



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 05:44 pm BST

PDB ID : 5TRY
Title : Structure of Mycobacterium tuberculosis proteasome in complex with N,C-capped dipeptide PKS2206
Authors : Hsu, H.-C.; Fan, H.; Singh, P.K.; Wang, R.; Sukenick, G.; Nathan, C.; Lin, G.; Li, H.
Deposited on : 2016-10-27
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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

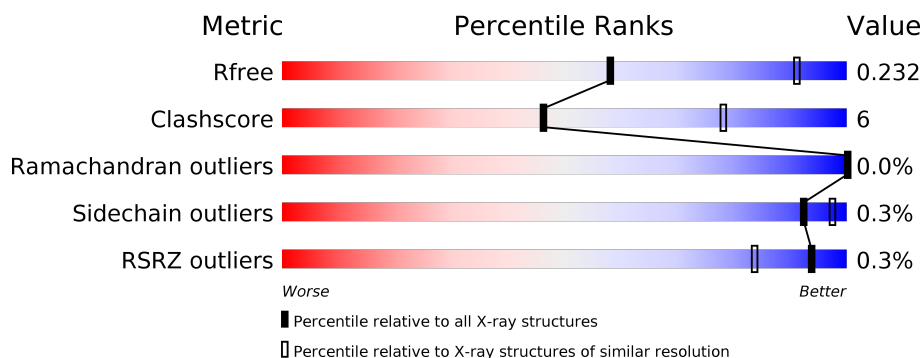
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.
























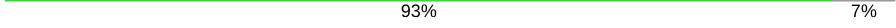
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	240	<div> <div>73%</div> <div>18%</div> <div>9%</div> </div>
1	B	240	<div> <div>73%</div> <div>16%</div> <div>10%</div> </div>
1	C	240	<div> <div>77%</div> <div>13%</div> <div>10%</div> </div>
1	D	240	<div> <div>78%</div> <div>12%</div> <div>10%</div> </div>
1	E	240	<div> <div>72%</div> <div>18%</div> <div>10%</div> </div>
1	F	240	<div> <div>66%</div> <div>25%</div> <div>9%</div> </div>

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

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 47136 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	216	Total	C	N	O	S	0	0	0
			1664	1043	304	313	4			
1	D	217	Total	C	N	O	S	0	0	0
			1670	1046	305	315	4			
1	E	217	Total	C	N	O	S	0	0	0
			1671	1047	305	315	4			
1	F	218	Total	C	N	O	S	0	0	0
			1678	1050	306	318	4			
1	G	216	Total	C	N	O	S	0	0	0
			1662	1040	304	314	4			
1	O	216	Total	C	N	O	S	0	0	0
			1662	1040	304	314	4			
1	P	217	Total	C	N	O	S	0	0	0
			1674	1050	305	315	4			
1	Q	218	Total	C	N	O	S	0	0	0
			1679	1051	306	318	4			
1	R	217	Total	C	N	O	S	0	0	0
			1671	1047	305	315	4			
1	S	219	Total	C	N	O	S	0	0	0
			1683	1053	307	319	4			
1	T	216	Total	C	N	O	S	0	0	0
			1664	1043	304	313	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	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	N	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	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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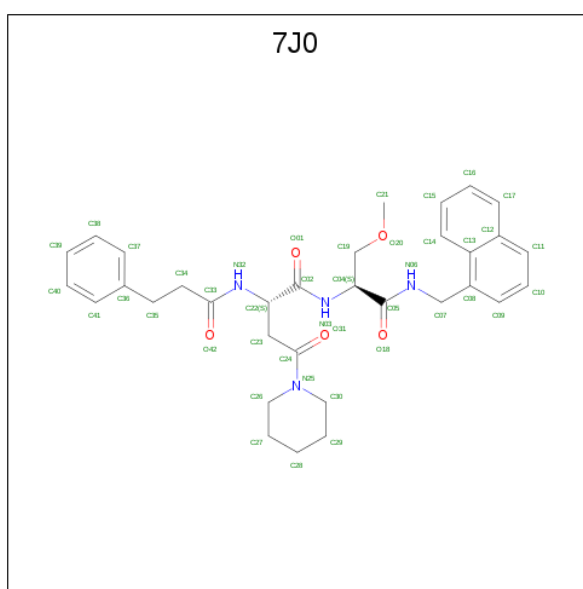
Chain	Residue	Modelled	Actual	Comment	Reference
N	235	HIS	-	expression tag	UNP A5U4D6
N	236	HIS	-	expression tag	UNP A5U4D6
N	237	HIS	-	expression tag	UNP A5U4D6
N	238	HIS	-	expression tag	UNP A5U4D6
N	239	HIS	-	expression tag	UNP A5U4D6
N	240	HIS	-	expression tag	UNP A5U4D6
V	235	HIS	-	expression tag	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 (2 {S})- {N}-[(2 {S})-3-methoxy-1-(naphthalen-1-ylmethylamino)-1-oxidanylidene-propan-2-yl]-4-oxidanylidene-2-(3-phenylpropanoylamino)-4-piperidin-1-yl-butanamide (three-letter code: 7J0) (formula: C₃₃H₄₀N₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	0
			42	33	4	5		
3	I	1	Total	C	N	O	0	0
			42	33	4	5		
3	J	1	Total	C	N	O	0	0
			42	33	4	5		
3	K	1	Total	C	N	O	0	0
			42	33	4	5		
3	L	1	Total	C	N	O	0	0
			42	33	4	5		
3	M	1	Total	C	N	O	0	0
			42	33	4	5		
3	N	1	Total	C	N	O	0	0
			42	33	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	V	1	Total	C	N	O	0	0
			42	33	4	5		
3	W	1	Total	C	N	O	0	0
			42	33	4	5		
3	X	1	Total	C	N	O	0	0
			42	33	4	5		
3	Y	1	Total	C	N	O	0	0
			42	33	4	5		
3	Z	1	Total	C	N	O	0	0
			42	33	4	5		
3	a	1	Total	C	N	O	0	0
			42	33	4	5		
3	b	1	Total	C	N	O	0	0
			42	33	4	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		
4	B	2	Total	O	0	0
			2	2		
4	C	5	Total	O	0	0
			5	5		
4	D	3	Total	O	0	0
			3	3		
4	E	5	Total	O	0	0
			5	5		
4	F	8	Total	O	0	0
			8	8		
4	G	7	Total	O	0	0
			7	7		
4	H	7	Total	O	0	0
			7	7		
4	I	8	Total	O	0	0
			8	8		
4	J	7	Total	O	0	0
			7	7		
4	K	12	Total	O	0	0
			12	12		
4	L	5	Total	O	0	0
			5	5		

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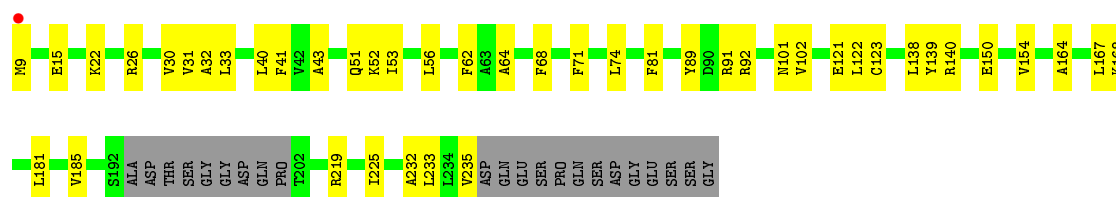
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	12	Total 12	O 12	0	0
4	N	7	Total 7	O 7	0	0
4	O	6	Total 6	O 6	0	0
4	P	6	Total 6	O 6	0	0
4	Q	5	Total 5	O 5	0	0
4	R	8	Total 8	O 8	0	0
4	S	9	Total 9	O 9	0	0
4	T	6	Total 6	O 6	0	0
4	U	7	Total 7	O 7	0	0
4	V	9	Total 9	O 9	0	0
4	W	8	Total 8	O 8	0	0
4	X	8	Total 8	O 8	0	0
4	Y	11	Total 11	O 11	0	0
4	Z	11	Total 11	O 11	0	0
4	a	6	Total 6	O 6	0	0
4	b	8	Total 8	O 8	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

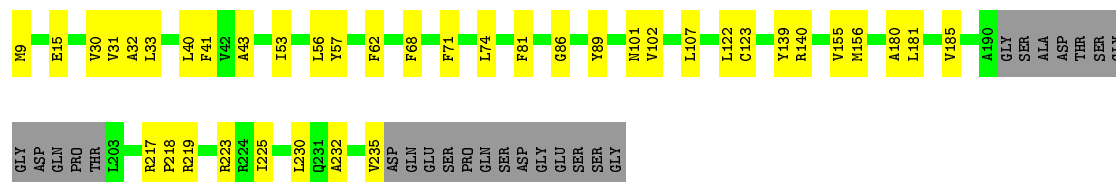
- Molecule 1: Proteasome subunit alpha

Chain A: 




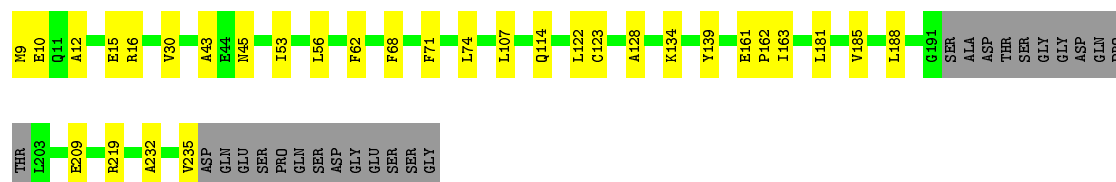
- Molecule 1: Proteasome subunit alpha

Chain B: 




- Molecule 1: Proteasome subunit alpha

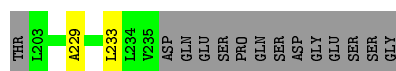
Chain C: 



- Molecule 1: Proteasome subunit alpha

Chain D: 





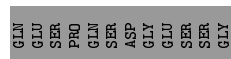
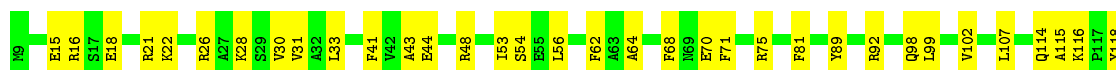
- Molecule 1: Proteasome subunit alpha

Chain E: 72% 18% 10%



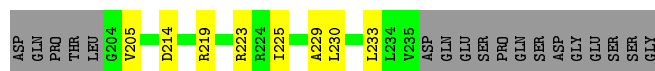
- Molecule 1: Proteasome subunit alpha

Chain F: 66% 25% 9%



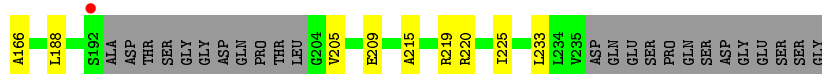
- Molecule 1: Proteasome subunit alpha

Chain G: 74% 16% 10%



- Molecule 1: Proteasome subunit alpha

Chain O: 71% 19% 10%



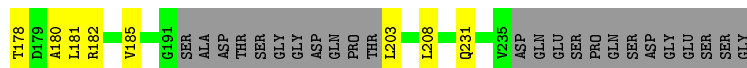
- Molecule 1: Proteasome subunit alpha

Chain P: 67% 23% 10%



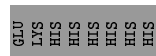
- Molecule 1: Proteasome subunit alpha

Chain U: 73% 18% 10%



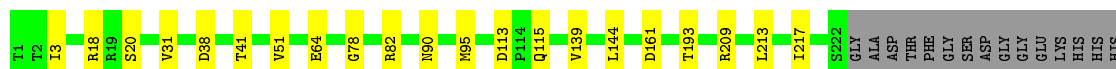
- Molecule 2: Proteasome subunit beta

Chain H: 82% 11% 8%



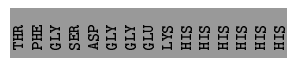
- Molecule 2: Proteasome subunit beta

Chain I: 84% 9% 8%



- Molecule 2: Proteasome subunit beta

Chain J: 81% 12% 8%




- Molecule 2: Proteasome subunit beta

Chain K: 82% 11% 7%




GLU
LYS
HIS
HIS
HIS
HIS
HIS
HIS

• Molecule 2: Proteasome subunit beta

Chain L:  86% 7% 7%


T1 R33 V51 E62 E64 K68 L69 E70 R82 L98 L101 D113 P114 Q115 L144 M150 Y154 D161 R209 G223 ALA ASP THR PHE GLY SER ASP GLY GLY GLU LYS HIS HIS HIS HIS HIS

• Molecule 2: Proteasome subunit beta

Chain M:  85% 7% 8%

T1 T2 I3 R18 R19 S20 M25 G28 D38 T41 V51 E64 K68 R82 N90 M95 L98 P114 V139 T193 S222 GLY ALA ASP THR PHE GLY SER ASP GLY LYS HIS HIS HIS HIS HIS


• Molecule 2: Proteasome subunit beta

Chain N:  79% 14% 7%

T1 T2 I3 V4 A5 V13 H14 A15 M25 D38 T41 G44 I45 V51 A52 R57 E64 T75 G78 R82 R88 G89 N90 L99 A100 V121 S122 A126 M130 I131 E132 Y136 Q137 L144 M150 L164 P192 T193

I210 G223 ALA ASP THR PHE GLY SER ASP GLY GLU LYS HIS HIS HIS HIS HIS


• Molecule 2: Proteasome subunit beta

Chain V:  83% 10% 7%

T1 T2 I3 V4 A5 V13 R18 R19 S20 R29 E30 V31 D38 T41 G44 H65 T75 G78 R82 V121 S122 M130 Q137 L144 Q156 R165 S179 T193 L213 G223 ALA ASP THR PHE GLY ASP GLY GLU

