



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 06:02 pm BST

PDB ID : 3UN4  
Title : Yeast 20S proteasome in complex with PR-957 (morpholine)  
Authors : Huber, E.; Basler, M.; Schwab, R.; Heinemeyer, W.; Kirk, C.; Groettrup, M.; Groll, M.  
Deposited on : 2011-11-15  
Resolution : 3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

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

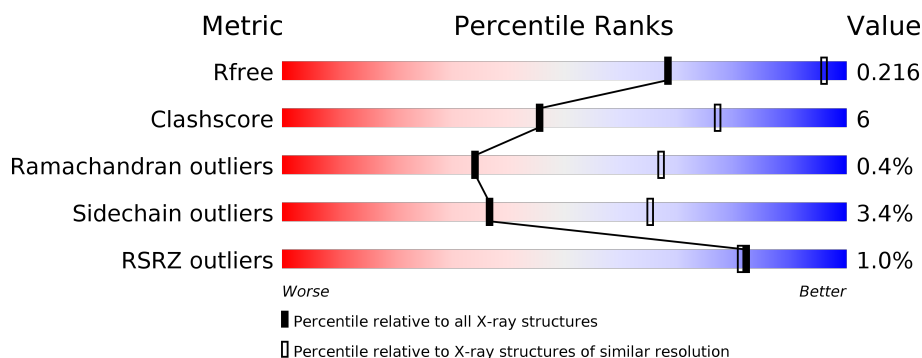
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	250	<div> <div>88%</div> <div>12%</div> </div>
1	O	250	<div> <div>%</div> <div>87%</div> <div>13%</div> </div>
2	B	258	<div> <div>75%</div> <div>18%</div> <div>• 5%</div> </div>
2	P	258	<div> <div>%</div> <div>75%</div> <div>18%</div> <div>• 5%</div> </div>
3	C	254	<div> <div>%</div> <div>72%</div> <div>20%</div> <div>• 5%</div> </div>
3	Q	254	<div> <div>2%</div> <div>74%</div> <div>19%</div> <div>• 5%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	233	
13	a	233	
14	N	196	
14	b	196	

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 51112 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 component Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			
2	P	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			

- Molecule 3 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			
4	R	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			

- Molecule 5 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
5	S	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			
6	T	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			

- Molecule 7 is a protein called Proteasome component C7-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
7	U	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

- Molecule 8 is a protein called Proteasome component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			

- Molecule 9 is a protein called Proteasome component PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome component C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- Molecule 11 is a protein called Proteasome component PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

- Molecule 12 is a protein called Proteasome component C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

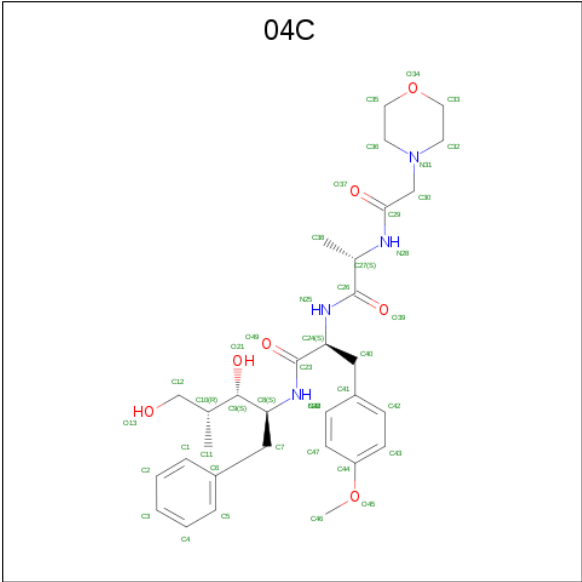
- Molecule 13 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	a	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome component PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	b	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is 1,2,4-trideoxy-4-methyl-2-{[N-(morpholin-4-ylacetyl)-L-alanyl-O-methyl-L-tyrosyl]amino}-1-phenyl-D-xylitol (three-letter code: 04C) (formula: C<sub>31</sub>H<sub>44</sub>N<sub>4</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	H	1	Total	C	N	O	0	0
			42	31	4	7		
15	K	1	Total	C	N	O	0	0
			42	31	4	7		
15	N	1	Total	C	N	O	0	0
			42	31	4	7		
15	V	1	Total	C	N	O	0	0
			42	31	4	7		
15	Y	1	Total	C	N	O	0	0
			42	31	4	7		
15	b	1	Total	C	N	O	0	0
			42	31	4	7		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	56	Total	O	0	0
			56	56		
16	B	38	Total	O	0	0
			38	38		
16	C	42	Total	O	0	0
			42	42		
16	D	38	Total	O	0	0
			38	38		
16	E	23	Total	O	0	0
			23	23		
16	F	48	Total	O	0	0
			48	48		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	61	Total O 61 61	0	0
16	H	49	Total O 49 49	0	0
16	I	62	Total O 62 62	0	0
16	J	54	Total O 54 54	0	0
16	K	46	Total O 46 46	0	0
16	L	55	Total O 55 55	0	0
16	M	72	Total O 72 72	0	0
16	N	51	Total O 51 51	0	0
16	O	32	Total O 32 32	0	0
16	P	30	Total O 30 30	0	0
16	Q	30	Total O 30 30	0	0
16	R	27	Total O 27 27	0	0
16	S	20	Total O 20 20	0	0
16	T	41	Total O 41 41	0	0
16	U	61	Total O 61 61	0	0
16	V	45	Total O 45 45	0	0
16	W	57	Total O 57 57	0	0
16	X	52	Total O 52 52	0	0
16	Y	49	Total O 49 49	0	0
16	Z	50	Total O 50 50	0	0
16	a	75	Total O 75 75	0	0

*Continued on next page...*




*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	b	58	Total	O	0	0
			58	58		

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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.

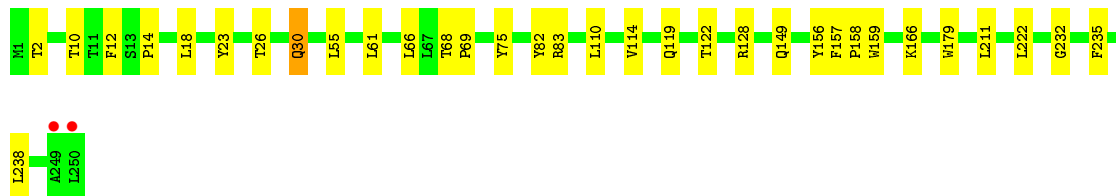
- Molecule 1: Proteasome component Y7

Chain A: 




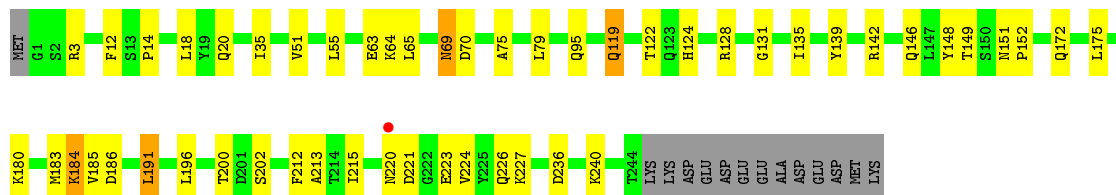
- Molecule 1: Proteasome component Y7

Chain O: 




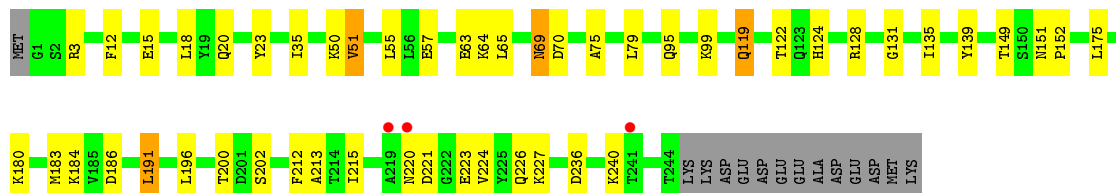
- Molecule 2: Proteasome component Y13

Chain B: 

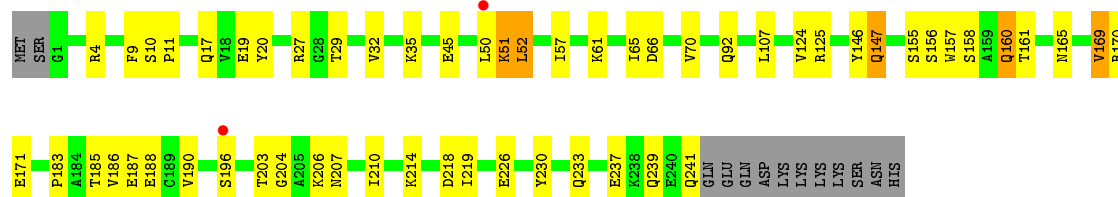
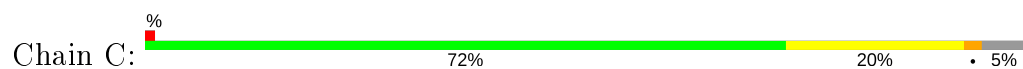


- Molecule 2: Proteasome component Y13

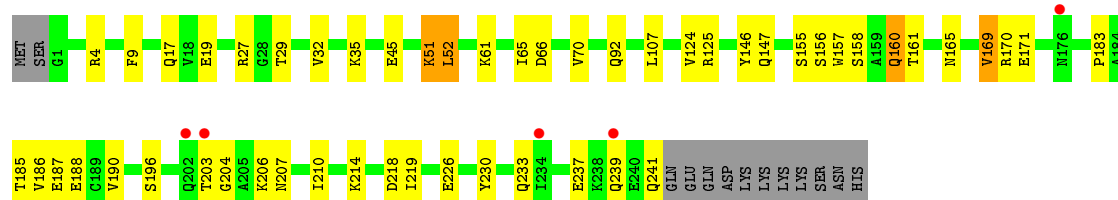
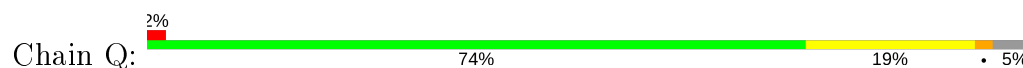
Chain P: 



