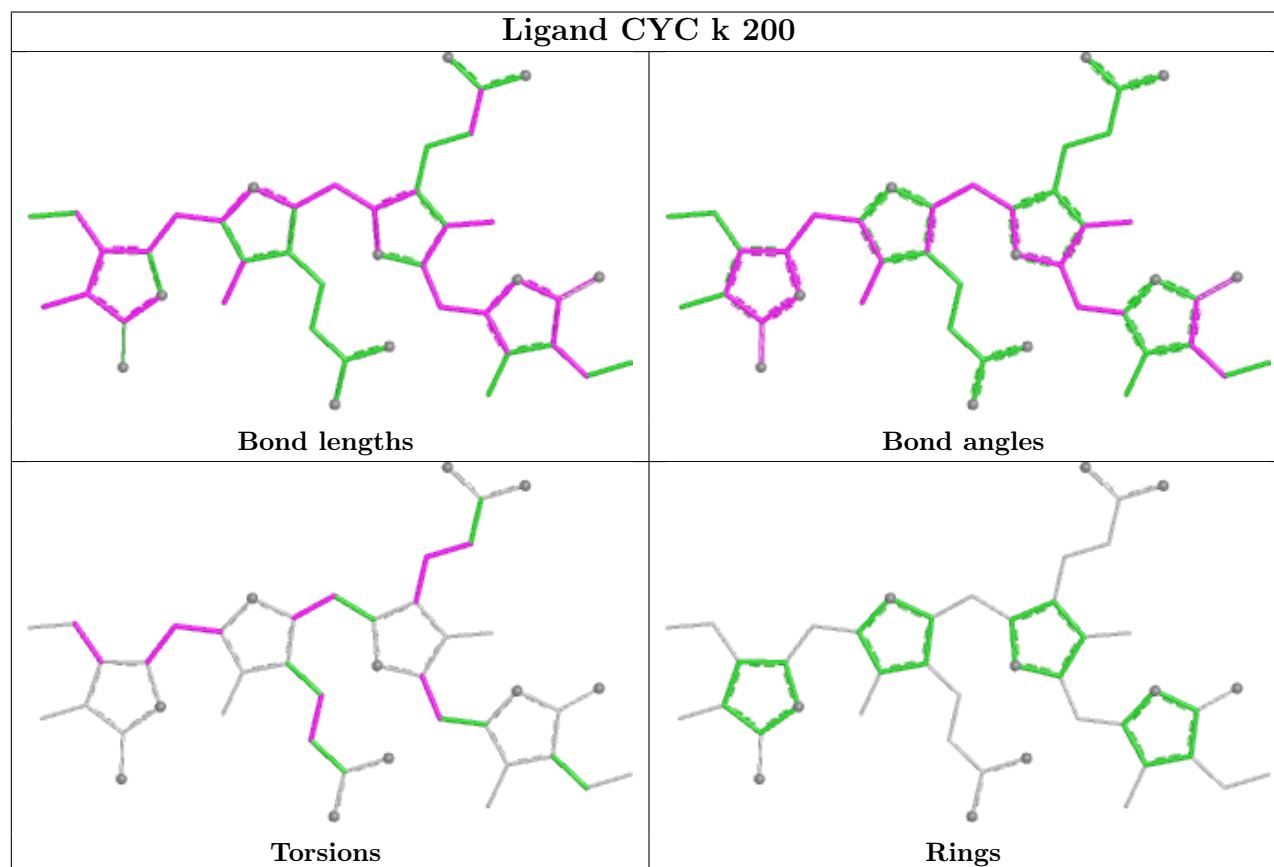
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	W	200	CYC	10	0
5	V	201	CYC	3	0
5	k	201	CYC	4	0
5	Y	201	CYC	5	0
5	A	200	CYC	3	0
5	I	201	CYC	4	0
5	l	201	CYC	7	0
5	Q	200	CYC	10	0
5	R	200	CYC	4	0
5	V	200	CYC	4	0
5	E	200	CYC	8	0
5	i	200	CYC	5	0
5	5	1202	CYC	12	0
5	i	201	CYC	4	0
5	f	200	CYC	6	0
5	5	1201	CYC	7	0
5	W	201	CYC	1	0
5	j	201	CYC	3	0
5	O	200	CYC	13	0
5	G	201	CYC	6	0
5	g	200	CYC	6	0
5	d	200	CYC	7	0
5	S	200	CYC	5	0
5	B	200	CYC	9	0
5	X	201	CYC	4	0
5	L	201	CYC	5	0
5	K	201	CYC	4	0
5	J	200	CYC	12	0
5	H	201	CYC	5	0
5	F	200	CYC	6	0
5	K	200	CYC	5	0
5	b	200	CYC	2	0
5	G	200	CYC	5	0
5	e	200	CYC	4	0
5	U	201	CYC	4	0
5	T	200	CYC	2	0
5	X	200	CYC	6	0
5	a	200	CYC	4	0
5	g	201	CYC	9	0
5	Y	200	CYC	8	0
5	C	200	CYC	7	0
5	H	200	CYC	15	0

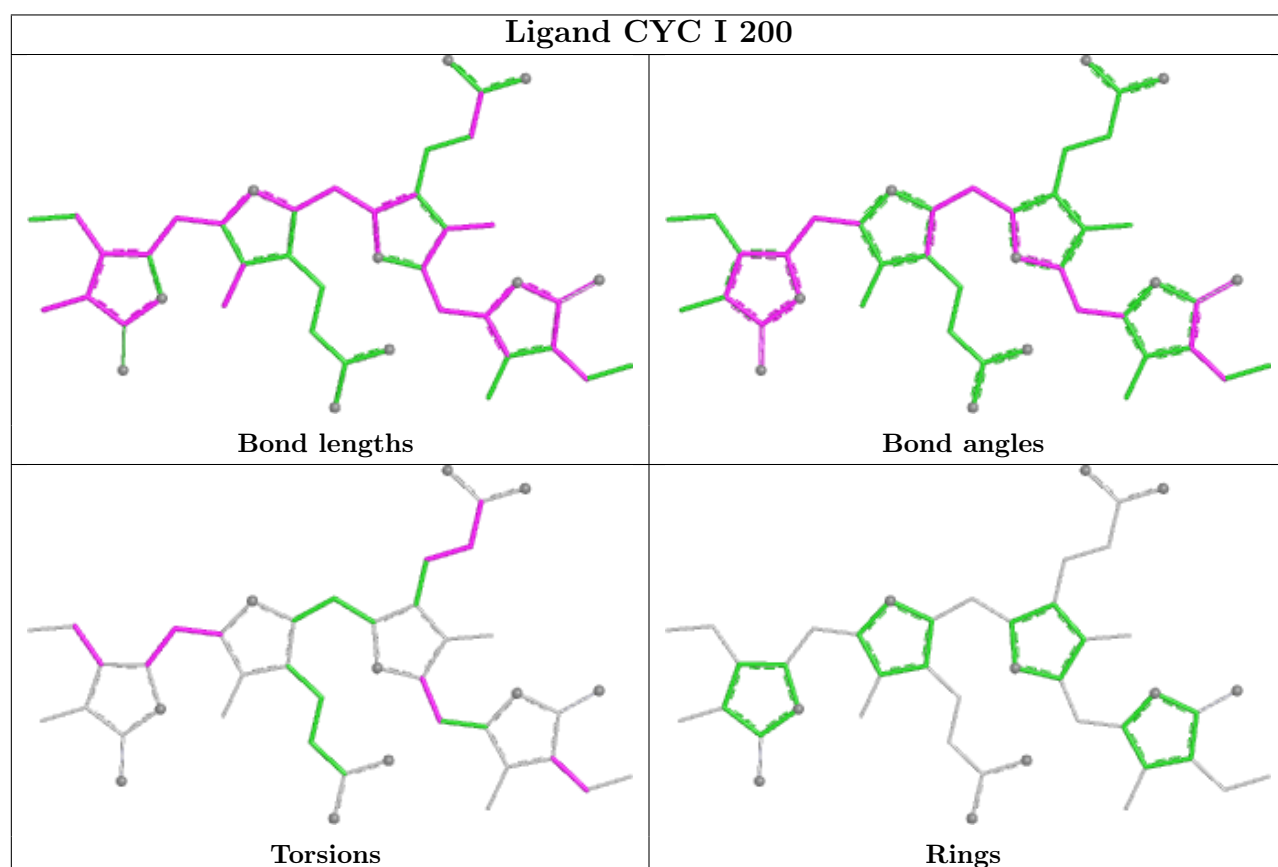
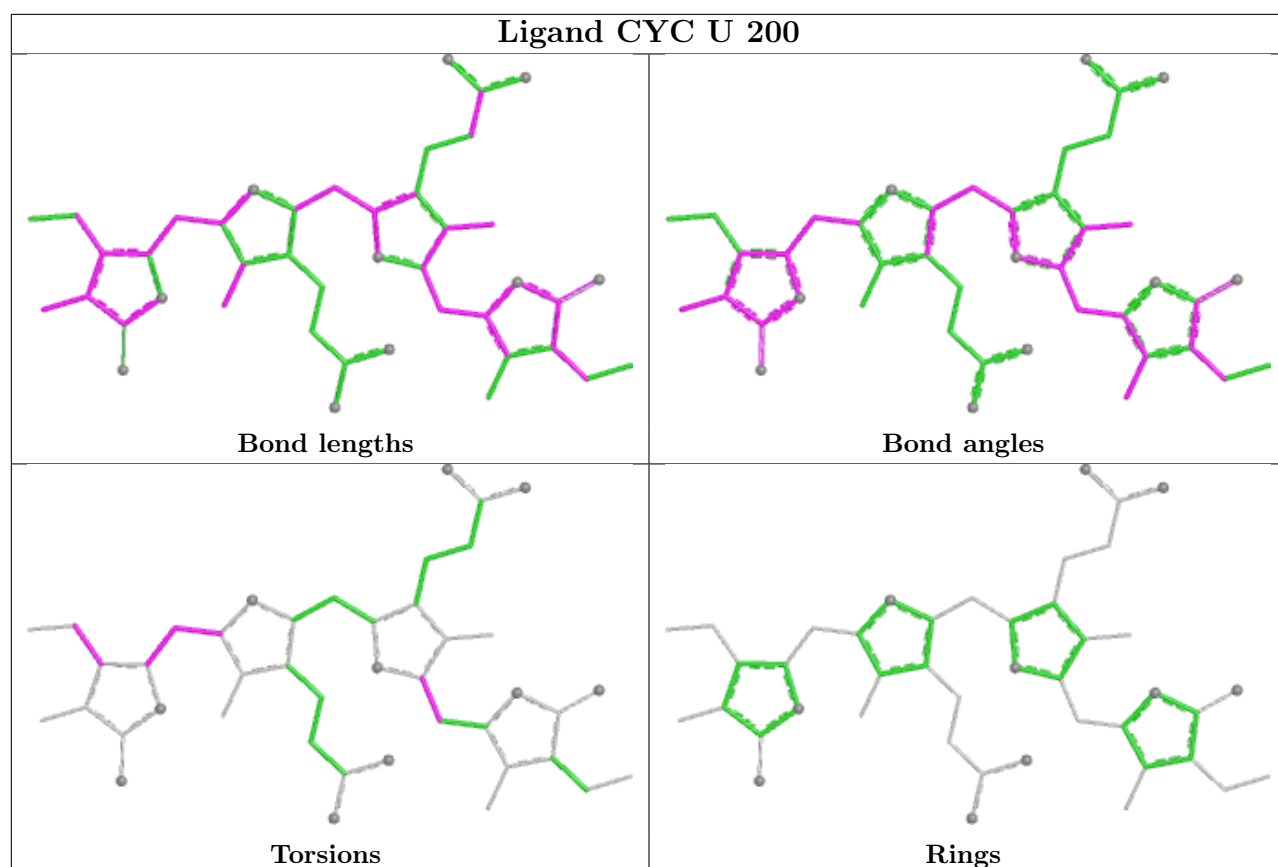
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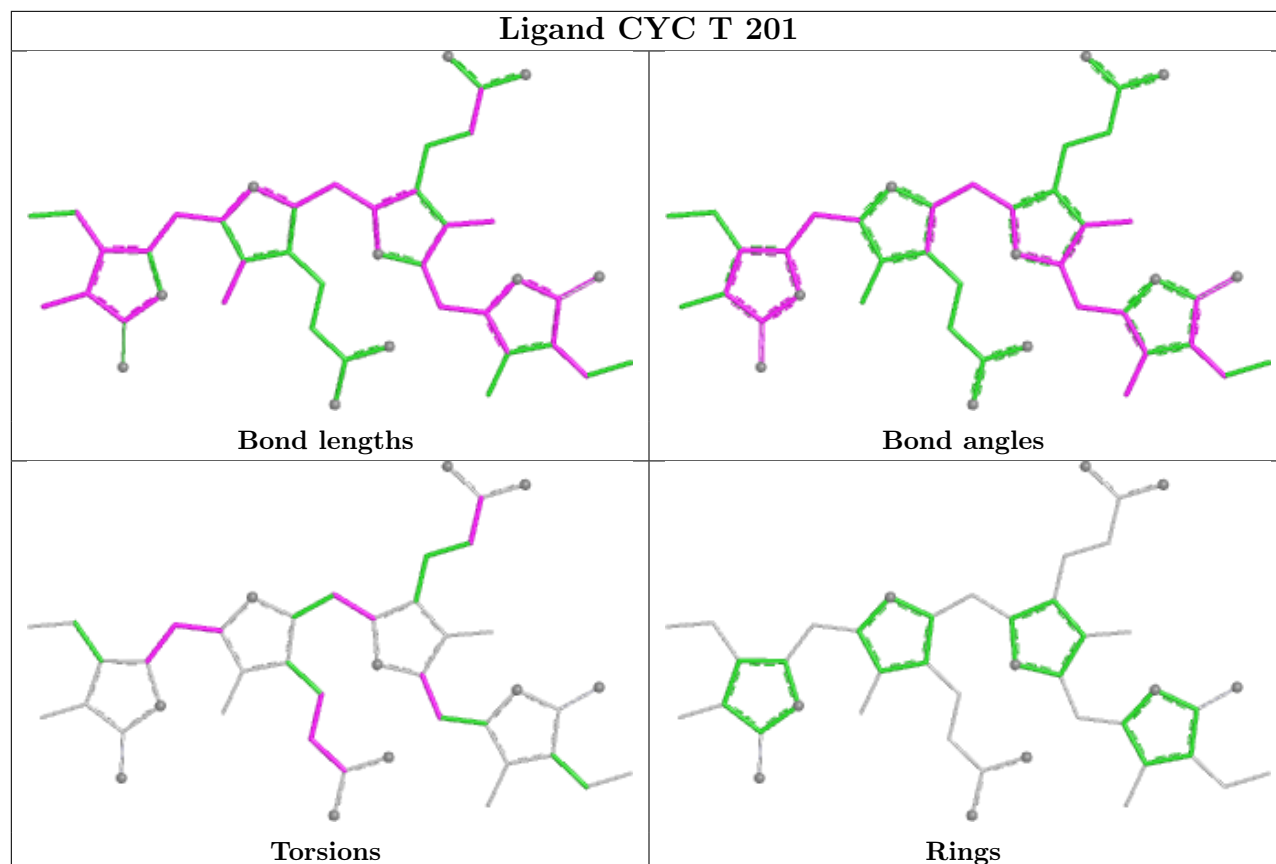
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	200	CYC	7	0
5	P	200	CYC	4	0
5	h	201	CYC	2	0
5	h	200	CYC	11	0
5	J	201	CYC	4	0

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.

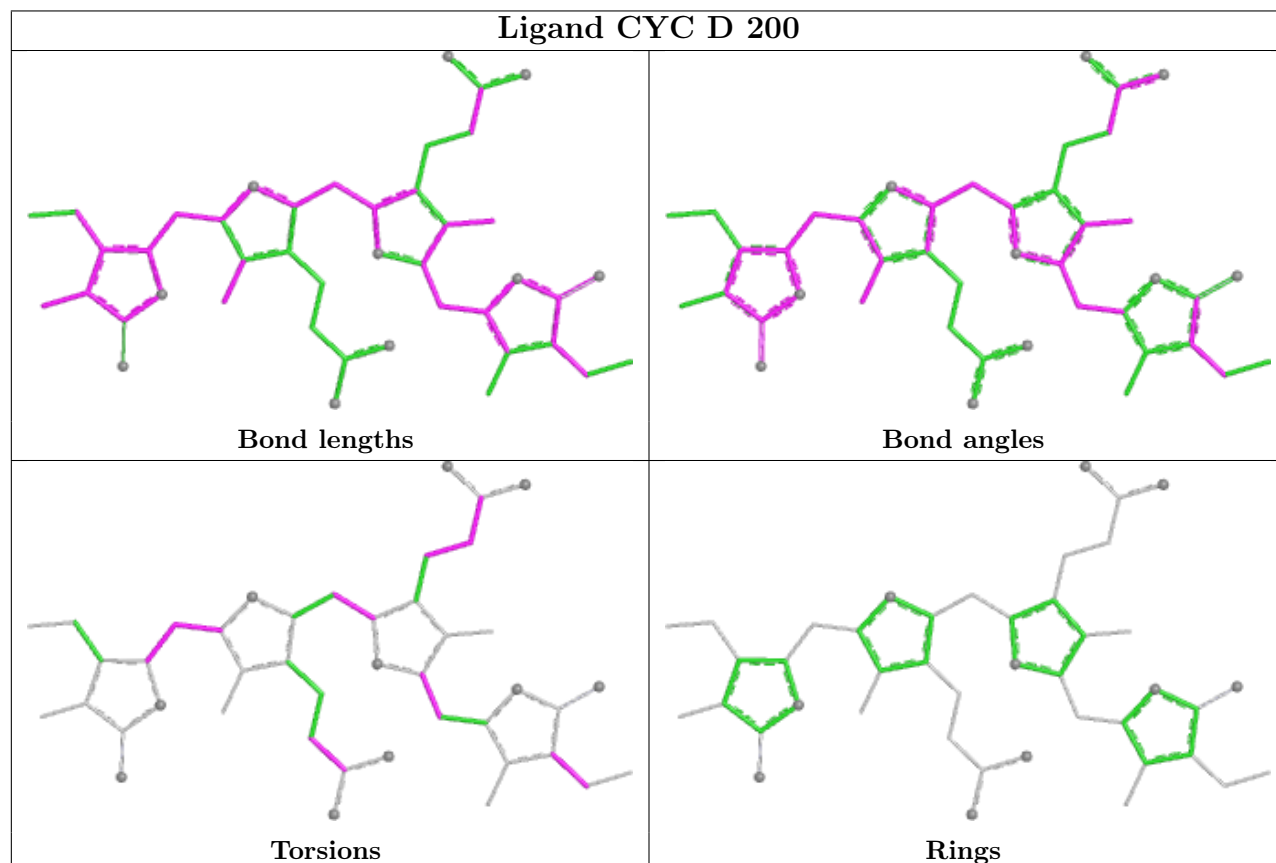




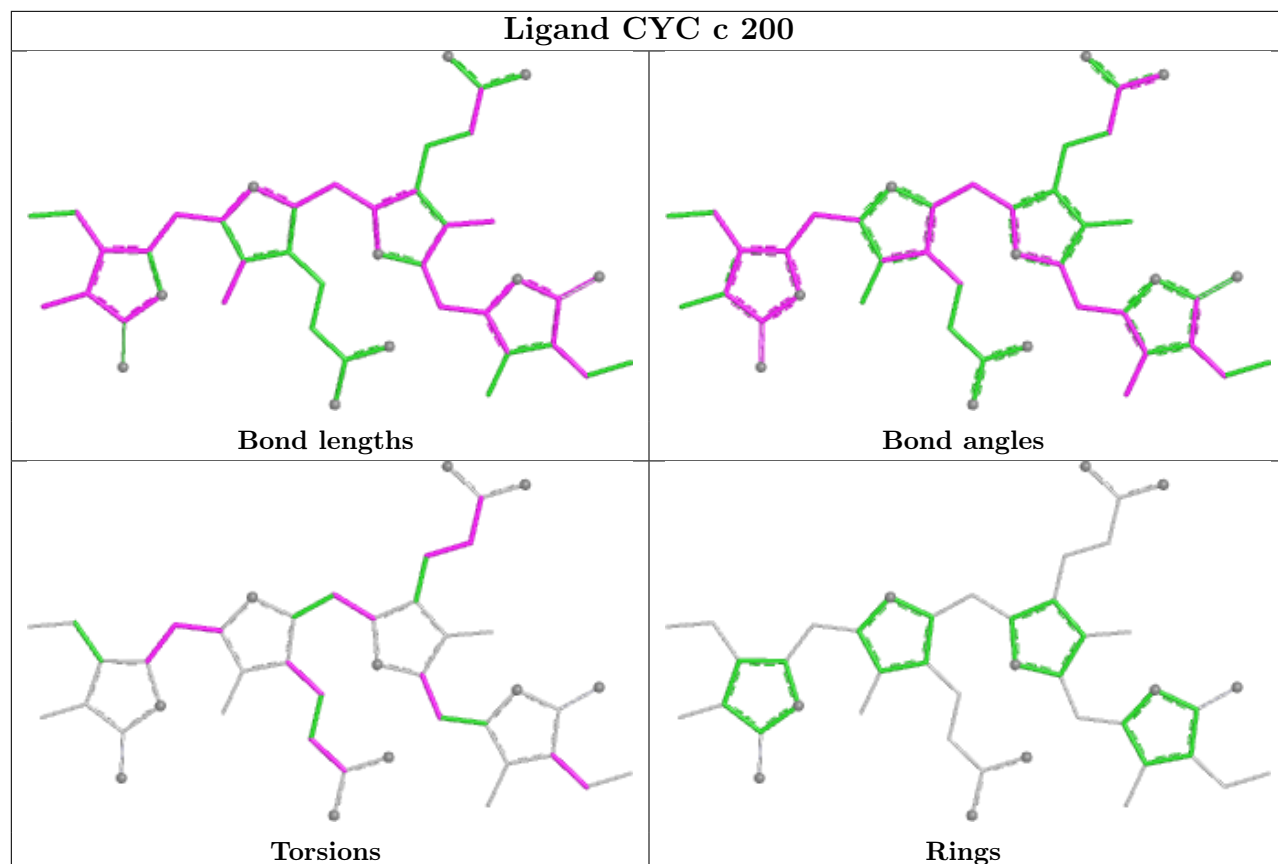
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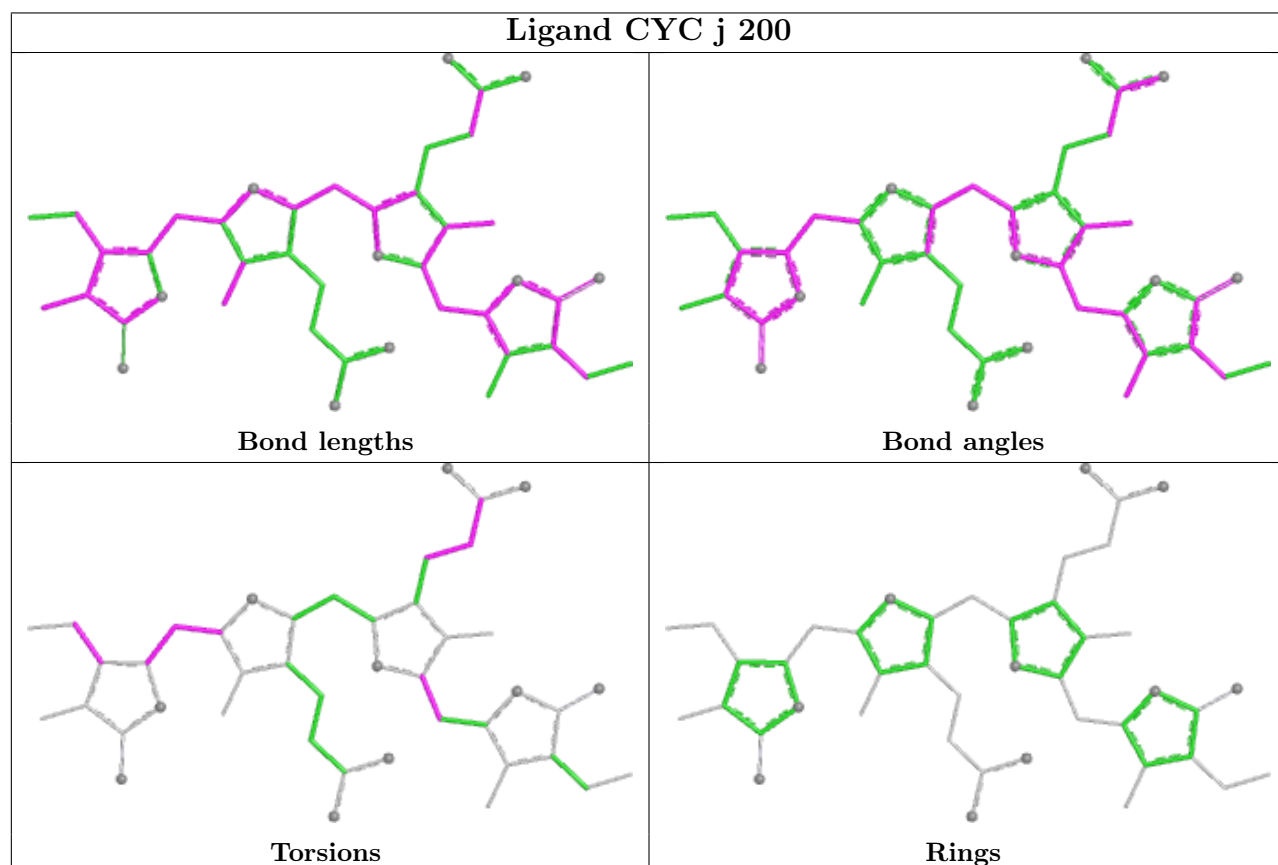
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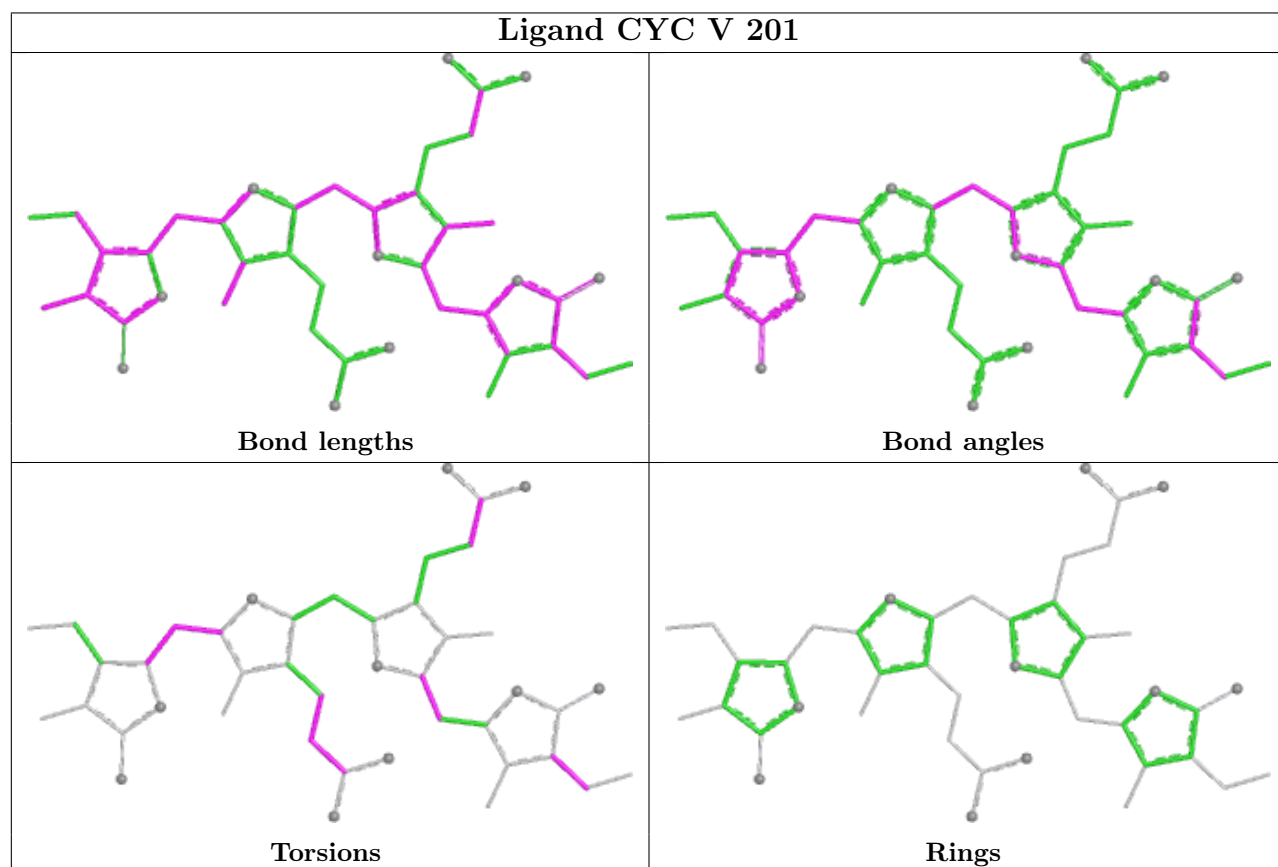
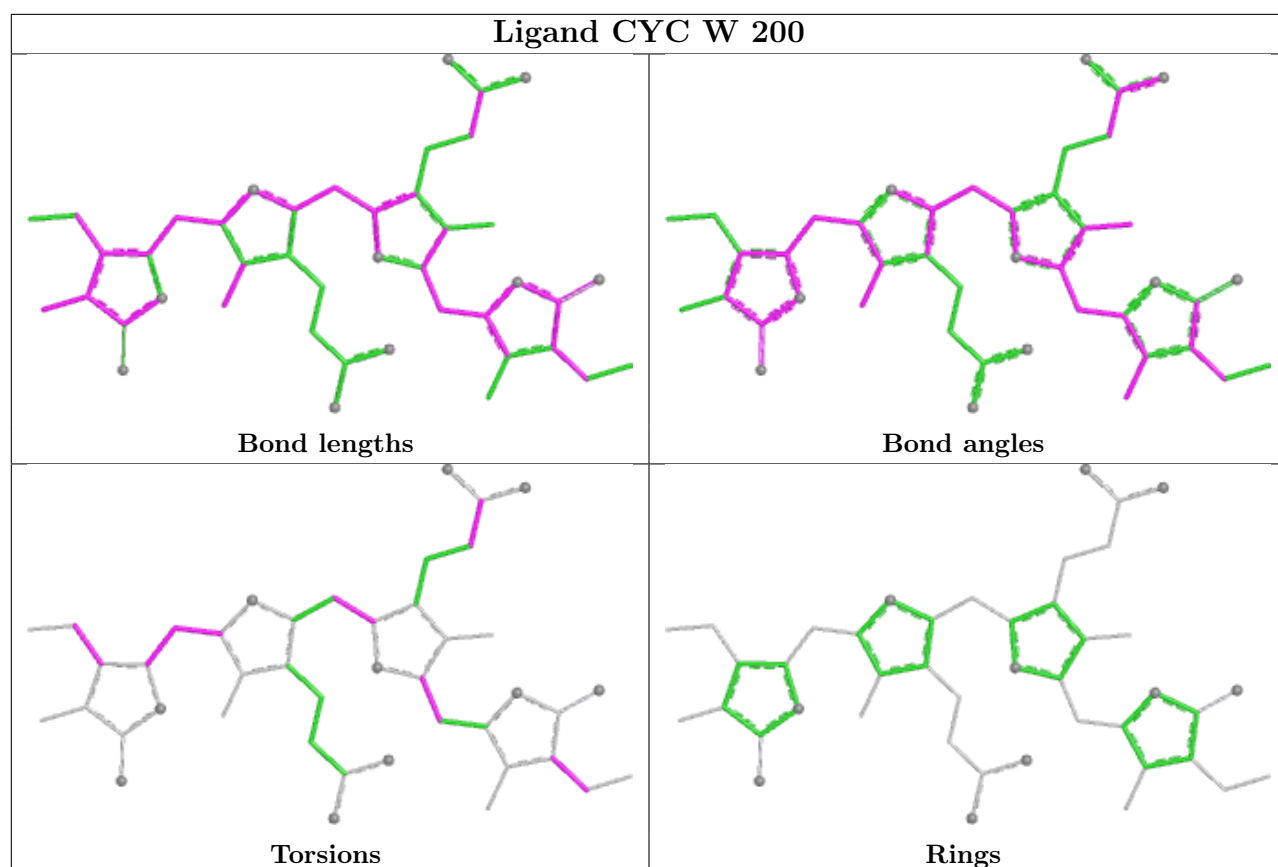


