



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2026 – 10:51 AM EDT

PDB ID : 11MI / pdb_000011mi
Title : Crystal Structure of M. tuberculosis ClpP1P2 bound to ADEP 19
Authors : Burnside, C.M.; Fei, F.; Schmitz, K.R.; Sello, J.K.
Deposited on : 2026-03-04
Resolution : 2.65 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

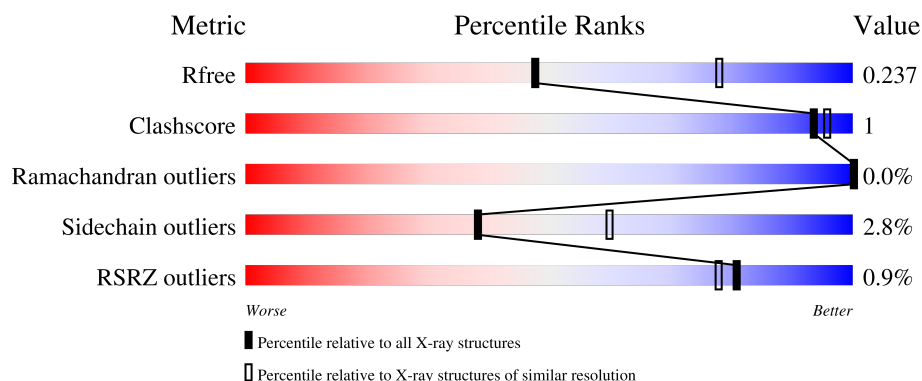
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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.



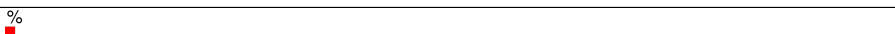
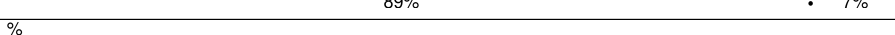
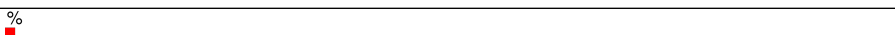
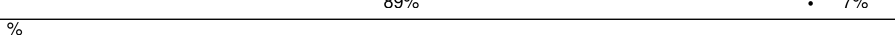
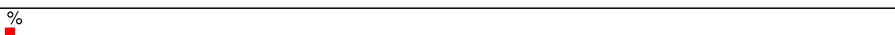
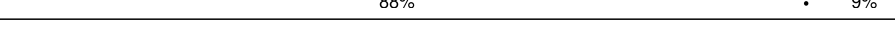
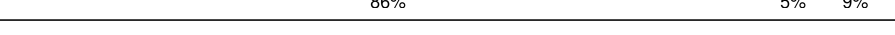
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	214	88% 8%
1	B	214	89% 7%
1	C	214	91% 6%
1	D	214	88% 5% 7%
1	E	214	91% 7%

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Mol	Chain	Length	Quality of chain
1	F	214	
1	G	214	
1	O	214	
1	P	214	
1	Q	214	
1	R	214	
1	S	214	
1	T	214	
1	U	214	
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 82314 atoms, of which 40660 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	197	Total	C	H	N	O	S	0	0	0
			2981	943	1482	254	294	8			
1	B	199	Total	C	H	N	O	S	0	0	0
			3026	951	1510	259	298	8			
1	C	202	Total	C	H	N	O	S	0	0	0
			3067	967	1527	262	303	8			
1	D	198	Total	C	H	N	O	S	0	0	0
			3005	949	1495	258	295	8			
1	E	200	Total	C	H	N	O	S	0	0	0
			3009	952	1494	257	298	8			
1	F	197	Total	C	H	N	O	S	0	0	0
			2978	943	1480	253	294	8			
1	G	198	Total	C	H	N	O	S	0	0	0
			3013	951	1501	255	298	8			
1	O	196	Total	C	H	N	O	S	0	0	0
			2976	940	1482	253	293	8			
1	P	199	Total	C	H	N	O	S	0	0	0
			3023	954	1506	256	299	8			
1	Q	197	Total	C	H	N	O	S	0	0	0
			2965	940	1472	251	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
			3003	949	1493	256	297	8			
1	T	198	Total	C	H	N	O	S	0	1	0
			2986	948	1481	254	295	8			
1	U	198	Total	C	H	N	O	S	0	0	0
			2993	946	1488	255	296	8			

There are 168 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
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
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
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
D	218	LEU	-	expression tag	UNP P9WPC3
D	219	GLU	-	expression tag	UNP P9WPC3
D	220	HIS	-	expression tag	UNP P9WPC3

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
Q	224	HIS	-	expression tag	UNP P9WPC3
Q	225	HIS	-	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

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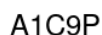
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Chain	Residue	Modelled	Actual	Comment	Reference
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R	222	HIS	-	expression tag	UNP P9WPC3
R	223	HIS	-	expression tag	UNP P9WPC3
R	224	HIS	-	expression tag	UNP P9WPC3
R	225	HIS	-	expression tag	UNP P9WPC3
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
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
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

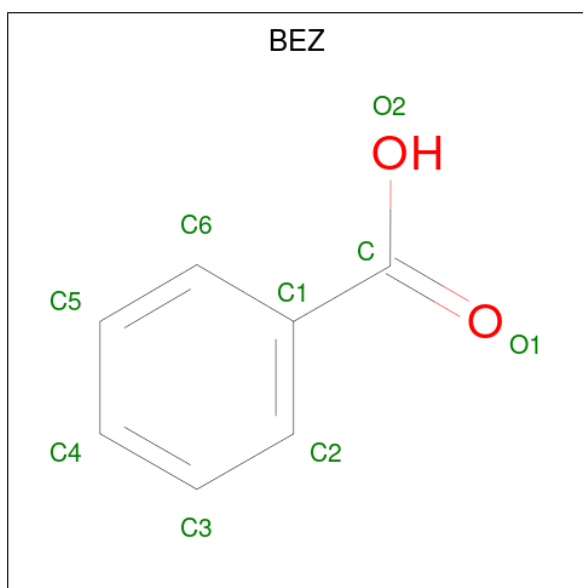
- Molecule 2 is a protein called ATP-dependent Clp protease proteolytic subunit 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	177	Total	C	H	N	O	S	0	0	0
			2661	849	1322	222	259	9			
2	I	177	Total	C	H	N	O	S	0	0	0
			2637	844	1308	219	257	9			
2	J	179	Total	C	H	N	O	S	0	0	0
			2658	850	1316	224	259	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
			2635	843	1305	222	256	9			
2	M	176	Total	C	H	N	O	S	0	0	0
			2627	840	1302	221	255	9			
2	N	177	Total	C	H	N	O	S	0	0	0
			2657	847	1321	222	258	9			
2	V	176	Total	C	H	N	O	S	0	0	0
			2628	840	1303	221	255	9			
2	W	176	Total	C	H	N	O	S	0	0	0
			2616	838	1298	218	253	9			
2	X	176	Total	C	H	N	O	S	0	0	0
			2611	837	1292	217	256	9			
2	Y	176	Total	C	H	N	O	S	0	0	0
			2608	836	1294	218	251	9			
2	Z	176	Total	C	H	N	O	S	0	0	0
			2624	840	1300	220	255	9			
2	a	176	Total	C	H	N	O	S	0	0	0
			2602	835	1287	218	253	9			
2	b	176	Total	C	H	N	O	S	0	0	0
			2563	828	1258	213	255	9			

- Molecule 3 is 3,5-difluoro-N-[(5R,6aS,8R,10R,12S,13S,15aS,19R,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)-3-[(1S,2R)-2-methylcyclopentyl]prop-2-enoyl}-L-phenylalaninamide (CCD ID: A1C9P) (formula: C₄₁H₅₃F₃N₆O₈) (labeled as "Ligand of Interest" by depositor).



- Molecule 4 is BENZOIC ACID (CCD ID: BEZ) (formula: $C_7H_6O_2$).



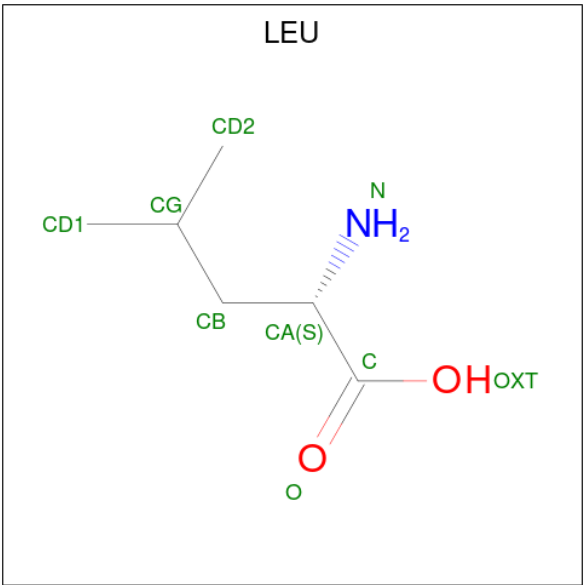
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			13	7	5	1		
4	B	1	Total	C	H	O	0	0
			13	7	5	1		
4	C	1	Total	C	H	O	0	0
			13	7	5	1		
4	D	1	Total	C	H	O	0	0
			13	7	5	1		
4	E	1	Total	C	H	O	0	0
			13	7	5	1		
4	F	1	Total	C	H	O	0	0
			13	7	5	1		
4	G	1	Total	C	H	O	0	0
			13	7	5	1		
4	H	1	Total	C	H	O	0	0
			13	7	5	1		
4	I	1	Total	C	H	O	0	0
			13	7	5	1		
4	J	1	Total	C	H	O	0	0
			13	7	5	1		
4	K	1	Total	C	H	O	0	0
			13	7	5	1		
4	L	1	Total	C	H	O	0	0
			13	7	5	1		
4	M	1	Total	C	H	O	0	0
			13	7	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	N	1	Total 13	C 7	H 5	O 1	0	0
4	O	1	Total 13	C 7	H 5	O 1	0	0
4	P	1	Total 13	C 7	H 5	O 1	0	0
4	Q	1	Total 13	C 7	H 5	O 1	0	0
4	R	1	Total 13	C 7	H 5	O 1	0	0
4	S	1	Total 13	C 7	H 5	O 1	0	0
4	T	1	Total 13	C 7	H 5	O 1	0	0
4	U	1	Total 13	C 7	H 5	O 1	0	0
4	V	1	Total 13	C 7	H 5	O 1	0	0
4	W	1	Total 13	C 7	H 5	O 1	0	0
4	X	1	Total 13	C 7	H 5	O 1	0	0
4	Y	1	Total 13	C 7	H 5	O 1	0	0
4	Z	1	Total 13	C 7	H 5	O 1	0	0
4	a	1	Total 13	C 7	H 5	O 1	0	0
4	b	1	Total 13	C 7	H 5	O 1	0	0

- Molecule 5 is LEUCINE (CCD ID: LEU) (formula: $C_6H_{13}NO_2$).



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

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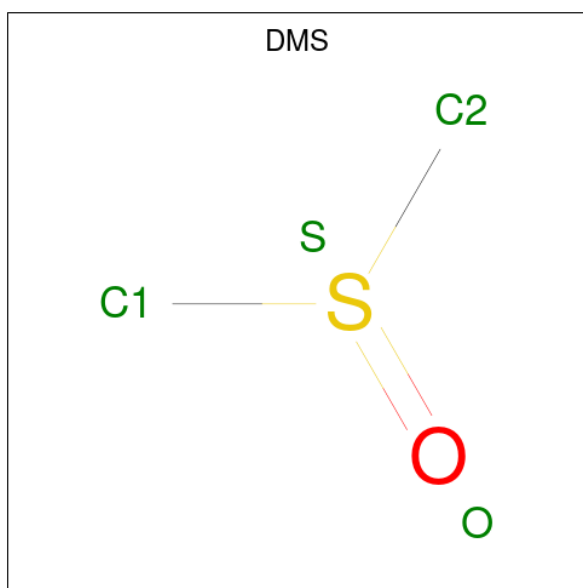
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	H	1	Total	C	H	N	O	0	0
			19	6	11	1	1		
5	H	1	Total	C	H	N	O	0	0
			19	6	11	1	1		
5	I	1	Total	C	H	N	O	0	0
			19	6	11	1	1		
5	I	1	Total	C	H	N	O	0	0
			19	6	11	1	1		
5	J	1	Total	C	H	N	O	0	0
			19	6	11	1	1		
5	J	1	Total	C	H	N	O	0	0
			19	6	11	1	1		
5	K	1	Total	C	H	N	O	0	0
			19	6	11	1	1		
5	K	1	Total	C	H	N	O	0	0
			19	6	11	1	1		
5	L	1	Total	C	H	N	O	0	0
			19	6	11	1	1		
5	L	1	Total	C	H	N	O	0	0
			19	6	11	1	1		
5	M	1	Total	C	H	N	O	0	0
			19	6	11	1	1		
5	M	1	Total	C	H	N	O	0	0
			19	6	11	1	1		
5	N	1	Total	C	H	N	O	0	0
			19	6	11	1	1		
5	N	1	Total	C	H	N	O	0	0
			19	6	11	1	1		
5	O	1	Total	C	H	N	O	0	0
			19	6	11	1	1		
5	O	1	Total	C	H	N	O	0	0
			20	6	11	1	2		
5	P	1	Total	C	H	N	O	0	0
			19	6	11	1	1		
5	P	1	Total	C	H	N	O	0	0
			20	6	11	1	2		
5	Q	1	Total	C	H	N	O	0	0
			19	6	11	1	1		
5	Q	1	Total	C	H	N	O	0	0
			20	6	11	1	2		
5	R	1	Total	C	H	N	O	0	0
			19	6	11	1	1		

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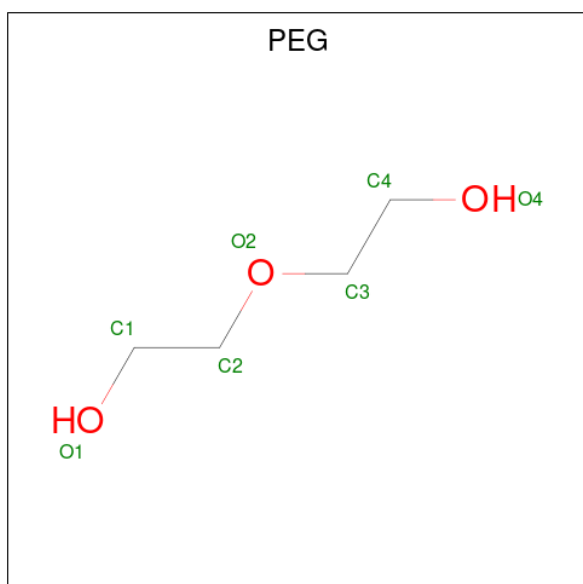
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	R	1	Total 20	C 6	H 11	N 1	O 2	0	0
5	S	1	Total 19	C 6	H 11	N 1	O 1	0	0
5	S	1	Total 20	C 6	H 11	N 1	O 2	0	0
5	T	1	Total 19	C 6	H 11	N 1	O 1	0	0
5	T	1	Total 20	C 6	H 11	N 1	O 2	0	0
5	U	1	Total 19	C 6	H 11	N 1	O 1	0	0
5	U	1	Total 20	C 6	H 11	N 1	O 2	0	0
5	V	1	Total 19	C 6	H 11	N 1	O 1	0	0
5	V	1	Total 19	C 6	H 11	N 1	O 1	0	0
5	W	1	Total 19	C 6	H 11	N 1	O 1	0	0
5	W	1	Total 19	C 6	H 11	N 1	O 1	0	0
5	X	1	Total 19	C 6	H 11	N 1	O 1	0	0
5	X	1	Total 19	C 6	H 11	N 1	O 1	0	0
5	Y	1	Total 19	C 6	H 11	N 1	O 1	0	0
5	Y	1	Total 19	C 6	H 11	N 1	O 1	0	0
5	Z	1	Total 19	C 6	H 11	N 1	O 1	0	0
5	Z	1	Total 19	C 6	H 11	N 1	O 1	0	0
5	a	1	Total 19	C 6	H 11	N 1	O 1	0	0
5	a	1	Total 19	C 6	H 11	N 1	O 1	0	0
5	b	1	Total 19	C 6	H 11	N 1	O 1	0	0
5	b	1	Total 19	C 6	H 11	N 1	O 1	0	0

- Molecule 6 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	F	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	O	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	Q	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	H	O	0	0
			17	4	10	3		
7	S	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	19	Total	O	0	0
			19	19		
8	B	18	Total	O	0	0
			18	18		
8	C	23	Total	O	0	0
			23	23		
8	D	17	Total	O	0	0
			17	17		
8	E	16	Total	O	0	0
			16	16		
8	F	21	Total	O	0	0
			21	21		
8	G	16	Total	O	0	0
			16	16		
8	H	16	Total	O	0	0
			16	16		
8	I	16	Total	O	0	0
			16	16		
8	J	15	Total	O	0	0
			15	15		
8	K	19	Total	O	0	0
			19	19		
8	L	19	Total	O	0	0
			19	19		
8	M	10	Total	O	0	0
			10	10		
8	N	17	Total	O	0	0
			17	17		
8	O	23	Total	O	0	0
			23	23		
8	P	17	Total	O	0	0
			17	17		
8	Q	18	Total	O	0	0
			18	18		
8	R	25	Total	O	0	0
			25	25		

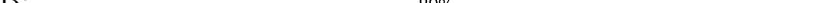
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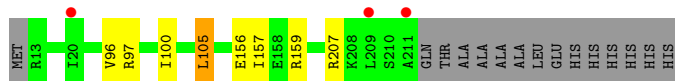
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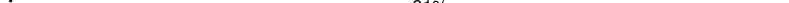
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	S	15	Total 15	O 15	0	0
8	T	18	Total 18	O 18	0	0
8	U	26	Total 26	O 26	0	0
8	V	11	Total 11	O 11	0	0
8	W	8	Total 8	O 8	0	0
8	X	12	Total 12	O 12	0	0
8	Y	9	Total 9	O 9	0	0
8	Z	11	Total 11	O 11	0	0
8	a	15	Total 15	O 15	0	0
8	b	8	Total 8	O 8	0	0

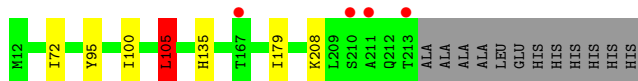
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

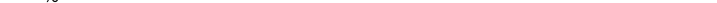


- Chain B:  89% 7%

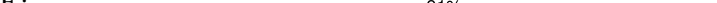


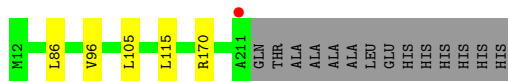
- Chain C:  2% 91% 6%



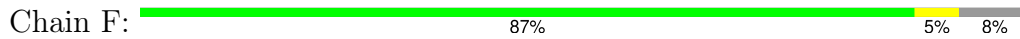
- Chain D:  88% 5% 7%



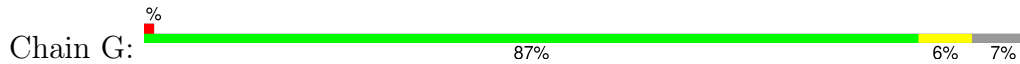
- Chain E:  91% • 7%



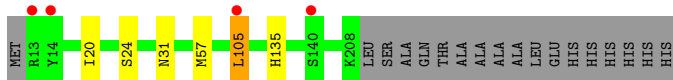
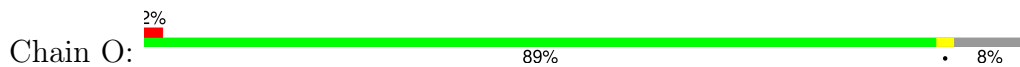
- 
- WORLD WIDE
PDB
PROTEIN DATA BANK



