



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 14, 2024 – 05:16 am GMT

PDB ID : 6HWB  
Title : Yeast 20S proteasome in complex with 44b  
Authors : Huber, E.M.; Groll, M.  
Deposited on : 2018-10-11  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

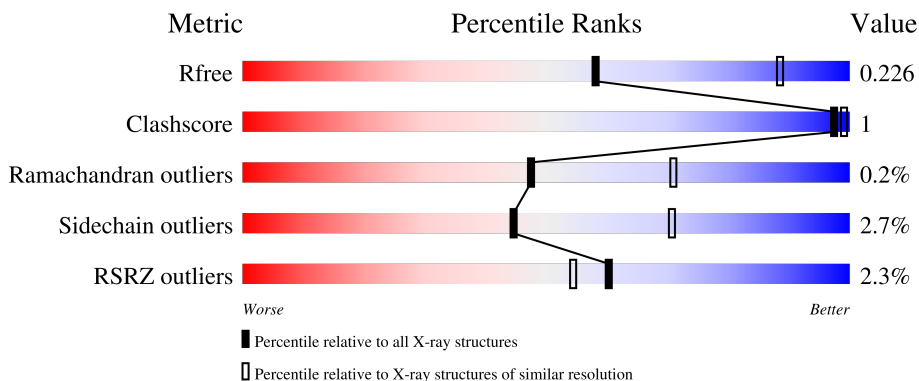
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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  $\geq 3$ , 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	 2% 98%
1	O	250	 3% 98%
2	B	258	 4% 91% 5%
2	P	258	 4% 91% 5%
3	C	254	 6% 91% 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	8% 91% 6%
4	D	260	% 87% 10%
4	R	260	2% 87% 10%
5	E	234	3% 95% ..
5	S	234	4% 95% ..
6	F	288	2% 81% .. 16%
6	T	288	3% 81% .. 16%
7	G	252	3% 92% ..
7	U	252	2% 92% ..
8	H	232	% 92% ..
8	V	232	% 94% ..
9	I	205	% 94% 5%
9	W	205	% 95% 5%
10	J	198	2% 92% 5% ..
10	X	198	2% 92% 5% ..
11	K	212	95% ..
11	Y	212	% 94% 5% .
12	L	222	96% .
12	Z	222	% 95% 5%
13	M	246	% 93% 5%
13	a	246	92% 5%
14	N	196	% 96% .
14	b	196	% 99% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	GWT	H	301	-	-	-	X
17	GWT	V	301	-	-	-	X

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 50234 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 type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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 subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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 subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			
3	Q	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			
4	R	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	231	Total 1773	C 1114	N 307	O 348	S 4	0	0	0
5	S	231	Total 1773	C 1114	N 307	O 348	S 4	0	0	0

- Molecule 6 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	243	Total 1892	C 1203	N 329	O 356	S 4	0	0	0
6	T	243	Total 1892	C 1203	N 329	O 356	S 4	0	0	0

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	241	Total 1907	C 1214	N 320	O 365	S 8	0	0	0
7	U	241	Total 1907	C 1214	N 320	O 365	S 8	0	0	0

- Molecule 8 is a protein called Proteasome subunit beta type-2.

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

- Molecule 9 is a protein called Proteasome subunit beta type-3.

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

- Molecule 10 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	195	Total 1561	C 992	N 264	O 299	S 6	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

- Molecule 11 is a protein called Proteasome subunit beta type-5.

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 subunit beta type-6.

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 subunit beta type-7.

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 subunit beta type-1.

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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	I	1	Total	Mg	0	0
			1	1		

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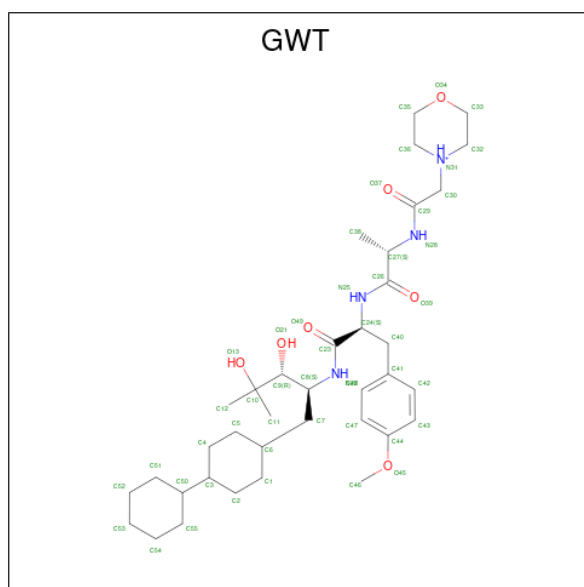
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	K	2	Total Mg 2 2	0	0
15	N	1	Total Mg 1 1	0	0
15	V	1	Total Mg 1 1	0	0
15	X	1	Total Mg 1 1	0	0
15	Y	2	Total Mg 2 2	0	0
15	Z	1	Total Mg 1 1	0	0

- Molecule 16 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

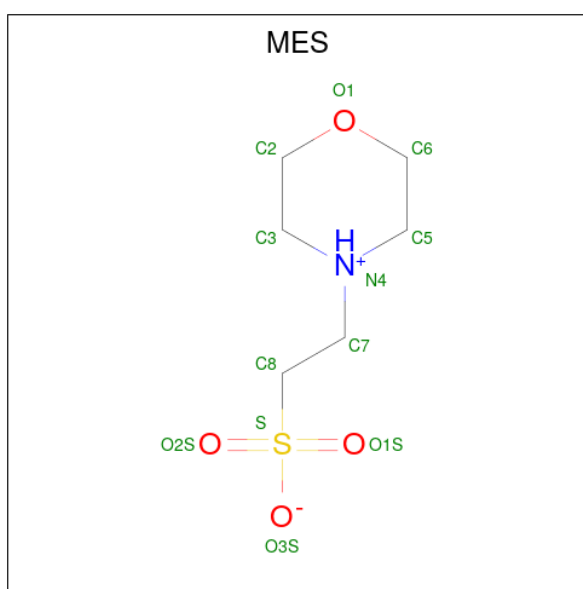
- Molecule 17 is (2 {S})- {N}-[(2 {S},3 {R})-1-(4-cyclohexylcyclohexyl)-4-methyl-3,4-bis(oxidanyl)pentan-2-yl]-3-(4-methoxyphenyl)-2-[[2 {S})-2-(2-morpholin-4-ium-4-ylethanoylamino)propanoyl]amino]propanamide (three-letter code: GWT) (formula: C<sub>37</sub>H<sub>61</sub>N<sub>4</sub>O<sub>7</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	H	1	Total	C	N	O	0	0
			48	37	4	7		
17	K	1	Total	C	N	O	0	0
			48	37	4	7		
17	V	1	Total	C	N	O	0	0
			48	37	4	7		
17	Y	1	Total	C	N	O	0	0
			48	37	4	7		

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	V	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	Y	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	31	Total	O	0	0
			31	31		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	B	29	Total O 29 29	0	0
19	C	24	Total O 24 24	0	0
19	D	11	Total O 11 11	0	0
19	E	13	Total O 13 13	0	0
19	F	24	Total O 24 24	0	0
19	G	36	Total O 36 36	0	0
19	H	28	Total O 28 28	0	0
19	I	36	Total O 36 36	0	0
19	J	32	Total O 32 32	0	0
19	K	36	Total O 36 36	0	0
19	L	25	Total O 25 25	0	0
19	M	26	Total O 26 26	0	0
19	N	23	Total O 23 23	0	0
19	O	19	Total O 19 19	0	0
19	P	12	Total O 12 12	0	0
19	Q	19	Total O 19 19	0	0
19	R	11	Total O 11 11	0	0
19	S	5	Total O 5 5	0	0
19	T	19	Total O 19 19	0	0
19	U	21	Total O 21 21	0	0
19	V	25	Total O 25 25	0	0

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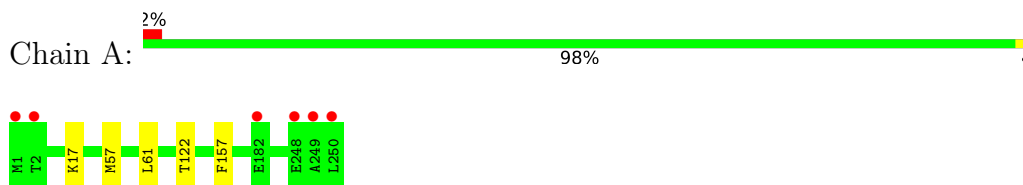
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
19	W	25	Total 25	O 25	0	0
19	X	31	Total 31	O 31	0	0
19	Y	30	Total 30	O 30	0	0
19	Z	31	Total 31	O 31	0	0
19	a	35	Total 35	O 35	0	0
19	b	29	Total 29	O 29	0	0

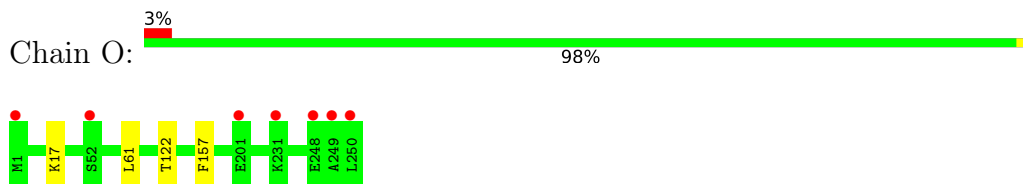
### 3 Residue-property plots [i](#)