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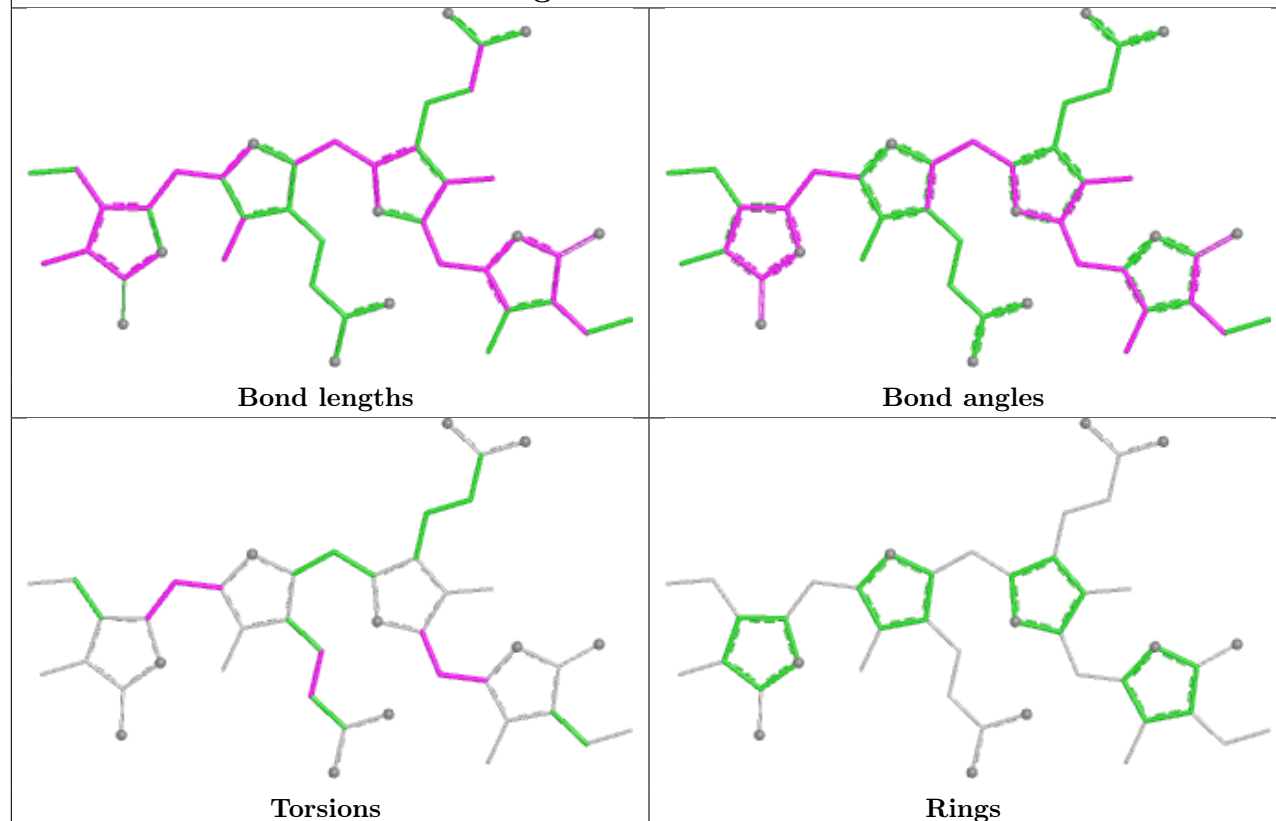


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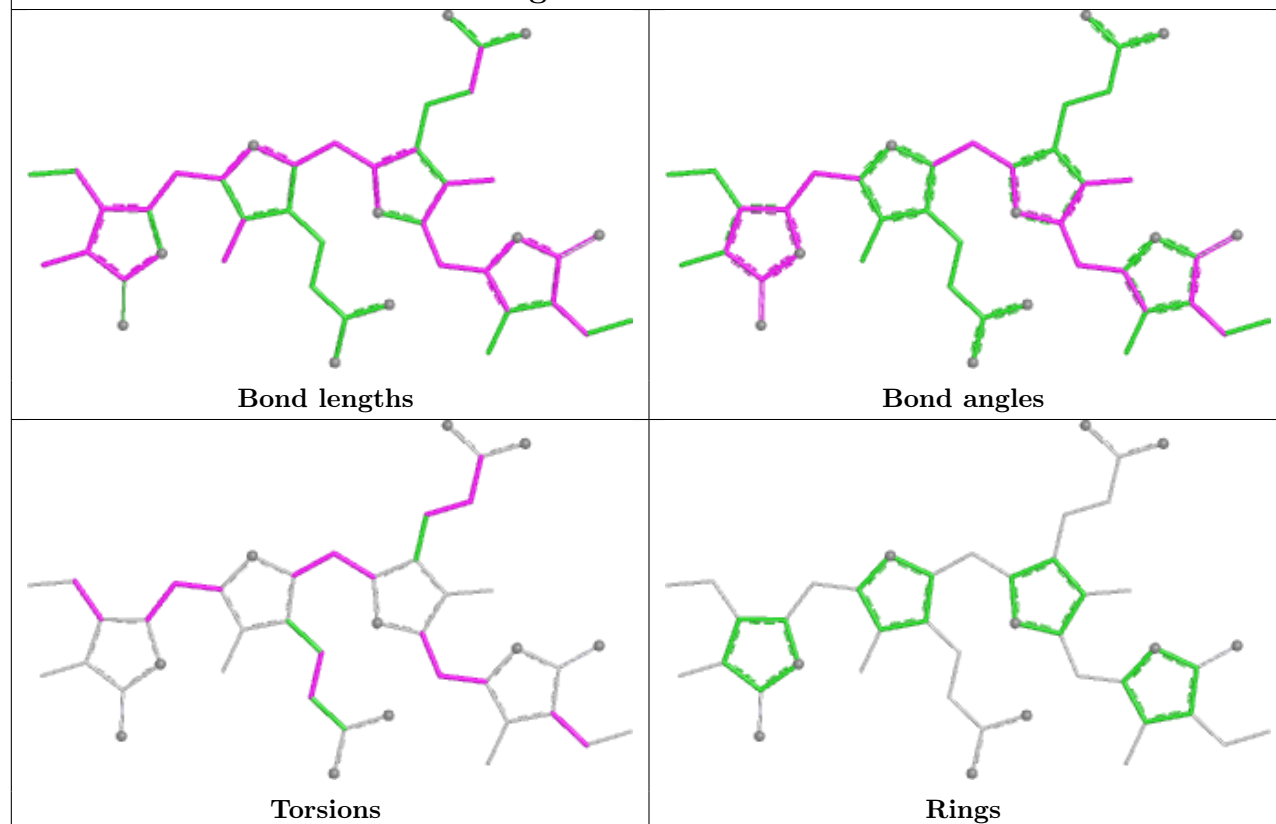


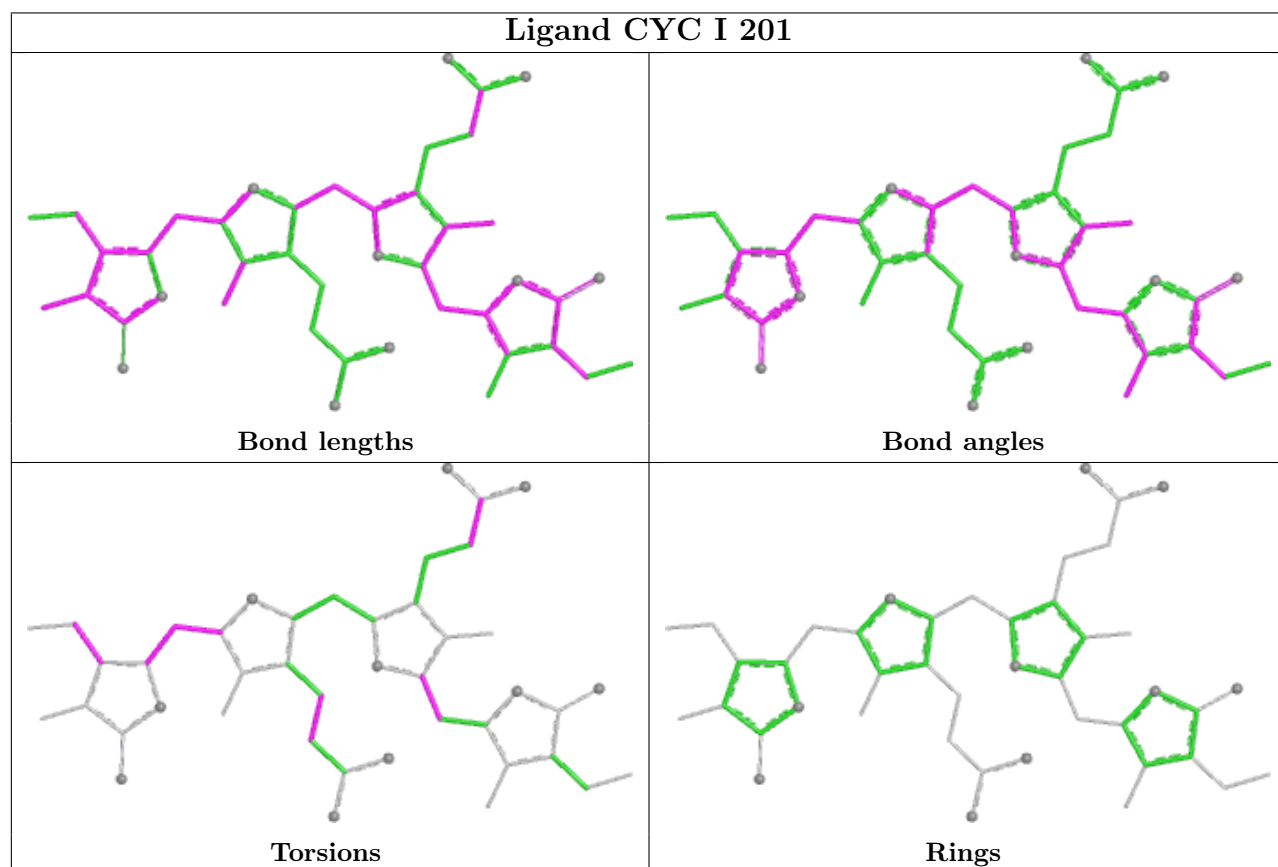
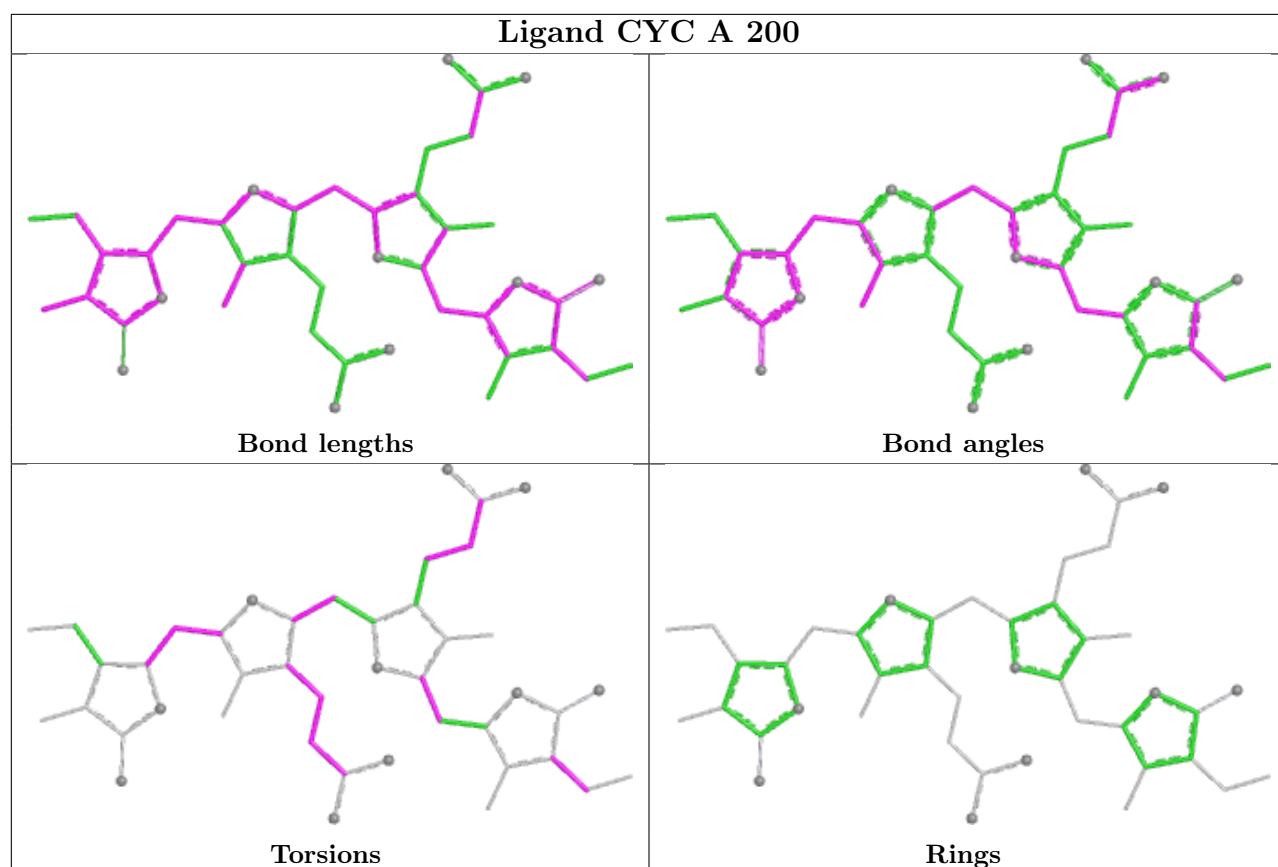


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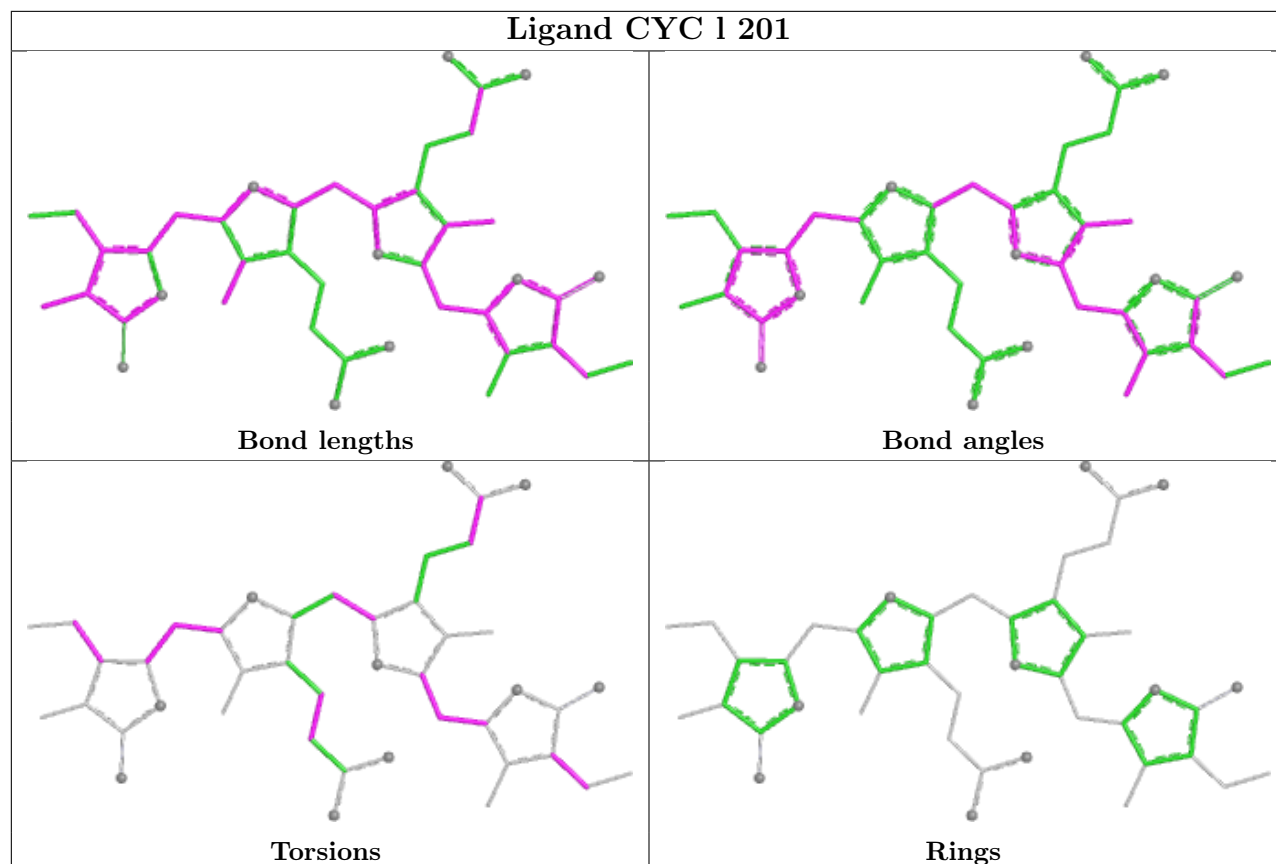


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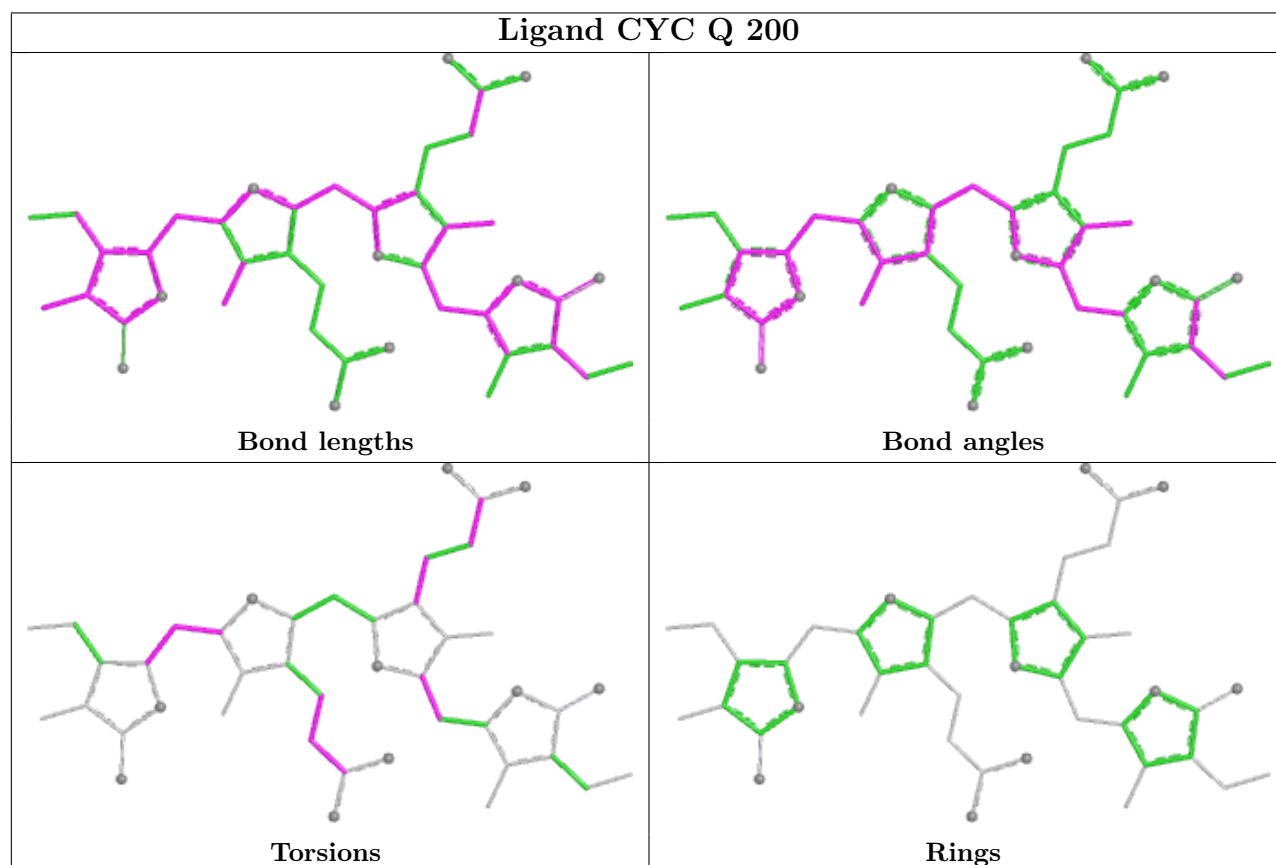


