W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Aug 16, 2020 – 08:44 PM BST

PDB ID	:	5TRG
Title	:	Structure of Mycobacterium tuberculosis proteasome in complex with N,C-capped dipeptide DPLG-2
Authors	:	Hsu, H.-C.; Fan, H.; Singh, R.K.; Wang, R.; Sukenick, G.; Nathan, C.; Lin, G.; Li, H.
Deposited on	:	2016-10-26
Resolution	:	2.80 Å(reported)

The following versions of software and data (see references (i)) 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	:	2.13.1
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)	:	2.13.1

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.80 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.
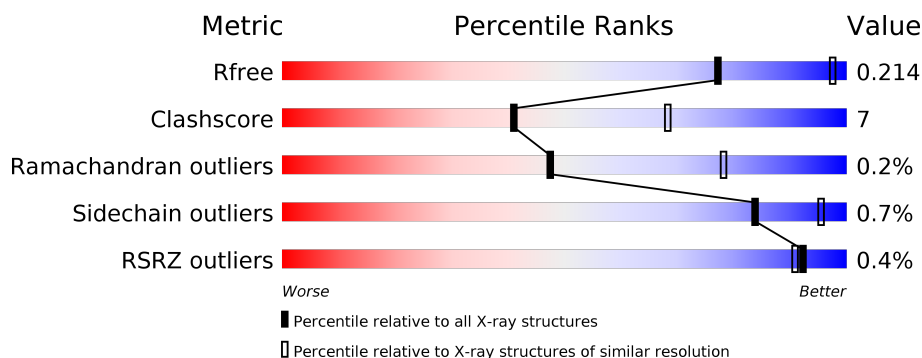
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	75% 16% 9%
1	B	240	4% 62% 27% • 10%
1	C	240	2% 70% 18% •• 10%
1	D	240	73% 20% 7%
1	E	240	84% 7% 9%
1	F	240	% 65% 23% • 10%

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Mol	Chain	Length	Quality of chain
1	G	240	71% · 19% · 10%
1	O	240	72% · 18% · 9%
1	P	240	69% · 22% · 9%
1	Q	240	73% · 18% · 10%
1	R	240	75% · 15% · 10%
1	S	240	79% · 11% · 9%
1	T	240	% · 75% · 15% · 10%
1	U	240	% · 68% · 21% · 10%
2	H	240	79% · 13% · 8%
2	I	240	85% · 8% · 8%
2	J	240	83% · 10% · 8%
2	K	240	82% · 11% · 7%
2	L	240	84% · 9% · 7%
2	M	240	85% · 7% · 8%
2	N	240	84% · 8% · 7%
2	V	240	85% · 8% · 7%
2	W	240	79% · 13% · 7%
2	X	240	83% · 9% · 8%
2	Y	240	84% · 9% · 7%
2	Z	240	81% · 11% · 8%
2	a	240	92% · 7%
2	b	240	92% · 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 47357 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	223	Total	C	N	O	S	0	0	0
			1716	1070	313	329	4			
1	E	218	Total	C	N	O	S	0	0	0
			1677	1050	306	317	4			
1	F	215	Total	C	N	O	S	0	0	0
			1655	1035	303	313	4			
1	G	216	Total	C	N	O	S	0	0	0
			1662	1040	304	314	4			
1	O	218	Total	C	N	O	S	0	0	0
			1677	1050	306	317	4			
1	P	219	Total	C	N	O	S	0	0	0
			1685	1054	307	320	4			
1	Q	217	Total	C	N	O	S	0	0	0
			1677	1050	306	317	4			
1	R	215	Total	C	N	O	S	0	0	0
			1657	1038	303	312	4			
1	S	218	Total	C	N	O	S	0	0	0
			1678	1050	306	318	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 1638	C 1027	N 282	O 324	S 5	0	0	0
2	I	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	J	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	K	223	Total 1642	C 1029	N 283	O 325	S 5	0	0	0
2	L	223	Total 1642	C 1029	N 283	O 325	S 5	0	0	0
2	M	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	N	223	Total 1642	C 1029	N 283	O 325	S 5	0	0	0
2	V	223	Total 1642	C 1029	N 283	O 325	S 5	0	0	0
2	W	223	Total 1642	C 1029	N 283	O 325	S 5	0	0	0
2	X	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	Y	223	Total 1642	C 1029	N 283	O 325	S 5	0	0	0
2	Z	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	a	223	Total 1642	C 1029	N 283	O 325	S 5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	b	223	1642	1029	283	325	5	0	0	0

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 -[(2E)-3-phenylprop-2-enoyl]-L-asparaginyl-4-fluoro-N-[(naphthalen-1-yl)methyl]-L-phenylalaninamide (three-letter code: 7HJ) (formula: $C_{37}H_{39}FN_4O_4$).
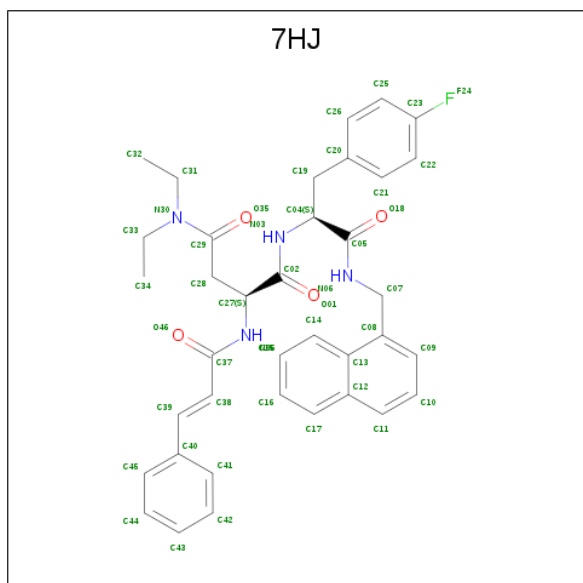
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	H	1	Total	C	F	N	O	0	0
			46	37	1	4	4		
3	I	1	Total	C	F	N	O	0	0
			46	37	1	4	4		
3	J	1	Total	C	F	N	O	0	0
			46	37	1	4	4		
3	K	1	Total	C	F	N	O	0	0
			46	37	1	4	4		
3	L	1	Total	C	F	N	O	0	0
			46	37	1	4	4		
3	M	1	Total	C	F	N	O	0	0
			46	37	1	4	4		
3	N	1	Total	C	F	N	O	0	0
			46	37	1	4	4		
3	V	1	Total	C	F	N	O	0	0
			46	37	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	W	1	Total	C	F	N	O	0	0
			46	37	1	4	4		
3	X	1	Total	C	F	N	O	0	0
			46	37	1	4	4		
3	Y	1	Total	C	F	N	O	0	0
			46	37	1	4	4		
3	Z	1	Total	C	F	N	O	0	0
			46	37	1	4	4		
3	a	1	Total	C	F	N	O	0	0
			46	37	1	4	4		
3	b	1	Total	C	F	N	O	0	0
			46	37	1	4	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	1	Total	O	0	0
			1	1		
4	C	4	Total	O	0	0
			4	4		
4	D	7	Total	O	0	0
			7	7		
4	E	16	Total	O	0	0
			16	16		
4	F	5	Total	O	0	0
			5	5		
4	G	14	Total	O	0	0
			14	14		
4	H	11	Total	O	0	0
			11	11		
4	I	19	Total	O	0	0
			19	19		
4	J	14	Total	O	0	0
			14	14		
4	K	14	Total	O	0	0
			14	14		
4	L	16	Total	O	0	0
			16	16		
4	M	14	Total	O	0	0
			14	14		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	N	9	Total 9	O 9	0	0
4	O	8	Total 8	O 8	0	0
4	P	9	Total 9	O 9	0	0
4	Q	8	Total 8	O 8	0	0
4	R	9	Total 9	O 9	0	0
4	S	15	Total 15	O 15	0	0
4	T	11	Total 11	O 11	0	0
4	U	13	Total 13	O 13	0	0
4	V	14	Total 14	O 14	0	0
4	W	17	Total 17	O 17	0	0
4	X	15	Total 15	O 15	0	0
4	Y	15	Total 15	O 15	0	0
4	Z	16	Total 16	O 16	0	0
4	a	7	Total 7	O 7	0	0
4	b	18	Total 18	O 18	0	0

3 Residue-property plots ⓘ

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

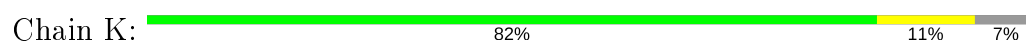- Molecule 1: Proteasome subunit alpha

- Molecule 1: Proteasome subunit alpha

- Molecule 1: Proteasome subunit alpha

Chain D:

73%　　20%　　7%

• Molecule 1: Proteasome subunit alpha

Chain E:

84%　　7%　　9%

• Molecule 1: Proteasome subunit alpha

Chain F:

%

65%　　23%　　•　　10%

• Molecule 1: Proteasome subunit alpha

Chain G:

71%　　19%　　10%

• Molecule 1: Proteasome subunit alpha

Chain O:

72%　　18%　　•　　9%

D179 A180 L181 R182 I183 R189 A190 G191 S192 ALA ASP SER GLY GLY ASP GLN PRO T202 L203 E209 V212 R219 R223 L234 V235 ASP GLN GLU SER PRO GLN SER ASP GLY GLU SER SER GLY

● Molecule 1: Proteasome subunit alpha

Chain P:

| 69% | 22% | 9% |

M9 R14 E18 K22 V30 V31 A32 L33 A36 L40 A43 R48 Q51 K52 I53 S54 E55 L56 F62 R75 F81 R85 G86 Y87 A88 Y89 D93 V94 T95 G96 R97 Q98 L99 A100 N101 V102 I110 Q114 E121 R140 E150

P151 H152 F153 V154 L167 Y171 N174 T178 D179 A180 I183 S192 ALA ASP THR SER GLY GLY ASP GLN PRO T202 V205 E209 D214 R217 R220 L230 Q231 A232 L233 L234 V235 D236 GLN GLU SER PRO GLN SER ASP GLU SER GLY

● Molecule 1: Proteasome subunit alpha

Chain Q:

| 73% | 18% | 10% |

M9 E10 R14 E15 R16 L19 A20 R21 R48 S49 I53 E70 Y87 A88 Y89 D90 D93 Q114 A115 K116 P117 Y118 E121 T133 E137 L138 Y139 R140 I141 T142 Y143 S146 P151 H152 L167 Y171 L177 R182 A187 A190 GLY

SER ALA ASP THR SER GLY GLY ASP GLN PRO THR L203 G204 V205 A206 S207 L208 E209 R217 P218 R219 R223 G227 L230 Q231 A232 L233 L234 V235 D236 Q237 GLU SER PRO GLN SER ASP GLY GLU SER SER GLY

● Molecule 1: Proteasome subunit alpha

Chain R:

| 75% | 15% | 10% |

M9 E10 Q11 E15 K22 R26 V30 A43 I53 L56 Y57 D58 F62 L74 Y89 D90 R91 R92 R97 Q98 V102 V120 E121 E137 R140 H152 E161 P162 I163 E173 N174 A187 L188 R189 A190 G191 SER ALA ASP THR SER

GLY GLY ASP GLN PRO THR L203 E209 D214 R217 R223 R224 L234 VAL ASP GLN GLU SER PRO GLN SER ASP GLY GLU SER SER GLY

● Molecule 1: Proteasome subunit alpha

Chain S:

| 79% | 11% | · | 9% |

M9 L33 R48 I53 Y57 D58 D72 R75 Y87 R91 R92 Q98 V102 E121 H129 E132 E137 R140 H152 V155 Y171 T178 D179 A180 L181 R182 S192 ALA ASP THR SER GLY GLY ASP GLN PRO THR L203 E209

R219 A229 L233 D236 GLN GLU SER PRO GLN SER ASP GLY GLU SER SER GLY

● Molecule 1: Proteasome subunit alpha

Chain T:

| 75% | 15% | 10% |

M9 E10 M13 R14 E15 R16 S17 E18 L19 A20 R21 K28 N45 P46 S47 R48 I53 S54 E55 L56 Y57 D58 F62 K67 F68 N69 R75 L99 V102 F111 E132 T133 E161 L167 N174 D179 R182 I183 G191 SER ALA ASP THR

