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 ⓘ

Sep 24, 2023 – 12:46 AM EDT

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)

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

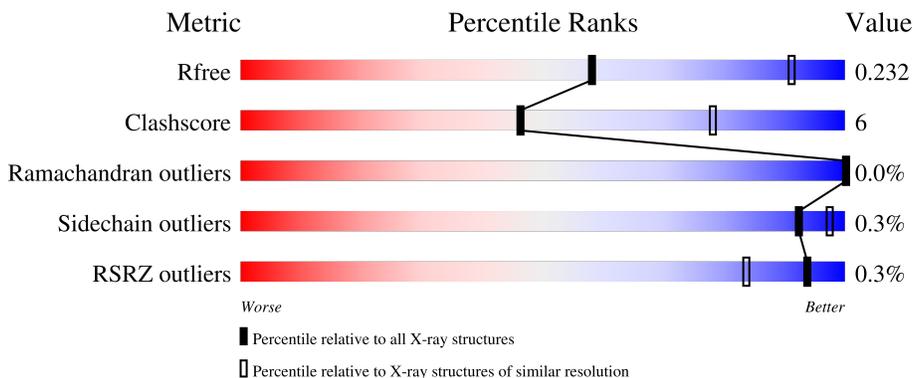|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 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.
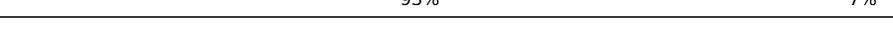
Metric	Percentile Ranks	Value
Rfree		0.232
Clashscore		6
Ramachandran outliers		0.0%
Sidechain outliers		0.3%
RSRZ outliers		0.3%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

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

Mol	Chain	Length	Quality of chain
1	A	240	72% 18% 9%
1	B	240	73% 16% 10%
1	C	240	77% 13% 10%
1	D	240	78% 12% 10%

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Mol	Chain	Length	Quality of chain
1	E	240	72% 18% 10%
1	F	240	% 66% 25% 9%
1	G	240	74% 16% 10%
1	O	240	71% 19% 10%
1	P	240	% 67% 22% · 10%
1	Q	240	% 70% 20% 9%
1	R	240	75% 16% 10%
1	S	240	% 78% 14% 9%
1	T	240	72% 18% 10%
1	U	240	72% 18% 10%
2	H	240	82% 11% 8%
2	I	240	84% 9% 8%
2	J	240	81% 12% 8%
2	K	240	82% 11% 7%
2	L	240	86% 7% 7%
2	M	240	85% 7% 8%
2	N	240	79% 14% 7%
2	V	240	83% 10% 7%
2	W	240	81% 12% 7%
2	X	240	80% 12% 8%
2	Y	240	78% 15% 7%
2	Z	240	81% 11% 8%
2	a	240	93% 7%
2	b	240	93% 7%

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 1677	C 1050	N 306	O 317	S 4	0	0	0
1	B	215	Total 1660	C 1041	N 303	O 312	S 4	0	0	0
1	C	216	Total 1664	C 1043	N 304	O 313	S 4	0	0	0
1	D	217	Total 1670	C 1046	N 305	O 315	S 4	0	0	0
1	E	217	Total 1671	C 1047	N 305	O 315	S 4	0	0	0
1	F	218	Total 1678	C 1050	N 306	O 318	S 4	0	0	0
1	G	216	Total 1662	C 1040	N 304	O 314	S 4	0	0	0
1	O	216	Total 1662	C 1040	N 304	O 314	S 4	0	0	0
1	P	217	Total 1674	C 1050	N 305	O 315	S 4	0	0	0
1	Q	218	Total 1679	C 1051	N 306	O 318	S 4	0	0	0
1	R	217	Total 1671	C 1047	N 305	O 315	S 4	0	0	0
1	S	219	Total 1683	C 1053	N 307	O 319	S 4	0	0	0
1	T	216	Total 1664	C 1043	N 304	O 313	S 4	0	0	0
1	U	216	Total 1664	C 1043	N 304	O 313	S 4	0	0	0

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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WORLDWIDE
wwPDB
PROTEIN DATA BANK

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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 (2 {S})- {N}-[(2 {S})-3-methoxy-1-(naphthalen-1-ylmethylamino)-1-oxidanyli dene-propan-2-yl]-4-oxidanylidene-2-(3-phenylpropanoylamino)-4-piperidin-1-yl-butanamide (three-letter code: 7J0) (formula: $C_{33}H_{40}N_4O_5$).
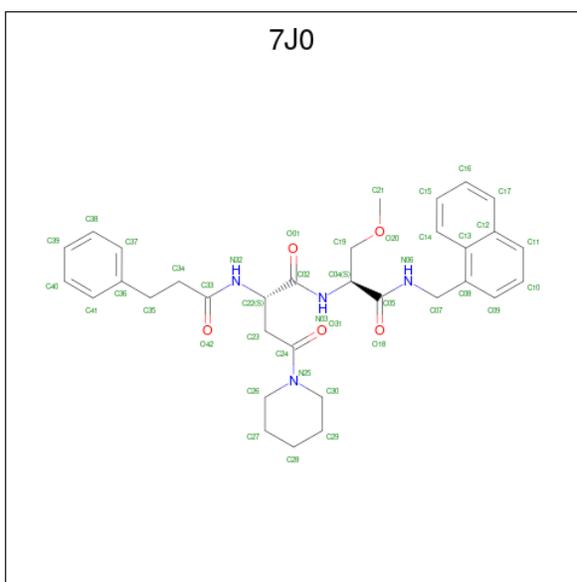
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	0
			42	33	4	5		
3	I	1	Total	C	N	O	0	0
			42	33	4	5		
3	J	1	Total	C	N	O	0	0
			42	33	4	5		
3	K	1	Total	C	N	O	0	0
			42	33	4	5		
3	L	1	Total	C	N	O	0	0
			42	33	4	5		
3	M	1	Total	C	N	O	0	0
			42	33	4	5		
3	N	1	Total	C	N	O	0	0
			42	33	4	5		

