wwPDB X-ray Structure Validation Summary Report (i)

Mar 1, 2026 – 12:08 AM UTC

PDB ID	:	5THO / pdb_00005tho
Title	:	Crystal Structure of Mycobacterium Tuberculosis Proteasome in complex with N,C-capped Dipeptide Inhibitor PKS2205
Authors	:	Hsu, H.C.; Li, H.
Deposited on	:	2016-09-30
Resolution	:	3.00 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 (i) 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 (i)) were used in the production of this report:

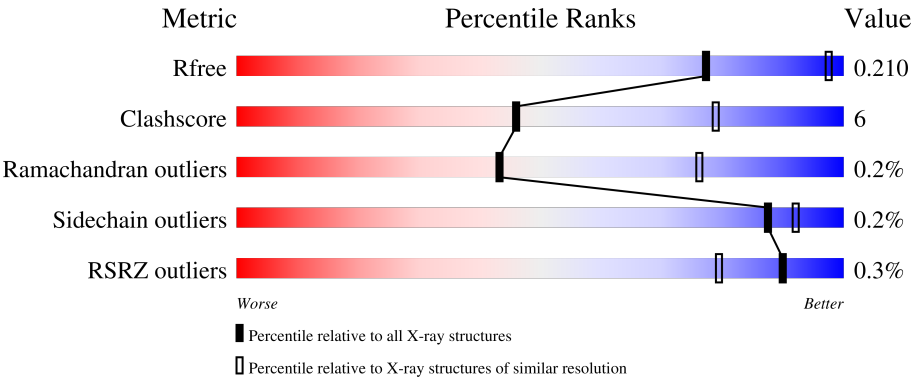
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 <=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	240	64% 27% 9%
1	B	240	69% 20% 10%
1	C	240	71% 19% 10%
1	D	240	73% 16% 10%
1	E	240	73% 17% 9%

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Mol	Chain	Length	Quality of chain
1	F	240	74% 16% 10%
1	G	240	% 69% 21% 9%
1	O	240	78% 13% 9%
1	P	240	% 72% 18% 10%
1	Q	240	73% 16% 10%
1	R	240	73% 17% 10%
1	S	240	76% 15% 8%
1	T	240	% 74% 16% 10%
1	U	240	75% 15% 10%
2	H	240	84% 8% 8%
2	I	240	89% 8%
2	J	240	82% 10% 8%
2	K	240	85% 8% 7%
2	L	240	86% 7% 7%
2	M	240	86% 7% 7%
2	N	240	82% 10% 8%
2	V	240	84% 9% 7%
2	W	240	85% 8% 7%
2	X	240	84% 9% 8%
2	Y	240	83% 10% 7%
2	Z	240	82% 11% 8%
2	a	240	84% 9% 7%
2	b	240	87% 6% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 47201 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	218	Total	C	N	O	S	0	0	0
			1677	1050	306	317	4			
1	B	215	Total	C	N	O	S	0	0	0
			1660	1041	303	312	4			
1	C	217	Total	C	N	O	S	0	0	0
			1672	1047	305	316	4			
1	D	216	Total	C	N	O	S	0	0	0
			1663	1041	304	314	4			
1	E	218	Total	C	N	O	S	0	0	0
			1677	1050	306	317	4			
1	F	217	Total	C	N	O	S	0	0	0
			1670	1046	305	315	4			
1	G	218	Total	C	N	O	S	0	0	0
			1677	1050	306	317	4			
1	O	218	Total	C	N	O	S	0	0	0
			1677	1050	306	317	4			
1	P	217	Total	C	N	O	S	0	0	0
			1671	1047	305	315	4			
1	Q	216	Total	C	N	O	S	0	0	0
			1668	1045	304	315	4			
1	R	217	Total	C	N	O	S	0	0	0
			1670	1046	305	315	4			
1	S	221	Total	C	N	O	S	0	0	0
			1701	1064	310	323	4			
1	T	217	Total	C	N	O	S	0	0	0
			1671	1047	305	315	4			
1	U	216	Total	C	N	O	S	0	0	0
			1664	1043	304	313	4			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	initiating methionine	UNP A5U4D5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	MET	-	initiating methionine	UNP A5U4D5
C	9	MET	-	initiating methionine	UNP A5U4D5
D	9	MET	-	initiating methionine	UNP A5U4D5
E	9	MET	-	initiating methionine	UNP A5U4D5
F	9	MET	-	initiating methionine	UNP A5U4D5
G	9	MET	-	initiating methionine	UNP A5U4D5
O	9	MET	-	initiating methionine	UNP A5U4D5
P	9	MET	-	initiating methionine	UNP A5U4D5
Q	9	MET	-	initiating methionine	UNP A5U4D5
R	9	MET	-	initiating methionine	UNP A5U4D5
S	9	MET	-	initiating methionine	UNP A5U4D5
T	9	MET	-	initiating methionine	UNP A5U4D5
U	9	MET	-	initiating methionine	UNP A5U4D5

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	I	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	K	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	L	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	M	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	V	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	W	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	X	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	Y	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	Z	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	a	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	b	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
H	235	HIS	-	expression tag	UNP A5U4D6
H	236	HIS	-	expression tag	UNP A5U4D6
H	237	HIS	-	expression tag	UNP A5U4D6
H	238	HIS	-	expression tag	UNP A5U4D6
H	239	HIS	-	expression tag	UNP A5U4D6
H	240	HIS	-	expression tag	UNP A5U4D6
I	235	HIS	-	expression tag	UNP A5U4D6
I	236	HIS	-	expression tag	UNP A5U4D6
I	237	HIS	-	expression tag	UNP A5U4D6
I	238	HIS	-	expression tag	UNP A5U4D6
I	239	HIS	-	expression tag	UNP A5U4D6
I	240	HIS	-	expression tag	UNP A5U4D6
J	235	HIS	-	expression tag	UNP A5U4D6
J	236	HIS	-	expression tag	UNP A5U4D6
J	237	HIS	-	expression tag	UNP A5U4D6
J	238	HIS	-	expression tag	UNP A5U4D6
J	239	HIS	-	expression tag	UNP A5U4D6
J	240	HIS	-	expression tag	UNP A5U4D6
K	235	HIS	-	expression tag	UNP A5U4D6
K	236	HIS	-	expression tag	UNP A5U4D6
K	237	HIS	-	expression tag	UNP A5U4D6
K	238	HIS	-	expression tag	UNP A5U4D6
K	239	HIS	-	expression tag	UNP A5U4D6
K	240	HIS	-	expression tag	UNP A5U4D6
L	235	HIS	-	expression tag	UNP A5U4D6
L	236	HIS	-	expression tag	UNP A5U4D6
L	237	HIS	-	expression tag	UNP A5U4D6
L	238	HIS	-	expression tag	UNP A5U4D6
L	239	HIS	-	expression tag	UNP A5U4D6
L	240	HIS	-	expression tag	UNP A5U4D6
M	235	HIS	-	expression tag	UNP A5U4D6
M	236	HIS	-	expression tag	UNP A5U4D6
M	237	HIS	-	expression tag	UNP A5U4D6
M	238	HIS	-	expression tag	UNP A5U4D6
M	239	HIS	-	expression tag	UNP A5U4D6
M	240	HIS	-	expression tag	UNP A5U4D6

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Chain	Residue	Modelled	Actual	Comment	Reference
N	235	HIS	-	expression tag	UNP A5U4D6
N	236	HIS	-	expression tag	UNP A5U4D6
N	237	HIS	-	expression tag	UNP A5U4D6
N	238	HIS	-	expression tag	UNP A5U4D6
N	239	HIS	-	expression tag	UNP A5U4D6
N	240	HIS	-	expression tag	UNP A5U4D6
V	235	HIS	-	expression tag	UNP A5U4D6
V	236	HIS	-	expression tag	UNP A5U4D6
V	237	HIS	-	expression tag	UNP A5U4D6
V	238	HIS	-	expression tag	UNP A5U4D6
V	239	HIS	-	expression tag	UNP A5U4D6
V	240	HIS	-	expression tag	UNP A5U4D6
W	235	HIS	-	expression tag	UNP A5U4D6
W	236	HIS	-	expression tag	UNP A5U4D6
W	237	HIS	-	expression tag	UNP A5U4D6
W	238	HIS	-	expression tag	UNP A5U4D6
W	239	HIS	-	expression tag	UNP A5U4D6
W	240	HIS	-	expression tag	UNP A5U4D6
X	235	HIS	-	expression tag	UNP A5U4D6
X	236	HIS	-	expression tag	UNP A5U4D6
X	237	HIS	-	expression tag	UNP A5U4D6
X	238	HIS	-	expression tag	UNP A5U4D6
X	239	HIS	-	expression tag	UNP A5U4D6
X	240	HIS	-	expression tag	UNP A5U4D6
Y	235	HIS	-	expression tag	UNP A5U4D6
Y	236	HIS	-	expression tag	UNP A5U4D6
Y	237	HIS	-	expression tag	UNP A5U4D6
Y	238	HIS	-	expression tag	UNP A5U4D6
Y	239	HIS	-	expression tag	UNP A5U4D6
Y	240	HIS	-	expression tag	UNP A5U4D6
Z	235	HIS	-	expression tag	UNP A5U4D6
Z	236	HIS	-	expression tag	UNP A5U4D6
Z	237	HIS	-	expression tag	UNP A5U4D6
Z	238	HIS	-	expression tag	UNP A5U4D6
Z	239	HIS	-	expression tag	UNP A5U4D6
Z	240	HIS	-	expression tag	UNP A5U4D6
a	235	HIS	-	expression tag	UNP A5U4D6
a	236	HIS	-	expression tag	UNP A5U4D6
a	237	HIS	-	expression tag	UNP A5U4D6
a	238	HIS	-	expression tag	UNP A5U4D6
a	239	HIS	-	expression tag	UNP A5U4D6
a	240	HIS	-	expression tag	UNP A5U4D6

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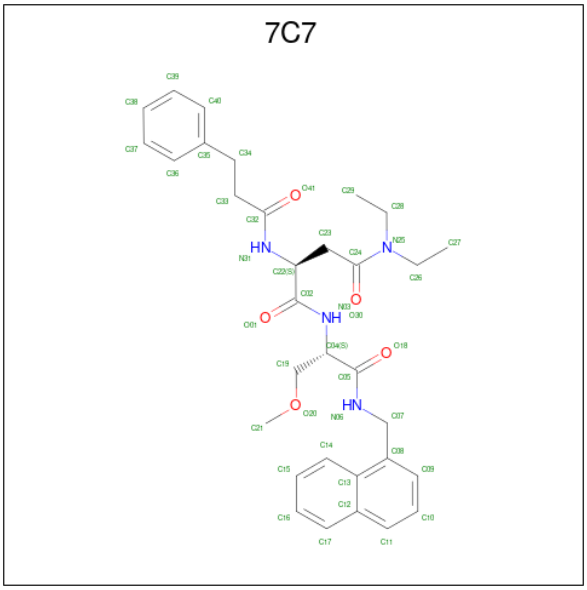
Chain	Residue	Modelled	Actual	Comment	Reference
b	235	HIS	-	expression tag	UNP A5U4D6
b	236	HIS	-	expression tag	UNP A5U4D6
b	237	HIS	-	expression tag	UNP A5U4D6
b	238	HIS	-	expression tag	UNP A5U4D6
b	239	HIS	-	expression tag	UNP A5U4D6
b	240	HIS	-	expression tag	UNP A5U4D6

- Molecule 3 is N,N-diethyl-N 2 -(3-phenylpropanoyl)-L-asparaginyl-O-methyl-N-[(naphthalen-1-yl)methyl]-L-serinamide (CCD ID: 7C7) (formula: $C_{32}H_{40}N_4O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	0
			41	32	4	5		
3	I	1	Total	C	N	O	0	0
			41	32	4	5		
3	J	1	Total	C	N	O	0	0
			41	32	4	5		
3	K	1	Total	C	N	O	0	0
			41	32	4	5		
3	L	1	Total	C	N	O	0	0
			41	32	4	5		
3	M	1	Total	C	N	O	0	0
			41	32	4	5		
3	N	1	Total	C	N	O	0	0
			41	32	4	5		
3	V	1	Total	C	N	O	0	0
			41	32	4	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	W	1	Total C N O 41 32 4 5	0	0
3	X	1	Total C N O 41 32 4 5	0	0
3	Y	1	Total C N O 41 32 4 5	0	0
3	Z	1	Total C N O 41 32 4 5	0	0
3	a	1	Total C N O 41 32 4 5	0	0
3	b	1	Total C N O 41 32 4 5	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total O 9 9	0	0
4	B	1	Total O 1 1	0	0
4	C	3	Total O 3 3	0	0
4	D	4	Total O 4 4	0	0
4	E	3	Total O 3 3	0	0
4	F	5	Total O 5 5	0	0
4	G	3	Total O 3 3	0	0
4	H	15	Total O 15 15	0	0
4	I	18	Total O 18 18	0	0
4	J	11	Total O 11 11	0	0
4	K	16	Total O 16 16	0	0
4	L	10	Total O 10 10	0	0
4	M	12	Total O 12 12	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	N	12	Total O 12 12	0	0
4	O	6	Total O 6 6	0	0
4	P	7	Total O 7 7	0	0
4	Q	3	Total O 3 3	0	0
4	R	5	Total O 5 5	0	0
4	S	8	Total O 8 8	0	0
4	T	6	Total O 6 6	0	0
4	U	3	Total O 3 3	0	0
4	V	20	Total O 20 20	0	0
4	W	13	Total O 13 13	0	0
4	X	10	Total O 10 10	0	0
4	Y	10	Total O 10 10	0	0
4	Z	12	Total O 12 12	0	0
4	a	10	Total O 10 10	0	0
4	b	10	Total O 10 10	0	0

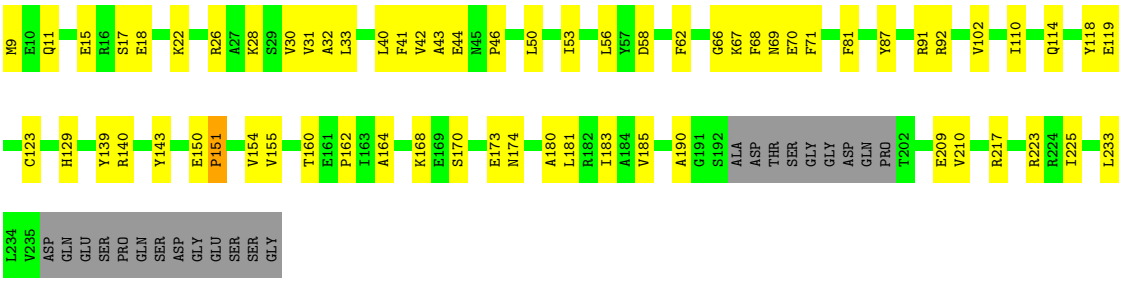
3 Residue-property plots (i)

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

- Molecule 1: Proteasome subunit alpha

Chain A:

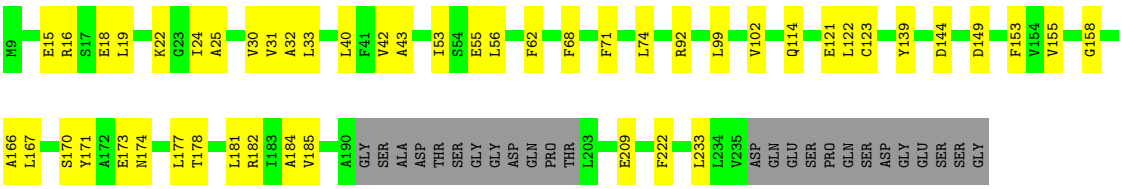




- Molecule 1: Proteasome subunit alpha

Chain B:

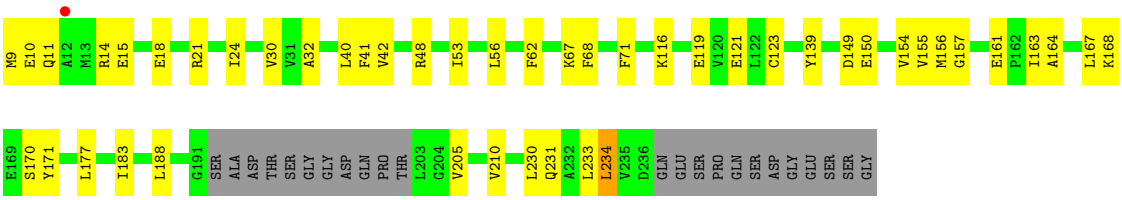




- Molecule 1: Proteasome subunit alpha

Chain C:

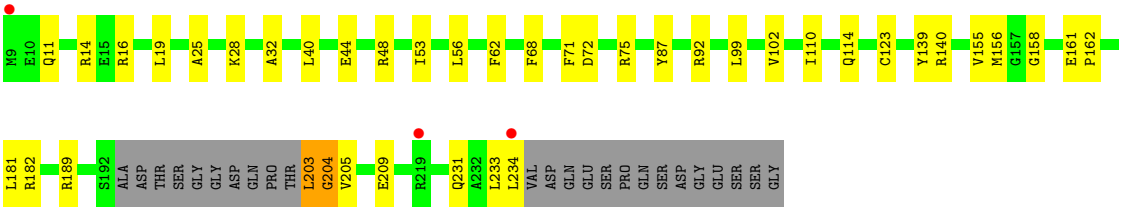




- Molecule 1: Proteasome subunit alpha

Chain D:

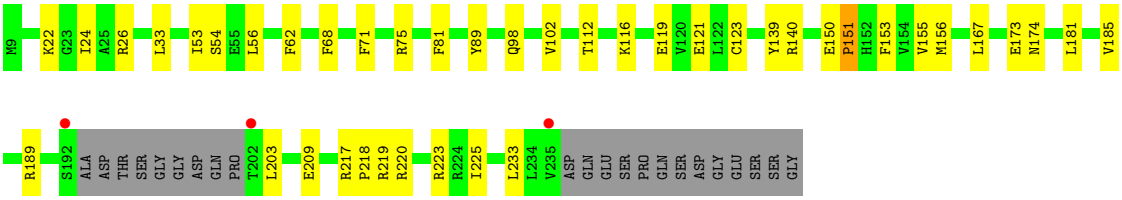




• Molecule 1: Proteasome subunit alpha

Chain E:

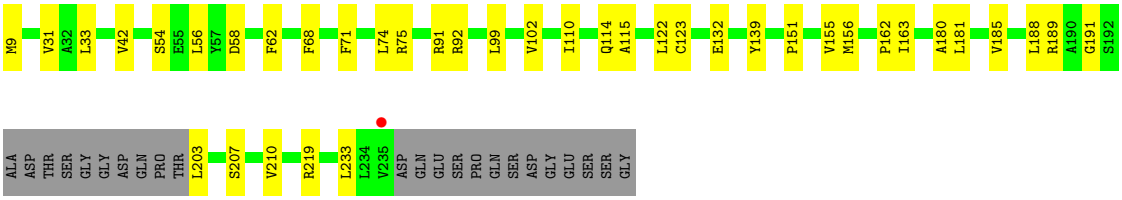




• Molecule 1: Proteasome subunit alpha

Chain F:

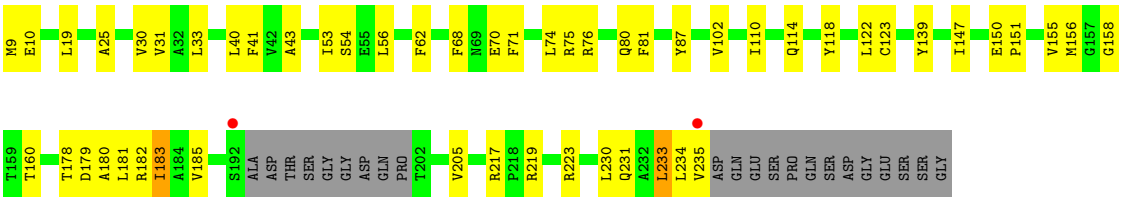




• Molecule 1: Proteasome subunit alpha

Chain G:

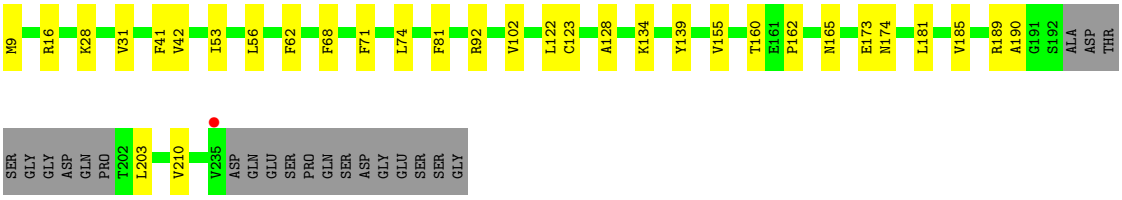




• Molecule 1: Proteasome subunit alpha

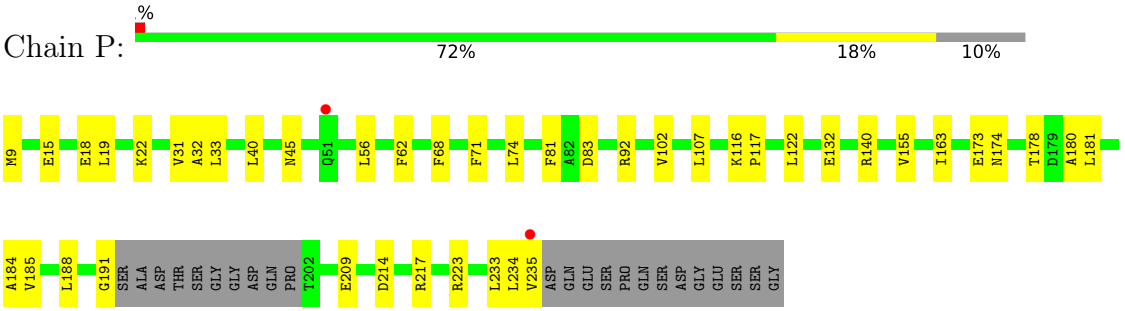
Chain O:





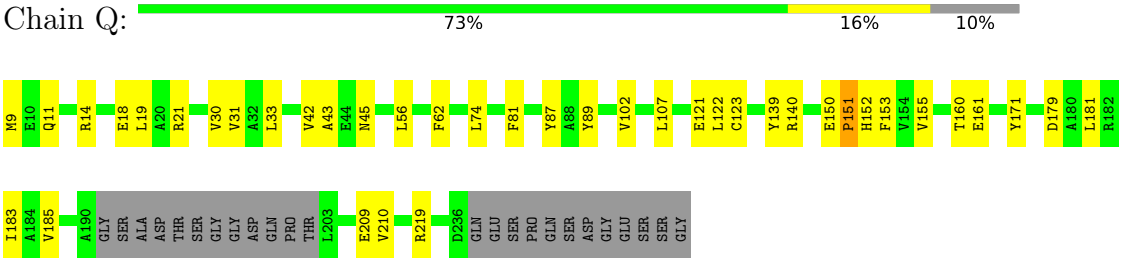
• Molecule 1: Proteasome subunit alpha

Chain P:



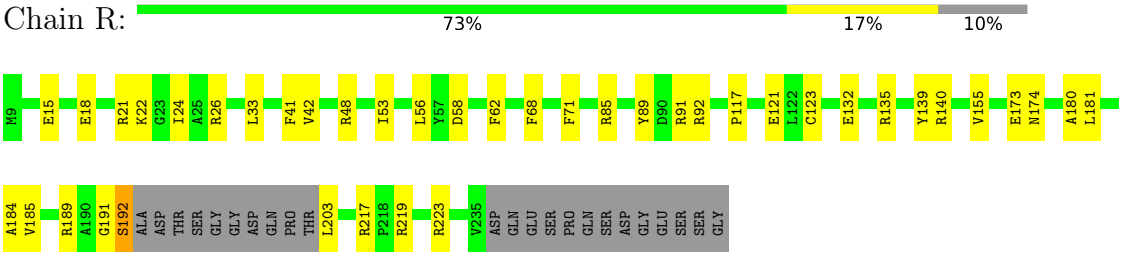
• Molecule 1: Proteasome subunit alpha

Chain Q:



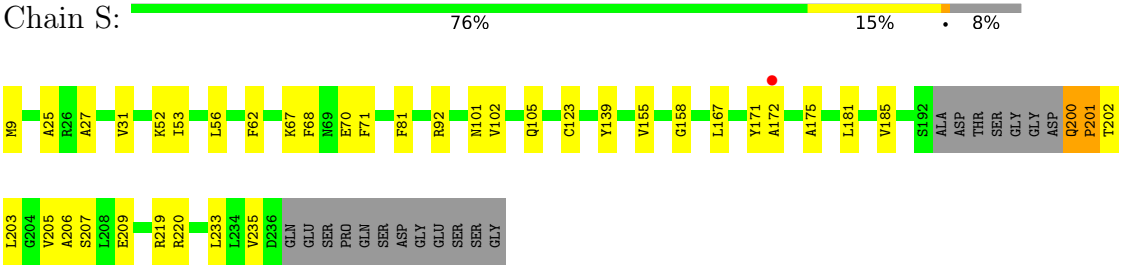
• Molecule 1: Proteasome subunit alpha

Chain R:



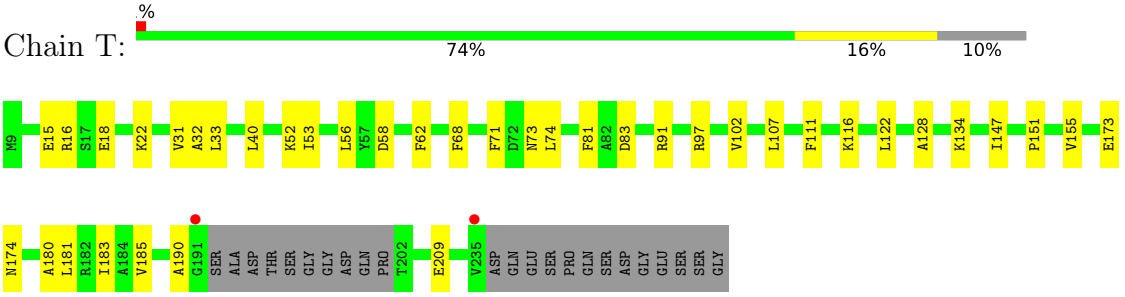
• Molecule 1: Proteasome subunit alpha

Chain S:



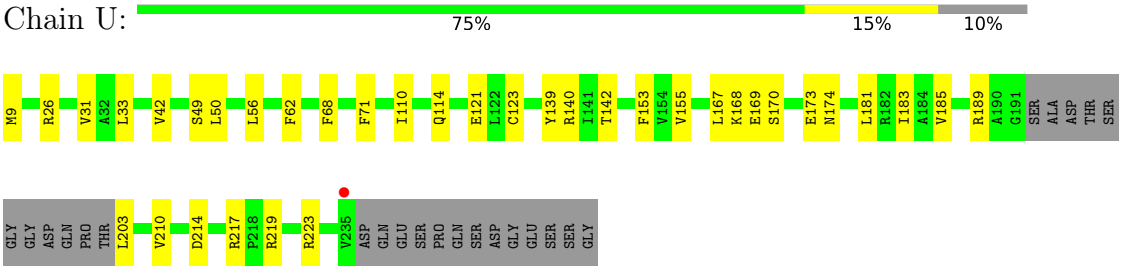
• Molecule 1: Proteasome subunit alpha

Chain T:



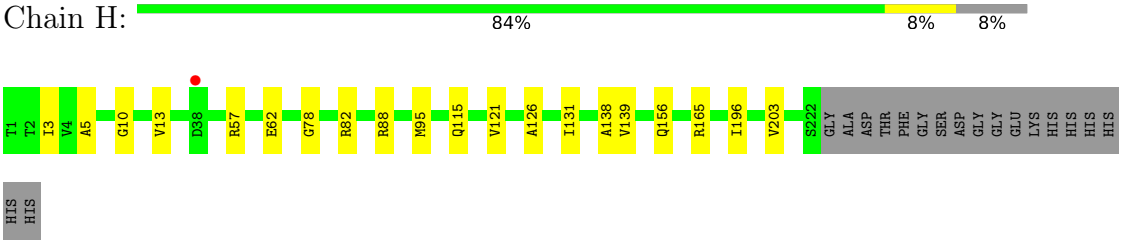
• Molecule 1: Proteasome subunit alpha

Chain U:



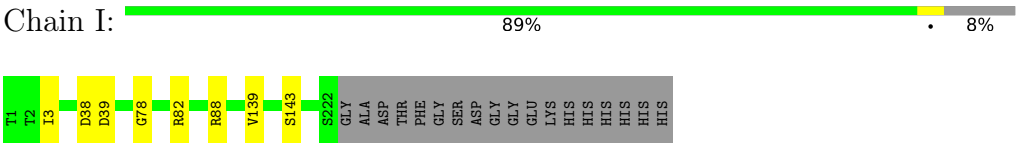
• Molecule 2: Proteasome subunit beta

Chain H:



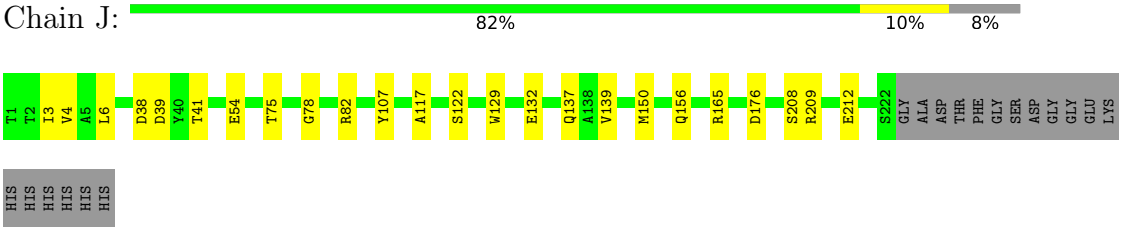
• Molecule 2: Proteasome subunit beta

Chain I:



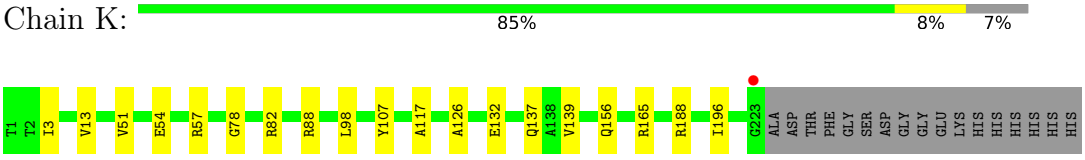
• Molecule 2: Proteasome subunit beta

Chain J:



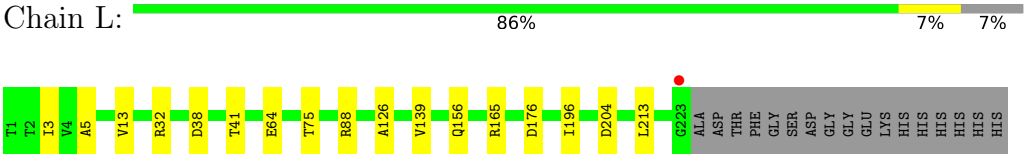
• Molecule 2: Proteasome subunit beta

Chain K:



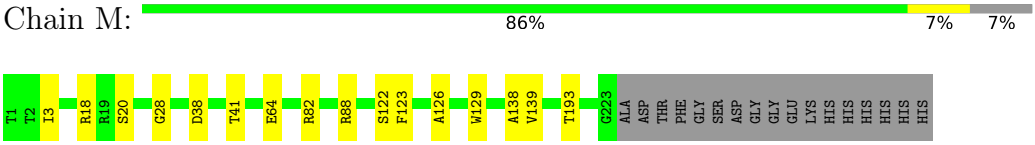
• Molecule 2: Proteasome subunit beta

Chain L:



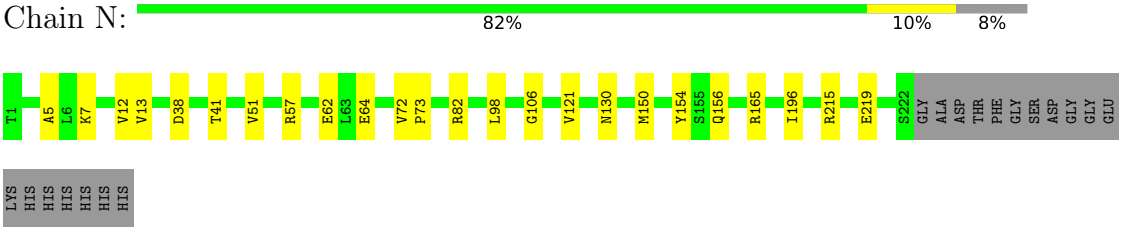
• Molecule 2: Proteasome subunit beta

Chain M:



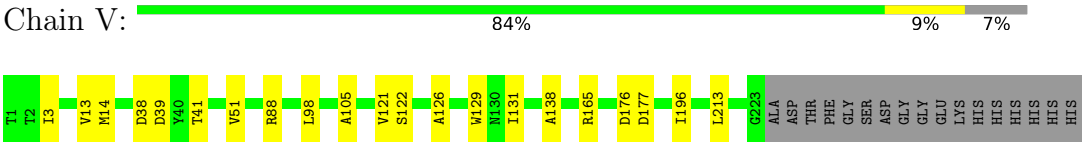
• Molecule 2: Proteasome subunit beta

Chain N:



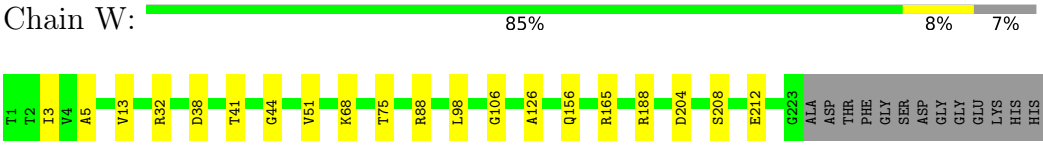
• Molecule 2: Proteasome subunit beta

Chain V:



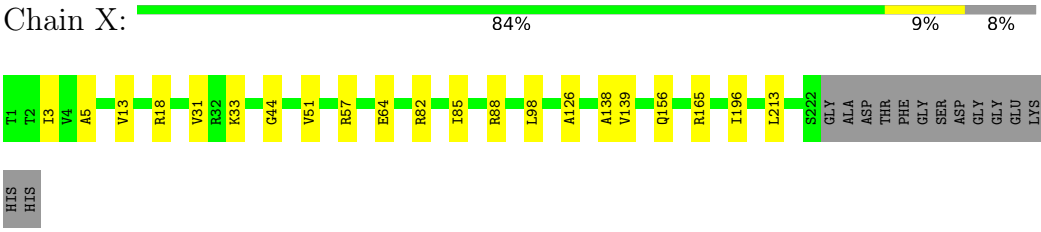
• Molecule 2: Proteasome subunit beta

Chain W:



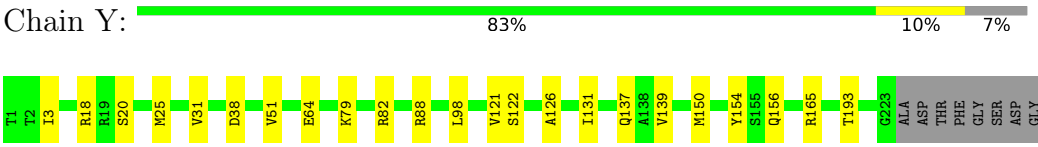
• Molecule 2: Proteasome subunit beta

Chain X:



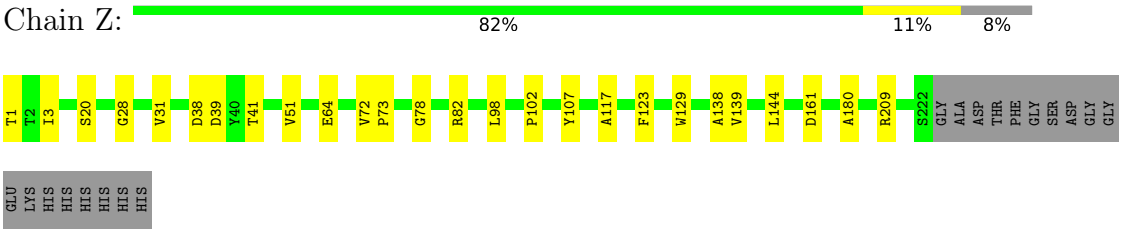
• Molecule 2: Proteasome subunit beta

Chain Y:



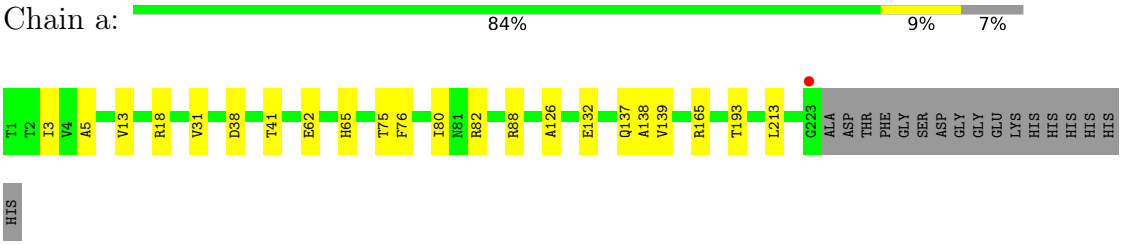
• Molecule 2: Proteasome subunit beta

Chain Z:



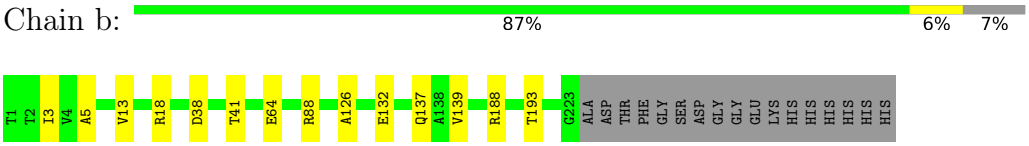
• Molecule 2: Proteasome subunit beta

Chain a:



• Molecule 2: Proteasome subunit beta

Chain b:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	120.16Å 198.19Å 166.24Å 90.00° 103.35° 90.00°	Depositor
Resolution (Å)	49.55 – 3.00 49.55 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.55-3.00) 93.3 (49.55-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.176 , 0.210 0.180 , 0.210	Depositor DCC
R_{free} test set	7272 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	59.5	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 27.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	47201	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 7C7

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	0.22	0/1701	0.49	0/2297
1	B	0.21	0/1684	0.46	0/2274
1	C	0.21	0/1696	0.48	0/2290
1	D	0.27	0/1687	0.52	1/2277 (0.0%)
1	E	0.22	0/1701	0.48	0/2297
1	F	0.24	0/1694	0.49	1/2287 (0.0%)
1	G	0.37	0/1701	0.51	0/2297
1	O	0.20	0/1701	0.45	0/2297
1	P	0.29	0/1695	0.46	0/2289
1	Q	0.22	0/1692	0.47	0/2285
1	R	0.21	0/1694	0.48	0/2287
1	S	0.29	0/1726	0.52	1/2332 (0.0%)
1	T	0.21	0/1695	0.47	0/2289
1	U	0.21	0/1688	0.52	0/2279
2	H	0.21	0/1662	0.45	0/2254
2	I	0.22	0/1662	0.42	0/2254
2	J	0.21	0/1662	0.42	0/2254
2	K	0.21	0/1666	0.44	0/2259
2	L	0.22	0/1666	0.44	0/2259
2	M	0.21	0/1666	0.43	0/2259
2	N	0.21	0/1662	0.43	0/2254
2	V	0.22	0/1666	0.43	0/2259
2	W	0.22	0/1666	0.42	0/2259
2	X	0.21	0/1662	0.43	0/2254
2	Y	0.22	0/1666	0.44	0/2259
2	Z	0.22	0/1662	0.44	0/2254
2	a	0.22	0/1666	0.42	0/2259
2	b	0.22	0/1666	0.45	0/2259
All	All	0.23	0/47055	0.46	3/63673 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	204	GLY	N-CA-C	6.65	121.42	111.18
1	S	202	THR	N-CA-C	6.05	118.31	108.26
1	F	207	SER	N-CA-C	-5.11	99.91	110.80

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	1677	0	1680	41	0
1	B	1660	0	1665	30	0
1	C	1672	0	1672	32	0
1	D	1663	0	1664	27	0
1	E	1677	0	1680	25	0
1	F	1670	0	1673	28	0
1	G	1677	0	1680	43	0
1	O	1677	0	1680	23	0
1	P	1671	0	1675	31	0
1	Q	1668	0	1669	29	0
1	R	1670	0	1673	30	0
1	S	1701	0	1699	33	0
1	T	1671	0	1675	26	0
1	U	1664	0	1668	25	0
2	H	1638	0	1633	12	0
2	I	1638	0	1633	5	0
2	J	1638	0	1633	16	0
2	K	1642	0	1636	11	0
2	L	1642	0	1636	11	0
2	M	1642	0	1636	11	0
2	N	1638	0	1633	15	0
2	V	1642	0	1636	12	0
2	W	1642	0	1636	12	0
2	X	1638	0	1633	14	0
2	Y	1642	0	1636	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Z	1638	0	1633	18	0
2	a	1642	0	1636	13	0
2	b	1642	0	1636	8	0
3	H	41	0	0	0	0
3	I	41	0	0	0	0
3	J	41	0	0	0	0
3	K	41	0	0	0	0
3	L	41	0	0	0	0
3	M	41	0	0	0	0
3	N	41	0	0	0	0
3	V	41	0	0	0	0
3	W	41	0	0	0	0
3	X	41	0	0	0	0
3	Y	41	0	0	0	0
3	Z	41	0	0	0	0
3	a	41	0	0	0	0
3	b	41	0	0	0	0
4	A	9	0	0	0	0
4	B	1	0	0	0	0
4	C	3	0	0	0	0
4	D	4	0	0	1	0
4	E	3	0	0	0	0
4	F	5	0	0	0	0
4	G	3	0	0	0	0
4	H	15	0	0	0	0
4	I	18	0	0	1	0
4	J	11	0	0	1	0
4	K	16	0	0	0	0
4	L	10	0	0	0	0
4	M	12	0	0	0	0
4	N	12	0	0	0	0
4	O	6	0	0	0	0
4	P	7	0	0	0	0
4	Q	3	0	0	0	0
4	R	5	0	0	0	0
4	S	8	0	0	2	0
4	T	6	0	0	1	0
4	U	3	0	0	2	0
4	V	20	0	0	1	0
4	W	13	0	0	0	0
4	X	10	0	0	1	0
4	Y	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Z	12	0	0	0	0
4	a	10	0	0	0	0
4	b	10	0	0	0	0
All	All	47201	0	46339	543	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 6.

The worst 5 of 543 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:S:200:GLN:HG3	1:S:201:PRO:CD	1.38	1.49
1:G:179:ASP:O	1:G:183:ILE:HG13	1.38	1.21
1:S:200:GLN:CG	1:S:201:PRO:CD	2.19	1.19
1:S:200:GLN:CG	1:S:201:PRO:HD2	1.74	1.18
1:F:189:ARG:HG3	1:F:203:LEU:CD2	1.85	1.05

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	214/240 (89%)	207 (97%)	6 (3%)	1 (0%)	24 60
1	B	211/240 (88%)	204 (97%)	7 (3%)	0	100 100
1	C	213/240 (89%)	209 (98%)	3 (1%)	1 (0%)	24 60
1	D	212/240 (88%)	204 (96%)	8 (4%)	0	100 100
1	E	214/240 (89%)	206 (96%)	7 (3%)	1 (0%)	24 60
1	F	213/240 (89%)	206 (97%)	6 (3%)	1 (0%)	24 60
1	G	214/240 (89%)	208 (97%)	6 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	214/240 (89%)	206 (96%)	8 (4%)	0	100	100
1	P	213/240 (89%)	206 (97%)	7 (3%)	0	100	100
1	Q	212/240 (88%)	207 (98%)	4 (2%)	1 (0%)	24	60
1	R	213/240 (89%)	205 (96%)	8 (4%)	0	100	100
1	S	217/240 (90%)	210 (97%)	4 (2%)	3 (1%)	9	36
1	T	213/240 (89%)	204 (96%)	7 (3%)	2 (1%)	14	48
1	U	212/240 (88%)	203 (96%)	9 (4%)	0	100	100
2	H	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
2	I	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
2	J	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
2	K	221/240 (92%)	217 (98%)	4 (2%)	0	100	100
2	L	221/240 (92%)	218 (99%)	3 (1%)	0	100	100
2	M	221/240 (92%)	216 (98%)	5 (2%)	0	100	100
2	N	220/240 (92%)	216 (98%)	4 (2%)	0	100	100
2	V	221/240 (92%)	218 (99%)	3 (1%)	0	100	100
2	W	221/240 (92%)	218 (99%)	3 (1%)	0	100	100
2	X	220/240 (92%)	216 (98%)	4 (2%)	0	100	100
2	Y	221/240 (92%)	218 (99%)	3 (1%)	0	100	100
2	Z	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
2	a	221/240 (92%)	217 (98%)	4 (2%)	0	100	100
2	b	221/240 (92%)	217 (98%)	4 (2%)	0	100	100
All	All	6073/6720 (90%)	5924 (98%)	139 (2%)	10 (0%)	43	76

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	201	PRO
1	T	190	ALA
1	S	206	ALA
1	C	234	LEU
1	F	151	PRO

5.3.2 Protein sidechains (i)

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	167/184 (91%)	167 (100%)	0	100 100
1	B	165/184 (90%)	165 (100%)	0	100 100
1	C	166/184 (90%)	166 (100%)	0	100 100
1	D	165/184 (90%)	164 (99%)	1 (1%)	78 88
1	E	167/184 (91%)	167 (100%)	0	100 100
1	F	166/184 (90%)	166 (100%)	0	100 100
1	G	167/184 (91%)	164 (98%)	3 (2%)	51 77
1	O	167/184 (91%)	167 (100%)	0	100 100
1	P	166/184 (90%)	165 (99%)	1 (1%)	78 88
1	Q	166/184 (90%)	166 (100%)	0	100 100
1	R	166/184 (90%)	165 (99%)	1 (1%)	78 88
1	S	170/184 (92%)	168 (99%)	2 (1%)	63 82
1	T	166/184 (90%)	166 (100%)	0	100 100
1	U	165/184 (90%)	164 (99%)	1 (1%)	78 88
2	H	165/178 (93%)	165 (100%)	0	100 100
2	I	165/178 (93%)	165 (100%)	0	100 100
2	J	165/178 (93%)	165 (100%)	0	100 100
2	K	165/178 (93%)	165 (100%)	0	100 100
2	L	165/178 (93%)	165 (100%)	0	100 100
2	M	165/178 (93%)	165 (100%)	0	100 100
2	N	165/178 (93%)	165 (100%)	0	100 100
2	V	165/178 (93%)	165 (100%)	0	100 100
2	W	165/178 (93%)	165 (100%)	0	100 100
2	X	165/178 (93%)	165 (100%)	0	100 100
2	Y	165/178 (93%)	165 (100%)	0	100 100
2	Z	165/178 (93%)	165 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	a	165/178 (93%)	165 (100%)	0	100 100
2	b	165/178 (93%)	165 (100%)	0	100 100
All	All	4639/5068 (92%)	4630 (100%)	9 (0%)	87 92

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	203	LEU
1	U	142	THR
1	G	235	VAL
1	P	234	LEU
1	R	192	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	S	231	GLN
2	X	115	GLN
2	b	130	ASN
2	X	137	GLN
2	V	137	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

14 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	7C7	H	301	-	43,43,43	1.25	7 (16%)	56,56,56	1.56	12 (21%)
3	7C7	I	301	-	43,43,43	1.14	5 (11%)	56,56,56	1.41	8 (14%)
3	7C7	K	301	-	43,43,43	1.14	6 (13%)	56,56,56	1.41	11 (19%)
3	7C7	M	301	-	43,43,43	1.10	5 (11%)	56,56,56	1.44	10 (17%)
3	7C7	X	301	-	43,43,43	1.18	6 (13%)	56,56,56	1.56	12 (21%)
3	7C7	J	301	-	43,43,43	1.21	5 (11%)	56,56,56	1.49	12 (21%)
3	7C7	b	301	-	43,43,43	1.13	6 (13%)	56,56,56	1.46	11 (19%)
3	7C7	V	301	-	43,43,43	1.24	6 (13%)	56,56,56	1.55	12 (21%)
3	7C7	Y	301	-	43,43,43	1.14	5 (11%)	56,56,56	1.40	11 (19%)
3	7C7	Z	301	-	43,43,43	1.00	3 (6%)	56,56,56	1.49	11 (19%)
3	7C7	L	301	-	43,43,43	1.09	6 (13%)	56,56,56	1.44	13 (23%)
3	7C7	N	301	-	43,43,43	1.07	4 (9%)	56,56,56	1.46	12 (21%)
3	7C7	W	301	-	43,43,43	1.07	4 (9%)	56,56,56	1.50	10 (17%)
3	7C7	a	301	-	43,43,43	0.99	4 (9%)	56,56,56	1.40	10 (17%)

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	7C7	H	301	-	-	3/41/41/41	0/3/3/3
3	7C7	I	301	-	-	4/41/41/41	0/3/3/3
3	7C7	K	301	-	-	2/41/41/41	0/3/3/3
3	7C7	M	301	-	-	5/41/41/41	0/3/3/3
3	7C7	X	301	-	-	1/41/41/41	0/3/3/3
3	7C7	J	301	-	-	3/41/41/41	0/3/3/3
3	7C7	b	301	-	-	4/41/41/41	0/3/3/3
3	7C7	V	301	-	-	4/41/41/41	0/3/3/3
3	7C7	Y	301	-	-	2/41/41/41	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	7C7	Z	301	-	-	5/41/41/41	0/3/3/3
3	7C7	L	301	-	-	4/41/41/41	0/3/3/3
3	7C7	N	301	-	-	2/41/41/41	0/3/3/3
3	7C7	W	301	-	-	3/41/41/41	0/3/3/3
3	7C7	a	301	-	-	3/41/41/41	0/3/3/3

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	301	7C7	C24-N25	3.62	1.42	1.35
3	V	301	7C7	C24-N25	3.54	1.42	1.35
3	K	301	7C7	C24-N25	3.52	1.42	1.35
3	N	301	7C7	C24-N25	3.47	1.41	1.35
3	H	301	7C7	C05-N06	3.41	1.41	1.33

The worst 5 of 155 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	301	7C7	C22-C23-C24	4.48	121.17	112.22
3	b	301	7C7	C22-C23-C24	4.36	120.94	112.22
3	W	301	7C7	C22-C23-C24	4.26	120.74	112.22
3	X	301	7C7	C22-C23-C24	4.22	120.66	112.22
3	J	301	7C7	C22-C23-C24	4.10	120.42	112.22

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	301	7C7	N03-C04-C19-O20
3	H	301	7C7	C05-C04-C19-O20
3	I	301	7C7	N03-C04-C19-O20
3	I	301	7C7	C05-C04-C19-O20
3	K	301	7C7	N03-C04-C19-O20

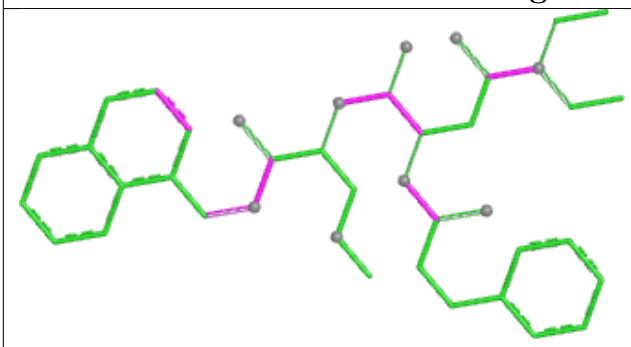
There are no ring outliers.

