



Full wwPDB EM Validation Report ⓘ

Oct 20, 2025 – 01:41 AM JST

PDB ID : 9V7L / pdb_00009v7l
EMDB ID : EMD-64817
Title : Phycobilisome rod R1 from *Gloeobacter violaceus* PCC 7421
Authors : Burtseva, A.D.; Baymukhametov, T.N.; Slonimskiy, Y.B.; Popov, V.O.;
Sluchanko, N.N.; Boyko, K.M.
Deposited on : 2025-05-28
Resolution : 3.76 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

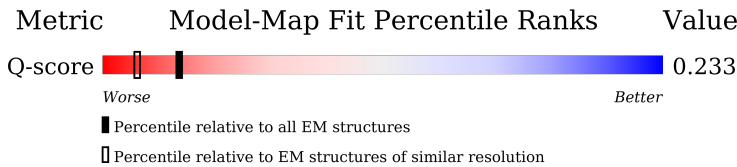
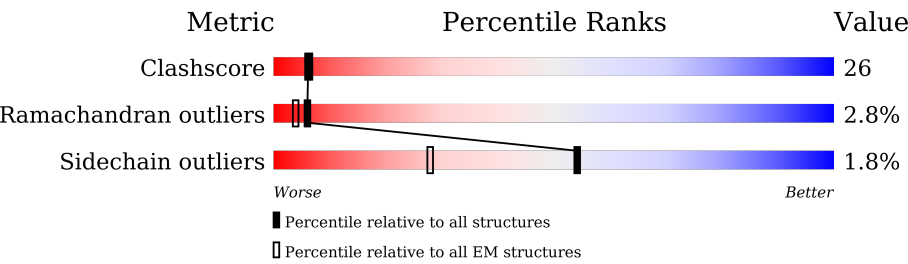
EMDB validation analysis : 0.0.1.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.76 Å.

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


























Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	10214 (3.26 - 4.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	824	<div><div>9%13%•</div><div>74%</div></div>
2	Z	275	<div><div>15%11%•</div><div>73%</div></div>
3	B	172	<div><div>•</div><div>59%37%•</div></div>
3	D	172	<div><div>•</div><div>56%39%••</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	172	
3	H	172	
3	J	172	
3	L	172	
3	O	172	
3	Q	172	
3	S	172	
3	U	172	
3	W	172	
3	Y	172	
4	C	162	
4	E	162	
4	G	162	
4	I	162	
4	K	162	
4	N	162	
4	P	162	
4	R	162	
4	T	162	
4	V	162	
4	X	162	
4	a	162	
5	M	274	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CYC	H	201	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 36440 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 Glr1262 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	216	Total	C	N	O	S	0	0
			1717	1070	311	333	3		

- Molecule 2 is a protein called Phycocyanin-associated rod linker protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Z	73	Total	C	N	O	S	0	0
			570	356	103	110	1		

- Molecule 3 is a protein called Phycocyanin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	D	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	F	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	H	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	J	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	L	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	O	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	Q	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	S	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	U	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	W	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Y	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		

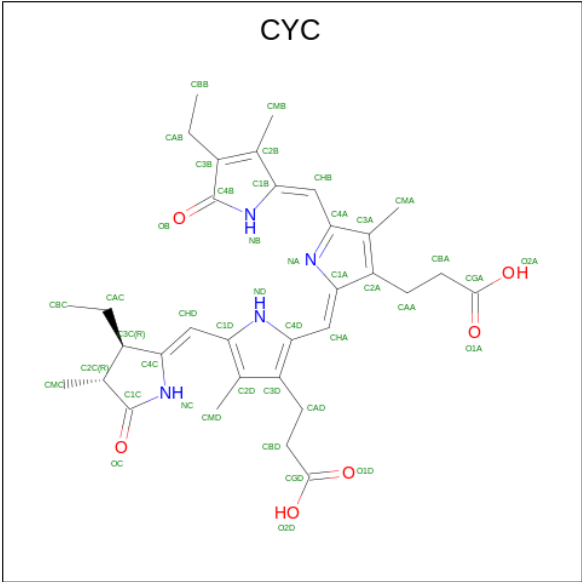
- Molecule 4 is a protein called Phycocyanin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
4	E	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
4	G	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
4	I	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
4	K	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
4	N	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
4	P	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
4	R	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
4	T	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
4	V	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
4	X	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
4	a	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		

- Molecule 5 is a protein called Phycocyanin-associated rod linker protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	273	Total	C	N	O	S	0	0
			2173	1378	376	414	5		

- Molecule 6 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			43	33	4	6	
6	B	1	Total	C	N	O	0
			43	33	4	6	
6	C	1	Total	C	N	O	0
			43	33	4	6	
6	D	1	Total	C	N	O	0
			43	33	4	6	
6	D	1	Total	C	N	O	0
			43	33	4	6	
6	E	1	Total	C	N	O	0
			43	33	4	6	
6	F	1	Total	C	N	O	0
			43	33	4	6	
6	F	1	Total	C	N	O	0
			43	33	4	6	
6	G	1	Total	C	N	O	0
			43	33	4	6	
6	H	1	Total	C	N	O	0
			43	33	4	6	
6	H	1	Total	C	N	O	0
			43	33	4	6	
6	I	1	Total	C	N	O	0
			43	33	4	6	
6	J	1	Total	C	N	O	0
			43	33	4	6	
6	J	1	Total	C	N	O	0
			43	33	4	6	

Continued on next page...

Continued from previous page...

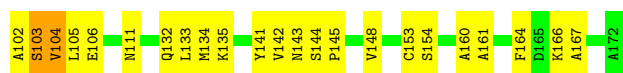
Mol	Chain	Residues	Atoms				AltConf
6	K	1	Total 43	C 33	N 4	O 6	0
6	L	1	Total 43	C 33	N 4	O 6	0
6	L	1	Total 43	C 33	N 4	O 6	0
6	N	1	Total 43	C 33	N 4	O 6	0
6	O	1	Total 43	C 33	N 4	O 6	0
6	O	1	Total 43	C 33	N 4	O 6	0
6	P	1	Total 43	C 33	N 4	O 6	0
6	Q	1	Total 43	C 33	N 4	O 6	0
6	Q	1	Total 43	C 33	N 4	O 6	0
6	R	1	Total 43	C 33	N 4	O 6	0
6	S	1	Total 43	C 33	N 4	O 6	0
6	S	1	Total 43	C 33	N 4	O 6	0
6	T	1	Total 43	C 33	N 4	O 6	0
6	U	1	Total 43	C 33	N 4	O 6	0
6	U	1	Total 43	C 33	N 4	O 6	0
6	V	1	Total 43	C 33	N 4	O 6	0
6	W	1	Total 43	C 33	N 4	O 6	0
6	W	1	Total 43	C 33	N 4	O 6	0
6	X	1	Total 43	C 33	N 4	O 6	0
6	Y	1	Total 43	C 33	N 4	O 6	0
6	Y	1	Total 43	C 33	N 4	O 6	0

Continued on next page...

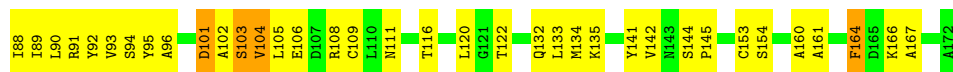
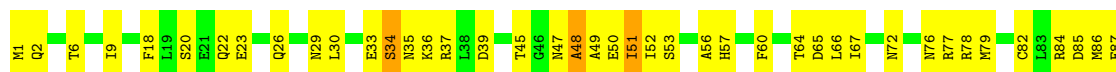
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	a	1	43	33	4	6	0

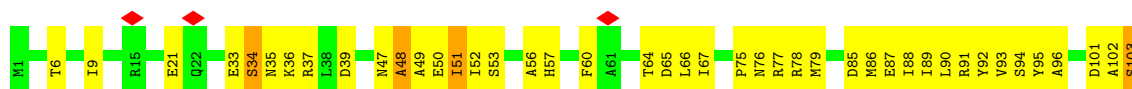




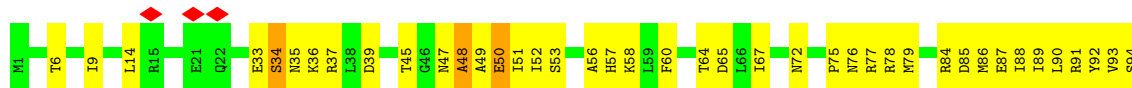
• Molecule 3: Phycocyanin beta chain



• Molecule 3: Phycocyanin beta chain



• Molecule 3: Phycocyanin beta chain

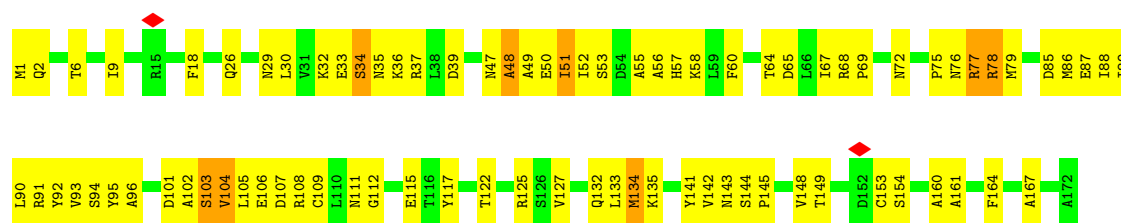


• Molecule 3: Phycocyanin beta chain

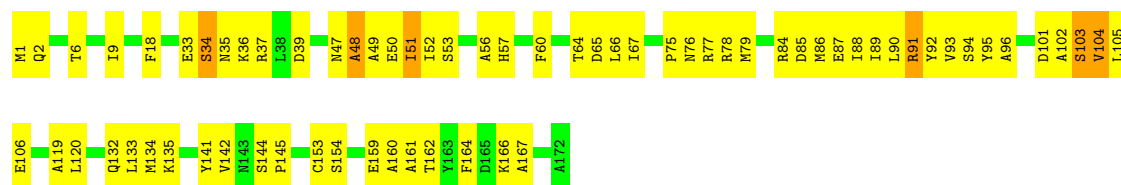


• Molecule 3: Phycocyanin beta chain

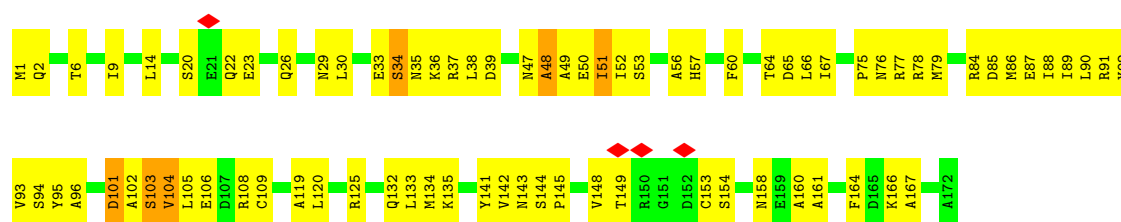




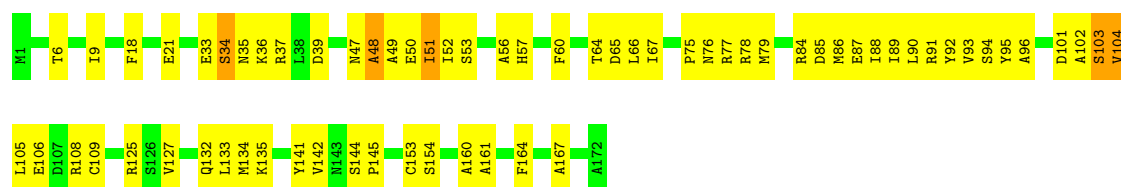
• Molecule 3: Phycocyanin beta chain



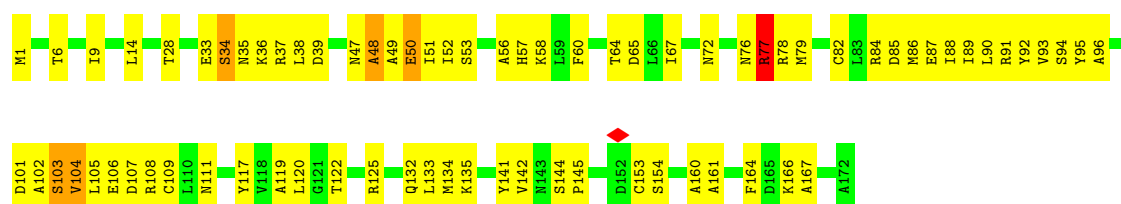
• Molecule 3: Phycocyanin beta chain



• Molecule 3: Phycocyanin beta chain

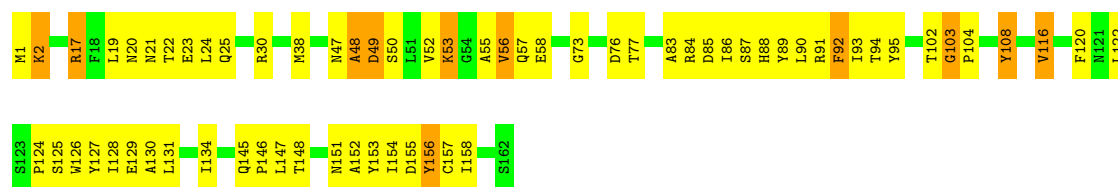


• Molecule 3: Phycocyanin beta chain



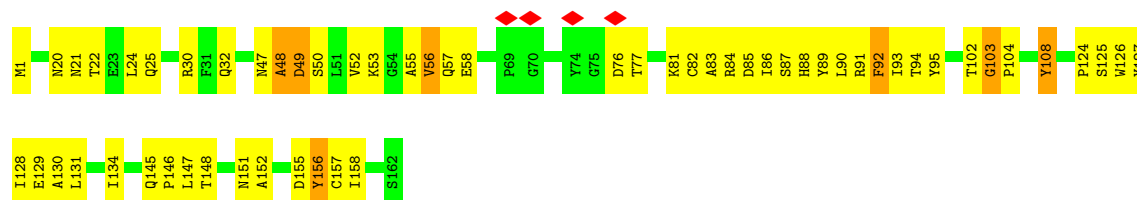
• Molecule 4: Phycocyanin alpha chain

Chain C: 



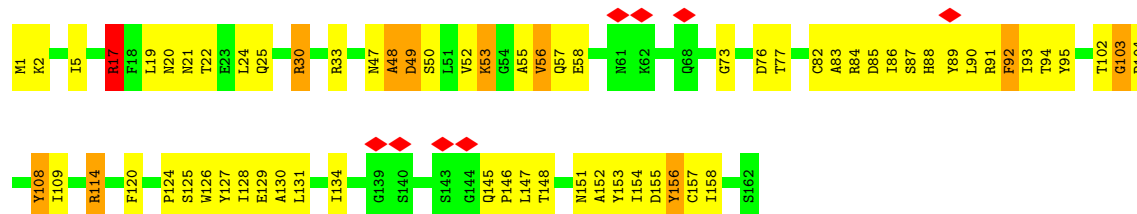
• Molecule 4: Phycocyanin alpha chain

Chain E: 



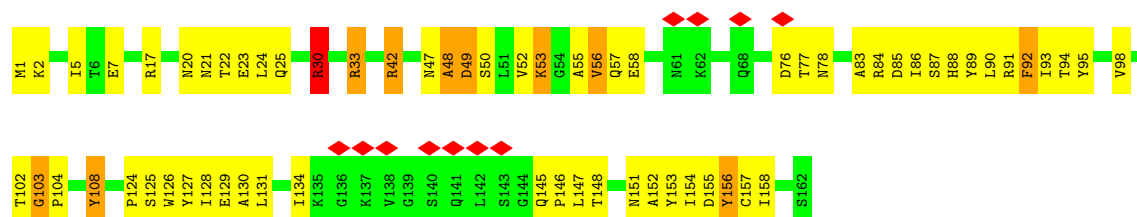
• Molecule 4: Phycocyanin alpha chain

Chain G: 



• Molecule 4: Phycocyanin alpha chain

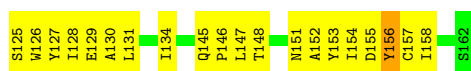
Chain I: 



• Molecule 4: Phycocyanin alpha chain

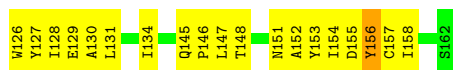
Chain K: 





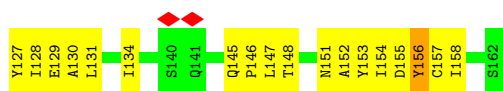
• Molecule 4: Phycocyanin alpha chain

Chain N: 60% 33% 5%



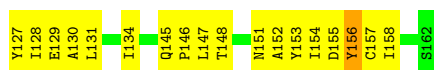
• Molecule 4: Phycocyanin alpha chain

Chain P: 61% 33% 6%



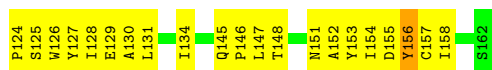
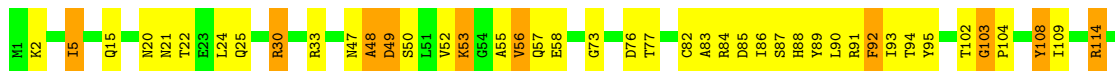
• Molecule 4: Phycocyanin alpha chain

Chain R: 62% 34% 4%



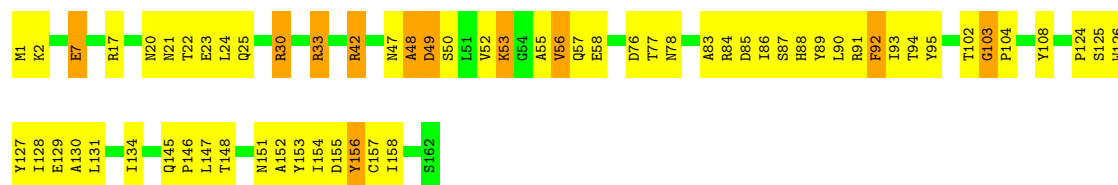
• Molecule 4: Phycocyanin alpha chain

Chain T: 60% 33% 7%

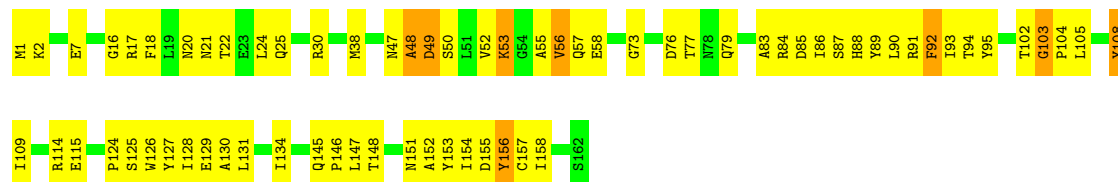


• Molecule 4: Phycocyanin alpha chain

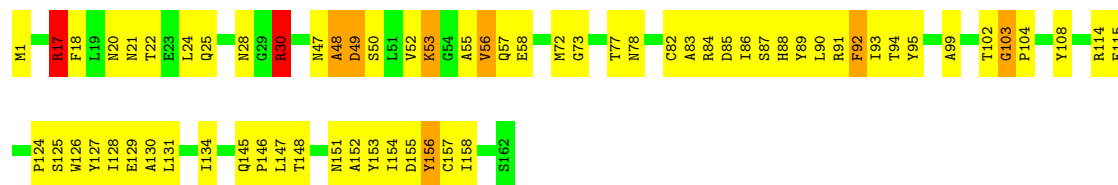
Chain V: 60% 33% 7%



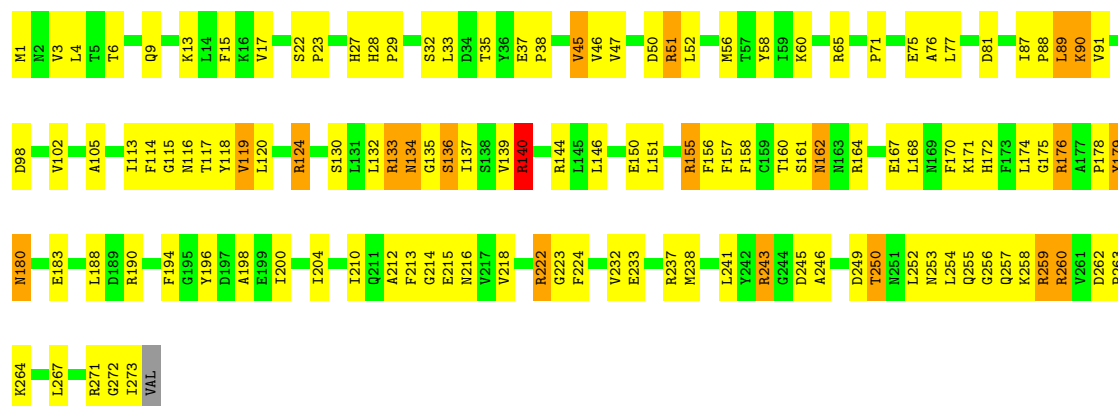
• Molecule 4: Phycocyanin alpha chain



• Molecule 4: Phycocyanin alpha chain



• Molecule 5: Phycocyanin-associated rod linker protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	746972	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	85000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.370	Depositor
Minimum map value	-1.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.2	Depositor
Map size (\AA)	840.0, 840.0, 840.0	wwPDB
Map dimensions	672, 672, 672	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.25, 1.25, 1.25	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	A	0.66	0/1748	1.42	16/2361 (0.7%)
2	Z	0.53	0/581	1.13	0/787
3	B	0.50	0/1307	1.14	2/1768 (0.1%)
3	D	0.54	0/1307	1.19	4/1768 (0.2%)
3	F	0.55	0/1307	1.17	1/1768 (0.1%)
3	H	0.51	0/1307	1.16	2/1768 (0.1%)
3	J	0.52	0/1307	1.15	1/1768 (0.1%)
3	L	0.54	0/1307	1.26	4/1768 (0.2%)
3	O	0.54	0/1307	1.17	2/1768 (0.1%)
3	Q	0.54	0/1307	1.19	3/1768 (0.2%)
3	S	0.51	0/1307	1.14	1/1768 (0.1%)
3	U	0.51	0/1307	1.17	1/1768 (0.1%)
3	W	0.53	0/1307	1.14	1/1768 (0.1%)
3	Y	0.55	0/1307	1.28	5/1768 (0.3%)
4	C	0.48	0/1265	1.12	5/1713 (0.3%)
4	E	0.48	0/1265	1.12	3/1713 (0.2%)
4	G	0.49	0/1265	1.17	6/1713 (0.4%)
4	I	0.48	0/1265	1.13	3/1713 (0.2%)
4	K	0.49	0/1265	1.10	2/1713 (0.1%)
4	N	0.49	0/1265	1.17	6/1713 (0.4%)
4	P	0.47	0/1265	1.11	4/1713 (0.2%)
4	R	0.49	0/1265	1.12	3/1713 (0.2%)
4	T	0.50	0/1265	1.12	3/1713 (0.2%)
4	V	0.48	0/1265	1.12	4/1713 (0.2%)
4	X	0.50	0/1265	1.11	3/1713 (0.2%)
4	a	0.49	0/1265	1.17	6/1713 (0.4%)
5	M	0.60	0/2220	1.22	4/3004 (0.1%)
All	All	0.52	0/35413	1.17	95/47924 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
2	Z	0	3
3	B	0	1
3	D	0	4
3	F	0	2
3	H	0	2
3	L	0	4
3	O	0	3
3	Q	0	3
3	S	0	1
3	U	0	2
3	W	0	1
3	Y	0	4
4	C	0	1
4	G	0	2
4	I	0	3
4	K	0	1
4	N	0	2
4	P	0	2
4	T	0	1
4	V	0	3
4	X	0	2
4	a	0	2
5	M	0	10
All	All	0	66

There are no bond length outliers.

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	50	GLU	CB-CA-C	14.25	132.90	110.96
3	L	50	GLU	CB-CA-C	14.21	132.84	110.96
4	G	17	ARG	CD-NE-CZ	12.36	141.70	124.40
1	A	147	ASN	CB-CA-C	-10.18	93.90	110.79
1	A	264	ASP	CA-CB-CG	8.34	120.94	112.60
4	N	92	PHE	CA-CB-CG	-8.00	105.80	113.80
3	Y	77	ARG	CD-NE-CZ	7.99	135.59	124.40
4	C	92	PHE	CA-CB-CG	-7.96	105.84	113.80
4	E	92	PHE	CA-CB-CG	-7.93	105.87	113.80
4	P	92	PHE	CA-CB-CG	-7.91	105.89	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	a	30	ARG	CG-CD-NE	7.90	129.37	112.00
4	N	30	ARG	CG-CD-NE	7.84	129.24	112.00
4	R	32	GLN	CB-CA-C	7.80	123.74	110.79
4	E	32	GLN	CB-CA-C	7.78	123.71	110.79
4	G	92	PHE	CA-CB-CG	-7.72	106.08	113.80
4	I	92	PHE	CA-CB-CG	-7.64	106.16	113.80
4	a	92	PHE	CA-CB-CG	-7.63	106.17	113.80
4	X	92	PHE	CA-CB-CG	-7.59	106.20	113.80
4	V	92	PHE	CA-CB-CG	-7.56	106.24	113.80
4	T	92	PHE	CA-CB-CG	-7.38	106.42	113.80
4	K	92	PHE	CA-CB-CG	-7.27	106.53	113.80
4	R	92	PHE	CA-CB-CG	-7.09	106.70	113.80
4	a	17	ARG	CA-CB-CG	6.90	127.89	114.10
4	G	17	ARG	NE-CZ-NH2	6.87	125.38	119.20
1	A	248	PHE	CA-CB-CG	-6.87	106.93	113.80
1	A	157	ARG	N-CA-CB	6.66	120.01	110.16
1	A	263	THR	CA-CB-OG1	-6.59	99.71	109.60
4	N	17	ARG	CA-CB-CG	6.54	127.17	114.10
1	A	178	PHE	N-CA-CB	6.40	120.20	110.28
1	A	281	PRO	N-CA-C	6.39	121.96	113.40
3	B	64	THR	CA-CB-OG1	-6.24	100.23	109.60
3	D	77	ARG	CG-CD-NE	-6.21	98.33	112.00
3	O	64	THR	CA-CB-OG1	-6.09	100.46	109.60
1	A	255	TYR	N-CA-CB	5.97	119.93	110.55
4	G	17	ARG	NE-CZ-NH1	-5.91	115.59	121.50
3	J	60	PHE	CA-CB-CG	-5.86	107.94	113.80
3	D	65	ASP	CA-CB-CG	5.85	118.45	112.60
1	A	157	ARG	CB-CA-C	-5.83	100.94	110.85
3	Q	65	ASP	CA-CB-CG	5.82	118.42	112.60
3	B	60	PHE	CA-CB-CG	-5.81	107.99	113.80
3	Y	65	ASP	CA-CB-CG	5.79	118.39	112.60
3	L	65	ASP	CA-CB-CG	5.77	118.37	112.60
4	X	108	TYR	CB-CA-C	5.77	120.38	110.86
3	Q	60	PHE	CA-CB-CG	-5.74	108.06	113.80
3	W	60	PHE	CA-CB-CG	-5.70	108.10	113.80
1	A	155	PHE	CB-CA-C	-5.70	101.93	110.88
3	H	60	PHE	CA-CB-CG	-5.69	108.11	113.80
3	S	60	PHE	CA-CB-CG	-5.67	108.12	113.80
3	Q	69	PRO	N-CA-CB	5.66	108.28	103.19
1	A	216	TYR	N-CA-CB	5.63	118.13	109.91
3	O	60	PHE	CA-CB-CG	-5.62	108.18	113.80
1	A	221	GLU	N-CA-CB	5.62	118.99	110.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	60	PHE	CA-CB-CG	-5.61	108.19	113.80
4	P	2	LYS	CD-CE-NZ	-5.60	93.97	111.90
3	L	111	ASN	CA-C-O	-5.59	115.00	121.15
4	a	108	TYR	CB-CA-C	5.56	120.03	110.86
4	C	2	LYS	CG-CD-CE	-5.54	98.55	111.30
5	M	157	PHE	N-CA-CB	-5.53	101.98	110.16
3	Y	60	PHE	CA-CB-CG	-5.53	108.27	113.80
4	K	108	TYR	CB-CA-C	5.50	119.94	110.86
4	V	108	TYR	CB-CA-C	5.50	119.94	110.86
4	I	108	TYR	CB-CA-C	5.48	119.91	110.86
4	N	108	TYR	CB-CA-C	5.47	119.89	110.86
3	D	60	PHE	CA-CB-CG	-5.47	108.33	113.80
4	C	2	LYS	CD-CE-NZ	-5.46	94.41	111.90
4	C	108	TYR	CB-CA-C	5.44	119.83	110.86
3	L	60	PHE	CA-CB-CG	-5.44	108.36	113.80
4	E	108	TYR	CB-CA-C	5.42	119.81	110.86
4	P	108	TYR	CB-CA-C	5.42	119.81	110.86
5	M	250	THR	CA-CB-OG1	-5.42	101.48	109.60
4	N	30	ARG	N-CA-C	-5.40	103.36	110.43
3	F	60	PHE	CA-CB-CG	-5.39	108.41	113.80
4	a	30	ARG	N-CA-C	-5.38	103.39	110.43
5	M	140	ARG	CG-CD-NE	5.36	123.78	112.00
4	R	108	TYR	CB-CA-C	5.34	119.67	110.86
4	T	108	TYR	CB-CA-C	5.33	119.65	110.86
1	A	258	ASP	CB-CA-C	5.28	119.25	110.81
3	D	69	PRO	N-CA-CB	5.27	107.94	103.19
4	G	108	TYR	CB-CA-C	5.25	119.52	110.86
4	G	53	LYS	CB-CA-C	-5.24	102.14	110.84
4	T	53	LYS	CB-CA-C	-5.23	102.16	110.84
1	A	165	TYR	N-CA-CB	-5.21	102.45	110.16
4	a	53	LYS	CB-CA-C	-5.21	102.19	110.84
3	H	164	PHE	CA-CB-CG	-5.20	108.60	113.80
4	N	53	LYS	CB-CA-C	-5.18	102.24	110.84
1	A	110	PHE	CA-CB-CG	5.14	118.94	113.80
5	M	157	PHE	N-CA-C	5.14	116.97	111.36
4	I	53	LYS	CB-CA-C	-5.08	102.41	110.84
4	V	53	LYS	CB-CA-C	-5.08	102.42	110.84
4	V	7	GLU	CB-CA-C	-5.07	102.92	110.88
4	C	53	LYS	CB-CA-C	-5.05	102.46	110.84
3	Y	77	ARG	NE-CZ-NH2	5.03	123.73	119.20
4	P	53	LYS	CB-CA-C	-5.03	102.49	110.84
4	X	53	LYS	CB-CA-C	-5.03	102.50	110.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	ASP	N-CA-C	-5.02	105.81	111.28

There are no chirality outliers.

All (66) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	ARG	Sidechain
1	A	171	ARG	Sidechain
1	A	189	ARG	Sidechain,Peptide
1	A	250	ARG	Sidechain
1	A	286	ARG	Sidechain
1	A	288	ARG	Sidechain
3	B	125	ARG	Sidechain
4	C	17	ARG	Sidechain
3	D	108	ARG	Sidechain
3	D	125	ARG	Sidechain
3	D	77	ARG	Sidechain
3	D	78	ARG	Sidechain
3	F	84	ARG	Sidechain
3	F	91	ARG	Sidechain
4	G	114	ARG	Sidechain
4	G	17	ARG	Sidechain
3	H	101	ASP	Sidechain
3	H	108	ARG	Sidechain
4	I	30	ARG	Sidechain
4	I	33	ARG	Sidechain
4	I	42	ARG	Sidechain
4	K	114	ARG	Sidechain
3	L	108	ARG	Sidechain
3	L	110	LEU	Mainchain
3	L	125	ARG	Sidechain
3	L	84	ARG	Sidechain
5	M	124	ARG	Sidechain
5	M	133	ARG	Sidechain
5	M	140	ARG	Sidechain
5	M	155	ARG	Sidechain
5	M	176	ARG	Sidechain
5	M	222	ARG	Sidechain
5	M	237	ARG	Sidechain
5	M	243	ARG	Sidechain
5	M	260	ARG	Sidechain
5	M	65	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
4	N	17	ARG	Sidechain
4	N	30	ARG	Sidechain
3	O	108	ARG	Sidechain
3	O	125	ARG	Sidechain
3	O	77	ARG	Sidechain
4	P	114	ARG	Sidechain
4	P	17	ARG	Sidechain
3	Q	125	ARG	Sidechain
3	Q	77	ARG	Sidechain
3	Q	78	ARG	Sidechain
3	S	91	ARG	Sidechain
4	T	114	ARG	Sidechain
3	U	101	ASP	Sidechain
3	U	125	ARG	Sidechain
4	V	30	ARG	Sidechain
4	V	33	ARG	Sidechain
4	V	42	ARG	Sidechain
3	W	108	ARG	Sidechain
4	X	114	ARG	Sidechain
4	X	17	ARG	Sidechain
3	Y	108	ARG	Sidechain
3	Y	125	ARG	Sidechain
3	Y	77	ARG	Sidechain
3	Y	84	ARG	Sidechain
2	Z	51	ARG	Sidechain
2	Z	58	ARG	Sidechain
2	Z	65	ARG	Sidechain
4	a	17	ARG	Sidechain
4	a	30	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1717	0	1662	188	0
2	Z	570	0	579	36	0
3	B	1293	0	1301	57	0
3	D	1293	0	1301	75	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1293	0	1301	68	0
3	H	1293	0	1301	73	0
3	J	1293	0	1301	58	0
3	L	1293	0	1301	67	0
3	O	1293	0	1301	71	0
3	Q	1293	0	1301	81	0
3	S	1293	0	1301	53	0
3	U	1293	0	1301	70	0
3	W	1293	0	1301	63	0
3	Y	1293	0	1301	81	0
4	C	1243	0	1225	61	0
4	E	1243	0	1225	45	0
4	G	1243	0	1225	70	0
4	I	1243	0	1225	52	0
4	K	1243	0	1225	59	0
4	N	1243	0	1225	56	0
4	P	1243	0	1225	54	0
4	R	1243	0	1225	45	0
4	T	1243	0	1225	57	0
4	V	1243	0	1225	53	0
4	X	1243	0	1225	59	0
4	a	1243	0	1225	53	0
5	M	2173	0	2145	165	0
6	B	86	0	74	15	0
6	C	43	0	37	8	0
6	D	86	0	74	23	0
6	E	43	0	37	3	0
6	F	86	0	74	21	0
6	G	43	0	37	18	0
6	H	86	0	74	29	0
6	I	43	0	37	7	0
6	J	86	0	74	19	0
6	K	43	0	37	11	0
6	L	86	0	74	7	0
6	N	43	0	37	5	0
6	O	86	0	74	25	0
6	P	43	0	37	6	0
6	Q	86	0	74	23	0
6	R	43	0	37	9	0
6	S	86	0	74	12	0
6	T	43	0	37	11	0
6	U	86	0	74	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	V	43	0	37	7	0
6	W	86	0	74	18	0
6	X	43	0	37	13	0
6	Y	86	0	74	21	0
6	a	43	0	37	7	0
All	All	36440	0	36030	1853	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 26.