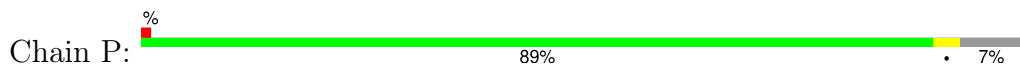
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



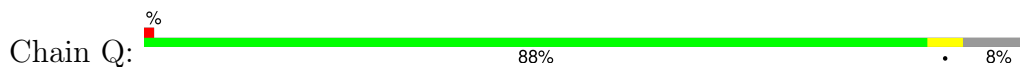
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



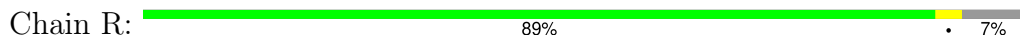
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



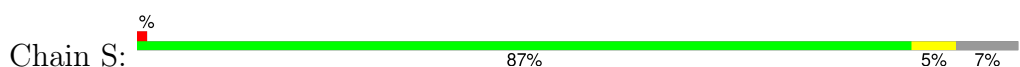
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



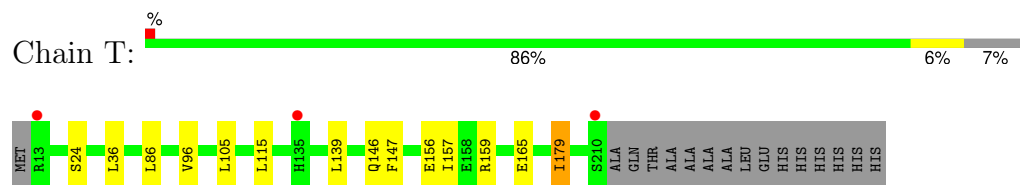
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



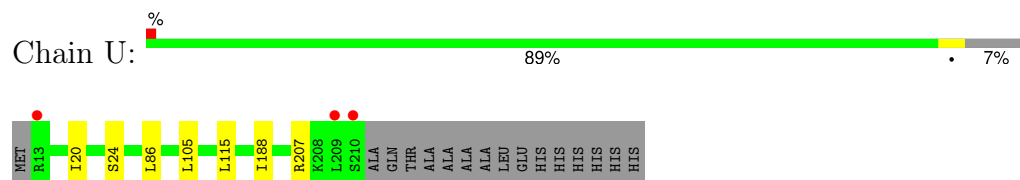
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



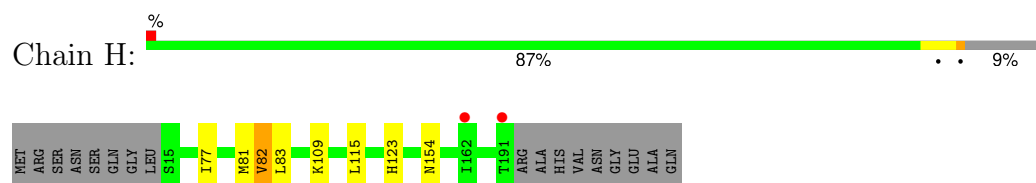
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



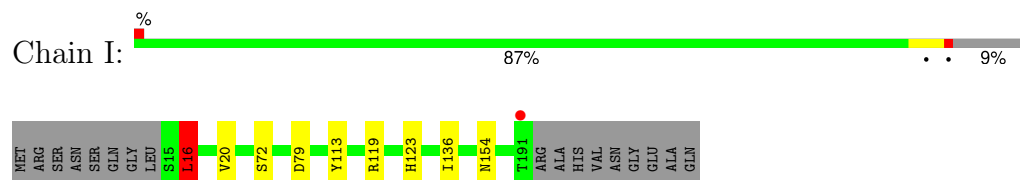
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



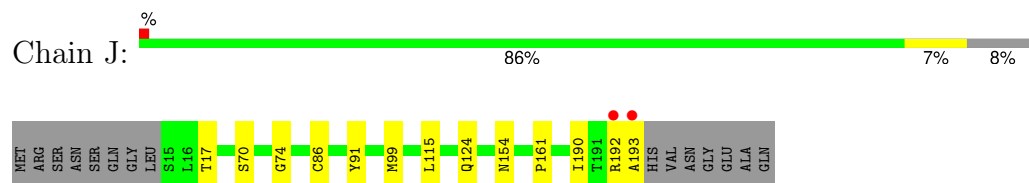
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1



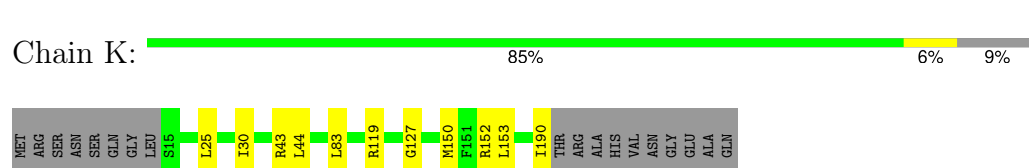
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1



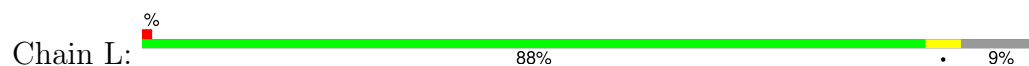
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1



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

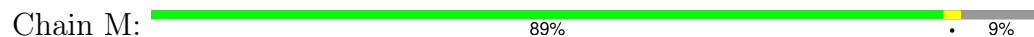


- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

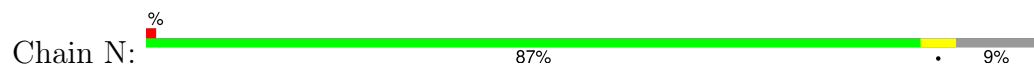




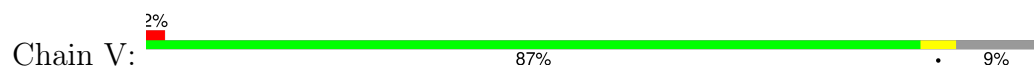
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1



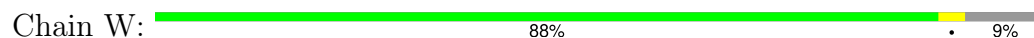
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1



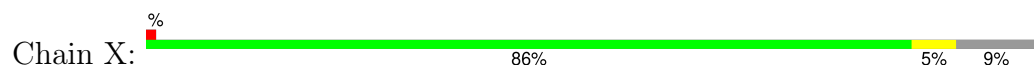
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1



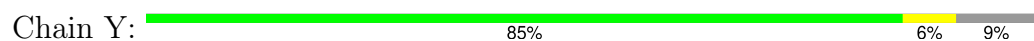
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1



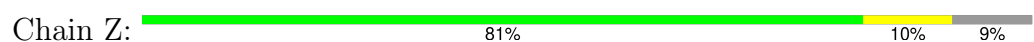
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1



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

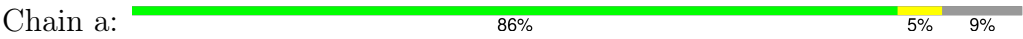


- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

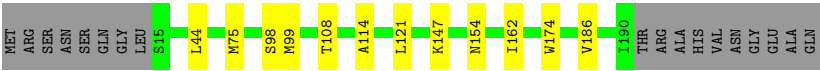
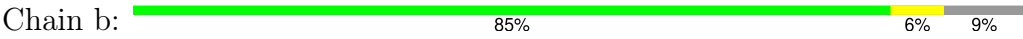




● Molecule 2: ATP-dependent Clp protease proteolytic subunit 1



● 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	211.46Å 183.69Å 191.70Å 90.00° 95.34° 90.00°	Depositor
Resolution (Å)	41.04 – 2.65 41.04 – 2.65	Depositor EDS
% Data completeness (in resolution range)	86.8 (41.04-2.65) 79.7 (41.04-2.65)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.200 , 0.237 0.200 , 0.237	Depositor DCC
R_{free} test set	9431 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	82314	wwPDB-VP
Average B, all atoms (Å ²)	50.0	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 41.80 % 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 2.2393e-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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BEZ, DMS, A1C9P, PEG

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	0.25	0/1521	0.44	0/2061
1	B	0.29	0/1537	0.45	0/2081
1	C	0.33	1/1562 (0.1%)	0.42	0/2116
1	D	0.39	1/1532 (0.1%)	0.50	0/2075
1	E	0.19	0/1537	0.36	0/2083
1	F	0.25	0/1520	0.44	0/2061
1	G	0.30	1/1534 (0.1%)	0.47	0/2078
1	O	0.32	0/1516	0.49	0/2054
1	P	0.26	0/1539	0.45	0/2085
1	Q	0.29	0/1515	0.47	0/2054
1	R	0.30	0/1527	0.48	0/2069
1	S	0.26	0/1532	0.46	0/2076
1	T	0.30	0/1531	0.40	0/2076
1	U	0.34	0/1527	0.50	0/2069
2	H	0.41	0/1361	0.65	0/1842
2	I	0.29	0/1351	0.51	1/1830 (0.1%)
2	J	0.42	1/1364 (0.1%)	0.61	0/1847
2	K	0.43	2/1350 (0.1%)	0.53	1/1827 (0.1%)
2	L	0.29	0/1352	0.52	0/1830
2	M	0.29	0/1347	0.50	0/1823
2	N	0.33	0/1358	0.50	0/1838
2	V	0.25	0/1347	0.46	0/1823
2	W	0.28	0/1340	0.44	0/1815
2	X	0.29	0/1341	0.42	0/1817
2	Y	0.36	0/1336	0.58	0/1810
2	Z	0.46	3/1346 (0.2%)	0.59	0/1823
2	a	0.35	0/1337	0.52	0/1811
2	b	0.36	1/1327 (0.1%)	0.59	1/1801 (0.1%)
All	All	0.32	10/40287 (0.0%)	0.49	3/54575 (0.0%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	105	LEU	C-N	9.72	1.47	1.33
2	K	152	ARG	C-N	-9.18	1.21	1.34
2	K	153	LEU	C-N	7.24	1.44	1.34
2	b	147	LYS	C-N	-7.17	1.24	1.34
2	Z	98	SER	C-N	-7.05	1.24	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	152	ARG	O-C-N	-7.12	114.74	122.07
2	I	16	LEU	N-CA-C	-5.89	105.93	113.23
2	b	98	SER	CA-CB-OG	5.04	121.19	111.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1499	1482	1482	5	0
1	B	1516	1510	1509	7	0
1	C	1540	1527	1527	4	0
1	D	1510	1495	1495	7	0
1	E	1515	1494	1494	1	0
1	F	1498	1480	1480	6	0
1	G	1512	1501	1500	5	0
1	O	1494	1482	1480	4	0
1	P	1517	1506	1505	8	0
1	Q	1493	1472	1471	4	0
1	R	1505	1488	1487	3	0
1	S	1510	1493	1492	6	0
1	T	1505	1481	1480	8	0
1	U	1505	1488	1487	4	0
2	H	1339	1322	1321	4	0
2	I	1329	1308	1306	5	0
2	J	1342	1316	1315	5	0
2	K	1328	1313	1310	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1330	1305	1303	3	0
2	M	1325	1302	1301	1	0
2	N	1336	1321	1320	3	0
2	V	1325	1303	1301	3	0
2	W	1318	1298	1295	4	0
2	X	1319	1292	1291	6	0
2	Y	1314	1294	1291	12	0
2	Z	1324	1300	1299	10	0
2	a	1315	1287	1286	6	0
2	b	1305	1258	1257	3	0
3	A	58	53	0	1	0
3	B	58	53	0	0	0
3	C	58	53	0	1	0
3	D	58	53	0	1	0
3	E	58	53	0	0	0
3	F	58	53	0	1	0
3	G	58	53	0	0	0
3	O	58	53	0	1	0
3	P	58	53	0	1	0
3	Q	58	53	0	1	0
3	R	58	53	0	1	0
3	S	58	53	0	1	0
3	T	58	53	0	0	0
3	U	58	53	0	0	0
4	A	8	5	5	0	0
4	B	8	5	5	0	0
4	C	8	5	5	0	0
4	D	8	5	5	0	0
4	E	8	5	5	0	0
4	F	8	5	5	0	0
4	G	8	5	5	0	0
4	H	8	5	5	0	0
4	I	8	5	5	0	0
4	J	8	5	5	0	0
4	K	8	5	5	0	0
4	L	8	5	5	0	0
4	M	8	5	5	0	0
4	N	8	5	5	0	0
4	O	8	5	5	0	0
4	P	8	5	5	0	0
4	Q	8	5	5	0	0
4	R	8	5	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	S	8	5	5	0	0
4	T	8	5	5	0	0
4	U	8	5	5	0	0
4	V	8	5	5	0	0
4	W	8	5	5	0	0
4	X	8	5	5	1	0
4	Y	8	5	5	0	0
4	Z	8	5	5	0	0
4	a	8	5	5	0	0
4	b	8	5	5	0	0
5	A	17	22	22	0	0
5	B	17	22	22	0	0
5	C	17	22	22	0	0
5	D	17	22	22	0	0
5	E	17	22	22	0	0
5	F	17	22	22	0	0
5	G	17	22	22	0	0
5	H	16	22	22	1	0
5	I	16	22	22	0	0
5	J	16	22	22	0	0
5	K	16	22	22	1	0
5	L	16	22	22	0	0
5	M	16	22	22	0	0
5	N	16	22	22	1	0
5	O	17	22	22	0	0
5	P	17	22	22	0	0
5	Q	17	22	22	0	0
5	R	17	22	22	0	0
5	S	17	22	22	0	0
5	T	17	22	22	0	0
5	U	17	22	22	0	0
5	V	16	22	22	0	0
5	W	16	22	22	0	0
5	X	16	22	22	1	0
5	Y	16	22	22	2	0
5	Z	16	22	22	0	0
5	a	16	22	22	0	0
5	b	16	22	22	0	0
6	C	4	6	6	0	0
6	F	4	6	6	3	0
6	O	4	6	6	0	0
6	Q	4	6	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	7	10	10	0	0
7	S	7	10	10	0	0
8	A	19	0	0	0	0
8	B	18	0	0	0	0
8	C	23	0	0	0	0
8	D	17	0	0	0	0
8	E	16	0	0	0	0
8	F	21	0	0	0	0
8	G	16	0	0	0	0
8	H	16	0	0	0	0
8	I	16	0	0	0	0
8	J	15	0	0	0	0
8	K	19	0	0	0	0
8	L	19	0	0	0	0
8	M	10	0	0	0	0
8	N	17	0	0	0	0
8	O	23	0	0	0	0
8	P	17	0	0	0	0
8	Q	18	0	0	0	0
8	R	25	0	0	0	0
8	S	15	0	0	0	0
8	T	18	0	0	0	0
8	U	26	0	0	0	0
8	V	11	0	0	0	0
8	W	8	0	0	0	0
8	X	12	0	0	0	0
8	Y	9	0	0	0	0
8	Z	11	0	0	0	0
8	a	15	0	0	0	0
8	b	8	0	0	0	0
All	All	41654	40660	39885	114	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 1.

The worst 5 of 114 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:17:THR:HG21	2:Z:43:ARG:NH1	2.02	0.74
2:Z:31:PHE:HE2	2:Z:93:MET:HE1	1.52	0.74
1:A:105:LEU:HD21	3:A:401:A1C9P:F37	1.82	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:105:LEU:HD21	3:P:401:A1C9P:F37	1.84	0.68
2:N:74:GLY:HA3	2:N:99:MET:HE2	1.77	0.66

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 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	195/214 (91%)	189 (97%)	5 (3%)	1 (0%)	24	39
1	B	197/214 (92%)	187 (95%)	10 (5%)	0	100	100
1	C	200/214 (94%)	194 (97%)	6 (3%)	0	100	100
1	D	196/214 (92%)	189 (96%)	7 (4%)	0	100	100
1	E	198/214 (92%)	190 (96%)	8 (4%)	0	100	100
1	F	195/214 (91%)	185 (95%)	10 (5%)	0	100	100
1	G	196/214 (92%)	188 (96%)	7 (4%)	1 (0%)	24	39
1	O	194/214 (91%)	187 (96%)	7 (4%)	0	100	100
1	P	197/214 (92%)	194 (98%)	3 (2%)	0	100	100
1	Q	195/214 (91%)	190 (97%)	5 (3%)	0	100	100
1	R	196/214 (92%)	189 (96%)	7 (4%)	0	100	100
1	S	197/214 (92%)	189 (96%)	8 (4%)	0	100	100
1	T	197/214 (92%)	192 (98%)	5 (2%)	0	100	100
1	U	196/214 (92%)	191 (97%)	5 (3%)	0	100	100
2	H	175/194 (90%)	169 (97%)	6 (3%)	0	100	100
2	I	175/194 (90%)	170 (97%)	5 (3%)	0	100	100
2	J	177/194 (91%)	173 (98%)	4 (2%)	0	100	100
2	K	174/194 (90%)	168 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	175/194 (90%)	171 (98%)	4 (2%)	0	100	100
2	M	174/194 (90%)	170 (98%)	4 (2%)	0	100	100
2	N	175/194 (90%)	174 (99%)	1 (1%)	0	100	100
2	V	174/194 (90%)	165 (95%)	9 (5%)	0	100	100
2	W	174/194 (90%)	166 (95%)	8 (5%)	0	100	100
2	X	174/194 (90%)	169 (97%)	5 (3%)	0	100	100
2	Y	174/194 (90%)	166 (95%)	8 (5%)	0	100	100
2	Z	174/194 (90%)	170 (98%)	4 (2%)	0	100	100
2	a	174/194 (90%)	166 (95%)	8 (5%)	0	100	100
2	b	174/194 (90%)	166 (95%)	8 (5%)	0	100	100
All	All	5192/5712 (91%)	5017 (97%)	173 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	GLY
1	G	106	GLY