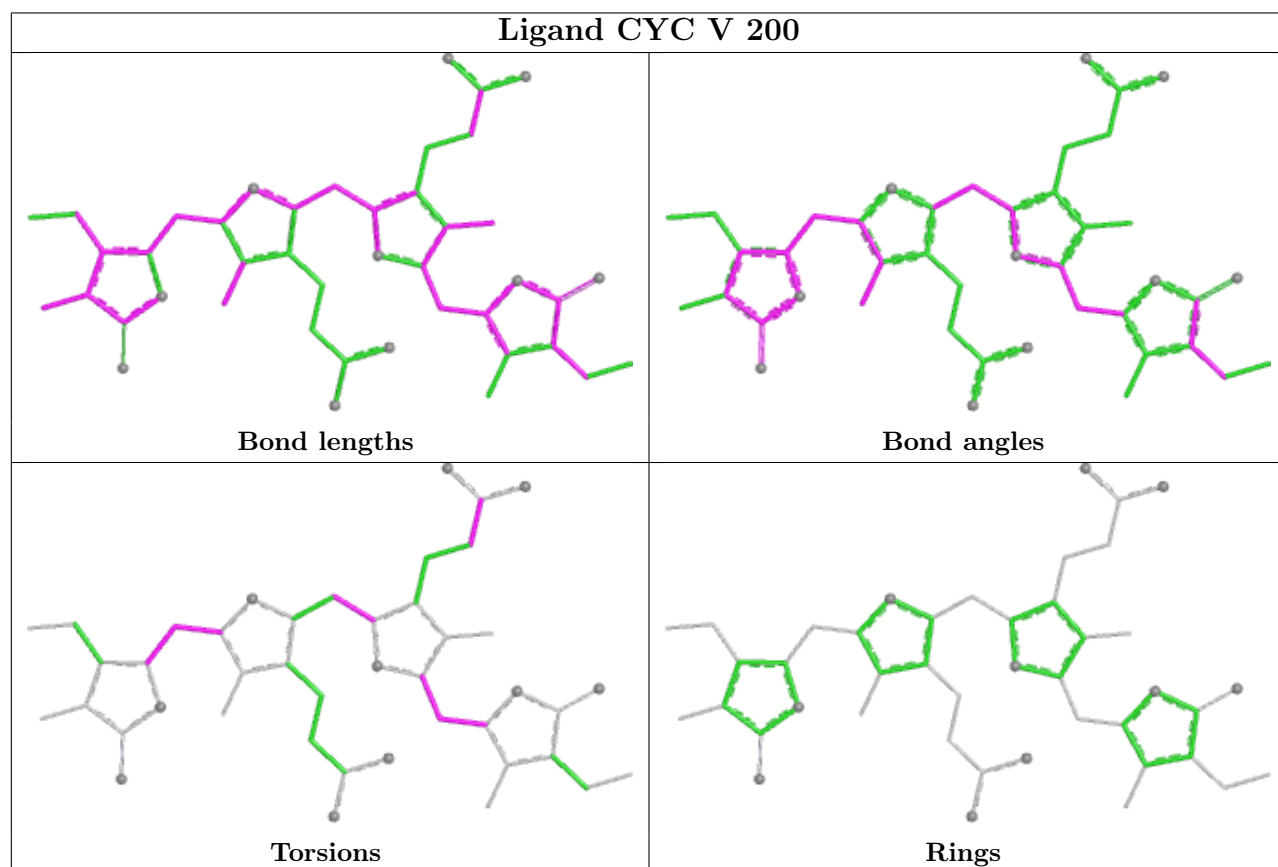
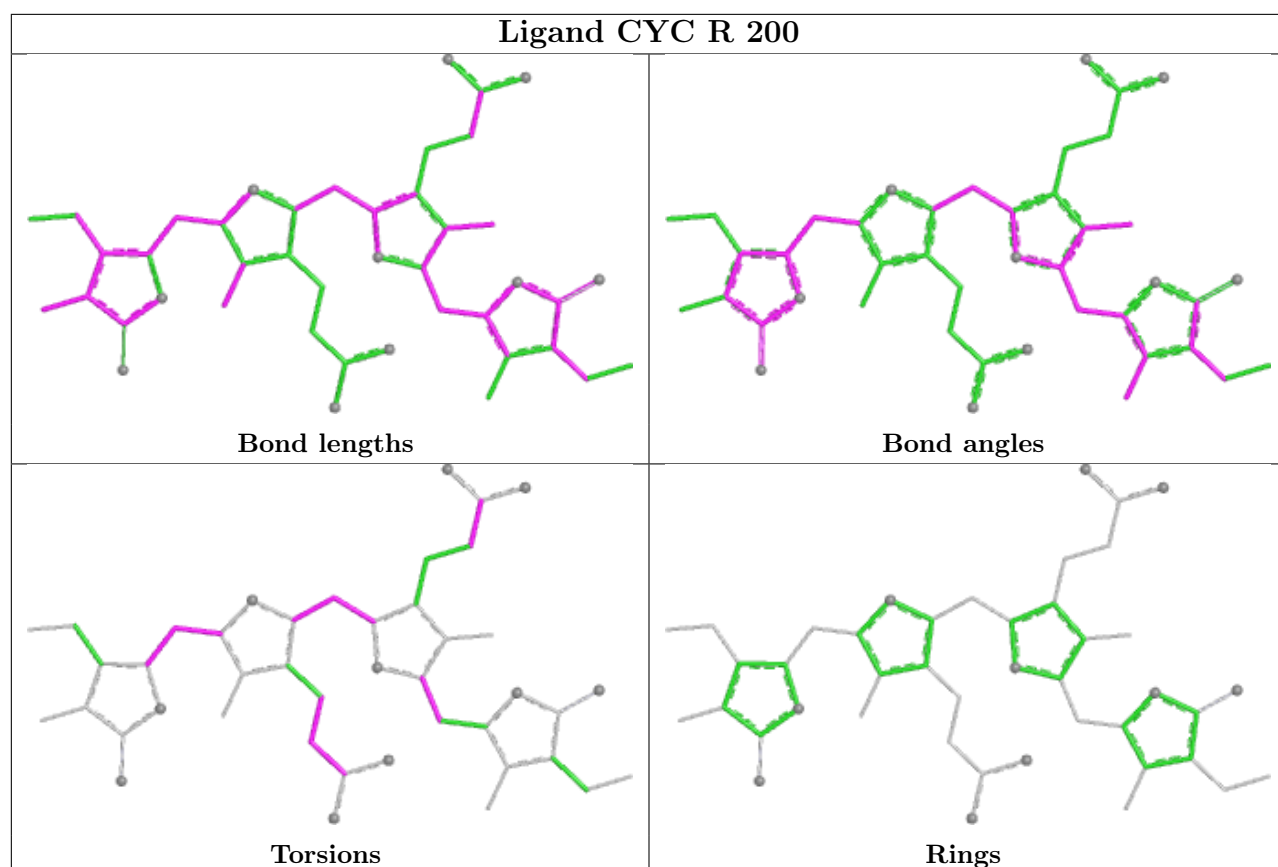


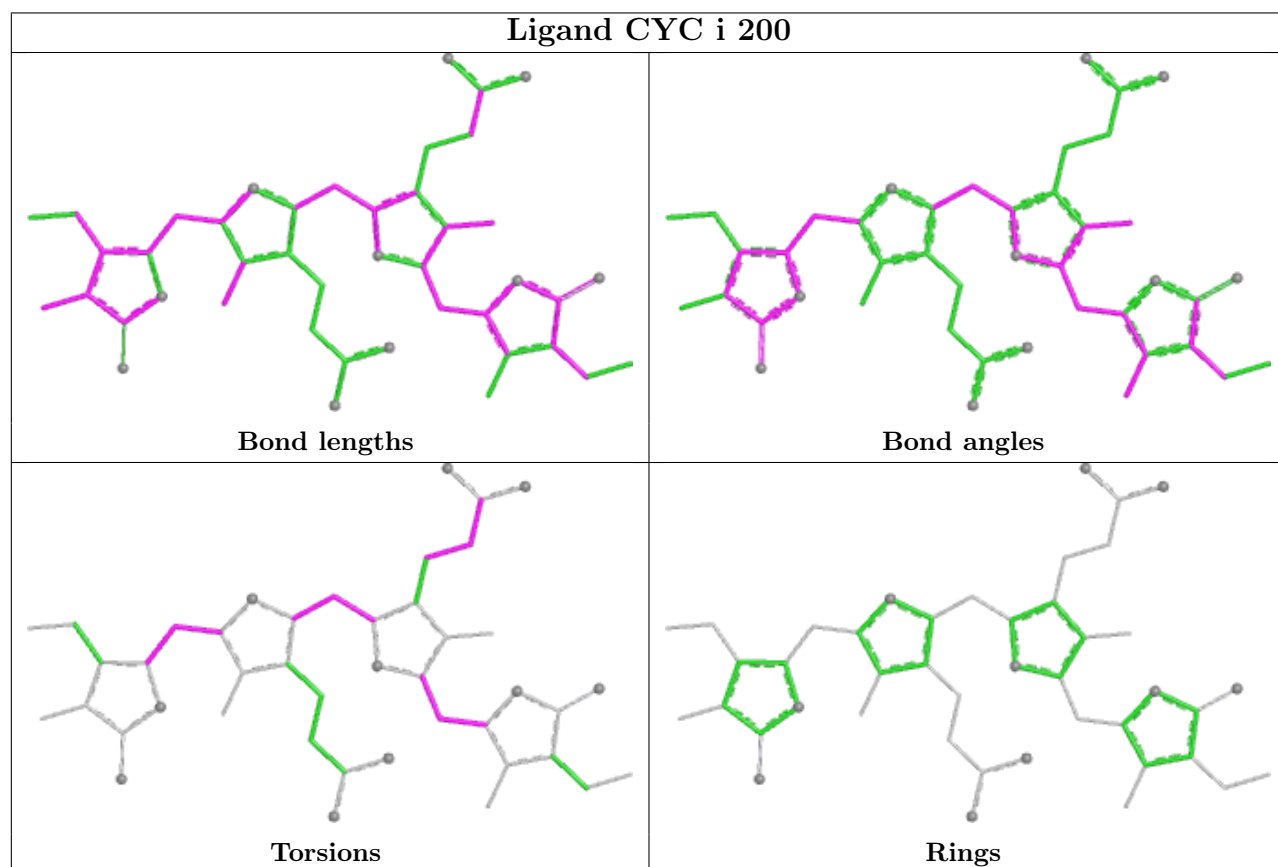
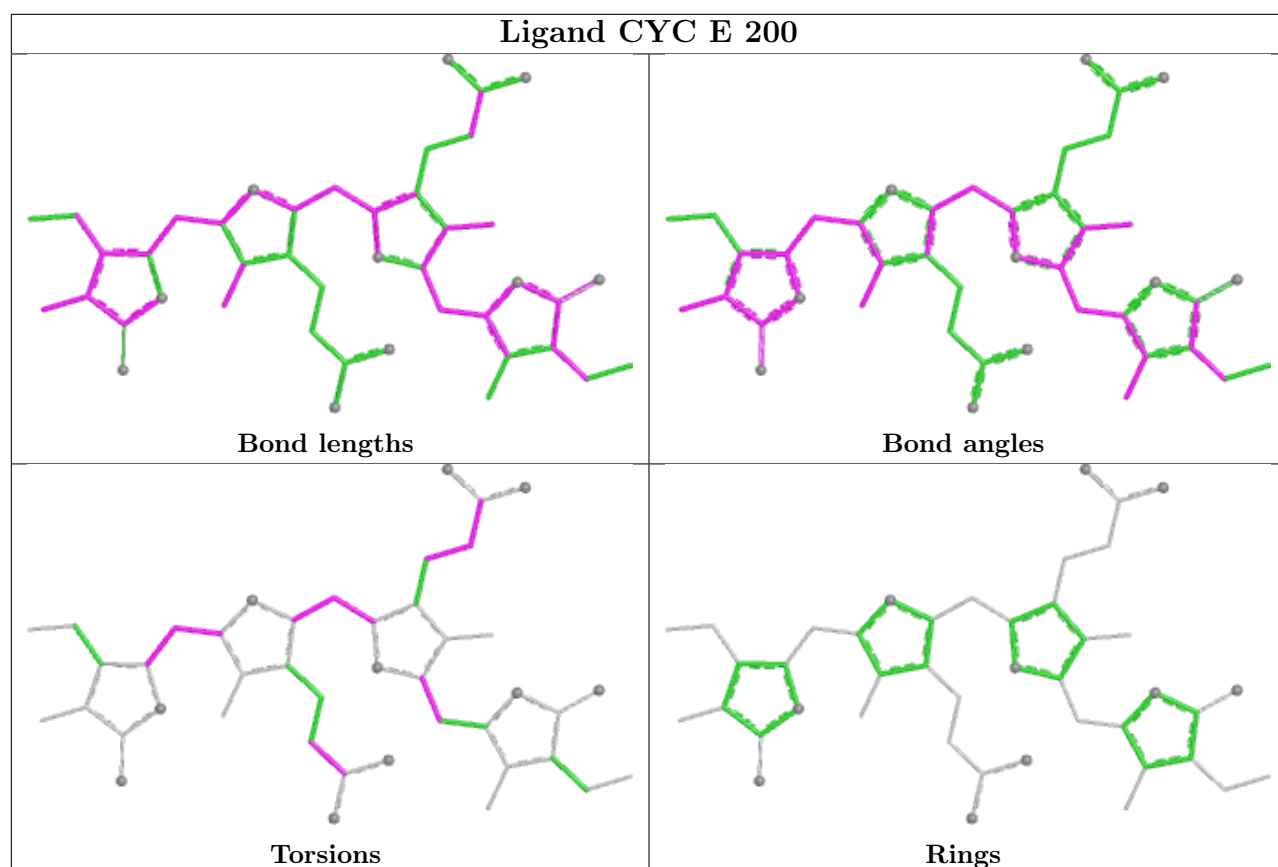
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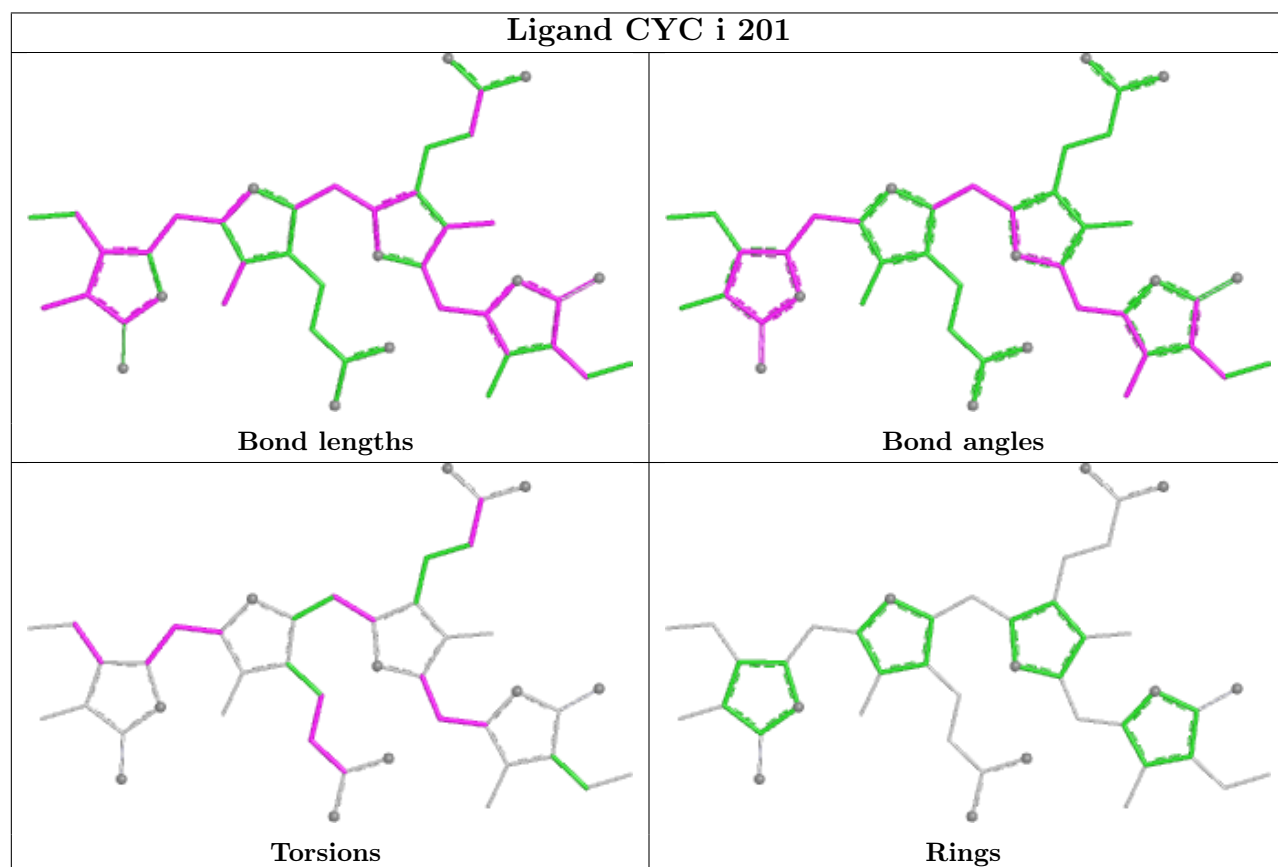
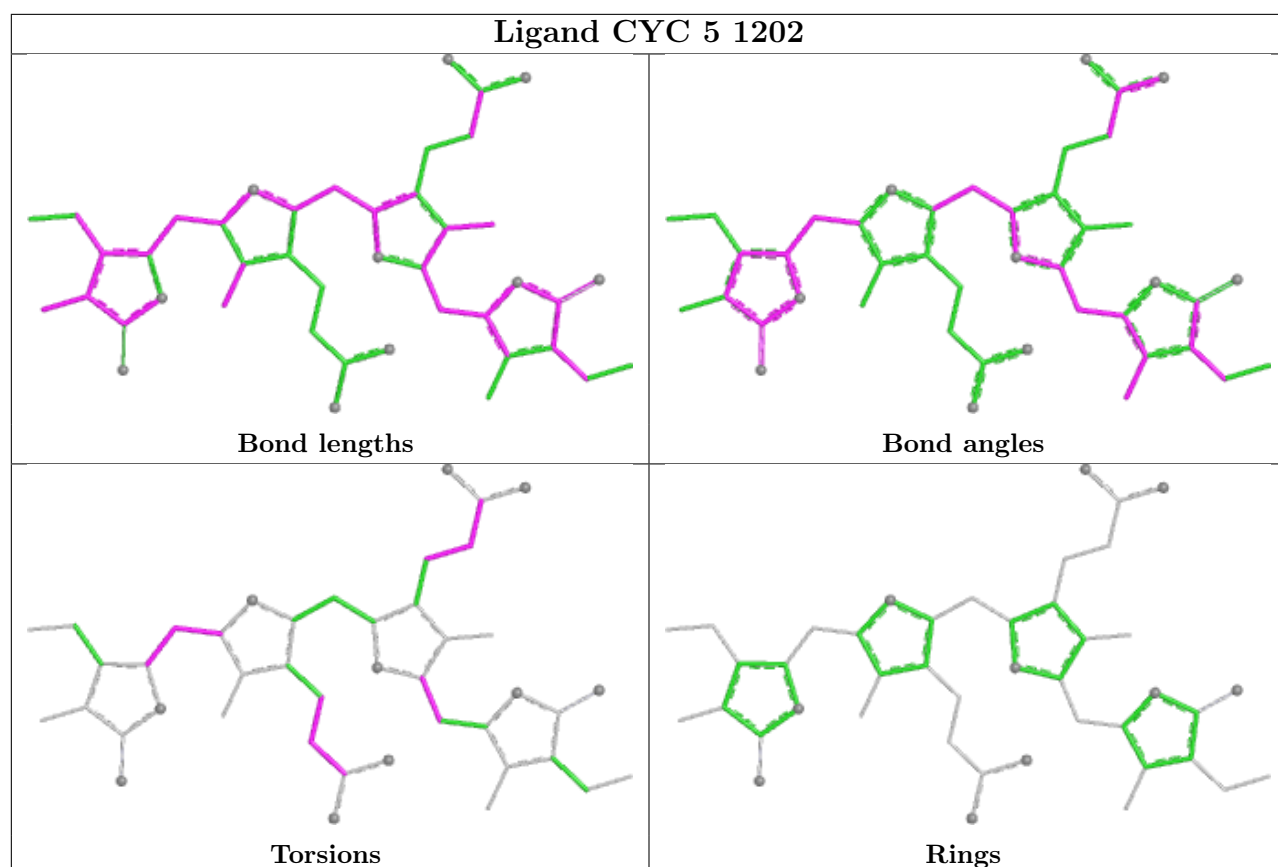


