



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:05 pm BST

PDB ID : 6HW3  
Title : Yeast 20S proteasome in complex with 13  
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.

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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 : 1.8.5 (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

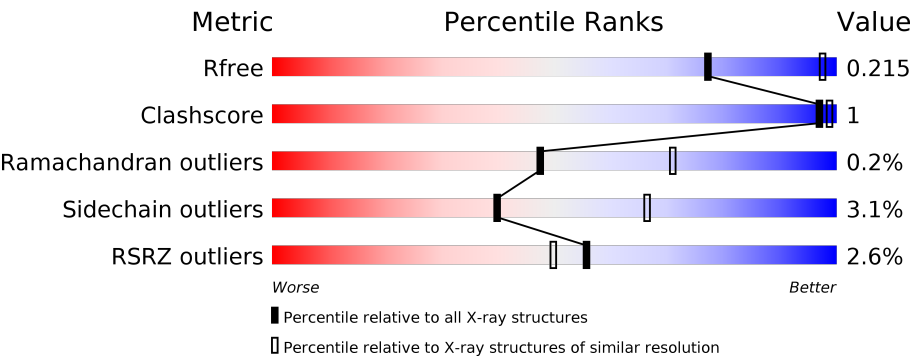
# 1 Overall quality at a glance i

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 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>4%</div><div>98%</div><div>•</div></div>
1	O	250	<div><div>4%</div><div>98%</div><div>•</div></div>
2	B	258	<div><div>4%</div><div>90%</div><div>• 5%</div></div>
2	P	258	<div><div>5%</div><div>91%</div><div>• 5%</div></div>
3	C	254	<div><div>6%</div><div>90%</div><div>• • 6%</div></div>
3	Q	254	<div><div>6%</div><div>90%</div><div>• • 6%</div></div>

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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	246	
13	a	246	
14	N	196	
14	b	196	

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 50171 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
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
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
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
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
5	E	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			
5	S	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			

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

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

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

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

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

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 subunit beta type-3.

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 subunit beta type-4.

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

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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	K	1	Total	Mg	0	0
			1	1		

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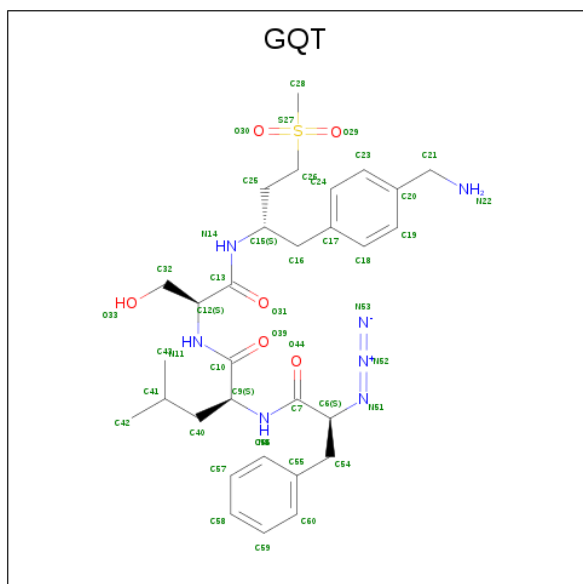
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	I	2	Total	Mg	0	0
			2	2		
15	Z	1	Total	Mg	0	0
			1	1		
15	N	1	Total	Mg	0	0
			1	1		
15	X	1	Total	Mg	0	0
			1	1		
15	L	1	Total	Mg	0	0
			1	1		

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

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

- Molecule 17 is (2 {S})- {N}-[(2 {S})-1-[(2 {S})-1-[4-(aminomethyl)phenyl]-4-methylsulfonylbutan-2-yl]amino]-3-oxidanyl-1-oxidanylidene-propan-2-yl]-2-[(2 {S})-2-azido-3-phenylpropanoyl]amino]-4-methylpentanamide (three-letter code: GQT) (formula: C<sub>30</sub>H<sub>43</sub>N<sub>7</sub>O<sub>6</sub>S).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	K	1	Total	C	N	O	S	0	0
			44	30	7	6	1		
17	V	1	Total	C	N	O	S	0	0
			44	30	7	6	1		
17	Y	1	Total	C	N	O	S	0	0
			44	30	7	6	1		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	23	Total	O	0	0
			23	23		
18	B	29	Total	O	0	0
			29	29		
18	C	19	Total	O	0	0
			19	19		
18	D	13	Total	O	0	0
			13	13		
18	E	12	Total	O	0	0
			12	12		
18	F	31	Total	O	0	0
			31	31		
18	G	31	Total	O	0	0
			31	31		
18	H	39	Total	O	0	0
			39	39		
18	I	23	Total	O	0	0
			23	23		
18	J	29	Total	O	0	0
			29	29		
18	K	32	Total	O	0	0
			32	32		
18	L	31	Total	O	0	0
			31	31		
18	M	31	Total	O	0	0
			31	31		
18	N	25	Total	O	0	0
			25	25		
18	O	23	Total	O	0	0
			23	23		
18	P	20	Total	O	0	0
			20	20		

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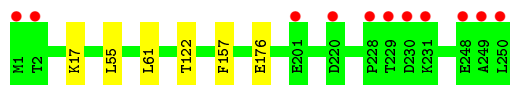
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	Q	14	Total 14	O 14	0	0
18	R	12	Total 12	O 12	0	0
18	S	10	Total 10	O 10	0	0
18	T	24	Total 24	O 24	0	0
18	U	31	Total 31	O 31	0	0
18	V	25	Total 25	O 25	0	0
18	W	16	Total 16	O 16	0	0
18	X	31	Total 31	O 31	0	0
18	Y	28	Total 28	O 28	0	0
18	Z	24	Total 24	O 24	0	0
18	a	31	Total 31	O 31	0	0
18	b	32	Total 32	O 32	0	0

### 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 ( $RSRZ > 2$ ). 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.

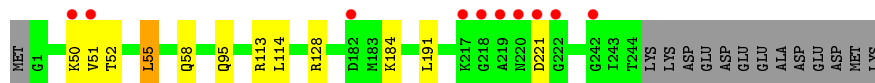
- Molecule 1: Proteasome subunit alpha type-2



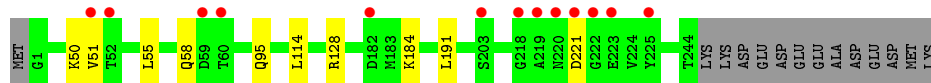
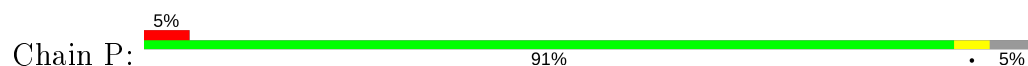
- Molecule 1: Proteasome subunit alpha type-2



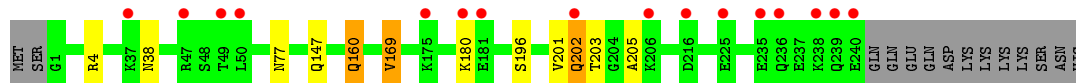
- Molecule 2: Proteasome subunit alpha type-3



