



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:11 AM UTC

PDB ID : 3MI0 / pdb_00003mi0
Title : Crystal Structure of Mycobacterium Tuberculosis Proteasome at 2.2 Å
Authors : Li, D.; Li, H.
Deposited on : 2010-04-09
Resolution : 2.20 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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

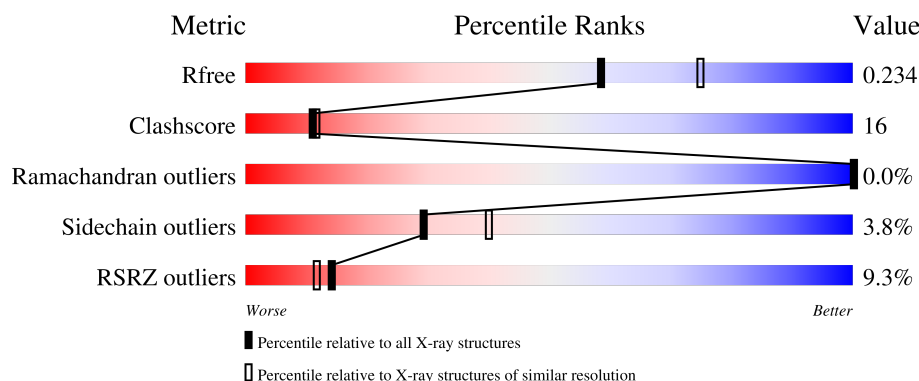
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	1	248	11% 62% 24% • 13%
1	A	248	19% 59% 24% • 13%
1	B	248	11% 59% 23% • 14%
1	D	248	38% 49% 35% • 14%
1	F	248	12% 59% 28% • 11%

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Mol	Chain	Length	Quality of chain
1	I	248	
1	K	248	
1	M	248	
1	O	248	
1	Q	248	
1	S	248	
1	U	248	
1	W	248	
1	Y	248	
2	2	240	
2	C	240	
2	E	240	
2	G	240	
2	H	240	
2	J	240	
2	L	240	
2	N	240	
2	P	240	
2	R	240	
2	T	240	
2	V	240	
2	X	240	
2	Z	240	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DMF	2	108	-	-	X	-
3	DMF	2	112	-	-	X	-
3	DMF	2	4	-	-	X	-
3	DMF	C	103	-	-	X	-
3	DMF	D	251	-	-	X	-
3	DMF	E	20	-	-	X	-
3	DMF	E	75	-	-	X	-
3	DMF	G	119	-	-	X	-
3	DMF	G	12	-	-	X	-
3	DMF	G	64	-	-	X	-
3	DMF	H	43	-	-	X	-
3	DMF	J	123	-	-	X	-
3	DMF	K	250	-	-	X	-
3	DMF	L	97	-	-	X	-
3	DMF	N	104	-	-	X	-
3	DMF	N	118	-	-	X	-
3	DMF	N	22	-	-	X	-
3	DMF	N	90	-	-	X	-
3	DMF	N	93	-	-	X	-
3	DMF	P	107	-	-	X	-
3	DMF	P	14	-	-	X	-
3	DMF	Q	250	-	-	X	-
3	DMF	R	59	-	-	X	-
3	DMF	T	113	-	-	X	-
3	DMF	U	250	-	-	X	-
3	DMF	V	116	-	-	X	-
3	DMF	V	120	-	-	X	-
3	DMF	V	27	-	-	X	-
3	DMF	V	32	-	-	X	-
3	DMF	V	42	-	-	X	-
3	DMF	V	83	-	-	X	-
3	DMF	W	250	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 50080 atoms, of which 0 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 Proteasome subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1654	1035	303	313	3			
1	B	213	Total	C	N	O	S	0	0	0
			1643	1028	301	311	3			
1	D	214	Total	C	N	O	S	0	0	0
			1650	1033	302	312	3			
1	F	220	Total	C	N	O	S	0	0	0
			1699	1068	308	320	3			
1	I	216	Total	C	N	O	S	0	0	0
			1669	1048	304	314	3			
1	K	216	Total	C	N	O	S	0	0	0
			1666	1045	304	314	3			
1	M	216	Total	C	N	O	S	0	0	0
			1666	1045	304	314	3			
1	O	216	Total	C	N	O	S	0	0	0
			1666	1045	304	314	3			
1	Q	215	Total	C	N	O	S	0	0	0
			1658	1039	303	313	3			
1	S	216	Total	C	N	O	S	0	0	0
			1665	1044	304	314	3			
1	U	216	Total	C	N	O	S	0	0	0
			1662	1041	304	314	3			
1	W	216	Total	C	N	O	S	0	0	0
			1669	1048	304	314	3			
1	Y	216	Total	C	N	O	S	0	0	0
			1666	1045	304	314	3			
1	1	215	Total	C	N	O	S	0	0	0
			1658	1039	303	313	3			

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	E	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	G	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	H	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	J	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	L	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	N	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	P	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	R	239	Total	C	N	O	S	0	0	0
			1767	1103	310	349	5			
2	T	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	V	239	Total	C	N	O	S	0	0	0
			1767	1103	310	349	5			
2	X	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	Z	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	2	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	535	HIS	-	expression tag	UNP O33245
C	536	HIS	-	expression tag	UNP O33245
C	537	HIS	-	expression tag	UNP O33245
C	538	HIS	-	expression tag	UNP O33245
C	539	HIS	-	expression tag	UNP O33245
C	540	HIS	-	expression tag	UNP O33245
E	535	HIS	-	expression tag	UNP O33245
E	536	HIS	-	expression tag	UNP O33245
E	537	HIS	-	expression tag	UNP O33245
E	538	HIS	-	expression tag	UNP O33245
E	539	HIS	-	expression tag	UNP O33245
E	540	HIS	-	expression tag	UNP O33245

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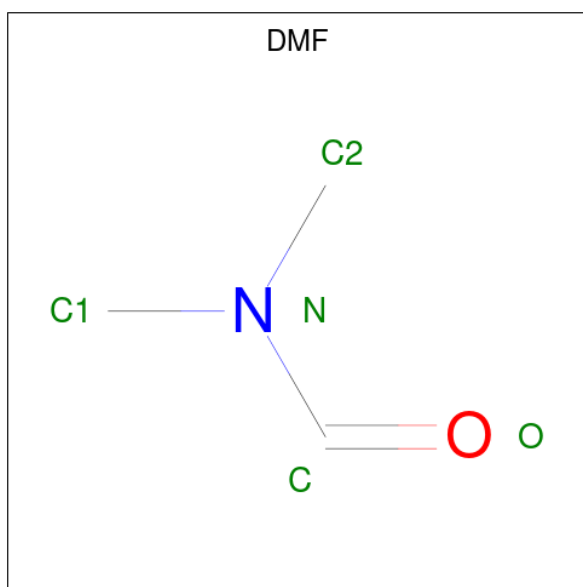
Chain	Residue	Modelled	Actual	Comment	Reference
G	535	HIS	-	expression tag	UNP O33245
G	536	HIS	-	expression tag	UNP O33245
G	537	HIS	-	expression tag	UNP O33245
G	538	HIS	-	expression tag	UNP O33245
G	539	HIS	-	expression tag	UNP O33245
G	540	HIS	-	expression tag	UNP O33245
H	535	HIS	-	expression tag	UNP O33245
H	536	HIS	-	expression tag	UNP O33245
H	537	HIS	-	expression tag	UNP O33245
H	538	HIS	-	expression tag	UNP O33245
H	539	HIS	-	expression tag	UNP O33245
H	540	HIS	-	expression tag	UNP O33245
J	535	HIS	-	expression tag	UNP O33245
J	536	HIS	-	expression tag	UNP O33245
J	537	HIS	-	expression tag	UNP O33245
J	538	HIS	-	expression tag	UNP O33245
J	539	HIS	-	expression tag	UNP O33245
J	540	HIS	-	expression tag	UNP O33245
L	535	HIS	-	expression tag	UNP O33245
L	536	HIS	-	expression tag	UNP O33245
L	537	HIS	-	expression tag	UNP O33245
L	538	HIS	-	expression tag	UNP O33245
L	539	HIS	-	expression tag	UNP O33245
L	540	HIS	-	expression tag	UNP O33245
N	535	HIS	-	expression tag	UNP O33245
N	536	HIS	-	expression tag	UNP O33245
N	537	HIS	-	expression tag	UNP O33245
N	538	HIS	-	expression tag	UNP O33245
N	539	HIS	-	expression tag	UNP O33245
N	540	HIS	-	expression tag	UNP O33245
P	535	HIS	-	expression tag	UNP O33245
P	536	HIS	-	expression tag	UNP O33245
P	537	HIS	-	expression tag	UNP O33245
P	538	HIS	-	expression tag	UNP O33245
P	539	HIS	-	expression tag	UNP O33245
P	540	HIS	-	expression tag	UNP O33245
R	535	HIS	-	expression tag	UNP O33245
R	536	HIS	-	expression tag	UNP O33245
R	537	HIS	-	expression tag	UNP O33245
R	538	HIS	-	expression tag	UNP O33245
R	539	HIS	-	expression tag	UNP O33245
R	540	HIS	-	expression tag	UNP O33245

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Chain	Residue	Modelled	Actual	Comment	Reference
T	535	HIS	-	expression tag	UNP O33245
T	536	HIS	-	expression tag	UNP O33245
T	537	HIS	-	expression tag	UNP O33245
T	538	HIS	-	expression tag	UNP O33245
T	539	HIS	-	expression tag	UNP O33245
T	540	HIS	-	expression tag	UNP O33245
V	535	HIS	-	expression tag	UNP O33245
V	536	HIS	-	expression tag	UNP O33245
V	537	HIS	-	expression tag	UNP O33245
V	538	HIS	-	expression tag	UNP O33245
V	539	HIS	-	expression tag	UNP O33245
V	540	HIS	-	expression tag	UNP O33245
X	535	HIS	-	expression tag	UNP O33245
X	536	HIS	-	expression tag	UNP O33245
X	537	HIS	-	expression tag	UNP O33245
X	538	HIS	-	expression tag	UNP O33245
X	539	HIS	-	expression tag	UNP O33245
X	540	HIS	-	expression tag	UNP O33245
Z	535	HIS	-	expression tag	UNP O33245
Z	536	HIS	-	expression tag	UNP O33245
Z	537	HIS	-	expression tag	UNP O33245
Z	538	HIS	-	expression tag	UNP O33245
Z	539	HIS	-	expression tag	UNP O33245
Z	540	HIS	-	expression tag	UNP O33245
2	535	HIS	-	expression tag	UNP O33245
2	536	HIS	-	expression tag	UNP O33245
2	537	HIS	-	expression tag	UNP O33245
2	538	HIS	-	expression tag	UNP O33245
2	539	HIS	-	expression tag	UNP O33245
2	540	HIS	-	expression tag	UNP O33245

- Molecule 3 is DIMETHYLFORMAMIDE (CCD ID: DMF) (formula: C₃H₇NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			5	3	1	1		
3	A	1	Total	C	N	O	0	0
			5	3	1	1		
3	B	1	Total	C	N	O	0	0
			5	3	1	1		
3	B	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	D	1	Total	C	N	O	0	0
			5	3	1	1		
3	D	1	Total	C	N	O	0	0
			5	3	1	1		
3	D	1	Total	C	N	O	0	0
			5	3	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			5	3	1	1		
3	D	1	Total	C	N	O	0	0
			5	3	1	1		
3	E	1	Total	C	N	O	0	0
			5	3	1	1		
3	E	1	Total	C	N	O	0	0
			5	3	1	1		
3	E	1	Total	C	N	O	0	0
			5	3	1	1		
3	E	1	Total	C	N	O	0	0
			5	3	1	1		
3	E	1	Total	C	N	O	0	0
			5	3	1	1		
3	F	1	Total	C	N	O	0	0
			5	3	1	1		
3	F	1	Total	C	N	O	0	0
			5	3	1	1		
3	F	1	Total	C	N	O	0	0
			5	3	1	1		
3	G	1	Total	C	N	O	0	0
			5	3	1	1		
3	G	1	Total	C	N	O	0	0
			5	3	1	1		
3	G	1	Total	C	N	O	0	0
			5	3	1	1		
3	G	1	Total	C	N	O	0	0
			5	3	1	1		
3	G	1	Total	C	N	O	0	0
			5	3	1	1		
3	G	1	Total	C	N	O	0	0
			5	3	1	1		
3	H	1	Total	C	N	O	0	0
			5	3	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total 5	C 3	N 1	O 1	0	0
3	H	1	Total 5	C 3	N 1	O 1	0	0
3	H	1	Total 5	C 3	N 1	O 1	0	0
3	H	1	Total 5	C 3	N 1	O 1	0	0
3	H	1	Total 5	C 3	N 1	O 1	0	0
3	I	1	Total 5	C 3	N 1	O 1	0	0
3	I	1	Total 5	C 3	N 1	O 1	0	0
3	J	1	Total 5	C 3	N 1	O 1	0	0
3	J	1	Total 5	C 3	N 1	O 1	0	0
3	J	1	Total 5	C 3	N 1	O 1	0	0
3	K	1	Total 5	C 3	N 1	O 1	0	0
3	K	1	Total 5	C 3	N 1	O 1	0	0
3	K	1	Total 5	C 3	N 1	O 1	0	0
3	K	1	Total 5	C 3	N 1	O 1	0	0
3	L	1	Total 5	C 3	N 1	O 1	0	0
3	L	1	Total 5	C 3	N 1	O 1	0	0
3	L	1	Total 5	C 3	N 1	O 1	0	0
3	L	1	Total 5	C 3	N 1	O 1	0	0
3	M	1	Total 5	C 3	N 1	O 1	0	0
3	M	1	Total 5	C 3	N 1	O 1	0	0
3	M	1	Total 5	C 3	N 1	O 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	M	1	Total	C	N	O	0	0
			5	3	1	1		
3	N	1	Total	C	N	O	0	0
			5	3	1	1		
3	N	1	Total	C	N	O	0	0
			5	3	1	1		
3	N	1	Total	C	N	O	0	0
			5	3	1	1		
3	N	1	Total	C	N	O	0	0
			5	3	1	1		
3	O	1	Total	C	N	O	0	0
			5	3	1	1		
3	O	1	Total	C	N	O	0	0
			5	3	1	1		
3	O	1	Total	C	N	O	0	0
			5	3	1	1		
3	P	1	Total	C	N	O	0	0
			5	3	1	1		
3	P	1	Total	C	N	O	0	0
			5	3	1	1		
3	P	1	Total	C	N	O	0	0
			5	3	1	1		
3	P	1	Total	C	N	O	0	0
			5	3	1	1		
3	P	1	Total	C	N	O	0	0
			5	3	1	1		
3	P	1	Total	C	N	O	0	0
			5	3	1	1		
3	P	1	Total	C	N	O	0	0
			5	3	1	1		
3	Q	1	Total	C	N	O	0	0
			5	3	1	1		
3	Q	1	Total	C	N	O	0	0
			5	3	1	1		
3	Q	1	Total	C	N	O	0	0
			5	3	1	1		
3	R	1	Total	C	N	O	0	0
			5	3	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	R	1	Total 5	C 3	N 1	O 1	0	0
3	R	1	Total 5	C 3	N 1	O 1	0	0
3	R	1	Total 5	C 3	N 1	O 1	0	0
3	R	1	Total 5	C 3	N 1	O 1	0	0
3	S	1	Total 5	C 3	N 1	O 1	0	0
3	S	1	Total 5	C 3	N 1	O 1	0	0
3	T	1	Total 5	C 3	N 1	O 1	0	0
3	T	1	Total 5	C 3	N 1	O 1	0	0
3	T	1	Total 5	C 3	N 1	O 1	0	0
3	T	1	Total 5	C 3	N 1	O 1	0	0
3	T	1	Total 5	C 3	N 1	O 1	0	0
3	T	1	Total 5	C 3	N 1	O 1	0	0
3	T	1	Total 5	C 3	N 1	O 1	0	0
3	U	1	Total 5	C 3	N 1	O 1	0	0
3	U	1	Total 5	C 3	N 1	O 1	0	0
3	V	1	Total 5	C 3	N 1	O 1	0	0
3	V	1	Total 5	C 3	N 1	O 1	0	0
3	V	1	Total 5	C 3	N 1	O 1	0	0
3	V	1	Total 5	C 3	N 1	O 1	0	0
3	V	1	Total 5	C 3	N 1	O 1	0	0
3	V	1	Total 5	C 3	N 1	O 1	0	0
3	V	1	Total 5	C 3	N 1	O 1	0	0

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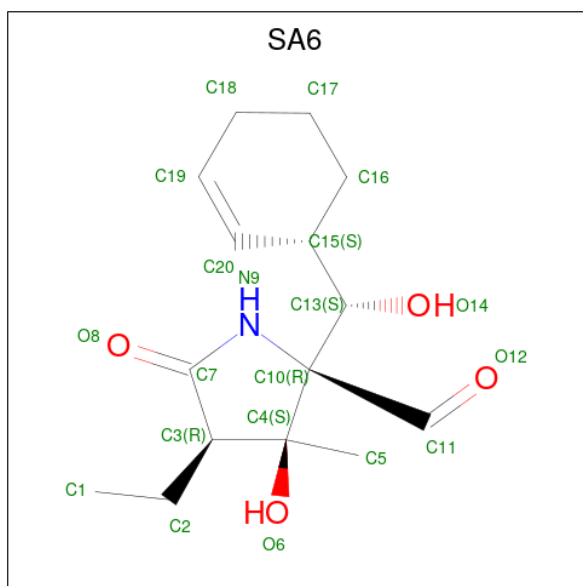
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	V	1	Total 5	C 3	N 1	O 1	0	0
3	V	1	Total 5	C 3	N 1	O 1	0	0
3	W	1	Total 5	C 3	N 1	O 1	0	0
3	W	1	Total 5	C 3	N 1	O 1	0	0
3	X	1	Total 5	C 3	N 1	O 1	0	0
3	X	1	Total 5	C 3	N 1	O 1	0	0
3	X	1	Total 5	C 3	N 1	O 1	0	0
3	X	1	Total 5	C 3	N 1	O 1	0	0
3	X	1	Total 5	C 3	N 1	O 1	0	0
3	Y	1	Total 5	C 3	N 1	O 1	0	0
3	Y	1	Total 5	C 3	N 1	O 1	0	0
3	Y	1	Total 5	C 3	N 1	O 1	0	0
3	Z	1	Total 5	C 3	N 1	O 1	0	0
3	Z	1	Total 5	C 3	N 1	O 1	0	0
3	Z	1	Total 5	C 3	N 1	O 1	0	0
3	Z	1	Total 5	C 3	N 1	O 1	0	0
3	1	1	Total 5	C 3	N 1	O 1	0	0
3	2	1	Total 5	C 3	N 1	O 1	0	0
3	2	1	Total 5	C 3	N 1	O 1	0	0
3	2	1	Total 5	C 3	N 1	O 1	0	0
3	2	1	Total 5	C 3	N 1	O 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	2	1	Total	C	N	O	0	0
			5	3	1	1		
3	2	1	Total	C	N	O	0	0
			5	3	1	1		
3	2	1	Total	C	N	O	0	0
			5	3	1	1		
3	2	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 4 is (2R,3S,4R)-2-[(S)-(1S)-cyclohex-2-en-1-yl(hydroxy)methyl]-4-ethyl-3-hydroxy-3-methyl-5-oxopyrrolidine-2-carbaldehyde (CCD ID: SA6) (formula: C₁₅H₂₃NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			20	15	1	4		
4	E	1	Total	C	N	O	0	0
			20	15	1	4		
4	G	1	Total	C	N	O	0	0
			20	15	1	4		
4	H	1	Total	C	N	O	0	0
			20	15	1	4		
4	J	1	Total	C	N	O	0	0
			20	15	1	4		
4	L	1	Total	C	N	O	0	0
			20	15	1	4		
4	N	1	Total	C	N	O	0	0
			20	15	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	P	1	Total	C	N	O	0	0
			20	15	1	4		
4	R	1	Total	C	N	O	0	0
			20	15	1	4		
4	T	1	Total	C	N	O	0	0
			20	15	1	4		
4	V	1	Total	C	N	O	0	0
			20	15	1	4		
4	X	1	Total	C	N	O	0	0
			20	15	1	4		
4	Z	1	Total	C	N	O	0	0
			20	15	1	4		
4	2	1	Total	C	N	O	0	0
			20	15	1	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	43	Total	O	0	0
			43	43		
5	B	41	Total	O	0	0
			41	41		
5	C	163	Total	O	0	0
			163	163		
5	D	40	Total	O	0	0
			40	40		
5	E	166	Total	O	0	0
			166	166		
5	F	58	Total	O	0	0
			58	58		
5	G	131	Total	O	0	0
			131	131		
5	H	148	Total	O	0	0
			148	148		
5	I	52	Total	O	0	0
			52	52		
5	J	142	Total	O	0	0
			142	142		
5	K	45	Total	O	0	0
			45	45		
5	L	153	Total	O	0	0
			153	153		