Ligand CYC Q 200

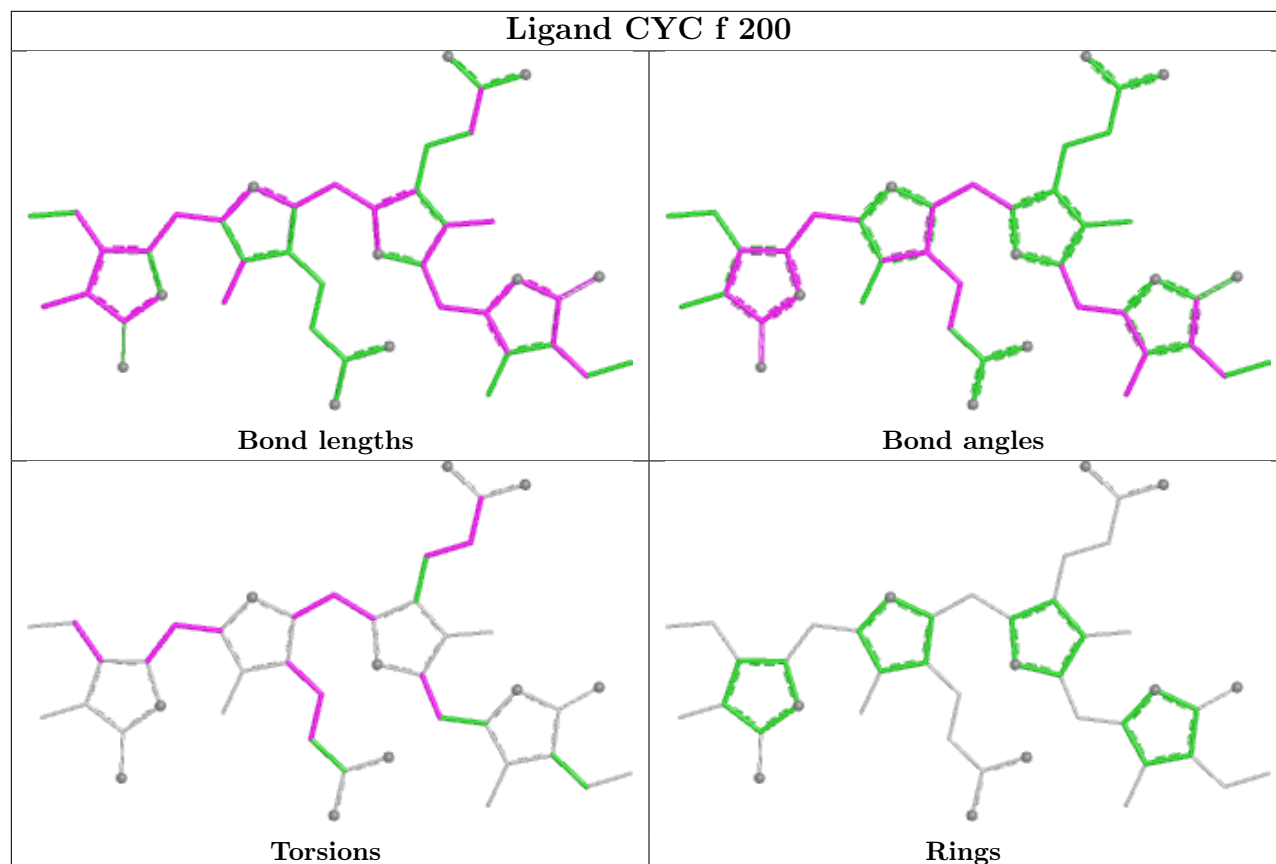




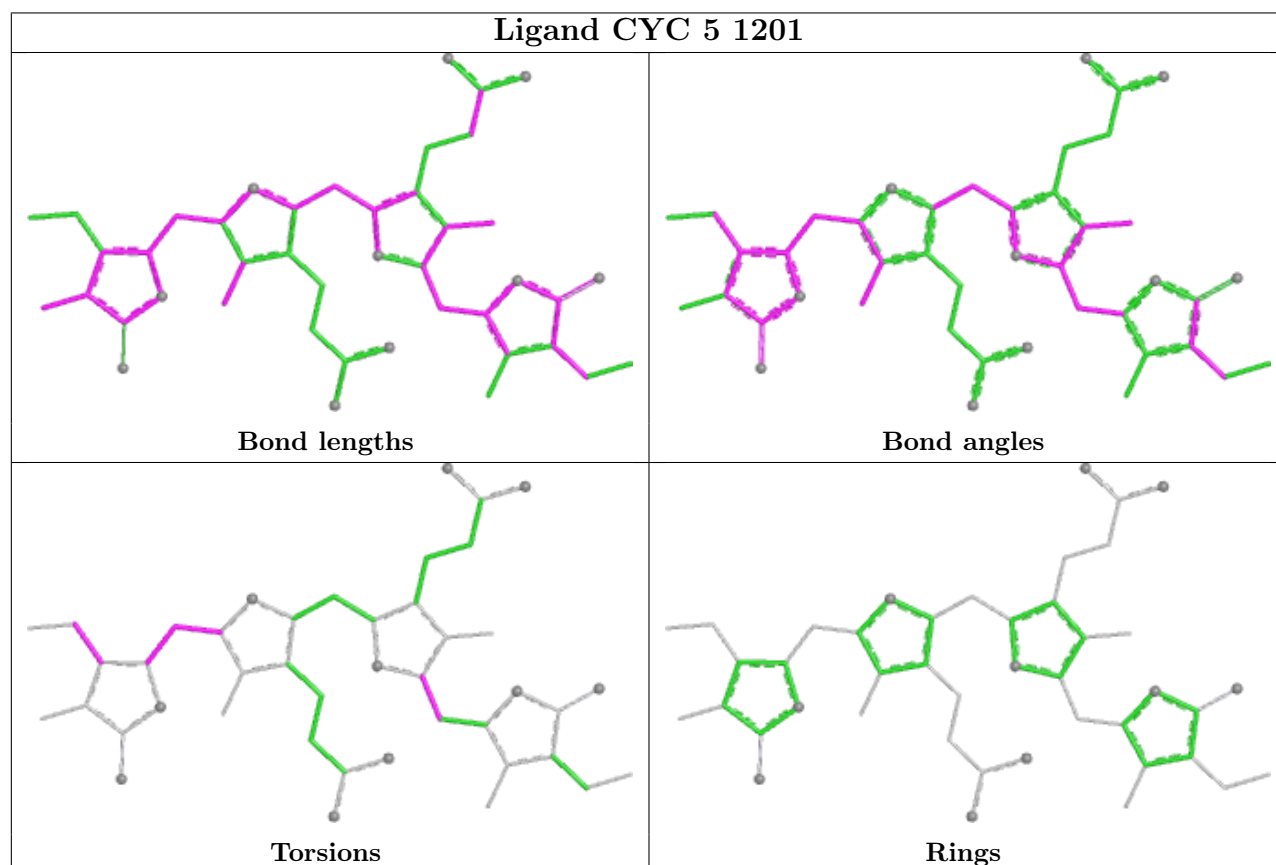


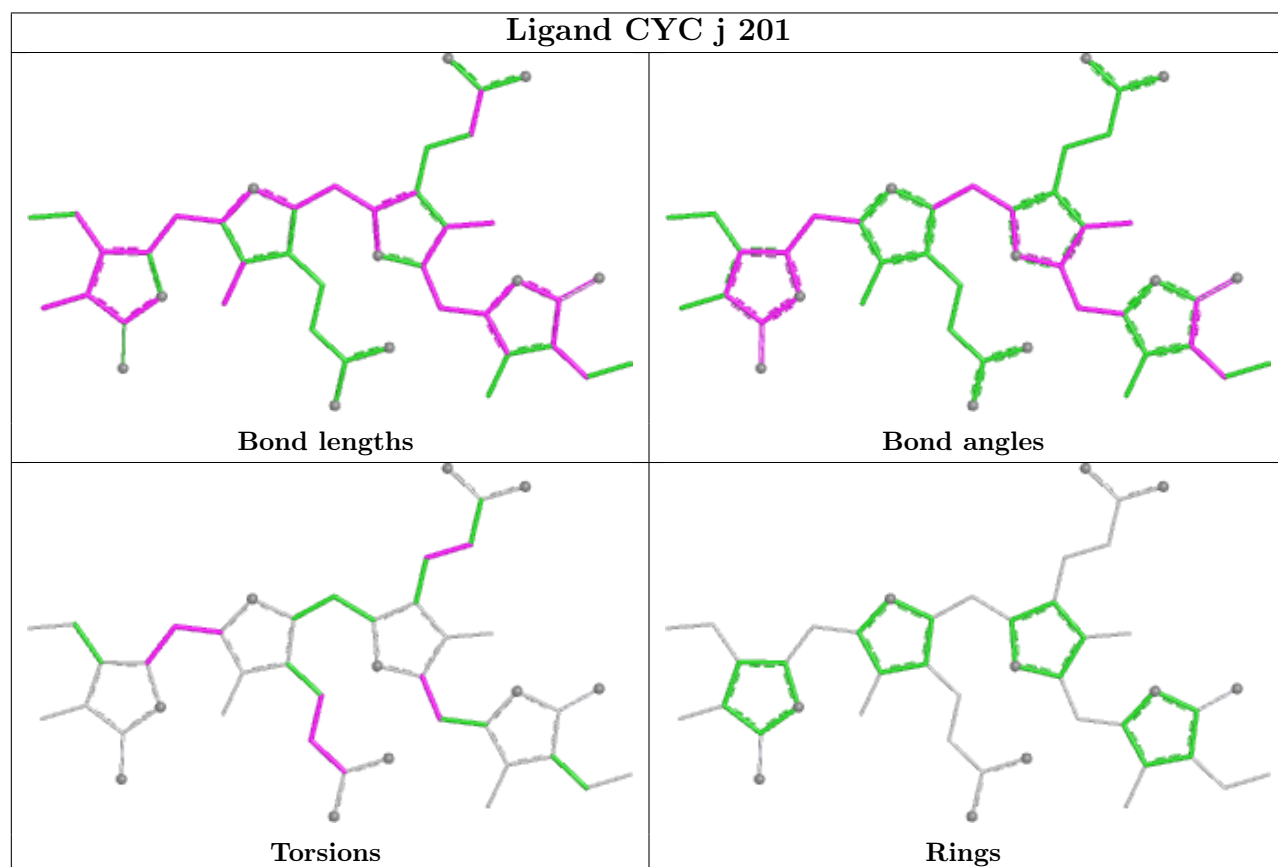
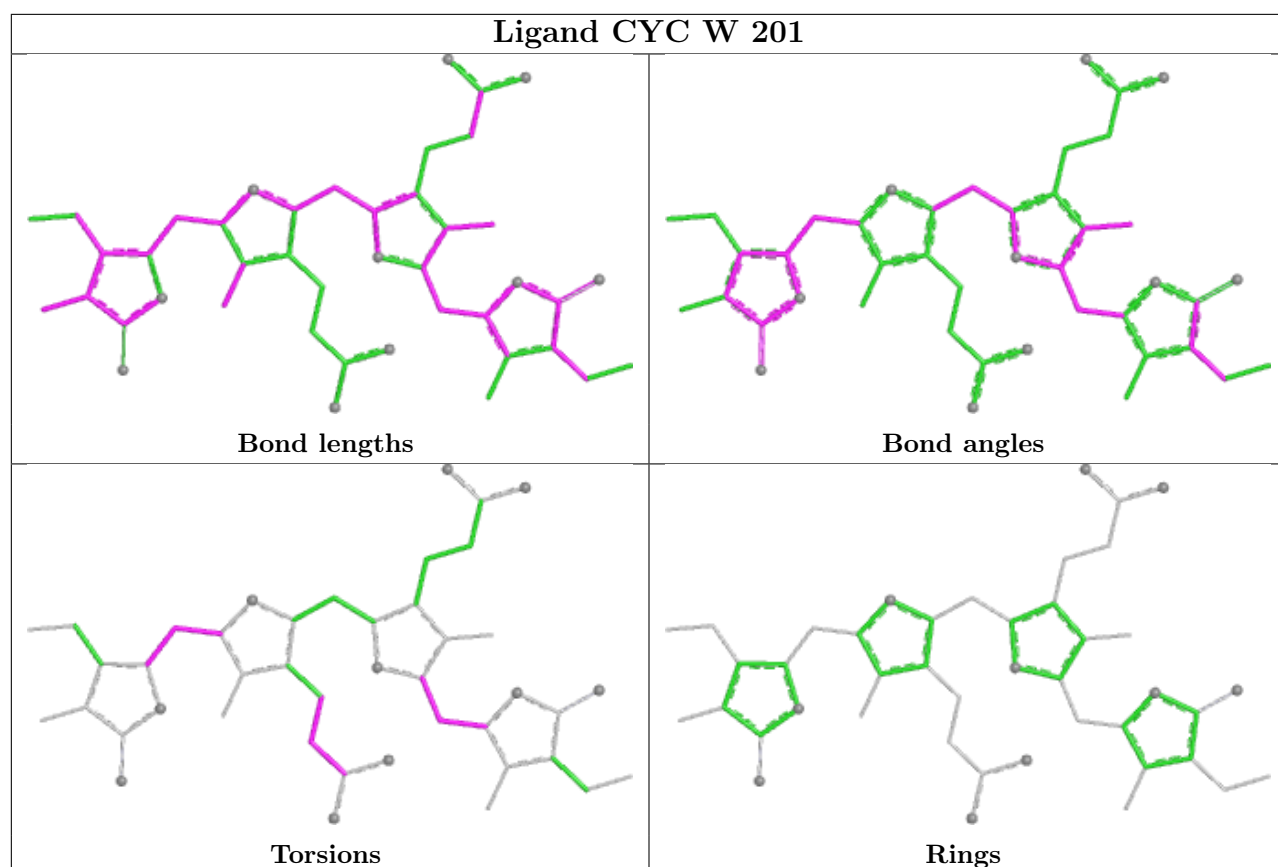


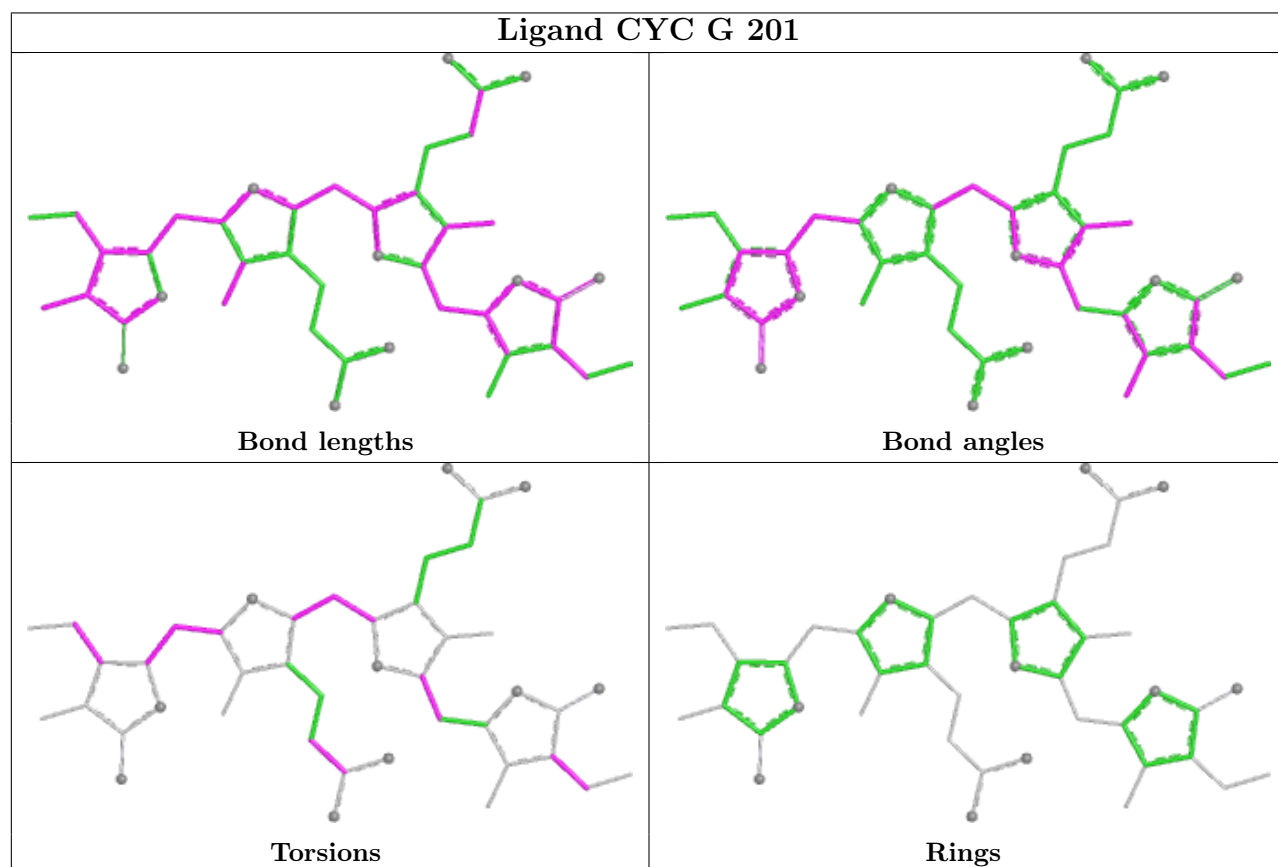
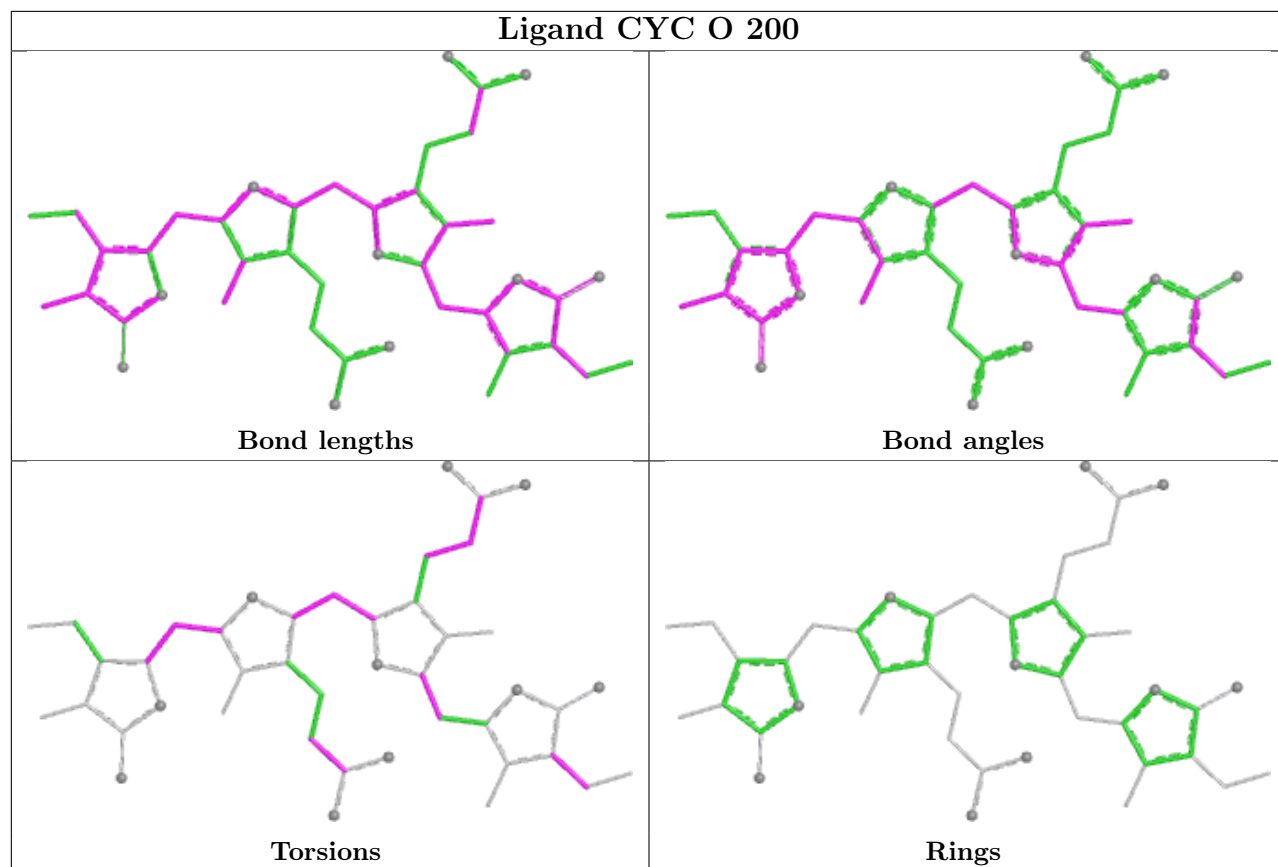
Ligand CYC f 200