SER GLY GLY ASP GLN PRO T202 E209 Q231 A232 L233 L234 V235 ASP GLN GLU SER PRO GLN SER ASP GLY GLU SER SER GLY

• Molecule 1: Proteasome subunit alpha

Chain U:

%

68%   21%   • 10%

M9 E10 Q11 R14 E15 E18 L19 K28 R48 I53 S54 E55 L56 V60 G61 F62 K67 F68 N69 E70 F71 D72 R75 R76 F81 R85 R92 R97 Q98 L99 V102 I110 Q114 E126 T133 K134 T142 D149 E150 P151

V155 T159 T160 E161 P162 N165 N174 T178 L181 R182 V185 L188 G191 SER ALA ASP THR SER GLY GLY ASP GLN PRO THR L203 E209 L213 R220 A221 F222 L234 V235 ASP GLN GLU SER PRO GLN SER ASP GLY GLU SER SER GLY

• Molecule 2: Proteasome subunit beta

Chain H:

79%   13%   8%

T1 T2 I3 K7 R18 K33 T37 D38 T41 G44 T48 V51 R57 V72 P73 L74 T75 R82 R88 L98 L104 S112 D113 P114 G118 V121 S122 W129 N130 I131 E132 Q137 A138 D173 T193 R209 E212

S222 GLY ALA ASP THR PHE GLY SER ASP GLY GLU LYS HIS HIS HIS HIS HIS HIS

• Molecule 2: Proteasome subunit beta

Chain I:

85%   8%   8%

T1 T2 I3 R18 R57 E64 K68 L74 S122 F123 G128 W129 Q137 A138 V139 K151 Q156 R165 T193 R215 E219 S222 GLY ALA ASP THR PHE GLY SER ASP GLY GLU LYS HIS HIS HIS HIS HIS
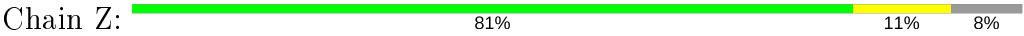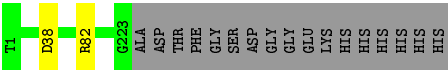
• Molecule 2: Proteasome subunit beta

Chain J:

83%   10%   8%

T1 V12 S20 T21 Q22 V31 T48 V51 T75 G78 N81 R82 R88 L98 S112 D113 A126 Q137 A138 Q156 R165 D176 A194 I197 I210 S222 GLY ALA ASP THR PHE GLY SER ASP GLY GLU LYS HIS

HIS HIS HIS HIS

• Molecule 2: Proteasome subunit beta

Chain K:

82%   11%   7%

T1 T2 R18 V31 D38 I45 T48 A52 R57 E62 R82 R88 L91 M95 L98 Y107 S112 D113 P114 A117 A126 E132 Q137 G142 A174 D177 T181 R209 G223 ALA ASP THR PHE GLY SER

ASP GLY GLU LYS HIS HIS HIS HIS HIS

● Molecule 2: Proteasome subunit beta

Chain L:

84% 9% 7%

T1 D30 D38 T41 T48 V51 R57 E62 L63 E64 K68 R82 I85 R88 A94 L98 L99 A126 E132 Q137 M150 Y154 S155 Q156 R165 G223 ALA ASP THR PHE GLY SER ASP GLY GLY GLU LYS HIS HIS HIS

HIS HIS HIS

● Molecule 2: Proteasome subunit beta

Chain M:

85% 7% 8%

T1 T2 I3 R18 D30 V31 T48 V51 G78 R82 L98 E132 E133 Q137 A138 Q156 R165 S208 E212 S222 GLY ALA ASP THR PHE GLY SER ASP GLY GLY GLU LYS HIS HIS HIS HIS HIS

● Molecule 2: Proteasome subunit beta

Chain N:

84% 8% · 7%

T1 T2 I3 V12 Q22 V31 D38 T41 G44 V51 R57 E64 K68 L69 R82 R88 L98 A126 D161 I197 E207 S208 R209 E212 G223 ALA ASP THR PHE GLY SER ASP GLY GLY GLU LYS HIS HIS HIS HIS HIS

HIS

● Molecule 2: Proteasome subunit beta

Chain V:

85% 8% 7%

T1 R29 R32 H33 V34 T48 R57 E64 V72 P73 L74 T75 G78 R82 G97 Y107 D113 P114 Q115 S116 A117 F123 G128 R188 G223 ALA ASP THR PHE GLY SER ASP GLY GLY GLU LYS HIS HIS HIS HIS HIS

● Molecule 2: Proteasome subunit beta

Chain W:

79% 13% 7%

T1 Y8 V12 S20 G28 V31 R32 K33 D38 G44 T48 V51 R57 R82 R88 L98 L101 P102 Q115 S116 R119 A126 E134 L153 Q156 D161 R165 R188 A194 V195 I196 I197 V205 R209

R215 E219 G223 ALA ASP THR PHE GLY SER ASP GLY GLY GLU LYS HIS HIS HIS HIS HIS

● Molecule 2: Proteasome subunit beta

Chain X:

83% 9% 8%

T1 S20 V31 R32 T37 D38 T41 R57 E64 K68 T75 N81 R82 I85 R88 L104 A126 E132 E133 E134 T193 S208 E212 E219 S222 GLY ALA ASP THR PHE GLY SER ASP GLY GLU LYS HIS HIS HIS HIS

HIS HIS

● Molecule 2: Proteasome subunit beta

Chain Y:

84% 9% 7%

T1 Y8 R18 R19 S20 D30 V31 R32 Y35 D38 T41 T75 R82 R88 A126 Q137 A138 D161 R165 D176 T193 I196 S208 R209 G223 ALA ASP THR PHE GLY SER ASP GLY GLU LYS HIS HIS HIS HIS HIS

● Molecule 2: Proteasome subunit beta

Chain Z:

81% 11% 8%

T1 R18 R19 S20 D30 V31 R32 D38 T41 V51 R57 L58 E64 T75 R82 R88 L98 S112 D113 P114 A126 E132 Q137 A138 K152 R165 S208 E212 L213 E219 S222 GLY ALA ASP THR PHE GLY SER ASP

GLY GLY GLU LYS HIS HIS HIS HIS HIS HIS

● Molecule 2: Proteasome subunit beta

Chain a:

92% • 7%

T1 D38 R82 G223 ALA ASP THR PHE GLY SER ASP GLY GLU LYS HIS HIS HIS HIS HIS

● Molecule 2: Proteasome subunit beta

Chain b:

92% • 7%

T1 V13 D38 T48 G223 ALA ASP THR PHE GLY SER ASP GLY GLU LYS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	120.05Å 219.09Å 137.89Å 90.00° 104.87° 90.00°	Depositor
Resolution (Å)	49.53 – 2.80 49.53 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.53-2.80) 99.4 (49.53-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.20 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.160 , 0.216 0.160 , 0.214	Depositor DCC
R_{free} test set	8302 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	48.5	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.9	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	0.95	EDS
Total number of atoms	47357	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: 7HJ

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	0.66	0/1701	0.76	0/2297
1	B	0.64	0/1684	0.80	1/2274 (0.0%)
1	C	0.66	0/1688	0.78	4/2279 (0.2%)
1	D	0.64	0/1741	0.74	0/2351
1	E	0.67	0/1701	0.75	0/2297
1	F	0.65	0/1679	0.81	3/2266 (0.1%)
1	G	0.67	0/1686	0.73	0/2276
1	O	0.66	0/1701	0.77	2/2297 (0.1%)
1	P	0.65	0/1709	0.76	2/2308 (0.1%)
1	Q	0.65	0/1701	0.75	2/2297 (0.1%)
1	R	0.70	1/1681 (0.1%)	0.75	0/2269
1	S	0.67	0/1702	0.73	0/2298
1	T	0.72	0/1695	0.78	0/2289
1	U	0.76	1/1688 (0.1%)	0.81	1/2279 (0.0%)
2	H	0.63	0/1662	0.76	1/2254 (0.0%)
2	I	0.63	0/1662	0.74	0/2254
2	J	0.60	0/1662	0.71	0/2254
2	K	0.65	0/1666	0.79	2/2259 (0.1%)
2	L	0.65	0/1666	0.77	1/2259 (0.0%)
2	M	0.64	0/1662	0.78	1/2254 (0.0%)
2	N	0.58	0/1666	0.74	1/2259 (0.0%)
2	V	0.66	0/1666	0.79	1/2259 (0.0%)
2	W	0.64	0/1666	0.75	1/2259 (0.0%)
2	X	0.66	2/1662 (0.1%)	0.74	0/2254
2	Y	0.64	0/1666	0.75	0/2259
2	Z	0.67	1/1662 (0.1%)	0.76	1/2254 (0.0%)
2	a	0.66	0/1666	0.79	2/2259 (0.1%)
2	b	0.63	0/1666	0.71	1/2259 (0.0%)
All	All	0.66	5/47057 (0.0%)	0.76	27/63673 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	U	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	219	GLU	CD-OE1	-7.73	1.17	1.25
2	Z	31	VAL	CB-CG1	-7.60	1.36	1.52
2	X	219	GLU	CD-OE2	-6.91	1.18	1.25
1	R	120	VAL	CB-CG1	-5.45	1.41	1.52
1	U	134	LYS	CB-CG	5.17	1.66	1.52

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	82	ARG	NE-CZ-NH2	7.94	124.27	120.30
1	Q	48	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	F	208	LEU	CA-CB-CG	7.19	131.84	115.30
2	M	82	ARG	NE-CZ-NH2	7.09	123.85	120.30
2	L	38	ASP	CB-CG-OD1	6.70	124.33	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	U	133	THR	Peptide

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	29	0
1	B	1660	0	1665	63	0
1	C	1664	0	1668	45	0
1	D	1716	0	1705	38	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1677	0	1680	11	0
1	F	1655	0	1653	56	0
1	G	1662	0	1662	33	0
1	O	1677	0	1680	41	0
1	P	1685	0	1684	39	0
1	Q	1677	0	1677	28	0
1	R	1657	0	1659	29	0
1	S	1678	0	1677	21	0
1	T	1671	0	1675	30	0
1	U	1664	0	1668	33	0
2	H	1638	0	1633	22	0
2	I	1638	0	1633	14	0
2	J	1638	0	1633	18	0
2	K	1642	0	1636	16	0
2	L	1642	0	1636	15	0
2	M	1638	0	1633	14	0
2	N	1642	0	1636	19	0
2	V	1642	0	1636	14	0
2	W	1642	0	1636	20	0
2	X	1638	0	1633	16	0
2	Y	1642	0	1636	14	0
2	Z	1638	0	1633	18	2
2	a	1642	0	1636	0	0
2	b	1642	0	1636	0	0
3	H	46	0	0	1	0
3	I	46	0	0	0	0
3	J	46	0	0	2	0
3	K	46	0	0	0	0
3	L	46	0	0	1	0
3	M	46	0	0	1	0
3	N	46	0	0	3	0
3	V	46	0	0	1	0
3	W	46	0	0	1	0
3	X	46	0	0	0	0
3	Y	46	0	0	0	0
3	Z	46	0	0	1	0
3	a	46	0	0	0	0
3	b	46	0	0	0	0
4	A	10	0	0	0	0
4	B	1	0	0	0	0
4	C	4	0	0	0	0
4	D	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	16	0	0	0	0
4	F	5	0	0	0	0
4	G	14	0	0	0	0
4	H	11	0	0	0	0
4	I	19	0	0	0	0
4	J	14	0	0	2	0
4	K	14	0	0	0	0
4	L	16	0	0	0	0
4	M	14	0	0	0	0
4	N	9	0	0	0	0
4	O	8	0	0	0	0
4	P	9	0	0	0	0
4	Q	8	0	0	0	0
4	R	9	0	0	0	0
4	S	15	0	0	1	0
4	T	11	0	0	0	0
4	U	13	0	0	2	0
4	V	14	0	0	0	0
4	W	17	0	0	1	0
4	X	15	0	0	0	0
4	Y	15	0	0	0	0
4	Z	16	0	0	0	0
4	a	7	0	0	0	0
4	b	18	0	0	0	0
All	All	47357	0	46319	618	2

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 7.