All (1853) 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)
6:X:201:CYC:HMA1	6:X:201:CYC:NB	1.58	1.18
1:A:95:ILE:HD12	1:A:97:ALA:H	1.01	1.12
1:A:254:LEU:HA	1:A:273:GLU:OE1	1.52	1.09
3:H:88:ILE:HD12	6:H:201:CYC:HMB2	1.09	1.09
1:A:201:LEU:HD13	6:S:202:CYC:HMA3	1.36	1.07
3:H:88:ILE:HD12	6:H:201:CYC:CMB	1.85	1.07
6:B:202:CYC:HMA3	6:B:202:CYC:HB	1.09	1.05
6:U:201:CYC:HMA1	6:U:201:CYC:NB	1.71	1.05
3:J:39:ASP:OD1	6:J:202:CYC:HHB	1.57	1.04
3:D:77:ARG:NE	5:M:273:ILE:HG22	1.73	1.04
6:U:201:CYC:HMA1	6:U:201:CYC:HB	0.89	1.03
1:A:278:LEU:HD13	1:A:282:ALA:O	1.57	1.03
6:D:202:CYC:NC	6:D:202:CYC:HMD1	1.72	1.02
6:S:202:CYC:HMA1	6:S:202:CYC:HB	1.24	1.02
5:M:160:THR:HB	5:M:257:GLN:HB3	1.39	1.01
6:U:201:CYC:NC	6:U:201:CYC:HMD1	1.74	1.01
5:M:262:ASP:OD1	5:M:263:PRO:HD2	1.60	1.00
3:Y:117:TYR:CD1	3:Y:122:THR:HG21	1.95	1.00
4:G:126:TRP:CZ3	6:G:201:CYC:HMC1	1.96	0.99
3:U:39:ASP:OD1	6:U:202:CYC:HHB	1.62	0.99
1:A:95:ILE:HD12	1:A:97:ALA:N	1.78	0.98
1:A:265:ARG:NH1	3:Y:77:ARG:HD3	1.78	0.98
3:D:77:ARG:CZ	5:M:273:ILE:HG22	1.95	0.97
1:A:143:SER:O	1:A:144:LEU:HB2	1.63	0.97
3:L:117:TYR:CD1	3:L:122:THR:HG21	1.99	0.97
6:Q:202:CYC:NC	6:Q:202:CYC:HMD1	1.80	0.97
4:C:2:LYS:HZ3	4:G:17:ARG:NH2	1.63	0.95
6:W:201:CYC:NC	6:W:201:CYC:HMD1	1.80	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:9:ILE:HD11	4:a:99:ALA:HB2	1.49	0.95
3:Q:145:PRO:HG2	6:Q:201:CYC:HMC1	1.48	0.95
6:O:202:CYC:NC	6:O:202:CYC:HMD1	1.82	0.94
3:H:39:ASP:OD1	6:H:202:CYC:HHB	1.67	0.94
1:A:278:LEU:HD13	1:A:282:ALA:C	1.93	0.93
1:A:265:ARG:CZ	3:Y:77:ARG:HD3	1.98	0.93
6:S:202:CYC:HMA1	6:S:202:CYC:NB	1.84	0.92
3:D:145:PRO:HG2	6:D:201:CYC:HMC1	1.49	0.92
5:M:262:ASP:OD1	5:M:263:PRO:CD	2.18	0.92
6:X:201:CYC:NB	6:X:201:CYC:CMA	2.34	0.91
4:X:126:TRP:CZ3	6:X:201:CYC:HMC1	2.07	0.90
1:A:166:LYS:O	1:A:170:PHE:HB3	1.71	0.89
6:J:201:CYC:HMA1	6:J:201:CYC:NB	1.87	0.89
3:D:119:ALA:CB	5:M:263:PRO:HB2	2.04	0.87
1:A:95:ILE:CD1	1:A:97:ALA:H	1.86	0.87
6:B:202:CYC:HB	6:B:202:CYC:CMA	1.87	0.86
3:F:14:LEU:HD22	3:O:125:ARG:HH22	1.39	0.86
5:M:132:LEU:O	5:M:133:ARG:HG2	1.73	0.86
6:F:202:CYC:HAB2	5:M:246:ALA:HB2	1.56	0.85
6:X:201:CYC:CMA	6:X:201:CYC:HB	1.87	0.85
6:B:202:CYC:HMA3	6:B:202:CYC:NB	1.90	0.85
6:H:201:CYC:HMA1	6:H:201:CYC:NB	1.92	0.84
3:B:9:ILE:CD1	4:a:99:ALA:HB2	2.07	0.84
6:U:201:CYC:HB	6:U:201:CYC:CMA	1.84	0.83
6:X:201:CYC:HMA1	6:X:201:CYC:HB	1.43	0.82
4:G:76:ASP:OD1	4:G:77:THR:N	2.13	0.82
1:A:186:LEU:C	1:A:187:LEU:HD12	2.04	0.82
4:P:76:ASP:OD1	4:P:77:THR:N	2.13	0.82
4:V:76:ASP:OD1	4:V:77:THR:N	2.13	0.82
4:C:76:ASP:OD1	4:C:77:THR:N	2.13	0.82
4:K:76:ASP:OD1	4:K:77:THR:N	2.13	0.82
4:X:76:ASP:OD1	4:X:77:THR:N	2.13	0.82
4:R:76:ASP:OD1	4:R:77:THR:N	2.13	0.81
4:T:76:ASP:OD1	4:T:77:THR:N	2.13	0.81
1:A:144:LEU:HB3	1:A:150:ILE:CD1	2.10	0.81
4:G:73:GLY:HA2	6:G:201:CYC:OC	1.80	0.81
4:G:120:PHE:CZ	6:G:201:CYC:HBA1	2.15	0.81
4:E:76:ASP:OD1	4:E:77:THR:N	2.13	0.81
5:M:160:THR:CB	5:M:257:GLN:HB3	2.11	0.81
3:J:145:PRO:CD	6:J:202:CYC:HMC3	2.10	0.81
6:F:202:CYC:NC	6:F:202:CYC:HMD1	1.96	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:39:ASP:OD1	6:Y:201:CYC:HHB	1.80	0.81
3:H:88:ILE:CD1	6:H:201:CYC:HMB2	2.03	0.81
4:T:108:TYR:CD1	3:W:75:PRO:HG3	2.15	0.81
1:A:156:ILE:HG22	1:A:217:ILE:HD11	1.62	0.80
1:A:144:LEU:CD2	1:A:150:ILE:HD11	2.11	0.80
4:N:99:ALA:HB2	3:O:9:ILE:HD11	1.63	0.80
3:Y:88:ILE:HG21	6:Y:202:CYC:HAB2	1.64	0.80
2:Z:1:SER:HB2	5:M:136:SER:HA	1.63	0.79
4:I:76:ASP:OD1	4:I:77:THR:N	2.13	0.79
2:Z:14:LEU:HD12	2:Z:72:GLY:HA3	1.63	0.79
3:F:145:PRO:HD2	6:F:201:CYC:HMC3	1.65	0.79
3:Q:145:PRO:CG	6:Q:201:CYC:HMC1	2.13	0.79
3:W:39:ASP:OD1	6:W:202:CYC:HHB	1.83	0.79
3:Y:88:ILE:HG21	6:Y:202:CYC:CAB	2.13	0.78
1:A:173:THR:HG23	1:A:270:GLN:OE1	1.83	0.78
3:L:14:LEU:HD13	3:W:125:ARG:CZ	2.13	0.78
4:N:99:ALA:HB2	3:O:9:ILE:CD1	2.14	0.78
6:V:201:CYC:HC	6:V:201:CYC:HMD3	1.47	0.78
6:J:201:CYC:NC	6:J:201:CYC:HMD1	1.98	0.78
4:a:77:THR:HG23	4:a:78:ASN:OD1	1.84	0.78
6:G:201:CYC:HMD3	6:G:201:CYC:NC	1.98	0.78
4:N:77:THR:HG23	4:N:78:ASN:OD1	1.84	0.78
1:A:263:THR:O	1:A:270:GLN:NE2	2.17	0.78
6:I:201:CYC:HC	6:I:201:CYC:HMD3	1.48	0.77
1:A:85:ALA:HB2	3:Y:14:LEU:HD21	1.65	0.77
4:R:73:GLY:HA2	6:R:201:CYC:OC	1.84	0.77
4:I:77:THR:HG23	4:I:78:ASN:OD1	1.84	0.77
2:Z:21:LEU:CD1	2:Z:25:LEU:HB2	2.14	0.77
3:F:14:LEU:HD22	3:O:125:ARG:NH2	2.01	0.76
4:V:77:THR:HG23	4:V:78:ASN:OD1	1.84	0.76
5:M:135:GLY:O	5:M:136:SER:OG	2.02	0.76
3:F:14:LEU:HD13	3:O:125:ARG:NH2	2.00	0.76
3:L:111:ASN:O	5:M:232:VAL:CG2	2.33	0.76
6:G:201:CYC:HMD3	6:G:201:CYC:HC	1.51	0.75
2:Z:21:LEU:HD11	2:Z:25:LEU:CB	2.16	0.75
3:H:65:ASP:OD1	3:H:66:LEU:N	2.20	0.75
5:M:254:LEU:O	5:M:255:GLN:CD	2.30	0.75
3:W:65:ASP:OD1	3:W:66:LEU:N	2.20	0.75
3:F:14:LEU:HD13	3:O:125:ARG:CZ	2.17	0.75
4:C:2:LYS:NZ	4:G:17:ARG:CZ	2.50	0.74
3:O:65:ASP:OD1	3:O:66:LEU:N	2.20	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:145:PRO:HD2	6:O:201:CYC:HMC3	1.69	0.74
6:T:201:CYC:C2A	6:T:201:CYC:O1A	2.35	0.74
1:A:106:LEU:HD13	1:A:152:VAL:HG21	1.68	0.74
6:R:201:CYC:CMA	6:R:201:CYC:NB	2.50	0.74
4:X:126:TRP:CE3	6:X:201:CYC:HMC1	2.21	0.74
3:S:65:ASP:OD1	3:S:66:LEU:N	2.20	0.74
3:J:65:ASP:OD1	3:J:66:LEU:N	2.20	0.74
5:M:160:THR:HB	5:M:257:GLN:CB	2.18	0.74
3:B:65:ASP:OD1	3:B:66:LEU:N	2.20	0.74
1:A:161:LYS:HE3	1:A:210:ASP:HB3	1.69	0.74
4:G:126:TRP:CE3	6:G:201:CYC:HMC1	2.22	0.74
3:D:145:PRO:CG	6:D:201:CYC:HMC1	2.18	0.74
3:F:65:ASP:OD1	3:F:66:LEU:N	2.20	0.73
4:X:73:GLY:HA2	6:X:201:CYC:OC	1.87	0.73
3:U:65:ASP:OD1	3:U:66:LEU:N	2.20	0.73
4:G:120:PHE:CE1	6:G:201:CYC:CBA	2.72	0.73
1:A:244:SER:O	1:A:245:ALA:CB	2.36	0.73
1:A:277:GLY:HA2	3:S:119:ALA:HB2	1.71	0.73
5:M:9:GLN:NE2	4:N:14:SER:HB3	2.04	0.73
5:M:245:ASP:O	5:M:246:ALA:HB3	1.88	0.72
1:A:126:LEU:HD12	1:A:127:PHE:N	2.03	0.72
1:A:144:LEU:HD23	1:A:150:ILE:HD11	1.68	0.72
3:D:75:PRO:HG3	4:K:108:TYR:CD1	2.24	0.72
3:O:145:PRO:CD	6:O:201:CYC:HMC3	2.19	0.72
1:A:254:LEU:CA	1:A:273:GLU:OE1	2.36	0.71
3:H:88:ILE:HG21	6:H:201:CYC:HAB1	1.72	0.71
1:A:286:ARG:HH12	1:A:287:ALA:HB3	1.53	0.71
3:D:39:ASP:OD1	6:D:201:CYC:HHB	1.90	0.71
1:A:187:LEU:N	1:A:187:LEU:CD1	2.54	0.71
4:C:17:ARG:HH22	4:C:23:GLU:CD	1.98	0.71
6:D:202:CYC:HMD1	6:D:202:CYC:HC	1.51	0.71
3:D:77:ARG:CZ	5:M:273:ILE:CG2	2.68	0.71
5:M:140:ARG:NH1	5:M:144:ARG:HH12	1.89	0.71
5:M:156:PHE:O	5:M:160:THR:HG22	1.91	0.71
1:A:89:ALA:O	1:A:93:LEU:HD13	1.90	0.71
3:S:145:PRO:HD2	6:S:201:CYC:HMC3	1.71	0.71
2:Z:21:LEU:HD11	2:Z:25:LEU:HB2	1.73	0.70
4:P:2:LYS:NZ	4:T:15:GLN:HE22	1.88	0.70
1:A:263:THR:HG22	6:Y:202:CYC:HAA1	1.74	0.70
4:I:17:ARG:HH22	4:I:23:GLU:CD	1.99	0.70
5:M:243:ARG:HG2	5:M:260:ARG:NH1	2.06	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:58:ARG:CZ	5:M:140:ARG:HH21	2.04	0.70
3:F:39:ASP:OD1	6:F:201:CYC:HHB	1.92	0.70
3:Q:75:PRO:HG3	4:X:108:TYR:CD1	2.27	0.70
3:Q:145:PRO:CD	6:Q:201:CYC:HMC1	2.22	0.70
1:A:169:PHE:CD2	1:A:169:PHE:O	2.45	0.69
5:M:190:ARG:HG3	5:M:194:PHE:HD2	1.55	0.69
3:F:145:PRO:CD	6:F:201:CYC:HMC3	2.21	0.69
6:X:201:CYC:NC	6:X:201:CYC:HMD1	2.07	0.69
4:V:17:ARG:HH22	4:V:23:GLU:CD	2.00	0.69
4:N:91:ARG:HA	3:O:18:PHE:CE2	2.27	0.69
4:P:17:ARG:HH22	4:P:23:GLU:CD	2.00	0.69
1:A:235:ARG:HG3	1:A:240:GLN:HE21	1.57	0.69
6:F:202:CYC:HMD1	6:F:202:CYC:HC	1.54	0.69
3:L:39:ASP:OD1	6:L:202:CYC:HHB	1.92	0.69
3:Y:107:ASP:O	3:Y:111:ASN:HB3	1.93	0.69
4:C:2:LYS:NZ	4:G:17:ARG:NH2	2.38	0.68
5:M:35:THR:HG22	6:W:201:CYC:O2A	1.93	0.68
4:C:2:LYS:HZ3	4:G:17:ARG:CZ	2.06	0.68
6:U:201:CYC:HMD1	6:U:201:CYC:HC	1.55	0.68
6:O:202:CYC:CMA	6:O:202:CYC:NB	2.57	0.68
5:M:132:LEU:O	5:M:133:ARG:CG	2.41	0.68
5:M:254:LEU:C	5:M:255:GLN:CD	2.62	0.68
4:G:120:PHE:CE1	6:G:201:CYC:HBA2	2.28	0.68
4:I:49:ASP:OD1	4:I:50:SER:N	2.26	0.68
4:T:49:ASP:OD1	4:T:50:SER:N	2.27	0.68
6:B:202:CYC:CMA	6:B:202:CYC:NB	2.53	0.67
6:V:201:CYC:HC	6:V:201:CYC:CMD	2.08	0.67
3:O:85:ASP:OD2	6:O:202:CYC:NA	2.28	0.67
6:F:202:CYC:CAB	5:M:246:ALA:HB2	2.25	0.67
6:I:201:CYC:HC	6:I:201:CYC:CMD	2.08	0.67
3:L:86:MET:HG3	6:L:201:CYC:HBC1	1.77	0.67
5:M:241:LEU:HD23	5:M:260:ARG:HB2	1.77	0.67
4:R:49:ASP:OD1	4:R:50:SER:N	2.27	0.67
2:Z:14:LEU:CD1	2:Z:72:GLY:HA3	2.24	0.67
4:C:49:ASP:OD1	4:C:50:SER:N	2.27	0.67
6:F:202:CYC:O2A	5:M:118:TYR:HD2	1.78	0.67
4:P:145:GLN:NE2	6:U:202:CYC:O1A	2.27	0.67
3:L:111:ASN:C	5:M:233:GLU:OE2	2.38	0.67
3:Q:39:ASP:OD1	6:Q:201:CYC:HHB	1.96	0.66
5:M:52:LEU:HD23	6:U:201:CYC:HAA1	1.77	0.66
1:A:144:LEU:CB	1:A:150:ILE:HD11	2.25	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ARG:CZ	1:A:181:LEU:HD21	2.25	0.66
2:Z:21:LEU:CD1	2:Z:25:LEU:CB	2.73	0.66
4:P:49:ASP:OD1	4:P:50:SER:N	2.27	0.66
4:T:108:TYR:HD1	3:W:75:PRO:HG3	1.61	0.66
4:V:49:ASP:OD1	4:V:50:SER:N	2.27	0.66
1:A:245:ALA:HB1	3:Q:111:ASN:O	1.95	0.66
1:A:248:PHE:CE2	6:Q:202:CYC:HMA2	2.30	0.66
4:E:49:ASP:OD1	4:E:50:SER:N	2.27	0.66
3:Q:145:PRO:HD2	6:Q:201:CYC:HMC1	1.77	0.65
3:S:39:ASP:OD1	6:S:201:CYC:HHB	1.95	0.65
1:A:85:ALA:O	3:Q:78:ARG:NH1	2.30	0.65
3:B:84:ARG:NH2	6:B:202:CYC:O2A	2.24	0.65
4:X:49:ASP:OD1	4:X:50:SER:N	2.27	0.65
1:A:248:PHE:O	1:A:252:ARG:HG3	1.95	0.65
3:D:75:PRO:HG3	4:K:108:TYR:HD1	1.60	0.65
4:K:49:ASP:OD1	4:K:50:SER:N	2.27	0.65
5:M:254:LEU:C	5:M:255:GLN:OE1	2.39	0.65
3:D:77:ARG:NE	5:M:273:ILE:CG2	2.56	0.65
3:H:85:ASP:CG	6:H:201:CYC:HHB	2.22	0.65
3:L:14:LEU:HD13	3:W:125:ARG:NH2	2.12	0.65
6:V:201:CYC:HHA	6:V:201:CYC:O1A	1.97	0.65
6:K:201:CYC:NB	6:K:201:CYC:HMA1	2.12	0.65
1:A:173:THR:HB	1:A:177:ARG:CG	2.27	0.65
6:G:201:CYC:C2A	6:G:201:CYC:O1A	2.44	0.64
5:M:88:PRO:O	5:M:89:LEU:HB2	1.96	0.64
4:G:120:PHE:CZ	6:G:201:CYC:CBA	2.81	0.64
3:F:14:LEU:HB3	3:O:125:ARG:NH2	2.12	0.64
4:G:49:ASP:OD1	4:G:50:SER:N	2.27	0.64
1:A:120:ARG:HG2	1:A:124:LYS:HZ1	1.62	0.64
1:A:126:LEU:HD12	1:A:126:LEU:C	2.23	0.64
1:A:186:LEU:C	1:A:187:LEU:CD1	2.71	0.64
1:A:244:SER:O	1:A:245:ALA:HB2	1.95	0.64
1:A:168:ARG:O	1:A:169:PHE:HB3	1.97	0.64
1:A:189:ARG:HG3	1:A:189:ARG:HH11	1.63	0.64
3:Q:109:CYS:HA	6:Q:202:CYC:HBB1	1.78	0.64
3:Y:120:LEU:HD22	6:Y:202:CYC:CGD	2.28	0.64
3:J:39:ASP:OD1	6:J:202:CYC:CHB	2.42	0.64
2:Z:21:LEU:HD23	2:Z:43:TYR:CE1	2.33	0.63
6:O:202:CYC:HMD1	6:O:202:CYC:C1C	2.28	0.63
6:X:201:CYC:HMA1	6:X:201:CYC:C1B	2.29	0.63
4:N:49:ASP:OD1	4:N:50:SER:N	2.27	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:U:201:CYC:C2A	6:U:201:CYC:O2A	2.47	0.63
5:M:140:ARG:HH12	5:M:144:ARG:HH12	1.47	0.63
3:Y:82:CYS:HA	6:Y:202:CYC:HHD	1.81	0.63
2:Z:21:LEU:HD11	2:Z:25:LEU:HB3	1.81	0.63
6:F:202:CYC:HAB2	5:M:246:ALA:CB	2.29	0.63
6:L:201:CYC:NC	6:L:201:CYC:HMD1	2.14	0.63
5:M:272:GLY:O	5:M:273:ILE:C	2.42	0.63
6:I:201:CYC:HHA	6:I:201:CYC:O1A	1.99	0.62
3:L:14:LEU:HD22	3:W:125:ARG:HH12	1.63	0.62
5:M:175:GLY:HA3	5:M:222:ARG:H	1.63	0.62
4:a:49:ASP:OD1	4:a:50:SER:N	2.27	0.62
3:J:127:VAL:HG22	6:J:201:CYC:H3C	1.81	0.62
6:J:201:CYC:HMD1	6:J:201:CYC:C1C	2.29	0.62
5:M:160:THR:OG1	5:M:164:ARG:HG2	1.99	0.62
4:T:82:CYS:HB2	6:T:201:CYC:NC	2.15	0.62
3:U:23:GLU:HA	3:U:26:GLN:OE1	2.00	0.62
1:A:144:LEU:CB	1:A:150:ILE:CD1	2.76	0.62
1:A:235:ARG:HG3	1:A:240:GLN:NE2	2.13	0.62
6:T:201:CYC:CMA	6:T:201:CYC:NB	2.63	0.62
1:A:173:THR:HB	1:A:177:ARG:HB3	1.82	0.62
3:D:125:ARG:HH22	3:U:14:LEU:CD1	2.13	0.62
3:J:145:PRO:HD2	6:J:202:CYC:HMC3	1.81	0.62
5:M:139:VAL:HB	5:M:216:ASN:HA	1.82	0.62
6:H:201:CYC:NC	6:H:201:CYC:HMD1	2.15	0.62
5:M:119:VAL:HG13	5:M:151:LEU:HD21	1.82	0.62
4:T:109:ILE:HD13	6:T:201:CYC:HAB1	1.82	0.62
1:A:120:ARG:CZ	4:X:16:GLY:HA3	2.30	0.61
1:A:286:ARG:NH1	1:A:287:ALA:H	1.97	0.61
6:W:201:CYC:HMD1	6:W:201:CYC:C1C	2.29	0.61
4:X:126:TRP:CZ3	6:X:201:CYC:CMC	2.81	0.61
3:H:23:GLU:HA	3:H:26:GLN:OE1	2.00	0.61
1:A:76:PHE:CE2	3:Q:68:ARG:HD3	2.35	0.61
3:D:109:CYS:HA	6:D:202:CYC:HBB1	1.80	0.61
3:U:52:ILE:O	3:U:53:SER:C	2.44	0.61
1:A:286:ARG:NH1	1:A:287:ALA:HB3	2.15	0.61
3:B:52:ILE:O	3:B:53:SER:C	2.44	0.61
4:G:108:TYR:O	3:J:76:ASN:HB2	2.00	0.61
5:M:114:PHE:CZ	5:M:151:LEU:HD23	2.36	0.61
3:W:52:ILE:O	3:W:53:SER:C	2.44	0.61
1:A:96:THR:HB	3:Y:107:ASP:HB3	1.82	0.61
1:A:175:ASN:HB2	6:S:202:CYC:HBB2	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:52:ILE:O	3:L:53:SER:C	2.44	0.61
3:O:39:ASP:OD1	6:O:201:CYC:HHB	2.01	0.61
3:W:145:PRO:HD2	6:W:202:CYC:HMC3	1.82	0.61
3:H:52:ILE:O	3:H:53:SER:C	2.44	0.61
6:I:201:CYC:HMD3	6:I:201:CYC:NC	2.16	0.61
6:J:201:CYC:HMA1	6:J:201:CYC:HB	1.64	0.61
5:M:37:GLU:HG3	5:M:38:PRO:HD2	1.81	0.61
3:D:52:ILE:O	3:D:53:SER:C	2.44	0.60
3:S:52:ILE:O	3:S:53:SER:C	2.44	0.60
3:U:38:LEU:HD13	6:U:202:CYC:C4B	2.31	0.60
1:A:265:ARG:CZ	3:Y:77:ARG:CD	2.76	0.60
4:R:18:PHE:CE2	3:S:91:ARG:HA	2.37	0.60
1:A:148:GLY:O	1:A:149:SER:CB	2.47	0.60
6:Y:202:CYC:HB	6:Y:202:CYC:HMA1	1.66	0.60
1:A:177:ARG:NE	1:A:181:LEU:HD11	2.16	0.60
3:O:52:ILE:O	3:O:53:SER:C	2.44	0.60
3:Q:57:HIS:NE2	6:X:201:CYC:O1D	2.34	0.60
4:C:91:ARG:HA	3:D:18:PHE:CE2	2.36	0.60
4:K:88:HIS:ND1	6:K:201:CYC:HBB3	2.17	0.60
3:U:39:ASP:OD1	6:U:202:CYC:CHB	2.45	0.60
3:Q:127:VAL:HG22	6:Q:202:CYC:H3C	1.82	0.60
1:A:126:LEU:HA	1:A:185:HIS:HB3	1.84	0.59
3:J:87:GLU:CD	3:J:87:GLU:C	2.70	0.59
6:J:201:CYC:HMA1	6:J:201:CYC:C1B	2.32	0.59
5:M:250:THR:CG2	5:M:252:LEU:HB2	2.32	0.59
6:R:201:CYC:NB	6:R:201:CYC:HMA3	2.16	0.59
4:K:73:GLY:HA2	6:K:201:CYC:OC	2.01	0.59
3:W:145:PRO:CD	6:W:202:CYC:HMC3	2.32	0.59
1:A:76:PHE:CD1	1:A:76:PHE:O	2.55	0.59
3:F:52:ILE:O	3:F:53:SER:C	2.44	0.59
4:G:109:ILE:O	3:J:76:ASN:ND2	2.35	0.59
3:J:52:ILE:O	3:J:53:SER:C	2.44	0.59
3:U:144:SER:N	3:U:145:PRO:HD3	2.18	0.59
3:F:72:ASN:HB3	6:F:202:CYC:OC	2.02	0.59
3:U:87:GLU:CD	3:U:87:GLU:C	2.70	0.59
3:W:87:GLU:C	3:W:87:GLU:CD	2.70	0.59
3:Y:52:ILE:O	3:Y:53:SER:C	2.44	0.59
1:A:166:LYS:HD2	1:A:209:TYR:CE2	2.37	0.59
3:B:144:SER:N	3:B:145:PRO:HD3	2.18	0.59
3:H:87:GLU:CD	3:H:87:GLU:C	2.70	0.59
6:K:201:CYC:NB	6:K:201:CYC:CMA	2.66	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:144:SER:N	3:W:145:PRO:HD3	2.18	0.59
4:a:72:MET:HE1	6:a:201:CYC:HBD2	1.84	0.59
1:A:144:LEU:HB3	1:A:150:ILE:HG13	1.83	0.59
1:A:173:THR:CG2	1:A:270:GLN:OE1	2.51	0.59
3:D:144:SER:N	3:D:145:PRO:HD3	2.18	0.59
3:O:33:GLU:O	3:O:34:SER:C	2.46	0.59
5:M:9:GLN:HE22	4:N:14:SER:HB3	1.68	0.59
4:T:108:TYR:O	3:W:76:ASN:HB2	2.03	0.59
2:Z:3:LEU:HB3	2:Z:46:ILE:HG13	1.84	0.59
3:D:33:GLU:O	3:D:34:SER:C	2.46	0.59
3:Q:52:ILE:O	3:Q:53:SER:C	2.44	0.59
6:Q:202:CYC:HMD1	6:Q:202:CYC:HC	1.65	0.59
6:R:201:CYC:HB	6:R:201:CYC:HMA2	1.68	0.59
1:A:144:LEU:HB3	1:A:150:ILE:CG1	2.33	0.58
3:W:127:VAL:HG22	6:W:201:CYC:H3C	1.85	0.58
1:A:257:GLY:CA	3:Y:111:ASN:HD21	2.16	0.58
3:D:119:ALA:HB3	5:M:263:PRO:HB2	1.85	0.58
4:X:105:LEU:HD23	4:X:109:ILE:HD12	1.85	0.58
3:F:144:SER:N	3:F:145:PRO:HD3	2.18	0.58
3:J:109:CYS:HA	6:J:201:CYC:HBB1	1.86	0.58
3:L:33:GLU:O	3:L:34:SER:C	2.46	0.58
3:Q:33:GLU:O	3:Q:34:SER:C	2.46	0.58
3:H:33:GLU:O	3:H:34:SER:C	2.46	0.58
4:G:120:PHE:CG	6:G:201:CYC:HAA2	2.39	0.58
3:H:144:SER:N	3:H:145:PRO:HD3	2.18	0.58
3:J:33:GLU:O	3:J:34:SER:C	2.47	0.58
3:J:144:SER:N	3:J:145:PRO:HD3	2.18	0.58
5:M:15:PHE:HD1	5:M:71:PRO:HA	1.68	0.58
3:O:144:SER:N	3:O:145:PRO:HD3	2.18	0.58
3:Y:144:SER:N	3:Y:145:PRO:HD3	2.18	0.58
2:Z:21:LEU:HD12	2:Z:22:SER:N	2.19	0.58
3:L:144:SER:N	3:L:145:PRO:HD3	2.18	0.58
5:M:160:THR:OG1	5:M:164:ARG:CB	2.52	0.58
3:B:33:GLU:O	3:B:34:SER:C	2.46	0.58
4:P:17:ARG:CZ	4:T:2:LYS:NZ	2.67	0.58
3:S:144:SER:N	3:S:145:PRO:HD3	2.18	0.58
3:Y:33:GLU:O	3:Y:34:SER:C	2.46	0.58
1:A:103:GLY:HA2	1:A:233:TYR:CE2	2.39	0.58
3:Y:117:TYR:HD1	3:Y:122:THR:HG21	1.63	0.58
1:A:204:TYR:HA	1:A:212:GLU:OE2	2.03	0.58
3:B:39:ASP:OD1	6:B:201:CYC:HHB	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1:MET:HG2	3:D:2:GLN:H	1.69	0.58
5:M:134:ASN:OD1	5:M:134:ASN:N	2.34	0.58
1:A:147:ASN:ND2	6:O:202:CYC:HAA1	2.19	0.57
3:D:145:PRO:CD	6:D:201:CYC:HMC1	2.34	0.57
3:F:14:LEU:CD2	3:O:125:ARG:HH22	2.14	0.57
5:M:224:PHE:CZ	5:M:238:MET:HG3	2.39	0.57
5:M:253:ASN:OD1	5:M:256:GLY:HA2	2.04	0.57
3:S:33:GLU:O	3:S:34:SER:C	2.47	0.57
3:W:33:GLU:O	3:W:34:SER:C	2.46	0.57
3:H:26:GLN:O	3:H:29:ASN:OD1	2.22	0.57
3:Q:26:GLN:O	3:Q:29:ASN:OD1	2.23	0.57
6:W:201:CYC:HMA1	6:W:201:CYC:NB	2.19	0.57
1:A:250:ARG:HH11	1:A:279:ALA:HA	1.68	0.57
3:B:26:GLN:O	3:B:29:ASN:OD1	2.23	0.57
4:K:88:HIS:CG	6:K:201:CYC:HBB3	2.39	0.57
1:A:99:ALA:HB3	1:A:100:PRO:HD3	1.86	0.57
3:F:33:GLU:O	3:F:34:SER:C	2.47	0.57
4:K:105:LEU:HD23	4:K:109:ILE:HD12	1.86	0.57
3:Q:144:SER:N	3:Q:145:PRO:HD3	2.18	0.57
6:C:201:CYC:NC	6:C:201:CYC:HMD1	2.19	0.57
4:G:91:ARG:HA	3:H:18:PHE:CE2	2.40	0.57
3:O:26:GLN:O	3:O:29:ASN:OD1	2.23	0.57
6:O:202:CYC:O2A	6:O:202:CYC:C2A	2.52	0.57
4:X:102:THR:O	4:X:103:GLY:C	2.48	0.57
1:A:191:PRO:O	1:A:250:ARG:NH2	2.38	0.57
5:M:215:GLU:O	5:M:216:ASN:OD1	2.23	0.57
3:Q:75:PRO:HG3	4:X:108:TYR:HD1	1.70	0.57
3:U:92:TYR:O	3:U:93:VAL:C	2.48	0.57
6:a:201:CYC:NC	6:a:201:CYC:HMD1	2.19	0.57
3:B:92:TYR:O	3:B:93:VAL:C	2.48	0.57
3:U:26:GLN:O	3:U:29:ASN:OD1	2.22	0.57
1:A:160:ALA:O	1:A:209:TYR:OH	2.22	0.57
4:C:17:ARG:CZ	4:G:2:LYS:NZ	2.67	0.57
1:A:80:ALA:HA	3:Q:68:ARG:HH12	1.69	0.56
1:A:173:THR:HB	1:A:177:ARG:CB	2.35	0.56
6:K:201:CYC:HMA1	6:K:201:CYC:C1B	2.34	0.56
4:C:102:THR:O	4:C:103:GLY:C	2.48	0.56
3:O:92:TYR:O	3:O:93:VAL:C	2.48	0.56
4:a:102:THR:O	4:a:103:GLY:C	2.49	0.56
4:I:17:ARG:CZ	4:K:2:LYS:HE2	2.36	0.56
4:R:102:THR:O	4:R:103:GLY:C	2.48	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:55:ALA:O	4:T:56:VAL:C	2.49	0.56
3:U:33:GLU:O	3:U:34:SER:C	2.46	0.56
3:Y:92:TYR:O	3:Y:93:VAL:C	2.48	0.56
3:L:14:LEU:HD22	3:W:125:ARG:NH1	2.21	0.56
4:P:17:ARG:CZ	4:T:2:LYS:HZ1	2.18	0.56
4:P:102:THR:O	4:P:103:GLY:C	2.48	0.56
4:P:108:TYR:CD1	3:S:75:PRO:HG3	2.40	0.56
3:S:1:MET:HG2	3:S:2:GLN:H	1.71	0.56
6:T:201:CYC:NC	6:T:201:CYC:HMD1	2.21	0.56
4:V:17:ARG:CZ	4:X:2:LYS:HE2	2.35	0.56
6:V:201:CYC:HMD3	6:V:201:CYC:NC	2.20	0.56
1:A:106:LEU:HD11	1:A:118:VAL:HG11	1.87	0.56
4:E:102:THR:O	4:E:103:GLY:C	2.48	0.56
3:F:148:VAL:HG11	6:F:201:CYC:CHD	2.35	0.56
3:H:88:ILE:CD1	6:H:201:CYC:CMB	2.73	0.56
6:N:201:CYC:HMD1	6:N:201:CYC:NC	2.21	0.56
1:A:136:GLU:HB3	1:A:164:LEU:HD11	1.88	0.56
3:D:26:GLN:O	3:D:29:ASN:OD1	2.23	0.56
3:Y:88:ILE:HD13	6:Y:202:CYC:HAB1	1.86	0.56
4:C:55:ALA:O	4:C:56:VAL:C	2.49	0.56
4:G:102:THR:O	4:G:103:GLY:C	2.48	0.56
4:I:55:ALA:O	4:I:56:VAL:C	2.49	0.56
5:M:132:LEU:HD12	5:M:137:ILE:HB	1.88	0.56
6:D:202:CYC:HB	6:D:202:CYC:HMA1	1.70	0.56
4:E:55:ALA:O	4:E:56:VAL:C	2.49	0.56
4:E:151:ASN:O	4:E:152:ALA:C	2.49	0.56
3:J:92:TYR:O	3:J:93:VAL:C	2.48	0.56
5:M:120:LEU:O	5:M:124:ARG:HG3	2.06	0.56
5:M:140:ARG:NH1	5:M:204:ILE:HG22	2.20	0.56
5:M:210:ILE:HA	5:M:214:GLY:HA2	1.86	0.56
4:P:17:ARG:NH2	4:T:2:LYS:NZ	2.53	0.56
1:A:266:ASN:HD21	3:Y:119:ALA:HB1	1.71	0.56
3:H:92:TYR:O	3:H:93:VAL:C	2.48	0.56
4:R:151:ASN:O	4:R:152:ALA:C	2.49	0.56
4:X:115:GLU:OE1	4:X:115:GLU:N	2.37	0.56
1:A:96:THR:O	1:A:97:ALA:HB3	2.06	0.56
1:A:277:GLY:CA	3:S:119:ALA:HB2	2.36	0.56
4:E:126:TRP:O	4:E:127:TYR:C	2.50	0.56
4:V:55:ALA:O	4:V:56:VAL:C	2.49	0.56
3:D:119:ALA:O	5:M:267:LEU:CD1	2.54	0.55
4:G:126:TRP:CZ3	6:G:201:CYC:CMC	2.81	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:102:THR:O	4:K:103:GLY:C	2.49	0.55
4:P:55:ALA:O	4:P:56:VAL:C	2.49	0.55
3:Y:117:TYR:CD1	3:Y:122:THR:CG2	2.81	0.55
4:a:17:ARG:HH11	4:a:17:ARG:HG2	1.70	0.55
4:a:151:ASN:O	4:a:152:ALA:C	2.49	0.55
1:A:160:ALA:CB	1:A:213:ILE:HD12	2.35	0.55
4:C:126:TRP:O	4:C:127:TYR:C	2.50	0.55
3:D:92:TYR:O	3:D:93:VAL:C	2.48	0.55
5:M:259:ARG:NH1	5:M:263:PRO:HG3	2.20	0.55
3:S:92:TYR:O	3:S:93:VAL:C	2.48	0.55
6:F:202:CYC:NB	5:M:118:TYR:OH	2.39	0.55
5:M:160:THR:HG21	5:M:164:ARG:HG3	1.87	0.55
3:Q:145:PRO:HD2	6:Q:201:CYC:CMC	2.37	0.55
4:a:126:TRP:O	4:a:127:TYR:C	2.49	0.55
4:C:151:ASN:O	4:C:152:ALA:C	2.49	0.55
3:F:92:TYR:O	3:F:93:VAL:C	2.48	0.55
4:K:151:ASN:O	4:K:152:ALA:C	2.49	0.55
4:T:102:THR:O	4:T:103:GLY:C	2.48	0.55
4:X:151:ASN:O	4:X:152:ALA:C	2.49	0.55
4:C:145:GLN:NE2	6:H:202:CYC:O1A	2.40	0.55
4:N:102:THR:O	4:N:103:GLY:C	2.48	0.55
4:V:102:THR:O	4:V:103:GLY:C	2.49	0.55
4:V:126:TRP:O	4:V:127:TYR:C	2.49	0.55
1:A:244:SER:CB	3:Q:108:ARG:HD3	2.36	0.55
5:M:223:GLY:O	5:M:224:PHE:HB2	2.06	0.55
4:T:126:TRP:O	4:T:127:TYR:C	2.49	0.55
6:F:201:CYC:NB	6:F:201:CYC:HMA1	2.22	0.55
5:M:245:ASP:O	5:M:246:ALA:CB	2.54	0.55
4:N:55:ALA:O	4:N:56:VAL:C	2.49	0.55
4:a:55:ALA:O	4:a:56:VAL:C	2.49	0.55
6:a:201:CYC:NB	6:a:201:CYC:CMA	2.69	0.55
1:A:134:GLU:HA	1:A:137:ARG:HD3	1.88	0.55
1:A:257:GLY:HA2	3:Y:111:ASN:HD21	1.71	0.55
4:N:151:ASN:O	4:N:152:ALA:C	2.49	0.55
4:R:155:ASP:O	4:R:158:ILE:N	2.40	0.55
3:Y:82:CYS:HA	6:Y:202:CYC:CHD	2.36	0.55
1:A:160:ALA:HB1	1:A:213:ILE:HD12	1.89	0.55
4:G:126:TRP:O	4:G:127:TYR:C	2.50	0.55
4:K:115:GLU:OE1	4:K:115:GLU:N	2.37	0.55
3:L:92:TYR:O	3:L:93:VAL:C	2.48	0.55
5:M:102:VAL:HG11	5:M:133:ARG:HB3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:151:ASN:O	4:V:152:ALA:C	2.49	0.55
3:B:103:SER:O	3:B:104:VAL:C	2.50	0.55
4:G:108:TYR:CD1	3:J:75:PRO:HG3	2.41	0.55
6:H:201:CYC:HMA1	6:H:201:CYC:C1B	2.37	0.55
4:I:102:THR:O	4:I:103:GLY:C	2.49	0.55
4:K:55:ALA:O	4:K:56:VAL:C	2.49	0.55
4:K:155:ASP:O	4:K:158:ILE:N	2.40	0.55
3:U:1:MET:HG2	3:U:2:GLN:H	1.72	0.55
4:V:155:ASP:O	4:V:158:ILE:N	2.40	0.55
4:X:55:ALA:O	4:X:56:VAL:C	2.49	0.55
4:E:155:ASP:O	4:E:158:ILE:N	2.41	0.54
4:I:126:TRP:O	4:I:127:TYR:C	2.50	0.54
4:T:151:ASN:O	4:T:152:ALA:C	2.49	0.54
4:X:126:TRP:O	4:X:127:TYR:C	2.50	0.54
4:G:151:ASN:O	4:G:152:ALA:C	2.49	0.54
3:L:117:TYR:CD1	3:L:122:THR:CG2	2.84	0.54
4:N:77:THR:HG23	4:N:78:ASN:N	2.23	0.54
4:N:82:CYS:HB2	6:N:201:CYC:NC	2.22	0.54
4:X:155:ASP:O	4:X:158:ILE:N	2.41	0.54
1:A:187:LEU:N	1:A:187:LEU:HD13	2.22	0.54
3:D:103:SER:O	3:D:104:VAL:C	2.50	0.54
3:F:14:LEU:HD22	3:O:125:ARG:HH12	1.71	0.54
3:F:111:ASN:ND2	5:M:81:ASP:OD1	2.40	0.54
4:G:155:ASP:O	4:G:158:ILE:N	2.41	0.54
3:J:103:SER:O	3:J:104:VAL:C	2.50	0.54
4:N:126:TRP:O	4:N:127:TYR:C	2.50	0.54
3:Q:1:MET:HG2	3:Q:2:GLN:H	1.71	0.54
4:R:55:ALA:O	4:R:56:VAL:C	2.49	0.54
3:W:92:TYR:O	3:W:93:VAL:C	2.48	0.54
4:C:17:ARG:NH2	4:G:2:LYS:HZ3	2.05	0.54
4:C:155:ASP:O	4:C:158:ILE:N	2.40	0.54
3:F:1:MET:HG2	3:F:2:GLN:H	1.72	0.54
4:G:55:ALA:O	4:G:56:VAL:C	2.49	0.54
3:J:145:PRO:HD3	6:J:202:CYC:HMC3	1.87	0.54
3:L:103:SER:O	3:L:104:VAL:C	2.50	0.54
4:N:155:ASP:O	4:N:158:ILE:N	2.40	0.54
3:U:120:LEU:HD22	6:U:201:CYC:HBD1	1.90	0.54
1:A:163:ASP:OD1	1:A:164:LEU:N	2.41	0.54
4:K:126:TRP:O	4:K:127:TYR:C	2.49	0.54
4:N:17:ARG:HG2	4:N:17:ARG:HH11	1.72	0.54
6:O:202:CYC:NB	6:O:202:CYC:HMA2	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:151:ASN:O	4:P:152:ALA:C	2.49	0.54
3:Q:92:TYR:O	3:Q:93:VAL:C	2.48	0.54
4:a:155:ASP:O	4:a:158:ILE:N	2.41	0.54
1:A:143:SER:O	1:A:144:LEU:CB	2.41	0.54
4:I:42:ARG:NH1	3:J:21:GLU:OE1	2.41	0.54
3:O:103:SER:O	3:O:104:VAL:C	2.50	0.54
4:T:155:ASP:O	4:T:158:ILE:N	2.41	0.54
1:A:173:THR:HB	1:A:177:ARG:HG2	1.90	0.54
4:I:151:ASN:O	4:I:152:ALA:C	2.49	0.54
4:V:77:THR:HG23	4:V:78:ASN:N	2.23	0.54
4:X:1:MET:SD	3:Y:6:THR:HG23	2.48	0.54
4:a:77:THR:HG23	4:a:78:ASN:N	2.23	0.54
4:C:86:ILE:O	4:C:87:SER:C	2.51	0.54
4:I:155:ASP:O	4:I:158:ILE:N	2.41	0.54
3:Y:103:SER:O	3:Y:104:VAL:C	2.51	0.54
3:S:145:PRO:CD	6:S:201:CYC:HMC3	2.37	0.54
4:X:86:ILE:O	4:X:87:SER:C	2.51	0.54
4:I:77:THR:HG23	4:I:78:ASN:N	2.23	0.54
6:O:202:CYC:HMA2	6:O:202:CYC:HB	1.72	0.54
4:P:126:TRP:O	4:P:127:TYR:C	2.50	0.54
4:P:155:ASP:O	4:P:158:ILE:N	2.41	0.54
3:Q:103:SER:O	3:Q:104:VAL:C	2.50	0.54
1:A:248:PHE:CE2	6:Q:202:CYC:CMA	2.91	0.53
2:Z:5:GLY:HA2	3:H:111:ASN:O	2.08	0.53
3:W:103:SER:O	3:W:104:VAL:C	2.51	0.53
4:C:17:ARG:NH2	4:G:2:LYS:NZ	2.56	0.53
6:H:201:CYC:HBA1	5:M:134:ASN:OD1	2.08	0.53
5:M:13:LYS:HE3	5:M:15:PHE:CE1	2.44	0.53
5:M:35:THR:HG22	3:W:84:ARG:CZ	2.39	0.53
3:W:78:ARG:O	3:W:79:MET:C	2.51	0.53
3:H:103:SER:O	3:H:104:VAL:C	2.50	0.53
3:S:50:GLU:O	3:S:51:ILE:C	2.52	0.53
3:U:103:SER:O	3:U:104:VAL:C	2.51	0.53
3:D:108:ARG:HG3	5:M:158:PHE:O	2.07	0.53
3:D:145:PRO:HD2	6:D:201:CYC:HMC1	1.90	0.53
6:D:202:CYC:O2D	5:M:271:ARG:NH1	2.41	0.53
3:F:14:LEU:CD1	3:O:125:ARG:NH2	2.71	0.53
3:H:35:ASN:HB3	6:H:202:CYC:C1A	2.39	0.53
5:M:135:GLY:O	5:M:136:SER:CB	2.56	0.53
3:W:87:GLU:CD	3:W:88:ILE:N	2.67	0.53
6:P:201:CYC:NC	6:P:201:CYC:HMD1	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:39:ASP:OD1	6:W:202:CYC:CHB	2.56	0.53
3:W:50:GLU:O	3:W:51:ILE:C	2.52	0.53
3:F:14:LEU:HD22	3:O:125:ARG:NH1	2.24	0.53
3:F:103:SER:O	3:F:104:VAL:C	2.51	0.53
5:M:174:LEU:HD13	5:M:176:ARG:HD3	1.89	0.53
6:R:201:CYC:NB	6:R:201:CYC:HMA2	2.24	0.53
6:R:201:CYC:NC	6:R:201:CYC:HMD1	2.22	0.53
4:T:86:ILE:O	4:T:87:SER:C	2.52	0.53
3:Y:50:GLU:O	3:Y:51:ILE:C	2.52	0.53
1:A:148:GLY:O	1:A:149:SER:HB3	2.09	0.53
3:B:47:ASN:O	3:B:48:ALA:C	2.52	0.53
4:G:82:CYS:HA	6:G:201:CYC:HHD	1.90	0.53
3:H:72:ASN:HB3	6:H:201:CYC:OC	2.09	0.53
5:M:170:PHE:CD1	5:M:176:ARG:NH1	2.77	0.53
3:Q:78:ARG:O	3:Q:79:MET:C	2.52	0.53
3:U:87:GLU:CD	3:U:88:ILE:N	2.67	0.53
4:a:115:GLU:OE1	4:a:115:GLU:N	2.38	0.53
4:I:86:ILE:O	4:I:87:SER:C	2.52	0.53
3:W:47:ASN:O	3:W:48:ALA:C	2.52	0.53
3:D:78:ARG:O	3:D:79:MET:C	2.51	0.53
3:O:50:GLU:O	3:O:51:ILE:C	2.52	0.53
3:Q:50:GLU:O	3:Q:51:ILE:C	2.52	0.53
3:S:78:ARG:O	3:S:79:MET:C	2.52	0.53
4:T:73:GLY:HA2	6:T:201:CYC:OC	2.09	0.53
1:A:250:ARG:HA	1:A:274:LEU:HD21	1.91	0.52
1:A:257:GLY:CA	3:Y:111:ASN:ND2	2.72	0.52
3:D:47:ASN:O	3:D:48:ALA:C	2.52	0.52
5:M:224:PHE:CE2	5:M:238:MET:HG3	2.43	0.52
4:P:86:ILE:O	4:P:87:SER:C	2.51	0.52
6:F:202:CYC:HB	6:F:202:CYC:CMA	2.22	0.52
3:H:87:GLU:CD	3:H:88:ILE:N	2.67	0.52
4:K:91:ARG:O	4:K:94:THR:OG1	2.22	0.52
3:L:78:ARG:O	3:L:79:MET:C	2.52	0.52
4:T:129:GLU:O	4:T:130:ALA:C	2.53	0.52
3:U:78:ARG:O	3:U:79:MET:C	2.52	0.52
4:V:86:ILE:O	4:V:87:SER:C	2.52	0.52
3:B:50:GLU:O	3:B:51:ILE:C	2.52	0.52
3:F:14:LEU:HD22	3:O:125:ARG:CZ	2.39	0.52
3:H:50:GLU:O	3:H:51:ILE:C	2.52	0.52
3:O:78:ARG:O	3:O:79:MET:C	2.52	0.52
3:B:78:ARG:O	3:B:79:MET:C	2.52	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:145:PRO:HD2	6:B:201:CYC:HMC3	1.92	0.52
3:F:47:ASN:O	3:F:48:ALA:C	2.52	0.52
3:J:87:GLU:CD	3:J:88:ILE:N	2.67	0.52
4:K:86:ILE:O	4:K:87:SER:C	2.52	0.52
4:R:126:TRP:O	4:R:127:TYR:C	2.50	0.52
3:S:103:SER:O	3:S:104:VAL:C	2.51	0.52
1:A:161:LYS:HZ1	1:A:213:ILE:HG23	1.75	0.52
1:A:187:LEU:HD12	1:A:187:LEU:N	2.19	0.52
4:G:86:ILE:O	4:G:87:SER:C	2.52	0.52
4:K:129:GLU:O	4:K:130:ALA:C	2.53	0.52
3:L:47:ASN:O	3:L:48:ALA:C	2.52	0.52
3:U:50:GLU:O	3:U:51:ILE:C	2.52	0.52
3:Y:103:SER:OG	3:Y:104:VAL:N	2.43	0.52
4:a:82:CYS:HB2	6:a:201:CYC:NC	2.25	0.52
4:a:129:GLU:O	4:a:130:ALA:C	2.53	0.52
1:A:244:SER:HA	3:Q:108:ARG:HD3	1.91	0.52
4:C:108:TYR:CD1	3:F:75:PRO:HG3	2.45	0.52
4:C:122:LEU:HD11	6:C:201:CYC:NA	2.25	0.52
6:E:201:CYC:NC	6:E:201:CYC:HMD1	2.24	0.52
3:F:14:LEU:HB3	3:O:125:ARG:HH22	1.75	0.52
3:H:84:ARG:NH2	6:H:201:CYC:O2A	2.27	0.52
3:J:47:ASN:O	3:J:48:ALA:C	2.52	0.52
6:K:201:CYC:NC	6:K:201:CYC:HMD1	2.23	0.52
3:L:50:GLU:O	3:L:51:ILE:C	2.52	0.52
3:S:47:ASN:O	3:S:48:ALA:C	2.52	0.52
4:X:129:GLU:O	4:X:130:ALA:C	2.53	0.52
1:A:250:ARG:NH1	1:A:279:ALA:HA	2.25	0.52
1:A:286:ARG:HH11	1:A:287:ALA:N	2.08	0.52
3:D:55:ALA:HA	3:D:58:LYS:HE2	1.92	0.52
3:F:134:MET:O	3:F:135:LYS:C	2.53	0.52
6:F:202:CYC:NB	6:F:202:CYC:HMA1	2.24	0.52
3:L:134:MET:O	3:L:135:LYS:C	2.53	0.52
5:M:168:LEU:HD11	5:M:249:ASP:OD2	2.10	0.52
4:N:129:GLU:O	4:N:130:ALA:C	2.53	0.52
3:Y:88:ILE:HG21	6:Y:202:CYC:HAB1	1.88	0.52
1:A:170:PHE:CD2	1:A:171:ARG:NH2	2.78	0.52
3:D:134:MET:O	3:D:135:LYS:C	2.53	0.52
4:E:91:ARG:HA	3:F:18:PHE:CE2	2.45	0.52
3:H:1:MET:HG2	3:H:2:GLN:H	1.75	0.52
3:O:47:ASN:O	3:O:48:ALA:C	2.52	0.52
1:A:278:LEU:O	1:A:279:ALA:HB3	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:103:SER:OG	3:B:104:VAL:N	2.43	0.52
4:E:129:GLU:O	4:E:130:ALA:C	2.53	0.52
3:H:78:ARG:O	3:H:79:MET:C	2.52	0.52
5:M:264:LYS:HA	5:M:267:LEU:HD12	1.92	0.52
3:O:134:MET:O	3:O:135:LYS:C	2.53	0.52
3:U:47:ASN:O	3:U:48:ALA:C	2.52	0.52
3:U:148:VAL:HG11	6:U:202:CYC:CHD	2.40	0.52
4:X:91:ARG:O	4:X:94:THR:OG1	2.22	0.52
3:B:134:MET:O	3:B:135:LYS:C	2.53	0.52
3:J:50:GLU:O	3:J:51:ILE:C	2.52	0.52
4:N:86:ILE:O	4:N:87:SER:C	2.52	0.52
4:V:129:GLU:O	4:V:130:ALA:C	2.53	0.52
4:C:129:GLU:O	4:C:130:ALA:C	2.53	0.51
3:F:50:GLU:O	3:F:51:ILE:C	2.52	0.51
4:G:120:PHE:CE2	6:G:201:CYC:HAA1	2.45	0.51
4:G:129:GLU:O	4:G:130:ALA:C	2.53	0.51
6:G:201:CYC:NC	6:G:201:CYC:CMD	2.71	0.51
3:H:47:ASN:O	3:H:48:ALA:C	2.52	0.51
3:Q:47:ASN:O	3:Q:48:ALA:C	2.52	0.51
3:Y:78:ARG:O	3:Y:79:MET:C	2.52	0.51
1:A:203:ARG:HA	1:A:206:GLN:HB2	1.91	0.51
3:D:77:ARG:CD	5:M:273:ILE:HG22	2.38	0.51
6:E:201:CYC:CMA	6:E:201:CYC:NB	2.73	0.51
3:F:78:ARG:O	3:F:79:MET:C	2.52	0.51
6:N:201:CYC:NB	6:N:201:CYC:CMA	2.74	0.51
3:U:6:THR:O	3:U:9:ILE:HB	2.10	0.51
4:a:86:ILE:O	4:a:87:SER:C	2.52	0.51
1:A:123:TYR:HE1	1:A:137:ARG:HG2	1.75	0.51
2:Z:52:LEU:HD21	2:Z:56:MET:SD	2.49	0.51
5:M:27:HIS:ND1	5:M:28:HIS:O	2.43	0.51
4:P:129:GLU:O	4:P:130:ALA:C	2.53	0.51
4:R:86:ILE:O	4:R:87:SER:C	2.52	0.51
6:R:201:CYC:CMA	6:R:201:CYC:HB	2.18	0.51
3:S:6:THR:O	3:S:9:ILE:HB	2.11	0.51
4:X:95:TYR:CG	3:Y:9:ILE:HG23	2.45	0.51
1:A:177:ARG:HA	1:A:272:THR:HG22	1.93	0.51
2:Z:47:VAL:HG12	2:Z:48:SER:O	2.11	0.51
4:E:86:ILE:O	4:E:87:SER:C	2.52	0.51
3:F:14:LEU:CD2	3:O:125:ARG:NH2	2.72	0.51
3:H:134:MET:O	3:H:135:LYS:C	2.53	0.51
3:J:78:ARG:O	3:J:79:MET:C	2.52	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:6:THR:O	3:Q:9:ILE:HB	2.11	0.51
3:Y:6:THR:O	3:Y:9:ILE:HB	2.10	0.51
4:I:33:ARG:HH12	4:I:145:GLN:HB3	1.75	0.51
5:M:190:ARG:HG3	5:M:194:PHE:CD2	2.42	0.51
3:S:134:MET:O	3:S:135:LYS:C	2.53	0.51
3:U:134:MET:O	3:U:135:LYS:C	2.53	0.51
2:Z:23:PRO:HA	2:Z:36:HIS:HB3	1.92	0.51
3:D:50:GLU:O	3:D:51:ILE:C	2.52	0.51
4:G:124:PRO:O	4:G:125:SER:C	2.54	0.51
4:I:129:GLU:O	4:I:130:ALA:C	2.53	0.51
3:J:6:THR:O	3:J:9:ILE:HB	2.11	0.51
3:J:103:SER:OG	3:J:104:VAL:N	2.43	0.51
4:N:124:PRO:O	4:N:125:SER:C	2.54	0.51
4:C:155:ASP:O	4:C:156:TYR:C	2.54	0.51
5:M:60:LYS:HE3	3:U:108:ARG:O	2.10	0.51
3:Y:47:ASN:O	3:Y:48:ALA:C	2.53	0.51
1:A:120:ARG:NH1	4:X:16:GLY:HA3	2.26	0.51
1:A:240:GLN:O	1:A:243:GLN:HG3	2.10	0.51
3:F:6:THR:O	3:F:9:ILE:HB	2.11	0.51
5:M:17:VAL:HB	5:M:45:VAL:HG12	1.93	0.51
4:R:129:GLU:O	4:R:130:ALA:C	2.53	0.51
3:U:103:SER:OG	3:U:104:VAL:N	2.43	0.51
4:V:91:ARG:HA	3:W:18:PHE:CE2	2.45	0.51
3:Y:117:TYR:CA	3:Y:122:THR:HG22	2.41	0.51
4:a:124:PRO:O	4:a:125:SER:C	2.54	0.51
4:a:155:ASP:O	4:a:156:TYR:C	2.54	0.51
1:A:176:ASN:HD21	6:S:202:CYC:CMA	2.23	0.51
3:W:134:MET:O	3:W:135:LYS:C	2.53	0.51
3:F:103:SER:OG	3:F:104:VAL:N	2.44	0.51
4:K:82:CYS:HB2	6:K:201:CYC:NC	2.26	0.51
3:L:48:ALA:O	3:L:49:ALA:C	2.54	0.51
3:Q:134:MET:O	3:Q:135:LYS:C	2.53	0.51
3:W:6:THR:O	3:W:9:ILE:HB	2.11	0.51
1:A:177:ARG:HD3	1:A:272:THR:HA	1.93	0.50
3:F:14:LEU:CG	3:O:125:ARG:NH2	2.74	0.50
3:L:103:SER:OG	3:L:104:VAL:N	2.44	0.50
3:Q:149:THR:HG21	6:Q:201:CYC:O2A	2.11	0.50
4:R:155:ASP:O	4:R:156:TYR:C	2.54	0.50
4:V:155:ASP:O	4:V:156:TYR:C	2.54	0.50
6:W:202:CYC:C1A	6:W:202:CYC:O1A	2.59	0.50
3:Y:86:MET:HG3	6:Y:202:CYC:HBC1	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ALA:HB3	1:A:213:ILE:CD1	2.41	0.50
3:B:91:ARG:HA	4:a:18:PHE:CE2	2.46	0.50
4:E:155:ASP:O	4:E:156:TYR:C	2.54	0.50
3:H:85:ASP:OD2	6:H:201:CYC:NA	2.44	0.50
3:J:134:MET:O	3:J:135:LYS:C	2.53	0.50
4:P:124:PRO:O	4:P:125:SER:C	2.54	0.50
4:X:18:PHE:CE2	3:Y:91:ARG:HA	2.45	0.50
1:A:90:GLN:HB3	1:A:95:ILE:CG1	2.42	0.50
1:A:170:PHE:CE1	1:A:178:PHE:CZ	2.99	0.50
4:N:19:LEU:O	3:O:45:THR:HG21	2.11	0.50
4:R:124:PRO:O	4:R:125:SER:C	2.54	0.50
3:Y:134:MET:O	3:Y:135:LYS:C	2.53	0.50
1:A:159:LEU:O	1:A:160:ALA:HB3	2.11	0.50
2:Z:1:SER:N	2:Z:44:SER:HB2	2.26	0.50
4:C:124:PRO:O	4:C:125:SER:C	2.54	0.50
6:G:201:CYC:CMA	6:G:201:CYC:NB	2.74	0.50
4:I:124:PRO:O	4:I:125:SER:C	2.54	0.50
4:K:88:HIS:HB3	6:K:201:CYC:HBB3	1.93	0.50
4:K:155:ASP:O	4:K:156:TYR:C	2.54	0.50
4:P:17:ARG:NH2	4:T:2:LYS:HZ1	2.08	0.50
1:A:280:ASP:HB3	1:A:281:PRO:HD3	1.94	0.50
3:L:6:THR:O	3:L:9:ILE:HB	2.11	0.50
5:M:175:GLY:HA3	5:M:222:ARG:N	2.27	0.50
3:O:48:ALA:O	3:O:49:ALA:C	2.55	0.50
4:T:124:PRO:O	4:T:125:SER:C	2.54	0.50
3:W:103:SER:OG	3:W:104:VAL:N	2.44	0.50
1:A:147:ASN:CG	6:O:202:CYC:HAA1	2.37	0.50
3:F:48:ALA:O	3:F:49:ALA:C	2.55	0.50
4:K:124:PRO:O	4:K:125:SER:C	2.55	0.50
5:M:160:THR:OG1	5:M:164:ARG:CG	2.59	0.50
3:U:76:ASN:O	3:U:77:ARG:C	2.55	0.50
1:A:205:CYS:SG	3:S:84:ARG:HG3	2.52	0.50
3:H:48:ALA:O	3:H:49:ALA:C	2.55	0.50
3:S:103:SER:OG	3:S:104:VAL:N	2.45	0.50
3:W:48:ALA:O	3:W:49:ALA:C	2.55	0.50
4:X:155:ASP:O	4:X:156:TYR:C	2.54	0.50
1:A:77:VAL:O	1:A:78:ARG:HB3	2.11	0.50
1:A:169:PHE:CZ	1:A:185:HIS:HD2	2.30	0.50
4:C:127:TYR:O	4:C:128:ILE:C	2.55	0.50
3:D:6:THR:O	3:D:9:ILE:HB	2.11	0.50
6:I:201:CYC:NB	6:I:201:CYC:HMA1	2.27	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:117:TYR:HD1	3:L:122:THR:HG21	1.71	0.50
6:O:202:CYC:C1B	6:O:202:CYC:HMA3	2.41	0.50
3:Q:103:SER:OG	3:Q:104:VAL:N	2.44	0.50
4:T:155:ASP:O	4:T:156:TYR:C	2.54	0.50
4:V:124:PRO:O	4:V:125:SER:C	2.54	0.50
4:C:120:PHE:CE2	6:C:201:CYC:HAA1	2.47	0.50
3:D:48:ALA:O	3:D:49:ALA:C	2.55	0.50
5:M:115:GLY:O	5:M:116:ASN:C	2.54	0.50
2:Z:21:LEU:HD23	2:Z:43:TYR:CD1	2.47	0.49
4:I:127:TYR:O	4:I:128:ILE:C	2.55	0.49
4:N:20:ASN:C	4:N:20:ASN:OD1	2.55	0.49
3:O:103:SER:OG	3:O:104:VAL:N	2.44	0.49
3:W:76:ASN:O	3:W:77:ARG:C	2.55	0.49
1:A:286:ARG:NH1	1:A:287:ALA:N	2.60	0.49
4:C:17:ARG:NH1	4:C:20:ASN:ND2	2.60	0.49
4:P:155:ASP:O	4:P:156:TYR:C	2.54	0.49
3:Q:48:ALA:O	3:Q:49:ALA:C	2.55	0.49
3:Q:57:HIS:CD2	6:X:201:CYC:O1D	2.66	0.49
3:Y:76:ASN:O	3:Y:77:ARG:C	2.54	0.49
1:A:244:SER:HB2	3:Q:108:ARG:HD3	1.94	0.49
4:E:124:PRO:O	4:E:125:SER:C	2.54	0.49
3:H:76:ASN:O	3:H:77:ARG:C	2.55	0.49
4:I:155:ASP:O	4:I:156:TYR:C	2.54	0.49
3:L:76:ASN:O	3:L:77:ARG:C	2.55	0.49
4:N:155:ASP:O	4:N:156:TYR:C	2.54	0.49
4:X:124:PRO:O	4:X:125:SER:C	2.54	0.49
3:B:6:THR:O	3:B:9:ILE:HB	2.12	0.49
4:C:1:MET:SD	3:D:6:THR:HG23	2.53	0.49
3:H:103:SER:OG	3:H:104:VAL:N	2.44	0.49
3:J:103:SER:O	3:J:106:GLU:N	2.46	0.49
3:L:117:TYR:CA	3:L:122:THR:HG22	2.42	0.49
3:W:36:LYS:O	3:W:37:ARG:C	2.56	0.49
3:H:103:SER:O	3:H:106:GLU:N	2.46	0.49
5:M:71:PRO:HD3	3:U:119:ALA:HB1	1.94	0.49
3:S:48:ALA:O	3:S:49:ALA:C	2.55	0.49
4:T:20:ASN:C	4:T:20:ASN:OD1	2.56	0.49
3:U:48:ALA:O	3:U:49:ALA:C	2.55	0.49
3:U:120:LEU:HD22	6:U:201:CYC:CBD	2.42	0.49
2:Z:21:LEU:HD12	2:Z:25:LEU:HB2	1.93	0.49
3:B:48:ALA:O	3:B:49:ALA:C	2.55	0.49
6:D:201:CYC:CMA	6:D:201:CYC:NB	2.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:155:ASP:O	4:G:156:TYR:C	2.54	0.49
4:I:91:ARG:O	4:I:94:THR:OG1	2.22	0.49
3:J:48:ALA:O	3:J:49:ALA:C	2.55	0.49
3:L:111:ASN:O	5:M:232:VAL:HG21	2.08	0.49
4:V:127:TYR:O	4:V:128:ILE:C	2.55	0.49
3:W:103:SER:O	3:W:106:GLU:N	2.45	0.49
3:Y:48:ALA:O	3:Y:49:ALA:C	2.54	0.49
1:A:138:VAL:HG23	1:A:138:VAL:O	2.11	0.49
3:B:76:ASN:O	3:B:77:ARG:C	2.55	0.49
3:B:103:SER:O	3:B:106:GLU:N	2.46	0.49
6:D:202:CYC:NB	5:M:188:LEU:CD1	2.76	0.49
3:F:94:SER:O	3:F:95:TYR:C	2.56	0.49
3:H:6:THR:O	3:H:9:ILE:HB	2.11	0.49
4:N:91:ARG:O	4:N:94:THR:OG1	2.22	0.49
3:O:76:ASN:O	3:O:77:ARG:C	2.55	0.49
3:O:94:SER:O	3:O:95:TYR:C	2.56	0.49
6:O:202:CYC:NA	6:O:202:CYC:ND	2.61	0.49
4:R:88:HIS:O	4:R:89:TYR:C	2.56	0.49
4:V:88:HIS:O	4:V:89:TYR:C	2.56	0.49
3:Y:103:SER:O	3:Y:106:GLU:N	2.45	0.49
3:D:103:SER:O	3:D:106:GLU:N	2.46	0.49
3:H:36:LYS:O	3:H:37:ARG:C	2.56	0.49
3:H:94:SER:O	3:H:95:TYR:C	2.56	0.49
3:L:103:SER:O	3:L:106:GLU:N	2.45	0.49
5:M:37:GLU:CG	5:M:38:PRO:HD2	2.42	0.49
4:N:115:GLU:OE1	4:N:115:GLU:N	2.37	0.49
3:Q:55:ALA:HA	3:Q:58:LYS:HE2	1.94	0.49
3:Q:94:SER:O	3:Q:95:TYR:C	2.56	0.49
3:S:120:LEU:HD13	6:S:202:CYC:CHA	2.42	0.49
4:X:127:TYR:O	4:X:128:ILE:C	2.55	0.49
4:E:127:TYR:O	4:E:128:ILE:C	2.55	0.49
3:F:76:ASN:O	3:F:77:ARG:C	2.55	0.49
4:G:20:ASN:C	4:G:20:ASN:OD1	2.56	0.49
4:K:20:ASN:C	4:K:20:ASN:OD1	2.56	0.49
3:Y:94:SER:O	3:Y:95:TYR:C	2.56	0.49
3:Y:117:TYR:CG	3:Y:122:THR:HG21	2.45	0.49
1:A:168:ARG:O	1:A:169:PHE:CB	2.61	0.49
2:Z:14:LEU:HD12	2:Z:14:LEU:O	2.12	0.49
2:Z:58:ARG:NH1	5:M:140:ARG:HH21	2.10	0.49
5:M:6:THR:HG23	3:O:111:ASN:CB	2.43	0.49
5:M:35:THR:CG2	3:W:84:ARG:CZ	2.91	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:88:HIS:O	4:N:89:TYR:C	2.56	0.49
4:N:127:TYR:O	4:N:128:ILE:C	2.55	0.49
4:P:88:HIS:O	4:P:89:TYR:C	2.56	0.49
4:R:20:ASN:C	4:R:20:ASN:OD1	2.56	0.49
3:S:76:ASN:O	3:S:77:ARG:C	2.55	0.49
6:T:201:CYC:CMA	6:T:201:CYC:HB	2.26	0.49
6:T:201:CYC:HB	6:T:201:CYC:HMA2	1.78	0.49
3:U:35:ASN:HB3	6:U:202:CYC:C1A	2.43	0.49
3:U:103:SER:O	3:U:106:GLU:N	2.46	0.49
6:U:201:CYC:O2A	6:U:201:CYC:C1A	2.61	0.49
4:a:20:ASN:C	4:a:20:ASN:OD1	2.56	0.49
2:Z:53:LEU:HB3	2:Z:54:PRO:HD3	1.95	0.48
3:B:36:LYS:O	3:B:37:ARG:C	2.56	0.48
4:C:73:GLY:HA2	6:C:201:CYC:OC	2.13	0.48
3:D:103:SER:OG	3:D:104:VAL:N	2.46	0.48
4:E:20:ASN:C	4:E:20:ASN:OD1	2.56	0.48
4:I:20:ASN:OD1	4:I:20:ASN:C	2.56	0.48
4:K:127:TYR:O	4:K:128:ILE:C	2.55	0.48
4:P:20:ASN:C	4:P:20:ASN:OD1	2.55	0.48
4:a:127:TYR:O	4:a:128:ILE:C	2.55	0.48
3:D:64:THR:O	3:D:67:ILE:HG12	2.13	0.48
3:H:64:THR:O	3:H:67:ILE:HG12	2.14	0.48
4:I:17:ARG:NH1	4:I:20:ASN:ND2	2.61	0.48
4:K:88:HIS:ND1	6:K:201:CYC:CBB	2.76	0.48
4:K:88:HIS:O	4:K:89:TYR:C	2.56	0.48
4:P:127:TYR:O	4:P:128:ILE:C	2.55	0.48
4:V:17:ARG:NH1	4:V:20:ASN:ND2	2.61	0.48
2:Z:19:ILE:O	2:Z:42:SER:HA	2.13	0.48
3:B:94:SER:O	3:B:95:TYR:C	2.56	0.48
4:G:88:HIS:O	4:G:89:TYR:C	2.56	0.48
3:L:36:LYS:O	3:L:37:ARG:C	2.56	0.48
5:M:35:THR:HA	6:W:201:CYC:O2A	2.13	0.48
4:N:114:ARG:H	4:N:114:ARG:HD2	1.78	0.48
6:Q:201:CYC:NB	6:Q:201:CYC:HMA1	2.29	0.48
6:Q:201:CYC:HMA1	4:T:33:ARG:HH12	1.79	0.48
4:X:88:HIS:O	4:X:89:TYR:C	2.56	0.48
3:Y:145:PRO:CD	6:Y:201:CYC:HMC3	2.43	0.48
1:A:203:ARG:O	1:A:204:TYR:C	2.56	0.48
3:F:103:SER:O	3:F:106:GLU:N	2.45	0.48
4:G:90:LEU:O	4:G:91:ARG:C	2.57	0.48
4:G:127:TYR:O	4:G:128:ILE:C	2.55	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:127:VAL:HG22	6:O:202:CYC:H3C	1.95	0.48
3:S:94:SER:O	3:S:95:TYR:C	2.56	0.48
3:S:103:SER:O	3:S:106:GLU:N	2.46	0.48
4:T:90:LEU:O	4:T:91:ARG:C	2.57	0.48
4:V:20:ASN:C	4:V:20:ASN:OD1	2.56	0.48
3:W:64:THR:O	3:W:67:ILE:HG12	2.12	0.48
3:W:94:SER:O	3:W:95:TYR:C	2.56	0.48
4:X:90:LEU:O	4:X:91:ARG:C	2.57	0.48
1:A:76:PHE:O	1:A:76:PHE:CG	2.66	0.48
1:A:223:ARG:HD3	5:M:58:TYR:CE2	2.48	0.48
4:C:20:ASN:C	4:C:20:ASN:OD1	2.56	0.48
3:D:36:LYS:O	3:D:37:ARG:C	2.56	0.48
6:D:202:CYC:HB	5:M:188:LEU:CD1	2.26	0.48
3:F:160:ALA:O	3:F:161:ALA:C	2.57	0.48
3:L:94:SER:O	3:L:95:TYR:C	2.56	0.48
3:O:1:MET:HE2	3:O:2:GLN:N	2.29	0.48
3:Q:36:LYS:O	3:Q:37:ARG:C	2.56	0.48
3:Q:103:SER:O	3:Q:106:GLU:N	2.46	0.48
3:U:36:LYS:O	3:U:37:ARG:C	2.56	0.48
3:W:160:ALA:O	3:W:161:ALA:C	2.57	0.48
3:Y:36:LYS:O	3:Y:37:ARG:C	2.56	0.48
3:H:102:ALA:O	3:H:103:SER:C	2.57	0.48
4:I:88:HIS:O	4:I:89:TYR:C	2.56	0.48
6:I:201:CYC:NB	6:I:201:CYC:CMA	2.77	0.48
5:M:4:LEU:O	3:O:111:ASN:O	2.32	0.48
3:O:103:SER:O	3:O:106:GLU:N	2.46	0.48
6:O:202:CYC:CMA	6:O:202:CYC:HB	2.25	0.48
3:L:145:PRO:CD	6:L:202:CYC:HMC3	2.44	0.48
3:S:36:LYS:O	3:S:37:ARG:C	2.56	0.48
3:W:88:ILE:HG21	6:W:201:CYC:HAB1	1.95	0.48
4:X:20:ASN:C	4:X:20:ASN:OD1	2.56	0.48
4:C:90:LEU:O	4:C:91:ARG:C	2.57	0.48
4:I:90:LEU:O	4:I:91:ARG:C	2.57	0.48
3:J:160:ALA:O	3:J:161:ALA:C	2.57	0.48
3:L:160:ALA:O	3:L:161:ALA:C	2.57	0.48
3:O:6:THR:O	3:O:9:ILE:HB	2.13	0.48
3:Q:64:THR:O	3:Q:67:ILE:HG12	2.13	0.48
4:T:127:TYR:O	4:T:128:ILE:C	2.55	0.48
4:a:90:LEU:O	4:a:91:ARG:C	2.57	0.48
4:a:114:ARG:H	4:a:114:ARG:HD2	1.78	0.48
1:A:113:ALA:HA	1:A:116:ILE:HD12	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:29:ASN:OD1	3:B:30:LEU:N	2.47	0.48
3:B:102:ALA:O	3:B:103:SER:C	2.57	0.48
3:D:76:ASN:O	3:D:77:ARG:C	2.55	0.48
3:D:94:SER:O	3:D:95:TYR:C	2.56	0.48
3:D:160:ALA:O	3:D:161:ALA:C	2.57	0.48
3:J:36:LYS:O	3:J:37:ARG:C	2.56	0.48
5:M:161:SER:O	5:M:164:ARG:HB3	2.13	0.48
3:Q:29:ASN:OD1	3:Q:30:LEU:N	2.47	0.48
3:Q:160:ALA:O	3:Q:161:ALA:C	2.57	0.48
1:A:161:LYS:NZ	1:A:214:ASP:OD1	2.47	0.48
1:A:169:PHE:CZ	1:A:181:LEU:HB3	2.49	0.48
3:B:6:THR:HG23	4:a:1:MET:SD	2.54	0.48
6:D:202:CYC:HMA1	6:D:202:CYC:NB	2.29	0.48
5:M:215:GLU:O	5:M:216:ASN:CG	2.56	0.48
3:O:29:ASN:OD1	3:O:30:LEU:N	2.47	0.48
3:Q:76:ASN:O	3:Q:77:ARG:C	2.57	0.48
3:U:94:SER:O	3:U:95:TYR:C	2.56	0.48
1:A:173:THR:HG22	1:A:270:GLN:HB2	1.96	0.47
1:A:278:LEU:HD22	1:A:282:ALA:H	1.79	0.47
3:H:132:GLN:O	3:H:133:LEU:C	2.57	0.47
3:H:160:ALA:O	3:H:161:ALA:C	2.57	0.47
3:O:1:MET:HE2	3:O:2:GLN:H	1.78	0.47
4:P:17:ARG:NH1	4:P:20:ASN:ND2	2.62	0.47
3:Y:102:ALA:O	3:Y:103:SER:C	2.57	0.47
1:A:192:TYR:C	1:A:250:ARG:HH22	2.22	0.47
2:Z:66:ILE:HD13	2:Z:69:ILE:HD11	1.95	0.47
6:H:201:CYC:HAA1	5:M:134:ASN:CG	2.39	0.47
4:K:1:MET:SD	3:L:6:THR:HG23	2.54	0.47
5:M:174:LEU:HB2	5:M:176:ARG:HG2	1.96	0.47
3:O:36:LYS:O	3:O:37:ARG:C	2.56	0.47
4:R:90:LEU:O	4:R:91:ARG:C	2.57	0.47
4:R:127:TYR:O	4:R:128:ILE:C	2.55	0.47
3:U:29:ASN:OD1	3:U:30:LEU:N	2.47	0.47
4:V:33:ARG:HH12	4:V:145:GLN:HB3	1.78	0.47
3:W:132:GLN:O	3:W:133:LEU:C	2.58	0.47
4:X:85:ASP:O	4:X:88:HIS:HB2	2.14	0.47
1:A:161:LYS:NZ	1:A:213:ILE:HG23	2.28	0.47
2:Z:4:THR:HG21	5:M:134:ASN:HD22	1.78	0.47
3:D:77:ARG:NH1	5:M:273:ILE:HG22	2.28	0.47
3:F:36:LYS:O	3:F:37:ARG:C	2.56	0.47
3:J:76:ASN:O	3:J:77:ARG:C	2.55	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:94:SER:O	3:J:95:TYR:C	2.56	0.47
5:M:6:THR:HG23	3:O:111:ASN:HB3	1.96	0.47
5:M:179:TYR:O	5:M:180:ASN:HB2	2.13	0.47
4:N:131:LEU:O	4:N:134:ILE:HB	2.15	0.47
3:Q:102:ALA:O	3:Q:103:SER:C	2.57	0.47
3:Y:160:ALA:O	3:Y:161:ALA:C	2.57	0.47
4:a:73:GLY:HA2	6:a:201:CYC:OC	2.14	0.47
1:A:186:LEU:O	1:A:187:LEU:HD12	2.12	0.47
1:A:136:GLU:HB3	1:A:164:LEU:CD1	2.45	0.47
2:Z:3:LEU:CD1	2:Z:3:LEU:H	2.27	0.47
3:D:29:ASN:OD1	3:D:30:LEU:N	2.47	0.47
4:G:52:VAL:O	4:G:53:LYS:C	2.58	0.47
3:J:109:CYS:HA	6:J:201:CYC:CBB	2.44	0.47
4:K:90:LEU:O	4:K:91:ARG:C	2.57	0.47
6:N:201:CYC:NC	6:N:201:CYC:CMD	2.77	0.47
3:O:102:ALA:O	3:O:103:SER:C	2.57	0.47
4:P:94:THR:O	4:P:95:TYR:C	2.58	0.47
3:S:160:ALA:O	3:S:161:ALA:C	2.57	0.47
4:T:88:HIS:O	4:T:89:TYR:C	2.56	0.47
6:U:201:CYC:HMD1	6:U:201:CYC:C1C	2.43	0.47
4:V:85:ASP:O	4:V:88:HIS:HB2	2.15	0.47
4:a:88:HIS:O	4:a:89:TYR:C	2.56	0.47
1:A:86:ASP:OD1	3:Q:75:PRO:HD2	2.15	0.47
1:A:173:THR:HG22	1:A:270:GLN:CB	2.44	0.47
3:D:132:GLN:O	3:D:133:LEU:C	2.58	0.47
4:G:85:ASP:O	4:G:88:HIS:HB2	2.14	0.47
4:I:94:THR:O	4:I:95:TYR:C	2.58	0.47
3:L:132:GLN:O	3:L:133:LEU:C	2.57	0.47
4:N:90:LEU:O	4:N:91:ARG:C	2.57	0.47
4:N:94:THR:O	4:N:95:TYR:C	2.58	0.47
6:O:202:CYC:CMA	6:O:202:CYC:C1B	2.92	0.47
4:T:94:THR:O	4:T:95:TYR:C	2.58	0.47
1:A:126:LEU:HD21	1:A:159:LEU:CD1	2.45	0.47
3:B:160:ALA:O	3:B:161:ALA:C	2.57	0.47
4:C:52:VAL:O	4:C:53:LYS:C	2.58	0.47
4:C:88:HIS:O	4:C:89:TYR:C	2.56	0.47
6:D:202:CYC:HMD1	6:D:202:CYC:C4C	2.41	0.47
3:F:39:ASP:OD1	6:F:201:CYC:CHB	2.61	0.47
3:F:90:LEU:HB2	3:F:134:MET:HE1	1.97	0.47
3:J:132:GLN:O	3:J:133:LEU:C	2.58	0.47
6:J:202:CYC:C1A	6:J:202:CYC:O1A	2.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:64:THR:O	3:L:67:ILE:HG12	2.15	0.47
5:M:88:PRO:O	5:M:89:LEU:CB	2.63	0.47
5:M:176:ARG:HH22	5:M:183:GLU:CD	2.22	0.47
4:P:90:LEU:O	4:P:91:ARG:C	2.57	0.47
4:V:90:LEU:O	4:V:91:ARG:C	2.57	0.47
6:V:201:CYC:NB	6:V:201:CYC:CMA	2.78	0.47
3:W:102:ALA:O	3:W:103:SER:C	2.57	0.47
4:X:94:THR:O	4:X:95:TYR:C	2.58	0.47
4:X:131:LEU:O	4:X:134:ILE:HB	2.15	0.47
1:A:120:ARG:HG2	1:A:124:LYS:NZ	2.29	0.47
3:B:1:MET:HE2	3:B:2:GLN:N	2.30	0.47
4:G:92:PHE:O	4:G:93:ILE:C	2.58	0.47
6:H:201:CYC:CBA	5:M:134:ASN:OD1	2.63	0.47
4:K:52:VAL:O	4:K:53:LYS:C	2.58	0.47
3:U:102:ALA:O	3:U:103:SER:C	2.57	0.47
4:a:92:PHE:O	4:a:93:ILE:C	2.58	0.47
3:B:82:CYS:HA	6:B:202:CYC:CHD	2.44	0.47
4:C:85:ASP:O	4:C:88:HIS:HB2	2.15	0.47
3:D:102:ALA:O	3:D:103:SER:C	2.57	0.47
4:E:52:VAL:O	4:E:53:LYS:C	2.58	0.47
4:E:88:HIS:O	4:E:89:TYR:C	2.56	0.47
4:E:91:ARG:O	4:E:94:THR:OG1	2.22	0.47
4:E:94:THR:O	4:E:95:TYR:C	2.58	0.47
3:F:102:ALA:O	3:F:103:SER:C	2.57	0.47
4:I:85:ASP:O	4:I:88:HIS:HB2	2.15	0.47
4:N:52:VAL:O	4:N:53:LYS:C	2.58	0.47
4:C:17:ARG:CZ	4:G:2:LYS:HZ1	2.28	0.47
4:C:131:LEU:O	4:C:134:ILE:HB	2.15	0.47
4:E:85:ASP:O	4:E:88:HIS:HB2	2.15	0.47
4:G:94:THR:O	4:G:95:TYR:C	2.58	0.47
3:J:122:THR:HG23	6:J:201:CYC:NC	2.30	0.47
5:M:117:THR:HG22	5:M:155:ARG:NH2	2.30	0.47
4:R:131:LEU:O	4:R:134:ILE:HB	2.15	0.47
4:T:94:THR:OG1	4:T:95:TYR:N	2.48	0.47
3:W:85:ASP:O	3:W:86:MET:C	2.58	0.47
4:a:94:THR:O	4:a:95:TYR:C	2.58	0.47
1:A:86:ASP:OD1	3:Q:75:PRO:CD	2.63	0.46
4:G:91:ARG:O	4:G:94:THR:OG1	2.22	0.46
3:J:102:ALA:O	3:J:103:SER:C	2.57	0.46
3:Q:85:ASP:O	3:Q:86:MET:C	2.58	0.46
3:S:132:GLN:O	3:S:133:LEU:C	2.58	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:85:ASP:O	4:a:88:HIS:HB2	2.15	0.46
1:A:257:GLY:HA3	3:Y:111:ASN:ND2	2.31	0.46
4:E:131:LEU:O	4:E:134:ILE:HB	2.15	0.46
3:H:29:ASN:OD1	3:H:30:LEU:N	2.47	0.46
3:H:164:PHE:O	3:H:167:ALA:HB3	2.16	0.46
6:H:201:CYC:O2A	6:H:201:CYC:C2A	2.62	0.46
4:K:94:THR:OG1	4:K:95:TYR:N	2.48	0.46
5:M:9:GLN:CD	4:N:14:SER:HB3	2.41	0.46
4:N:145:GLN:O	4:N:146:PRO:C	2.59	0.46
3:O:160:ALA:O	3:O:161:ALA:C	2.57	0.46
4:P:145:GLN:O	4:P:146:PRO:C	2.59	0.46
4:R:20:ASN:OD1	4:R:22:THR:N	2.48	0.46
4:R:52:VAL:O	4:R:53:LYS:C	2.57	0.46
3:S:102:ALA:O	3:S:103:SER:C	2.58	0.46
4:T:131:LEU:O	4:T:134:ILE:HB	2.15	0.46
3:F:132:GLN:O	3:F:133:LEU:C	2.57	0.46
4:I:94:THR:OG1	4:I:95:TYR:N	2.49	0.46
4:I:131:LEU:O	4:I:134:ILE:HB	2.15	0.46
3:L:102:ALA:O	3:L:103:SER:C	2.58	0.46
3:L:117:TYR:O	3:L:122:THR:HG22	2.16	0.46
4:P:94:THR:OG1	4:P:95:TYR:N	2.49	0.46
6:R:201:CYC:HMA3	6:R:201:CYC:C1B	2.44	0.46
3:U:160:ALA:O	3:U:161:ALA:C	2.57	0.46
3:B:132:GLN:O	3:B:133:LEU:C	2.58	0.46
4:E:145:GLN:O	4:E:146:PRO:C	2.59	0.46
4:I:20:ASN:OD1	4:I:22:THR:N	2.49	0.46
3:J:164:PHE:O	3:J:167:ALA:HB3	2.16	0.46
5:M:139:VAL:CG2	5:M:216:ASN:HA	2.46	0.46
3:Q:77:ARG:HH22	6:Q:202:CYC:CGD	2.28	0.46
3:Q:91:ARG:O	3:Q:94:SER:OG	2.24	0.46
3:U:64:THR:O	3:U:67:ILE:HG12	2.15	0.46
4:V:52:VAL:O	4:V:53:LYS:C	2.58	0.46
4:X:145:GLN:O	4:X:146:PRO:C	2.59	0.46
4:a:131:LEU:O	4:a:134:ILE:HB	2.15	0.46
1:A:166:LYS:HD2	1:A:209:TYR:HE2	1.81	0.46
1:A:244:SER:HA	3:Q:108:ARG:HA	1.97	0.46
4:C:20:ASN:OD1	4:C:22:THR:N	2.48	0.46
4:C:94:THR:O	4:C:95:TYR:C	2.58	0.46
3:D:88:ILE:O	3:D:89:ILE:C	2.58	0.46
3:D:164:PHE:O	3:D:167:ALA:HB3	2.15	0.46
6:H:201:CYC:HMD1	6:H:201:CYC:C1C	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:52:VAL:O	4:I:53:LYS:C	2.58	0.46
4:N:92:PHE:O	4:N:93:ILE:C	2.58	0.46
4:P:85:ASP:O	4:P:88:HIS:HB2	2.15	0.46
4:P:131:LEU:O	4:P:134:ILE:HB	2.15	0.46
4:R:85:ASP:O	4:R:88:HIS:HB2	2.15	0.46
4:R:94:THR:O	4:R:95:TYR:C	2.58	0.46
3:S:153:CYS:O	3:S:154:SER:C	2.59	0.46
3:U:149:THR:O	6:U:202:CYC:HMD2	2.15	0.46
4:V:2:LYS:HG3	4:V:7:GLU:OE2	2.14	0.46
4:V:131:LEU:O	4:V:134:ILE:HB	2.15	0.46
3:F:88:ILE:O	3:F:89:ILE:C	2.59	0.46
4:I:2:LYS:HG3	4:I:7:GLU:OE2	2.15	0.46
4:K:88:HIS:CB	6:K:201:CYC:HBB3	2.46	0.46
3:L:153:CYS:O	3:L:154:SER:C	2.59	0.46
4:N:20:ASN:OD1	4:N:22:THR:N	2.49	0.46
6:Q:202:CYC:HB	6:Q:202:CYC:HMA1	1.81	0.46
4:T:20:ASN:OD1	4:T:22:THR:N	2.49	0.46
4:T:85:ASP:O	4:T:88:HIS:HB2	2.15	0.46
4:V:92:PHE:O	4:V:93:ILE:C	2.58	0.46
6:W:201:CYC:HHA	6:W:201:CYC:HBD1	1.97	0.46
4:X:52:VAL:O	4:X:53:LYS:C	2.58	0.46
3:Y:153:CYS:O	3:Y:154:SER:C	2.59	0.46
3:Y:164:PHE:O	3:Y:167:ALA:HB3	2.15	0.46
4:a:94:THR:OG1	4:a:95:TYR:N	2.48	0.46
1:A:78:ARG:HG3	1:A:80:ALA:H	1.79	0.46
2:Z:51:ARG:C	2:Z:54:PRO:HD2	2.41	0.46
3:F:78:ARG:HD3	6:F:202:CYC:O1D	2.16	0.46
3:H:85:ASP:O	3:H:86:MET:C	2.59	0.46
3:H:120:LEU:HD13	6:H:201:CYC:HBD1	1.97	0.46
3:J:88:ILE:O	3:J:89:ILE:C	2.59	0.46
3:L:85:ASP:O	3:L:86:MET:C	2.59	0.46
3:Q:76:ASN:HB2	4:X:108:TYR:O	2.16	0.46
3:Q:88:ILE:O	3:Q:89:ILE:C	2.59	0.46
3:S:85:ASP:O	3:S:86:MET:C	2.59	0.46
4:T:52:VAL:O	4:T:53:LYS:C	2.58	0.46
4:a:20:ASN:OD1	4:a:22:THR:N	2.49	0.46
1:A:244:SER:CA	3:Q:108:ARG:HD3	2.46	0.46
1:A:278:LEU:HA	1:A:281:PRO:HD2	1.97	0.46
2:Z:52:LEU:CD2	2:Z:56:MET:SD	3.04	0.46
4:E:90:LEU:O	4:E:91:ARG:C	2.57	0.46
4:G:94:THR:OG1	4:G:95:TYR:N	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:85:ASP:O	4:K:88:HIS:HB2	2.15	0.46
4:K:92:PHE:O	4:K:93:ILE:C	2.58	0.46
5:M:116:ASN:O	5:M:117:THR:C	2.58	0.46
4:N:85:ASP:O	4:N:88:HIS:HB2	2.15	0.46
6:O:202:CYC:O2A	6:O:202:CYC:C1A	2.63	0.46
4:P:52:VAL:O	4:P:53:LYS:C	2.58	0.46
4:R:91:ARG:O	4:R:94:THR:OG1	2.22	0.46
4:R:145:GLN:O	4:R:146:PRO:C	2.59	0.46
3:Y:132:GLN:O	3:Y:133:LEU:C	2.57	0.46
6:a:201:CYC:NC	6:a:201:CYC:CMD	2.78	0.46
3:B:153:CYS:O	3:B:154:SER:C	2.59	0.46
4:C:92:PHE:O	4:C:93:ILE:C	2.58	0.46
3:D:85:ASP:O	3:D:86:MET:C	2.59	0.46
4:K:94:THR:O	4:K:95:TYR:C	2.58	0.46
3:L:117:TYR:CB	3:L:122:THR:CG2	2.93	0.46
4:R:92:PHE:O	4:R:93:ILE:C	2.58	0.46
3:S:164:PHE:O	3:S:167:ALA:HB3	2.16	0.46
4:T:114:ARG:H	4:T:114:ARG:HD2	1.80	0.46
4:V:94:THR:O	4:V:95:TYR:C	2.58	0.46
3:W:164:PHE:O	3:W:167:ALA:HB3	2.16	0.46
4:a:145:GLN:O	4:a:146:PRO:C	2.59	0.46
4:C:116:VAL:HG13	6:C:201:CYC:HMA2	1.98	0.46
6:C:201:CYC:HMA1	6:C:201:CYC:C1B	2.46	0.46
3:D:119:ALA:HB2	5:M:263:PRO:HB2	1.93	0.46
4:K:20:ASN:OD1	4:K:22:THR:N	2.49	0.46
4:K:145:GLN:O	4:K:146:PRO:C	2.59	0.46
4:K:157:CYS:O	4:K:158:ILE:C	2.59	0.46
3:O:153:CYS:O	3:O:154:SER:C	2.59	0.46
6:Q:201:CYC:NB	6:Q:201:CYC:CMA	2.79	0.46
4:R:94:THR:OG1	4:R:95:TYR:N	2.49	0.46
3:U:153:CYS:O	3:U:154:SER:C	2.59	0.46
1:A:265:ARG:NH2	3:Y:77:ARG:NH2	2.63	0.45
6:H:202:CYC:CMA	6:H:202:CYC:NB	2.79	0.45
3:Q:164:PHE:O	3:Q:167:ALA:HB3	2.16	0.45
4:T:157:CYS:O	4:T:158:ILE:C	2.59	0.45
3:U:164:PHE:O	3:U:167:ALA:HB3	2.16	0.45
4:X:94:THR:OG1	4:X:95:TYR:N	2.49	0.45
1:A:126:LEU:HD21	1:A:159:LEU:HD12	1.99	0.45
2:Z:16:LYS:N	2:Z:70:THR:O	2.49	0.45
3:F:153:CYS:O	3:F:154:SER:C	2.59	0.45
4:G:127:TYR:O	4:G:130:ALA:HB3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:145:GLN:O	4:G:146:PRO:C	2.59	0.45
3:J:153:CYS:O	3:J:154:SER:C	2.59	0.45
3:L:164:PHE:O	3:L:167:ALA:HB3	2.16	0.45
3:U:132:GLN:O	3:U:133:LEU:C	2.58	0.45
4:V:94:THR:OG1	4:V:95:TYR:N	2.49	0.45
3:F:141:TYR:O	3:F:142:VAL:C	2.60	0.45
3:J:64:THR:O	3:J:67:ILE:HG12	2.15	0.45
5:M:75:GLU:O	5:M:76:ALA:C	2.58	0.45
4:P:92:PHE:O	4:P:93:ILE:C	2.58	0.45
6:P:201:CYC:CMA	6:P:201:CYC:NB	2.79	0.45
4:a:52:VAL:O	4:a:53:LYS:C	2.58	0.45
1:A:82:GLN:HB3	1:A:84:THR:HG23	1.99	0.45
3:F:64:THR:O	3:F:67:ILE:HG12	2.17	0.45
4:I:92:PHE:O	4:I:93:ILE:C	2.58	0.45
3:L:88:ILE:O	3:L:89:ILE:C	2.59	0.45
5:M:140:ARG:HH11	5:M:204:ILE:CG2	2.29	0.45
5:M:262:ASP:OD1	5:M:263:PRO:HD3	2.12	0.45
3:U:141:TYR:O	3:U:142:VAL:C	2.59	0.45
4:V:20:ASN:OD1	4:V:22:THR:N	2.49	0.45
4:V:145:GLN:O	4:V:146:PRO:C	2.59	0.45
6:V:201:CYC:NB	6:V:201:CYC:HMA1	2.32	0.45
3:W:153:CYS:O	3:W:154:SER:C	2.59	0.45
1:A:99:ALA:HB2	1:A:237:PHE:HB3	1.98	0.45
2:Z:4:THR:HA	3:H:116:THR:OG1	2.16	0.45
6:B:201:CYC:OB	4:a:28:ASN:CG	2.59	0.45
4:E:94:THR:OG1	4:E:95:TYR:N	2.49	0.45
4:I:157:CYS:O	4:I:158:ILE:C	2.59	0.45
4:V:83:ALA:O	4:V:84:ARG:C	2.60	0.45
1:A:278:LEU:HD11	1:A:282:ALA:HB3	1.99	0.45
3:D:141:TYR:O	3:D:142:VAL:C	2.59	0.45
3:D:153:CYS:O	3:D:154:SER:C	2.59	0.45
4:E:83:ALA:O	4:E:84:ARG:C	2.59	0.45
3:F:14:LEU:CB	3:O:125:ARG:NH2	2.80	0.45
3:J:86:MET:HG3	6:J:201:CYC:HBC1	1.97	0.45
4:K:131:LEU:O	4:K:134:ILE:HB	2.15	0.45
5:M:87:ILE:HD12	5:M:87:ILE:O	2.16	0.45
6:Y:201:CYC:CHA	6:Y:201:CYC:CGA	2.95	0.45
4:a:157:CYS:O	4:a:158:ILE:C	2.59	0.45
1:A:138:VAL:HG23	1:A:141:ALA:HB3	1.99	0.45
1:A:153:ARG:HH12	1:A:223:ARG:NH1	2.15	0.45
3:F:85:ASP:O	3:F:86:MET:C	2.59	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:141:TYR:O	3:J:142:VAL:C	2.60	0.45
6:J:201:CYC:NA	6:J:201:CYC:ND	2.63	0.45
5:M:255:GLN:HB2	5:M:258:LYS:HE3	1.99	0.45
3:Q:141:TYR:O	3:Q:142:VAL:C	2.59	0.45
4:V:91:ARG:O	4:V:94:THR:OG1	2.22	0.45
1:A:195:GLY:O	1:A:198:ALA:HB3	2.16	0.45
4:E:20:ASN:OD1	4:E:22:THR:N	2.48	0.45
6:F:202:CYC:HB	6:F:202:CYC:HMA1	1.81	0.45
4:G:20:ASN:OD1	4:G:22:THR:N	2.49	0.45
3:L:72:ASN:ND2	3:L:122:THR:OG1	2.50	0.45
4:N:157:CYS:O	4:N:158:ILE:C	2.59	0.45
4:T:92:PHE:O	4:T:93:ILE:C	2.58	0.45
4:V:157:CYS:O	4:V:158:ILE:C	2.59	0.45
3:Y:85:ASP:O	3:Y:86:MET:C	2.59	0.45
1:A:147:ASN:HD21	6:O:202:CYC:HAA1	1.82	0.45
3:B:85:ASP:O	3:B:86:MET:C	2.58	0.45
6:B:202:CYC:NC	6:B:202:CYC:HMD1	2.31	0.45
4:C:94:THR:OG1	4:C:95:TYR:N	2.49	0.45
3:F:84:ARG:HD2	3:F:84:ARG:HA	1.65	0.45
4:G:157:CYS:O	4:G:158:ILE:C	2.59	0.45
4:I:145:GLN:O	4:I:146:PRO:C	2.59	0.45
3:O:132:GLN:O	3:O:133:LEU:C	2.58	0.45
6:O:201:CYC:O2A	6:O:201:CYC:C1A	2.65	0.45
3:Q:132:GLN:O	3:Q:133:LEU:C	2.58	0.45
3:S:141:TYR:O	3:S:142:VAL:C	2.60	0.45
4:V:90:LEU:HD12	4:V:90:LEU:HA	1.84	0.45
4:X:38:MET:HE2	3:Y:28:THR:OG1	2.17	0.45
3:Y:120:LEU:HD21	6:Y:202:CYC:HAA2	1.99	0.45
1:A:223:ARG:O	1:A:227:GLY:HA3	2.16	0.45
1:A:244:SER:O	3:Q:107:ASP:O	2.35	0.45
1:A:263:THR:HA	6:Y:202:CYC:O1A	2.16	0.45
3:D:119:ALA:O	5:M:267:LEU:HD11	2.17	0.45
3:F:87:GLU:O	3:F:88:ILE:C	2.60	0.45
3:H:88:ILE:O	3:H:89:ILE:C	2.59	0.45
4:I:127:TYR:O	4:I:130:ALA:HB3	2.17	0.45
4:N:108:TYR:O	3:U:76:ASN:HB2	2.16	0.45
4:P:115:GLU:OE1	4:P:115:GLU:N	2.38	0.45
3:Q:58:LYS:HE3	3:Q:133:LEU:HD22	1.99	0.45
3:U:88:ILE:O	3:U:89:ILE:C	2.59	0.45
3:W:88:ILE:O	3:W:89:ILE:C	2.59	0.45
4:X:127:TYR:O	4:X:130:ALA:HB3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:88:ILE:O	3:Y:89:ILE:C	2.59	0.45
3:Y:117:TYR:CB	3:Y:122:THR:CG2	2.94	0.45
1:A:188:GLY:HA2	1:A:234:PHE:HA	1.99	0.44
1:A:190:ALA:HB1	1:A:191:PRO:HD2	1.97	0.44
3:B:1:MET:HE2	3:B:2:GLN:H	1.80	0.44
3:B:164:PHE:O	3:B:167:ALA:HB3	2.16	0.44
4:C:145:GLN:O	4:C:146:PRO:C	2.59	0.44
3:H:122:THR:HG23	6:H:201:CYC:NC	2.32	0.44
3:J:85:ASP:O	3:J:86:MET:C	2.59	0.44
4:K:19:LEU:O	3:L:45:THR:HG21	2.17	0.44
3:O:85:ASP:O	3:O:86:MET:C	2.58	0.44
4:P:83:ALA:O	4:P:84:ARG:C	2.60	0.44
4:P:157:CYS:O	4:P:158:ILE:C	2.59	0.44
4:R:83:ALA:O	4:R:84:ARG:C	2.60	0.44
4:V:127:TYR:O	4:V:130:ALA:HB3	2.17	0.44
3:Y:64:THR:O	3:Y:67:ILE:HG12	2.17	0.44
4:a:83:ALA:O	4:a:84:ARG:C	2.60	0.44
1:A:254:LEU:HD23	1:A:273:GLU:HB2	1.98	0.44
4:C:91:ARG:O	4:C:94:THR:OG1	2.22	0.44
4:C:157:CYS:O	4:C:158:ILE:C	2.59	0.44
3:F:164:PHE:O	3:F:167:ALA:HB3	2.17	0.44
3:H:120:LEU:HD22	6:H:201:CYC:CGD	2.47	0.44
3:H:122:THR:HG23	6:H:201:CYC:HC	1.82	0.44
4:K:127:TYR:O	4:K:130:ALA:HB3	2.17	0.44
3:O:141:TYR:O	3:O:142:VAL:C	2.60	0.44
3:Q:153:CYS:O	3:Q:154:SER:C	2.59	0.44
3:S:88:ILE:O	3:S:89:ILE:C	2.59	0.44
3:S:90:LEU:HB2	3:S:134:MET:HE1	1.98	0.44
4:T:127:TYR:O	4:T:130:ALA:HB3	2.18	0.44
6:T:201:CYC:O1A	6:T:201:CYC:C1A	2.66	0.44
3:Y:72:ASN:ND2	3:Y:122:THR:OG1	2.51	0.44
3:Y:141:TYR:O	3:Y:142:VAL:C	2.60	0.44
1:A:263:THR:HB	6:Y:202:CYC:O1A	2.17	0.44
3:B:85:ASP:OD2	6:B:202:CYC:ND	2.48	0.44
3:D:72:ASN:OD1	3:D:122:THR:HG22	2.17	0.44
3:H:87:GLU:O	3:H:88:ILE:C	2.61	0.44
3:J:87:GLU:O	3:J:88:ILE:C	2.60	0.44
5:M:56:MET:HE3	6:U:201:CYC:OB	2.17	0.44
4:P:2:LYS:HZ1	4:T:15:GLN:HE22	1.62	0.44
4:V:42:ARG:NH1	3:W:21:GLU:OE1	2.50	0.44
4:C:83:ALA:O	4:C:84:ARG:C	2.60	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:131:LEU:O	4:G:134:ILE:HB	2.16	0.44
3:H:153:CYS:O	3:H:154:SER:C	2.59	0.44
5:M:139:VAL:CB	5:M:216:ASN:HA	2.47	0.44
4:N:127:TYR:O	4:N:130:ALA:HB3	2.17	0.44
3:O:87:GLU:O	3:O:88:ILE:C	2.61	0.44
4:R:91:ARG:HA	3:S:18:PHE:CE2	2.53	0.44
1:A:196:GLU:HA	1:A:199:GLU:CD	2.43	0.44
3:B:141:TYR:O	3:B:142:VAL:C	2.60	0.44
4:C:90:LEU:HD12	4:C:90:LEU:HA	1.84	0.44
4:G:83:ALA:O	4:G:84:ARG:C	2.60	0.44
4:T:88:HIS:CD2	4:T:91:ARG:HH21	2.36	0.44
3:U:90:LEU:O	3:U:91:ARG:C	2.61	0.44
6:U:202:CYC:CMA	6:U:202:CYC:NB	2.80	0.44
4:a:47:ASN:O	4:a:48:ALA:C	2.61	0.44
6:B:202:CYC:O2A	6:B:202:CYC:C2A	2.65	0.44
6:B:202:CYC:ND	6:B:202:CYC:NA	2.66	0.44
3:D:87:GLU:O	3:D:88:ILE:C	2.61	0.44
4:E:47:ASN:O	4:E:48:ALA:C	2.61	0.44
3:F:102:ALA:O	3:F:105:LEU:HB3	2.18	0.44
3:H:82:CYS:HA	6:H:201:CYC:HHD	1.99	0.44
4:I:47:ASN:O	4:I:48:ALA:C	2.61	0.44
3:J:90:LEU:O	3:J:91:ARG:C	2.61	0.44
5:M:51:ARG:O	5:M:52:LEU:C	2.59	0.44
5:M:140:ARG:HH11	5:M:204:ILE:HG22	1.83	0.44
5:M:212:ALA:O	5:M:213:PHE:CG	2.70	0.44
4:P:127:TYR:O	4:P:130:ALA:HB3	2.18	0.44
6:P:201:CYC:NB	6:P:201:CYC:HMA1	2.32	0.44
4:R:127:TYR:O	4:R:130:ALA:HB3	2.17	0.44
4:X:92:PHE:O	4:X:93:ILE:C	2.58	0.44
1:A:144:LEU:HB3	1:A:150:ILE:HD11	1.85	0.44
3:O:164:PHE:O	3:O:167:ALA:HB3	2.17	0.44
4:P:20:ASN:OD1	4:P:22:THR:N	2.49	0.44
4:P:90:LEU:HD12	4:P:90:LEU:HA	1.84	0.44
4:R:157:CYS:O	4:R:158:ILE:C	2.59	0.44
3:S:87:GLU:O	3:S:88:ILE:C	2.60	0.44
4:T:83:ALA:O	4:T:84:ARG:C	2.60	0.44
3:U:87:GLU:OE1	3:U:88:ILE:N	2.51	0.44
3:Y:88:ILE:HD13	6:Y:202:CYC:CAB	2.48	0.44
1:A:169:PHE:O	1:A:169:PHE:CG	2.71	0.44
4:K:83:ALA:O	4:K:84:ARG:C	2.60	0.44
6:L:202:CYC:CMA	6:L:202:CYC:NB	2.80	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:115:GLY:C	5:M:117:THR:N	2.76	0.44
4:P:73:GLY:HA2	6:P:201:CYC:OC	2.18	0.44
4:P:91:ARG:O	4:P:94:THR:OG1	2.22	0.44
3:W:90:LEU:O	3:W:91:ARG:C	2.61	0.44
4:X:93:ILE:O	4:X:94:THR:C	2.61	0.44
3:Y:38:LEU:HD13	6:Y:201:CYC:C4B	2.48	0.44
3:Y:145:PRO:HD2	6:Y:201:CYC:HMC3	1.99	0.44
3:B:88:ILE:O	3:B:89:ILE:C	2.59	0.44
3:B:102:ALA:O	3:B:105:LEU:HB3	2.18	0.44
4:G:88:HIS:CD2	4:G:91:ARG:HH21	2.36	0.44
4:I:147:LEU:O	4:I:148:THR:C	2.61	0.44
3:J:87:GLU:OE1	3:J:88:ILE:N	2.51	0.44
3:L:117:TYR:CG	3:L:122:THR:CG2	3.01	0.44
3:L:141:TYR:O	3:L:142:VAL:C	2.60	0.44
4:N:94:THR:OG1	4:N:95:TYR:N	2.49	0.44
4:N:147:LEU:O	4:N:148:THR:C	2.61	0.44
3:O:1:MET:HE2	3:O:2:GLN:O	2.18	0.44
3:O:90:LEU:O	3:O:91:ARG:C	2.61	0.44
4:P:147:LEU:O	4:P:148:THR:C	2.61	0.44
3:Q:78:ARG:HD2	6:Q:202:CYC:HBD2	2.00	0.44
3:Q:87:GLU:O	3:Q:88:ILE:C	2.61	0.44
4:T:93:ILE:O	4:T:94:THR:C	2.61	0.44
3:U:85:ASP:O	3:U:86:MET:C	2.59	0.44
1:A:120:ARG:HG2	1:A:124:LYS:CE	2.47	0.43
1:A:266:ASN:HD21	3:Y:119:ALA:CB	2.30	0.43
4:C:127:TYR:O	4:C:130:ALA:HB3	2.18	0.43
3:D:58:LYS:HE3	3:D:133:LEU:HD22	1.99	0.43
3:H:39:ASP:OD1	6:H:202:CYC:CHB	2.53	0.43
3:L:14:LEU:HB3	3:W:125:ARG:HH22	1.83	0.43
3:L:117:TYR:CG	3:L:122:THR:HG21	2.49	0.43
4:N:83:ALA:O	4:N:84:ARG:C	2.60	0.43
4:X:20:ASN:OD1	4:X:22:THR:N	2.49	0.43
1:A:223:ARG:HA	1:A:227:GLY:HA2	2.00	0.43
3:D:145:PRO:HD2	6:D:201:CYC:CMC	2.47	0.43
4:E:127:TYR:O	4:E:130:ALA:HB3	2.18	0.43
4:E:147:LEU:O	4:E:148:THR:C	2.61	0.43
4:G:47:ASN:O	4:G:48:ALA:C	2.61	0.43
4:I:83:ALA:O	4:I:84:ARG:C	2.60	0.43
3:J:102:ALA:O	3:J:105:LEU:HB3	2.19	0.43
5:M:171:LYS:O	5:M:174:LEU:O	2.35	0.43
4:R:93:ILE:O	4:R:94:THR:C	2.62	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:83:ALA:O	4:X:84:ARG:C	2.60	0.43
4:a:127:TYR:O	4:a:130:ALA:HB3	2.17	0.43
1:A:157:ARG:HD3	1:A:214:ASP:OD1	2.18	0.43
4:C:147:LEU:O	4:C:148:THR:C	2.61	0.43
6:F:202:CYC:C4B	5:M:118:TYR:OH	2.65	0.43
3:H:87:GLU:OE1	3:H:88:ILE:N	2.51	0.43
5:M:250:THR:HG22	5:M:253:ASN:H	1.83	0.43
4:N:57:GLN:O	4:N:58:GLU:C	2.62	0.43
3:Q:56:ALA:O	3:Q:57:HIS:C	2.61	0.43
4:T:47:ASN:O	4:T:48:ALA:C	2.61	0.43
4:X:157:CYS:O	4:X:158:ILE:C	2.59	0.43
6:C:201:CYC:NB	6:C:201:CYC:CMA	2.81	0.43
3:D:56:ALA:O	3:D:57:HIS:C	2.61	0.43
3:D:108:ARG:HH22	5:M:162:ASN:HB2	1.83	0.43
4:E:57:GLN:O	4:E:58:GLU:C	2.62	0.43
4:E:103:GLY:O	4:E:104:PRO:C	2.61	0.43
4:E:157:CYS:O	4:E:158:ILE:C	2.59	0.43
3:L:104:VAL:HG13	3:L:105:LEU:N	2.34	0.43
5:M:174:LEU:CB	5:M:176:ARG:HG2	2.48	0.43
3:S:64:THR:O	3:S:67:ILE:HG12	2.19	0.43
4:T:5:ILE:HD11	4:T:30:ARG:HH11	1.83	0.43
4:T:145:GLN:O	4:T:146:PRO:C	2.59	0.43
6:T:201:CYC:NC	6:T:201:CYC:CMD	2.80	0.43
3:U:56:ALA:O	3:U:57:HIS:C	2.61	0.43
4:V:47:ASN:O	4:V:48:ALA:C	2.61	0.43
1:A:73:TYR:CZ	4:X:79:GLN:HB3	2.53	0.43
4:C:93:ILE:O	4:C:94:THR:C	2.62	0.43
3:D:90:LEU:O	3:D:91:ARG:C	2.61	0.43
3:F:90:LEU:O	3:F:91:ARG:C	2.61	0.43
4:I:103:GLY:O	4:I:104:PRO:C	2.62	0.43
5:M:196:TYR:CE1	5:M:200:ILE:HD11	2.54	0.43
3:O:111:ASN:HD22	3:O:111:ASN:HA	1.56	0.43
4:P:103:GLY:O	4:P:104:PRO:C	2.62	0.43
6:R:201:CYC:CMA	6:R:201:CYC:C1B	2.97	0.43
3:S:86:MET:HG3	6:S:202:CYC:HBC1	2.00	0.43
4:T:103:GLY:O	4:T:104:PRO:C	2.62	0.43
3:U:102:ALA:O	3:U:105:LEU:HB3	2.19	0.43
3:W:141:TYR:O	3:W:142:VAL:C	2.60	0.43
4:X:103:GLY:O	4:X:104:PRO:C	2.61	0.43
3:Y:56:ALA:O	3:Y:57:HIS:C	2.61	0.43
1:A:108:PRO:HD3	5:M:37:GLU:OE1	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:125:ARG:NH2	3:U:14:LEU:HD13	2.33	0.43
3:F:56:ALA:O	3:F:57:HIS:C	2.61	0.43
4:G:147:LEU:O	4:G:148:THR:C	2.61	0.43
3:H:102:ALA:O	3:H:105:LEU:HB3	2.18	0.43
4:K:57:GLN:O	4:K:58:GLU:C	2.62	0.43
3:L:87:GLU:O	3:L:88:ILE:C	2.61	0.43
4:N:103:GLY:O	4:N:104:PRO:C	2.62	0.43
6:Q:201:CYC:C1A	6:Q:201:CYC:CGA	2.95	0.43
3:S:90:LEU:O	3:S:91:ARG:C	2.61	0.43
3:U:87:GLU:O	3:U:88:ILE:C	2.60	0.43
4:V:93:ILE:O	4:V:94:THR:C	2.62	0.43
4:X:57:GLN:O	4:X:58:GLU:C	2.62	0.43
3:Y:93:VAL:O	3:Y:94:SER:C	2.62	0.43
3:Y:105:LEU:O	3:Y:109:CYS:HB3	2.19	0.43
3:B:56:ALA:O	3:B:57:HIS:C	2.62	0.43
4:G:93:ILE:O	4:G:94:THR:C	2.62	0.43
3:J:122:THR:HG23	6:J:201:CYC:HC	1.83	0.43
3:L:145:PRO:HD2	6:L:202:CYC:HMC3	2.01	0.43
5:M:150:GLU:O	5:M:151:LEU:C	2.61	0.43
3:O:88:ILE:O	3:O:89:ILE:C	2.59	0.43
4:P:57:GLN:O	4:P:58:GLU:C	2.62	0.43
4:R:57:GLN:O	4:R:58:GLU:C	2.62	0.43
4:T:57:GLN:O	4:T:58:GLU:C	2.61	0.43
4:T:90:LEU:HD12	4:T:90:LEU:HA	1.85	0.43
3:U:20:SER:OG	3:U:23:GLU:HB2	2.19	0.43
3:W:56:ALA:O	3:W:57:HIS:C	2.62	0.43
6:W:202:CYC:CMA	6:W:202:CYC:NB	2.82	0.43
4:X:155:ASP:O	4:X:157:CYS:N	2.52	0.43
4:a:91:ARG:O	4:a:94:THR:OG1	2.22	0.43
1:A:175:ASN:HB2	6:S:202:CYC:CBB	2.48	0.43
3:B:87:GLU:O	3:B:88:ILE:C	2.61	0.43
3:D:95:TYR:O	3:D:96:ALA:C	2.62	0.43
3:D:102:ALA:O	3:D:105:LEU:HB3	2.19	0.43
4:E:92:PHE:O	4:E:93:ILE:C	2.58	0.43
3:H:105:LEU:O	3:H:109:CYS:HB3	2.19	0.43
3:H:141:TYR:O	3:H:142:VAL:C	2.60	0.43
4:K:147:LEU:O	4:K:148:THR:C	2.61	0.43
5:M:255:GLN:HB2	5:M:258:LYS:CE	2.49	0.43
4:N:108:TYR:CD1	3:U:75:PRO:HG3	2.53	0.43
3:O:145:PRO:HD2	6:O:201:CYC:CMC	2.44	0.43
3:Q:95:TYR:O	3:Q:96:ALA:C	2.62	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:93:VAL:O	3:U:94:SER:C	2.62	0.43
4:X:47:ASN:O	4:X:48:ALA:C	2.61	0.43
1:A:147:ASN:HD21	6:O:202:CYC:CMA	2.32	0.43
6:C:201:CYC:NC	6:C:201:CYC:CMD	2.82	0.43
4:G:120:PHE:CE1	6:G:201:CYC:HBA1	2.42	0.43
4:I:155:ASP:O	4:I:157:CYS:N	2.52	0.43
4:K:47:ASN:O	4:K:48:ALA:C	2.61	0.43
3:L:56:ALA:O	3:L:57:HIS:C	2.62	0.43
5:M:22:SER:OG	5:M:23:PRO:HD2	2.19	0.43
4:N:93:ILE:O	4:N:94:THR:C	2.62	0.43
3:O:56:ALA:O	3:O:57:HIS:C	2.61	0.43
4:P:1:MET:SD	3:Q:6:THR:HG23	2.59	0.43
4:P:47:ASN:O	4:P:48:ALA:C	2.61	0.43
3:S:39:ASP:OD1	6:S:201:CYC:CHB	2.65	0.43
3:S:95:TYR:O	3:S:96:ALA:C	2.62	0.43
4:T:147:LEU:O	4:T:148:THR:C	2.61	0.43
3:W:93:VAL:O	3:W:94:SER:C	2.62	0.43
3:Y:90:LEU:O	3:Y:91:ARG:C	2.61	0.43
4:a:93:ILE:O	4:a:94:THR:C	2.62	0.43
1:A:160:ALA:HA	1:A:165:TYR:CG	2.54	0.43
4:C:103:GLY:O	4:C:104:PRO:C	2.62	0.43
4:G:1:MET:SD	3:H:6:THR:HG23	2.59	0.43
5:M:3:VAL:HG22	5:M:76:ALA:HB2	2.00	0.43
5:M:45:VAL:HG13	5:M:47:VAL:HG13	2.00	0.43
5:M:117:THR:HG21	5:M:155:ARG:HD3	2.01	0.43
4:R:147:LEU:O	4:R:148:THR:C	2.61	0.43
3:S:56:ALA:O	3:S:57:HIS:C	2.62	0.43
3:U:95:TYR:O	3:U:96:ALA:C	2.62	0.43
4:V:147:LEU:O	4:V:148:THR:C	2.61	0.43
3:W:102:ALA:O	3:W:105:LEU:HB3	2.19	0.43
6:X:201:CYC:NC	6:X:201:CYC:CMD	2.81	0.43
4:G:57:GLN:O	4:G:58:GLU:C	2.62	0.42
3:H:93:VAL:O	3:H:94:SER:C	2.62	0.42
3:L:93:VAL:O	3:L:94:SER:C	2.62	0.42
4:N:155:ASP:O	4:N:157:CYS:N	2.52	0.42
3:Q:90:LEU:O	3:Q:91:ARG:C	2.61	0.42
6:T:201:CYC:NB	6:T:201:CYC:HMA2	2.33	0.42
3:W:87:GLU:OE1	3:W:88:ILE:N	2.52	0.42
4:X:2:LYS:HG3	4:X:7:GLU:OE2	2.19	0.42
3:Y:95:TYR:O	3:Y:96:ALA:C	2.62	0.42
4:a:103:GLY:O	4:a:104:PRO:C	2.61	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:THR:CB	6:Y:202:CYC:O1A	2.67	0.42
2:Z:58:ARG:HH11	5:M:210:ILE:CD1	2.32	0.42
3:B:95:TYR:O	3:B:96:ALA:C	2.62	0.42
6:B:202:CYC:HMD1	6:B:202:CYC:C1C	2.49	0.42
3:F:78:ARG:HD3	6:F:202:CYC:CGD	2.49	0.42
4:G:155:ASP:O	4:G:157:CYS:N	2.53	0.42
3:H:56:ALA:O	3:H:57:HIS:C	2.61	0.42
4:I:30:ARG:NH2	4:I:98:VAL:O	2.52	0.42
4:I:153:TYR:O	4:I:154:ILE:C	2.63	0.42
3:L:102:ALA:O	3:L:105:LEU:HB3	2.19	0.42
4:N:47:ASN:O	4:N:48:ALA:C	2.61	0.42
4:R:48:ALA:O	4:R:49:ASP:C	2.62	0.42
4:R:155:ASP:O	4:R:157:CYS:N	2.52	0.42
3:U:105:LEU:O	3:U:109:CYS:HB3	2.19	0.42
3:Y:87:GLU:O	3:Y:88:ILE:C	2.61	0.42
3:Y:117:TYR:HB3	3:Y:122:THR:CG2	2.49	0.42
1:A:126:LEU:C	1:A:126:LEU:CD1	2.92	0.42
2:Z:14:LEU:HD12	2:Z:72:GLY:CA	2.42	0.42
4:C:47:ASN:O	4:C:48:ALA:C	2.61	0.42
3:D:76:ASN:HB2	4:K:108:TYR:O	2.19	0.42
3:F:93:VAL:O	3:F:94:SER:C	2.62	0.42
4:I:48:ALA:O	4:I:49:ASP:C	2.63	0.42
3:J:95:TYR:O	3:J:96:ALA:C	2.62	0.42
5:M:56:MET:CE	6:U:201:CYC:OB	2.67	0.42
5:M:146:LEU:HD23	5:M:146:LEU:HA	1.91	0.42
5:M:255:GLN:O	5:M:255:GLN:HG2	2.19	0.42
3:Q:102:ALA:O	3:Q:105:LEU:HB3	2.19	0.42
4:R:47:ASN:O	4:R:48:ALA:C	2.61	0.42
4:T:155:ASP:O	4:T:157:CYS:N	2.52	0.42
3:U:104:VAL:HG13	3:U:105:LEU:N	2.35	0.42
4:V:24:LEU:O	4:V:25:GLN:C	2.63	0.42
4:V:57:GLN:O	4:V:58:GLU:C	2.62	0.42
4:a:48:ALA:O	4:a:49:ASP:C	2.62	0.42
6:a:201:CYC:NB	6:a:201:CYC:HMA3	2.34	0.42
4:C:57:GLN:O	4:C:58:GLU:C	2.62	0.42
3:D:104:VAL:HG13	3:D:105:LEU:N	2.34	0.42
4:G:120:PHE:CD2	6:G:201:CYC:CAA	3.02	0.42
3:H:104:VAL:HG13	3:H:105:LEU:N	2.35	0.42
6:H:201:CYC:O2A	6:H:201:CYC:C1A	2.67	0.42
4:K:103:GLY:O	4:K:104:PRO:C	2.61	0.42
3:L:90:LEU:O	3:L:91:ARG:C	2.61	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:168:LEU:CD1	5:M:172:HIS:CE1	3.02	0.42
5:M:194:PHE:HB3	5:M:198:ALA:CB	2.49	0.42
3:O:95:TYR:O	3:O:96:ALA:C	2.62	0.42
4:P:155:ASP:O	4:P:157:CYS:N	2.52	0.42
3:W:104:VAL:HG13	3:W:105:LEU:N	2.35	0.42
6:W:201:CYC:HB	6:W:201:CYC:CMA	2.32	0.42
4:X:147:LEU:O	4:X:148:THR:C	2.61	0.42
2:Z:21:LEU:CD1	2:Z:25:LEU:HB3	2.46	0.42
3:D:34:SER:O	3:D:35:ASN:C	2.63	0.42
4:E:95:TYR:CG	3:F:9:ILE:HG23	2.55	0.42
4:E:155:ASP:O	4:E:157:CYS:N	2.53	0.42
3:F:92:TYR:O	3:F:95:TYR:N	2.53	0.42
4:G:114:ARG:H	4:G:114:ARG:HD2	1.84	0.42
4:I:93:ILE:O	4:I:94:THR:C	2.62	0.42
5:M:89:LEU:O	5:M:90:LYS:HB2	2.20	0.42
3:O:34:SER:O	3:O:35:ASN:C	2.62	0.42
3:O:102:ALA:O	3:O:105:LEU:HB3	2.18	0.42
4:P:93:ILE:O	4:P:94:THR:C	2.62	0.42
3:Q:72:ASN:OD1	3:Q:122:THR:HG22	2.20	0.42
3:Q:93:VAL:O	3:Q:94:SER:C	2.62	0.42
4:R:90:LEU:HD12	4:R:90:LEU:HA	1.84	0.42
4:V:153:TYR:O	4:V:154:ILE:C	2.63	0.42
3:Y:92:TYR:O	3:Y:95:TYR:N	2.53	0.42
3:B:104:VAL:HG13	3:B:105:LEU:N	2.35	0.42
4:C:48:ALA:O	4:C:49:ASP:C	2.62	0.42
4:C:155:ASP:O	4:C:157:CYS:N	2.52	0.42
3:D:93:VAL:O	3:D:94:SER:C	2.62	0.42
3:H:20:SER:OG	3:H:23:GLU:HB2	2.19	0.42
4:N:1:MET:HE3	4:N:1:MET:HB2	1.95	0.42
4:N:90:LEU:HD12	4:N:90:LEU:HA	1.84	0.42
3:Q:92:TYR:O	3:Q:95:TYR:N	2.53	0.42
4:R:88:HIS:CD2	4:R:91:ARG:HH21	2.37	0.42
6:W:202:CYC:O1A	6:W:202:CYC:C2A	2.68	0.42
3:B:1:MET:HB2	3:B:2:GLN:H	1.72	0.42
3:B:111:ASN:HD22	3:B:111:ASN:HA	1.58	0.42
3:F:95:TYR:O	3:F:96:ALA:C	2.62	0.42
3:H:92:TYR:O	3:H:95:TYR:N	2.53	0.42
3:H:95:TYR:O	3:H:96:ALA:C	2.62	0.42
4:K:24:LEU:O	4:K:25:GLN:C	2.62	0.42
3:L:117:TYR:HB3	3:L:122:THR:CG2	2.50	0.42
6:L:202:CYC:CGA	6:L:202:CYC:CHA	2.98	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:104:VAL:HG13	3:O:105:LEU:N	2.35	0.42
6:Q:201:CYC:CGA	6:Q:201:CYC:CHA	2.97	0.42
3:S:102:ALA:O	3:S:105:LEU:HB3	2.19	0.42
3:U:101:ASP:OD2	3:U:103:SER:CB	2.68	0.42
3:W:34:SER:O	3:W:35:ASN:C	2.63	0.42
3:W:87:GLU:O	3:W:88:ILE:C	2.60	0.42
3:Y:117:TYR:CG	3:Y:122:THR:CG2	3.02	0.42
4:a:57:GLN:O	4:a:58:GLU:C	2.62	0.42
1:A:138:VAL:O	1:A:138:VAL:CG2	2.67	0.42
1:A:177:ARG:O	1:A:181:LEU:HG	2.20	0.42
1:A:286:ARG:HA	1:A:286:ARG:HD2	1.77	0.42
3:H:90:LEU:O	3:H:91:ARG:C	2.61	0.42
4:K:88:HIS:CD2	4:K:91:ARG:HH21	2.37	0.42
3:L:110:LEU:O	3:L:111:ASN:C	2.58	0.42
5:M:91:VAL:HG11	5:M:105:ALA:HA	2.02	0.42
3:O:93:VAL:O	3:O:94:SER:C	2.62	0.42
4:P:24:LEU:O	4:P:25:GLN:C	2.63	0.42
6:Q:202:CYC:HMA1	6:Q:202:CYC:NB	2.34	0.42
4:R:153:TYR:O	4:R:154:ILE:C	2.62	0.42
3:U:92:TYR:O	3:U:95:TYR:N	2.53	0.42
4:a:147:LEU:O	4:a:148:THR:C	2.61	0.42
4:C:38:MET:HE3	4:C:38:MET:HB3	1.96	0.42
4:C:125:SER:O	4:C:126:TRP:C	2.63	0.42
3:D:101:ASP:OD1	3:D:102:ALA:N	2.53	0.42
6:D:201:CYC:CGA	6:D:201:CYC:CHA	2.98	0.42
4:E:24:LEU:O	4:E:25:GLN:C	2.62	0.42
4:E:48:ALA:O	4:E:49:ASP:C	2.62	0.42
4:G:19:LEU:O	3:H:45:THR:HG21	2.20	0.42
3:H:101:ASP:OD2	3:H:103:SER:CB	2.68	0.42
4:K:48:ALA:O	4:K:49:ASP:C	2.63	0.42
4:K:155:ASP:O	4:K:157:CYS:N	2.53	0.42
4:N:48:ALA:O	4:N:49:ASP:C	2.62	0.42
4:R:24:LEU:O	4:R:25:GLN:C	2.62	0.42
3:S:93:VAL:O	3:S:94:SER:C	2.62	0.42
4:T:48:ALA:O	4:T:49:ASP:C	2.63	0.42
4:V:48:ALA:O	4:V:49:ASP:C	2.62	0.42
4:V:77:THR:CG2	4:V:78:ASN:N	2.83	0.42
4:X:88:HIS:CD2	4:X:91:ARG:HH21	2.37	0.42
3:Y:102:ALA:O	3:Y:105:LEU:HB3	2.19	0.42
4:a:155:ASP:O	4:a:157:CYS:N	2.52	0.42
1:A:140:GLN:O	1:A:143:SER:O	2.38	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1:MET:HE2	3:B:2:GLN:O	2.20	0.42
3:B:92:TYR:O	3:B:95:TYR:N	2.53	0.42
3:B:93:VAL:O	3:B:94:SER:C	2.62	0.42
4:C:21:ASN:O	4:C:22:THR:C	2.63	0.42
4:C:24:LEU:O	4:C:25:GLN:C	2.62	0.42
4:C:153:TYR:O	4:C:154:ILE:C	2.63	0.42
4:G:153:TYR:O	4:G:154:ILE:C	2.63	0.42
3:J:34:SER:O	3:J:35:ASN:C	2.63	0.42
3:J:78:ARG:HD3	6:J:201:CYC:CGD	2.49	0.42
3:J:92:TYR:O	3:J:95:TYR:N	2.53	0.42
4:K:153:TYR:O	4:K:154:ILE:C	2.63	0.42
3:S:34:SER:O	3:S:35:ASN:C	2.63	0.42
3:S:87:GLU:O	3:S:90:LEU:HB3	2.19	0.42
3:S:104:VAL:HG13	3:S:105:LEU:N	2.35	0.42
4:T:125:SER:O	4:T:126:TRP:C	2.63	0.42
3:U:101:ASP:OD2	3:U:103:SER:HB3	2.20	0.42
4:V:155:ASP:O	4:V:157:CYS:N	2.52	0.42
3:W:105:LEU:O	3:W:109:CYS:HB3	2.20	0.42
3:Y:1:MET:SD	3:Y:104:VAL:HG23	2.60	0.42
4:a:77:THR:CG2	4:a:78:ASN:N	2.83	0.42
4:E:82:CYS:HB2	6:E:201:CYC:NC	2.35	0.41
3:F:1:MET:O	3:F:2:GLN:OE1	2.38	0.41
6:F:201:CYC:NB	6:F:201:CYC:CMA	2.83	0.41
4:K:2:LYS:HG3	4:K:7:GLU:OE2	2.20	0.41
3:L:95:TYR:O	3:L:96:ALA:C	2.62	0.41
3:L:101:ASP:OD1	3:L:102:ALA:N	2.53	0.41
3:L:117:TYR:HA	3:L:122:THR:HG22	2.01	0.41
5:M:178:PRO:HD2	5:M:241:LEU:HD11	2.02	0.41
5:M:233:GLU:OE1	5:M:233:GLU:N	2.51	0.41
4:N:153:TYR:O	4:N:154:ILE:C	2.62	0.41
3:U:34:SER:O	3:U:35:ASN:C	2.63	0.41
6:U:201:CYC:ND	6:U:201:CYC:NA	2.68	0.41
4:X:24:LEU:O	4:X:25:GLN:C	2.62	0.41
1:A:130:THR:OG1	1:A:262:ASP:O	2.38	0.41
1:A:161:LYS:HD2	1:A:210:ASP:OD1	2.19	0.41
3:B:87:GLU:O	3:B:90:LEU:HB3	2.20	0.41
4:E:88:HIS:CD2	4:E:91:ARG:HH21	2.37	0.41
4:E:93:ILE:O	4:E:94:THR:C	2.62	0.41
4:G:24:LEU:O	4:G:25:GLN:C	2.63	0.41
4:G:48:ALA:O	4:G:49:ASP:C	2.63	0.41
6:I:201:CYC:HMA1	6:I:201:CYC:C1B	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:104:VAL:HG13	3:J:105:LEU:N	2.35	0.41
5:M:164:ARG:HD3	5:M:258:LYS:O	2.19	0.41
5:M:196:TYR:CZ	5:M:200:ILE:HD11	2.55	0.41
3:Q:112:GLY:HA2	3:Q:115:GLU:OE1	2.20	0.41
3:S:159:GLU:O	3:S:162:THR:OG1	2.34	0.41
3:U:84:ARG:NH2	6:U:201:CYC:O2A	2.34	0.41
4:a:153:TYR:O	4:a:154:ILE:C	2.62	0.41
1:A:114:ASP:O	1:A:118:VAL:HG23	2.20	0.41
6:D:201:CYC:CMD	6:D:201:CYC:NC	2.84	0.41
4:E:125:SER:O	4:E:126:TRP:C	2.63	0.41
3:F:104:VAL:HG13	3:F:105:LEU:N	2.35	0.41
4:G:103:GLY:O	4:G:104:PRO:C	2.62	0.41
3:H:34:SER:O	3:H:35:ASN:C	2.63	0.41
3:J:56:ALA:O	3:J:57:HIS:C	2.62	0.41
4:K:21:ASN:O	4:K:22:THR:C	2.63	0.41
3:L:92:TYR:O	3:L:95:TYR:N	2.53	0.41
4:N:21:ASN:O	4:N:22:THR:C	2.63	0.41
4:P:48:ALA:O	4:P:49:ASP:C	2.62	0.41
6:P:201:CYC:HMA1	6:P:201:CYC:C1B	2.50	0.41
3:Q:104:VAL:HG13	3:Q:105:LEU:N	2.34	0.41
3:S:92:TYR:O	3:S:95:TYR:N	2.53	0.41
3:U:34:SER:OG	3:U:35:ASN:N	2.54	0.41
4:V:21:ASN:O	4:V:22:THR:C	2.63	0.41
3:W:87:GLU:O	3:W:90:LEU:HB3	2.21	0.41
6:W:201:CYC:NB	6:W:201:CYC:CMA	2.83	0.41
4:a:125:SER:O	4:a:126:TRP:C	2.63	0.41
3:B:34:SER:O	3:B:35:ASN:C	2.63	0.41
4:I:21:ASN:O	4:I:22:THR:C	2.63	0.41
3:J:93:VAL:O	3:J:94:SER:C	2.62	0.41
4:K:90:LEU:HD12	4:K:90:LEU:HA	1.84	0.41
4:K:125:SER:O	4:K:126:TRP:C	2.63	0.41
3:L:34:SER:O	3:L:35:ASN:C	2.63	0.41
3:O:92:TYR:O	3:O:95:TYR:N	2.53	0.41
4:P:153:TYR:O	4:P:154:ILE:C	2.63	0.41
3:Y:34:SER:OG	3:Y:35:ASN:N	2.54	0.41
3:Y:104:VAL:HG13	3:Y:105:LEU:N	2.35	0.41
3:Y:120:LEU:HD13	6:Y:202:CYC:CHA	2.50	0.41
3:B:101:ASP:OD1	3:B:102:ALA:N	2.54	0.41
3:D:125:ARG:HH22	3:U:14:LEU:HD13	1.83	0.41
3:L:34:SER:OG	3:L:35:ASN:N	2.54	0.41
3:L:112:GLY:N	5:M:233:GLU:OE2	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:1:MET:HE2	5:M:1:MET:HB2	1.95	0.41
4:P:2:LYS:HZ3	4:T:15:GLN:HE22	1.66	0.41
3:U:87:GLU:O	3:U:90:LEU:HB3	2.21	0.41
3:W:95:TYR:O	3:W:96:ALA:C	2.62	0.41
1:A:150:ILE:HG21	1:A:150:ILE:HD13	1.74	0.41
1:A:278:LEU:CD1	1:A:282:ALA:C	2.79	0.41
1:A:283:GLN:HG2	3:Q:115:GLU:HG2	2.03	0.41
3:B:75:PRO:HG3	4:I:108:TYR:CD1	2.56	0.41
3:D:119:ALA:C	5:M:267:LEU:HD11	2.45	0.41
6:D:202:CYC:C4B	5:M:188:LEU:HD11	2.51	0.41
3:H:101:ASP:OD2	3:H:103:SER:HB3	2.20	0.41
3:H:145:PRO:HD2	6:H:202:CYC:HMC3	2.03	0.41
4:I:57:GLN:O	4:I:58:GLU:C	2.62	0.41
3:L:105:LEU:O	3:L:109:CYS:HB3	2.20	0.41
4:N:82:CYS:HB2	6:N:201:CYC:C1C	2.51	0.41
6:P:201:CYC:NC	6:P:201:CYC:CMD	2.84	0.41
3:Q:34:SER:OG	3:Q:35:ASN:N	2.53	0.41
3:Q:34:SER:O	3:Q:35:ASN:C	2.63	0.41
4:R:125:SER:O	4:R:126:TRP:C	2.63	0.41
4:V:103:GLY:O	4:V:104:PRO:C	2.62	0.41
3:W:101:ASP:OD1	3:W:102:ALA:N	2.53	0.41
6:W:201:CYC:NC	6:W:201:CYC:CMD	2.67	0.41
4:X:48:ALA:O	4:X:49:ASP:C	2.63	0.41
4:a:24:LEU:O	4:a:25:GLN:C	2.63	0.41
2:Z:1:SER:H3	2:Z:44:SER:HB2	1.85	0.41
3:B:34:SER:OG	3:B:35:ASN:N	2.53	0.41
3:B:90:LEU:O	3:B:91:ARG:C	2.61	0.41
4:E:1:MET:HE3	4:E:1:MET:HB2	1.97	0.41
4:G:21:ASN:O	4:G:22:THR:C	2.63	0.41
4:K:93:ILE:O	4:K:94:THR:C	2.61	0.41
6:O:202:CYC:NB	6:O:202:CYC:HMA3	2.33	0.41
4:P:38:MET:HE3	4:P:38:MET:HB3	1.96	0.41
3:Q:101:ASP:OD1	3:Q:102:ALA:N	2.53	0.41
3:S:101:ASP:OD1	3:S:102:ALA:N	2.54	0.41
3:W:92:TYR:O	3:W:95:TYR:N	2.53	0.41
4:X:90:LEU:HD12	4:X:90:LEU:HA	1.84	0.41
4:X:125:SER:O	4:X:128:ILE:HB	2.21	0.41
3:Y:101:ASP:OD1	3:Y:102:ALA:N	2.53	0.41
1:A:141:ALA:HB2	1:A:158:ILE:HG21	2.02	0.41
3:D:92:TYR:O	3:D:95:TYR:N	2.53	0.41
3:H:34:SER:OG	3:H:35:ASN:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:17:ARG:NH2	4:I:23:GLU:OE2	2.51	0.41
4:I:77:THR:CG2	4:I:78:ASN:N	2.83	0.41
3:O:101:ASP:OD1	3:O:102:ALA:N	2.53	0.41
3:U:145:PRO:HD2	6:U:202:CYC:HMC3	2.01	0.41
4:V:33:ARG:HA	4:V:33:ARG:HD2	1.91	0.41
4:X:125:SER:O	4:X:126:TRP:C	2.63	0.41
4:X:153:TYR:O	4:X:154:ILE:C	2.62	0.41
3:B:127:VAL:HG22	6:B:202:CYC:H3C	2.03	0.41
3:D:78:ARG:HD2	6:D:202:CYC:HBD2	2.03	0.41
3:D:108:ARG:NH2	5:M:162:ASN:HB2	2.36	0.41
4:E:21:ASN:O	4:E:22:THR:C	2.63	0.41
4:E:125:SER:O	4:E:128:ILE:HB	2.21	0.41
3:F:101:ASP:OD1	3:F:102:ALA:N	2.53	0.41
4:G:108:TYR:HD1	3:J:75:PRO:HG3	1.83	0.41
4:G:125:SER:O	4:G:128:ILE:HB	2.21	0.41
4:I:1:MET:HE3	4:I:1:MET:HB2	1.96	0.41
4:I:33:ARG:HA	4:I:33:ARG:HD2	1.91	0.41
3:J:101:ASP:OD1	3:J:102:ALA:N	2.54	0.41
3:L:75:PRO:O	3:L:76:ASN:C	2.64	0.41
5:M:167:GLU:HB3	5:M:178:PRO:HG3	2.03	0.41
4:N:125:SER:O	4:N:128:ILE:HB	2.21	0.41
3:O:39:ASP:OD1	6:O:201:CYC:CHB	2.68	0.41
3:Q:117:TYR:HD1	3:Q:122:THR:OG1	2.04	0.41
3:Q:148:VAL:HG11	6:Q:201:CYC:CHD	2.51	0.41
4:R:21:ASN:O	4:R:22:THR:C	2.64	0.41
3:S:34:SER:OG	3:S:35:ASN:N	2.53	0.41
4:T:153:TYR:O	4:T:154:ILE:C	2.62	0.41
3:U:143:ASN:C	3:U:145:PRO:HD3	2.46	0.41
4:V:1:MET:HE3	4:V:1:MET:HB2	1.95	0.41
4:V:125:SER:O	4:V:126:TRP:C	2.63	0.41
4:a:21:ASN:O	4:a:22:THR:C	2.63	0.41
4:C:17:ARG:NH2	4:C:23:GLU:OE2	2.49	0.41
6:D:201:CYC:HB	6:D:201:CYC:HMA2	1.85	0.41
6:D:202:CYC:NB	5:M:188:LEU:HD11	2.35	0.41
4:E:108:TYR:CD1	3:L:75:PRO:HG3	2.56	0.41
3:H:91:ARG:O	3:H:94:SER:OG	2.24	0.41
3:H:101:ASP:OD1	3:H:102:ALA:N	2.54	0.41
3:O:64:THR:O	3:O:67:ILE:HG12	2.21	0.41
3:Q:117:TYR:CD1	3:Q:122:THR:OG1	2.73	0.41
4:R:103:GLY:O	4:R:104:PRO:C	2.61	0.41
4:R:125:SER:O	4:R:128:ILE:HB	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:24:LEU:O	4:T:25:GLN:C	2.63	0.41
4:T:108:TYR:HD1	3:W:75:PRO:CG	2.31	0.41
3:U:22:GLN:NE2	3:U:26:GLN:OE1	2.54	0.41
4:a:17:ARG:NH1	4:a:18:PHE:O	2.54	0.41
1:A:105:GLU:HA	1:A:229:ASN:O	2.20	0.40
3:B:64:THR:O	3:B:67:ILE:HG12	2.21	0.40
3:D:34:SER:OG	3:D:35:ASN:N	2.53	0.40
3:J:75:PRO:O	3:J:76:ASN:C	2.64	0.40
5:M:33:LEU:HB2	3:W:84:ARG:HD3	2.03	0.40
4:V:125:SER:O	4:V:128:ILE:HB	2.21	0.40
6:V:201:CYC:HMA1	6:V:201:CYC:C1B	2.51	0.40
4:X:21:ASN:O	4:X:22:THR:C	2.63	0.40
1:A:223:ARG:HD3	5:M:58:TYR:CZ	2.56	0.40
3:B:18:PHE:CE2	4:a:91:ARG:HA	2.56	0.40
4:G:5:ILE:HD11	4:G:30:ARG:HH11	1.86	0.40
4:I:24:LEU:O	4:I:25:GLN:C	2.63	0.40
4:K:55:ALA:O	4:K:58:GLU:HB3	2.21	0.40
4:K:87:SER:O	4:K:88:HIS:C	2.65	0.40
4:K:125:SER:O	4:K:128:ILE:HB	2.21	0.40
5:M:13:LYS:HE3	5:M:15:PHE:CZ	2.55	0.40
5:M:35:THR:HG22	3:W:84:ARG:NH1	2.36	0.40
5:M:130:SER:O	5:M:134:ASN:OD1	2.39	0.40
3:O:145:PRO:CD	6:O:201:CYC:CMC	2.93	0.40
4:P:125:SER:O	4:P:128:ILE:HB	2.22	0.40
4:T:21:ASN:O	4:T:22:THR:C	2.63	0.40
1:A:156:ILE:HD13	1:A:232:PRO:HD3	2.04	0.40
1:A:245:ALA:HB2	3:Q:107:ASP:O	2.22	0.40
2:Z:27:HIS:CE1	5:M:213:PHE:H	2.39	0.40
4:E:55:ALA:O	4:E:58:GLU:HB3	2.21	0.40
4:I:125:SER:O	4:I:126:TRP:C	2.63	0.40
5:M:77:LEU:HD23	5:M:77:LEU:HA	1.83	0.40
3:Q:87:GLU:O	3:Q:90:LEU:HB3	2.20	0.40
3:U:75:PRO:O	3:U:76:ASN:C	2.64	0.40
3:U:101:ASP:OD1	3:U:102:ALA:N	2.54	0.40
3:U:158:ASN:O	3:U:161:ALA:HB3	2.22	0.40
4:V:128:ILE:O	4:V:129:GLU:C	2.65	0.40
3:Y:34:SER:O	3:Y:35:ASN:C	2.63	0.40
3:Y:87:GLU:O	3:Y:90:LEU:HB3	2.21	0.40
1:A:171:ARG:HH11	4:R:10:ALA:HB1	1.86	0.40
2:Z:58:ARG:HH11	5:M:210:ILE:HD12	1.86	0.40
4:C:19:LEU:O	3:D:45:THR:HG21	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:125:SER:O	4:C:128:ILE:HB	2.21	0.40
6:D:201:CYC:HMA3	4:G:33:ARG:HH12	1.87	0.40
3:F:87:GLU:O	3:F:90:LEU:HB3	2.21	0.40
3:L:111:ASN:O	5:M:232:VAL:HG23	2.20	0.40
5:M:156:PHE:CD2	5:M:168:LEU:HD21	2.56	0.40
5:M:176:ARG:HH11	5:M:176:ARG:HG3	1.86	0.40
4:N:77:THR:CG2	4:N:78:ASN:N	2.83	0.40
4:P:91:ARG:HA	3:Q:18:PHE:CE2	2.57	0.40
1:A:98:ILE:HG12	1:A:255:TYR:CE1	2.57	0.40
1:A:170:PHE:HD2	1:A:171:ARG:HH21	1.67	0.40
3:D:87:GLU:O	3:D:90:LEU:HB3	2.22	0.40
3:F:34:SER:O	3:F:35:ASN:C	2.63	0.40
3:F:143:ASN:C	3:F:145:PRO:HD3	2.46	0.40
3:H:22:GLN:NE2	3:H:26:GLN:OE1	2.54	0.40
3:J:87:GLU:O	3:J:90:LEU:HB3	2.21	0.40
5:M:22:SER:OG	5:M:23:PRO:CD	2.69	0.40
4:N:24:LEU:O	4:N:25:GLN:C	2.63	0.40
3:Q:143:ASN:C	3:Q:145:PRO:HD3	2.47	0.40
4:T:87:SER:O	4:T:88:HIS:C	2.64	0.40
3:W:75:PRO:O	3:W:76:ASN:C	2.64	0.40
3:Y:117:TYR:O	3:Y:122:THR:HG22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	214/824 (26%)	195 (91%)	14 (6%)	5 (2%)	5	31
2	Z	71/275 (26%)	67 (94%)	4 (6%)	0	100	100
3	B	170/172 (99%)	133 (78%)	32 (19%)	5 (3%)	3	27
3	D	170/172 (99%)	132 (78%)	34 (20%)	4 (2%)	5	30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	170/172 (99%)	131 (77%)	34 (20%)	5 (3%)	3	27
3	H	170/172 (99%)	129 (76%)	36 (21%)	5 (3%)	3	27
3	J	170/172 (99%)	132 (78%)	33 (19%)	5 (3%)	3	27
3	L	170/172 (99%)	131 (77%)	35 (21%)	4 (2%)	5	30
3	O	170/172 (99%)	133 (78%)	32 (19%)	5 (3%)	3	27
3	Q	170/172 (99%)	132 (78%)	33 (19%)	5 (3%)	3	27
3	S	170/172 (99%)	133 (78%)	32 (19%)	5 (3%)	3	27
3	U	170/172 (99%)	132 (78%)	33 (19%)	5 (3%)	3	27
3	W	170/172 (99%)	133 (78%)	32 (19%)	5 (3%)	3	27
3	Y	170/172 (99%)	129 (76%)	37 (22%)	4 (2%)	5	30
4	C	160/162 (99%)	129 (81%)	25 (16%)	6 (4%)	2	23
4	E	160/162 (99%)	130 (81%)	25 (16%)	5 (3%)	3	27
4	G	160/162 (99%)	128 (80%)	27 (17%)	5 (3%)	3	27
4	I	160/162 (99%)	130 (81%)	25 (16%)	5 (3%)	3	27
4	K	160/162 (99%)	127 (79%)	28 (18%)	5 (3%)	3	27
4	N	160/162 (99%)	128 (80%)	27 (17%)	5 (3%)	3	27
4	P	160/162 (99%)	129 (81%)	26 (16%)	5 (3%)	3	27
4	R	160/162 (99%)	127 (79%)	28 (18%)	5 (3%)	3	27
4	T	160/162 (99%)	128 (80%)	27 (17%)	5 (3%)	3	27
4	V	160/162 (99%)	130 (81%)	25 (16%)	5 (3%)	3	27
4	X	160/162 (99%)	127 (79%)	28 (18%)	5 (3%)	3	27
4	a	160/162 (99%)	129 (81%)	26 (16%)	5 (3%)	3	27
5	M	271/274 (99%)	256 (94%)	10 (4%)	5 (2%)	7	35
All	All	4516/5381 (84%)	3640 (81%)	748 (17%)	128 (3%)	6	28