No monomer is involved in short contacts.

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 then 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 7C7 H 301



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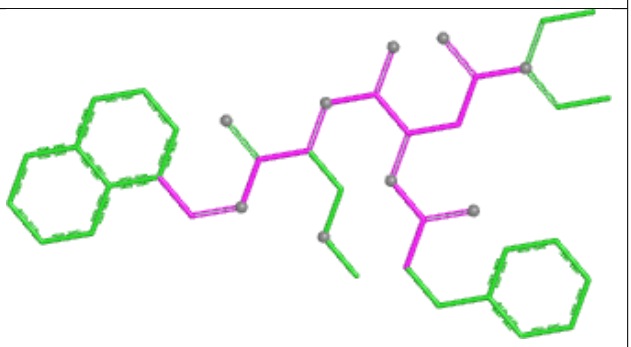
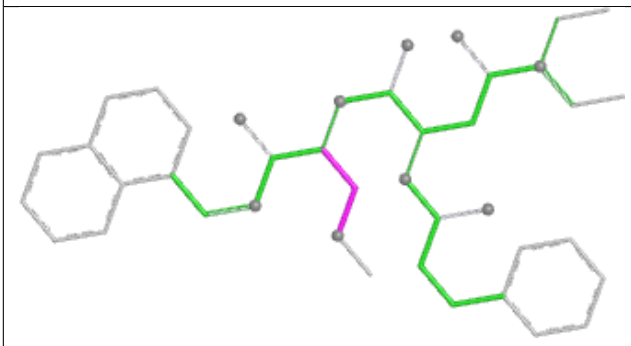


Bond angles



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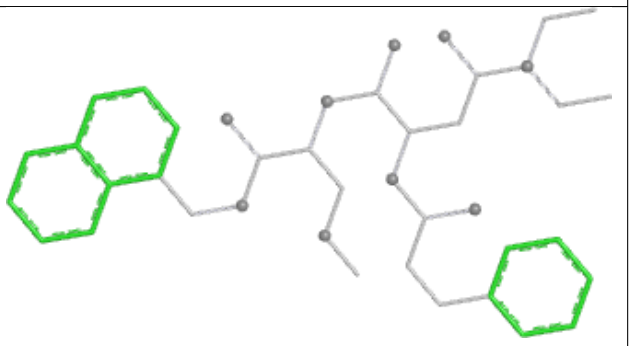
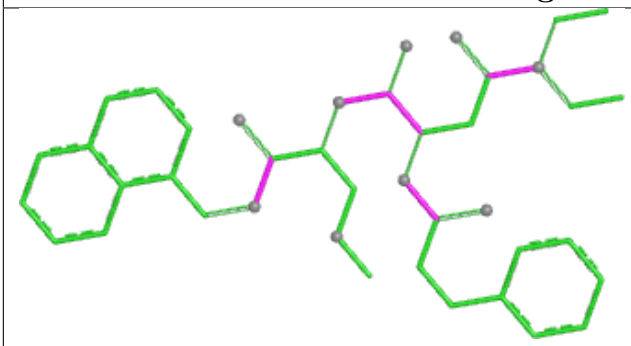


Rings

Ligand 7C7 I 301



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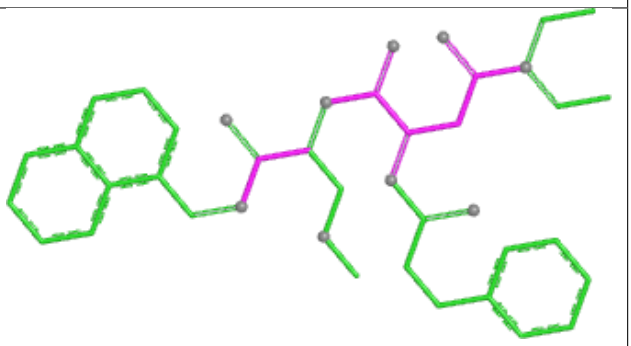

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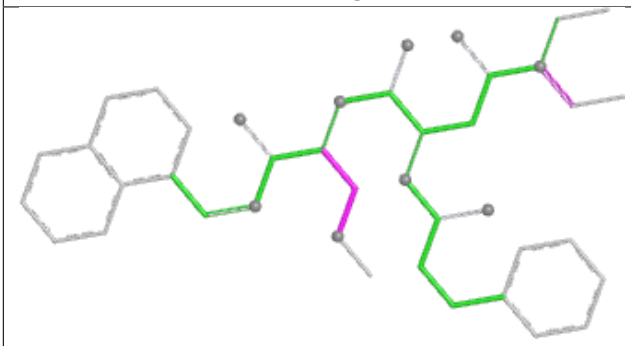

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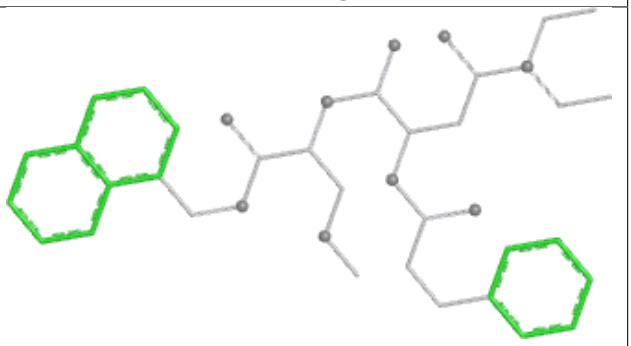
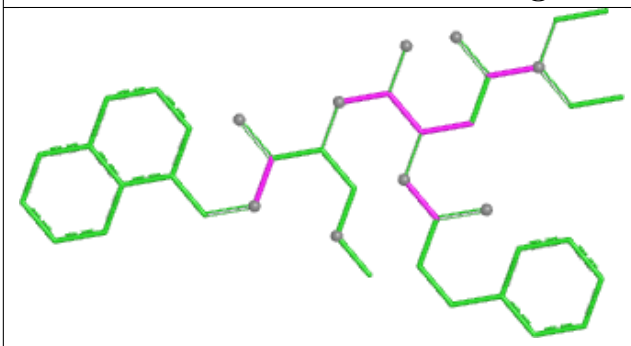


Rings

Ligand 7C7 K 301



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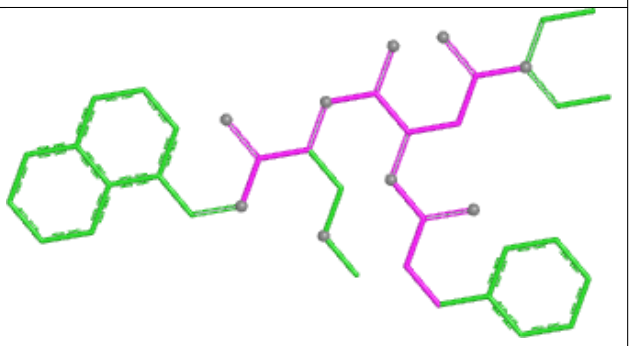

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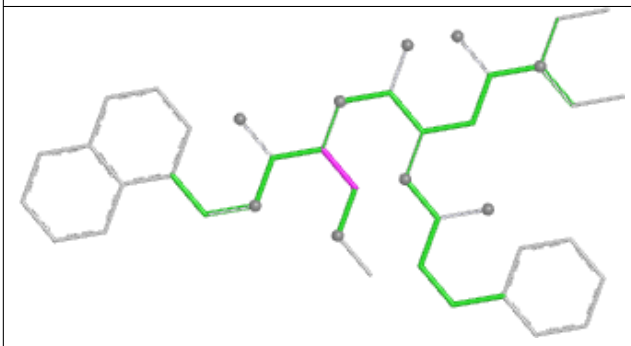

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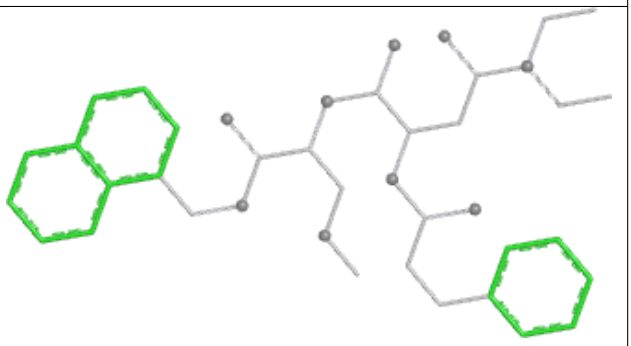
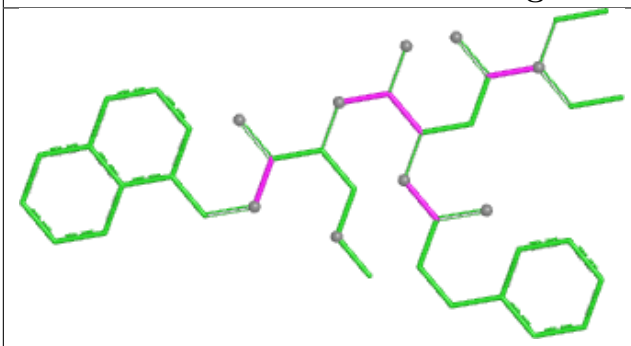


Rings

Ligand 7C7 M 301



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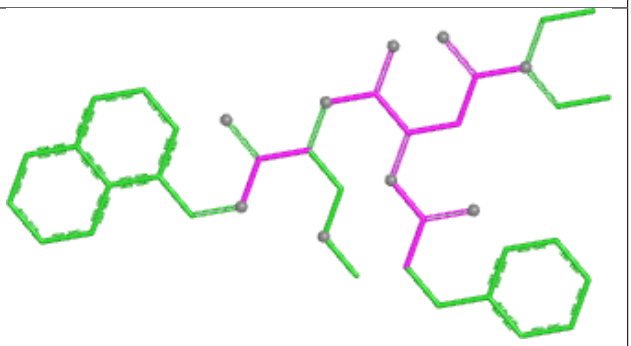

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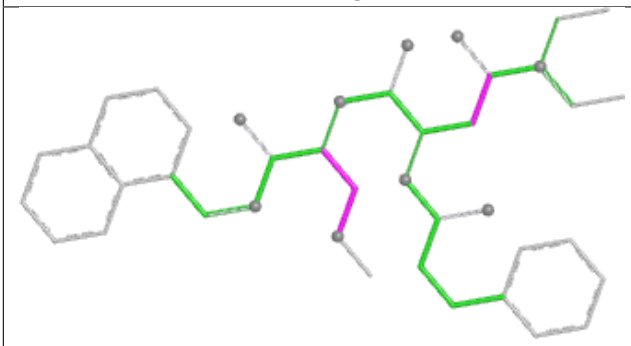

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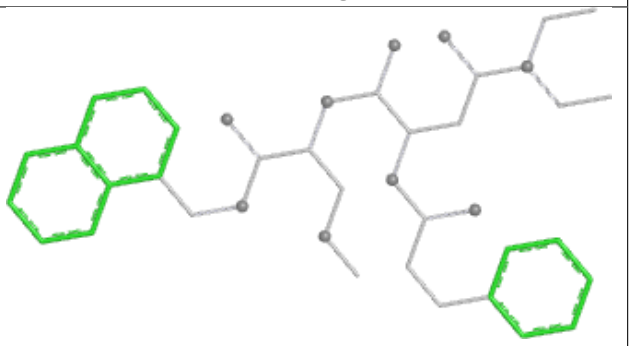
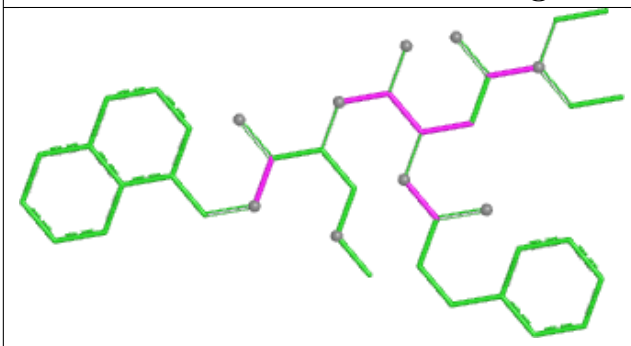


Rings

Ligand 7C7 X 301



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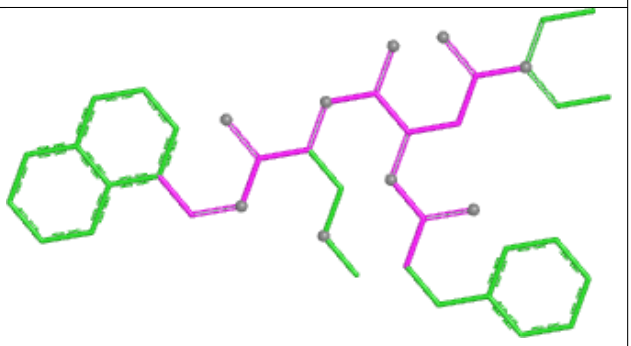

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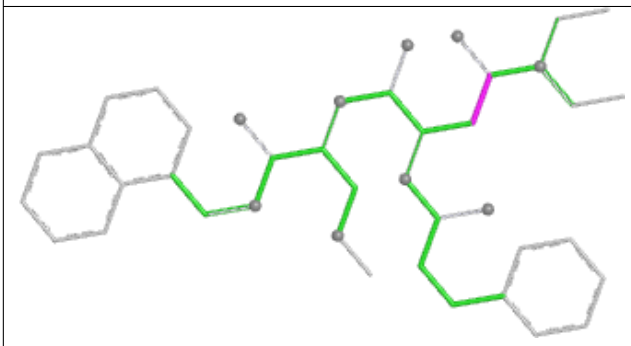

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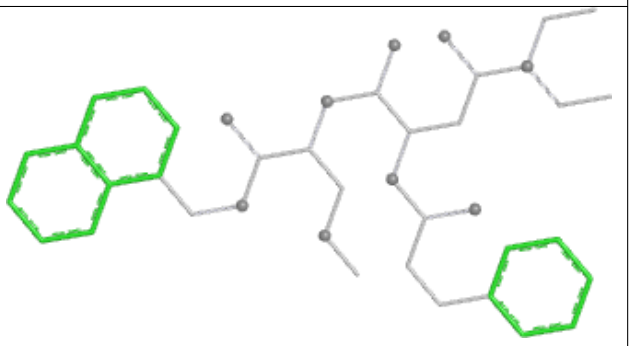
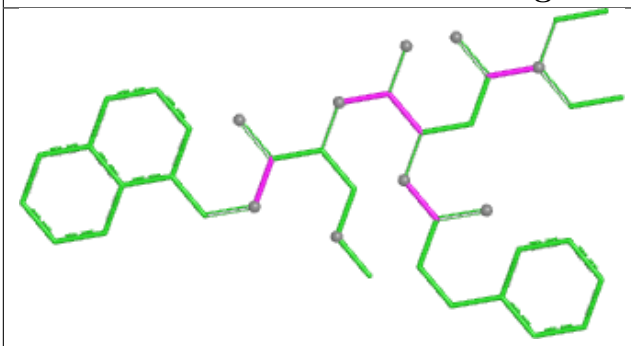


Rings

Ligand 7C7 J 301



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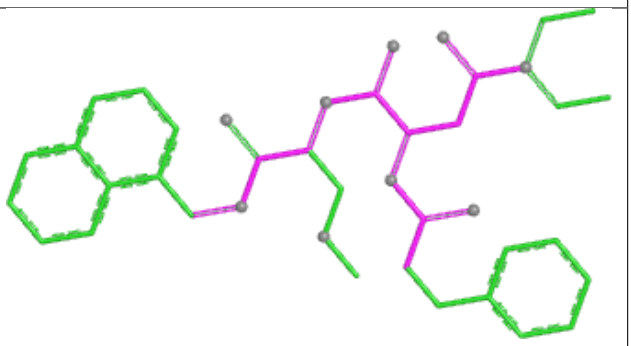