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

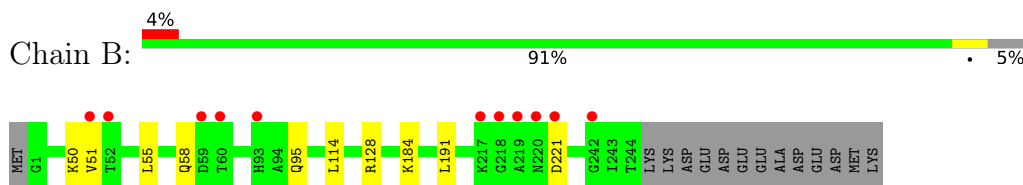
- Molecule 1: Proteasome subunit alpha type-2



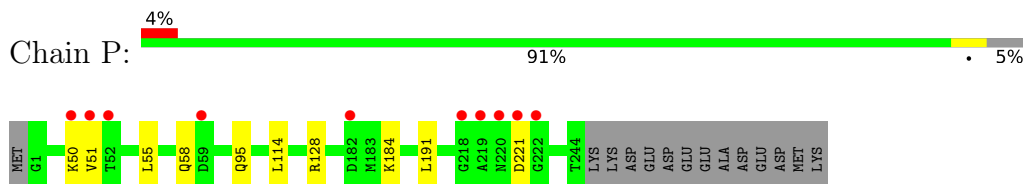
- Molecule 1: Proteasome subunit alpha type-2



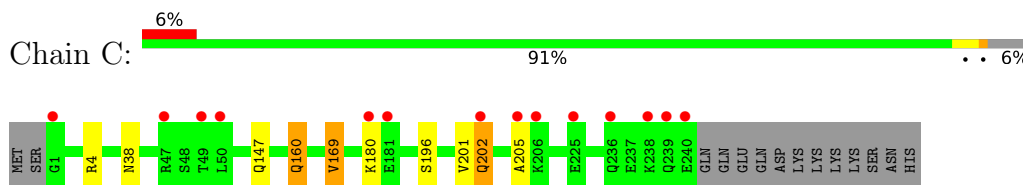
- Molecule 2: Proteasome subunit alpha type-3



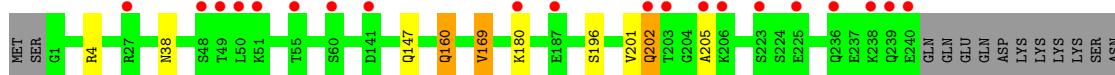
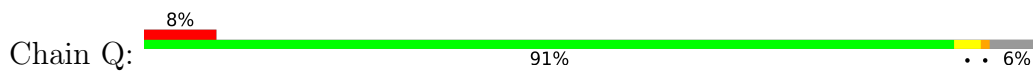
- Molecule 2: Proteasome subunit alpha type-3



- Molecule 3: Proteasome subunit alpha type-4

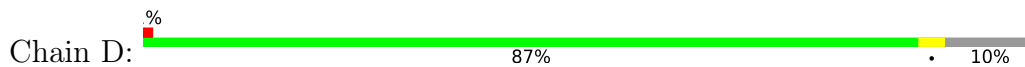


- Molecule 3: Proteasome subunit alpha type-4

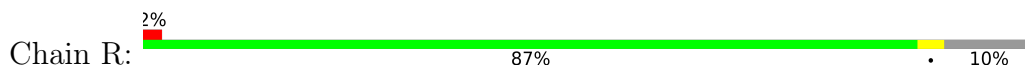


HIS

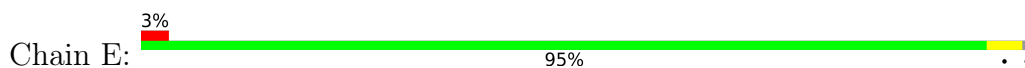
- Molecule 4: Proteasome subunit alpha type-5



- Molecule 4: Proteasome subunit alpha type-5



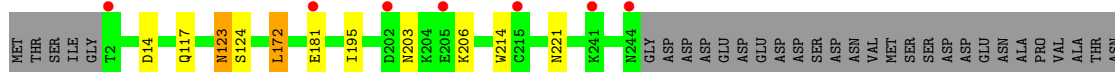
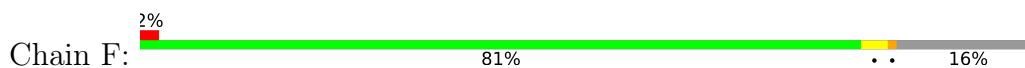
- Molecule 5: Proteasome subunit alpha type-6



- Molecule 5: Proteasome subunit alpha type-6



- Molecule 6: Probable proteasome subunit alpha type-7



ALA, ASN, THR, THR, ASP, GLN, GLU, GLY, ASP, ILE, HIS, LEU, LEU, GLU

- Molecule 6: Probable proteasome subunit alpha type-7

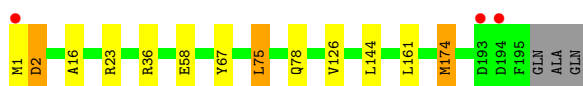
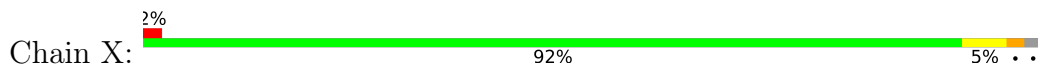




- Molecule 10: Proteasome subunit beta type-4



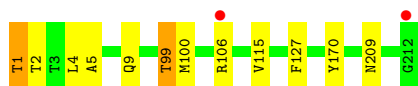
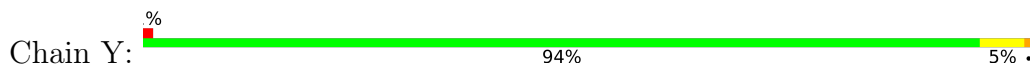
- Molecule 10: Proteasome subunit beta type-4



- Molecule 11: Proteasome subunit beta type-5



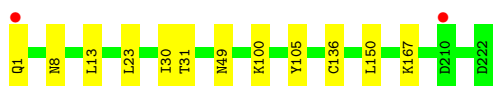
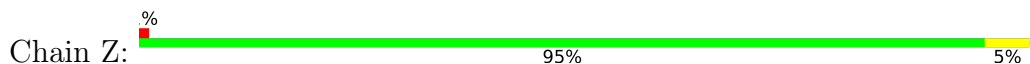
- Molecule 11: Proteasome subunit beta type-5



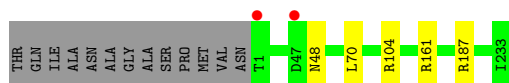
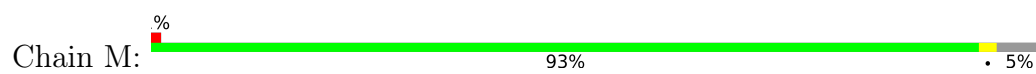
- Molecule 12: Proteasome subunit beta type-6



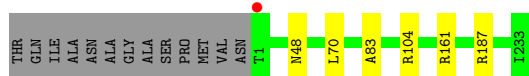
- Molecule 12: Proteasome subunit beta type-6



- Molecule 13: Proteasome subunit beta type-7



- Molecule 13: Proteasome subunit beta type-7



- Molecule 14: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.61Å 299.92Å 145.63Å 90.00° 113.16° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 15.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.3 (15.00-2.60) 97.8 (15.00-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.189 , 0.221 0.195 , 0.226	Depositor DCC
$R_{free}$ test set	15998 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.5	Xtrriage
Anisotropy	0.273	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 34.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	50234	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MES, CL, MG, GWT