All (128) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	245	ALA
4	C	48	ALA
4	C	49	ASP
4	E	48	ALA
4	E	49	ASP
4	G	48	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	G	49	ASP
4	I	48	ALA
4	I	49	ASP
4	K	48	ALA
4	K	49	ASP
5	M	89	LEU
4	N	48	ALA
4	N	49	ASP
4	P	48	ALA
4	P	49	ASP
4	R	48	ALA
4	R	49	ASP
4	T	48	ALA
4	T	49	ASP
4	V	48	ALA
4	V	49	ASP
4	X	48	ALA
4	X	49	ASP
4	a	48	ALA
4	a	49	ASP
1	A	144	LEU
4	C	103	GLY
4	E	103	GLY
4	G	103	GLY
4	I	103	GLY
4	K	103	GLY
5	M	136	SER
4	N	103	GLY
3	O	103	SER
4	P	103	GLY
4	R	103	GLY
4	T	103	GLY
4	V	103	GLY
3	W	103	SER
4	X	103	GLY
4	a	103	GLY
1	A	160	ALA
1	A	280	ASP
3	B	48	ALA
3	B	103	SER
3	D	48	ALA
3	D	103	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	34	SER
3	F	48	ALA
3	F	103	SER
3	H	48	ALA
3	H	103	SER
3	J	48	ALA
3	J	103	SER
3	L	48	ALA
3	L	103	SER
5	M	32	SER
3	Q	48	ALA
3	Q	103	SER
3	S	34	SER
3	S	48	ALA
3	S	103	SER
3	U	48	ALA
3	U	103	SER
3	Y	34	SER
3	Y	48	ALA
3	Y	103	SER
3	B	34	SER
3	D	34	SER
3	H	34	SER
3	L	34	SER
5	M	90	LYS
3	O	34	SER
3	O	48	ALA
3	Q	34	SER
3	U	34	SER
3	W	48	ALA
1	A	78	ARG
4	G	156	TYR
3	J	34	SER
5	M	180	ASN
4	N	156	TYR
4	P	156	TYR
4	R	156	TYR
3	U	104	VAL
3	W	34	SER
3	W	104	VAL
4	X	156	TYR
4	a	156	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	104	VAL
4	C	156	TYR
3	D	104	VAL
4	E	156	TYR
3	F	104	VAL
3	H	104	VAL
4	I	156	TYR
3	J	104	VAL
4	K	156	TYR
3	L	104	VAL
3	O	104	VAL
3	Q	104	VAL
3	S	104	VAL
4	T	156	TYR
4	V	156	TYR
3	Y	104	VAL
3	F	51	ILE
4	K	56	VAL
4	R	56	VAL
3	S	51	ILE
4	T	56	VAL
4	C	56	VAL
4	C	116	VAL
4	E	56	VAL
4	G	56	VAL
3	H	51	ILE
4	I	56	VAL
3	J	51	ILE
4	N	56	VAL
3	O	51	ILE
4	P	56	VAL
3	Q	51	ILE
4	V	56	VAL
3	W	51	ILE
4	X	56	VAL
4	a	56	VAL
3	U	51	ILE
3	B	51	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	177/670 (26%)	159 (90%)	18 (10%)	6	25
2	Z	65/240 (27%)	60 (92%)	5 (8%)	10	35
3	B	134/134 (100%)	132 (98%)	2 (2%)	60	76
3	D	134/134 (100%)	132 (98%)	2 (2%)	60	76
3	F	134/134 (100%)	132 (98%)	2 (2%)	60	76
3	H	134/134 (100%)	133 (99%)	1 (1%)	81	88
3	J	134/134 (100%)	134 (100%)	0	100	100
3	L	134/134 (100%)	133 (99%)	1 (1%)	81	88
3	O	134/134 (100%)	133 (99%)	1 (1%)	81	88
3	Q	134/134 (100%)	132 (98%)	2 (2%)	60	76
3	S	134/134 (100%)	133 (99%)	1 (1%)	81	88
3	U	134/134 (100%)	133 (99%)	1 (1%)	81	88
3	W	134/134 (100%)	134 (100%)	0	100	100
3	Y	134/134 (100%)	132 (98%)	2 (2%)	60	76
4	C	130/130 (100%)	129 (99%)	1 (1%)	79	85
4	E	130/130 (100%)	128 (98%)	2 (2%)	60	76
4	G	130/130 (100%)	129 (99%)	1 (1%)	79	85
4	I	130/130 (100%)	128 (98%)	2 (2%)	60	76
4	K	130/130 (100%)	129 (99%)	1 (1%)	79	85
4	N	130/130 (100%)	129 (99%)	1 (1%)	79	85
4	P	130/130 (100%)	129 (99%)	1 (1%)	79	85
4	R	130/130 (100%)	128 (98%)	2 (2%)	60	76
4	T	130/130 (100%)	128 (98%)	2 (2%)	60	76
4	V	130/130 (100%)	129 (99%)	1 (1%)	79	85
4	X	130/130 (100%)	129 (99%)	1 (1%)	79	85
4	a	130/130 (100%)	129 (99%)	1 (1%)	79	85