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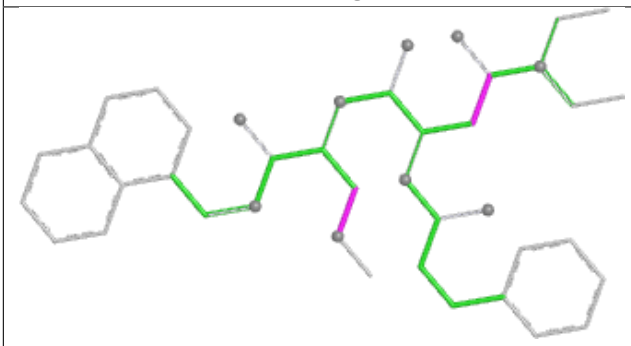

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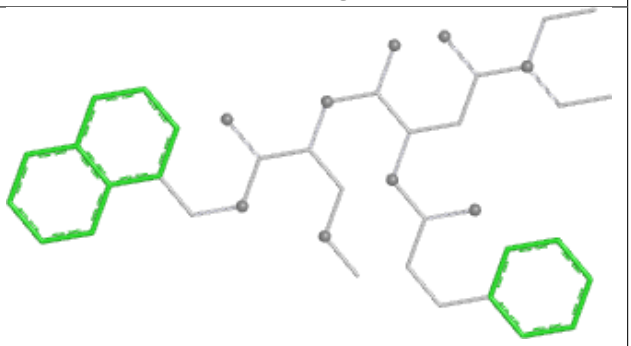
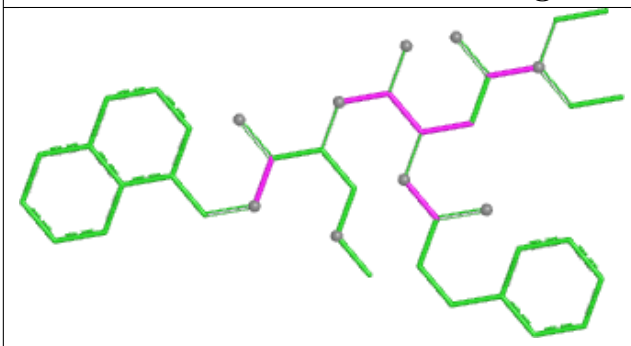


Rings

Ligand 7C7 b 301



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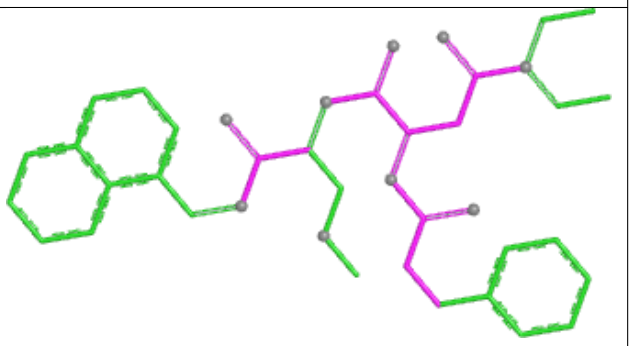

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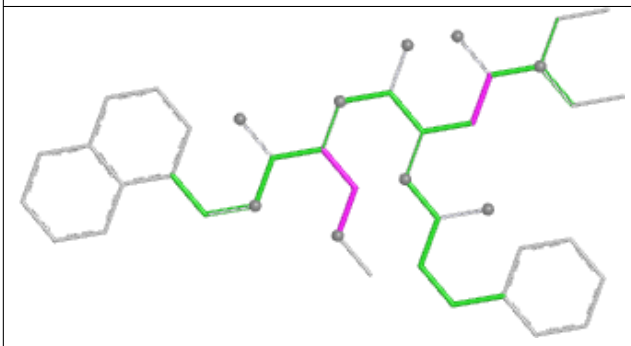

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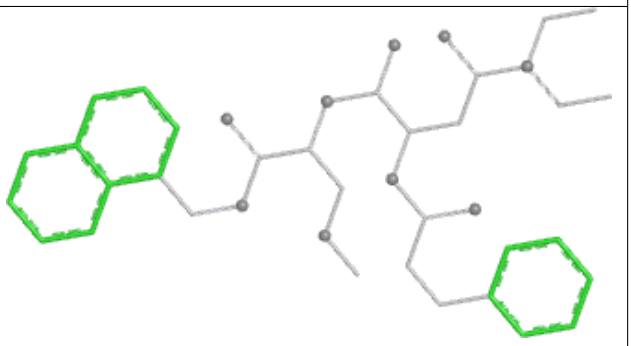
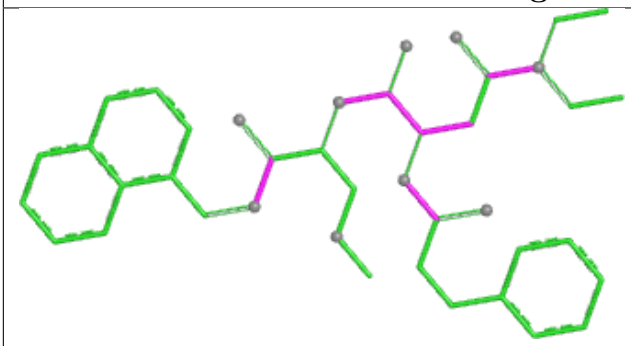


Rings

Ligand 7C7 V 301



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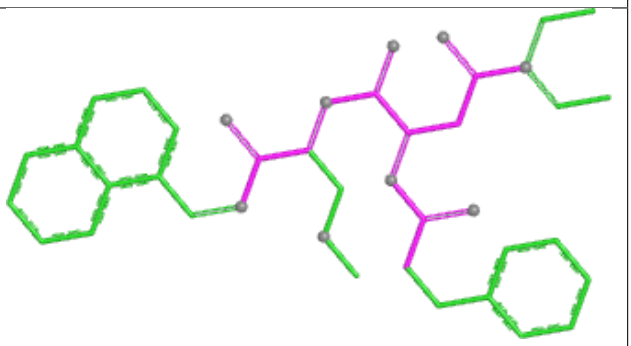

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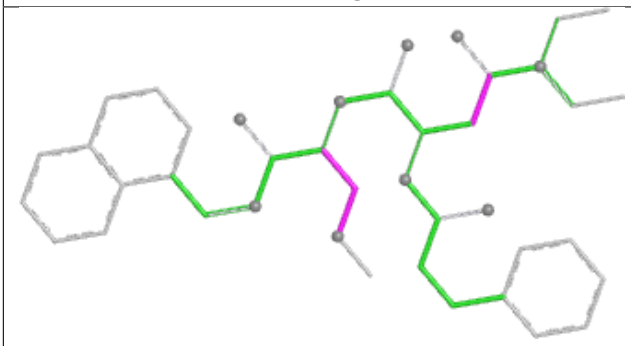

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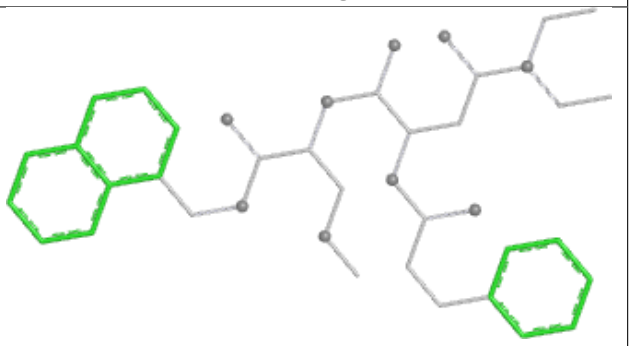
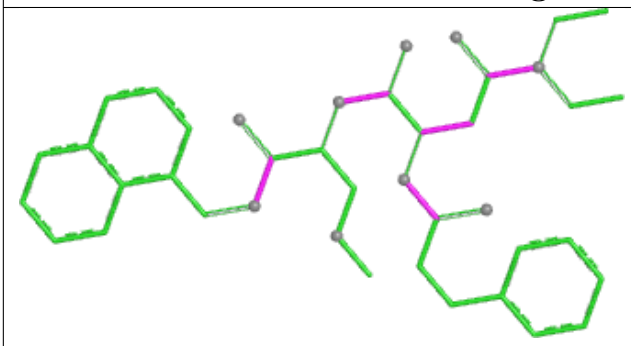


Rings

Ligand 7C7 Y 301



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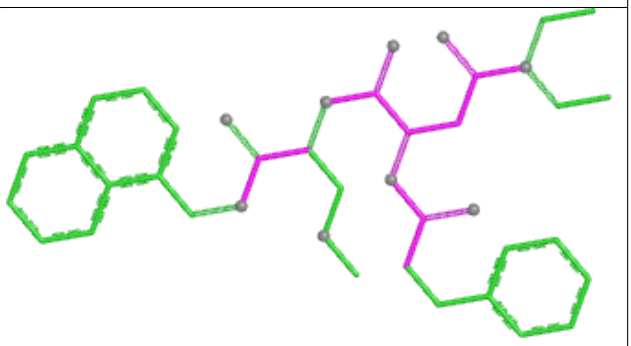

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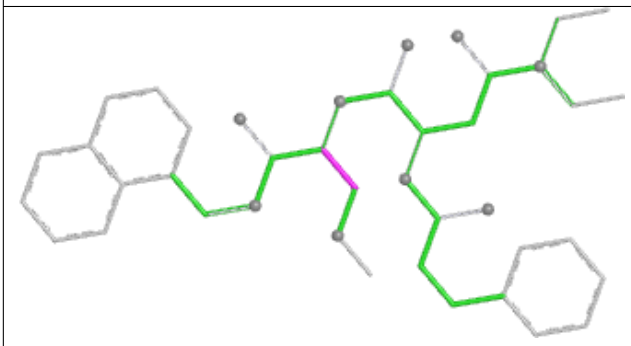

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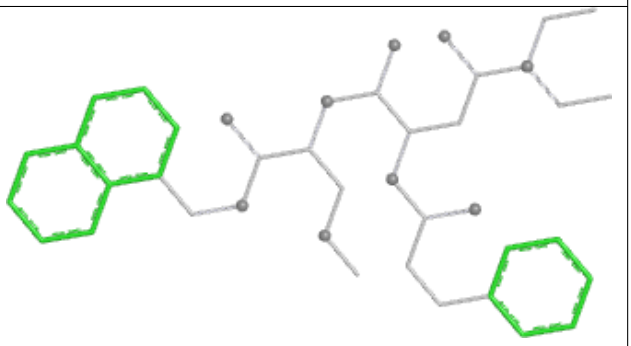
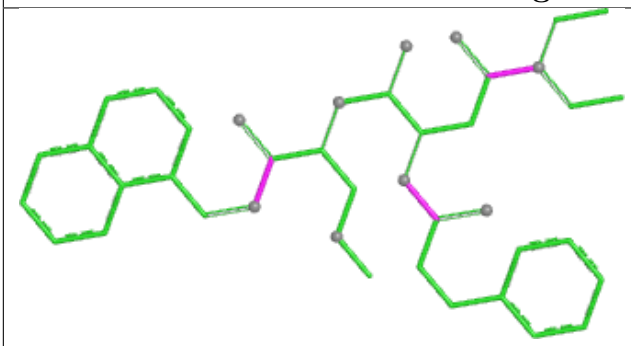


Rings

Ligand 7C7 Z 301



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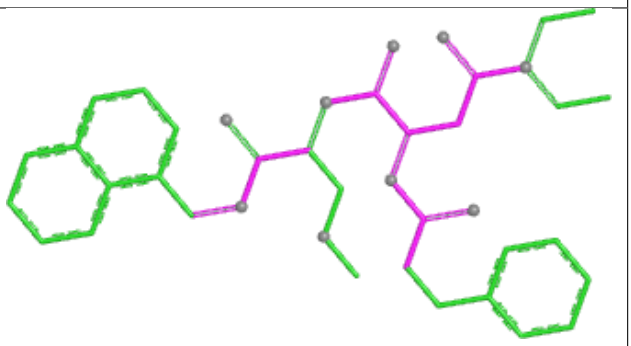

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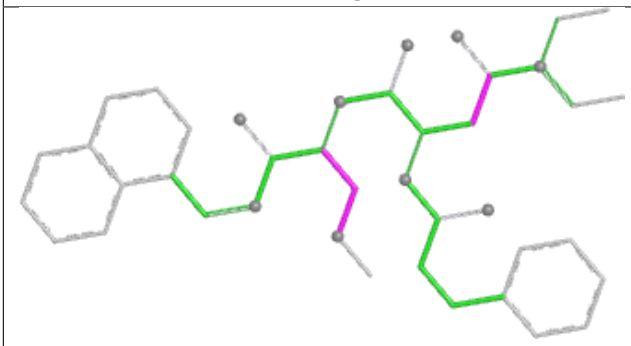

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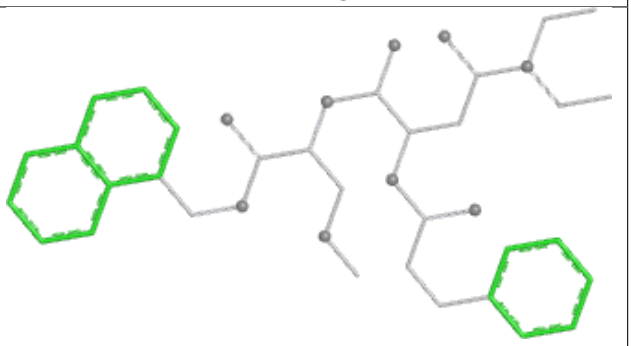
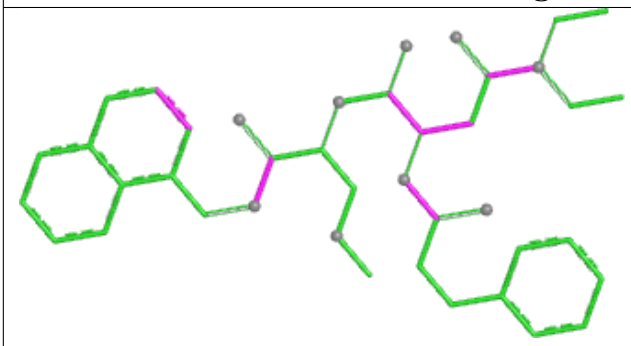


Rings

Ligand 7C7 L 301



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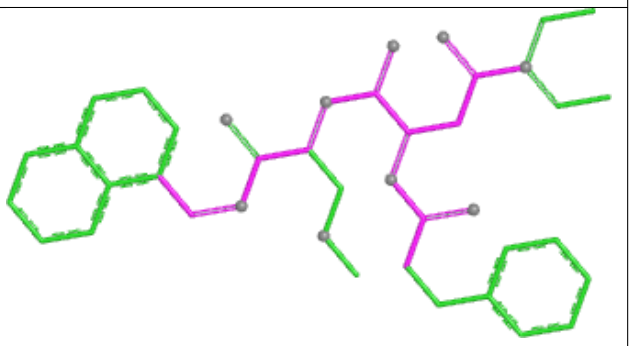

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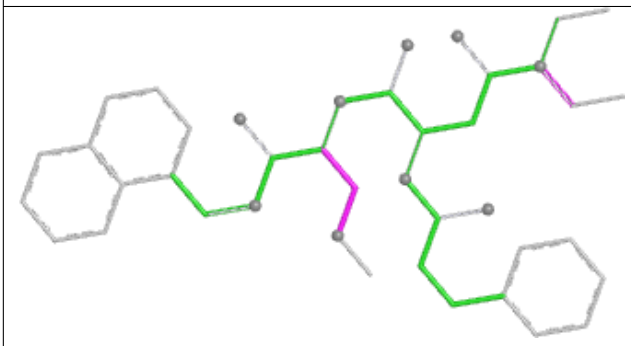

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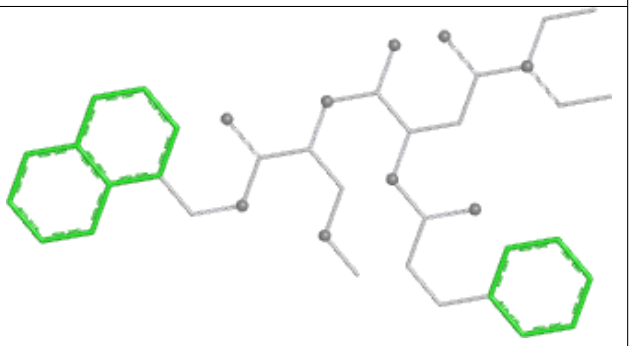
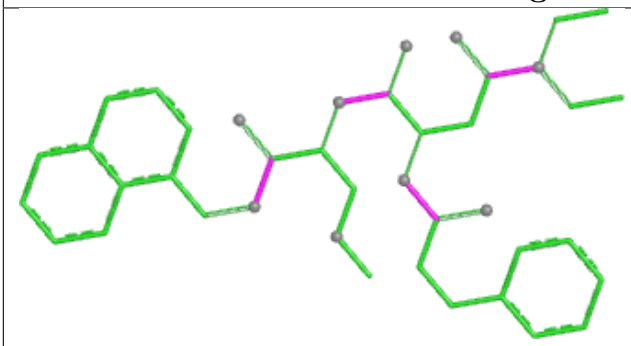


