



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2026 – 10:36 AM EDT

PDB ID : 11PA / pdb_000011pa
Title : Crystal Structure of M. tuberculosis ClpP1P2 bound to ADEP AB
Authors : Burnside, C.M.; Fei, F.; Schmitz, K.R.; Sello, J.K.
Deposited on : 2026-03-06
Resolution : 2.75 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

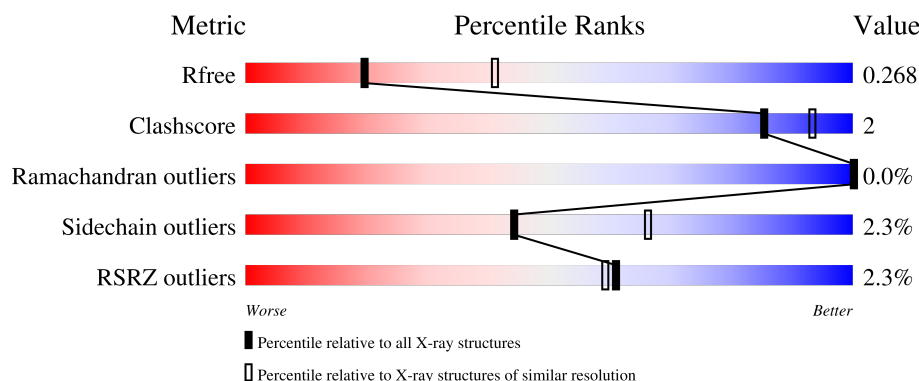
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	215	3% 85% 7% 8%
1	B	215	2% 89% • 7%
1	C	215	3% 84% 11% 5%
1	D	215	2% 87% • 9%
1	E	215	2% 87% 6% 7%

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Mol	Chain	Length	Quality of chain
1	F	215	
1	G	215	
1	O	215	
1	P	215	
1	Q	215	
1	R	215	
1	S	215	
1	T	215	
1	U	215	
2	H	194	
2	I	194	
2	J	194	
2	K	194	
2	L	194	
2	M	194	
2	N	194	
2	V	194	
2	W	194	
2	X	194	
2	Y	194	
2	Z	194	
2	a	194	
2	b	194	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 81232 atoms, of which 40226 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 ATP-dependent Clp protease proteolytic subunit 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	198	Total	C	H	N	O	S	0	0	0
			2957	937	1466	252	294	8			
1	B	199	Total	C	H	N	O	S	0	0	0
			3015	948	1502	259	298	8			
1	C	204	Total	C	H	N	O	S	0	0	0
			3060	964	1523	261	304	8			
1	D	196	Total	C	H	N	O	S	0	0	0
			2962	934	1475	253	292	8			
1	E	200	Total	C	H	N	O	S	0	0	0
			2996	946	1488	257	297	8			
1	F	198	Total	C	H	N	O	S	0	0	0
			2963	937	1471	252	295	8			
1	G	200	Total	C	H	N	O	S	0	0	0
			3034	954	1513	260	299	8			
1	O	197	Total	C	H	N	O	S	0	0	0
			2968	937	1476	254	293	8			
1	P	199	Total	C	H	N	O	S	0	0	0
			3023	954	1506	256	299	8			
1	Q	198	Total	C	H	N	O	S	0	0	0
			2959	937	1468	252	294	8			
1	R	198	Total	C	H	N	O	S	0	0	0
			2993	946	1488	255	296	8			
1	S	199	Total	C	H	N	O	S	0	0	0
			2986	946	1482	253	297	8			
1	T	199	Total	C	H	N	O	S	0	1	0
			3006	953	1491	255	299	8			
1	U	198	Total	C	H	N	O	S	0	0	0
			3019	951	1504	258	298	8			

There are 182 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP P9WPC3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	215	ALA	-	expression tag	UNP P9WPC3
A	216	ALA	-	expression tag	UNP P9WPC3
A	217	ALA	-	expression tag	UNP P9WPC3
A	218	LEU	-	expression tag	UNP P9WPC3
A	219	GLU	-	expression tag	UNP P9WPC3
A	220	HIS	-	expression tag	UNP P9WPC3
A	221	HIS	-	expression tag	UNP P9WPC3
A	222	HIS	-	expression tag	UNP P9WPC3
A	223	HIS	-	expression tag	UNP P9WPC3
A	224	HIS	-	expression tag	UNP P9WPC3
A	225	HIS	-	expression tag	UNP P9WPC3
A	226	ALA	-	expression tag	UNP P9WPC3
B	12	MET	-	initiating methionine	UNP P9WPC3
B	215	ALA	-	expression tag	UNP P9WPC3
B	216	ALA	-	expression tag	UNP P9WPC3
B	217	ALA	-	expression tag	UNP P9WPC3
B	218	LEU	-	expression tag	UNP P9WPC3
B	219	GLU	-	expression tag	UNP P9WPC3
B	220	HIS	-	expression tag	UNP P9WPC3
B	221	HIS	-	expression tag	UNP P9WPC3
B	222	HIS	-	expression tag	UNP P9WPC3
B	223	HIS	-	expression tag	UNP P9WPC3
B	224	HIS	-	expression tag	UNP P9WPC3
B	225	HIS	-	expression tag	UNP P9WPC3
B	226	ALA	-	expression tag	UNP P9WPC3
C	12	MET	-	initiating methionine	UNP P9WPC3
C	215	ALA	-	expression tag	UNP P9WPC3
C	216	ALA	-	expression tag	UNP P9WPC3
C	217	ALA	-	expression tag	UNP P9WPC3
C	218	LEU	-	expression tag	UNP P9WPC3
C	219	GLU	-	expression tag	UNP P9WPC3
C	220	HIS	-	expression tag	UNP P9WPC3
C	221	HIS	-	expression tag	UNP P9WPC3
C	222	HIS	-	expression tag	UNP P9WPC3
C	223	HIS	-	expression tag	UNP P9WPC3
C	224	HIS	-	expression tag	UNP P9WPC3
C	225	HIS	-	expression tag	UNP P9WPC3
C	226	ALA	-	expression tag	UNP P9WPC3
D	12	MET	-	initiating methionine	UNP P9WPC3
D	215	ALA	-	expression tag	UNP P9WPC3
D	216	ALA	-	expression tag	UNP P9WPC3
D	217	ALA	-	expression tag	UNP P9WPC3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	218	LEU	-	expression tag	UNP P9WPC3
D	219	GLU	-	expression tag	UNP P9WPC3
D	220	HIS	-	expression tag	UNP P9WPC3
D	221	HIS	-	expression tag	UNP P9WPC3
D	222	HIS	-	expression tag	UNP P9WPC3
D	223	HIS	-	expression tag	UNP P9WPC3
D	224	HIS	-	expression tag	UNP P9WPC3
D	225	HIS	-	expression tag	UNP P9WPC3
D	226	ALA	-	expression tag	UNP P9WPC3
E	12	MET	-	initiating methionine	UNP P9WPC3
E	215	ALA	-	expression tag	UNP P9WPC3
E	216	ALA	-	expression tag	UNP P9WPC3
E	217	ALA	-	expression tag	UNP P9WPC3
E	218	LEU	-	expression tag	UNP P9WPC3
E	219	GLU	-	expression tag	UNP P9WPC3
E	220	HIS	-	expression tag	UNP P9WPC3
E	221	HIS	-	expression tag	UNP P9WPC3
E	222	HIS	-	expression tag	UNP P9WPC3
E	223	HIS	-	expression tag	UNP P9WPC3
E	224	HIS	-	expression tag	UNP P9WPC3
E	225	HIS	-	expression tag	UNP P9WPC3
E	226	ALA	-	expression tag	UNP P9WPC3
F	12	MET	-	initiating methionine	UNP P9WPC3
F	215	ALA	-	expression tag	UNP P9WPC3
F	216	ALA	-	expression tag	UNP P9WPC3
F	217	ALA	-	expression tag	UNP P9WPC3
F	218	LEU	-	expression tag	UNP P9WPC3
F	219	GLU	-	expression tag	UNP P9WPC3
F	220	HIS	-	expression tag	UNP P9WPC3
F	221	HIS	-	expression tag	UNP P9WPC3
F	222	HIS	-	expression tag	UNP P9WPC3
F	223	HIS	-	expression tag	UNP P9WPC3
F	224	HIS	-	expression tag	UNP P9WPC3
F	225	HIS	-	expression tag	UNP P9WPC3
F	226	ALA	-	expression tag	UNP P9WPC3
G	12	MET	-	initiating methionine	UNP P9WPC3
G	215	ALA	-	expression tag	UNP P9WPC3
G	216	ALA	-	expression tag	UNP P9WPC3
G	217	ALA	-	expression tag	UNP P9WPC3
G	218	LEU	-	expression tag	UNP P9WPC3
G	219	GLU	-	expression tag	UNP P9WPC3
G	220	HIS	-	expression tag	UNP P9WPC3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	221	HIS	-	expression tag	UNP P9WPC3
G	222	HIS	-	expression tag	UNP P9WPC3
G	223	HIS	-	expression tag	UNP P9WPC3
G	224	HIS	-	expression tag	UNP P9WPC3
G	225	HIS	-	expression tag	UNP P9WPC3
G	226	ALA	-	expression tag	UNP P9WPC3
O	12	MET	-	initiating methionine	UNP P9WPC3
O	215	ALA	-	expression tag	UNP P9WPC3
O	216	ALA	-	expression tag	UNP P9WPC3
O	217	ALA	-	expression tag	UNP P9WPC3
O	218	LEU	-	expression tag	UNP P9WPC3
O	219	GLU	-	expression tag	UNP P9WPC3
O	220	HIS	-	expression tag	UNP P9WPC3
O	221	HIS	-	expression tag	UNP P9WPC3
O	222	HIS	-	expression tag	UNP P9WPC3
O	223	HIS	-	expression tag	UNP P9WPC3
O	224	HIS	-	expression tag	UNP P9WPC3
O	225	HIS	-	expression tag	UNP P9WPC3
O	226	ALA	-	expression tag	UNP P9WPC3
P	12	MET	-	initiating methionine	UNP P9WPC3
P	215	ALA	-	expression tag	UNP P9WPC3
P	216	ALA	-	expression tag	UNP P9WPC3
P	217	ALA	-	expression tag	UNP P9WPC3
P	218	LEU	-	expression tag	UNP P9WPC3
P	219	GLU	-	expression tag	UNP P9WPC3
P	220	HIS	-	expression tag	UNP P9WPC3
P	221	HIS	-	expression tag	UNP P9WPC3
P	222	HIS	-	expression tag	UNP P9WPC3
P	223	HIS	-	expression tag	UNP P9WPC3
P	224	HIS	-	expression tag	UNP P9WPC3
P	225	HIS	-	expression tag	UNP P9WPC3
P	226	ALA	-	expression tag	UNP P9WPC3
Q	12	MET	-	initiating methionine	UNP P9WPC3
Q	215	ALA	-	expression tag	UNP P9WPC3
Q	216	ALA	-	expression tag	UNP P9WPC3
Q	217	ALA	-	expression tag	UNP P9WPC3
Q	218	LEU	-	expression tag	UNP P9WPC3
Q	219	GLU	-	expression tag	UNP P9WPC3
Q	220	HIS	-	expression tag	UNP P9WPC3
Q	221	HIS	-	expression tag	UNP P9WPC3
Q	222	HIS	-	expression tag	UNP P9WPC3
Q	223	HIS	-	expression tag	UNP P9WPC3

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	224	HIS	-	expression tag	UNP P9WPC3
Q	225	HIS	-	expression tag	UNP P9WPC3
Q	226	ALA	-	expression tag	UNP P9WPC3
R	12	MET	-	initiating methionine	UNP P9WPC3
R	215	ALA	-	expression tag	UNP P9WPC3
R	216	ALA	-	expression tag	UNP P9WPC3
R	217	ALA	-	expression tag	UNP P9WPC3
R	218	LEU	-	expression tag	UNP P9WPC3
R	219	GLU	-	expression tag	UNP P9WPC3
R	220	HIS	-	expression tag	UNP P9WPC3
R	221	HIS	-	expression tag	UNP P9WPC3
R	222	HIS	-	expression tag	UNP P9WPC3
R	223	HIS	-	expression tag	UNP P9WPC3
R	224	HIS	-	expression tag	UNP P9WPC3
R	225	HIS	-	expression tag	UNP P9WPC3
R	226	ALA	-	expression tag	UNP P9WPC3
S	12	MET	-	initiating methionine	UNP P9WPC3
S	215	ALA	-	expression tag	UNP P9WPC3
S	216	ALA	-	expression tag	UNP P9WPC3
S	217	ALA	-	expression tag	UNP P9WPC3
S	218	LEU	-	expression tag	UNP P9WPC3
S	219	GLU	-	expression tag	UNP P9WPC3
S	220	HIS	-	expression tag	UNP P9WPC3
S	221	HIS	-	expression tag	UNP P9WPC3
S	222	HIS	-	expression tag	UNP P9WPC3
S	223	HIS	-	expression tag	UNP P9WPC3
S	224	HIS	-	expression tag	UNP P9WPC3
S	225	HIS	-	expression tag	UNP P9WPC3
S	226	ALA	-	expression tag	UNP P9WPC3
T	12	MET	-	initiating methionine	UNP P9WPC3
T	215	ALA	-	expression tag	UNP P9WPC3
T	216	ALA	-	expression tag	UNP P9WPC3
T	217	ALA	-	expression tag	UNP P9WPC3
T	218	LEU	-	expression tag	UNP P9WPC3
T	219	GLU	-	expression tag	UNP P9WPC3
T	220	HIS	-	expression tag	UNP P9WPC3
T	221	HIS	-	expression tag	UNP P9WPC3
T	222	HIS	-	expression tag	UNP P9WPC3
T	223	HIS	-	expression tag	UNP P9WPC3
T	224	HIS	-	expression tag	UNP P9WPC3
T	225	HIS	-	expression tag	UNP P9WPC3
T	226	ALA	-	expression tag	UNP P9WPC3

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Chain	Residue	Modelled	Actual	Comment	Reference
U	12	MET	-	initiating methionine	UNP P9WPC3
U	215	ALA	-	expression tag	UNP P9WPC3
U	216	ALA	-	expression tag	UNP P9WPC3
U	217	ALA	-	expression tag	UNP P9WPC3
U	218	LEU	-	expression tag	UNP P9WPC3
U	219	GLU	-	expression tag	UNP P9WPC3
U	220	HIS	-	expression tag	UNP P9WPC3
U	221	HIS	-	expression tag	UNP P9WPC3
U	222	HIS	-	expression tag	UNP P9WPC3
U	223	HIS	-	expression tag	UNP P9WPC3
U	224	HIS	-	expression tag	UNP P9WPC3
U	225	HIS	-	expression tag	UNP P9WPC3
U	226	ALA	-	expression tag	UNP P9WPC3

- Molecule 2 is a protein called ATP-dependent Clp protease proteolytic subunit 1.

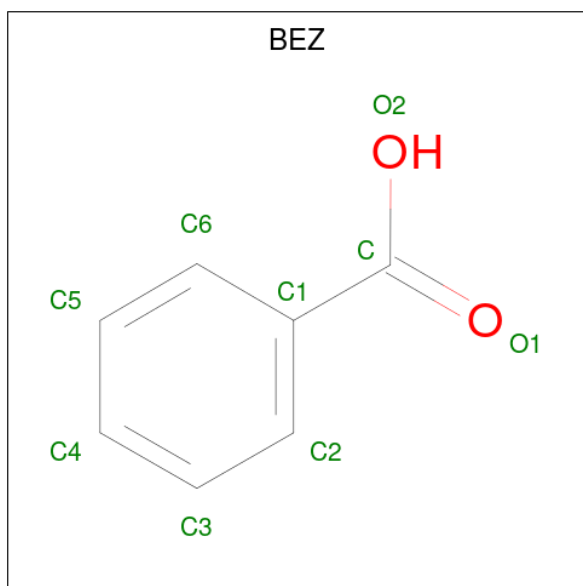
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	177	Total	C	H	N	O	S	0	0	0
			2662	849	1323	222	259	9			
2	I	177	Total	C	H	N	O	S	0	0	0
			2655	847	1320	222	257	9			
2	J	177	Total	C	H	N	O	S	0	0	0
			2643	844	1311	222	257	9			
2	K	176	Total	C	H	N	O	S	0	0	0
			2641	843	1313	221	255	9			
2	L	177	Total	C	H	N	O	S	0	0	0
			2636	843	1306	222	256	9			
2	M	176	Total	C	H	N	O	S	0	0	0
			2628	840	1303	221	255	9			
2	N	177	Total	C	H	N	O	S	0	0	0
			2658	847	1322	222	258	9			
2	V	176	Total	C	H	N	O	S	0	0	0
			2612	837	1293	218	255	9			
2	W	177	Total	C	H	N	O	S	0	0	0
			2630	842	1305	219	255	9			
2	X	176	Total	C	H	N	O	S	0	0	0
			2613	837	1294	217	256	9			
2	Y	180	Total	C	H	N	O	S	0	0	0
			2656	852	1315	224	256	9			
2	Z	176	Total	C	H	N	O	S	0	0	0
			2608	837	1290	217	255	9			
2	a	176	Total	C	H	N	O	S	0	0	0
			2603	835	1288	218	253	9			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	b	176	Total	C	H	N	O	S	0	0	0
			2579	831	1270	214	255	9			

- Molecule 3 is BENZOIC ACID (CCD ID: BEZ) (formula: C₇H₆O₂).