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	M	237/238 (100%)	224 (94%)	13 (6%)	18	45
All	All	3647/4316 (84%)	3580 (98%)	67 (2%)	54	72

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	ARG
1	A	81	ASP
1	A	93	LEU
1	A	105	GLU
1	A	109	ASN
1	A	110	PHE
1	A	111	THR
1	A	112	GLU
1	A	132	ILE
1	A	134	GLU
1	A	187	LEU
1	A	209	TYR
1	A	213	ILE
1	A	229	ASN
1	A	238	LYS
1	A	267	GLN
1	A	283	GLN
1	A	288	ARG
2	Z	3	LEU
2	Z	13	LYS
2	Z	21	LEU
2	Z	59	ILE
2	Z	73	GLU
3	B	1	MET
3	B	166	LYS
4	C	30	ARG
3	D	32	LYS
3	D	108	ARG
4	E	30	ARG
4	E	81	LYS
3	F	84	ARG
3	F	166	LYS
4	G	30	ARG
3	H	166	LYS
4	I	5	ILE
4	I	30	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	K	30	ARG
3	L	58	LYS
5	M	29	PRO
5	M	45	VAL
5	M	46	VAL
5	M	50	ASP
5	M	51	ARG
5	M	98	ASP
5	M	113	ILE
5	M	119	VAL
5	M	134	ASN
5	M	162	ASN
5	M	179	TYR
5	M	218	VAL
5	M	259	ARG
4	N	30	ARG
3	O	1	MET
4	P	30	ARG
3	Q	32	LYS
3	Q	134	MET
4	R	30	ARG
4	R	81	LYS
3	S	166	LYS
4	T	5	ILE
4	T	30	ARG
3	U	166	LYS
4	V	30	ARG
4	X	30	ARG
3	Y	58	LYS
3	Y	166	LYS
4	a	30	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	125	GLN
1	A	147	ASN
1	A	175	ASN
1	A	176	ASN
1	A	185	HIS
1	A	229	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	243	GLN
1	A	266	ASN
1	A	267	GLN
2	Z	8	GLN
3	B	47	ASN
3	B	111	ASN
4	C	28	ASN
4	C	68	GLN
3	D	47	ASN
4	E	15	GLN
4	E	21	ASN
4	E	25	GLN
4	E	68	GLN
4	E	88	HIS
3	F	2	GLN
3	F	47	ASN
4	G	21	ASN
4	G	25	GLN
4	G	28	ASN
4	G	68	GLN
4	G	88	HIS
4	G	159	ASN
3	H	2	GLN
3	H	22	GLN
3	H	47	ASN
3	H	111	ASN
4	I	21	ASN
4	I	25	GLN
4	I	32	GLN
4	I	68	GLN
4	I	159	ASN
3	J	47	ASN
4	K	21	ASN
4	K	25	GLN
4	K	28	ASN
4	K	32	GLN
4	K	68	GLN
3	L	47	ASN
3	L	72	ASN
5	M	28	HIS
5	M	134	ASN
5	M	163	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	M	181	GLN
4	N	21	ASN
4	N	25	GLN
4	N	68	GLN
3	O	2	GLN
3	O	47	ASN
3	O	111	ASN
4	P	21	ASN
4	P	25	GLN
4	P	28	ASN
4	P	68	GLN
3	Q	47	ASN
4	R	15	GLN
4	R	28	ASN
4	R	68	GLN
4	R	88	HIS
3	S	2	GLN
3	S	47	ASN
4	T	15	GLN
4	T	21	ASN
4	T	25	GLN
4	T	28	ASN
4	T	68	GLN
4	T	88	HIS
3	U	2	GLN
3	U	22	GLN
3	U	47	ASN
4	V	21	ASN
4	V	25	GLN
4	V	68	GLN
3	W	47	ASN
4	X	21	ASN
4	X	25	GLN
4	X	28	ASN
4	X	32	GLN
4	X	68	GLN
3	Y	2	GLN
3	Y	47	ASN
3	Y	72	ASN
3	Y	111	ASN
4	a	21	ASN
4	a	25	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	a	68	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

36 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	CYC	C	201	4	42,46,46	0.93	2 (4%)	50,67,67	1.18	4 (8%)
6	CYC	H	201	3	42,46,46	1.01	2 (4%)	50,67,67	1.35	4 (8%)
6	CYC	J	201	3	42,46,46	0.79	0	50,67,67	1.35	3 (6%)
6	CYC	Q	201	3	42,46,46	1.04	2 (4%)	50,67,67	1.24	6 (12%)
6	CYC	O	202	3	42,46,46	1.00	2 (4%)	50,67,67	1.43	4 (8%)
6	CYC	B	201	3	42,46,46	1.00	1 (2%)	50,67,67	1.10	4 (8%)
6	CYC	P	201	4	42,46,46	0.96	3 (7%)	50,67,67	1.16	2 (4%)
6	CYC	T	201	4	42,46,46	1.13	3 (7%)	50,67,67	1.42	6 (12%)
6	CYC	G	201	4	42,46,46	1.05	4 (9%)	50,67,67	1.20	5 (10%)
6	CYC	D	202	3	42,46,46	1.17	2 (4%)	50,67,67	1.53	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CYC	L	201	3	42,46,46	1.09	1 (2%)	50,67,67	1.28	5 (10%)
6	CYC	S	201	3	42,46,46	0.99	1 (2%)	50,67,67	1.04	2 (4%)
6	CYC	D	201	3	42,46,46	1.06	2 (4%)	50,67,67	1.25	5 (10%)
6	CYC	R	201	4	42,46,46	1.06	2 (4%)	50,67,67	1.19	4 (8%)
6	CYC	U	202	3	42,46,46	1.12	2 (4%)	50,67,67	1.04	3 (6%)
6	CYC	W	202	3	42,46,46	0.96	1 (2%)	50,67,67	0.99	2 (4%)
6	CYC	X	201	4	42,46,46	1.24	4 (9%)	50,67,67	1.21	6 (12%)
6	CYC	Q	202	3	42,46,46	0.84	0	50,67,67	1.70	11 (22%)
6	CYC	V	201	4	42,46,46	0.99	2 (4%)	50,67,67	1.13	2 (4%)
6	CYC	I	201	4	42,46,46	0.97	1 (2%)	50,67,67	1.09	2 (4%)
6	CYC	N	201	4	42,46,46	0.90	3 (7%)	50,67,67	1.06	3 (6%)
6	CYC	a	201	4	42,46,46	0.99	3 (7%)	50,67,67	1.13	3 (6%)
6	CYC	E	201	4	42,46,46	1.00	3 (7%)	50,67,67	1.09	3 (6%)
6	CYC	S	202	3	42,46,46	0.79	0	50,67,67	1.11	3 (6%)
6	CYC	O	201	3	42,46,46	1.12	1 (2%)	50,67,67	1.23	4 (8%)
6	CYC	H	202	3	42,46,46	1.01	1 (2%)	50,67,67	1.02	2 (4%)
6	CYC	J	202	3	42,46,46	0.92	1 (2%)	50,67,67	1.15	2 (4%)
6	CYC	Y	201	3	42,46,46	0.98	1 (2%)	50,67,67	1.01	2 (4%)
6	CYC	F	201	3	42,46,46	0.95	1 (2%)	50,67,67	1.11	2 (4%)
6	CYC	B	202	3	42,46,46	0.93	1 (2%)	50,67,67	1.38	3 (6%)
6	CYC	W	201	3	42,46,46	1.12	4 (9%)	50,67,67	1.85	9 (18%)
6	CYC	Y	202	3	42,46,46	1.18	1 (2%)	50,67,67	1.56	6 (12%)
6	CYC	K	201	4	42,46,46	1.06	2 (4%)	50,67,67	1.18	5 (10%)
6	CYC	L	202	3	42,46,46	0.98	2 (4%)	50,67,67	0.95	2 (4%)
6	CYC	F	202	3	42,46,46	0.92	1 (2%)	50,67,67	1.38	6 (12%)
6	CYC	U	201	3	42,46,46	1.19	4 (9%)	50,67,67	1.30	5 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CYC	C	201	4	-	11/25/74/74	0/4/4/4
6	CYC	H	201	3	-	10/25/74/74	0/4/4/4
6	CYC	J	201	3	-	15/25/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CYC	Q	201	3	-	6/25/74/74	0/4/4/4
6	CYC	O	202	3	-	12/25/74/74	0/4/4/4
6	CYC	B	201	3	-	11/25/74/74	0/4/4/4
6	CYC	P	201	4	-	12/25/74/74	0/4/4/4
6	CYC	T	201	4	-	7/25/74/74	0/4/4/4
6	CYC	G	201	4	-	6/25/74/74	0/4/4/4
6	CYC	D	202	3	-	12/25/74/74	0/4/4/4
6	CYC	L	201	3	-	9/25/74/74	0/4/4/4
6	CYC	S	201	3	-	10/25/74/74	0/4/4/4
6	CYC	D	201	3	-	7/25/74/74	0/4/4/4
6	CYC	R	201	4	-	10/25/74/74	0/4/4/4
6	CYC	U	202	3	-	9/25/74/74	0/4/4/4
6	CYC	W	202	3	-	5/25/74/74	0/4/4/4
6	CYC	X	201	4	-	10/25/74/74	0/4/4/4
6	CYC	Q	202	3	-	16/25/74/74	0/4/4/4
6	CYC	V	201	4	-	8/25/74/74	0/4/4/4
6	CYC	I	201	4	-	11/25/74/74	0/4/4/4
6	CYC	N	201	4	-	12/25/74/74	0/4/4/4
6	CYC	a	201	4	-	11/25/74/74	0/4/4/4
6	CYC	E	201	4	-	9/25/74/74	0/4/4/4
6	CYC	S	202	3	-	8/25/74/74	0/4/4/4
6	CYC	O	201	3	-	11/25/74/74	0/4/4/4
6	CYC	H	202	3	-	8/25/74/74	0/4/4/4
6	CYC	J	202	3	-	5/25/74/74	0/4/4/4
6	CYC	Y	201	3	-	7/25/74/74	0/4/4/4
6	CYC	F	201	3	-	10/25/74/74	0/4/4/4
6	CYC	B	202	3	-	11/25/74/74	0/4/4/4
6	CYC	W	201	3	-	14/25/74/74	0/4/4/4
6	CYC	Y	202	3	-	11/25/74/74	0/4/4/4
6	CYC	K	201	4	-	10/25/74/74	0/4/4/4
6	CYC	L	202	3	-	9/25/74/74	0/4/4/4
6	CYC	F	202	3	-	13/25/74/74	0/4/4/4
6	CYC	U	201	3	-	11/25/74/74	0/4/4/4