The worst 5 of 618 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:T:10:GLU:O	1:T:14:ARG:HG3	1.45	1.15
1:S:92:ARG:NH1	1:S:132:GLU:OE2	1.82	1.12
1:T:182:ARG:NH2	1:T:233:LEU:O	1.91	1.02
1:R:58:ASP:OD1	1:R:91:ARG:NH1	1.95	0.99
1:O:182:ARG:HH22	1:O:234:LEU:HA	1.25	0.99

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:LYS:CE	2:Z:219:GLU:OE1[2_555]	1.89	0.31
1:D:22:LYS:NZ	2:Z:219:GLU:OE1[2_555]	2.19	0.01

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%)	209 (98%)	4 (2%)	1 (0%)	29	61
1	B	211/240 (88%)	204 (97%)	6 (3%)	1 (0%)	29	61
1	C	212/240 (88%)	206 (97%)	5 (2%)	1 (0%)	29	61
1	D	219/240 (91%)	210 (96%)	8 (4%)	1 (0%)	29	61
1	E	214/240 (89%)	208 (97%)	6 (3%)	0	100	100
1	F	211/240 (88%)	204 (97%)	7 (3%)	0	100	100
1	G	212/240 (88%)	208 (98%)	4 (2%)	0	100	100
1	O	214/240 (89%)	206 (96%)	6 (3%)	2 (1%)	17	46
1	P	215/240 (90%)	210 (98%)	5 (2%)	0	100	100
1	Q	213/240 (89%)	210 (99%)	2 (1%)	1 (0%)	29	61
1	R	211/240 (88%)	203 (96%)	6 (3%)	2 (1%)	17	46
1	S	214/240 (89%)	208 (97%)	6 (3%)	0	100	100
1	T	213/240 (89%)	207 (97%)	5 (2%)	1 (0%)	29	61
1	U	212/240 (88%)	204 (96%)	6 (3%)	2 (1%)	17	46
2	H	220/240 (92%)	216 (98%)	4 (2%)	0	100	100
2	I	220/240 (92%)	216 (98%)	4 (2%)	0	100	100
2	J	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
2	K	221/240 (92%)	218 (99%)	3 (1%)	0	100	100
2	L	221/240 (92%)	217 (98%)	4 (2%)	0	100	100
2	M	220/240 (92%)	217 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	221/240 (92%)	218 (99%)	3 (1%)	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%)	217 (99%)	3 (1%)	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%)	218 (99%)	3 (1%)	0	100	100
2	b	221/240 (92%)	217 (98%)	4 (2%)	0	100	100
All	All	6073/6720 (90%)	5939 (98%)	122 (2%)	12 (0%)	47	78

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	174	ASN
1	T	174	ASN
1	U	174	ASN
1	R	174	ASN
1	A	174	ASN

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%)	162 (98%)	3 (2%)	59	86
1	C	165/184 (90%)	160 (97%)	5 (3%)	41	75
1	D	172/184 (94%)	172 (100%)	0	100	100
1	E	167/184 (91%)	166 (99%)	1 (1%)	86	96
1	F	164/184 (89%)	162 (99%)	2 (1%)	71	92
1	G	165/184 (90%)	164 (99%)	1 (1%)	86	96
1	O	167/184 (91%)	162 (97%)	5 (3%)	41	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	168/184 (91%)	167 (99%)	1 (1%)	86	96
1	Q	167/184 (91%)	167 (100%)	0	100	100
1	R	164/184 (89%)	162 (99%)	2 (1%)	71	92
1	S	167/184 (91%)	165 (99%)	2 (1%)	71	92
1	T	166/184 (90%)	166 (100%)	0	100	100
1	U	165/184 (90%)	164 (99%)	1 (1%)	86	96
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%)	164 (99%)	1 (1%)	86	96
2	V	165/178 (93%)	165 (100%)	0	100	100
2	W	165/178 (93%)	162 (98%)	3 (2%)	59	86
2	X	165/178 (93%)	165 (100%)	0	100	100
2	Y	165/178 (93%)	163 (99%)	2 (1%)	71	92
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%)	162 (98%)	3 (2%)	59	86
All	All	4639/5068 (92%)	4607 (99%)	32 (1%)	84	95

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	101	ASN
1	O	182	ARG
2	b	13	VAL
1	O	135	ARG
1	P	101	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	73	ASN
2	I	156	GLN
1	P	73	ASN
1	F	231	GLN
2	N	137	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	7HJ	b	301	-	49,49,49	1.78	7 (14%)	64,65,65	1.44	6 (9%)
3	7HJ	a	301	-	49,49,49	1.70	3 (6%)	64,65,65	1.53	11 (17%)
3	7HJ	X	301	-	49,49,49	1.88	5 (10%)	64,65,65	1.40	7 (10%)
3	7HJ	Z	301	-	49,49,49	1.71	8 (16%)	64,65,65	1.37	5 (7%)
3	7HJ	Y	301	-	49,49,49	1.68	4 (8%)	64,65,65	1.28	6 (9%)
3	7HJ	V	301	-	49,49,49	1.60	3 (6%)	64,65,65	1.62	8 (12%)
3	7HJ	W	301	-	49,49,49	1.56	6 (12%)	64,65,65	1.53	9 (14%)
3	7HJ	L	301	-	49,49,49	1.69	4 (8%)	64,65,65	1.42	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	7HJ	N	301	-	49,49,49	1.54	6 (12%)	64,65,65	1.45	8 (12%)
3	7HJ	M	301	-	49,49,49	1.90	7 (14%)	64,65,65	1.31	9 (14%)
3	7HJ	H	301	-	49,49,49	1.72	7 (14%)	64,65,65	1.42	8 (12%)
3	7HJ	J	301	-	49,49,49	1.85	9 (18%)	64,65,65	1.34	7 (10%)
3	7HJ	I	301	-	49,49,49	1.78	3 (6%)	64,65,65	1.32	7 (10%)
3	7HJ	K	301	-	49,49,49	1.44	5 (10%)	64,65,65	1.35	6 (9%)

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	7HJ	b	301	-	-	4/42/42/42	0/4/4/4
3	7HJ	a	301	-	-	6/42/42/42	0/4/4/4
3	7HJ	X	301	-	-	4/42/42/42	0/4/4/4
3	7HJ	Z	301	-	-	5/42/42/42	0/4/4/4
3	7HJ	Y	301	-	-	6/42/42/42	0/4/4/4
3	7HJ	V	301	-	-	8/42/42/42	0/4/4/4
3	7HJ	W	301	-	-	7/42/42/42	0/4/4/4
3	7HJ	L	301	-	-	5/42/42/42	0/4/4/4
3	7HJ	N	301	-	-	8/42/42/42	0/4/4/4
3	7HJ	M	301	-	-	6/42/42/42	0/4/4/4
3	7HJ	H	301	-	-	4/42/42/42	0/4/4/4
3	7HJ	J	301	-	-	7/42/42/42	0/4/4/4
3	7HJ	I	301	-	-	6/42/42/42	0/4/4/4
3	7HJ	K	301	-	-	6/42/42/42	0/4/4/4

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	301	7HJ	C38-C39	9.04	1.56	1.33
3	J	301	7HJ	C38-C39	8.85	1.56	1.33
3	X	301	7HJ	C38-C39	8.60	1.55	1.33
3	M	301	7HJ	C38-C39	8.33	1.54	1.33
3	V	301	7HJ	C38-C39	8.01	1.53	1.33

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	301	7HJ	C40-C39-C38	-6.17	112.78	126.91
3	X	301	7HJ	C40-C39-C38	-5.83	113.56	126.91
3	b	301	7HJ	C40-C39-C38	-5.74	113.78	126.91
3	Z	301	7HJ	C40-C39-C38	-5.72	113.82	126.91
3	W	301	7HJ	C07-N06-C05	5.51	130.27	122.34

There are no chirality outliers.

5 of 82 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Y	301	7HJ	C34-C33-N30-C29
3	W	301	7HJ	C32-C31-N30-C29
3	W	301	7HJ	C32-C31-N30-C33
3	a	301	7HJ	O46-C37-C38-C39
3	Y	301	7HJ	O46-C37-C38-C39

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Z	301	7HJ	1	0
3	V	301	7HJ	1	0
3	W	301	7HJ	1	0
3	L	301	7HJ	1	0
3	N	301	7HJ	3	0
3	M	301	7HJ	1	0
3	H	301	7HJ	1	0
3	J	301	7HJ	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 7HJ b 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 7HJ a 301

Bond lengths

Bond angles
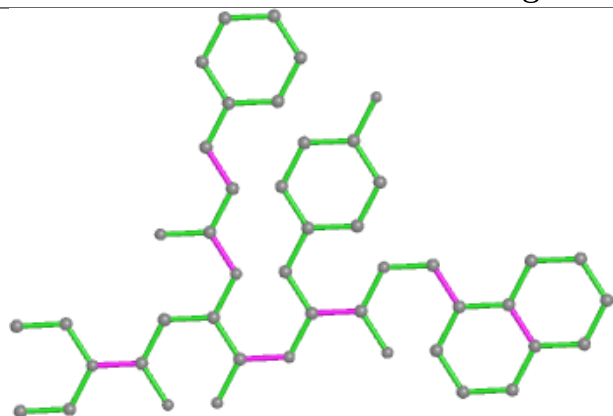
Torsions
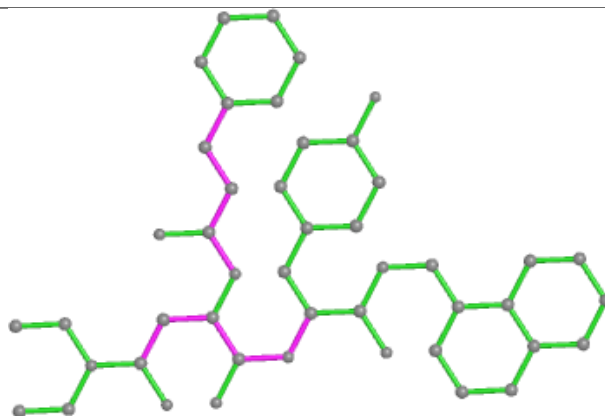
Rings