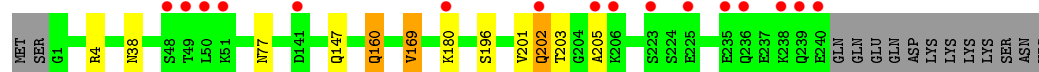
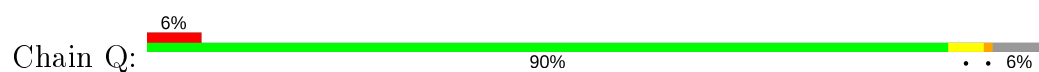
- Molecule 2: Proteasome subunit alpha type-3



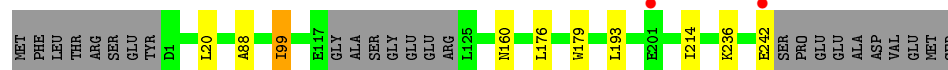
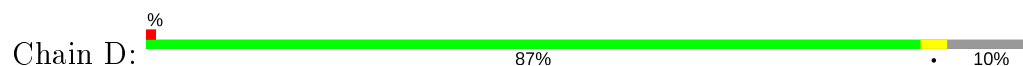
- Molecule 3: Proteasome subunit alpha type-4



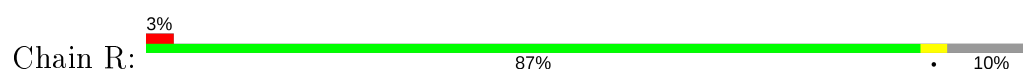
- Molecule 3: Proteasome subunit alpha type-4



- Molecule 4: Proteasome subunit alpha type-5



- Molecule 4: Proteasome subunit alpha type-5



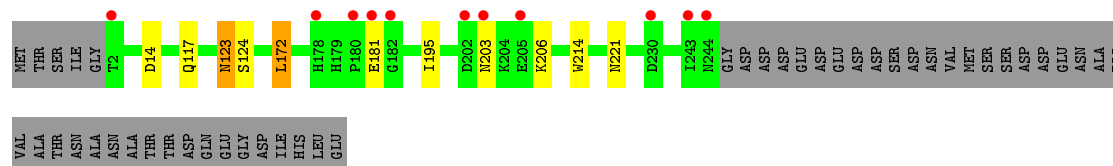
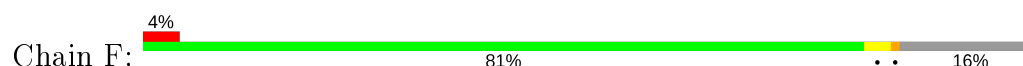
- Molecule 5: Proteasome subunit alpha type-6



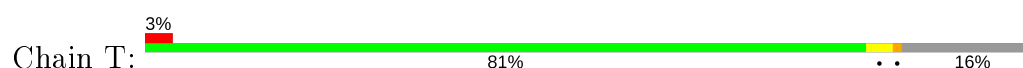
- Molecule 5: Proteasome subunit alpha type-6

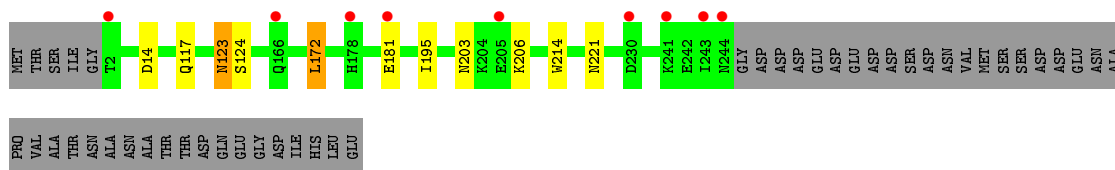


- Molecule 6: Probable proteasome subunit alpha type-7

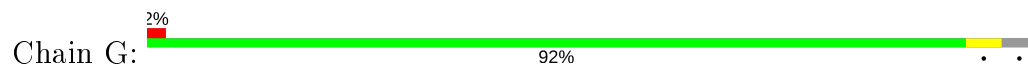


- Molecule 6: Probable proteasome subunit alpha type-7

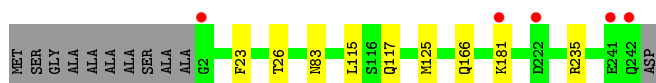




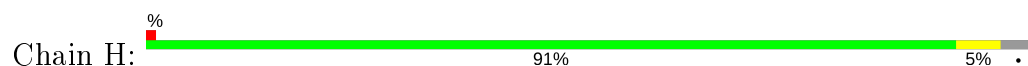
- Molecule 7: Proteasome subunit alpha type-1



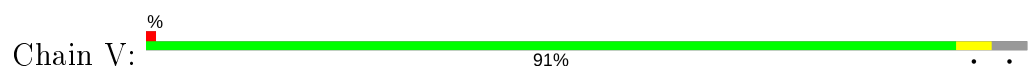
- Molecule 7: Proteasome subunit alpha type-1



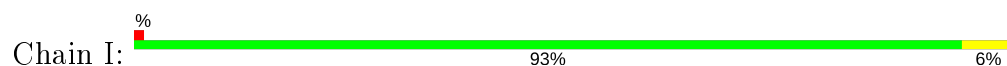
- Molecule 8: Proteasome subunit beta type-2



- Molecule 8: Proteasome subunit beta type-2



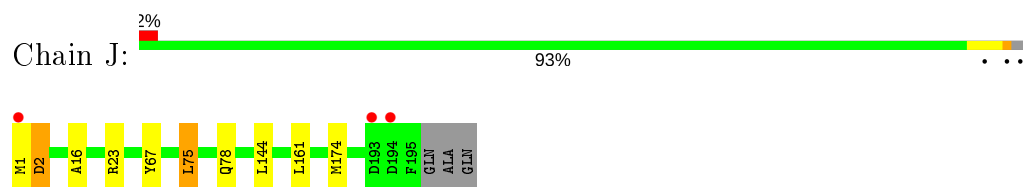
- Molecule 9: Proteasome subunit beta type-3



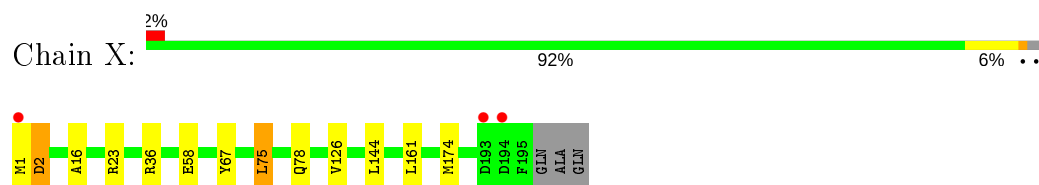
- Molecule 9: Proteasome subunit beta type-3



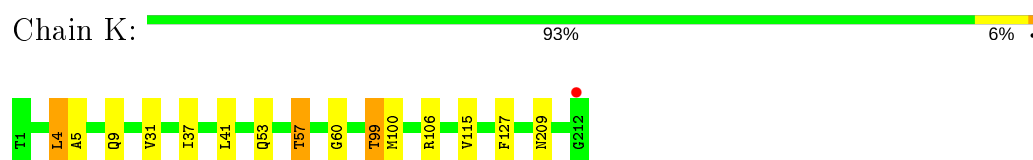
- Molecule 10: Proteasome subunit beta type-4