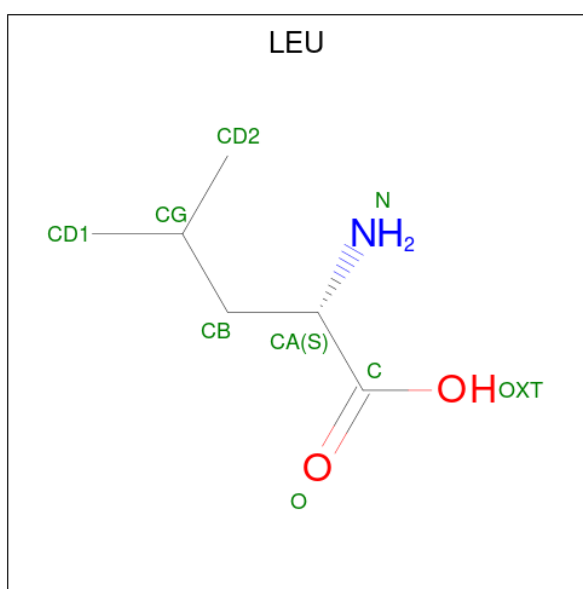
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			13	7	5	1		
3	B	1	Total	C	H	O	0	0
			13	7	5	1		
3	C	1	Total	C	H	O	0	0
			13	7	5	1		
3	D	1	Total	C	H	O	0	0
			13	7	5	1		
3	E	1	Total	C	H	O	0	0
			13	7	5	1		
3	F	1	Total	C	H	O	0	0
			13	7	5	1		
3	G	1	Total	C	H	O	0	0
			13	7	5	1		
3	O	1	Total	C	H	O	0	0
			13	7	5	1		
3	P	1	Total	C	H	O	0	0
			13	7	5	1		
3	Q	1	Total	C	H	O	0	0
			13	7	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	R	1	Total	C	H	O	0	0
			13	7	5	1		
3	S	1	Total	C	H	O	0	0
			13	7	5	1		
3	T	1	Total	C	H	O	0	0
			13	7	5	1		
3	U	1	Total	C	H	O	0	0
			13	7	5	1		

- Molecule 4 is LEUCINE (CCD ID: LEU) (formula: C₆H₁₃NO₂).



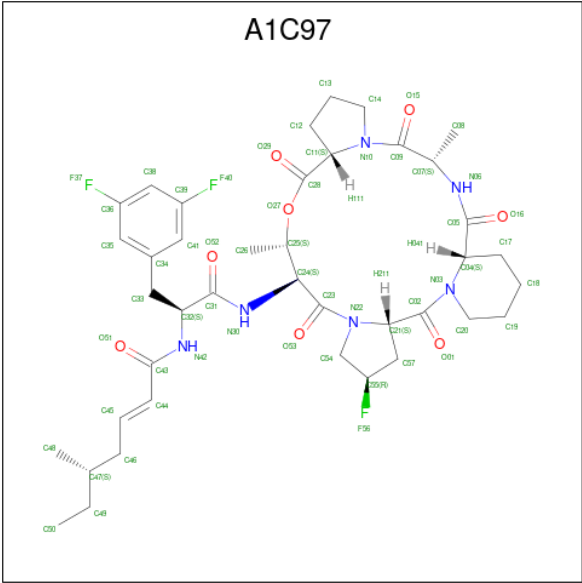
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			19	6	11	1	1		
4	A	1	Total	C	H	N	O	0	0
			20	6	11	1	2		
4	B	1	Total	C	H	N	O	0	0
			19	6	11	1	1		
4	B	1	Total	C	H	N	O	0	0
			20	6	11	1	2		
4	C	1	Total	C	H	N	O	0	0
			19	6	11	1	1		
4	C	1	Total	C	H	N	O	0	0
			20	6	11	1	2		
4	D	1	Total	C	H	N	O	0	0
			19	6	11	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total 20	C 6	H 11	N 1	O 2	0	0
4	E	1	Total 19	C 6	H 11	N 1	O 1	0	0
4	E	1	Total 20	C 6	H 11	N 1	O 2	0	0
4	F	1	Total 19	C 6	H 11	N 1	O 1	0	0
4	F	1	Total 20	C 6	H 11	N 1	O 2	0	0
4	G	1	Total 19	C 6	H 11	N 1	O 1	0	0
4	G	1	Total 20	C 6	H 11	N 1	O 2	0	0
4	O	1	Total 19	C 6	H 11	N 1	O 1	0	0
4	O	1	Total 20	C 6	H 11	N 1	O 2	0	0
4	P	1	Total 19	C 6	H 11	N 1	O 1	0	0
4	P	1	Total 20	C 6	H 11	N 1	O 2	0	0
4	Q	1	Total 19	C 6	H 11	N 1	O 1	0	0
4	Q	1	Total 20	C 6	H 11	N 1	O 2	0	0
4	R	1	Total 19	C 6	H 11	N 1	O 1	0	0
4	R	1	Total 20	C 6	H 11	N 1	O 2	0	0
4	S	1	Total 19	C 6	H 11	N 1	O 1	0	0
4	S	1	Total 20	C 6	H 11	N 1	O 2	0	0
4	T	1	Total 19	C 6	H 11	N 1	O 1	0	0
4	T	1	Total 20	C 6	H 11	N 1	O 2	0	0
4	U	1	Total 19	C 6	H 11	N 1	O 1	0	0
4	U	1	Total 20	C 6	H 11	N 1	O 2	0	0

- Molecule 5 is 3,5-difluoro-N-[(5R,6aS,8R,10R,12S,13S,15aS,19S,21S,23aS)-8-fluoro-13,21-dimethyl-6,11,15,20,23-pentaoxooctadecahydro-2H,6H,11H,15H-pyrido[2,1-i]dipyrrolo[2,1-c:2',1'-l][1,4,7,10,13]oxatetraazacyclohexadecin-12-yl]-Nalpha-[(2E,5S)-5-methylhept-2-enoyl]-L-phenylalaninamide (CCD ID: A1C97) (formula: C₄₀H₅₃F₃N₆O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	F	H	N	O	0	0
			110	40	3	53	6	8		
5	B	1	Total	C	F	H	N	O	0	0
			110	40	3	53	6	8		
5	C	1	Total	C	F	H	N	O	0	0
			110	40	3	53	6	8		
5	D	1	Total	C	F	H	N	O	0	0
			110	40	3	53	6	8		
5	E	1	Total	C	F	H	N	O	0	0
			110	40	3	53	6	8		
5	E	1	Total	C	F	H	N	O	0	0
			110	40	3	53	6	8		
5	G	1	Total	C	F	H	N	O	0	0
			110	40	3	53	6	8		
5	O	1	Total	C	F	H	N	O	0	0
			110	40	3	53	6	8		
5	P	1	Total	C	F	H	N	O	0	0
			110	40	3	53	6	8		
5	Q	1	Total	C	F	H	N	O	0	0
			110	40	3	53	6	8		
5	R	1	Total	C	F	H	N	O	0	0
			110	40	3	53	6	8		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	S	1	Total 110	C 40	F 3	H 53	N 6	O 8	0	0
5	T	1	Total 110	C 40	F 3	H 53	N 6	O 8	0	0
5	U	1	Total 110	C 40	F 3	H 53	N 6	O 8	0	0

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	Cl 1	0	0
6	B	1	Total 1	Cl 1	0	0
6	C	1	Total 1	Cl 1	0	0
6	D	1	Total 1	Cl 1	0	0
6	E	1	Total 1	Cl 1	0	0
6	G	1	Total 1	Cl 1	0	0
6	Q	1	Total 1	Cl 1	0	0

- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	P	1	Total 1	K 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	13	Total 13	O 13	0	0
8	B	17	Total 17	O 17	0	0
8	C	10	Total 10	O 10	0	0
8	D	10	Total 10	O 10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	3	Total O 3 3	0	0
8	F	11	Total O 11 11	0	0
8	G	8	Total O 8 8	0	0
8	H	10	Total O 10 10	0	0
8	I	3	Total O 3 3	0	0
8	J	5	Total O 5 5	0	0
8	K	6	Total O 6 6	0	0
8	L	4	Total O 4 4	0	0
8	M	6	Total O 6 6	0	0
8	N	9	Total O 9 9	0	0
8	O	8	Total O 8 8	0	0
8	P	8	Total O 8 8	0	0
8	Q	2	Total O 2 2	0	0
8	R	9	Total O 9 9	0	0
8	S	5	Total O 5 5	0	0
8	T	5	Total O 5 5	0	0
8	U	10	Total O 10 10	0	0
8	V	6	Total O 6 6	0	0
8	W	5	Total O 5 5	0	0
8	X	2	Total O 2 2	0	0
8	Y	4	Total O 4 4	0	0

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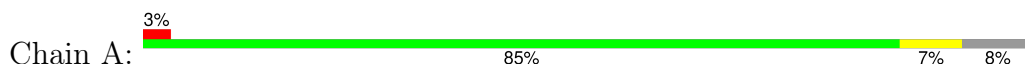
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	Z	3	Total 3	O 3	0	0
8	a	2	Total 2	O 2	0	0
8	b	7	Total 7	O 7	0	0

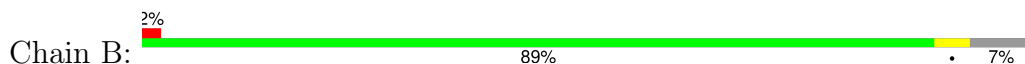
3 Residue-property plots [i](#)

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

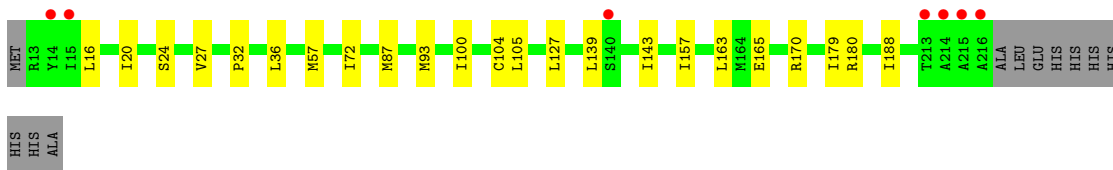
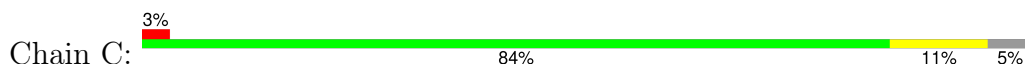
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



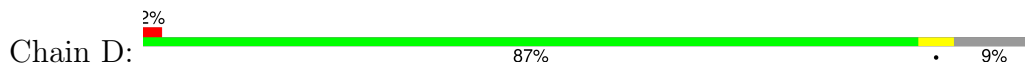
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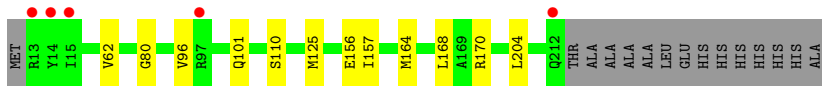
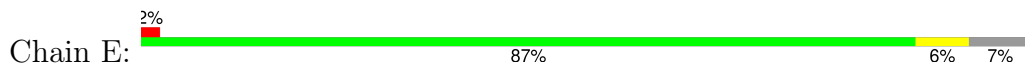
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



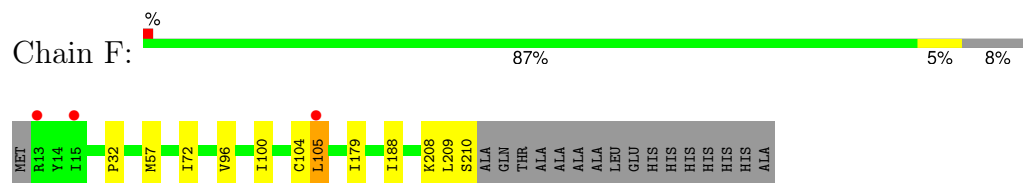
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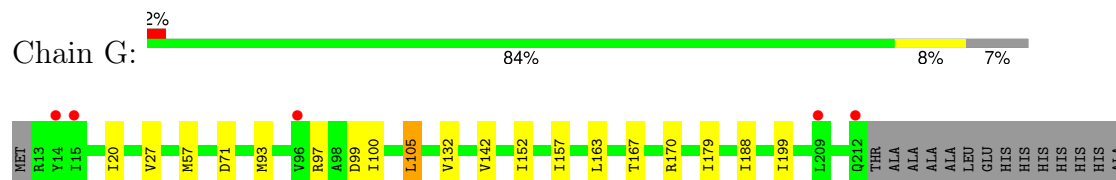
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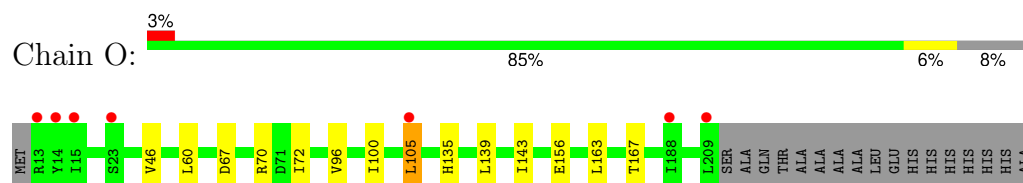
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



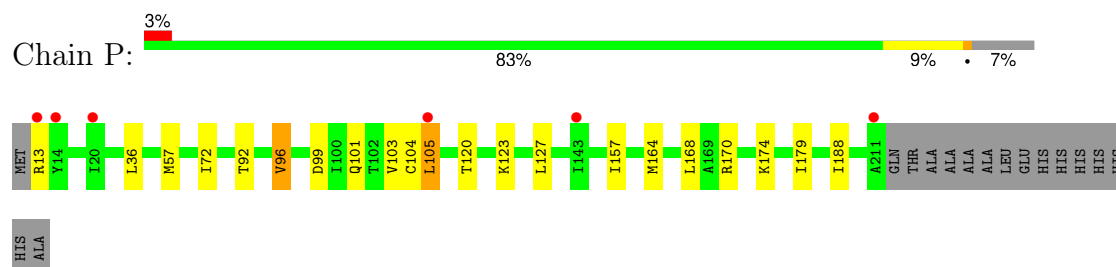
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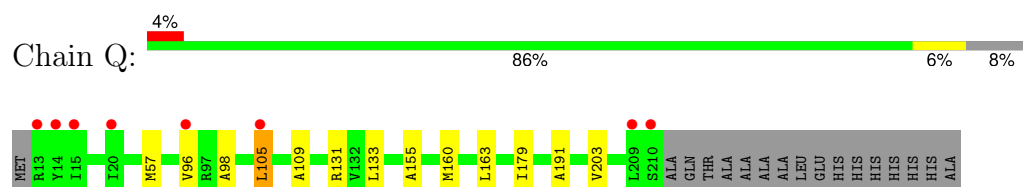
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



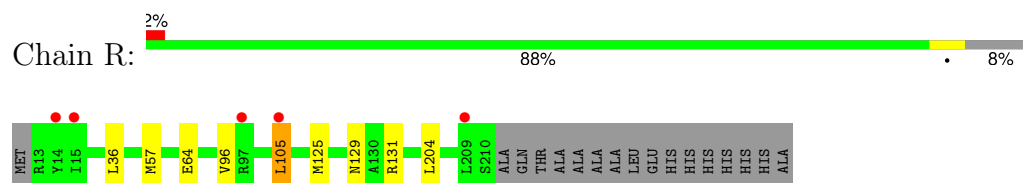
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



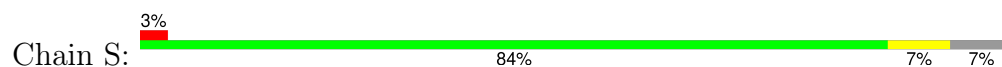
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

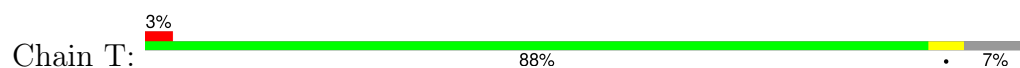


- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

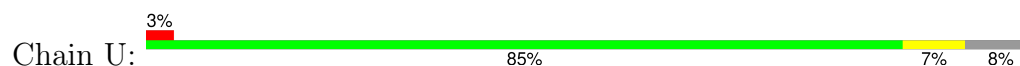




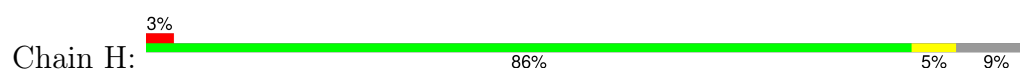
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



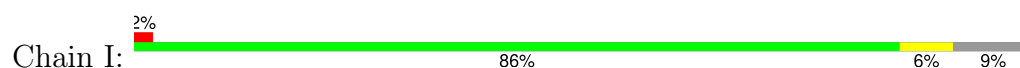
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



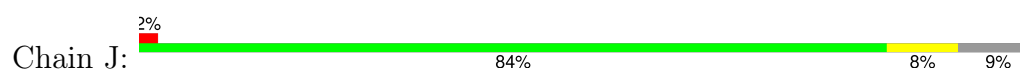
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1



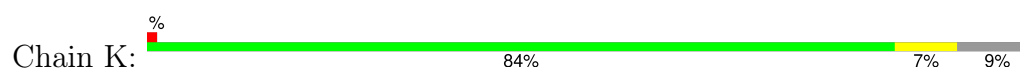
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1



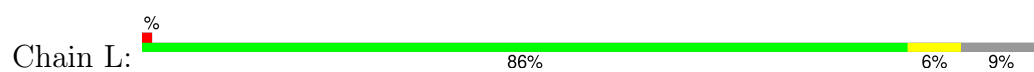
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1



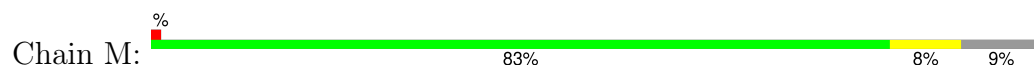
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1



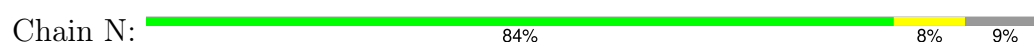
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1



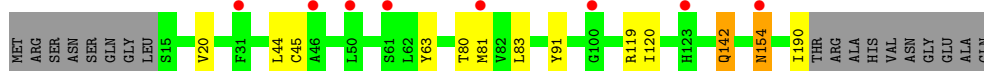
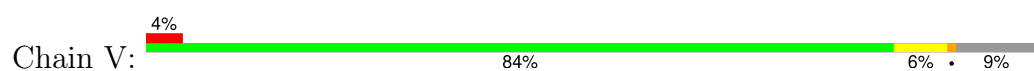
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1



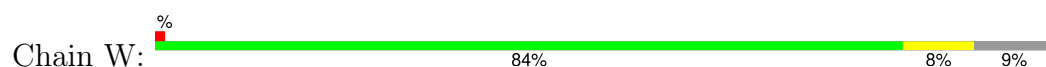
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1