Ligand 7HJ X 301
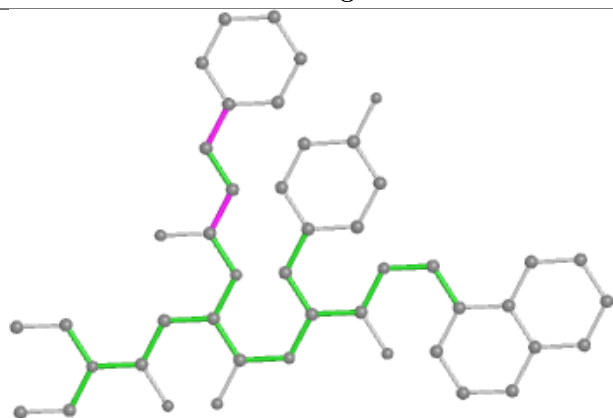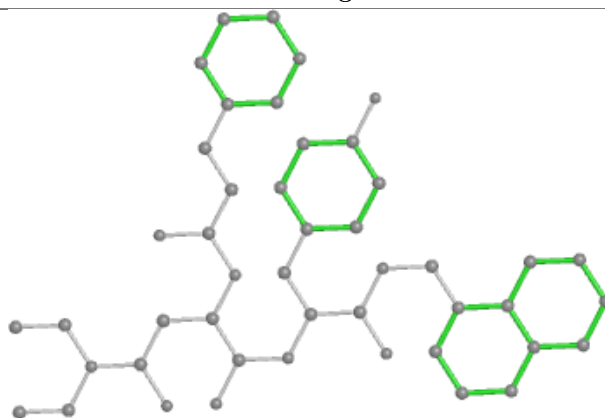
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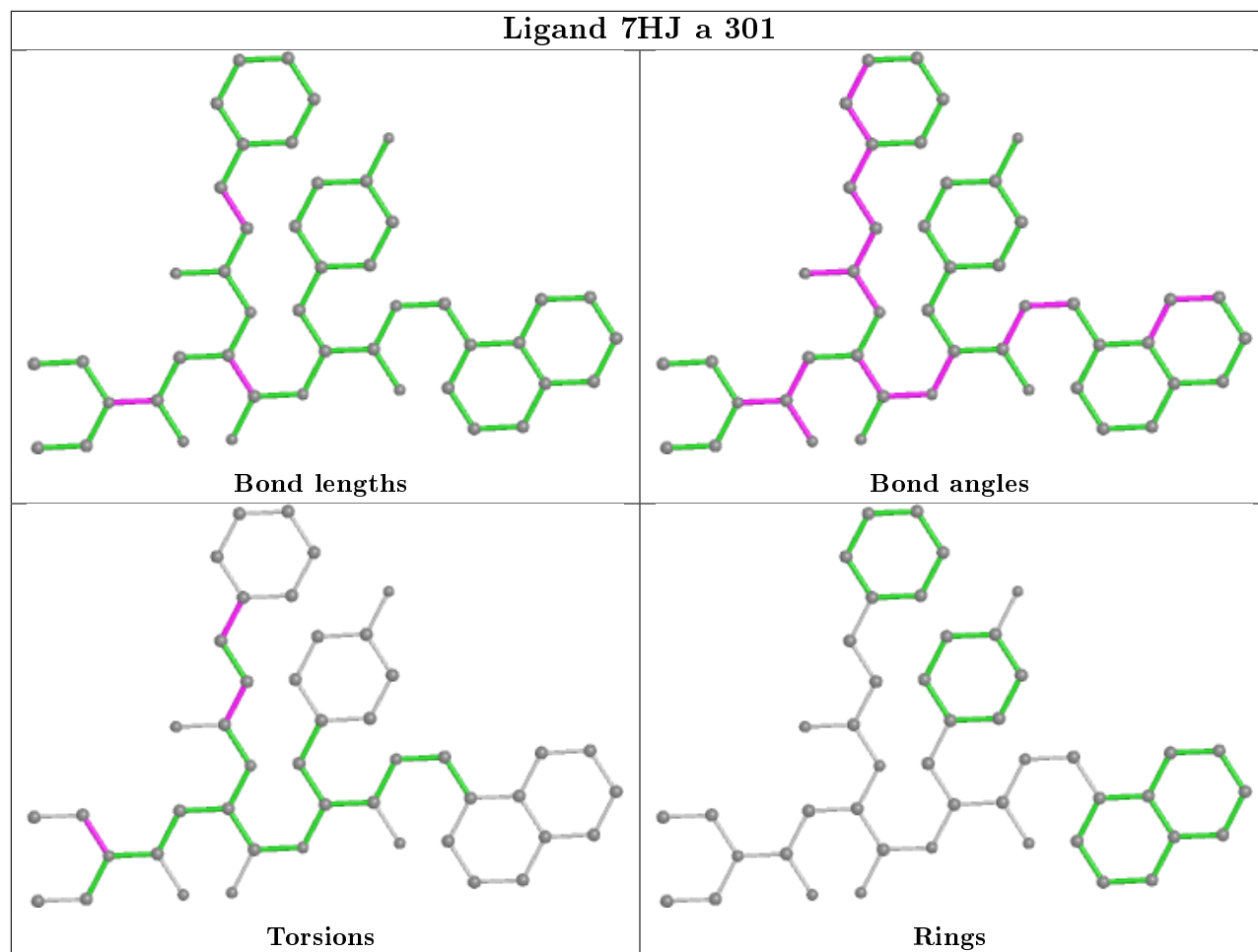
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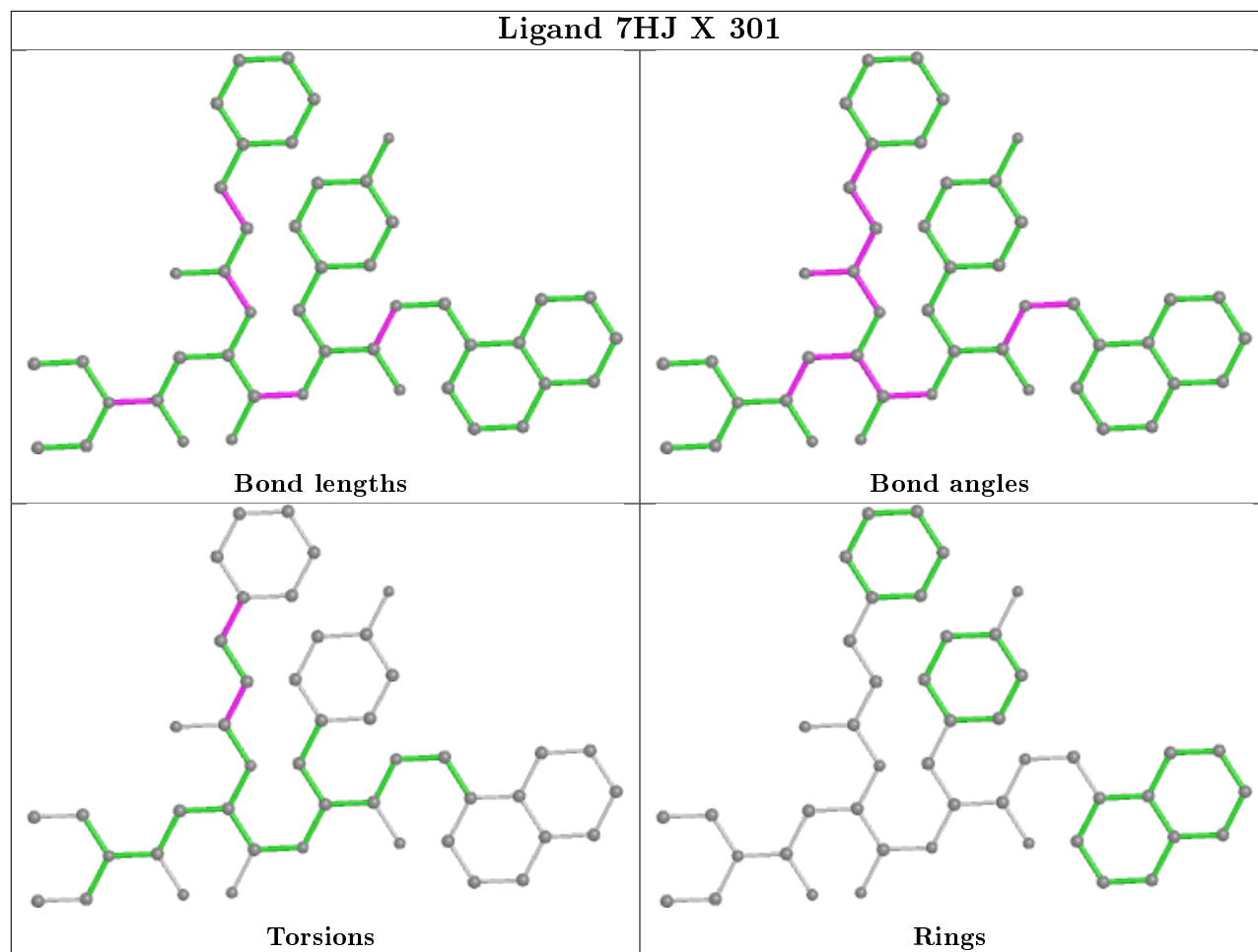
Torsions

Rings

Ligand 7HJ Z 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 7HJ Y 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 7HJ V 301

Bond lengths
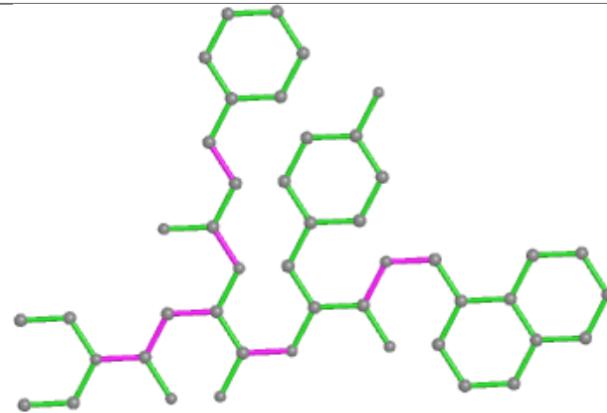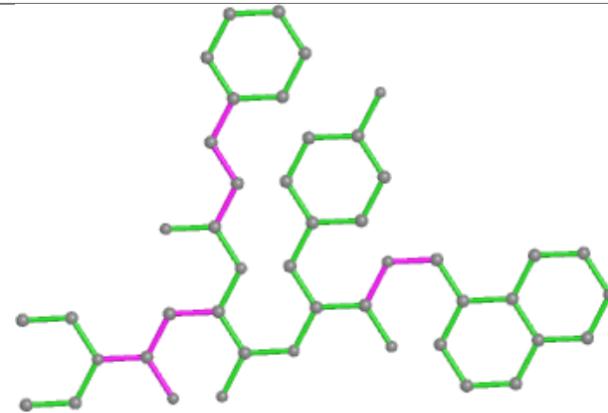
Bond angles

Torsions
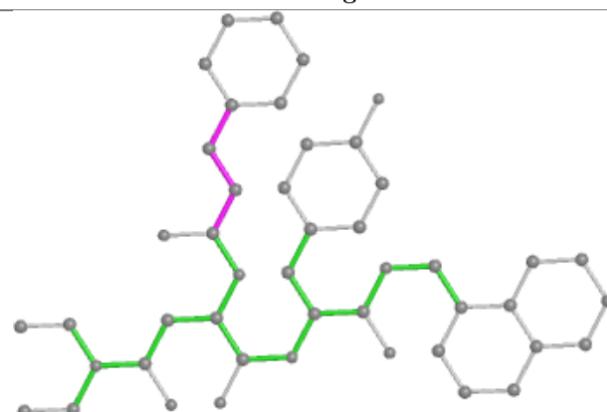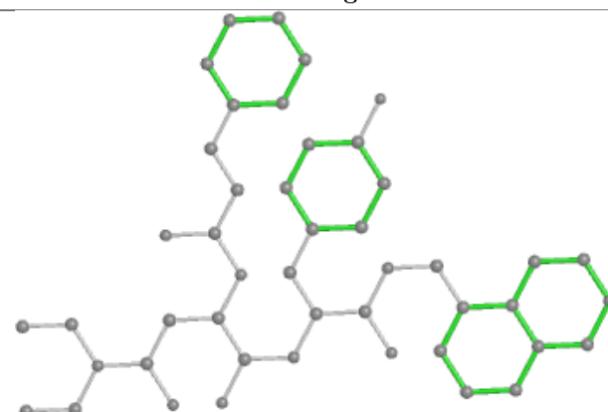
Rings