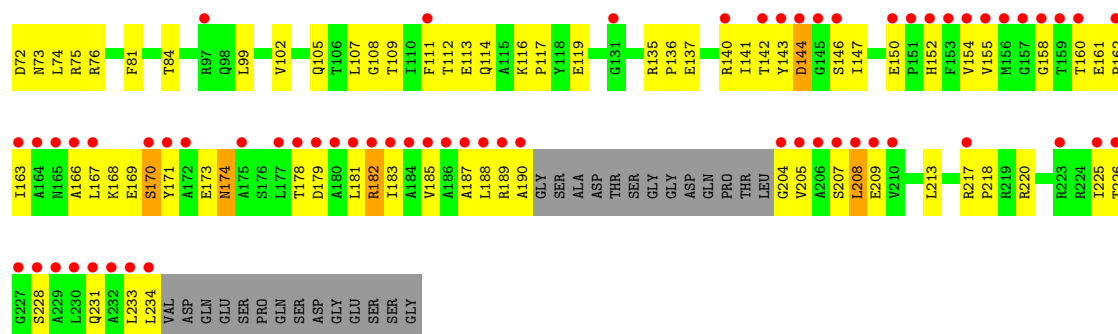
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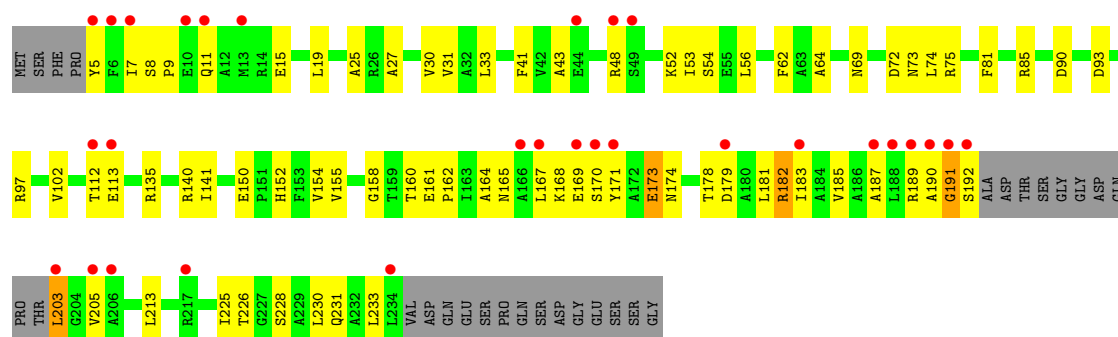
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	40	Total 40	O 40	0	0
5	N	154	Total 154	O 154	0	0
5	O	47	Total 47	O 47	0	0
5	P	139	Total 139	O 139	0	0
5	Q	38	Total 38	O 38	0	0
5	R	170	Total 170	O 170	0	0
5	S	42	Total 42	O 42	0	0
5	T	116	Total 116	O 116	0	0
5	U	49	Total 49	O 49	0	0
5	V	177	Total 177	O 177	0	0
5	W	35	Total 35	O 35	0	0
5	X	150	Total 150	O 150	0	0
5	Y	28	Total 28	O 28	0	0
5	Z	123	Total 123	O 123	0	0
5	1	47	Total 47	O 47	0	0
5	2	143	Total 143	O 143	0	0

- Molecule 1: Proteasome subunit alpha

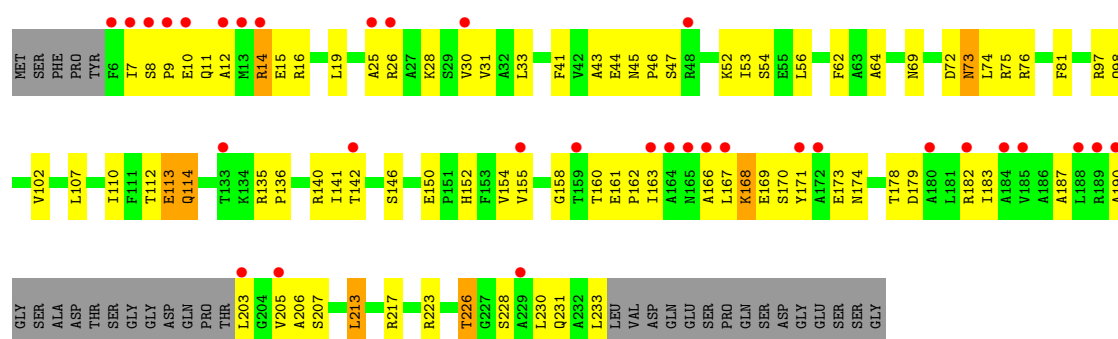




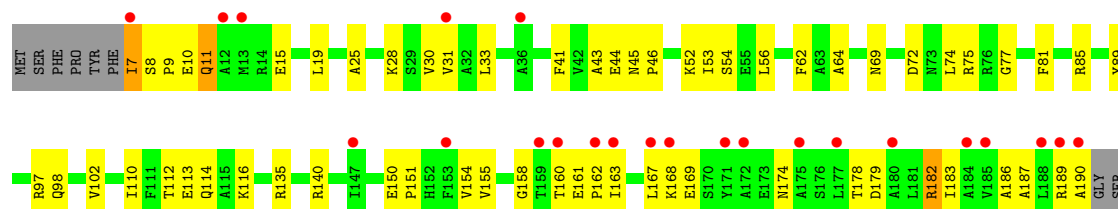
• Molecule 1: Proteasome subunit alpha



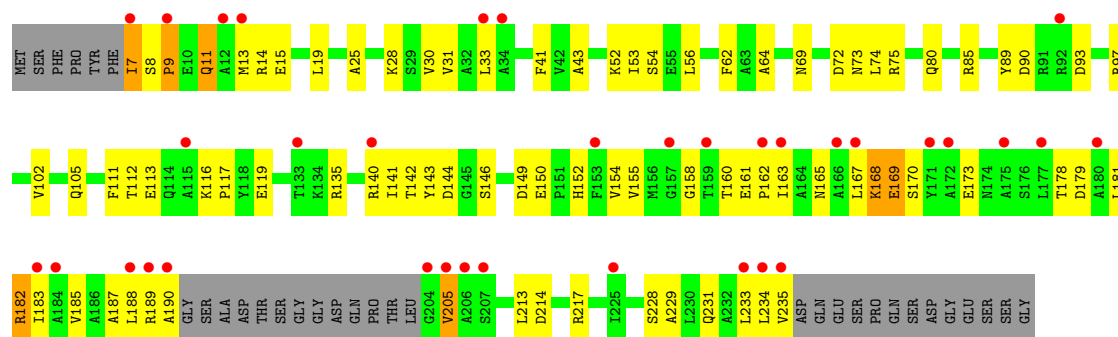
• Molecule 1: Proteasome subunit alpha



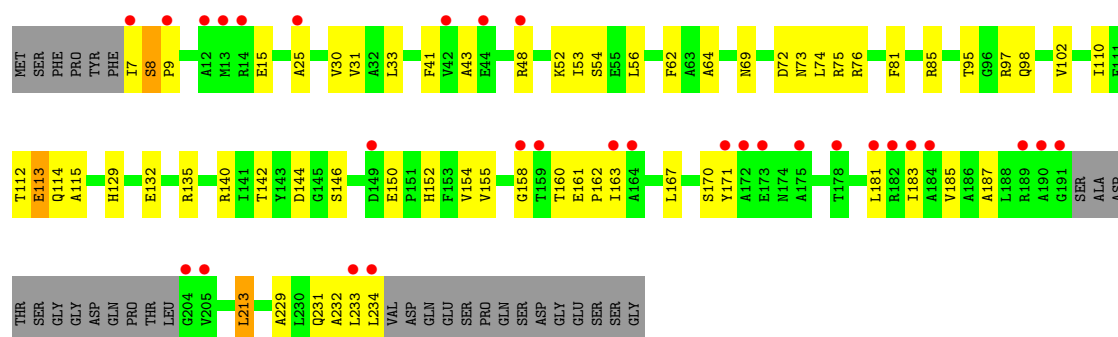
• Molecule 1: Proteasome subunit alpha



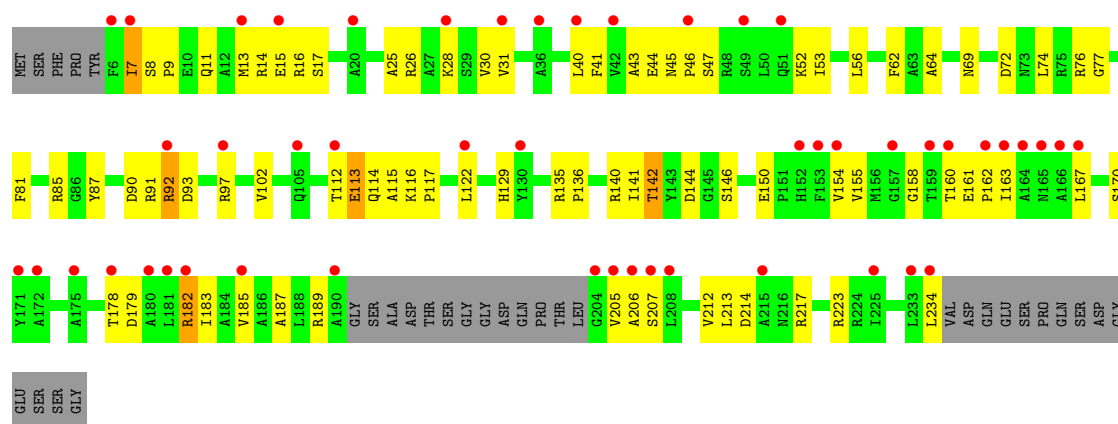




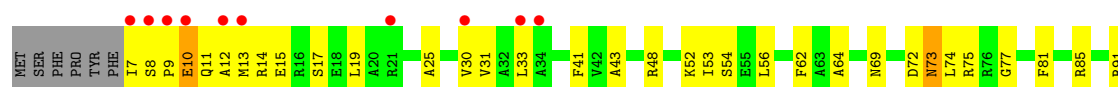
• Molecule 1: Proteasome subunit alpha

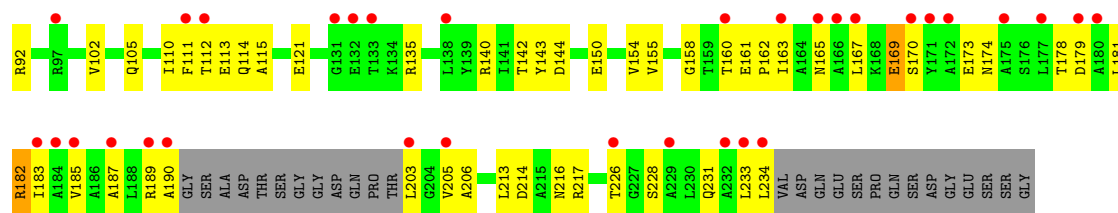


• Molecule 1: Proteasome subunit alpha

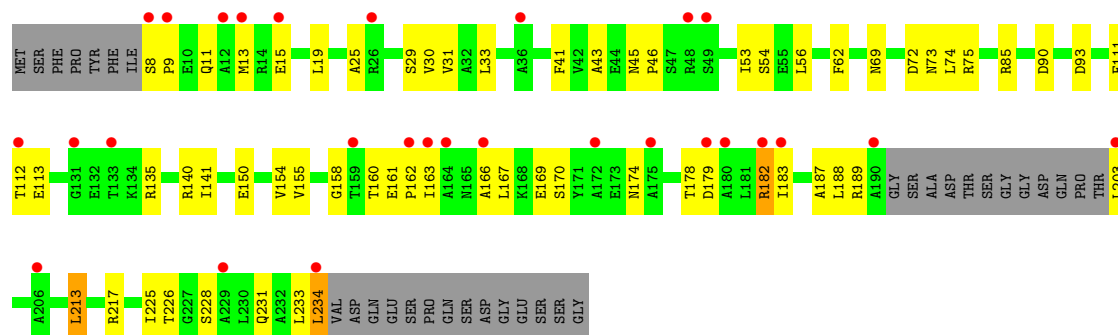


• Molecule 1: Proteasome subunit alpha

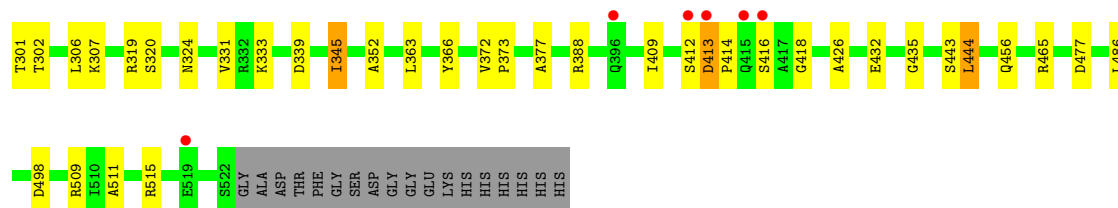
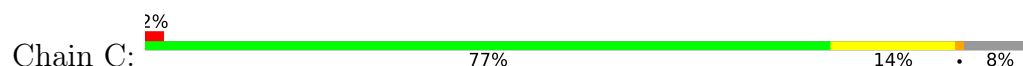




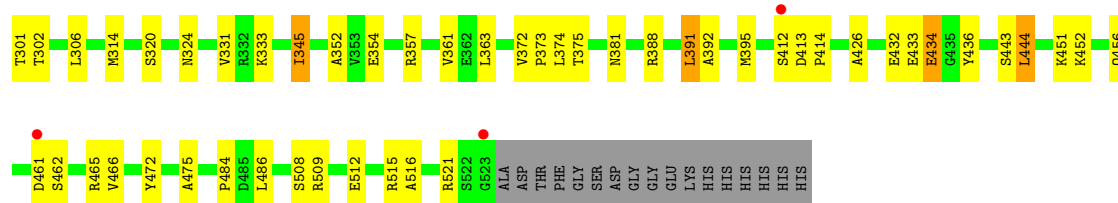
• Molecule 1: Proteasome subunit alpha



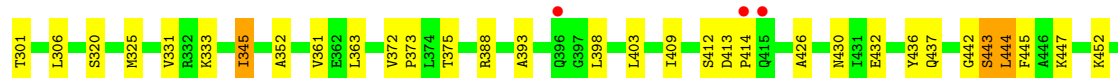
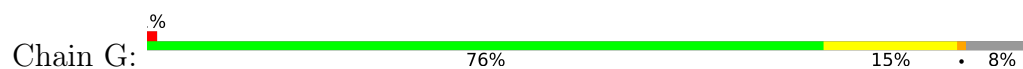
• Molecule 2: Proteasome subunit beta

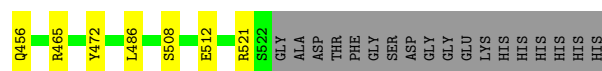


• Molecule 2: Proteasome subunit beta

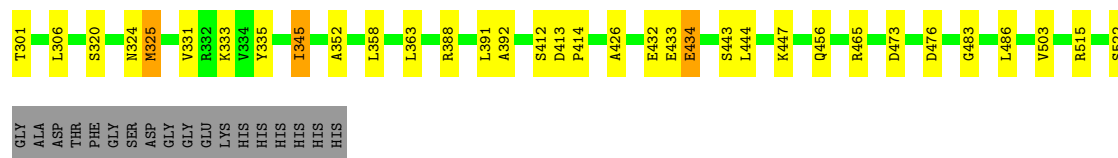
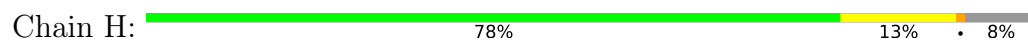


• Molecule 2: Proteasome subunit beta

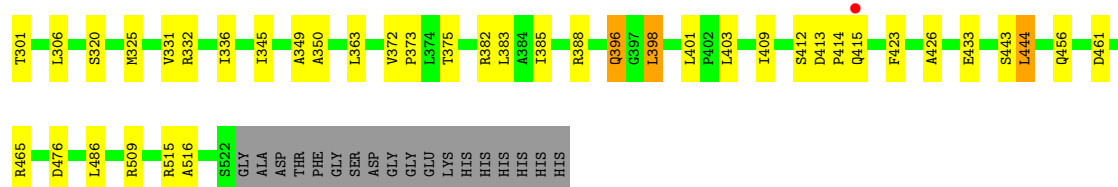




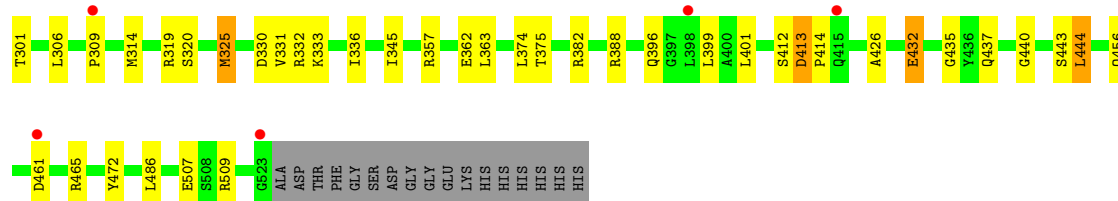
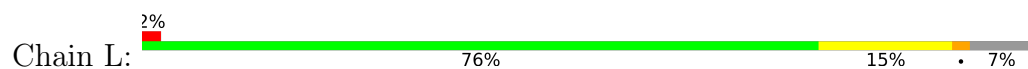
• Molecule 2: Proteasome subunit beta



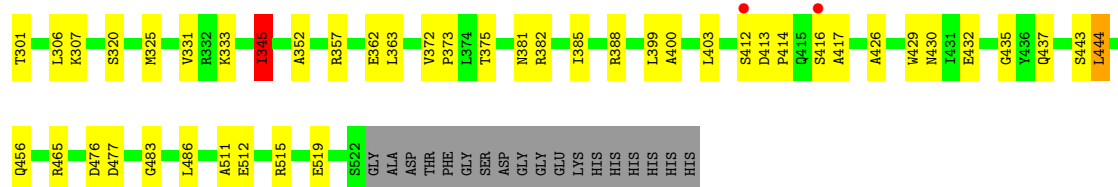
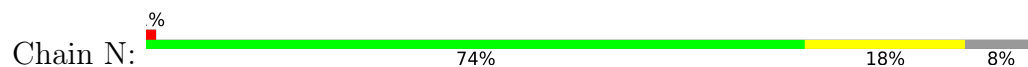
• Molecule 2: Proteasome subunit beta



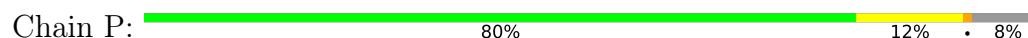
• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta



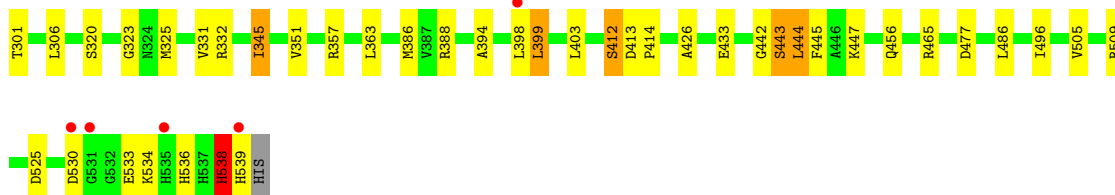
• Molecule 2: Proteasome subunit beta



THR
PHE
GLY
SER
ASP
GLY
GLY
GLY
LYS
HIS
HIS
HIS
HIS
HIS

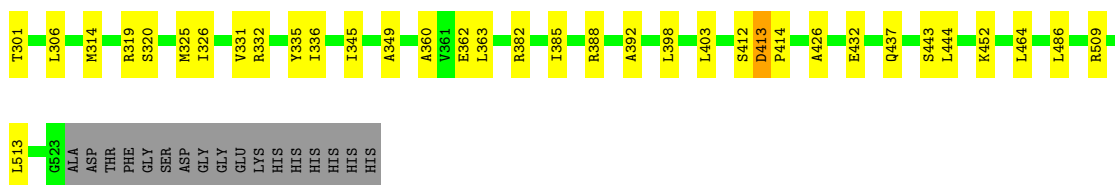
• Molecule 2: Proteasome subunit beta

Chain R:  2% 82% 15%



• Molecule 2: Proteasome subunit beta

Chain T:  78% 14% 7%



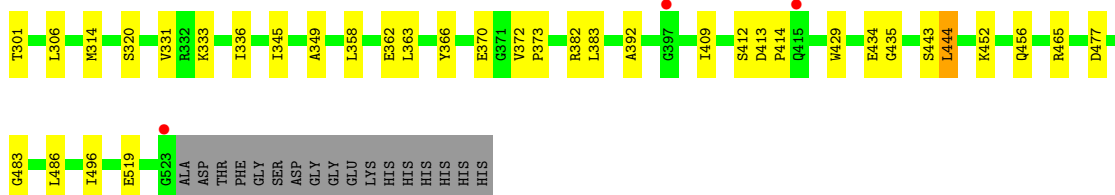
• Molecule 2: Proteasome subunit beta

Chain V:  2% 82% 17%



• Molecule 2: Proteasome subunit beta

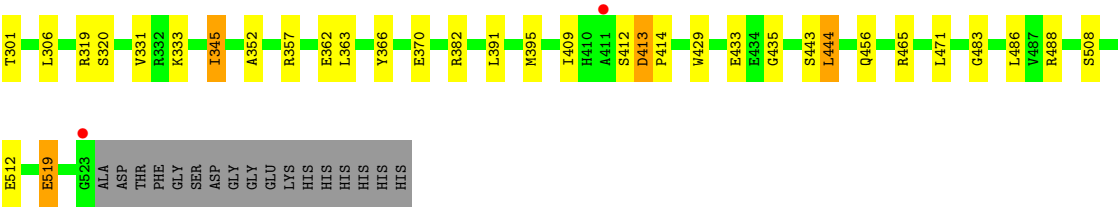
Chain X:  78% 15% 7%



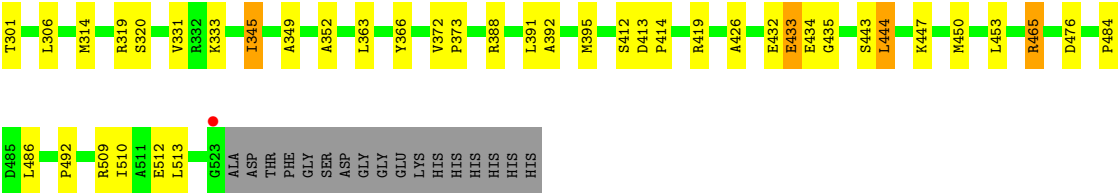
• Molecule 2: Proteasome subunit beta

Chain Z:  79% 12% 7%





● Molecule 2: Proteasome subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	170.37Å 118.44Å 195.25Å 90.00° 113.02° 90.00°	Depositor
Resolution (Å)	24.95 – 2.20 24.95 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.0 (24.95-2.20) 92.0 (24.95-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.11Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.234 0.205 , 0.234	Depositor DCC
R_{free} test set	18918 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	50080	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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: DMF, SA6

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	1	0.63	0/1683	0.99	3/2274 (0.1%)
1	A	0.58	0/1679	0.97	5/2268 (0.2%)
1	B	0.64	0/1668	0.99	4/2253 (0.2%)
1	D	0.55	0/1675	0.98	5/2263 (0.2%)
1	F	0.63	0/1726	1.00	4/2332 (0.2%)
1	I	0.62	0/1695	0.99	6/2290 (0.3%)
1	K	0.61	0/1691	0.99	6/2285 (0.3%)
1	M	0.61	0/1691	1.00	7/2285 (0.3%)
1	O	0.65	1/1691 (0.1%)	0.99	5/2285 (0.2%)
1	Q	0.58	0/1683	0.97	5/2274 (0.2%)
1	S	0.61	0/1690	1.00	4/2284 (0.2%)
1	U	0.60	0/1687	1.02	6/2279 (0.3%)
1	W	0.53	0/1695	0.96	2/2290 (0.1%)
1	Y	0.59	0/1691	1.04	6/2285 (0.3%)
2	2	0.83	2/1666 (0.1%)	1.05	6/2259 (0.3%)
2	C	0.89	0/1662	1.08	5/2254 (0.2%)
2	E	0.95	1/1666 (0.1%)	1.08	6/2259 (0.3%)
2	G	0.84	0/1662	1.05	5/2254 (0.2%)
2	H	0.90	2/1662 (0.1%)	1.06	4/2254 (0.2%)
2	J	0.89	0/1662	1.07	6/2254 (0.3%)
2	L	0.88	2/1666 (0.1%)	1.08	8/2259 (0.4%)
2	N	0.88	1/1662 (0.1%)	1.06	6/2254 (0.3%)
2	P	0.87	1/1662 (0.1%)	1.07	5/2254 (0.2%)
2	R	0.88	0/1797	1.09	7/2435 (0.3%)
2	T	0.85	2/1666 (0.1%)	1.06	6/2259 (0.3%)
2	V	0.88	1/1797 (0.1%)	1.05	6/2435 (0.2%)
2	X	0.83	1/1666 (0.1%)	1.07	6/2259 (0.3%)
2	Z	0.79	0/1666	1.03	5/2259 (0.2%)
All	All	0.75	14/47207 (0.0%)	1.03	149/63895 (0.2%)

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	314	MET	SD-CE	-8.32	1.58	1.79
1	O	7	ILE	C-N	7.92	1.44	1.33
2	L	325	MET	SD-CE	7.29	1.97	1.79
2	L	314	MET	SD-CE	-6.71	1.62	1.79
2	T	325	MET	SD-CE	6.42	1.95	1.79

The worst 5 of 149 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	538	HIS	N-CA-C	-10.33	96.61	110.55
1	Y	169	GLU	N-CA-C	8.88	120.73	111.14
2	H	443	SER	N-CA-C	8.08	120.08	111.28
2	V	413	ASP	CA-C-N	7.83	128.25	119.32
2	V	413	ASP	C-N-CA	7.83	128.25	119.32

There are no chirality outliers.