LYS
HIS
HIS
HIS
HIS
HIS
HIS


• Molecule 2: Proteasome subunit beta

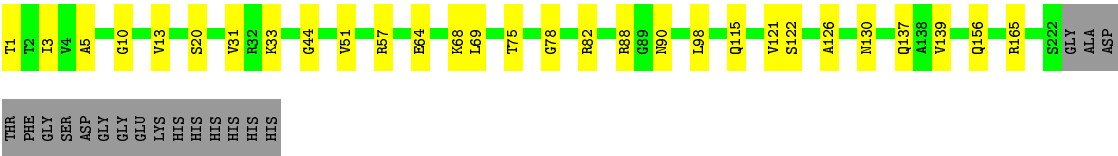
Chain W:  81% 12% 7%

T1 T2 V4 V13 S20 G28 G44 I45 V51 A52 R57 E64 G78 R82 R88 G89 N90 L98 A126 E132 E133 E134 G135 Y136 V139 M150 Y154 E169 R188 I196 D204 I217 G223 ALA ASP THR PHE

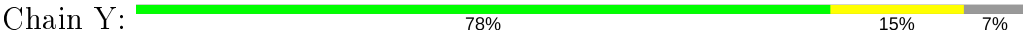
GLY
SER
ASP
GLY
GLY
GLU
LYS
HIS
HIS
HIS
HIS
HIS

• Molecule 2: Proteasome subunit beta

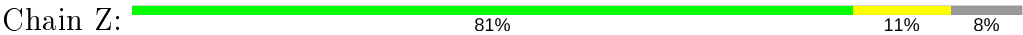
Chain X:  80% 12% 8%



• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta



• 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	120.65Å 197.48Å 164.81Å 90.00° 103.05° 90.00°	Depositor
Resolution (Å)	51.09 – 3.00 51.09 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (51.09-3.00) 92.7 (51.09-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.182 , 0.234 0.184 , 0.232	Depositor DCC
R_{free} test set	7376 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	47136	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 7J0

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	0.28	0/1701	0.50	0/2297
1	B	0.26	0/1684	0.46	0/2274
1	C	0.26	0/1688	0.46	0/2279
1	D	0.26	0/1694	0.48	1/2287 (0.0%)
1	E	0.29	0/1695	0.50	1/2289 (0.0%)
1	F	0.27	0/1702	0.48	0/2298
1	G	0.26	0/1686	0.48	0/2276
1	O	0.27	0/1686	0.48	0/2276
1	P	0.27	0/1699	0.49	0/2295
1	Q	0.26	0/1703	0.48	0/2300
1	R	0.29	0/1695	0.46	0/2289
1	S	0.27	0/1707	0.47	0/2305
1	T	0.27	0/1688	0.48	0/2279
1	U	0.26	0/1688	0.50	1/2279 (0.0%)
2	H	0.26	0/1662	0.49	0/2254
2	I	0.26	0/1662	0.48	0/2254
2	J	0.26	0/1662	0.50	0/2254
2	K	0.27	0/1666	0.50	0/2259
2	L	0.27	0/1666	0.50	0/2259
2	M	0.26	0/1662	0.49	0/2254
2	N	0.27	0/1666	0.50	0/2259
2	V	0.27	0/1666	0.51	0/2259
2	W	0.27	0/1666	0.50	0/2259
2	X	0.26	0/1662	0.49	0/2254
2	Y	0.27	0/1666	0.49	0/2259
2	Z	0.26	0/1662	0.49	0/2254
2	a	0.27	0/1666	0.49	0/2259
2	b	0.26	0/1666	0.48	0/2259
All	All	0.27	0/47016	0.49	3/63619 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	203	LEU	CA-CB-CG	7.12	131.69	115.30
1	D	40	LEU	CA-CB-CG	5.23	127.34	115.30
1	E	33	LEU	CA-CB-CG	5.09	127.00	115.30

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	A	1677	0	1680	29	0
1	B	1660	0	1665	27	0
1	C	1664	0	1668	22	0
1	D	1670	0	1673	16	0
1	E	1671	0	1675	32	0
1	F	1678	0	1677	40	0
1	G	1662	0	1662	24	0
1	O	1662	0	1662	28	0
1	P	1674	0	1680	38	0
1	Q	1679	0	1679	36	0
1	R	1671	0	1675	21	0
1	S	1683	0	1682	21	0
1	T	1664	0	1668	25	0
1	U	1664	0	1668	26	0
2	H	1638	0	1633	19	0
2	I	1638	0	1633	14	0
2	J	1638	0	1633	21	0
2	K	1642	0	1636	15	0
2	L	1642	0	1636	12	0
2	M	1638	0	1633	13	0
2	N	1642	0	1636	22	0
2	V	1642	0	1636	15	0
2	W	1642	0	1636	20	0
2	X	1638	0	1633	20	0
2	Y	1642	0	1636	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Z	1638	0	1633	19	0
2	a	1642	0	1636	0	0
2	b	1642	0	1636	0	0
3	H	42	0	0	0	0
3	I	42	0	0	1	0
3	J	42	0	0	1	0
3	K	42	0	0	0	0
3	L	42	0	0	0	0
3	M	42	0	0	0	0
3	N	42	0	0	0	0
3	V	42	0	0	0	0
3	W	42	0	0	0	0
3	X	42	0	0	0	0
3	Y	42	0	0	0	0
3	Z	42	0	0	0	0
3	a	42	0	0	0	0
3	b	42	0	0	0	0
4	A	9	0	0	0	0
4	B	2	0	0	0	0
4	C	5	0	0	0	0
4	D	3	0	0	0	0
4	E	5	0	0	0	0
4	F	8	0	0	0	0
4	G	7	0	0	0	0
4	H	7	0	0	0	0
4	I	8	0	0	0	0
4	J	7	0	0	0	0
4	K	12	0	0	0	0
4	L	5	0	0	0	0
4	M	12	0	0	0	0
4	N	7	0	0	0	0
4	O	6	0	0	0	0
4	P	6	0	0	0	0
4	Q	5	0	0	0	0
4	R	8	0	0	1	0
4	S	9	0	0	0	0
4	T	6	0	0	0	0
4	U	7	0	0	0	0
4	V	9	0	0	0	0
4	W	8	0	0	1	0
4	X	8	0	0	1	0
4	Y	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Z	11	0	0	0	0
4	a	6	0	0	0	0
4	b	8	0	0	0	0
All	All	47136	0	46300	544	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 544 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:MET:N	1:E:15:GLU:OE1	2.14	0.81
1:R:16:ARG:NH2	1:R:114:GLN:O	2.13	0.80
2:V:29:ARG:NH1	2:W:134:GLU:OE2	2.15	0.80
1:P:219:ARG:NH2	2:W:64:GLU:OE1	2.14	0.79
1:Q:140:ARG:NH2	1:Q:155:VAL:O	2.13	0.78

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%)	7 (3%)	0	100	100
1	B	211/240 (88%)	206 (98%)	5 (2%)	0	100	100
1	C	212/240 (88%)	206 (97%)	6 (3%)	0	100	100
1	D	213/240 (89%)	206 (97%)	7 (3%)	0	100	100
1	E	213/240 (89%)	206 (97%)	7 (3%)	0	100	100
1	F	214/240 (89%)	206 (96%)	8 (4%)	0	100	100
1	G	212/240 (88%)	207 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	212/240 (88%)	205 (97%)	6 (3%)	1 (0%)	29	68
1	P	213/240 (89%)	205 (96%)	8 (4%)	0	100	100
1	Q	214/240 (89%)	207 (97%)	7 (3%)	0	100	100
1	R	213/240 (89%)	205 (96%)	8 (4%)	0	100	100
1	S	215/240 (90%)	205 (95%)	10 (5%)	0	100	100
1	T	212/240 (88%)	204 (96%)	8 (4%)	0	100	100
1	U	212/240 (88%)	206 (97%)	6 (3%)	0	100	100
2	H	220/240 (92%)	216 (98%)	4 (2%)	0	100	100
2	I	220/240 (92%)	214 (97%)	6 (3%)	0	100	100
2	J	220/240 (92%)	216 (98%)	4 (2%)	0	100	100
2	K	221/240 (92%)	216 (98%)	5 (2%)	0	100	100
2	L	221/240 (92%)	217 (98%)	4 (2%)	0	100	100
2	M	220/240 (92%)	215 (98%)	4 (2%)	1 (0%)	29	68
2	N	221/240 (92%)	217 (98%)	4 (2%)	0	100	100
2	V	221/240 (92%)	217 (98%)	4 (2%)	0	100	100
2	W	221/240 (92%)	216 (98%)	5 (2%)	0	100	100
2	X	220/240 (92%)	216 (98%)	4 (2%)	0	100	100
2	Y	221/240 (92%)	215 (97%)	6 (3%)	0	100	100
2	Z	220/240 (92%)	213 (97%)	7 (3%)	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	6068/6720 (90%)	5903 (97%)	163 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	205	VAL
2	M	114	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	167/184 (91%)	166 (99%)	1 (1%)	86	95
1	B	165/184 (90%)	164 (99%)	1 (1%)	86	95
1	C	165/184 (90%)	165 (100%)	0	100	100
1	D	166/184 (90%)	163 (98%)	3 (2%)	59	85
1	E	166/184 (90%)	165 (99%)	1 (1%)	86	95
1	F	167/184 (91%)	167 (100%)	0	100	100
1	G	165/184 (90%)	165 (100%)	0	100	100
1	O	165/184 (90%)	164 (99%)	1 (1%)	86	95
1	P	167/184 (91%)	165 (99%)	2 (1%)	71	90
1	Q	167/184 (91%)	166 (99%)	1 (1%)	86	95
1	R	166/184 (90%)	165 (99%)	1 (1%)	86	95
1	S	167/184 (91%)	166 (99%)	1 (1%)	86	95
1	T	165/184 (90%)	165 (100%)	0	100	100
1	U	165/184 (90%)	164 (99%)	1 (1%)	86	95
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
2	a	165/178 (93%)	165 (100%)	0	100	100
2	b	165/178 (93%)	165 (100%)	0	100	100
All	All	4633/5068 (91%)	4620 (100%)	13 (0%)	92	97

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	33	LEU
1	O	33	LEU
1	R	101	ASN
1	D	179	ASP
1	Q	75	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	X	90	ASN
2	a	115	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 carbohydrates 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	7J0	V	301	-	45,45,45	1.84	11 (24%)	59,59,59	1.47	9 (15%)
3	7J0	W	301	-	45,45,45	1.86	11 (24%)	59,59,59	1.47	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	7J0	J	301	-	45,45,45	1.86	11 (24%)	59,59,59	1.54	10 (16%)
3	7J0	H	301	-	45,45,45	1.86	11 (24%)	59,59,59	1.48	10 (16%)
3	7J0	K	301	-	45,45,45	1.87	11 (24%)	59,59,59	1.49	9 (15%)
3	7J0	N	301	-	45,45,45	1.85	11 (24%)	59,59,59	1.48	10 (16%)
3	7J0	I	301	-	45,45,45	1.85	11 (24%)	59,59,59	1.47	9 (15%)
3	7J0	L	301	-	45,45,45	1.84	11 (24%)	59,59,59	1.47	9 (15%)
3	7J0	b	301	-	45,45,45	1.84	11 (24%)	59,59,59	1.49	9 (15%)
3	7J0	M	301	-	45,45,45	1.85	11 (24%)	59,59,59	1.48	9 (15%)
3	7J0	a	301	-	45,45,45	1.85	11 (24%)	59,59,59	1.48	9 (15%)
3	7J0	Z	301	-	45,45,45	1.85	11 (24%)	59,59,59	1.47	8 (13%)
3	7J0	X	301	-	45,45,45	1.85	11 (24%)	59,59,59	1.47	9 (15%)
3	7J0	Y	301	-	45,45,45	1.85	11 (24%)	59,59,59	1.47	8 (13%)

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	7J0	V	301	-	-	5/37/45/45	0/4/4/4
3	7J0	W	301	-	-	2/37/45/45	0/4/4/4
3	7J0	J	301	-	-	6/37/45/45	0/4/4/4
3	7J0	H	301	-	-	8/37/45/45	0/4/4/4
3	7J0	K	301	-	-	7/37/45/45	0/4/4/4
3	7J0	N	301	-	-	4/37/45/45	0/4/4/4
3	7J0	I	301	-	-	3/37/45/45	0/4/4/4
3	7J0	L	301	-	-	3/37/45/45	0/4/4/4
3	7J0	b	301	-	-	3/37/45/45	0/4/4/4
3	7J0	M	301	-	-	5/37/45/45	0/4/4/4
3	7J0	a	301	-	-	7/37/45/45	0/4/4/4
3	7J0	Z	301	-	-	5/37/45/45	0/4/4/4
3	7J0	X	301	-	-	3/37/45/45	0/4/4/4
3	7J0	Y	301	-	-	3/37/45/45	0/4/4/4

The worst 5 of 154 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	301	7J0	C33-N32	6.24	1.47	1.34
3	K	301	7J0	C33-N32	6.21	1.47	1.34
3	W	301	7J0	C33-N32	6.20	1.47	1.34
3	M	301	7J0	C33-N32	6.20	1.47	1.34
3	N	301	7J0	C33-N32	6.20	1.47	1.34

The worst 5 of 127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	301	7J0	C34-C33-N32	4.57	123.76	115.83
3	K	301	7J0	C34-C33-N32	4.53	123.68	115.83
3	I	301	7J0	C34-C33-N32	4.51	123.66	115.83
3	a	301	7J0	C34-C33-N32	4.51	123.65	115.83
3	L	301	7J0	C34-C33-N32	4.51	123.65	115.83

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	V	301	7J0	C33-C34-C35-C36
3	V	301	7J0	C05-C04-C19-O20
3	W	301	7J0	N03-C04-C19-O20
3	W	301	7J0	C05-C04-C19-O20
3	J	301	7J0	C33-C34-C35-C36