Rings

Ligand 7C7 N 301



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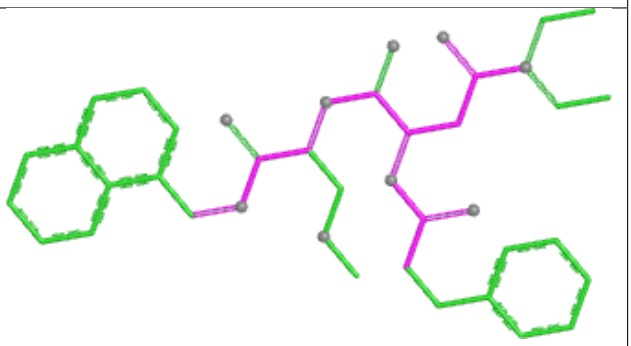

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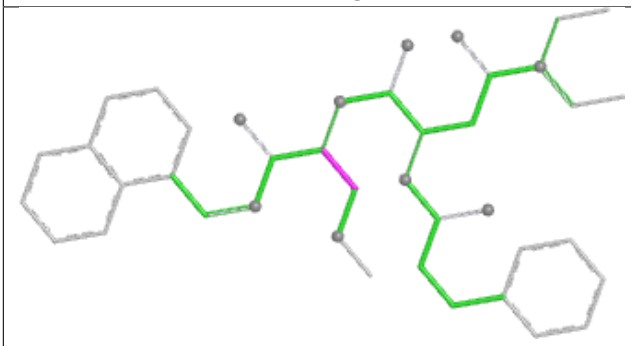
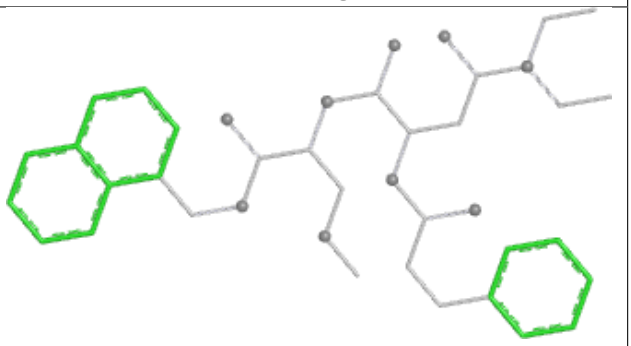
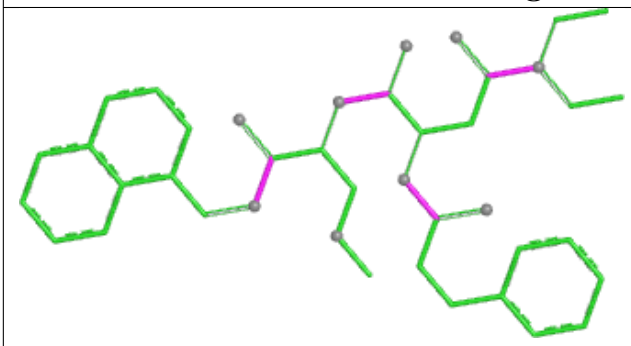


Torsions

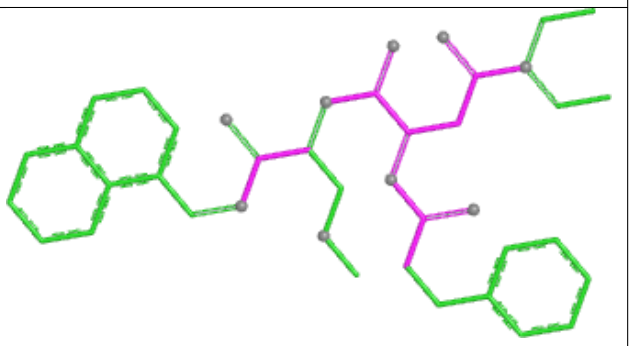


Rings

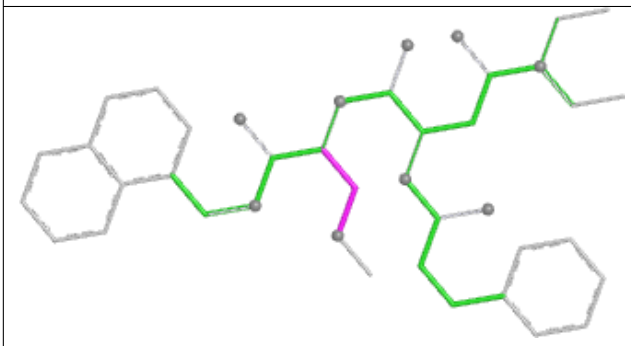
Ligand 7C7 W 301



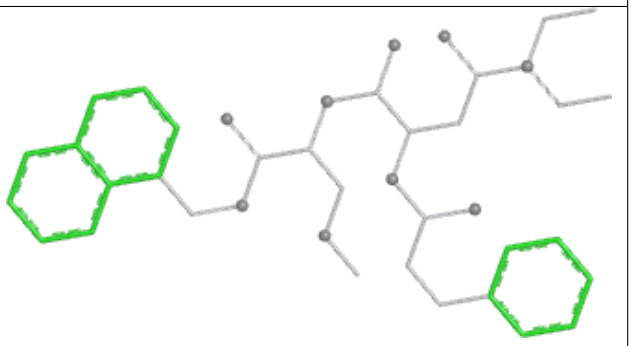
Bond lengths



Bond angles

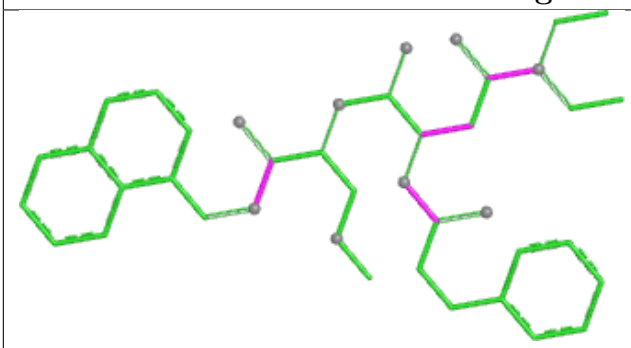


Torsions

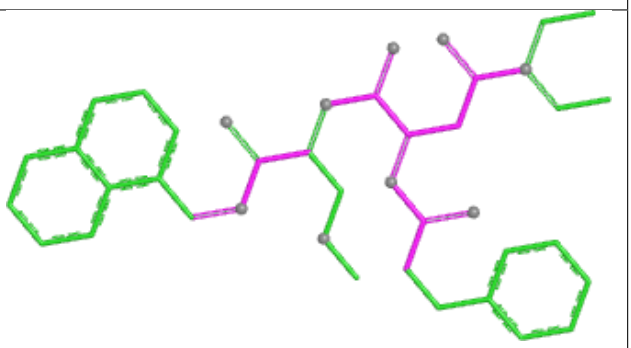


Rings

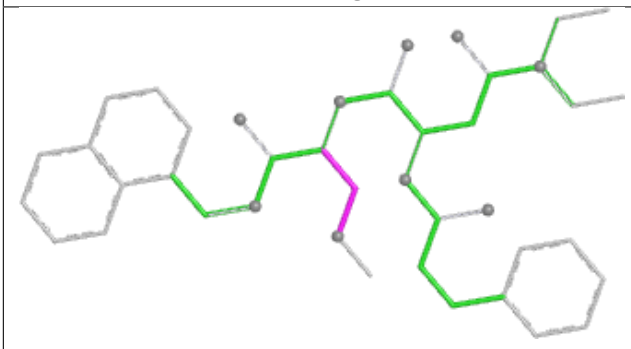
Ligand 7C7 a 301



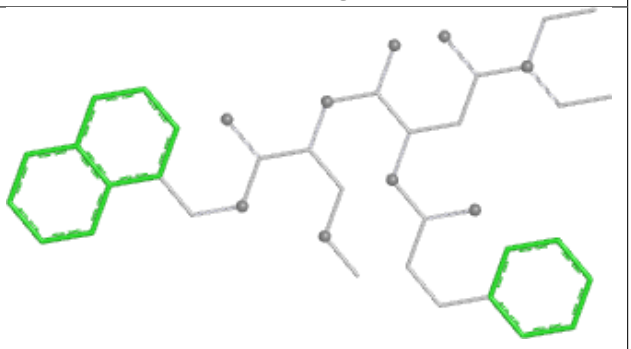
Bond lengths



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	A	218/240 (90%)	-0.35	0 100 100	42, 56, 84, 107	0
1	B	215/240 (89%)	-0.12	0 100 100	40, 69, 102, 124	0
1	C	217/240 (90%)	0.03	1 (0%) 87 72	44, 73, 111, 140	0
1	D	216/240 (90%)	-0.18	3 (1%) 73 51	46, 69, 103, 121	0
1	E	218/240 (90%)	-0.16	3 (1%) 73 51	43, 64, 96, 129	0
1	F	217/240 (90%)	-0.17	1 (0%) 87 72	44, 67, 101, 132	0
1	G	218/240 (90%)	-0.32	2 (0%) 81 61	41, 59, 94, 118	0
1	O	218/240 (90%)	-0.08	1 (0%) 87 72	43, 69, 113, 131	0
1	P	217/240 (90%)	-0.20	2 (0%) 81 61	40, 65, 99, 128	0
1	Q	216/240 (90%)	-0.30	0 100 100	41, 62, 88, 129	0
1	R	217/240 (90%)	-0.26	0 100 100	38, 60, 89, 128	0
1	S	221/240 (92%)	-0.24	1 (0%) 87 72	39, 57, 98, 160	0
1	T	217/240 (90%)	-0.20	2 (0%) 81 61	44, 66, 96, 114	0
1	U	216/240 (90%)	-0.27	1 (0%) 87 72	41, 61, 92, 119	0
2	H	222/240 (92%)	-0.51	1 (0%) 87 72	39, 49, 71, 96	0
2	I	222/240 (92%)	-0.55	0 100 100	38, 46, 66, 93	0
2	J	222/240 (92%)	-0.59	0 100 100	40, 48, 71, 92	0
2	K	223/240 (92%)	-0.57	1 (0%) 88 76	39, 47, 66, 86	0
2	L	223/240 (92%)	-0.60	1 (0%) 88 76	38, 47, 73, 107	0
2	M	223/240 (92%)	-0.52	0 100 100	37, 49, 71, 97	0
2	N	222/240 (92%)	-0.47	0 100 100	41, 51, 75, 96	0
2	V	223/240 (92%)	-0.66	0 100 100	38, 45, 66, 79	0
2	W	223/240 (92%)	-0.64	0 100 100	39, 46, 66, 93	0
2	X	222/240 (92%)	-0.61	0 100 100	39, 48, 68, 85	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
2	Y	223/240 (92%)	-0.57	0 100 100	38, 47, 67, 90	0
2	Z	222/240 (92%)	-0.55	0 100 100	38, 49, 70, 94	0
2	a	223/240 (92%)	-0.54	1 (0%) 88 76	40, 50, 73, 94	0
2	b	223/240 (92%)	-0.56	0 100 100	37, 49, 72, 84	0
All	All	6157/6720 (91%)	-0.39	21 (0%) 90 79	37, 54, 93, 160	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	235	VAL	4.4
1	O	235	VAL	3.6
1	P	235	VAL	3.4
1	G	192	SER	3.4
1	F	235	VAL	3.1

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	7C7	J	301	41/41	0.94	0.10	38,42,49,56	0
3	7C7	I	301	41/41	0.95	0.09	36,43,50,57	0
3	7C7	H	301	41/41	0.95	0.09	38,43,52,59	0
3	7C7	K	301	41/41	0.95	0.09	42,46,55,61	0
3	7C7	L	301	41/41	0.95	0.09	38,44,53,57	0
3	7C7	N	301	41/41	0.95	0.09	39,46,56,59	0
3	7C7	W	301	41/41	0.95	0.09	37,42,53,65	0

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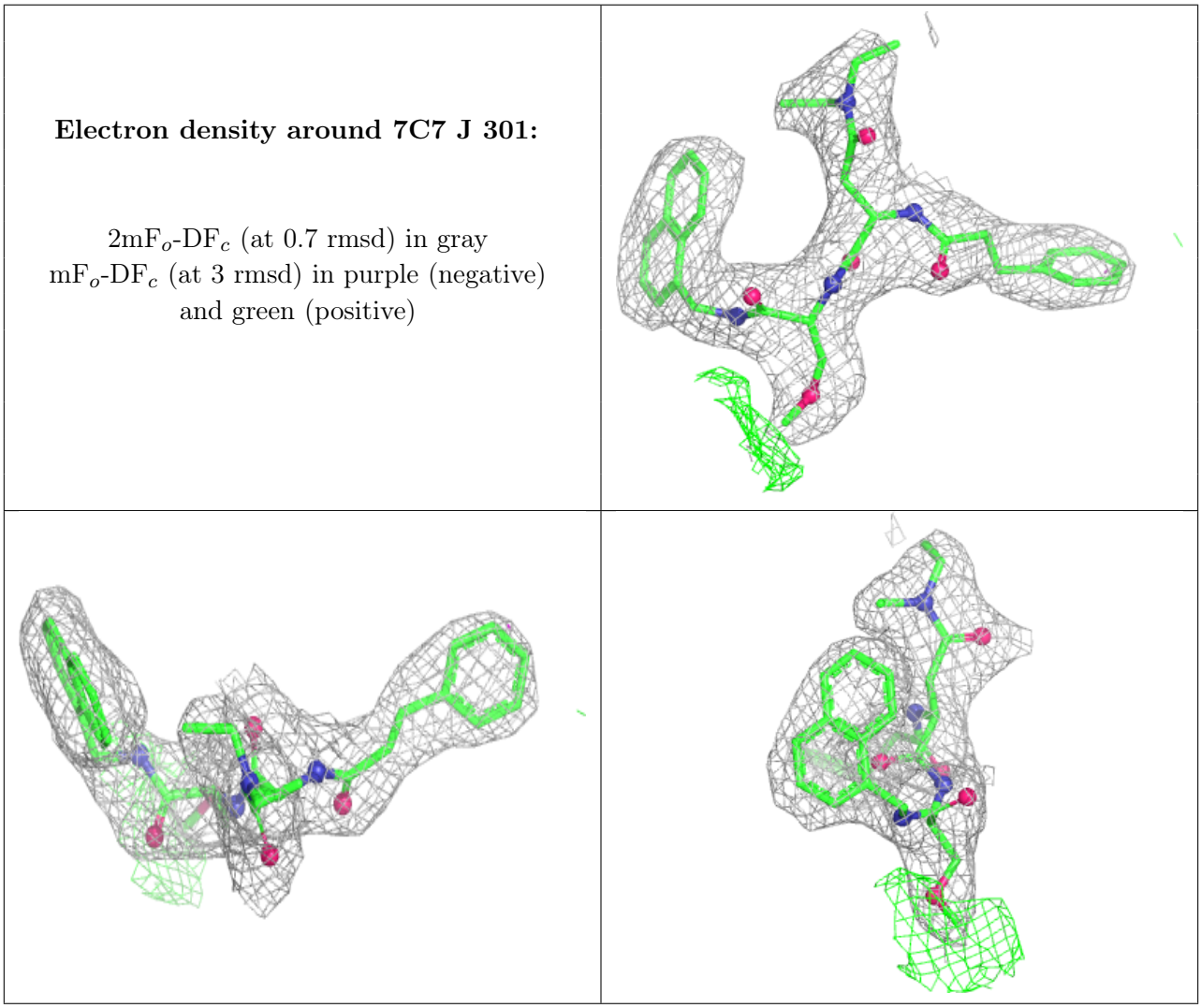
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	7C7	X	301	41/41	0.95	0.10	39,44,58,67	0
3	7C7	Y	301	41/41	0.95	0.09	33,43,48,52	0
3	7C7	a	301	41/41	0.95	0.08	42,44,55,57	0
3	7C7	b	301	41/41	0.95	0.09	40,44,48,55	0
3	7C7	Z	301	41/41	0.96	0.08	40,44,55,60	0
3	7C7	V	301	41/41	0.96	0.08	38,42,46,59	0
3	7C7	M	301	41/41	0.96	0.09	36,45,52,60	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.