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

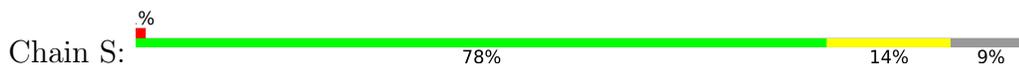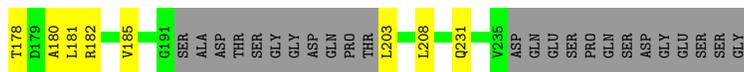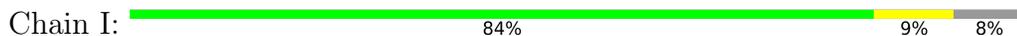• Molecule 1: Proteasome subunit alpha

Chain A:

• Molecule 1: Proteasome subunit alpha

Chain B:

• Molecule 1: Proteasome subunit alpha

Chain C:

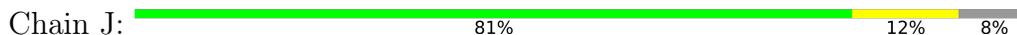• Molecule 1: Proteasome subunit alpha

Chain D:

• Molecule 1: Proteasome subunit alpha

Chain E: 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%   22%   10%

M9 E10 Q11 A12 M13 R14 E15 R16 S17 E18 K22 A25 V31 A32 L40 F41 Q51 K52 I53 S54 E55 L56 F62 F68 F71 L74 R75 F81 Y87 R92 R97 V102 L107 I110 L114 Q114 E121 L122 C123 A128 E132

T133 K134 Y139 R140 I141 V155 G158 E161 N165 L181 V185 A190 GLY SER ALA ASP THR SER GLY ASP GLN P201 T202 L203 G204 V205 L208 D214 R217 P218 R219 R223 R224 I225 L230 L233 L234 V235 ASP GLN GLU SER PRO GLN SER

ASP GLY GLU SER SER GLY

• Molecule 1: Proteasome subunit alpha

Chain Q:

M9 E10 E18 R21 K22 K28 S29 V30 V31 A32 L33 A34 Y35 A43 S49 L50 Q51 L56 F62 F68 F71 L74 R75 F81 Y87 A88 Y89 R92 V102 L107 T112 E113 E121 L122 C123 A128 K134 E137 L138 Y139

R140 V155 P162 I163 L177 A180 L181 V185 L188 R189 A190 G191 SER ALA ASP THR SER GLY ASP GLN PRO T202 V212 R219 R220 R223 L233 L234 V235 D236 GLN GLU SER PRO GLN SER ASP GLY GLU SER SER GLY

• Molecule 1: Proteasome subunit alpha

Chain R:

M9 E10 Q11 A12 R16 V30 V31 A32 L40 F41 V42 A43 I53 L56 G61 F62 F68 F71 F81 Y89 N101 V102 L107 Q114 E121 L122 C123 A128 K134 Y139 R140 P162 L181 V185 R189 A190 G191 SER ALA

ASP THR SER GLY ASP GLN PRO T202 L203 L213 R219 R220 L233 L234 V235 ASP GLN GLU SER PRO GLN SER ASP GLY GLU SER SER GLY

• Molecule 1: Proteasome subunit alpha

Chain S:

M9 E10 R16 S17 E18 R21 K22 V30 V31 F41 V42 A43 I53 L56 F62 F68 N69 E70 F71 N101 I110 F111 Q114 A115 K116 L122 R140 V155 L167 Y171 A172 A175 L181 R182 V185 S192 A193 ASP THR SER

GLY GLY ASP GLN PRO THR L203 R219 Q231 V235 D236 GLN GLU SER PRO GLN SER ASP GLY GLU SER SER GLY

• Molecule 1: Proteasome subunit alpha

Chain T:

M9 K28 A32 L40 N45 L56 F62 A65 G66 K67 F68 F71 L74 R97 Q98 L99 V102 G108 T112 E113 E119 V120 E121 L122 C123 A128 K134 E137 L138 Y139 R140 H152 F153 V154 Y171 T178 D179 A180 L181

V185 G191 SER ALA ASP THR SER GLY GLY ASP GLN PRO THR L203 E209 D214 R219 R220 R223 A229 L233 L234 V235 ASP GLN GLU SER PRO GLN SER ASP GLY GLU SER SER GLY

• Molecule 1: Proteasome subunit alpha

Chain U: ████████████████████████████████ 72%   18%   10%

M9 E18 K22 K28 S29 V30 V31 A32 L33 L40 A43 E44 R48 S49 L56 F62 F68 F71 L74 F81 R92 L99 V102 L122 C123 L138 Y139 R140 E150 P151 H152 V155 E161 P162 N165 A166 Y171

T178 D179 A180 L181 R182 V185 G191 SER ALA ASP THR SER GLY GLY ASP GLN PRO THR L203 L208 Q231 V235 ASP GLN GLU SER PRO GLN SER ASP GLY GLU SER SER GLY

• Molecule 2: Proteasome subunit beta

Chain H: ████████████████████████████████████ 82%   11%   8%

T1 T2 I3 Y8 P9 G10 G11 G44 I45 V51 A52 E62 L63 E64 K68 T75 G78 R82 L98 Q115 S122 F123 G128 W129 L144 M150 Y154 L164 D176 L213 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 I: ████████████████████████████████████ 84%   9%   8%

T1 T2 I3 R18 R19 S20 V31 D38 T41 V51 E64 G78 R82 N90 M95 D113 P114 Q115 V139 L144 D161 T193 R209 L213 I217 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 J: ████████████████████████████████ 81%   12%   8%

T1 T2 I3 V4 G10 S20 T21 Q22 V31 T37 D38 T41 G44 V51 Y59 E64 K68 G78 R82 L91 L98 Q115 S122 E132 E133 E134 Q137 A138 V139 M150 L164 D176 V205 S222 GLY ALA ASP

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

• Molecule 2: Proteasome subunit beta

Chain K: ████████████████████████████████████ 82%   11%   7%

T1 T2 I3 K7 S20 V31 R32 K33 T37 G44 Y59 H65 G78 R82 V121 S122 N130 G135 Y136 Q137 A138 V139 L164 E169 S179 D204 V205 L213 I217 R221 S222 G223 ALA ASP THR PHE GLY SER ASP GLY GLY

GLU LYS HIS HIS HIS HIS HIS

- Molecule 2: Proteasome subunit beta

Chain L:

86% 7% 7%

T1 K33 V51 E62 L63 E64 K68 L69 E70 R82 L98 L101 D113 P114 Q115 L144 M150 Y154 D161 R209 G223 ALA ASP THR PHE GLY SER ASP GLY GLU LYS HIS 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 GLU LYS HIS HIS HIS HIS HIS HIS

- Molecule 2: Proteasome subunit beta

Chain N:

79% 14% 7%

T1 T2 I3 V4 A5 V13 M14 A15 M25 D38 T41 G44 I45 V51 A52 R57 E64 T75 G78 R82 R88 G89 N90 L99 A100 V121 S122 A126 N130 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 HIS

- Molecule 2: Proteasome subunit beta

Chain V:

83% 10% 7%

T1 T2 I3 V4 A5 V13 R18 R19 S20 R29 D30 V31 D38 T41 G44 H65 T75 G78 R82 V121 S122 N130 Q137 L144 Q156 R165 S179 T193 L213 G223 ALA ASP THR PHE GLY SER ASP GLY GLU

LYS HIS HIS HIS HIS HIS

- Molecule 2: Proteasome subunit beta

Chain W:

81% 12% 7%

T1 T2 I3 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 GLU LYS HIS HIS HIS HIS HIS HIS

- Molecule 2: Proteasome subunit beta

Chain X:

80% 12% 8%

T1 T2 I3 V4 A5 G10 V13 S20 V31 R32 K33 G44 V51 R57 E64 K68 L69 T75 G78 R82 R88 G89 N90 L98 Q115 V121 S122 A126 N130 Q137 A138 V139 Q156 R165 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:

78%	15%	7%

T1 T2 I3 L6 V13 R18 R19 S20 M25 G28 V31 D38 T41 V51 F55 L58 E64 K68 T75 G78 R82 M86 V87 R88 G89 N90 L98 Q115 S116 V121 S122 A126 N130 Q137 A138 V139

F145 R165 E169 T193 I217 G223 ALA ASP THR PHE GLY SER ASP GLY GLU LYS HIS HIS HIS HIS HIS HIS

• Molecule 2: Proteasome subunit beta

Chain Z:

81%	11%	8%

T1 R18 R19 S20 G28 V31 R32 K33 V51 E64 K68 G78 R82 N90 L98 Y107 A117 V121 S122 N130 Q137 L144 M150 K151 Y154 D161 T193 D204 R209 S222 GLY ALA ASP THR PHE GLY SER

ASP GLY GLU LYS HIS HIS HIS HIS HIS HIS

• Molecule 2: Proteasome subunit beta

Chain a:

93%	7%

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

• Molecule 2: Proteasome subunit beta

Chain b:

93%	7%

T1 G223 ALA ASP THR PHE GLY SER ASP GLY GLU LYS HIS 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	120.65Å 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
$< I/\sigma(I) >$ [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]	$< |L| > = 0.48, < L^2 > = 0.31$	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.*

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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 ⓘ

5.1   Standard geometry ⓘ

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(^{o})	Ideal(^{o})
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 ⓘ

5.3.1 Protein backbone ⓘ

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	P	10	GLU
1	P	92	ARG
1	U	231	GLN
1	R	101	ASN
1	S	101	ASN

Sometimes 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 ⓘ

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	7J0	N	301	-	45,45,45	1.85	11 (24%)	59,59,59	1.48	10 (16%)
3	7J0	J	301	-	45,45,45	1.86	11 (24%)	59,59,59	1.54	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	7J0	a	301	-	45,45,45	1.85	11 (24%)	59,59,59	1.48	9 (15%)
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	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	M	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	b	301	-	45,45,45	1.84	11 (24%)	59,59,59	1.49	9 (15%)
3	7J0	Y	301	-	45,45,45	1.85	11 (24%)	59,59,59	1.47	8 (13%)
3	7J0	V	301	-	45,45,45	1.84	11 (24%)	59,59,59	1.47	9 (15%)
3	7J0	X	301	-	45,45,45	1.85	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%)

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	N	301	-	-	4/37/45/45	0/4/4/4
3	7J0	J	301	-	-	6/37/45/45	0/4/4/4
3	7J0	a	301	-	-	7/37/45/45	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	I	301	-	-	3/37/45/45	0/4/4/4
3	7J0	L	301	-	-	3/37/45/45	0/4/4/4
3	7J0	M	301	-	-	5/37/45/45	0/4/4/4
3	7J0	Z	301	-	-	5/37/45/45	0/4/4/4
3	7J0	b	301	-	-	3/37/45/45	0/4/4/4
3	7J0	Y	301	-	-	3/37/45/45	0/4/4/4
3	7J0	V	301	-	-	5/37/45/45	0/4/4/4
3	7J0	X	301	-	-	3/37/45/45	0/4/4/4
3	7J0	W	301	-	-	2/37/45/45	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(^{o})	Ideal(^{o})
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	H	301	7J0	C33-C34-C35-C36
3	H	301	7J0	N03-C04-C19-O20
3	H	301	7J0	C05-C04-C19-O20
3	I	301	7J0	C04-C19-O20-C21
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 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 7J0 N 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 7J0 J 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 7J0 a 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 7J0 H 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 7J0 K 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 7J0 I 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 7J0 L 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 7J0 M 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 7J0 Z 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 7J0 b 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 7J0 Y 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 7J0 V 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 7J0 X 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 7J0 W 301