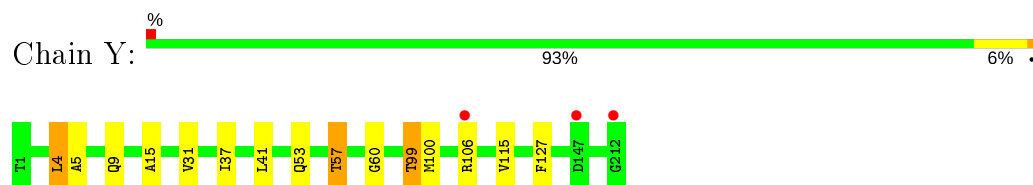
- Molecule 10: Proteasome subunit beta type-4



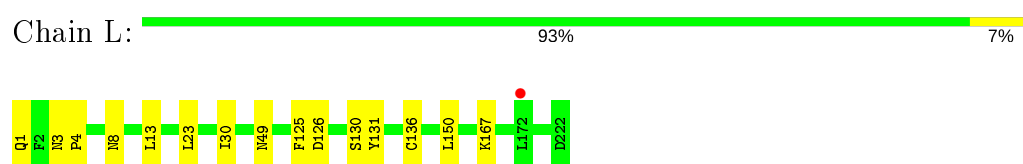
- Molecule 11: PROTEASOME SUBUNIT BETA TYPE-5



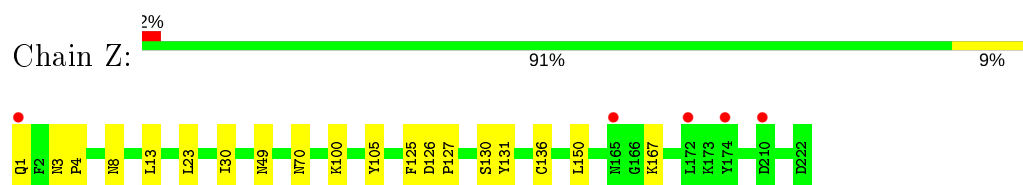
- Molecule 11: PROTEASOME SUBUNIT BETA TYPE-5



- Molecule 12: Proteasome subunit beta type-6

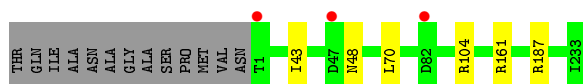


- Molecule 12: Proteasome subunit beta type-6



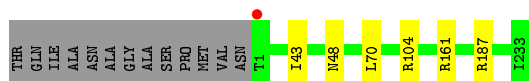
- Molecule 13: Proteasome subunit beta type-7





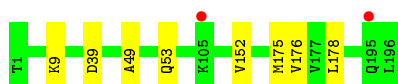
- Molecule 13: Proteasome subunit beta type-7

Chain a: 92% • 5%



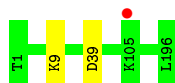
- Molecule 14: Proteasome subunit beta type-1

Chain N: 96% •



- Molecule 14: Proteasome subunit beta type-1

Chain b: 99% •



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.51Å 299.28Å 145.42Å 90.00° 112.95° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 15.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.1 (15.00-2.60) 98.7 (15.00-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.78 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.191 , 0.215 0.195 , 0.215	Depositor DCC
$R_{free}$ test set	15981 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.2	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 34.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	50171	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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: MG, GQT, CL

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	0.56	0/2642
1	O	0.35	0/1952	0.56	0/2642
2	B	0.35	0/1934	0.59	0/2618
2	P	0.34	0/1934	0.58	0/2618
3	C	0.35	0/1910	0.61	0/2586
3	Q	0.34	0/1910	0.62	0/2586
4	D	0.34	0/1837	0.57	0/2475
4	R	0.33	0/1837	0.57	0/2475
5	E	0.34	0/1800	0.56	0/2433
5	S	0.34	0/1800	0.56	0/2433
6	F	0.34	0/1932	0.54	0/2609
6	T	0.34	0/1932	0.54	0/2609
7	G	0.34	0/1945	0.56	0/2634
7	U	0.35	0/1945	0.55	0/2634
8	H	0.34	0/1715	0.57	0/2326
8	V	0.33	0/1715	0.57	0/2326
9	I	0.34	0/1611	0.58	0/2174
9	W	0.34	0/1611	0.59	0/2174
10	J	0.34	0/1589	0.59	0/2142
10	X	0.34	0/1589	0.59	0/2142
11	K	0.34	0/1681	0.66	2/2274 (0.1%)
11	Y	0.34	0/1681	0.66	2/2274 (0.1%)
12	L	0.34	0/1795	0.58	0/2420
12	Z	0.34	0/1795	0.58	0/2420
13	M	0.34	0/1855	0.63	0/2514
13	a	0.34	0/1855	0.63	0/2514
14	N	0.32	0/1541	0.57	0/2087
14	b	0.32	0/1541	0.57	0/2087
All	All	0.34	0/50194	0.58	4/67868 (0.0%)

There are no bond length outliers.



All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	4	LEU	CD1-CG-CD2	-11.21	76.88	110.50
11	K	4	LEU	CD1-CG-CD2	-10.56	78.82	110.50
11	K	4	LEU	CB-CG-CD2	9.98	127.97	111.00
11	Y	4	LEU	CB-CG-CD1	9.86	127.76	111.00