There are no planarity outliers.

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	1	1658	0	1659	59	0
1	A	1654	0	1651	70	0
1	B	1643	0	1639	82	0
1	D	1650	0	1648	102	0
1	F	1699	0	1696	69	0
1	I	1669	0	1668	98	0
1	K	1666	0	1670	70	0
1	M	1666	0	1670	78	0
1	O	1666	0	1670	67	0
1	Q	1658	0	1659	84	0
1	S	1665	0	1668	90	0
1	U	1662	0	1662	52	0
1	W	1669	0	1668	71	0
1	Y	1666	0	1670	83	0
2	2	1642	0	1632	40	0
2	C	1638	0	1629	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1642	0	1632	51	0
2	G	1638	0	1629	43	0
2	H	1638	0	1629	35	0
2	J	1638	0	1629	44	0
2	L	1642	0	1632	32	0
2	N	1638	0	1629	47	0
2	P	1638	0	1629	31	0
2	R	1767	0	1729	45	0
2	T	1642	0	1632	22	0
2	V	1767	0	1729	42	0
2	X	1642	0	1632	26	0
2	Z	1642	0	1632	25	0
3	1	5	0	7	0	0
3	2	40	0	56	28	0
3	A	10	0	14	1	0
3	B	10	0	14	2	0
3	C	35	0	49	16	0
3	D	25	0	35	7	0
3	E	30	0	42	16	0
3	F	15	0	21	1	0
3	G	45	0	63	31	0
3	H	30	0	42	12	0
3	I	10	0	14	2	0
3	J	15	0	21	7	0
3	K	20	0	28	11	0
3	L	20	0	28	5	0
3	M	20	0	28	0	0
3	N	25	0	35	26	0
3	O	15	0	21	1	0
3	P	40	0	56	14	0
3	Q	15	0	21	9	0
3	R	25	0	35	13	0
3	S	10	0	14	1	0
3	T	30	0	42	15	0
3	U	10	0	14	8	0
3	V	45	0	63	47	0
3	W	10	0	14	7	0
3	X	25	0	35	8	0
3	Y	15	0	21	4	0
3	Z	20	0	28	8	0
4	2	20	0	22	4	0
4	C	20	0	22	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	20	0	22	3	0
4	G	20	0	22	3	0
4	H	20	0	22	5	0
4	J	20	0	22	2	0
4	L	20	0	22	3	0
4	N	20	0	22	3	0
4	P	20	0	22	4	0
4	R	20	0	22	3	0
4	T	20	0	22	3	0
4	V	20	0	22	4	0
4	X	20	0	22	4	0
4	Z	20	0	22	3	0
5	1	47	0	0	1	0
5	2	143	0	0	7	0
5	A	43	0	0	4	0
5	B	41	0	0	6	0
5	C	163	0	0	10	0
5	D	40	0	0	8	0
5	E	166	0	0	9	0
5	F	58	0	0	4	0
5	G	131	0	0	2	0
5	H	148	0	0	7	0
5	I	52	0	0	9	0
5	J	142	0	0	10	0
5	K	45	0	0	5	0
5	L	153	0	0	12	0
5	M	40	0	0	4	0
5	N	154	0	0	6	0
5	O	47	0	0	4	0
5	P	139	0	0	6	0
5	Q	38	0	0	9	0
5	R	170	0	0	7	0
5	S	42	0	0	8	0
5	T	116	0	0	7	0
5	U	49	0	0	4	0
5	V	177	0	0	14	0
5	W	35	0	0	4	0
5	X	150	0	0	7	0
5	Y	28	0	0	6	0
5	Z	123	0	0	4	0
All	All	50080	0	47491	1555	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 16.

The worst 5 of 1555 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:B:7:ILE:HG21	1:B:11:GLN:CG	1.63	1.27
1:F:7:ILE:CG2	1:F:11:GLN:HB3	1.65	1.27
1:A:80:GLN:HE21	1:A:80:GLN:C	1.45	1.24
3:R:92:DMF:H21	5:R:1869:HOH:O	1.30	1.23
1:O:9:PRO:HD2	1:U:15:GLU:CG	1.69	1.21

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	1	211/248 (85%)	199 (94%)	12 (6%)	0	100	100
1	A	211/248 (85%)	203 (96%)	8 (4%)	0	100	100
1	B	209/248 (84%)	201 (96%)	8 (4%)	0	100	100
1	D	210/248 (85%)	201 (96%)	9 (4%)	0	100	100
1	F	216/248 (87%)	209 (97%)	6 (3%)	1 (0%)	24	27
1	I	212/248 (86%)	201 (95%)	11 (5%)	0	100	100
1	K	212/248 (86%)	202 (95%)	10 (5%)	0	100	100
1	M	212/248 (86%)	201 (95%)	11 (5%)	0	100	100
1	O	212/248 (86%)	199 (94%)	13 (6%)	0	100	100
1	Q	211/248 (85%)	198 (94%)	13 (6%)	0	100	100
1	S	212/248 (86%)	203 (96%)	9 (4%)	0	100	100
1	U	212/248 (86%)	200 (94%)	12 (6%)	0	100	100
1	W	212/248 (86%)	199 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	212/248 (86%)	202 (95%)	10 (5%)	0	100	100
2	2	221/240 (92%)	220 (100%)	1 (0%)	0	100	100
2	C	220/240 (92%)	219 (100%)	1 (0%)	0	100	100
2	E	221/240 (92%)	219 (99%)	2 (1%)	0	100	100
2	G	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	H	220/240 (92%)	219 (100%)	1 (0%)	0	100	100
2	J	220/240 (92%)	219 (100%)	1 (0%)	0	100	100
2	L	221/240 (92%)	218 (99%)	3 (1%)	0	100	100
2	N	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	P	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	R	237/240 (99%)	236 (100%)	1 (0%)	0	100	100
2	T	221/240 (92%)	220 (100%)	1 (0%)	0	100	100
2	V	237/240 (99%)	234 (99%)	3 (1%)	0	100	100
2	X	221/240 (92%)	219 (99%)	2 (1%)	0	100	100
2	Z	221/240 (92%)	218 (99%)	3 (1%)	0	100	100
All	All	6084/6832 (89%)	5913 (97%)	170 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	191	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	1	165/192 (86%)	159 (96%)	6 (4%)	31	42
1	A	164/192 (85%)	155 (94%)	9 (6%)	19	24
1	B	163/192 (85%)	154 (94%)	9 (6%)	19	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	164/192 (85%)	153 (93%)	11 (7%)	15	17
1	F	169/192 (88%)	162 (96%)	7 (4%)	27	37
1	I	166/192 (86%)	161 (97%)	5 (3%)	36	49
1	K	166/192 (86%)	158 (95%)	8 (5%)	23	30
1	M	166/192 (86%)	156 (94%)	10 (6%)	17	21
1	O	166/192 (86%)	161 (97%)	5 (3%)	36	49
1	Q	165/192 (86%)	158 (96%)	7 (4%)	26	36
1	S	166/192 (86%)	157 (95%)	9 (5%)	20	25
1	U	165/192 (86%)	161 (98%)	4 (2%)	43	58
1	W	166/192 (86%)	161 (97%)	5 (3%)	36	49
1	Y	166/192 (86%)	159 (96%)	7 (4%)	26	36
2	2	165/178 (93%)	158 (96%)	7 (4%)	26	36
2	C	165/178 (93%)	161 (98%)	4 (2%)	43	58
2	E	165/178 (93%)	159 (96%)	6 (4%)	31	42
2	G	165/178 (93%)	161 (98%)	4 (2%)	43	58
2	H	165/178 (93%)	158 (96%)	7 (4%)	26	36
2	J	165/178 (93%)	159 (96%)	6 (4%)	31	42
2	L	165/178 (93%)	160 (97%)	5 (3%)	36	49
2	N	165/178 (93%)	160 (97%)	5 (3%)	36	49
2	P	165/178 (93%)	161 (98%)	4 (2%)	43	58
2	R	177/178 (99%)	170 (96%)	7 (4%)	28	38
2	T	165/178 (93%)	159 (96%)	6 (4%)	31	42
2	V	177/178 (99%)	172 (97%)	5 (3%)	38	52
2	X	165/178 (93%)	160 (97%)	5 (3%)	36	49
2	Z	165/178 (93%)	159 (96%)	6 (4%)	31	42
All	All	4651/5180 (90%)	4472 (96%)	179 (4%)	29	40

5 of 179 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	R	433	GLU
1	W	7	ILE
1	S	7	ILE

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Mol	Chain	Res	Type
2	T	398	LEU
2	X	444	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	174	ASN
1	U	101	ASN
2	R	456	GLN
1	S	80	GLN
2	V	430	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](#)

137 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	DMF	J	45	-	4,4,4	0.30	0	4,4,4	0.33	0
3	DMF	N	90	-	4,4,4	0.31	0	4,4,4	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DMF	L	81	-	4,4,4	0.30	0	4,4,4	0.35	0
3	DMF	Q	250	-	4,4,4	0.27	0	4,4,4	0.55	0
4	SA6	X	300	2	16,21,21	3.04	8 (50%)	21,32,32	1.66	2 (9%)
3	DMF	E	28	-	4,4,4	0.30	0	4,4,4	0.22	0
3	DMF	F	250	-	4,4,4	0.30	0	4,4,4	0.37	0
3	DMF	H	71	-	4,4,4	0.52	0	4,4,4	0.39	0
3	DMF	A	249	-	4,4,4	0.60	0	4,4,4	0.28	0
3	DMF	G	64	-	4,4,4	0.32	0	4,4,4	0.39	0
3	DMF	H	117	-	4,4,4	0.42	0	4,4,4	0.82	0
3	DMF	V	39	-	4,4,4	0.33	0	4,4,4	0.39	0
3	DMF	W	250	-	4,4,4	0.30	0	4,4,4	0.46	0
3	DMF	D	253	-	4,4,4	0.27	0	4,4,4	0.34	0
3	DMF	X	122	-	4,4,4	0.31	0	4,4,4	0.36	0
3	DMF	E	100	-	4,4,4	0.31	0	4,4,4	0.48	0
3	DMF	C	103	-	4,4,4	0.32	0	4,4,4	0.37	0
3	DMF	E	75	-	4,4,4	0.28	0	4,4,4	0.43	0
3	DMF	Y	250	-	4,4,4	0.68	0	4,4,4	0.33	0
3	DMF	G	111	-	4,4,4	0.25	0	4,4,4	0.36	0
3	DMF	P	2	-	4,4,4	0.28	0	4,4,4	0.55	0
3	DMF	F	251	-	4,4,4	0.21	0	4,4,4	0.41	0
3	DMF	P	33	-	4,4,4	0.29	0	4,4,4	0.26	0
3	DMF	N	104	-	4,4,4	0.35	0	4,4,4	0.42	0
3	DMF	P	60	-	4,4,4	0.29	0	4,4,4	0.41	0
3	DMF	X	15	-	4,4,4	0.32	0	4,4,4	0.48	0
3	DMF	R	95	-	4,4,4	0.35	0	4,4,4	0.40	0
3	DMF	N	93	-	4,4,4	0.33	0	4,4,4	0.41	0
3	DMF	K	251	-	4,4,4	0.32	0	4,4,4	0.17	0
3	DMF	Z	94	-	4,4,4	0.27	0	4,4,4	0.40	0
3	DMF	I	249	-	4,4,4	0.32	0	4,4,4	0.41	0
3	DMF	R	80	-	4,4,4	0.30	0	4,4,4	0.39	0
3	DMF	E	20	-	4,4,4	0.31	0	4,4,4	0.46	0
3	DMF	K	252	-	4,4,4	0.28	0	4,4,4	0.38	0
3	DMF	G	77	-	4,4,4	0.45	0	4,4,4	0.43	0
3	DMF	M	249	-	4,4,4	0.31	0	4,4,4	0.45	0
3	DMF	Z	114	-	4,4,4	0.34	0	4,4,4	0.47	0
3	DMF	2	4	-	4,4,4	0.32	0	4,4,4	0.48	0
4	SA6	E	300	2	16,21,21	2.81	7 (43%)	21,32,32	1.79	5 (23%)
3	DMF	V	109	-	4,4,4	0.23	0	4,4,4	0.32	0
3	DMF	T	29	-	4,4,4	0.30	0	4,4,4	0.41	0
3	DMF	G	119	-	4,4,4	0.28	0	4,4,4	0.37	0
3	DMF	C	38	-	4,4,4	0.18	0	4,4,4	0.53	0
3	DMF	Q	251	-	4,4,4	0.32	0	4,4,4	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DMF	P	14	-	4,4,4	0.28	0	4,4,4	0.43	0
3	DMF	J	110	-	4,4,4	0.34	0	4,4,4	0.61	0
3	DMF	N	118	-	4,4,4	0.38	0	4,4,4	0.68	0
3	DMF	K	249	-	4,4,4	0.29	0	4,4,4	0.41	0
3	DMF	D	250	-	4,4,4	0.34	0	4,4,4	0.41	0
4	SA6	2	300	2	16,21,21	2.48	4 (25%)	21,32,32	1.83	6 (28%)
3	DMF	M	252	-	4,4,4	0.33	0	4,4,4	0.39	0
4	SA6	N	300	2	16,21,21	2.77	6 (37%)	21,32,32	1.74	5 (23%)
3	DMF	O	249	-	4,4,4	0.26	0	4,4,4	0.53	0
3	DMF	2	87	-	4,4,4	0.30	0	4,4,4	0.45	0
3	DMF	O	251	-	4,4,4	0.41	0	4,4,4	0.81	0
3	DMF	X	16	-	4,4,4	0.29	0	4,4,4	0.41	0
3	DMF	R	59	-	4,4,4	0.32	0	4,4,4	0.42	0
3	DMF	R	89	-	4,4,4	0.41	0	4,4,4	0.70	0
3	DMF	G	12	-	4,4,4	0.30	0	4,4,4	0.45	0
4	SA6	G	300	2	16,21,21	3.07	7 (43%)	21,32,32	1.53	3 (14%)
4	SA6	Z	300	2	16,21,21	3.30	10 (62%)	21,32,32	1.52	1 (4%)
4	SA6	J	300	2	16,21,21	3.04	8 (50%)	21,32,32	1.51	3 (14%)
3	DMF	U	249	-	4,4,4	0.29	0	4,4,4	0.35	0
3	DMF	E	53	-	4,4,4	0.30	0	4,4,4	0.41	0
3	DMF	V	82	-	4,4,4	0.35	0	4,4,4	0.43	0
3	DMF	G	62	-	4,4,4	0.31	0	4,4,4	0.43	0
3	DMF	Z	18	-	4,4,4	0.24	0	4,4,4	0.44	0
3	DMF	H	66	-	4,4,4	0.31	0	4,4,4	0.44	0
3	DMF	F	249	-	4,4,4	0.28	0	4,4,4	0.39	0
3	DMF	T	115	-	4,4,4	0.32	0	4,4,4	0.51	0
3	DMF	Z	54	-	4,4,4	0.35	0	4,4,4	0.49	0
3	DMF	W	249	-	4,4,4	0.31	0	4,4,4	0.43	0
3	DMF	X	41	-	4,4,4	0.56	0	4,4,4	0.36	0
3	DMF	B	250	-	4,4,4	0.30	0	4,4,4	0.36	0
3	DMF	L	97	-	4,4,4	0.30	0	4,4,4	0.45	0
4	SA6	L	300	2	16,21,21	3.09	7 (43%)	21,32,32	1.90	6 (28%)
3	DMF	P	86	-	4,4,4	0.30	0	4,4,4	0.42	0
3	DMF	T	102	-	4,4,4	0.16	0	4,4,4	0.13	0
3	DMF	2	52	-	4,4,4	0.33	0	4,4,4	0.44	0
4	SA6	R	300	2	16,21,21	3.73	7 (43%)	21,32,32	1.77	5 (23%)
3	DMF	R	92	-	4,4,4	0.30	0	4,4,4	0.42	0
3	DMF	V	42	-	4,4,4	0.30	0	4,4,4	0.49	0
3	DMF	1	249	-	4,4,4	0.30	0	4,4,4	0.39	0
3	DMF	S	249	-	4,4,4	0.29	0	4,4,4	0.38	0
3	DMF	C	63	-	4,4,4	0.29	0	4,4,4	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DMF	T	84	-	4,4,4	0.08	0	4,4,4	0.15	0
3	DMF	V	32	-	4,4,4	0.31	0	4,4,4	0.49	0
3	DMF	N	22	-	4,4,4	0.32	0	4,4,4	0.37	0
3	DMF	V	83	-	4,4,4	0.24	0	4,4,4	0.44	0
3	DMF	C	69	-	4,4,4	0.29	0	4,4,4	0.47	0
3	DMF	P	56	-	4,4,4	0.31	0	4,4,4	0.46	0
3	DMF	C	88	-	4,4,4	0.33	0	4,4,4	0.51	0
3	DMF	V	27	-	4,4,4	0.30	0	4,4,4	0.36	0
4	SA6	T	300	2	16,21,21	3.23	8 (50%)	21,32,32	1.81	4 (19%)
3	DMF	C	121	-	4,4,4	0.31	0	4,4,4	0.45	0
3	DMF	T	113	-	4,4,4	0.25	0	4,4,4	0.44	0
3	DMF	Y	249	-	4,4,4	0.32	0	4,4,4	0.44	0
4	SA6	V	300	2	16,21,21	3.11	10 (62%)	21,32,32	1.41	2 (9%)
3	DMF	H	72	-	4,4,4	0.33	0	4,4,4	0.42	0
3	DMF	J	123	-	4,4,4	0.31	0	4,4,4	0.42	0
3	DMF	V	120	-	4,4,4	0.35	0	4,4,4	0.46	0
4	SA6	C	300	2	16,21,21	2.89	6 (37%)	21,32,32	1.93	6 (28%)
3	DMF	P	51	-	4,4,4	0.26	0	4,4,4	0.37	0
3	DMF	U	250	-	4,4,4	0.71	0	4,4,4	0.34	0
3	DMF	2	101	-	4,4,4	0.34	0	4,4,4	0.43	0
3	DMF	L	36	-	4,4,4	0.33	0	4,4,4	0.48	0
3	DMF	I	250	-	4,4,4	0.28	0	4,4,4	0.35	0
3	DMF	H	91	-	4,4,4	0.29	0	4,4,4	0.47	0
3	DMF	D	249	-	4,4,4	0.60	0	4,4,4	0.37	0
3	DMF	Q	249	-	4,4,4	0.31	0	4,4,4	0.42	0
3	DMF	H	43	-	4,4,4	0.37	0	4,4,4	0.75	0
3	DMF	M	250	-	4,4,4	0.32	0	4,4,4	0.37	0
4	SA6	P	300	2	16,21,21	2.82	6 (37%)	21,32,32	1.71	4 (19%)
3	DMF	Y	251	-	4,4,4	0.31	0	4,4,4	0.43	0
3	DMF	2	57	-	4,4,4	0.31	0	4,4,4	0.34	0
3	DMF	D	251	-	4,4,4	0.31	0	4,4,4	0.43	0
3	DMF	2	49	-	4,4,4	0.25	0	4,4,4	0.51	0
3	DMF	S	250	-	4,4,4	0.70	0	4,4,4	0.37	0
3	DMF	E	73	-	4,4,4	0.29	0	4,4,4	0.45	0
3	DMF	V	116	-	4,4,4	0.45	0	4,4,4	1.07	0
3	DMF	C	47	-	4,4,4	0.57	0	4,4,4	0.24	0
4	SA6	H	300	2	16,21,21	3.09	7 (43%)	21,32,32	1.58	4 (19%)
3	DMF	D	252	-	4,4,4	0.30	0	4,4,4	0.40	0
3	DMF	2	108	-	4,4,4	0.32	0	4,4,4	0.46	0
3	DMF	G	98	-	4,4,4	0.32	0	4,4,4	0.43	0
3	DMF	O	250	-	4,4,4	0.35	0	4,4,4	0.40	0
3	DMF	G	70	-	4,4,4	0.73	0	4,4,4	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DMF	K	250	-	4,4,4	0.28	0	4,4,4	0.35	0
3	DMF	M	251	-	4,4,4	0.32	0	4,4,4	0.34	0
3	DMF	P	107	-	4,4,4	0.23	0	4,4,4	0.46	0
3	DMF	2	112	-	4,4,4	0.19	0	4,4,4	0.40	0
3	DMF	L	50	-	4,4,4	0.24	0	4,4,4	0.30	0
3	DMF	X	40	-	4,4,4	0.32	0	4,4,4	0.42	0
3	DMF	B	249	-	4,4,4	0.29	0	4,4,4	0.43	0
3	DMF	G	24	-	4,4,4	0.31	0	4,4,4	0.42	0
3	DMF	T	10	-	4,4,4	0.35	0	4,4,4	0.53	0
3	DMF	A	250	-	4,4,4	0.48	0	4,4,4	0.53	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	DMF	J	45	-	-	0/2/2/2	-
3	DMF	N	90	-	-	2/2/2/2	-
3	DMF	L	81	-	-	0/2/2/2	-
3	DMF	Q	250	-	-	2/2/2/2	-
4	SA6	X	300	2	-	0/6/47/47	0/2/2/2
3	DMF	E	28	-	-	2/2/2/2	-
3	DMF	F	250	-	-	2/2/2/2	-
3	DMF	H	71	-	-	0/2/2/2	-
3	DMF	A	249	-	-	0/2/2/2	-
3	DMF	G	64	-	-	2/2/2/2	-
3	DMF	H	117	-	-	2/2/2/2	-
3	DMF	V	39	-	-	2/2/2/2	-
3	DMF	W	250	-	-	2/2/2/2	-
3	DMF	D	253	-	-	2/2/2/2	-
3	DMF	X	122	-	-	0/2/2/2	-
3	DMF	E	100	-	-	2/2/2/2	-
3	DMF	C	103	-	-	2/2/2/2	-
3	DMF	E	75	-	-	2/2/2/2	-
3	DMF	Y	250	-	-	0/2/2/2	-
3	DMF	G	111	-	-	2/2/2/2	-
3	DMF	P	2	-	-	2/2/2/2	-
3	DMF	F	251	-	-	2/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMF	P	33	-	-	1/2/2/2	-
3	DMF	N	104	-	-	1/2/2/2	-
3	DMF	P	60	-	-	2/2/2/2	-
3	DMF	X	15	-	-	2/2/2/2	-
3	DMF	R	95	-	-	2/2/2/2	-
3	DMF	N	93	-	-	2/2/2/2	-
3	DMF	K	251	-	-	2/2/2/2	-
3	DMF	Z	94	-	-	2/2/2/2	-
3	DMF	I	249	-	-	2/2/2/2	-
3	DMF	R	80	-	-	2/2/2/2	-
3	DMF	E	20	-	-	2/2/2/2	-
3	DMF	K	252	-	-	2/2/2/2	-
3	DMF	G	77	-	-	0/2/2/2	-
3	DMF	M	249	-	-	0/2/2/2	-
3	DMF	Z	114	-	-	0/2/2/2	-
3	DMF	2	4	-	-	0/2/2/2	-
4	SA6	E	300	2	-	1/6/47/47	0/2/2/2
3	DMF	V	109	-	-	0/2/2/2	-
3	DMF	T	29	-	-	2/2/2/2	-
3	DMF	G	119	-	-	2/2/2/2	-
3	DMF	C	38	-	-	2/2/2/2	-
3	DMF	Q	251	-	-	2/2/2/2	-
3	DMF	P	14	-	-	2/2/2/2	-
3	DMF	J	110	-	-	2/2/2/2	-
3	DMF	N	118	-	-	2/2/2/2	-
3	DMF	K	249	-	-	1/2/2/2	-
3	DMF	D	250	-	-	2/2/2/2	-
4	SA6	2	300	2	-	0/6/47/47	0/2/2/2
3	DMF	M	252	-	-	2/2/2/2	-
4	SA6	N	300	2	-	1/6/47/47	0/2/2/2
3	DMF	O	249	-	-	2/2/2/2	-
3	DMF	2	87	-	-	2/2/2/2	-
3	DMF	O	251	-	-	2/2/2/2	-
3	DMF	X	16	-	-	2/2/2/2	-
3	DMF	R	59	-	-	0/2/2/2	-
3	DMF	R	89	-	-	0/2/2/2	-
3	DMF	G	12	-	-	2/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SA6	G	300	2	-	1/6/47/47	0/2/2/2
4	SA6	Z	300	2	-	0/6/47/47	0/2/2/2
4	SA6	J	300	2	-	0/6/47/47	0/2/2/2
3	DMF	U	249	-	-	2/2/2/2	-
3	DMF	E	53	-	-	0/2/2/2	-
3	DMF	V	82	-	-	0/2/2/2	-
3	DMF	G	62	-	-	2/2/2/2	-
3	DMF	Z	18	-	-	2/2/2/2	-
3	DMF	H	66	-	-	2/2/2/2	-
3	DMF	F	249	-	-	0/2/2/2	-
3	DMF	T	115	-	-	2/2/2/2	-
3	DMF	Z	54	-	-	2/2/2/2	-
3	DMF	W	249	-	-	2/2/2/2	-
3	DMF	X	41	-	-	0/2/2/2	-
3	DMF	B	250	-	-	2/2/2/2	-
3	DMF	L	97	-	-	2/2/2/2	-
4	SA6	L	300	2	-	2/6/47/47	0/2/2/2
3	DMF	P	86	-	-	2/2/2/2	-
3	DMF	T	102	-	-	0/2/2/2	-
3	DMF	2	52	-	-	2/2/2/2	-
4	SA6	R	300	2	-	0/6/47/47	0/2/2/2
3	DMF	R	92	-	-	0/2/2/2	-
3	DMF	V	42	-	-	2/2/2/2	-
3	DMF	1	249	-	-	0/2/2/2	-
3	DMF	S	249	-	-	2/2/2/2	-
3	DMF	C	63	-	-	2/2/2/2	-
3	DMF	T	84	-	-	2/2/2/2	-
3	DMF	V	32	-	-	2/2/2/2	-
3	DMF	N	22	-	-	2/2/2/2	-
3	DMF	V	83	-	-	0/2/2/2	-
3	DMF	C	69	-	-	2/2/2/2	-
3	DMF	P	56	-	-	2/2/2/2	-
3	DMF	C	88	-	-	2/2/2/2	-
3	DMF	V	27	-	-	2/2/2/2	-
4	SA6	T	300	2	-	0/6/47/47	0/2/2/2
3	DMF	C	121	-	-	2/2/2/2	-
3	DMF	T	113	-	-	2/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMF	Y	249	-	-	2/2/2/2	-
4	SA6	V	300	2	-	0/6/47/47	0/2/2/2
3	DMF	H	72	-	-	2/2/2/2	-
3	DMF	J	123	-	-	0/2/2/2	-
3	DMF	V	120	-	-	2/2/2/2	-
4	SA6	C	300	2	-	1/6/47/47	0/2/2/2
3	DMF	P	51	-	-	2/2/2/2	-
3	DMF	U	250	-	-	0/2/2/2	-
3	DMF	2	101	-	-	2/2/2/2	-
3	DMF	L	36	-	-	2/2/2/2	-
3	DMF	I	250	-	-	0/2/2/2	-
3	DMF	H	91	-	-	2/2/2/2	-
3	DMF	D	249	-	-	0/2/2/2	-
3	DMF	Q	249	-	-	0/2/2/2	-
3	DMF	H	43	-	-	2/2/2/2	-
3	DMF	M	250	-	-	2/2/2/2	-
4	SA6	P	300	2	-	0/6/47/47	0/2/2/2
3	DMF	Y	251	-	-	2/2/2/2	-
3	DMF	2	57	-	-	0/2/2/2	-
3	DMF	D	251	-	-	2/2/2/2	-
3	DMF	2	49	-	-	0/2/2/2	-
3	DMF	S	250	-	-	0/2/2/2	-
3	DMF	E	73	-	-	2/2/2/2	-
3	DMF	V	116	-	-	0/2/2/2	-
3	DMF	C	47	-	-	0/2/2/2	-
4	SA6	H	300	2	-	0/6/47/47	0/2/2/2
3	DMF	D	252	-	-	2/2/2/2	-
3	DMF	2	108	-	-	0/2/2/2	-
3	DMF	G	98	-	-	0/2/2/2	-
3	DMF	O	250	-	-	0/2/2/2	-
3	DMF	G	70	-	-	0/2/2/2	-
3	DMF	K	250	-	-	2/2/2/2	-
3	DMF	M	251	-	-	2/2/2/2	-
3	DMF	P	107	-	-	2/2/2/2	-
3	DMF	2	112	-	-	2/2/2/2	-
3	DMF	L	50	-	-	0/2/2/2	-
3	DMF	X	40	-	-	0/2/2/2	-
3	DMF	B	249	-	-	0/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMF	G	24	-	-	0/2/2/2	-
3	DMF	T	10	-	-	2/2/2/2	-
3	DMF	A	250	-	-	0/2/2/2	-