Ligand 7HJ W 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 7HJ L 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 7HJ N 301
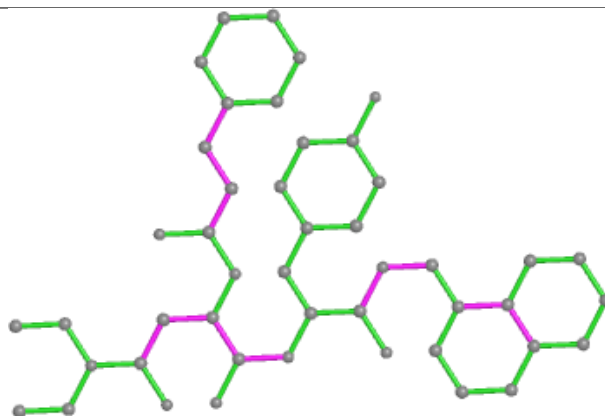
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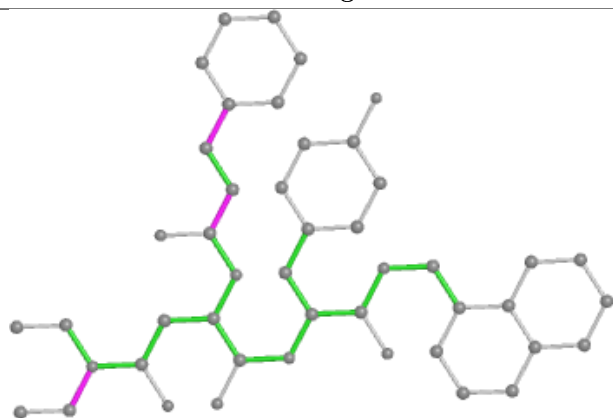
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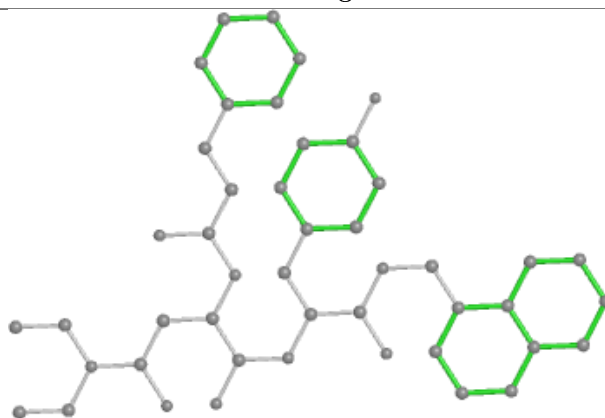
Torsions

Rings
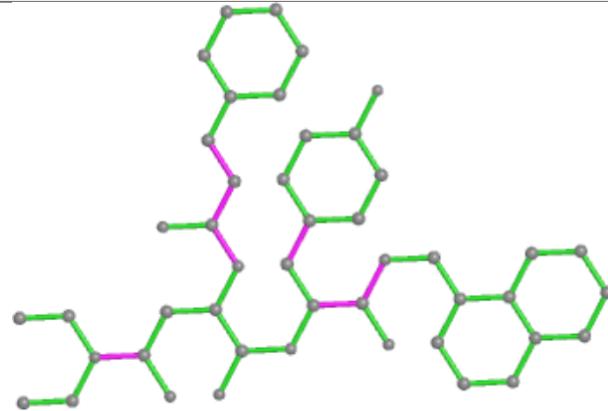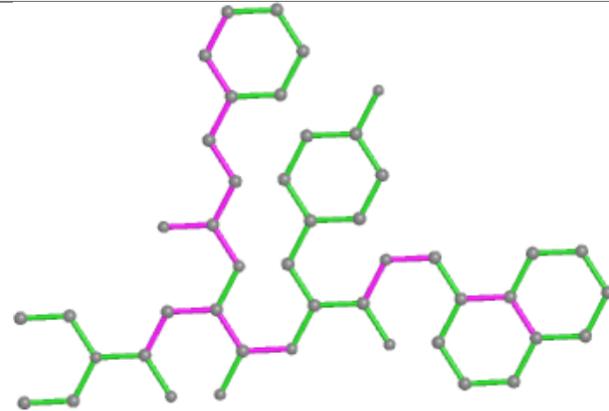
Ligand 7HJ M 301

Bond lengths

Bond angles
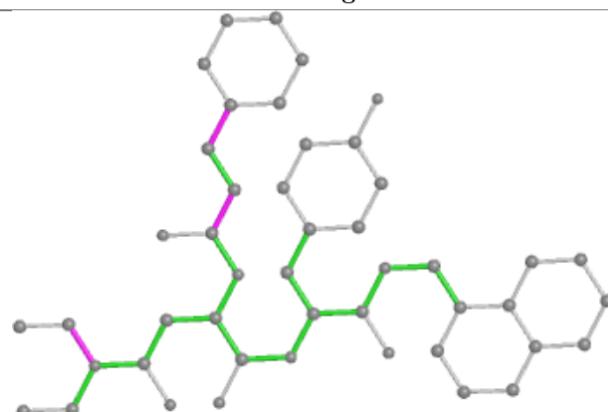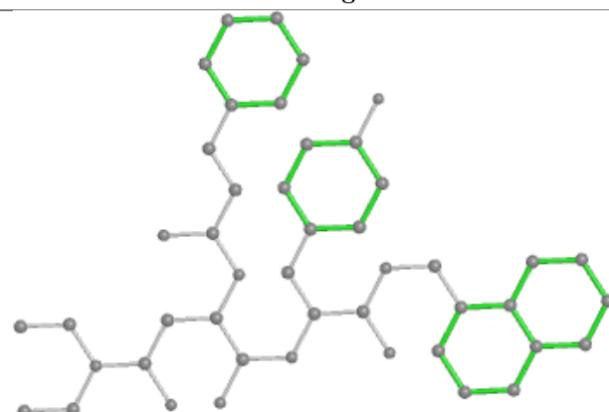
Torsions

Rings

Ligand 7HJ H 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 7HJ J 301
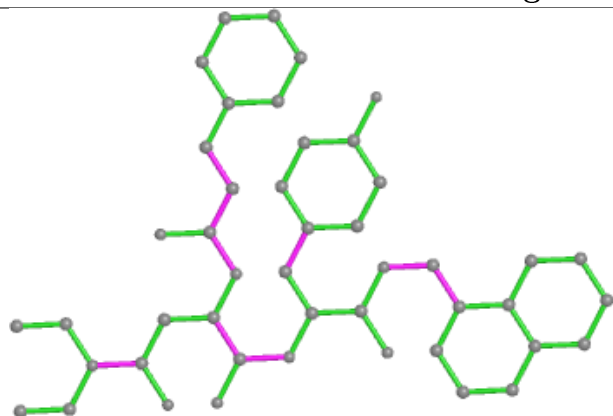
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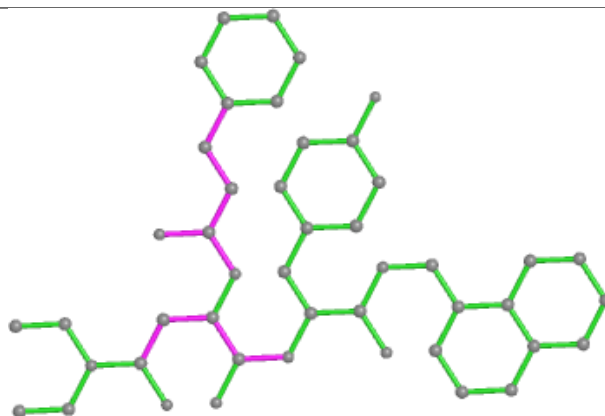
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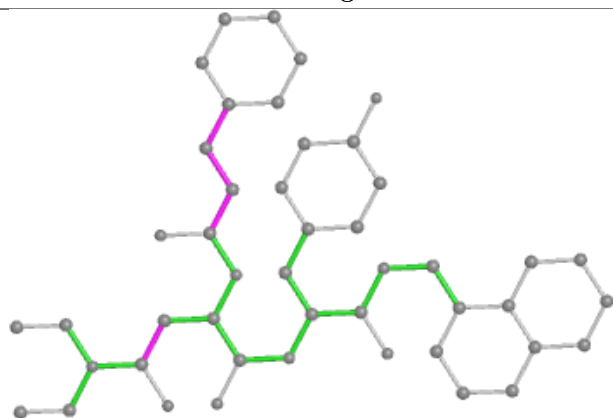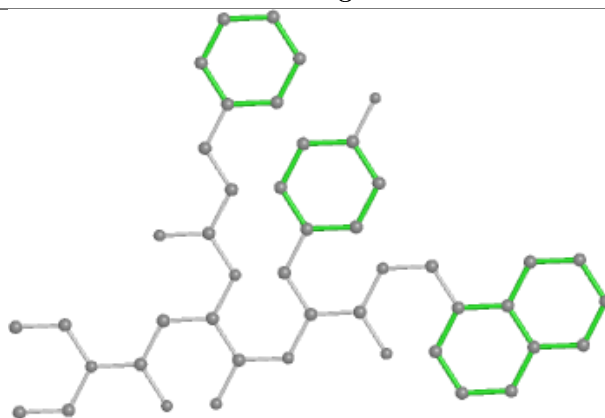
Torsions