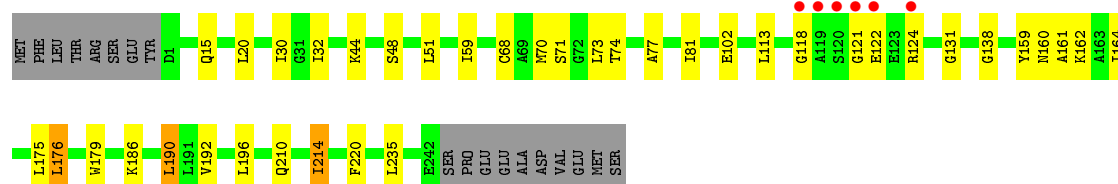
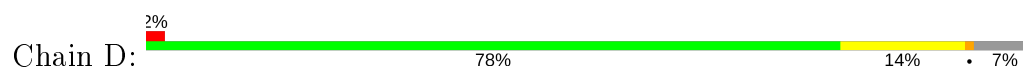
- Molecule 3: Proteasome component PRE6



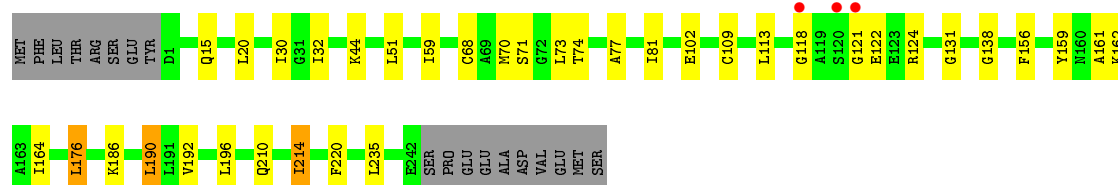
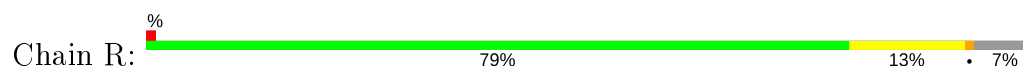
- Molecule 3: Proteasome component PRE6



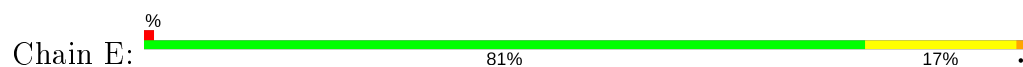
- Molecule 4: Proteasome component PUP2



- Molecule 4: Proteasome component PUP2

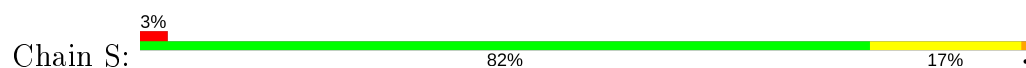


- Molecule 5: Proteasome component PRE5

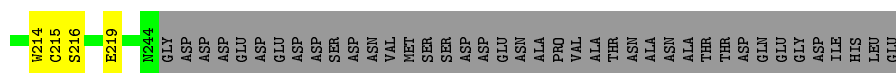
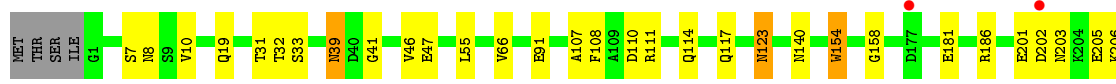
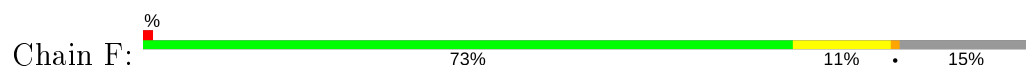




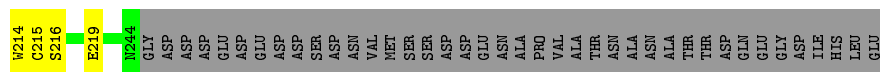
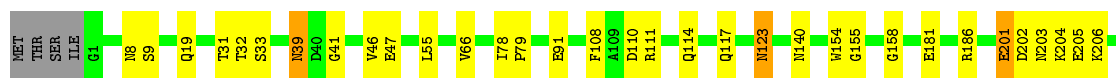
• Molecule 5: Proteasome component PRE5



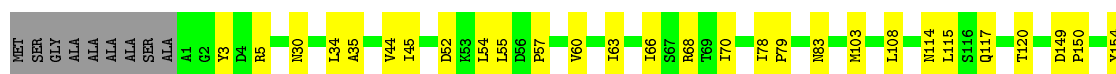
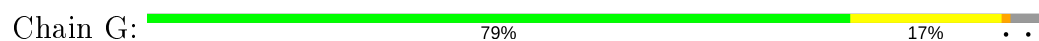
• Molecule 6: Proteasome component C1



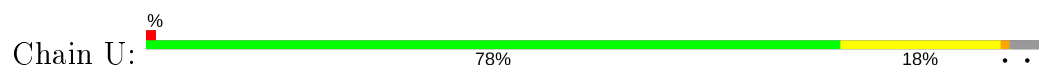
• Molecule 6: Proteasome component C1

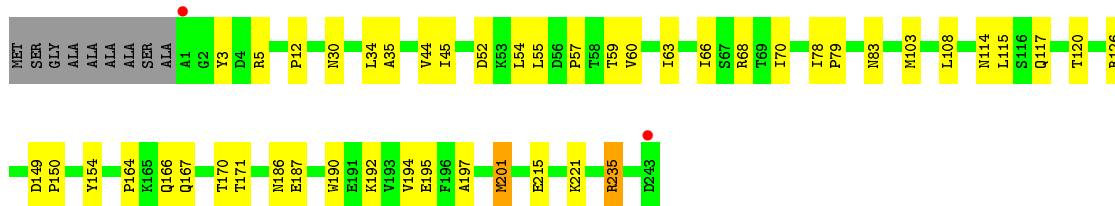


• Molecule 7: Proteasome component C7-alpha



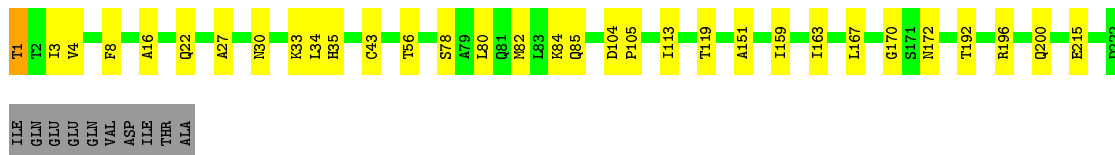
• Molecule 7: Proteasome component C7-alpha