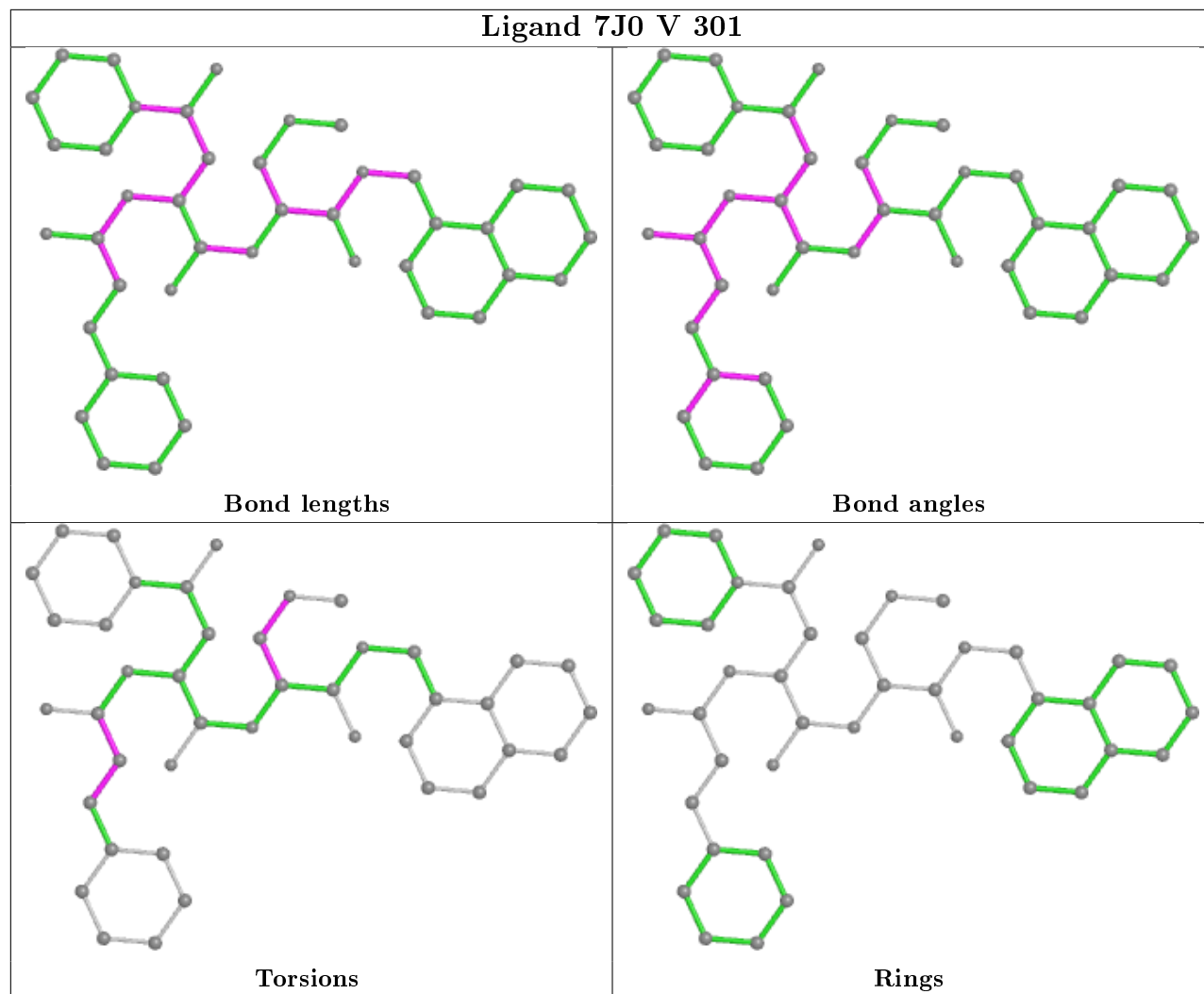
There are no ring outliers.

2 monomers are involved in 2 short contacts:

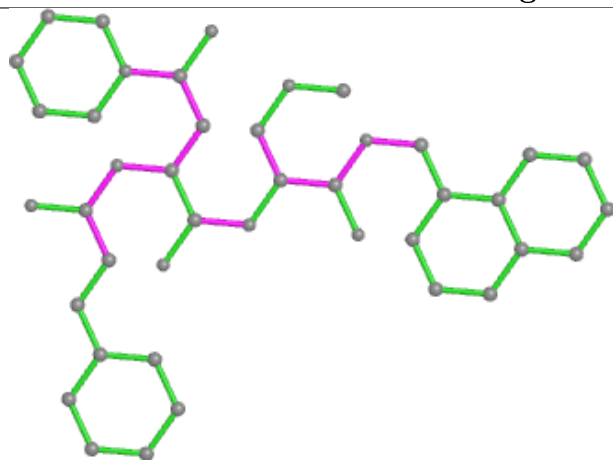
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	301	7J0	1	0
3	I	301	7J0	1	0

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

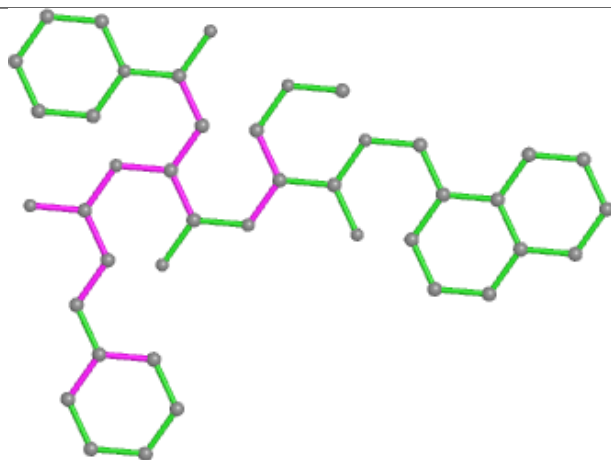
equivalents in the CSD to analyse the geometry.



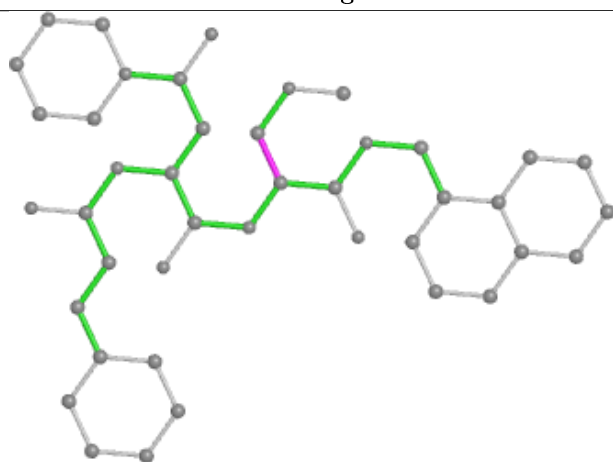
Ligand 7J0 W 301



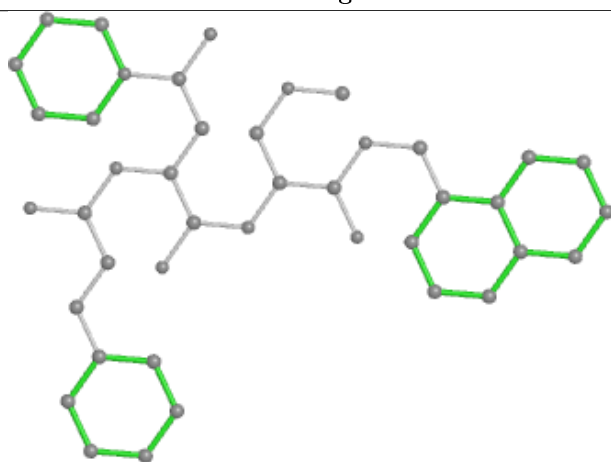
Bond lengths



Bond angles

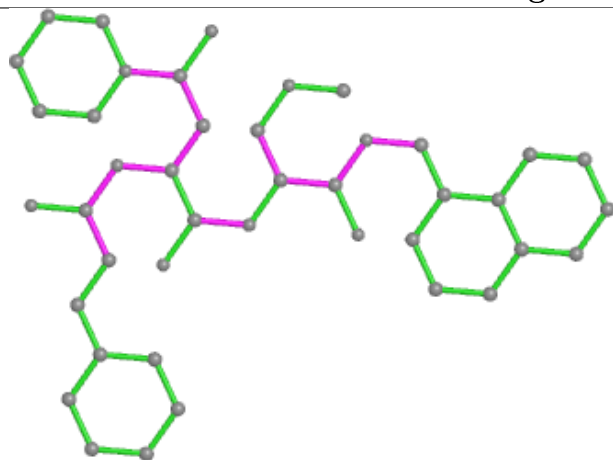


Torsions

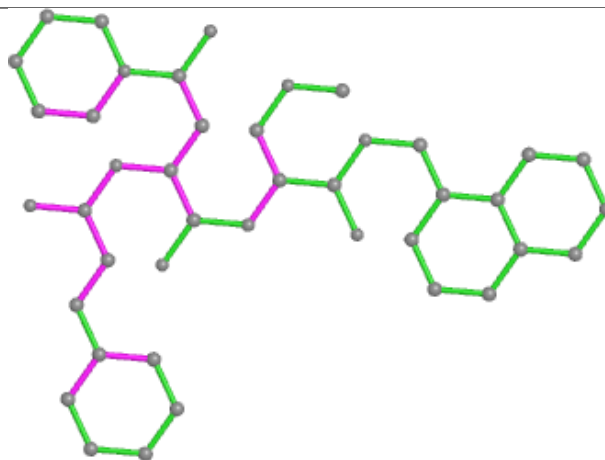


Rings

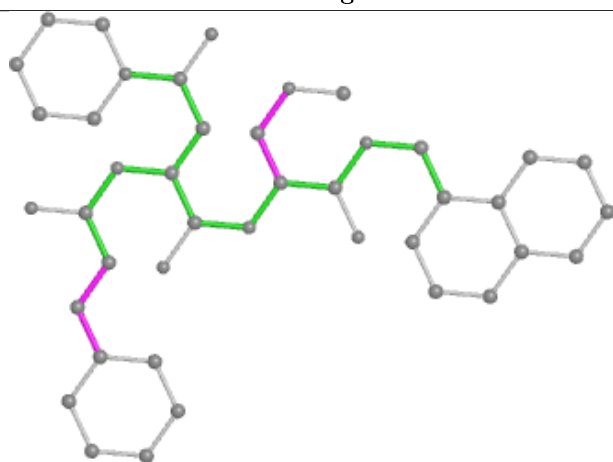
Ligand 7J0 J 301



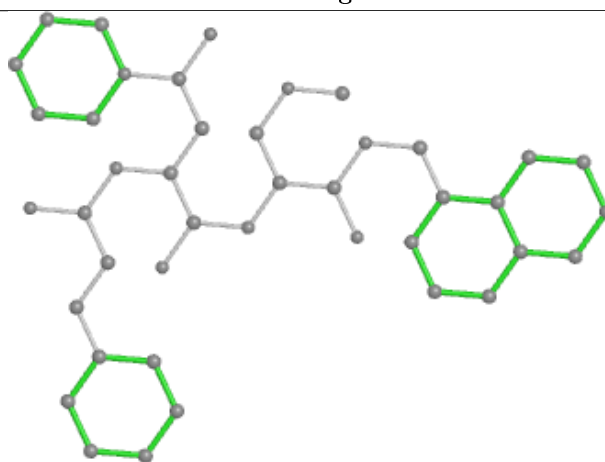
Bond lengths



Bond angles

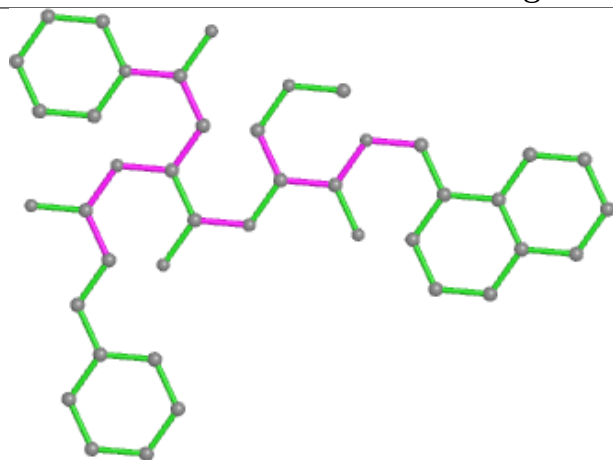


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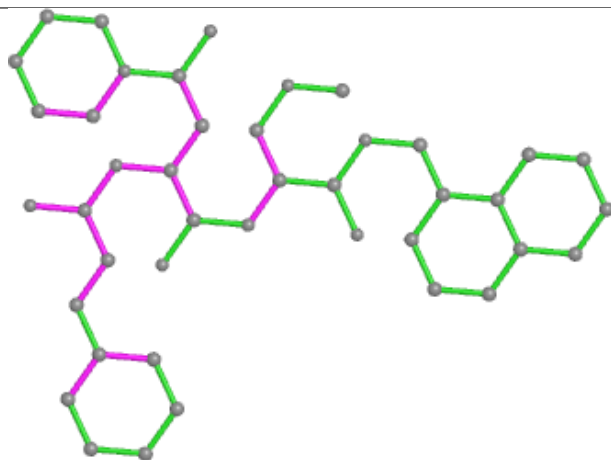