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	3	0
1	O	1915	0	1929	1	0
2	B	1904	0	1904	4	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	2	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	3	0
7	G	1907	0	1901	2	0
7	U	1907	0	1901	1	0
8	H	1684	0	1687	4	0
8	V	1684	0	1687	2	0
9	I	1581	0	1574	6	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	3	0
10	X	1561	0	1569	5	0
11	K	1644	0	1594	9	0
11	Y	1644	0	1594	9	0
12	L	1757	0	1711	5	0
12	Z	1757	0	1711	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	1824	0	1832	0	0
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	2	0	0	0	0
15	K	1	0	0	0	0
15	L	1	0	0	0	0
15	N	1	0	0	0	0
15	X	1	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	44	0	0	1	0
17	K	44	0	0	2	0
17	V	44	0	0	0	0
17	Y	44	0	0	2	0
18	A	23	0	0	0	0
18	B	29	0	0	1	0
18	C	19	0	0	0	0
18	D	13	0	0	0	0
18	E	12	0	0	0	0
18	F	31	0	0	0	0
18	G	31	0	0	0	0
18	H	39	0	0	0	0
18	I	23	0	0	0	0
18	J	29	0	0	0	0
18	K	32	0	0	0	0
18	L	31	0	0	0	0
18	M	31	0	0	0	0
18	N	25	0	0	0	0
18	O	23	0	0	0	0
18	P	20	0	0	0	0
18	Q	14	0	0	0	0
18	R	12	0	0	0	0
18	S	10	0	0	0	0
18	T	24	0	0	0	0
18	U	31	0	0	0	0
18	V	25	0	0	0	0
18	W	16	0	0	0	0
18	X	31	0	0	0	0
18	Y	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	Z	24	0	0	0	0
18	a	31	0	0	0	0
18	b	32	0	0	0	0
All	All	50171	0	49064	84	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 (84) 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)
8:H:3:ILE:HG22	8:H:99:ILE:HD12	1.81	0.61
8:V:3:ILE:HG22	8:V:99:ILE:HD12	1.81	0.61
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.85	0.59
11:Y:53:GLN:O	11:Y:57:THR:OG1	2.21	0.58
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.86	0.57
14:N:152:VAL:HA	14:N:175:MET:HE1	1.86	0.57
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.86	0.57
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.89	0.55
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.71	0.55
10:X:1:MET:O	10:X:2:ASP:HB2	2.07	0.55
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.71	0.55
11:K:53:GLN:O	11:K:57:THR:OG1	2.26	0.54
11:K:99:THR:HG22	11:K:115:VAL:HB	1.90	0.54
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.42	0.54
10:J:1:MET:O	10:J:2:ASP:HB2	2.07	0.54
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.43	0.54
11:Y:99:THR:HG22	11:Y:115:VAL:HB	1.90	0.54
14:N:49:ALA:O	14:N:53:GLN:HB2	2.07	0.54
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.91	0.53
8:H:19:ARG:NH1	8:H:167:LEU:O	2.44	0.50
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.58	0.49
17:Y:301:GQT:C57	12:Z:127:PRO:HB2	2.43	0.49
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	1.96	0.48
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.96	0.47
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.96	0.47
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.96	0.47
8:H:50:ALA:HB2	9:I:128:CYS:HB2	1.96	0.47
8:V:19:ARG:NH1	8:V:167:LEU:O	2.47	0.46
6:F:123:ASN:HD22	6:F:123:ASN:C	2.18	0.46
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.98	0.46
6:T:123:ASN:C	6:T:123:ASN:HD22	2.19	0.46
12:L:8:ASN:HA	12:L:30:ILE:O	2.16	0.46
8:H:22:GLN:NE2	17:H:301:GQT:N53	2.64	0.45
7:U:23:PHE:O	7:U:26:THR:HB	2.17	0.45
11:Y:4:LEU:HD11	11:Y:15:ALA:HB3	1.98	0.45
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.98	0.45
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.99	0.45
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.80	0.45
6:F:123:ASN:HD22	6:F:124:SER:N	2.14	0.45
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.99	0.45
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.64	0.45
1:A:176:GLU:HG2	2:B:55:LEU:HD13	1.99	0.44
7:G:23:PHE:O	7:G:26:THR:HB	2.17	0.44
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.99	0.44
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.99	0.44
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.98	0.44
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.17	0.44
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.00	0.44
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.00	0.44
9:I:98:ARG:O	9:I:126:ILE:HD11	2.19	0.43
11:K:37:ILE:HB	11:K:41:LEU:HB3	2.01	0.43
10:X:36:ARG:NH1	10:X:58:GLU:OE2	2.52	0.43
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	2.00	0.43
10:X:16:ALA:HB2	10:X:161:LEU:HD21	2.00	0.43
2:B:113:ARG:HD2	18:B:327:HOH:O	2.17	0.43
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.49	0.43
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.49	0.43
6:T:123:ASN:HD22	6:T:124:SER:N	2.17	0.43
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.67	0.43
17:K:301:GQT:N51	17:K:301:GQT:C56	2.82	0.43
11:Y:31:VAL:HG11	17:Y:301:GQT:C23	2.50	0.42
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.54	0.42
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	2.17	0.42
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.84	0.42
3:C:201:VAL:O	3:C:202:GLN:CB	2.67	0.42
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.01	0.42
11:K:100:MET:CE	11:K:127:PHE:HB2	2.49	0.42
11:K:31:VAL:HG11	17:K:301:GQT:C23	2.50	0.42
1:A:55:LEU:HD12	7:G:170:THR:HG23	2.02	0.42
11:K:209:ASN:O	9:W:37:ASN:ND2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.50	0.41
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.01	0.41
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.55	0.41
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.01	0.41
9:W:98:ARG:O	9:W:126:ILE:HD11	2.21	0.41
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.50	0.41
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.56	0.41
12:Z:100:LYS:HD3	12:Z:105:TYR:CZ	2.56	0.41
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.02	0.41
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.50	0.40
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.57	0.40
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.85	0.40
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
1	O	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
2	B	242/258 (94%)	234 (97%)	6 (2%)	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%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	222 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
6	T	241/288 (84%)	237 (98%)	4 (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%)	215 (98%)	5 (2%)	0	100	100
8	V	220/232 (95%)	215 (98%)	5 (2%)	0	100	100
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%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
13	a	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
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%)	6114 (97%)	152 (2%)	10 (0%)	47	71

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
10	J	2	ASP
2	P	51	VAL
3	Q	202	GLN
10	X	2	ASP
3	C	205	ALA
3	Q	205	ALA
2	B	221	ASP
2	P	221	ASP

### 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	85
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	85
2	B	203/216 (94%)	196 (97%)	7 (3%)	37	63
2	P	203/216 (94%)	197 (97%)	6 (3%)	41	67
3	C	212/226 (94%)	204 (96%)	8 (4%)	33	59
3	Q	212/226 (94%)	204 (96%)	8 (4%)	33	59
4	D	194/215 (90%)	187 (96%)	7 (4%)	35	61
4	R	194/215 (90%)	187 (96%)	7 (4%)	35	61
5	E	190/193 (98%)	182 (96%)	8 (4%)	30	55
5	S	190/193 (98%)	182 (96%)	8 (4%)	30	55
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%)	175 (97%)	6 (3%)	38	64
8	V	181/190 (95%)	175 (97%)	6 (3%)	38	64
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%)	164 (97%)	5 (3%)	41	67
11	Y	169/169 (100%)	165 (98%)	4 (2%)	49	74
12	L	185/185 (100%)	178 (96%)	7 (4%)	33	59
12	Z	185/185 (100%)	178 (96%)	7 (4%)	33	59
13	M	199/208 (96%)	193 (97%)	6 (3%)	41	67
13	a	199/208 (96%)	193 (97%)	6 (3%)	41	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	162/162 (100%)	160 (99%)	2 (1%)	71	87
14	b	162/162 (100%)	160 (99%)	2 (1%)	71	87
All	All	5312/5540 (96%)	5148 (97%)	164 (3%)	40	66

All (164) 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	52	THR
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	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	203	THR
4	D	20	LEU
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	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
6	F	14	ASP

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Mol	Chain	Res	Type
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
7	G	235	ARG
8	H	30	ASN
8	H	34	LEU
8	H	36	ARG
8	H	38	SER
8	H	56	THR
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	57	THR
11	K	99	THR
11	K	106	ARG
12	L	1	GLN
12	L	23	LEU
12	L	49	ASN
12	L	126	ASP
12	L	130	SER
12	L	136	CYS
12	L	167	LYS
13	M	43	ILE

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Mol	Chain	Res	Type
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	9	LYS
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	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	203	THR
4	R	20	LEU
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	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
6	T	14	ASP
6	T	117	GLN
6	T	123	ASN

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Mol	Chain	Res	Type
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	34	LEU
8	V	36	ARG
8	V	38	SER
8	V	56	THR
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
10	X	174	MET
11	Y	9	GLN
11	Y	57	THR
11	Y	99	THR
11	Y	106	ARG
12	Z	1	GLN
12	Z	23	LEU
12	Z	49	ASN
12	Z	126	ASP
12	Z	130	SER
12	Z	136	CYS
12	Z	167	LYS
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG

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Mol	Chain	Res	Type
13	a	161	ARG
13	a	187	ARG
14	b	9	LYS
14	b	39	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
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
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	22	GLN
8	H	30	ASN