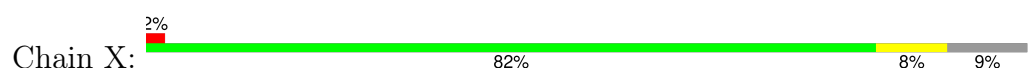
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1



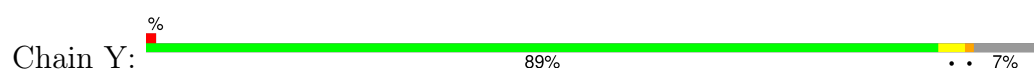
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1



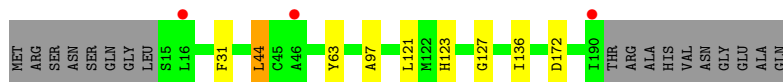
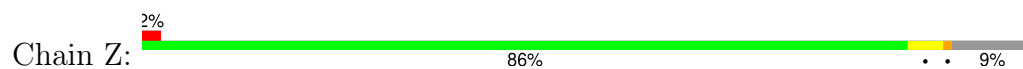
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1



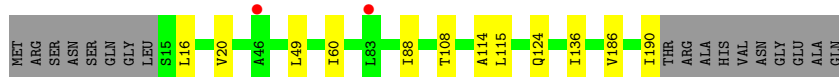
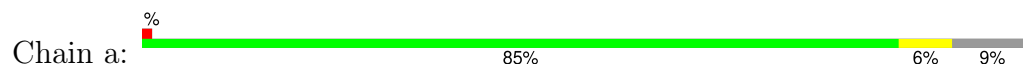
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1



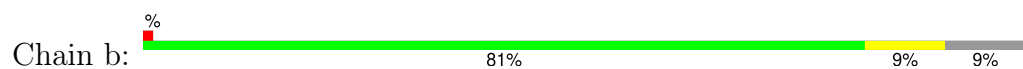
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1



- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1



- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	209.12Å 182.32Å 188.78Å 90.00° 94.89° 90.00°	Depositor
Resolution (Å)	49.05 – 2.75 49.05 – 2.75	Depositor EDS
% Data completeness (in resolution range)	58.2 (49.05-2.75) 88.0 (49.05-2.75)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.194 , 0.239 0.226 , 0.268	Depositor DCC
R_{free} test set	8229 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	45.4	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 18.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	81232	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.10 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8533e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BEZ, CL, A1C97, K

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	0.40	2/1512 (0.1%)	0.53	0/2050
1	B	0.33	0/1534	0.51	0/2077
1	C	0.43	1/1558 (0.1%)	0.62	0/2112
1	D	0.28	0/1508	0.47	0/2043
1	E	0.34	0/1529	0.53	0/2072
1	F	0.32	0/1513	0.53	0/2051
1	G	0.35	0/1542	0.56	0/2088
1	O	0.37	0/1513	0.58	0/2050
1	P	0.42	0/1539	0.62	0/2085
1	Q	0.46	1/1512 (0.1%)	0.62	0/2050
1	R	0.34	0/1527	0.53	0/2069
1	S	0.39	2/1526 (0.1%)	0.55	0/2069
1	T	0.44	0/1541	0.60	0/2089
1	U	0.38	0/1537	0.59	0/2081
2	H	0.28	0/1361	0.51	0/1842
2	I	0.40	1/1357 (0.1%)	0.53	0/1837
2	J	0.39	1/1354 (0.1%)	0.59	0/1833
2	K	0.37	0/1350	0.59	0/1827
2	L	0.39	1/1352 (0.1%)	0.56	0/1830
2	M	0.35	1/1347 (0.1%)	0.51	0/1823
2	N	0.39	1/1358 (0.1%)	0.63	0/1838
2	V	0.48	2/1341 (0.1%)	0.70	0/1816
2	W	0.43	1/1347 (0.1%)	0.65	0/1825
2	X	0.37	2/1341 (0.1%)	0.52	0/1817
2	Y	0.40	0/1364	0.64	0/1849
2	Z	0.30	0/1340	0.48	0/1816
2	a	0.30	0/1337	0.49	0/1811
2	b	0.37	2/1331 (0.2%)	0.55	0/1805
All	All	0.38	18/40271 (0.0%)	0.57	0/54555

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	B	0	2
1	E	0	1
1	G	0	2
1	Q	0	1
1	S	0	2
1	T	0	1
1	U	0	1
2	M	0	1
All	All	0	11

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	16	LEU	C-N	7.77	1.43	1.33
2	V	81	MET	C-N	7.42	1.42	1.33
2	V	154	ASN	C-N	7.30	1.43	1.33
2	X	122	MET	C-N	-6.94	1.24	1.33
2	b	75	MET	C-N	6.86	1.42	1.33

There are no bond angle outliers.

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	131	ARG	Sidechain
1	B	207	ARG	Sidechain
1	E	170	ARG	Sidechain
1	G	170	ARG	Sidechain
1	G	97	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	1491	1466	1466	10	0
1	B	1513	1502	1500	2	0
1	C	1537	1523	1522	12	0
1	D	1487	1475	1473	9	0
1	E	1508	1488	1487	7	0
1	F	1492	1471	1469	10	0
1	G	1521	1513	1511	12	0
1	O	1492	1476	1475	8	0
1	P	1517	1506	1505	12	0
1	Q	1491	1468	1466	8	0
1	R	1505	1488	1487	6	0
1	S	1504	1482	1481	9	0
1	T	1515	1491	1492	5	0
1	U	1515	1504	1502	8	0
2	H	1339	1323	1322	6	0
2	I	1335	1320	1318	5	0
2	J	1332	1311	1309	9	0
2	K	1328	1313	1311	7	0
2	L	1330	1306	1304	6	0
2	M	1325	1303	1302	6	0
2	N	1336	1322	1321	8	0
2	V	1319	1293	1291	8	0
2	W	1325	1305	1303	8	0
2	X	1319	1294	1292	5	0
2	Y	1341	1315	1313	3	0
2	Z	1318	1290	1289	6	0
2	a	1315	1288	1287	8	0
2	b	1309	1270	1269	11	0
3	A	8	5	5	0	0
3	B	8	5	5	0	0
3	C	8	5	5	0	0
3	D	8	5	5	0	0
3	E	8	5	5	1	0
3	F	8	5	5	0	0
3	G	8	5	5	0	0
3	O	8	5	5	0	0
3	P	8	5	5	0	0
3	Q	8	5	5	0	0
3	R	8	5	5	0	0
3	S	8	5	5	0	0
3	T	8	5	5	0	0
3	U	8	5	5	0	0
4	A	17	22	22	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	17	22	22	0	0
4	C	17	22	22	1	0
4	D	17	22	22	0	0
4	E	17	22	22	1	0
4	F	17	22	22	0	0
4	G	17	22	22	0	0
4	O	17	22	22	0	0
4	P	17	22	22	0	0
4	Q	17	22	22	0	0
4	R	17	22	22	0	0
4	S	17	22	22	0	0
4	T	17	22	22	0	0
4	U	17	22	22	0	0
5	A	57	53	0	1	0
5	B	57	53	0	0	0
5	C	57	53	0	1	0
5	D	57	53	0	3	0
5	E	114	106	0	0	0
5	G	57	53	0	0	0
5	O	57	53	0	0	0
5	P	57	53	0	1	0
5	Q	57	53	0	0	0
5	R	57	53	0	0	0
5	S	57	53	0	0	0
5	T	57	53	0	2	0
5	U	57	53	0	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	Q	1	0	0	0	0
7	P	1	0	0	0	0
8	A	13	0	0	0	0
8	B	17	0	0	0	0
8	C	10	0	0	0	0
8	D	10	0	0	0	0
8	E	3	0	0	0	0
8	F	11	0	0	0	0
8	G	8	0	0	0	0
8	H	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	I	3	0	0	0	0
8	J	5	0	0	0	0
8	K	6	0	0	0	0
8	L	4	0	0	0	0
8	M	6	0	0	0	0
8	N	9	0	0	0	0
8	O	8	0	0	0	0
8	P	8	0	0	0	0
8	Q	2	0	0	0	0
8	R	9	0	0	0	0
8	S	5	0	0	0	0
8	T	5	0	0	0	0
8	U	10	0	0	0	0
8	V	6	0	0	0	0
8	W	5	0	0	0	0
8	X	2	0	0	0	0
8	Y	4	0	0	0	0
8	Z	3	0	0	0	0
8	a	2	0	0	0	0
8	b	7	0	0	0	0
All	All	41006	40226	39445	173	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 2.

The worst 5 of 173 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)
1:D:105:LEU:HD23	1:D:127:LEU:HD12	1.71	0.72
1:C:57:MET:SD	1:D:105:LEU:HD22	2.31	0.71
1:D:105:LEU:HD21	5:D:804:A1C97:F37	1.82	0.70
2:W:31:PHE:HE1	2:W:93:MET:HE1	1.57	0.70
1:B:93:MET:HE3	1:B:100:ILE:HG21	1.79	0.65

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	196/215 (91%)	187 (95%)	9 (5%)	0	100	100
1	B	197/215 (92%)	188 (95%)	9 (5%)	0	100	100
1	C	202/215 (94%)	197 (98%)	5 (2%)	0	100	100
1	D	194/215 (90%)	187 (96%)	7 (4%)	0	100	100
1	E	198/215 (92%)	187 (94%)	11 (6%)	0	100	100
1	F	196/215 (91%)	186 (95%)	10 (5%)	0	100	100
1	G	198/215 (92%)	191 (96%)	7 (4%)	0	100	100
1	O	195/215 (91%)	187 (96%)	8 (4%)	0	100	100
1	P	197/215 (92%)	192 (98%)	4 (2%)	1 (0%)	24	43
1	Q	196/215 (91%)	188 (96%)	8 (4%)	0	100	100
1	R	196/215 (91%)	188 (96%)	8 (4%)	0	100	100
1	S	197/215 (92%)	190 (96%)	7 (4%)	0	100	100
1	T	198/215 (92%)	192 (97%)	6 (3%)	0	100	100
1	U	196/215 (91%)	192 (98%)	4 (2%)	0	100	100
2	H	175/194 (90%)	169 (97%)	6 (3%)	0	100	100
2	I	175/194 (90%)	169 (97%)	6 (3%)	0	100	100
2	J	175/194 (90%)	173 (99%)	2 (1%)	0	100	100
2	K	174/194 (90%)	167 (96%)	7 (4%)	0	100	100
2	L	175/194 (90%)	165 (94%)	10 (6%)	0	100	100
2	M	174/194 (90%)	168 (97%)	6 (3%)	0	100	100
2	N	175/194 (90%)	169 (97%)	6 (3%)	0	100	100
2	V	174/194 (90%)	166 (95%)	8 (5%)	0	100	100
2	W	175/194 (90%)	169 (97%)	6 (3%)	0	100	100
2	X	174/194 (90%)	166 (95%)	8 (5%)	0	100	100
2	Y	178/194 (92%)	168 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Z	174/194 (90%)	166 (95%)	8 (5%)	0	100	100
2	a	174/194 (90%)	165 (95%)	9 (5%)	0	100	100
2	b	174/194 (90%)	168 (97%)	6 (3%)	0	100	100
All	All	5202/5726 (91%)	5000 (96%)	201 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	96	VAL

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 X-ray entries followed by that with respect to entries of similar resolution.

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	156/176 (89%)	153 (98%)	3 (2%)	50	70
1	B	160/176 (91%)	158 (99%)	2 (1%)	61	76
1	C	161/176 (92%)	156 (97%)	5 (3%)	35	59
1	D	157/176 (89%)	157 (100%)	0	100	100
1	E	158/176 (90%)	156 (99%)	2 (1%)	61	76
1	F	157/176 (89%)	154 (98%)	3 (2%)	50	70
1	G	161/176 (92%)	159 (99%)	2 (1%)	63	78
1	O	157/176 (89%)	154 (98%)	3 (2%)	50	70
1	P	161/176 (92%)	157 (98%)	4 (2%)	42	64
1	Q	156/176 (89%)	154 (99%)	2 (1%)	61	76
1	R	159/176 (90%)	155 (98%)	4 (2%)	42	64
1	S	158/176 (90%)	153 (97%)	5 (3%)	34	58
1	T	160/176 (91%)	157 (98%)	3 (2%)	50	70
1	U	161/176 (92%)	157 (98%)	4 (2%)	42	64
2	H	136/151 (90%)	135 (99%)	1 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	135/151 (89%)	132 (98%)	3 (2%)	45	67
2	J	134/151 (89%)	131 (98%)	3 (2%)	45	67
2	K	134/151 (89%)	130 (97%)	4 (3%)	36	60
2	L	133/151 (88%)	132 (99%)	1 (1%)	73	84
2	M	133/151 (88%)	131 (98%)	2 (2%)	57	74
2	N	136/151 (90%)	133 (98%)	3 (2%)	45	67
2	V	132/151 (87%)	128 (97%)	4 (3%)	36	60
2	W	133/151 (88%)	130 (98%)	3 (2%)	44	66
2	X	133/151 (88%)	127 (96%)	6 (4%)	24	46
2	Y	133/151 (88%)	129 (97%)	4 (3%)	36	60
2	Z	132/151 (87%)	131 (99%)	1 (1%)	73	84
2	a	131/151 (87%)	129 (98%)	2 (2%)	57	74
2	b	130/151 (86%)	126 (97%)	4 (3%)	35	59
All	All	4087/4578 (89%)	4004 (98%)	83 (2%)	44	69

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	105	LEU
2	X	162	ILE
2	V	20	VAL
2	W	154	ASN
2	Y	191	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 64 ligands modelled in this entry, 8 are monoatomic - leaving 56 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	A1C97	S	804	-	61,61,61	1.45	9 (14%)	85,87,87	1.60	17 (20%)
4	LEU	D	802	3,4	5,7,8	0.62	0	6,8,10	0.51	0
4	LEU	R	803	4	6,8,8	0.89	0	5,10,10	1.09	1 (20%)
4	LEU	B	802	3,4	5,7,8	0.48	0	6,8,10	0.76	0
3	BEZ	Q	801	4	8,8,9	0.70	0	9,9,11	0.74	0
4	LEU	R	802	3,4	5,7,8	0.66	0	6,8,10	0.36	0
5	A1C97	C	804	-	61,61,61	1.45	9 (14%)	85,87,87	1.60	18 (21%)
4	LEU	P	803	4	6,8,8	0.88	0	5,10,10	1.01	1 (20%)
3	BEZ	P	801	4	8,8,9	0.60	0	9,9,11	0.66	0
4	LEU	Q	802	3,4	5,7,8	0.53	0	6,8,10	0.54	0
4	LEU	T	802	3,4	5,7,8	0.58	0	6,8,10	0.63	0
4	LEU	U	802	3,4	5,7,8	0.63	0	6,8,10	0.42	0
5	A1C97	U	804	-	61,61,61	1.48	9 (14%)	85,87,87	1.70	19 (22%)
4	LEU	S	803	4	6,8,8	0.82	0	5,10,10	0.25	0
3	BEZ	E	801	4	8,8,9	0.74	0	9,9,11	0.72	0
5	A1C97	B	804	-	61,61,61	1.45	9 (14%)	85,87,87	1.60	17 (20%)
4	LEU	O	802	3,4	5,7,8	0.54	0	6,8,10	0.38	0
5	A1C97	O	804	-	61,61,61	1.45	9 (14%)	85,87,87	1.60	17 (20%)
5	A1C97	D	804	-	61,61,61	1.46	9 (14%)	85,87,87	1.60	17 (20%)
3	BEZ	B	801	4	8,8,9	0.54	0	9,9,11	0.77	0
5	A1C97	Q	804	-	61,61,61	1.39	8 (13%)	85,87,87	1.64	19 (22%)
4	LEU	G	802	3,4	5,7,8	0.67	0	6,8,10	0.61	0
3	BEZ	R	801	4	8,8,9	0.65	0	9,9,11	0.52	0
4	LEU	F	803	4	6,8,8	0.93	1 (16%)	5,10,10	1.07	1 (20%)
3	BEZ	U	801	4	8,8,9	0.59	0	9,9,11	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	A1C97	E	805	-	61,61,61	1.45	9 (14%)	85,87,87	1.60	17 (20%)
4	LEU	A	803	4	6,8,8	0.94	1 (16%)	5,10,10	1.26	1 (20%)
3	BEZ	S	801	4	8,8,9	0.61	0	9,9,11	0.88	0
3	BEZ	C	801	4	8,8,9	0.56	0	9,9,11	0.75	0
4	LEU	C	802	3,4	5,7,8	0.66	0	6,8,10	1.23	1 (16%)
4	LEU	T	803	4	6,8,8	0.89	1 (16%)	5,10,10	1.09	1 (20%)
4	LEU	F	802	3,4	5,7,8	0.70	0	6,8,10	0.67	0
3	BEZ	A	801	4	8,8,9	0.60	0	9,9,11	1.04	1 (11%)
5	A1C97	E	804	-	61,61,61	1.46	9 (14%)	85,87,87	1.60	17 (20%)
4	LEU	U	803	4	6,8,8	0.90	1 (16%)	5,10,10	0.96	1 (20%)
4	LEU	B	803	4	6,8,8	0.91	1 (16%)	5,10,10	1.07	1 (20%)
3	BEZ	D	801	4	8,8,9	0.67	0	9,9,11	0.58	0
3	BEZ	T	801	4	8,8,9	0.61	0	9,9,11	0.76	0
4	LEU	C	803	4	6,8,8	0.92	1 (16%)	5,10,10	1.38	1 (20%)
5	A1C97	G	804	-	61,61,61	1.45	9 (14%)	85,87,87	1.60	17 (20%)
4	LEU	E	802	3,4	5,7,8	0.50	0	6,8,10	0.30	0
5	A1C97	R	804	-	61,61,61	1.45	9 (14%)	85,87,87	1.60	17 (20%)
4	LEU	S	802	3,4	5,7,8	0.64	0	6,8,10	0.41	0
3	BEZ	G	801	4	8,8,9	0.72	0	9,9,11	0.49	0
4	LEU	Q	803	4	6,8,8	0.88	0	5,10,10	1.09	1 (20%)
4	LEU	D	803	4	6,8,8	0.91	1 (16%)	5,10,10	0.98	1 (20%)
4	LEU	O	803	4	6,8,8	0.89	0	5,10,10	1.11	1 (20%)
4	LEU	A	802	3,4	5,7,8	0.54	0	6,8,10	0.21	0
4	LEU	G	803	4	6,8,8	0.89	0	5,10,10	1.31	1 (20%)
5	A1C97	P	804	-	61,61,61	1.45	9 (14%)	85,87,87	1.60	17 (20%)
3	BEZ	F	801	4	8,8,9	0.64	0	9,9,11	0.58	0
5	A1C97	A	804	-	61,61,61	1.45	9 (14%)	85,87,87	1.60	17 (20%)
4	LEU	P	802	3,4	5,7,8	0.53	0	6,8,10	0.49	0
4	LEU	E	803	4	6,8,8	0.89	0	5,10,10	1.07	1 (20%)
3	BEZ	O	801	4	8,8,9	0.60	0	9,9,11	0.68	0
5	A1C97	T	804	-	61,61,61	1.45	9 (14%)	85,87,87	1.60	17 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	A1C97	S	804	-	-	8/68/101/101	0/4/5/5
4	LEU	D	802	3,4	-	3/5/6/8	-
4	LEU	R	803	4	-	1/8/8/8	-
4	LEU	B	802	3,4	-	2/5/6/8	-
3	BEZ	Q	801	4	-	0/2/2/4	0/1/1/1
4	LEU	R	802	3,4	-	2/5/6/8	-
5	A1C97	C	804	-	-	8/68/101/101	0/4/5/5
4	LEU	P	803	4	-	1/8/8/8	-
3	BEZ	P	801	4	-	0/2/2/4	0/1/1/1
4	LEU	Q	802	3,4	-	2/5/6/8	-
4	LEU	T	802	3,4	-	2/5/6/8	-
4	LEU	U	802	3,4	-	2/5/6/8	-
5	A1C97	U	804	-	-	11/68/101/101	0/4/5/5
4	LEU	S	803	4	-	1/8/8/8	-
3	BEZ	E	801	4	-	0/2/2/4	0/1/1/1
5	A1C97	B	804	-	-	8/68/101/101	0/4/5/5
4	LEU	O	802	3,4	-	2/5/6/8	-
5	A1C97	O	804	-	-	8/68/101/101	0/4/5/5
5	A1C97	D	804	-	-	8/68/101/101	0/4/5/5
3	BEZ	B	801	4	-	2/2/2/4	0/1/1/1
5	A1C97	Q	804	-	-	8/68/101/101	0/4/5/5
4	LEU	G	802	3,4	-	2/5/6/8	-
3	BEZ	R	801	4	-	0/2/2/4	0/1/1/1
4	LEU	F	803	4	-	0/8/8/8	-
3	BEZ	U	801	4	-	0/2/2/4	0/1/1/1
5	A1C97	E	805	-	-	8/68/101/101	0/4/5/5
4	LEU	A	803	4	-	2/8/8/8	-
3	BEZ	S	801	4	-	0/2/2/4	0/1/1/1
3	BEZ	C	801	4	-	0/2/2/4	0/1/1/1
4	LEU	C	802	3,4	-	2/5/6/8	-
4	LEU	T	803	4	-	0/8/8/8	-
4	LEU	F	802	3,4	-	2/5/6/8	-
3	BEZ	A	801	4	-	0/2/2/4	0/1/1/1
5	A1C97	E	804	-	-	8/68/101/101	0/4/5/5
4	LEU	U	803	4	-	1/8/8/8	-
4	LEU	B	803	4	-	1/8/8/8	-
3	BEZ	D	801	4	-	2/2/2/4	0/1/1/1
3	BEZ	T	801	4	-	2/2/2/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LEU	C	803	4	-	0/8/8/8	-
5	A1C97	G	804	-	-	8/68/101/101	0/4/5/5
4	LEU	E	802	3,4	-	3/5/6/8	-
5	A1C97	R	804	-	-	8/68/101/101	0/4/5/5
4	LEU	S	802	3,4	-	2/5/6/8	-
3	BEZ	G	801	4	-	0/2/2/4	0/1/1/1
4	LEU	Q	803	4	-	1/8/8/8	-
4	LEU	D	803	4	-	1/8/8/8	-
4	LEU	O	803	4	-	1/8/8/8	-
4	LEU	A	802	3,4	-	1/5/6/8	-
4	LEU	G	803	4	-	0/8/8/8	-
5	A1C97	P	804	-	-	8/68/101/101	0/4/5/5
3	BEZ	F	801	4	-	0/2/2/4	0/1/1/1
5	A1C97	A	804	-	-	8/68/101/101	0/4/5/5
4	LEU	P	802	3,4	-	2/5/6/8	-
4	LEU	E	803	4	-	0/8/8/8	-
3	BEZ	O	801	4	-	0/2/2/4	0/1/1/1
5	A1C97	T	804	-	-	8/68/101/101	0/4/5/5