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	0.35	0/1952	0.55	0/2642
1	O	0.35	0/1952	0.55	0/2642
2	B	0.35	0/1934	0.57	0/2618
2	P	0.35	0/1934	0.57	0/2618
3	C	0.35	0/1910	0.61	0/2586
3	Q	0.35	0/1910	0.60	0/2586
4	D	0.34	0/1837	0.55	0/2475
4	R	0.34	0/1837	0.55	0/2475
5	E	0.35	0/1800	0.55	0/2433
5	S	0.34	0/1800	0.55	0/2433
6	F	0.35	0/1932	0.53	0/2609
6	T	0.34	0/1932	0.53	0/2609
7	G	0.35	0/1945	0.54	0/2634
7	U	0.35	0/1945	0.54	0/2634
8	H	0.33	0/1715	0.57	1/2326 (0.0%)
8	V	0.32	0/1715	0.55	0/2326
9	I	0.34	0/1611	0.59	0/2174
9	W	0.33	0/1611	0.58	0/2174
10	J	0.34	0/1589	0.57	0/2142
10	X	0.33	0/1589	0.58	0/2142
11	K	0.34	0/1681	0.60	1/2274 (0.0%)
11	Y	0.35	0/1681	0.59	1/2274 (0.0%)
12	L	0.34	0/1795	0.57	0/2420
12	Z	0.35	0/1795	0.57	0/2420
13	M	0.34	0/1855	0.61	0/2514
13	a	0.34	0/1855	0.61	0/2514
14	N	0.32	0/1541	0.55	0/2087
14	b	0.32	0/1541	0.55	0/2087
All	All	0.34	0/50194	0.57	3/67868 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	1	THR	CA-CB-OG1	6.43	122.51	109.00
11	K	1	THR	CA-CB-OG1	6.10	121.82	109.00
11	Y	1	THR	CA-CB-OG1	5.62	120.80	109.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	2	0
1	O	1915	0	1929	1	0
2	B	1904	0	1904	2	0
2	P	1904	0	1904	2	0
3	C	1881	0	1895	3	0
3	Q	1881	0	1895	3	0
4	D	1813	0	1797	2	0
4	R	1813	0	1797	2	0
5	E	1773	0	1775	1	0
5	S	1773	0	1775	1	0
6	F	1892	0	1883	2	0
6	T	1892	0	1883	3	0
7	G	1907	0	1901	1	0
7	U	1907	0	1901	2	0
8	H	1684	0	1686	3	0
8	V	1684	0	1686	0	0
9	I	1581	0	1574	8	0
9	W	1581	0	1574	5	0
10	J	1561	0	1569	7	0
10	X	1561	0	1569	6	0
11	K	1644	0	1593	6	0
11	Y	1644	0	1593	7	0
12	L	1757	0	1711	2	0
12	Z	1757	0	1711	4	0
13	M	1824	0	1832	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	a	1824	0	1832	0	0
14	N	1512	0	1481	3	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	I	1	0	0	0	0
15	K	2	0	0	0	0
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	X	1	0	0	0	0
15	Y	2	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	H	48	0	0	1	0
17	K	48	0	0	2	0
17	V	48	0	0	1	0
17	Y	48	0	0	1	0
18	H	12	0	13	0	0
18	K	12	0	13	1	0
18	V	12	0	13	0	0
18	Y	12	0	13	0	0
19	A	31	0	0	0	0
19	B	29	0	0	0	0
19	C	24	0	0	0	0
19	D	11	0	0	0	0
19	E	13	0	0	0	0
19	F	24	0	0	0	0
19	G	36	0	0	1	0
19	H	28	0	0	0	0
19	I	36	0	0	0	0
19	J	32	0	0	0	0
19	K	36	0	0	0	0
19	L	25	0	0	0	0
19	M	26	0	0	0	0
19	N	23	0	0	0	0
19	O	19	0	0	0	0
19	P	12	0	0	0	0
19	Q	19	0	0	0	0
19	R	11	0	0	0	0
19	S	5	0	0	0	0
19	T	19	0	0	0	0
19	U	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	V	25	0	0	0	0
19	W	25	0	0	0	0
19	X	31	0	0	0	0
19	Y	30	0	0	0	0
19	Z	31	0	0	0	0
19	a	35	0	0	0	0
19	b	29	0	0	0	0
All	All	50234	0	49112	72	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 1.

All (72) 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)
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.80	0.64
8:H:1:THR:HG22	8:H:2:THR:N	2.13	0.62
8:H:1:THR:CG2	8:H:2:THR:N	2.63	0.61
14:N:152:VAL:HA	14:N:175:MET:HE1	1.84	0.59
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.86	0.58
11:K:1:THR:HG22	11:K:2:THR:N	2.19	0.58
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.85	0.58
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.86	0.57
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.88	0.56
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.70	0.56
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.70	0.55
14:N:49:ALA:O	14:N:53:GLN:HB2	2.05	0.55
11:K:99:THR:HG22	11:K:115:VAL:HB	1.90	0.53
11:Y:99:THR:HG22	11:Y:115:VAL:HB	1.91	0.53
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.93	0.51
17:V:301:GWT:C23	17:V:301:GWT:C12	2.89	0.51
10:J:174:MET:HA	10:X:174:MET:HA	1.92	0.51
11:K:1:THR:CG2	11:K:2:THR:N	2.73	0.50
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.49	0.48
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.43	0.48
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.43	0.48
17:H:301:GWT:N22	17:H:301:GWT:O13	2.46	0.48
7:G:23:PHE:O	7:G:26:THR:HB	2.14	0.47
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.63	0.47
7:U:23:PHE:O	7:U:26:THR:HB	2.15	0.47
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.97	0.47
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.64	0.46
10:J:23:ARG:NH2	18:K:304:MES:O1	2.47	0.46
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.98	0.45
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.98	0.45
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.99	0.45
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.98	0.45
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.82	0.44
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.99	0.44
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.99	0.44
10:J:16:ALA:HB2	10:J:161:LEU:HD21	2.00	0.43
10:J:1:MET:O	10:J:2:ASP:HB2	2.19	0.43
3:C:201:VAL:O	3:C:202:GLN:CB	2.66	0.43
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.67	0.43
17:K:301:GWT:O13	17:K:301:GWT:N22	2.52	0.43
10:X:1:MET:O	10:X:2:ASP:HB2	2.19	0.43
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.00	0.42
9:W:36:SER:HB2	10:X:126:VAL:HG11	2.01	0.42
11:Y:170:TYR:O	17:Y:301:GWT:C11	2.67	0.42
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.55	0.42
11:K:170:TYR:O	17:K:301:GWT:C11	2.67	0.42
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.01	0.42
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.54	0.42
9:I:37:ASN:ND2	11:Y:209:ASN:O	2.53	0.42
9:I:98:ARG:O	9:I:126:ILE:HD11	2.20	0.42
9:I:101:PRO:HB3	9:I:126:ILE:HD12	2.02	0.42
10:X:16:ALA:HB2	10:X:161:LEU:HD21	2.00	0.42
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.50	0.42
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.01	0.41
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.03	0.41
9:W:101:PRO:HB3	9:W:126:ILE:HD12	2.03	0.41
6:T:123:ASN:HD22	6:T:124:SER:N	2.19	0.41
8:H:50:ALA:CB	9:I:126:ILE:HG23	2.50	0.41
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.86	0.41
6:F:123:ASN:HD22	6:F:124:SER:N	2.19	0.41
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.51	0.41
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.51	0.41
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.21	0.41
1:A:57:MET:HE1	19:G:407:HOH:O	2.20	0.41
6:T:123:ASN:HD22	6:T:123:ASN:C	2.25	0.40
7:U:26:THR:HG21	7:U:131:ILE:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:1:THR:HG22	11:Y:2:THR:N	2.35	0.40
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.02	0.40
10:X:36:ARG:NH1	10:X:58:GLU:OE2	2.55	0.40
12:Z:100:LYS:HD3	12:Z:105:TYR:CE2	2.56	0.40
10:J:36:ARG:NH1	10:J:58:GLU:OE2	2.54	0.40

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%)	243 (98%)	5 (2%)	0	100	100
1	O	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
2	B	242/258 (94%)	233 (96%)	7 (3%)	2 (1%)	19	39
2	P	242/258 (94%)	233 (96%)	7 (3%)	2 (1%)	19	39
3	C	238/254 (94%)	231 (97%)	5 (2%)	2 (1%)	19	39
3	Q	238/254 (94%)	231 (97%)	5 (2%)	2 (1%)	19	39
4	D	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
4	R	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
5	E	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
7	G	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
7	U	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
8	H	220/232 (95%)	214 (97%)	5 (2%)	1 (0%)	29	52
8	V	220/232 (95%)	214 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	52
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	52
11	K	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
11	Y	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
12	L	220/222 (99%)	217 (99%)	3 (1%)	0	100	100
12	Z	220/222 (99%)	217 (99%)	3 (1%)	0	100	100
13	M	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
13	a	231/246 (94%)	223 (96%)	7 (3%)	1 (0%)	34	57
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
All	All	6276/6614 (95%)	6108 (97%)	156 (2%)	12 (0%)	47	71

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
2	P	51	VAL
3	Q	202	GLN
10	J	2	ASP
10	X	2	ASP
2	B	221	ASP
3	C	205	ALA
2	P	221	ASP
3	Q	205	ALA
8	H	9	ASN
13	a	83	ALA

### 5.3.2 Protein sidechains [i](#)

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

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	206 (99%)	3 (1%)	67	85
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	85
2	B	203/216 (94%)	197 (97%)	6 (3%)	41	67
2	P	203/216 (94%)	197 (97%)	6 (3%)	41	67
3	C	212/226 (94%)	206 (97%)	6 (3%)	43	69
3	Q	212/226 (94%)	206 (97%)	6 (3%)	43	69
4	D	194/215 (90%)	188 (97%)	6 (3%)	40	66
4	R	194/215 (90%)	188 (97%)	6 (3%)	40	66
5	E	190/193 (98%)	183 (96%)	7 (4%)	34	60
5	S	190/193 (98%)	183 (96%)	7 (4%)	34	60
6	F	201/239 (84%)	192 (96%)	9 (4%)	27	52
6	T	201/239 (84%)	192 (96%)	9 (4%)	27	52
7	G	206/210 (98%)	199 (97%)	7 (3%)	37	63
7	U	206/210 (98%)	199 (97%)	7 (3%)	37	63
8	H	181/190 (95%)	177 (98%)	4 (2%)	52	76
8	V	181/190 (95%)	177 (98%)	4 (2%)	52	76
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	81
9	W	172/173 (99%)	169 (98%)	3 (2%)	60	81
10	J	173/175 (99%)	168 (97%)	5 (3%)	42	68
10	X	173/175 (99%)	168 (97%)	5 (3%)	42	68
11	K	169/169 (100%)	165 (98%)	4 (2%)	49	74
11	Y	169/169 (100%)	165 (98%)	4 (2%)	49	74
12	L	185/185 (100%)	179 (97%)	6 (3%)	39	65
12	Z	185/185 (100%)	179 (97%)	6 (3%)	39	65
13	M	199/208 (96%)	194 (98%)	5 (2%)	47	73
13	a	199/208 (96%)	194 (98%)	5 (2%)	47	73
14	N	162/162 (100%)	161 (99%)	1 (1%)	86	95
14	b	162/162 (100%)	161 (99%)	1 (1%)	86	95
All	All	5312/5540 (96%)	5168 (97%)	144 (3%)	44	71