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Mol	Chain	Res	Type
8	H	86	HIS
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	158	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
1	O	94	HIS
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
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

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Mol	Chain	Res	Type
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	66	HIS
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
10	X	55	GLN
10	X	86	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	158	ASN
12	Z	159	GLN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
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 ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 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	GQT	K	301	11	44,45,45	1.52	5 (11%)	56,60,60	2.24	18 (32%)
17	GQT	H	301	8	44,45,45	1.77	8 (18%)	56,60,60	1.42	9 (16%)
17	GQT	Y	301	11	44,45,45	1.59	7 (15%)	56,60,60	2.17	17 (30%)
17	GQT	V	301	8	44,45,45	1.72	8 (18%)	56,60,60	1.51	11 (19%)

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	GQT	K	301	11	-	7/49/49/49	0/2/2/2
17	GQT	H	301	8	-	11/49/49/49	0/2/2/2
17	GQT	Y	301	11	-	6/49/49/49	0/2/2/2
17	GQT	V	301	8	-	12/49/49/49	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	301	GQT	N52-N51	-5.57	1.08	1.23
17	Y	301	GQT	C16-C17	-5.33	1.38	1.51
17	K	301	GQT	C16-C17	-5.19	1.38	1.51
17	V	301	GQT	N52-N51	-4.69	1.11	1.23
17	H	301	GQT	C16-C17	-4.67	1.40	1.51
17	V	301	GQT	C16-C17	-4.64	1.40	1.51
17	Y	301	GQT	C54-C55	-4.07	1.41	1.51
17	V	301	GQT	O30-S27	4.05	1.53	1.44
17	K	301	GQT	C54-C55	-4.00	1.41	1.51
17	H	301	GQT	O29-S27	3.97	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	301	GQT	O30-S27	3.94	1.53	1.44
17	V	301	GQT	O29-S27	3.93	1.53	1.44
17	Y	301	GQT	O29-S27	3.81	1.52	1.44
17	V	301	GQT	C54-C55	-3.78	1.42	1.51
17	K	301	GQT	O29-S27	3.73	1.52	1.44
17	H	301	GQT	C54-C55	-3.59	1.42	1.51
17	Y	301	GQT	O30-S27	3.48	1.52	1.44
17	Y	301	GQT	C21-C20	-3.38	1.39	1.51
17	K	301	GQT	O30-S27	3.38	1.51	1.44
17	H	301	GQT	C21-C20	-3.35	1.39	1.51
17	V	301	GQT	C21-C20	-3.32	1.39	1.51
17	K	301	GQT	C21-C20	-3.31	1.39	1.51
17	V	301	GQT	C26-S27	3.14	1.82	1.78
17	H	301	GQT	C25-C26	2.80	1.55	1.52
17	H	301	GQT	C26-S27	2.67	1.82	1.78
17	V	301	GQT	C25-C26	2.38	1.55	1.52
17	Y	301	GQT	N52-N51	-2.31	1.17	1.23
17	Y	301	GQT	C26-S27	2.14	1.81	1.78

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	301	GQT	C56-C55-C60	-6.00	108.73	118.17
17	Y	301	GQT	C57-C58-C59	-6.00	108.78	119.93
17	K	301	GQT	O29-S27-C26	-5.96	104.17	108.34
17	K	301	GQT	C57-C58-C59	-5.95	108.88	119.93
17	Y	301	GQT	C56-C55-C60	-5.75	109.12	118.17
17	Y	301	GQT	O29-S27-C26	-5.68	104.37	108.34
17	Y	301	GQT	C58-C57-C56	4.98	127.78	120.19
17	K	301	GQT	C58-C57-C56	4.19	126.58	120.19
17	V	301	GQT	O29-S27-C26	-4.09	105.48	108.34
17	K	301	GQT	O30-S27-O29	-3.92	108.70	117.09
17	Y	301	GQT	O30-S27-O29	-3.79	109.00	117.09
17	H	301	GQT	O30-S27-O29	-3.74	109.09	117.09
17	K	301	GQT	C58-C59-C60	3.65	125.75	120.19
17	K	301	GQT	O30-S27-C26	3.65	110.90	108.34
17	V	301	GQT	O30-S27-O29	-3.60	109.40	117.09
17	H	301	GQT	O29-S27-C26	-3.54	105.87	108.34
17	K	301	GQT	C54-C6-N51	3.29	114.73	109.30
17	Y	301	GQT	O30-S27-C26	3.20	110.59	108.34
17	K	301	GQT	C57-C56-C55	3.19	125.53	120.63
17	K	301	GQT	C32-C12-N11	-3.13	103.50	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Y	301	GQT	C58-C59-C60	3.12	124.95	120.19
17	Y	301	GQT	C32-C12-N11	-3.08	103.61	110.56
17	K	301	GQT	C6-N51-N52	3.00	118.40	115.24
17	V	301	GQT	O30-S27-C26	2.99	110.44	108.34
17	Y	301	GQT	C59-C60-C55	2.96	125.17	120.63
17	Y	301	GQT	C6-N51-N52	2.83	118.21	115.24
17	K	301	GQT	C16-C17-C18	-2.76	115.43	120.91
17	Y	301	GQT	C9-C10-N11	-2.71	110.76	116.70
17	Y	301	GQT	C16-C17-C18	-2.70	115.54	120.91
17	Y	301	GQT	C54-C55-C56	2.66	126.18	120.91
17	K	301	GQT	C16-C17-C24	2.66	126.18	120.91
17	K	301	GQT	C9-C10-N11	-2.63	110.93	116.70
17	K	301	GQT	C54-C55-C56	2.62	126.11	120.91
17	V	301	GQT	C6-N51-N52	2.60	117.98	115.24
17	V	301	GQT	C16-C17-C24	2.59	126.05	120.91
17	Y	301	GQT	C16-C17-C24	2.56	126.00	120.91
17	H	301	GQT	C28-S27-C26	2.56	115.09	105.21
17	K	301	GQT	C59-C60-C55	2.54	124.53	120.63
17	V	301	GQT	C28-S27-C26	2.52	114.92	105.21
17	V	301	GQT	C25-C15-C16	2.52	115.24	111.14
17	H	301	GQT	C16-C17-C24	2.51	125.89	120.91
17	H	301	GQT	O30-S27-C26	2.49	110.09	108.34
17	Y	301	GQT	C54-C6-N51	2.46	113.36	109.30
17	V	301	GQT	C54-C55-C56	2.45	125.78	120.91
17	H	301	GQT	C54-C55-C56	2.40	125.67	120.91
17	Y	301	GQT	C28-S27-C26	2.34	114.23	105.21
17	Y	301	GQT	C57-C56-C55	2.32	124.20	120.63
17	V	301	GQT	C16-C17-C18	-2.31	116.31	120.91
17	H	301	GQT	C25-C15-C16	2.23	114.77	111.14
17	H	301	GQT	C16-C17-C18	-2.17	116.61	120.91
17	K	301	GQT	C28-S27-C26	2.15	113.50	105.21
17	K	301	GQT	C54-C55-C60	2.14	125.15	120.91
17	H	301	GQT	C12-C13-N14	-2.06	112.19	116.70
17	V	301	GQT	O29-S27-C28	-2.05	106.85	108.91
17	V	301	GQT	C12-C13-N14	-2.03	112.25	116.70