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	158/176 (90%)	154 (98%)	4 (2%)	42	64
1	B	161/176 (92%)	160 (99%)	1 (1%)	78	88
1	C	163/176 (93%)	160 (98%)	3 (2%)	51	72
1	D	159/176 (90%)	158 (99%)	1 (1%)	78	88
1	E	159/176 (90%)	156 (98%)	3 (2%)	50	71
1	F	158/176 (90%)	155 (98%)	3 (2%)	50	71
1	G	161/176 (92%)	159 (99%)	2 (1%)	63	79
1	O	158/176 (90%)	154 (98%)	4 (2%)	42	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	161/176 (92%)	157 (98%)	4 (2%)	42	64
1	Q	157/176 (89%)	151 (96%)	6 (4%)	29	49
1	R	159/176 (90%)	155 (98%)	4 (2%)	42	64
1	S	159/176 (90%)	155 (98%)	4 (2%)	42	64
1	T	158/176 (90%)	152 (96%)	6 (4%)	29	49
1	U	159/176 (90%)	156 (98%)	3 (2%)	50	71
2	H	136/151 (90%)	133 (98%)	3 (2%)	45	67
2	I	134/151 (89%)	130 (97%)	4 (3%)	36	57
2	J	134/151 (89%)	130 (97%)	4 (3%)	36	57
2	K	134/151 (89%)	132 (98%)	2 (2%)	57	75
2	L	133/151 (88%)	130 (98%)	3 (2%)	44	66
2	M	133/151 (88%)	130 (98%)	3 (2%)	44	66
2	N	136/151 (90%)	133 (98%)	3 (2%)	45	67
2	V	133/151 (88%)	130 (98%)	3 (2%)	44	66
2	W	132/151 (87%)	130 (98%)	2 (2%)	57	75
2	X	133/151 (88%)	130 (98%)	3 (2%)	44	66
2	Y	131/151 (87%)	129 (98%)	2 (2%)	57	75
2	Z	133/151 (88%)	129 (97%)	4 (3%)	36	57
2	a	131/151 (87%)	129 (98%)	2 (2%)	57	75
2	b	129/151 (85%)	123 (95%)	6 (5%)	23	40
All	All	4092/4578 (89%)	4000 (98%)	92 (2%)	38	67

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	32	PRO
2	V	44	LEU
1	S	105	LEU
1	T	139	LEU
2	X	20	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	54	ASN
1	D	77	ASN
1	G	77	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

104 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
3	A1C9P	A	401	-	63,63,63	2.60	28 (44%)	87,91,91	2.19	27 (31%)
5	LEU	P	403	5,4	5,7,8	0.98	0	6,8,10	1.38	1 (16%)
4	BEZ	E	402	5	8,8,9	1.38	1 (12%)	9,9,11	1.61	2 (22%)
4	BEZ	L	801	5	8,8,9	2.52	5 (62%)	9,9,11	0.83	0
5	LEU	H	803	5	5,7,8	1.30	1 (20%)	6,8,10	1.17	1 (16%)
3	A1C9P	R	401	-	63,63,63	2.65	28 (44%)	87,91,91	2.12	27 (31%)
5	LEU	X	802	5,4	5,7,8	1.40	1 (20%)	6,8,10	0.80	0
5	LEU	b	803	5	5,7,8	0.73	0	6,8,10	0.79	0
6	DMS	C	405	-	3,3,3	0.59	0	3,3,3	0.54	0
4	BEZ	A	402	5	8,8,9	1.39	1 (12%)	9,9,11	1.59	2 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	LEU	A	403	5,4	5,7,8	1.17	1 (20%)	6,8,10	1.29	2 (33%)
5	LEU	a	803	5	5,7,8	0.21	0	6,8,10	0.53	0
5	LEU	C	403	5,4	5,7,8	0.98	0	6,8,10	1.38	1 (16%)
5	LEU	O	404	5	6,8,8	0.87	1 (16%)	5,10,10	0.45	0
4	BEZ	R	402	5	8,8,9	1.39	1 (12%)	9,9,11	1.60	2 (22%)
5	LEU	L	802	5,4	5,7,8	0.84	0	6,8,10	0.96	0
5	LEU	E	403	5,4	5,7,8	0.99	0	6,8,10	1.37	1 (16%)
5	LEU	K	803	5	5,7,8	0.95	0	6,8,10	1.11	0
3	A1C9P	S	401	-	63,63,63	2.62	28 (44%)	87,91,91	2.08	29 (33%)
3	A1C9P	D	401	-	63,63,63	2.59	26 (41%)	87,91,91	2.12	29 (33%)
4	BEZ	V	801	5	8,8,9	2.51	5 (62%)	9,9,11	0.85	0
4	BEZ	Z	801	5	8,8,9	2.52	5 (62%)	9,9,11	0.84	0
5	LEU	D	403	5,4	5,7,8	0.99	0	6,8,10	1.37	1 (16%)
5	LEU	G	404	5	6,8,8	0.83	0	5,10,10	0.42	0
5	LEU	J	803	5	5,7,8	0.67	0	6,8,10	1.55	1 (16%)
5	LEU	R	404	5	6,8,8	0.79	0	5,10,10	0.43	0
3	A1C9P	C	401	-	63,63,63	2.60	29 (46%)	87,91,91	2.17	29 (33%)
6	DMS	Q	405	-	3,3,3	0.60	0	3,3,3	0.52	0
5	LEU	T	403	5,4	5,7,8	0.97	0	6,8,10	1.37	1 (16%)
5	LEU	Z	803	5	5,7,8	0.25	0	6,8,10	0.39	0
3	A1C9P	T	401	-	63,63,63	2.63	27 (42%)	87,91,91	2.14	27 (31%)
4	BEZ	S	402	5	8,8,9	1.39	1 (12%)	9,9,11	1.62	2 (22%)
5	LEU	S	404	5	6,8,8	0.79	0	5,10,10	0.40	0
4	BEZ	X	801	5	8,8,9	2.51	5 (62%)	9,9,11	0.84	0
7	PEG	D	405	-	6,6,6	0.10	0	5,5,5	0.10	0
5	LEU	b	802	5,4	5,7,8	1.38	0	6,8,10	0.90	1 (16%)
4	BEZ	M	801	5	8,8,9	2.52	5 (62%)	9,9,11	0.84	0
5	LEU	N	802	5,4	5,7,8	0.72	0	6,8,10	0.49	0
4	BEZ	Q	402	5	8,8,9	1.41	2 (25%)	9,9,11	1.58	2 (22%)
5	LEU	L	803	5	5,7,8	1.00	0	6,8,10	1.54	1 (16%)
5	LEU	W	802	5,4	5,7,8	1.04	0	6,8,10	1.52	1 (16%)
5	LEU	Q	403	5,4	5,7,8	0.98	0	6,8,10	1.37	1 (16%)
3	A1C9P	Q	401	-	63,63,63	2.60	26 (41%)	87,91,91	2.19	27 (31%)
6	DMS	O	405	-	3,3,3	0.60	0	3,3,3	0.51	0
5	LEU	K	802	5,4	5,7,8	1.33	1 (20%)	6,8,10	1.03	0
5	LEU	I	802	5,4	5,7,8	1.52	1 (20%)	6,8,10	0.95	0
5	LEU	Y	803	5	5,7,8	1.00	0	6,8,10	1.71	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BEZ	b	801	5	8,8,9	2.52	5 (62%)	9,9,11	0.86	0
4	BEZ	a	801	5	8,8,9	2.50	5 (62%)	9,9,11	0.85	0
5	LEU	B	404	5	6,8,8	0.83	0	5,10,10	0.37	0
3	A1C9P	G	401	-	63,63,63	2.59	27 (42%)	87,91,91	2.08	27 (31%)
5	LEU	E	404	5	6,8,8	0.83	0	5,10,10	0.40	0
5	LEU	U	404	5	6,8,8	0.83	0	5,10,10	0.42	0
3	A1C9P	P	401	-	63,63,63	2.60	27 (42%)	87,91,91	2.13	29 (33%)
4	BEZ	W	801	5	8,8,9	2.50	5 (62%)	9,9,11	0.86	0
5	LEU	N	803	5	5,7,8	0.82	0	6,8,10	1.14	0
5	LEU	O	403	5,4	5,7,8	0.98	0	6,8,10	1.38	1 (16%)
5	LEU	M	802	5,4	5,7,8	1.43	1 (20%)	6,8,10	1.63	2 (33%)
4	BEZ	J	801	5	8,8,9	2.53	5 (62%)	9,9,11	0.84	0
4	BEZ	C	402	5	8,8,9	1.39	1 (12%)	9,9,11	1.61	2 (22%)
5	LEU	A	404	5	6,8,8	0.82	0	5,10,10	0.43	0
5	LEU	C	404	5	6,8,8	0.82	0	5,10,10	0.41	0
5	LEU	I	803	5	5,7,8	0.82	0	6,8,10	1.33	1 (16%)
3	A1C9P	O	401	-	63,63,63	2.57	28 (44%)	87,91,91	2.07	26 (29%)
5	LEU	G	403	5,4	5,7,8	0.99	0	6,8,10	1.37	1 (16%)
7	PEG	S	405	-	6,6,6	0.11	0	5,5,5	0.07	0
5	LEU	Z	802	5,4	5,7,8	1.05	0	6,8,10	1.55	1 (16%)
4	BEZ	D	402	5	8,8,9	1.39	2 (25%)	9,9,11	1.61	2 (22%)
5	LEU	D	404	5	6,8,8	0.83	0	5,10,10	0.46	0
5	LEU	B	403	5,4	5,7,8	0.97	0	6,8,10	1.38	1 (16%)
5	LEU	F	404	5	6,8,8	0.84	1 (16%)	5,10,10	0.42	0
5	LEU	S	403	5,4	5,7,8	0.99	0	6,8,10	1.38	1 (16%)
5	LEU	F	403	5,4	5,7,8	0.98	0	6,8,10	1.38	1 (16%)
5	LEU	M	803	5	5,7,8	0.38	0	6,8,10	0.25	0
5	LEU	J	802	5,4	5,7,8	1.56	1 (20%)	6,8,10	0.86	0
3	A1C9P	B	401	-	63,63,63	2.64	27 (42%)	87,91,91	2.14	28 (32%)
4	BEZ	H	801	5	8,8,9	2.50	5 (62%)	9,9,11	0.86	0
5	LEU	P	404	5	6,8,8	0.86	1 (16%)	5,10,10	0.44	0
4	BEZ	Y	801	5	8,8,9	2.51	5 (62%)	9,9,11	0.85	0
4	BEZ	B	402	5	8,8,9	1.38	1 (12%)	9,9,11	1.64	2 (22%)
6	DMS	F	405	-	3,3,3	0.23	0	3,3,3	0.07	0
4	BEZ	G	402	5	8,8,9	1.40	1 (12%)	9,9,11	1.62	2 (22%)
5	LEU	V	803	5	5,7,8	1.01	0	6,8,10	2.16	2 (33%)
5	LEU	V	802	5,4	5,7,8	1.56	2 (40%)	6,8,10	1.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	LEU	W	803	5	5,7,8	0.91	0	6,8,10	1.18	0
5	LEU	Y	802	5,4	5,7,8	1.17	0	6,8,10	1.26	1 (16%)
5	LEU	T	404	5	6,8,8	0.79	0	5,10,10	0.37	0
4	BEZ	P	402	5	8,8,9	1.39	1 (12%)	9,9,11	1.61	2 (22%)
5	LEU	H	802	5,4	5,7,8	0.78	0	6,8,10	1.49	2 (33%)
4	BEZ	F	402	5	8,8,9	1.38	2 (25%)	9,9,11	1.58	2 (22%)
4	BEZ	N	801	5	8,8,9	2.51	5 (62%)	9,9,11	0.86	0
3	A1C9P	U	401	-	63,63,63	2.60	28 (44%)	87,91,91	2.08	28 (32%)
5	LEU	X	803	5	5,7,8	0.95	0	6,8,10	1.56	1 (16%)
5	LEU	a	802	5,4	5,7,8	1.53	1 (20%)	6,8,10	0.93	0
3	A1C9P	F	401	-	63,63,63	2.62	27 (42%)	87,91,91	2.11	28 (32%)
5	LEU	U	403	5,4	5,7,8	0.98	0	6,8,10	1.37	1 (16%)
4	BEZ	K	801	5	8,8,9	2.52	5 (62%)	9,9,11	0.81	0
5	LEU	R	403	5,4	5,7,8	0.98	0	6,8,10	1.38	1 (16%)
3	A1C9P	E	401	-	63,63,63	2.63	28 (44%)	87,91,91	2.16	28 (32%)
4	BEZ	I	801	5	8,8,9	2.51	5 (62%)	9,9,11	0.85	0
4	BEZ	T	402	5	8,8,9	1.39	2 (25%)	9,9,11	1.59	2 (22%)
4	BEZ	O	402	5	8,8,9	1.38	1 (12%)	9,9,11	1.62	2 (22%)
4	BEZ	U	402	5	8,8,9	1.39	1 (12%)	9,9,11	1.61	2 (22%)
5	LEU	Q	404	5	6,8,8	0.82	0	5,10,10	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1C9P	A	401	-	-	10/65/108/108	0/5/6/6
5	LEU	P	403	5,4	-	2/5/6/8	-
4	BEZ	E	402	5	-	0/2/2/4	0/1/1/1
4	BEZ	L	801	5	-	2/2/2/4	0/1/1/1
5	LEU	H	803	5	-	3/5/6/8	-
3	A1C9P	R	401	-	-	8/65/108/108	0/5/6/6
5	LEU	X	802	5,4	-	2/5/6/8	-
5	LEU	b	803	5	-	4/5/6/8	-
4	BEZ	A	402	5	-	0/2/2/4	0/1/1/1
5	LEU	A	403	5,4	-	2/5/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LEU	a	803	5	-	3/5/6/8	-
5	LEU	C	403	5,4	-	2/5/6/8	-
5	LEU	O	404	5	-	0/8/8/8	-
4	BEZ	R	402	5	-	0/2/2/4	0/1/1/1
5	LEU	L	802	5,4	-	2/5/6/8	-
5	LEU	E	403	5,4	-	2/5/6/8	-
5	LEU	K	803	5	-	3/5/6/8	-
3	A1C9P	S	401	-	-	8/65/108/108	0/5/6/6
3	A1C9P	D	401	-	-	8/65/108/108	0/5/6/6
4	BEZ	V	801	5	-	2/2/2/4	0/1/1/1
4	BEZ	Z	801	5	-	2/2/2/4	0/1/1/1
5	LEU	D	403	5,4	-	2/5/6/8	-
5	LEU	G	404	5	-	0/8/8/8	-
5	LEU	J	803	5	-	3/5/6/8	-
5	LEU	R	404	5	-	0/8/8/8	-
3	A1C9P	C	401	-	-	11/65/108/108	0/5/6/6
5	LEU	T	403	5,4	-	2/5/6/8	-
5	LEU	Z	803	5	-	1/5/6/8	-
3	A1C9P	T	401	-	-	13/65/108/108	0/5/6/6
4	BEZ	S	402	5	-	0/2/2/4	0/1/1/1
5	LEU	S	404	5	-	0/8/8/8	-
4	BEZ	X	801	5	-	2/2/2/4	0/1/1/1
7	PEG	D	405	-	-	2/4/4/4	-
5	LEU	b	802	5,4	-	2/5/6/8	-
4	BEZ	M	801	5	-	2/2/2/4	0/1/1/1
5	LEU	N	802	5,4	-	0/5/6/8	-
4	BEZ	Q	402	5	-	0/2/2/4	0/1/1/1
5	LEU	L	803	5	-	3/5/6/8	-
5	LEU	W	802	5,4	-	2/5/6/8	-
5	LEU	Q	403	5,4	-	2/5/6/8	-
3	A1C9P	Q	401	-	-	13/65/108/108	0/5/6/6
5	LEU	K	802	5,4	-	3/5/6/8	-
5	LEU	I	802	5,4	-	2/5/6/8	-
5	LEU	Y	803	5	-	3/5/6/8	-
4	BEZ	b	801	5	-	2/2/2/4	0/1/1/1
4	BEZ	a	801	5	-	2/2/2/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LEU	B	404	5	-	0/8/8/8	-
3	A1C9P	G	401	-	-	8/65/108/108	0/5/6/6
5	LEU	E	404	5	-	0/8/8/8	-
5	LEU	U	404	5	-	0/8/8/8	-
3	A1C9P	P	401	-	-	7/65/108/108	0/5/6/6
4	BEZ	W	801	5	-	2/2/2/4	0/1/1/1
5	LEU	N	803	5	-	3/5/6/8	-
5	LEU	O	403	5,4	-	2/5/6/8	-
5	LEU	M	802	5,4	-	2/5/6/8	-
4	BEZ	J	801	5	-	2/2/2/4	0/1/1/1
4	BEZ	C	402	5	-	0/2/2/4	0/1/1/1
5	LEU	A	404	5	-	0/8/8/8	-
5	LEU	C	404	5	-	0/8/8/8	-
5	LEU	I	803	5	-	3/5/6/8	-
3	A1C9P	O	401	-	-	6/65/108/108	0/5/6/6
5	LEU	G	403	5,4	-	2/5/6/8	-
7	PEG	S	405	-	-	1/4/4/4	-
5	LEU	Z	802	5,4	-	2/5/6/8	-
4	BEZ	D	402	5	-	0/2/2/4	0/1/1/1
5	LEU	D	404	5	-	0/8/8/8	-
5	LEU	B	403	5,4	-	2/5/6/8	-
5	LEU	F	404	5	-	0/8/8/8	-
5	LEU	S	403	5,4	-	2/5/6/8	-
5	LEU	F	403	5,4	-	2/5/6/8	-
5	LEU	M	803	5	-	5/5/6/8	-
5	LEU	J	802	5,4	-	3/5/6/8	-
3	A1C9P	B	401	-	-	10/65/108/108	0/5/6/6
4	BEZ	H	801	5	-	2/2/2/4	0/1/1/1
5	LEU	P	404	5	-	0/8/8/8	-
4	BEZ	Y	801	5	-	2/2/2/4	0/1/1/1
4	BEZ	B	402	5	-	0/2/2/4	0/1/1/1
4	BEZ	G	402	5	-	0/2/2/4	0/1/1/1
5	LEU	V	803	5	-	3/5/6/8	-
5	LEU	V	802	5,4	-	2/5/6/8	-
5	LEU	W	803	5	-	3/5/6/8	-
5	LEU	Y	802	5,4	-	3/5/6/8	-
5	LEU	T	404	5	-	1/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BEZ	P	402	5	-	0/2/2/4	0/1/1/1
5	LEU	H	802	5,4	-	3/5/6/8	-
4	BEZ	F	402	5	-	0/2/2/4	0/1/1/1
4	BEZ	N	801	5	-	2/2/2/4	0/1/1/1
3	A1C9P	U	401	-	-	8/65/108/108	0/5/6/6
5	LEU	X	803	5	-	3/5/6/8	-
5	LEU	a	802	5,4	-	2/5/6/8	-
3	A1C9P	F	401	-	-	9/65/108/108	0/5/6/6
5	LEU	U	403	5,4	-	2/5/6/8	-
4	BEZ	K	801	5	-	2/2/2/4	0/1/1/1
5	LEU	R	403	5,4	-	2/5/6/8	-
3	A1C9P	E	401	-	-	9/65/108/108	0/5/6/6
4	BEZ	I	801	5	-	2/2/2/4	0/1/1/1
4	BEZ	T	402	5	-	0/2/2/4	0/1/1/1
4	BEZ	O	402	5	-	0/2/2/4	0/1/1/1
4	BEZ	U	402	5	-	0/2/2/4	0/1/1/1
5	LEU	Q	404	5	-	0/8/8/8	-

The worst 5 of 485 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	A1C9P	C02-N03	6.02	1.48	1.34
3	R	401	A1C9P	C02-N03	5.88	1.47	1.34
3	E	401	A1C9P	C02-N03	5.87	1.47	1.34
3	P	401	A1C9P	C02-N03	5.86	1.47	1.34
3	A	401	A1C9P	C02-N03	5.85	1.47	1.34

The worst 5 of 448 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	401	A1C9P	C44-C43-N42	9.15	130.27	114.61
3	Q	401	A1C9P	C44-C43-N42	8.96	129.94	114.61
3	A	401	A1C9P	C44-C43-N42	8.69	129.48	114.61
3	C	401	A1C9P	C44-C43-N42	8.48	129.13	114.61
3	B	401	A1C9P	C44-C43-N42	8.33	128.87	114.61

There are no chirality outliers.