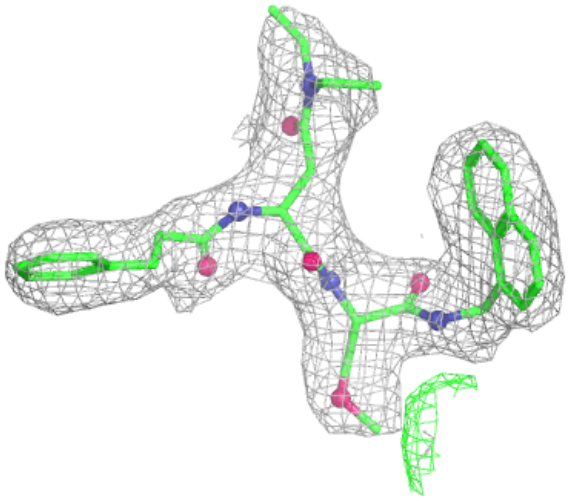
Electron density around 7C7 J 301:

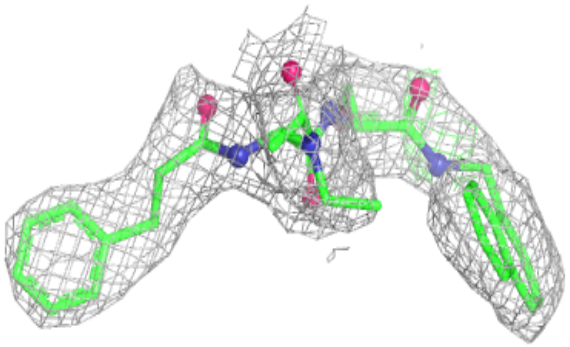
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

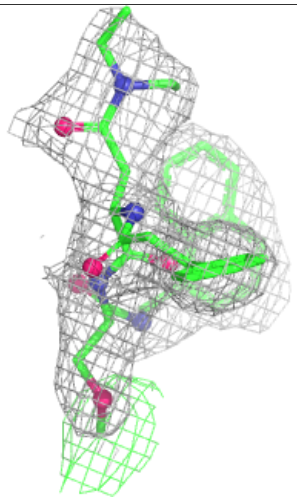


Electron density around 7C7 I 301:

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

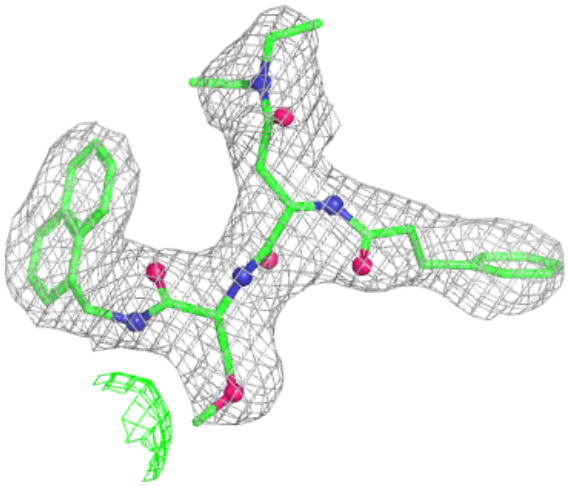


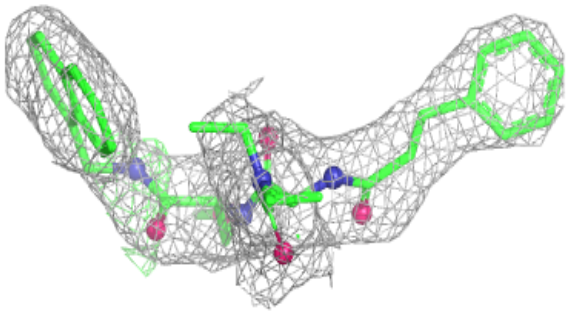


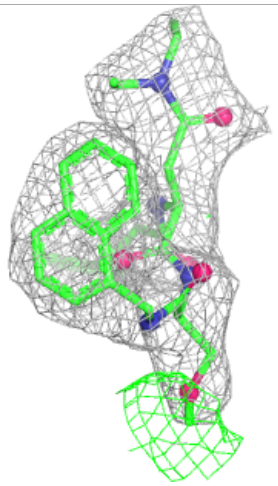


Electron density around 7C7 H 301:

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

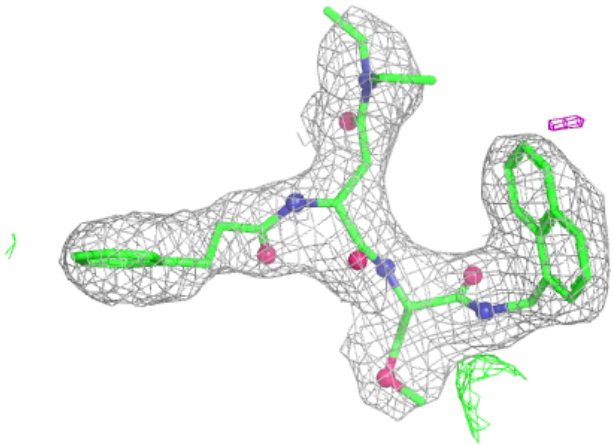


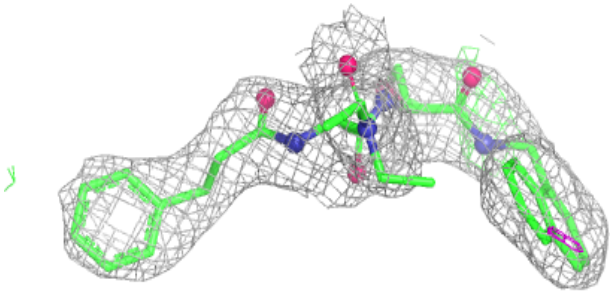




Electron density around 7C7 K 301:

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

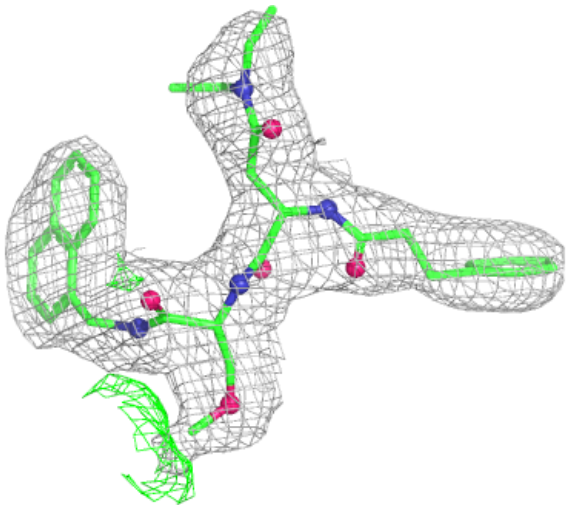


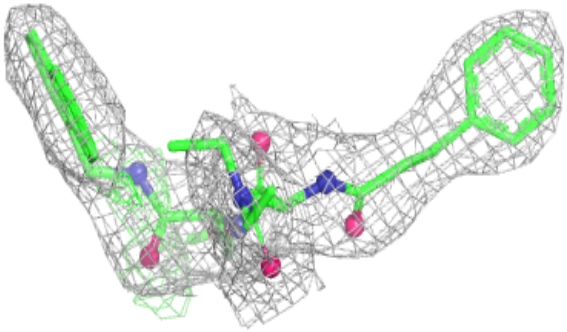


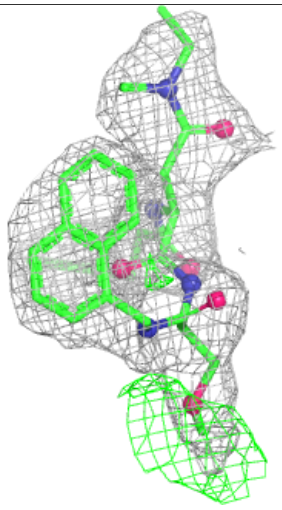


Electron density around 7C7 L 301:

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

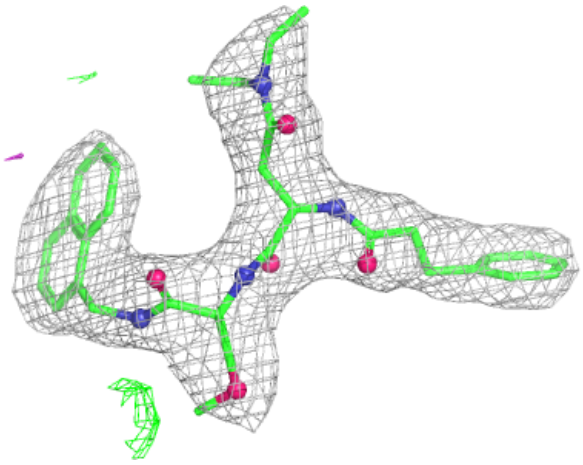


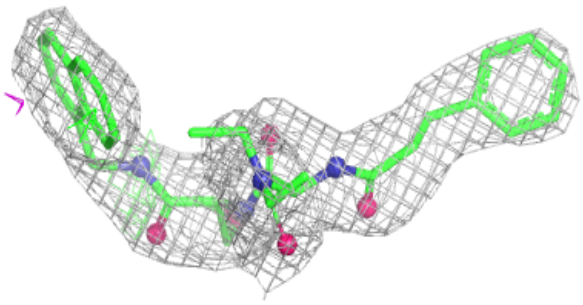


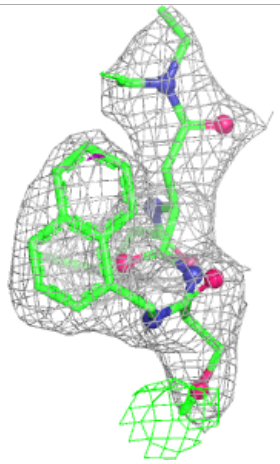


Electron density around 7C7 N 301:

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

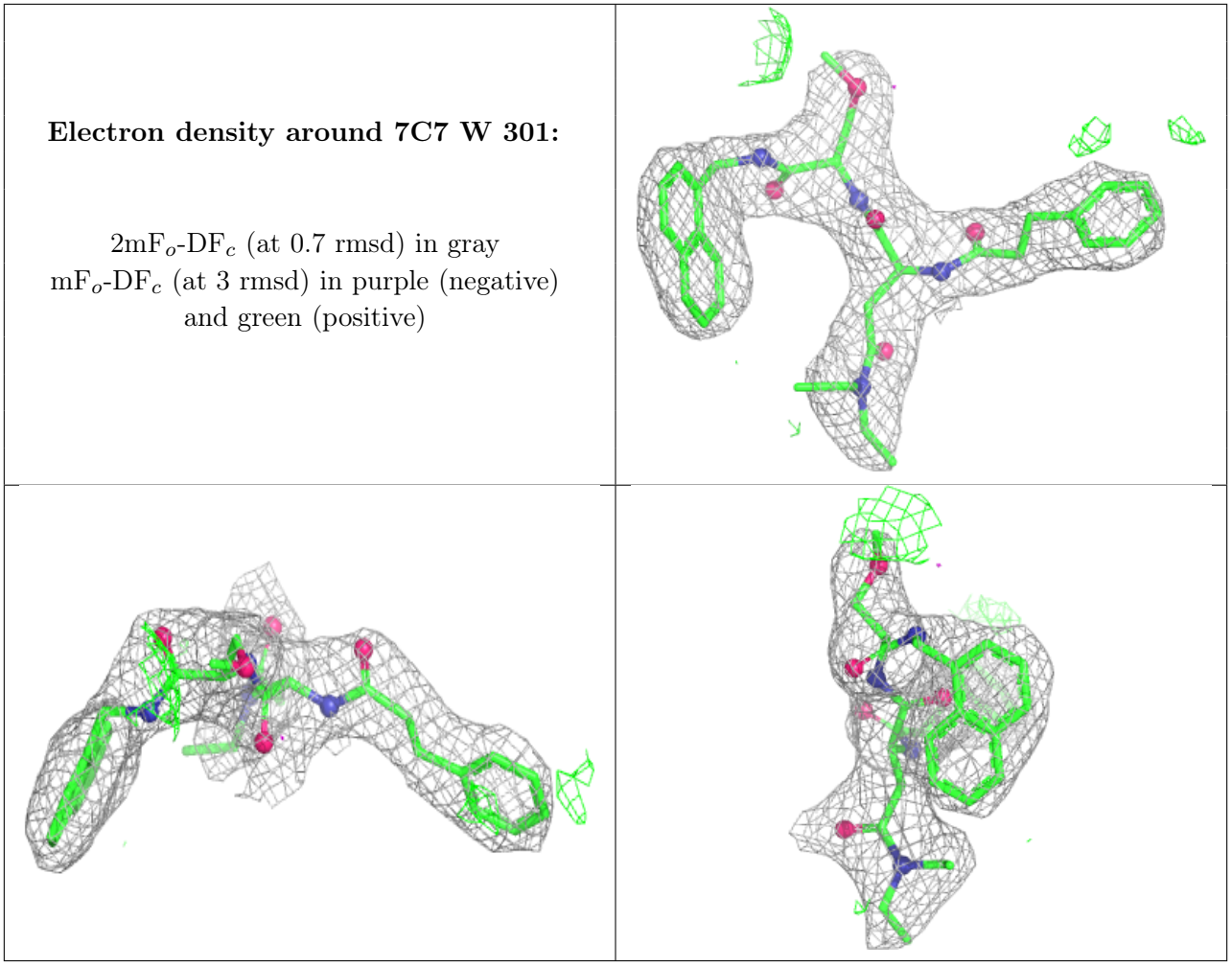






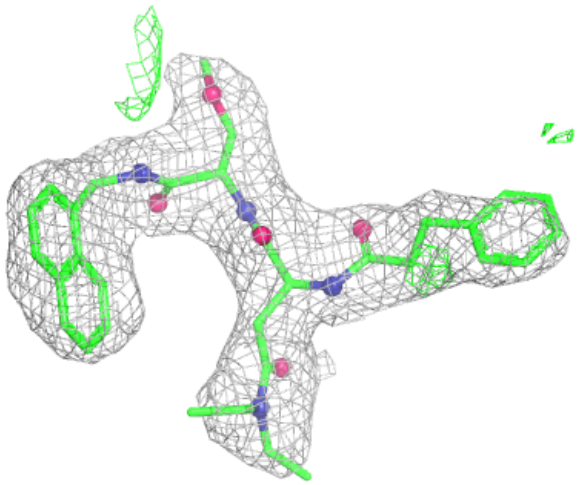
Electron density around 7C7 W 301:

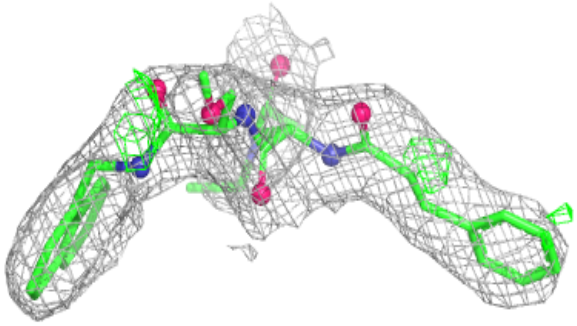
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

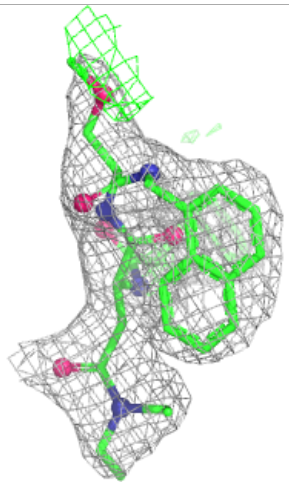


Electron density around 7C7 X 301:

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

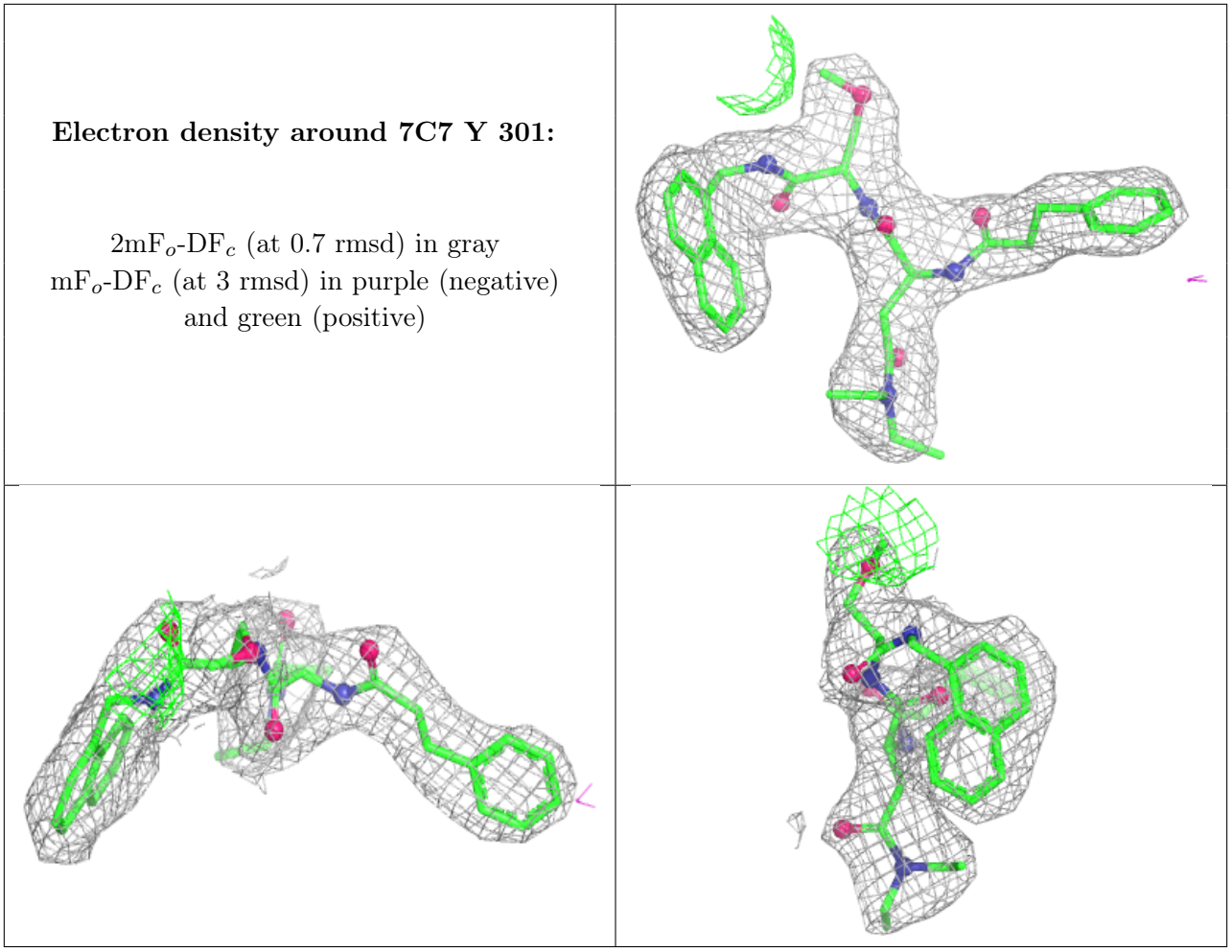






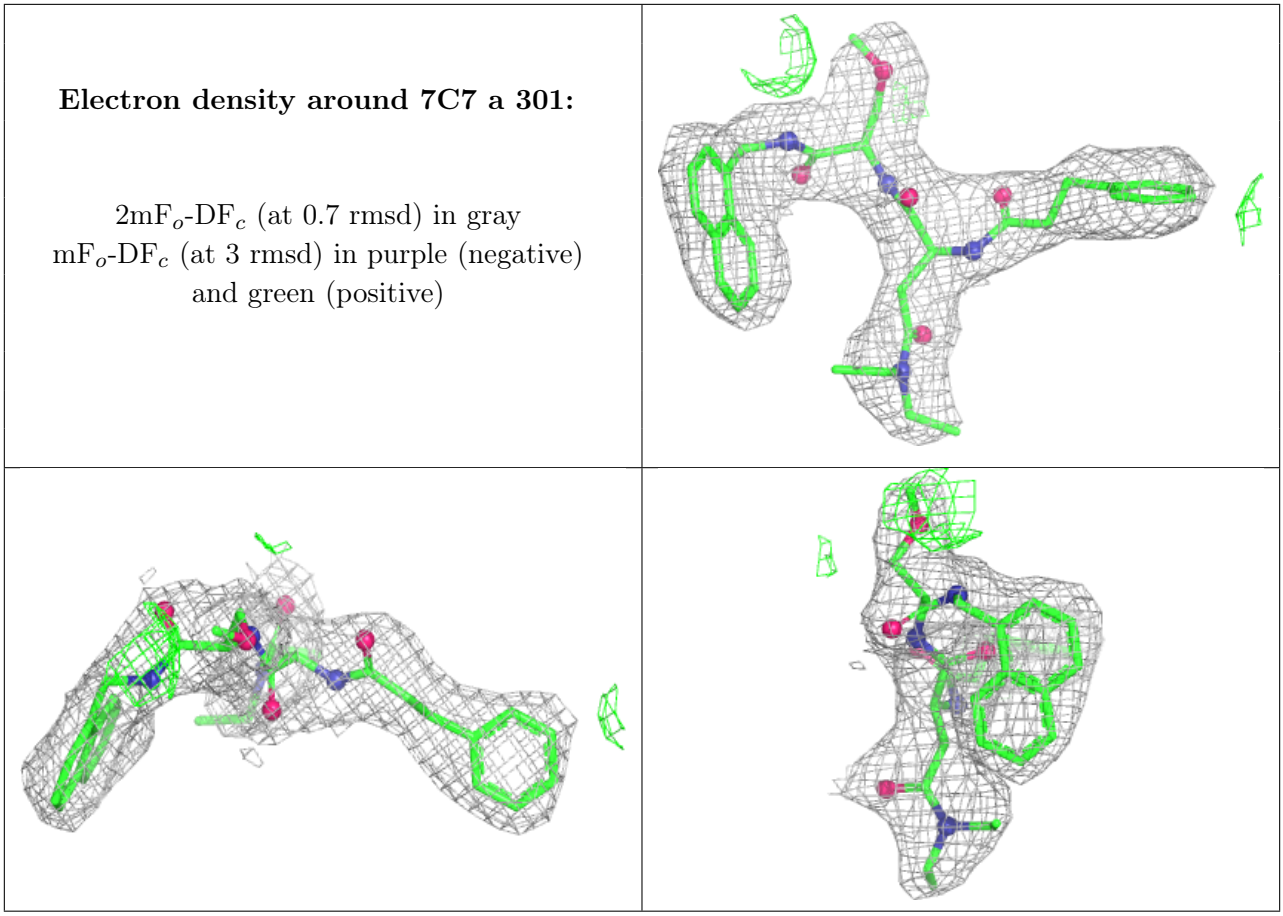
Electron density around 7C7 Y 301:

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



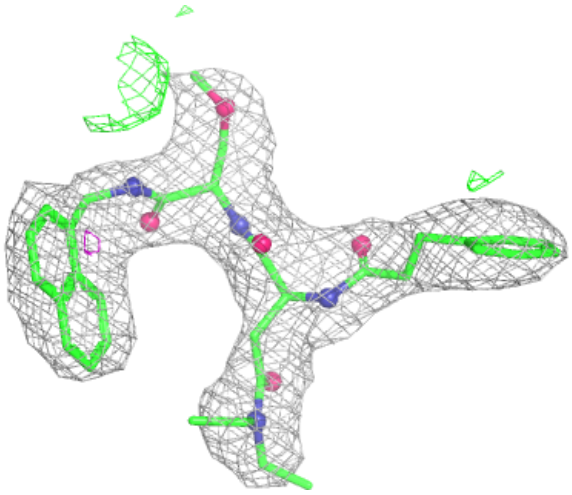
Electron density around 7C7 a 301:

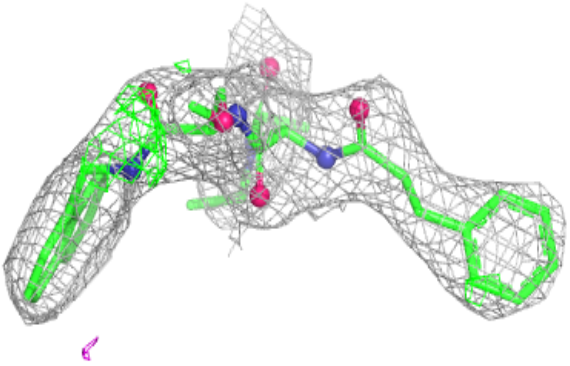
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

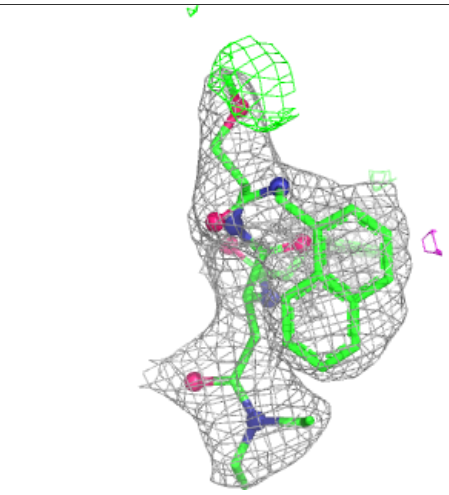


Electron density around 7C7 b 301:

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

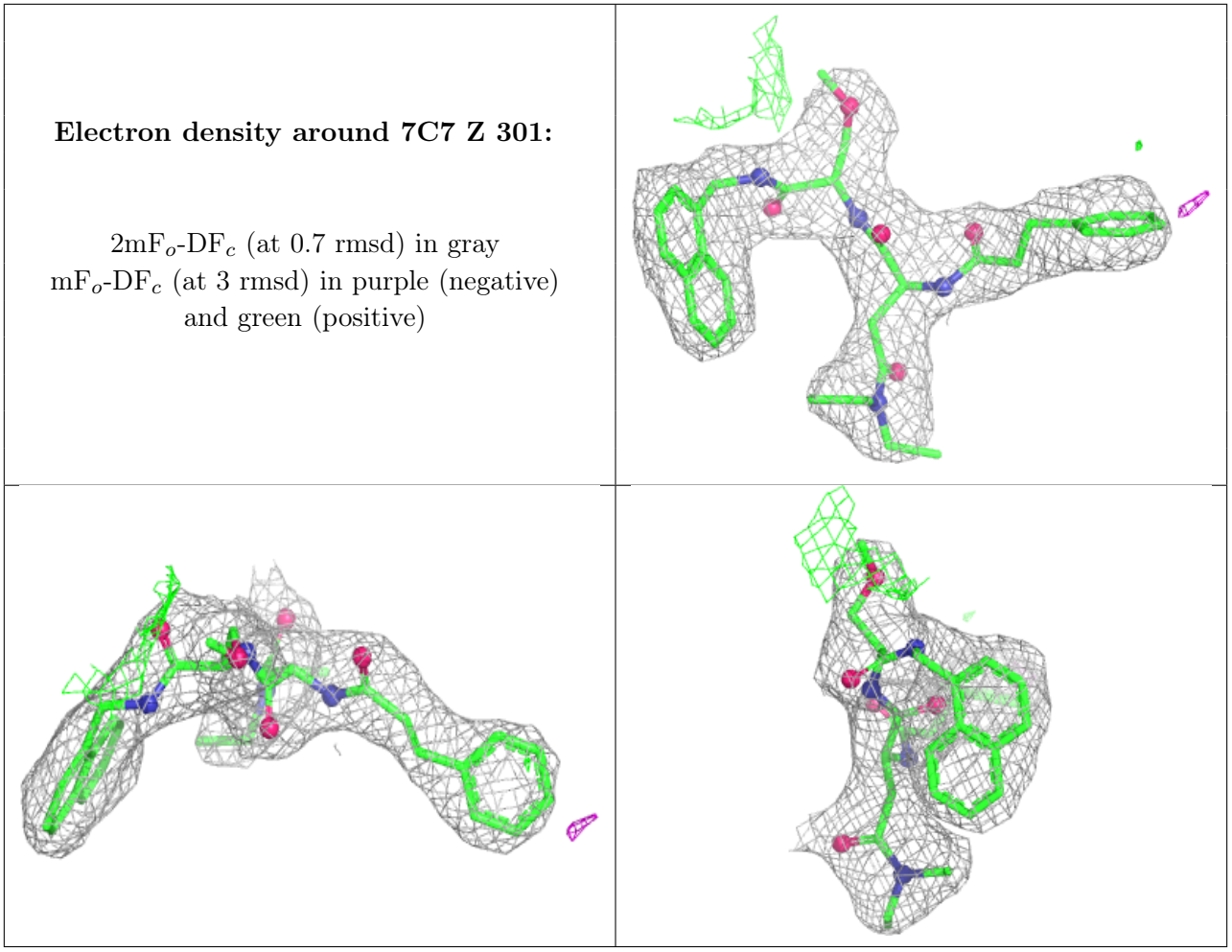






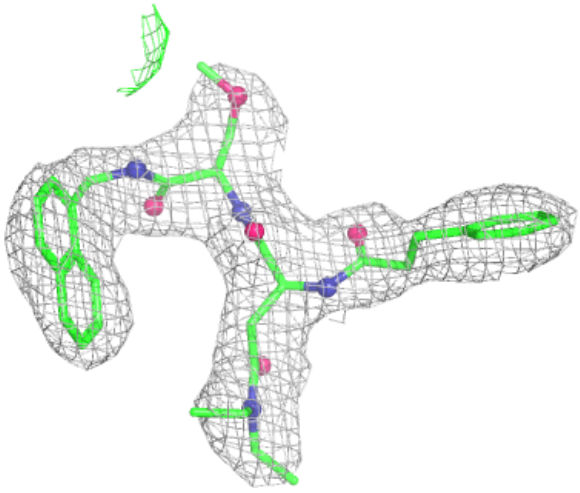
Electron density around 7C7 Z 301:

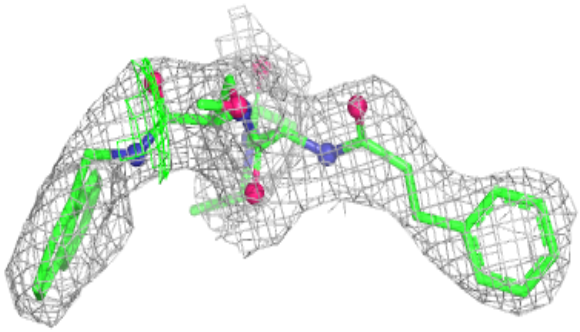
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

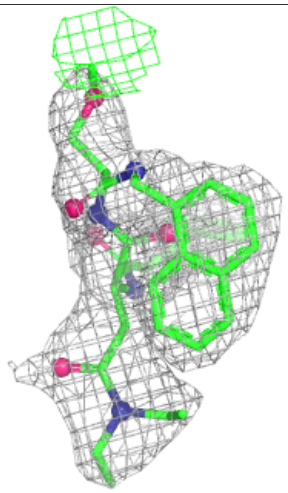


Electron density around 7C7 V 301:

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

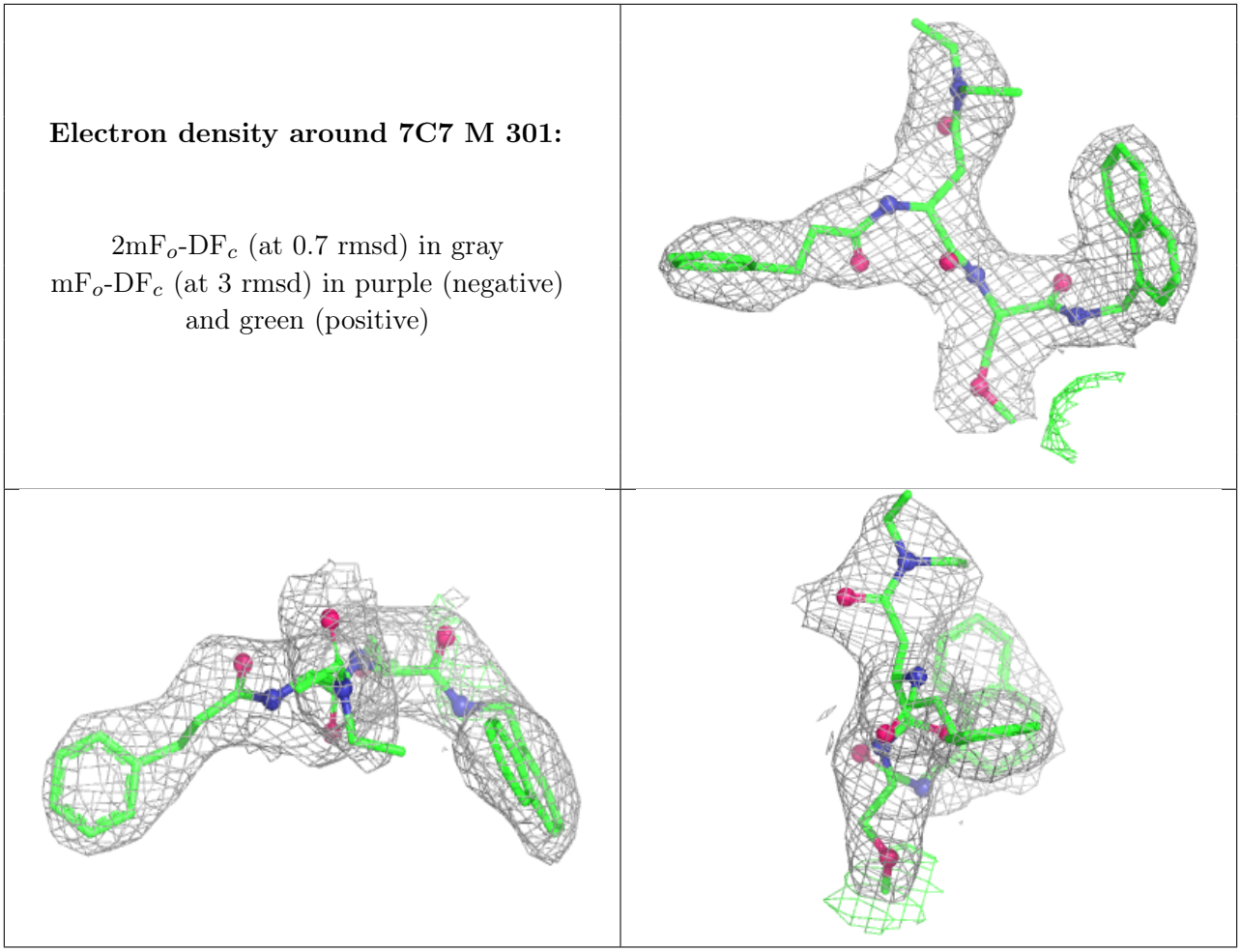






Electron density around 7C7 M 301:

$2mF_o$-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.