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	61	LEU
1	A	157	PHE
2	B	50	LYS
2	B	55	LEU
2	B	58	GLN
2	B	114	LEU
2	B	184	LYS
2	B	191	LEU
3	C	4	ARG
3	C	38	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
4	D	99	ILE
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	54	GLU
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
6	F	14	ASP
6	F	117	GLN
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	125	MET
7	G	166	GLN
7	G	181	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	G	235	ARG
8	H	30	ASN
8	H	68	LEU
8	H	84	LYS
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
10	J	23	ARG
10	J	75	LEU
10	J	78	GLN
10	J	144	LEU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	99	THR
11	K	106	ARG
12	L	1	GLN
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	136	CYS
12	L	167	LYS
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	39	ASP
1	O	17	LYS
1	O	61	LEU
1	O	157	PHE
2	P	50	LYS
2	P	55	LEU
2	P	58	GLN
2	P	114	LEU
2	P	184	LYS
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	147	GLN
3	Q	160	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	Q	169	VAL
3	Q	180	LYS
4	R	99	ILE
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	54	GLU
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
6	T	14	ASP
6	T	117	GLN
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	125	MET
7	U	166	GLN
7	U	181	LYS
7	U	235	ARG
8	V	30	ASN
8	V	68	LEU
8	V	84	LYS
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
10	X	23	ARG
10	X	75	LEU
10	X	78	GLN
10	X	144	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	99	THR
11	Y	106	ARG
12	Z	1	GLN
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	136	CYS
12	Z	167	LYS
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	39	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	20	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	38	ASN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	E	184	ASN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	175	ASN
8	H	30	ASN
8	H	172	ASN
8	H	189	ASN
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	94	GLN
12	L	158	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
2	P	20	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN

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Mol	Chain	Res	Type
4	R	91	HIS
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	184	ASN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	175	ASN
8	V	30	ASN
8	V	172	ASN
8	V	189	ASN
10	X	55	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	94	GLN
12	Z	158	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	179	ASN
14	b	161	GLN

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 for Mogul analysis.

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
17	GWT	K	301	11	51,51,51	2.06	7 (13%)	67,70,70	2.70	14 (20%)
18	MES	V	303	-	12,12,12	2.15	1 (8%)	14,16,16	1.51	2 (14%)
17	GWT	V	301	8	51,51,51	1.11	4 (7%)	67,70,70	1.77	13 (19%)
18	MES	K	304	-	12,12,12	2.48	1 (8%)	14,16,16	1.49	1 (7%)
17	GWT	Y	301	11	51,51,51	2.23	7 (13%)	67,70,70	2.80	16 (23%)
18	MES	Y	304	-	12,12,12	2.43	1 (8%)	14,16,16	1.52	2 (14%)
18	MES	H	302	-	12,12,12	2.13	1 (8%)	14,16,16	1.51	2 (14%)
17	GWT	H	301	8	51,51,51	1.78	4 (7%)	67,70,70	2.64	11 (16%)

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
17	GWT	K	301	11	-	4/48/74/74	0/4/4/4
18	MES	V	303	-	-	0/6/14/14	0/1/1/1
17	GWT	V	301	8	-	9/48/74/74	0/4/4/4
18	MES	K	304	-	-	0/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	GWT	Y	301	11	-	8/48/74/74	0/4/4/4
18	MES	Y	304	-	-	0/6/14/14	0/1/1/1
18	MES	H	302	-	-	3/6/14/14	0/1/1/1
17	GWT	H	301	8	-	7/48/74/74	0/4/4/4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	301	GWT	C10-C9	8.51	1.71	1.54
18	K	304	MES	C8-S	-8.39	1.65	1.77
18	Y	304	MES	C8-S	-8.21	1.65	1.77
17	Y	301	GWT	C10-C9	8.17	1.70	1.54
17	H	301	GWT	C10-C9	7.93	1.70	1.54
18	V	303	MES	C8-S	-7.09	1.67	1.77
18	H	302	MES	C8-S	-7.01	1.67	1.77
17	Y	301	GWT	C40-C41	-6.42	1.35	1.51
17	H	301	GWT	C40-C41	-6.27	1.36	1.51
17	K	301	GWT	C40-C41	-6.00	1.36	1.51
17	Y	301	GWT	C2-C3	-5.97	1.38	1.53
17	K	301	GWT	C2-C3	-5.96	1.38	1.53
17	Y	301	GWT	O13-C10	-4.82	1.36	1.44
17	H	301	GWT	C2-C3	-4.80	1.41	1.53
17	V	301	GWT	C40-C41	-4.79	1.39	1.51
17	Y	301	GWT	C12-C10	-3.05	1.47	1.52
17	K	301	GWT	O13-C10	-2.66	1.39	1.44
17	Y	301	GWT	C23-N22	-2.51	1.28	1.34
17	V	301	GWT	C11-C10	2.45	1.56	1.52
17	Y	301	GWT	C55-C50	-2.39	1.47	1.53
17	V	301	GWT	C54-C55	-2.36	1.47	1.53
17	K	301	GWT	C12-C10	-2.34	1.48	1.52
17	K	301	GWT	C51-C50	-2.32	1.47	1.53
17	H	301	GWT	C55-C50	-2.16	1.47	1.53
17	K	301	GWT	C1-C2	-2.13	1.47	1.52
17	V	301	GWT	C55-C50	-2.04	1.48	1.53

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Y	301	GWT	O13-C10-C11	16.10	142.47	107.90
17	K	301	GWT	O13-C10-C11	15.43	141.04	107.90
17	H	301	GWT	O13-C10-C11	15.36	140.88	107.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	301	GWT	O13-C10-C9	-9.32	85.72	107.64
17	Y	301	GWT	O13-C10-C9	-8.88	86.76	107.64
17	H	301	GWT	O13-C10-C9	-8.75	87.05	107.64
17	V	301	GWT	C12-C10-C11	-6.64	101.07	110.56
17	V	301	GWT	C30-N31-C32	-5.09	103.20	111.09
17	K	301	GWT	C8-N22-C23	4.99	131.90	123.07
17	Y	301	GWT	O21-C9-C8	-4.94	97.58	109.41
17	K	301	GWT	C12-C10-C11	-4.61	103.96	110.56
17	H	301	GWT	O21-C9-C8	-4.61	98.37	109.41
17	V	301	GWT	C32-N31-C36	-4.33	99.07	108.83
17	Y	301	GWT	C12-C10-C11	-4.20	104.56	110.56
18	H	302	MES	O2S-S-C8	4.17	111.94	106.92
17	K	301	GWT	O21-C9-C8	-4.10	99.58	109.41
18	Y	304	MES	O3S-S-C8	4.09	112.39	105.77
17	H	301	GWT	C12-C10-C11	-4.05	104.76	110.56
18	V	303	MES	O1S-S-C8	3.96	111.69	106.92
18	K	304	MES	O3S-S-C8	3.85	112.00	105.77
17	Y	301	GWT	O21-C9-C10	3.84	118.73	109.36
17	K	301	GWT	O21-C9-C10	3.73	118.46	109.36
17	V	301	GWT	C33-C32-N31	3.71	115.73	110.10
17	Y	301	GWT	C8-N22-C23	3.60	129.43	123.07
17	H	301	GWT	O21-C9-C10	3.58	118.09	109.36
17	V	301	GWT	C52-C51-C50	-3.55	105.87	111.93
17	V	301	GWT	C11-C10-C9	3.37	117.59	111.28
17	Y	301	GWT	C11-C10-C9	-3.35	105.00	111.28
17	H	301	GWT	C7-C8-N22	3.27	114.42	110.18
17	V	301	GWT	C4-C5-C6	-3.20	107.12	112.42
17	K	301	GWT	C24-C23-N22	-2.99	110.14	116.70
17	V	301	GWT	C29-C30-N31	-2.95	106.50	113.36
17	Y	301	GWT	C24-C23-N22	-2.94	110.26	116.70
17	H	301	GWT	C11-C10-C9	-2.90	105.85	111.28
17	K	301	GWT	C2-C1-C6	-2.72	107.92	112.42
17	K	301	GWT	C11-C10-C9	-2.59	106.43	111.28
17	Y	301	GWT	C2-C1-C6	-2.50	108.29	112.42
17	H	301	GWT	C24-C23-N22	-2.50	111.23	116.70
18	V	303	MES	O3S-S-C8	2.49	109.79	105.77
17	K	301	GWT	C38-C27-N28	-2.43	105.81	110.38
17	Y	301	GWT	O49-C23-C24	2.37	125.44	120.45
17	Y	301	GWT	C26-C27-N28	2.36	117.46	111.60
17	H	301	GWT	C8-N22-C23	2.31	127.16	123.07
17	V	301	GWT	C7-C6-C1	-2.31	106.72	111.73
17	V	301	GWT	C55-C50-C3	-2.30	107.74	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Y	301	GWT	C38-C27-N28	-2.28	106.09	110.38
17	V	301	GWT	C2-C3-C50	-2.27	107.79	112.59
17	K	301	GWT	C4-C5-C6	-2.27	108.67	112.42
17	H	301	GWT	C46-O45-C44	-2.23	112.68	117.51
17	Y	301	GWT	C30-N31-C32	-2.18	107.71	111.09
17	V	301	GWT	C5-C4-C3	-2.17	107.35	112.24
17	H	301	GWT	C4-C5-C6	-2.13	108.90	112.42
18	Y	304	MES	C6-O1-C2	2.12	116.95	109.89
17	K	301	GWT	C40-C24-N25	2.09	115.19	110.79
17	Y	301	GWT	C23-C24-N25	-2.08	105.49	111.16
18	H	302	MES	O1S-S-C8	2.07	109.40	106.92
17	Y	301	GWT	C4-C5-C6	-2.05	109.02	112.42
17	Y	301	GWT	C40-C41-C42	-2.04	116.86	120.91
17	V	301	GWT	O13-C10-C11	2.04	112.27	107.90
17	K	301	GWT	C23-C24-N25	-2.02	105.67	111.16
17	K	301	GWT	O49-C23-C24	2.01	124.68	120.45