Rings

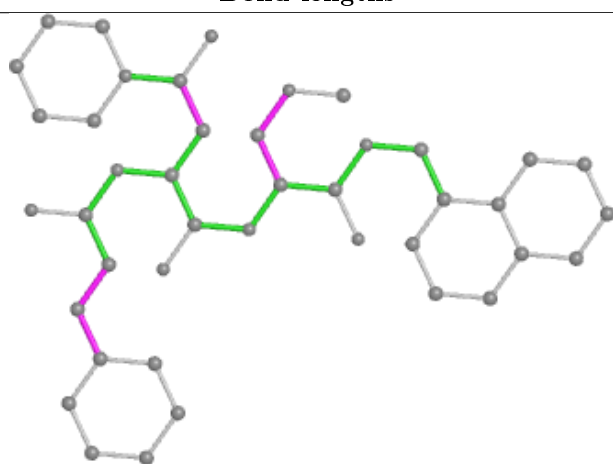
Ligand 7J0 H 301



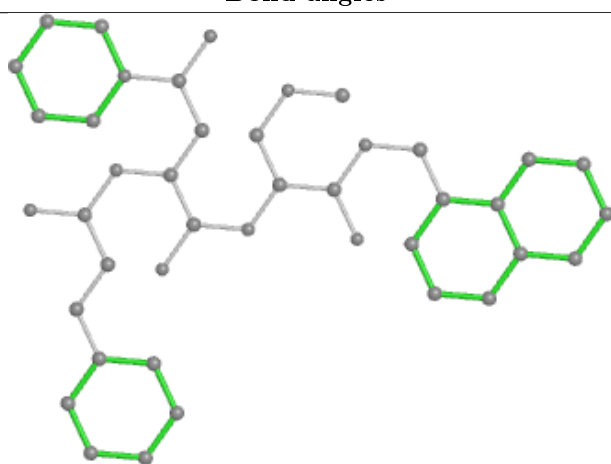
Bond lengths



Bond angles

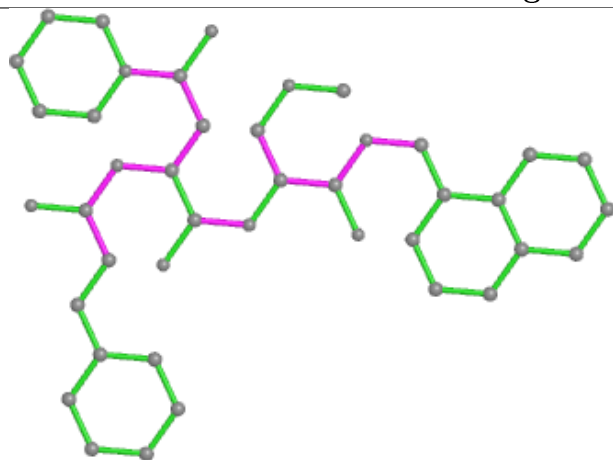


Torsions

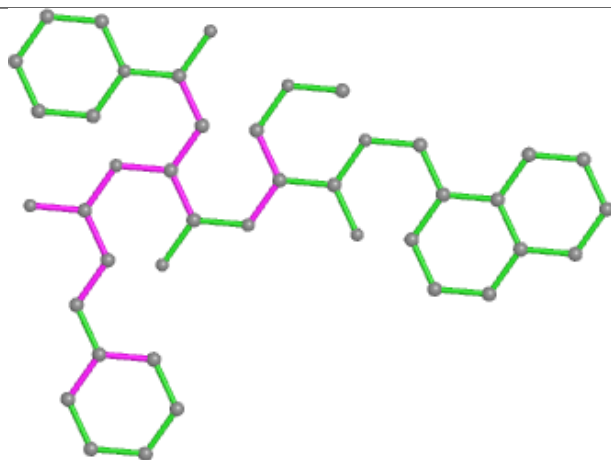


Rings

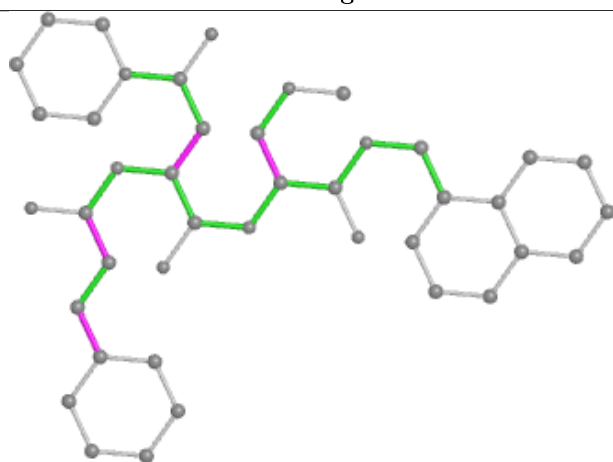
Ligand 7J0 K 301



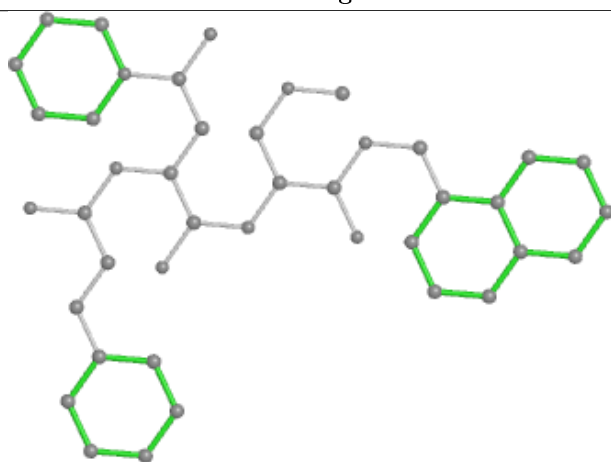
Bond lengths



Bond angles

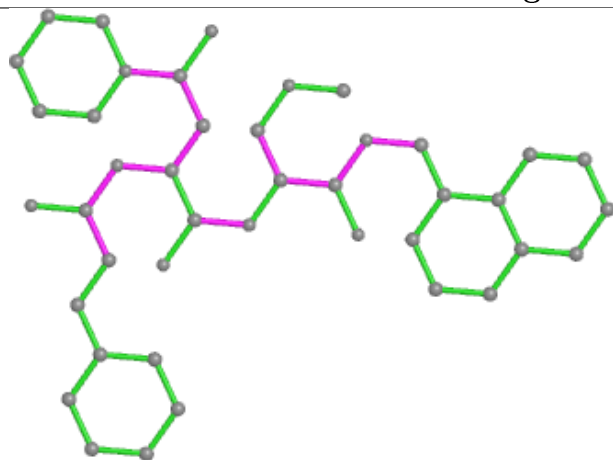


Torsions

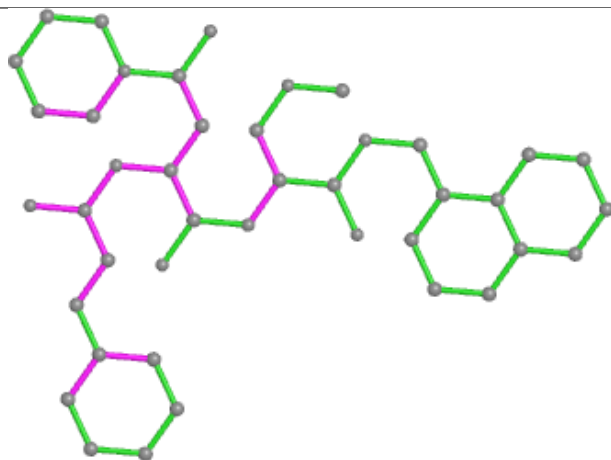


Rings

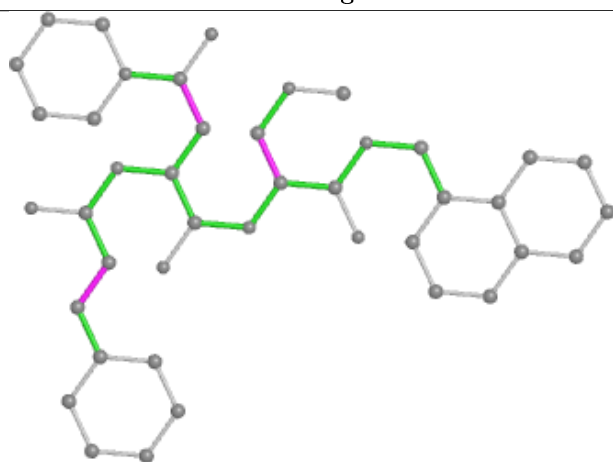
Ligand 7J0 N 301



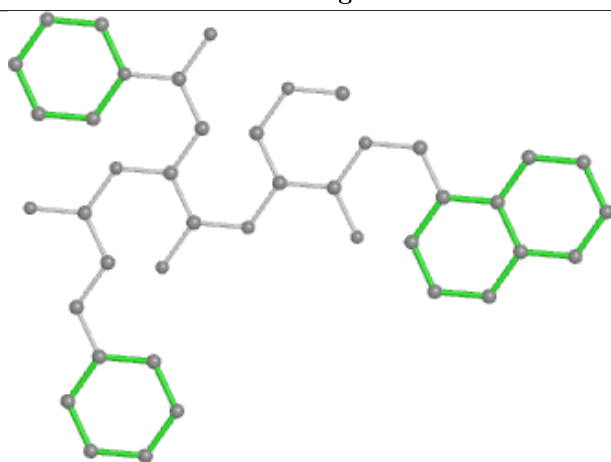
Bond lengths



Bond angles

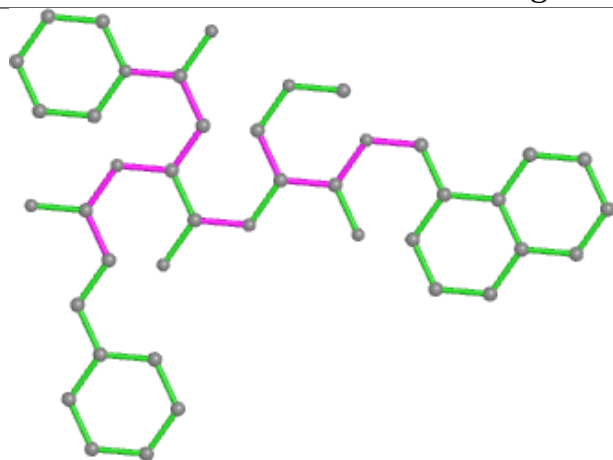


Torsions

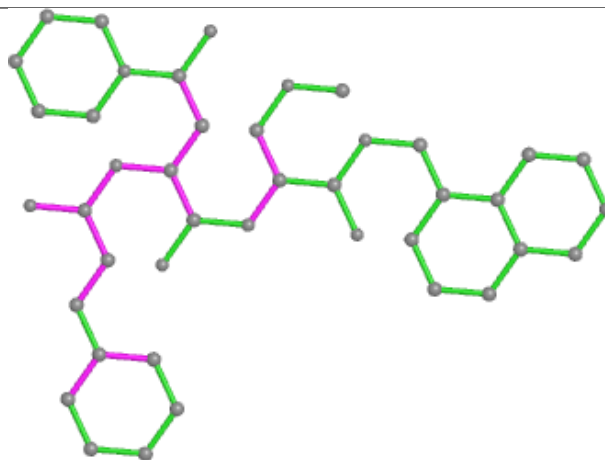


Rings

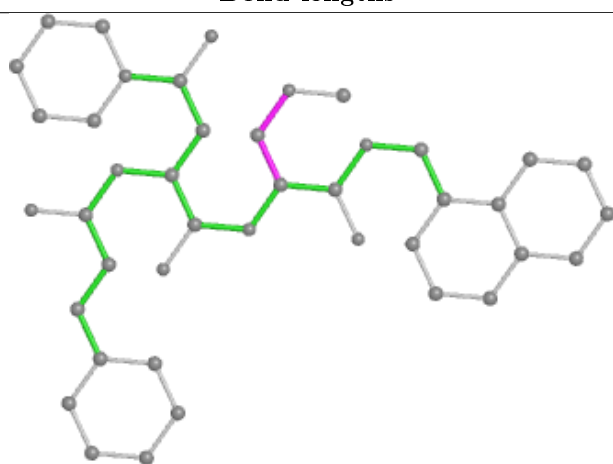
Ligand 7J0 I 301



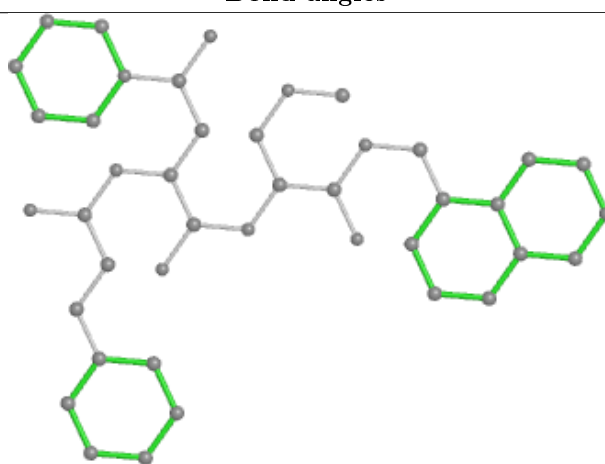
Bond lengths



Bond angles

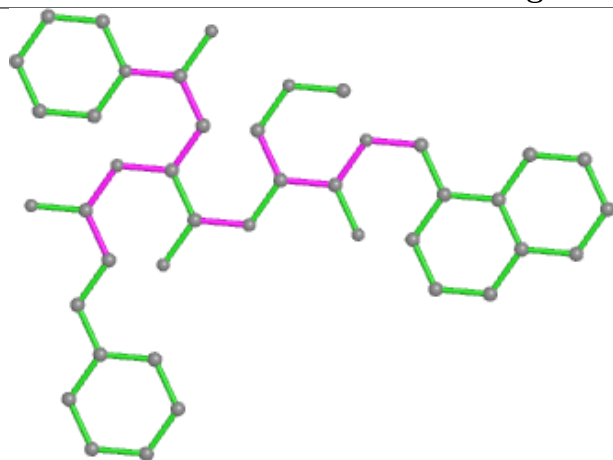


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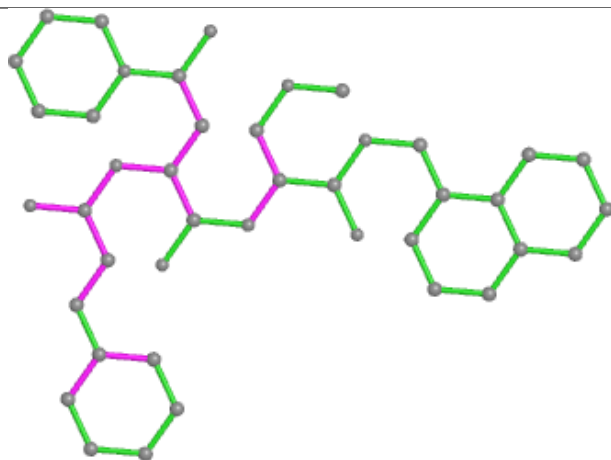