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	O	201	CYC	CHA-C1A	5.44	1.39	1.35
6	Y	202	CYC	CHA-C1A	5.38	1.39	1.35
6	L	201	CYC	CHA-C1A	5.14	1.39	1.35
6	D	202	CYC	CHA-C1A	4.98	1.39	1.35
6	U	202	CYC	CHA-C1A	4.89	1.39	1.35
6	B	201	CYC	CHA-C1A	4.25	1.38	1.35
6	H	202	CYC	CHA-C1A	3.68	1.38	1.35
6	X	201	CYC	C1B-C2B	-3.53	1.38	1.45
6	D	201	CYC	CHA-C1A	3.51	1.38	1.35
6	Y	201	CYC	CHA-C1A	3.49	1.38	1.35
6	X	201	CYC	CHB-C4A	-3.48	1.32	1.40
6	R	201	CYC	C1B-C2B	-3.44	1.38	1.45
6	S	201	CYC	CHA-C1A	3.44	1.38	1.35
6	E	201	CYC	CHA-C1A	3.38	1.37	1.35
6	T	201	CYC	CHB-C4A	-3.35	1.32	1.40
6	K	201	CYC	C1B-C2B	-3.27	1.39	1.45
6	U	201	CYC	C1B-C2B	-3.27	1.39	1.45
6	K	201	CYC	CHB-C4A	-3.23	1.32	1.40
6	F	202	CYC	C1B-C2B	-3.21	1.39	1.45
6	T	201	CYC	C1B-C2B	-3.21	1.39	1.45
6	L	202	CYC	CHA-C1A	3.18	1.37	1.35
6	F	201	CYC	CHA-C1A	3.13	1.37	1.35
6	J	202	CYC	CHA-C1A	3.09	1.37	1.35
6	W	201	CYC	C1B-C2B	-3.08	1.39	1.45
6	R	201	CYC	CHB-C4A	-3.06	1.33	1.40
6	X	201	CYC	CHA-C1A	3.04	1.37	1.35
6	a	201	CYC	C1B-C2B	-3.04	1.39	1.45
6	U	201	CYC	CHA-C1A	-3.02	1.32	1.35
6	B	202	CYC	CHA-C1A	2.99	1.37	1.35
6	W	202	CYC	CHA-C1A	2.93	1.37	1.35
6	Q	201	CYC	CHA-C1A	2.93	1.37	1.35
6	V	201	CYC	C1B-C2B	-2.91	1.39	1.45
6	P	201	CYC	C1B-C2B	-2.88	1.39	1.45
6	U	201	CYC	CHB-C1B	-2.79	1.31	1.38
6	X	201	CYC	CHB-C1B	-2.79	1.31	1.38
6	H	201	CYC	C1B-C2B	-2.72	1.40	1.45
6	I	201	CYC	C1B-C2B	-2.69	1.40	1.45
6	a	201	CYC	CHB-C4A	-2.67	1.34	1.40
6	C	201	CYC	C1B-C2B	-2.66	1.40	1.45
6	G	201	CYC	CHB-C4A	-2.58	1.34	1.40
6	N	201	CYC	C1B-C2B	-2.58	1.40	1.45
6	O	202	CYC	C1B-C2B	-2.55	1.40	1.45
6	W	201	CYC	CHB-C4A	-2.48	1.34	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Q	201	CYC	C1B-C2B	-2.44	1.40	1.45
6	T	201	CYC	CHB-C1B	-2.43	1.32	1.38
6	U	201	CYC	CHB-C4A	-2.36	1.34	1.40
6	G	201	CYC	CHA-C1A	2.34	1.37	1.35
6	E	201	CYC	C1B-C2B	-2.30	1.41	1.45
6	N	201	CYC	CHB-C4A	-2.29	1.35	1.40
6	C	201	CYC	CHB-C4A	-2.25	1.35	1.40
6	G	201	CYC	CHB-C1B	-2.21	1.32	1.38
6	W	201	CYC	O2A-CGA	-2.19	1.23	1.30
6	G	201	CYC	C1B-C2B	-2.17	1.41	1.45
6	a	201	CYC	CHB-C1B	-2.13	1.32	1.38
6	P	201	CYC	CHA-C1A	2.13	1.36	1.35
6	O	202	CYC	CHB-C4A	-2.13	1.35	1.40
6	V	201	CYC	CHB-C4A	-2.12	1.35	1.40
6	H	201	CYC	CHB-C1B	-2.11	1.32	1.38
6	W	201	CYC	C4D-CHA	-2.09	1.32	1.41
6	U	202	CYC	CHB-C4A	-2.09	1.35	1.40
6	E	201	CYC	CHB-C4A	-2.09	1.35	1.40
6	D	201	CYC	C1B-C2B	-2.07	1.41	1.45
6	L	202	CYC	CHB-C4A	-2.06	1.35	1.40
6	D	202	CYC	CHB-C4A	-2.04	1.35	1.40
6	P	201	CYC	CHB-C4A	-2.01	1.35	1.40
6	N	201	CYC	CHB-C1B	-2.00	1.33	1.38

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	W	201	CYC	CMB-C2B-C1B	7.96	134.10	124.17
6	Y	202	CYC	CMB-C2B-C1B	6.71	132.54	124.17
6	D	202	CYC	CMB-C2B-C1B	5.60	131.16	124.17
6	O	201	CYC	CMB-C2B-C1B	5.39	130.89	124.17
6	O	202	CYC	CMB-C2B-C1B	5.30	130.79	124.17
6	Q	202	CYC	CMB-C2B-C1B	5.18	130.64	124.17
6	W	201	CYC	CAB-C3B-C4B	5.14	129.50	121.38
6	B	202	CYC	CMB-C2B-C1B	5.01	130.42	124.17
6	H	201	CYC	CMB-C2B-C1B	4.75	130.09	124.17
6	Q	202	CYC	CHA-C1A-NA	-4.60	122.44	128.83
6	C	201	CYC	CHA-C1A-NA	-4.52	122.56	128.83
6	T	201	CYC	CMB-C2B-C1B	4.48	129.76	124.17
6	T	201	CYC	CHA-C1A-NA	-4.42	122.69	128.83
6	J	201	CYC	C4D-CHA-C1A	-4.34	123.62	128.81
6	P	201	CYC	CHA-C1A-NA	-4.31	122.85	128.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	202	CYC	CHA-C1A-NA	-4.30	122.86	128.83
6	O	202	CYC	C4D-CHA-C1A	-4.26	123.72	128.81
6	J	202	CYC	CMB-C2B-C1B	4.19	129.40	124.17
6	J	201	CYC	CMB-C2B-C1B	4.18	129.38	124.17
6	F	202	CYC	CHA-C1A-NA	-4.17	123.04	128.83
6	V	201	CYC	CHA-C1A-NA	-4.16	123.06	128.83
6	L	201	CYC	CHB-C1B-C2B	-4.11	118.80	126.95
6	B	202	CYC	C4D-CHA-C1A	-4.04	123.98	128.81
6	D	201	CYC	C2C-C1C-NC	-3.90	104.91	108.27
6	U	201	CYC	CHA-C1A-NA	-3.89	123.43	128.83
6	I	201	CYC	CHA-C1A-NA	-3.88	123.45	128.83
6	K	201	CYC	CHA-C1A-NA	-3.82	123.53	128.83
6	N	201	CYC	CHA-C1A-NA	-3.81	123.54	128.83
6	J	201	CYC	CHA-C1A-NA	-3.81	123.54	128.83
6	E	201	CYC	CHA-C1A-NA	-3.79	123.58	128.83
6	Q	201	CYC	C2C-C1C-NC	-3.70	105.08	108.27
6	Y	202	CYC	CHA-C1A-NA	-3.67	123.73	128.83
6	F	201	CYC	CMB-C2B-C1B	3.67	128.74	124.17
6	F	202	CYC	CMA-C3A-C4A	3.66	130.70	125.06
6	W	201	CYC	CMB-C2B-C3B	-3.63	116.27	126.12
6	a	201	CYC	CHA-C1A-NA	-3.62	123.81	128.83
6	G	201	CYC	CHA-C1A-NA	-3.59	123.84	128.83
6	X	201	CYC	CHA-C1A-NA	-3.59	123.84	128.83
6	D	202	CYC	CHB-C1B-C2B	-3.57	119.86	126.95
6	L	201	CYC	CHA-C1A-NA	-3.57	123.87	128.83
6	U	201	CYC	C4D-CHA-C1A	-3.57	124.54	128.81
6	D	202	CYC	CHA-C1A-NA	-3.45	124.04	128.83
6	F	201	CYC	CHA-C1A-NA	-3.42	124.09	128.83
6	S	201	CYC	CHA-C1A-NA	-3.36	124.16	128.83
6	G	201	CYC	CMB-C2B-C1B	3.33	128.33	124.17
6	D	201	CYC	CMB-C2B-C1B	3.29	128.27	124.17
6	Q	202	CYC	CBA-CAA-C2A	3.21	121.55	112.63
6	U	202	CYC	CMB-C2B-C1B	3.18	128.13	124.17
6	G	201	CYC	CAC-C3C-C2C	3.16	122.16	114.26
6	B	201	CYC	CMB-C2B-C1B	3.11	128.05	124.17
6	H	202	CYC	CHA-C1A-NA	-3.11	124.51	128.83
6	W	201	CYC	CHB-C1B-C2B	-3.06	120.88	126.95
6	H	201	CYC	C4D-CHA-C1A	-3.04	125.18	128.81
6	P	201	CYC	C4D-CHA-C1A	-3.04	125.18	128.81
6	Y	201	CYC	CMB-C2B-C1B	3.01	127.92	124.17
6	Y	201	CYC	CHA-C1A-NA	-3.01	124.66	128.83
6	R	201	CYC	CHA-C1A-NA	-2.96	124.72	128.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	W	202	CYC	CMB-C2B-C1B	2.93	127.83	124.17
6	U	202	CYC	CHA-C1A-NA	-2.93	124.76	128.83
6	J	202	CYC	CHA-C1A-NA	-2.92	124.78	128.83
6	U	201	CYC	CMA-C3A-C4A	2.91	129.55	125.06
6	C	201	CYC	C4D-CHA-C1A	-2.90	125.35	128.81
6	X	201	CYC	CMB-C2B-C1B	2.83	127.70	124.17
6	S	202	CYC	CMA-C3A-C4A	2.80	129.38	125.06
6	O	202	CYC	CHA-C1A-NA	-2.79	124.95	128.83
6	B	201	CYC	CAC-C3C-C4C	-2.79	105.51	112.67
6	Y	202	CYC	CMB-C2B-C3B	-2.78	118.57	126.12
6	D	201	CYC	CHA-C1A-NA	-2.78	124.97	128.83
6	L	202	CYC	CHA-C1A-NA	-2.77	124.98	128.83
6	D	202	CYC	C1B-CHB-C4A	2.77	134.84	128.08
6	S	201	CYC	CMB-C2B-C1B	2.74	127.59	124.17
6	H	202	CYC	CMB-C2B-C1B	2.74	127.58	124.17
6	S	202	CYC	CHA-C1A-NA	-2.70	125.08	128.83
6	T	201	CYC	CAC-C3C-C2C	2.69	120.98	114.26
6	E	201	CYC	CMB-C2B-C1B	2.69	127.52	124.17
6	B	201	CYC	CHA-C1A-NA	-2.67	125.13	128.83
6	L	201	CYC	CHB-C1B-NB	2.65	131.75	126.06
6	X	201	CYC	C1B-CHB-C4A	-2.64	121.63	128.08
6	R	201	CYC	CAC-C3C-C2C	2.63	120.84	114.26
6	L	201	CYC	CMB-C2B-C1B	2.60	127.42	124.17
6	D	202	CYC	CHB-C1B-NB	2.59	131.62	126.06
6	W	202	CYC	CHA-C1A-NA	-2.59	125.24	128.83
6	R	201	CYC	CHB-C1B-C2B	-2.58	121.83	126.95
6	H	201	CYC	CAA-C2A-C3A	2.58	132.69	127.88
6	W	201	CYC	CAB-C3B-C2B	-2.56	123.15	127.53
6	C	201	CYC	CHD-C4C-NC	2.55	128.24	125.20
6	Q	201	CYC	CMA-C3A-C4A	2.54	128.97	125.06
6	K	201	CYC	CMB-C2B-C1B	2.53	127.32	124.17
6	S	202	CYC	CHB-C1B-C2B	-2.51	121.98	126.95
6	Y	202	CYC	CHB-C1B-C2B	-2.51	121.98	126.95
6	U	201	CYC	C3B-C4B-NB	-2.49	104.76	106.78
6	Q	202	CYC	C4D-CHA-C1A	-2.49	125.83	128.81
6	O	201	CYC	CAC-C3C-C4C	-2.48	106.30	112.67
6	K	201	CYC	CAC-C3C-C2C	2.47	120.43	114.26
6	Q	201	CYC	CMB-C2B-C1B	2.46	127.23	124.17
6	Q	202	CYC	C1A-C2A-C3A	-2.44	104.08	106.78
6	a	201	CYC	C4D-CHA-C1A	-2.42	125.92	128.81
6	D	202	CYC	CMB-C2B-C3B	-2.41	119.56	126.12
6	Q	202	CYC	C2C-C1C-NC	-2.41	106.19	108.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	201	CYC	C1B-CHB-C4A	-2.40	122.21	128.08
6	L	202	CYC	CMB-C2B-C1B	2.40	127.16	124.17
6	Q	201	CYC	OC-C1C-NC	2.36	127.80	124.94
6	B	201	CYC	CAC-C3C-C2C	2.35	120.13	114.26
6	X	201	CYC	C4D-CHA-C1A	-2.35	126.00	128.81
6	Q	202	CYC	C1B-CHB-C4A	2.34	133.81	128.08
6	O	201	CYC	CHA-C1A-NA	-2.32	125.61	128.83
6	Q	202	CYC	CHD-C4C-NC	2.32	127.97	125.20
6	V	201	CYC	CMB-C2B-C1B	2.30	127.04	124.17
6	K	201	CYC	C4D-CHA-C1A	-2.30	126.06	128.81
6	X	201	CYC	C2B-C1B-NB	2.29	110.34	106.99
6	N	201	CYC	C4D-CHA-C1A	-2.29	126.08	128.81
6	E	201	CYC	CHD-C4C-NC	2.28	127.92	125.20
6	O	202	CYC	CMB-C2B-C3B	-2.27	119.97	126.12
6	W	201	CYC	C4D-CHA-C1A	-2.26	126.11	128.81
6	Q	202	CYC	CMB-C2B-C3B	-2.26	119.98	126.12
6	D	201	CYC	OC-C1C-NC	2.25	127.67	124.94
6	H	201	CYC	CHA-C1A-NA	-2.25	125.71	128.83
6	D	202	CYC	C2C-C3C-C4C	2.23	104.68	101.34
6	T	201	CYC	CAB-C3B-C4B	2.22	124.89	121.38
6	F	202	CYC	CAB-C3B-C4B	2.22	124.88	121.38
6	Y	202	CYC	CBD-CAD-C3D	2.21	116.39	112.62
6	Q	202	CYC	C4A-C3A-C2A	2.21	109.04	106.51
6	F	202	CYC	CHB-C1B-C2B	-2.19	122.62	126.95
6	Q	201	CYC	CAC-C3C-C2C	2.17	119.69	114.26
6	W	201	CYC	C2C-C1C-NC	-2.17	106.41	108.27
6	Q	201	CYC	CHA-C1A-NA	-2.15	125.85	128.83
6	D	201	CYC	CMA-C3A-C4A	2.14	128.37	125.06
6	N	201	CYC	CAB-C3B-C2B	2.14	131.19	127.53
6	F	202	CYC	C2C-C3C-C4C	2.14	104.54	101.34
6	O	201	CYC	CAC-C3C-C2C	2.14	119.60	114.26
6	T	201	CYC	C1B-CHB-C4A	-2.13	122.89	128.08
6	G	201	CYC	C4D-CHA-C1A	-2.12	126.28	128.81
6	C	201	CYC	C1B-CHB-C4A	-2.11	122.92	128.08
6	W	201	CYC	C3B-C4B-NB	-2.11	105.07	106.78
6	T	201	CYC	C4D-CHA-C1A	-2.10	126.30	128.81
6	G	201	CYC	C2B-C1B-NB	2.08	110.03	106.99
6	F	202	CYC	O1A-CGA-CBA	-2.08	116.40	123.08
6	W	201	CYC	CHB-C1B-NB	2.07	130.51	126.06
6	U	202	CYC	CMA-C3A-C4A	2.07	128.25	125.06
6	Q	202	CYC	C2C-C3C-C4C	2.07	104.44	101.34
6	I	201	CYC	CMA-C3A-C4A	2.05	128.22	125.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Y	202	CYC	CMA-C3A-C4A	2.05	128.22	125.06
6	R	201	CYC	CBD-CAD-C3D	2.03	116.09	112.62
6	L	201	CYC	C1B-CHB-C4A	2.02	133.02	128.08
6	X	201	CYC	CAC-C3C-C2C	2.02	119.29	114.26
6	a	201	CYC	CHB-C1B-C2B	-2.01	122.96	126.95
6	U	201	CYC	CMB-C2B-C1B	2.00	126.67	124.17

There are no chirality outliers.

All (357) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	201	CYC	NA-C4A-CHB-C1B
6	B	201	CYC	C3A-C4A-CHB-C1B
6	B	201	CYC	C2C-C3C-CAC-CBC
6	B	201	CYC	C4C-C3C-CAC-CBC
6	B	202	CYC	C2A-CAA-CBA-CGA
6	B	202	CYC	C4C-C3C-CAC-CBC
6	C	201	CYC	NA-C4A-CHB-C1B
6	C	201	CYC	C3A-C4A-CHB-C1B
6	C	201	CYC	C2A-CAA-CBA-CGA
6	C	201	CYC	ND-C1D-CHD-C4C
6	C	201	CYC	C2D-C1D-CHD-C4C
6	D	201	CYC	NA-C4A-CHB-C1B
6	D	201	CYC	C3A-C4A-CHB-C1B
6	D	201	CYC	ND-C1D-CHD-C4C
6	D	201	CYC	C2D-C1D-CHD-C4C
6	D	202	CYC	NA-C4A-CHB-C1B
6	D	202	CYC	C3A-C4A-CHB-C1B
6	D	202	CYC	C4C-C3C-CAC-CBC
6	D	202	CYC	ND-C1D-CHD-C4C
6	D	202	CYC	C2D-C1D-CHD-C4C
6	D	202	CYC	C3D-CAD-CBD-CGD
6	E	201	CYC	NA-C4A-CHB-C1B
6	E	201	CYC	NC-C4C-CHD-C1D
6	E	201	CYC	ND-C1D-CHD-C4C
6	E	201	CYC	C2D-C1D-CHD-C4C
6	F	201	CYC	NA-C4A-CHB-C1B
6	F	201	CYC	C3A-C4A-CHB-C1B
6	F	201	CYC	C2C-C3C-CAC-CBC
6	F	201	CYC	C4C-C3C-CAC-CBC
6	F	201	CYC	ND-C1D-CHD-C4C
6	F	202	CYC	NA-C4A-CHB-C1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	F	202	CYC	C2B-C3B-CAB-CBB
6	F	202	CYC	C2C-C3C-CAC-CBC
6	F	202	CYC	C4C-C3C-CAC-CBC
6	F	202	CYC	ND-C1D-CHD-C4C
6	F	202	CYC	C2D-C1D-CHD-C4C
6	F	202	CYC	C3D-CAD-CBD-CGD
6	G	201	CYC	NA-C4A-CHB-C1B
6	G	201	CYC	C3A-C4A-CHB-C1B
6	G	201	CYC	C2A-CAA-CBA-CGA
6	G	201	CYC	NC-C4C-CHD-C1D
6	G	201	CYC	ND-C1D-CHD-C4C
6	G	201	CYC	C2D-C1D-CHD-C4C
6	H	202	CYC	NA-C4A-CHB-C1B
6	H	202	CYC	C3A-C4A-CHB-C1B
6	H	202	CYC	C2A-CAA-CBA-CGA
6	H	202	CYC	ND-C1D-CHD-C4C
6	I	201	CYC	NA-C4A-CHB-C1B
6	I	201	CYC	C4C-C3C-CAC-CBC
6	I	201	CYC	NC-C4C-CHD-C1D
6	I	201	CYC	ND-C1D-CHD-C4C
6	I	201	CYC	C2D-C1D-CHD-C4C
6	J	201	CYC	C2B-C3B-CAB-CBB
6	J	201	CYC	C2C-C3C-CAC-CBC
6	J	201	CYC	C4C-C3C-CAC-CBC
6	J	201	CYC	ND-C1D-CHD-C4C
6	J	201	CYC	C2D-C1D-CHD-C4C
6	J	202	CYC	NA-C4A-CHB-C1B
6	J	202	CYC	C3A-C4A-CHB-C1B
6	K	201	CYC	NA-C4A-CHB-C1B
6	K	201	CYC	C3A-C4A-CHB-C1B
6	K	201	CYC	NC-C4C-CHD-C1D
6	K	201	CYC	ND-C1D-CHD-C4C
6	K	201	CYC	C2D-C1D-CHD-C4C
6	L	201	CYC	NA-C4A-CHB-C1B
6	L	201	CYC	C3A-C4A-CHB-C1B
6	L	201	CYC	C4C-C3C-CAC-CBC
6	L	201	CYC	ND-C1D-CHD-C4C
6	L	201	CYC	C2D-C1D-CHD-C4C
6	L	202	CYC	NA-C4A-CHB-C1B
6	L	202	CYC	C3A-C4A-CHB-C1B
6	L	202	CYC	ND-C1D-CHD-C4C
6	N	201	CYC	NA-C4A-CHB-C1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	N	201	CYC	NC-C4C-CHD-C1D
6	N	201	CYC	ND-C1D-CHD-C4C
6	N	201	CYC	C2D-C1D-CHD-C4C
6	O	201	CYC	NA-C4A-CHB-C1B
6	O	201	CYC	C3A-C4A-CHB-C1B
6	O	201	CYC	C2C-C3C-CAC-CBC
6	O	201	CYC	C4C-C3C-CAC-CBC
6	O	202	CYC	C2B-C3B-CAB-CBB
6	O	202	CYC	C2C-C3C-CAC-CBC
6	O	202	CYC	C4C-C3C-CAC-CBC
6	O	202	CYC	ND-C1D-CHD-C4C
6	O	202	CYC	C2D-C1D-CHD-C4C
6	P	201	CYC	NA-C4A-CHB-C1B
6	P	201	CYC	C3A-C4A-CHB-C1B
6	P	201	CYC	C4C-C3C-CAC-CBC
6	P	201	CYC	NC-C4C-CHD-C1D
6	P	201	CYC	ND-C1D-CHD-C4C
6	P	201	CYC	C2D-C1D-CHD-C4C
6	Q	201	CYC	NA-C4A-CHB-C1B
6	Q	201	CYC	C3A-C4A-CHB-C1B
6	Q	201	CYC	ND-C1D-CHD-C4C
6	Q	202	CYC	NA-C4A-CHB-C1B
6	Q	202	CYC	C3A-C4A-CHB-C1B
6	Q	202	CYC	NB-C1B-CHB-C4A
6	Q	202	CYC	C2B-C1B-CHB-C4A
6	Q	202	CYC	C4B-C3B-CAB-CBB
6	Q	202	CYC	C4C-C3C-CAC-CBC
6	Q	202	CYC	ND-C1D-CHD-C4C
6	Q	202	CYC	C2D-C1D-CHD-C4C
6	Q	202	CYC	C3D-CAD-CBD-CGD
6	R	201	CYC	NA-C4A-CHB-C1B
6	R	201	CYC	NC-C4C-CHD-C1D
6	R	201	CYC	ND-C1D-CHD-C4C
6	R	201	CYC	C2D-C1D-CHD-C4C
6	S	201	CYC	NA-C4A-CHB-C1B
6	S	201	CYC	C3A-C4A-CHB-C1B
6	S	201	CYC	C4C-C3C-CAC-CBC
6	S	201	CYC	ND-C1D-CHD-C4C
6	S	202	CYC	C4C-C3C-CAC-CBC
6	S	202	CYC	ND-C1D-CHD-C4C
6	S	202	CYC	C2D-C1D-CHD-C4C
6	T	201	CYC	NA-C4A-CHB-C1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	T	201	CYC	C3A-C4A-CHB-C1B
6	T	201	CYC	C2A-CAA-CBA-CGA
6	T	201	CYC	NC-C4C-CHD-C1D
6	T	201	CYC	ND-C1D-CHD-C4C
6	T	201	CYC	C2D-C1D-CHD-C4C
6	U	201	CYC	NA-C4A-CHB-C1B
6	U	201	CYC	C3A-C4A-CHB-C1B
6	U	201	CYC	C4C-C3C-CAC-CBC
6	U	201	CYC	ND-C1D-CHD-C4C
6	U	201	CYC	C2D-C1D-CHD-C4C
6	U	202	CYC	NA-C4A-CHB-C1B
6	U	202	CYC	C3A-C4A-CHB-C1B
6	U	202	CYC	C2A-CAA-CBA-CGA
6	U	202	CYC	ND-C1D-CHD-C4C
6	U	202	CYC	C2D-C1D-CHD-C4C
6	V	201	CYC	NA-C4A-CHB-C1B
6	V	201	CYC	C4C-C3C-CAC-CBC
6	V	201	CYC	NC-C4C-CHD-C1D
6	V	201	CYC	ND-C1D-CHD-C4C
6	V	201	CYC	C2D-C1D-CHD-C4C
6	W	201	CYC	NA-C4A-CHB-C1B
6	W	201	CYC	C3A-C4A-CHB-C1B
6	W	201	CYC	C2B-C3B-CAB-CBB
6	W	201	CYC	C4B-C3B-CAB-CBB
6	W	201	CYC	ND-C1D-CHD-C4C
6	W	201	CYC	C2D-C1D-CHD-C4C
6	W	201	CYC	C2D-C3D-CAD-CBD
6	W	202	CYC	NA-C4A-CHB-C1B
6	W	202	CYC	C3A-C4A-CHB-C1B
6	X	201	CYC	NA-C4A-CHB-C1B
6	X	201	CYC	C3A-C4A-CHB-C1B
6	X	201	CYC	NC-C4C-CHD-C1D
6	X	201	CYC	ND-C1D-CHD-C4C
6	X	201	CYC	C2D-C1D-CHD-C4C
6	Y	201	CYC	NA-C4A-CHB-C1B
6	Y	201	CYC	C3A-C4A-CHB-C1B
6	Y	201	CYC	ND-C1D-CHD-C4C
6	Y	202	CYC	NA-C4A-CHB-C1B
6	Y	202	CYC	C3A-C4A-CHB-C1B
6	Y	202	CYC	C2B-C1B-CHB-C4A
6	a	201	CYC	NA-C4A-CHB-C1B
6	a	201	CYC	NC-C4C-CHD-C1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	a	201	CYC	ND-C1D-CHD-C4C
6	a	201	CYC	C2D-C1D-CHD-C4C
6	B	202	CYC	C2B-C3B-CAB-CBB
6	Q	202	CYC	C2B-C3B-CAB-CBB
6	H	201	CYC	C2A-CAA-CBA-CGA
6	J	201	CYC	C2A-CAA-CBA-CGA
6	N	201	CYC	C2A-CAA-CBA-CGA
6	O	202	CYC	NA-C4A-CHB-C1B
6	W	201	CYC	C2A-CAA-CBA-CGA
6	a	201	CYC	C2A-CAA-CBA-CGA
6	N	201	CYC	C3A-C4A-CHB-C1B
6	V	201	CYC	C3A-C4A-CHB-C1B
6	a	201	CYC	C3A-C4A-CHB-C1B
6	I	201	CYC	C2B-C3B-CAB-CBB
6	H	201	CYC	NB-C1B-CHB-C4A
6	L	201	CYC	C3D-CAD-CBD-CGD
6	Y	202	CYC	C3D-CAD-CBD-CGD
6	B	202	CYC	C4B-C3B-CAB-CBB
6	F	202	CYC	C4B-C3B-CAB-CBB
6	J	201	CYC	C4B-C3B-CAB-CBB
6	O	202	CYC	C4B-C3B-CAB-CBB
6	B	202	CYC	NB-C1B-CHB-C4A
6	J	201	CYC	NB-C1B-CHB-C4A
6	L	201	CYC	NB-C1B-CHB-C4A
6	Y	202	CYC	NB-C1B-CHB-C4A
6	B	202	CYC	C2B-C1B-CHB-C4A
6	B	201	CYC	C2A-CAA-CBA-CGA
6	O	201	CYC	C2A-CAA-CBA-CGA
6	O	202	CYC	C2A-CAA-CBA-CGA
6	P	201	CYC	C2A-CAA-CBA-CGA
6	Y	202	CYC	C2B-C3B-CAB-CBB
6	H	201	CYC	C2B-C3B-CAB-CBB
6	K	201	CYC	C2B-C3B-CAB-CBB
6	L	201	CYC	C2B-C1B-CHB-C4A
6	T	201	CYC	C2B-C3B-CAB-CBB
6	B	202	CYC	NA-C4A-CHB-C1B
6	H	201	CYC	NA-C4A-CHB-C1B
6	J	201	CYC	NA-C4A-CHB-C1B
6	S	202	CYC	NA-C4A-CHB-C1B
6	B	202	CYC	C3A-C4A-CHB-C1B
6	E	201	CYC	C3A-C4A-CHB-C1B
6	F	202	CYC	C3A-C4A-CHB-C1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	H	201	CYC	C3A-C4A-CHB-C1B
6	I	201	CYC	C3A-C4A-CHB-C1B
6	J	201	CYC	C3A-C4A-CHB-C1B
6	O	202	CYC	C3A-C4A-CHB-C1B
6	R	201	CYC	C3A-C4A-CHB-C1B
6	S	202	CYC	C3A-C4A-CHB-C1B
6	V	201	CYC	C2B-C3B-CAB-CBB
6	I	201	CYC	C2B-C1B-CHB-C4A
6	H	201	CYC	C2B-C1B-CHB-C4A
6	J	201	CYC	C2B-C1B-CHB-C4A
6	D	201	CYC	C2A-CAA-CBA-CGA
6	Q	201	CYC	C2A-CAA-CBA-CGA
6	U	201	CYC	C2A-CAA-CBA-CGA
6	U	201	CYC	C2B-C3B-CAB-CBB
6	F	201	CYC	NC-C4C-CHD-C1D
6	C	201	CYC	C3D-CAD-CBD-CGD
6	I	201	CYC	C2C-C3C-CAC-CBC
6	Q	202	CYC	C2C-C3C-CAC-CBC
6	S	201	CYC	C2C-C3C-CAC-CBC
6	X	201	CYC	C2B-C3B-CAB-CBB
6	O	202	CYC	NB-C1B-CHB-C4A
6	S	201	CYC	C2B-C3B-CAB-CBB
6	F	201	CYC	C3D-CAD-CBD-CGD
6	L	202	CYC	C2A-CAA-CBA-CGA
6	Y	201	CYC	C2A-CAA-CBA-CGA
6	Y	202	CYC	C4B-C3B-CAB-CBB
6	V	201	CYC	C2B-C1B-CHB-C4A
6	F	201	CYC	C2B-C3B-CAB-CBB
6	L	202	CYC	C4C-C3C-CAC-CBC
6	Y	202	CYC	C4C-C3C-CAC-CBC
6	W	202	CYC	C2A-CAA-CBA-CGA
6	D	202	CYC	NB-C1B-CHB-C4A
6	O	201	CYC	C2B-C3B-CAB-CBB
6	S	202	CYC	C2B-C3B-CAB-CBB
6	I	201	CYC	C4B-C3B-CAB-CBB
6	P	201	CYC	C2B-C3B-CAB-CBB
6	B	201	CYC	NC-C4C-CHD-C1D
6	C	201	CYC	NC-C4C-CHD-C1D
6	L	201	CYC	NC-C4C-CHD-C1D
6	O	201	CYC	NC-C4C-CHD-C1D
6	S	201	CYC	NC-C4C-CHD-C1D
6	B	202	CYC	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	P	201	CYC	C3D-CAD-CBD-CGD
6	U	201	CYC	C2C-C3C-CAC-CBC
6	U	201	CYC	C4B-C3B-CAB-CBB
6	E	201	CYC	C2B-C1B-CHB-C4A
6	a	201	CYC	C2B-C3B-CAB-CBB
6	B	201	CYC	C2B-C3B-CAB-CBB
6	H	201	CYC	C3D-CAD-CBD-CGD
6	W	201	CYC	C1A-C2A-CAA-CBA
6	E	201	CYC	C2B-C3B-CAB-CBB
6	D	202	CYC	C2A-CAA-CBA-CGA
6	W	202	CYC	CAD-CBD-CGD-O1D
6	X	201	CYC	CAA-CBA-CGA-O1A
6	K	201	CYC	CAD-CBD-CGD-O1D
6	N	201	CYC	CAA-CBA-CGA-O1A
6	a	201	CYC	CAA-CBA-CGA-O2A
6	N	201	CYC	CAA-CBA-CGA-O2A
6	R	201	CYC	CAA-CBA-CGA-O1A
6	B	201	CYC	CAA-CBA-CGA-O2A
6	O	201	CYC	CAA-CBA-CGA-O1A
6	K	201	CYC	CAA-CBA-CGA-O1A
6	C	201	CYC	CAA-CBA-CGA-O1A
6	B	201	CYC	CAA-CBA-CGA-O1A
6	E	201	CYC	CAA-CBA-CGA-O1A
6	P	201	CYC	CAA-CBA-CGA-O1A
6	C	201	CYC	C2B-C3B-CAB-CBB
6	B	201	CYC	CAD-CBD-CGD-O1D
6	J	202	CYC	CAD-CBD-CGD-O1D
6	O	201	CYC	CAD-CBD-CGD-O1D
6	D	202	CYC	CAA-CBA-CGA-O2A
6	B	202	CYC	CAA-CBA-CGA-O1A
6	X	201	CYC	CAA-CBA-CGA-O2A
6	D	202	CYC	CAA-CBA-CGA-O1A
6	K	201	CYC	CAA-CBA-CGA-O2A
6	Q	202	CYC	CAA-CBA-CGA-O1A
6	O	201	CYC	CAD-CBD-CGD-O2D
6	U	202	CYC	CAA-CBA-CGA-O1A
6	B	201	CYC	CAD-CBD-CGD-O2D
6	J	202	CYC	CAD-CBD-CGD-O2D
6	R	201	CYC	CAA-CBA-CGA-O2A
6	H	201	CYC	CAD-CBD-CGD-O1D
6	K	201	CYC	CAD-CBD-CGD-O2D
6	P	201	CYC	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	W	202	CYC	CAD-CBD-CGD-O2D
6	H	201	CYC	CAD-CBD-CGD-O2D
6	H	202	CYC	CAA-CBA-CGA-O1A
6	Q	202	CYC	NC-C4C-CHD-C1D
6	U	201	CYC	NC-C4C-CHD-C1D
6	C	201	CYC	CAA-CBA-CGA-O2A
6	a	201	CYC	CAA-CBA-CGA-O1A
6	L	202	CYC	C2C-C3C-CAC-CBC
6	C	201	CYC	C2B-C1B-CHB-C4A
6	F	201	CYC	CAA-CBA-CGA-O1A
6	F	201	CYC	CAA-CBA-CGA-O2A
6	O	201	CYC	CAA-CBA-CGA-O2A
6	E	201	CYC	CAA-CBA-CGA-O2A
6	H	202	CYC	CAA-CBA-CGA-O2A
6	Q	202	CYC	CAD-CBD-CGD-O2D
6	U	202	CYC	CAA-CBA-CGA-O2A
6	H	201	CYC	C4C-C3C-CAC-CBC
6	D	202	CYC	CAD-CBD-CGD-O2D
6	L	202	CYC	CAA-CBA-CGA-O2A
6	S	201	CYC	CAA-CBA-CGA-O2A
6	S	202	CYC	CAA-CBA-CGA-O2A
6	J	201	CYC	CAD-CBD-CGD-O2D
6	W	201	CYC	CAD-CBD-CGD-O2D
6	F	202	CYC	CAA-CBA-CGA-O2A
6	Q	202	CYC	CAA-CBA-CGA-O2A
6	L	202	CYC	CAA-CBA-CGA-O1A
6	W	201	CYC	CAA-CBA-CGA-O2A
6	a	201	CYC	CAD-CBD-CGD-O2D
6	N	201	CYC	C2B-C3B-CAB-CBB
6	J	201	CYC	CAA-CBA-CGA-O2A
6	S	202	CYC	CAA-CBA-CGA-O1A
6	P	201	CYC	C2B-C1B-CHB-C4A
6	S	201	CYC	CAA-CBA-CGA-O1A
6	D	201	CYC	CAA-CBA-CGA-O2A
6	O	202	CYC	CAD-CBD-CGD-O2D
6	Y	201	CYC	CAA-CBA-CGA-O2A
6	B	202	CYC	CAA-CBA-CGA-O2A
6	F	202	CYC	CAD-CBD-CGD-O2D
6	S	201	CYC	C3D-CAD-CBD-CGD
6	W	201	CYC	C3D-CAD-CBD-CGD
6	D	201	CYC	CAA-CBA-CGA-O1A
6	F	202	CYC	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	Q	201	CYC	CAA-CBA-CGA-O1A
6	Q	202	CYC	CAD-CBD-CGD-O1D
6	W	201	CYC	CAD-CBD-CGD-O1D
6	J	201	CYC	CAA-CBA-CGA-O1A
6	N	201	CYC	CAD-CBD-CGD-O2D
6	W	201	CYC	CAA-CBA-CGA-O1A
6	D	202	CYC	CAD-CBD-CGD-O1D
6	F	202	CYC	CAD-CBD-CGD-O1D
6	J	201	CYC	CAD-CBD-CGD-O1D
6	Q	201	CYC	CAA-CBA-CGA-O2A
6	N	201	CYC	CAD-CBD-CGD-O1D
6	O	202	CYC	CAD-CBD-CGD-O1D
6	R	201	CYC	CAD-CBD-CGD-O2D
6	Y	202	CYC	CAD-CBD-CGD-O2D
6	a	201	CYC	CAD-CBD-CGD-O1D
6	Y	201	CYC	CAA-CBA-CGA-O1A
6	I	201	CYC	NB-C1B-CHB-C4A
6	U	202	CYC	CAD-CBD-CGD-O1D
6	N	201	CYC	C2B-C1B-CHB-C4A
6	R	201	CYC	C2B-C3B-CAB-CBB
6	H	202	CYC	CAD-CBD-CGD-O1D
6	X	201	CYC	CAD-CBD-CGD-O2D
6	Y	202	CYC	CAD-CBD-CGD-O1D
6	R	201	CYC	CAD-CBD-CGD-O1D
6	H	202	CYC	CAD-CBD-CGD-O2D
6	U	201	CYC	CAA-CBA-CGA-O2A
6	Y	201	CYC	NC-C4C-CHD-C1D
6	U	202	CYC	CAD-CBD-CGD-O2D
6	X	201	CYC	CAD-CBD-CGD-O1D
6	Y	202	CYC	C2C-C3C-CAC-CBC
6	J	202	CYC	C2A-CAA-CBA-CGA
6	L	202	CYC	CAD-CBD-CGD-O2D

There are no ring outliers.

36 monomers are involved in 342 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	201	CYC	8	0
6	H	201	CYC	23	0
6	J	201	CYC	13	0
6	Q	201	CYC	13	0
6	O	202	CYC	18	0

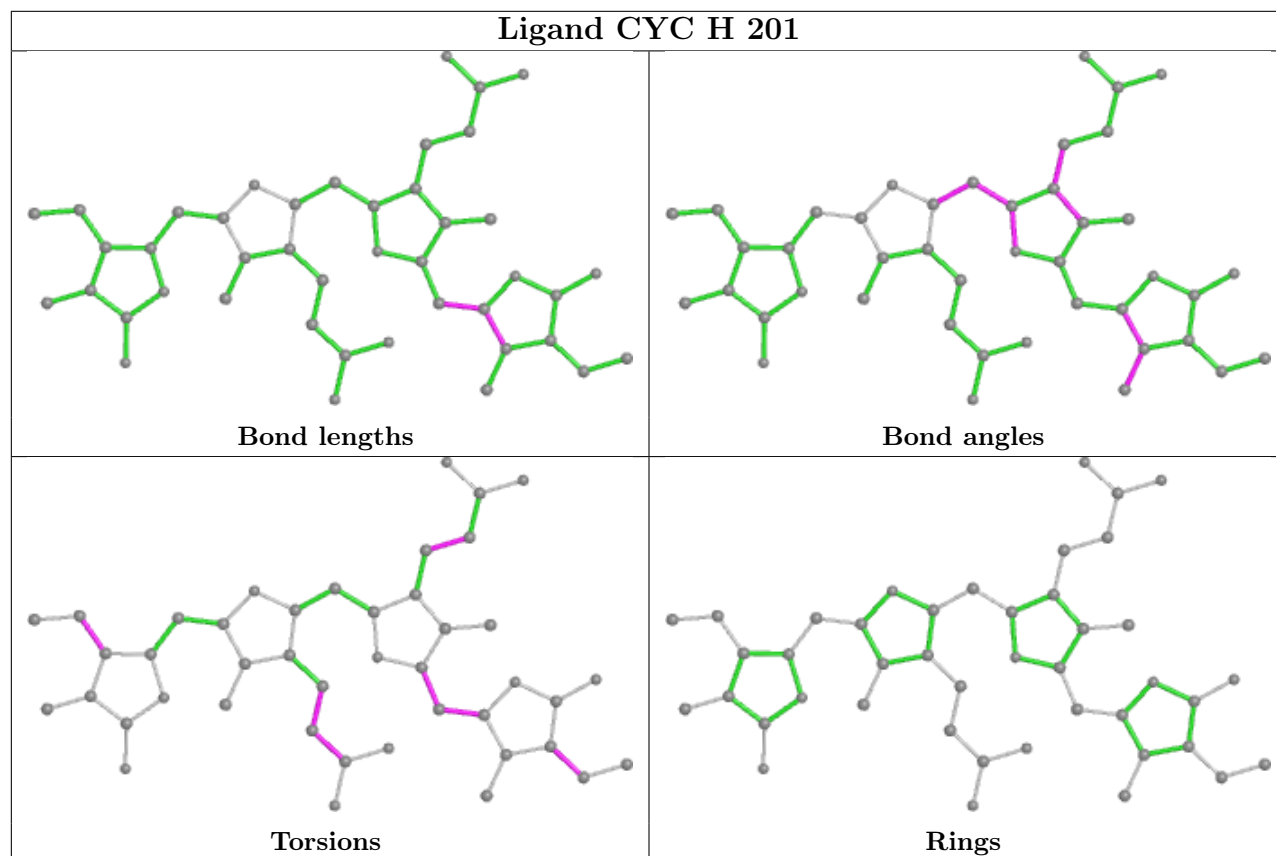
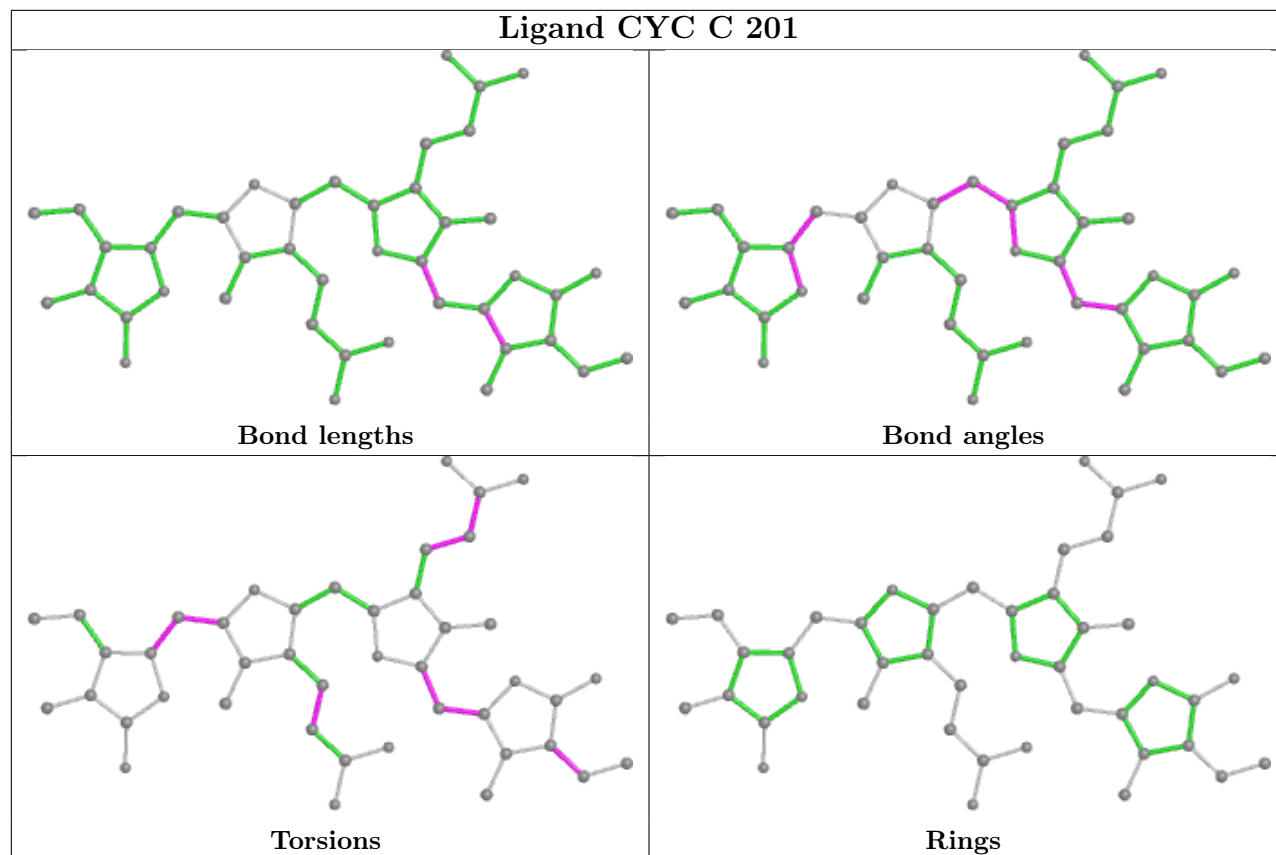
Continued on next page...

Continued from previous page...

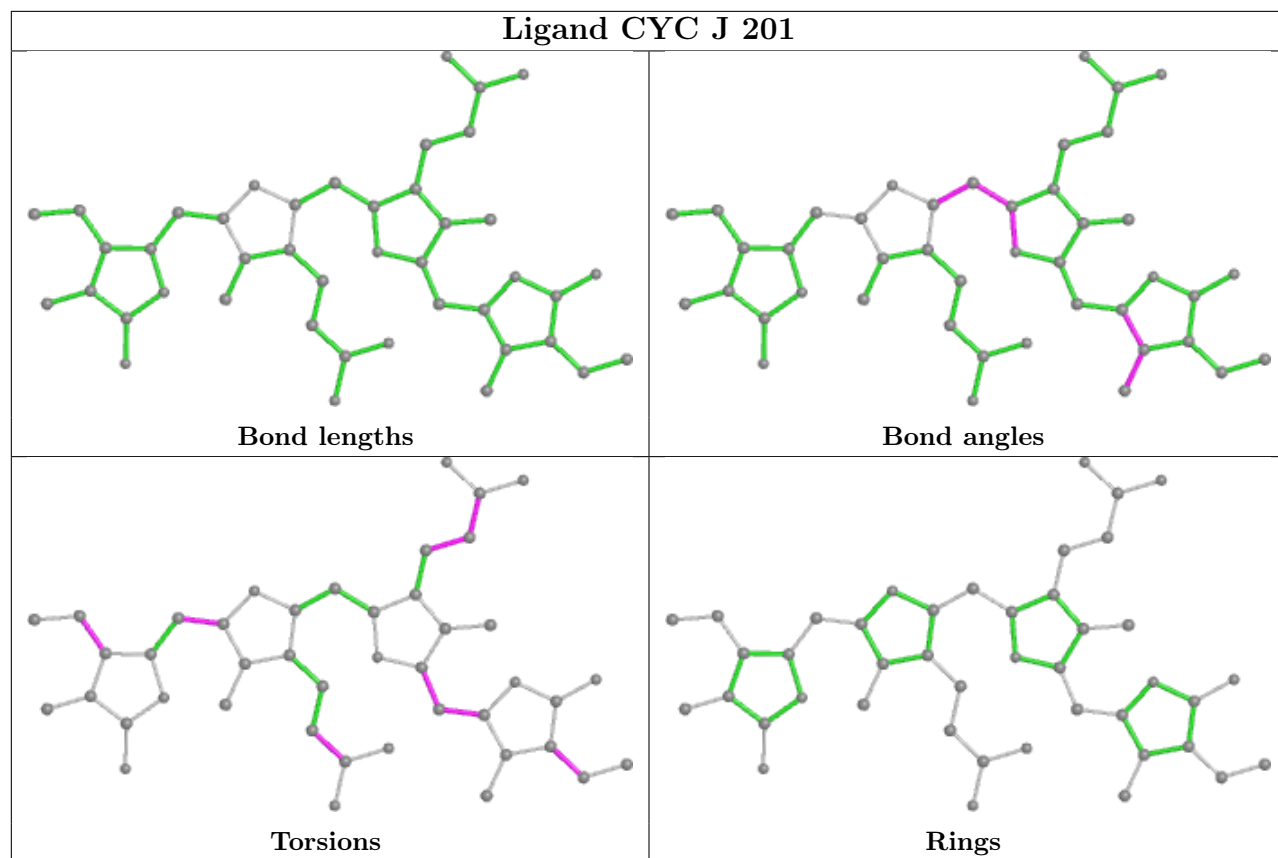
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	201	CYC	3	0
6	P	201	CYC	6	0
6	T	201	CYC	11	0
6	G	201	CYC	18	0
6	D	202	CYC	12	0
6	L	201	CYC	2	0
6	S	201	CYC	4	0
6	D	201	CYC	11	0
6	R	201	CYC	9	0
6	U	202	CYC	9	0
6	W	202	CYC	7	0
6	X	201	CYC	13	0
6	Q	202	CYC	10	0
6	V	201	CYC	7	0
6	I	201	CYC	7	0
6	N	201	CYC	5	0
6	a	201	CYC	7	0
6	E	201	CYC	3	0
6	S	202	CYC	8	0
6	O	201	CYC	7	0
6	H	202	CYC	6	0
6	J	202	CYC	6	0
6	Y	201	CYC	5	0
6	F	201	CYC	7	0
6	B	202	CYC	12	0
6	W	201	CYC	11	0
6	Y	202	CYC	16	0
6	K	201	CYC	11	0
6	L	202	CYC	5	0
6	F	202	CYC	14	0
6	U	201	CYC	15	0

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

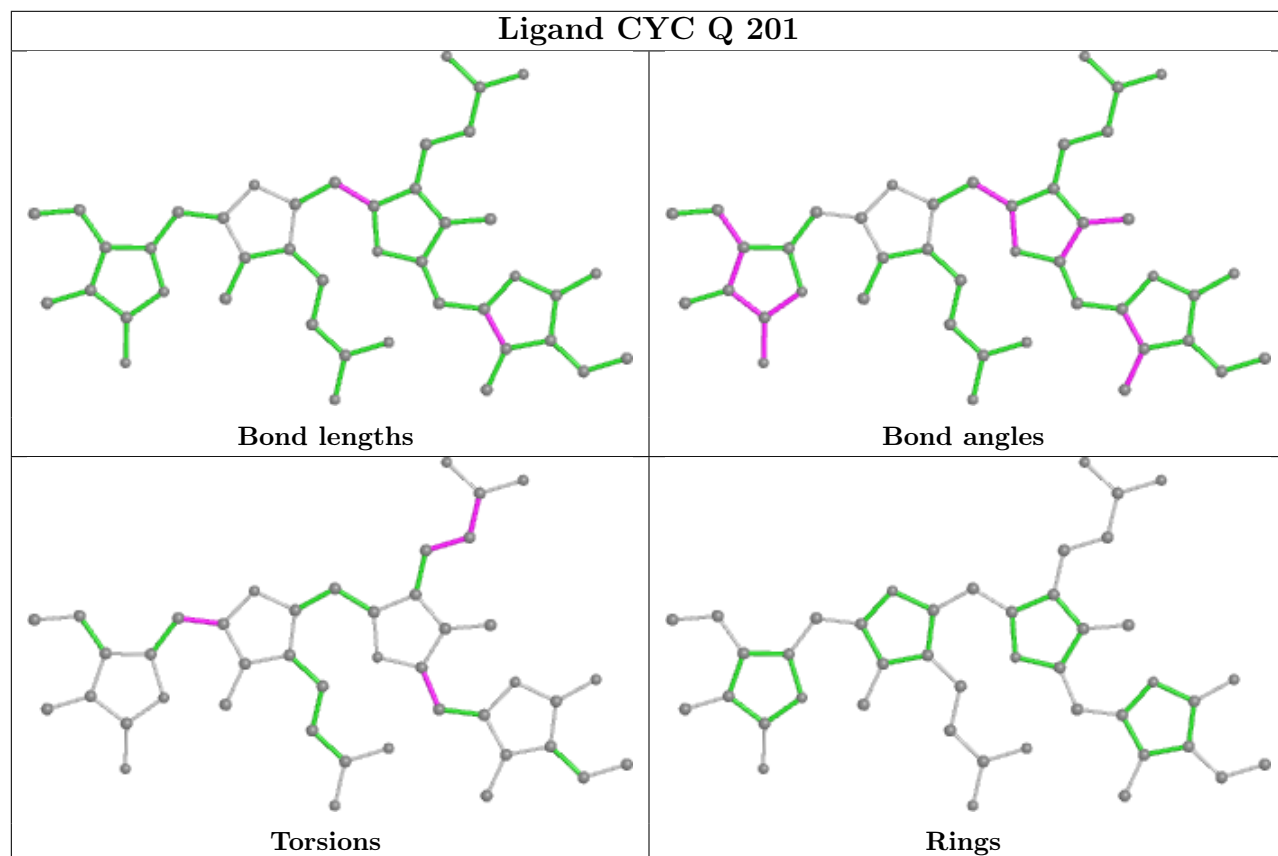
equivalents in the CSD to analyse the geometry.