The worst 5 of 132 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	804	A1C97	C43-N42	4.37	1.43	1.34
5	D	804	A1C97	C09-N10	4.30	1.44	1.34
5	O	804	A1C97	C09-N10	4.29	1.44	1.34
5	G	804	A1C97	C09-N10	4.28	1.44	1.34
5	P	804	A1C97	C09-N10	4.28	1.44	1.34

The worst 5 of 258 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	804	A1C97	O27-C25-C24	4.56	115.75	105.77
5	S	804	A1C97	O27-C25-C24	4.56	115.74	105.77
5	O	804	A1C97	O27-C25-C24	4.56	115.73	105.77
5	E	805	A1C97	O27-C25-C24	4.55	115.73	105.77
5	E	804	A1C97	O27-C25-C24	4.55	115.72	105.77

There are no chirality outliers.

5 of 160 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	802	LEU	O-C-CA-CB
4	B	802	LEU	N-CA-CB-CG
4	B	802	LEU	C-CA-CB-CG
4	D	802	LEU	O-C-CA-CB
4	D	802	LEU	C-CA-CB-CG

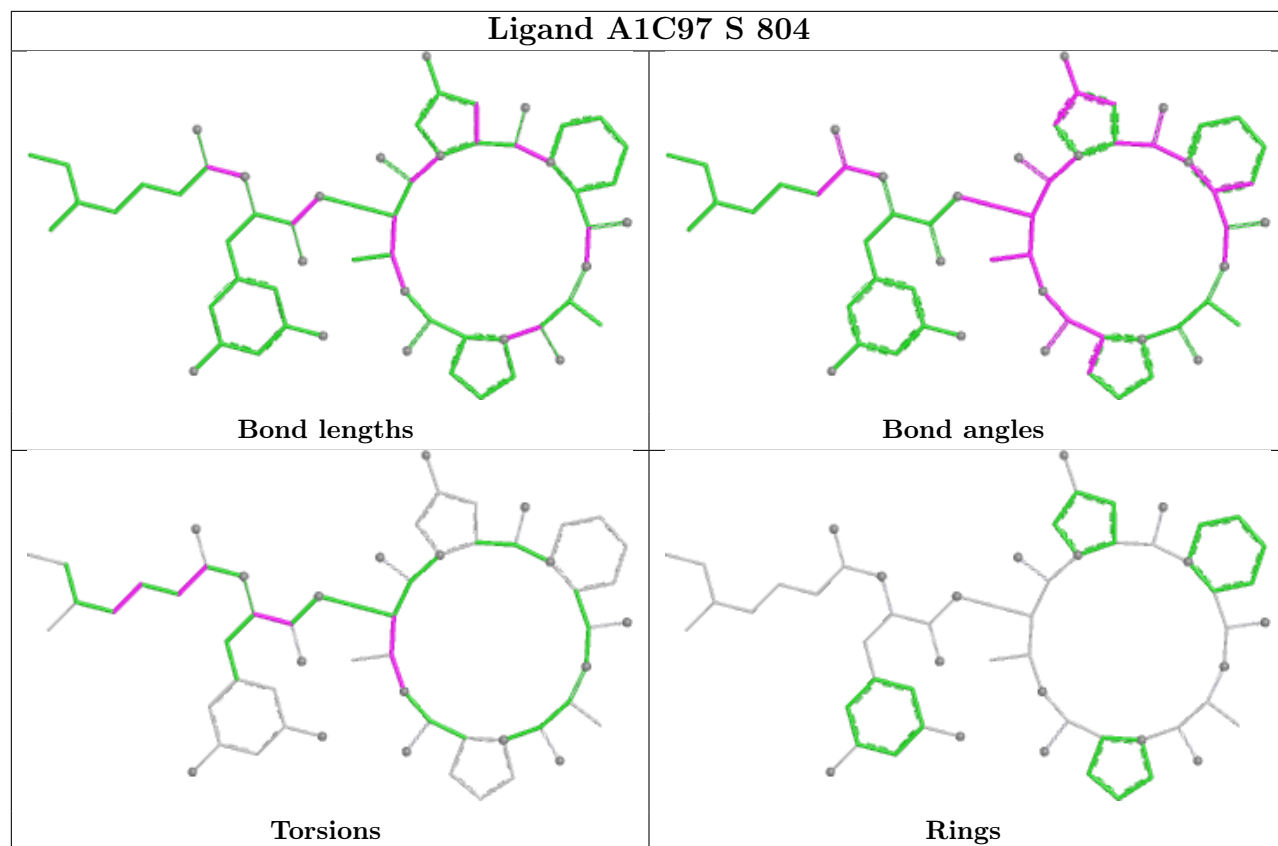
There are no ring outliers.

10 monomers are involved in 14 short contacts:

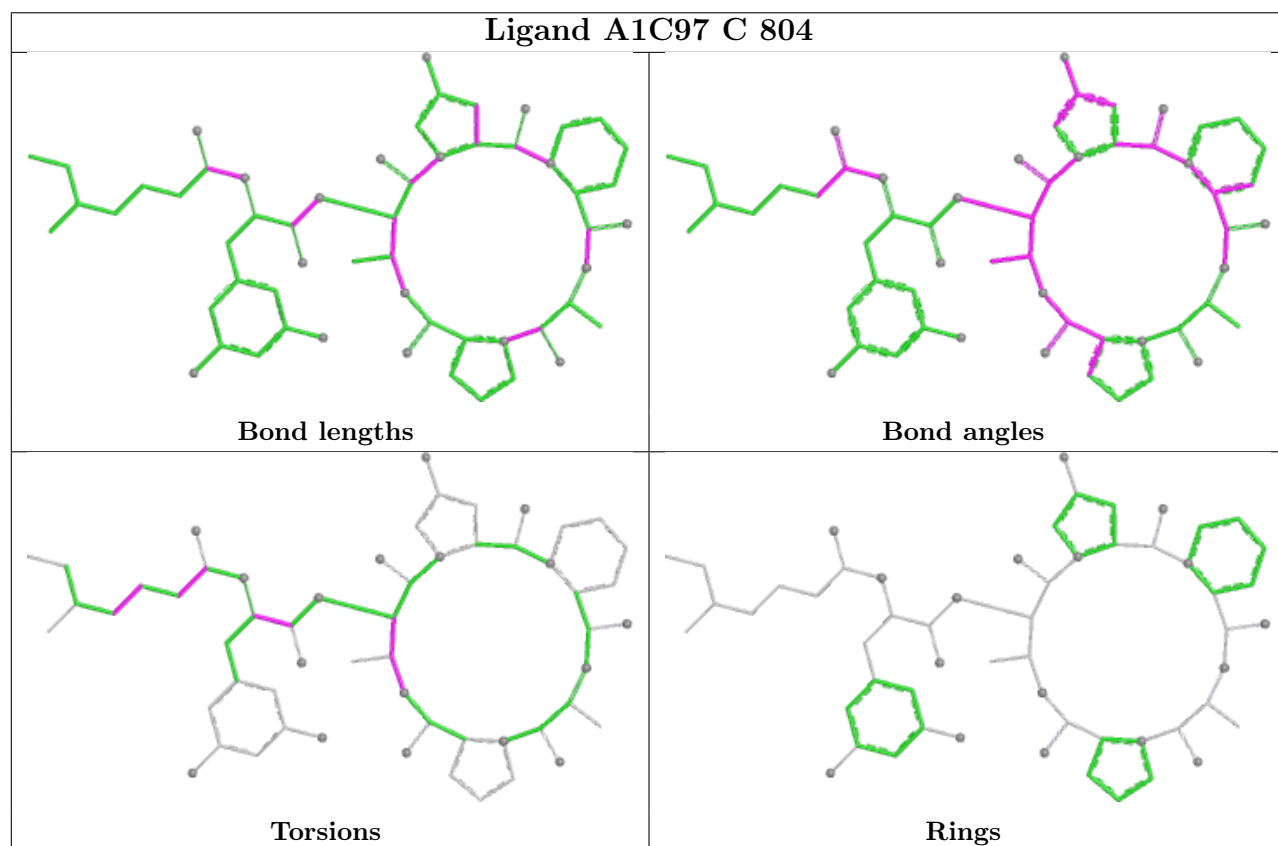
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	804	A1C97	1	0
5	U	804	A1C97	2	0
3	E	801	BEZ	1	0
5	D	804	A1C97	3	0
4	A	803	LEU	2	0
4	C	803	LEU	1	0
4	E	802	LEU	1	0
5	P	804	A1C97	1	0
5	A	804	A1C97	1	0
5	T	804	A1C97	2	0

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.