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	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, 30, 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(Å²)	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 ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	7J0	K	301	42/42	0.94	0.20	21,31,52,64	0
3	7J0	M	301	42/42	0.94	0.20	14,24,49,63	0
3	7J0	N	301	42/42	0.94	0.23	20,29,53,59	0
3	7J0	H	301	42/42	0.95	0.21	15,25,45,66	0
3	7J0	L	301	42/42	0.95	0.20	14,24,39,52	0
3	7J0	I	301	42/42	0.95	0.19	16,26,46,64	0
3	7J0	J	301	42/42	0.95	0.21	19,26,60,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
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	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
3	7J0	Z	301	42/42	0.95	0.19	19,25,38,50	0
3	7J0	a	301	42/42	0.95	0.20	21,27,48,62	0
3	7J0	b	301	42/42	0.95	0.21	16,24,38,41	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.
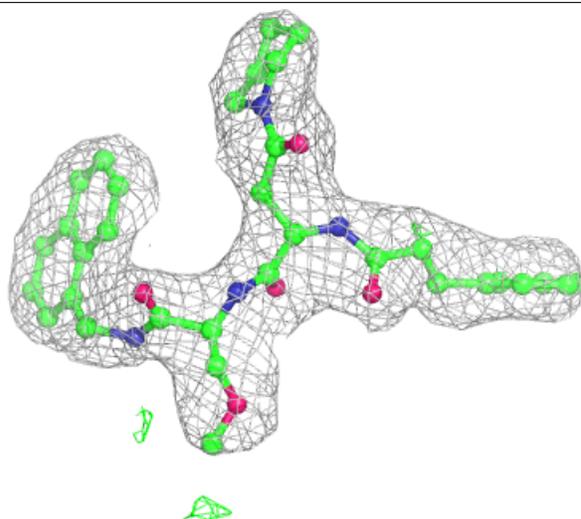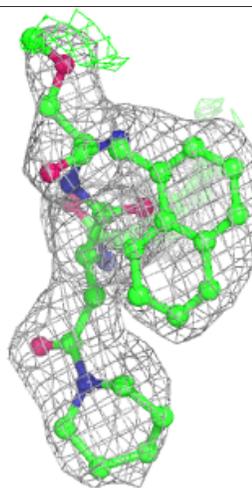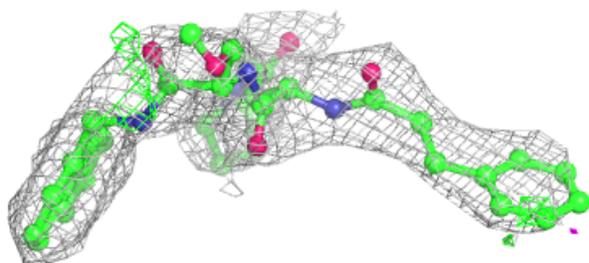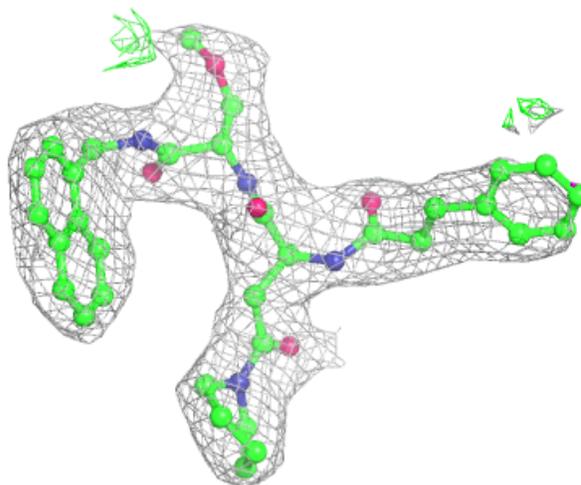