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	V	301	GQT	C25-C26-S27-O30
17	V	301	GQT	C13-C12-C32-O33

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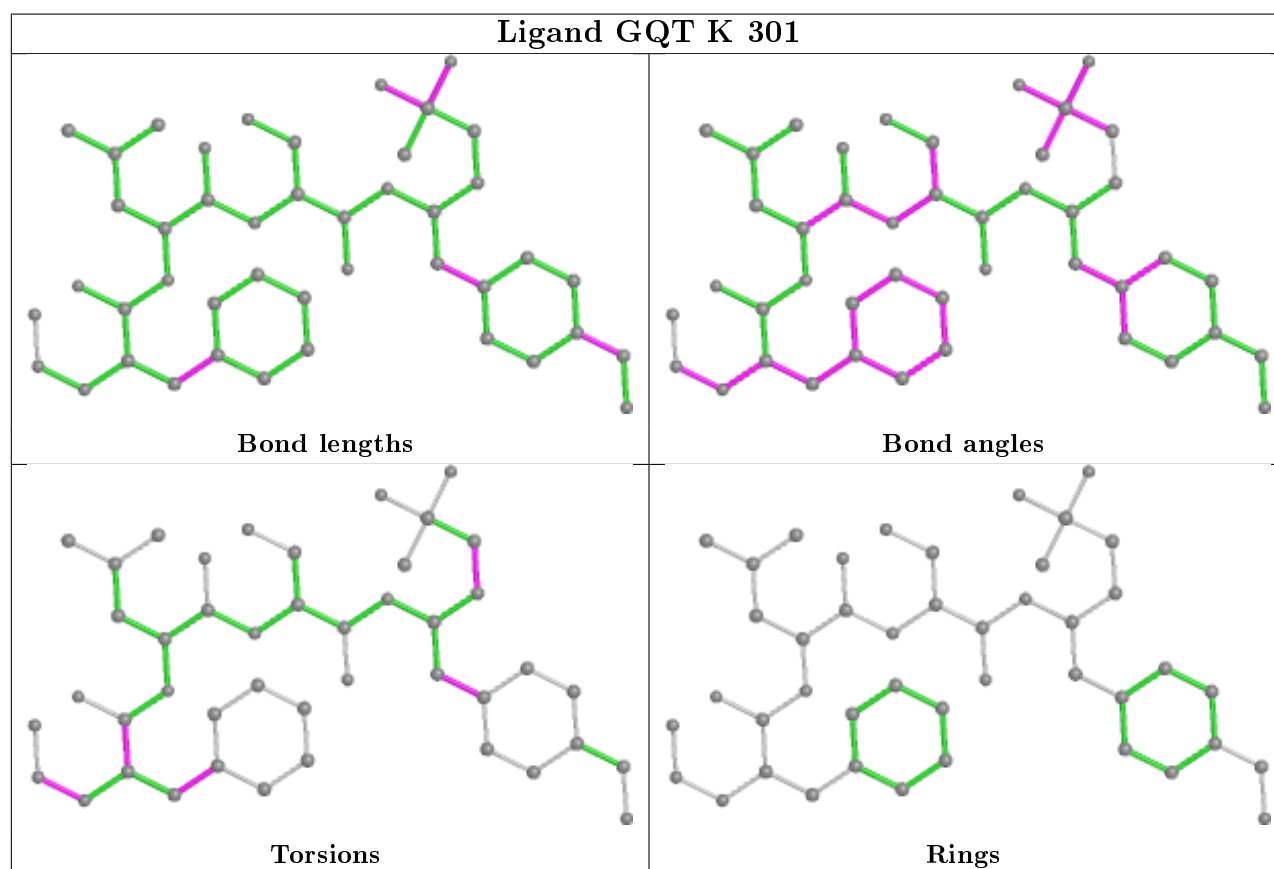
Mol	Chain	Res	Type	Atoms
17	K	301	GQT	N51-C6-C7-N8
17	K	301	GQT	C6-N51-N52-N53
17	H	301	GQT	C13-C12-C32-O33
17	Y	301	GQT	N51-C6-C7-N8
17	V	301	GQT	N11-C12-C32-O33
17	H	301	GQT	N11-C12-C32-O33
17	Y	301	GQT	C6-C54-C55-C56
17	Y	301	GQT	C15-C16-C17-C24
17	K	301	GQT	C15-C16-C17-C24
17	Y	301	GQT	C6-C54-C55-C60
17	Y	301	GQT	C15-C16-C17-C18
17	K	301	GQT	C15-C16-C17-C18
17	V	301	GQT	C15-C16-C17-C24
17	H	301	GQT	C15-C16-C17-C24
17	H	301	GQT	C15-C16-C17-C18
17	V	301	GQT	C15-C16-C17-C18
17	K	301	GQT	C6-C54-C55-C56
17	V	301	GQT	C6-C54-C55-C56
17	H	301	GQT	C6-C54-C55-C56
17	K	301	GQT	C6-C54-C55-C60
17	H	301	GQT	C6-C54-C55-C60
17	V	301	GQT	C6-C54-C55-C60
17	V	301	GQT	C25-C26-S27-C28
17	H	301	GQT	C25-C26-S27-C28
17	V	301	GQT	C6-N51-N52-N53
17	V	301	GQT	C7-C6-N51-N52
17	H	301	GQT	C7-C6-N51-N52
17	V	301	GQT	C25-C26-S27-O29
17	H	301	GQT	C25-C26-S27-O30
17	V	301	GQT	C15-C25-C26-S27
17	H	301	GQT	C15-C25-C26-S27
17	H	301	GQT	C25-C26-S27-O29
17	Y	301	GQT	C15-C25-C26-S27
17	K	301	GQT	C15-C25-C26-S27