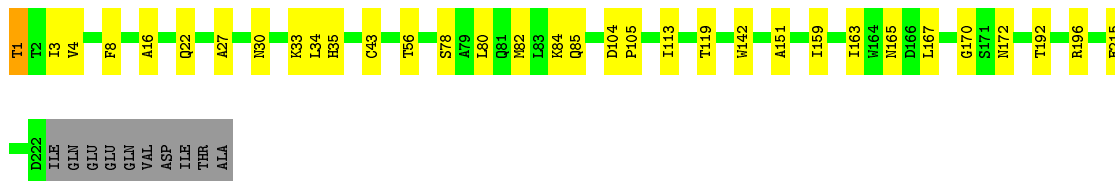
• Molecule 8: Proteasome component PUP1

Chain H: 82% 13% •



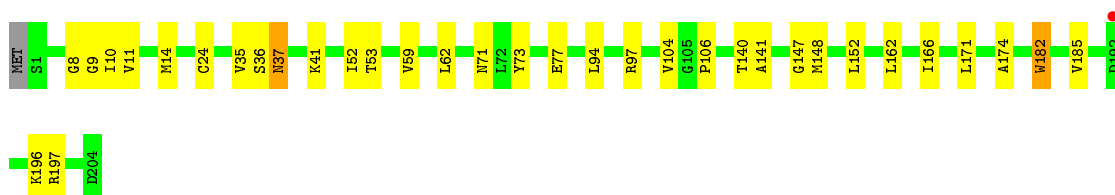
• Molecule 8: Proteasome component PUP1

Chain V: 81% 14% •



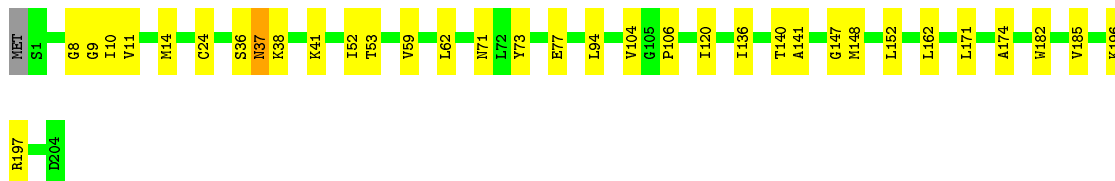
• Molecule 9: Proteasome component PUP3

Chain I: 83% 16% •

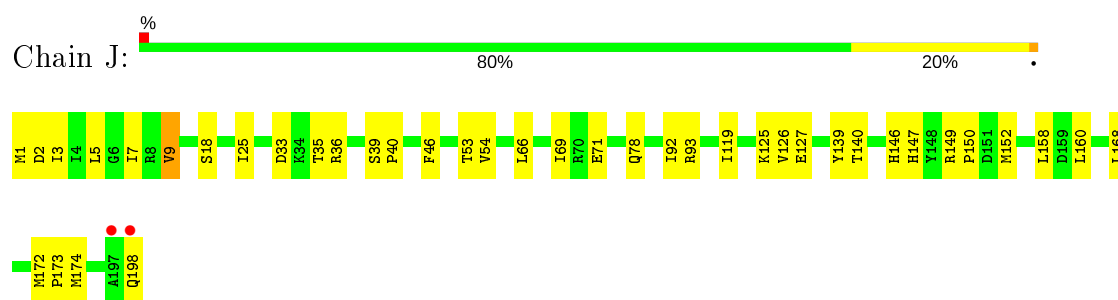


• Molecule 9: Proteasome component PUP3

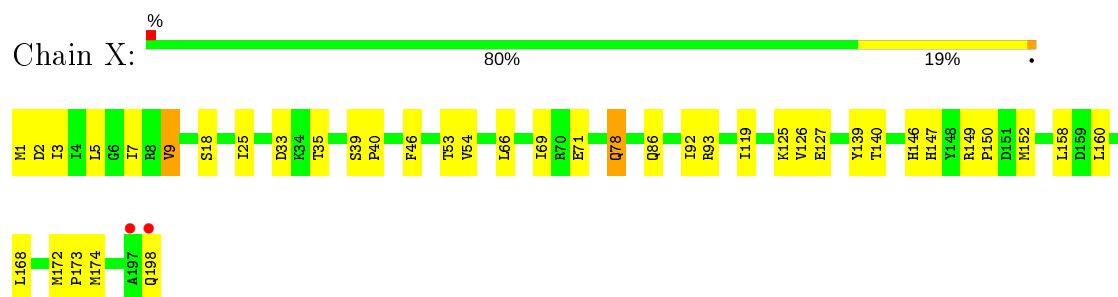
Chain W: 83% 16%



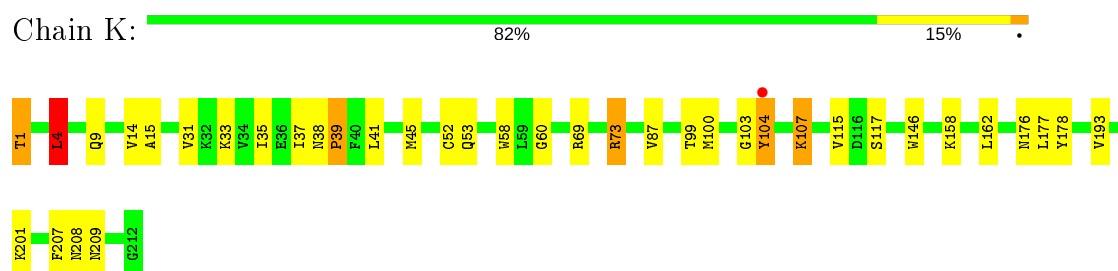
• Molecule 10: Proteasome component C11



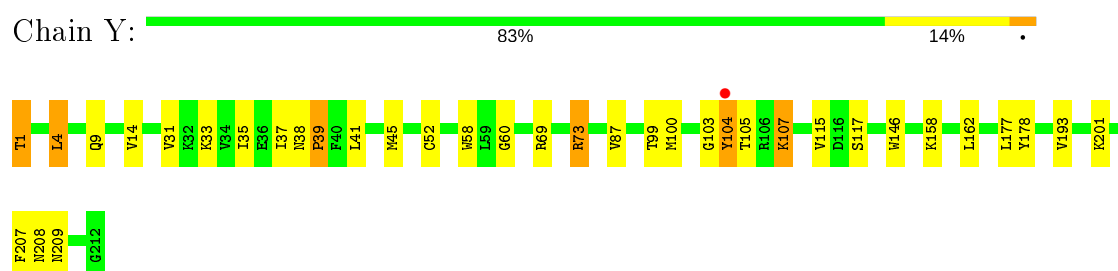
- Molecule 10: Proteasome component C11



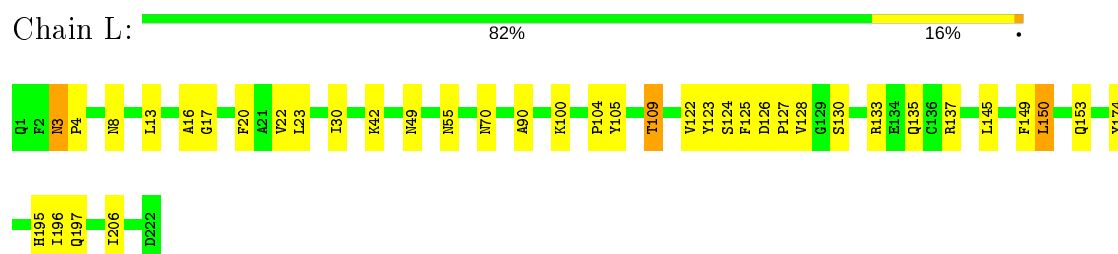
- Molecule 11: Proteasome component PRE2



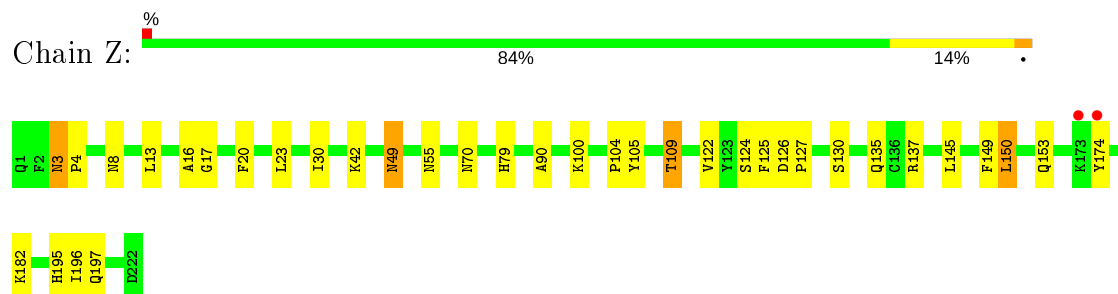
- Molecule 11: Proteasome component PRE2



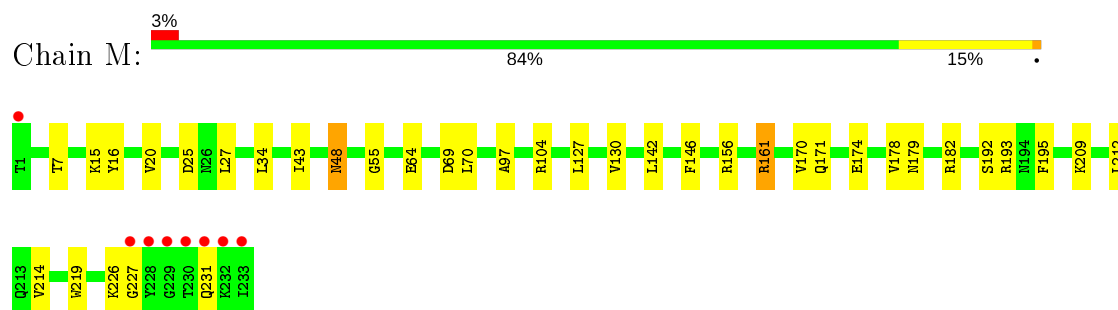
- Molecule 12: Proteasome component C5



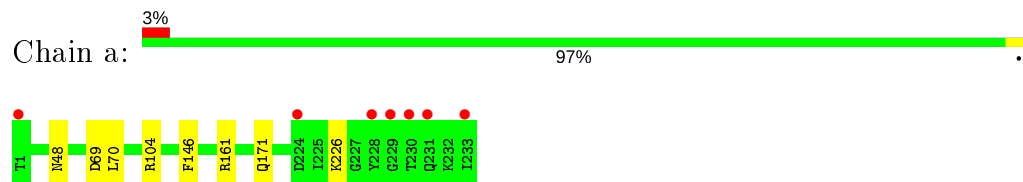
- Molecule 12: Proteasome component C5



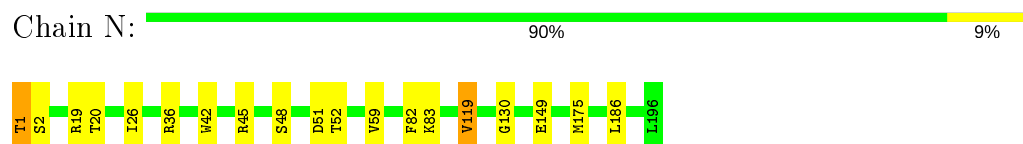
- Molecule 13: Proteasome component PRE4



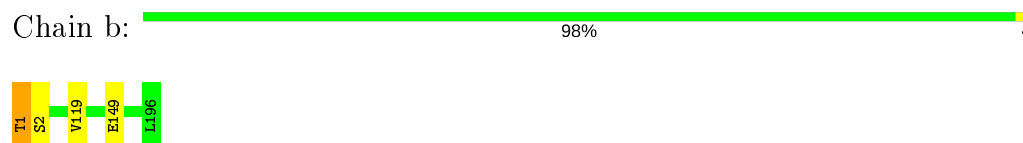
- Molecule 13: Proteasome component PRE4



- Molecule 14: Proteasome component PRE3



- Molecule 14: Proteasome component PRE3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.41Å 300.78Å 143.82Å 90.00° 112.75° 90.00°	Depositor
Resolution (Å)	15.00 – 3.40 49.31 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.3 (15.00-3.40) 98.3 (49.31-3.40)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.67 (at 3.40Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.179 , 0.219 0.176 , 0.216	Depositor DCC
$R_{free}$ test set	7082 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.8	Xtriage
Anisotropy	0.786	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 64.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	51112	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 04C