5 of 261 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	A1C9P	C24-C25-O27-C28
3	A	401	A1C9P	C26-C25-O27-C28
3	B	401	A1C9P	C24-C25-O27-C28
3	B	401	A1C9P	C26-C25-O27-C28
3	C	401	A1C9P	C24-C25-O27-C28

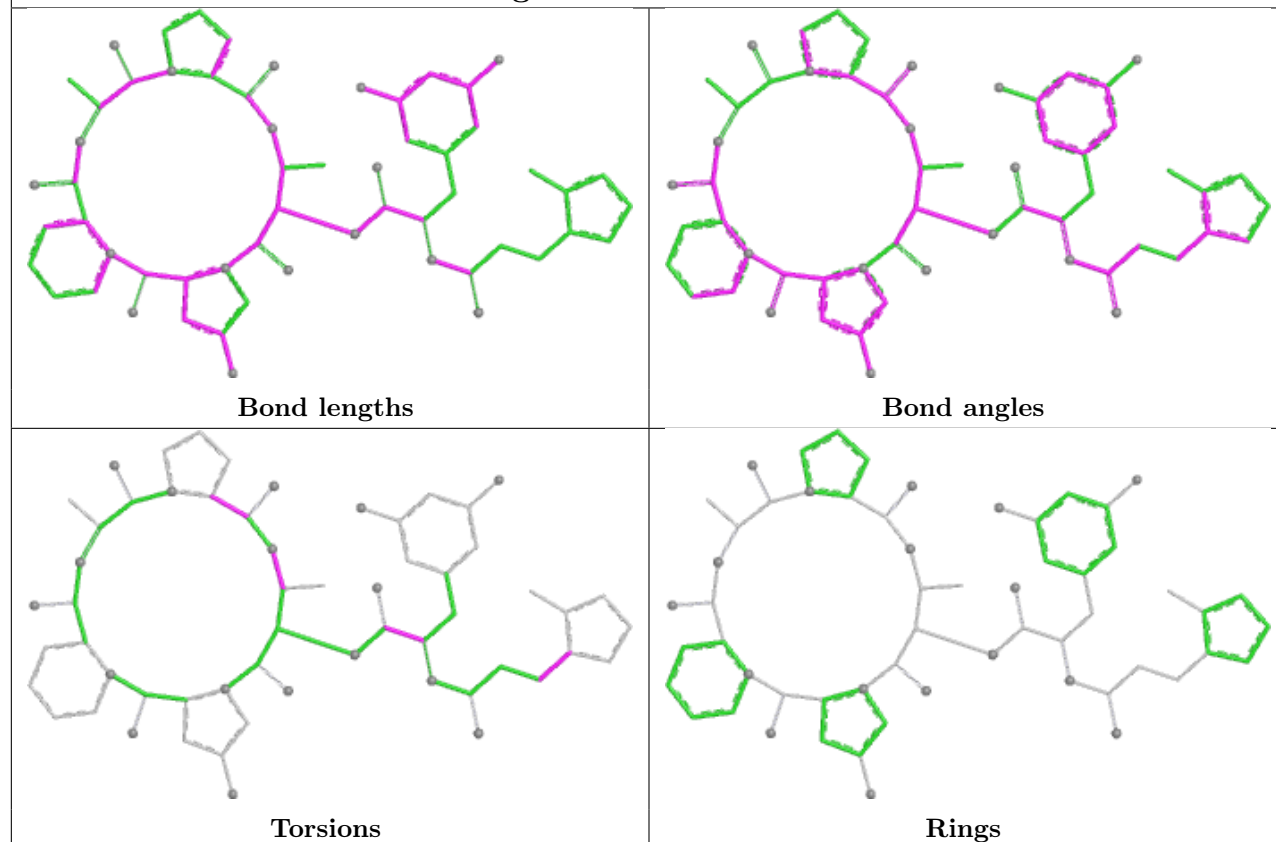
There are no ring outliers.

17 monomers are involved in 19 short contacts:

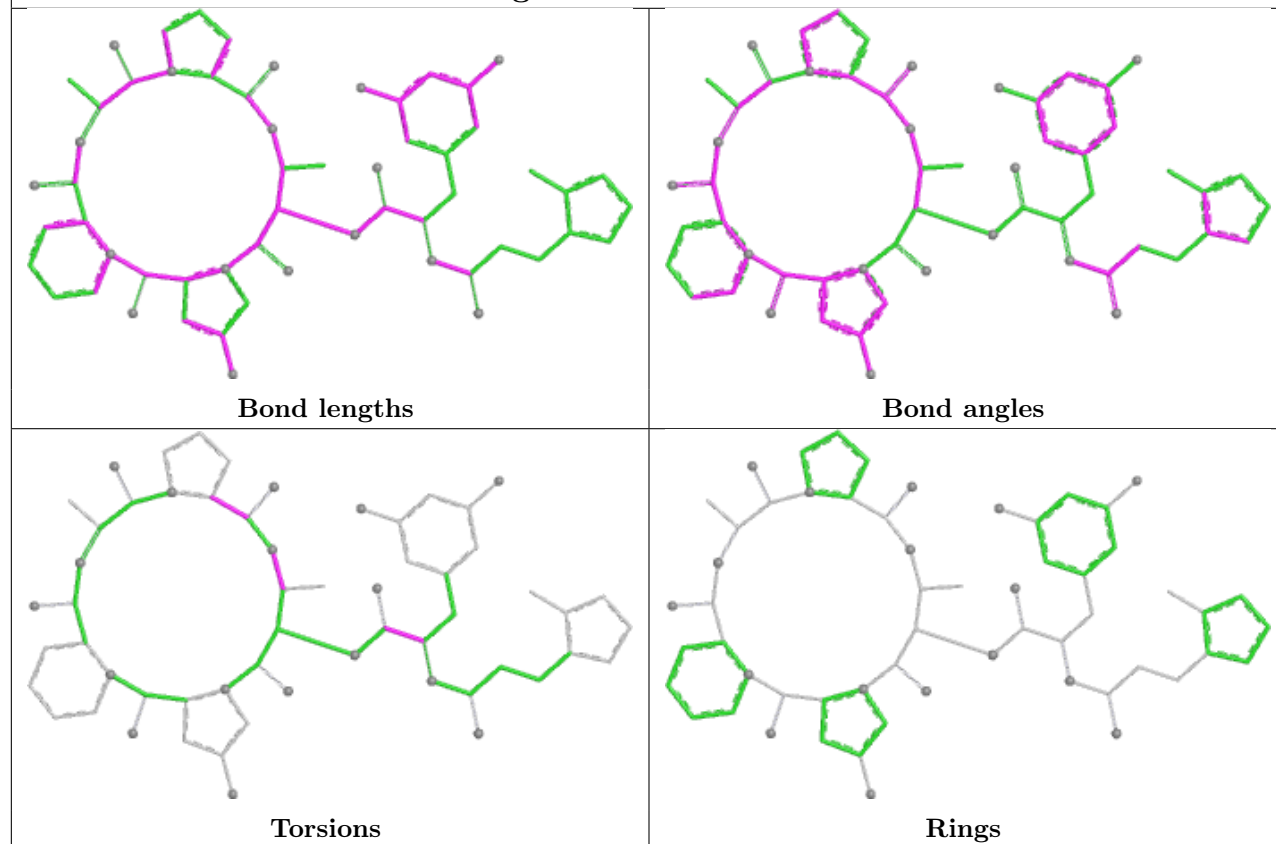
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	A1C9P	1	0
5	H	803	LEU	1	0
3	R	401	A1C9P	1	0
5	K	803	LEU	1	0
3	S	401	A1C9P	1	0
3	D	401	A1C9P	1	0
3	C	401	A1C9P	1	0
4	X	801	BEZ	1	0
5	N	802	LEU	1	0
3	Q	401	A1C9P	1	0
5	Y	803	LEU	1	0
3	P	401	A1C9P	1	0
3	O	401	A1C9P	1	0
6	F	405	DMS	3	0
5	Y	802	LEU	1	0
5	X	803	LEU	1	0
3	F	401	A1C9P	1	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.