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	301	GWT	C11-C10-C9-O21
17	K	301	GWT	C6-C7-C8-C9
17	K	301	GWT	C11-C10-C9-O21
17	V	301	GWT	C11-C10-C9-C8
17	V	301	GWT	C11-C10-C9-O21
17	V	301	GWT	C12-C10-C9-C8
17	V	301	GWT	C12-C10-C9-O21
17	V	301	GWT	O13-C10-C9-C8
17	V	301	GWT	O13-C10-C9-O21
17	Y	301	GWT	C6-C7-C8-C9
17	Y	301	GWT	C11-C10-C9-O21
17	Y	301	GWT	C29-C30-N31-C36
18	H	302	MES	C7-C8-S-O1S
18	H	302	MES	C7-C8-S-O3S
17	Y	301	GWT	N28-C29-C30-N31
17	Y	301	GWT	O37-C29-C30-N31
17	H	301	GWT	N28-C29-C30-N31
17	V	301	GWT	N28-C29-C30-N31
17	V	301	GWT	C6-C7-C8-N22
17	H	301	GWT	O37-C29-C30-N31
17	V	301	GWT	O37-C29-C30-N31

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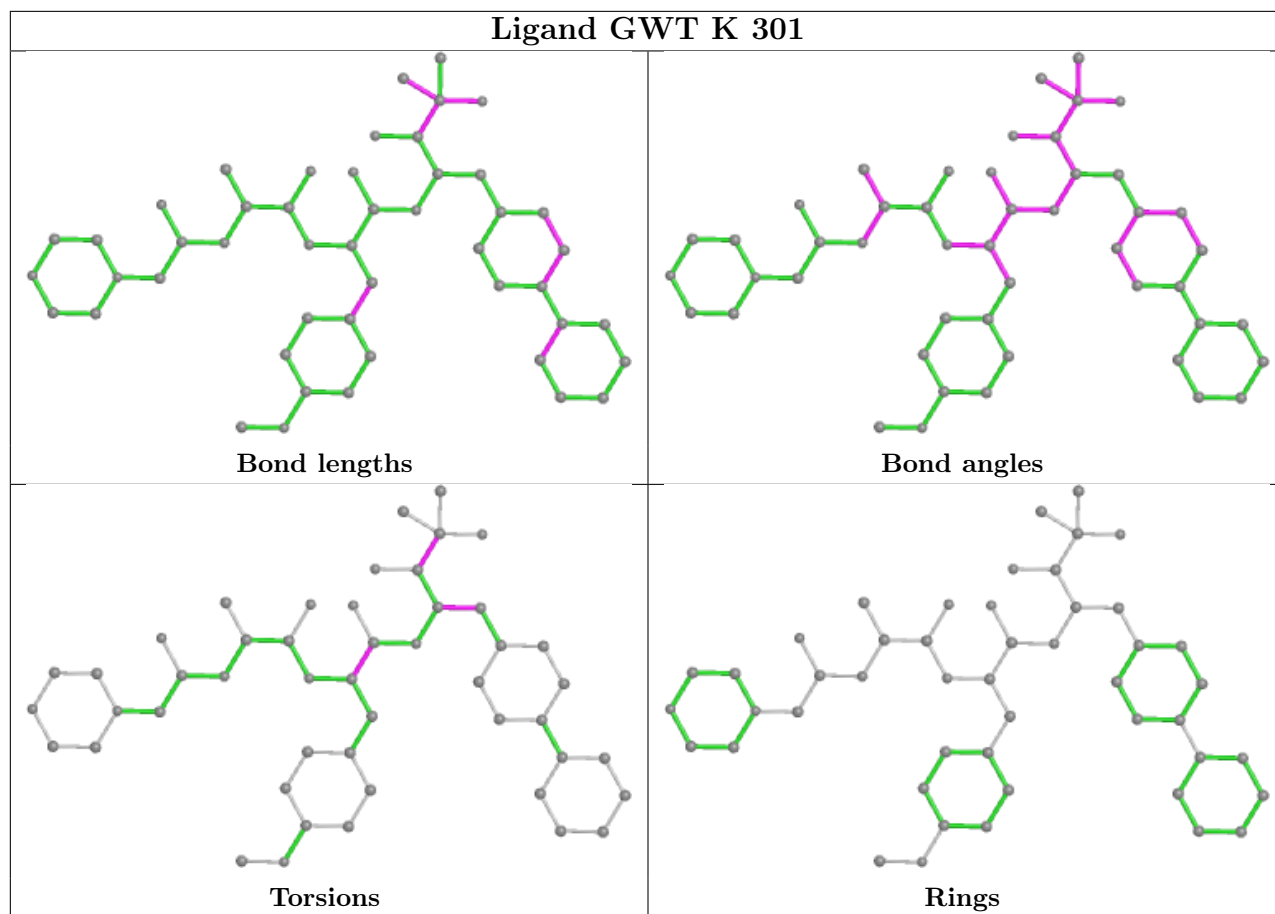
Mol	Chain	Res	Type	Atoms
17	Y	301	GWT	C11-C10-C9-C8
18	H	302	MES	C7-C8-S-O2S
17	H	301	GWT	C6-C7-C8-C9
17	K	301	GWT	O49-C23-C24-N25
17	H	301	GWT	C11-C10-C9-C8
17	K	301	GWT	C11-C10-C9-C8
17	H	301	GWT	N22-C8-C9-C10
17	H	301	GWT	C12-C10-C9-O21
17	Y	301	GWT	C12-C10-C9-O21
17	Y	301	GWT	O49-C23-C24-N25

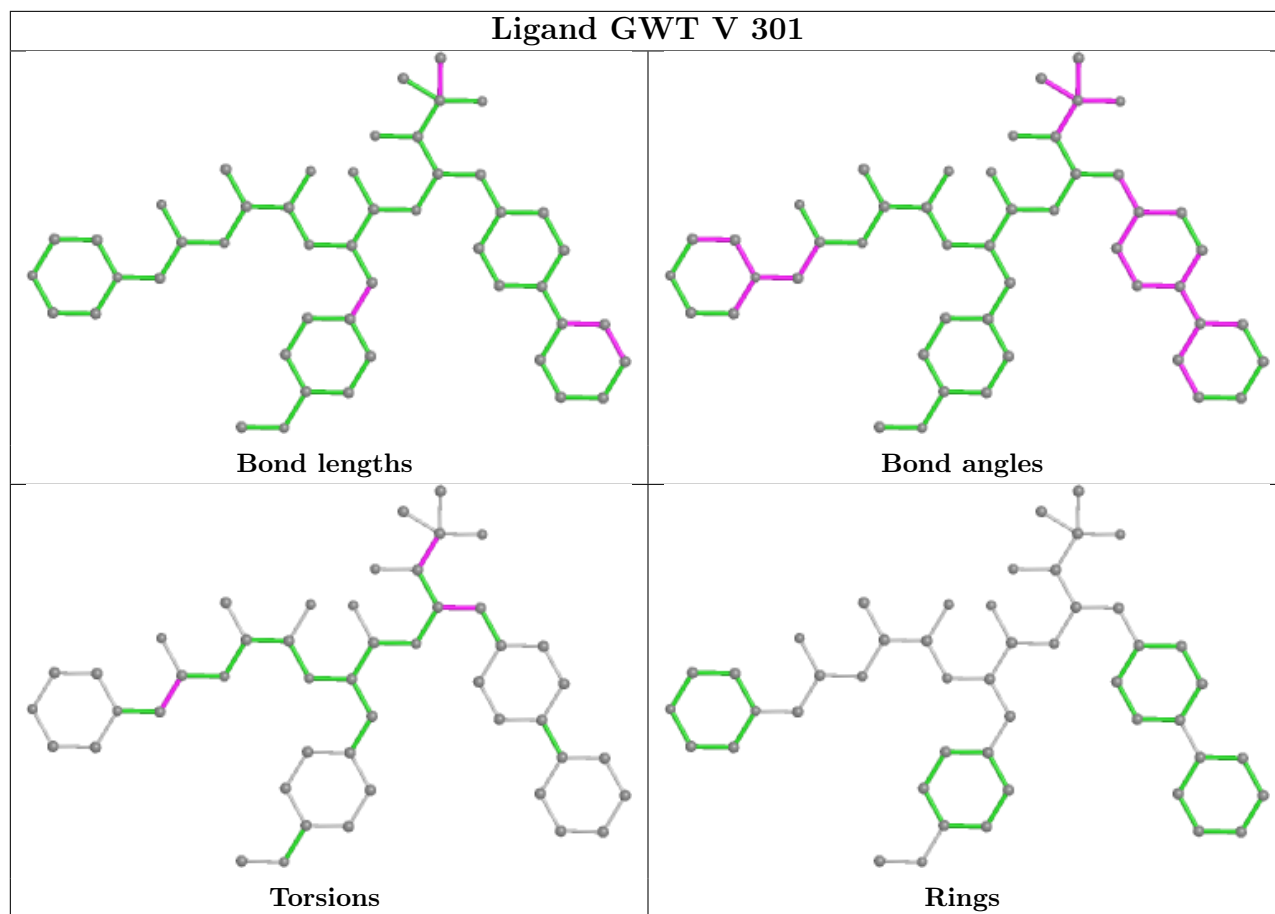
There are no ring outliers.