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	0.36	2/1952 (0.1%)	0.48	0/2642
1	O	0.36	2/1952 (0.1%)	0.48	0/2642
2	B	0.33	0/1934	0.48	0/2618
2	P	0.33	0/1934	0.48	0/2618
3	C	0.34	0/1919	0.49	0/2598
3	Q	0.33	0/1919	0.49	0/2598
4	D	0.36	0/1886	0.50	0/2541
4	R	0.35	0/1886	0.50	0/2541
5	E	0.31	0/1823	0.48	0/2463
5	S	0.30	0/1823	0.48	0/2463
6	F	0.41	1/1936 (0.1%)	0.47	0/2614
6	T	0.40	0/1936	0.47	0/2614
7	G	0.34	0/1959	0.48	0/2652
7	U	0.34	0/1959	0.48	0/2652
8	H	0.46	1/1715 (0.1%)	0.48	0/2326
8	V	0.46	2/1715 (0.1%)	0.49	0/2326
9	I	0.35	1/1611 (0.1%)	0.49	0/2174
9	W	0.34	0/1611	0.49	0/2174
10	J	0.31	0/1613	0.48	0/2173
10	X	0.31	0/1613	0.48	0/2173
11	K	0.52	3/1681 (0.2%)	0.52	1/2274 (0.0%)
11	Y	0.52	3/1681 (0.2%)	0.52	1/2274 (0.0%)
12	L	0.36	0/1795	0.50	0/2420
12	Z	0.36	0/1795	0.50	0/2420
13	M	0.36	1/1855 (0.1%)	0.50	0/2514
13	a	0.36	0/1855	0.50	0/2514
14	N	0.43	1/1541 (0.1%)	0.49	1/2087 (0.0%)
14	b	0.43	1/1541 (0.1%)	0.51	1/2087 (0.0%)
All	All	0.38	18/50440 (0.0%)	0.49	4/68192 (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
14	b	0	1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1	THR	C-N	6.64	1.49	1.34
14	N	1	THR	C-N	6.25	1.48	1.34
8	V	1	THR	C-N	5.61	1.47	1.34
11	K	1	THR	C-N	5.37	1.46	1.34
8	H	1	THR	C-N	5.34	1.46	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	1	THR	N-CA-C	6.01	127.24	111.00
11	Y	4	LEU	CA-CB-CG	5.22	127.30	115.30
11	K	4	LEU	CA-CB-CG	5.21	127.27	115.30
14	N	1	THR	N-CA-C	5.11	124.79	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	b	1	THR	Mainchain

## 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	1915	0	1929	17	0
1	O	1915	0	1929	20	0
2	B	1904	0	1904	33	0
2	P	1904	0	1904	31	0
3	C	1890	0	1903	40	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	1890	0	1903	34	0
4	D	1861	0	1839	19	0
4	R	1861	0	1839	20	0
5	E	1795	0	1800	31	0
5	S	1795	0	1800	30	0
6	F	1896	0	1889	21	0
6	T	1896	0	1889	22	0
7	G	1921	0	1913	25	0
7	U	1921	0	1913	30	0
8	H	1684	0	1686	18	0
8	V	1684	0	1686	18	0
9	I	1581	0	1574	25	0
9	W	1581	0	1574	23	0
10	J	1585	0	1590	41	0
10	X	1585	0	1590	38	0
11	K	1644	0	1593	24	0
11	Y	1644	0	1593	20	0
12	L	1757	0	1711	28	0
12	Z	1757	0	1711	29	0
13	M	1824	0	1832	24	0
13	a	1824	0	1832	0	0
14	N	1512	0	1479	11	0
14	b	1512	0	1479	0	0
15	H	42	0	42	0	0
15	K	42	0	42	4	0
15	N	42	0	42	4	0
15	V	42	0	42	0	0
15	Y	42	0	42	2	0
15	b	42	0	42	0	0
16	A	56	0	0	0	0
16	B	38	0	0	1	0
16	C	42	0	0	0	0
16	D	38	0	0	0	0
16	E	23	0	0	0	0
16	F	48	0	0	0	0
16	G	61	0	0	0	0
16	H	49	0	0	0	0
16	I	62	0	0	1	0
16	J	54	0	0	3	0
16	K	46	0	0	0	0
16	L	55	0	0	0	0
16	M	72	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	N	51	0	0	0	0
16	O	32	0	0	0	0
16	P	30	0	0	0	0
16	Q	30	0	0	0	0
16	R	27	0	0	2	0
16	S	20	0	0	0	0
16	T	41	0	0	0	0
16	U	61	0	0	0	0
16	V	45	0	0	0	0
16	W	57	0	0	0	0
16	X	52	0	0	3	0
16	Y	49	0	0	0	0
16	Z	50	0	0	0	0
16	a	75	0	0	0	0
16	b	58	0	0	0	0
All	All	51112	0	49536	582	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 582 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)
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.13	0.91
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.19	0.91
11:K:209:ASN:HB3	16:X:234:HOH:O	1.77	0.85
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.63	0.80
1:O:12:PHE:H	2:P:20:GLN:HE22	1.27	0.80

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	239 (96%)	7 (3%)	2 (1%)	19	51
1	O	248/250 (99%)	239 (96%)	7 (3%)	2 (1%)	19	51
2	B	242/258 (94%)	230 (95%)	10 (4%)	2 (1%)	19	51
2	P	242/258 (94%)	231 (96%)	9 (4%)	2 (1%)	19	51
3	C	239/254 (94%)	227 (95%)	9 (4%)	3 (1%)	12	39
3	Q	239/254 (94%)	227 (95%)	9 (4%)	3 (1%)	12	39
4	D	240/260 (92%)	230 (96%)	7 (3%)	3 (1%)	12	39
4	R	240/260 (92%)	230 (96%)	7 (3%)	3 (1%)	12	39
5	E	231/234 (99%)	218 (94%)	12 (5%)	1 (0%)	34	67
5	S	231/234 (99%)	218 (94%)	12 (5%)	1 (0%)	34	67
6	F	242/288 (84%)	232 (96%)	10 (4%)	0	100	100
6	T	242/288 (84%)	232 (96%)	10 (4%)	0	100	100
7	G	241/252 (96%)	232 (96%)	9 (4%)	0	100	100
7	U	241/252 (96%)	231 (96%)	10 (4%)	0	100	100
8	H	220/232 (95%)	212 (96%)	8 (4%)	0	100	100
8	V	220/232 (95%)	210 (96%)	10 (4%)	0	100	100
9	I	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	196/198 (99%)	187 (95%)	8 (4%)	1 (0%)	29	61
10	X	196/198 (99%)	187 (95%)	8 (4%)	1 (0%)	29	61
11	K	210/212 (99%)	202 (96%)	7 (3%)	1 (0%)	29	61
11	Y	210/212 (99%)	201 (96%)	8 (4%)	1 (0%)	29	61
12	L	220/222 (99%)	210 (96%)	10 (4%)	0	100	100
12	Z	220/222 (99%)	210 (96%)	10 (4%)	0	100	100
13	M	231/233 (99%)	221 (96%)	10 (4%)	0	100	100
13	a	231/233 (99%)	221 (96%)	10 (4%)	0	100	100
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	186 (96%)	7 (4%)	1 (0%)	29	61
All	All	6312/6588 (96%)	6042 (96%)	243 (4%)	27 (0%)	34	67

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	52	LEU
3	Q	52	LEU
1	A	166	LYS
3	C	203	THR
4	D	122	GLU

### 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	209/209 (100%)	206 (99%)	3 (1%)	67	83
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	83
2	B	203/216 (94%)	193 (95%)	10 (5%)	25	55
2	P	203/216 (94%)	193 (95%)	10 (5%)	25	55
3	C	213/226 (94%)	204 (96%)	9 (4%)	30	59
3	Q	213/226 (94%)	204 (96%)	9 (4%)	30	59
4	D	198/215 (92%)	190 (96%)	8 (4%)	31	60
4	R	198/215 (92%)	190 (96%)	8 (4%)	31	60
5	E	192/193 (100%)	183 (95%)	9 (5%)	26	57
5	S	192/193 (100%)	183 (95%)	9 (5%)	26	57
6	F	201/239 (84%)	191 (95%)	10 (5%)	24	54
6	T	201/239 (84%)	191 (95%)	10 (5%)	24	54
7	G	207/210 (99%)	198 (96%)	9 (4%)	29	59
7	U	207/210 (99%)	198 (96%)	9 (4%)	29	59
8	H	181/190 (95%)	177 (98%)	4 (2%)	52	75
8	V	181/190 (95%)	177 (98%)	4 (2%)	52	75
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	80
9	W	172/173 (99%)	169 (98%)	3 (2%)	60	80
10	J	175/175 (100%)	172 (98%)	3 (2%)	60	80
10	X	175/175 (100%)	172 (98%)	3 (2%)	60	80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	169/169 (100%)	161 (95%)	8 (5%)	26	57
11	Y	169/169 (100%)	161 (95%)	8 (5%)	26	57
12	L	185/185 (100%)	180 (97%)	5 (3%)	44	70
12	Z	185/185 (100%)	180 (97%)	5 (3%)	44	70
13	M	199/199 (100%)	191 (96%)	8 (4%)	31	60
13	a	199/199 (100%)	191 (96%)	8 (4%)	31	60
14	N	162/162 (100%)	160 (99%)	2 (1%)	71	85
14	b	162/162 (100%)	160 (99%)	2 (1%)	71	85
All	All	5332/5522 (97%)	5150 (97%)	182 (3%)	37	65

5 of 182 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	69	ASP
2	P	191	LEU
12	Z	23	LEU
13	M	104	ARG
1	O	61	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 179 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	48	ASN
3	Q	17	GLN
12	Z	158	ASN
13	M	171	GLN
1	O	30	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 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$
15	04C	H	301	8	44,44,44	1.33	3 (6%)	56,58,58	0.92	4 (7%)
15	04C	V	301	8	44,44,44	1.40	3 (6%)	56,58,58	0.85	3 (5%)
15	04C	K	301	11	44,44,44	1.25	2 (4%)	56,58,58	1.22	5 (8%)
15	04C	N	201	14	44,44,44	1.42	2 (4%)	56,58,58	1.19	3 (5%)
15	04C	Y	301	11	44,44,44	1.36	2 (4%)	56,58,58	1.13	3 (5%)
15	04C	b	201	14	44,44,44	1.49	5 (11%)	56,58,58	1.45	8 (14%)

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
15	04C	H	301	8	-	13/44/52/52	0/3/3/3
15	04C	V	301	8	-	15/44/52/52	0/3/3/3
15	04C	K	301	11	-	13/44/52/52	0/3/3/3
15	04C	N	201	14	-	15/44/52/52	0/3/3/3
15	04C	Y	301	11	-	14/44/52/52	0/3/3/3
15	04C	b	201	14	-	12/44/52/52	0/3/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Y	301	04C	C12-C10	4.42	1.57	1.52

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b	201	04C	C12-C10	4.15	1.57	1.52
15	b	201	04C	C10-C9	3.95	1.60	1.53
15	K	301	04C	C12-C10	3.88	1.57	1.52
15	N	201	04C	C10-C9	3.76	1.60	1.53

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	b	201	04C	C11-C10-C12	-5.44	102.74	109.88
15	N	201	04C	C11-C10-C12	-4.92	103.41	109.88
15	Y	301	04C	C6-C7-C8	4.34	120.88	113.33
15	K	301	04C	C11-C10-C12	-4.00	104.62	109.88
15	K	301	04C	C6-C7-C8	3.93	120.17	113.33

There are no chirality outliers.