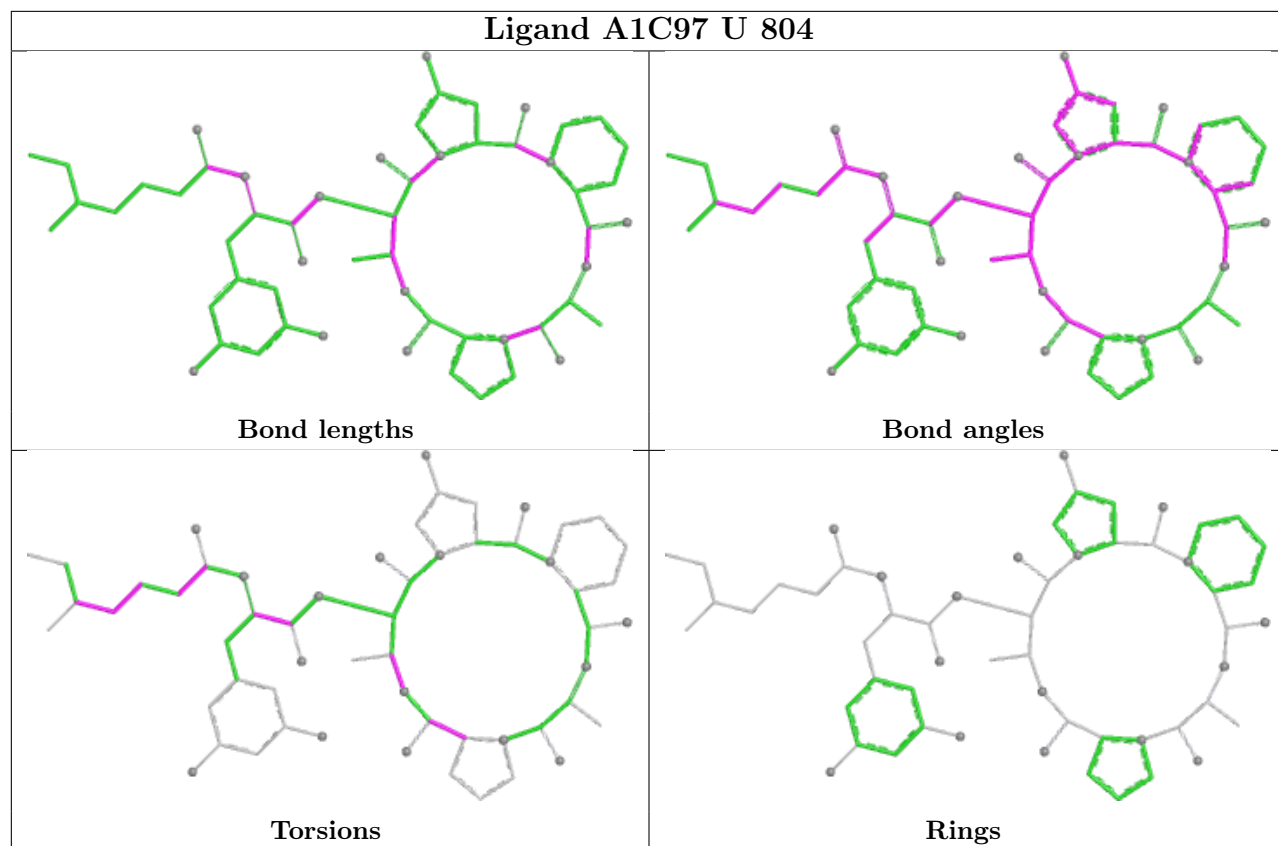
Ligand A1C97 S 804



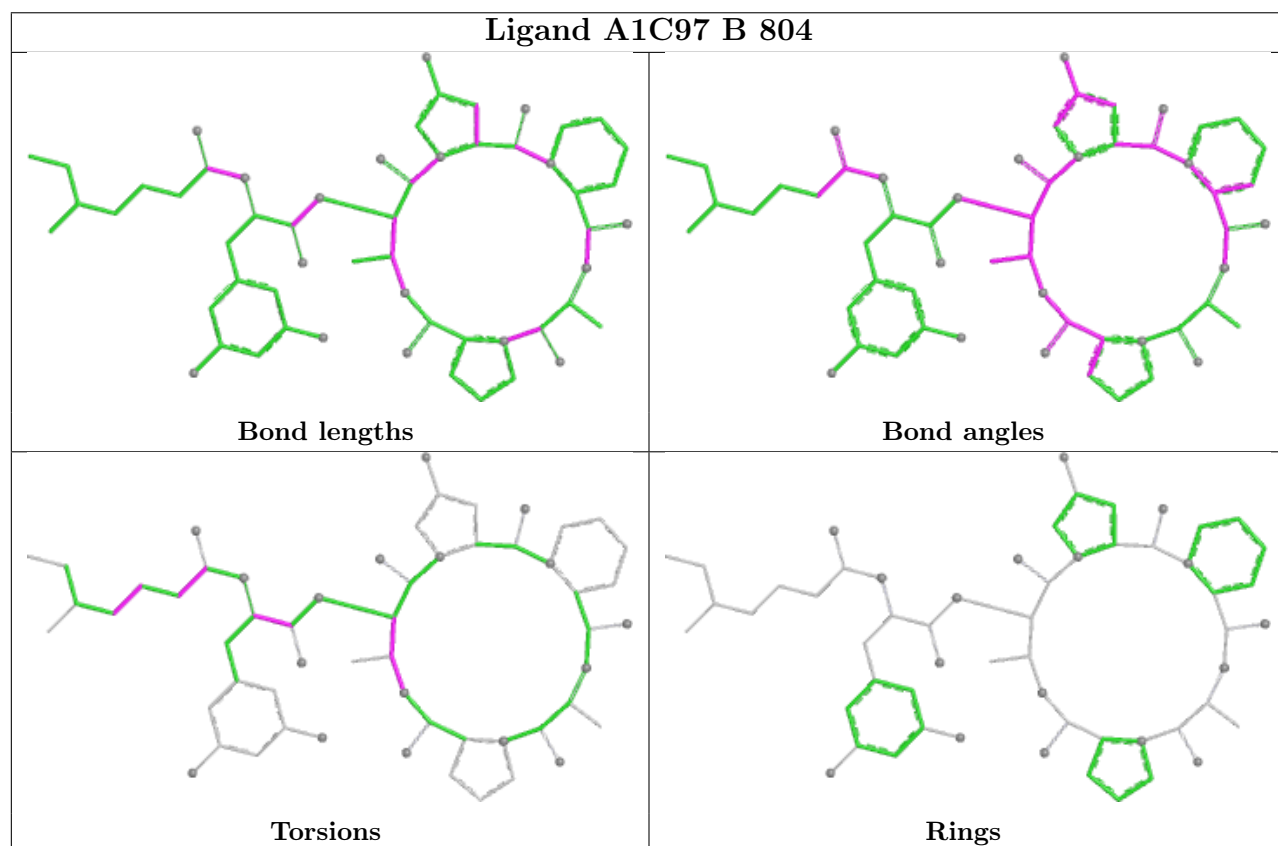
Ligand A1C97 C 804



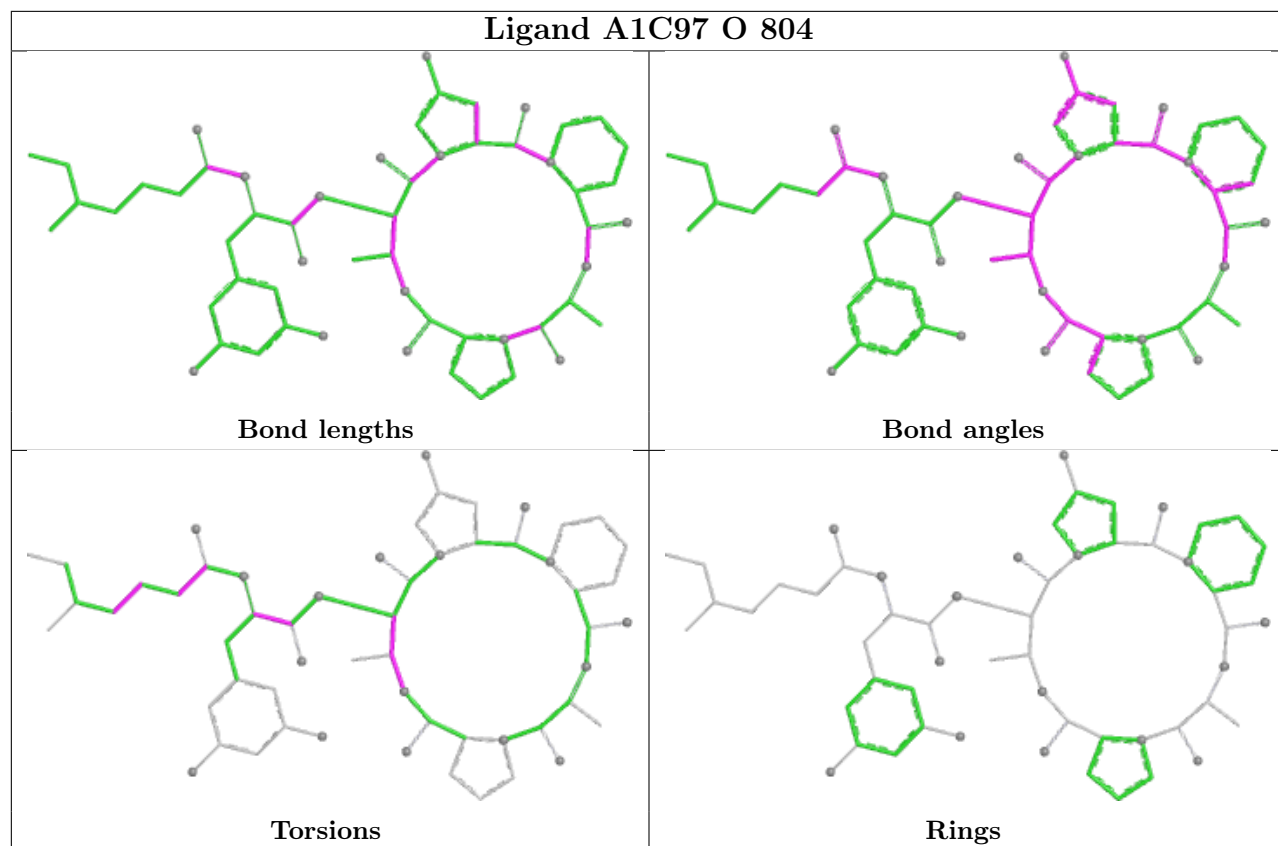
Ligand A1C97 U 804



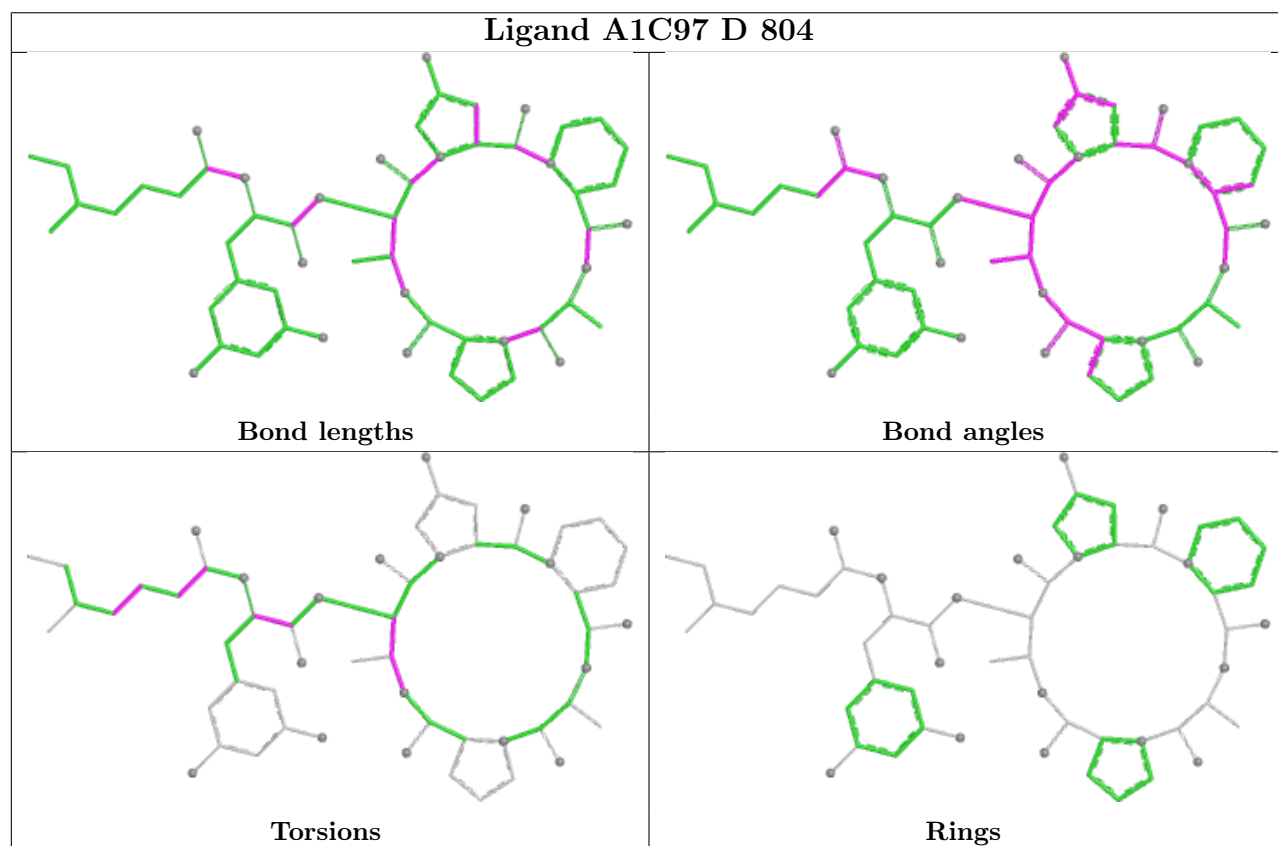
Ligand A1C97 B 804



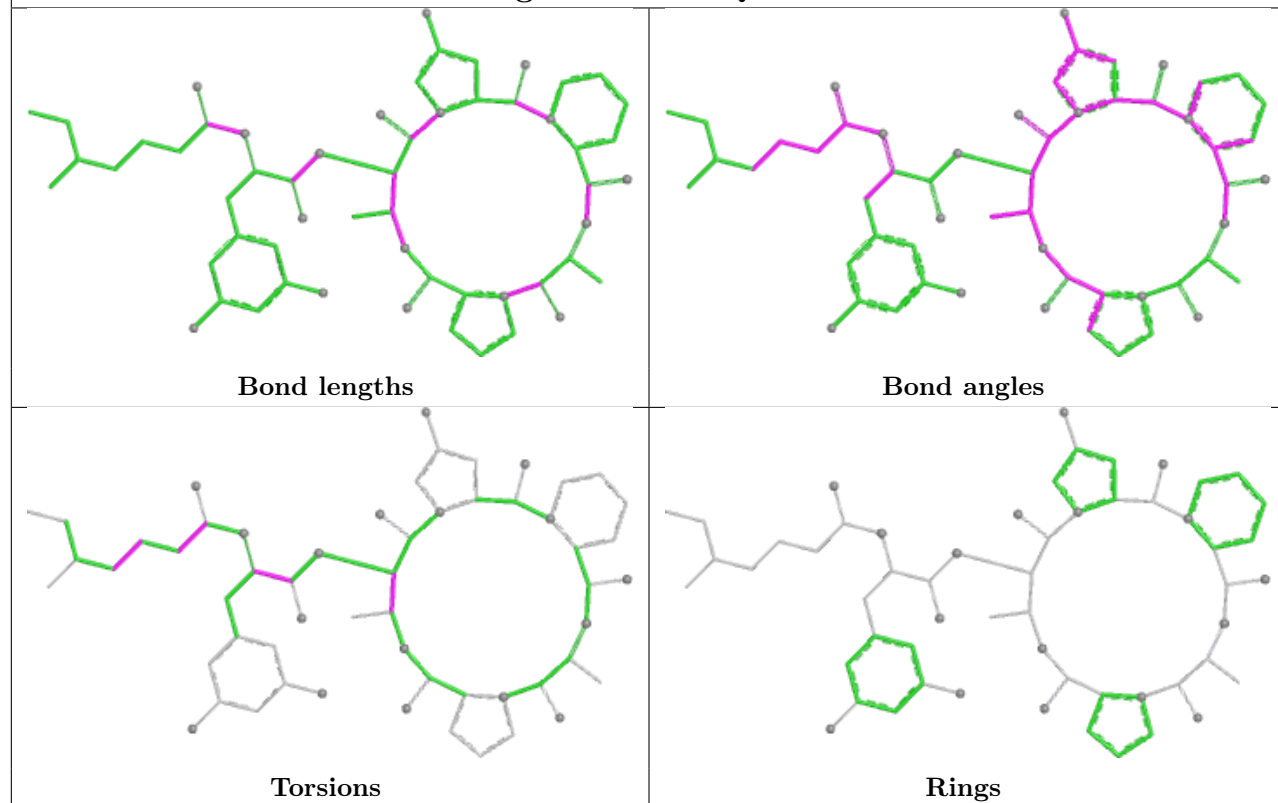
Ligand A1C97 O 804



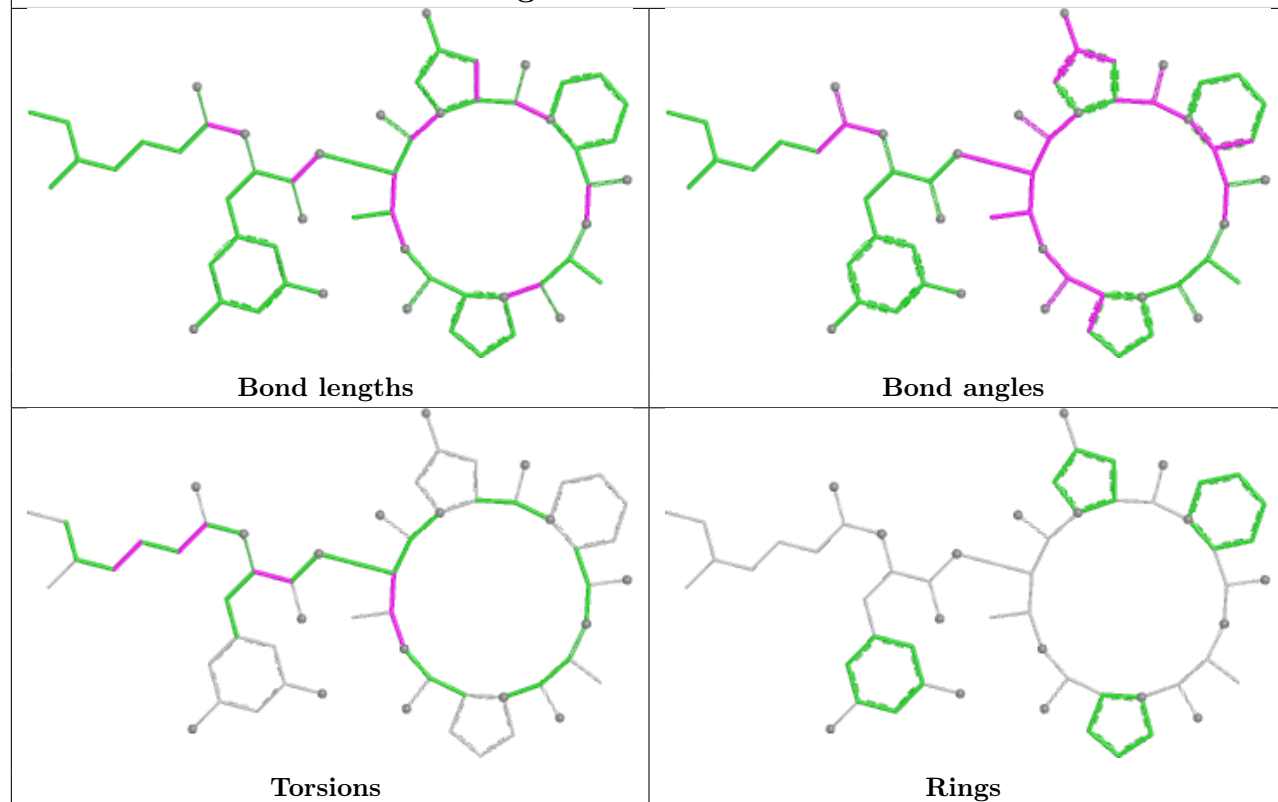
Ligand A1C97 D 804



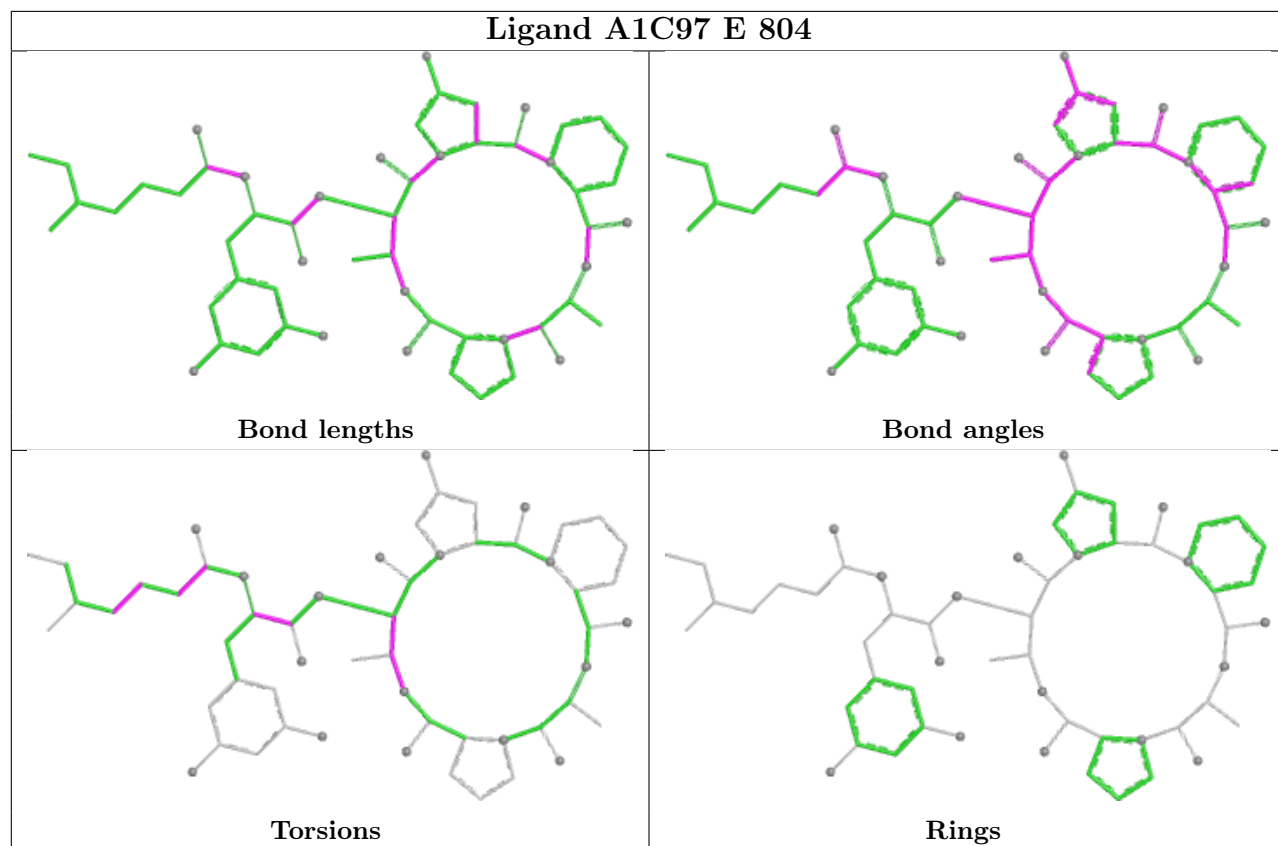
Ligand A1C97 Q 804



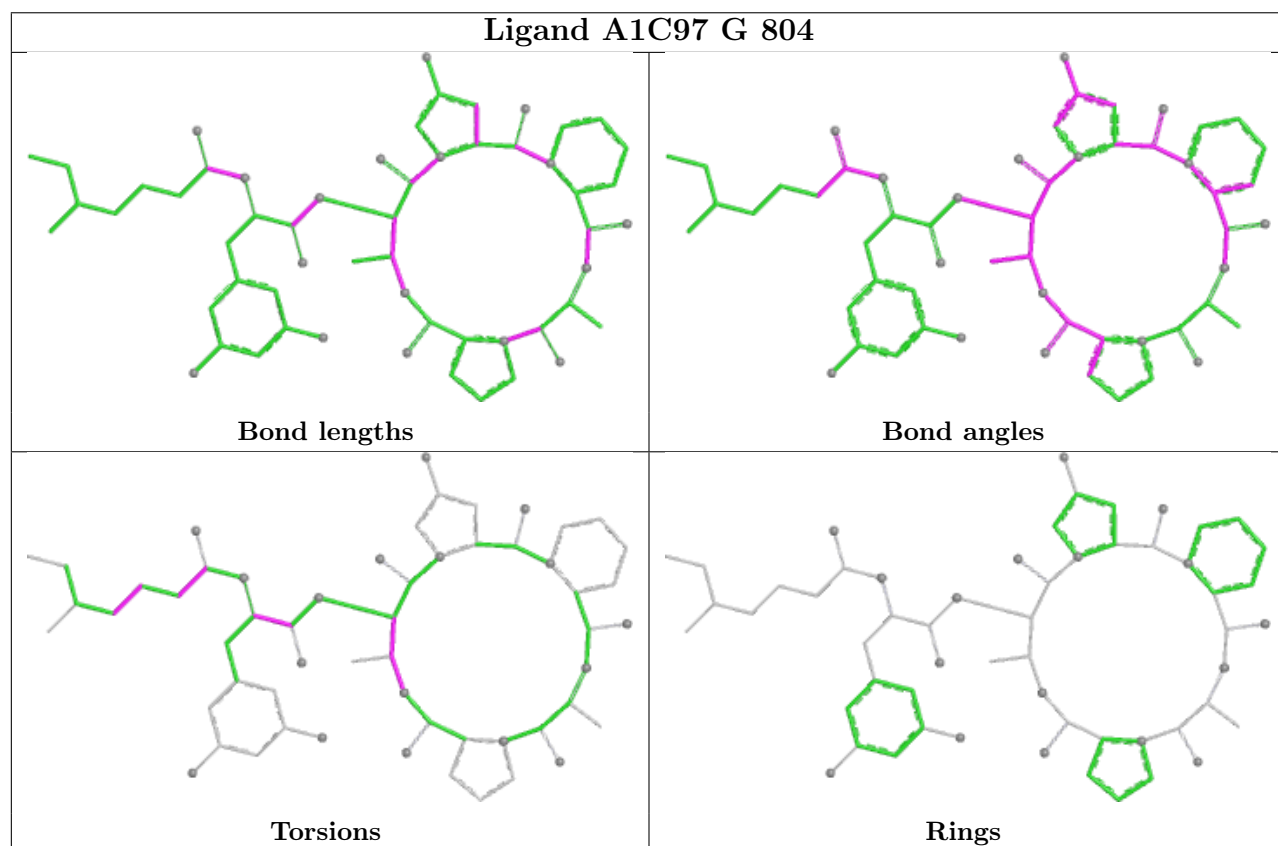
Ligand A1C97 E 805



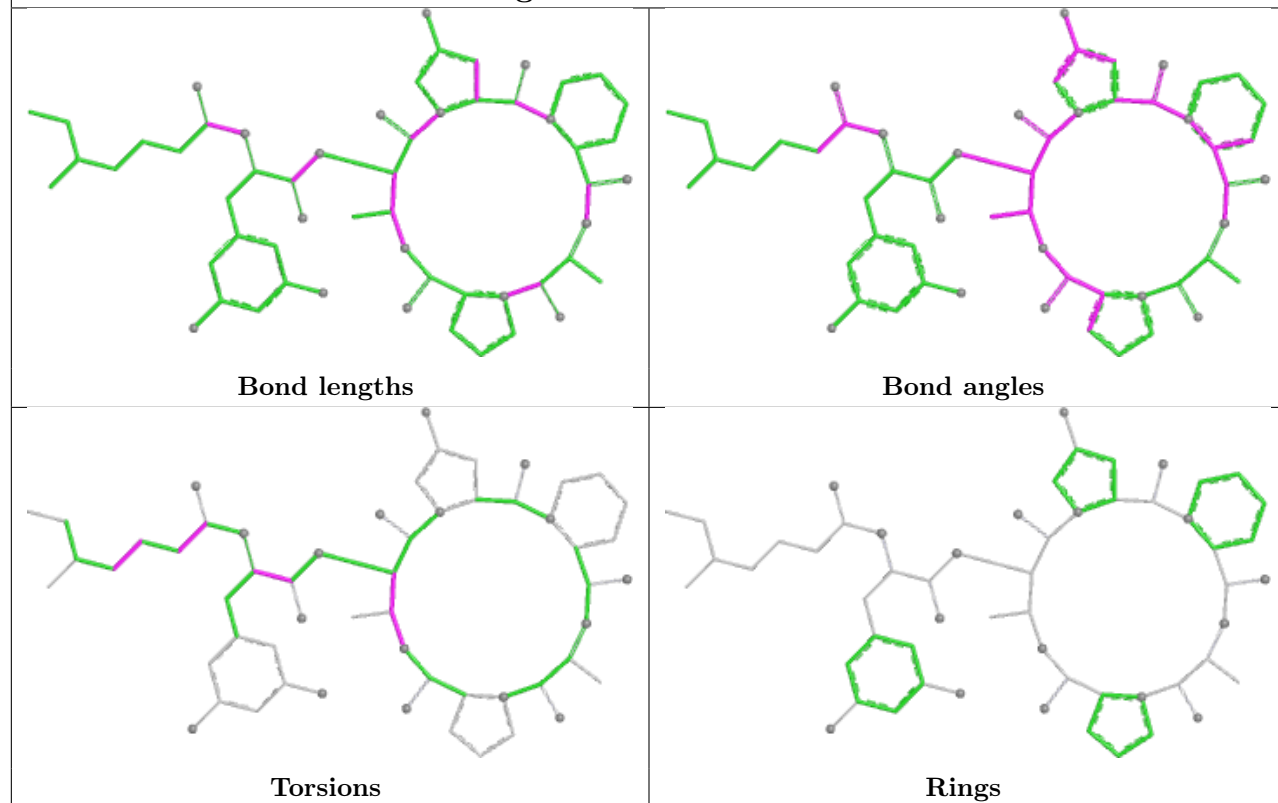
Ligand A1C97 E 804



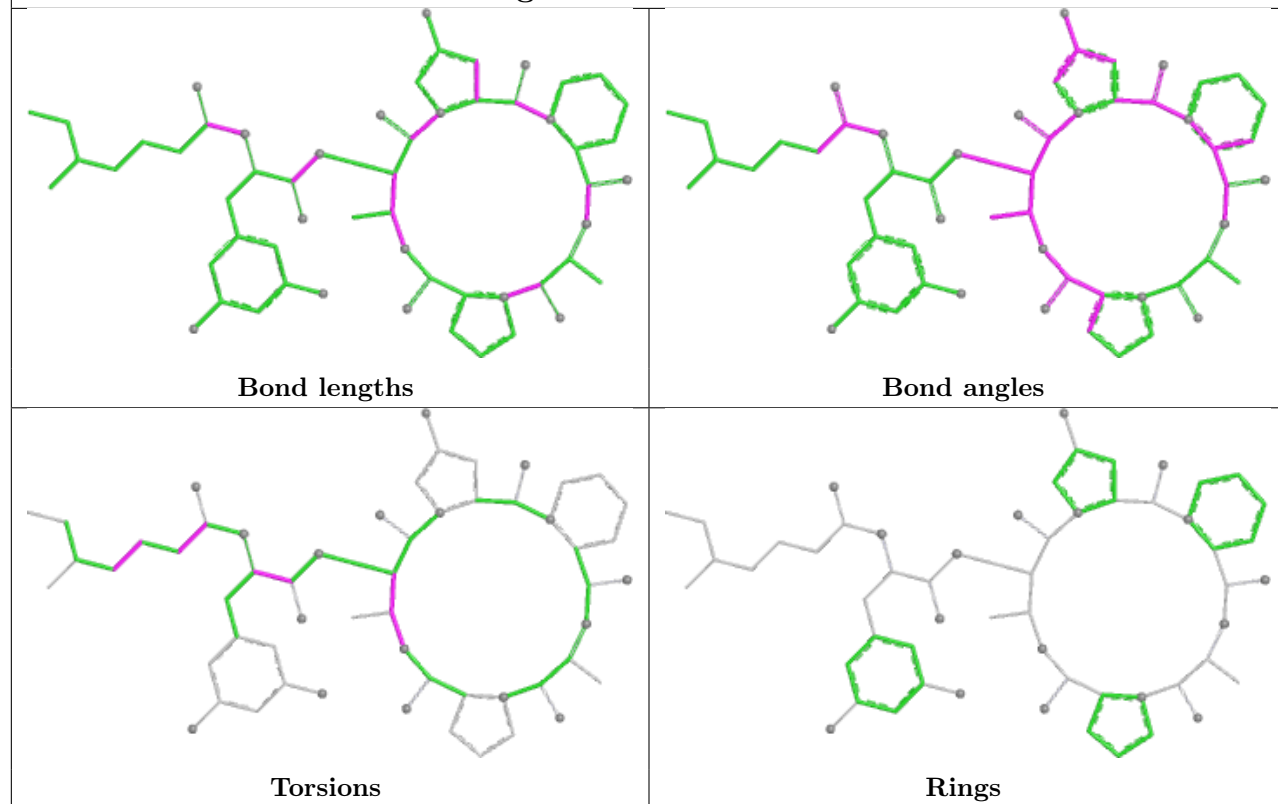
Ligand A1C97 G 804



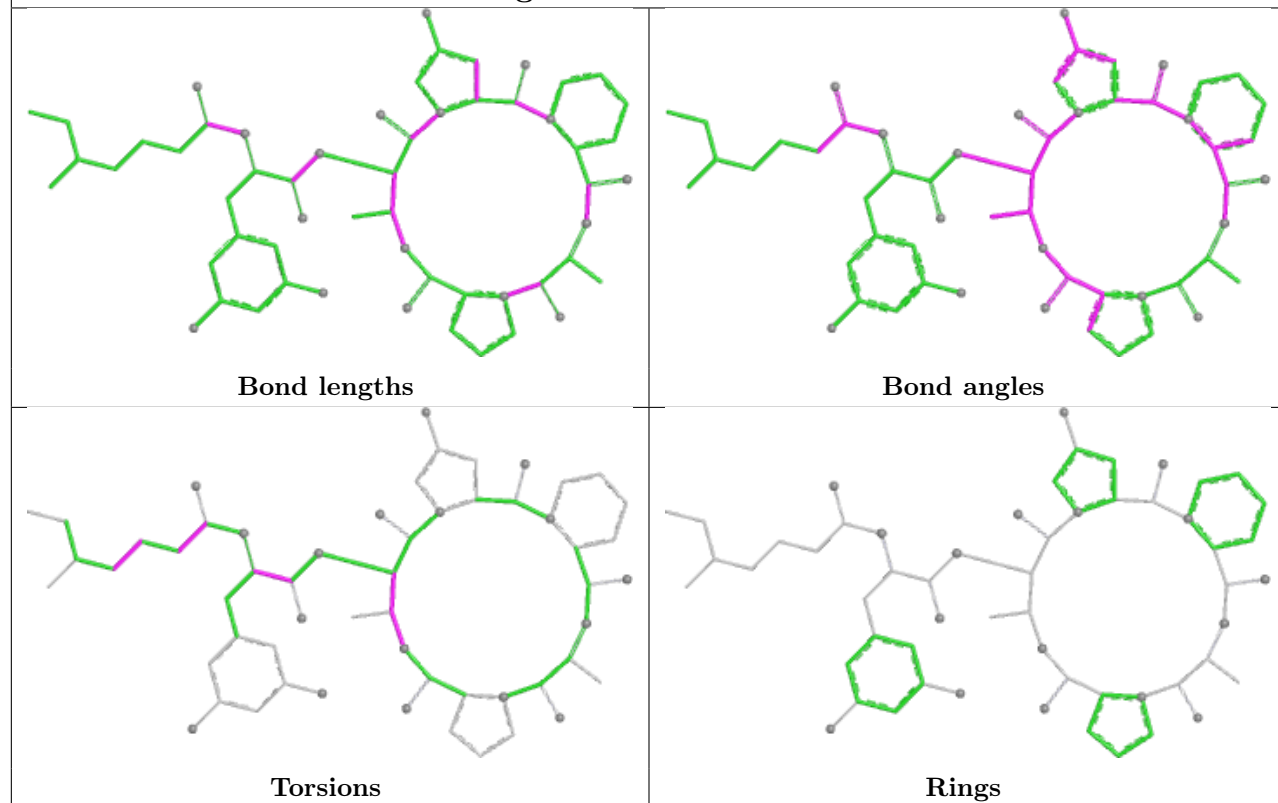
Ligand A1C97 R 804



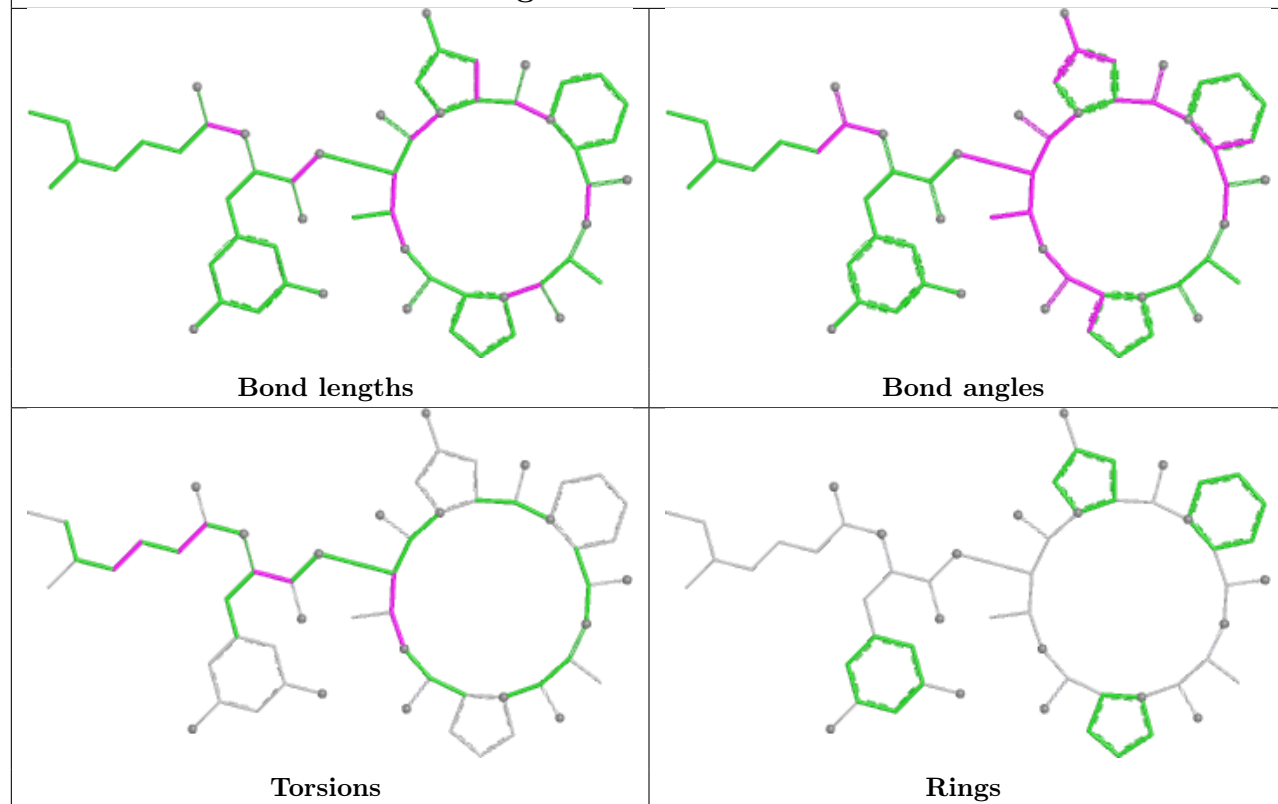
Ligand A1C97 P 804



Ligand A1C97 A 804



Ligand A1C97 T 804



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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	198/215 (92%)	0.12	7 (3%) 47 44	33, 50, 66, 93	0
1	B	199/215 (92%)	0.07	4 (2%) 65 63	33, 51, 68, 95	0
1	C	204/215 (94%)	0.01	7 (3%) 48 46	32, 48, 67, 96	0
1	D	196/215 (91%)	0.02	4 (2%) 65 63	34, 49, 63, 85	0
1	E	200/215 (93%)	0.22	5 (2%) 58 56	36, 55, 70, 104	0
1	F	198/215 (92%)	0.16	3 (1%) 72 71	36, 53, 69, 87	0
1	G	200/215 (93%)	0.15	5 (2%) 58 56	34, 51, 67, 94	0