Rings

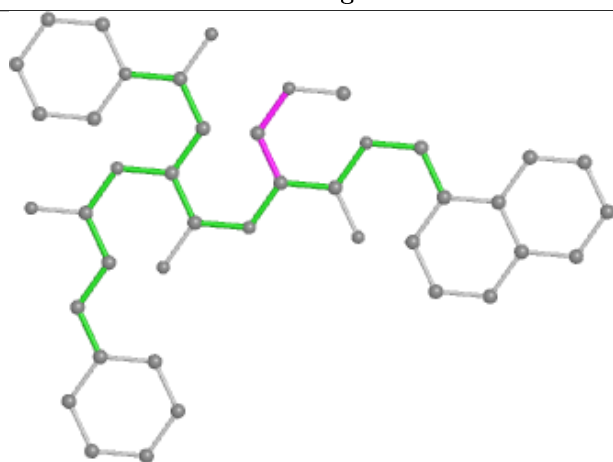
Ligand 7J0 L 301



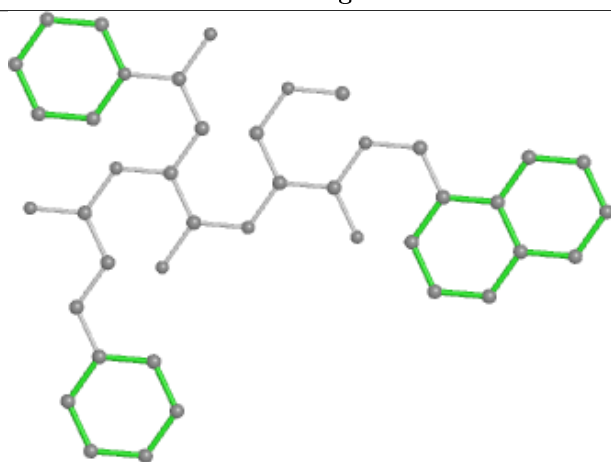
Bond lengths



Bond angles

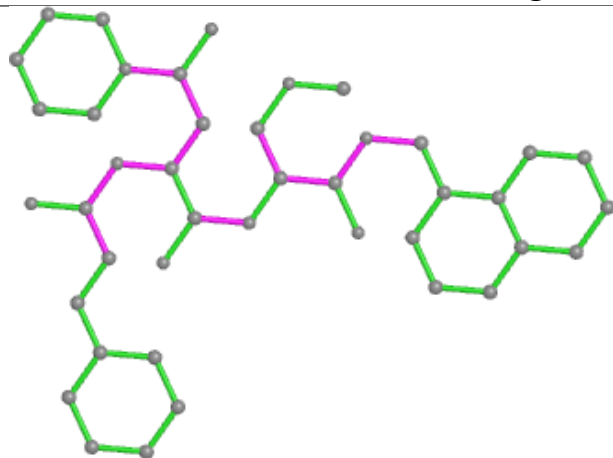


Torsions

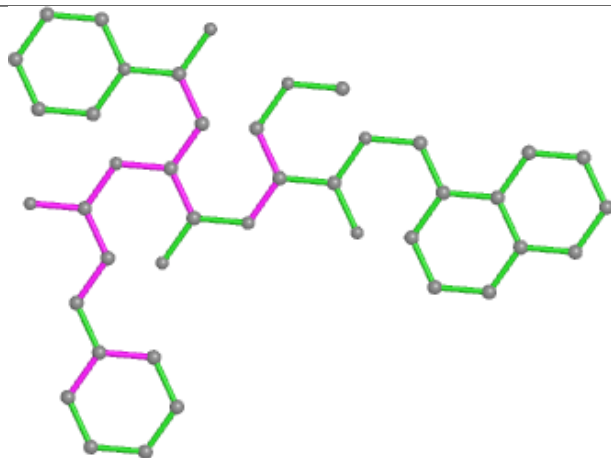


Rings

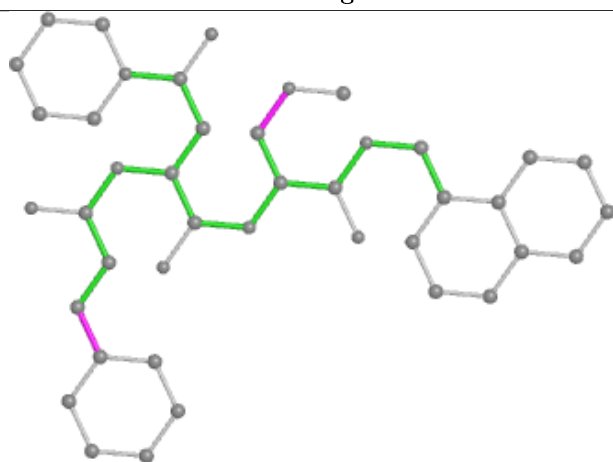
Ligand 7J0 b 301



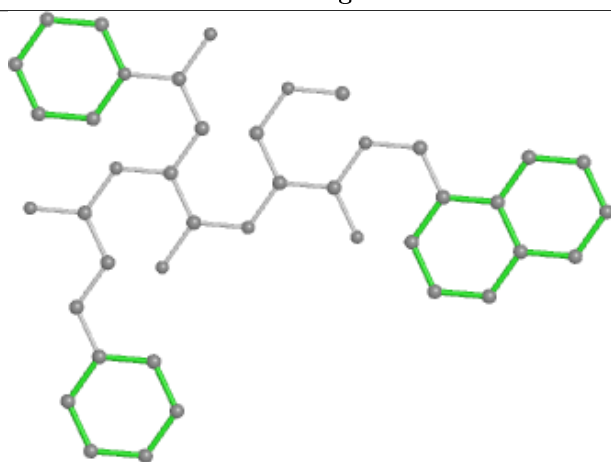
Bond lengths



Bond angles

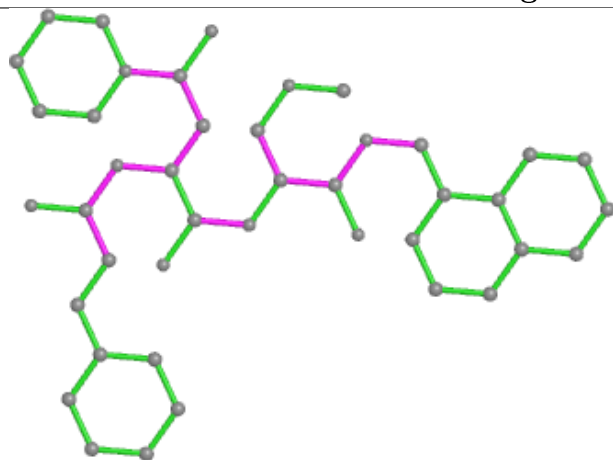


Torsions

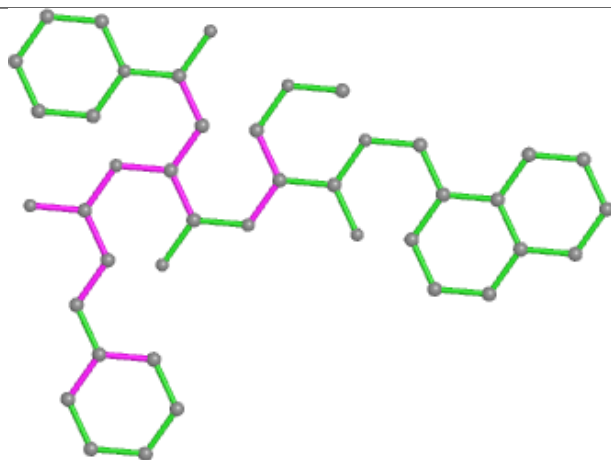


Rings

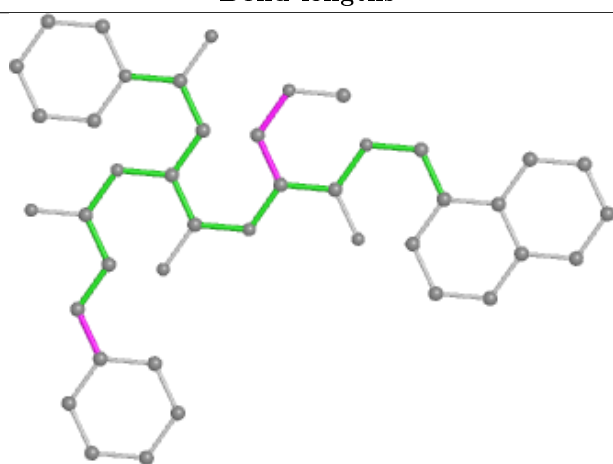
Ligand 7J0 M 301



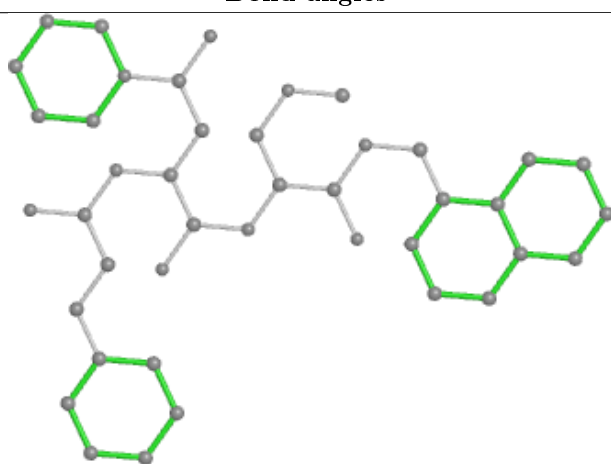
Bond lengths



Bond angles

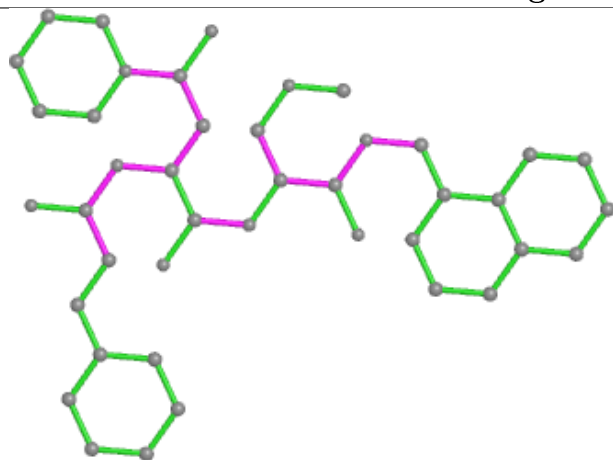


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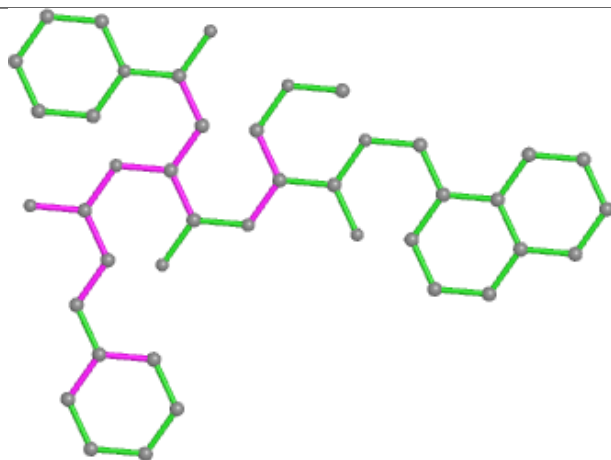