5 of 82 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	H	301	04C	C6-C7-C8-N22
15	H	301	04C	C6-C7-C8-C9
15	V	301	04C	C6-C7-C8-C9
15	V	301	04C	C11-C10-C9-O21
15	K	301	04C	C9-C10-C12-O13

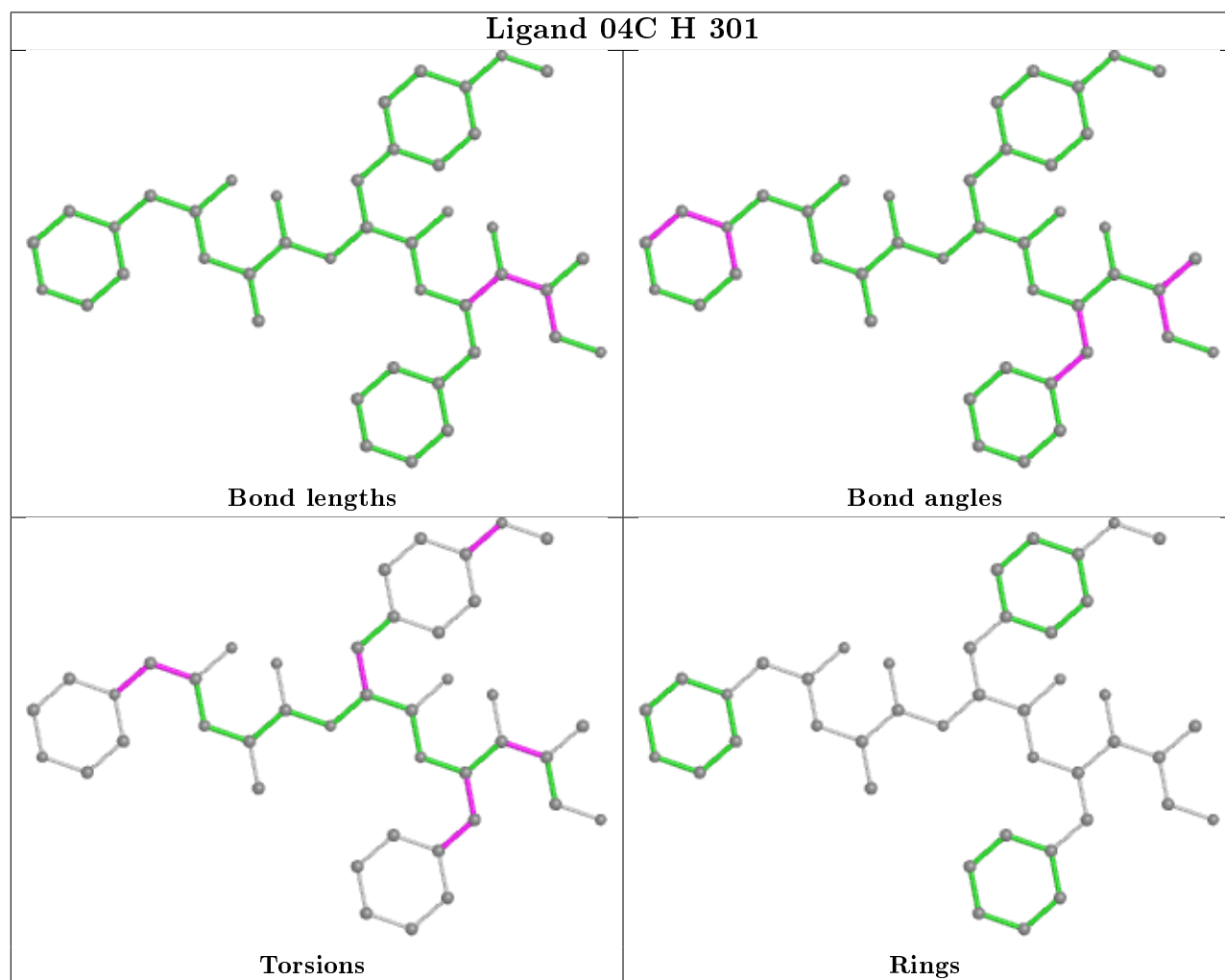
There are no ring outliers.

3 monomers are involved in 10 short contacts:

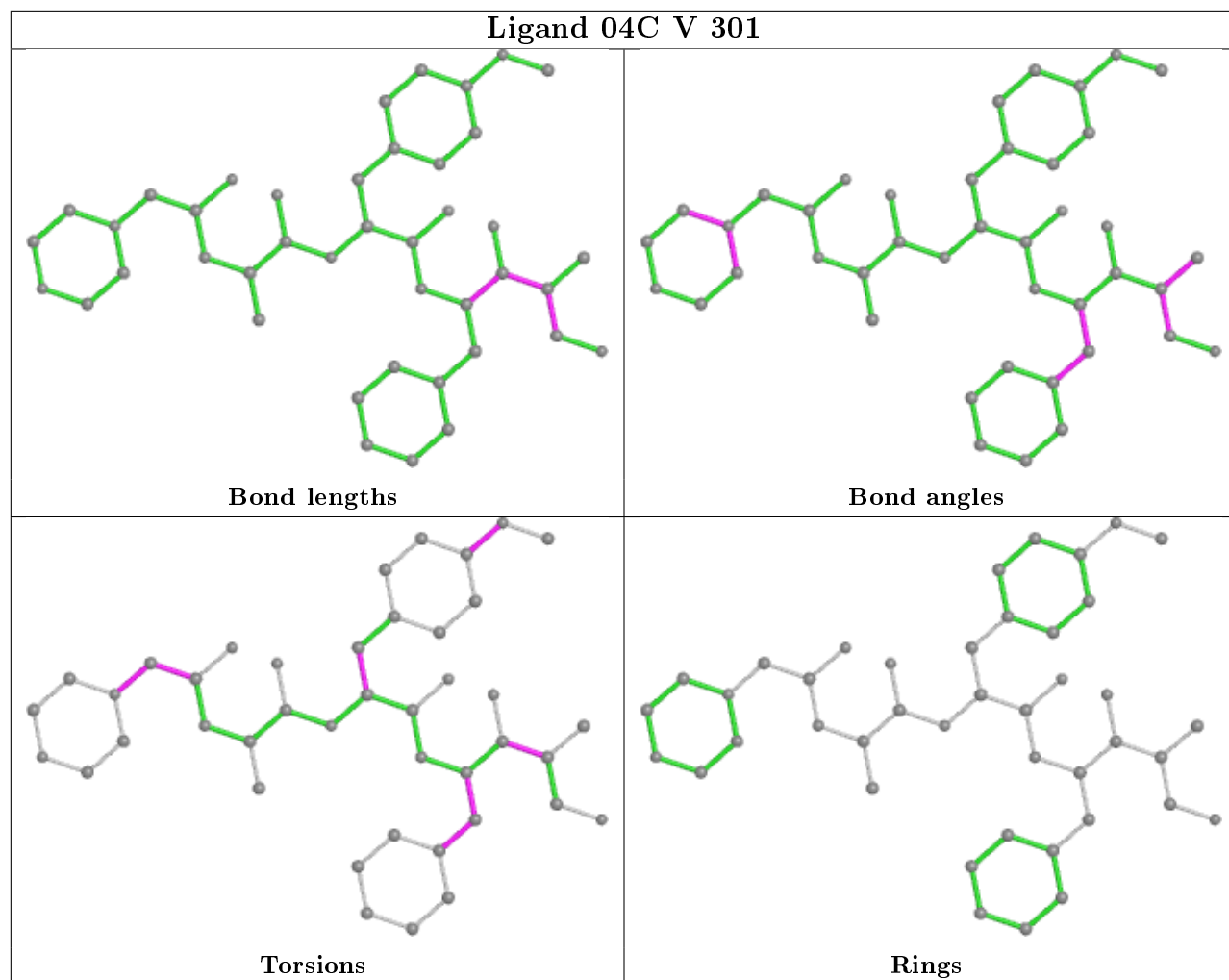
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	K	301	04C	4	0
15	N	201	04C	4	0
15	Y	301	04C	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