1	O	197/215 (91%)	0.03	7 (3%) 46 44	32, 48, 62, 89	0
1	P	199/215 (92%)	0.12	6 (3%) 52 50	32, 50, 65, 104	0
1	Q	198/215 (92%)	0.10	8 (4%) 42 40	35, 50, 68, 106	0
1	R	198/215 (92%)	0.09	5 (2%) 58 56	33, 51, 65, 100	0
1	S	199/215 (92%)	0.16	7 (3%) 47 44	34, 53, 69, 106	0
1	T	199/215 (92%)	0.09	6 (3%) 52 50	37, 50, 68, 96	1 (0%)
1	U	198/215 (92%)	0.04	6 (3%) 52 50	32, 48, 65, 93	0
2	H	177/194 (91%)	0.12	6 (3%) 48 46	35, 53, 70, 95	0
2	I	177/194 (91%)	0.08	3 (1%) 69 67	40, 54, 74, 91	0
2	J	177/194 (91%)	0.12	3 (1%) 69 67	36, 53, 69, 82	0
2	K	176/194 (90%)	0.17	1 (0%) 85 86	39, 56, 69, 79	0
2	L	177/194 (91%)	0.21	2 (1%) 78 77	38, 58, 74, 82	0
2	M	176/194 (90%)	0.24	2 (1%) 78 77	40, 58, 74, 94	0
2	N	177/194 (91%)	0.11	0 100 100	39, 54, 70, 86	0
2	V	176/194 (90%)	0.30	8 (4%) 38 37	40, 55, 69, 77	0
2	W	177/194 (91%)	0.21	2 (1%) 78 77	38, 55, 68, 84	0
2	X	176/194 (90%)	0.12	3 (1%) 69 67	39, 54, 68, 78	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	Y	180/194 (92%)	0.17	2 (1%) 78 77	37, 55, 72, 84	0
2	Z	176/194 (90%)	0.11	3 (1%) 69 67	38, 54, 67, 86	0
2	a	176/194 (90%)	0.27	2 (1%) 78 77	39, 58, 73, 85	0
2	b	176/194 (90%)	0.20	2 (1%) 78 77	40, 56, 74, 82	0
All	All	5257/5726 (91%)	0.13	119 (2%) 61 59	32, 53, 70, 106	1 (0%)