The worst 5 of 101 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	300	SA6	C5-C4	8.58	1.62	1.52
4	T	300	SA6	C5-C4	8.00	1.61	1.52
4	Z	300	SA6	C5-C4	7.61	1.61	1.52
4	H	300	SA6	C5-C4	7.40	1.61	1.52
4	L	300	SA6	C5-C4	7.32	1.61	1.52

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	300	SA6	C4-C3-C7	-5.24	99.79	104.23
4	T	300	SA6	C4-C3-C7	-5.06	99.95	104.23
4	R	300	SA6	C4-C3-C7	-4.61	100.32	104.23
4	C	300	SA6	C4-C3-C7	-4.60	100.34	104.23
4	P	300	SA6	C4-C3-C7	-4.58	100.35	104.23

There are no chirality outliers.

5 of 169 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	300	SA6	C1-C2-C3-C4
4	E	300	SA6	C1-C2-C3-C4
4	G	300	SA6	C1-C2-C3-C4
4	L	300	SA6	C1-C2-C3-C4
4	N	300	SA6	C1-C2-C3-C4

There are no ring outliers.

105 monomers are involved in 317 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	45	DMF	1	0
3	N	90	DMF	7	0
3	L	81	DMF	1	0
3	Q	250	DMF	6	0
4	X	300	SA6	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	28	DMF	1	0
3	F	250	DMF	1	0
3	H	71	DMF	1	0
3	A	249	DMF	1	0
3	G	64	DMF	9	0
3	H	117	DMF	2	0
3	V	39	DMF	1	0
3	W	250	DMF	5	0
3	D	253	DMF	2	0
3	X	122	DMF	1	0
3	E	100	DMF	2	0
3	C	103	DMF	8	0
3	E	75	DMF	4	0
3	Y	250	DMF	1	0
3	G	111	DMF	1	0
3	P	2	DMF	1	0
3	P	33	DMF	3	0
3	N	104	DMF	7	0
3	X	15	DMF	2	0
3	R	95	DMF	1	0
3	N	93	DMF	4	0
3	K	251	DMF	3	0
3	Z	94	DMF	3	0
3	R	80	DMF	1	0
3	E	20	DMF	4	0
3	K	252	DMF	3	0
3	2	4	DMF	8	0
4	E	300	SA6	3	0
3	T	29	DMF	3	0
3	G	119	DMF	11	0
3	C	38	DMF	3	0
3	Q	251	DMF	1	0
3	P	14	DMF	5	0
3	N	118	DMF	4	0
3	K	249	DMF	1	0
4	2	300	SA6	4	0
4	N	300	SA6	3	0
3	2	87	DMF	2	0
3	X	16	DMF	3	0
3	R	59	DMF	9	0
3	G	12	DMF	4	0
4	G	300	SA6	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Z	300	SA6	3	0
4	J	300	SA6	2	0
3	E	53	DMF	2	0
3	V	82	DMF	2	0
3	G	62	DMF	1	0
3	Z	18	DMF	2	0
3	H	66	DMF	3	0
3	T	115	DMF	1	0
3	Z	54	DMF	3	0
3	W	249	DMF	2	0
3	X	41	DMF	1	0
3	L	97	DMF	4	0
4	L	300	SA6	3	0
3	T	102	DMF	3	0
3	2	52	DMF	2	0
4	R	300	SA6	3	0
3	R	92	DMF	2	0
3	V	42	DMF	7	0
3	S	249	DMF	1	0
3	C	63	DMF	1	0
3	T	84	DMF	3	0
3	V	32	DMF	5	0
3	N	22	DMF	4	0
3	V	83	DMF	10	0
3	C	69	DMF	1	0
3	C	88	DMF	2	0
3	V	27	DMF	8	0
4	T	300	SA6	3	0
3	T	113	DMF	5	0
3	Y	249	DMF	1	0
4	V	300	SA6	4	0
3	J	123	DMF	6	0
3	V	120	DMF	8	0
4	C	300	SA6	3	0
3	U	250	DMF	8	0
3	2	101	DMF	3	0
3	I	250	DMF	2	0
3	H	91	DMF	2	0
3	Q	249	DMF	2	0
3	H	43	DMF	4	0
4	P	300	SA6	4	0
3	Y	251	DMF	2	0

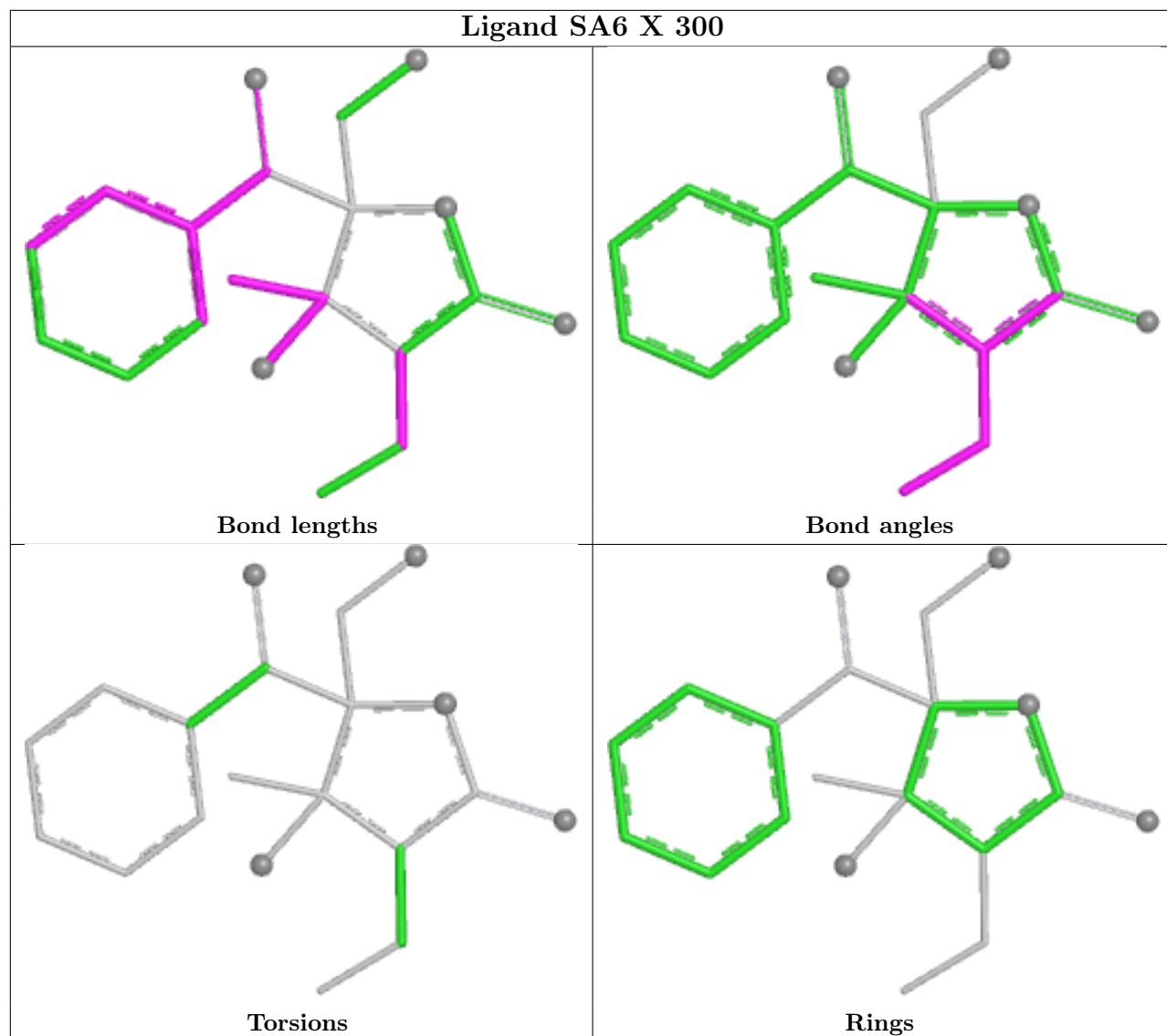
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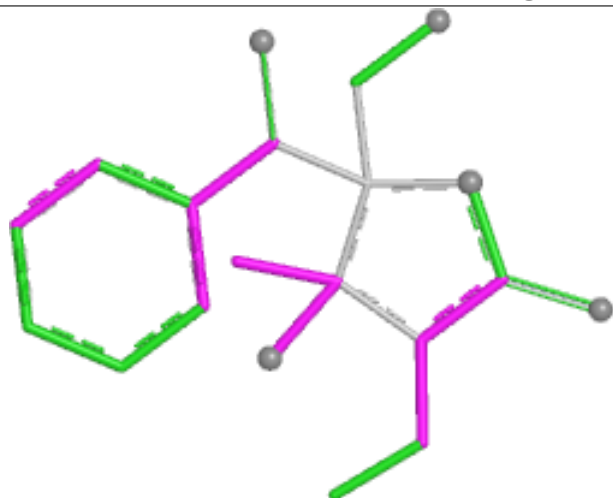
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	251	DMF	5	0
3	2	49	DMF	1	0
3	E	73	DMF	3	0
3	V	116	DMF	6	0
3	C	47	DMF	1	0
4	H	300	SA6	5	0
3	2	108	DMF	5	0
3	G	98	DMF	2	0
3	O	250	DMF	1	0
3	G	70	DMF	1	0
3	K	250	DMF	4	0
3	P	107	DMF	5	0
3	2	112	DMF	7	0
3	X	40	DMF	1	0
3	B	249	DMF	2	0
3	G	24	DMF	2	0

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.