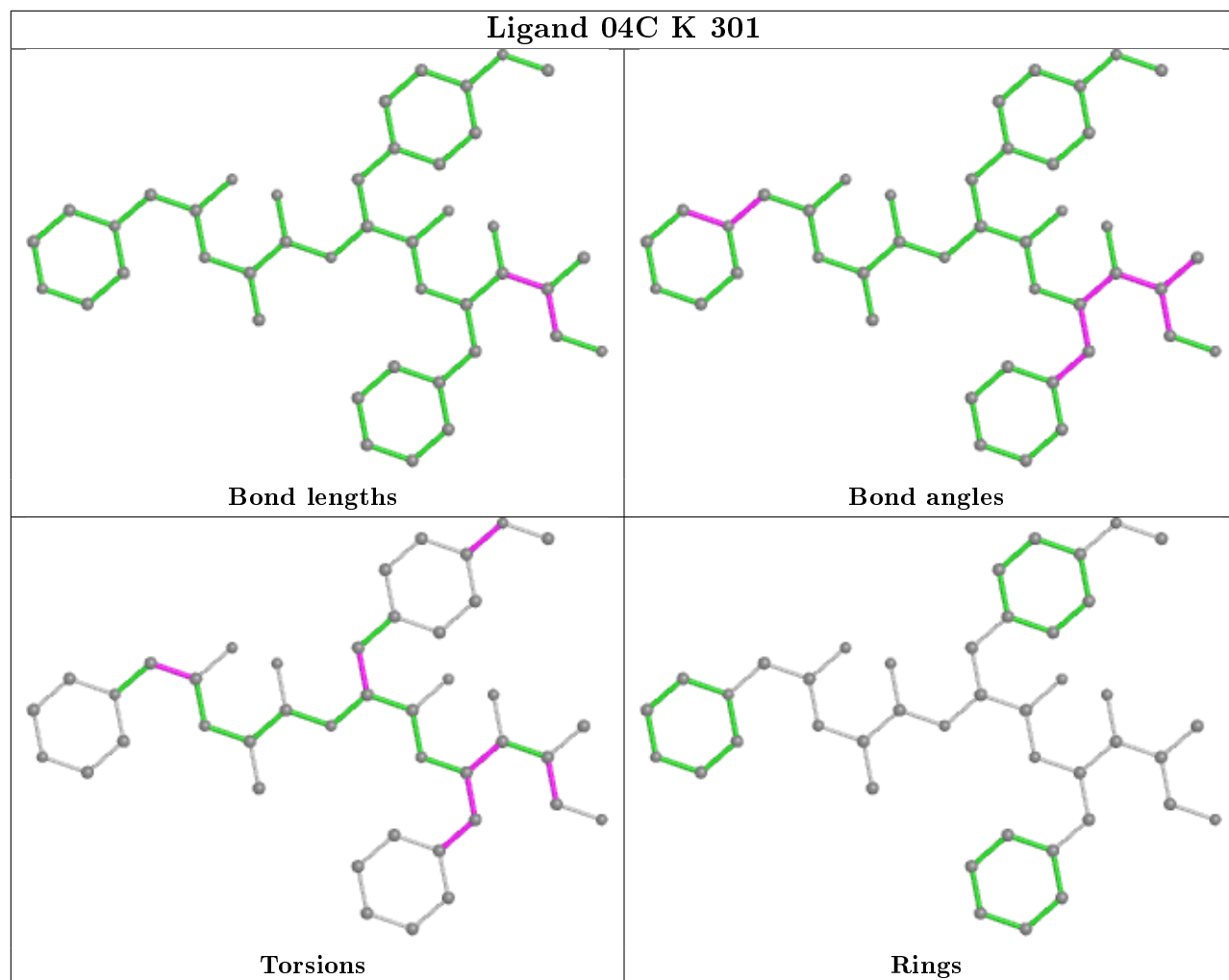
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