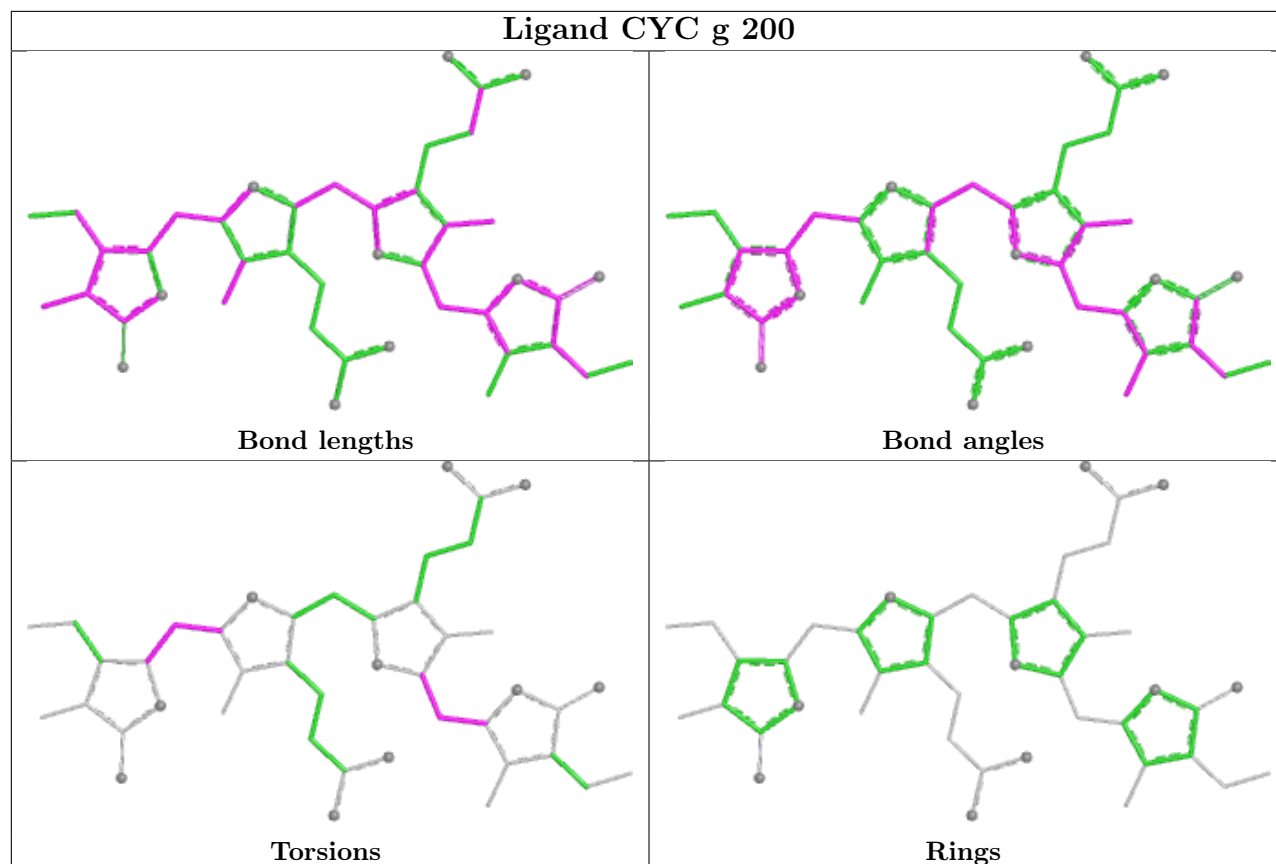
Ligand CYC 5 1201



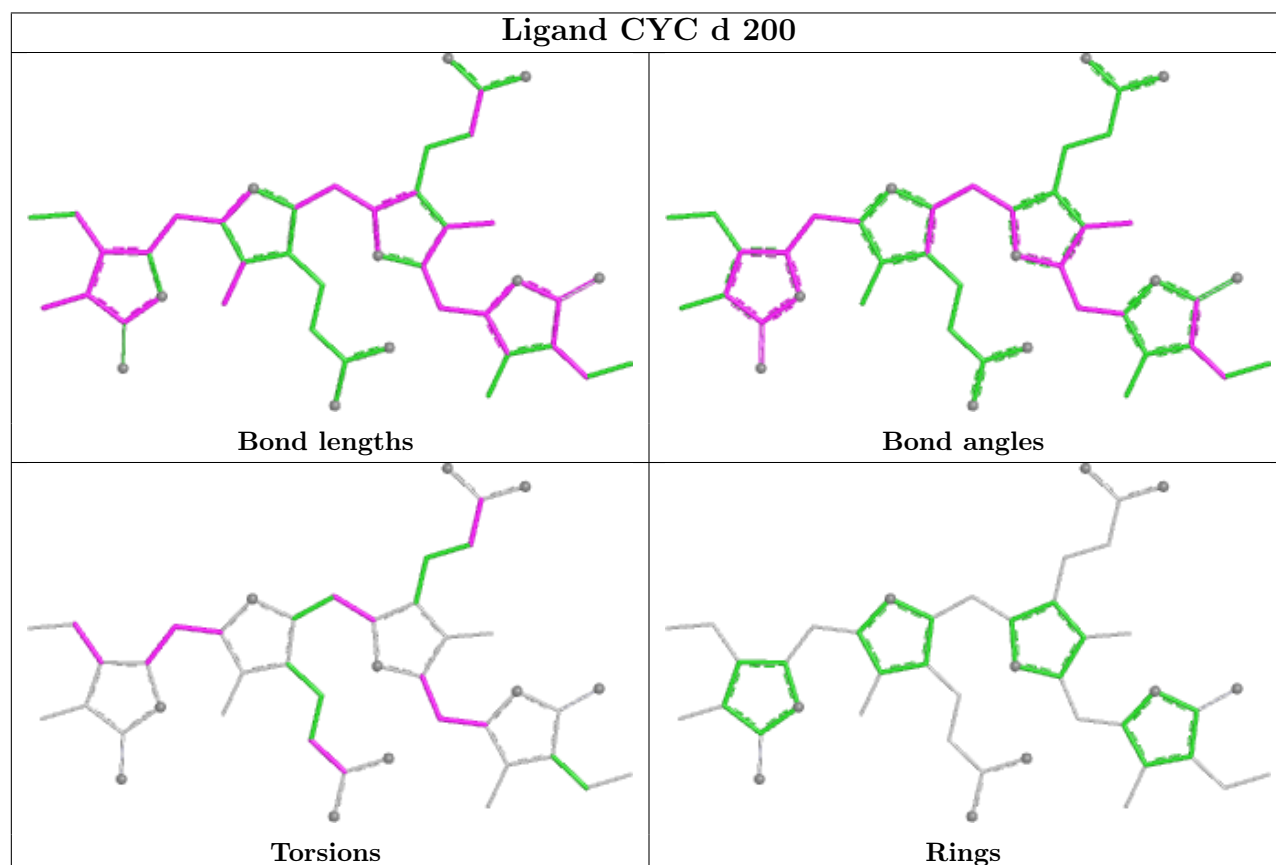




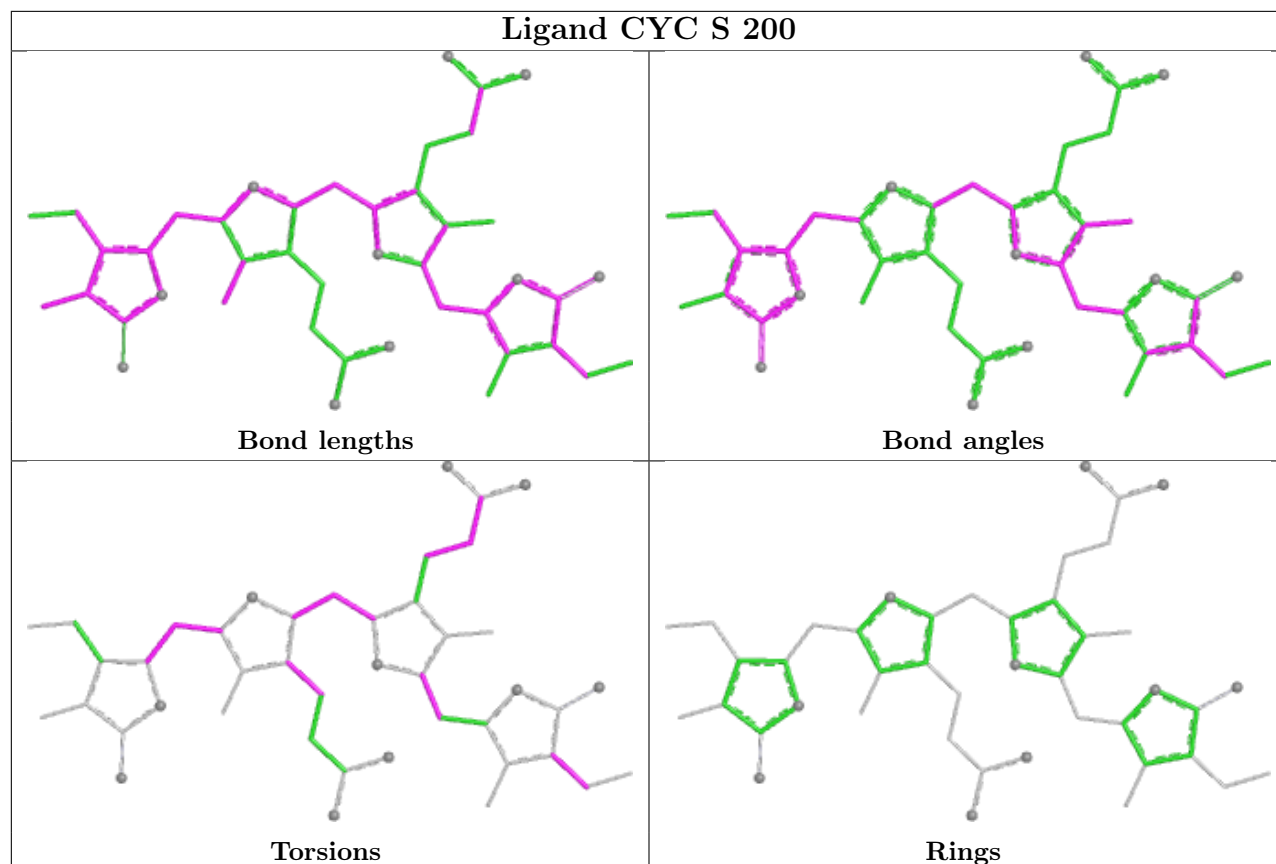
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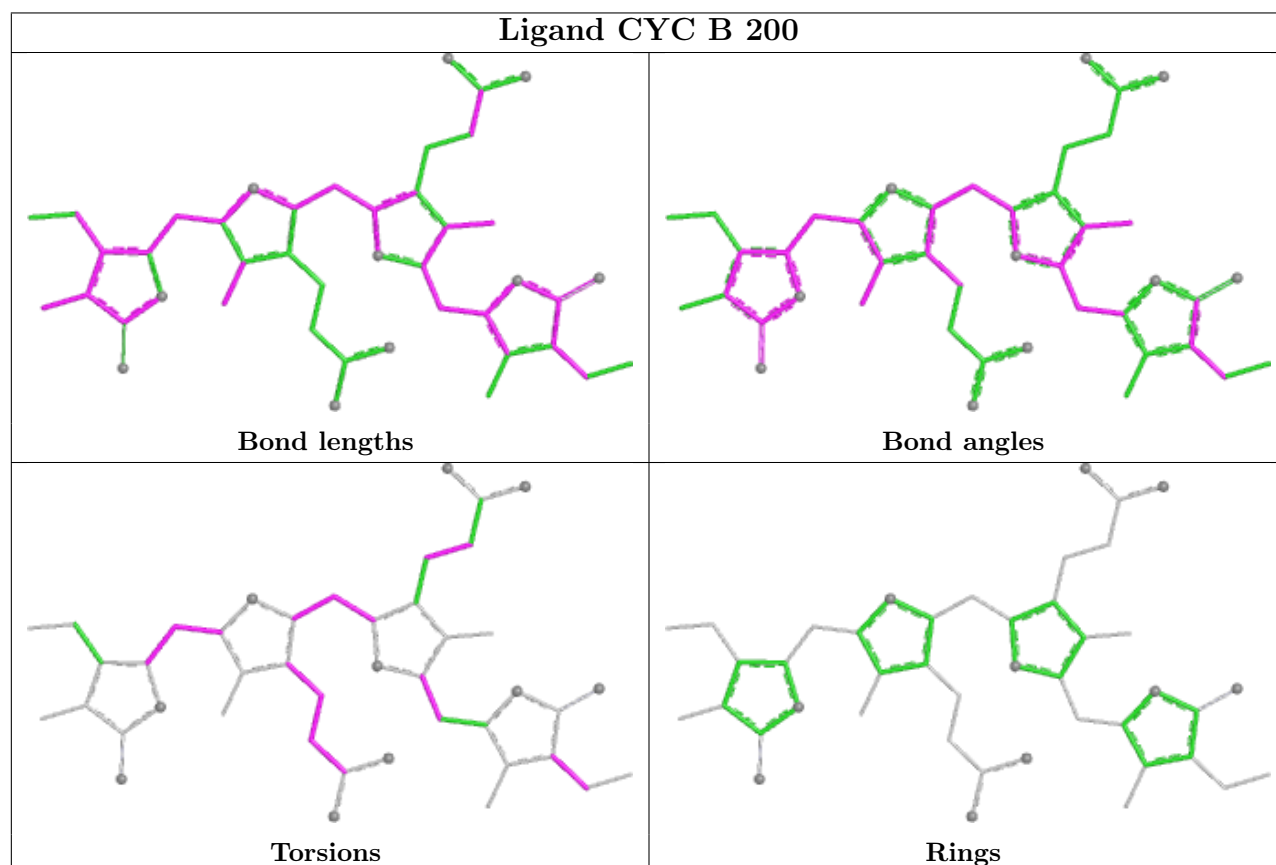
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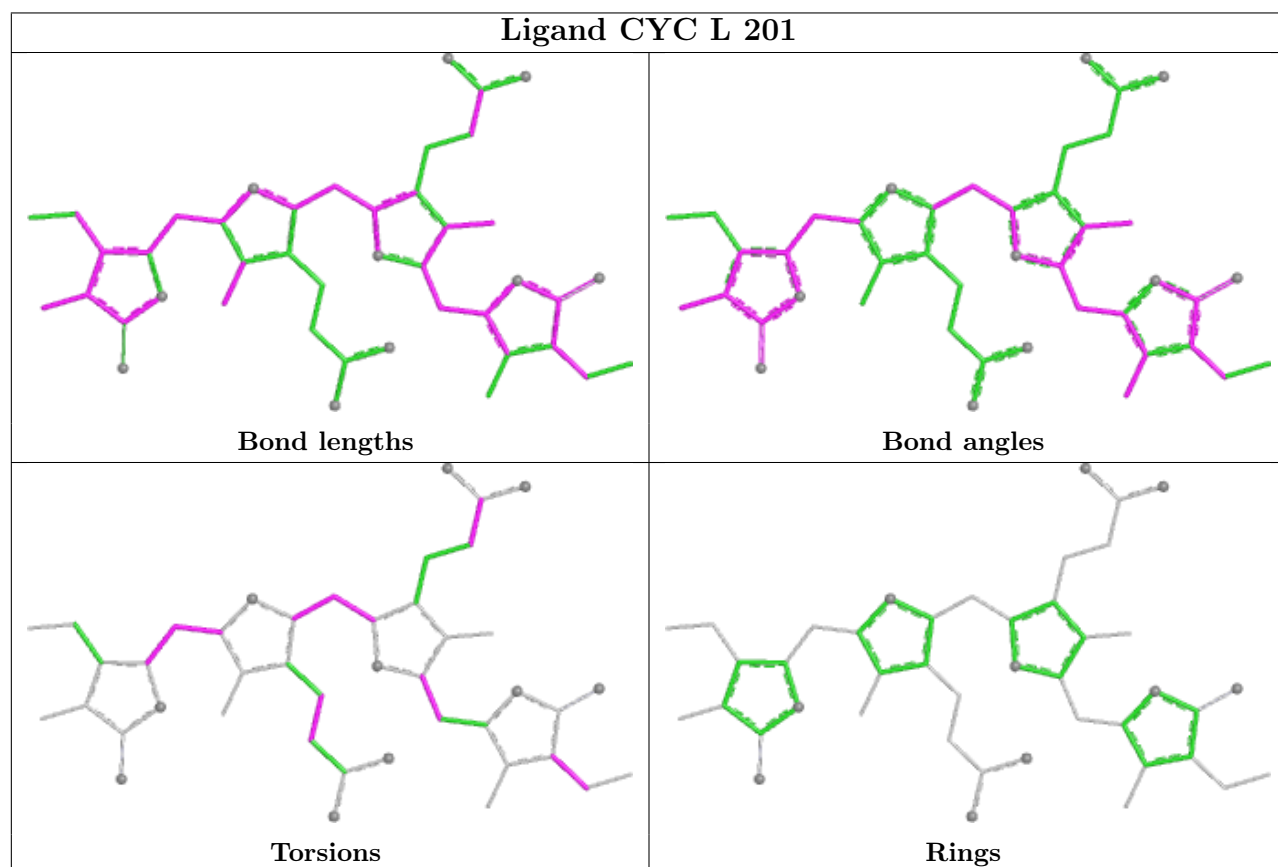
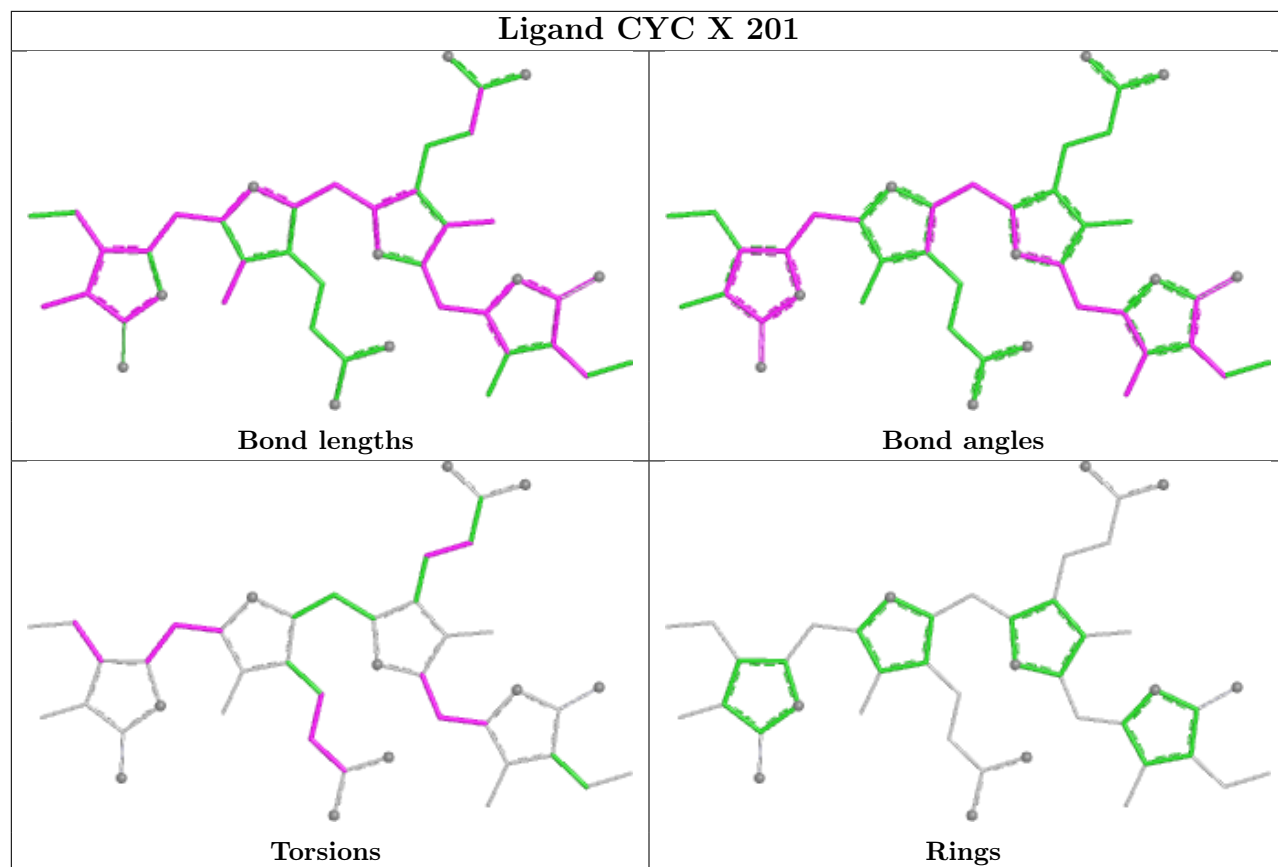


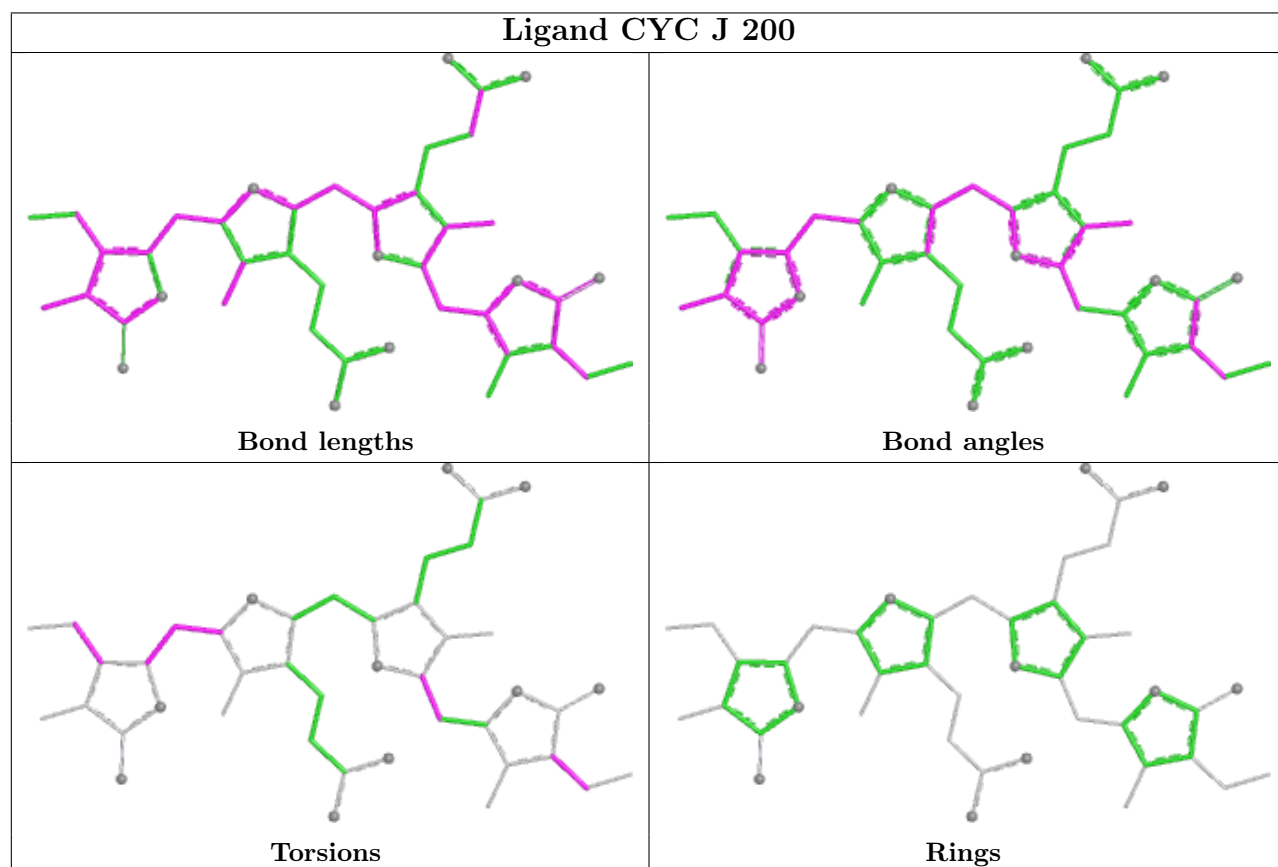
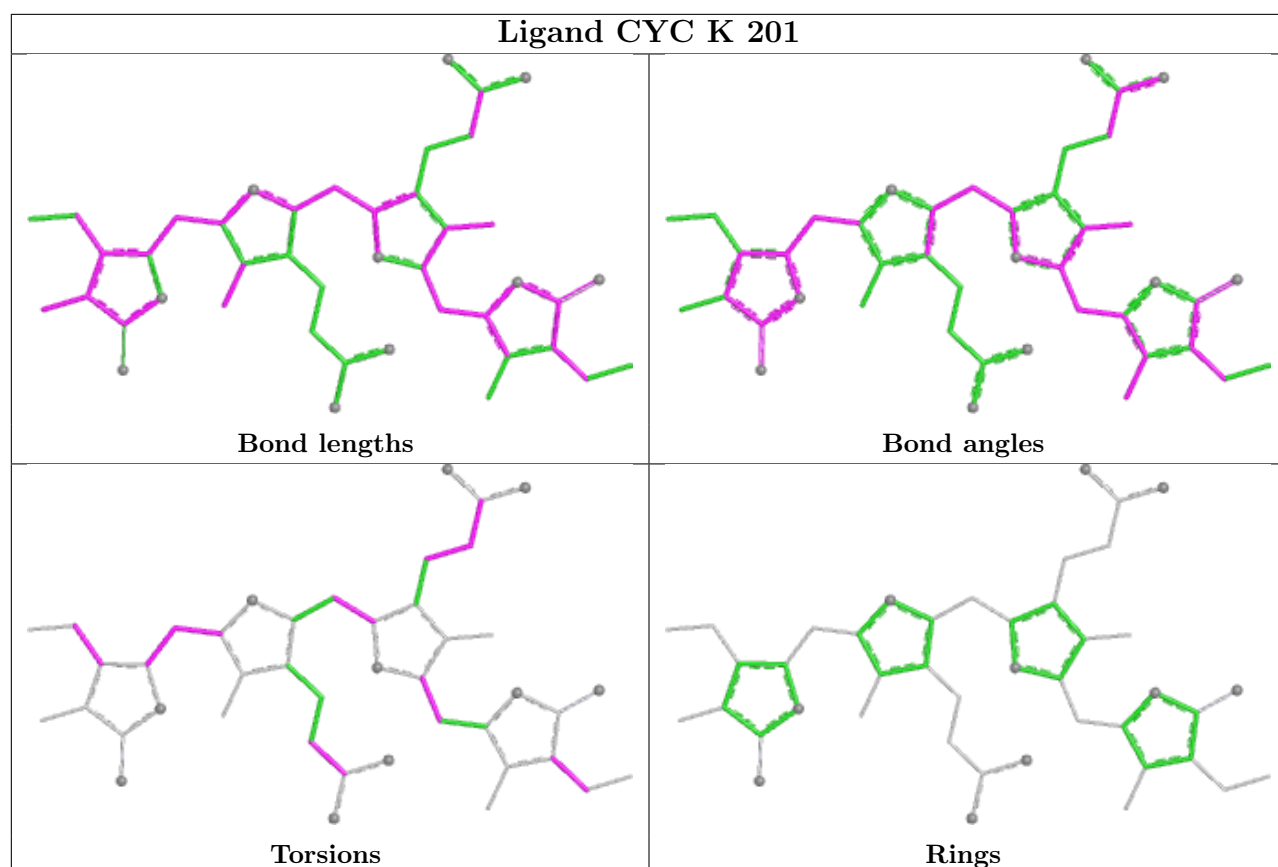
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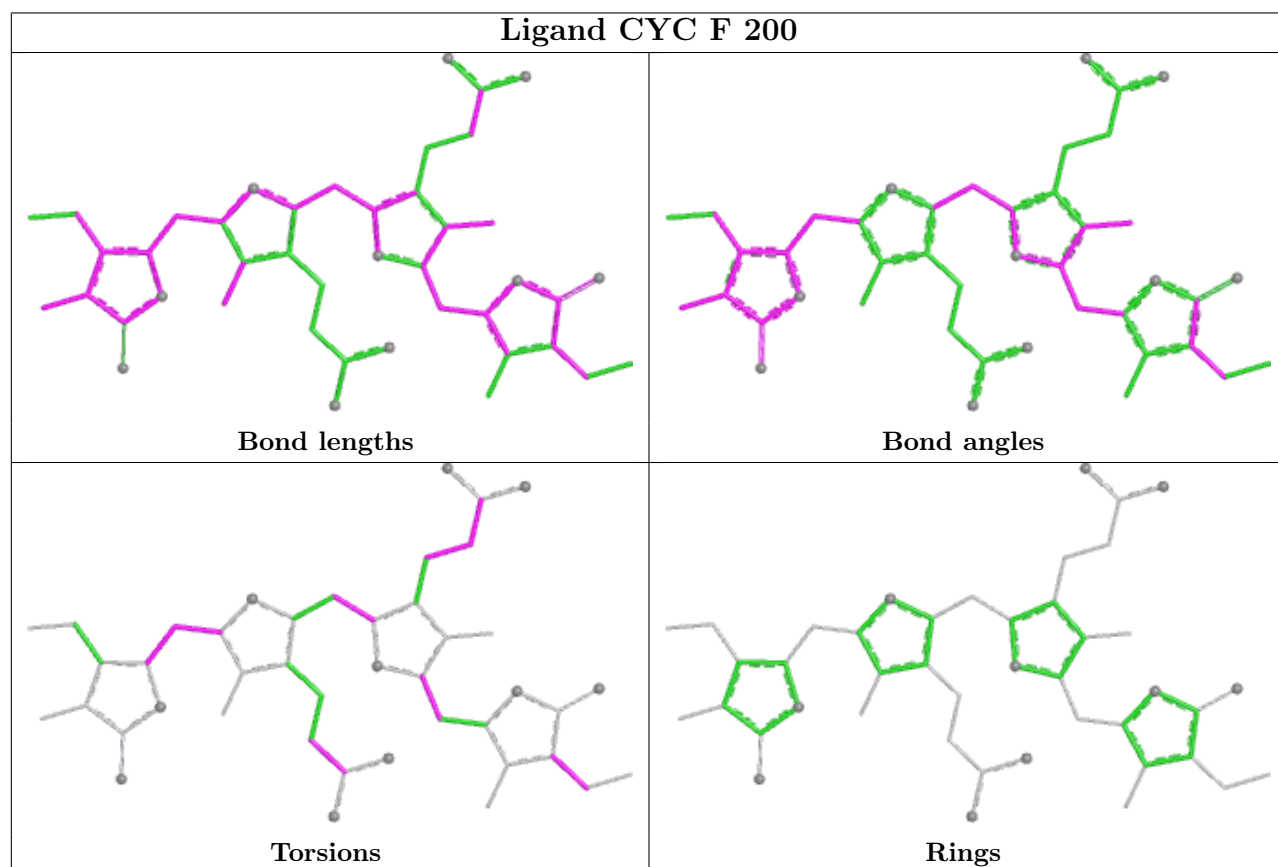
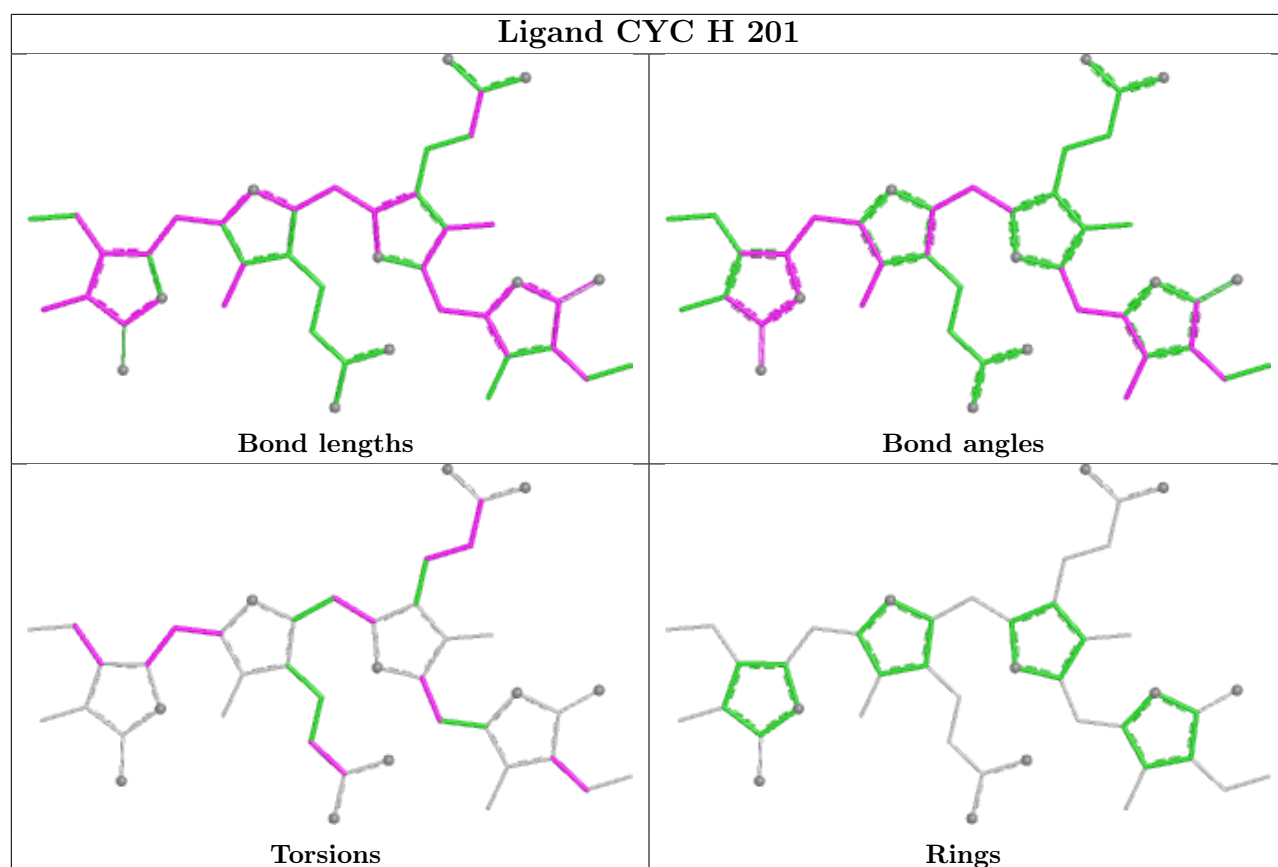


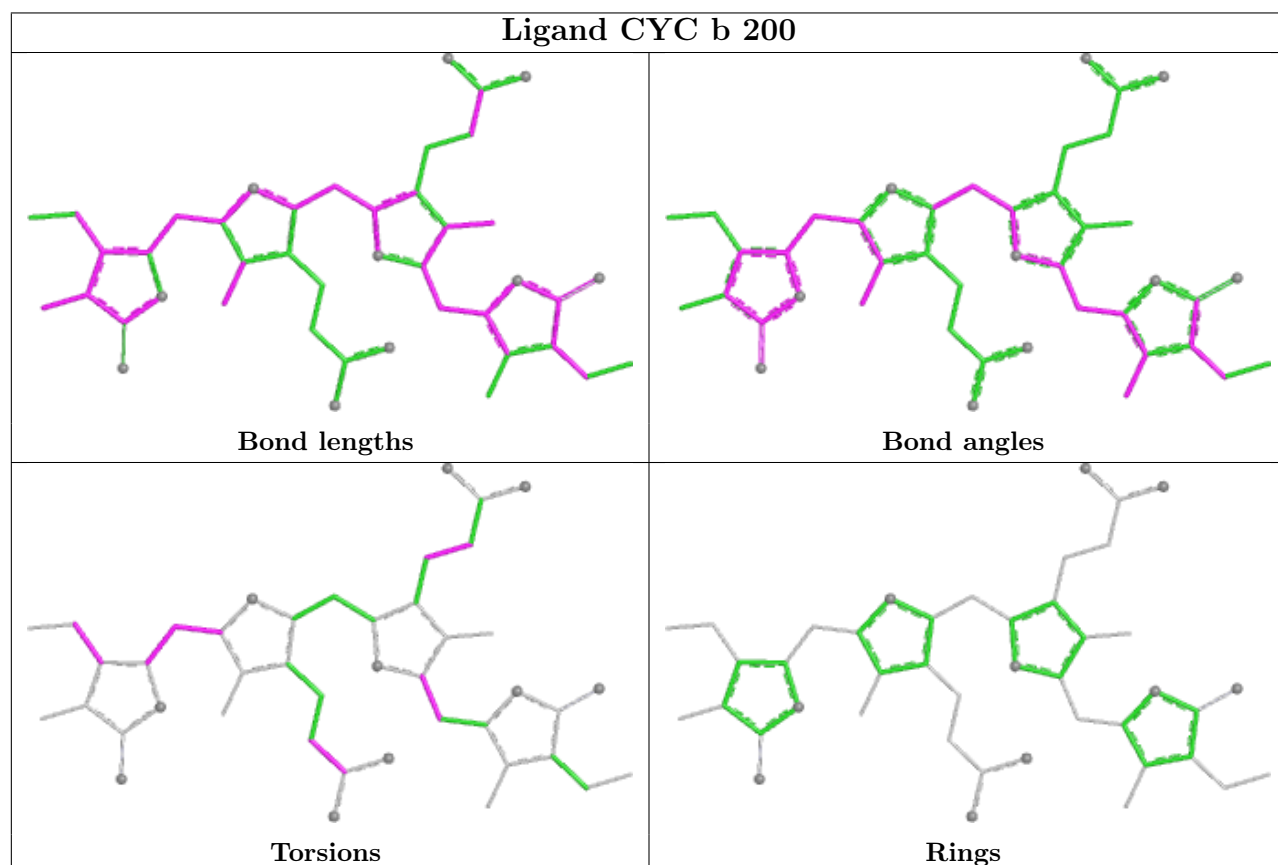
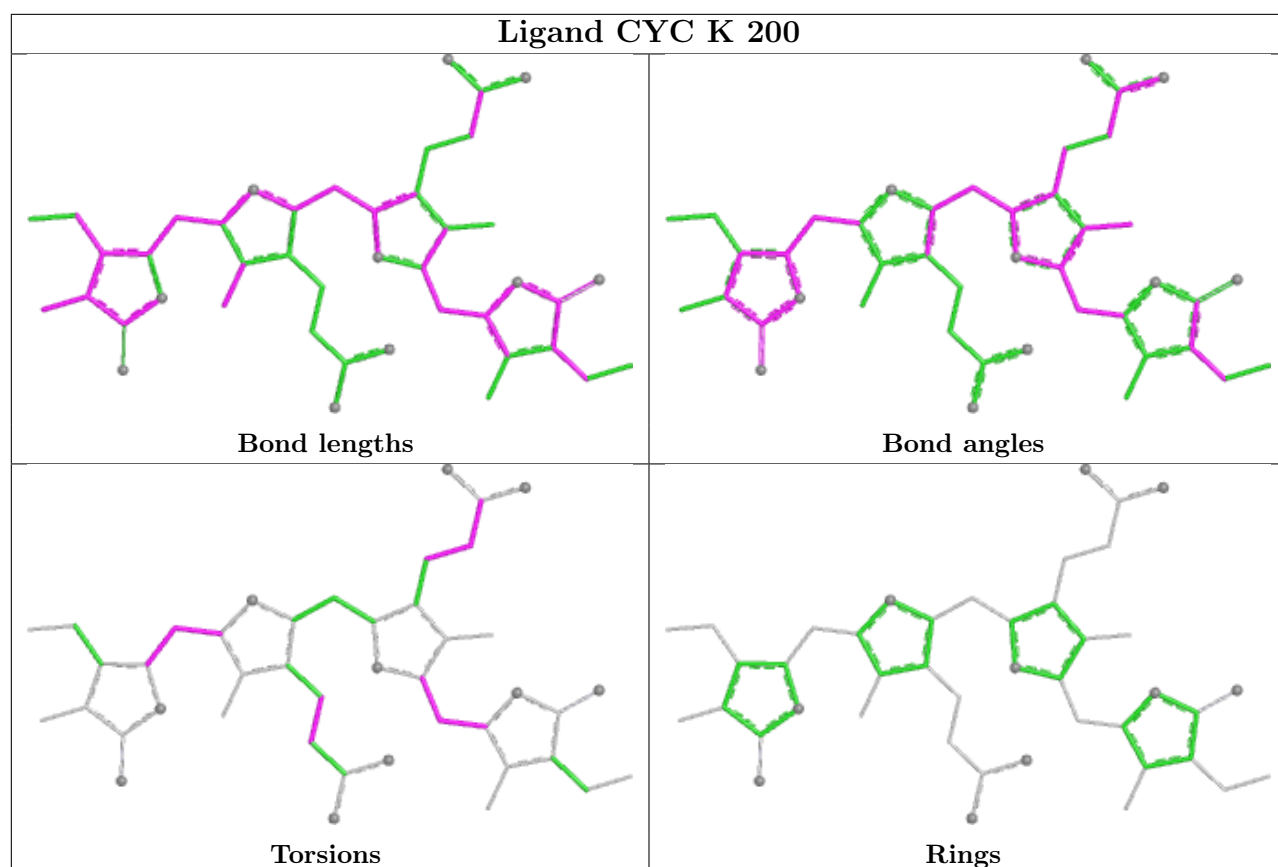
Ligand CYC B 200