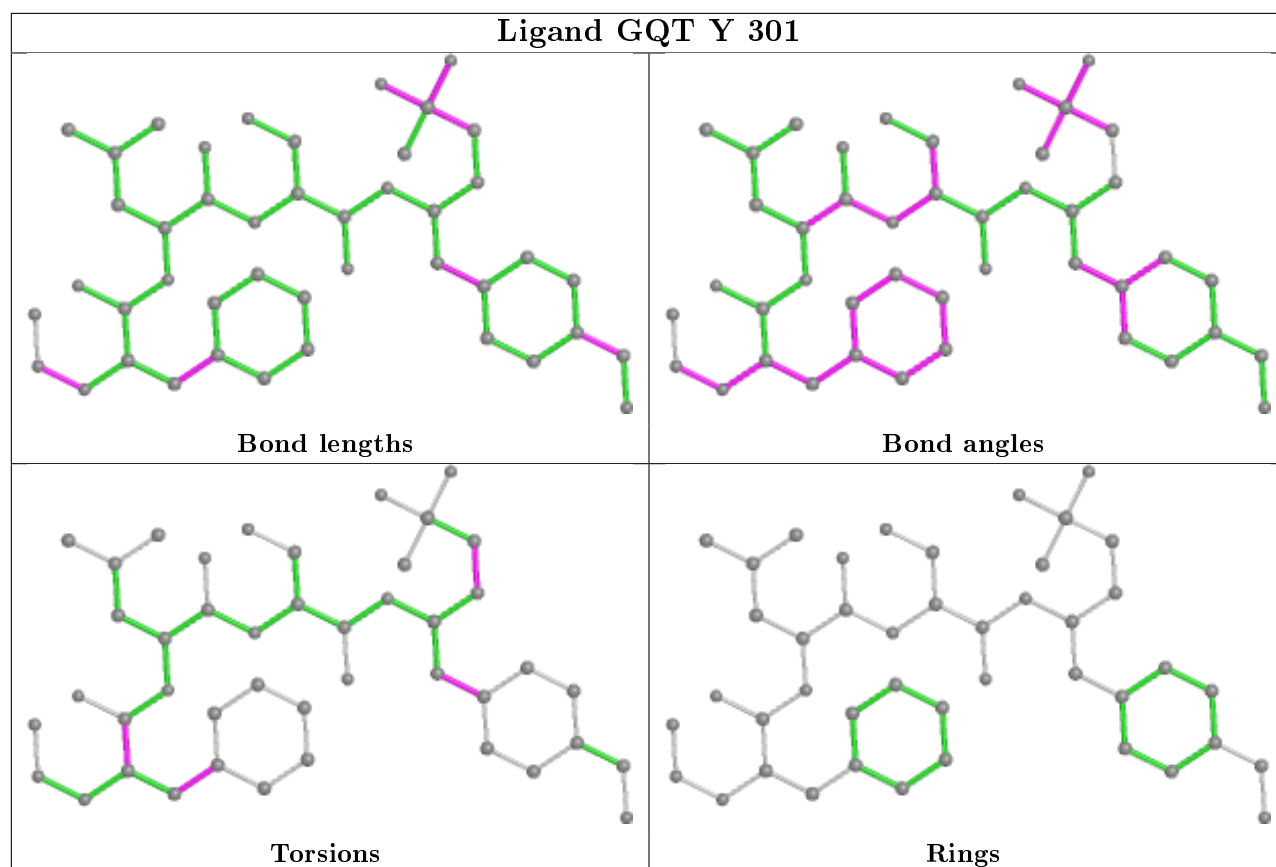
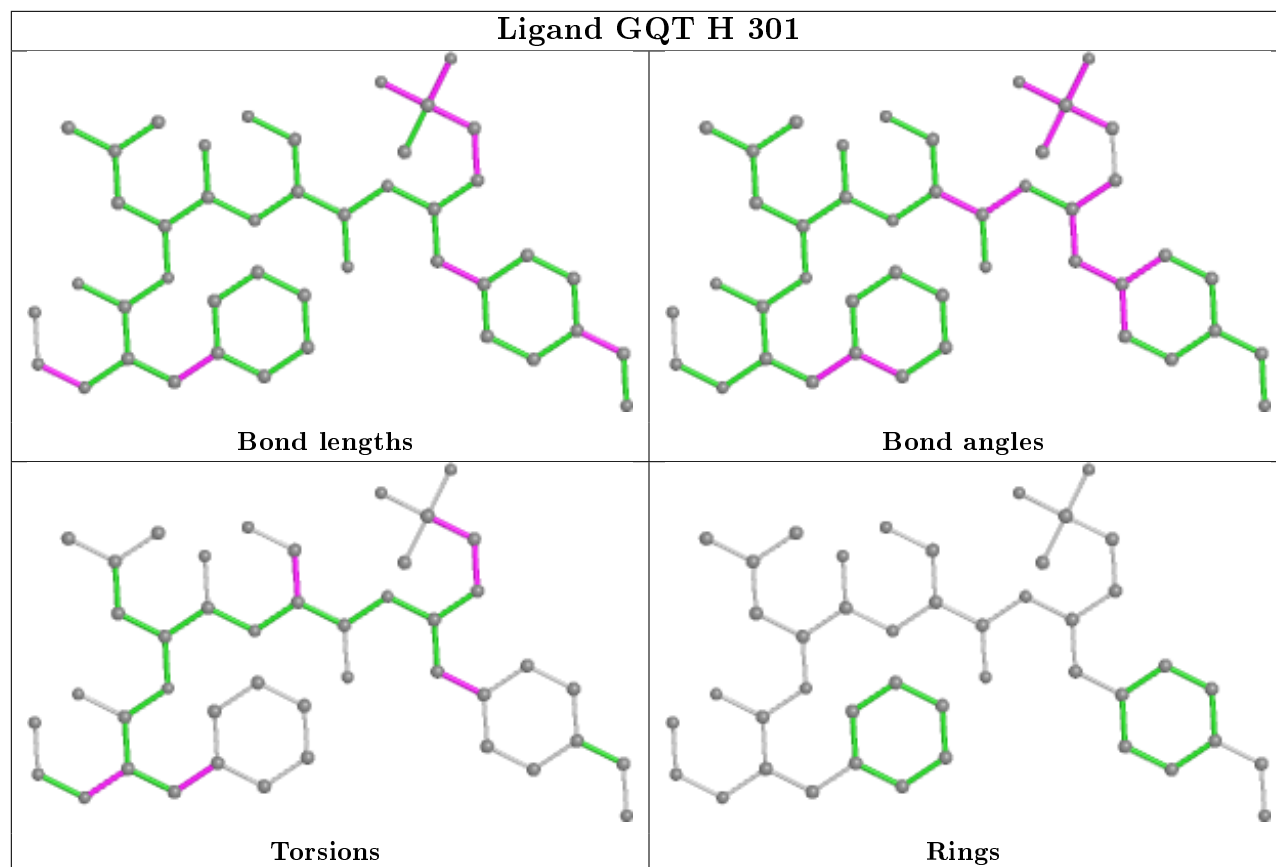
There are no ring outliers.