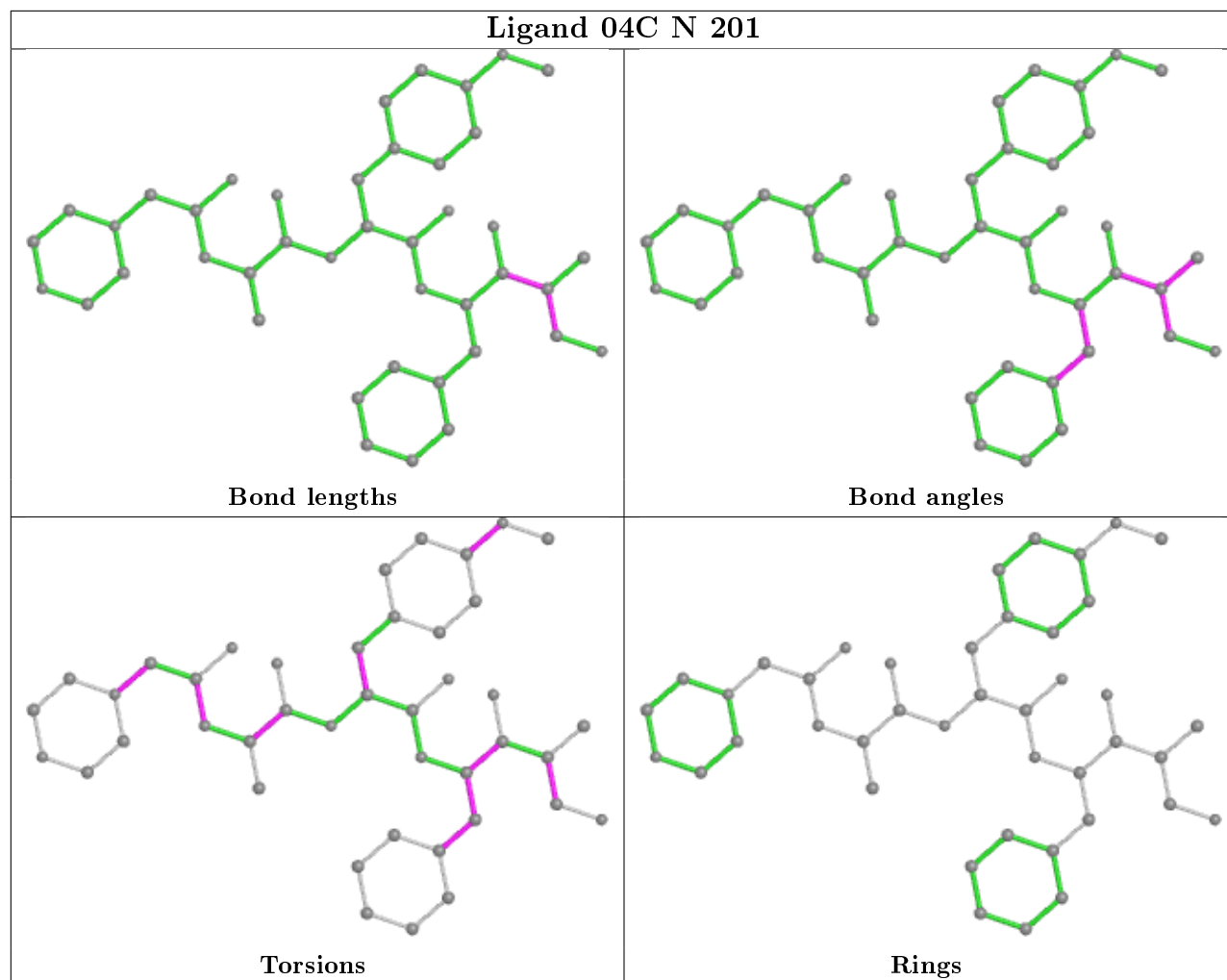
## Ligand 04C V 301



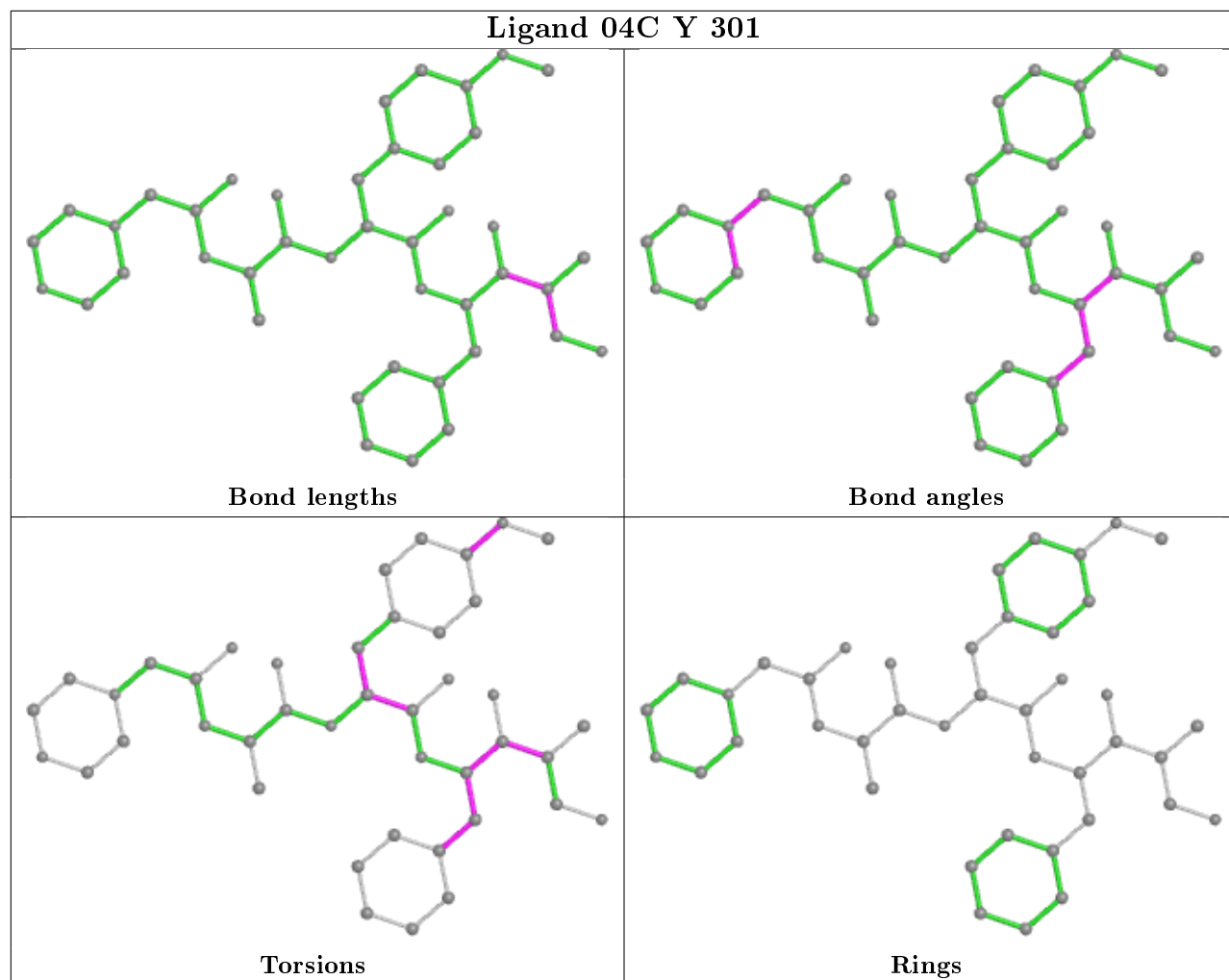
## Ligand 04C K 301

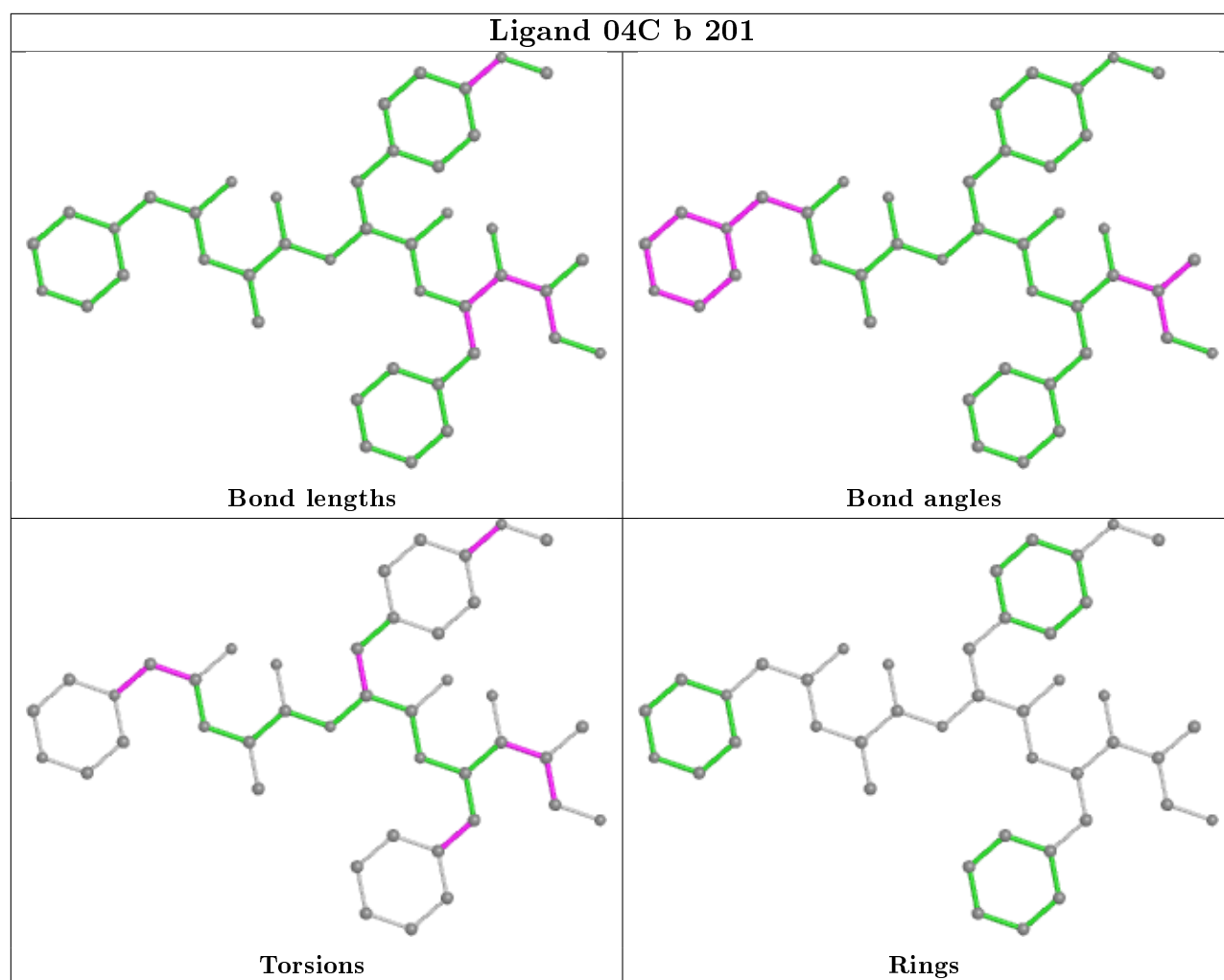


## Ligand 04C N 201



## Ligand 04C Y 301





## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	250/250 (100%)	-0.47	1 (0%) 92 92	46, 72, 111, 148	0
1	O	250/250 (100%)	-0.30	2 (0%) 86 85	59, 80, 119, 157	0
2	B	244/258 (94%)	-0.33	1 (0%) 92 92	54, 80, 132, 166	0
2	P	244/258 (94%)	-0.25	3 (1%) 79 77	55, 80, 123, 174	0
3	C	241/254 (94%)	-0.26	2 (0%) 86 85	50, 79, 133, 170	0
3	Q	241/254 (94%)	-0.03	5 (2%) 63 62	62, 94, 160, 208	0
4	D	242/260 (93%)	-0.33	6 (2%) 57 55	58, 82, 128, 160	0
4	R	242/260 (93%)	-0.27	3 (1%) 79 77	66, 92, 141, 182	0
5	E	233/234 (99%)	-0.13	3 (1%) 77 76	60, 88, 131, 155	0
5	S	233/234 (99%)	-0.02	7 (3%) 50 49	67, 98, 146, 184	0
6	F	244/288 (84%)	-0.36	2 (0%) 86 85	61, 83, 132, 154	0
6	T	244/288 (84%)	-0.26	0 100 100	63, 91, 142, 177	0
7	G	243/252 (96%)	-0.43	1 (0%) 92 92	53, 76, 118, 184	0
7	U	243/252 (96%)	-0.41	2 (0%) 86 85	59, 78, 113, 163	0
8	H	222/232 (95%)	-0.48	0 100 100	18, 70, 104, 147	0
8	V	222/232 (95%)	-0.50	0 100 100	10, 72, 105, 148	0
9	I	204/205 (99%)	-0.43	1 (0%) 91 90	43, 65, 96, 117	0
9	W	204/205 (99%)	-0.50	0 100 100	46, 64, 98, 117	0
10	J	198/198 (100%)	-0.45	2 (1%) 82 81	44, 64, 94, 164	0
10	X	198/198 (100%)	-0.43	2 (1%) 82 81	50, 67, 95, 168	0
11	K	212/212 (100%)	-0.41	1 (0%) 91 90	18, 65, 100, 116	0
11	Y	212/212 (100%)	-0.46	1 (0%) 91 90	14, 69, 102, 126	0
12	L	222/222 (100%)	-0.39	0 100 100	48, 69, 104, 134	0
12	Z	222/222 (100%)	-0.31	2 (0%) 84 83	50, 69, 106, 132	0

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/233 (100%)	-0.35	8 (3%) 45 44	49, 72, 107, 149	0
13	a	233/233 (100%)	-0.38	7 (3%) 50 49	47, 68, 100, 142	0
14	N	196/196 (100%)	-0.50	0 100 100	11, 66, 97, 117	0
14	b	196/196 (100%)	-0.50	0 100 100	6, 66, 96, 115	0
All	All	6368/6588 (96%)	-0.35	62 (0%) 82 81	6, 75, 126, 208	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	198	GLN	6.0
4	R	121	GLY	5.5
13	M	231	GLN	5.4
4	D	121	GLY	5.2
4	D	118	GLY	5.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

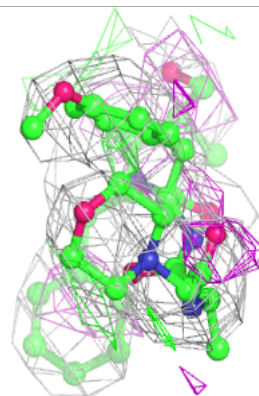
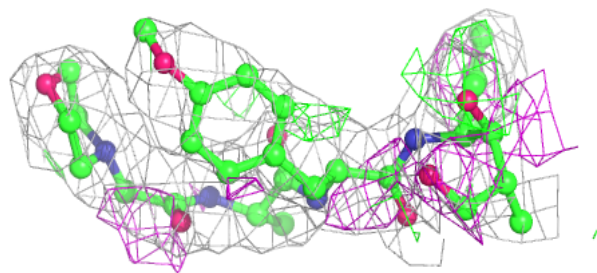
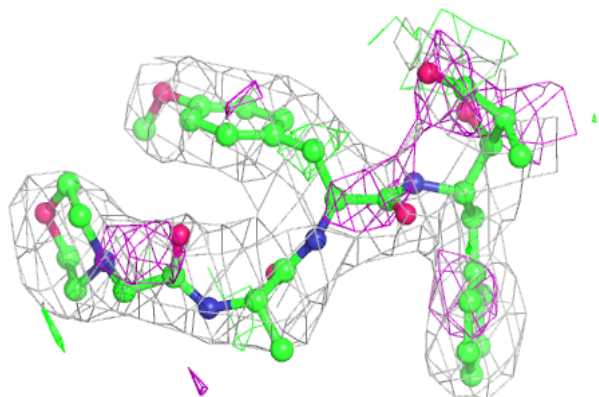
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
15	04C	K	301	42/42	0.94	0.22	17,31,47,55	0
15	04C	V	301	42/42	0.95	0.25	9,13,54,141	0
15	04C	H	301	42/42	0.95	0.20	13,26,45,51	0
15	04C	N	201	42/42	0.95	0.24	6,10,19,25	0
15	04C	Y	301	42/42	0.95	0.20	11,31,53,59	0
15	04C	b	201	42/42	0.95	0.24	4,11,27,40	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.