Rings

Ligand 7HJ I 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 7HJ K 301
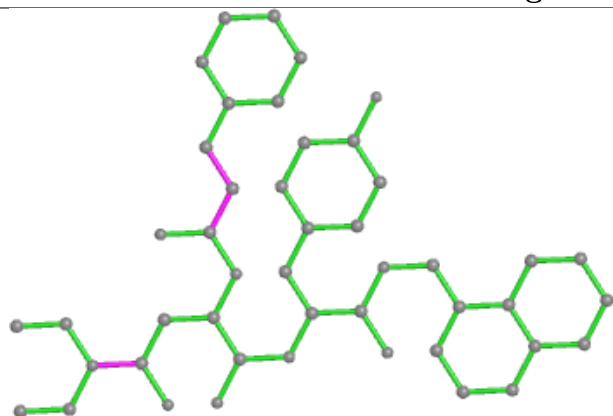
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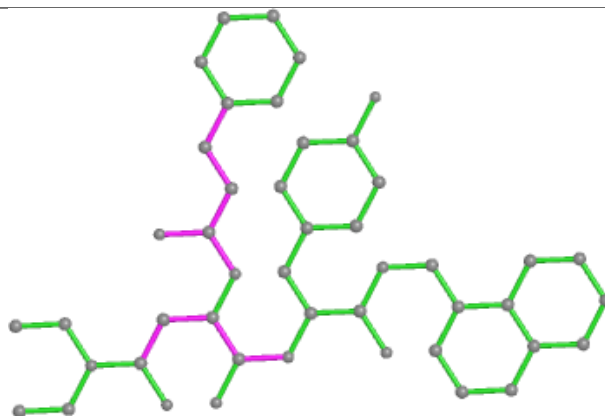
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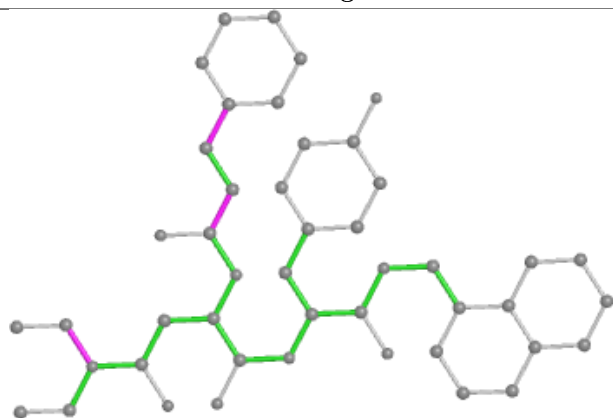
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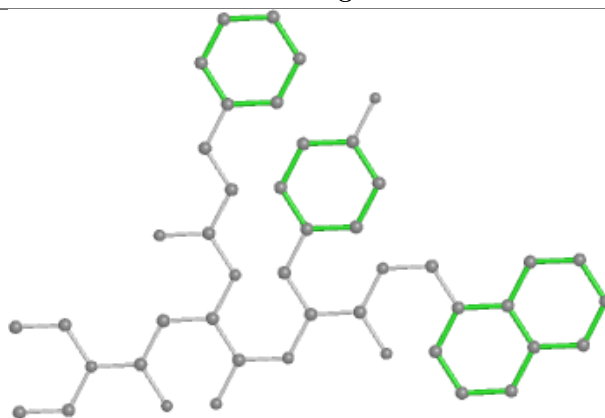
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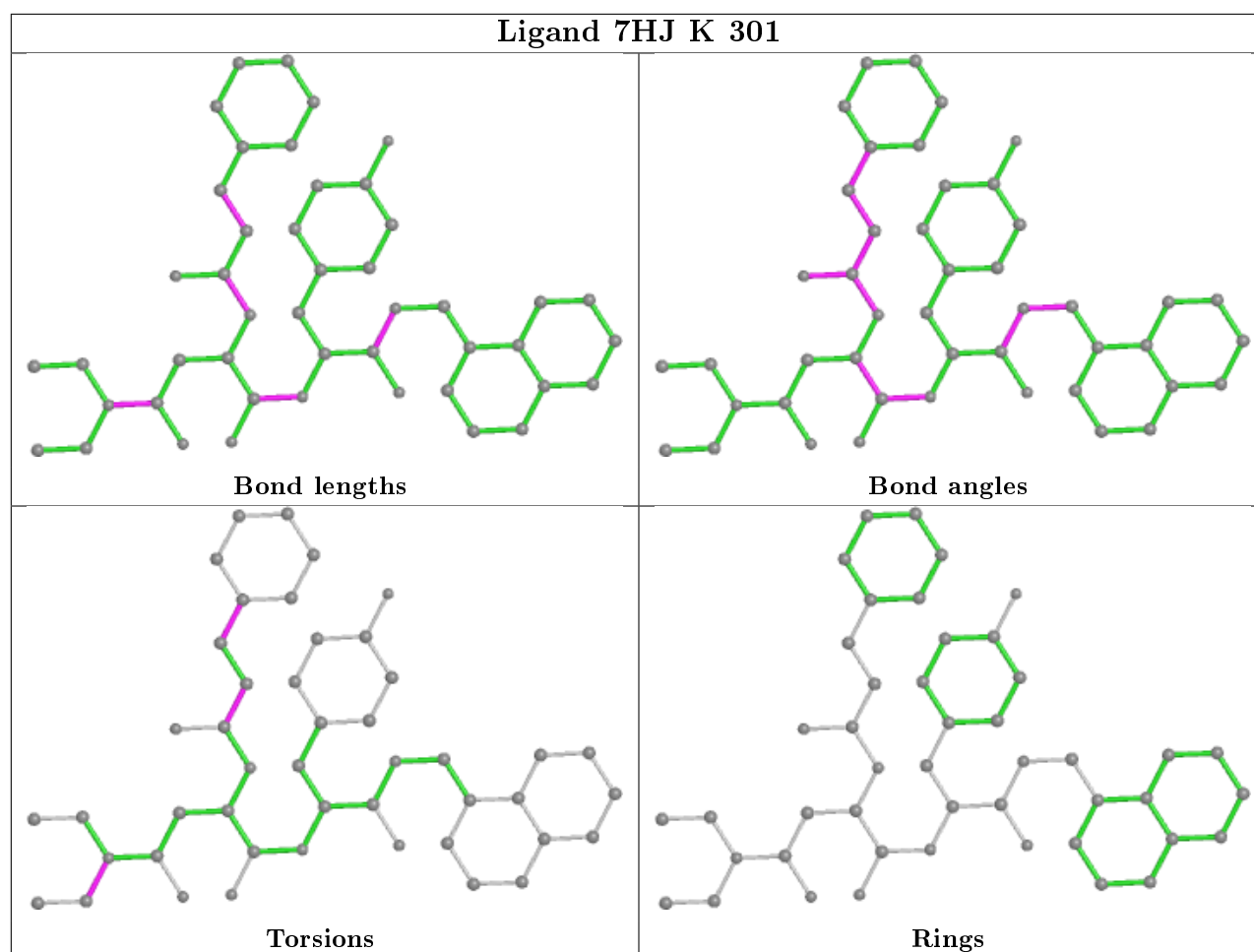
5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	218/240 (90%)	-0.55	1 (0%)	91	88	25, 39, 65, 98	0
1	B	215/240 (89%)	-0.04	9 (4%)	36	26	30, 58, 99, 159	0
1	C	216/240 (90%)	-0.19	4 (1%)	66	59	27, 54, 93, 111	0
1	D	223/240 (92%)	-0.41	1 (0%)	92	91	25, 45, 82, 117	0
1	E	218/240 (90%)	-0.60	0	100	100	24, 38, 68, 103	0
1	F	215/240 (89%)	-0.18	2 (0%)	84	80	27, 57, 117, 144	0
1	G	216/240 (90%)	-0.45	0	100	100	23, 42, 76, 91	0
1	O	218/240 (90%)	-0.43	1 (0%)	91	88	22, 44, 83, 117	0
1	P	219/240 (91%)	-0.49	1 (0%)	91	88	25, 43, 79, 107	0
1	Q	217/240 (90%)	-0.38	1 (0%)	91	88	25, 48, 87, 114	0
1	R	215/240 (89%)	-0.50	0	100	100	24, 41, 72, 88	0
1	S	218/240 (90%)	-0.60	0	100	100	22, 36, 66, 107	0
1	T	217/240 (90%)	-0.48	2 (0%)	84	80	23, 35, 70, 134	0
1	U	216/240 (90%)	-0.44	2 (0%)	84	80	23, 38, 73, 91	0
2	H	222/240 (92%)	-0.48	0	100	100	23, 33, 56, 78	0
2	I	222/240 (92%)	-0.60	0	100	100	23, 33, 52, 72	0
2	J	222/240 (92%)	-0.64	0	100	100	25, 35, 55, 74	0
2	K	223/240 (92%)	-0.69	0	100	100	22, 32, 52, 66	0
2	L	223/240 (92%)	-0.66	0	100	100	20, 30, 50, 74	0
2	M	222/240 (92%)	-0.62	0	100	100	22, 32, 53, 82	0
2	N	223/240 (92%)	-0.60	0	100	100	24, 35, 62, 84	0
2	V	223/240 (92%)	-0.63	0	100	100	21, 29, 48, 69	0
2	W	223/240 (92%)	-0.66	0	100	100	23, 32, 56, 68	0
2	X	222/240 (92%)	-0.65	0	100	100	24, 33, 54, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
2	Y	223/240 (92%)	-0.65	0	100	100	20, 32, 53, 85	0
2	Z	222/240 (92%)	-0.65	0	100	100	22, 34, 55, 70	0
2	a	223/240 (92%)	-0.68	0	100	100	22, 31, 53, 68	0
2	b	223/240 (92%)	-0.60	0	100	100	21, 30, 52, 77	0
All	All	6157/6720 (91%)	-0.52	24 (0%)	92	91	20, 36, 76, 159	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	9	MET	4.0
1	F	205	VAL	3.8
1	F	169	GLU	3.8
1	B	234	LEU	3.7
1	T	9	MET	3.6

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 monosaccharides 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(Å²)	Q<0.9
3	7HJ	X	301	46/46	0.95	0.15	29,43,61,64	0
3	7HJ	Z	301	46/46	0.95	0.17	21,34,44,49	0
3	7HJ	Y	301	46/46	0.95	0.15	20,36,49,57	0
3	7HJ	W	301	46/46	0.95	0.16	20,33,49,51	0
3	7HJ	L	301	46/46	0.95	0.17	24,40,54,57	0
3	7HJ	M	301	46/46	0.95	0.17	25,39,55,68	0
3	7HJ	H	301	46/46	0.95	0.17	22,41,53,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	7HJ	I	301	46/46	0.95	0.15	29,39,50,65	0
3	7HJ	a	301	46/46	0.96	0.15	21,34,44,51	0
3	7HJ	b	301	46/46	0.96	0.15	22,34,42,53	0
3	7HJ	J	301	46/46	0.96	0.17	23,36,45,55	0
3	7HJ	N	301	46/46	0.96	0.15	21,34,45,49	0
3	7HJ	K	301	46/46	0.96	0.15	24,33,47,53	0
3	7HJ	V	301	46/46	0.97	0.14	19,31,46,53	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.
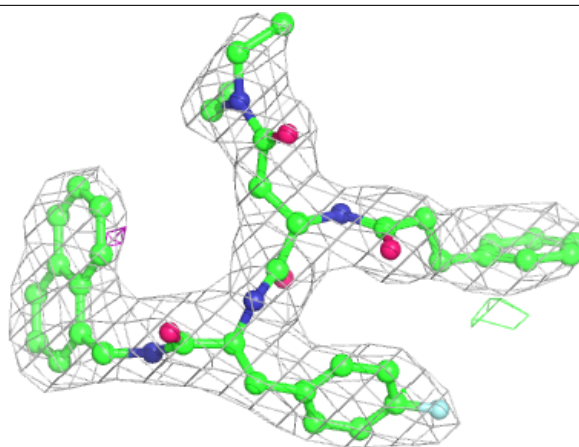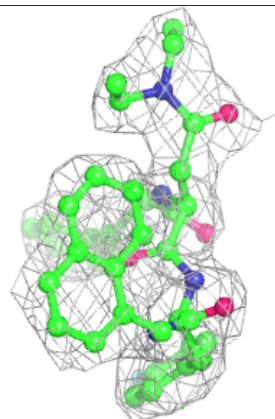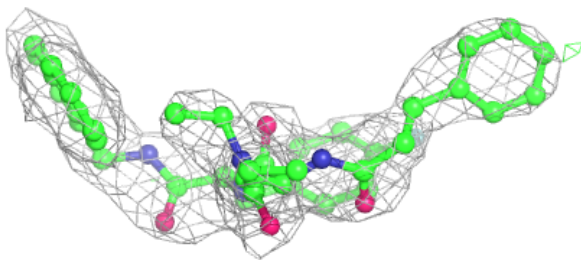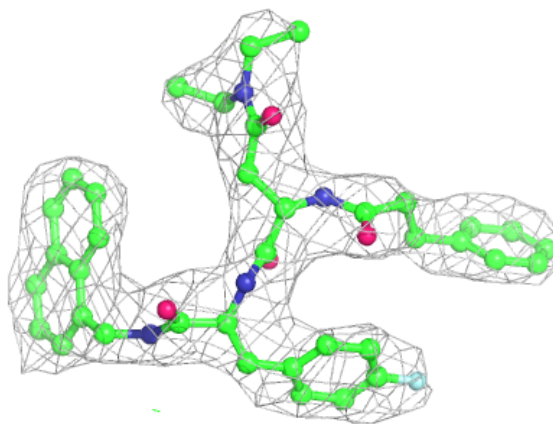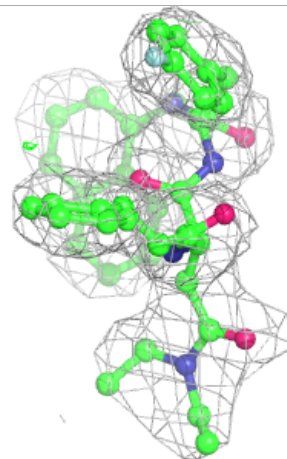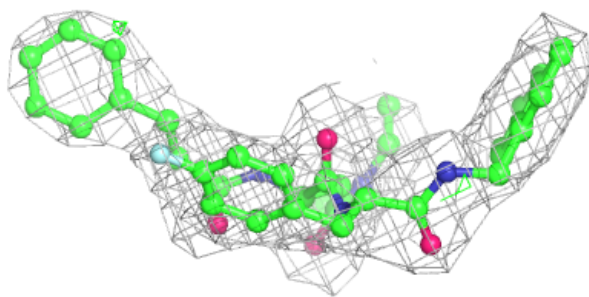
Electron density around 7HJ X 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)
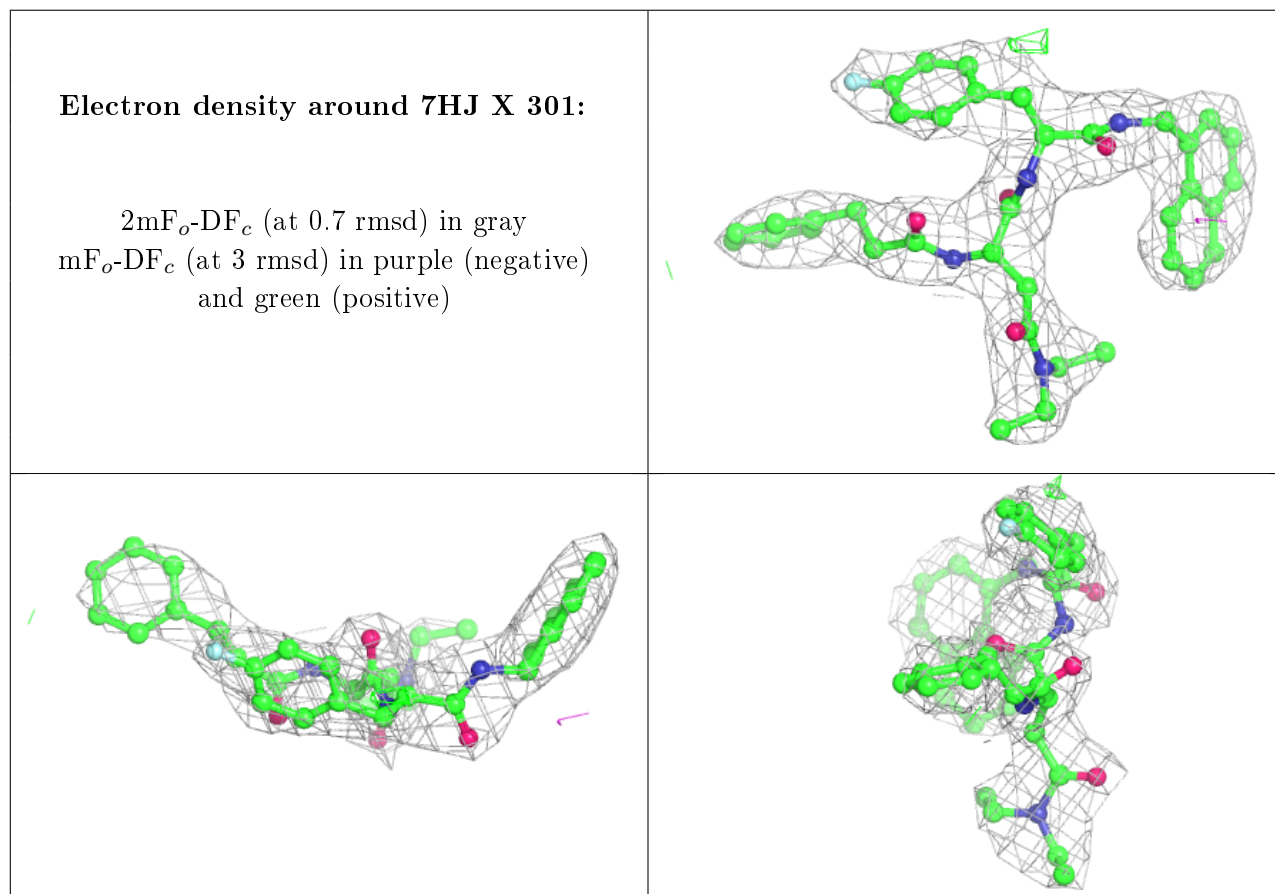
Electron density around 7HJ Z 301:

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$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
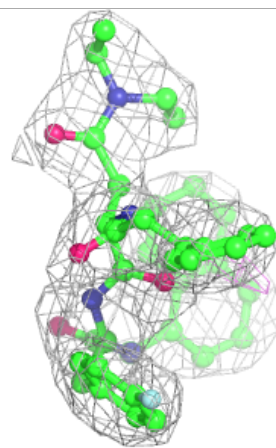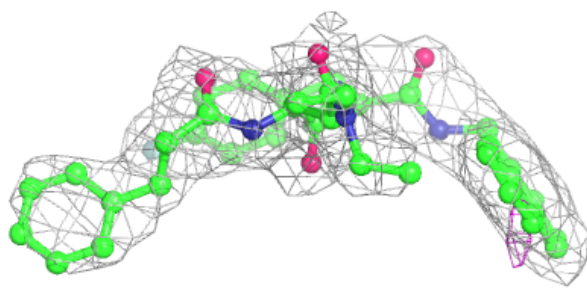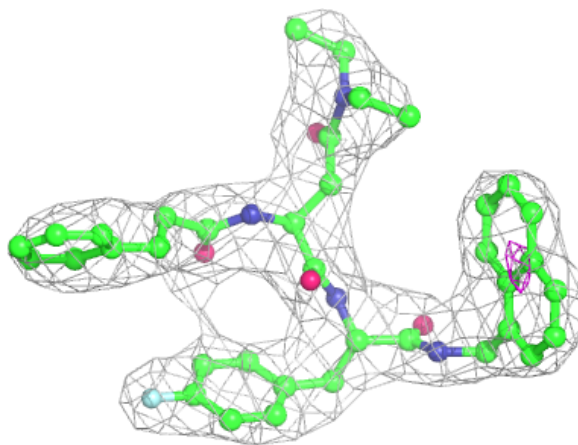
Electron density around 7HJ Y 301:

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and green (positive)
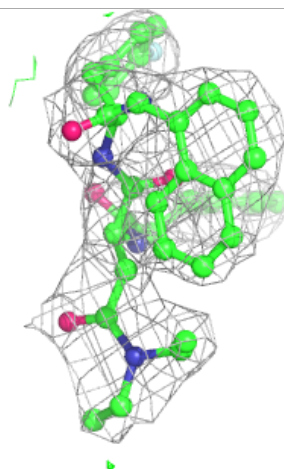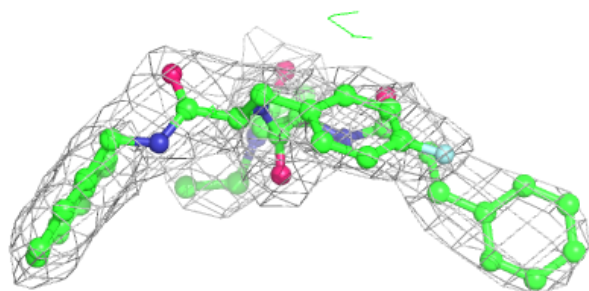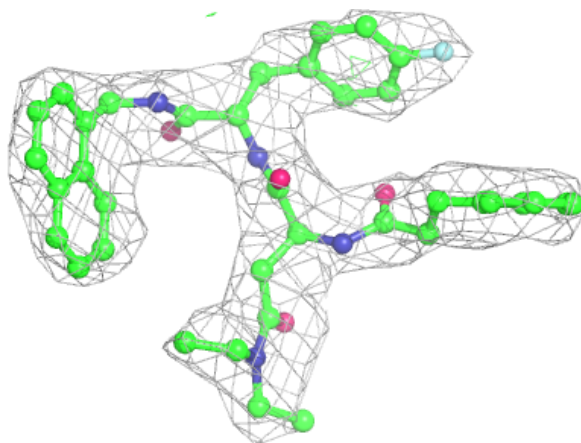
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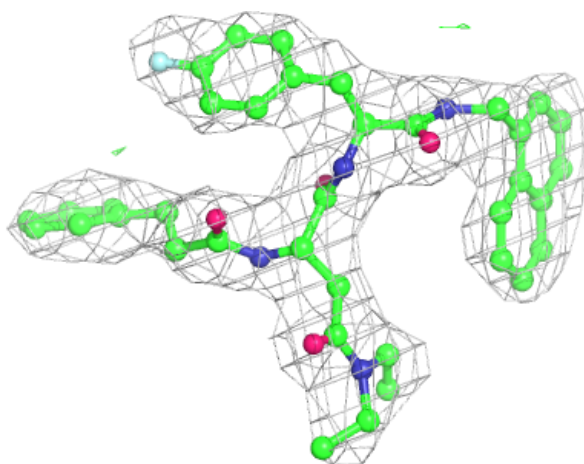$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
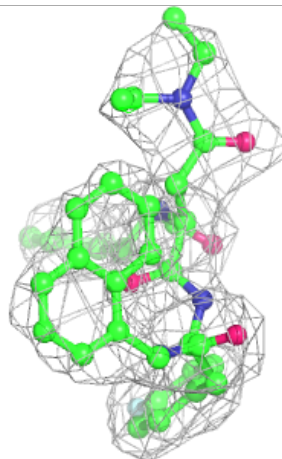and green (positive)
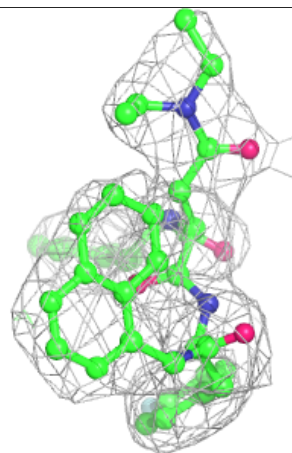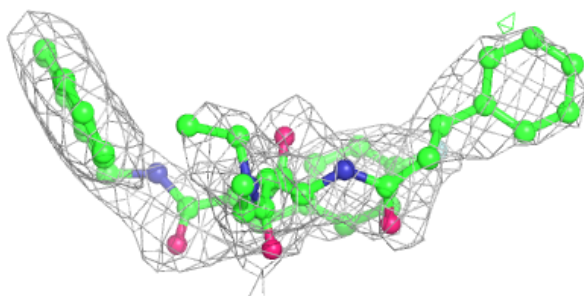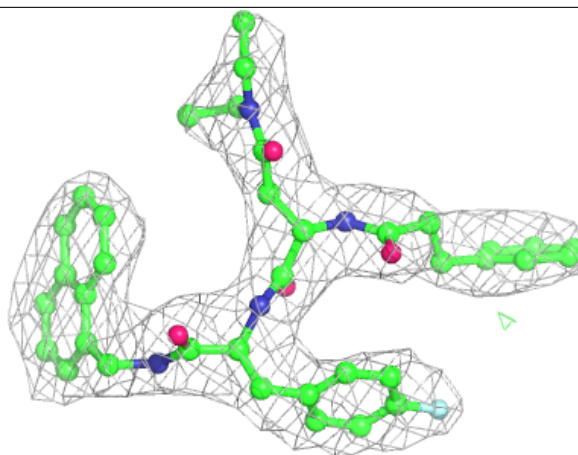
Electron density around 7HJ L 301:

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and green (positive)
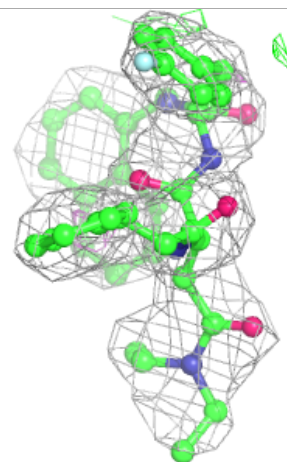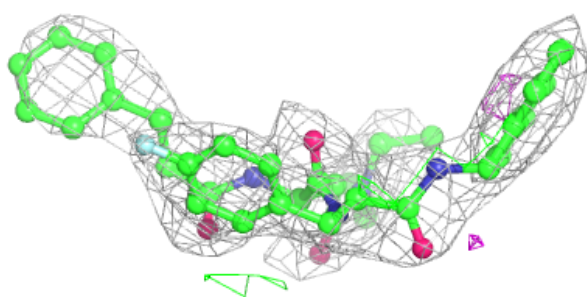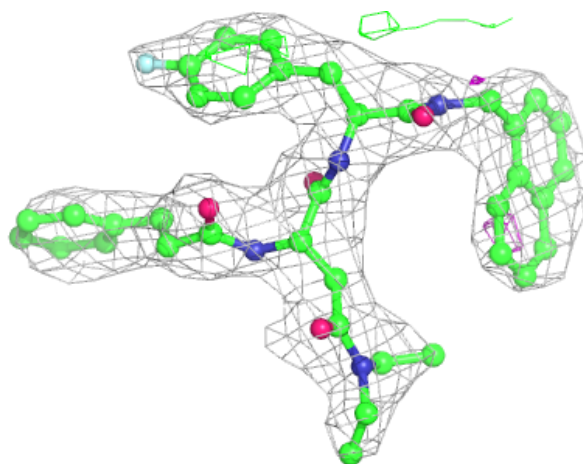
Electron density around 7HJ M 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
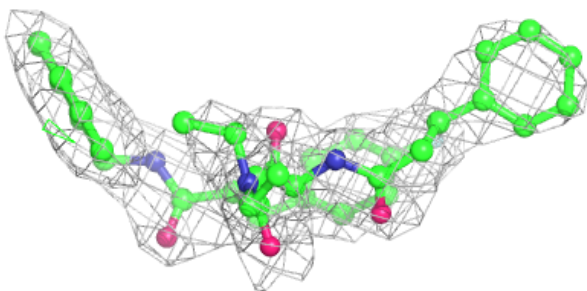and green (positive)
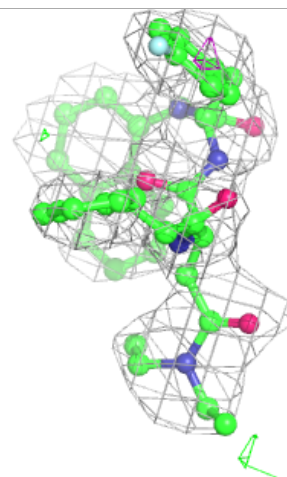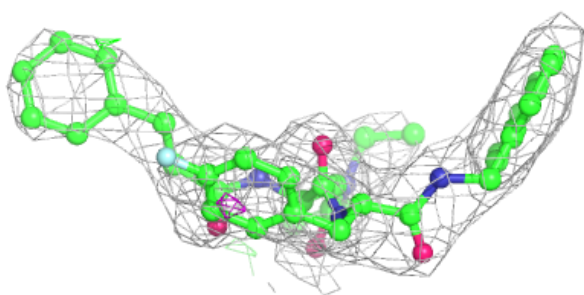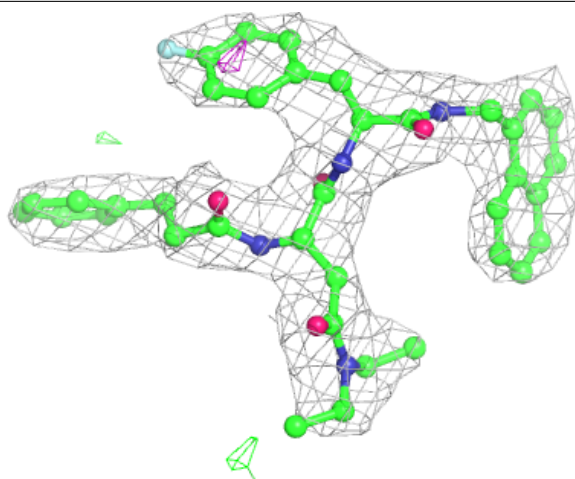
Electron density around 7HJ H 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
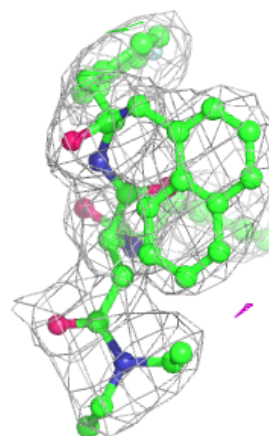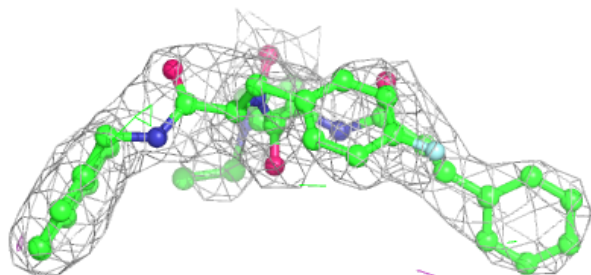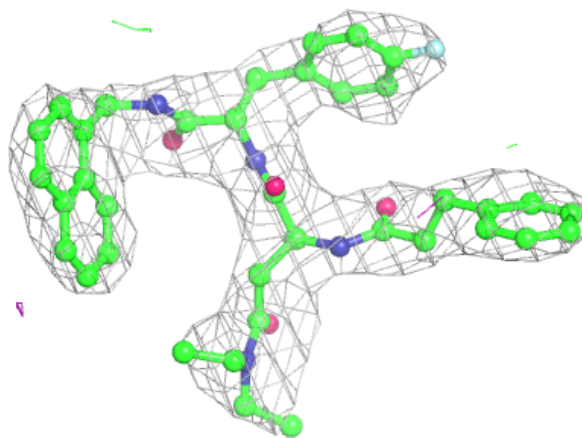
Electron density around 7HJ I 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
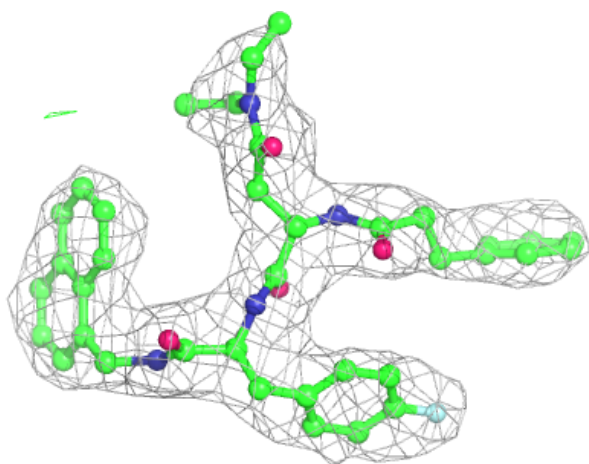and green (positive)
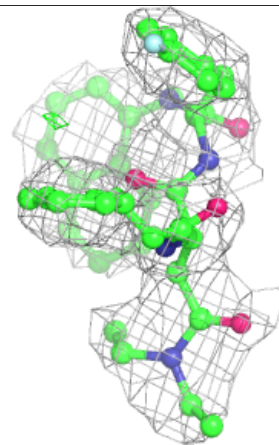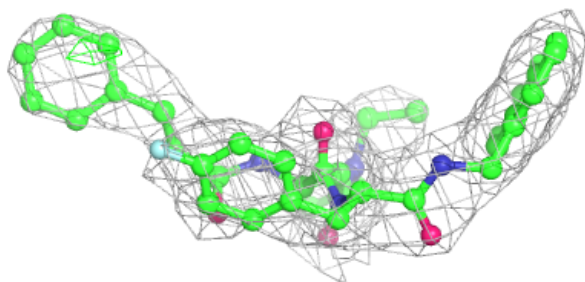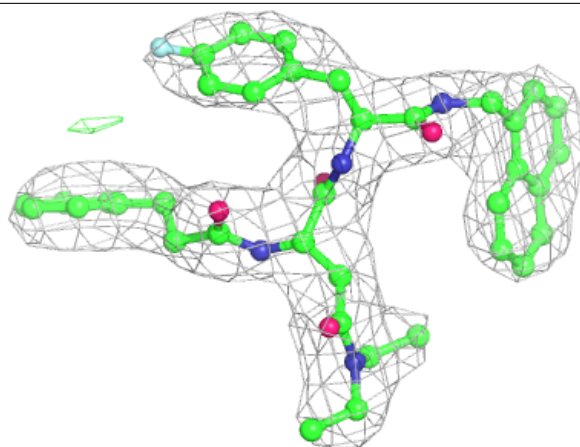
Electron density around 7HJ a 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
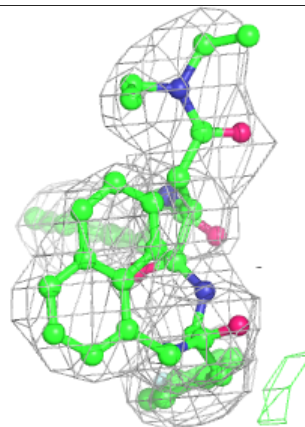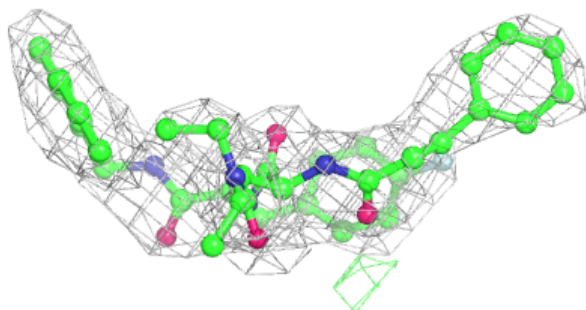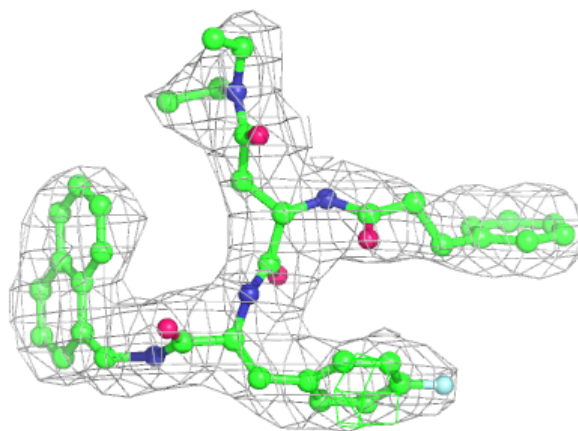
Electron density around 7HJ b 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
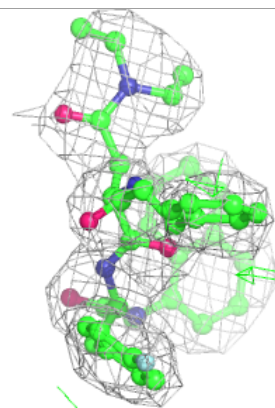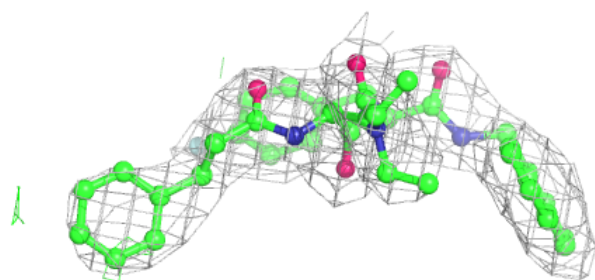and green (positive)
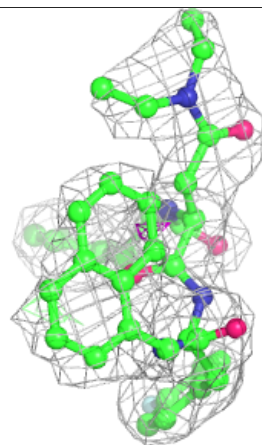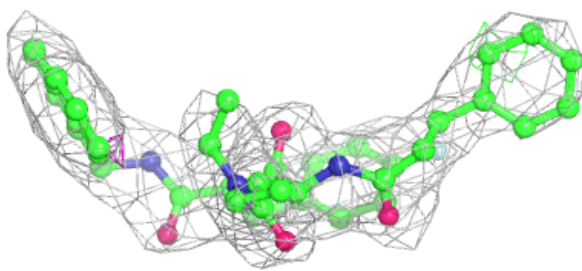
Electron density around 7HJ J 301:

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

Electron density around 7HJ N 301:

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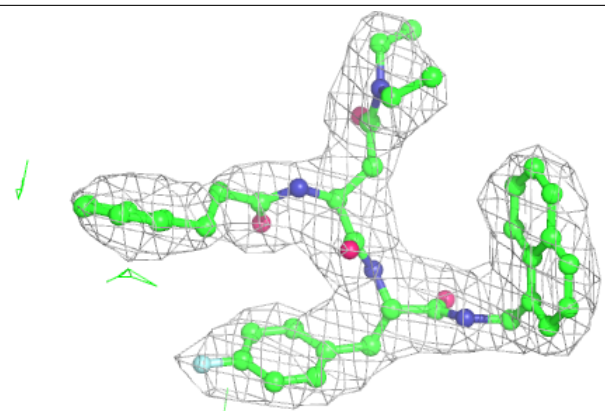and green (positive)

Electron density around 7HJ 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 7HJ V 301:

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

6.5 Other polymers (i)

There are no such residues in this entry.