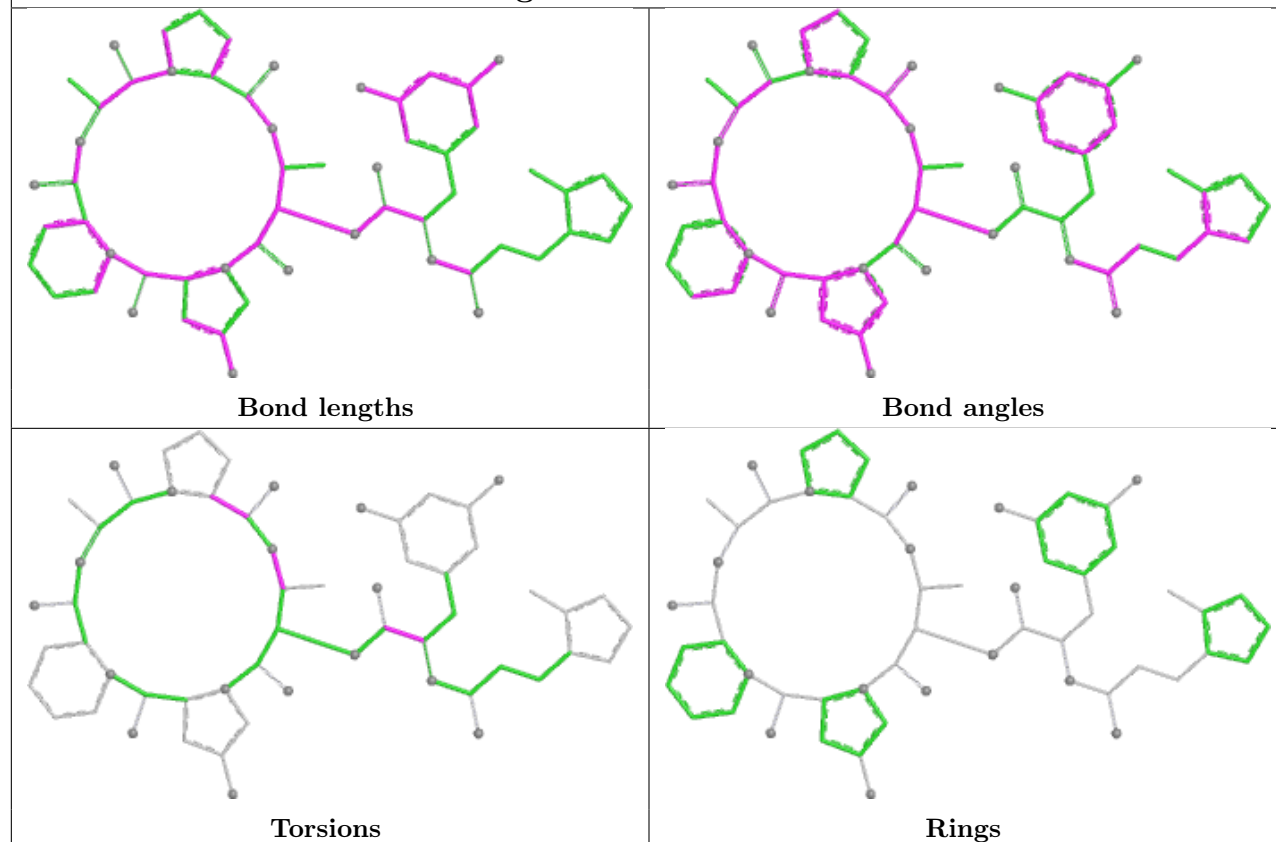
Ligand A1C9P A 401



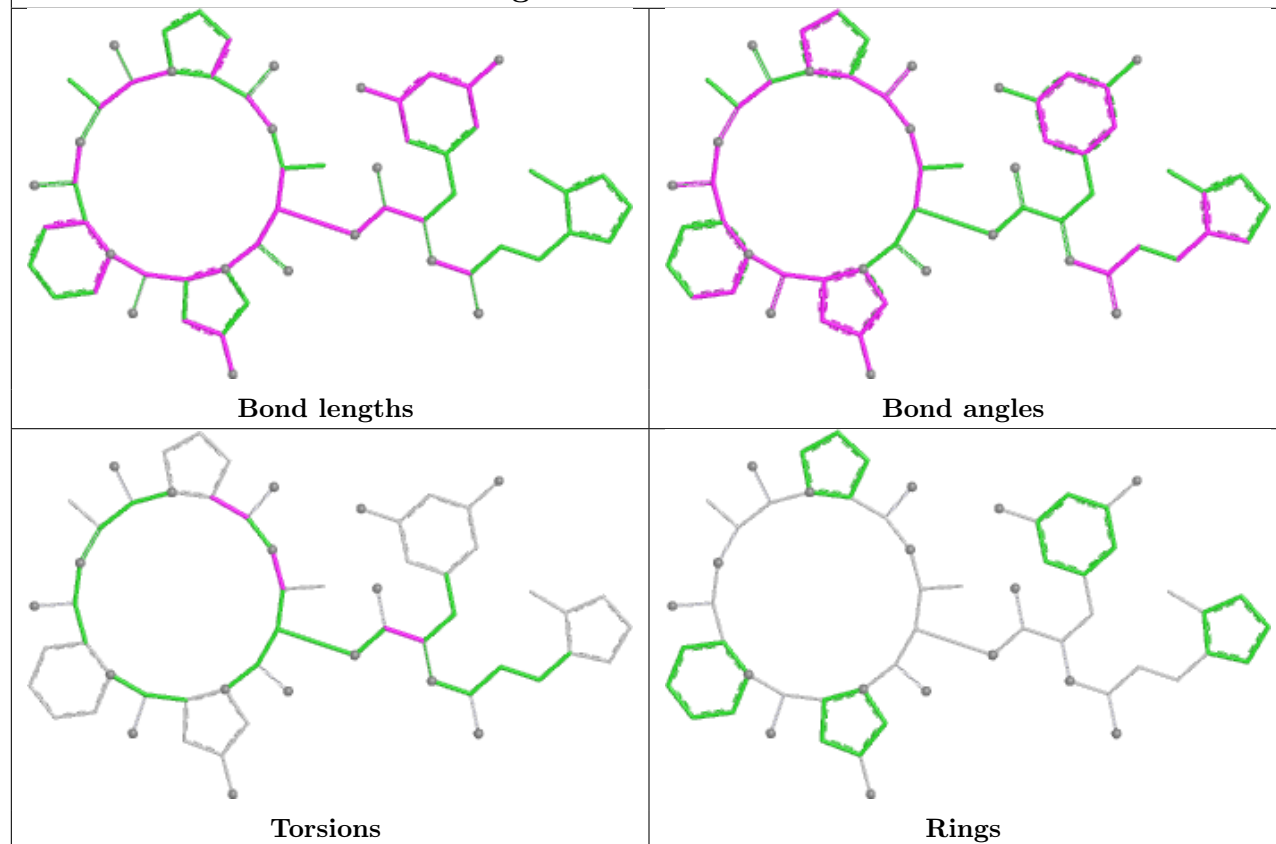
Ligand A1C9P R 401



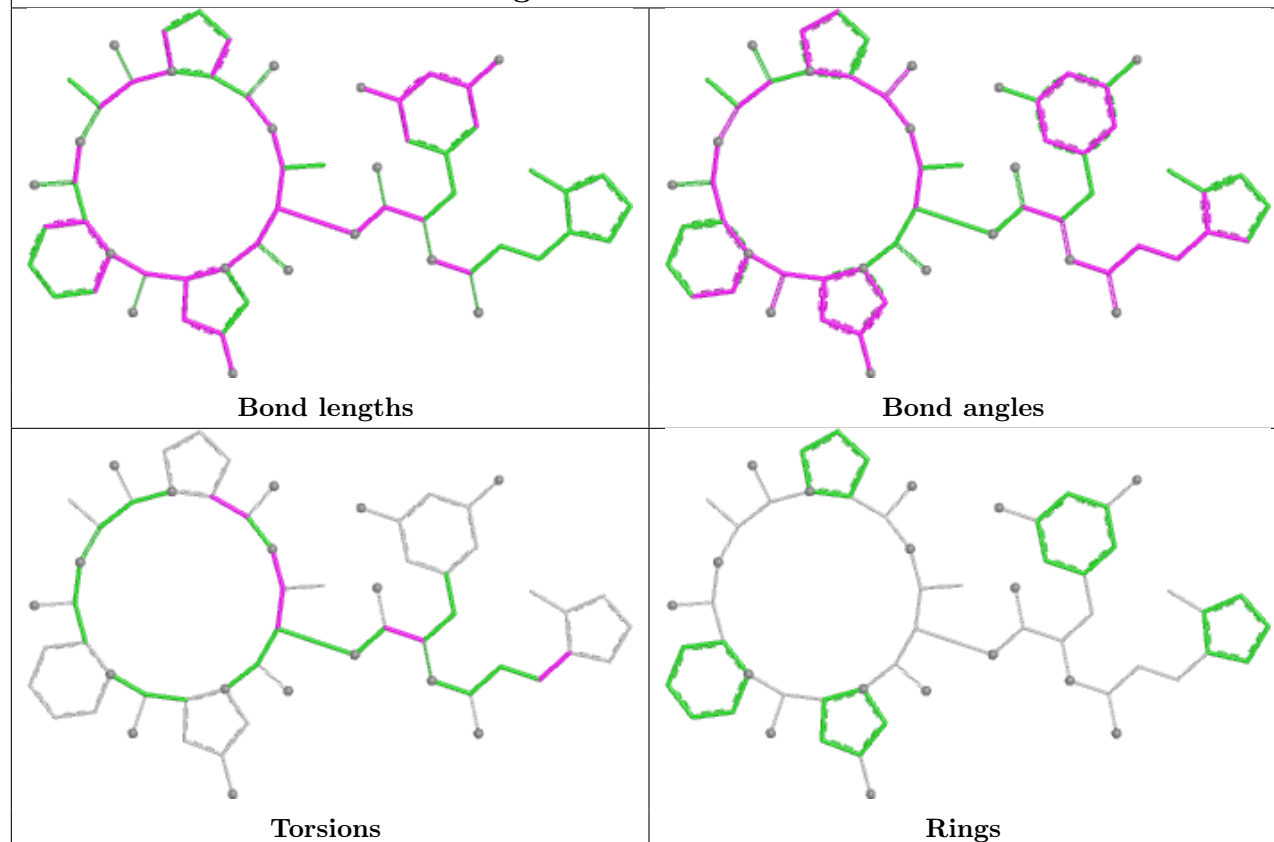
Ligand A1C9P S 401



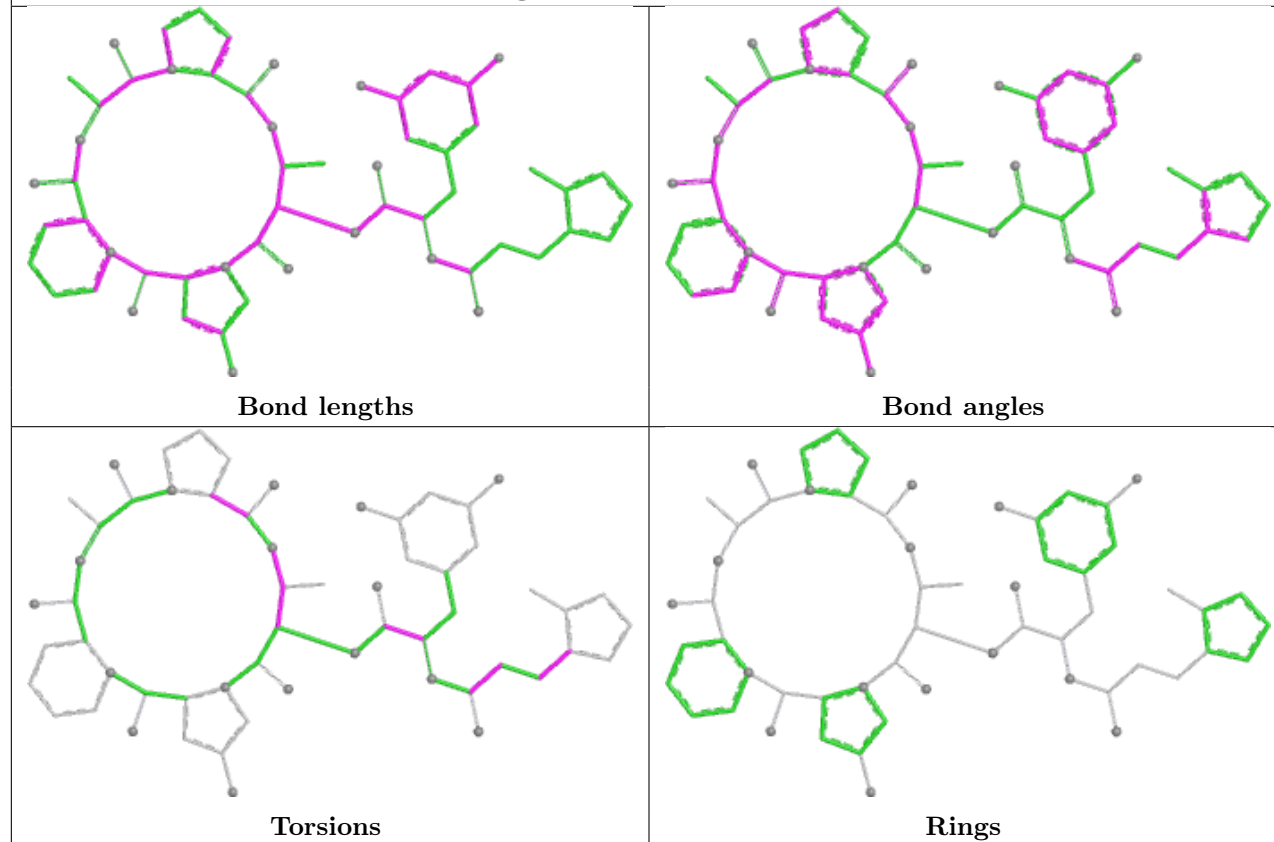
Ligand A1C9P D 401



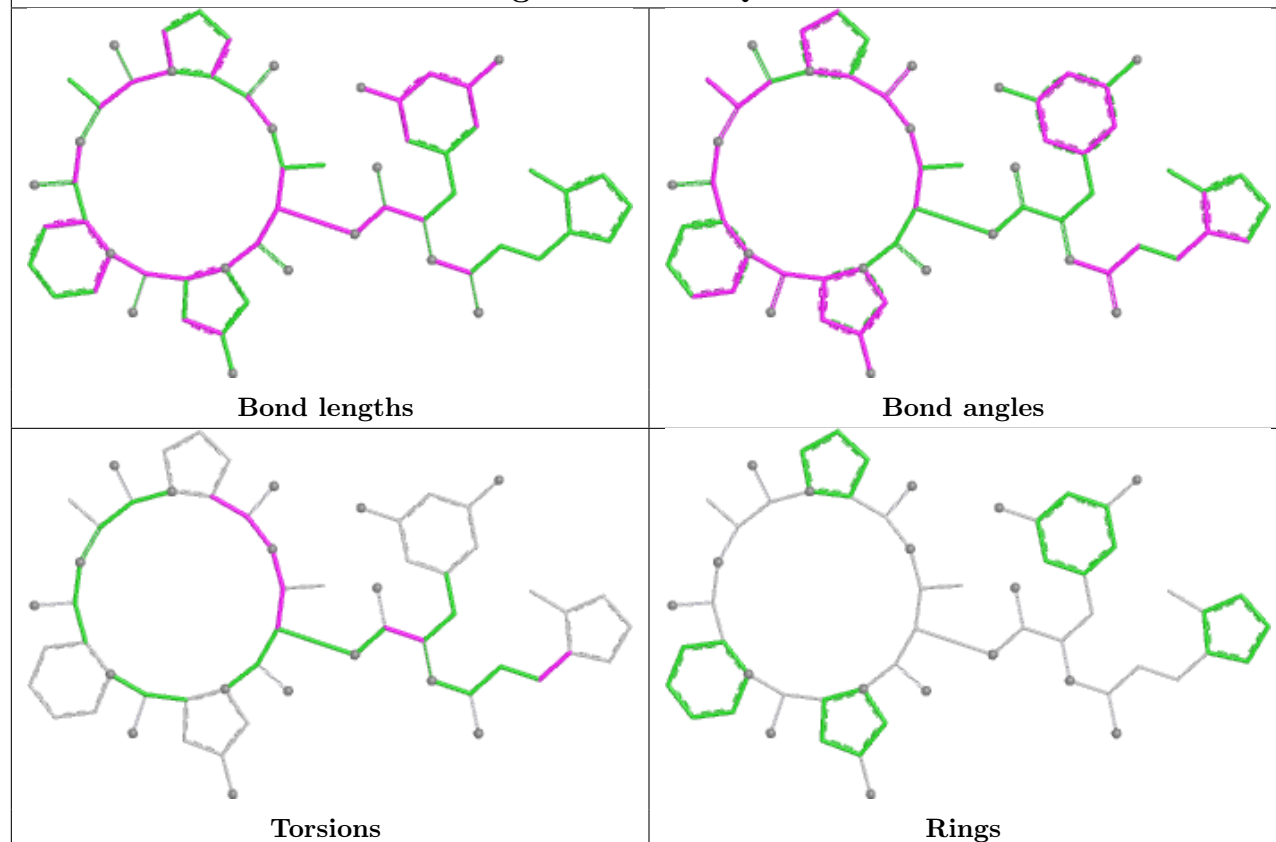
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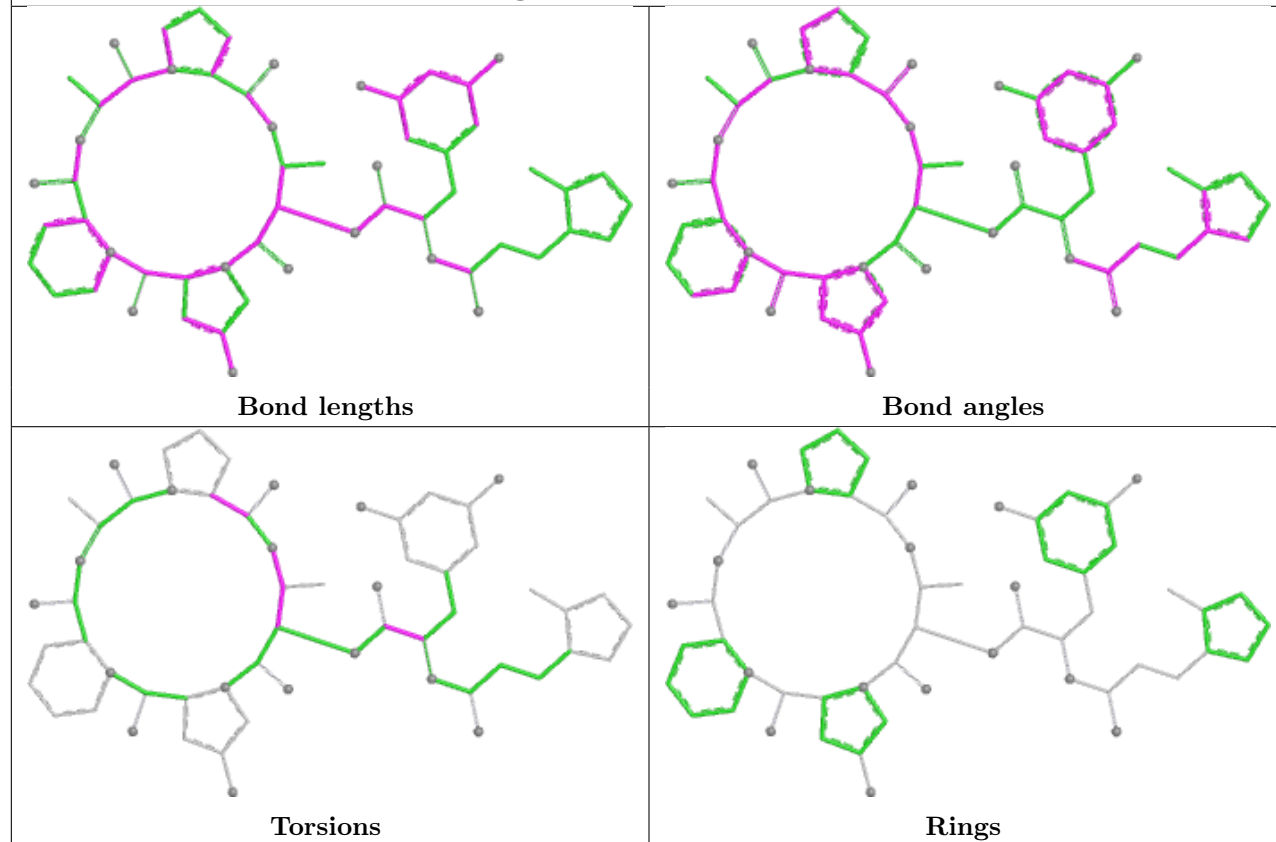
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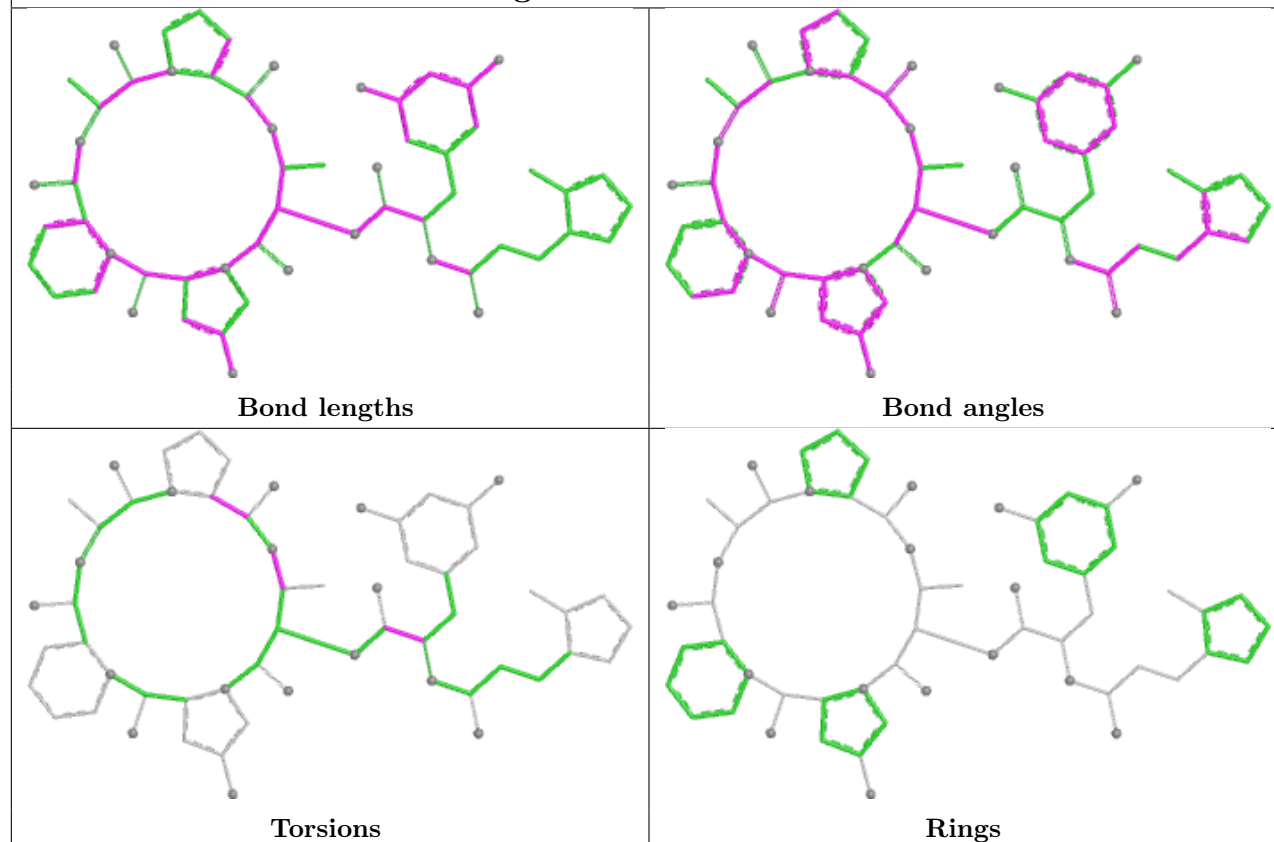
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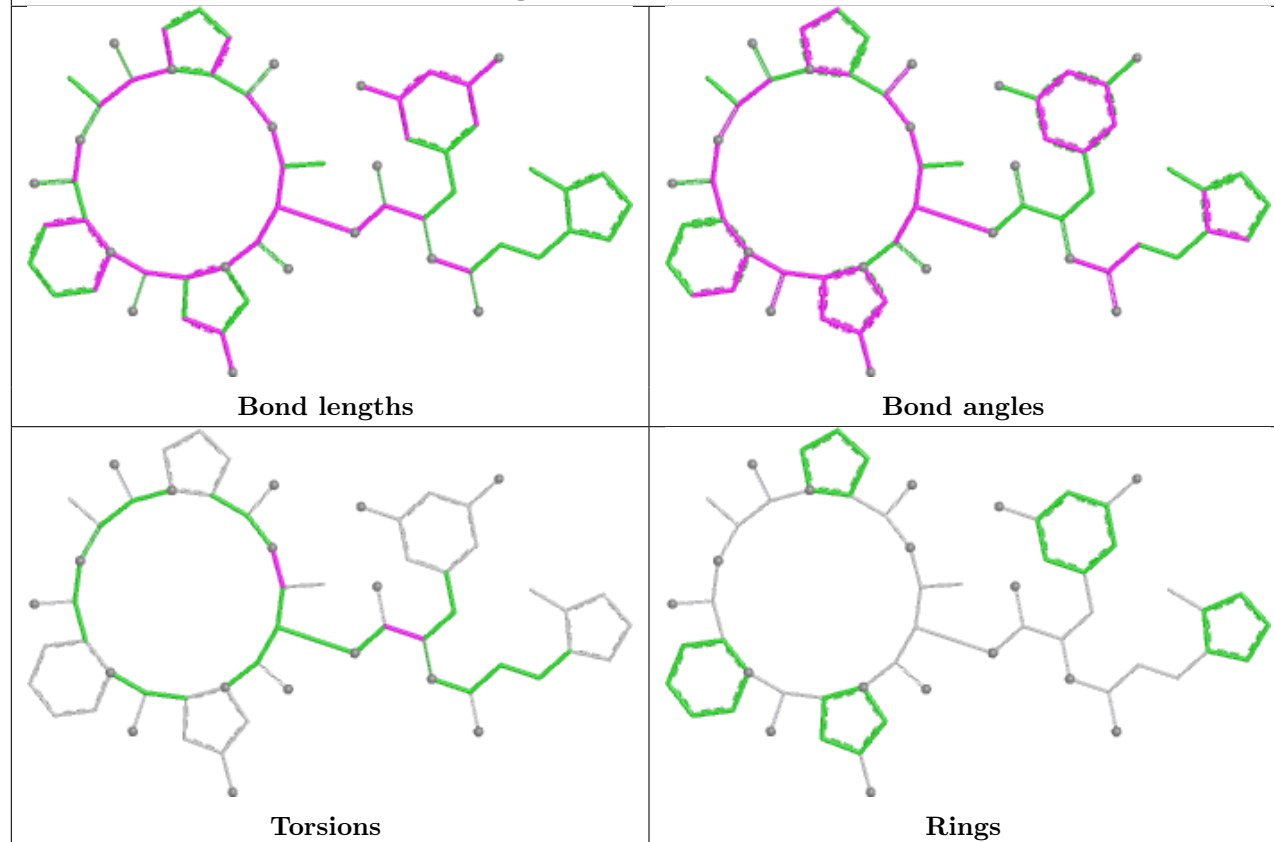
Ligand A1C9P G 401