Electron density around 7J0 K 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
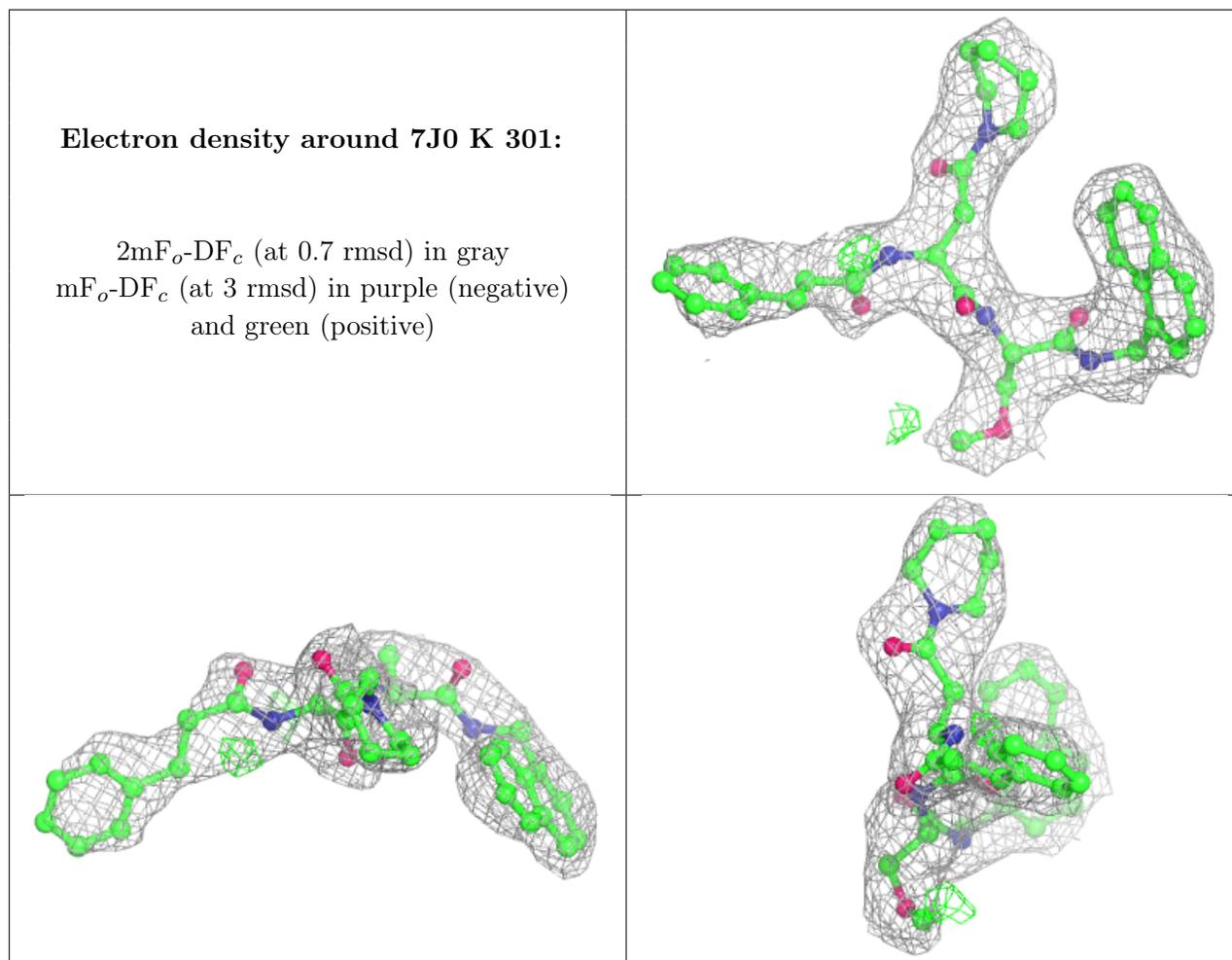
Electron density around 7J0 M 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
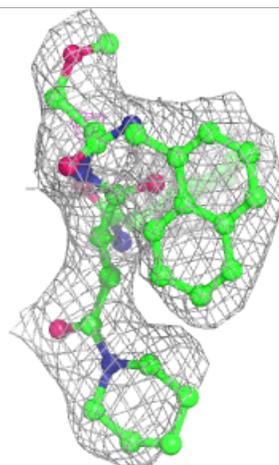and green (positive)
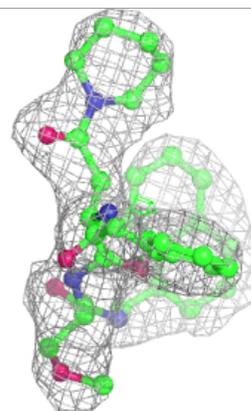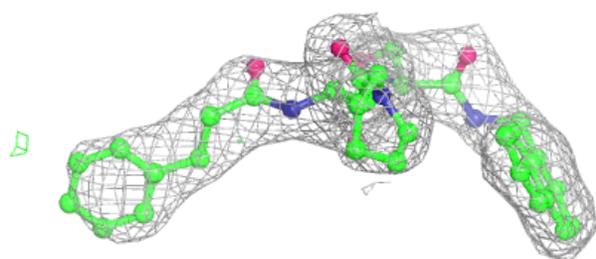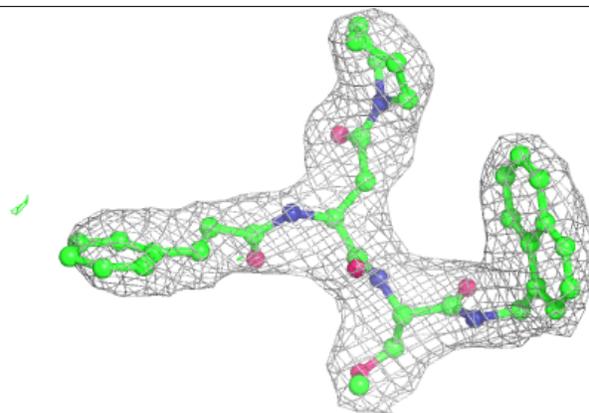
Electron density around 7J0 N 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
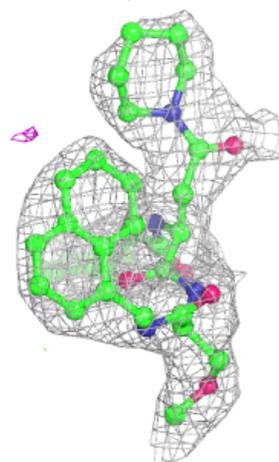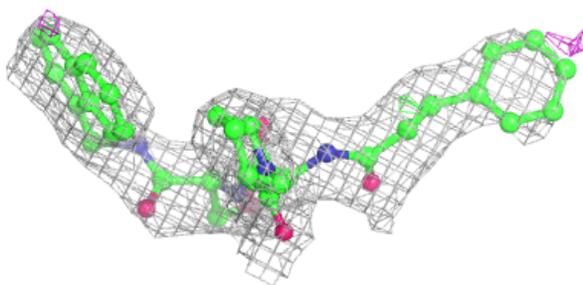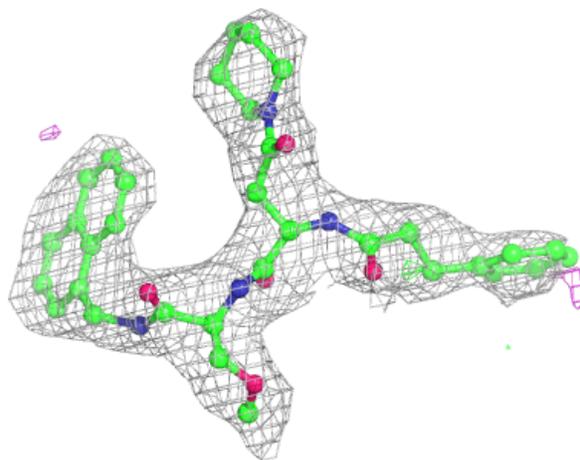
Electron density around 7J0 H 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
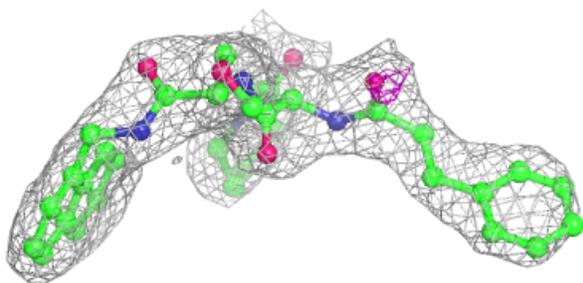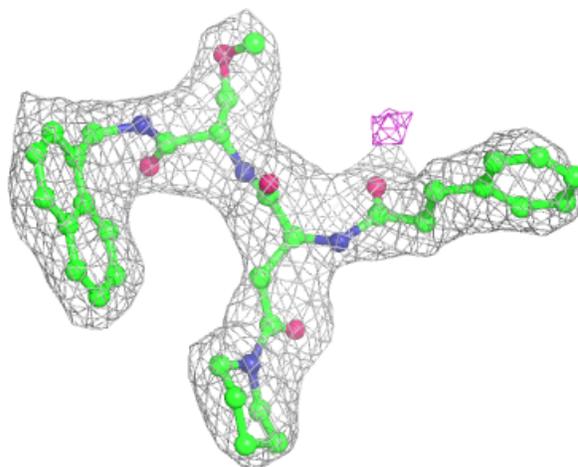and green (positive)
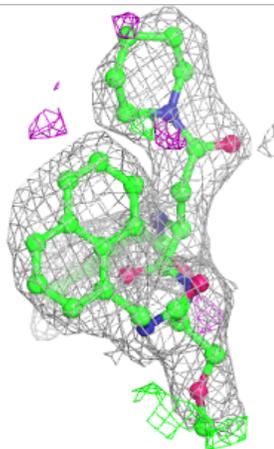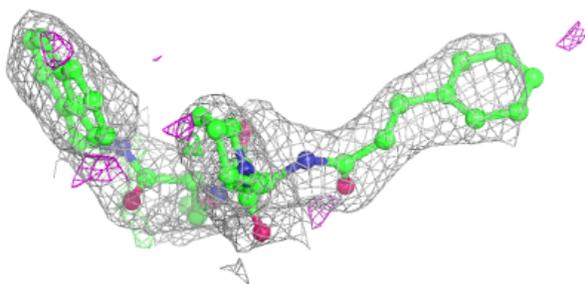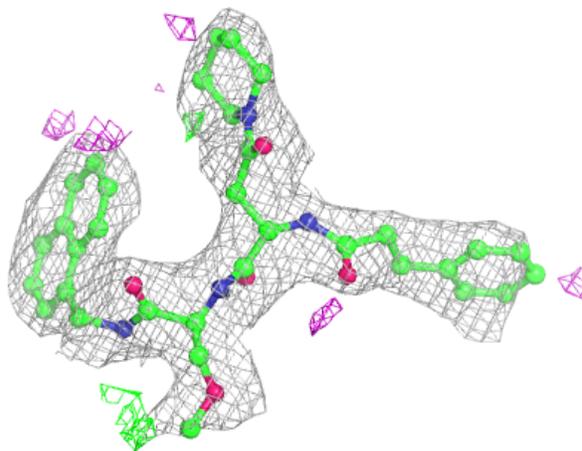
Electron density around 7J0 L 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
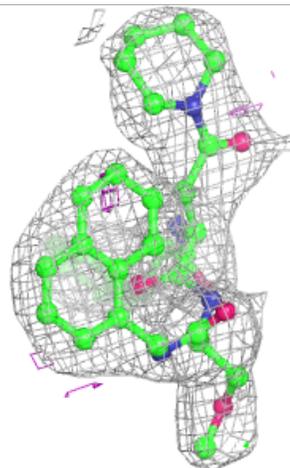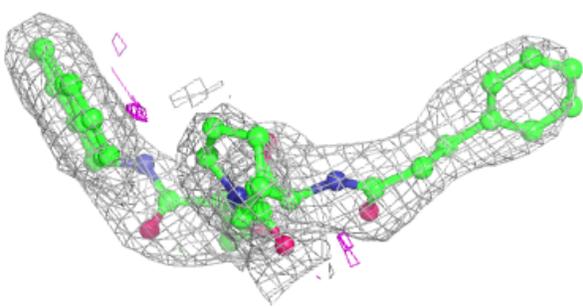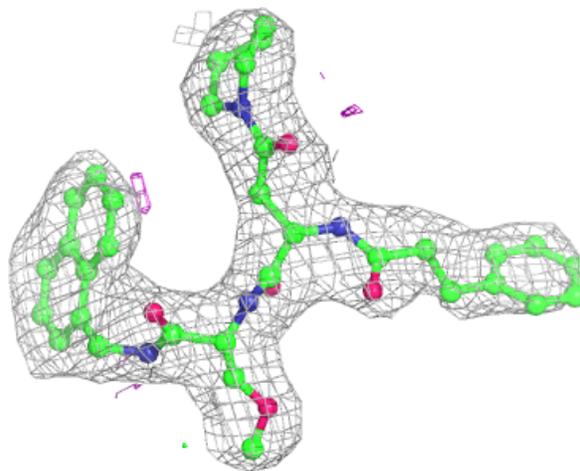
Electron density around 7J0 I 301:

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$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
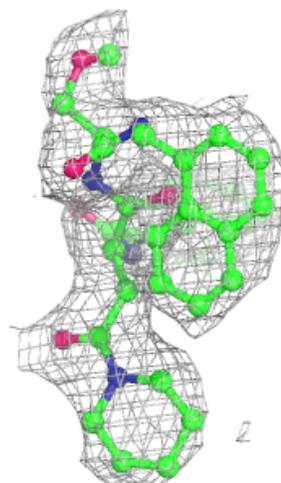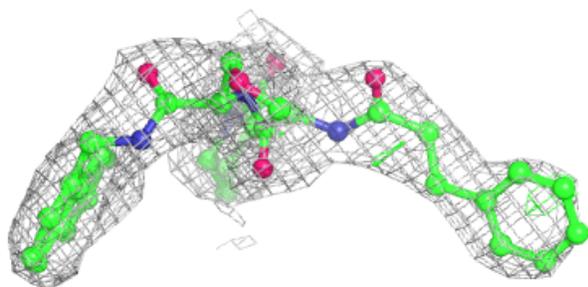and green (positive)
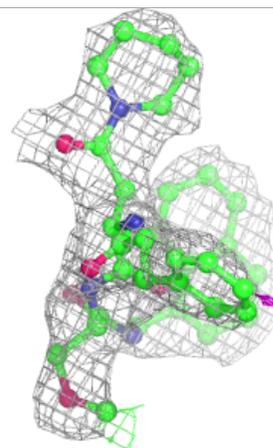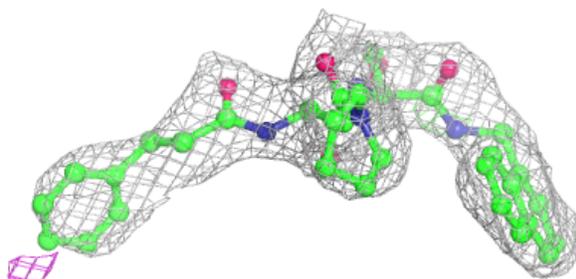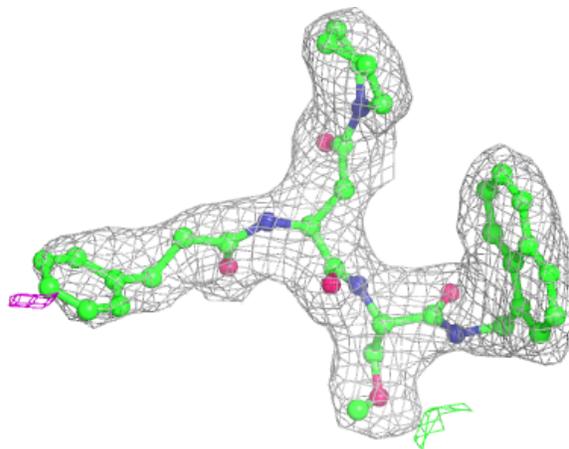
Electron density around 7J0 J 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
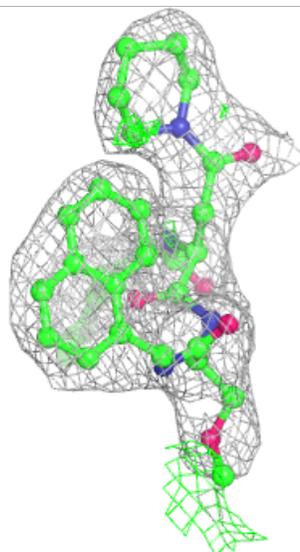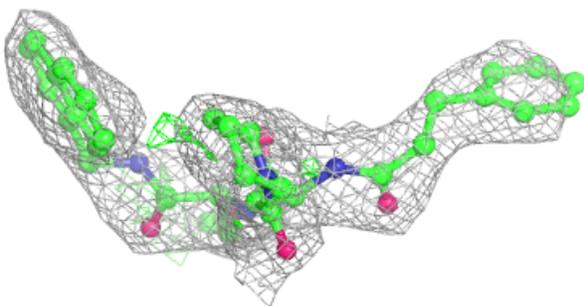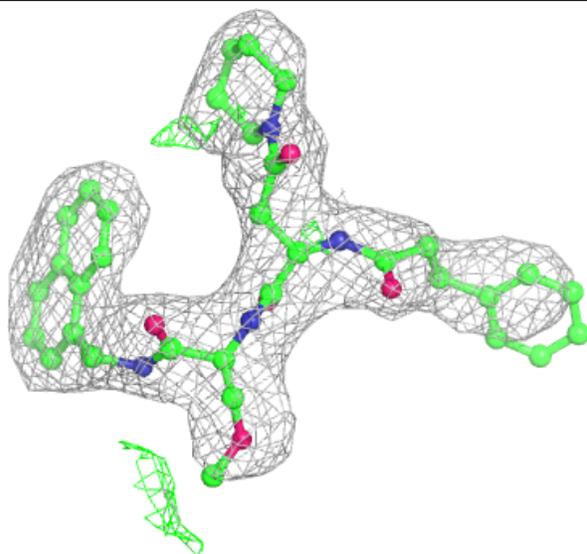
Electron density around 7J0 V 301:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
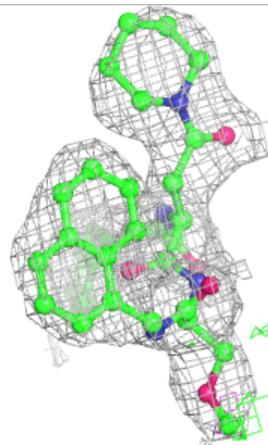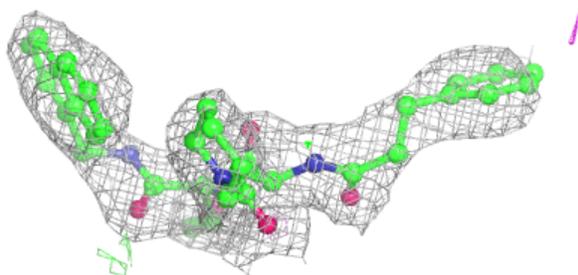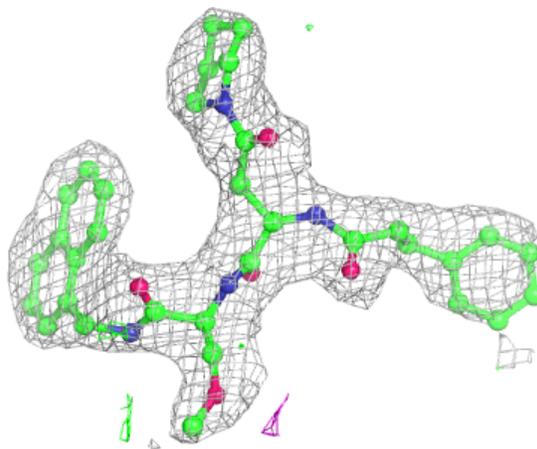
Electron density around 7J0 W 301:

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$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
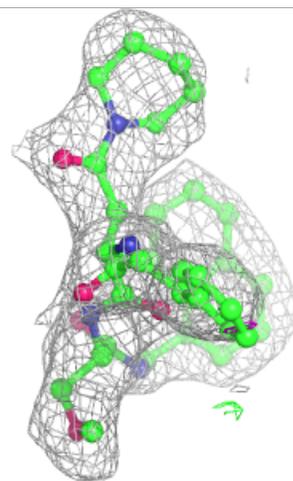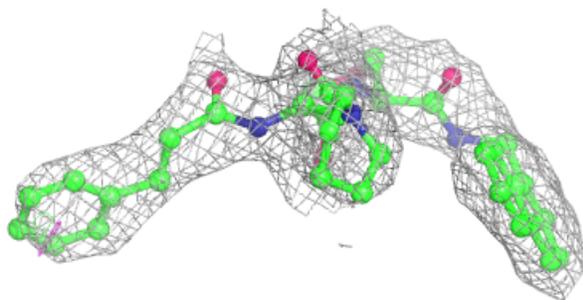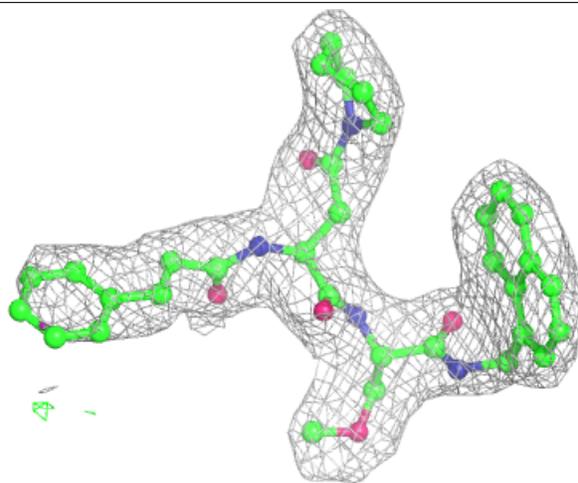
Electron density around 7J0 X 301:

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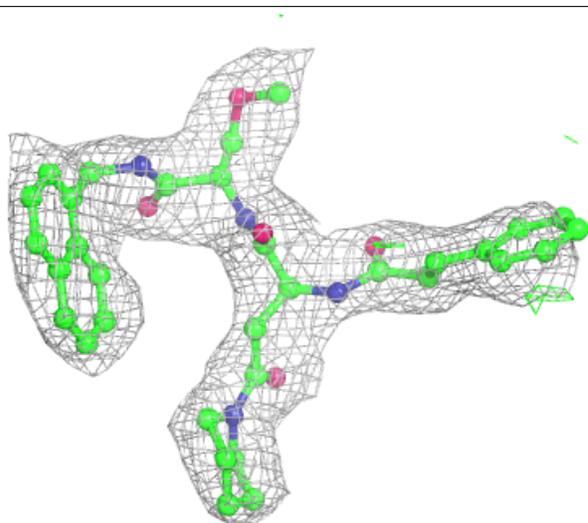and green (positive)
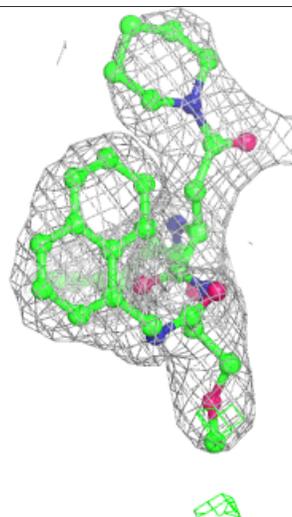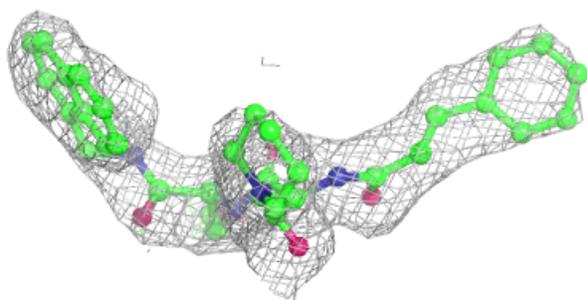
Electron density around 7J0 Y 301:

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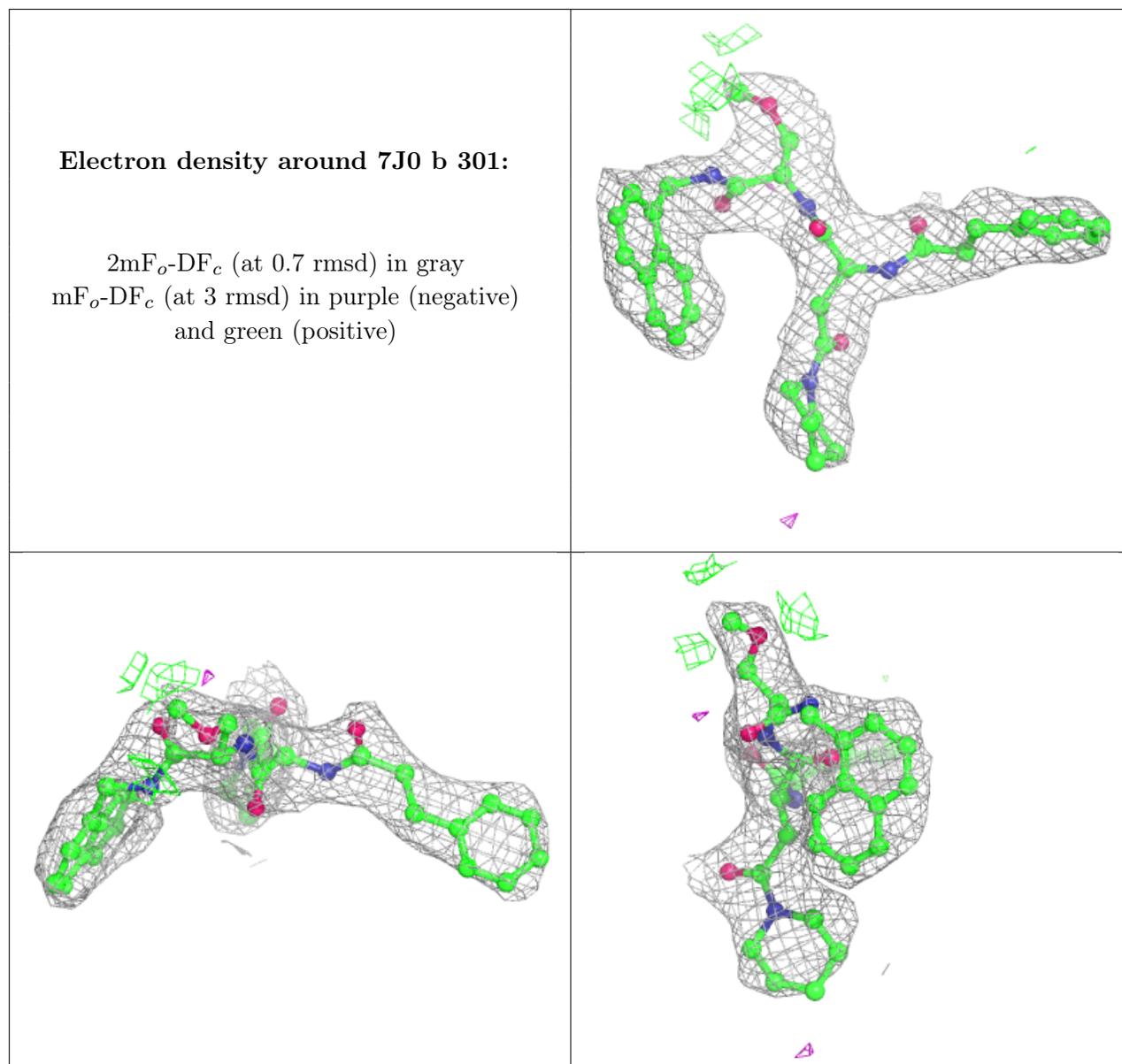and green (positive)

Electron density around 7J0 Z 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 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 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)

6.5 Other polymers ⓘ

There are no such residues in this entry.