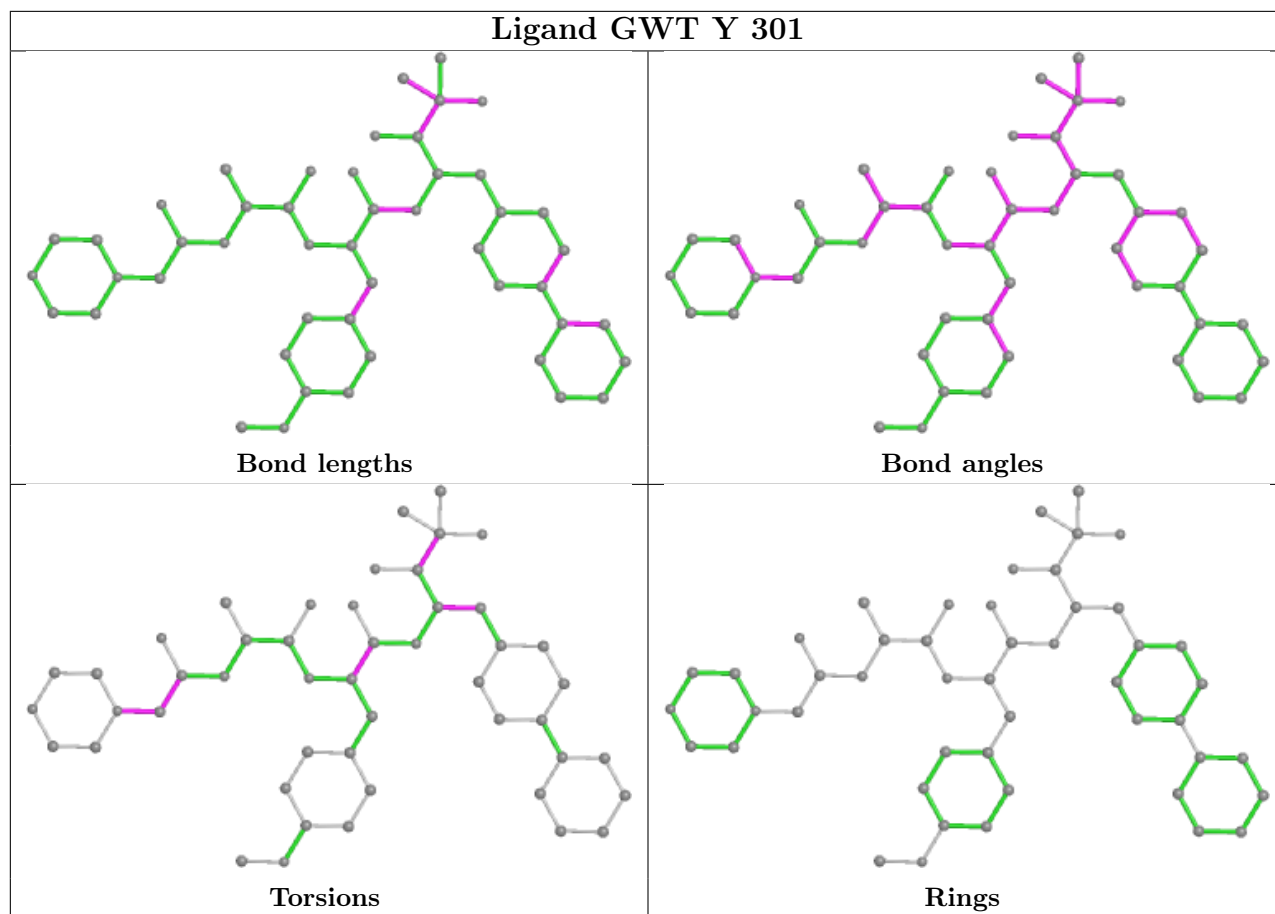
5 monomers are involved in 6 short contacts:

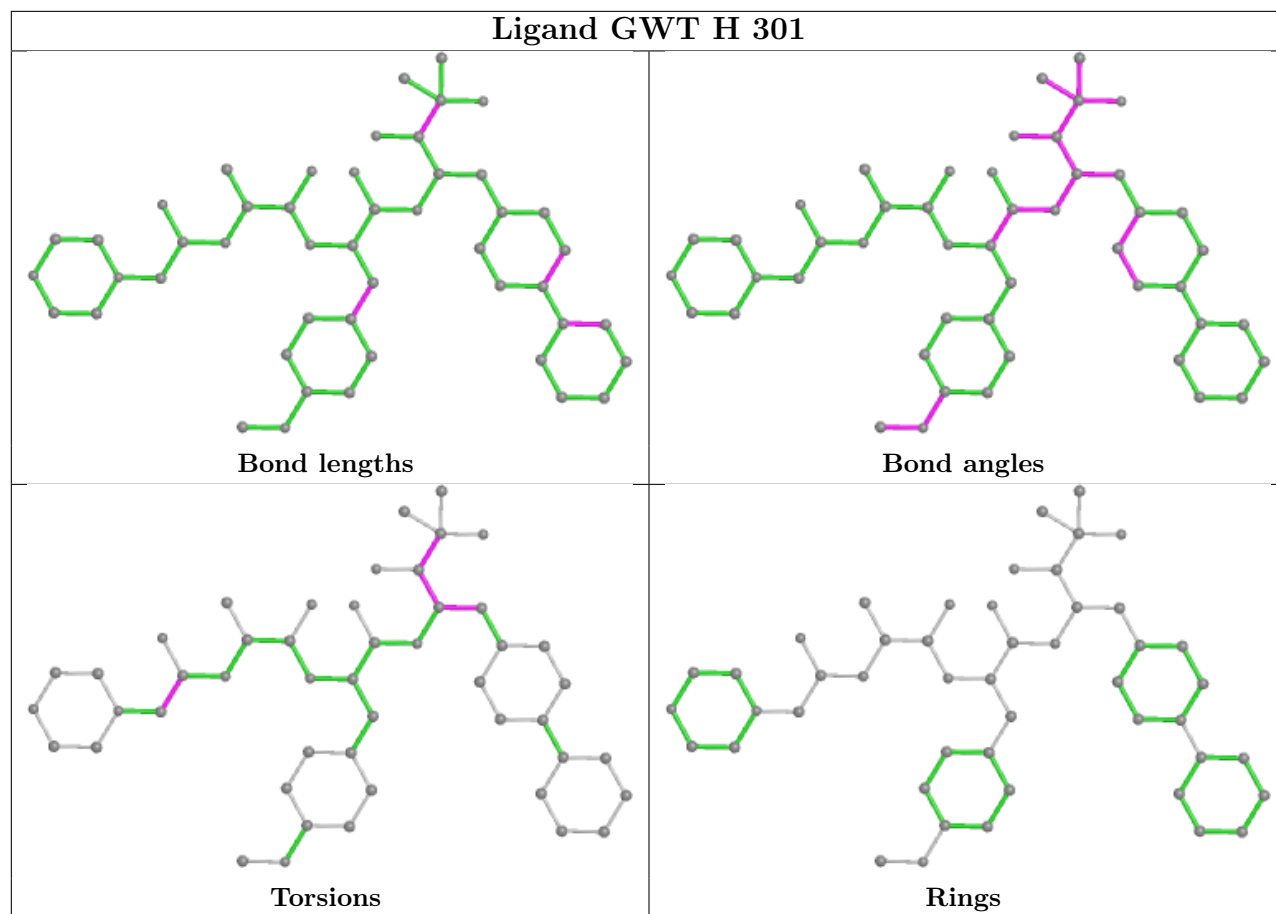
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	K	301	GWT	2	0
17	V	301	GWT	1	0
18	K	304	MES	1	0
17	Y	301	GWT	1	0
17	H	301	GWT	1	0