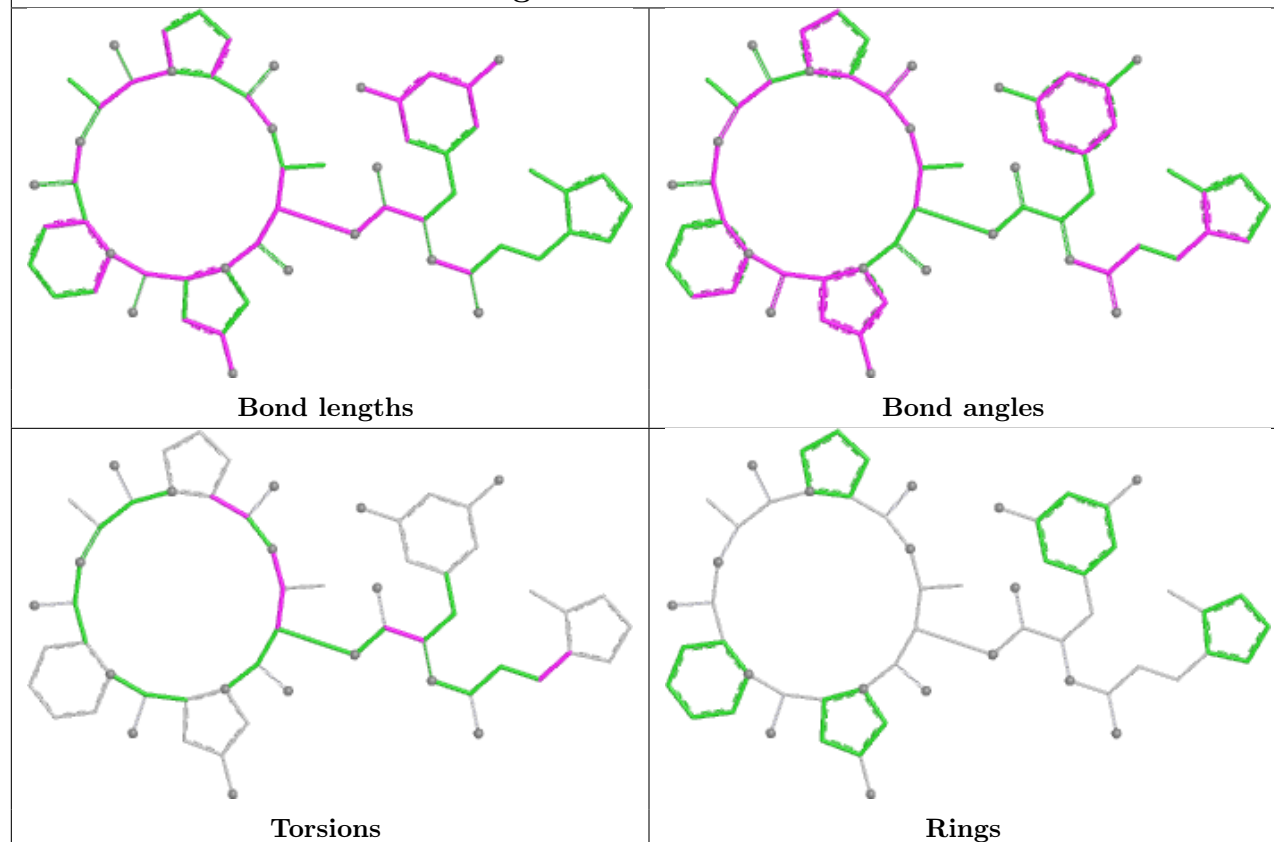
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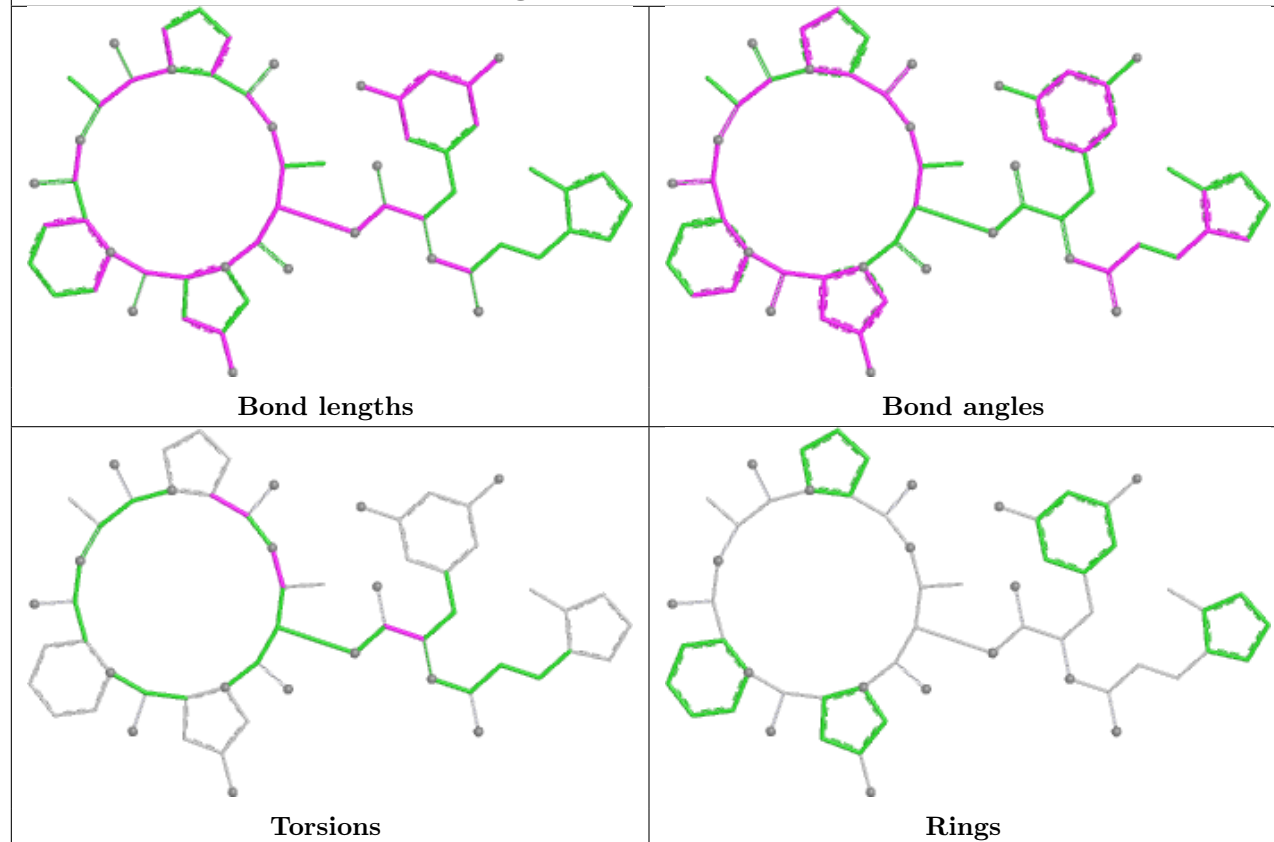
Ligand A1C9P O 401



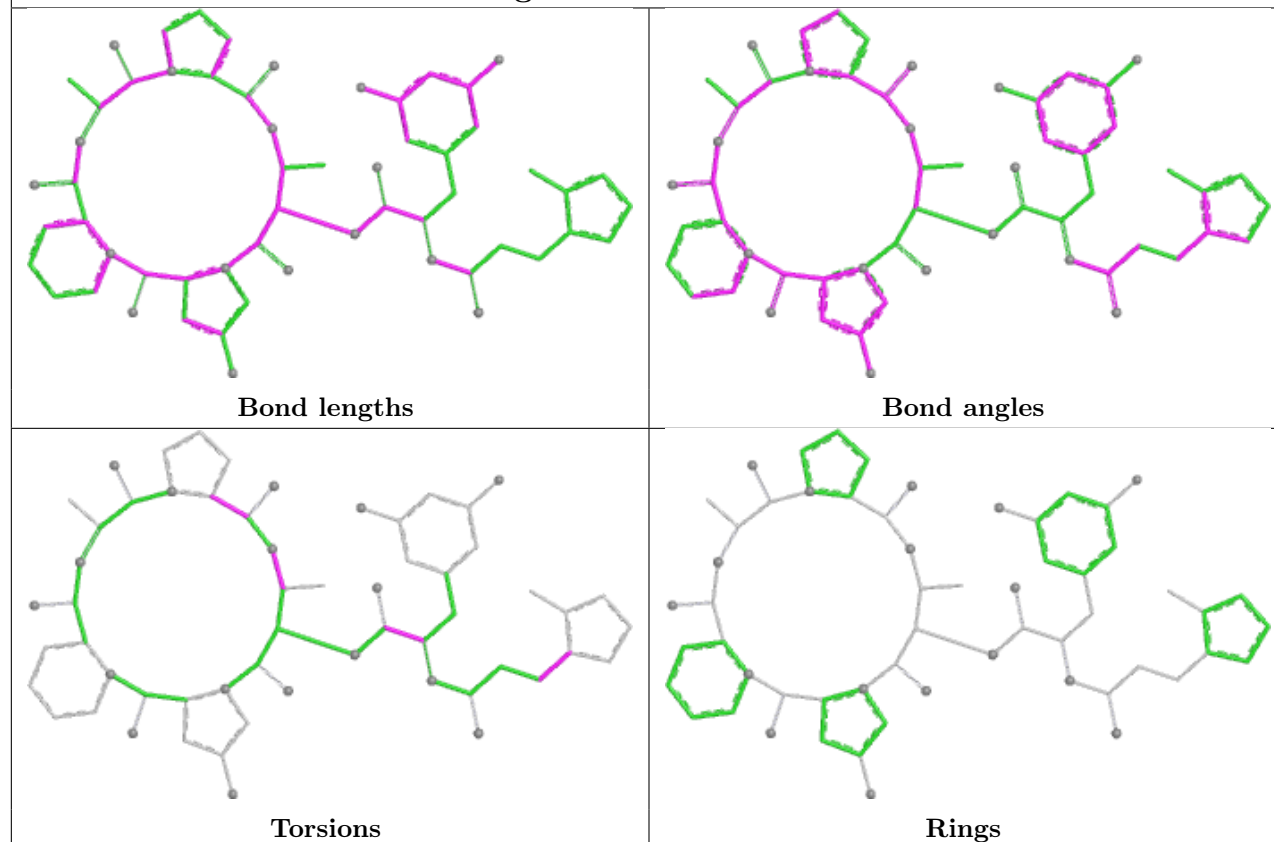
Ligand A1C9P B 401



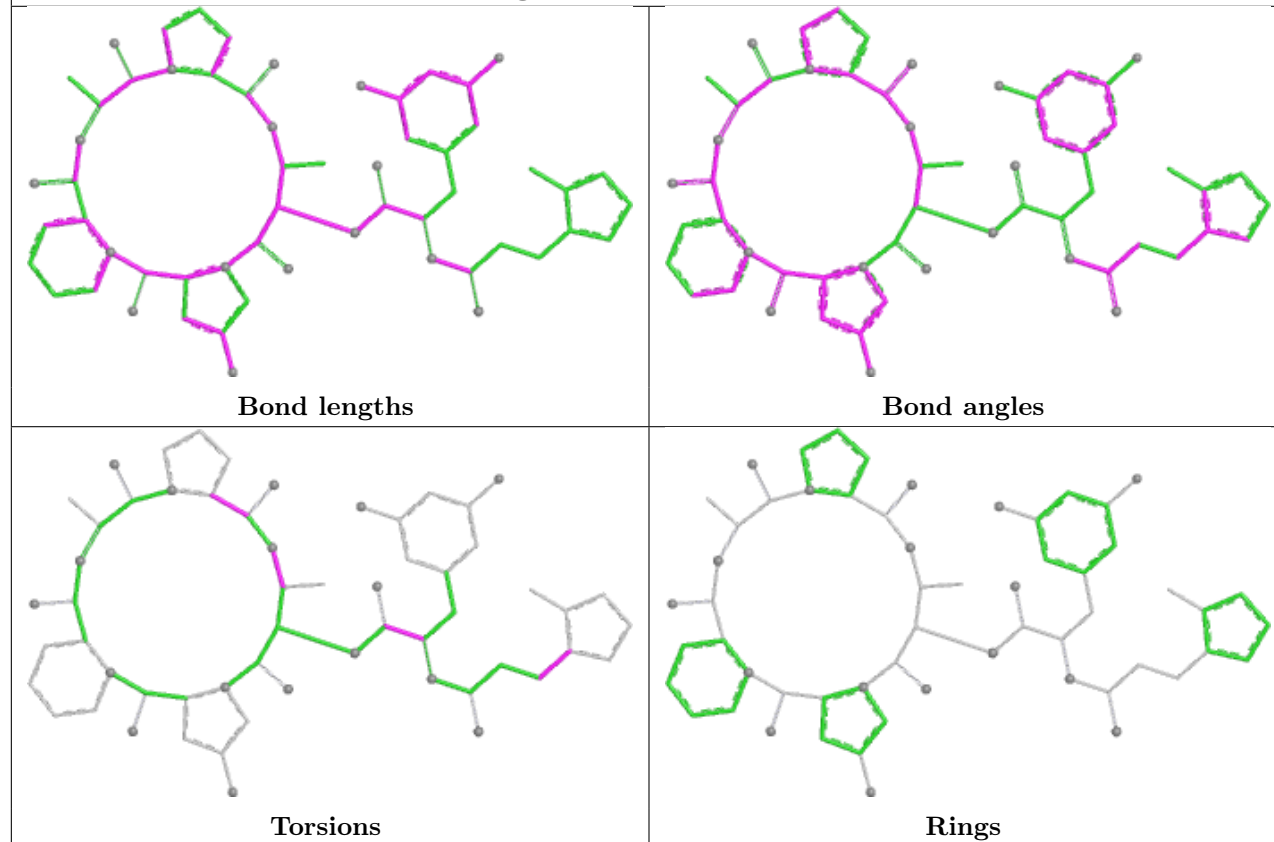
Ligand A1C9P U 401



Ligand A1C9P F 401



Ligand A1C9P E 401



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	197/214 (92%)	-0.24	2 (1%) 79 76	30, 45, 59, 82	0
1	B	199/214 (92%)	-0.24	3 (1%) 72 67	32, 47, 66, 87	0
1	C	202/214 (94%)	-0.28	4 (1%) 65 59	28, 44, 66, 92	0
1	D	198/214 (92%)	-0.25	2 (1%) 79 76	30, 43, 61, 87	0
1	E	200/214 (93%)	-0.22	1 (0%) 87 85	34, 48, 65, 85	0
1	F	197/214 (92%)	-0.18	1 (0%) 87 85	31, 48, 65, 83	0
1	G	198/214 (92%)	-0.17	3 (1%) 72 67	26, 46, 64, 94	0
1	O	196/214 (91%)	-0.37	4 (2%) 65 59	27, 41, 58, 84	0
1	P	199/214 (92%)	-0.32	2 (1%) 79 76	31, 44, 62, 80	0
1	Q	197/214 (92%)	-0.23	2 (1%) 79 76	33, 46, 61, 77	0
1	R	198/214 (92%)	-0.15	0 100 100	36, 49, 66, 101	0
1	S	199/214 (92%)	-0.04	3 (1%) 72 67	32, 53, 71, 98	0
1	T	198/214 (92%)	-0.17	3 (1%) 72 67	33, 48, 65, 93	1 (0%)
1	U	198/214 (92%)	-0.29	3 (1%) 72 67	27, 43, 63, 87	0
2	H	177/194 (91%)	-0.11	2 (1%) 78 75	34, 50, 65, 91	0
2	I	177/194 (91%)	-0.16	1 (0%) 85 83	35, 49, 71, 90	0
2	J	179/194 (92%)	-0.11	2 (1%) 78 75	33, 48, 69, 90	0
2	K	176/194 (90%)	-0.19	0 100 100	33, 50, 65, 73	0
2	L	177/194 (91%)	-0.03	2 (1%) 78 75	34, 53, 71, 83	0
2	M	176/194 (90%)	-0.10	0 100 100	37, 52, 67, 83	0
2	N	177/194 (91%)	-0.19	1 (0%) 85 83	36, 48, 67, 78	0
2	V	176/194 (90%)	-0.11	3 (1%) 69 64	33, 49, 68, 88	0
2	W	176/194 (90%)	-0.15	0 100 100	31, 51, 66, 75	0
2	X	176/194 (90%)	-0.12	1 (0%) 85 83	34, 51, 67, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	Y	176/194 (90%)	0.04	0 100 100	36, 55, 71, 84	0
2	Z	176/194 (90%)	0.05	0 100 100	41, 55, 71, 83	0
2	a	176/194 (90%)	0.09	0 100 100	37, 55, 72, 84	0
2	b	176/194 (90%)	-0.10	0 100 100	36, 53, 67, 78	0
All	All	5247/5712 (91%)	-0.16	45 (0%) 81 78	26, 49, 68, 101	1 (0%)

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	191	THR	5.9
1	D	209	LEU	5.1
1	T	135[A]	HIS	4.7
1	S	211	ALA	4.4
1	B	211	ALA	4.0

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	DMS	C	405	4/4	0.38	0.29	67,82,82,118	0
6	DMS	Q	405	4/4	0.43	0.29	58,70,76,116	0
6	DMS	O	405	4/4	0.50	0.31	65,78,83,113	0
6	DMS	F	405	4/4	0.72	0.33	54,70,86,99	0
5	LEU	a	803	8/9	0.73	0.23	30,30,69,69	0
5	LEU	Z	803	8/9	0.77	0.18	30,30,71,71	0
5	LEU	M	803	8/9	0.77	0.20	30,30,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	LEU	N	802	8/9	0.77	0.19	30,30,64,72	0
5	LEU	S	404	9/9	0.80	0.18	57,73,87,87	0
5	LEU	I	802	8/9	0.82	0.27	55,71,85,85	0
7	PEG	S	405	7/7	0.84	0.15	55,71,86,86	0
5	LEU	A	404	9/9	0.85	0.18	44,54,62,65	0
4	BEZ	b	801	8/9	0.86	0.19	56,68,81,96	0
5	LEU	T	404	9/9	0.86	0.18	56,71,82,82	0
5	LEU	M	802	8/9	0.86	0.18	49,77,98,98	0
5	LEU	C	404	9/9	0.87	0.15	39,56,68,70	0
5	LEU	G	404	9/9	0.87	0.14	51,62,73,77	0
5	LEU	H	803	8/9	0.87	0.18	51,65,78,81	0
4	BEZ	a	801	8/9	0.87	0.20	53,59,71,80	0
5	LEU	L	802	8/9	0.87	0.13	53,67,72,81	0
5	LEU	V	802	8/9	0.87	0.17	48,58,74,82	0
5	LEU	Z	802	8/9	0.87	0.17	53,65,81,81	0
4	BEZ	H	801	8/9	0.88	0.19	50,63,77,88	0
5	LEU	a	802	8/9	0.88	0.20	52,69,81,85	0
5	LEU	R	404	9/9	0.88	0.15	56,68,79,79	0
4	BEZ	M	801	8/9	0.88	0.20	50,60,79,81	0
5	LEU	X	803	8/9	0.89	0.15	50,67,75,84	0
5	LEU	J	802	8/9	0.89	0.12	51,61,71,72	0
5	LEU	O	404	9/9	0.89	0.17	38,56,63,65	0
5	LEU	Q	404	9/9	0.89	0.16	43,59,66,66	0
5	LEU	K	803	8/9	0.89	0.14	41,69,86,86	0
4	BEZ	T	402	8/9	0.89	0.15	48,60,72,75	0
5	LEU	D	404	9/9	0.89	0.13	43,60,65,71	0
5	LEU	U	404	9/9	0.89	0.15	47,57,74,75	0
5	LEU	F	404	9/9	0.89	0.14	45,68,79,79	0
7	PEG	D	405	7/7	0.89	0.17	51,68,82,82	0
5	LEU	W	802	8/9	0.89	0.18	44,58,82,82	0
5	LEU	V	803	8/9	0.90	0.14	53,66,87,87	0
3	A1C9P	F	401	58/58	0.90	0.13	33,53,74,96	0
5	LEU	W	803	8/9	0.90	0.15	58,71,85,85	0
5	LEU	X	802	8/9	0.90	0.16	54,71,82,82	0
5	LEU	E	404	9/9	0.90	0.15	42,56,67,72	0
5	LEU	Y	802	8/9	0.90	0.16	57,69,86,89	0
5	LEU	Y	803	8/9	0.90	0.13	53,64,77,77	0
5	LEU	F	403	8/9	0.90	0.14	44,54,88,88	0
4	BEZ	Z	801	8/9	0.90	0.18	50,63,75,79	0
5	LEU	N	803	8/9	0.90	0.14	56,70,87,87	0
3	A1C9P	Q	401	58/58	0.90	0.13	35,54,67,84	0
3	A1C9P	C	401	58/58	0.90	0.12	30,51,69,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BEZ	K	801	8/9	0.90	0.17	52,61,73,73	0
5	LEU	I	803	8/9	0.90	0.15	58,74,81,85	0
5	LEU	B	404	9/9	0.90	0.14	48,60,72,72	0
5	LEU	K	802	8/9	0.90	0.14	53,68,80,84	0
3	A1C9P	E	401	58/58	0.90	0.12	28,51,67,73	0
3	A1C9P	A	401	58/58	0.91	0.11	31,50,63,70	0
5	LEU	H	802	8/9	0.91	0.14	57,69,75,77	0
3	A1C9P	G	401	58/58	0.91	0.12	21,53,69,88	0
3	A1C9P	P	401	58/58	0.91	0.11	29,45,58,65	0
5	LEU	P	404	9/9	0.91	0.16	44,59,66,66	0
4	BEZ	Q	402	8/9	0.91	0.12	39,55,67,68	0
3	A1C9P	B	401	58/58	0.91	0.11	26,50,68,72	0
5	LEU	S	403	8/9	0.91	0.16	48,65,96,96	0
5	LEU	J	803	8/9	0.91	0.13	52,64,77,84	0
5	LEU	b	802	8/9	0.91	0.14	49,61,73,80	0
5	LEU	E	403	8/9	0.91	0.15	44,58,91,91	0
5	LEU	U	403	8/9	0.91	0.13	47,58,77,77	0
4	BEZ	X	801	8/9	0.91	0.19	47,61,76,81	0
3	A1C9P	R	401	58/58	0.91	0.12	31,54,71,98	0
5	LEU	L	803	8/9	0.91	0.15	56,69,81,83	0
3	A1C9P	S	401	58/58	0.91	0.12	35,55,75,86	0
5	LEU	R	403	8/9	0.92	0.13	43,55,91,91	0
3	A1C9P	U	401	58/58	0.92	0.12	23,48,63,70	0
4	BEZ	G	402	8/9	0.92	0.14	46,53,64,73	0
3	A1C9P	D	401	58/58	0.92	0.13	32,54,71,94	0
5	LEU	T	403	8/9	0.92	0.12	43,57,88,88	0
4	BEZ	J	801	8/9	0.92	0.16	49,65,81,85	0
5	LEU	P	403	8/9	0.92	0.11	41,52,80,80	0
3	A1C9P	T	401	58/58	0.92	0.12	29,53,70,85	0
5	LEU	G	403	8/9	0.92	0.14	42,61,74,74	0
5	LEU	A	403	8/9	0.93	0.12	41,56,85,85	0
4	BEZ	V	801	8/9	0.93	0.17	46,60,79,89	0
5	LEU	B	403	8/9	0.93	0.11	37,52,68,68	0
5	LEU	Q	403	8/9	0.93	0.11	42,58,77,77	0
4	BEZ	U	402	8/9	0.93	0.12	38,46,62,70	0
5	LEU	C	403	8/9	0.93	0.11	35,54,75,75	0
4	BEZ	Y	801	8/9	0.93	0.14	51,63,76,77	0
5	LEU	D	403	8/9	0.93	0.14	46,56,95,95	0
4	BEZ	W	801	8/9	0.94	0.17	46,62,81,83	0
3	A1C9P	O	401	58/58	0.94	0.09	24,42,63,75	0
4	BEZ	N	801	8/9	0.94	0.17	38,58,69,70	0
4	BEZ	O	402	8/9	0.94	0.10	40,49,59,60	0