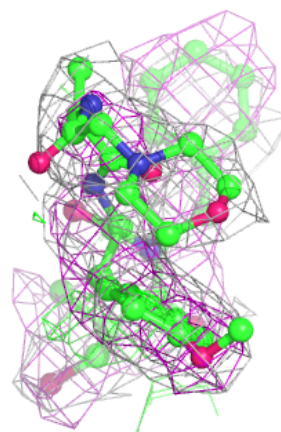
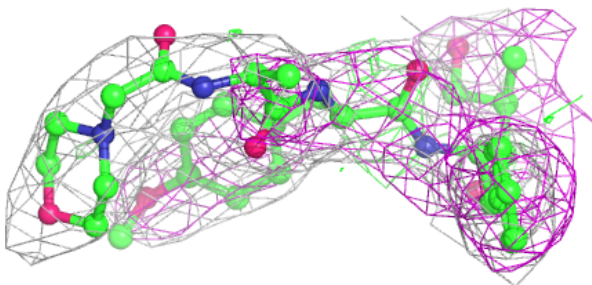
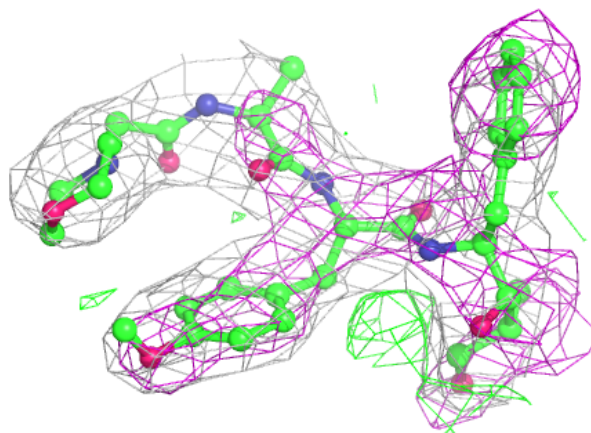
**Electron density around 04C K 301:**

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



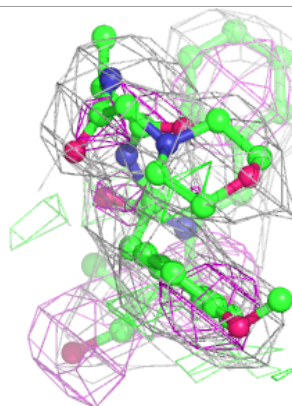
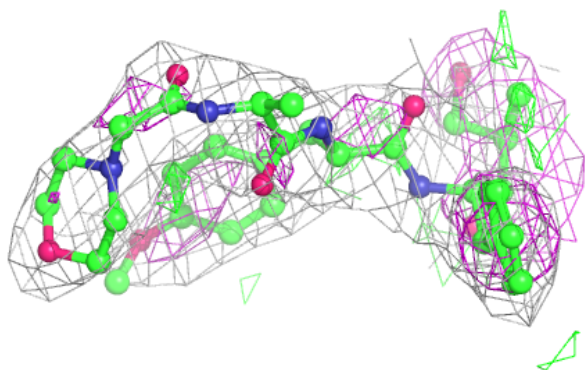
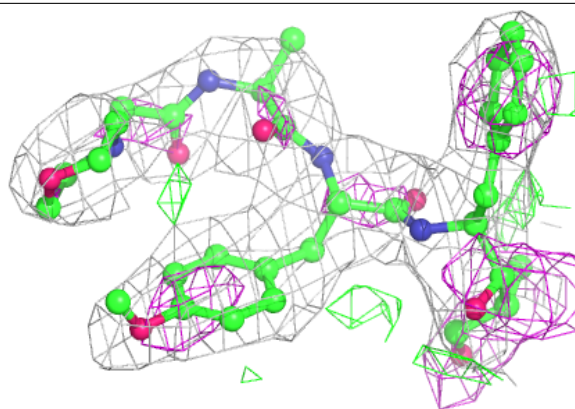
**Electron density around 04C V 301:**

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



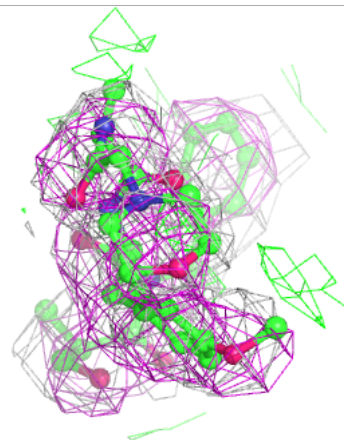
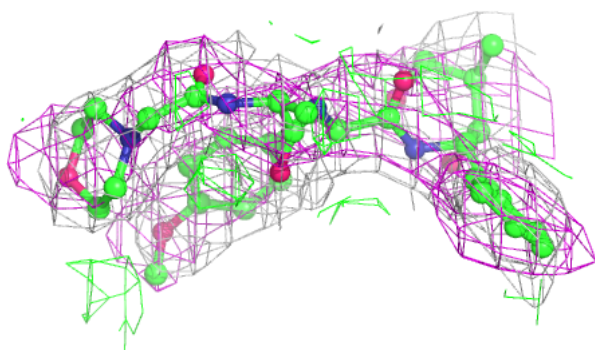
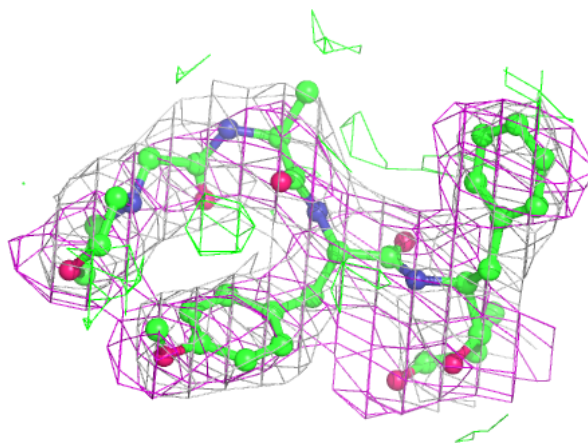
**Electron density around 04C H 301:**

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



**Electron density around 04C N 201:**

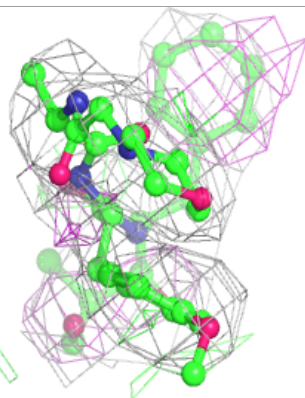
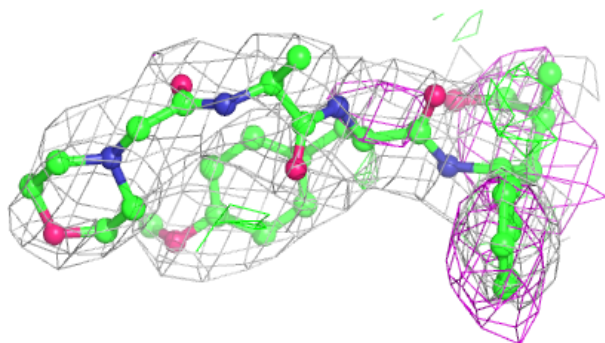
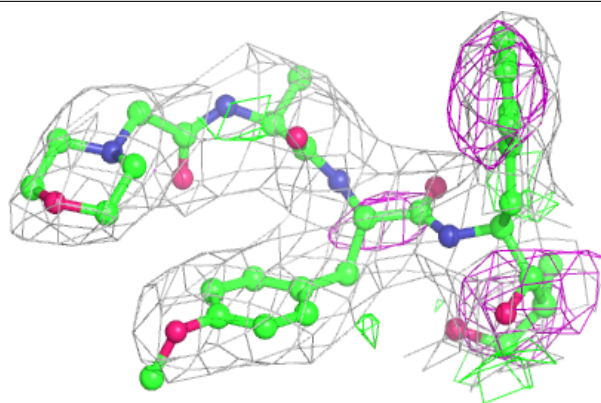
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



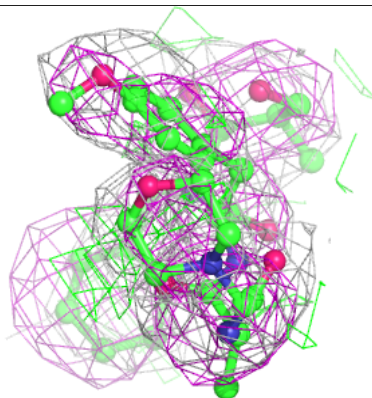
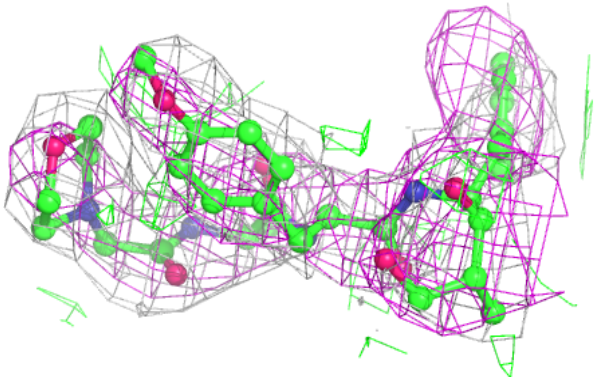
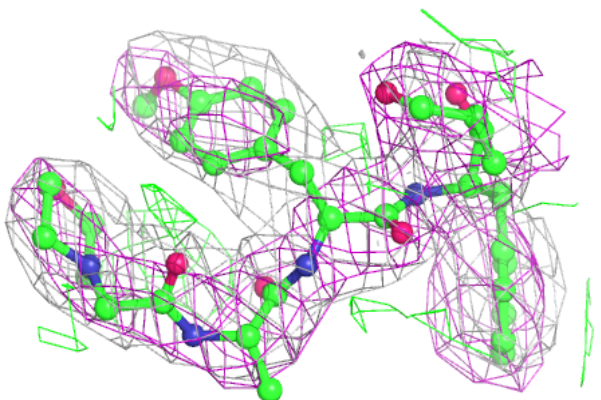


**Electron density around 04C Y 301:**

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

**Electron density around 04C b 201:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.