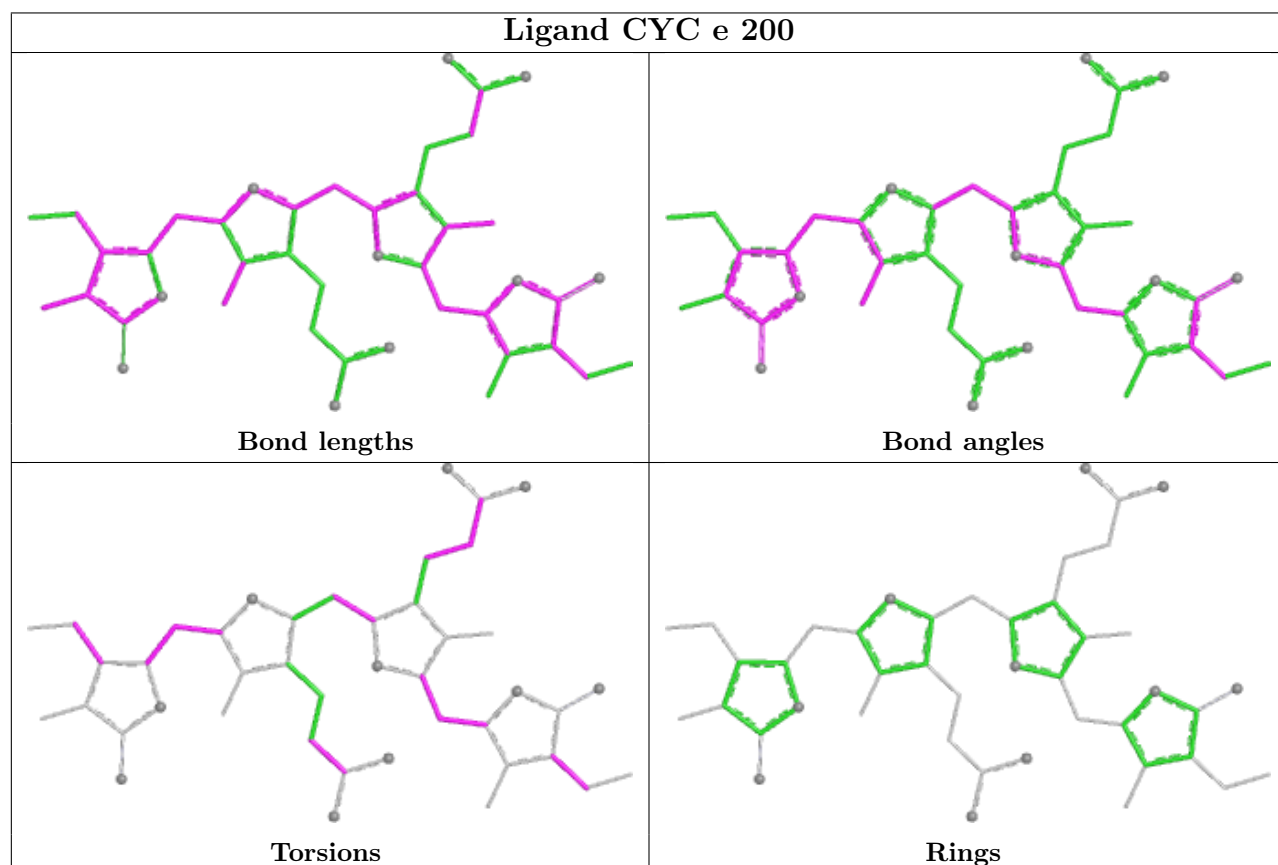
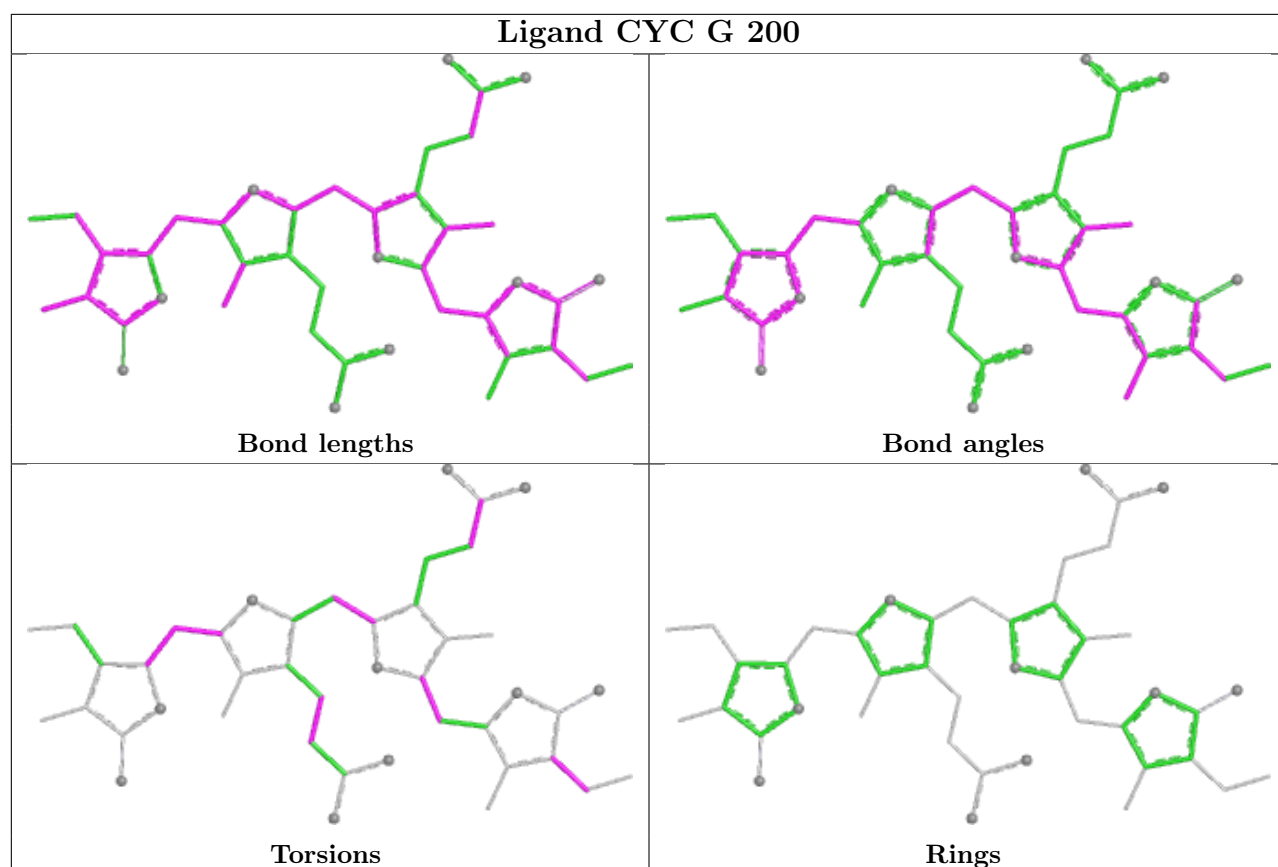


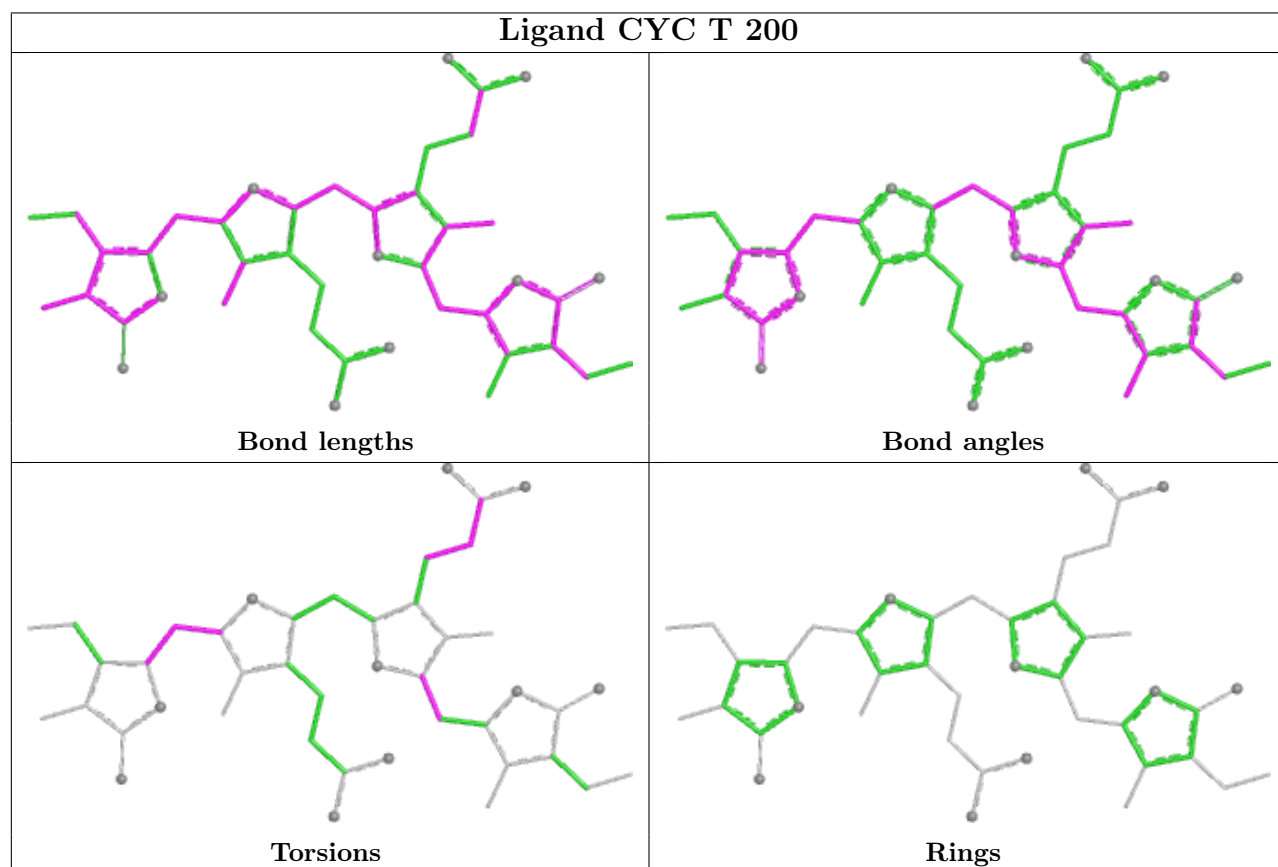
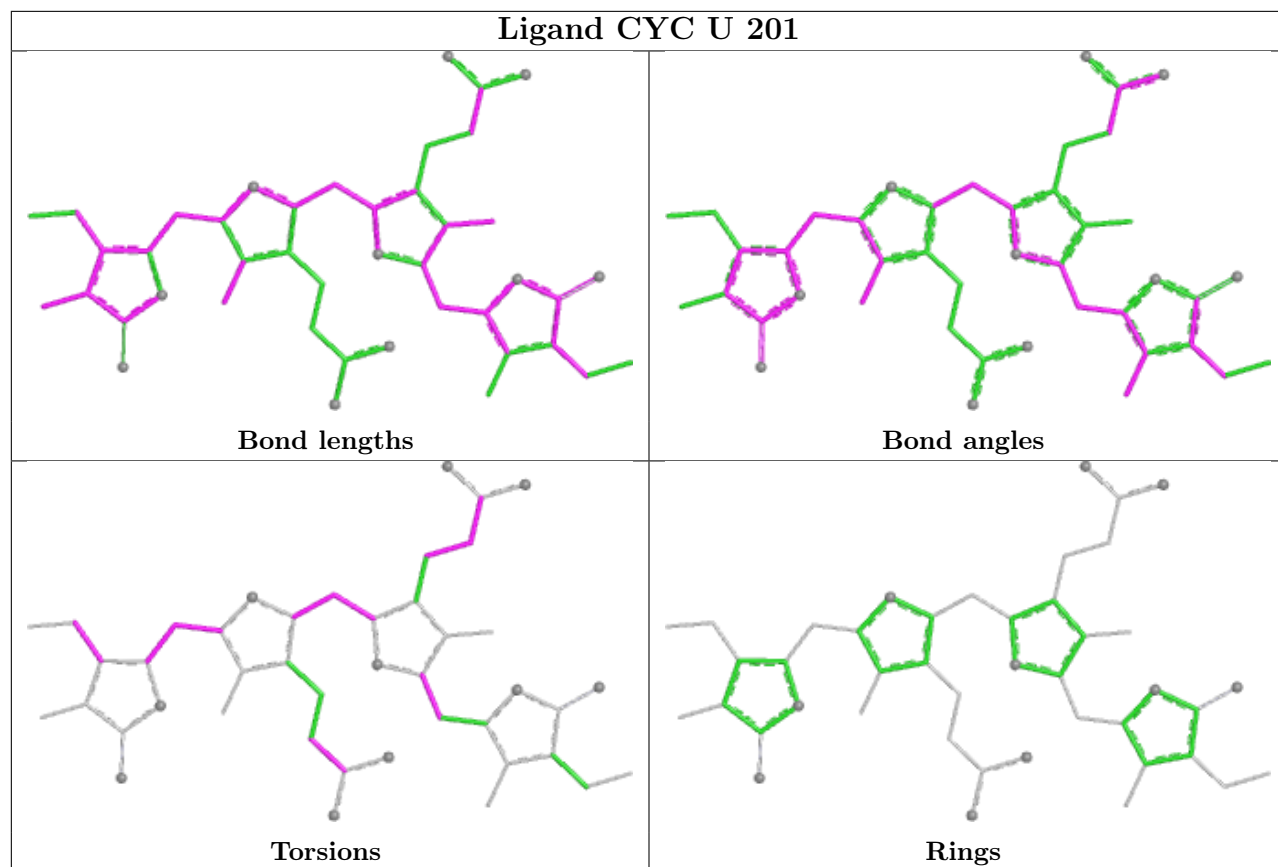


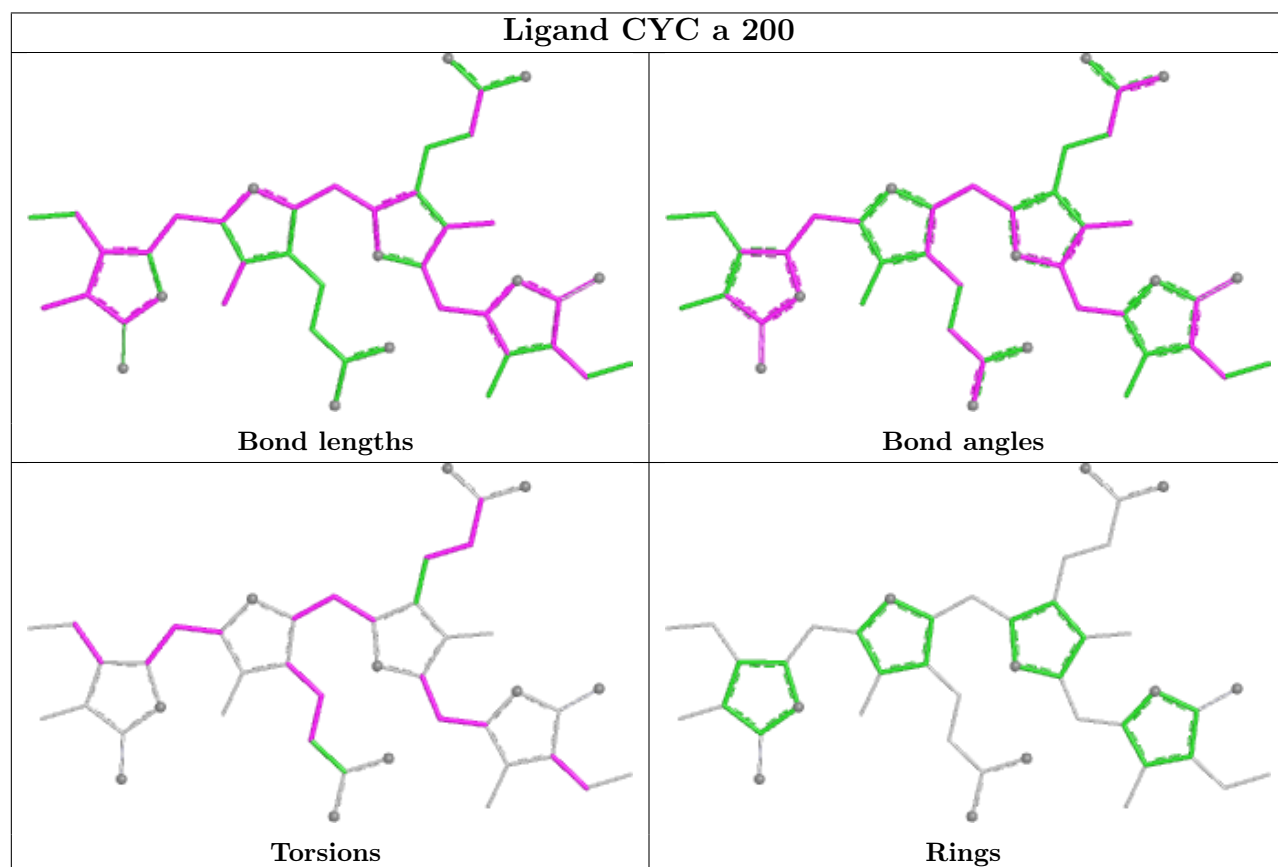
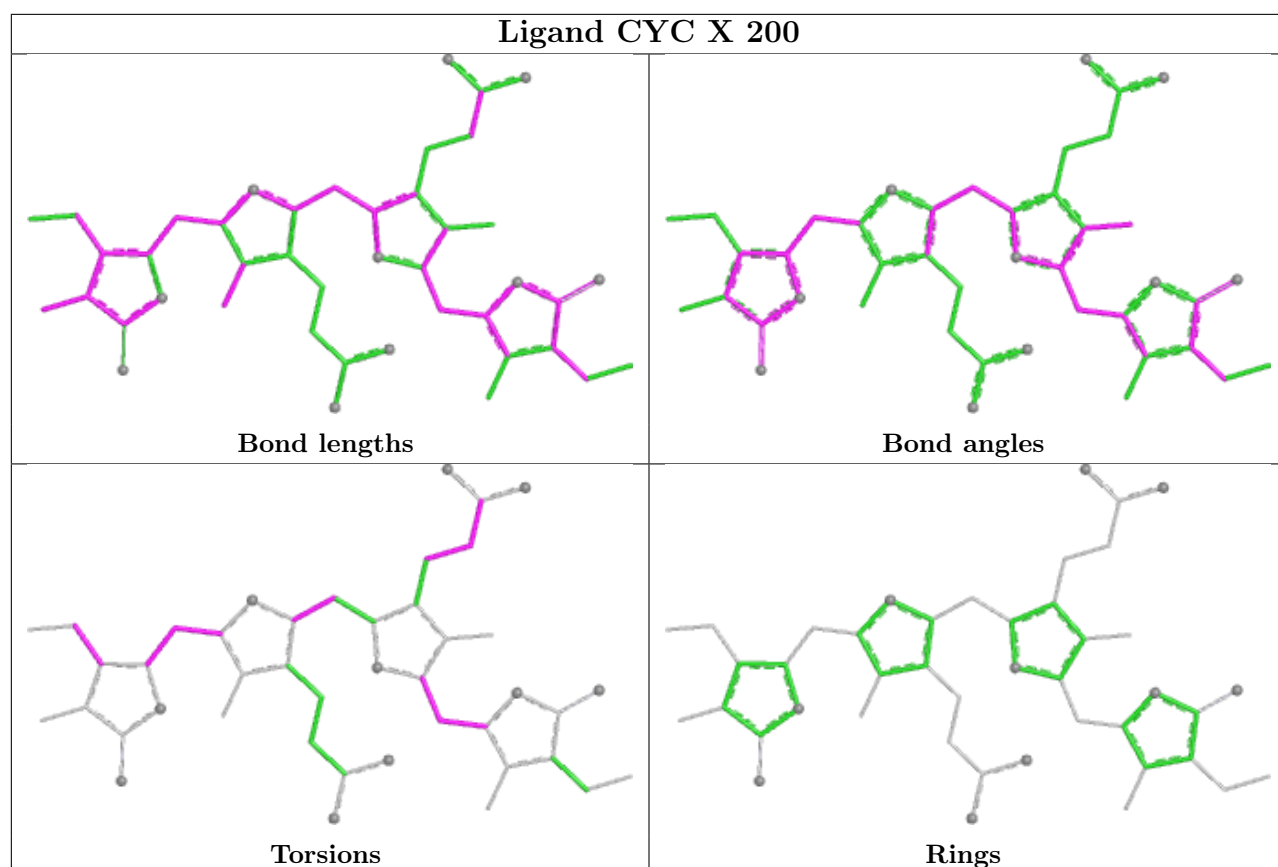