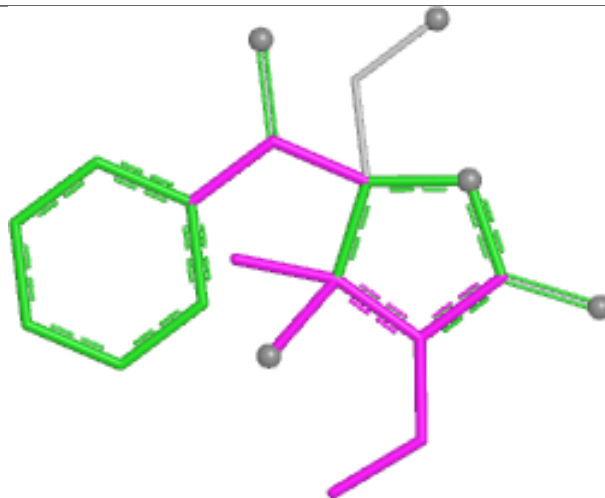
Ligand SA6 X 300



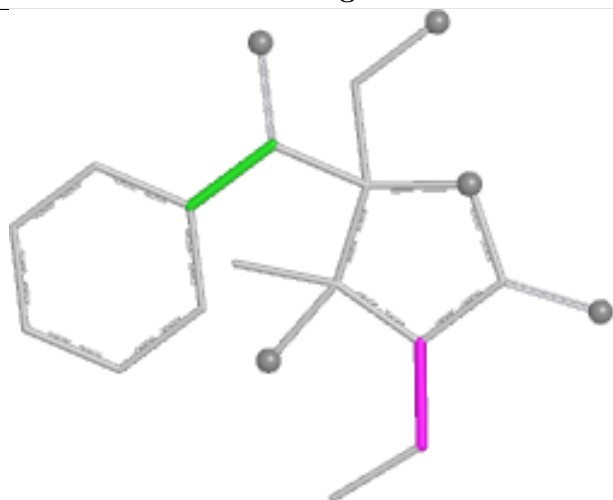
Ligand SA6 E 300



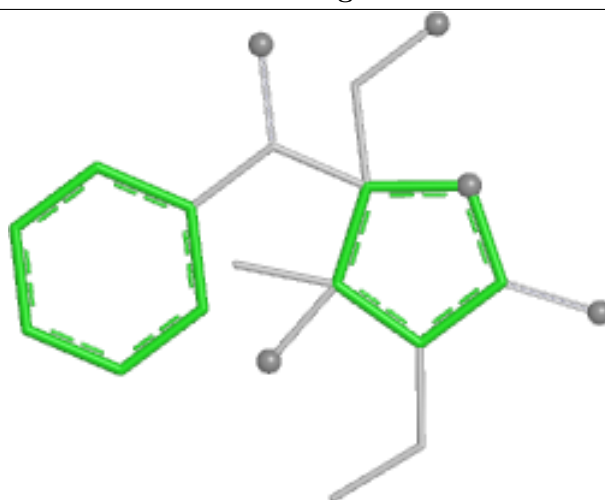
Bond lengths



Bond angles

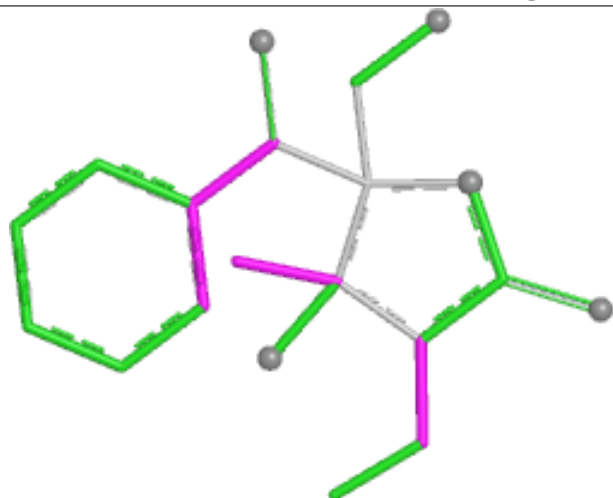


Torsions

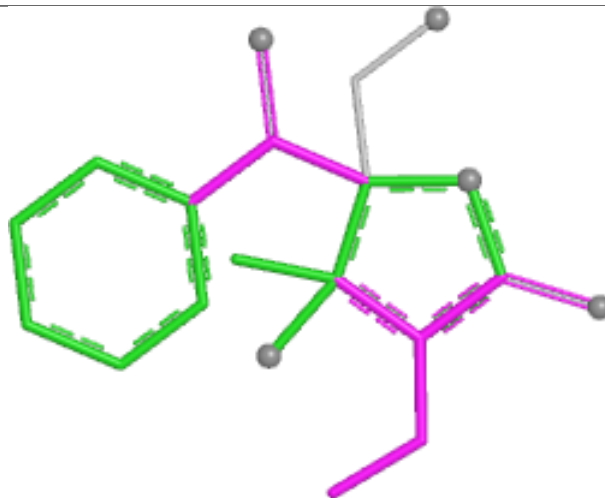


Rings

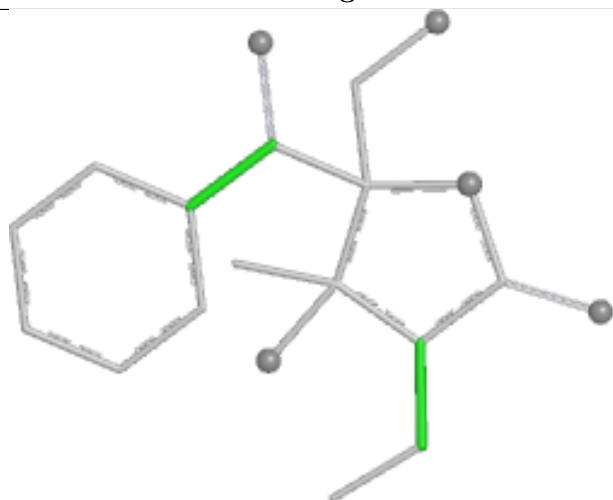
Ligand SA6 2 300



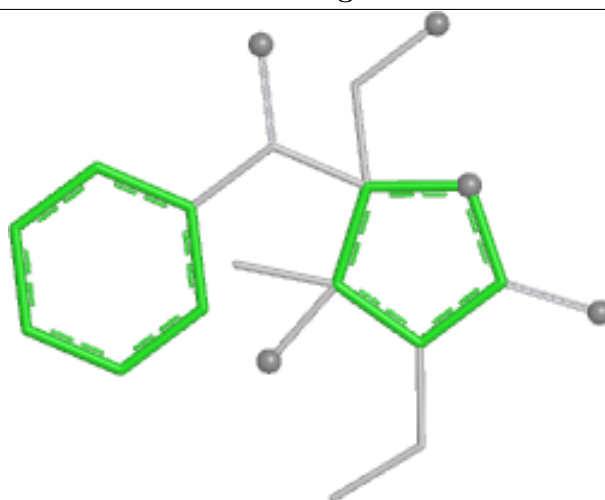
Bond lengths



Bond angles

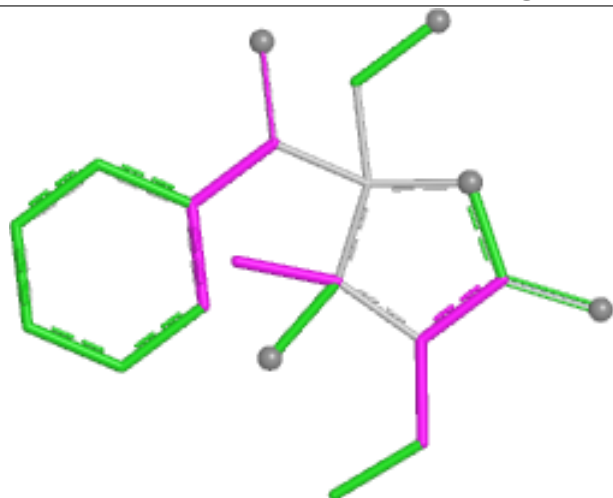


Torsions

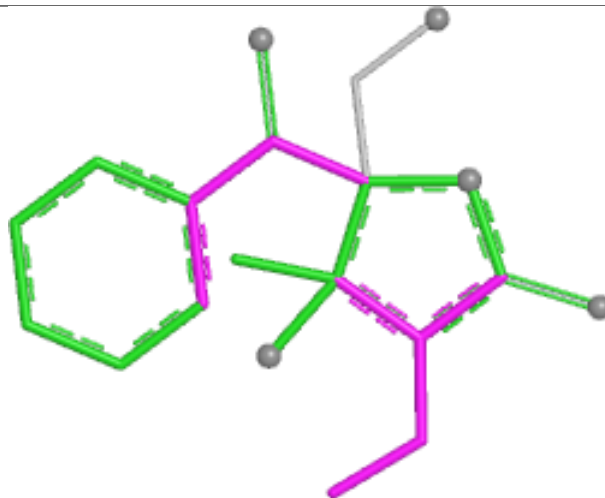


Rings

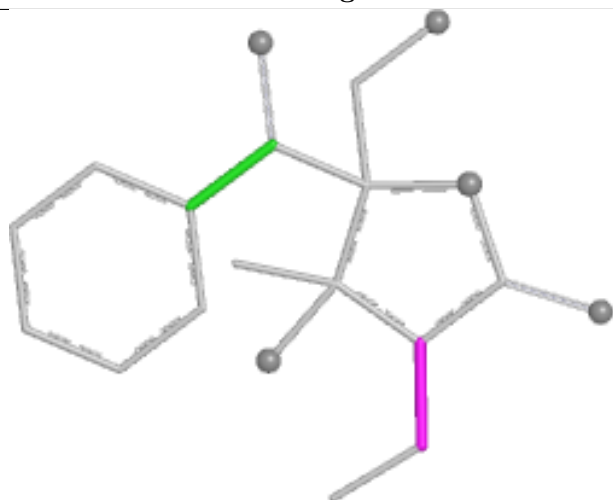
Ligand SA6 N 300



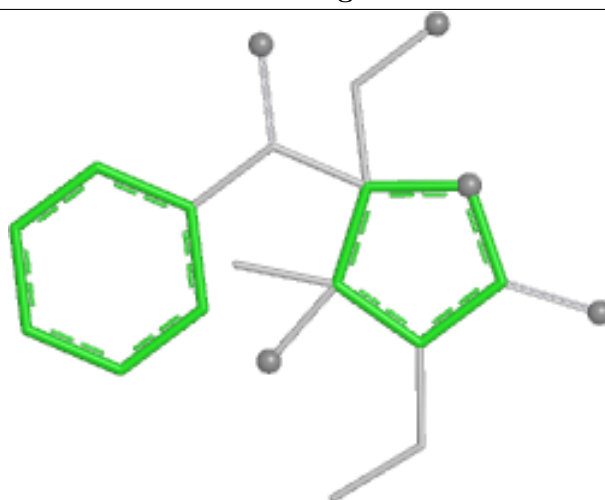
Bond lengths



Bond angles

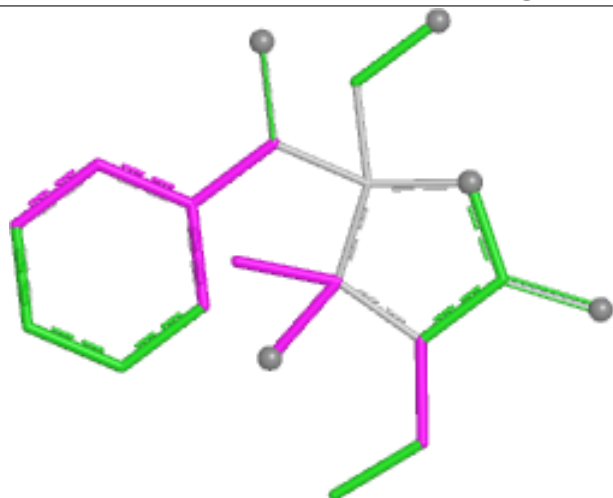


Torsions

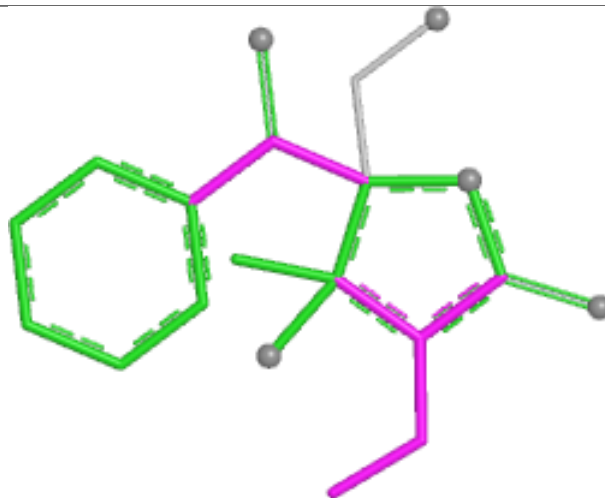


Rings

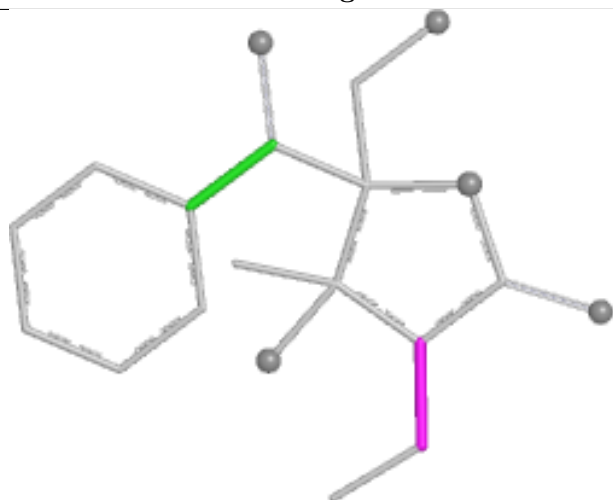
Ligand SA6 G 300



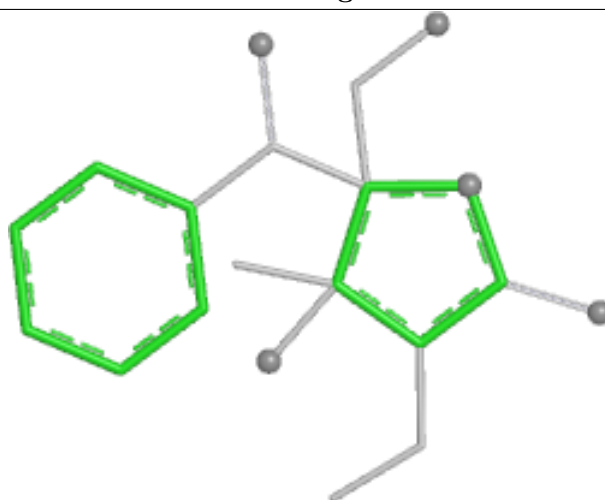
Bond lengths



Bond angles

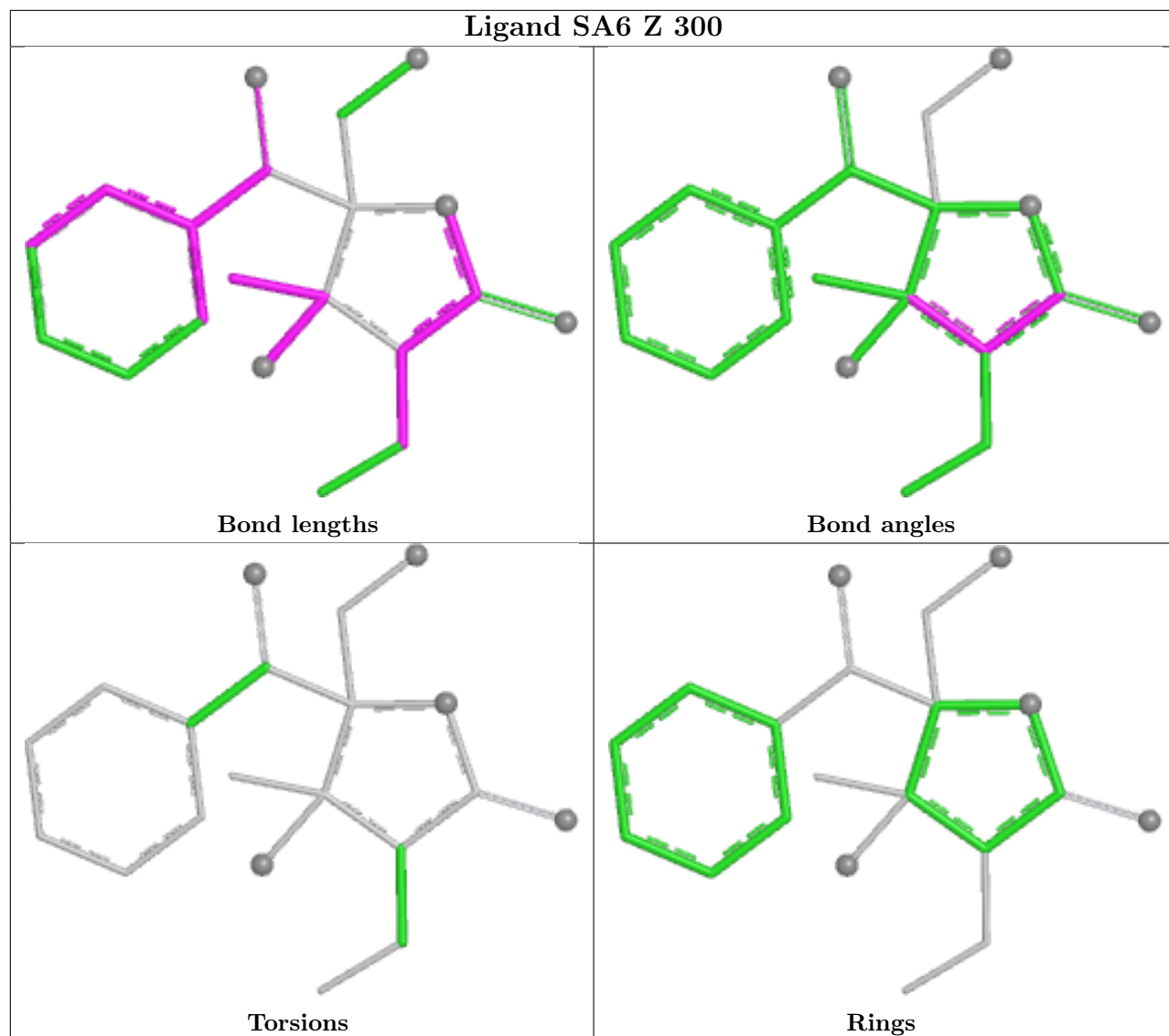


Torsions

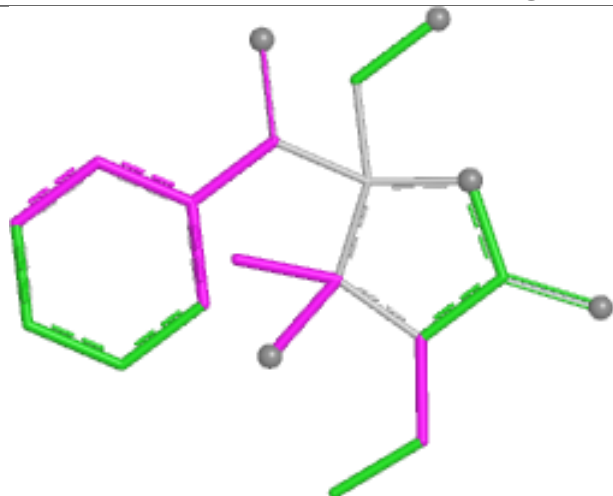


Rings

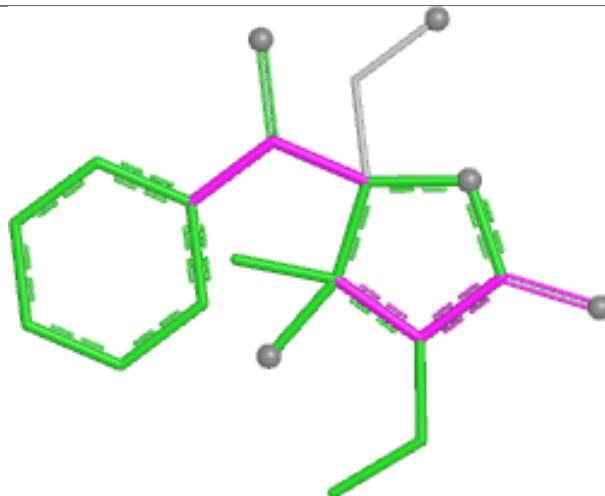
Ligand SA6 Z 300



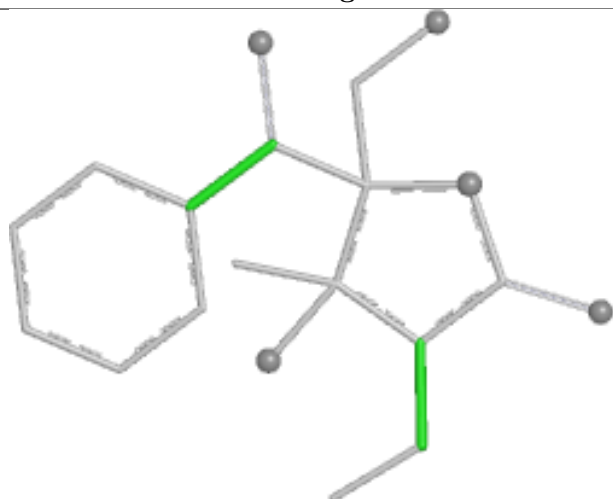
Ligand SA6 J 300



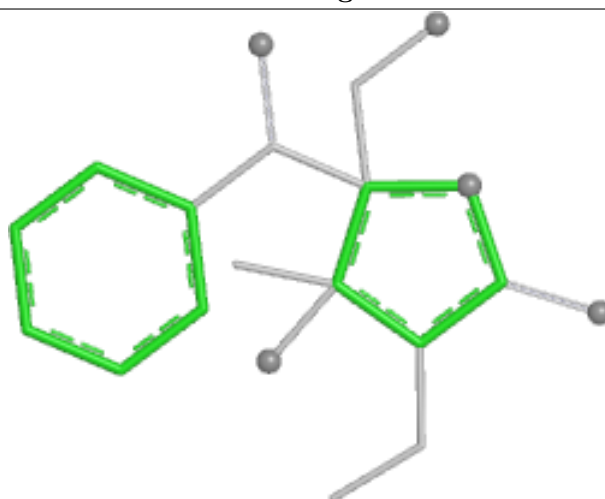
Bond lengths



Bond angles

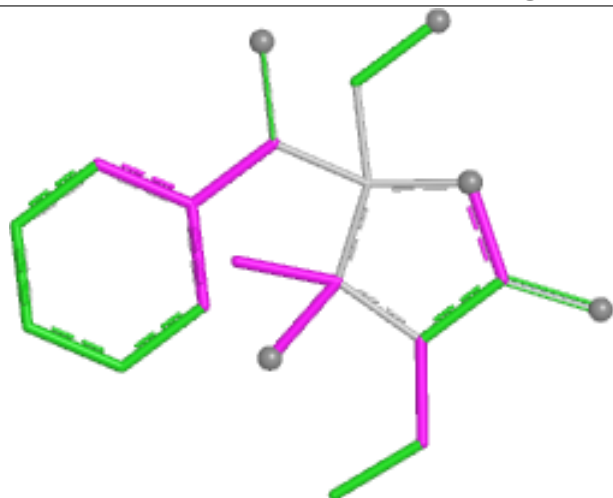


Torsions

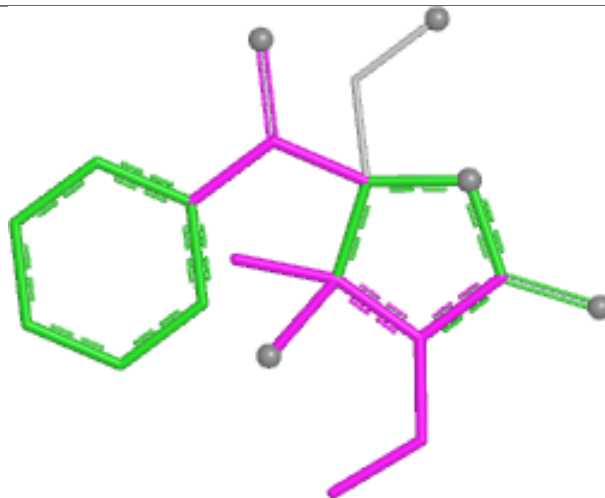


Rings

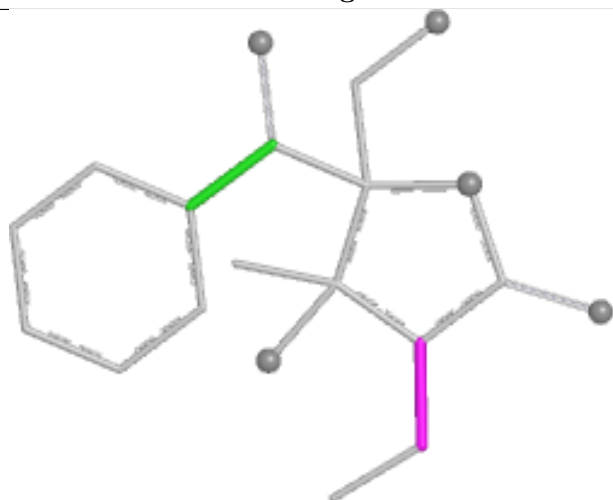
Ligand SA6 L 300



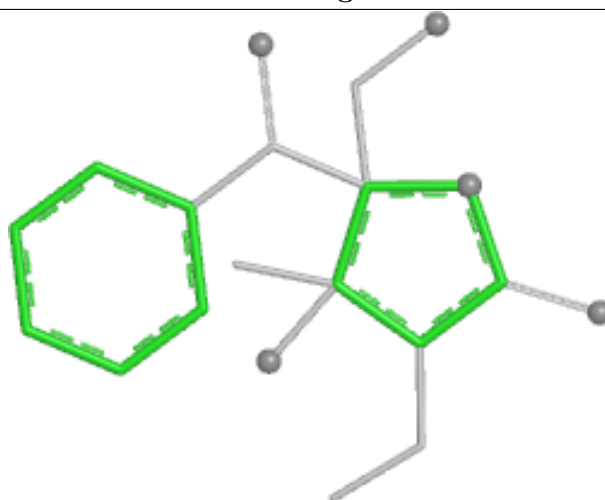
Bond lengths



Bond angles

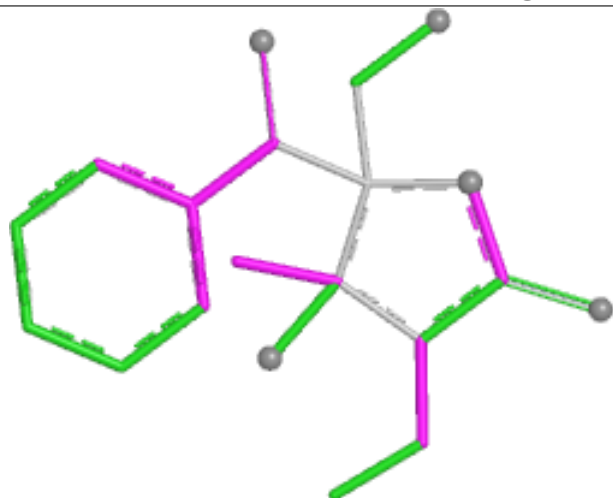


Torsions

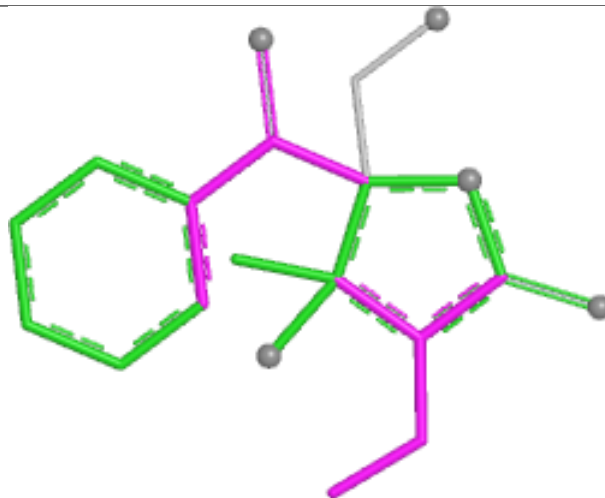


Rings

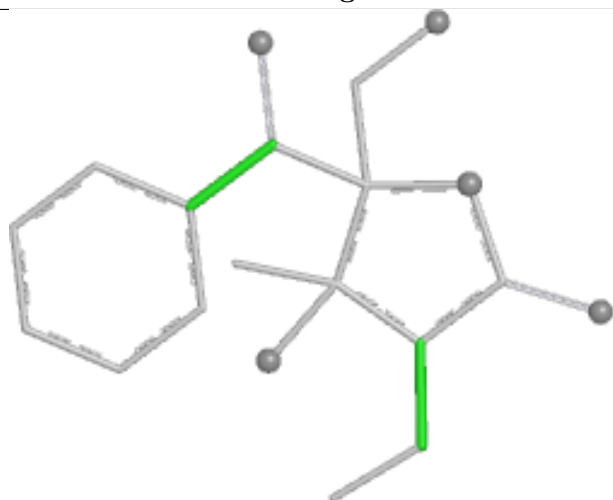
Ligand SA6 R 300



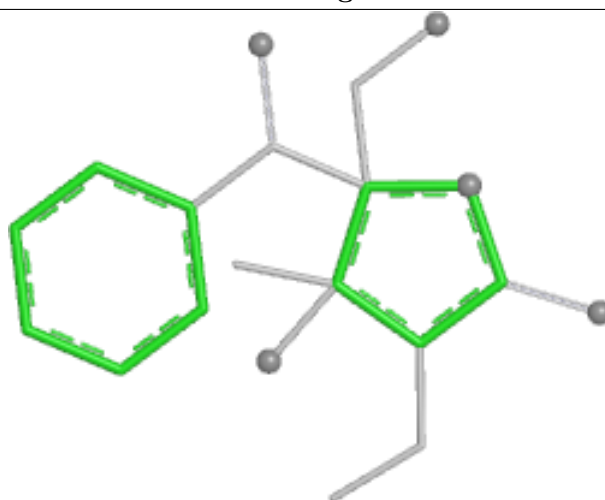
Bond lengths



Bond angles

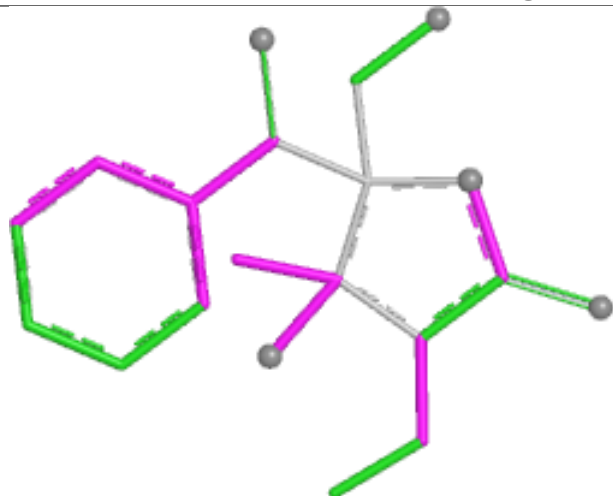


Torsions

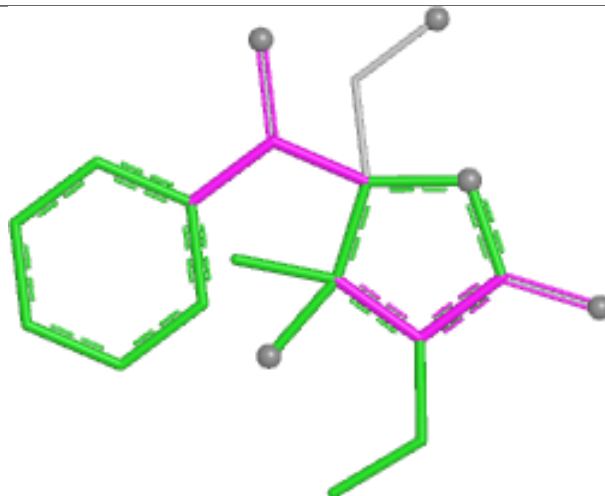


Rings

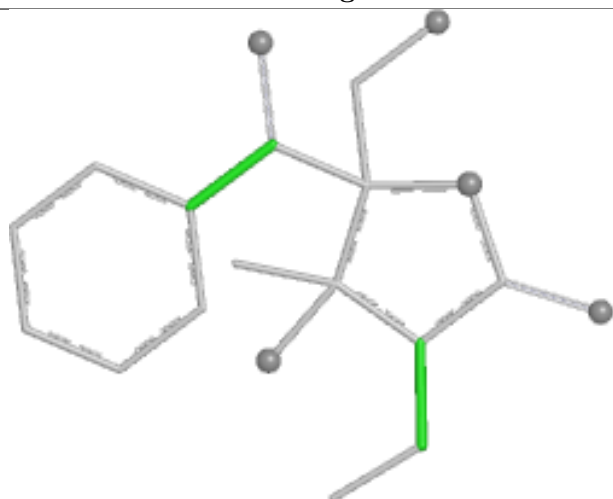
Ligand SA6 T 300



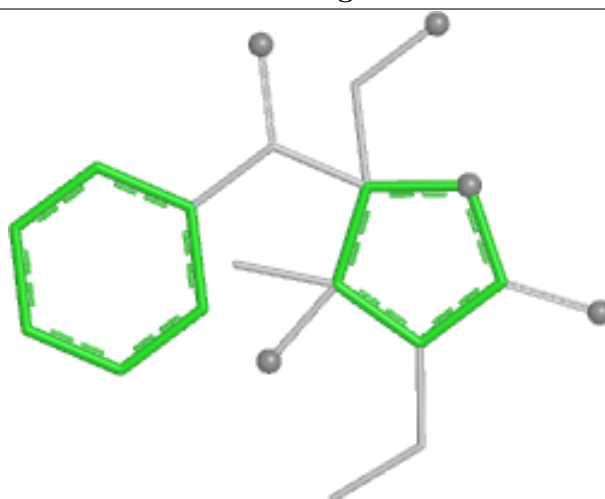
Bond lengths



Bond angles

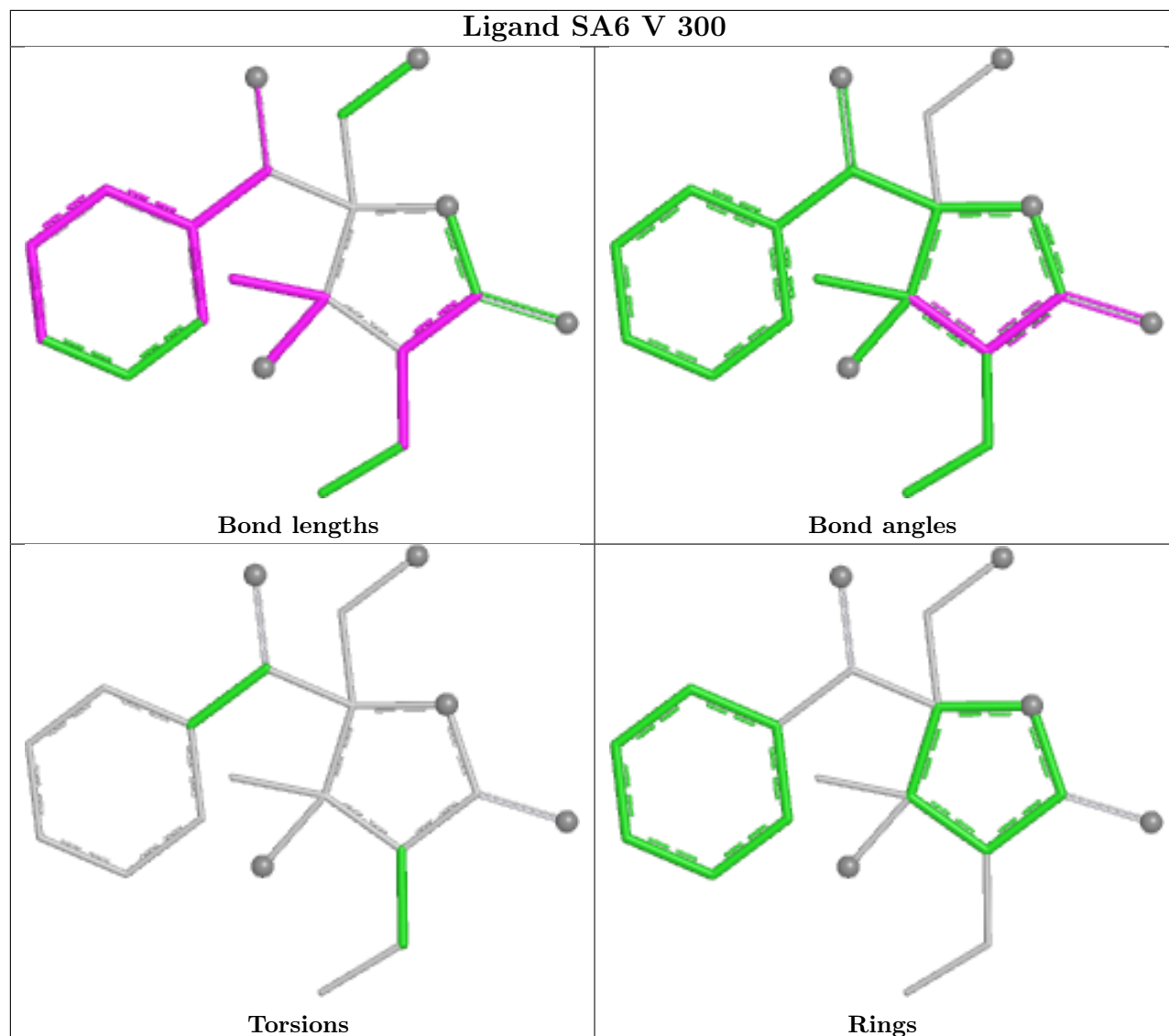


Torsions

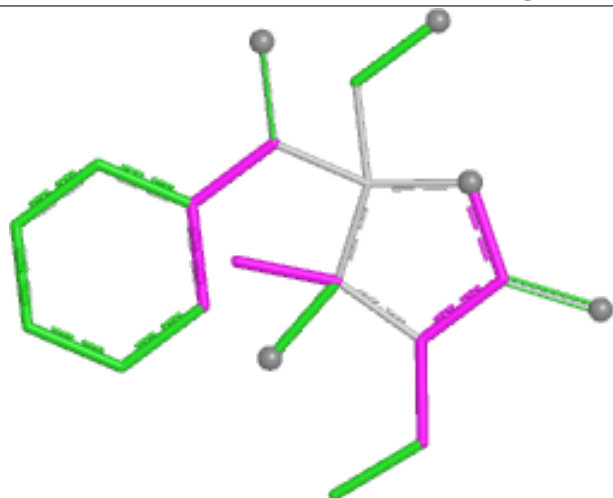


Rings

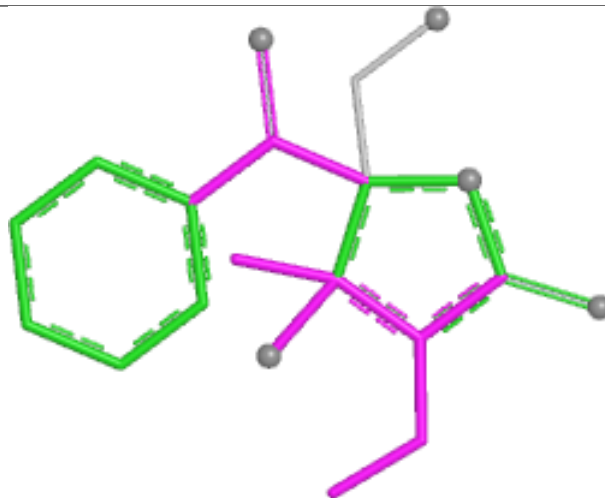
Ligand SA6 V 300



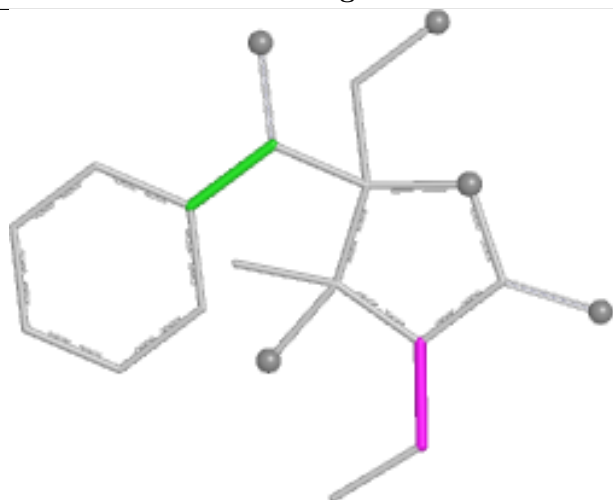
Ligand SA6 C 300



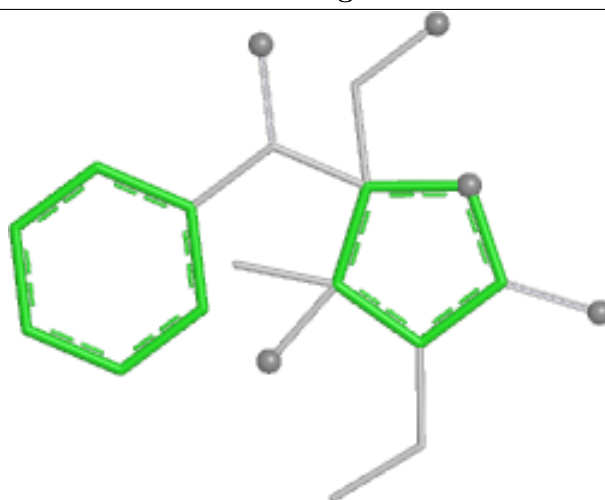
Bond lengths



Bond angles

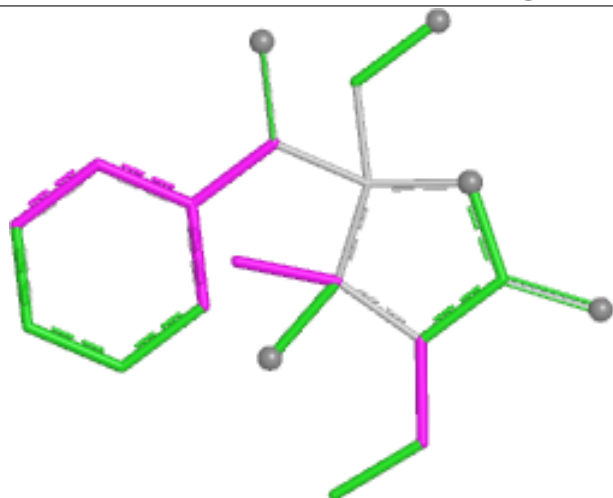


Torsions

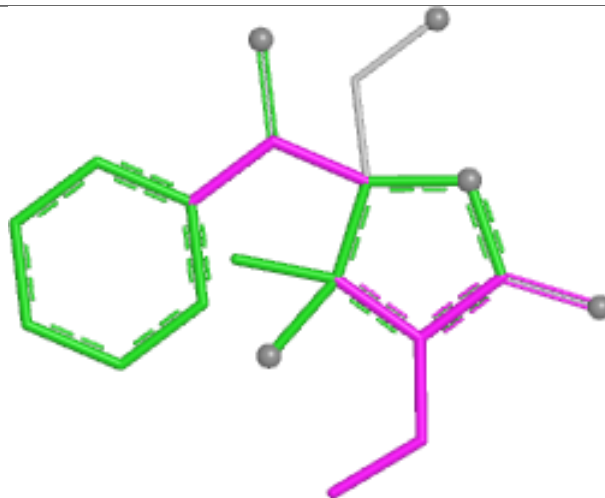


Rings

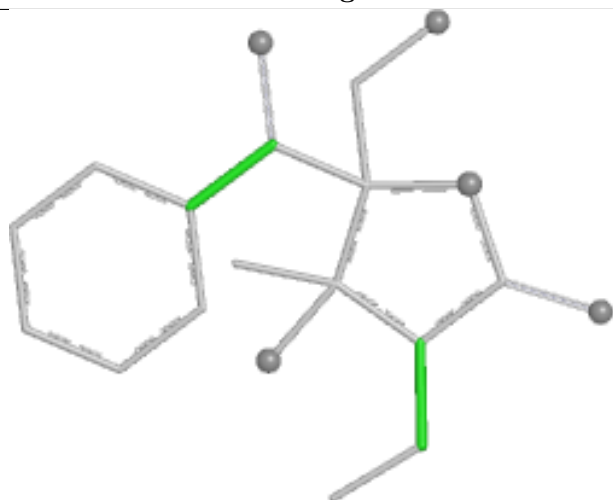
Ligand SA6 P 300



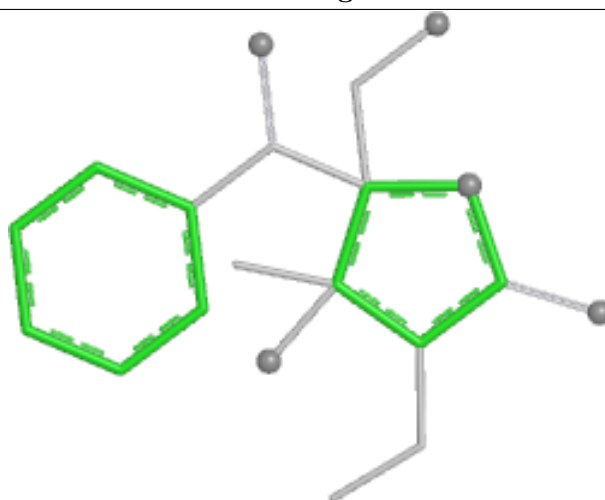
Bond lengths



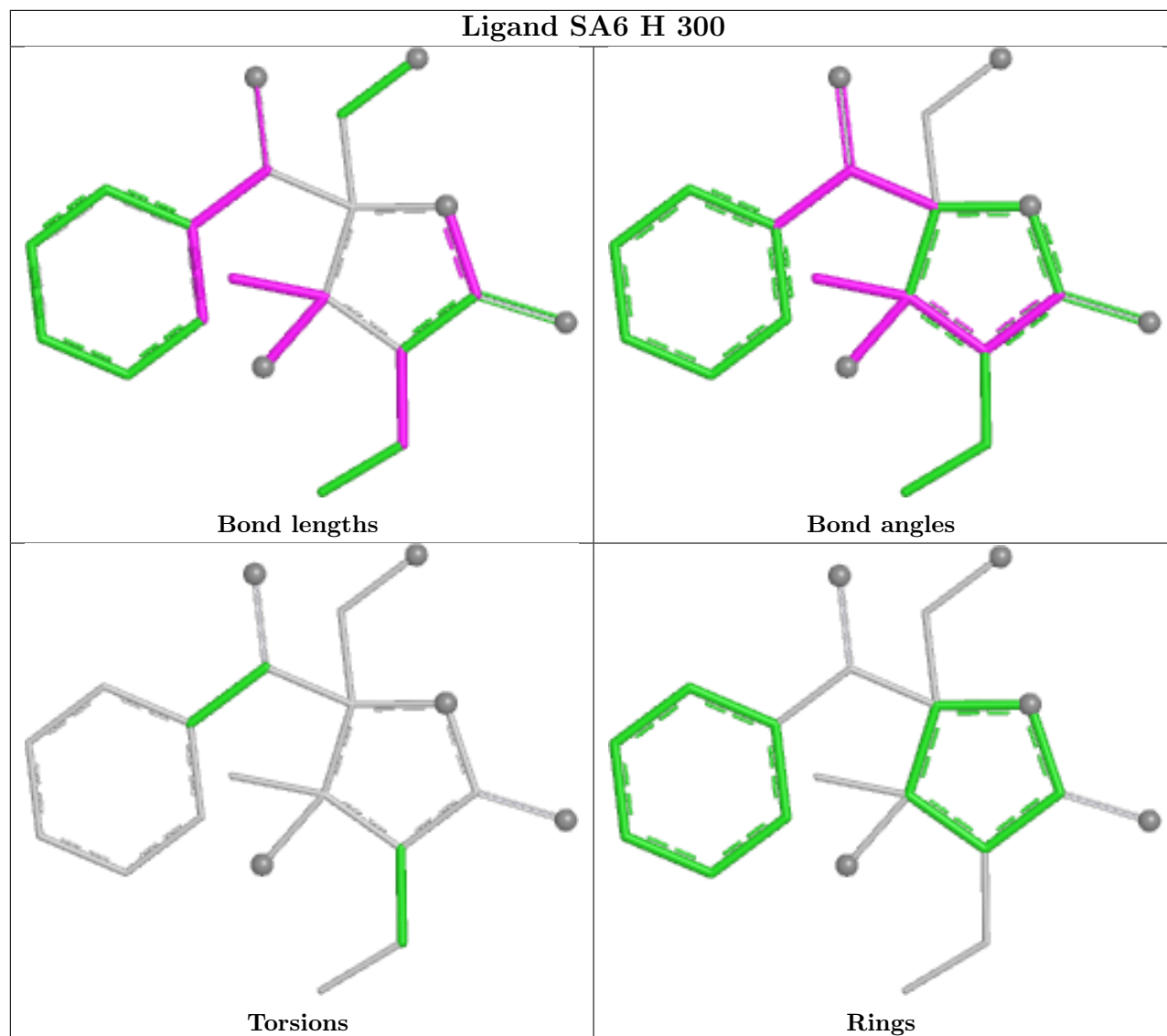
Bond angles



Torsions



Rings



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	1	215/248 (86%)	0.82	28 (13%) 7 5	19, 48, 88, 109	0
1	A	215/248 (86%)	1.05	46 (21%) 2 2	20, 54, 91, 107	0
1	B	213/248 (85%)	0.84	28 (13%) 7 5	20, 49, 88, 106	0
1	D	214/248 (86%)	1.76	93 (43%) 0 0	20, 65, 98, 110	0
1	F	220/248 (88%)	0.87	29 (13%) 7 5	17, 48, 86, 104	0
1	I	216/248 (87%)	0.96	33 (15%) 5 4	18, 52, 92, 108	0
1	K	216/248 (87%)	0.97	30 (13%) 6 5	21, 55, 92, 107	0
1	M	216/248 (87%)	1.11	47 (21%) 2 1	18, 53, 92, 104	0
1	O	216/248 (87%)	0.87	27 (12%) 8 6	17, 49, 87, 102	0
1	Q	215/248 (86%)	0.91	23 (10%) 11 8	22, 50, 86, 99	0
1	S	216/248 (87%)	1.05	35 (16%) 4 3	20, 56, 91, 104	0
1	U	216/248 (87%)	0.90	30 (13%) 6 5	16, 49, 86, 102	0
1	W	216/248 (87%)	1.37	49 (22%) 2 1	20, 63, 94, 107	0
1	Y	216/248 (87%)	1.22	42 (19%) 3 2	22, 58, 94, 123	0
2	2	223/240 (92%)	-0.39	1 (0%) 88 87	11, 21, 45, 65	0
2	C	222/240 (92%)	-0.39	6 (2%) 56 53	8, 20, 48, 79	0
2	E	223/240 (92%)	-0.41	3 (1%) 75 73	8, 20, 46, 63	0
2	G	222/240 (92%)	-0.34	3 (1%) 73 71	10, 23, 53, 75	0