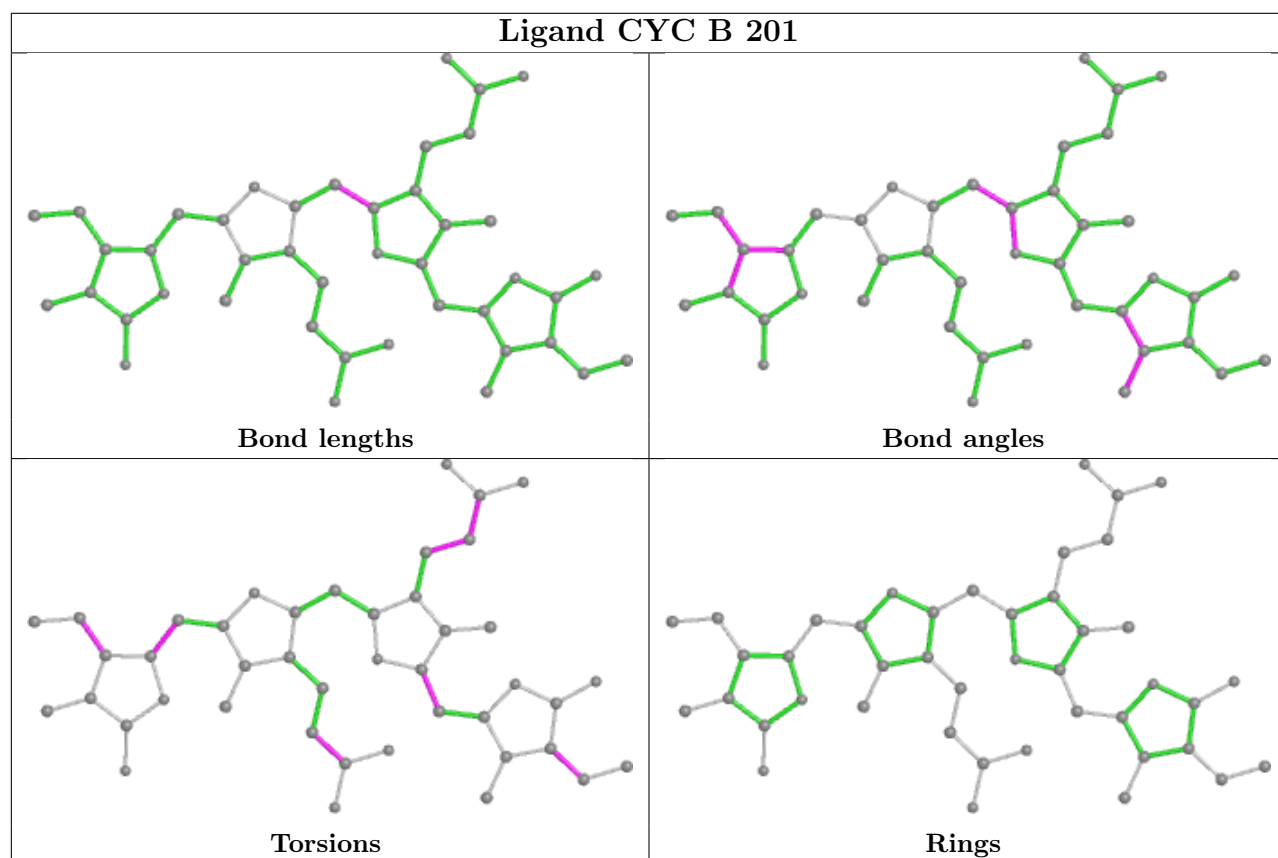
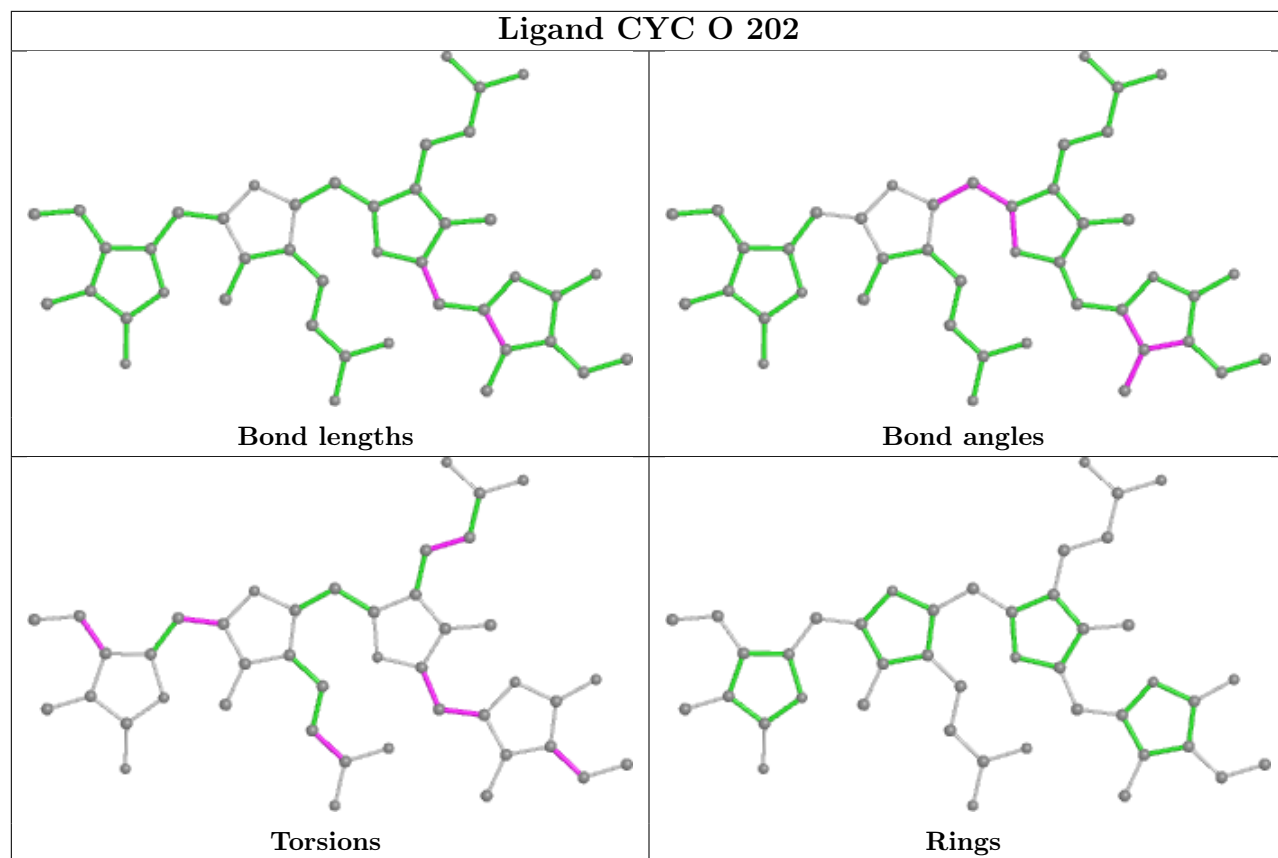


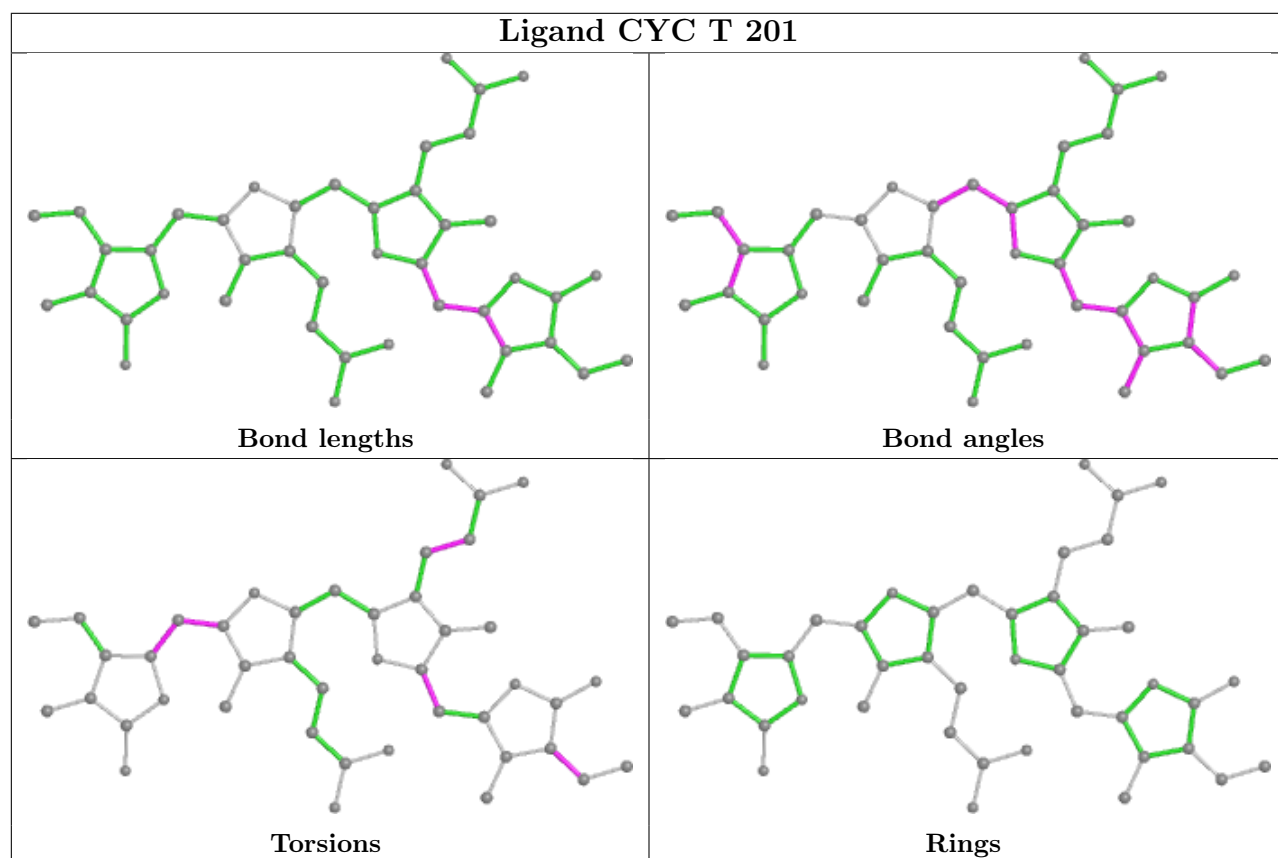
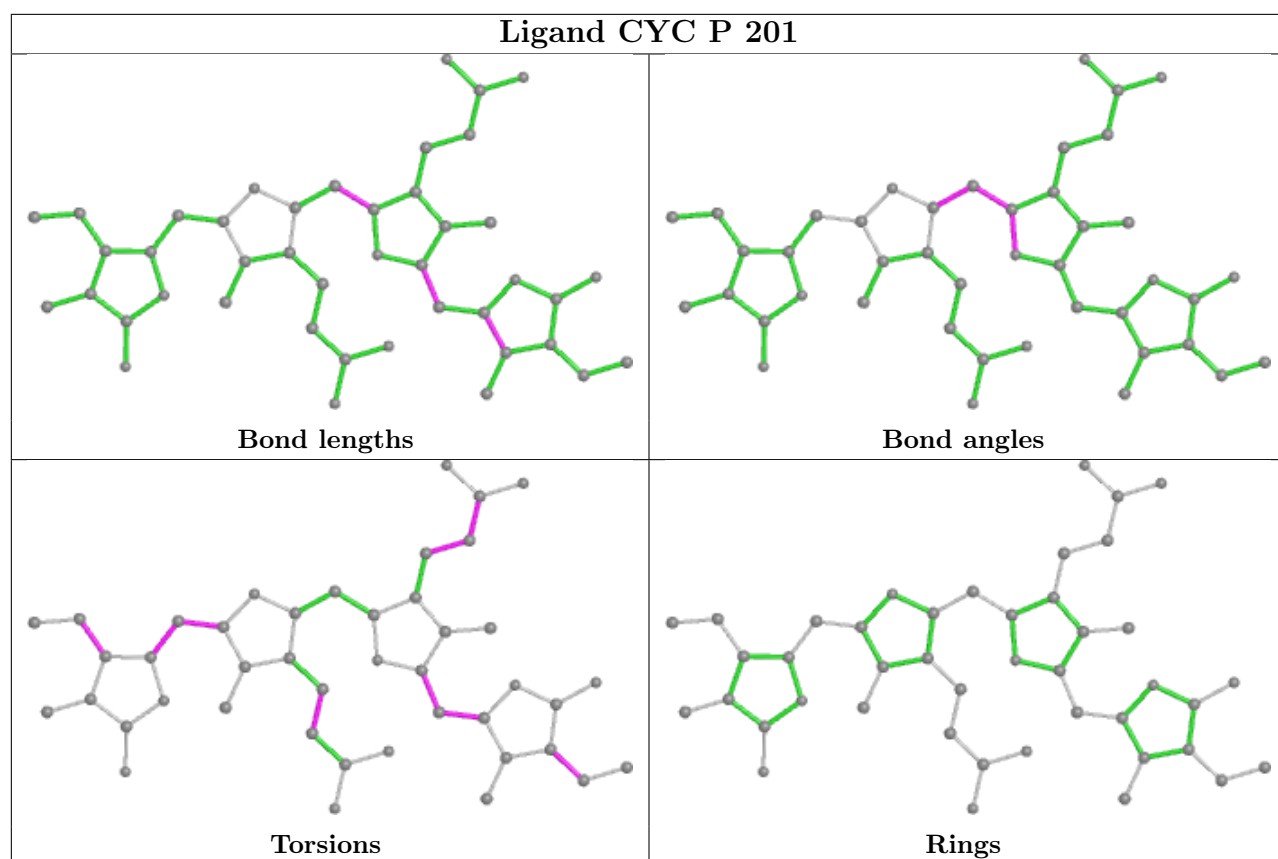
Ligand CYC J 201

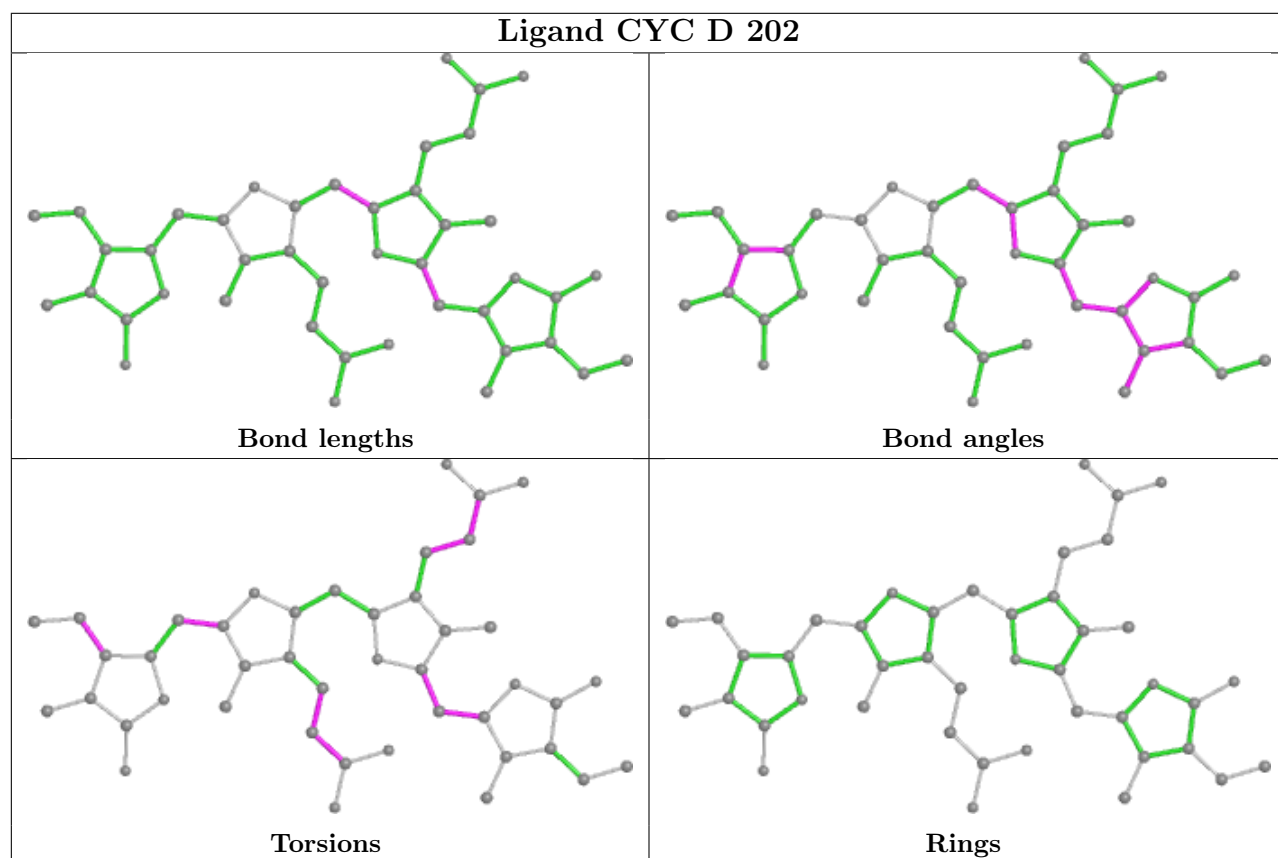
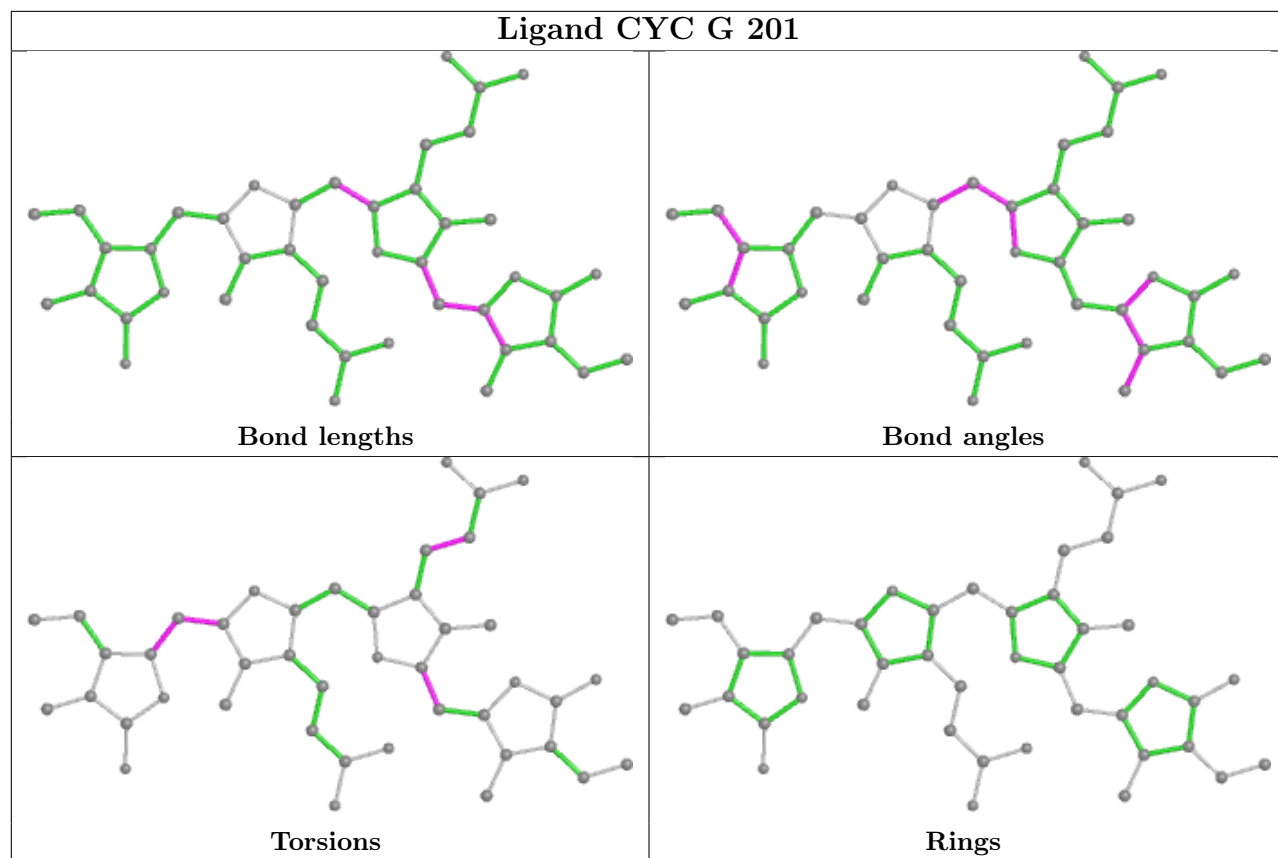


Ligand CYC Q 201

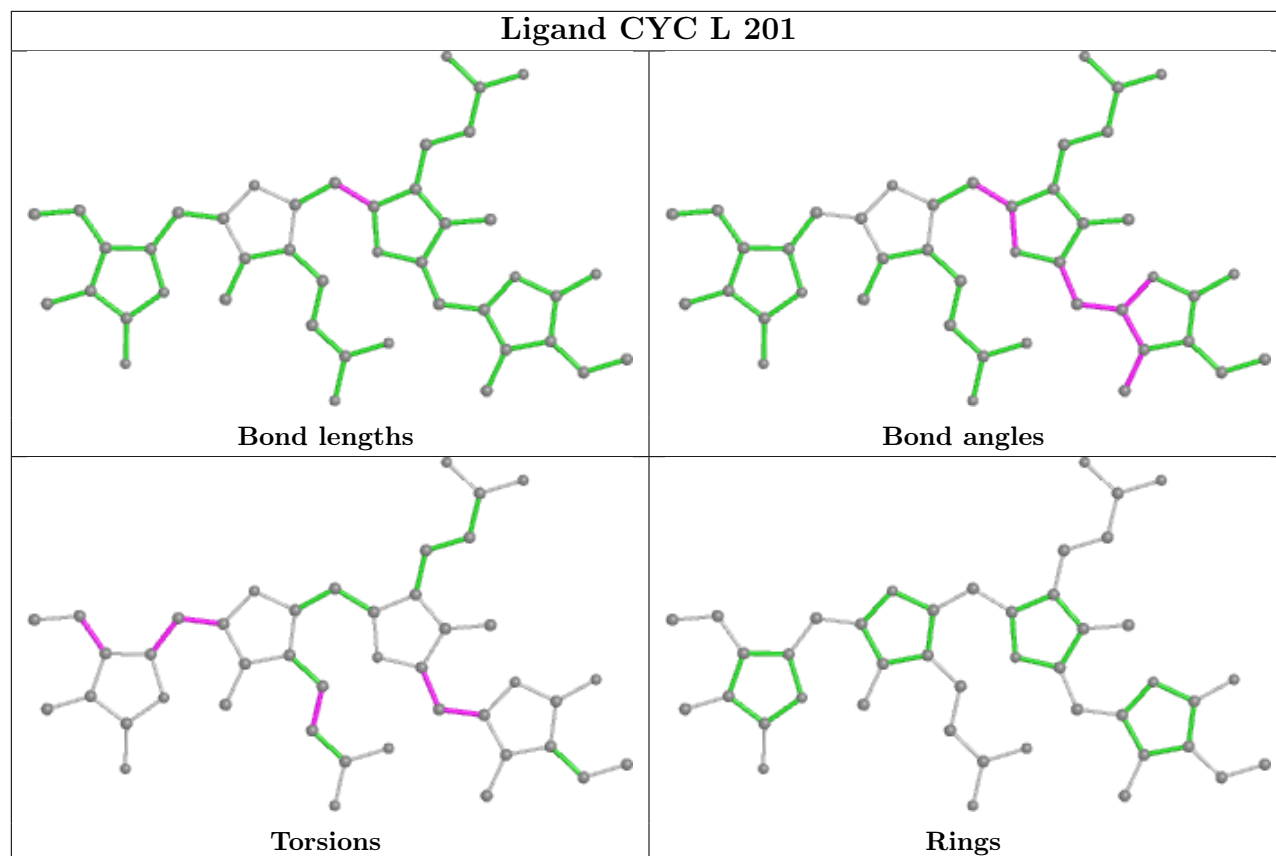




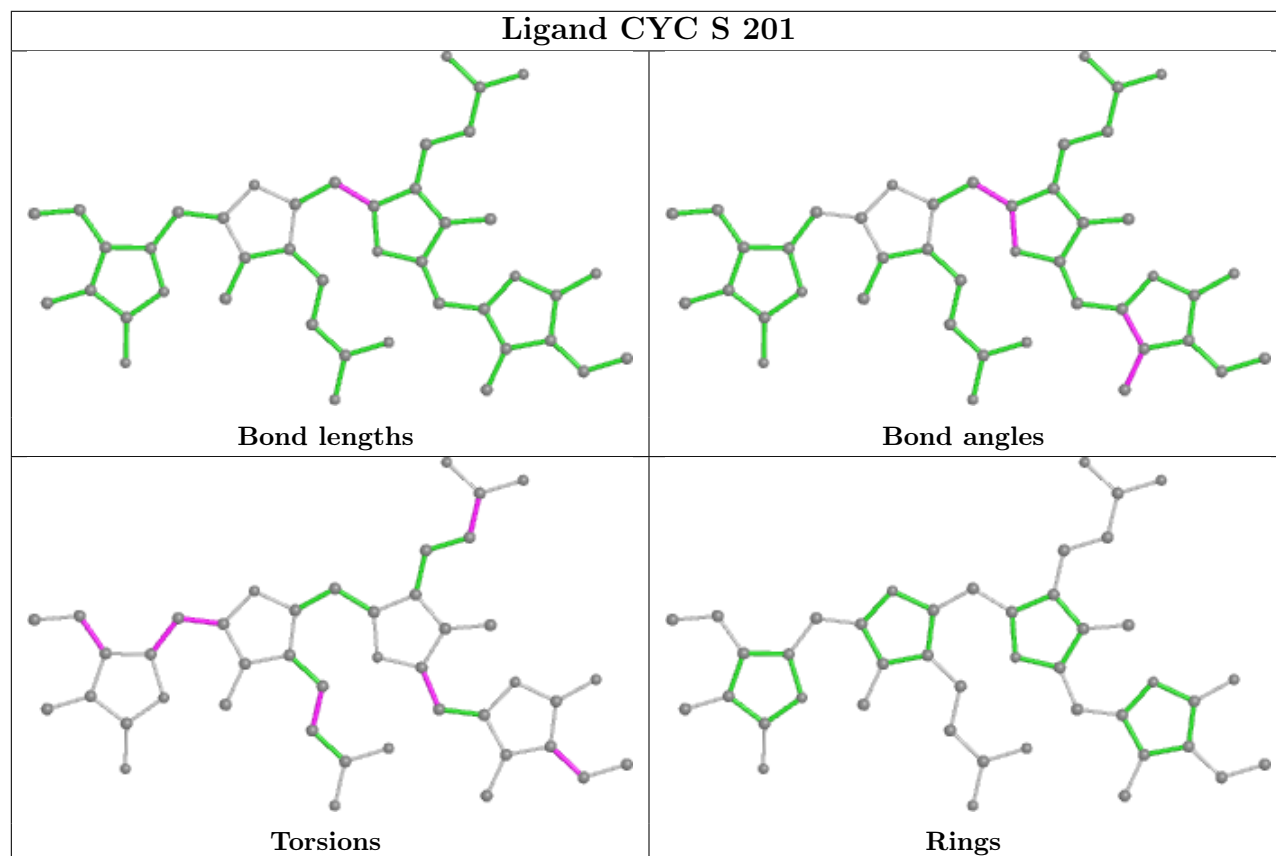


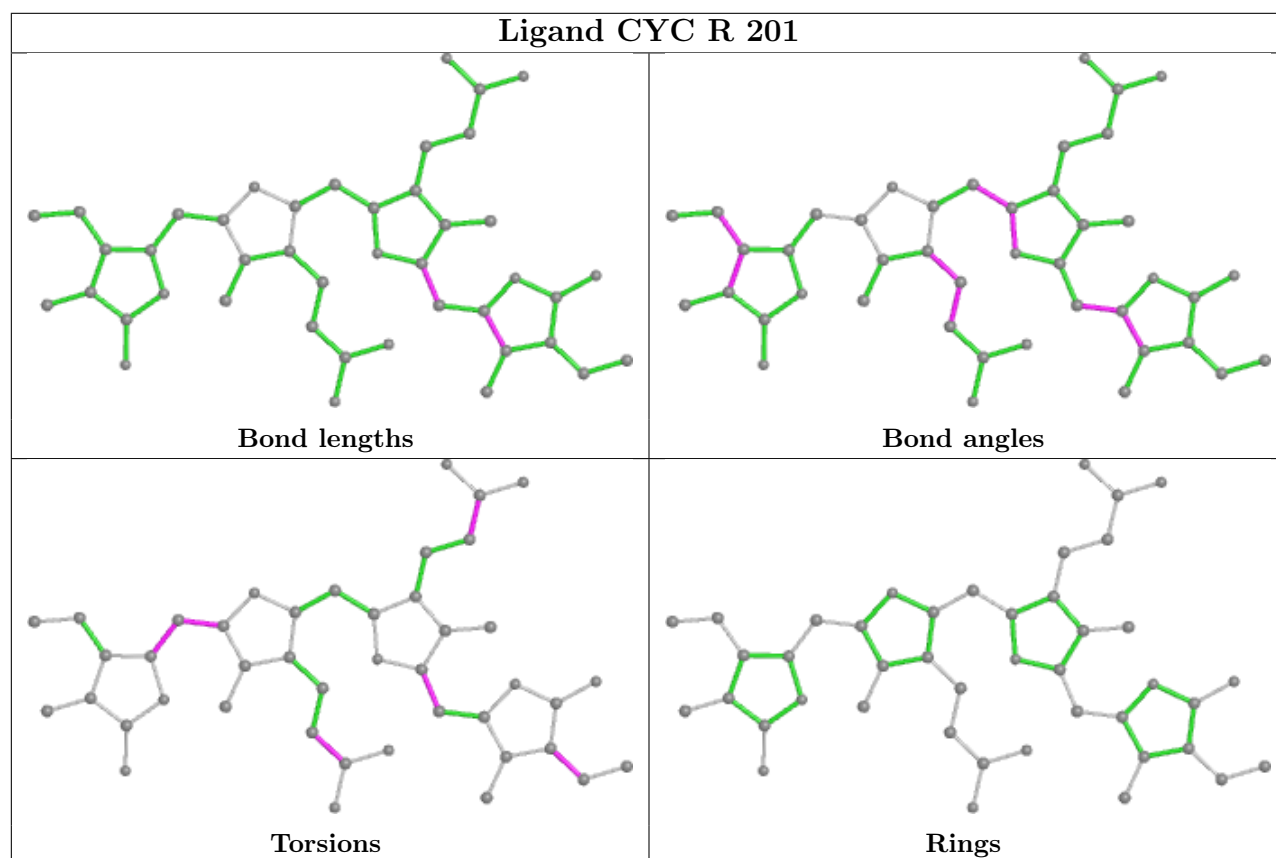
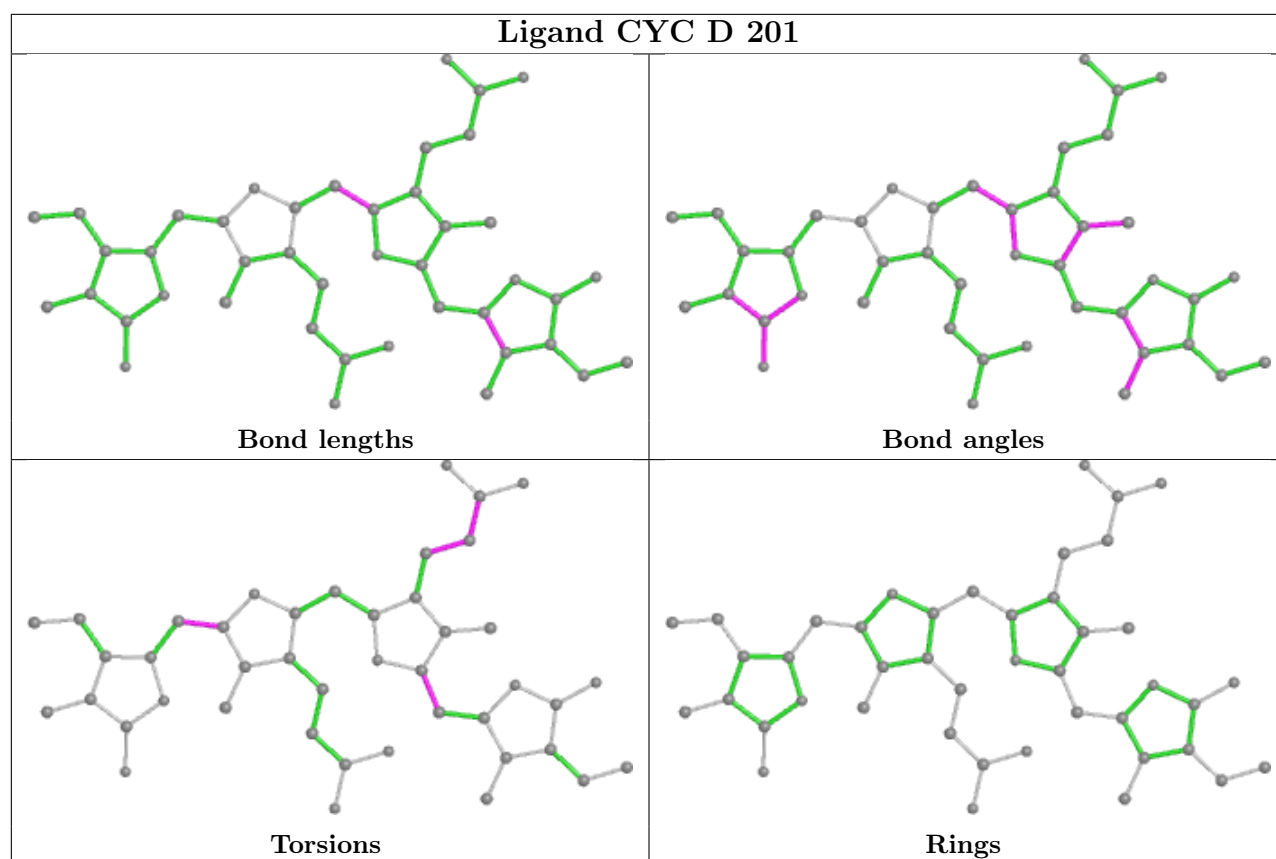


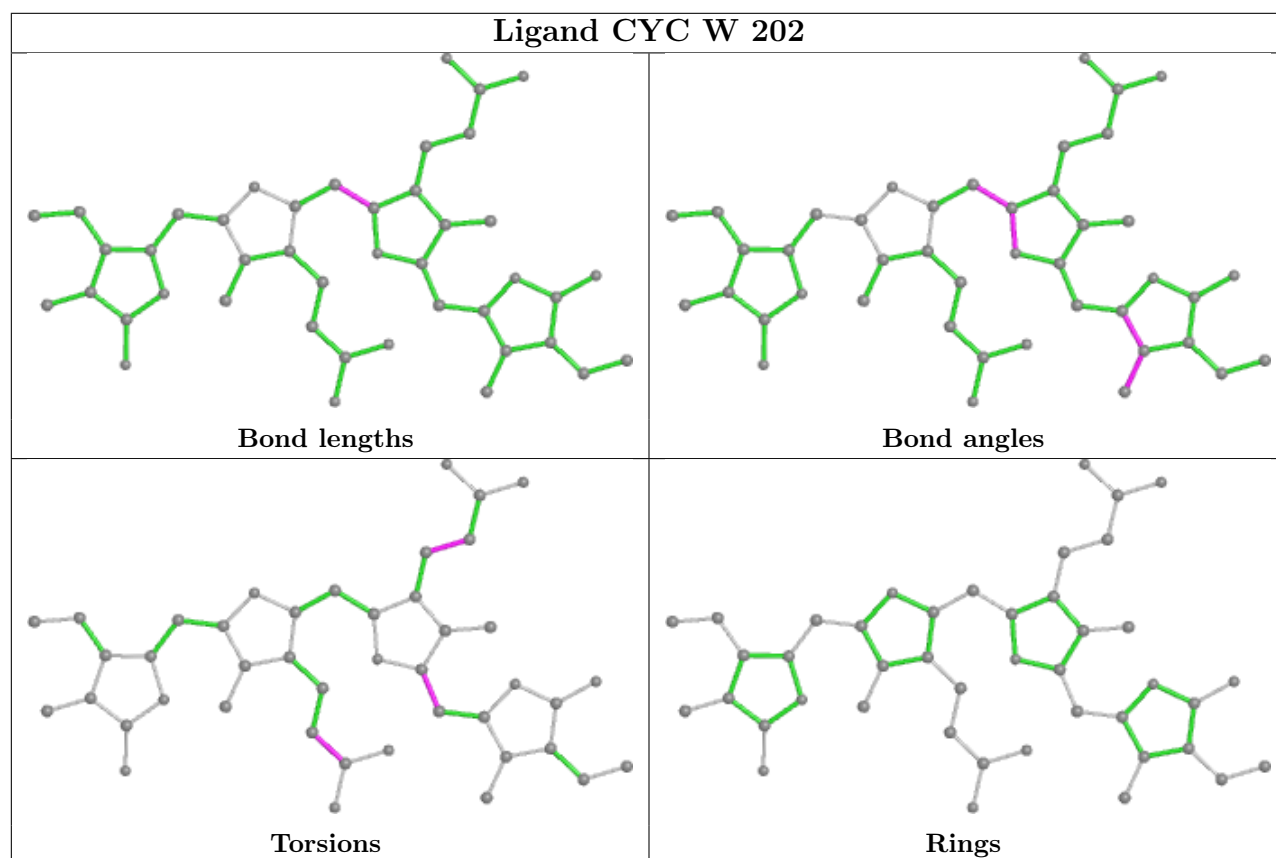
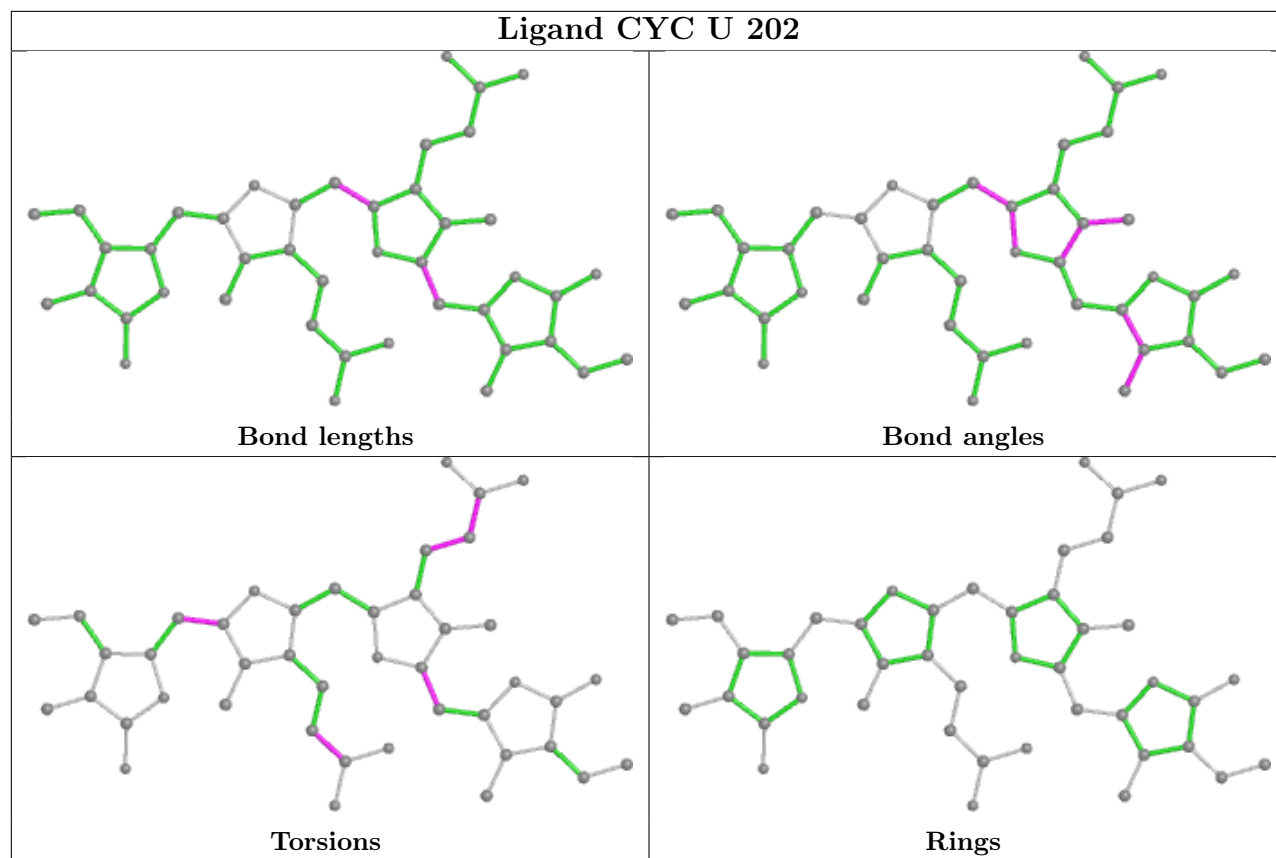
Ligand CYC L 201

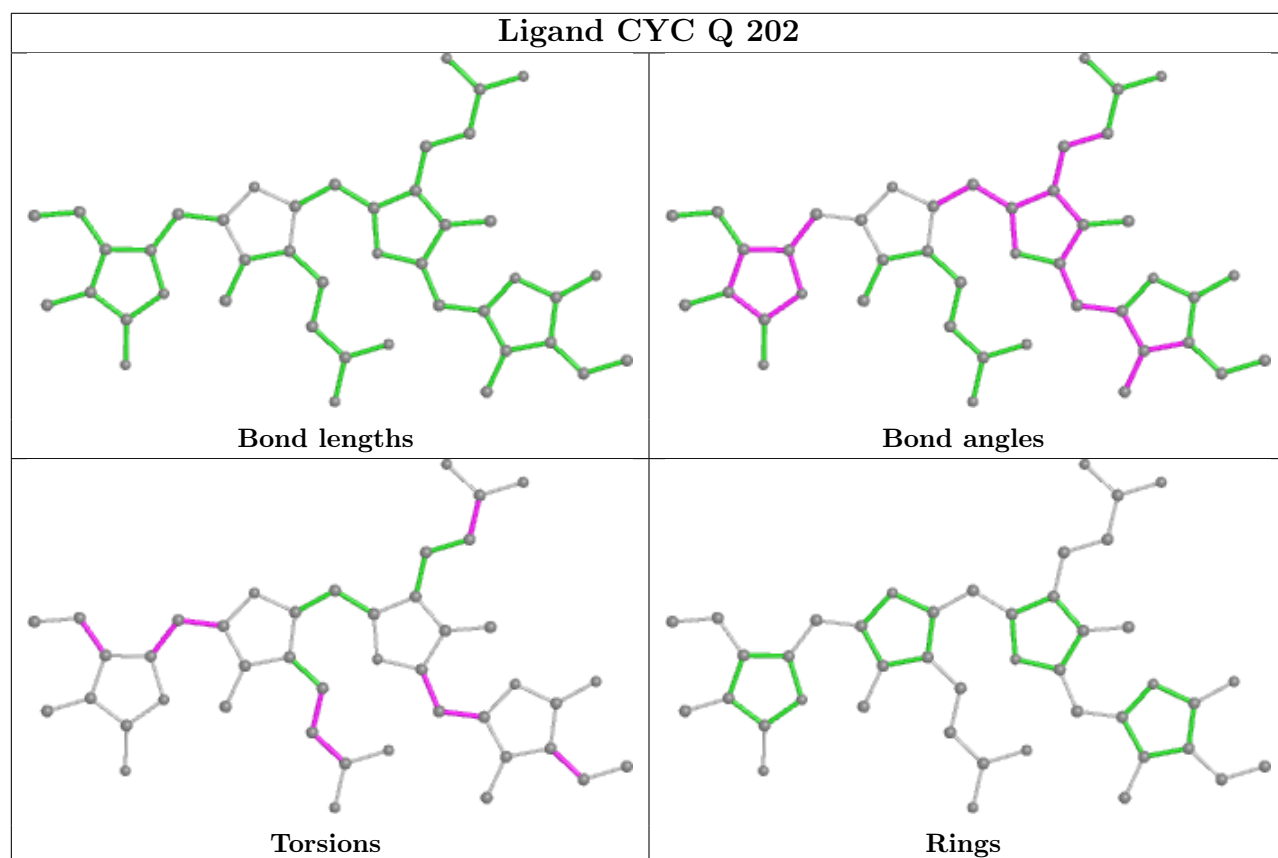
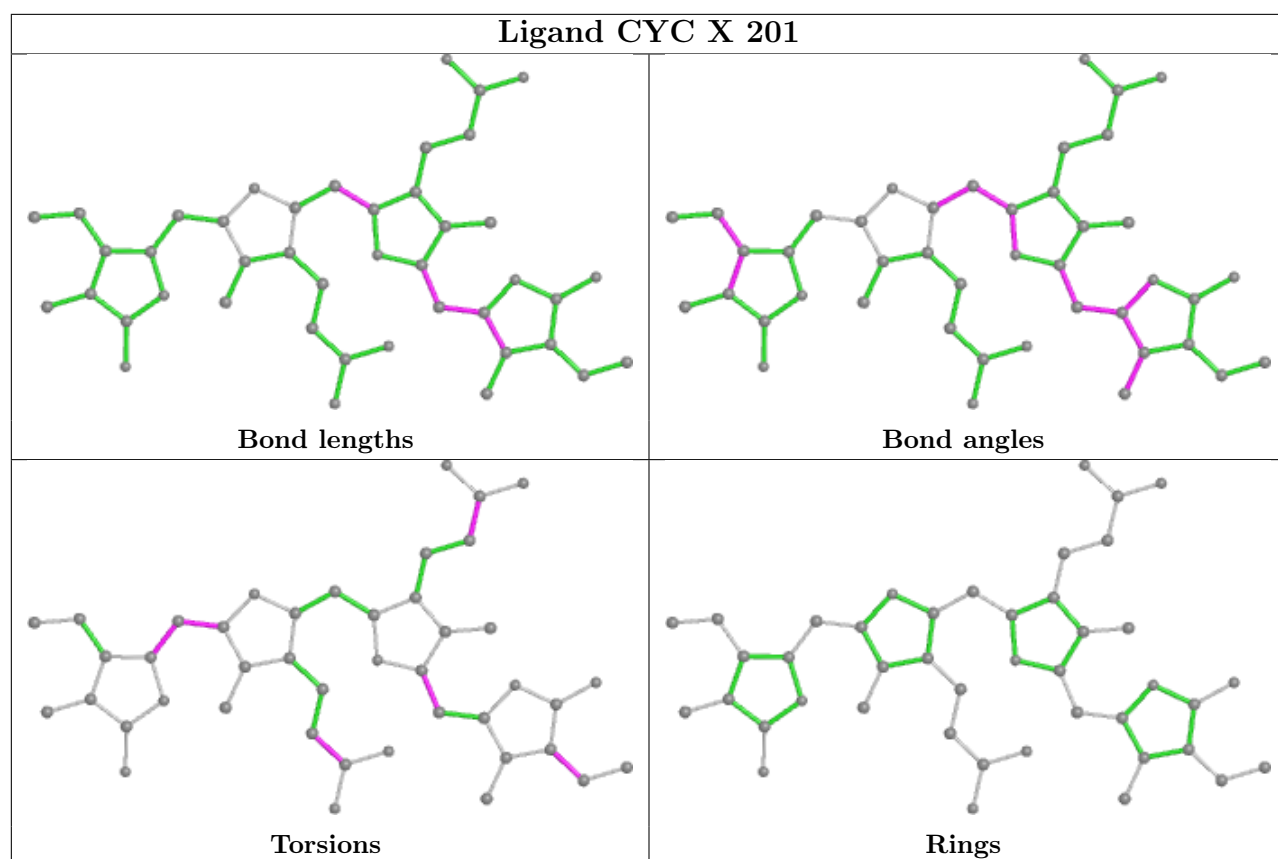