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









## 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%)	-0.36	6 (2%) 59 53	39, 52, 90, 147	0
1	O	250/250 (100%)	-0.30	7 (2%) 53 46	43, 61, 102, 153	0
2	B	244/258 (94%)	-0.22	11 (4%) 33 26	40, 60, 105, 154	0
2	P	244/258 (94%)	-0.21	10 (4%) 37 30	42, 63, 110, 152	0
3	C	240/254 (94%)	-0.13	14 (5%) 23 17	39, 64, 127, 156	0
3	Q	240/254 (94%)	0.11	20 (8%) 11 8	46, 76, 157, 188	0
4	D	235/260 (90%)	-0.37	2 (0%) 84 82	44, 65, 99, 141	0
4	R	235/260 (90%)	-0.26	5 (2%) 63 58	45, 66, 103, 154	0
5	E	231/234 (98%)	-0.17	7 (3%) 50 43	46, 69, 106, 146	0
5	S	231/234 (98%)	-0.04	10 (4%) 35 28	50, 76, 123, 158	0
6	F	243/288 (84%)	-0.37	7 (2%) 51 45	34, 62, 112, 144	0
6	T	243/288 (84%)	-0.23	8 (3%) 46 39	41, 70, 130, 164	0
7	G	241/252 (95%)	-0.37	8 (3%) 46 39	37, 56, 98, 143	0
7	U	241/252 (95%)	-0.39	6 (2%) 57 51	41, 57, 92, 127	0
8	H	222/232 (95%)	-0.44	2 (0%) 84 82	41, 54, 82, 106	0
8	V	222/232 (95%)	-0.40	3 (1%) 75 71	42, 57, 85, 112	0
9	I	204/205 (99%)	-0.69	2 (0%) 82 80	34, 49, 77, 102	0
9	W	204/205 (99%)	-0.62	2 (0%) 82 80	35, 53, 80, 110	0
10	J	195/198 (98%)	-0.52	3 (1%) 73 70	35, 51, 79, 118	0
10	X	195/198 (98%)	-0.55	3 (1%) 73 70	38, 53, 80, 133	0
11	K	212/212 (100%)	-0.57	1 (0%) 91 89	36, 51, 77, 99	0
11	Y	212/212 (100%)	-0.58	2 (0%) 84 82	34, 51, 78, 107	0
12	L	222/222 (100%)	-0.60	0 100 100	36, 56, 84, 101	0
12	Z	222/222 (100%)	-0.56	2 (0%) 84 82	35, 54, 82, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/246 (94%)	-0.53	2 (0%) 84 82	32, 57, 82, 98	0
13	a	233/246 (94%)	-0.55	1 (0%) 92 91	31, 54, 81, 102	0
14	N	196/196 (100%)	-0.59	1 (0%) 91 89	37, 51, 81, 105	0
14	b	196/196 (100%)	-0.57	2 (1%) 82 80	37, 51, 82, 106	0
All	All	6336/6614 (95%)	-0.38	147 (2%) 60 54	31, 58, 105, 188	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	49	THR	8.5
1	O	1	MET	8.0
3	Q	206	LYS	7.7
1	A	1	MET	7.5
3	C	206	LYS	7.3
5	S	202	ASP	6.8
2	B	218	GLY	6.3
2	P	51	VAL	5.8
2	B	220	ASN	5.5
10	J	1	MET	5.4
2	P	219	ALA	5.3
3	Q	50	LEU	5.3
3	Q	48	SER	5.2
10	X	1	MET	4.6
5	E	202	ASP	4.5
3	Q	239	GLN	4.5
3	C	238	LYS	4.5
3	C	49	THR	4.4
2	B	221	ASP	4.4
2	B	219	ALA	4.3
1	O	249	ALA	4.3
10	J	194	ASP	4.1
8	V	222	ASP	4.1
2	P	220	ASN	4.0
4	R	241	ALA	3.9
1	O	52	SER	3.9
3	C	202	GLN	3.9
2	B	51	VAL	3.8
3	Q	240	GLU	3.8
2	P	221	ASP	3.8
6	T	241	LYS	3.8
3	Q	205	ALA	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
7	U	242	GLN	3.8
10	X	194	ASP	3.7
1	A	250	LEU	3.7
3	Q	238	LYS	3.7
3	C	50	LEU	3.7
2	P	218	GLY	3.5
7	U	222	ASP	3.4
4	R	242	GLU	3.4
8	V	221	CYS	3.3
13	a	1	THR	3.3
3	Q	202	GLN	3.3
6	T	244	ASN	3.3
13	M	1	THR	3.3
9	W	1	SER	3.2
4	D	241	ALA	3.2
6	F	181	GLU	3.2
8	H	221	CYS	3.2
3	Q	225	GLU	3.2
3	Q	51	LYS	3.2
1	O	201	GLU	3.2
7	G	2	GLY	3.2
1	A	249	ALA	3.1
6	T	243	ILE	3.1
10	X	193	ASP	3.1
5	E	123	GLY	3.1
3	C	225	GLU	3.1
4	D	242	GLU	3.1
4	R	125	LEU	3.1
6	F	215	CYS	3.1
6	F	205	GLU	3.1
7	G	242	GLN	3.1
3	C	205	ALA	3.1
1	O	231	LYS	3.1
8	H	222	ASP	3.0
8	V	145	ASP	3.0
6	F	244	ASN	3.0
6	F	202	ASP	3.0
2	B	59	ASP	3.0
6	F	241	LYS	2.9
3	Q	236	GLN	2.9
5	E	233	ILE	2.9
13	M	47	ASP	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
6	T	2	THR	2.9
5	S	233	ILE	2.9
5	S	180	LYS	2.8
6	F	2	THR	2.8
3	Q	203	THR	2.8
2	P	59	ASP	2.8
5	E	201	ARG	2.8
7	G	179	LYS	2.8
7	G	181	LYS	2.7
11	K	212	GLY	2.7
5	S	54	GLU	2.7
3	C	236	GLN	2.7
11	Y	106	ARG	2.7
3	Q	223	SER	2.7
3	Q	180	LYS	2.7
2	P	222	GLY	2.7
9	I	133	LYS	2.6
9	I	1	SER	2.6
7	U	2	GLY	2.6
2	B	217	LYS	2.5
3	C	180	LYS	2.5
2	P	52	THR	2.5
1	A	248	GLU	2.5
1	A	182	GLU	2.5
5	S	52	ALA	2.5
3	Q	55	THR	2.4
4	R	1	ASP	2.4
5	S	225	ASP	2.4
7	U	181	LYS	2.4
5	S	173	ARG	2.4
11	Y	212	GLY	2.4
1	O	248	GLU	2.4
5	E	54	GLU	2.4
5	E	217	LYS	2.3
3	C	240	GLU	2.3
2	P	50	LYS	2.3
7	U	241	GLU	2.2
2	P	182	ASP	2.2
6	T	181	GLU	2.2
7	G	241	GLU	2.2
2	B	60	THR	2.2
1	O	250	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
6	T	180	PRO	2.2
6	T	53	LYS	2.2
3	C	47	ARG	2.2
3	C	239	GLN	2.2
7	G	51	PRO	2.2
12	Z	210	ASP	2.2
5	S	204	SER	2.1
7	G	208	GLU	2.1
2	B	242	GLY	2.1
6	T	205	GLU	2.1
5	S	218	ASP	2.1
3	C	181	GLU	2.1
3	Q	60	SER	2.1
3	Q	27	ARG	2.1
7	U	206	GLY	2.1
5	S	3	ASN	2.1
10	J	193	ASP	2.1
7	G	230	GLU	2.1
3	Q	141	ASP	2.1
14	b	104	ASP	2.1
5	E	207	VAL	2.1
14	N	105	LYS	2.1
3	C	1	GLY	2.1
3	Q	187	GLU	2.1
1	A	2	THR	2.1
2	B	93	HIS	2.0
12	Z	1	GLN	2.0
2	B	52	THR	2.0
14	b	195	GLN	2.0
4	R	230	GLU	2.0
9	W	191	LYS	2.0

## 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 monosaccharides in this entry.

## 6.4 Ligands

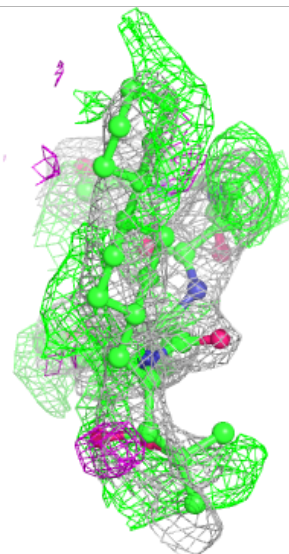
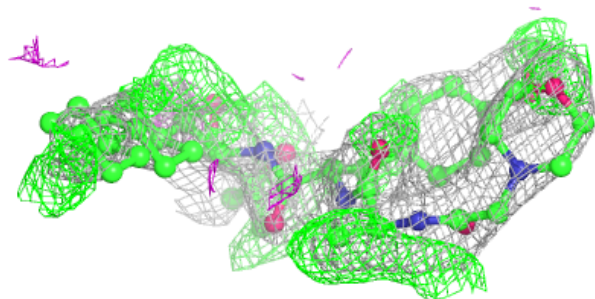
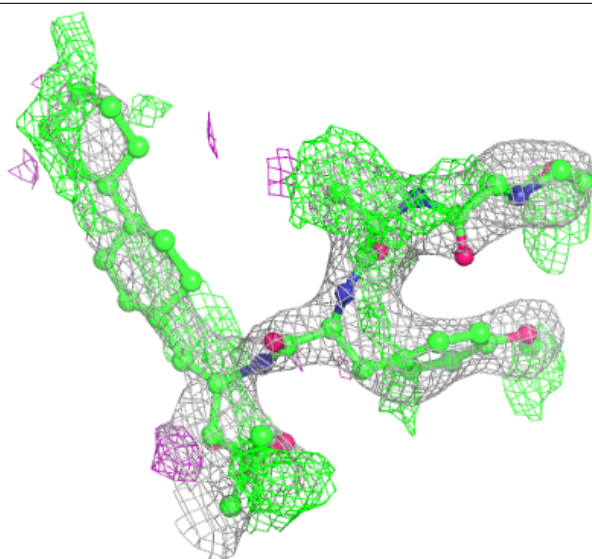
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
17	GWT	H	301	48/48	0.75	0.41	38,45,48,49	48
17	GWT	V	301	48/48	0.79	0.41	37,44,47,48	48
18	MES	V	303	12/12	0.83	0.38	75,77,92,98	12
18	MES	H	302	12/12	0.90	0.30	74,75,81,82	12
17	GWT	K	301	48/48	0.92	0.15	41,45,51,55	0
15	MG	Z	301	1/1	0.93	0.21	65,65,65,65	0
17	GWT	Y	301	48/48	0.93	0.14	42,46,50,55	0
15	MG	G	301	1/1	0.93	0.13	57,57,57,57	0
15	MG	V	302	1/1	0.93	0.26	84,84,84,84	0
15	MG	I	301	1/1	0.94	0.14	60,60,60,60	0
15	MG	K	303	1/1	0.95	0.12	47,47,47,47	0
15	MG	Y	302	1/1	0.96	0.14	64,64,64,64	0
15	MG	N	201	1/1	0.97	0.10	53,53,53,53	0
18	MES	K	304	12/12	0.97	0.16	43,45,53,54	12
15	MG	K	302	1/1	0.97	0.10	70,70,70,70	0
18	MES	Y	304	12/12	0.97	0.14	43,46,50,51	12
15	MG	Y	303	1/1	0.98	0.22	45,45,45,45	0
16	CL	U	301	1/1	0.98	0.09	48,48,48,48	0
16	CL	G	302	1/1	0.99	0.08	48,48,48,48	0
15	MG	X	201	1/1	0.99	0.32	45,45,45,45	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.