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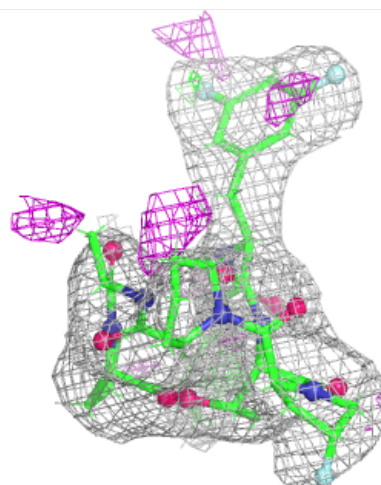
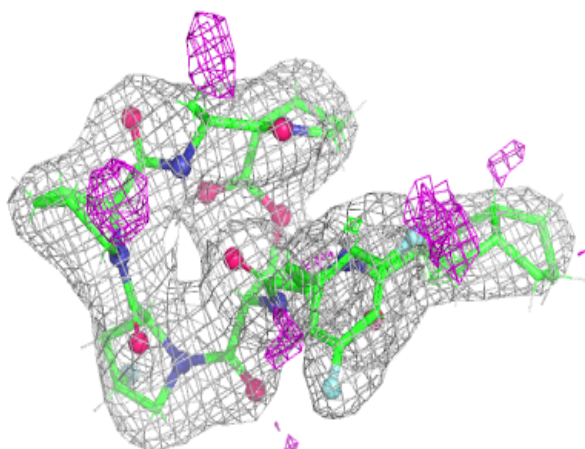
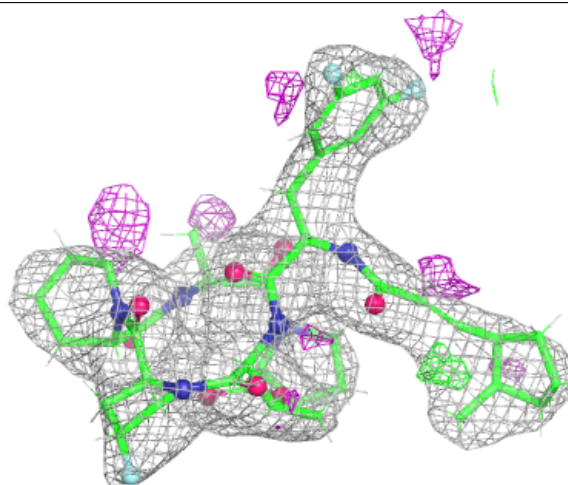
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	LEU	b	803	8/9	0.94	0.12	55,67,74,75	0
4	BEZ	P	402	8/9	0.94	0.09	36,45,54,57	0
4	BEZ	B	402	8/9	0.94	0.09	41,50,60,65	0
4	BEZ	D	402	8/9	0.94	0.09	35,40,48,51	0
5	LEU	O	403	8/9	0.94	0.11	38,57,76,76	0
4	BEZ	F	402	8/9	0.94	0.11	35,54,66,67	0
4	BEZ	L	801	8/9	0.94	0.14	59,66,79,79	0
4	BEZ	S	402	8/9	0.95	0.10	51,61,74,83	0
4	BEZ	E	402	8/9	0.95	0.10	45,51,60,61	0
4	BEZ	I	801	8/9	0.95	0.12	44,53,64,65	0
4	BEZ	A	402	8/9	0.96	0.08	36,49,56,61	0
4	BEZ	C	402	8/9	0.96	0.07	32,40,47,49	0
4	BEZ	R	402	8/9	0.97	0.07	42,49,59,61	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.

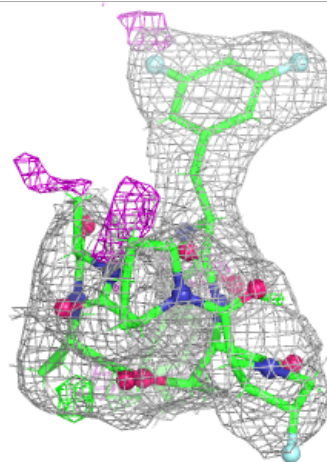
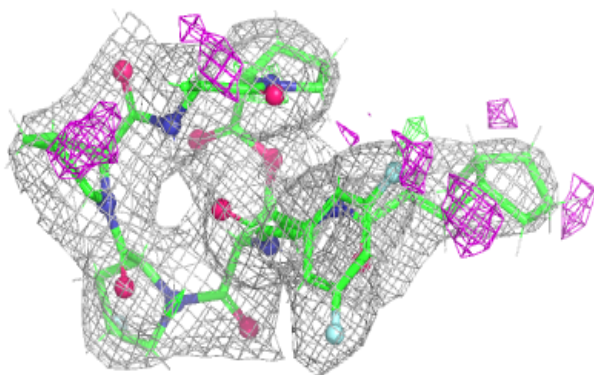
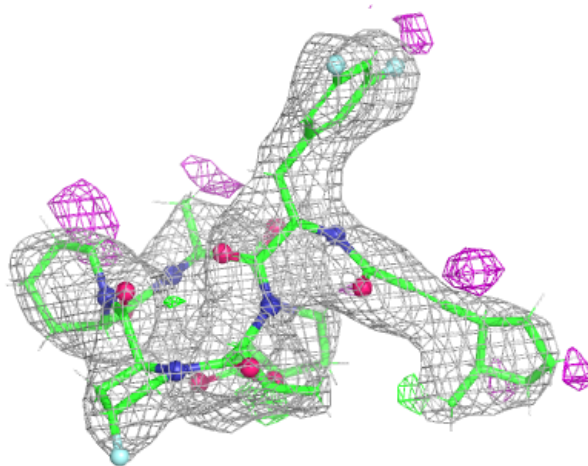
Electron density around A1C9P F 401:

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



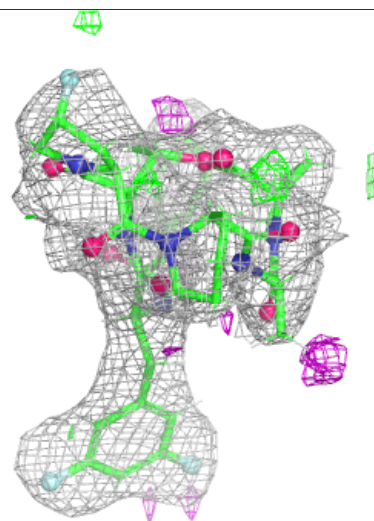
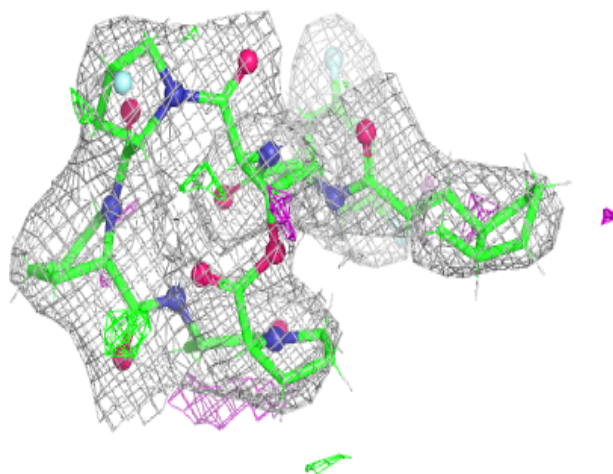
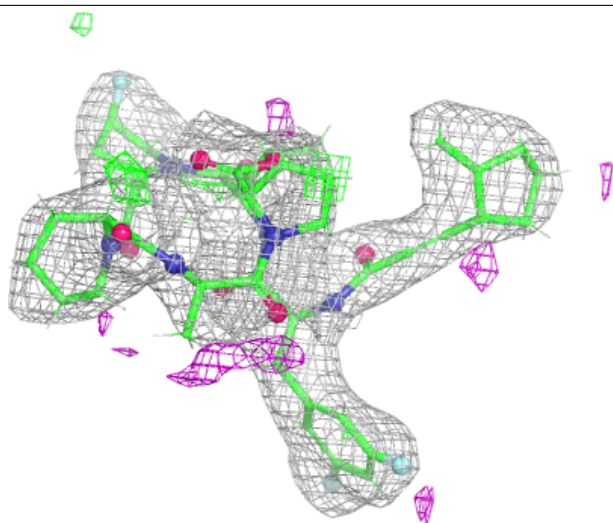
Electron density around A1C9P Q 401:

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and green (positive)



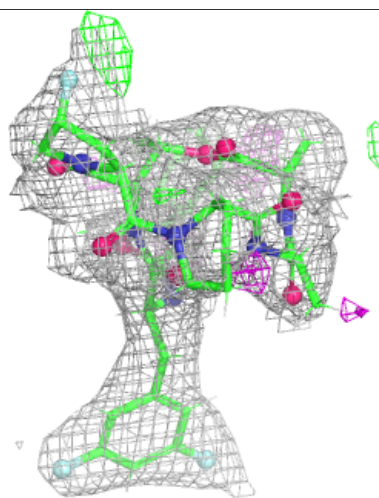
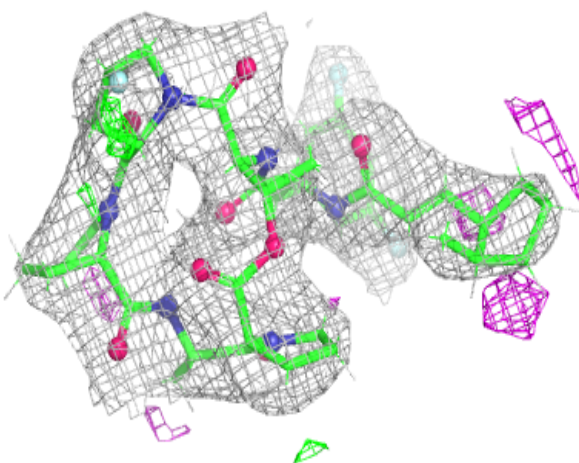
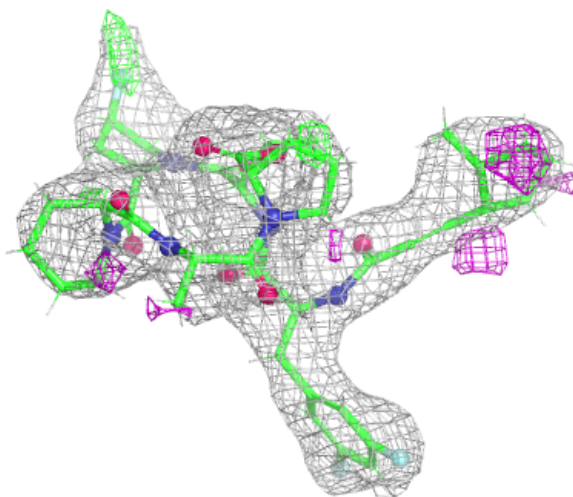
Electron density around A1C9P C 401:

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and green (positive)



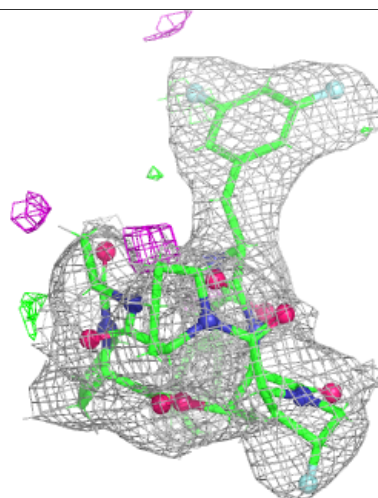
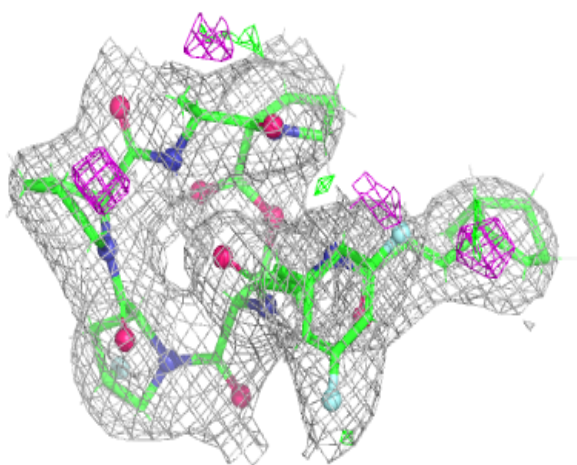
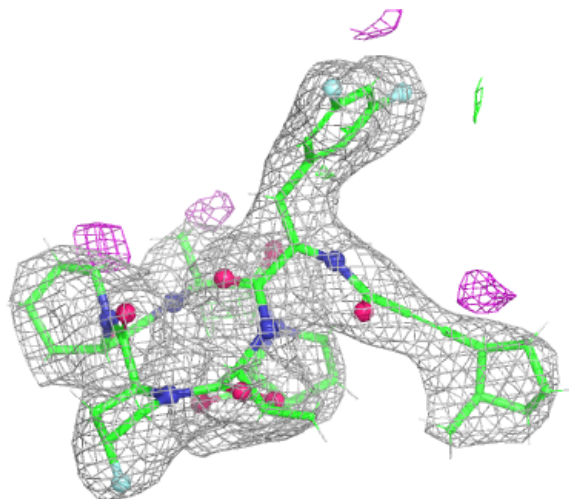
Electron density around A1C9P E 401:

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



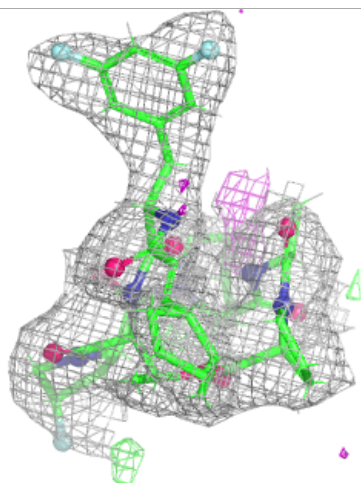
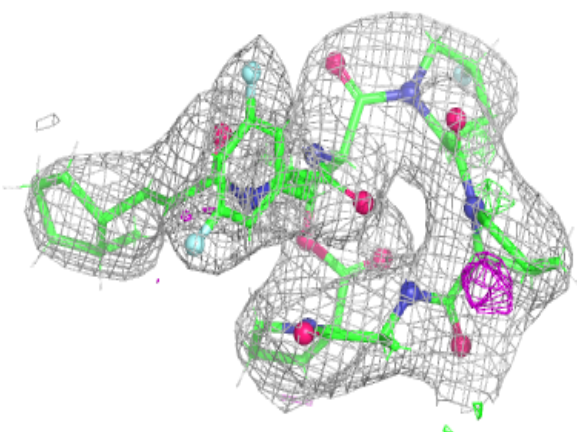
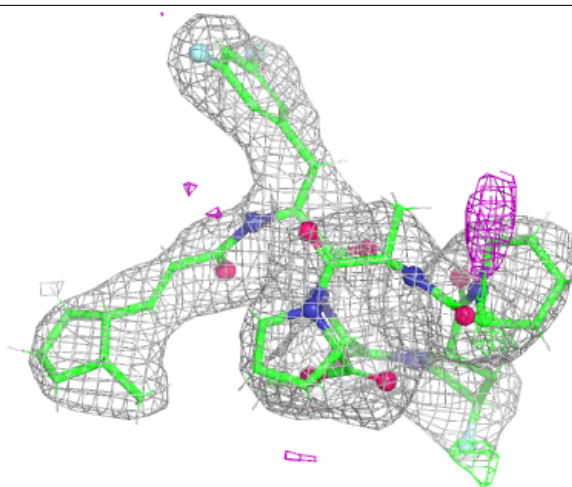
Electron density around A1C9P A 401:

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and green (positive)