The worst 5 of 119 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	135[A]	HIS	6.3
2	L	191	THR	5.6
1	E	14	TYR	4.9
1	G	212	GLN	4.8
1	U	13	ARG	4.7

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	CL	Q	805	1/1	0.76	0.14	51,51,51,51	0
7	K	P	805	1/1	0.76	0.20	79,79,79,79	0
4	LEU	C	802	8/9	0.79	0.18	38,50,80,80	0
6	CL	B	805	1/1	0.79	0.11	53,53,53,53	0
4	LEU	S	803	9/9	0.83	0.19	55,68,95,95	0
4	LEU	T	802	8/9	0.84	0.19	46,64,84,84	0
4	LEU	P	803	9/9	0.86	0.16	57,70,78,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	LEU	R	803	9/9	0.87	0.16	57,69,83,83	0
6	CL	G	805	1/1	0.87	0.11	51,51,51,51	0
4	LEU	O	803	9/9	0.87	0.18	43,64,71,74	0
4	LEU	B	803	9/9	0.87	0.18	48,66,81,81	0
4	LEU	E	803	9/9	0.88	0.15	51,65,83,83	0
4	LEU	U	803	9/9	0.88	0.15	49,62,71,80	0
4	LEU	Q	803	9/9	0.88	0.17	47,73,88,88	0
6	CL	C	805	1/1	0.89	0.10	49,49,49,49	0
4	LEU	A	803	9/9	0.89	0.15	49,64,77,77	0
6	CL	A	805	1/1	0.89	0.14	55,55,55,55	0
4	LEU	F	802	8/9	0.89	0.17	57,73,94,94	0
4	LEU	G	802	8/9	0.90	0.13	54,65,78,78	0
3	BEZ	A	801	8/9	0.90	0.11	44,52,57,63	0
4	LEU	P	802	8/9	0.90	0.17	55,68,88,88	0
4	LEU	B	802	8/9	0.90	0.15	47,60,76,76	0
3	BEZ	F	801	8/9	0.90	0.18	48,58,69,74	0
5	A1C97	T	804	57/57	0.91	0.12	31,54,76,91	0
5	A1C97	U	804	57/57	0.91	0.12	31,50,72,81	0
4	LEU	Q	802	8/9	0.91	0.12	49,62,77,77	0
4	LEU	U	802	8/9	0.91	0.14	45,54,71,71	0
4	LEU	D	803	9/9	0.91	0.12	50,62,77,77	0
5	A1C97	E	804	57/57	0.91	0.13	36,55,72,74	0
5	A1C97	Q	804	57/57	0.91	0.13	34,56,72,85	0
5	A1C97	S	804	57/57	0.91	0.13	28,53,75,82	0
5	A1C97	B	804	57/57	0.92	0.12	30,50,72,78	0
5	A1C97	C	804	57/57	0.92	0.13	32,48,71,86	0
5	A1C97	D	804	57/57	0.92	0.12	32,53,90,96	0
4	LEU	E	802	8/9	0.92	0.17	49,63,76,76	0
5	A1C97	E	805	57/57	0.92	0.11	34,55,80,99	0
5	A1C97	G	804	57/57	0.92	0.13	35,58,81,89	0
5	A1C97	O	804	57/57	0.92	0.11	31,46,66,79	0
3	BEZ	B	801	8/9	0.92	0.13	45,52,62,67	0
3	BEZ	T	801	8/9	0.92	0.18	51,61,76,80	0
4	LEU	R	802	8/9	0.92	0.16	46,64,83,83	0
4	LEU	A	802	8/9	0.92	0.14	48,60,77,77	0
4	LEU	G	803	9/9	0.92	0.12	59,71,75,77	0
4	LEU	O	802	8/9	0.92	0.14	50,63,85,85	0
4	LEU	T	803	9/9	0.92	0.15	58,72,84,86	0
4	LEU	C	803	9/9	0.92	0.14	49,60,72,72	0
3	BEZ	E	801	8/9	0.92	0.15	45,55,66,72	0
5	A1C97	A	804	57/57	0.92	0.12	35,51,64,74	0
5	A1C97	R	804	57/57	0.93	0.11	31,56,90,97	0

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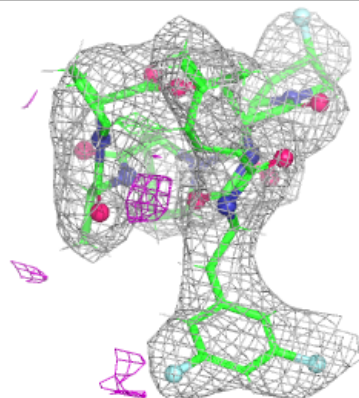
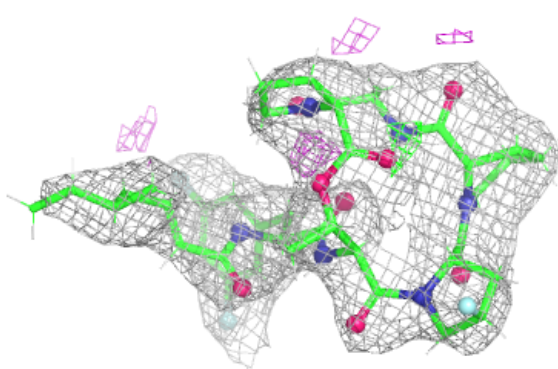
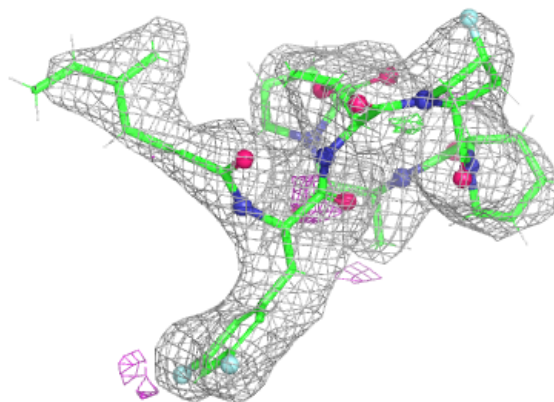
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	LEU	S	802	8/9	0.93	0.23	52,73,106,106	0
3	BEZ	G	801	8/9	0.93	0.11	47,56,69,79	0
5	A1C97	P	804	57/57	0.93	0.12	34,50,72,87	0
4	LEU	F	803	9/9	0.93	0.14	60,74,93,93	0
3	BEZ	S	801	8/9	0.94	0.16	47,59,71,75	0
3	BEZ	O	801	8/9	0.94	0.11	40,48,57,61	0
6	CL	E	806	1/1	0.94	0.09	59,59,59,59	0
3	BEZ	R	801	8/9	0.95	0.10	50,56,68,68	0
6	CL	D	805	1/1	0.95	0.09	57,57,57,57	0
3	BEZ	P	801	8/9	0.95	0.15	44,55,68,70	0
4	LEU	D	802	8/9	0.95	0.11	39,52,83,83	0
3	BEZ	Q	801	8/9	0.95	0.11	47,58,71,75	0
3	BEZ	U	801	8/9	0.95	0.09	35,46,56,59	0
3	BEZ	C	801	8/9	0.96	0.07	39,44,55,56	0
3	BEZ	D	801	8/9	0.97	0.07	39,48,60,61	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

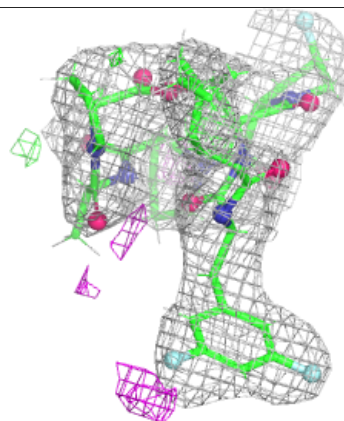
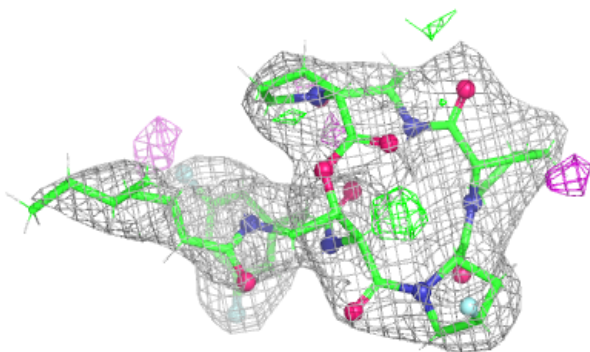
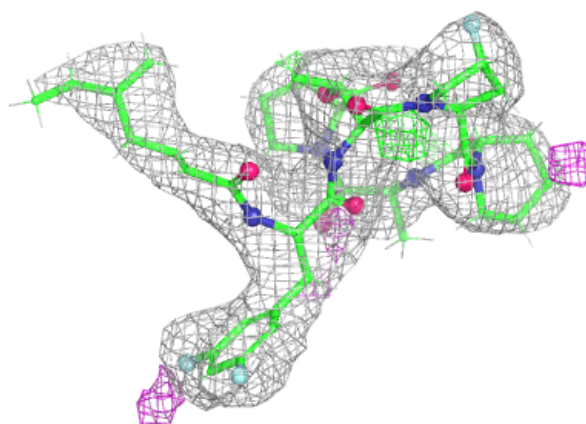
Electron density around A1C97 T 804:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



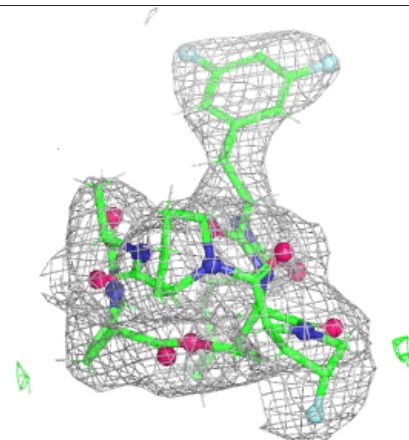
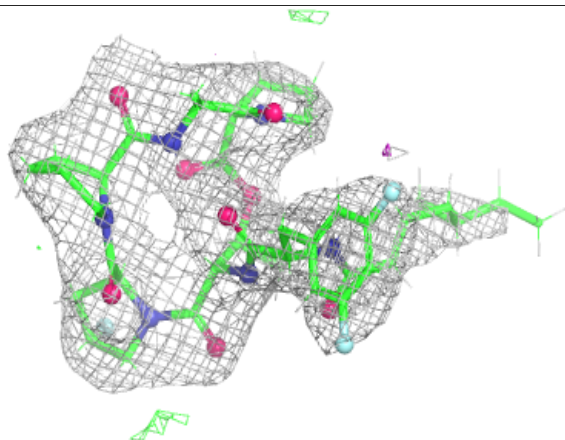
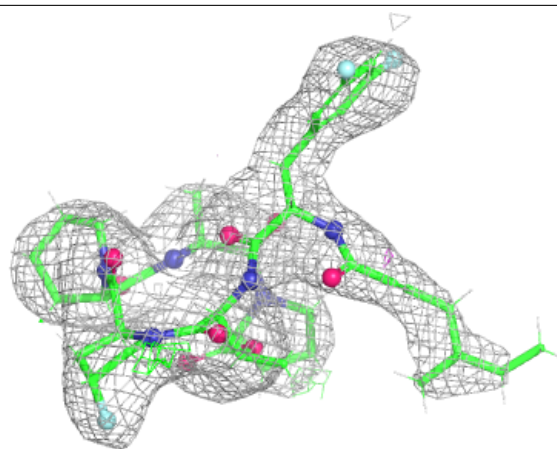
Electron density around A1C97 U 804:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



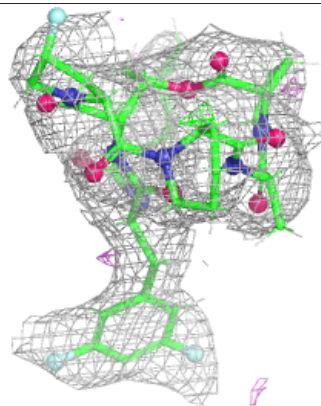
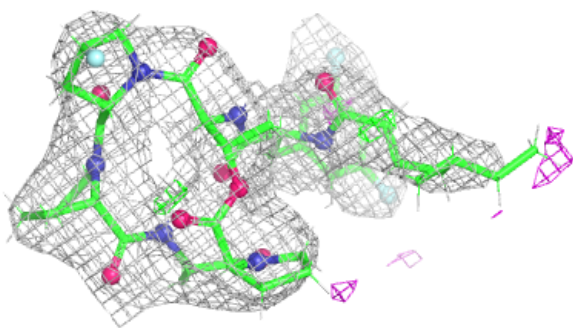
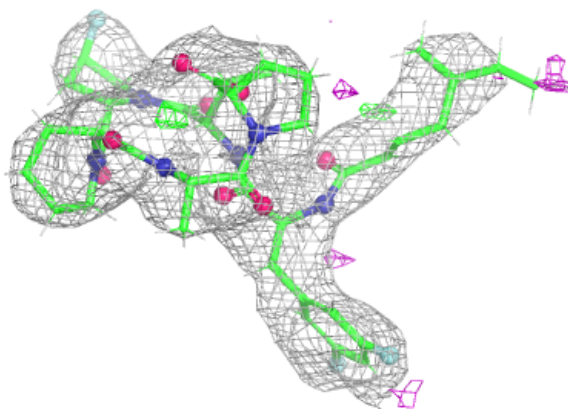
Electron density around A1C97 E 804:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



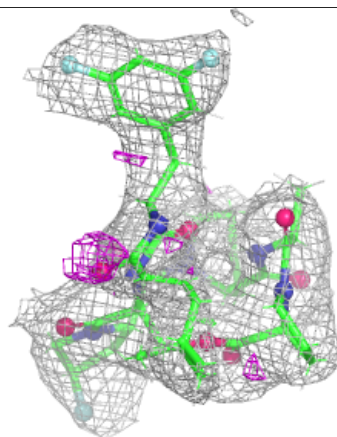
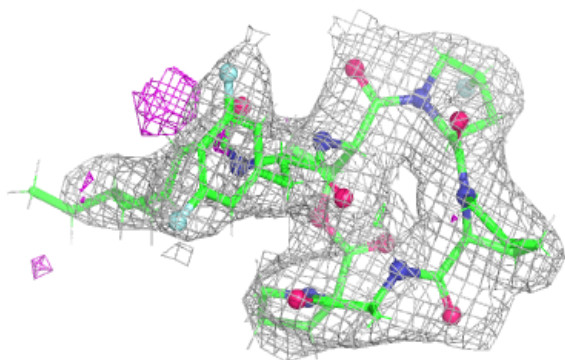
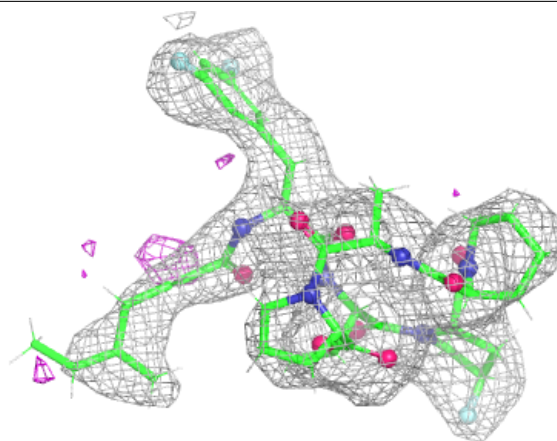
Electron density around A1C97 Q 804:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