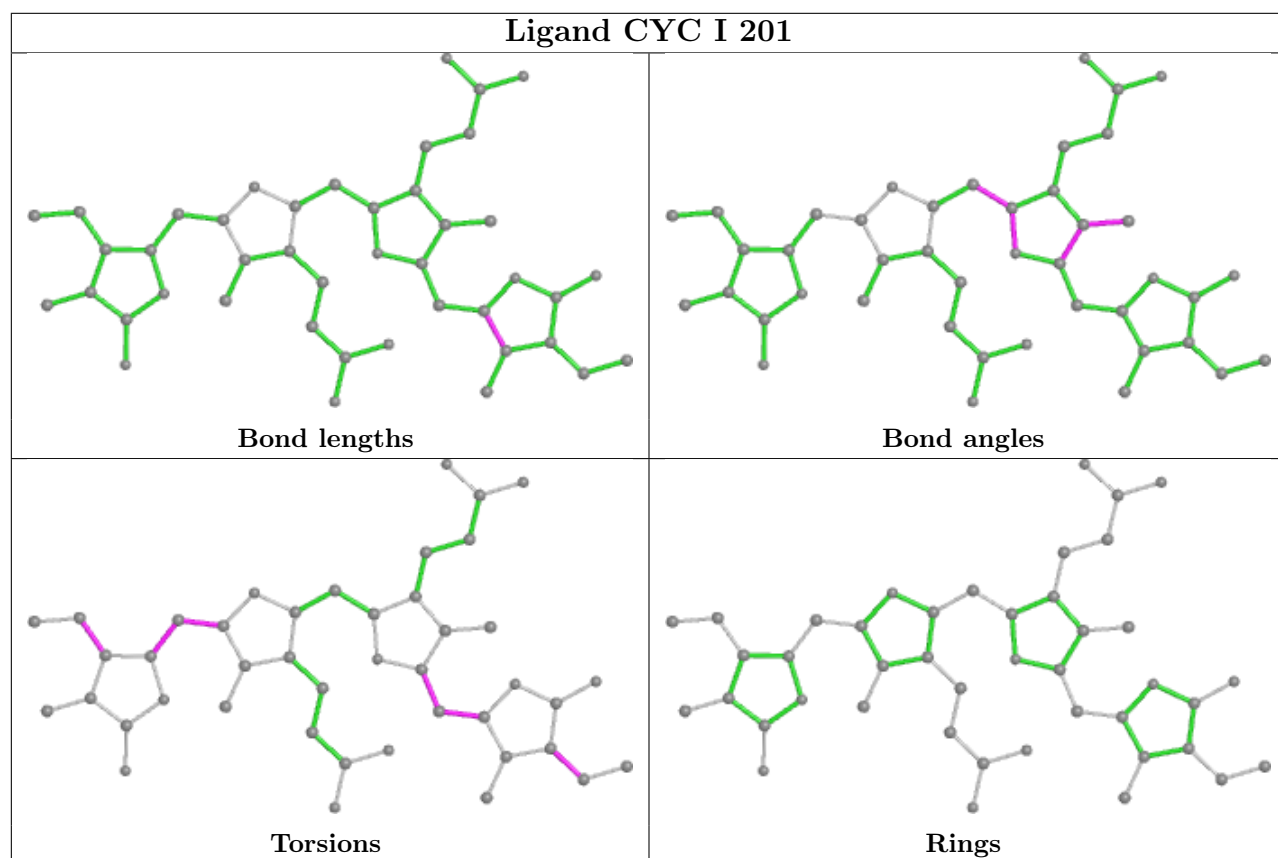
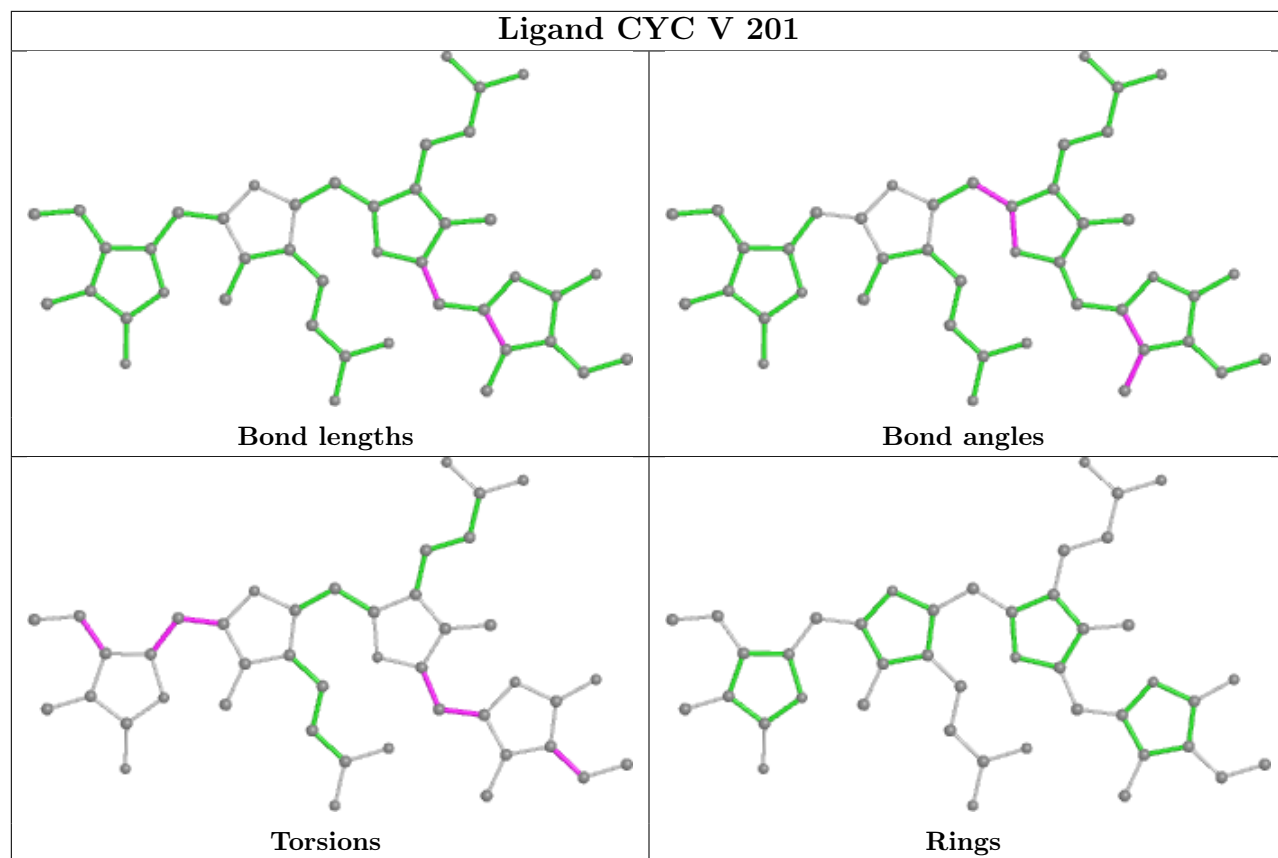
Ligand CYC S 201

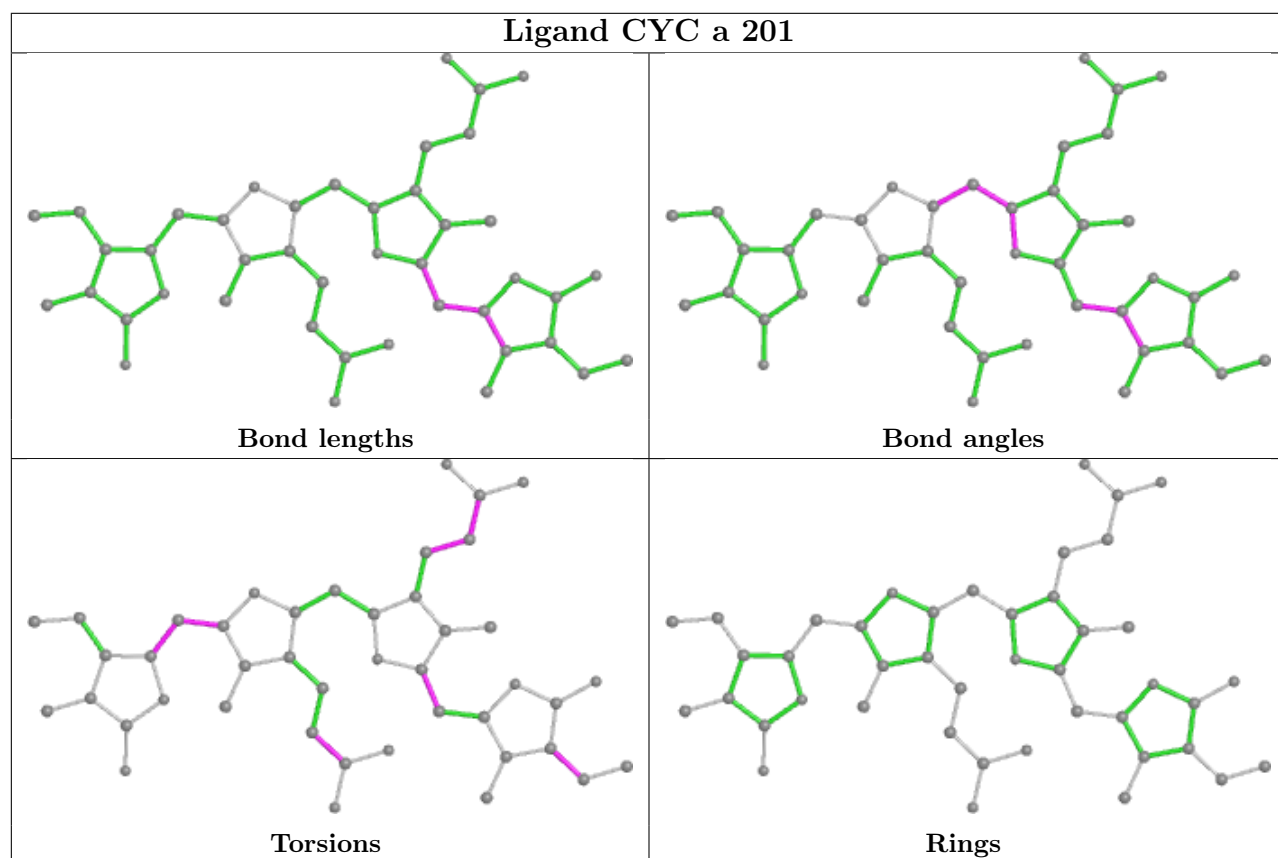
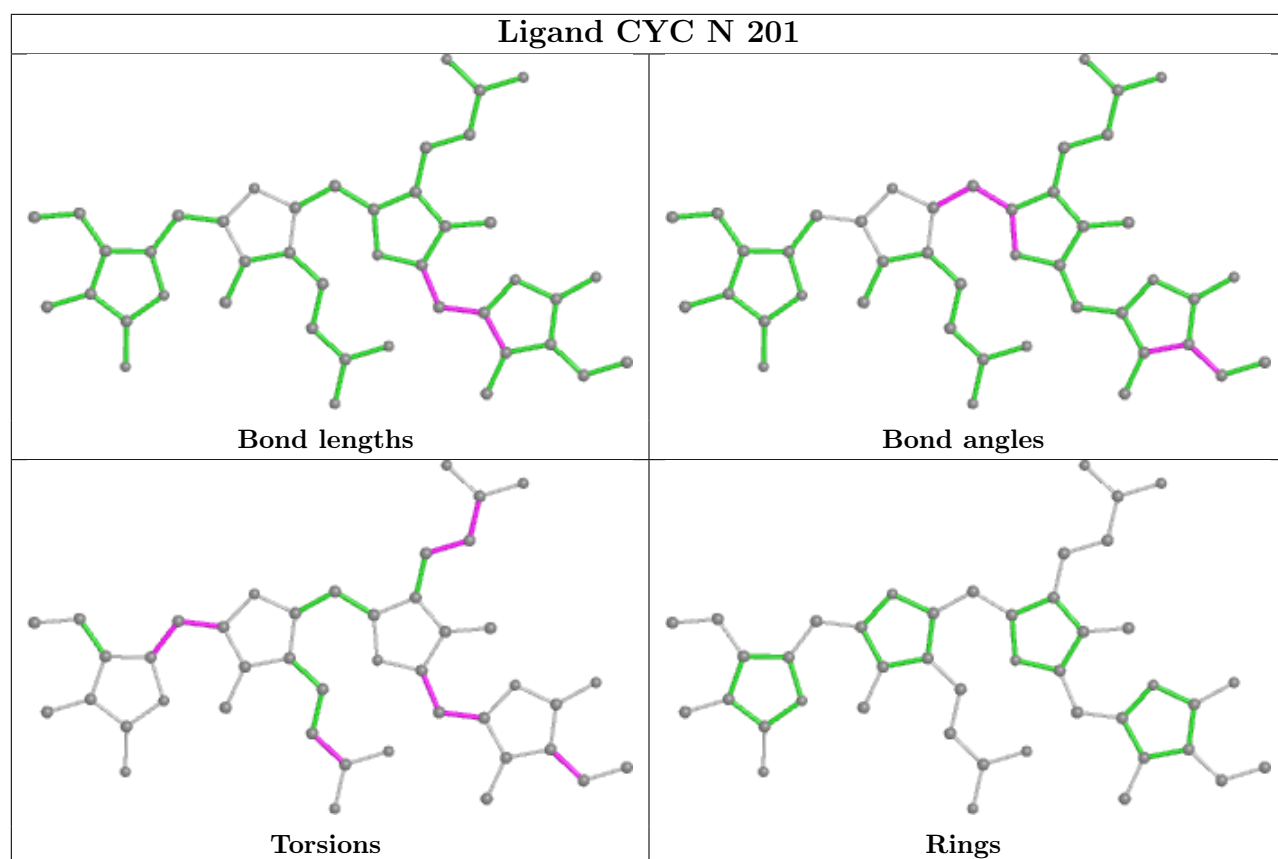


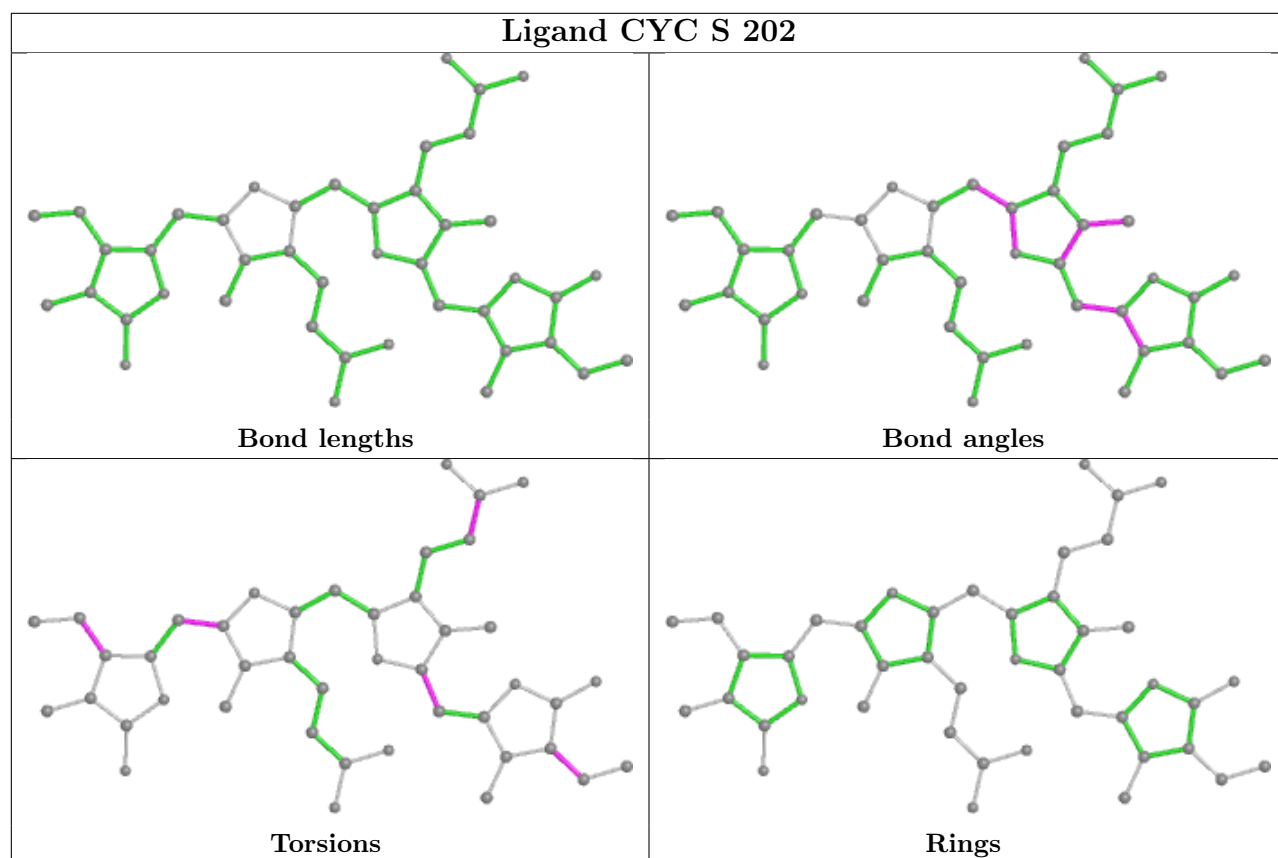
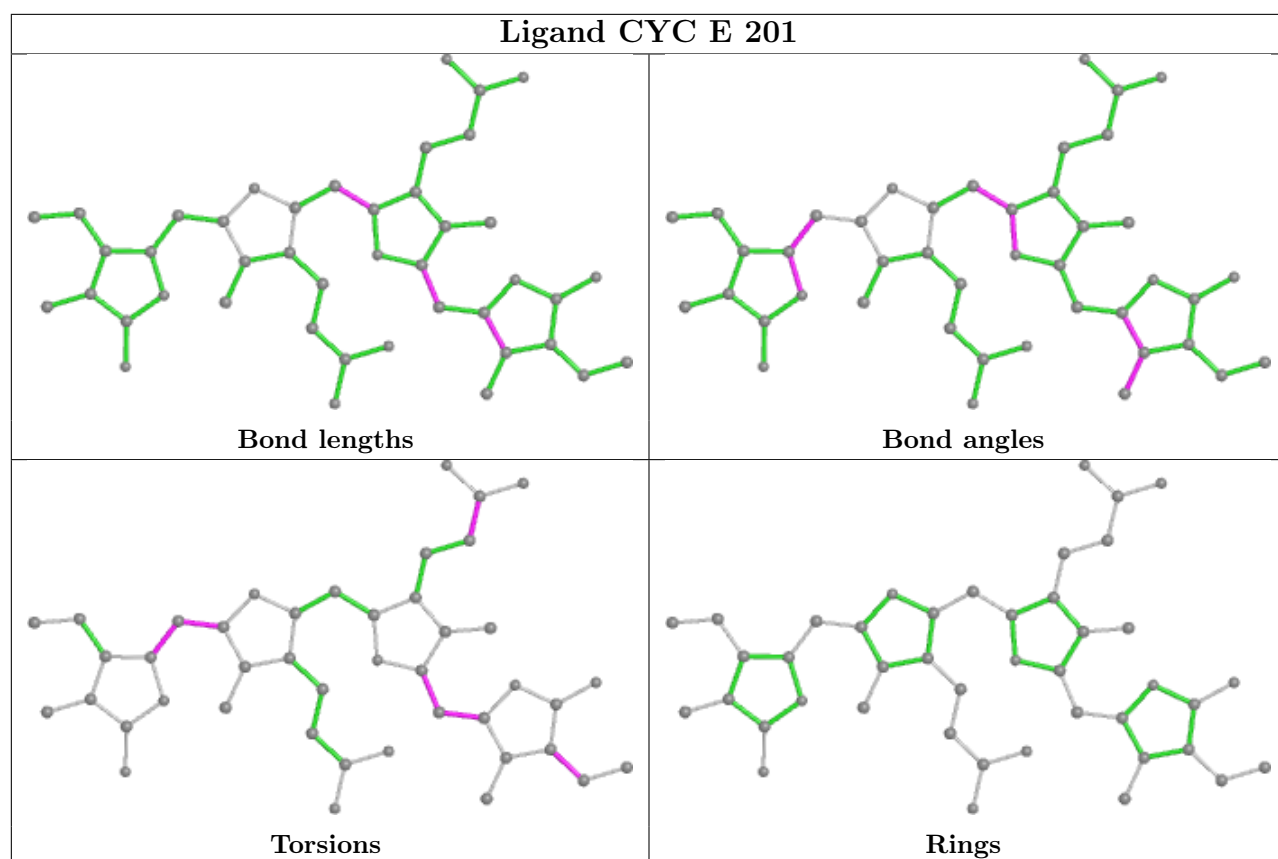


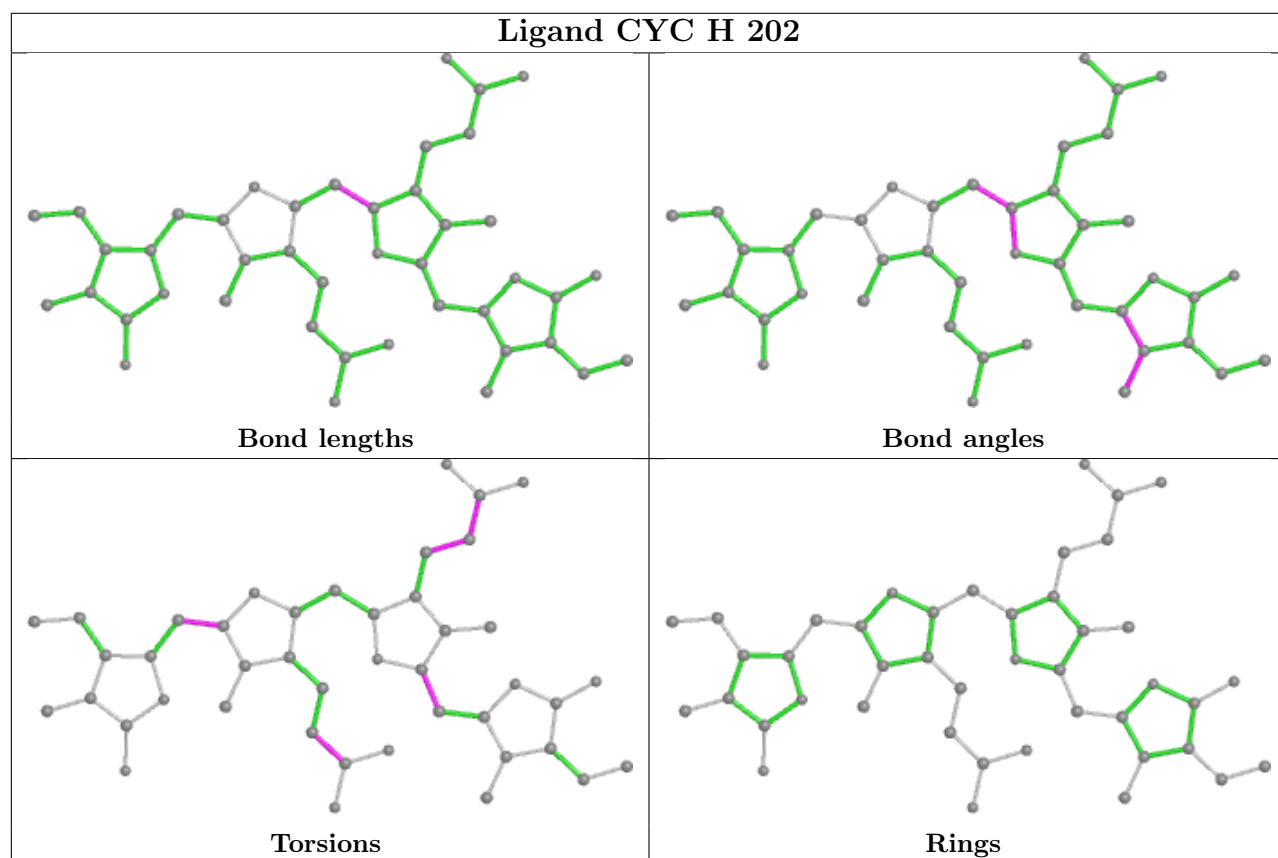
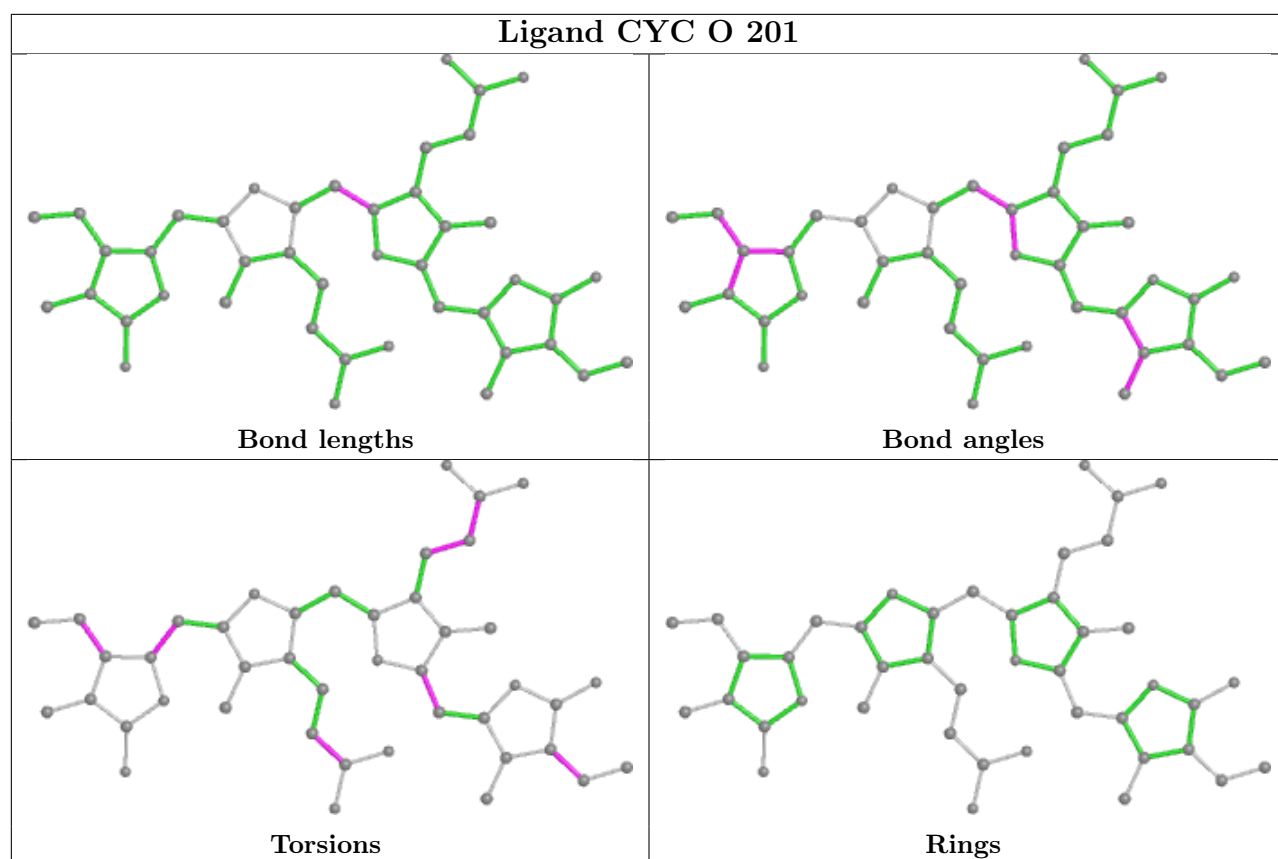




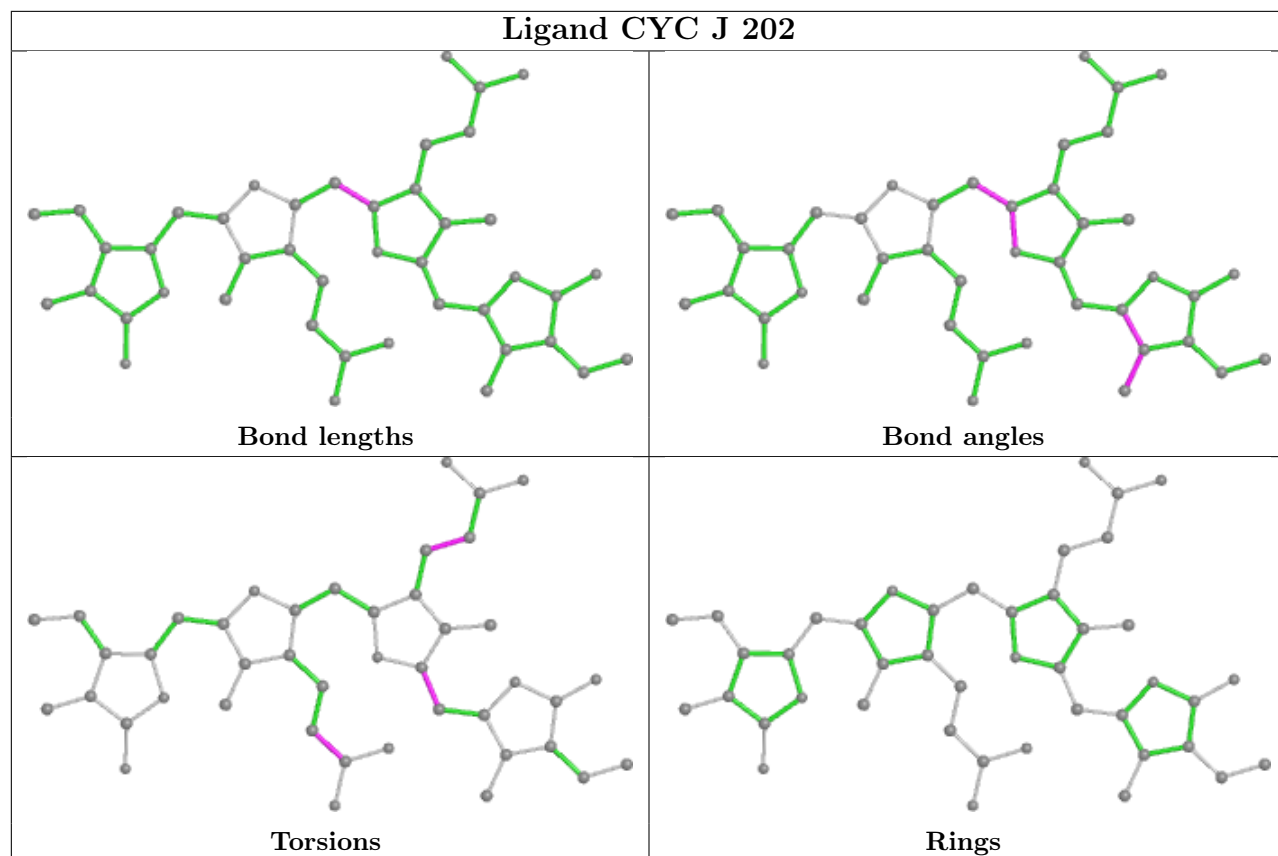




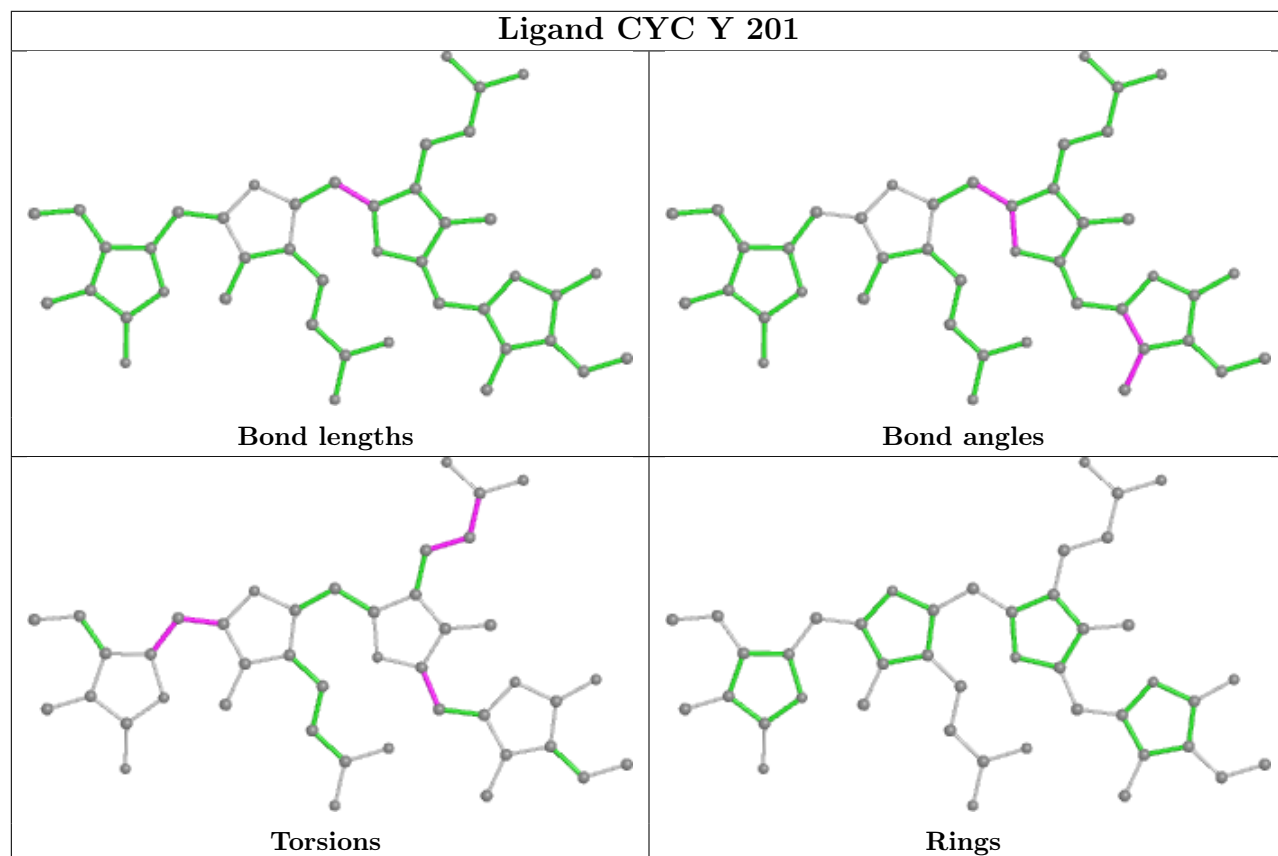




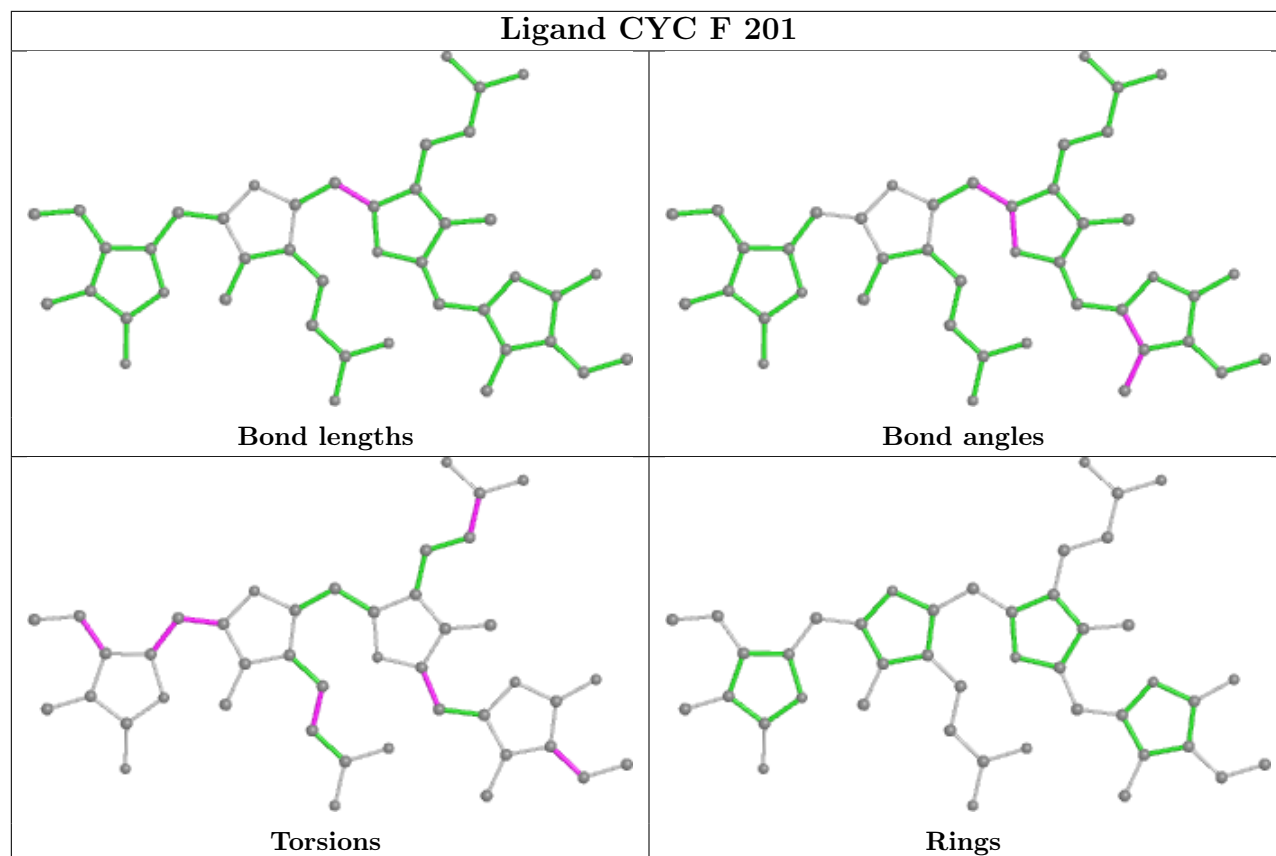
Ligand CYC J 202



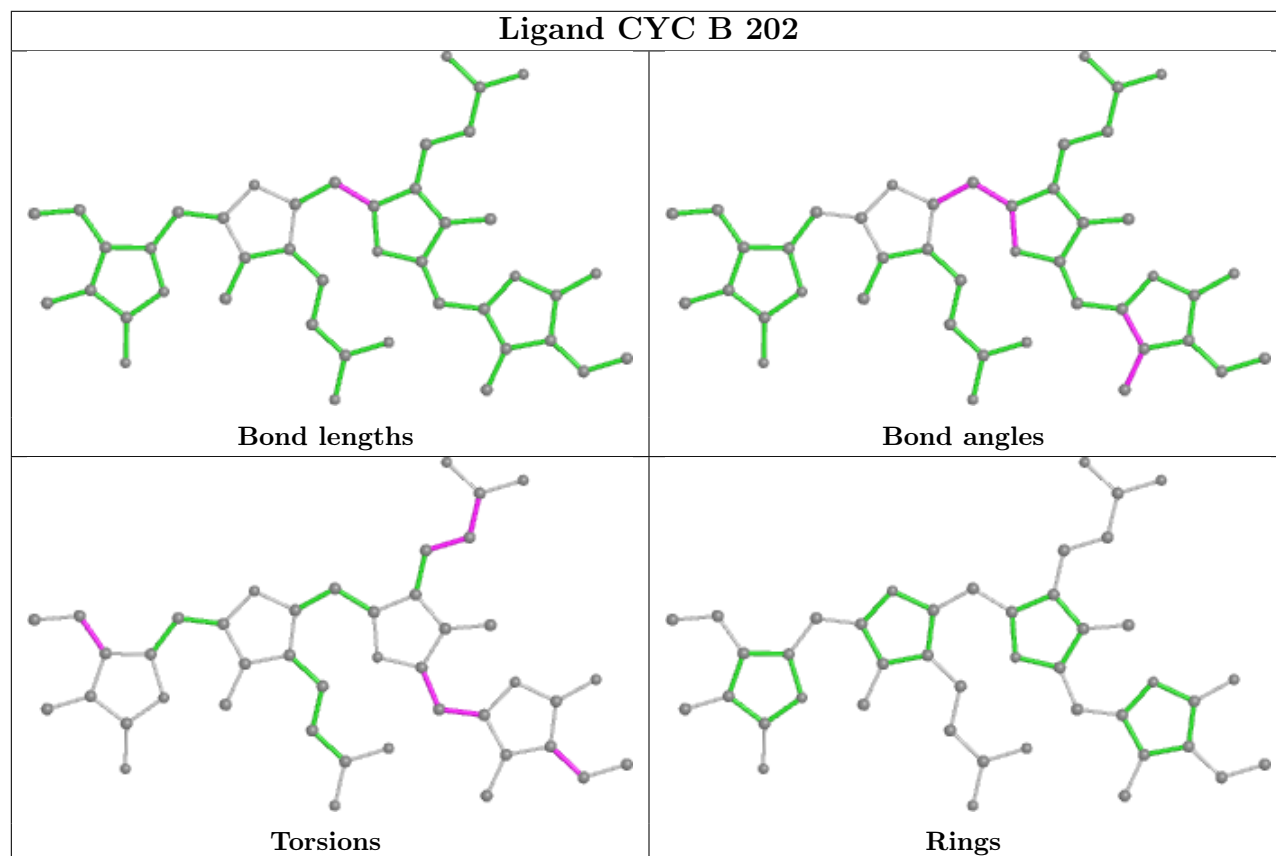
Ligand CYC Y 201

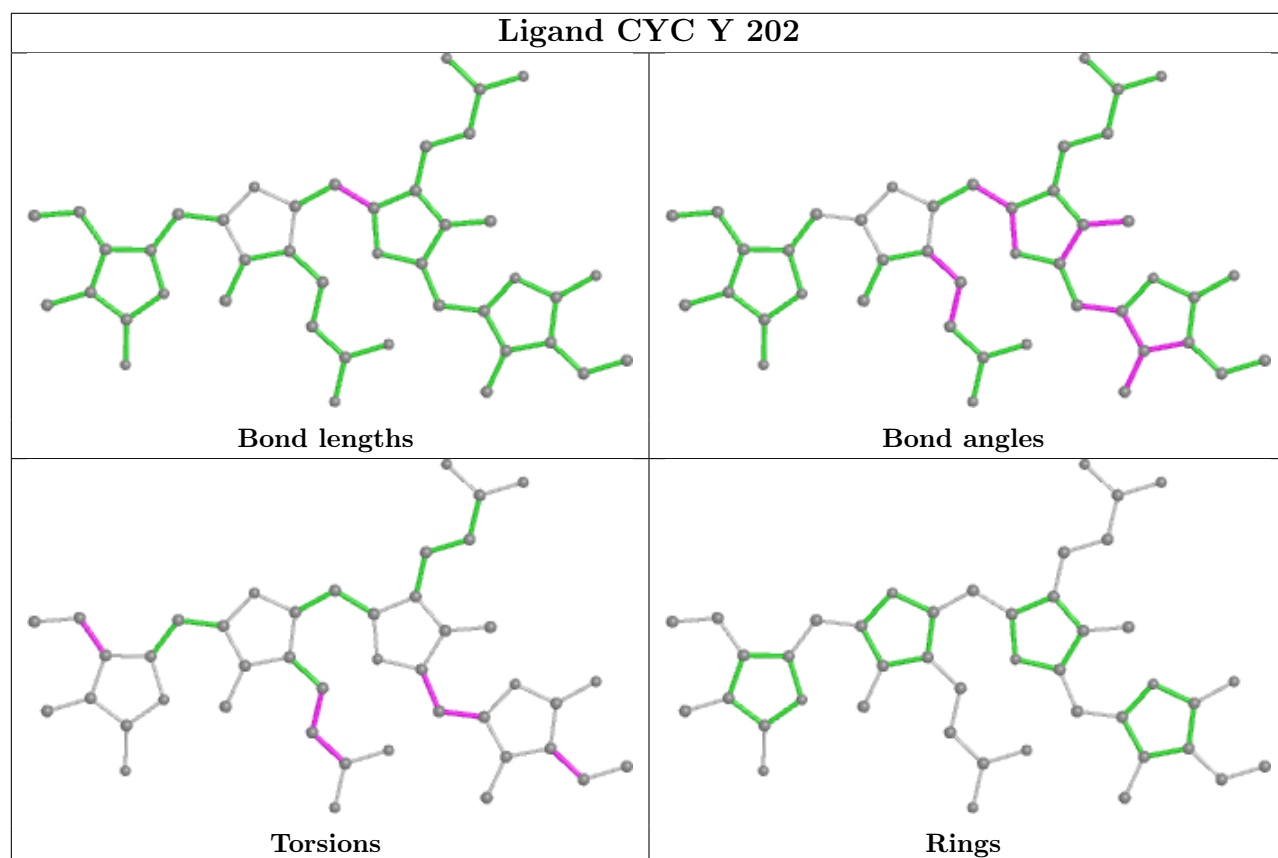
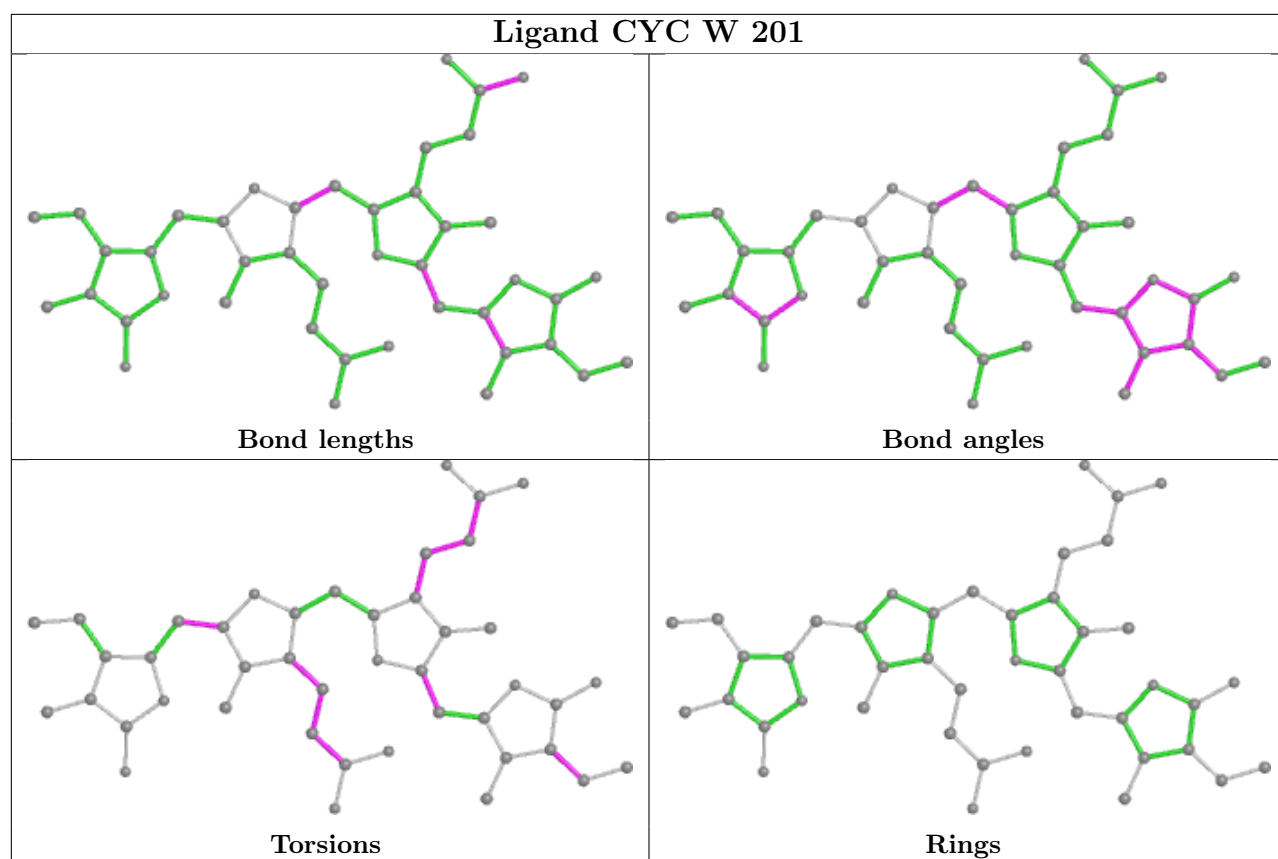