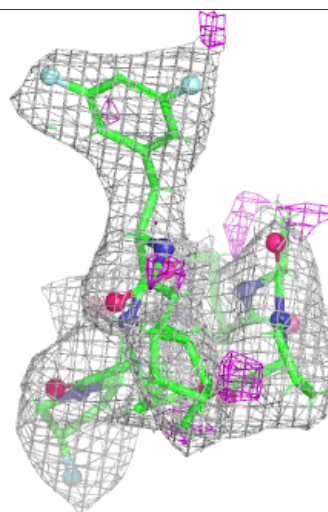
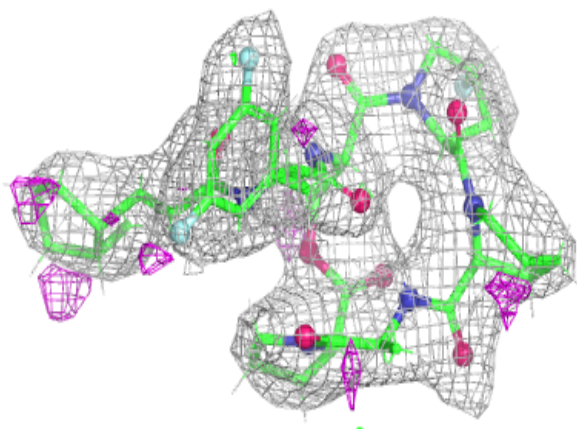
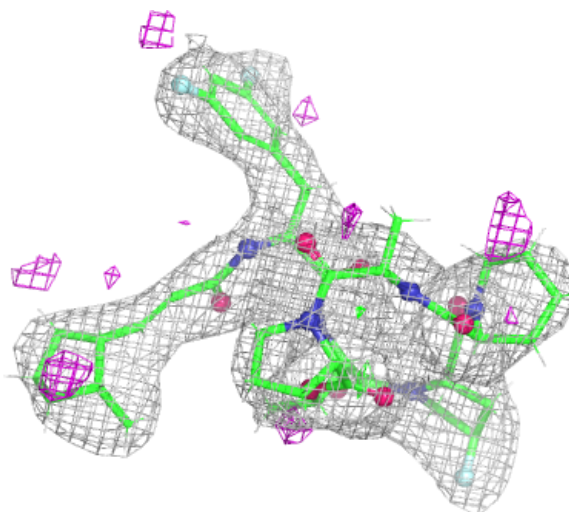
Electron density around A1C9P G 401:

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and green (positive)



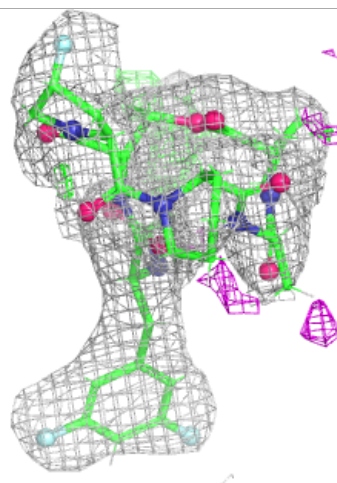
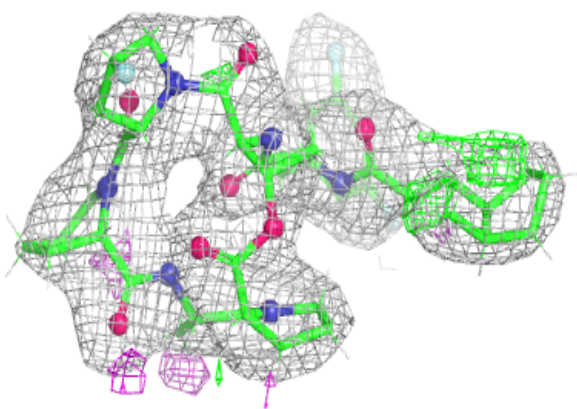
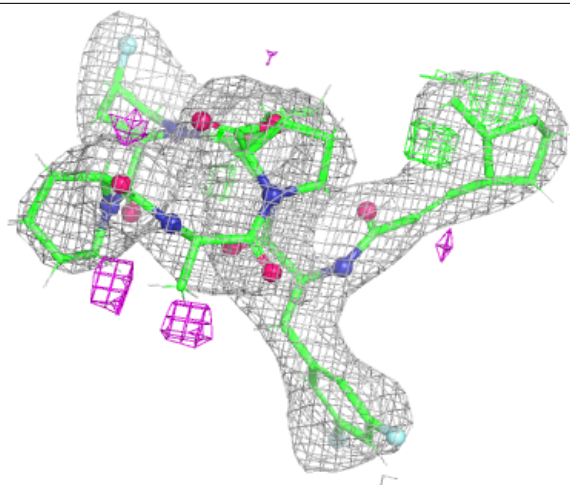
Electron density around A1C9P P 401:

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and green (positive)



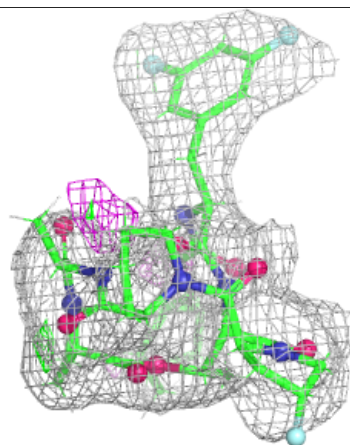
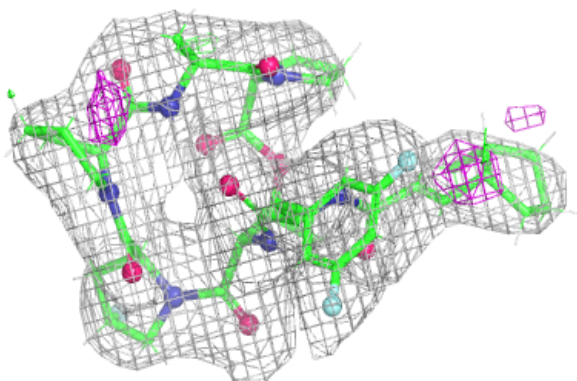
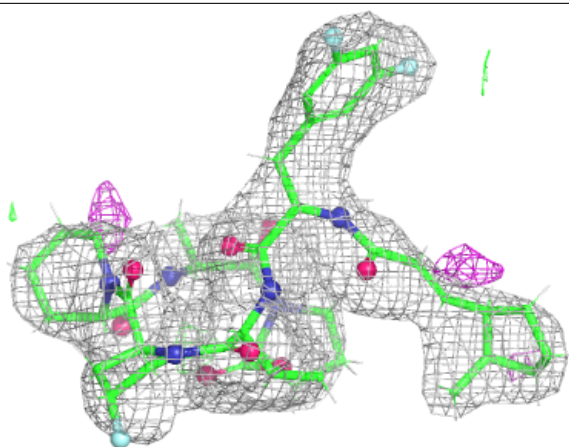
Electron density around A1C9P B 401:

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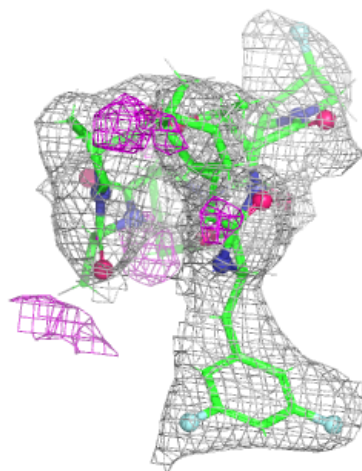
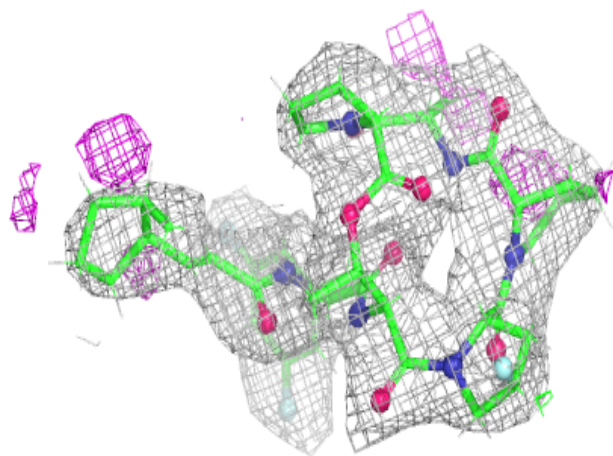
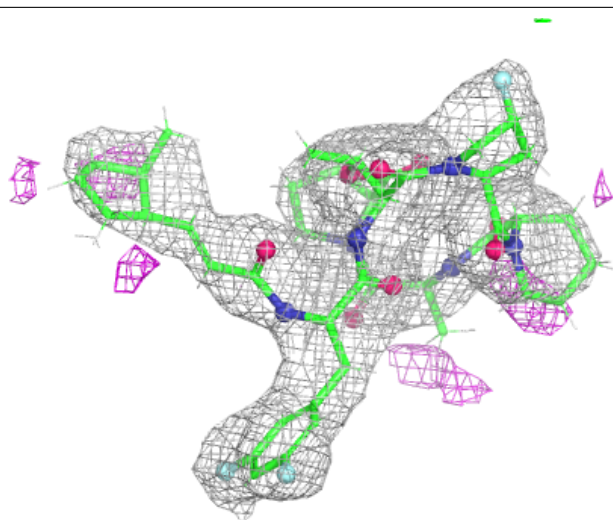
Electron density around A1C9P R 401:

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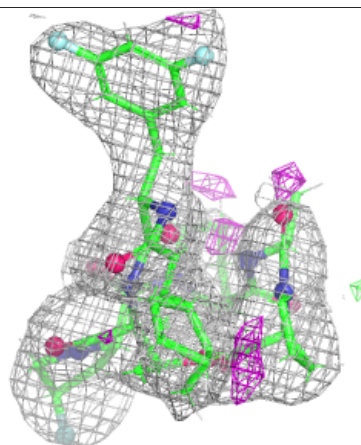
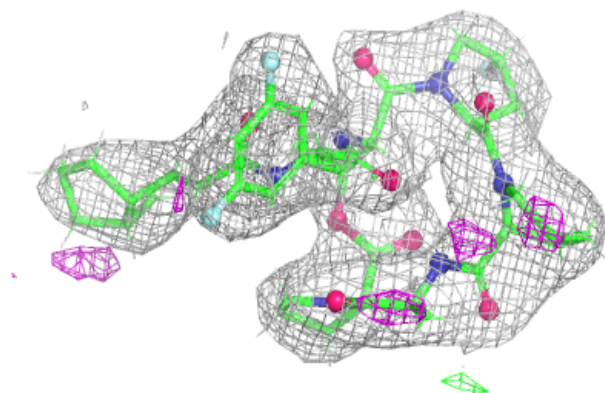
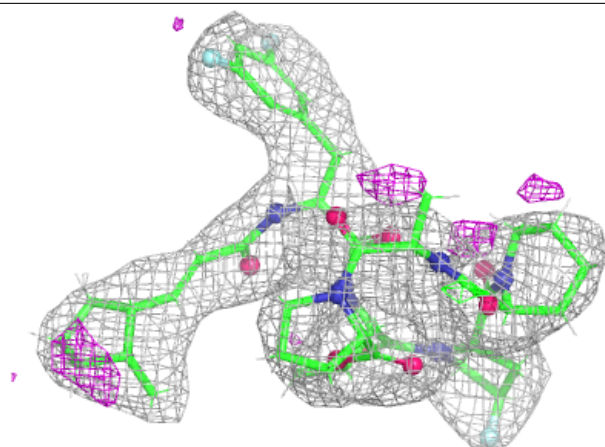
Electron density around A1C9P S 401:

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and green (positive)



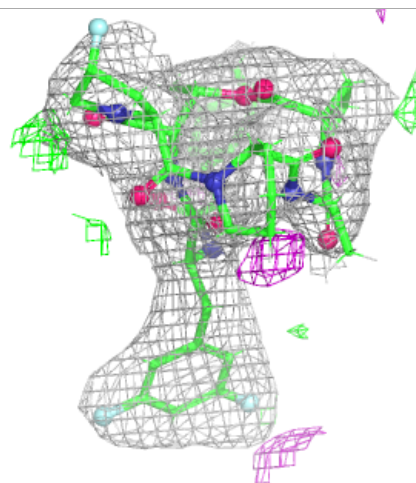
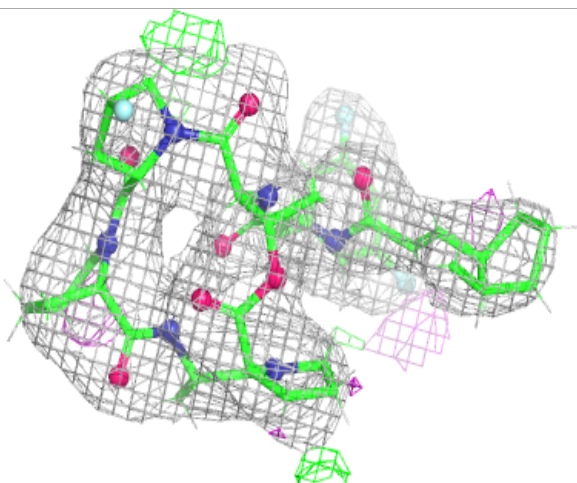
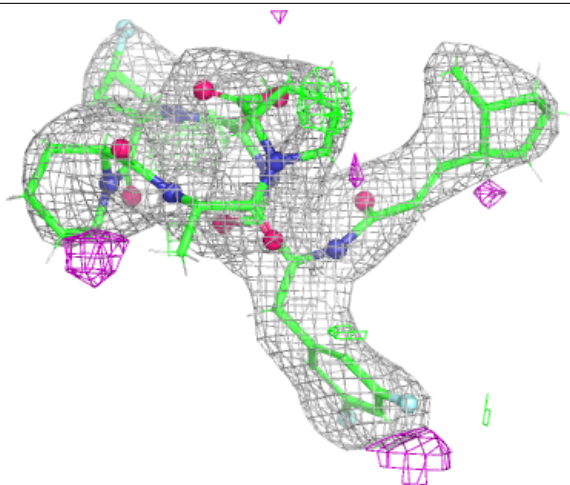
Electron density around A1C9P U 401:

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and green (positive)



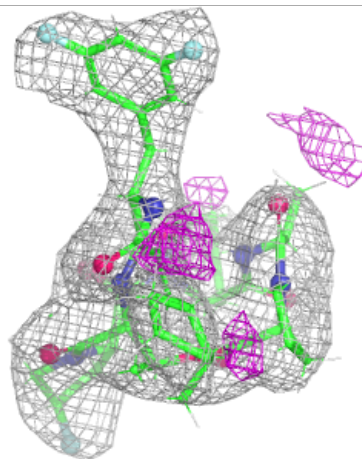
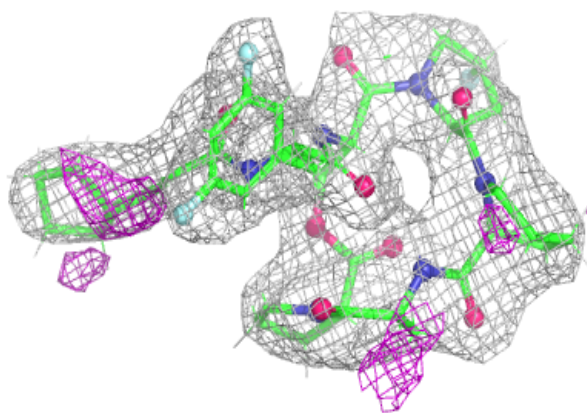
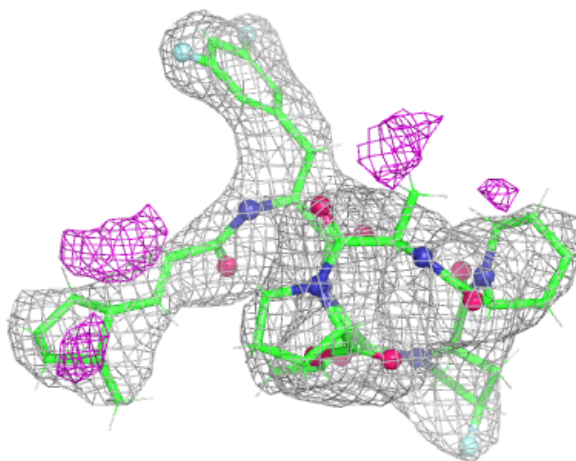
Electron density around A1C9P D 401:

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and green (positive)



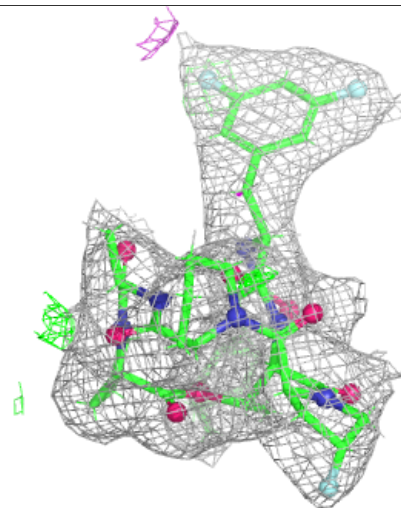
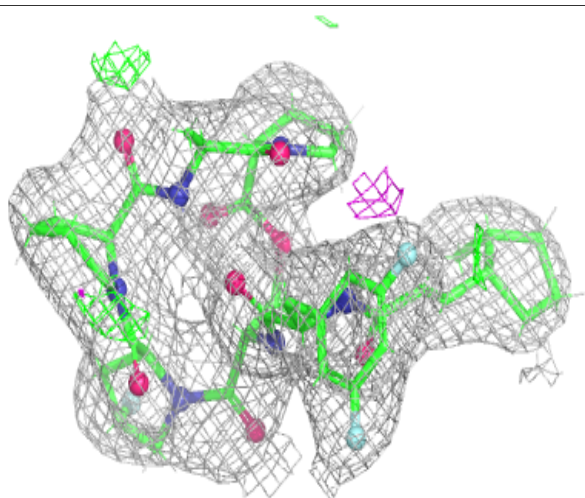
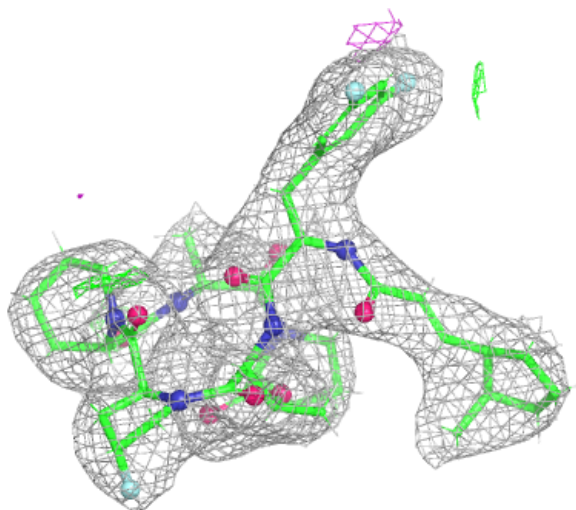
Electron density around A1C9P T 401:

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



Electron density around A1C9P O 401:

$2mF_o-DF_c$ (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.