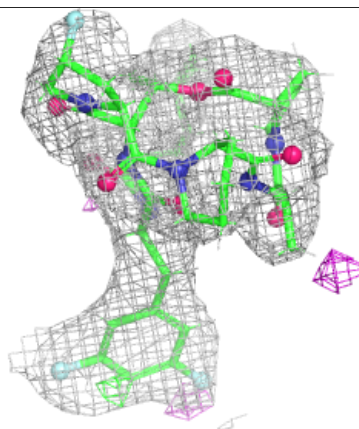
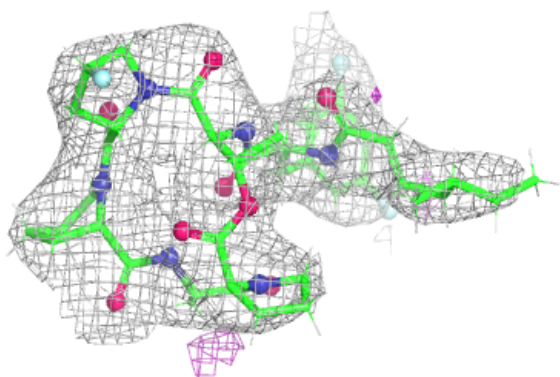
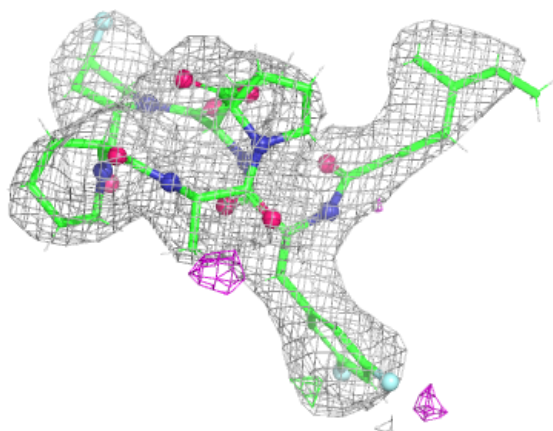
Electron density around A1C97 S 804:

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and green (positive)



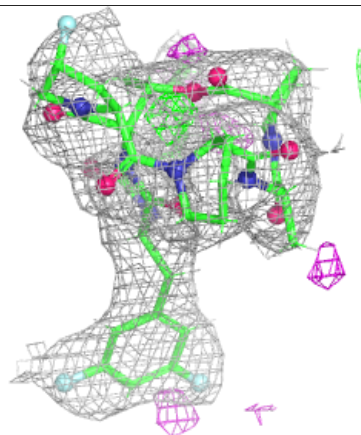
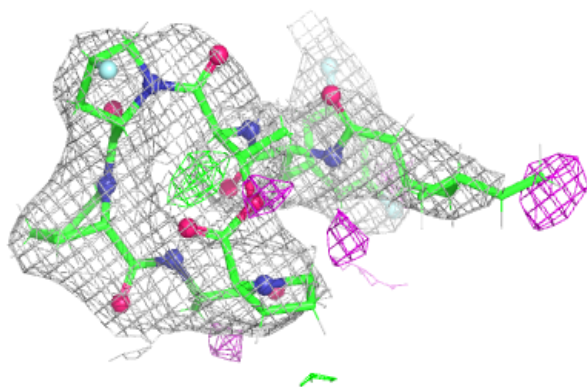
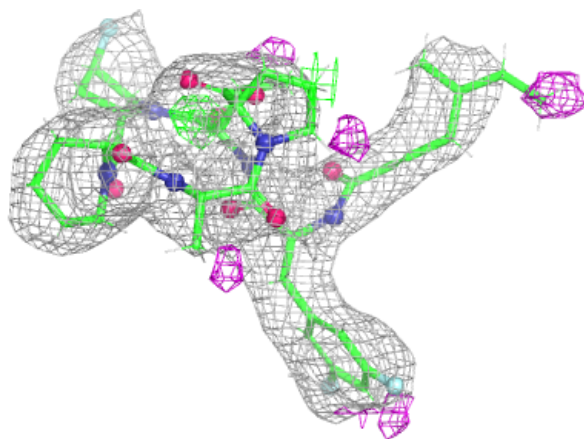
Electron density around A1C97 B 804:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



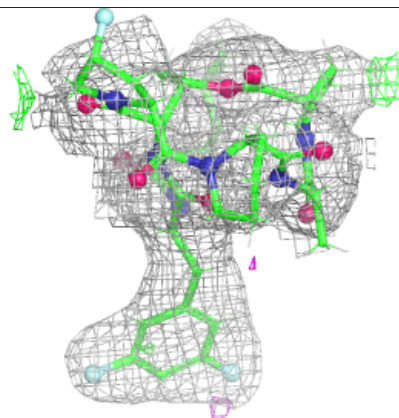
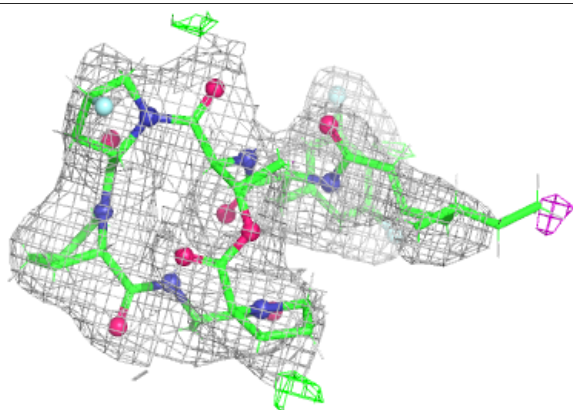
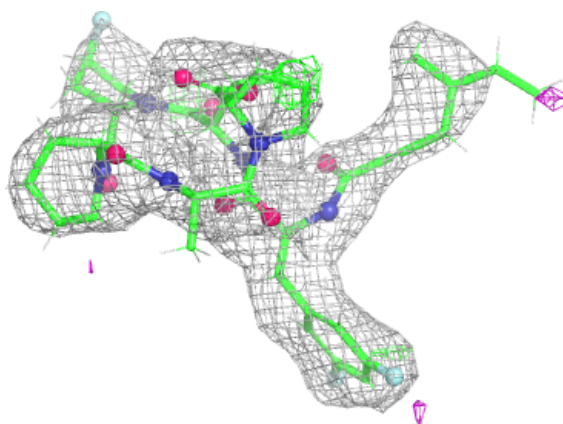
Electron density around A1C97 C 804:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



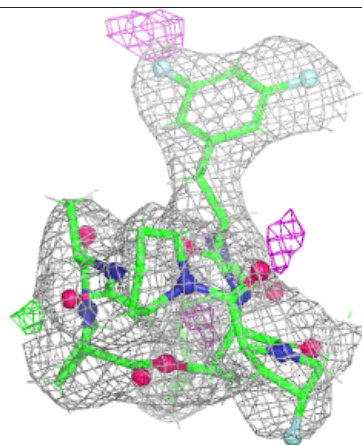
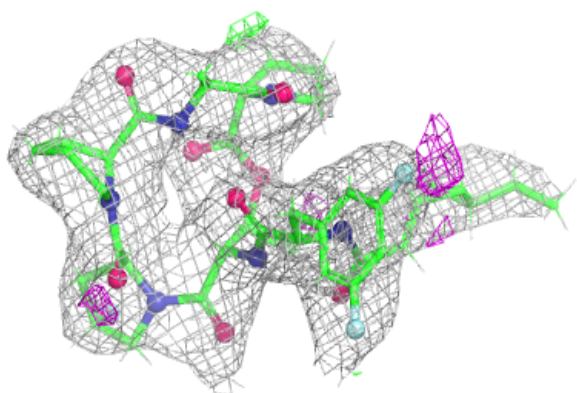
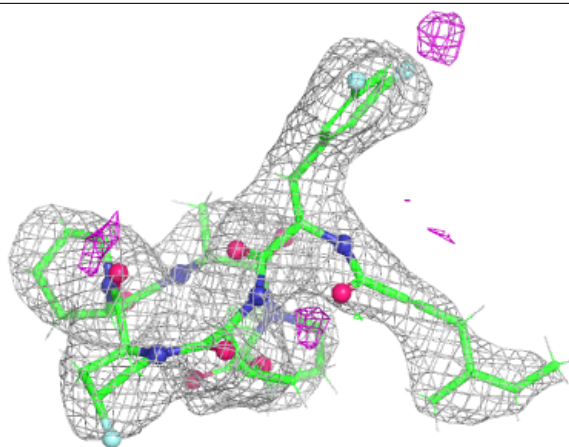
Electron density around A1C97 D 804:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



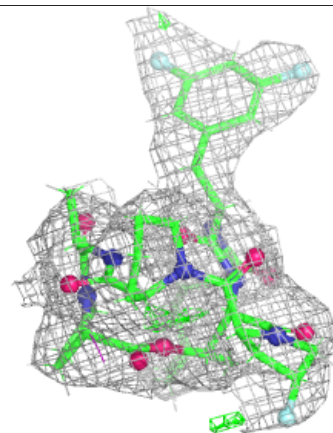
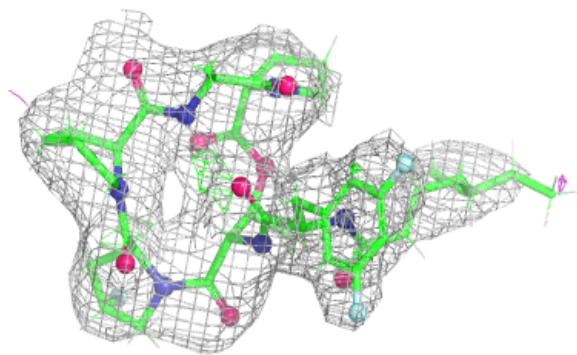
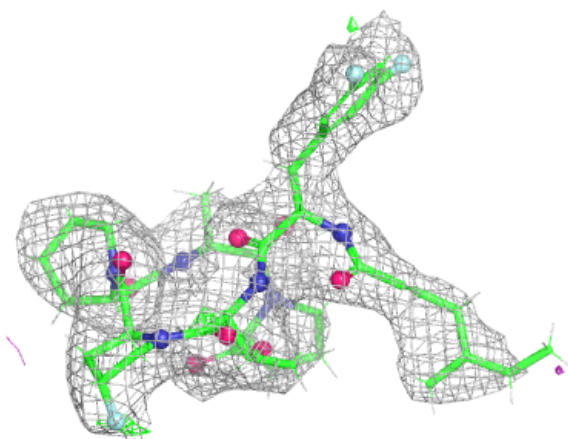
Electron density around A1C97 E 805:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



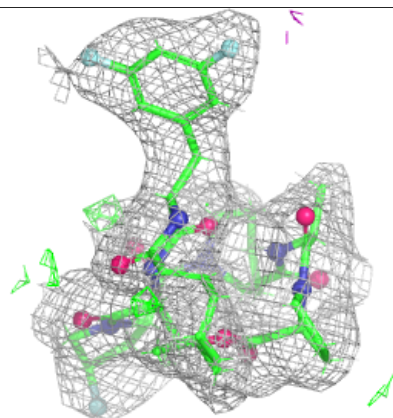
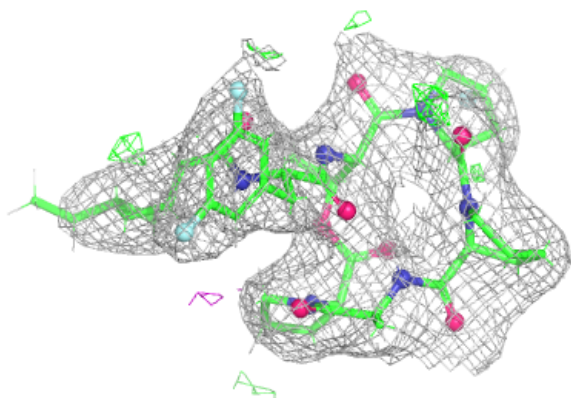
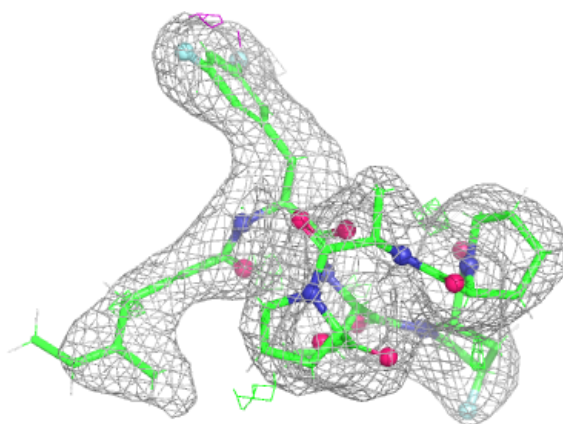
Electron density around A1C97 G 804:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



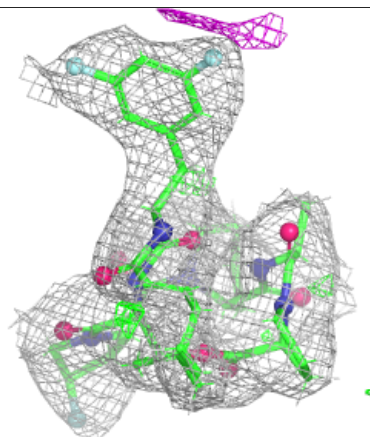
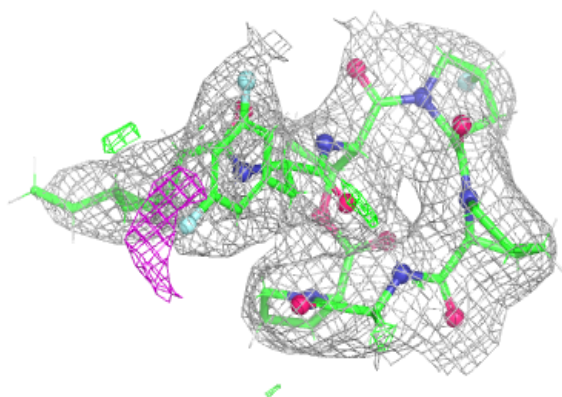
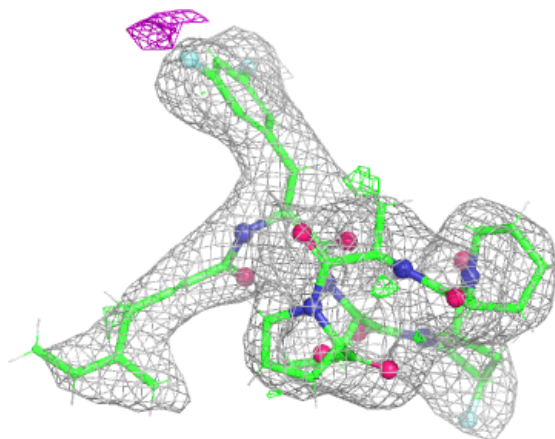
Electron density around A1C97 O 804:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



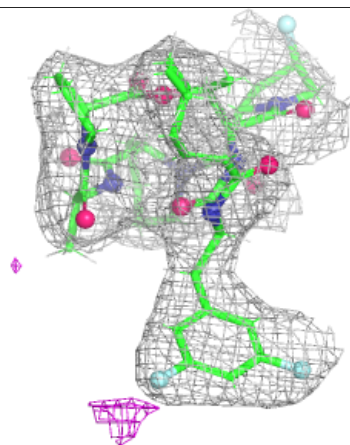
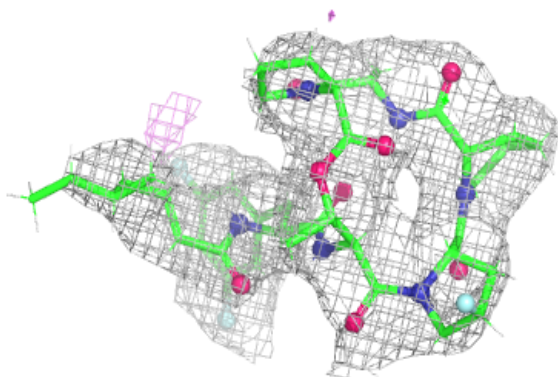
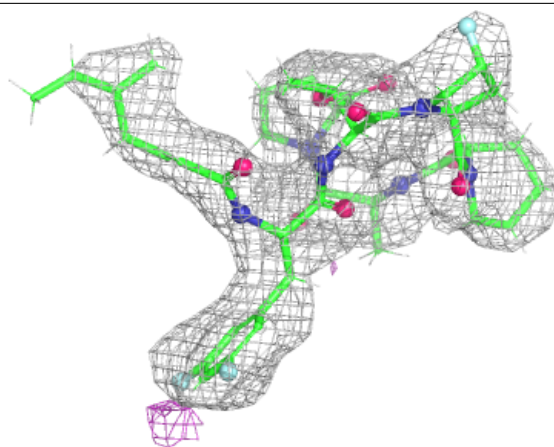
Electron density around A1C97 A 804:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



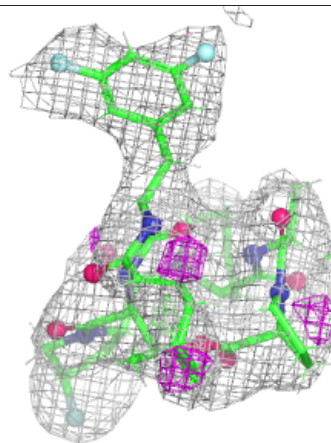
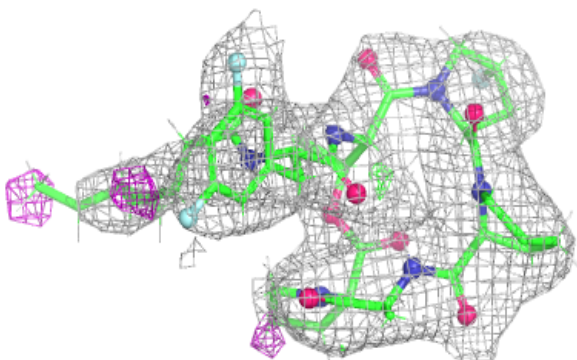
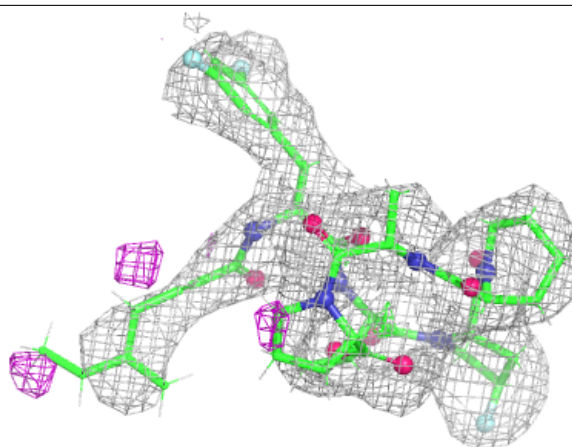
Electron density around A1C97 R 804:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around A1C97 P 804:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.