2	H	222/240 (92%)	-0.38	0 100 100	9, 23, 50, 71	0
2	J	222/240 (92%)	-0.39	1 (0%) 87 85	9, 21, 49, 70	0
2	L	223/240 (92%)	-0.31	5 (2%) 62 59	8, 21, 46, 66	0
2	N	222/240 (92%)	-0.42	2 (0%) 81 79	8, 21, 47, 79	0
2	P	222/240 (92%)	-0.38	0 100 100	10, 23, 49, 73	0
2	R	239/240 (99%)	-0.39	5 (2%) 63 60	8, 20, 55, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	T	223/240 (92%)	-0.25	0 100 100	10, 24, 53, 72	0
2	V	239/240 (99%)	-0.38	5 (2%) 63 60	8, 20, 63, 91	0
2	X	223/240 (92%)	-0.32	3 (1%) 75 73	10, 24, 56, 73	0
2	Z	223/240 (92%)	-0.29	2 (0%) 81 79	11, 24, 52, 69	0
All	All	6168/6832 (90%)	0.33	576 (9%) 14 12	8, 33, 84, 123	0

The worst 5 of 576 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	GLY	6.8
1	Y	9	PRO	6.3
1	M	203	LEU	5.7
1	O	203	LEU	5.5
1	I	203	LEU	5.4

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
3	DMF	D	253	5/5	0.54	0.32	20,20,20,20	0
3	DMF	O	251	5/5	0.54	0.26	20,20,20,20	0
3	DMF	K	251	5/5	0.62	0.29	63,63,64,64	0
3	DMF	2	57	5/5	0.63	0.24	54,56,57,57	0
3	DMF	V	39	5/5	0.64	0.23	60,60,61,61	0
3	DMF	E	28	5/5	0.66	0.28	61,61,63,64	0
3	DMF	H	66	5/5	0.66	0.25	69,69,69,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DMF	M	251	5/5	0.67	0.27	64,64,66,66	0
3	DMF	K	252	5/5	0.68	0.22	80,81,82,82	0
3	DMF	2	112	5/5	0.68	0.36	20,20,20,20	0
3	DMF	J	45	5/5	0.69	0.23	41,43,45,46	0
3	DMF	Z	114	5/5	0.69	0.36	20,20,20,20	0
3	DMF	X	40	5/5	0.71	0.28	84,85,85,85	0
3	DMF	P	60	5/5	0.71	0.28	68,69,69,69	0
3	DMF	P	51	5/5	0.72	0.25	75,76,76,77	0
3	DMF	Y	251	5/5	0.72	0.35	20,20,20,20	0
3	DMF	H	117	5/5	0.72	0.28	20,20,20,20	0
3	DMF	2	52	5/5	0.72	0.28	77,77,78,78	0
3	DMF	U	249	5/5	0.72	0.22	40,40,44,45	0
3	DMF	P	33	5/5	0.72	0.23	65,66,66,66	0
3	DMF	N	104	5/5	0.73	0.34	20,20,20,20	0
3	DMF	T	102	5/5	0.73	0.28	20,20,20,20	0
3	DMF	V	82	5/5	0.73	0.25	45,47,47,48	0
3	DMF	J	110	5/5	0.74	0.30	20,20,20,20	0
3	DMF	L	36	5/5	0.74	0.22	41,42,43,43	0
3	DMF	Z	54	5/5	0.74	0.24	58,59,60,61	0
3	DMF	M	250	5/5	0.74	0.24	60,61,61,62	0
3	DMF	R	95	5/5	0.74	0.29	20,20,20,20	0
3	DMF	V	120	5/5	0.74	0.29	20,20,20,20	0
3	DMF	W	249	5/5	0.74	0.23	69,70,71,72	0
3	DMF	C	121	5/5	0.75	0.23	20,20,20,20	0
3	DMF	2	49	5/5	0.75	0.26	57,57,57,58	0
3	DMF	G	62	5/5	0.75	0.26	72,73,73,74	0
3	DMF	T	10	5/5	0.75	0.27	71,72,72,74	0
3	DMF	C	103	5/5	0.75	0.31	20,20,20,20	0
3	DMF	G	24	5/5	0.76	0.24	65,67,68,68	0
3	DMF	2	108	5/5	0.76	0.32	20,20,20,20	0
3	DMF	J	123	5/5	0.76	0.31	20,20,20,20	0
3	DMF	P	86	5/5	0.77	0.31	20,20,20,20	0
3	DMF	X	122	5/5	0.77	0.23	20,20,20,20	0
3	DMF	N	93	5/5	0.77	0.26	20,20,20,20	0
3	DMF	Z	18	5/5	0.77	0.25	55,55,55,55	0
3	DMF	D	251	5/5	0.77	0.25	94,95,96,96	0
3	DMF	Z	94	5/5	0.77	0.33	20,20,20,20	0
3	DMF	G	98	5/5	0.78	0.30	20,20,20,20	0
3	DMF	G	111	5/5	0.78	0.28	20,20,20,20	0
3	DMF	T	113	5/5	0.78	0.34	20,20,20,20	0
3	DMF	G	119	5/5	0.78	0.33	20,20,20,20	0
3	DMF	D	250	5/5	0.78	0.22	61,63,64,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DMF	H	72	5/5	0.78	0.31	20,20,20,20	0
3	DMF	L	81	5/5	0.78	0.25	59,60,61,62	0
3	DMF	C	63	5/5	0.78	0.24	58,59,59,60	0
3	DMF	D	249	5/5	0.78	0.17	53,53,53,54	0
3	DMF	S	250	5/5	0.78	0.20	59,59,60,61	0
3	DMF	K	250	5/5	0.79	0.25	77,78,79,79	0
3	DMF	B	249	5/5	0.79	0.20	50,51,51,53	0
3	DMF	C	88	5/5	0.79	0.34	20,20,20,20	0
3	DMF	R	59	5/5	0.80	0.29	54,55,57,57	0
3	DMF	R	89	5/5	0.80	0.29	20,20,20,20	0
3	DMF	L	50	5/5	0.80	0.23	55,56,57,57	0
3	DMF	T	29	5/5	0.81	0.23	76,76,76,76	0
3	DMF	H	91	5/5	0.81	0.29	20,20,20,20	0
3	DMF	G	70	5/5	0.81	0.21	37,38,41,41	0
3	DMF	T	115	5/5	0.81	0.28	20,20,20,20	0
3	DMF	M	249	5/5	0.81	0.17	46,47,48,48	0
3	DMF	E	53	5/5	0.81	0.20	56,57,58,59	0