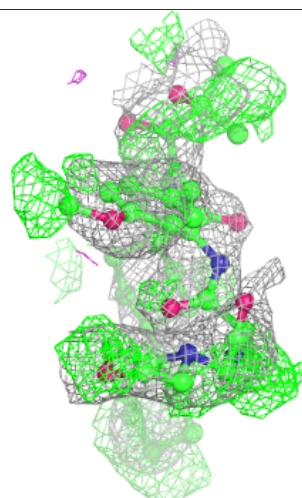
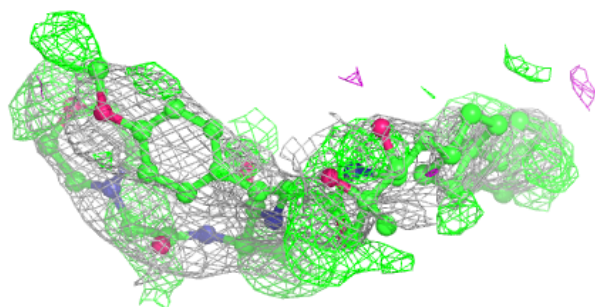
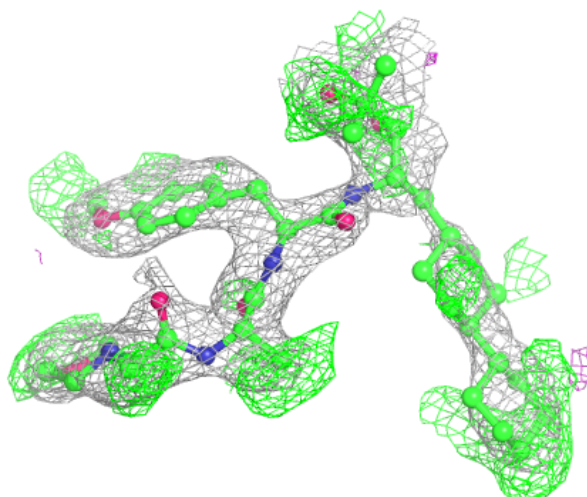
**Electron density around GWT H 301:**

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



**Electron density around GWT V 301:**

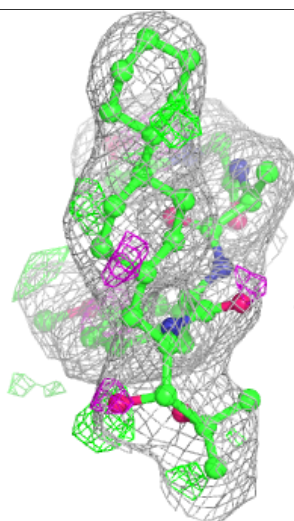
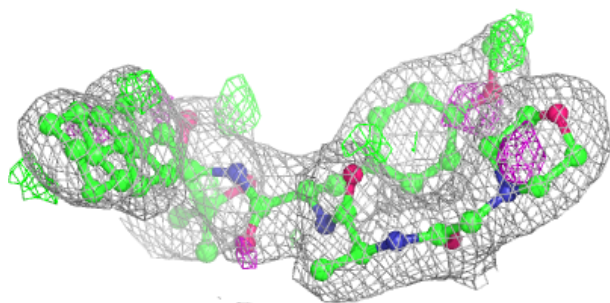
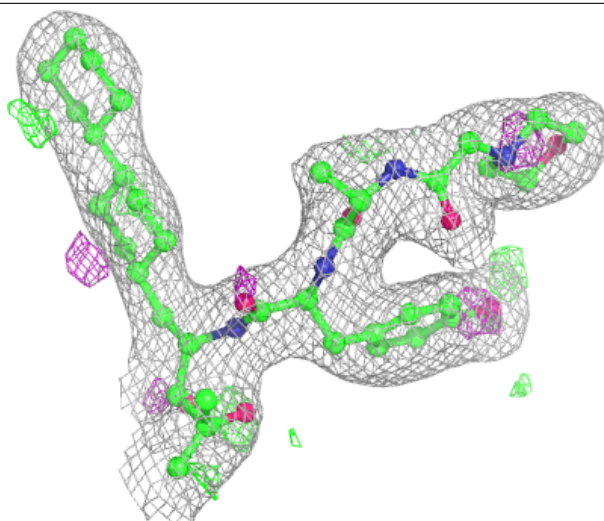
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

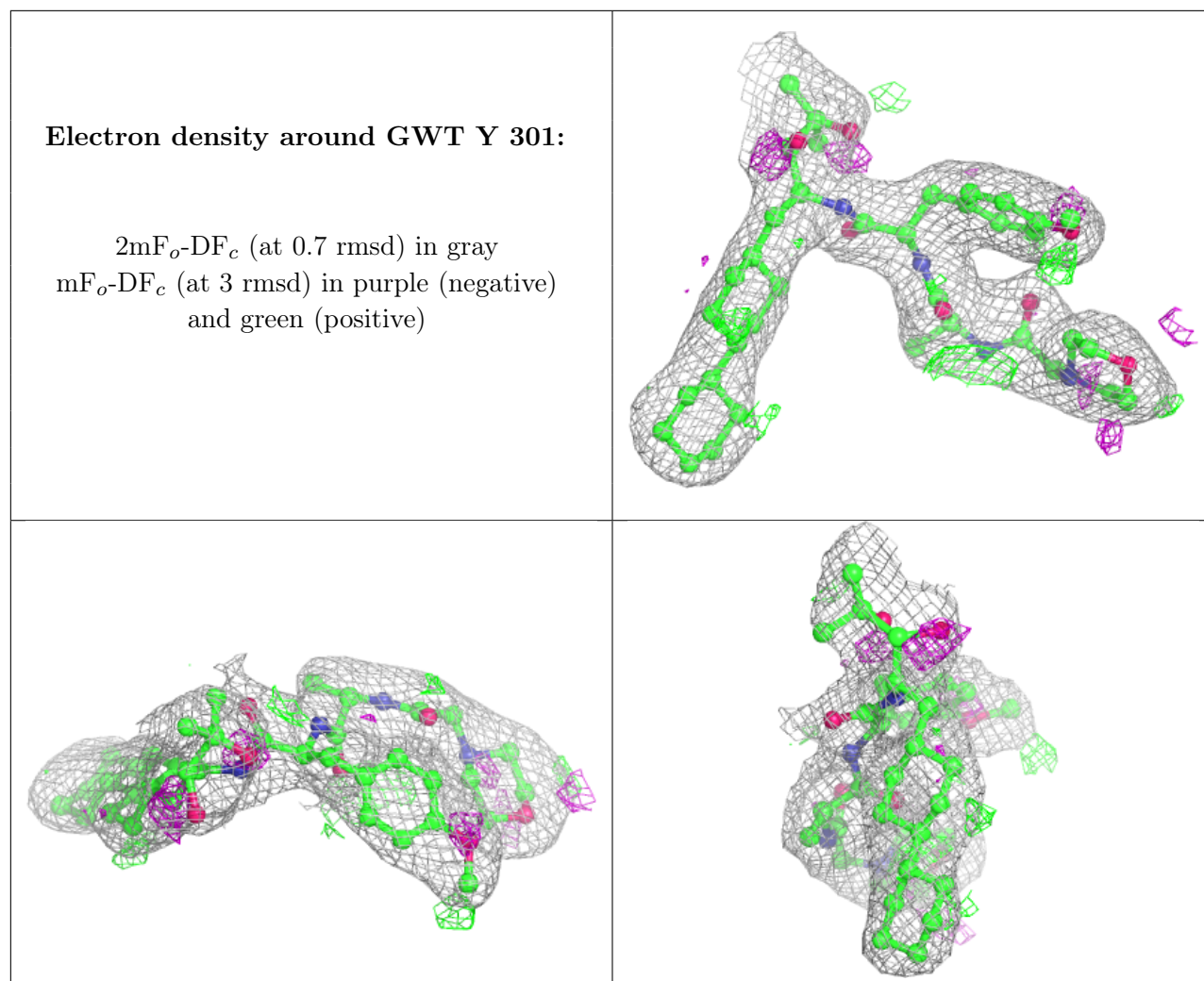




**Electron density around GWT K 301:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.