Rings

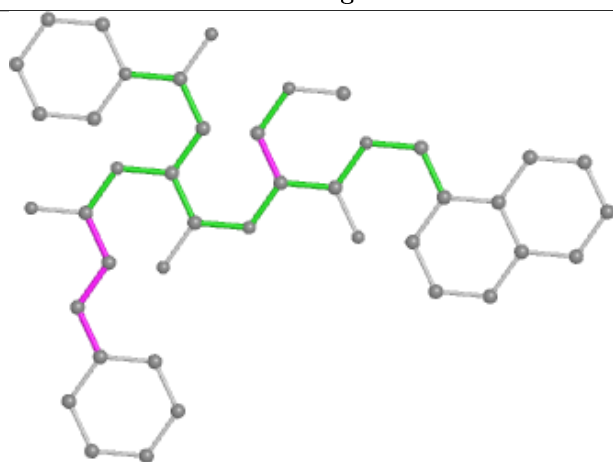
Ligand 7J0 a 301



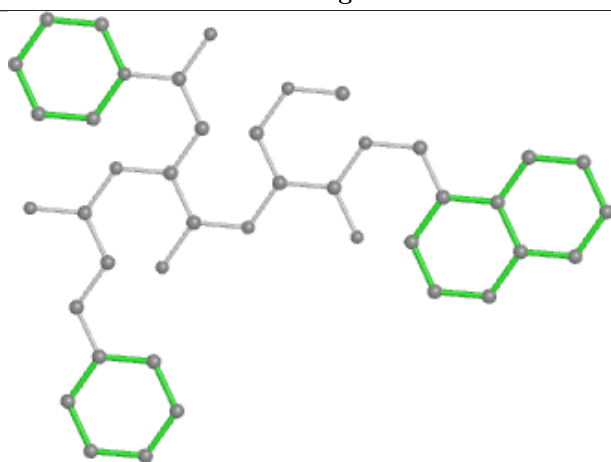
Bond lengths



Bond angles

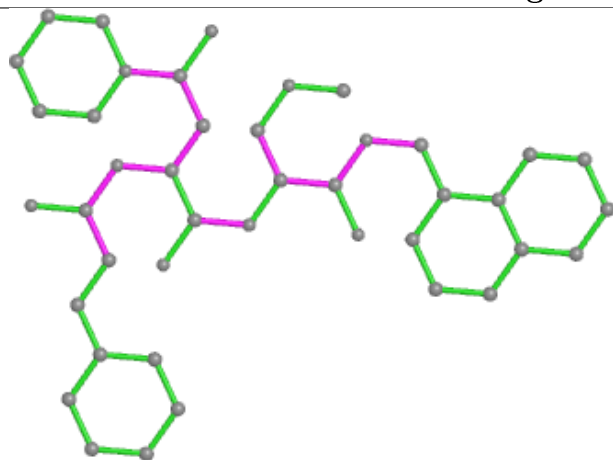


Torsions

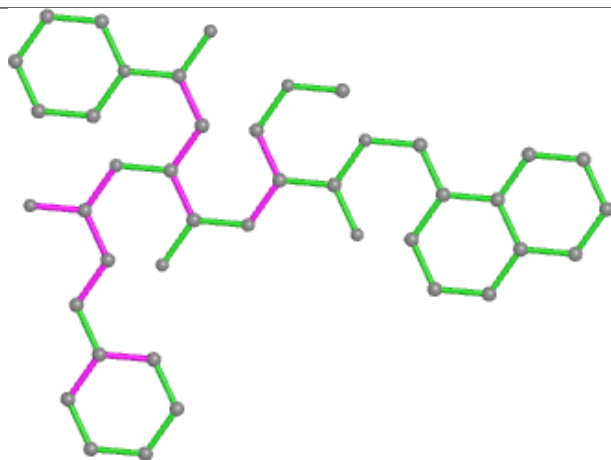


Rings

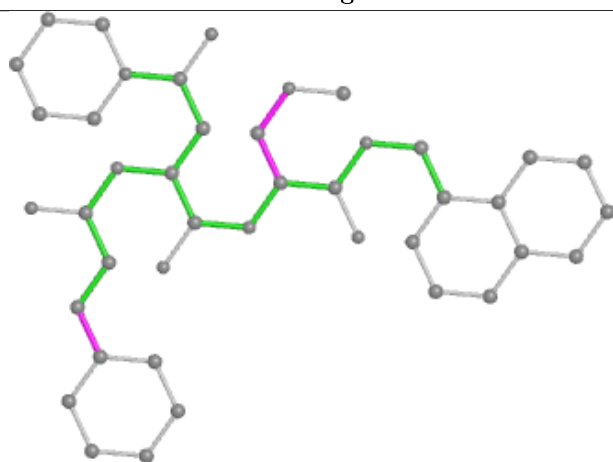
Ligand 7J0 Z 301



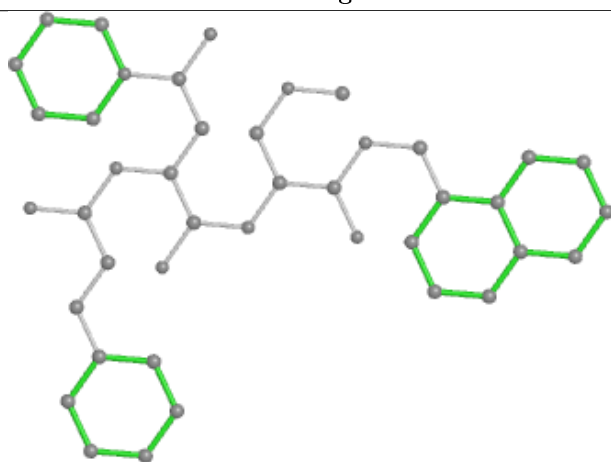
Bond lengths



Bond angles

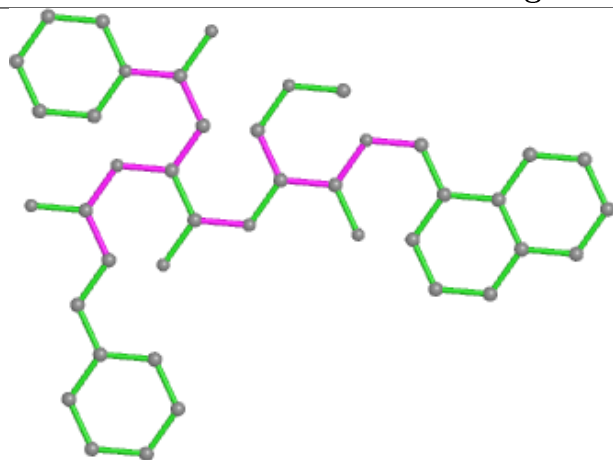


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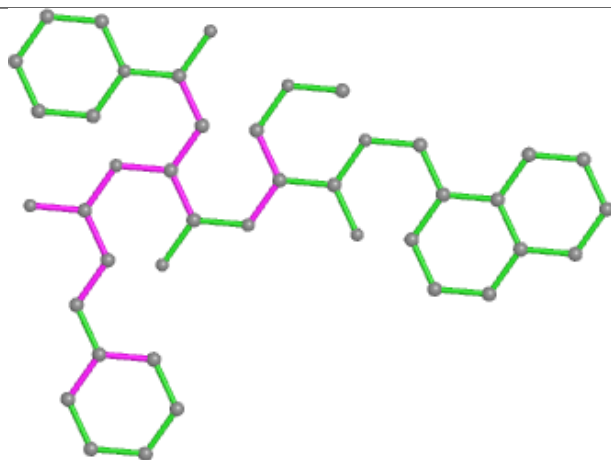


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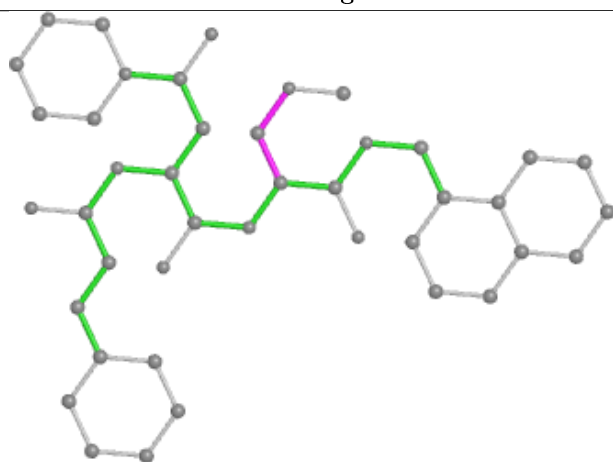
Ligand 7J0 X 301



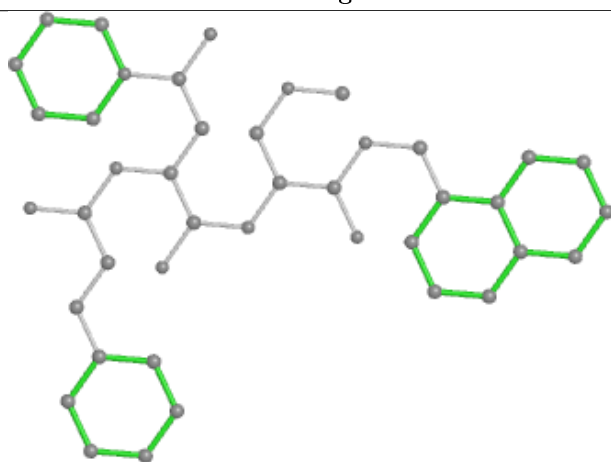
Bond lengths



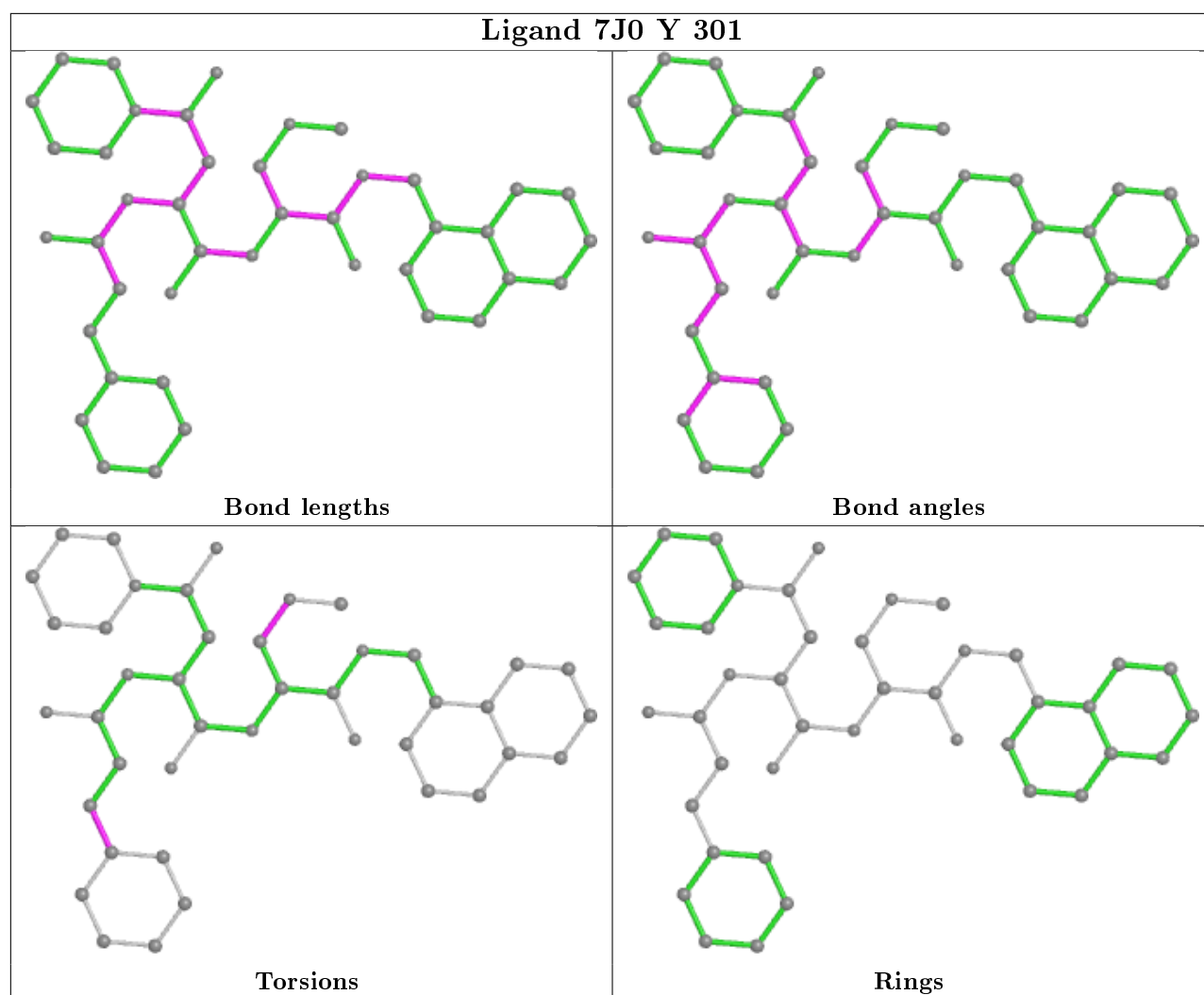
Bond angles



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%)	-0.41	1 (0%) 91 75	17, 36, 59, 80	0
1	B	215/240 (89%)	-0.23	0 100 100	21, 45, 77, 92	0
1	C	216/240 (90%)	-0.22	0 100 100	19, 49, 81, 101	0
1	D	217/240 (90%)	-0.28	0 100 100	21, 45, 75, 83	0
1	E	217/240 (90%)	-0.41	0 100 100	16, 42, 65, 95	0
1	F	218/240 (90%)	-0.23	3 (1%) 75 49	19, 47, 81, 113	0
1	G	216/240 (90%)	-0.45	0 100 100	15, 37, 66, 82	0
1	O	216/240 (90%)	-0.09	1 (0%) 91 75	20, 51, 87, 102	0
1	P	217/240 (90%)	-0.24	2 (0%) 84 63	20, 47, 77, 111	0
1	Q	218/240 (90%)	-0.27	3 (1%) 75 49	23, 44, 75, 115	0
1	R	217/240 (90%)	-0.32	1 (0%) 91 75	17, 45, 71, 92	0
1	S	219/240 (91%)	-0.37	3 (1%) 75 49	19, 38, 76, 101	0
1	T	216/240 (90%)	-0.20	1 (0%) 91 75	21, 46, 76, 85	0
1	U	216/240 (90%)	-0.31	1 (0%) 91 75	20, 41, 73, 101	0
2	H	222/240 (92%)	-0.51	0 100 100	19, 29, 50, 81	0
2	I	222/240 (92%)	-0.53	0 100 100	16, 27, 47, 65	0
2	J	222/240 (92%)	-0.57	0 100 100	19, 30, 54, 86	0
2	K	223/240 (92%)	-0.61	0 100 100	18, 30, 53, 70	0
2	L	223/240 (92%)	-0.55	0 100 100	17, 27, 51, 72	0
2	M	222/240 (92%)	-0.51	0 100 100	18, 30, 53, 82	0
2	N	223/240 (92%)	-0.53	1 (0%) 92 79	18, 32, 59, 85	0
2	V	223/240 (92%)	-0.54	0 100 100	19, 28, 48, 64	0
2	W	223/240 (92%)	-0.51	0 100 100	18, 31, 57, 73	0
2	X	222/240 (92%)	-0.54	0 100 100	19, 30, 54, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	Y	223/240 (92%)	-0.56	0 100 100	17, 29, 55, 87	0
2	Z	222/240 (92%)	-0.57	0 100 100	16, 28, 53, 76	0
2	a	223/240 (92%)	-0.50	0 100 100	19, 32, 58, 77	0
2	b	223/240 (92%)	-0.42	0 100 100	18, 30, 56, 77	0
All	All	6152/6720 (91%)	-0.41	17 (0%) 94 84	15, 35, 71, 115	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	169	GLU	3.5
1	S	193	ALA	3.3
1	Q	236	ASP	3.3
1	P	201	PRO	3.2
1	F	236	ASP	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 carbohydrates 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	7J0	K	301	42/42	0.94	0.20	21,31,52,64	0
3	7J0	N	301	42/42	0.94	0.23	20,29,53,59	0
3	7J0	M	301	42/42	0.94	0.20	14,24,49,63	0
3	7J0	H	301	42/42	0.95	0.21	15,25,45,66	0
3	7J0	V	301	42/42	0.95	0.20	21,30,51,62	0
3	7J0	W	301	42/42	0.95	0.19	14,24,43,55	0
3	7J0	I	301	42/42	0.95	0.19	16,26,46,64	0

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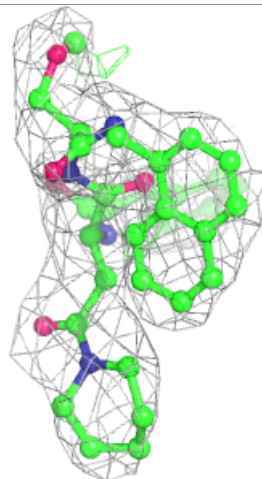
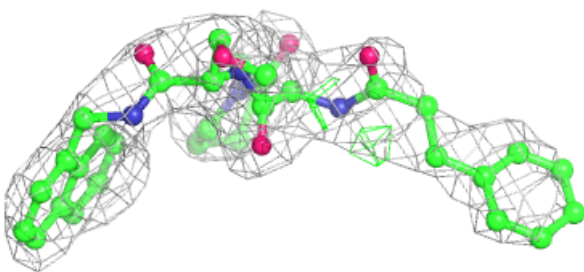
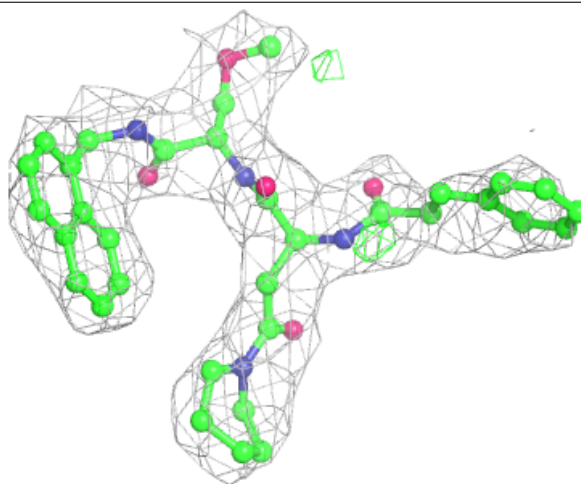
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	7J0	L	301	42/42	0.95	0.20	14,24,39,52	0
3	7J0	b	301	42/42	0.95	0.21	16,24,38,41	0
3	7J0	J	301	42/42	0.95	0.21	19,26,60,81	0
3	7J0	a	301	42/42	0.95	0.20	21,27,48,62	0
3	7J0	Z	301	42/42	0.95	0.19	19,25,38,50	0
3	7J0	X	301	42/42	0.95	0.19	15,25,41,47	0
3	7J0	Y	301	42/42	0.95	0.20	14,24,53,75	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.