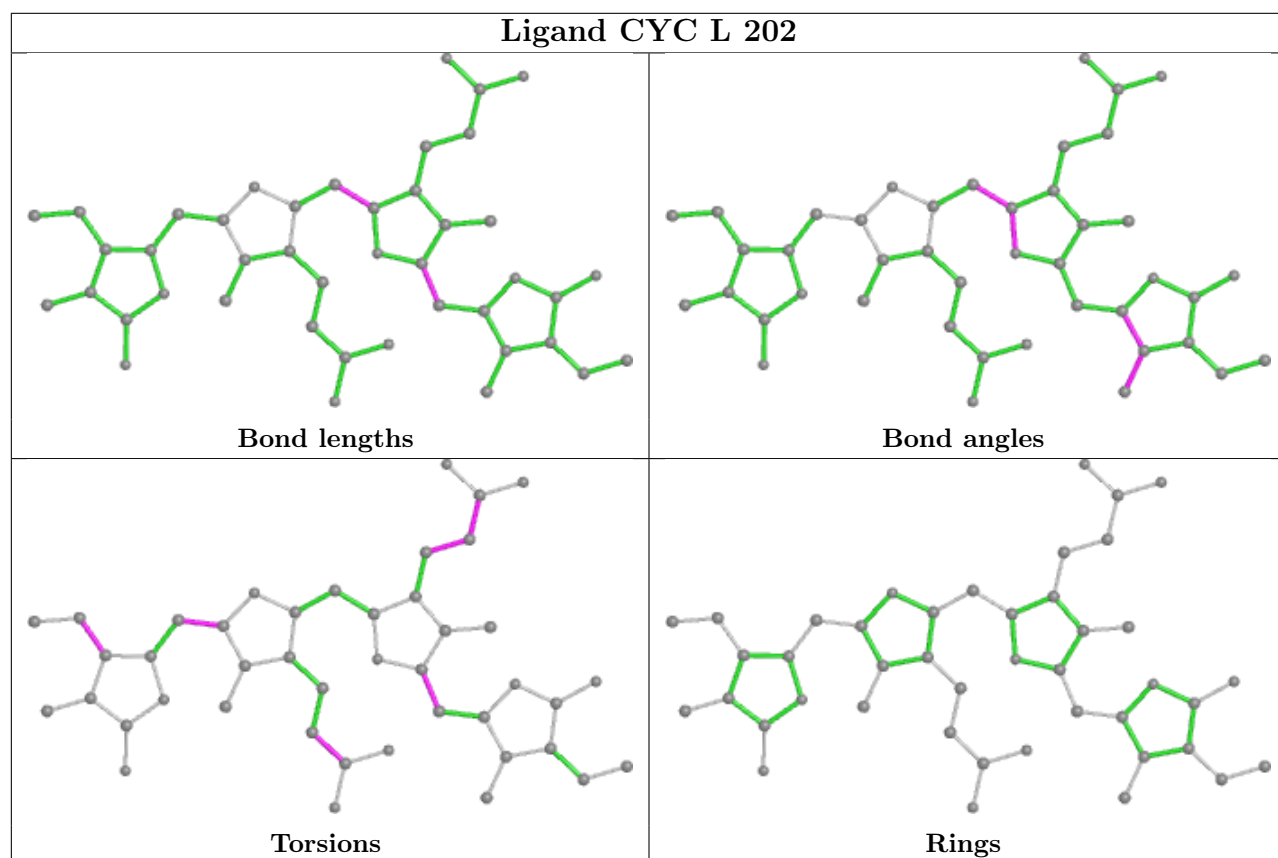
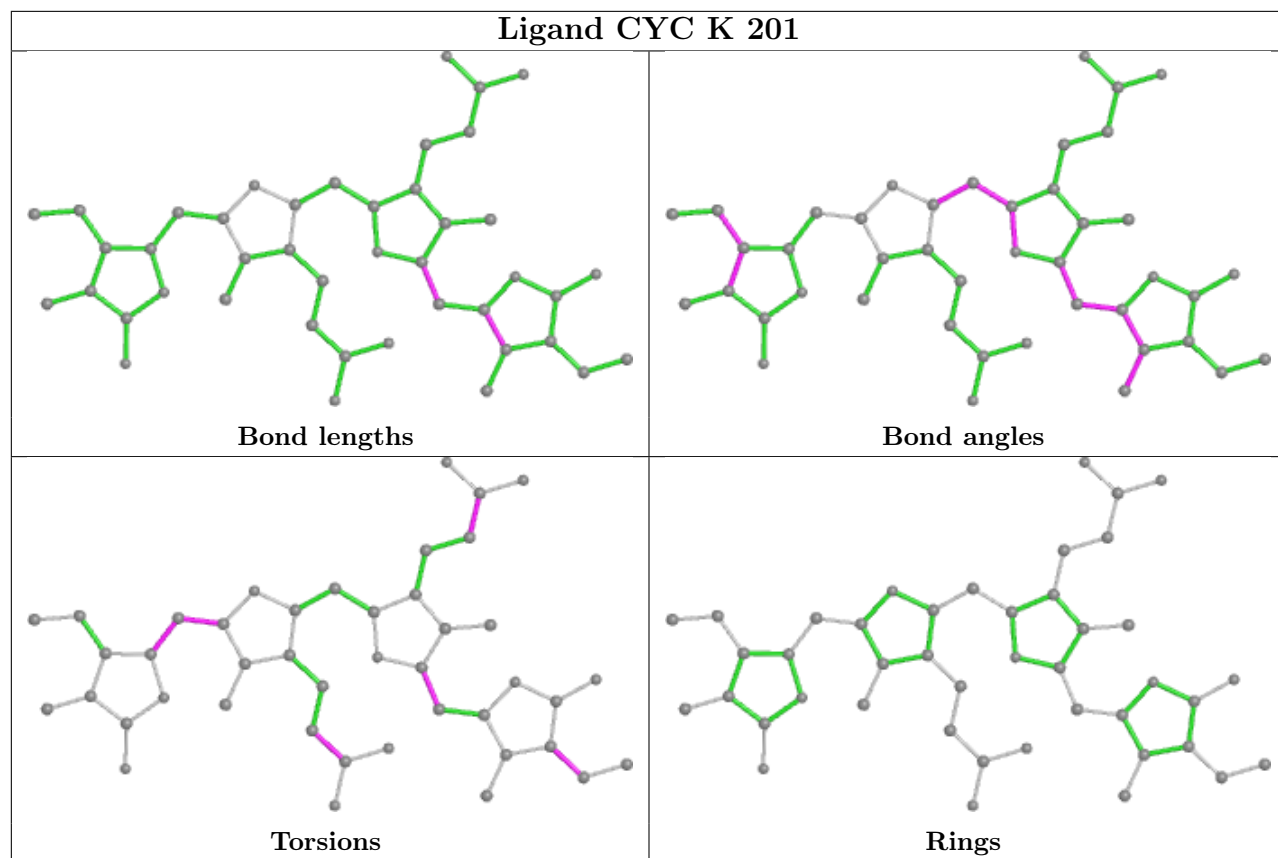
Ligand CYC F 201

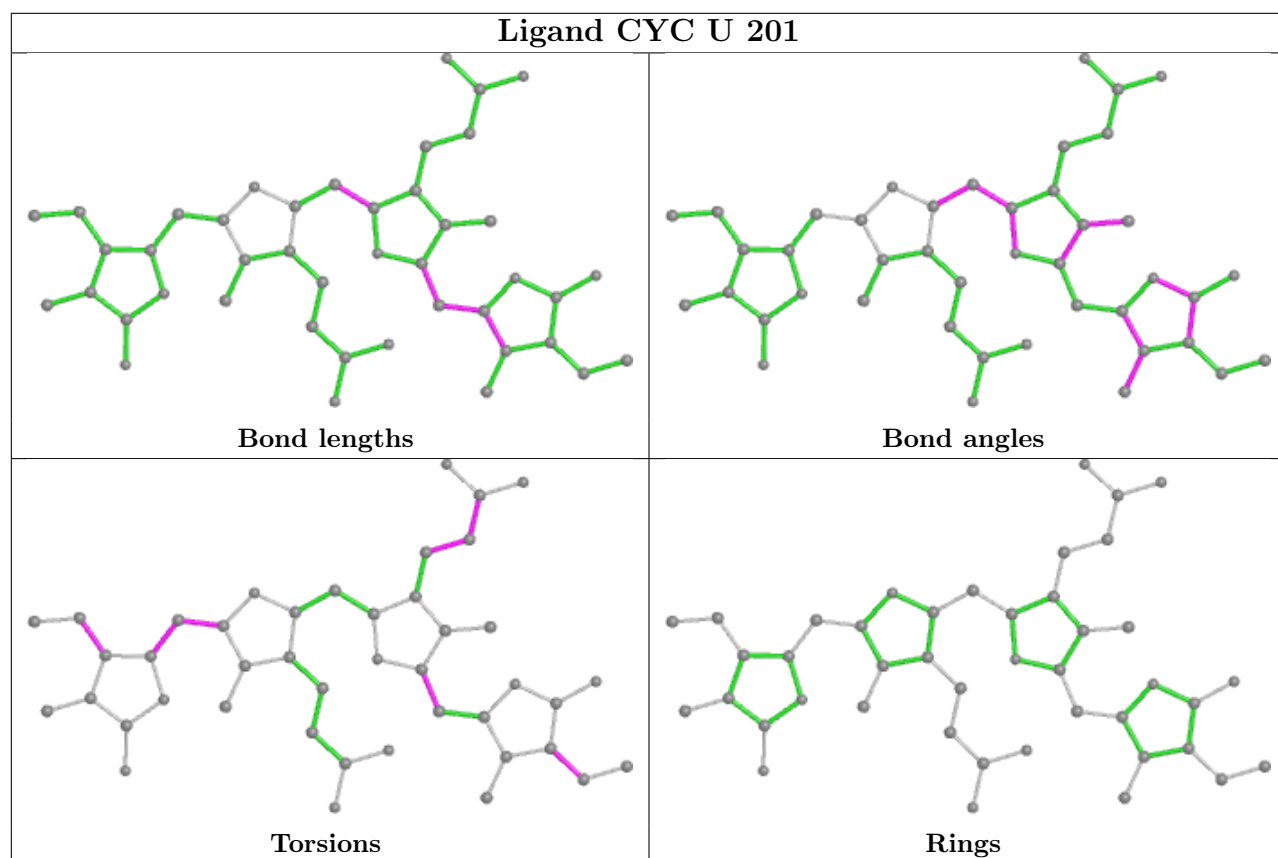
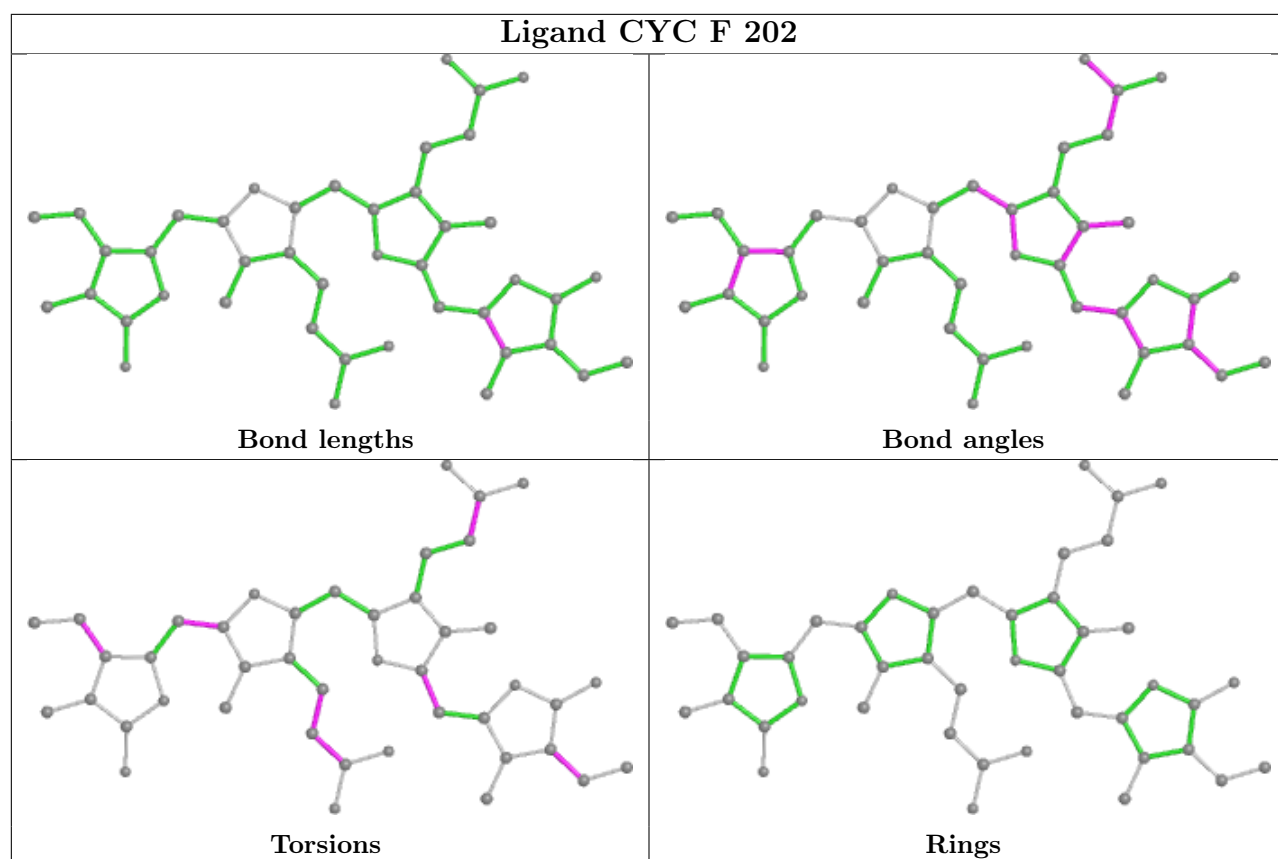


Ligand CYC B 202









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.

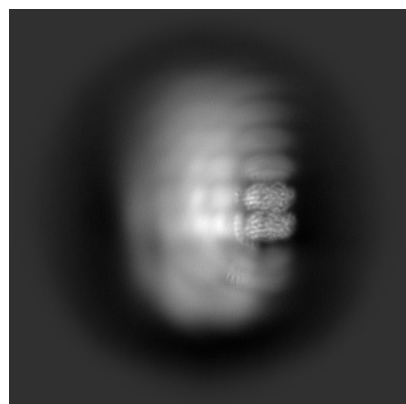
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64817. These allow visual inspection of the internal detail of the map and identification of artifacts.

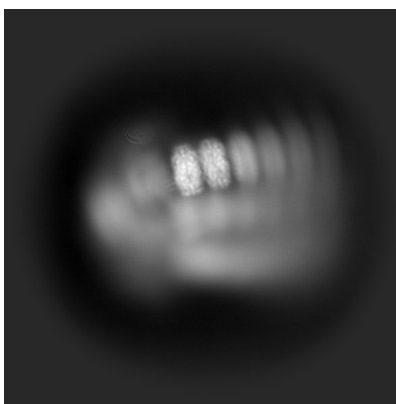
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

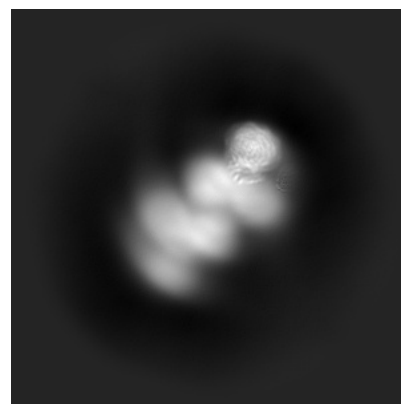
6.1.1 Primary map



X

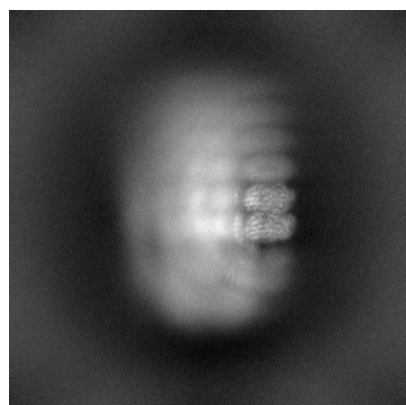


Y

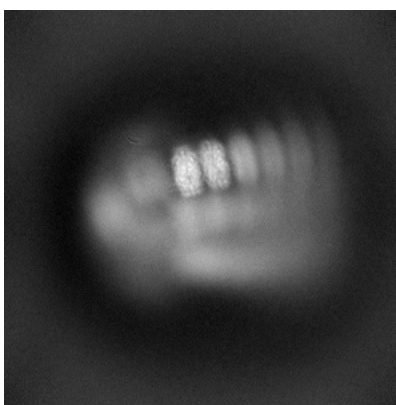


Z

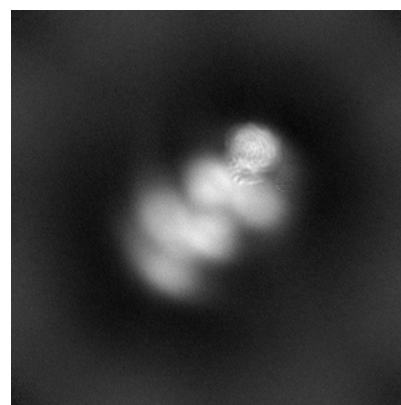
6.1.2 Raw map



X



Y

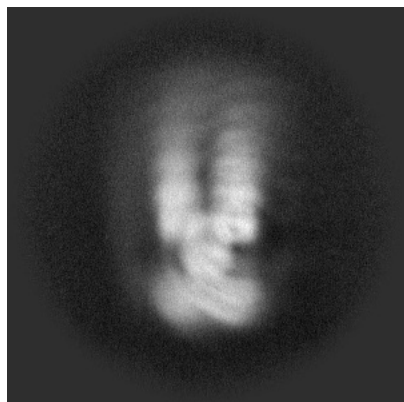


Z

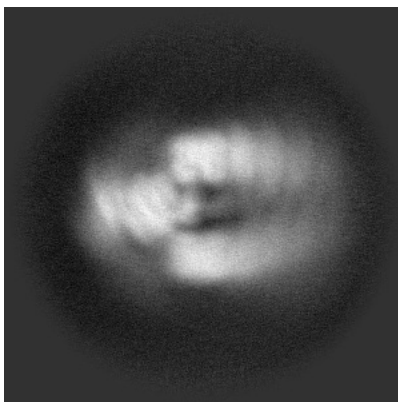
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

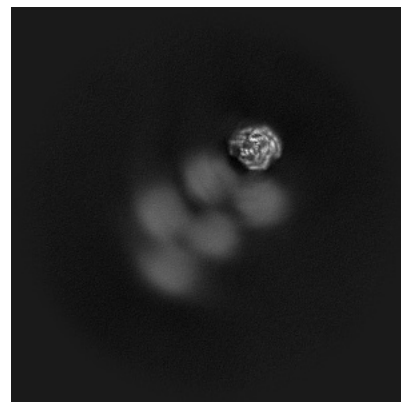
6.2.1 Primary map



X Index: 336

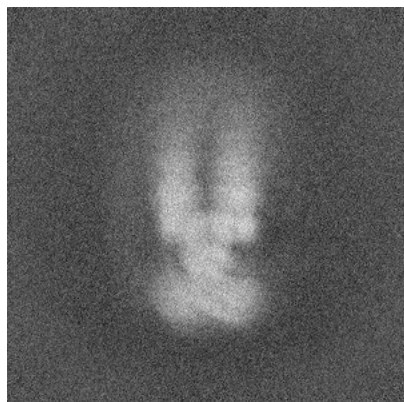


Y Index: 336

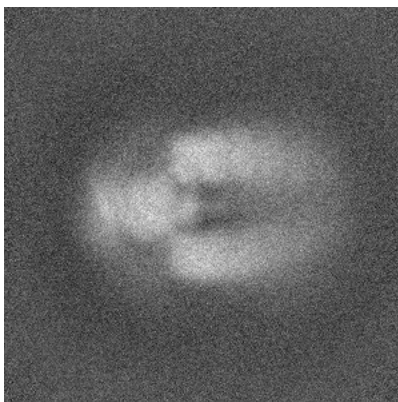


Z Index: 336

6.2.2 Raw map



X Index: 336



Y Index: 336

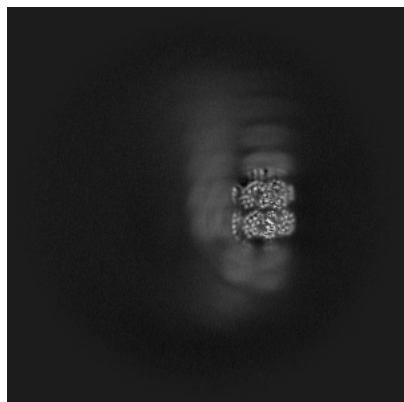


Z Index: 336

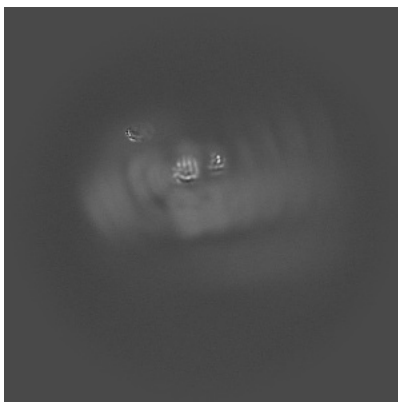
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

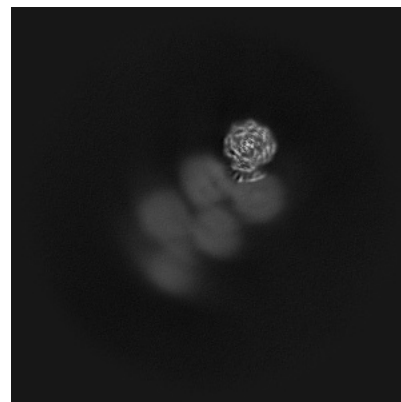
6.3.1 Primary map



X Index: 404

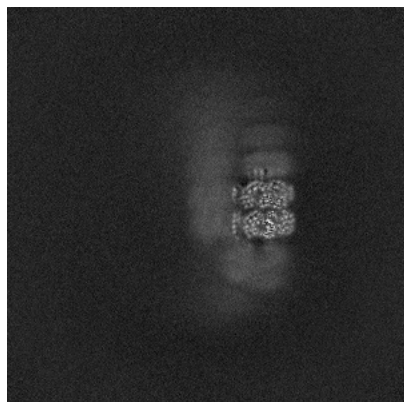


Y Index: 382



Z Index: 301

6.3.2 Raw map



X Index: 404



Y Index: 382

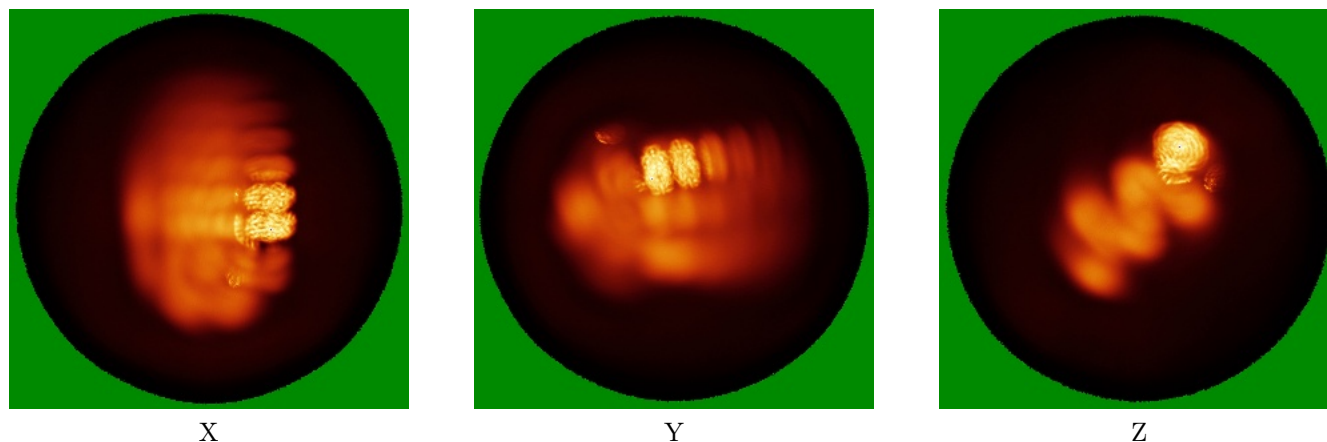


Z Index: 301

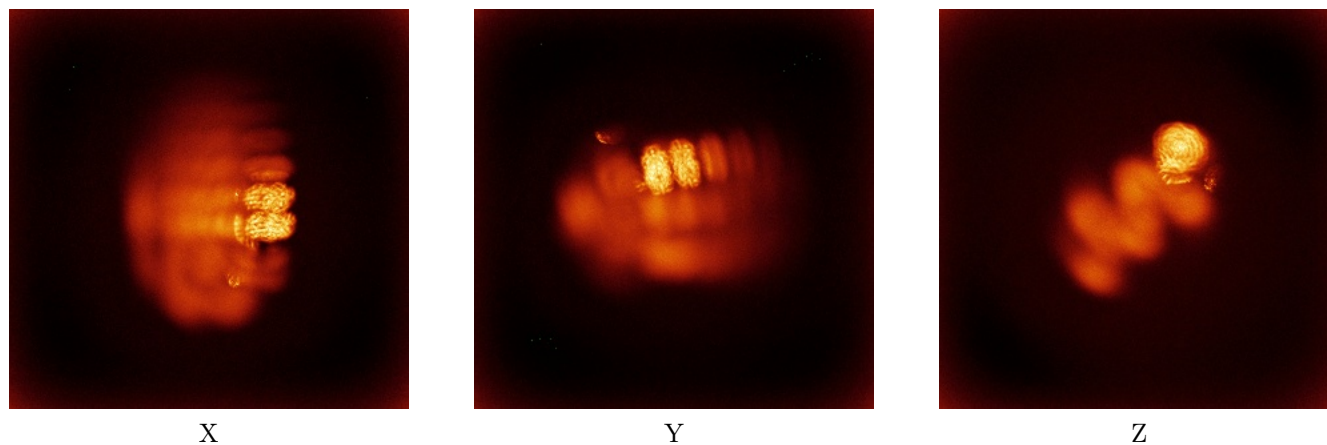
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



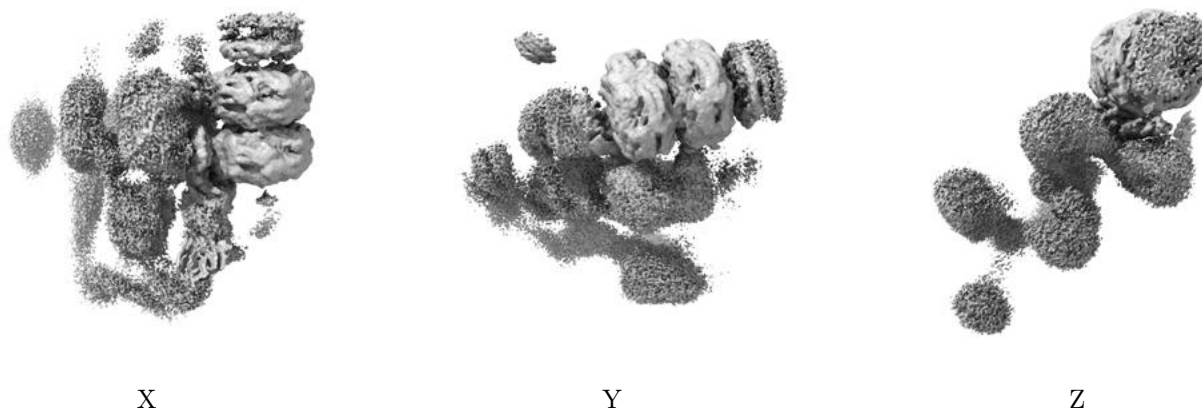
6.4.2 Raw map



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

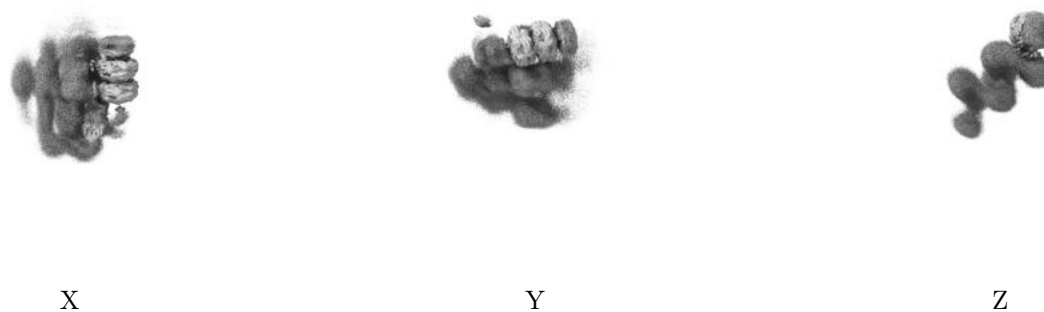
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

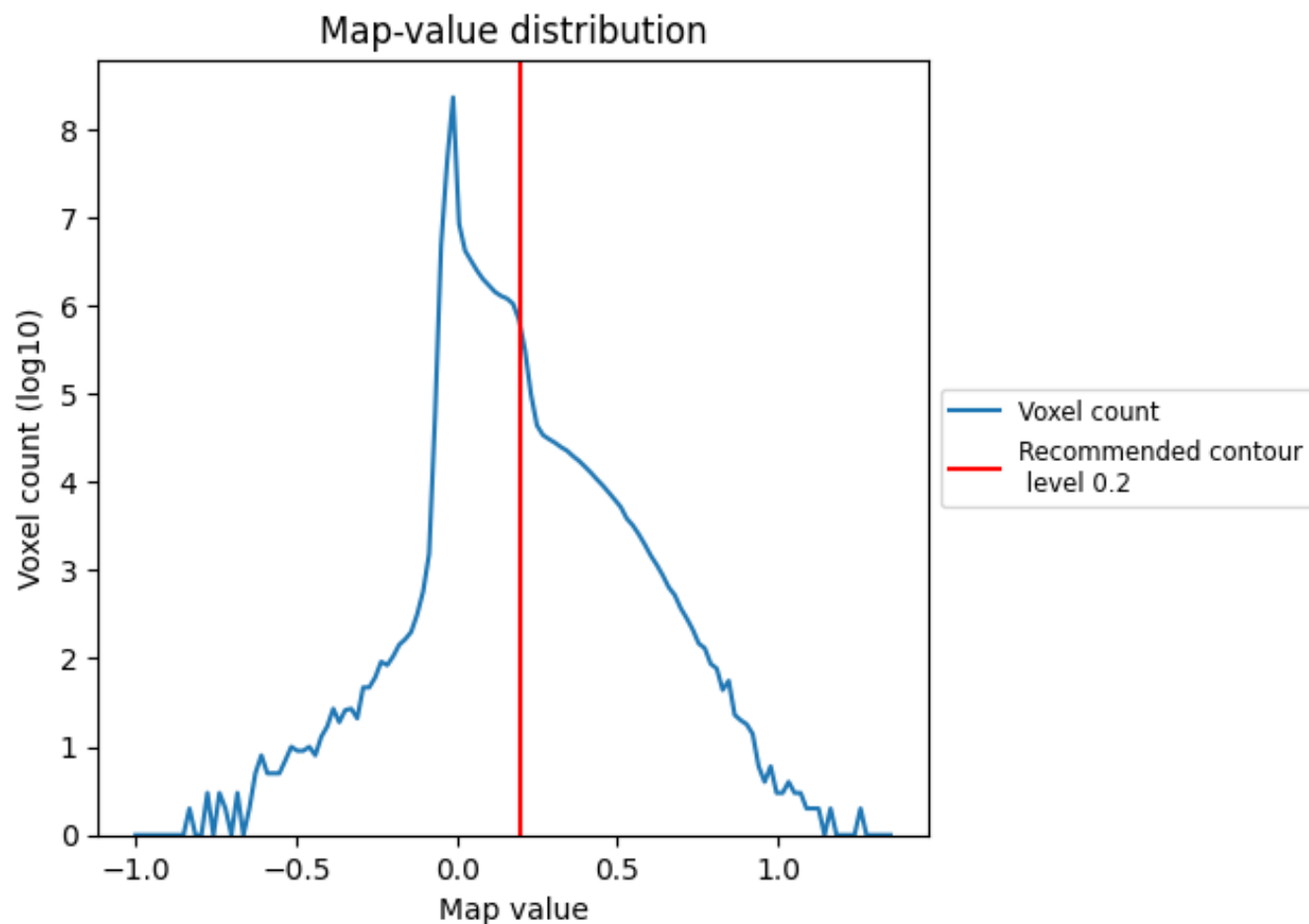
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

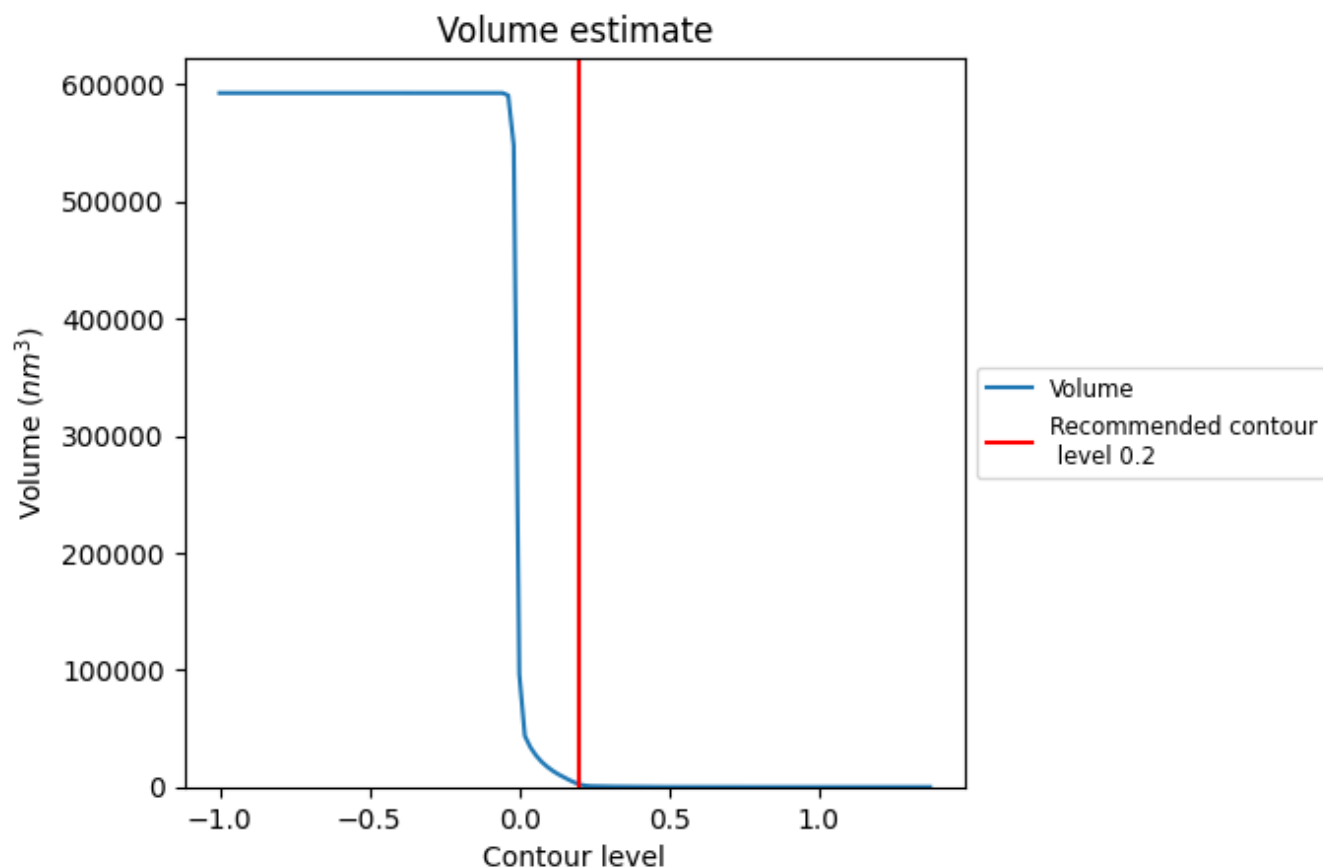
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

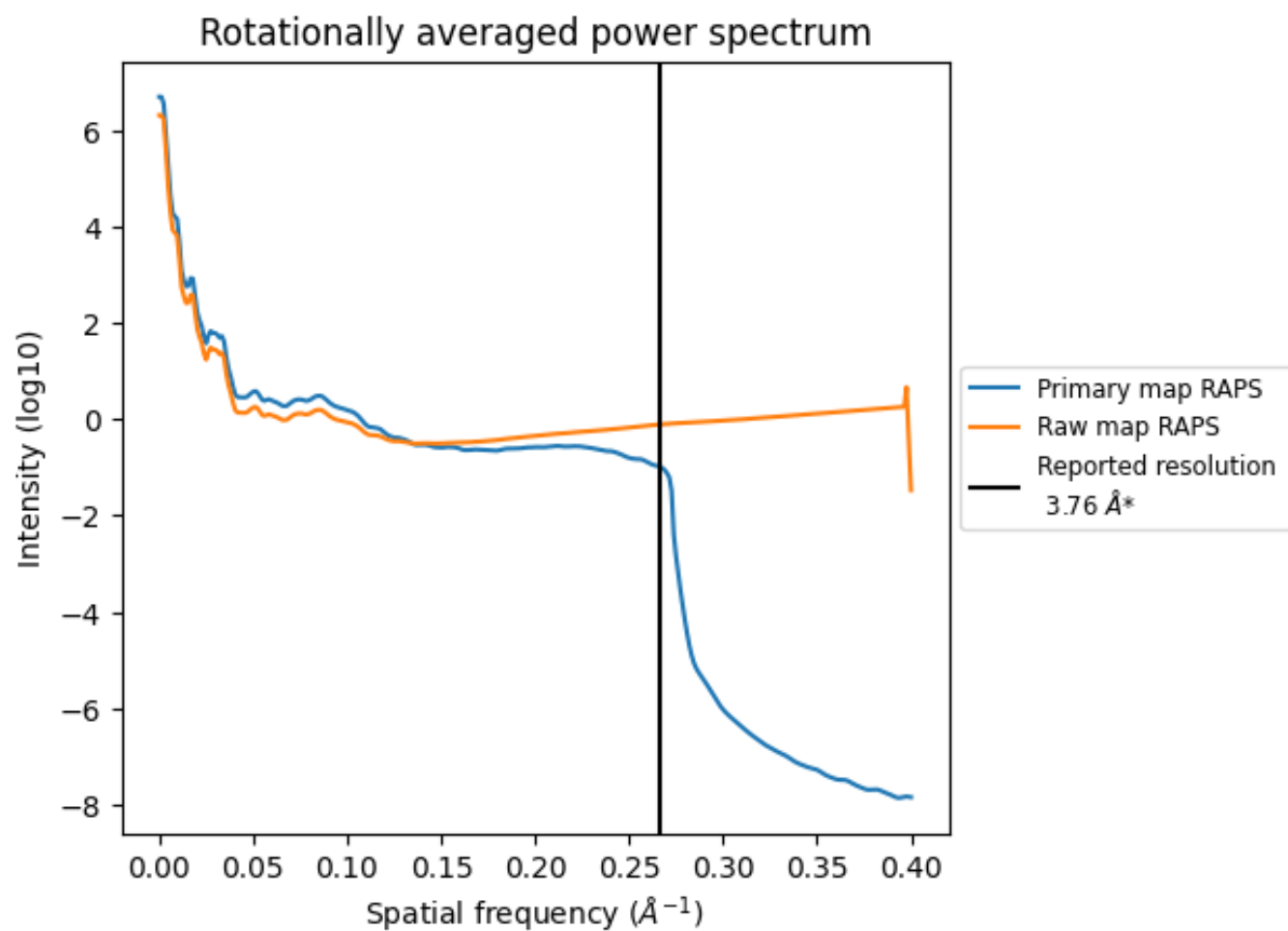
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2325 nm^3 ; this corresponds to an approximate mass of 2100 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 ⓘ

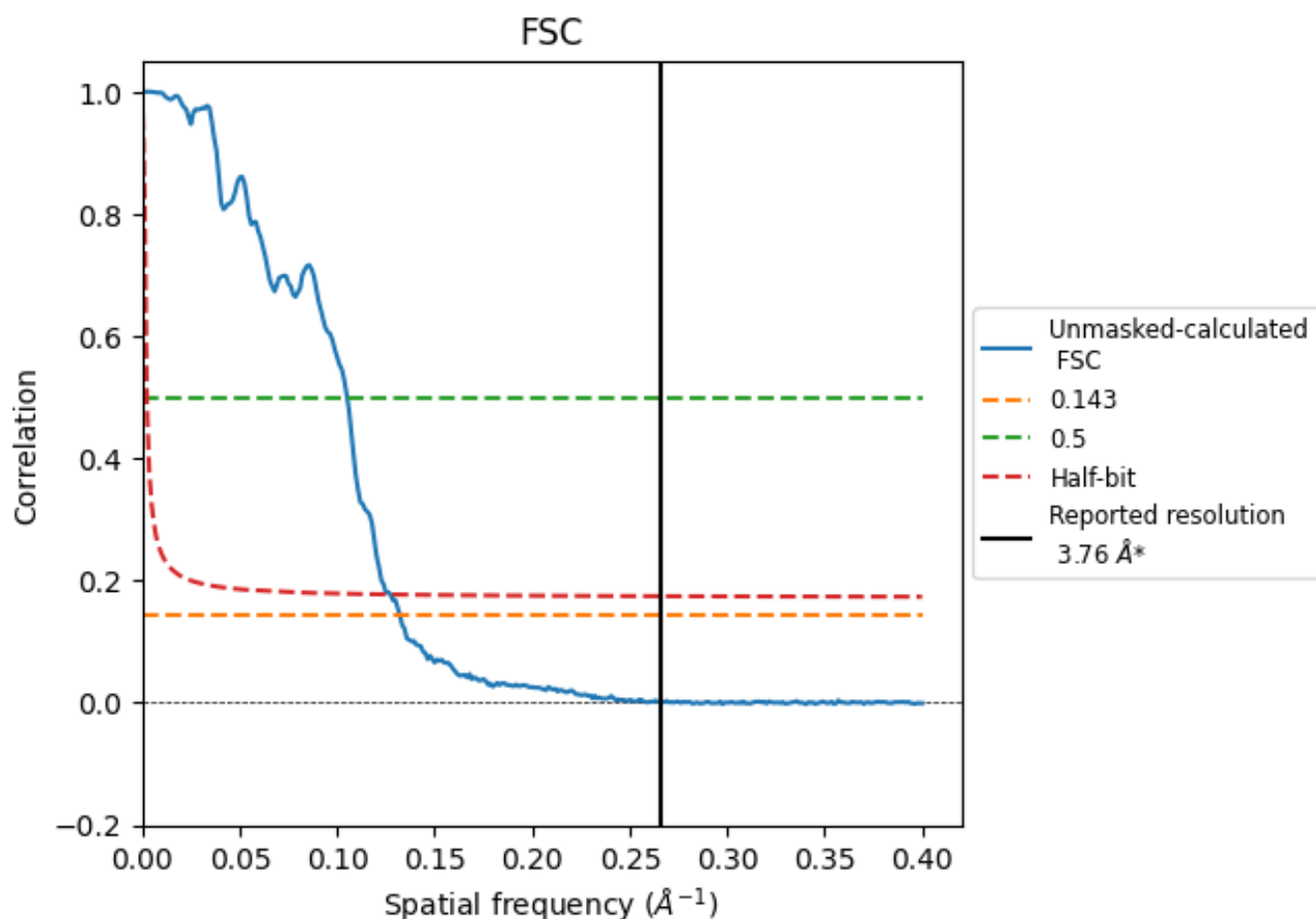


*Reported resolution corresponds to spatial frequency of 0.266 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.266 \AA^{-1}

8.2 Resolution estimates [i](#)

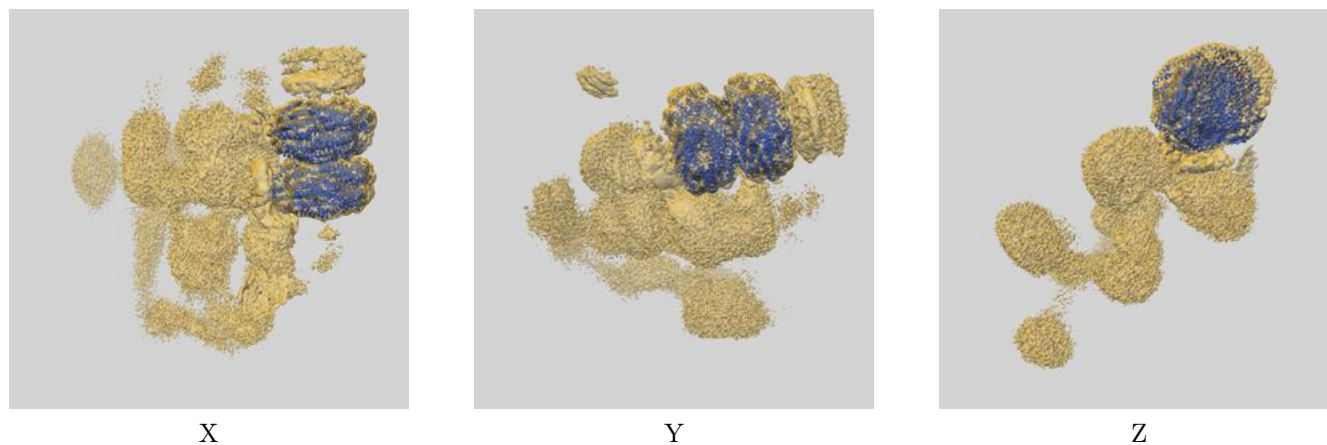
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.76	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.56	9.52	7.86

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.56 differs from the reported value 3.76 by more than 10 %

9 Map-model fit [i](#)

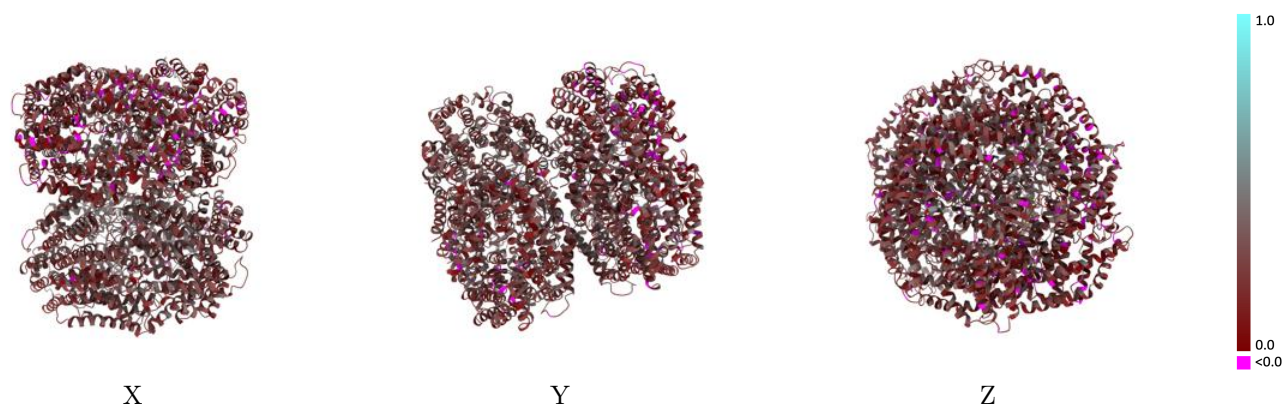
This section contains information regarding the fit between EMDB map EMD-64817 and PDB model 9V7L. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



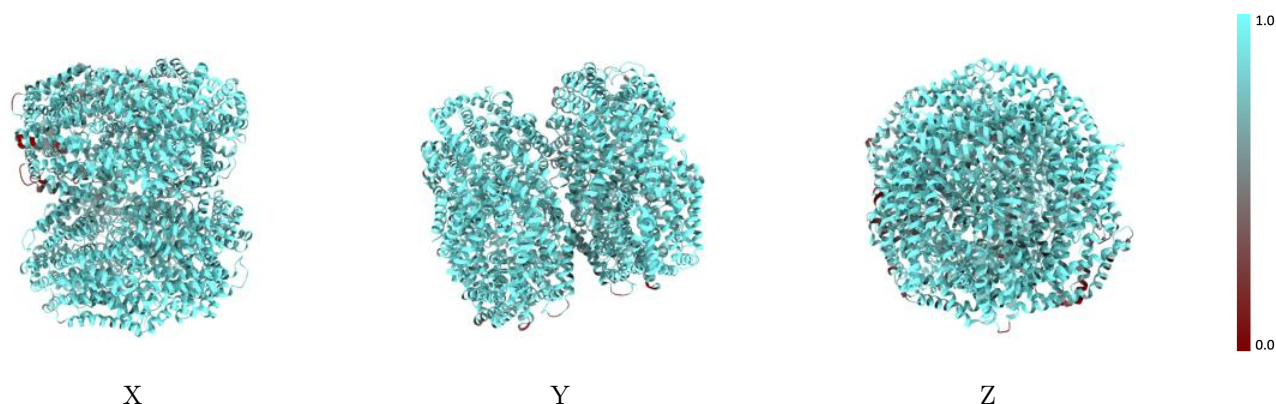
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



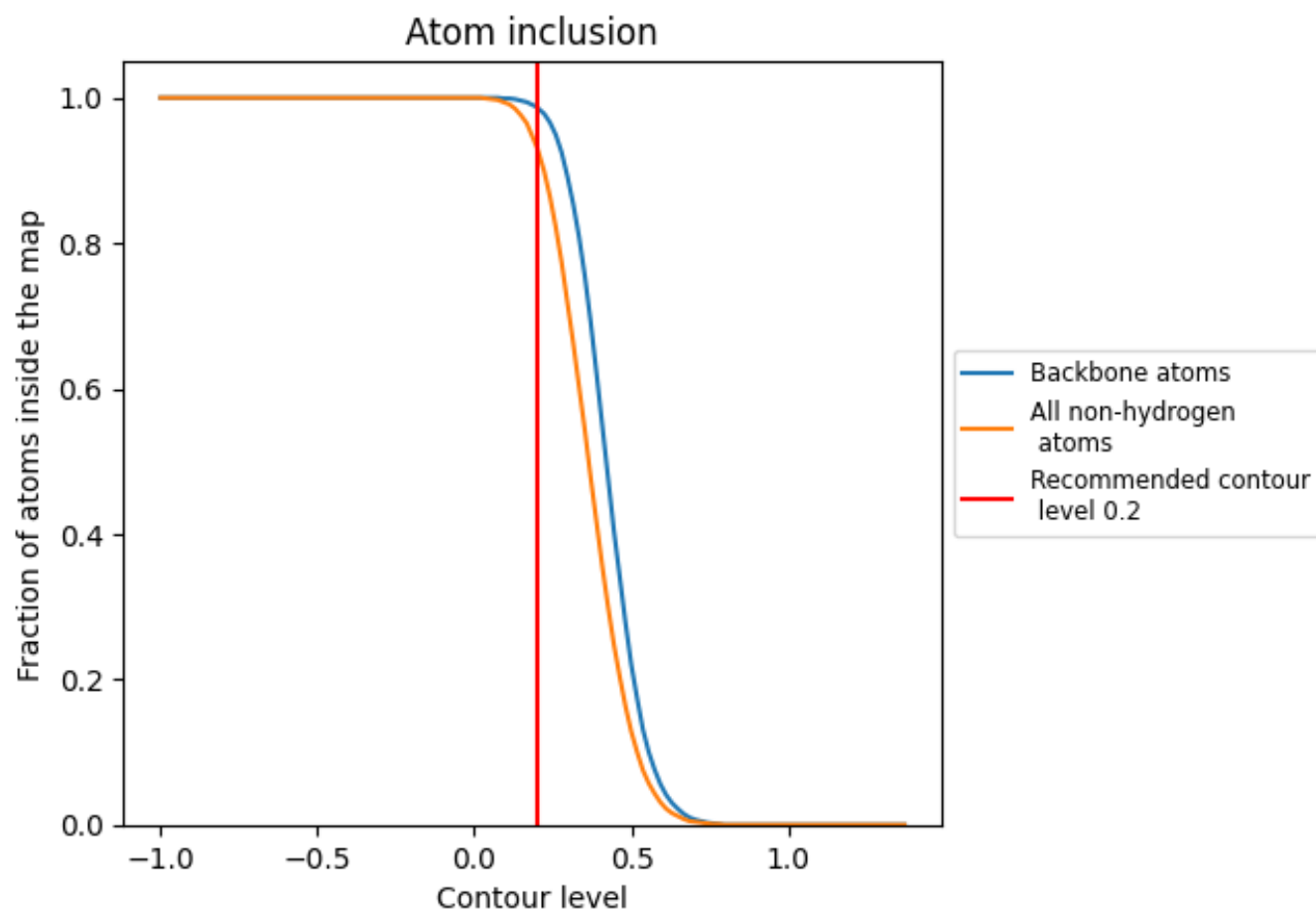
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

























































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	 0.9310	 0.2330
A	 0.9590	 0.2750
B	 0.9370	 0.1720
C	 0.9630	 0.2150
D	 0.8730	 0.2680
E	 0.9400	 0.1990
F	 0.9360	 0.2200
G	 0.8660	 0.2030
H	 0.9270	 0.1830
I	 0.8700	 0.1740
J	 0.8740	 0.1900
K	 0.9200	 0.2100
L	 0.8170	 0.1880
M	 0.9490	 0.2790
N	 0.9710	 0.2330
O	 0.9750	 0.2860
P	 0.9240	 0.2230
Q	 0.9160	 0.2730
R	 0.9960	 0.2660
S	 0.9760	 0.2380
T	 0.9280	 0.2640
U	 0.8940	 0.2540
V	 0.9790	 0.2360
W	 0.9480	 0.2520
X	 0.9660	 0.2490
Y	 0.9430	 0.2670
Z	 0.8780	 0.1930
a	 0.9750	 0.1970