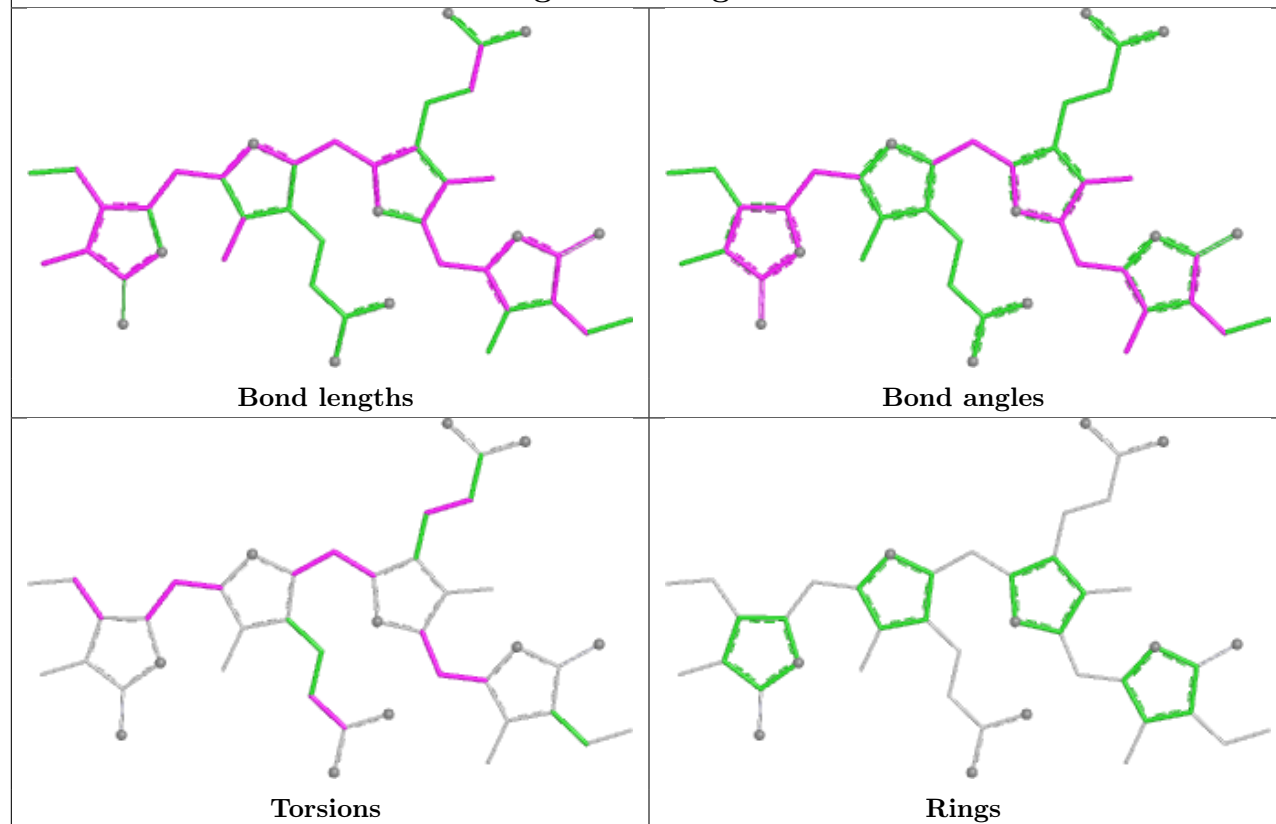




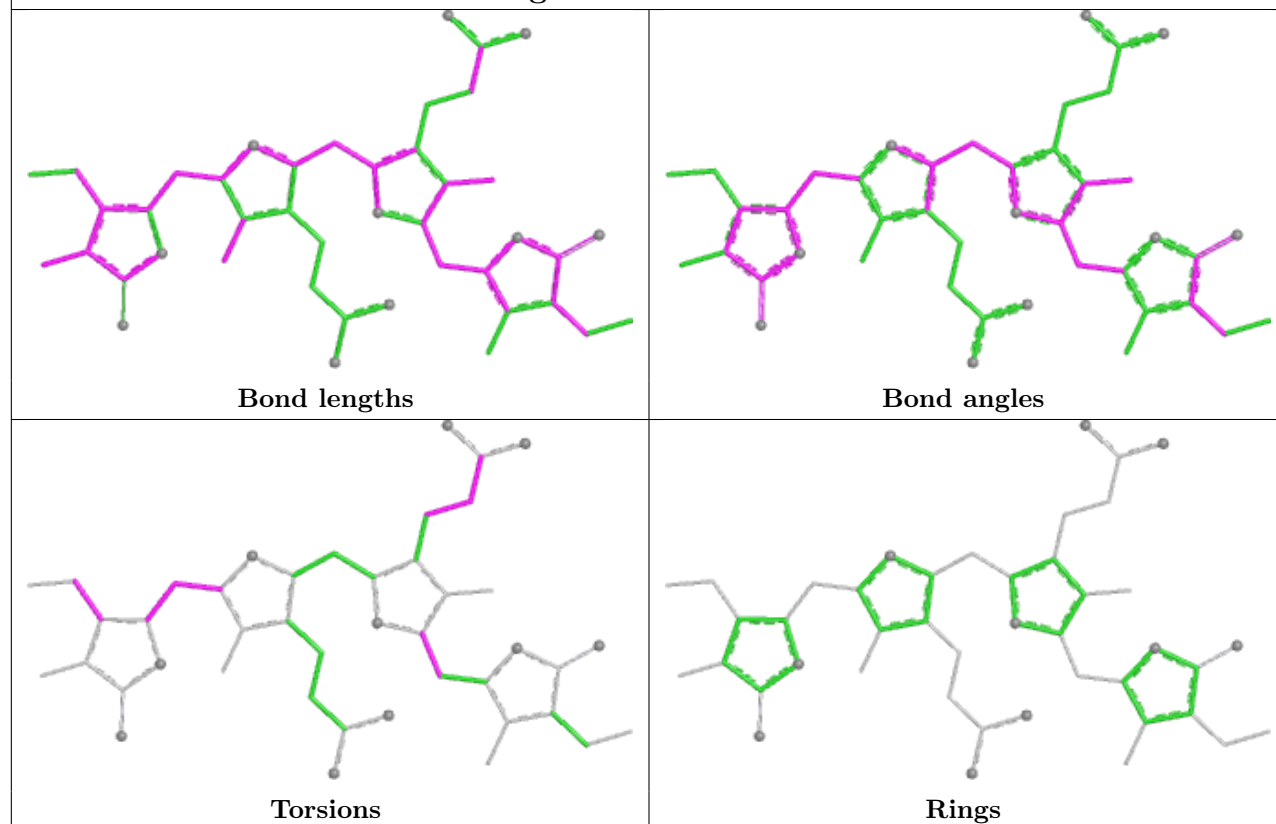


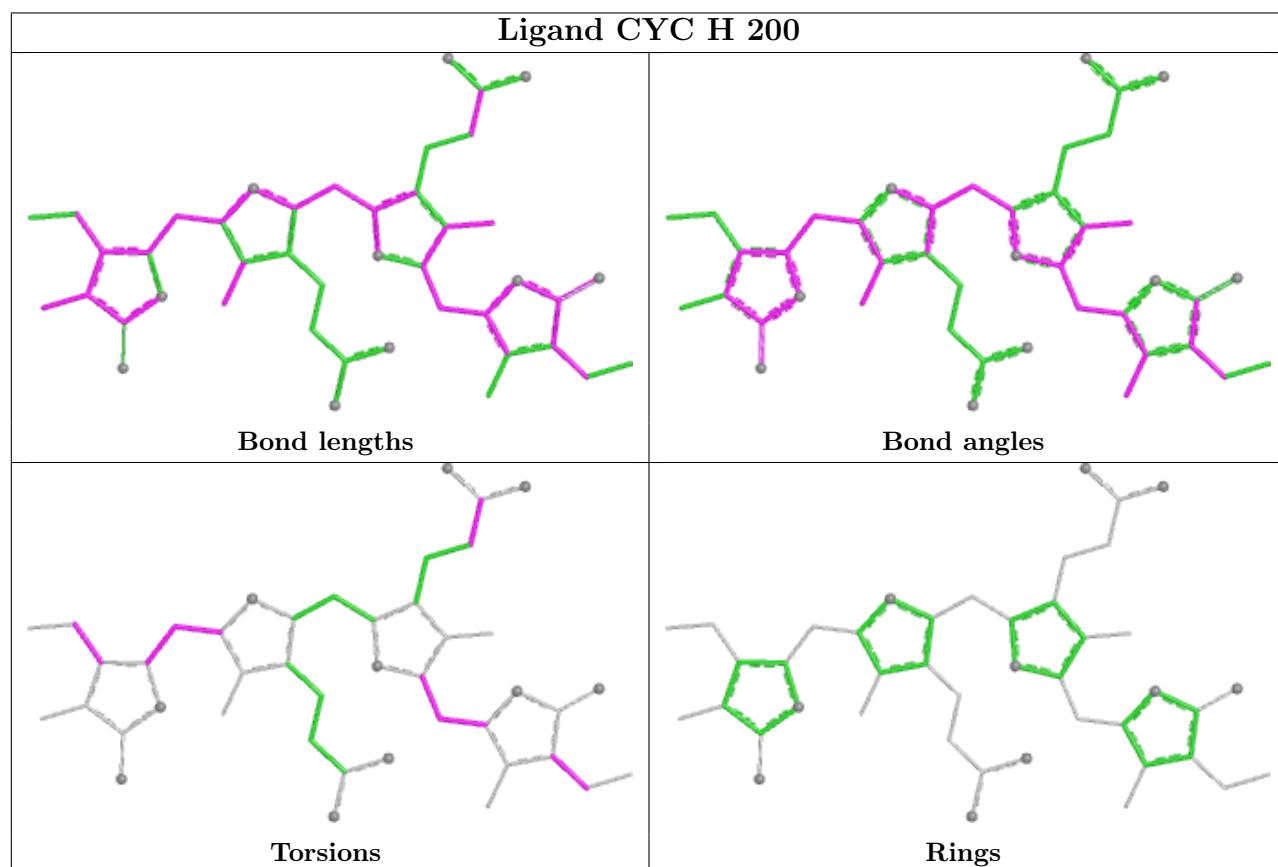
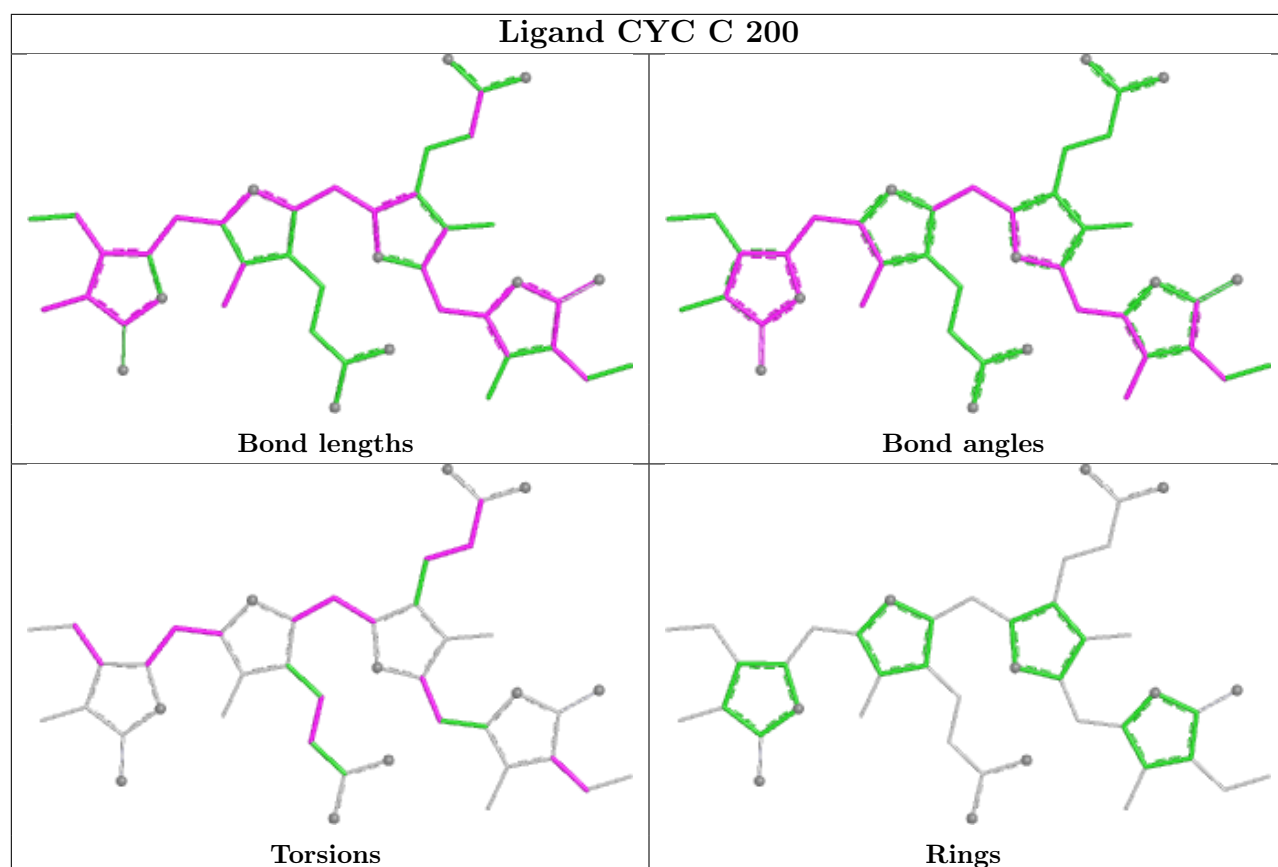


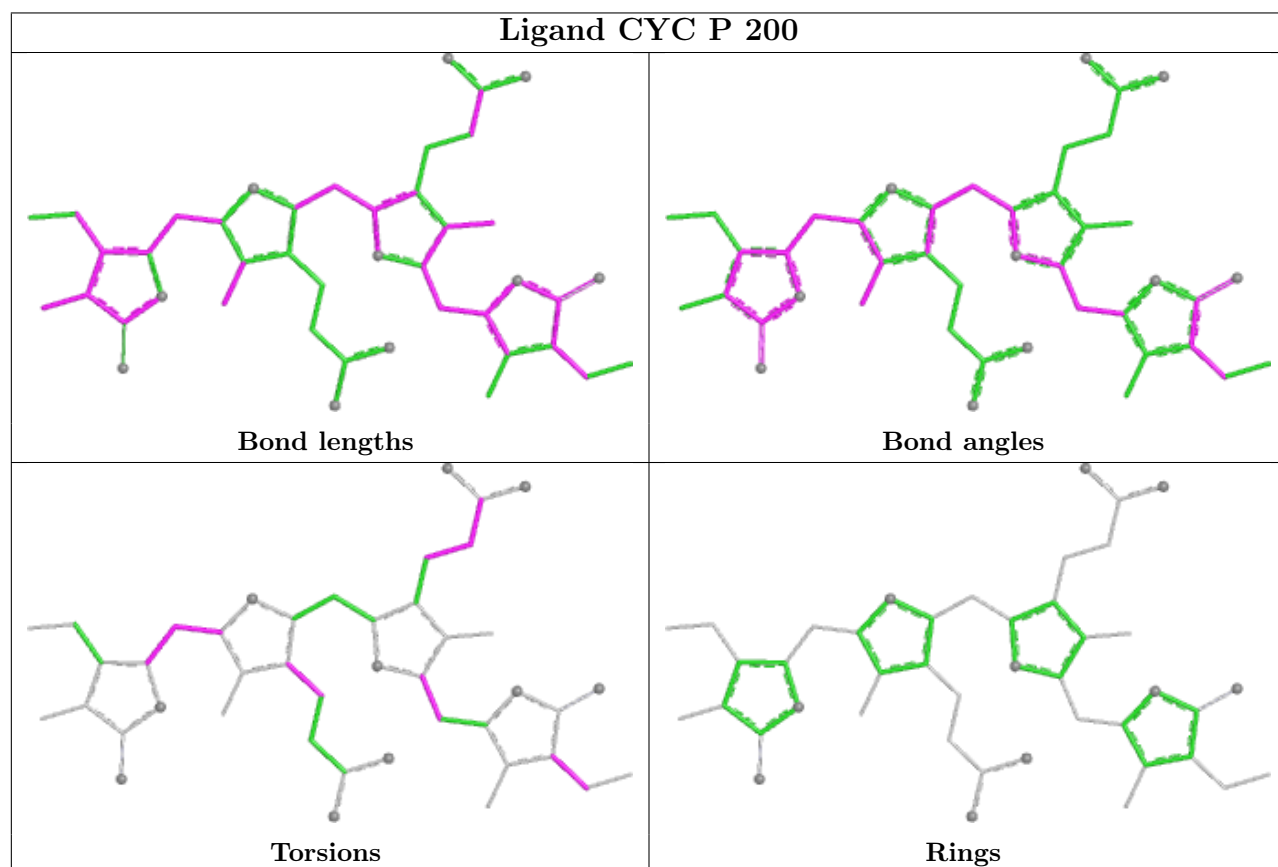
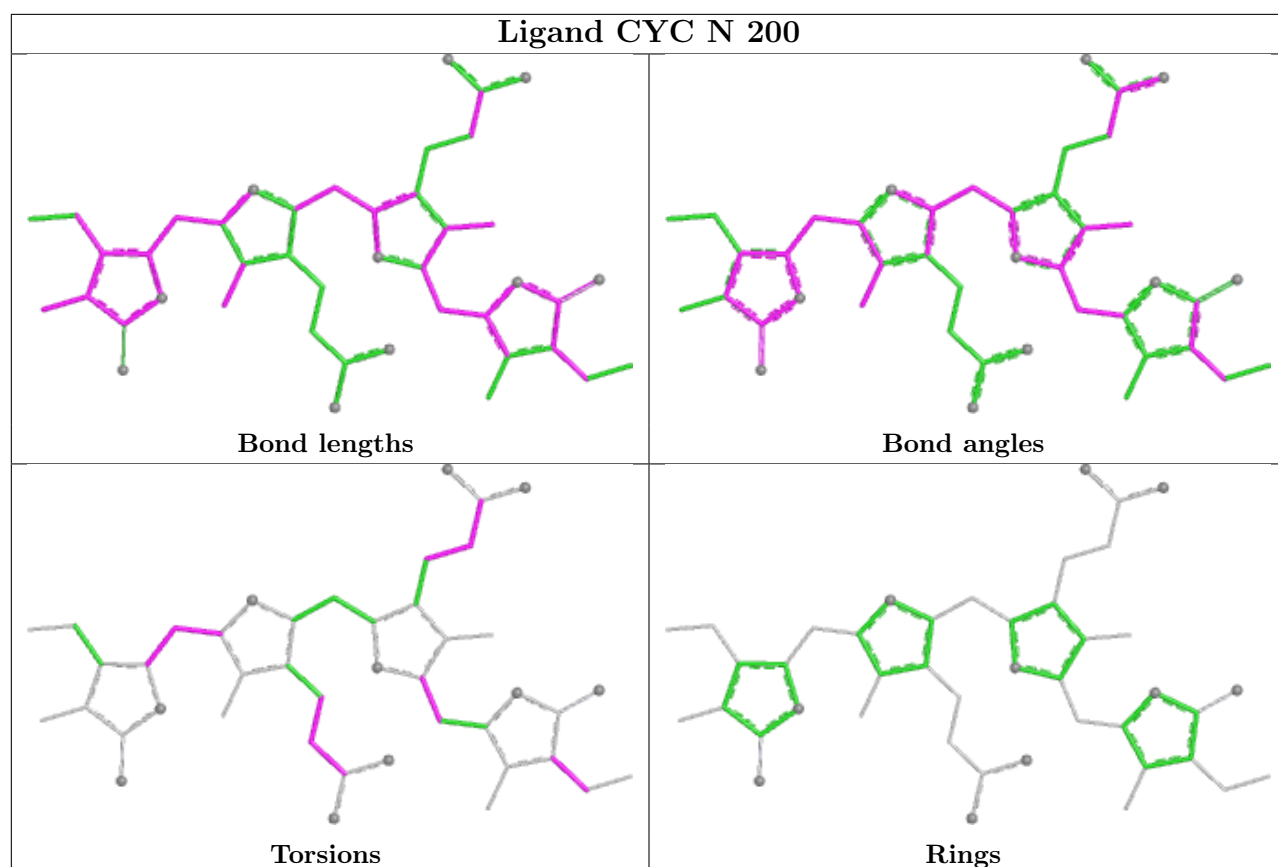
Ligand CYC g 201



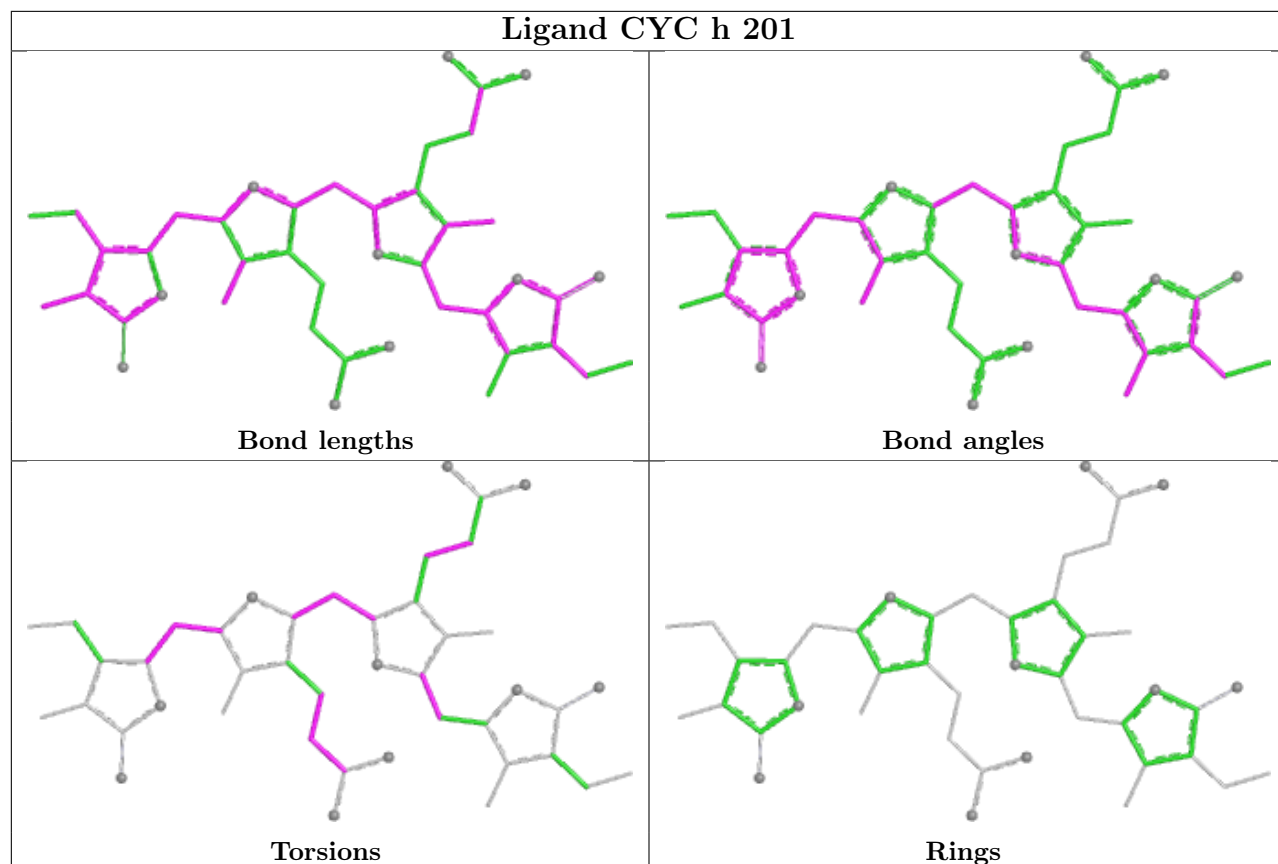
Ligand CYC Y 200



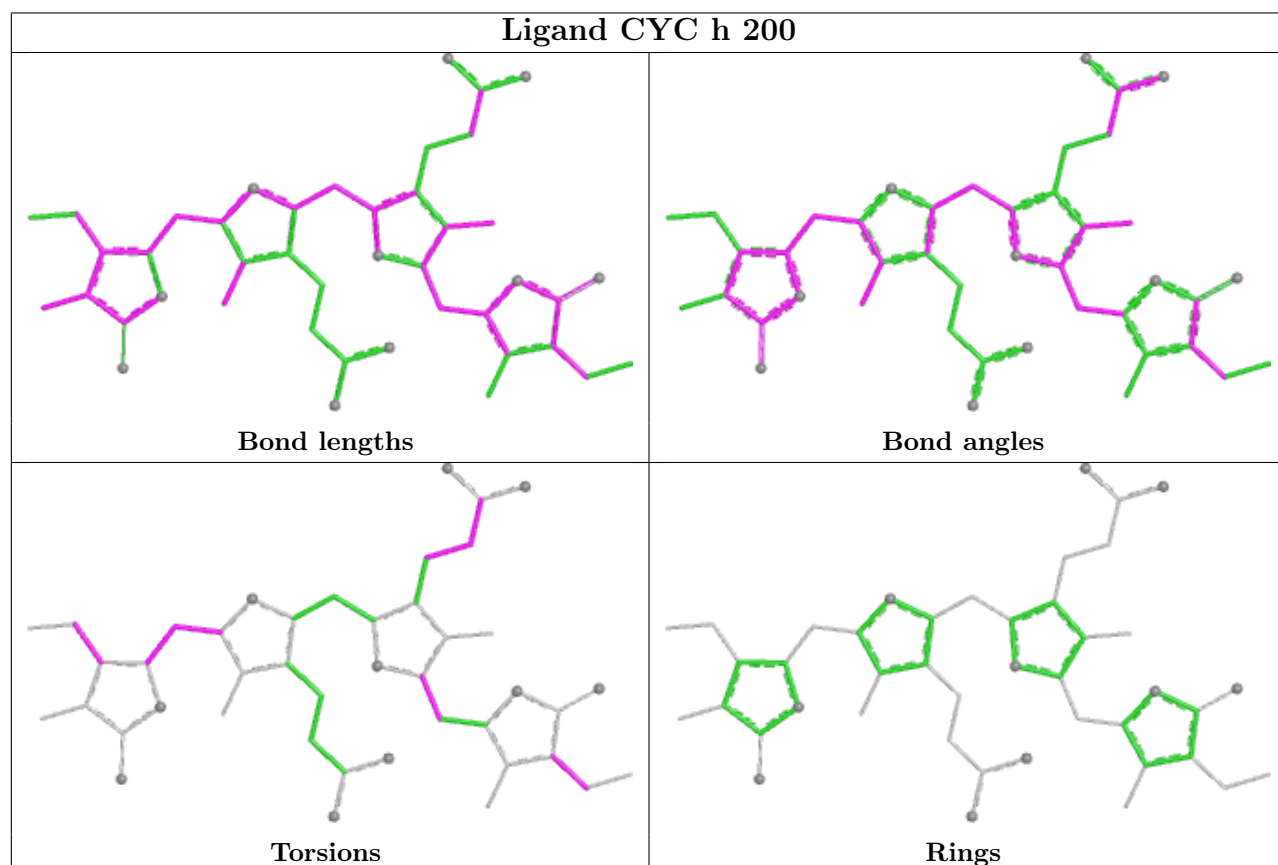


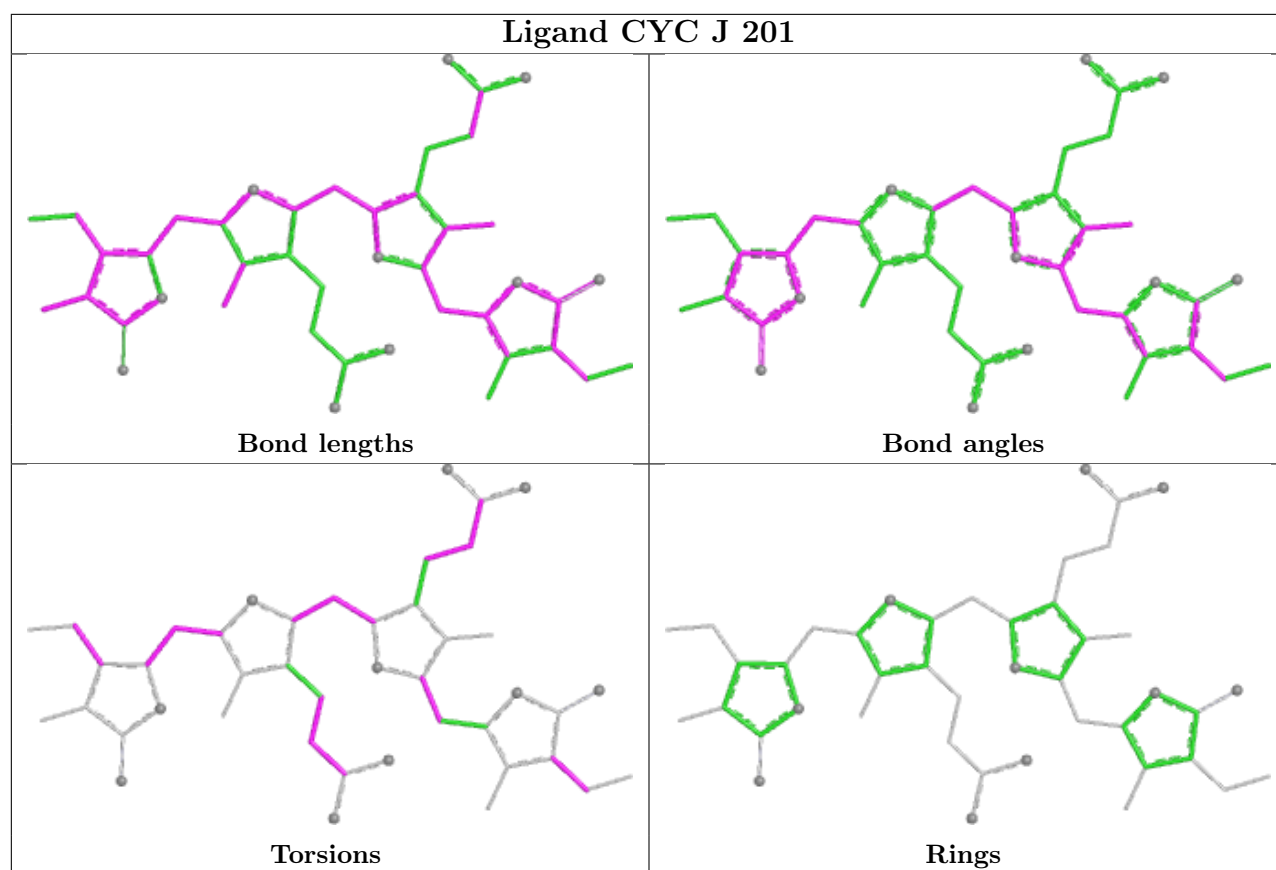


Ligand CYC h 201



Ligand CYC h 200





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.