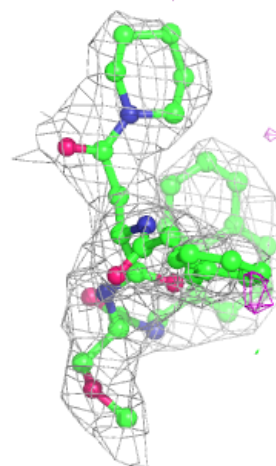
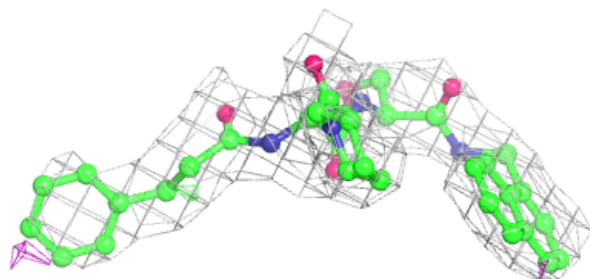
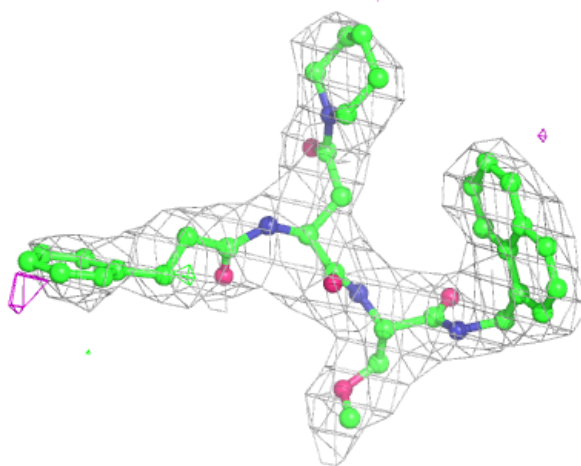
Electron density around 7J0 K 301:

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



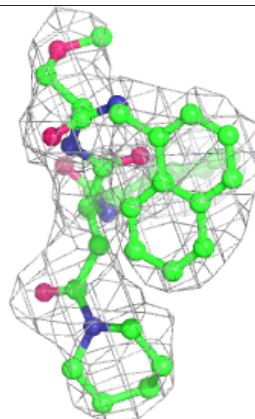
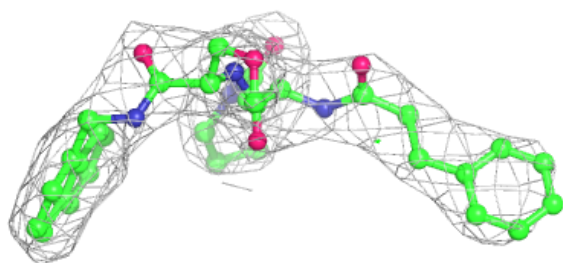
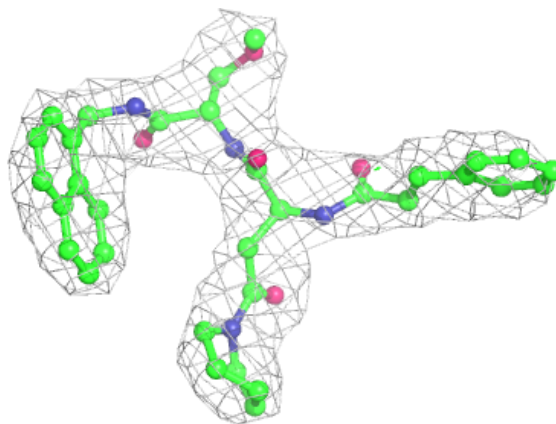
Electron density around 7J0 N 301:

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



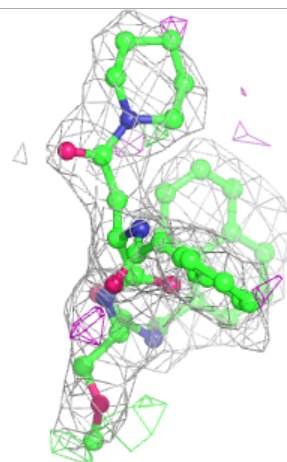
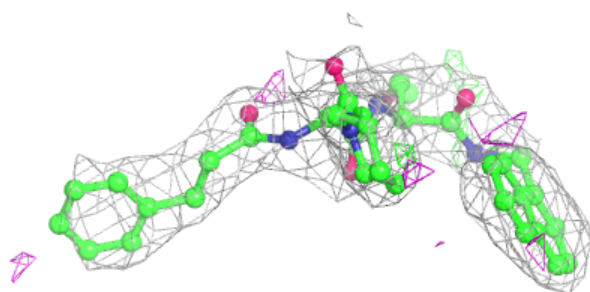
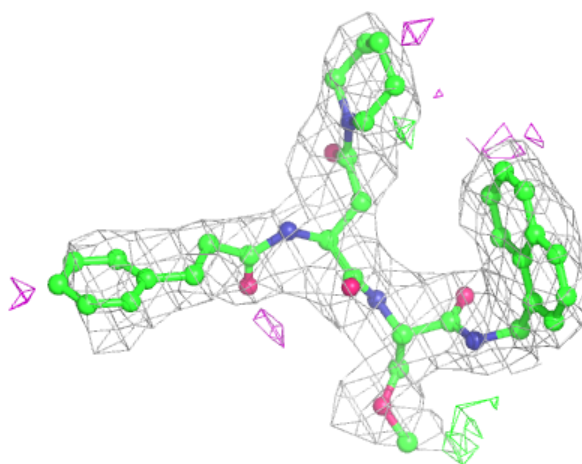
Electron density around 7J0 M 301:

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



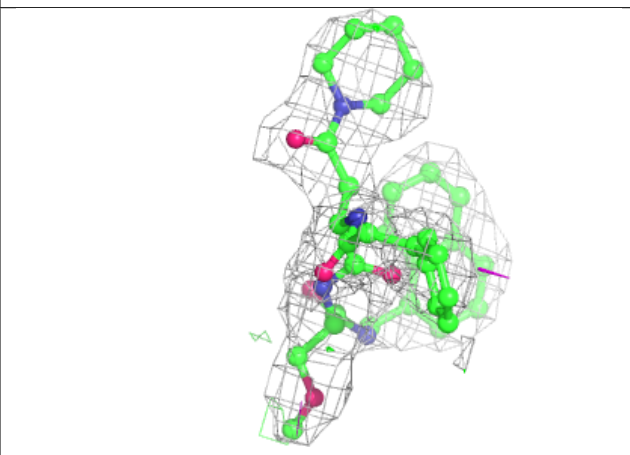
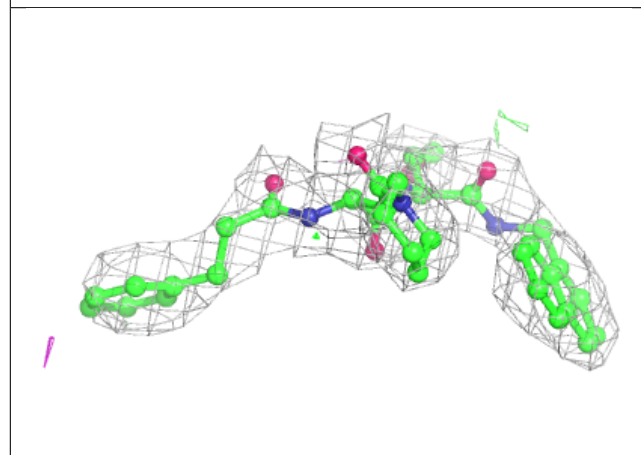
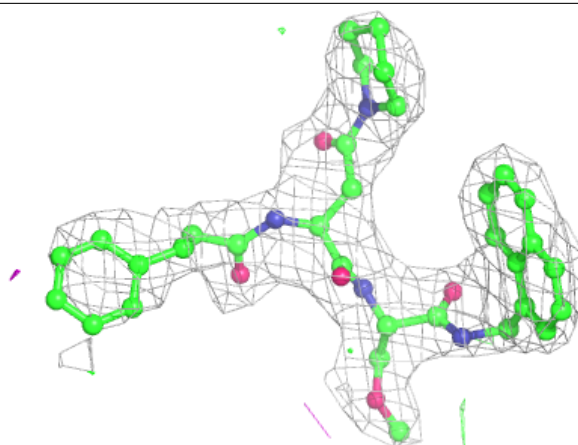
Electron density around 7J0 H 301:

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



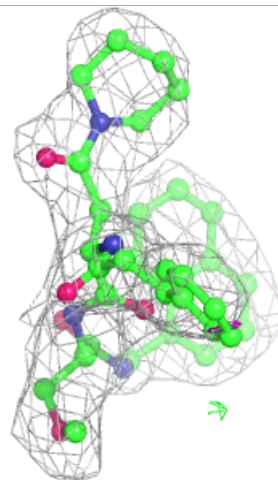
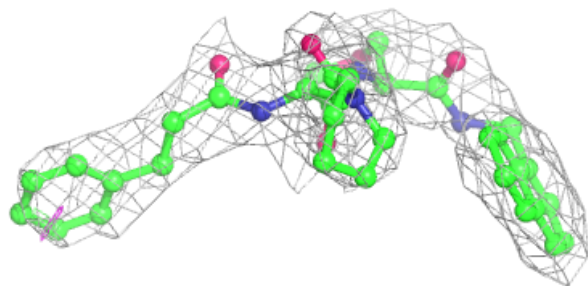
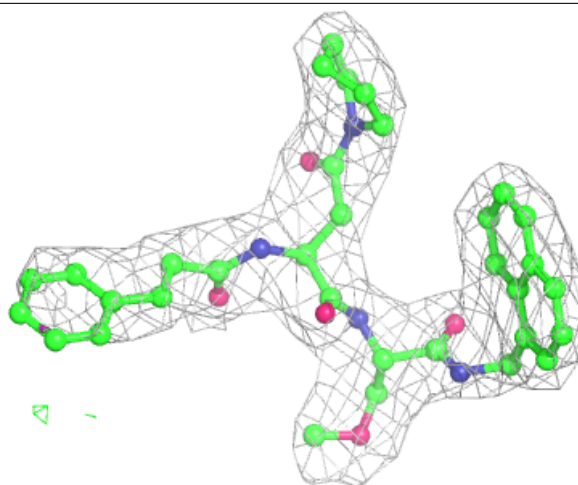
Electron density around 7J0 V 301:

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



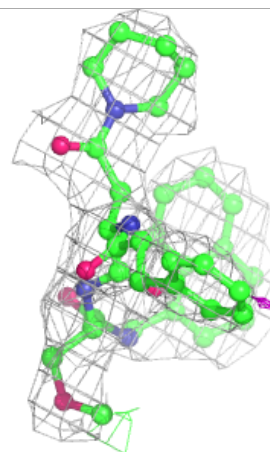
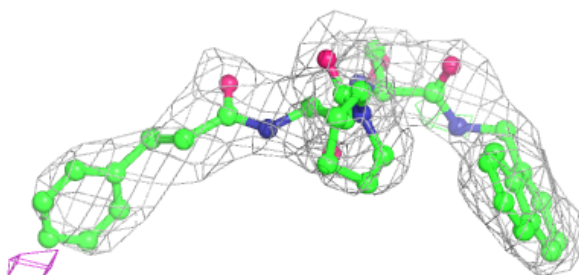
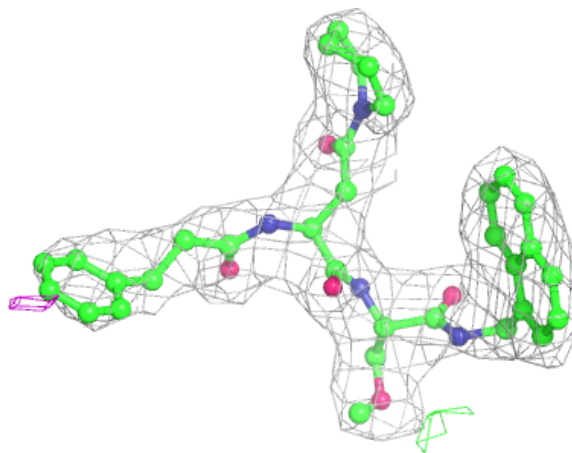
Electron density around 7J0 W 301:

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



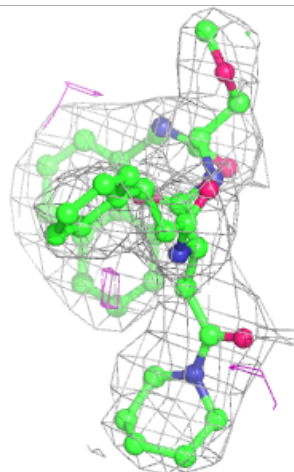
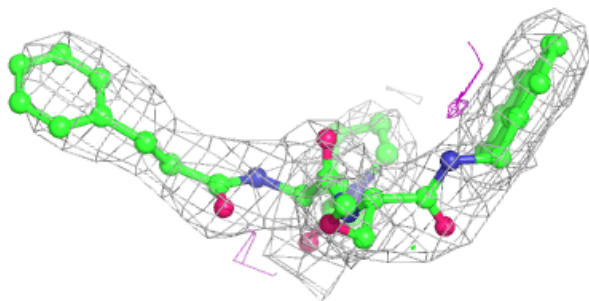
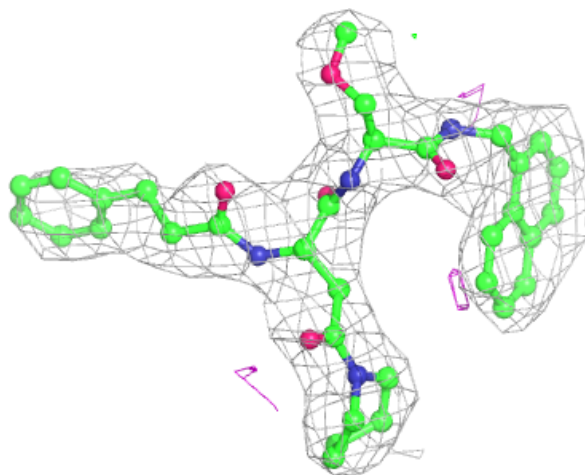
Electron density around 7J0 I 301:

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



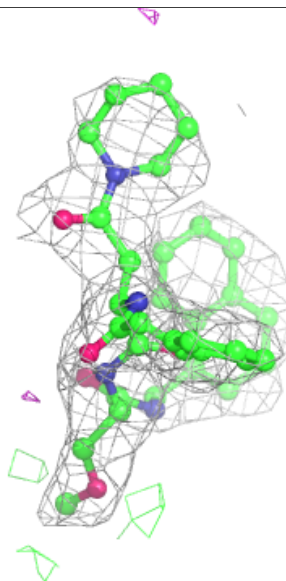
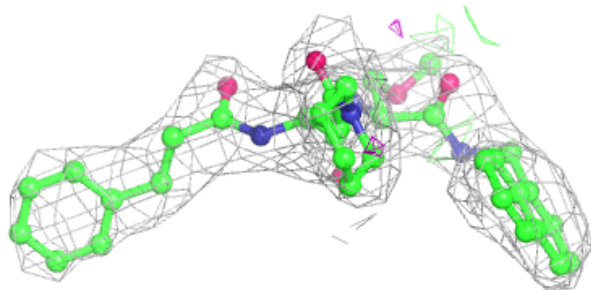
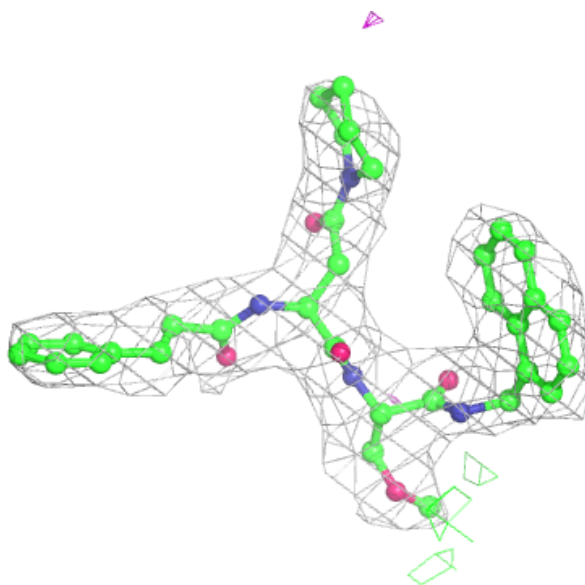
Electron density around 7J0 L 301:

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



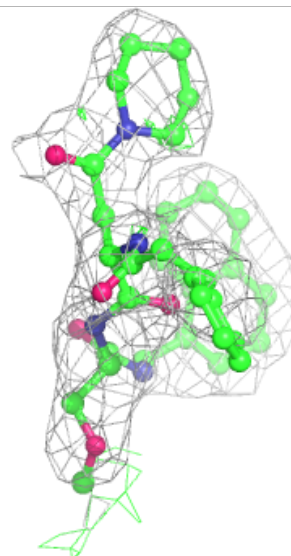
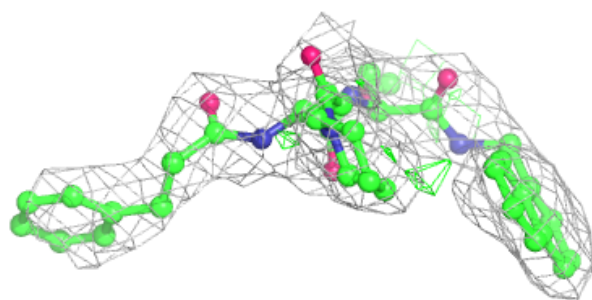
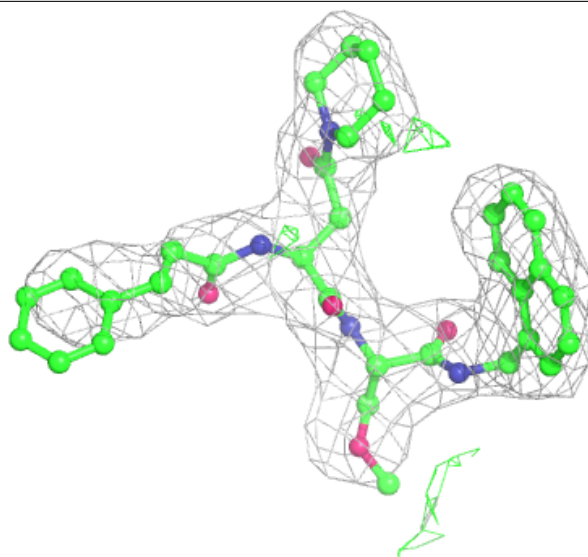
Electron density around 7J0 b 301:

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



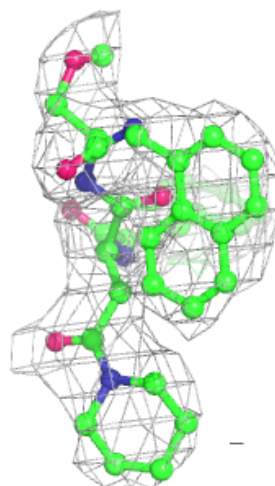
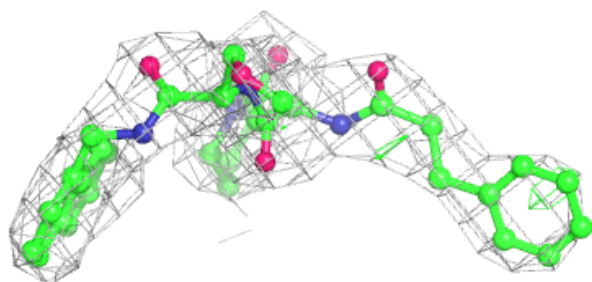
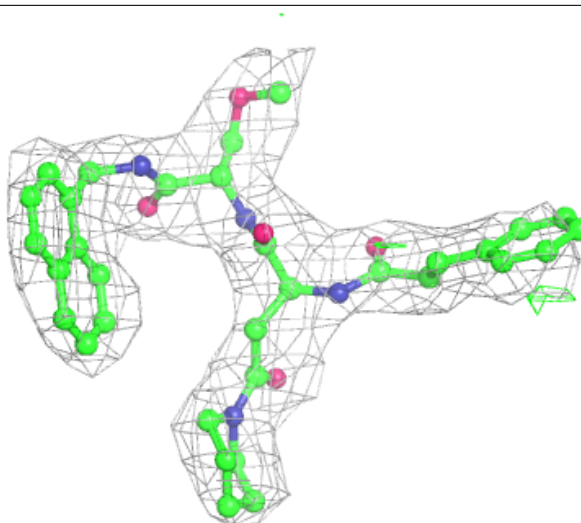
Electron density around 7J0 J 301:

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



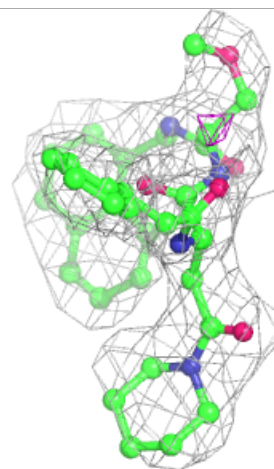
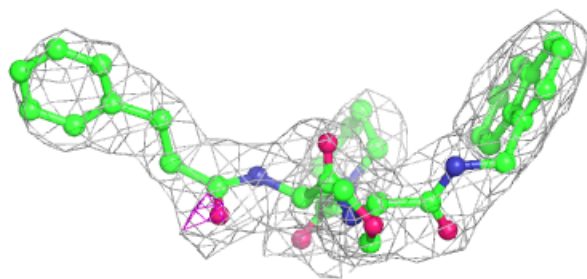
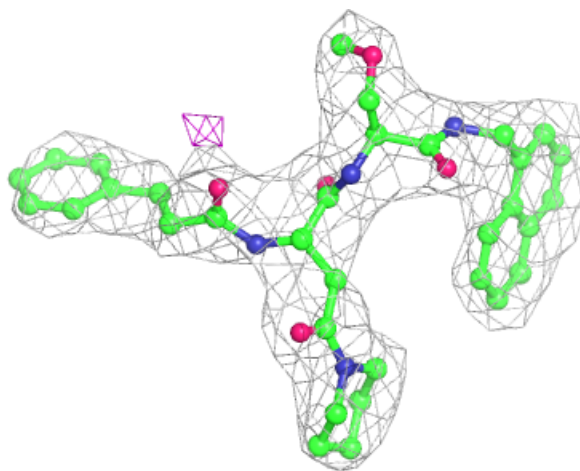
Electron density around 7J0 a 301:

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



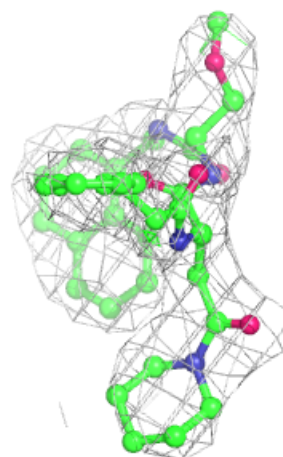
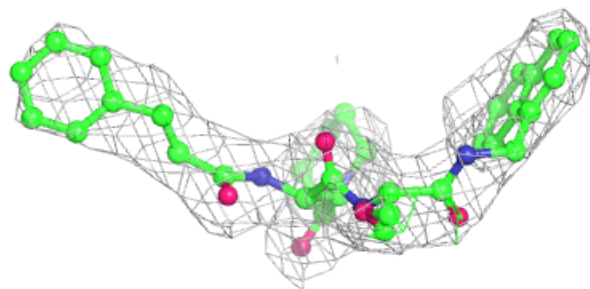
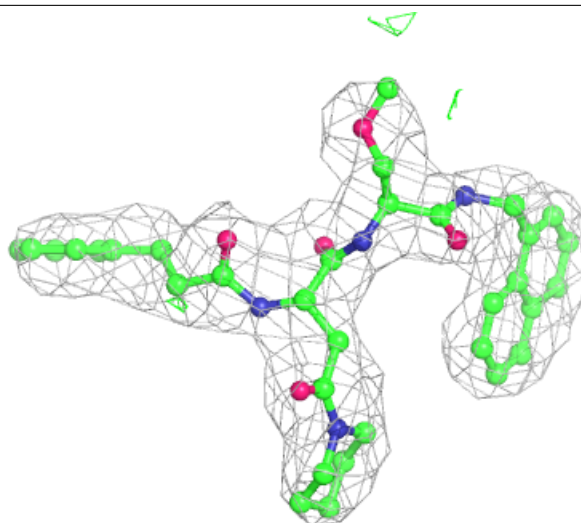
Electron density around 7J0 Z 301:

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



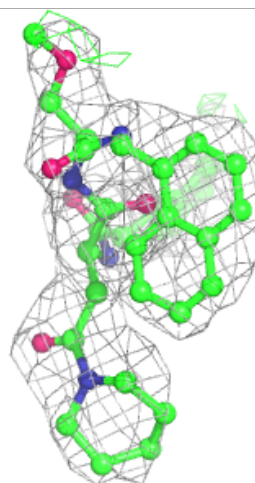
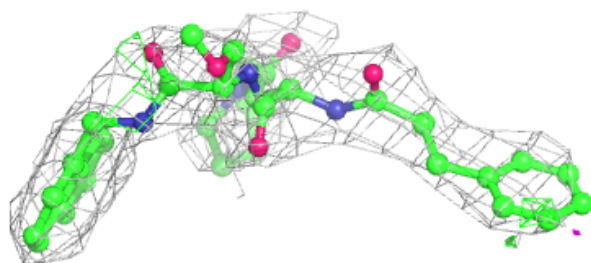
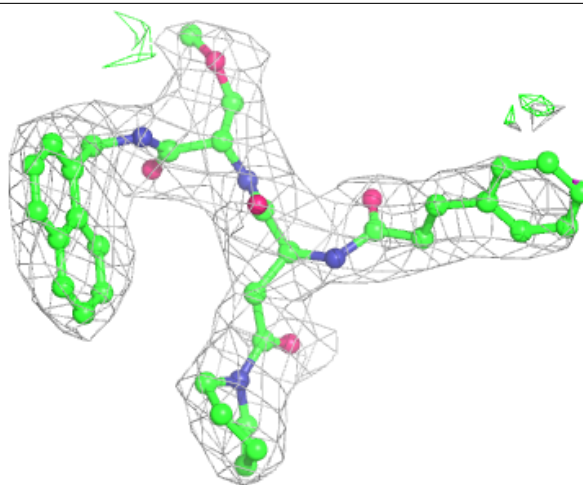
Electron density around 7J0 X 301:

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



Electron density around 7J0 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.