3	DMF	Q	251	5/5	0.81	0.18	53,53,56,57	0
3	DMF	A	250	5/5	0.82	0.16	39,41,42,44	0
3	DMF	E	100	5/5	0.82	0.31	20,20,20,20	0
3	DMF	D	252	5/5	0.82	0.25	20,20,20,20	0
3	DMF	P	2	5/5	0.82	0.25	62,62,64,64	0
3	DMF	N	22	5/5	0.82	0.14	44,45,49,50	0
3	DMF	G	77	5/5	0.83	0.18	49,50,50,51	0
3	DMF	E	73	5/5	0.83	0.45	120,120,121,121	0
3	DMF	Q	250	5/5	0.83	0.19	84,85,85,86	0
3	DMF	C	38	5/5	0.83	0.17	64,64,65,65	0
3	DMF	P	14	5/5	0.83	0.25	56,58,58,59	0
3	DMF	X	41	5/5	0.83	0.21	61,61,62,62	0
3	DMF	K	249	5/5	0.83	0.16	49,50,51,52	0
3	DMF	2	101	5/5	0.83	0.24	20,20,20,20	0
3	DMF	Y	250	5/5	0.83	0.13	42,42,44,44	0
3	DMF	F	249	5/5	0.83	0.30	90,91,91,91	0
3	DMF	E	75	5/5	0.84	0.20	64,64,64,65	0
3	DMF	I	250	5/5	0.84	0.17	41,41,42,42	0
3	DMF	C	47	5/5	0.84	0.21	61,62,62,62	0
3	DMF	H	43	5/5	0.84	0.27	82,82,83,83	0
3	DMF	R	80	5/5	0.84	0.20	74,75,76,76	0
3	DMF	V	42	5/5	0.84	0.27	58,58,59,61	0
3	DMF	F	250	5/5	0.85	0.18	56,56,58,59	0
3	DMF	G	64	5/5	0.85	0.26	66,68,68,69	0
3	DMF	F	251	5/5	0.85	0.20	54,54,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DMF	B	250	5/5	0.85	0.20	53,53,55,55	0
3	DMF	P	107	5/5	0.85	0.26	20,20,20,20	0
3	DMF	X	16	5/5	0.85	0.24	86,86,86,86	0
3	DMF	I	249	5/5	0.85	0.14	40,42,42,43	0
3	DMF	X	15	5/5	0.86	0.20	66,67,68,70	0
3	DMF	H	71	5/5	0.86	0.17	54,55,55,56	0
3	DMF	P	56	5/5	0.86	0.18	59,60,60,61	0
3	DMF	2	4	5/5	0.86	0.21	62,62,62,62	0
3	DMF	V	83	5/5	0.86	0.18	58,59,60,62	0
3	DMF	V	109	5/5	0.86	0.31	20,20,20,20	0
3	DMF	Y	249	5/5	0.86	0.19	62,64,64,65	0
3	DMF	T	84	5/5	0.86	0.21	59,59,60,62	0
3	DMF	C	69	5/5	0.86	0.19	48,48,50,50	0
3	DMF	W	250	5/5	0.86	0.18	63,63,64,64	0
3	DMF	N	118	5/5	0.87	0.29	20,20,20,20	0
3	DMF	N	90	5/5	0.87	0.27	20,20,20,20	0
3	DMF	U	250	5/5	0.87	0.15	49,50,51,51	0
3	DMF	V	32	5/5	0.88	0.21	73,74,74,74	0
3	DMF	Q	249	5/5	0.88	0.16	48,48,49,49	0
3	DMF	R	92	5/5	0.88	0.25	20,20,20,20	0
3	DMF	V	27	5/5	0.88	0.22	63,63,64,64	0
3	DMF	S	249	5/5	0.89	0.15	54,54,55,56	0
3	DMF	L	97	5/5	0.89	0.21	20,20,20,20	0
3	DMF	V	116	5/5	0.89	0.23	20,20,20,20	0
3	DMF	G	12	5/5	0.89	0.21	60,61,62,63	0
3	DMF	2	87	5/5	0.89	0.26	20,20,20,20	0
3	DMF	O	250	5/5	0.89	0.14	44,45,46,48	0
3	DMF	M	252	5/5	0.89	0.20	20,20,20,20	0
3	DMF	1	249	5/5	0.89	0.12	45,47,48,49	0
3	DMF	A	249	5/5	0.90	0.14	44,44,44,44	0
3	DMF	O	249	5/5	0.90	0.15	39,40,41,41	0
3	DMF	E	20	5/5	0.92	0.23	76,77,77,78	0
4	SA6	H	300	20/20	0.92	0.08	16,21,23,24	0
4	SA6	L	300	20/20	0.93	0.08	16,19,26,27	0
4	SA6	E	300	20/20	0.94	0.07	12,18,21,24	0
4	SA6	N	300	20/20	0.94	0.07	13,18,23,26	0
4	SA6	V	300	20/20	0.94	0.07	15,17,21,22	0
4	SA6	2	300	20/20	0.94	0.08	17,20,28,29	0
4	SA6	R	300	20/20	0.95	0.07	12,21,24,31	0
4	SA6	T	300	20/20	0.95	0.07	17,22,28,29	0
4	SA6	G	300	20/20	0.95	0.07	11,19,22,24	0
4	SA6	X	300	20/20	0.95	0.06	15,17,23,25	0

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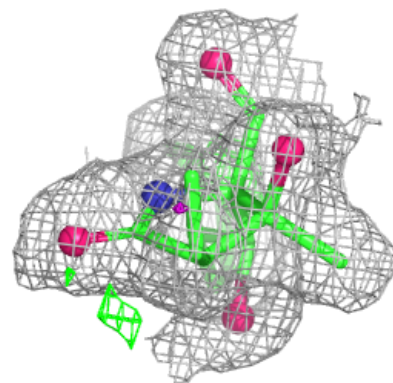
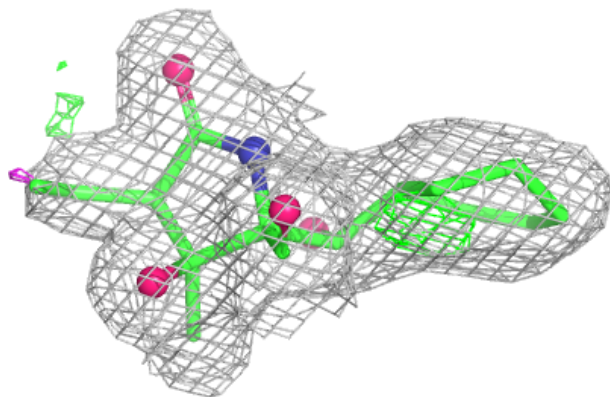
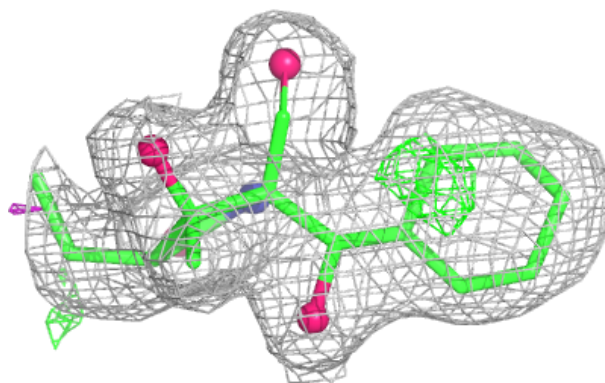
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SA6	Z	300	20/20	0.95	0.06	17,19,22,25	0
4	SA6	C	300	20/20	0.95	0.06	16,19,24,24	0
4	SA6	J	300	20/20	0.96	0.06	12,19,24,27	0
4	SA6	P	300	20/20	0.96	0.06	16,20,28,29	0

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.

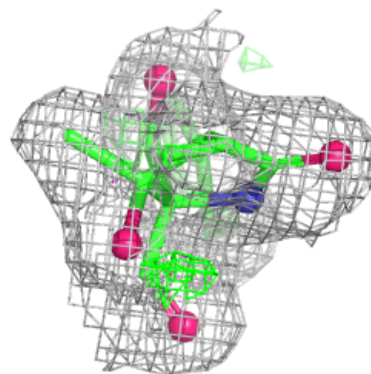
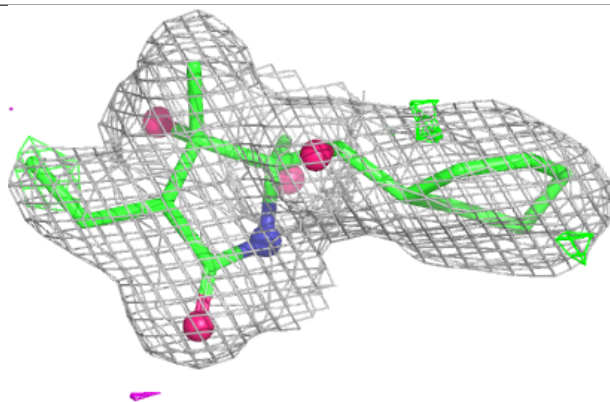
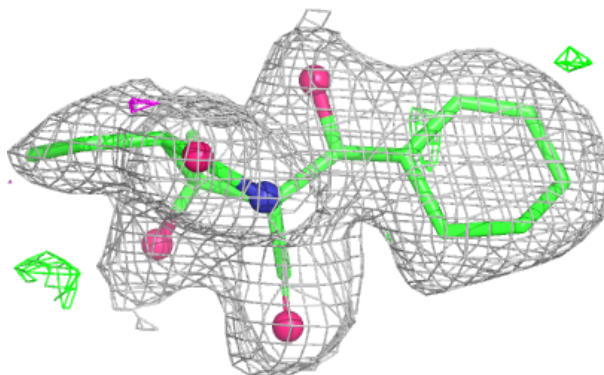
Electron density around SA6 H 300:

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

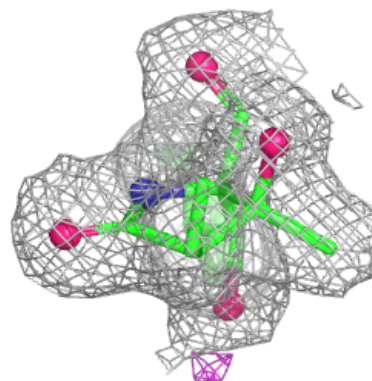
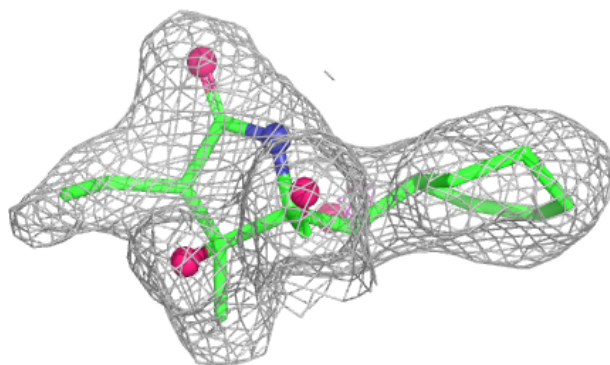
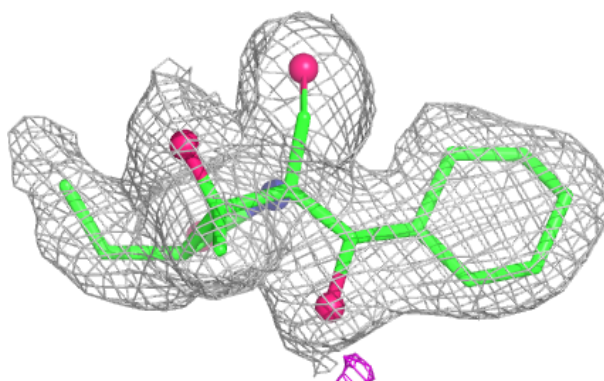