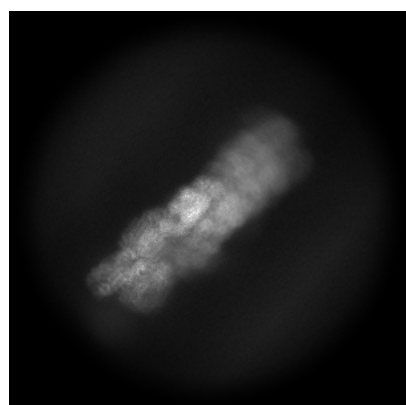
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35570. These allow visual inspection of the internal detail of the map and identification of artifacts.

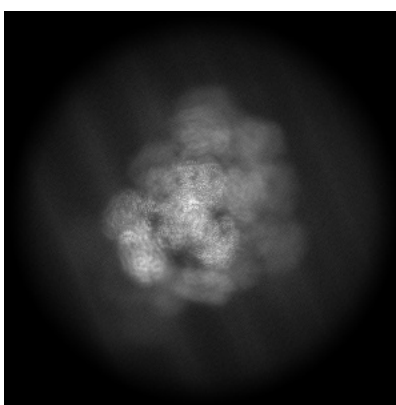
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

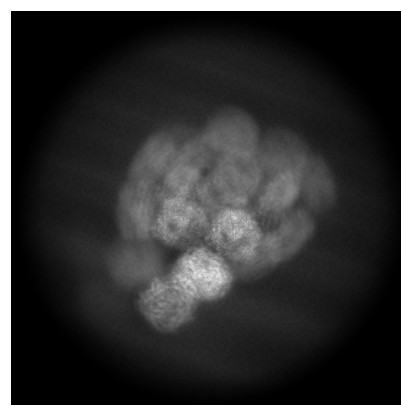
6.1.1 Primary map



X



Y

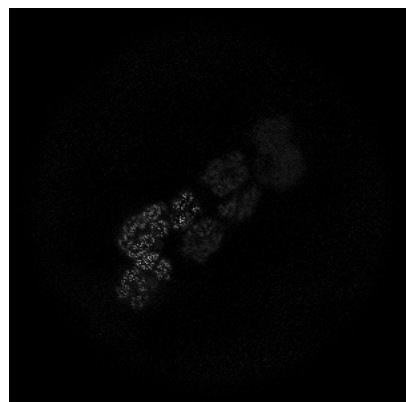


Z

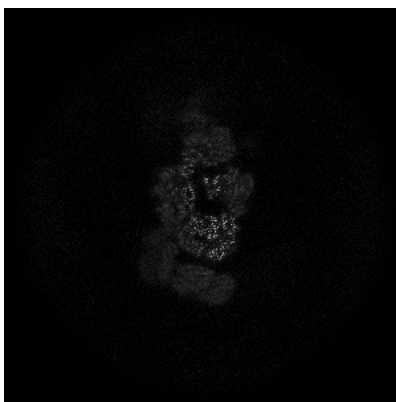
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

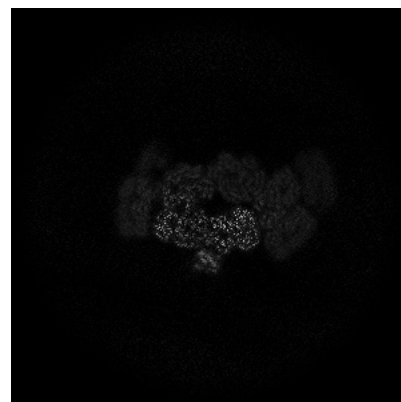
6.2.1 Primary map



X Index: 340



Y Index: 340

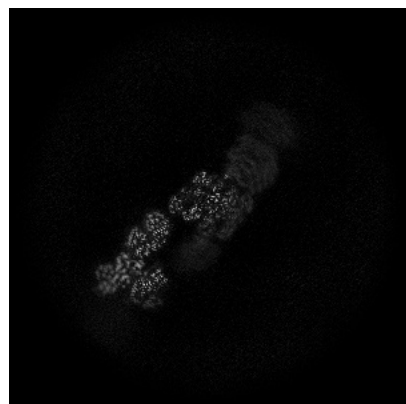


Z Index: 340

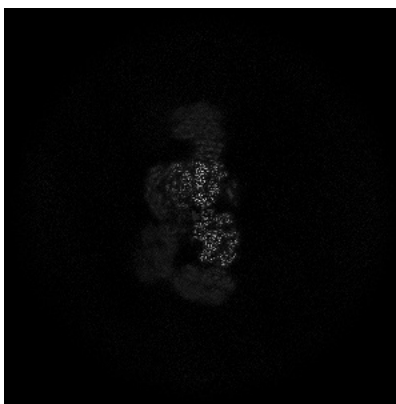
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

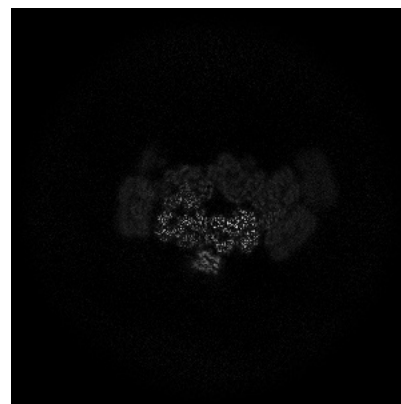
6.3.1 Primary map



X Index: 298



Y Index: 320



Z Index: 337

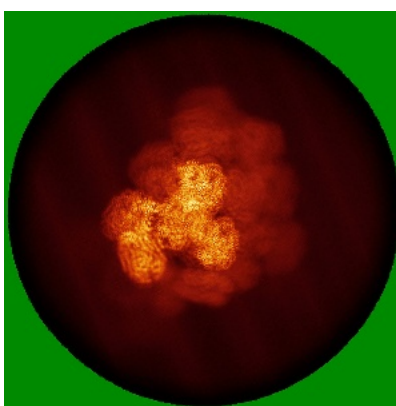
The images above show the largest variance slices of the map in three orthogonal directions.

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

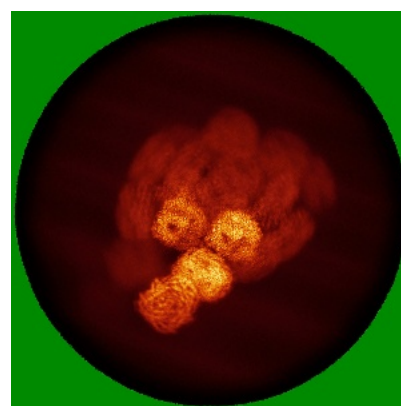
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

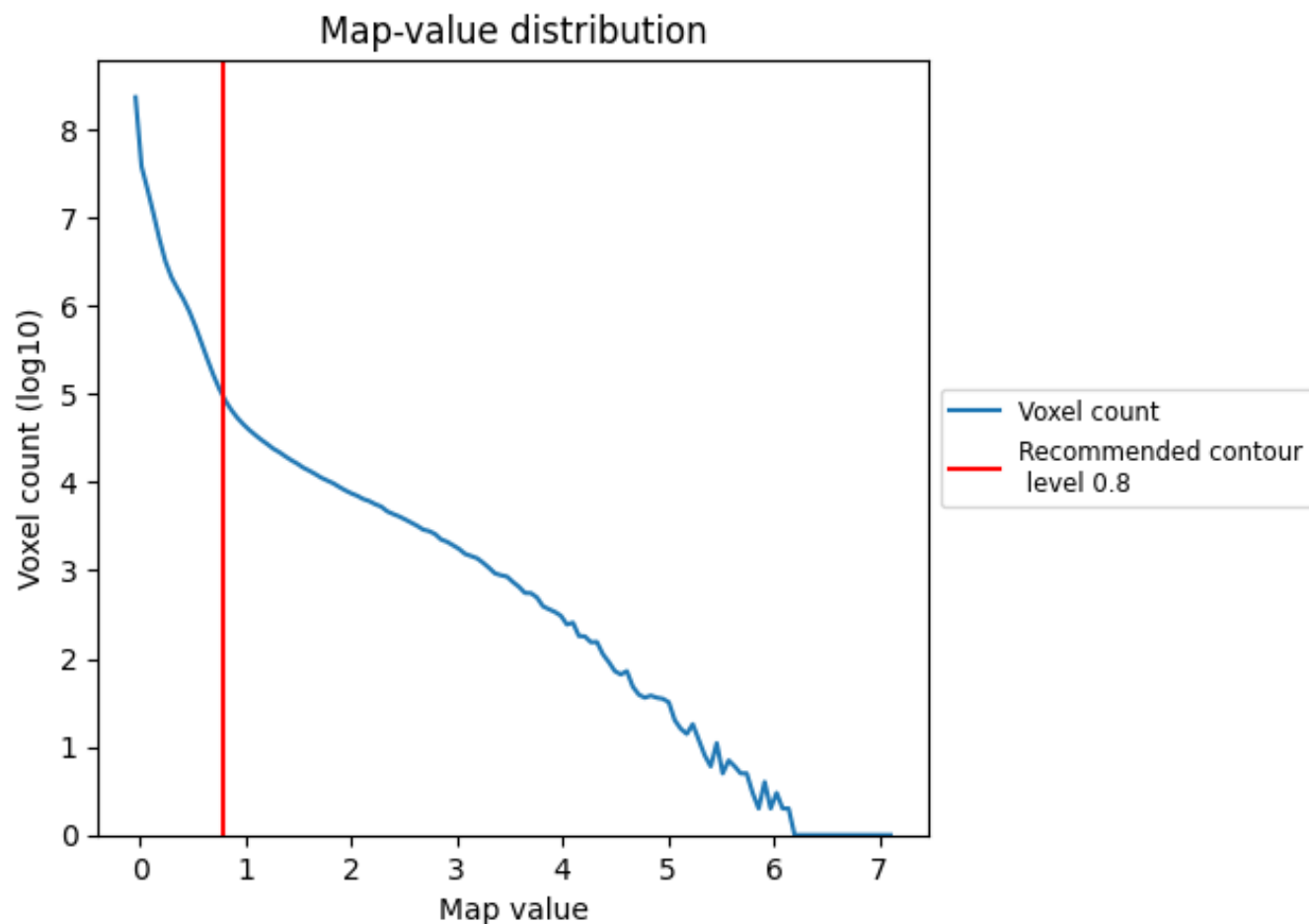
6.6 Mask visualisation

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

7 Map analysis [i](#)

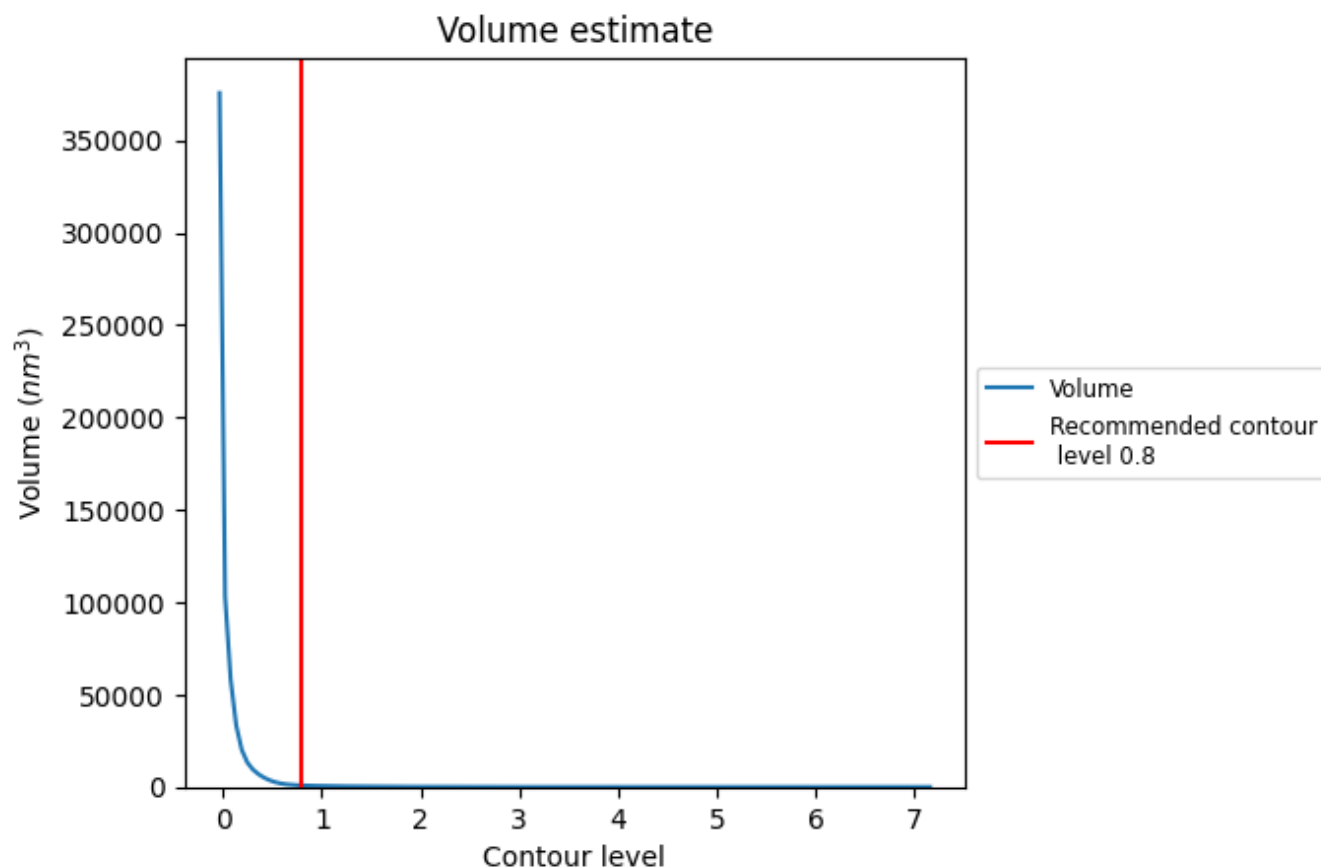
This section contains the results of statistical analysis of the map.

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.

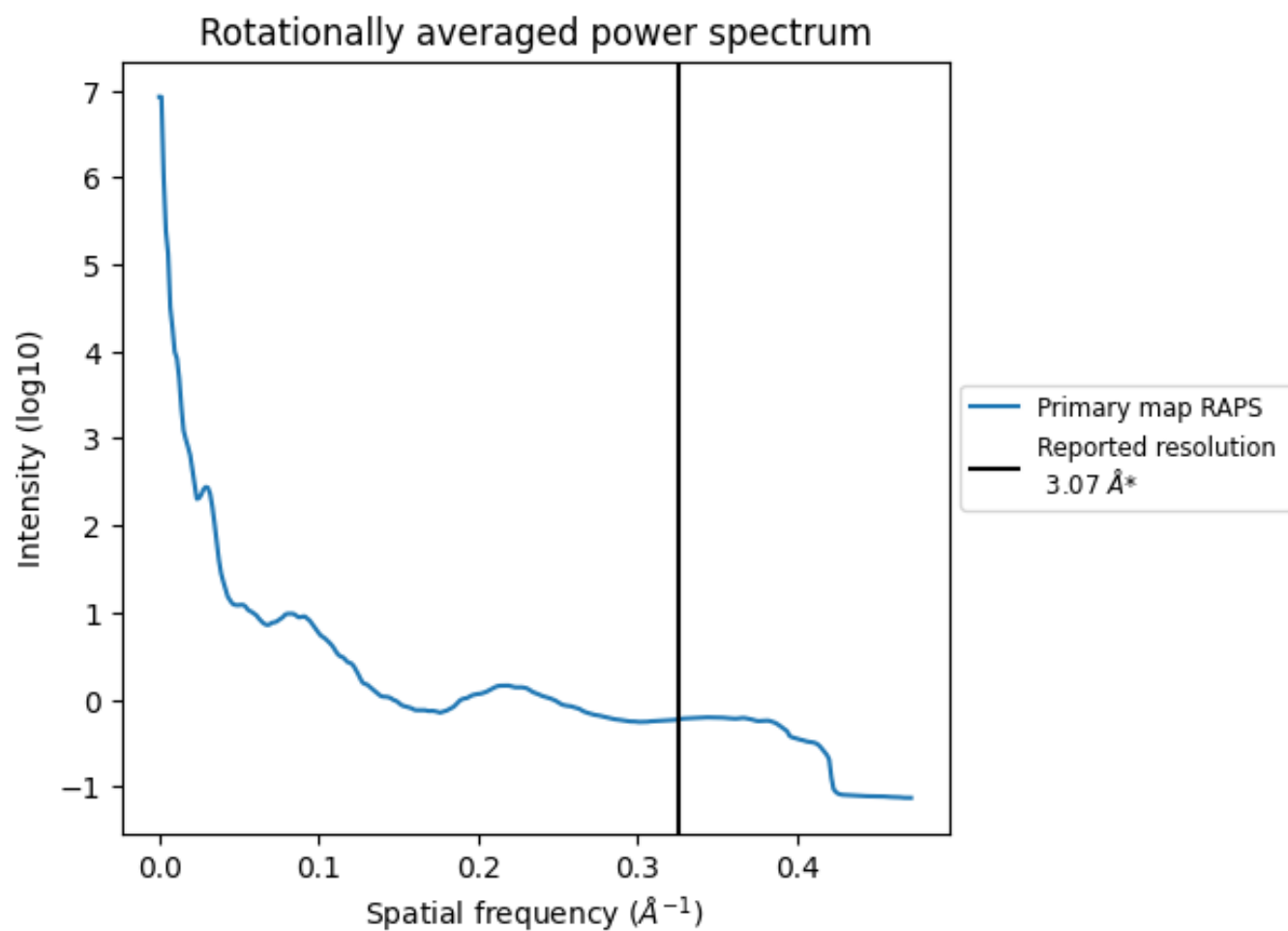
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 815 nm^3 ; this corresponds to an approximate mass of 736 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 0.326 Å⁻¹

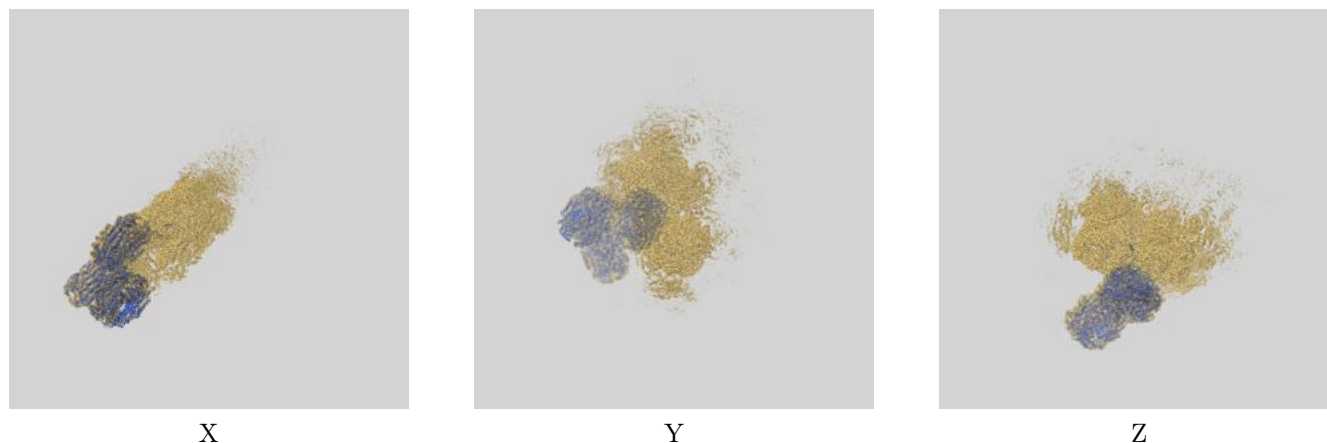
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

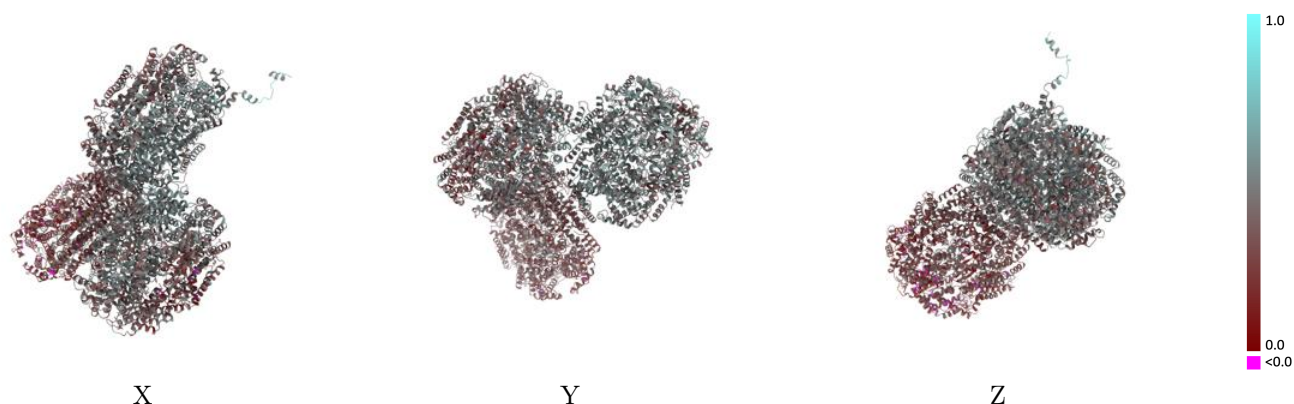
This section contains information regarding the fit between EMDB map EMD-35570 and PDB model 8IMN. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.8 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](#)

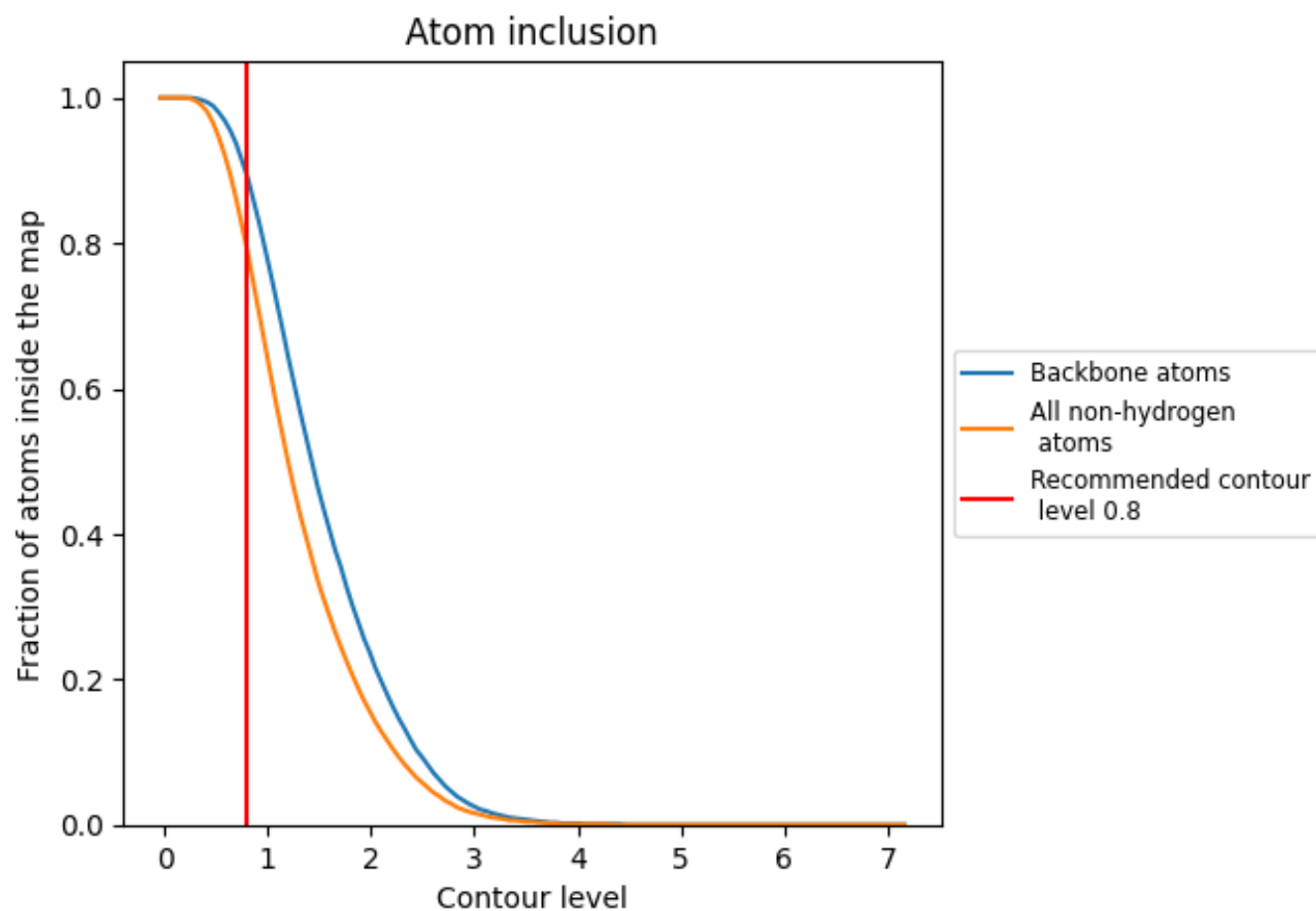


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 79% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7910	 0.3970
5	 0.8500	 0.4540
A	 0.9390	 0.4340
B	 0.9400	 0.4870
C	 0.8590	 0.4420
D	 0.9220	 0.5150
E	 0.9220	 0.4720
F	 0.9100	 0.5040
G	 0.9210	 0.4320
H	 0.8160	 0.4020
I	 0.8720	 0.4500
J	 0.9170	 0.5150
K	 0.9180	 0.5200
L	 0.8680	 0.5080
M	 0.5730	 0.3850
N	 0.7860	 0.4440
O	 0.7730	 0.4600
P	 0.2910	 0.3400
Q	 0.7440	 0.4660
R	 0.6520	 0.4330
S	 0.9270	 0.5170
T	 0.7730	 0.4070
U	 0.4110	 0.3550
V	 0.4600	 0.3910
W	 0.9250	 0.5130
X	 0.7780	 0.4660
Y	 0.8300	 0.4950
Z	 0.0700	 0.3000
a	 0.8620	 0.2810
b	 0.8270	 0.2670
c	 0.6320	 0.2060
d	 0.8700	 0.2620
e	 0.8890	 0.2670
f	 0.9300	 0.3340
g	 0.8680	 0.2740



Continued on next page...

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Chain	Atom inclusion	Q-score
h	 0.6360	 0.2190
i	 0.6710	 0.2130
j	 0.7710	 0.2990
k	 0.8330	 0.2670
l	 0.8970	 0.3290
m	 0.2480	 0.1930