Electron density around SA6 L 300:

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

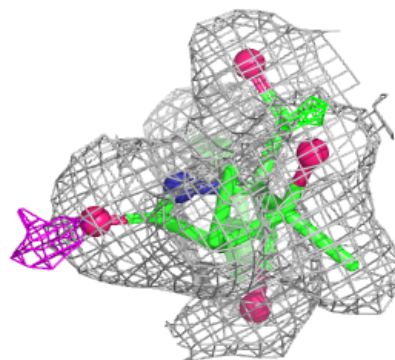
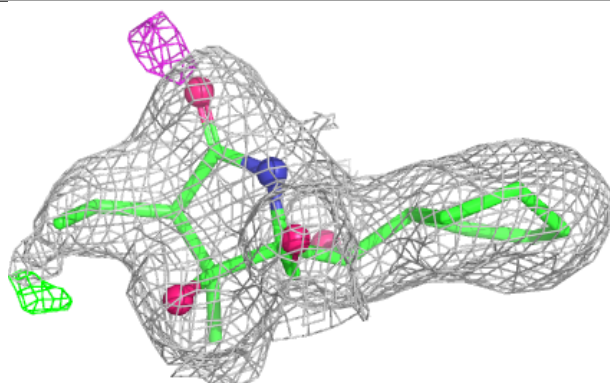
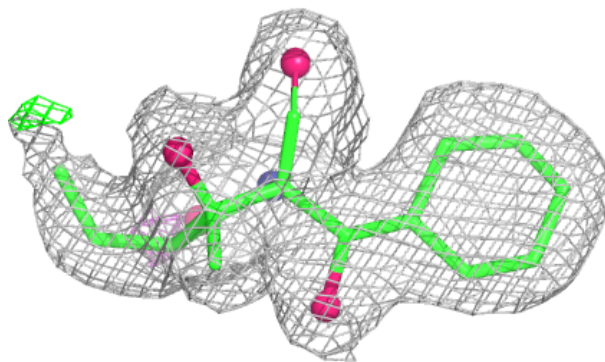
**Electron density around SA6 E 300:**

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

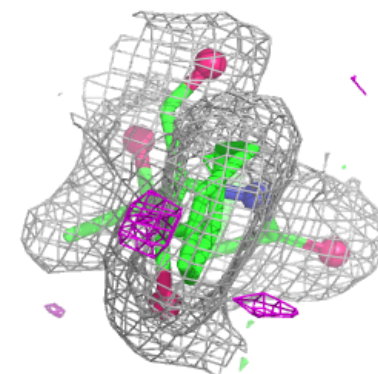
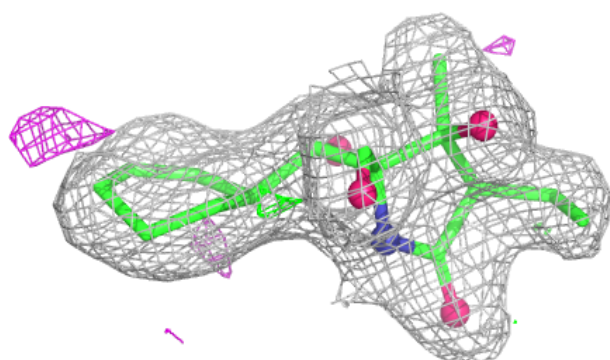
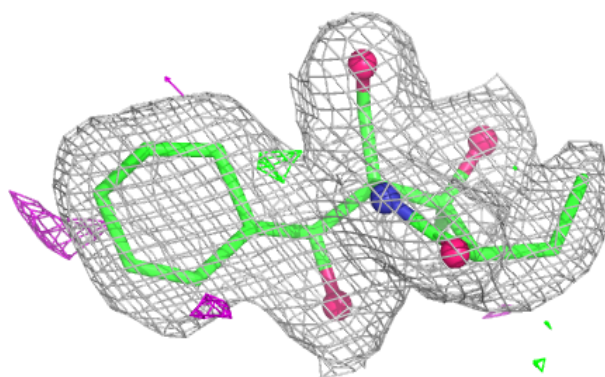


Electron density around SA6 N 300:

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

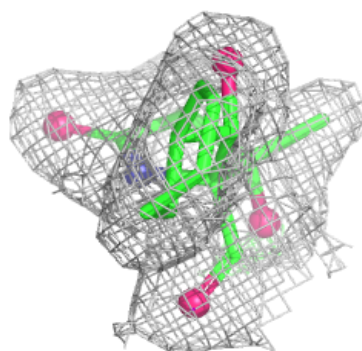
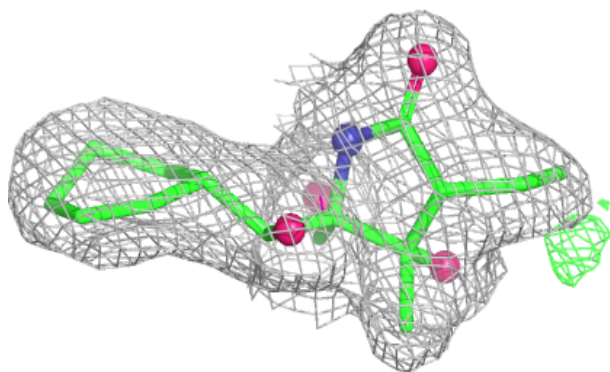
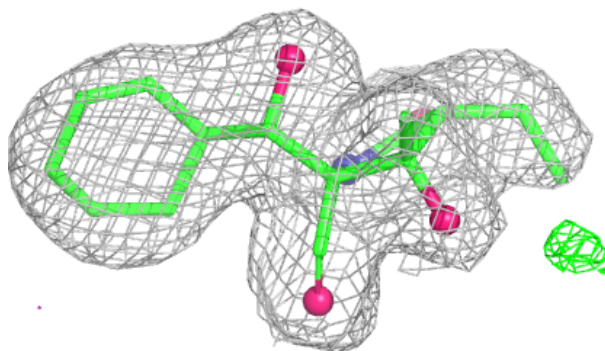
**Electron density around SA6 V 300:**

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

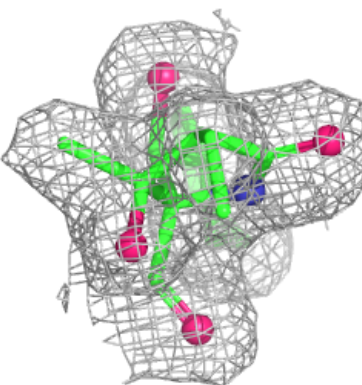
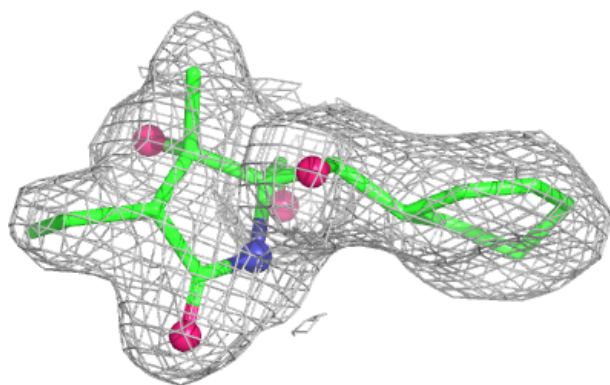
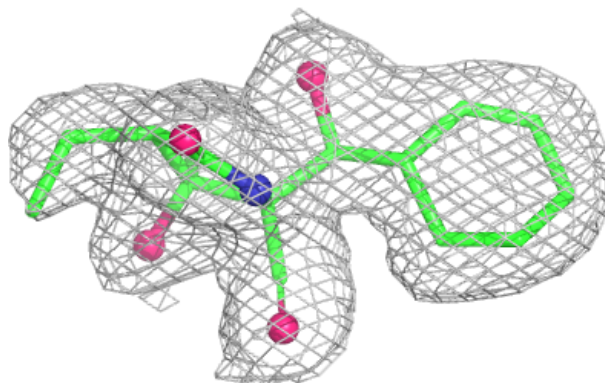


Electron density around SA6 2 300:

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

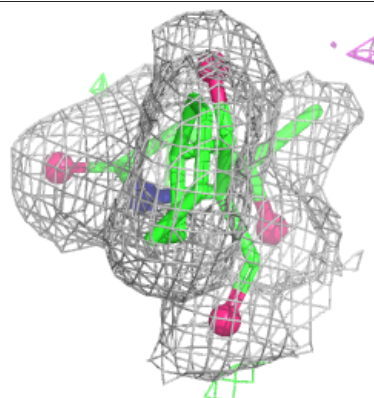
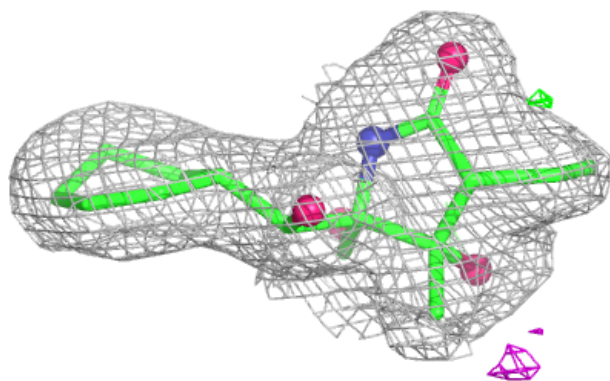
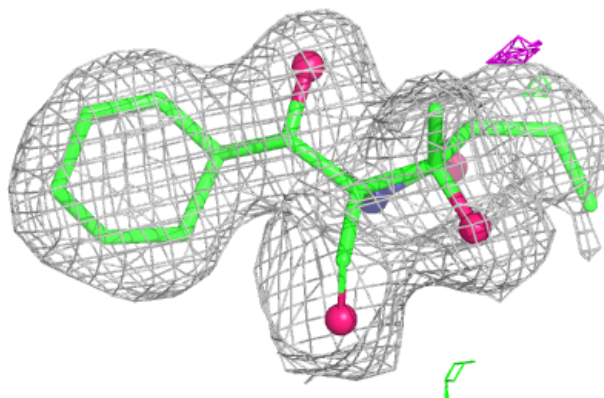
**Electron density around SA6 R 300:**

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

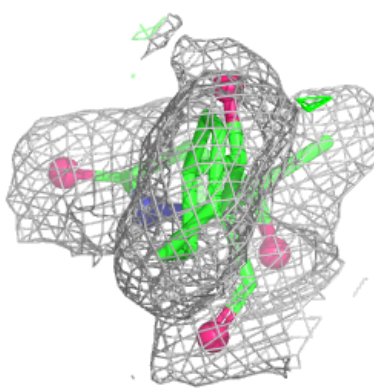
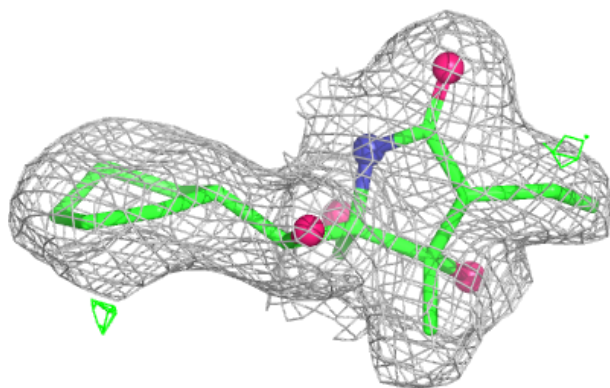
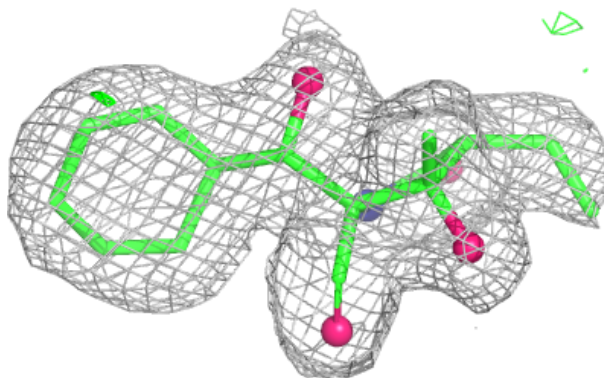


Electron density around SA6 T 300:

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

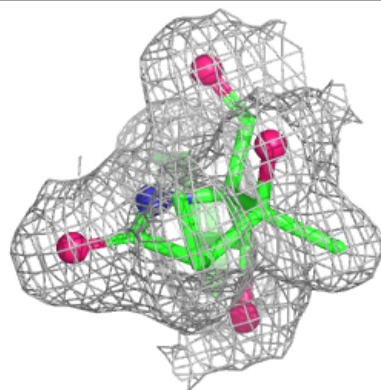
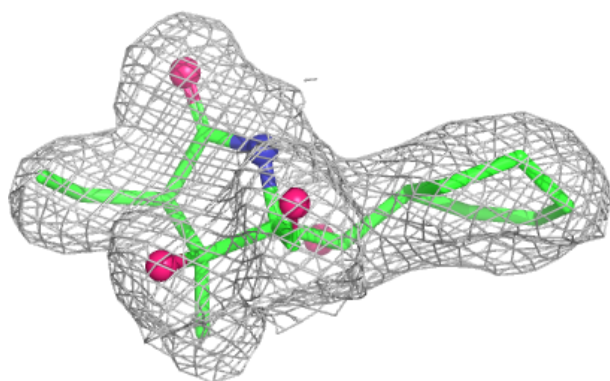
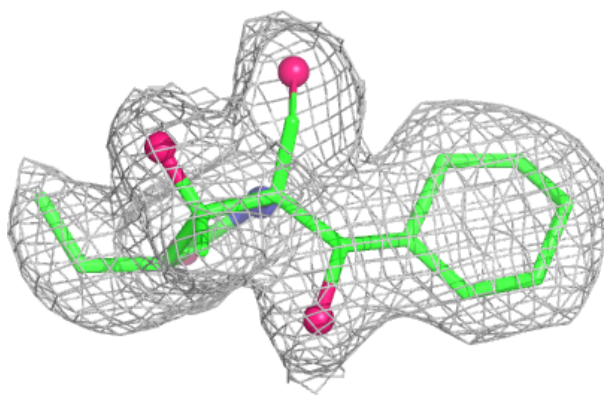
**Electron density around SA6 G 300:**

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

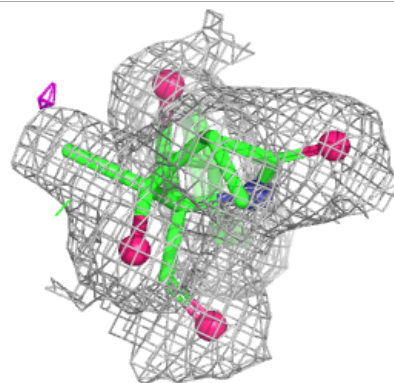
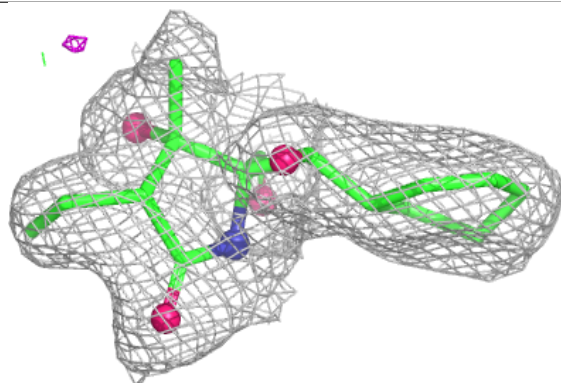
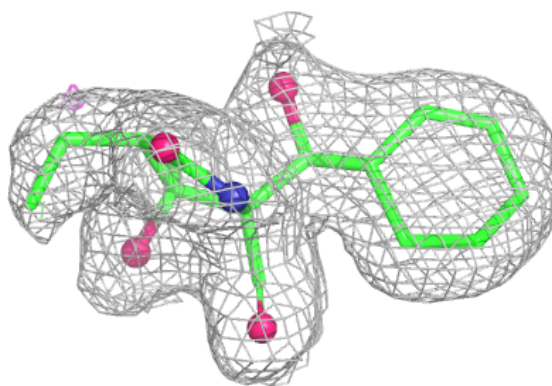


Electron density around SA6 X 300:

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

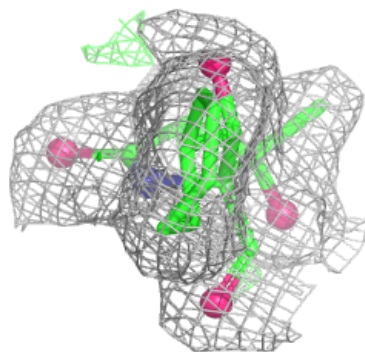
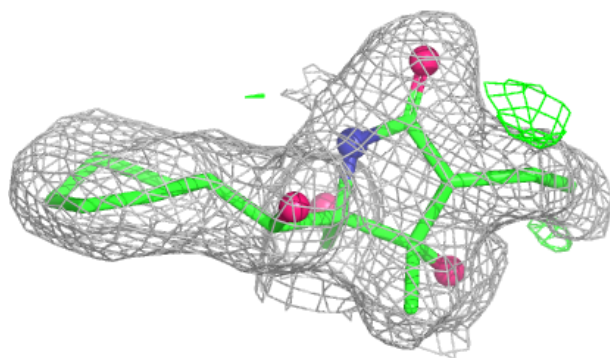
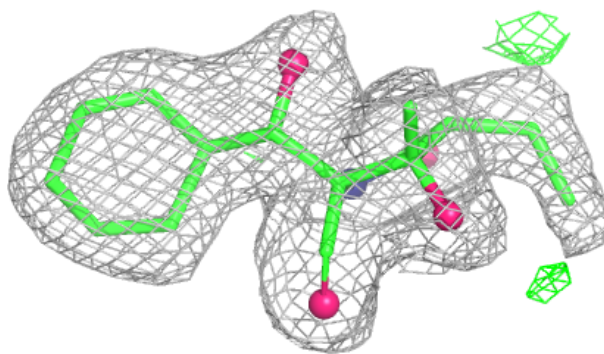
**Electron density around SA6 Z 300:**

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

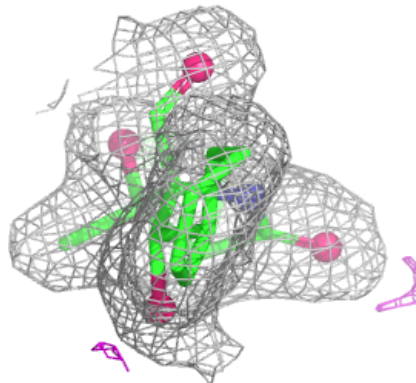
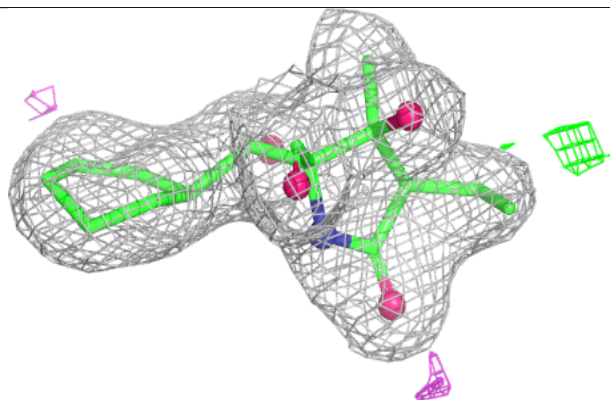
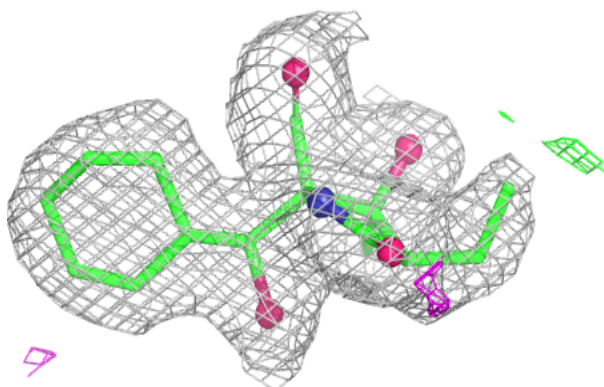


Electron density around SA6 C 300:

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

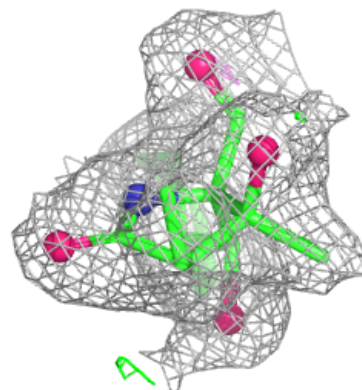
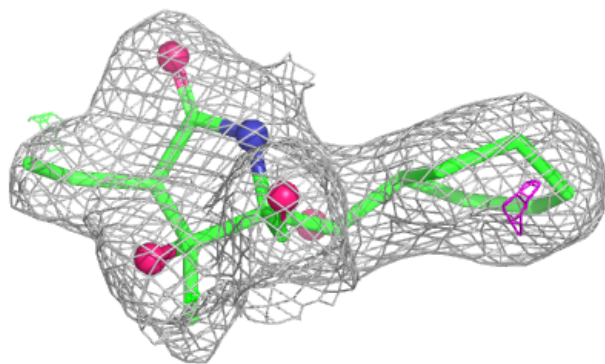
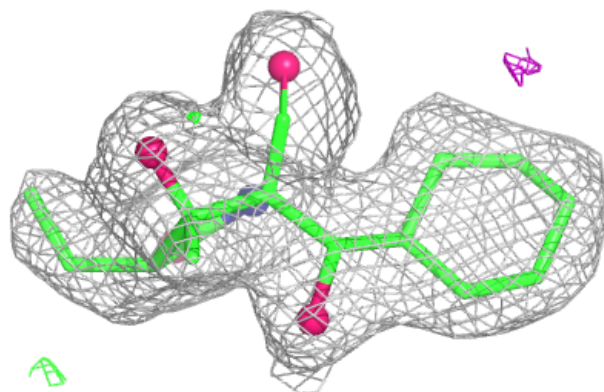
**Electron density around SA6 J 300:**

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



Electron density around SA6 P 300:

$2mF_o-DF_c$ (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.