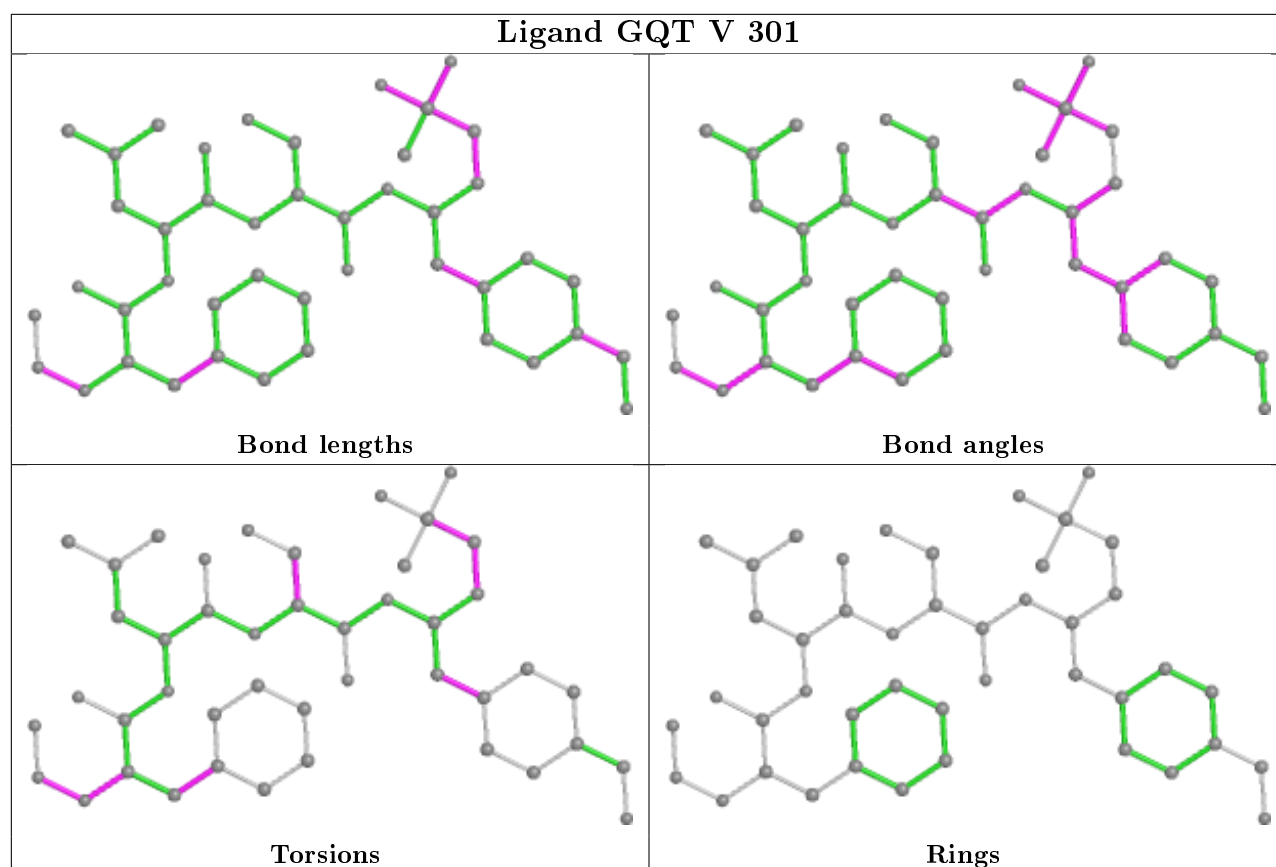
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	K	301	GQT	2	0
17	H	301	GQT	1	0
17	Y	301	GQT	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.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å²)	Q<0.9
1	A	250/250 (100%)	-0.21	11 (4%)	34	27	44, 61, 106, 154	0
1	O	250/250 (100%)	-0.16	10 (4%)	38	31	46, 68, 112, 159	0
2	B	244/258 (94%)	-0.17	10 (4%)	37	30	44, 67, 114, 167	0
2	P	244/258 (94%)	-0.17	13 (5%)	26	20	46, 68, 115, 161	0
3	C	240/254 (94%)	-0.10	16 (6%)	17	13	43, 70, 133, 163	0
3	Q	240/254 (94%)	0.19	16 (6%)	17	13	51, 83, 164, 198	0
4	D	235/260 (90%)	-0.25	2 (0%)	84	82	49, 72, 104, 150	0
4	R	235/260 (90%)	-0.14	8 (3%)	45	38	53, 75, 118, 165	0
5	E	231/234 (98%)	-0.16	6 (2%)	56	50	48, 74, 113, 158	0
5	S	231/234 (98%)	-0.10	12 (5%)	27	21	50, 77, 126, 157	0
6	F	243/288 (84%)	-0.30	11 (4%)	33	26	44, 67, 119, 146	0
6	T	243/288 (84%)	-0.24	9 (3%)	41	34	45, 71, 123, 159	0
7	G	241/252 (95%)	-0.30	6 (2%)	57	51	41, 61, 108, 156	0
7	U	241/252 (95%)	-0.37	5 (2%)	63	58	45, 61, 97, 134	0
8	H	222/232 (95%)	-0.16	2 (0%)	84	82	47, 62, 104, 136	0
8	V	222/232 (95%)	-0.11	3 (1%)	75	71	50, 65, 105, 142	0
9	I	204/205 (99%)	-0.58	2 (0%)	82	80	40, 56, 86, 114	0
9	W	204/205 (99%)	-0.54	2 (0%)	82	80	41, 59, 89, 120	0
10	J	195/198 (98%)	-0.44	3 (1%)	73	70	40, 57, 88, 130	0
10	X	195/198 (98%)	-0.49	3 (1%)	73	70	42, 59, 88, 139	0
11	K	212/212 (100%)	-0.47	1 (0%)	91	89	42, 59, 90, 117	0
11	Y	212/212 (100%)	-0.50	3 (1%)	75	71	41, 58, 89, 117	0
12	L	222/222 (100%)	-0.44	1 (0%)	91	89	41, 61, 99, 122	0
12	Z	222/222 (100%)	-0.38	5 (2%)	60	54	37, 60, 96, 117	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/246 (94%)	-0.48	3 (1%)	77	73	37, 60, 88, 98	0
13	a	233/246 (94%)	-0.50	1 (0%)	92	91	35, 58, 85, 108	0
14	N	196/196 (100%)	-0.51	2 (1%)	82	80	29, 54, 86, 111	0
14	b	196/196 (100%)	-0.47	1 (0%)	91	89	31, 55, 87, 109	0
All	All	6336/6614 (95%)	-0.30	167 (2%)	56	50	29, 64, 111, 198	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	1	MET	8.5
2	P	219	ALA	8.4
1	O	231	LYS	7.1
2	B	220	ASN	6.8
1	A	1	MET	6.6
3	Q	49	THR	6.5
2	B	51	VAL	6.1
2	B	219	ALA	5.9
3	Q	50	LEU	5.9
1	O	249	ALA	5.7
2	P	51	VAL	5.5
3	C	206	LYS	5.5
2	B	221	ASP	5.4
5	E	202	ASP	5.3
10	X	1	MET	5.2
5	S	202	ASP	5.2
1	A	229	THR	4.9
3	Q	206	LYS	4.8
3	Q	238	LYS	4.7
2	P	220	ASN	4.7
3	Q	239	GLN	4.6
8	H	222	ASP	4.5
10	J	194	ASP	4.5
8	H	221	CYS	4.5
3	Q	202	GLN	4.5
10	J	1	MET	4.5
8	V	222	ASP	4.4
1	O	229	THR	4.4
2	B	218	GLY	4.3
3	Q	48	SER	4.3
1	A	231	LYS	4.2
2	P	221	ASP	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	C	202	GLN	4.2
3	Q	51	LYS	4.1
10	X	194	ASP	4.1
4	D	242	GLU	4.0
5	E	233	ILE	4.0
3	C	238	LYS	3.9
3	Q	240	GLU	3.9
2	P	222	GLY	3.8
3	C	235	GLU	3.7
4	R	241	ALA	3.7
8	V	221	CYS	3.7
6	F	202	ASP	3.6
1	A	250	LEU	3.6
3	Q	141	ASP	3.5
3	C	239	GLN	3.5
9	W	1	SER	3.4
6	F	205	GLU	3.4
5	E	123	GLY	3.4
3	C	49	THR	3.3
13	a	1	THR	3.3
3	C	240	GLU	3.3
4	R	242	GLU	3.3
7	U	242	GLN	3.3
7	G	3	TYR	3.3
3	C	50	LEU	3.2
5	S	54	GLU	3.2
5	S	233	ILE	3.2
1	A	220	ASP	3.2
2	P	59	ASP	3.2
5	E	201	ARG	3.1
3	Q	236	GLN	3.1
10	J	193	ASP	3.1
1	O	250	LEU	3.1
7	G	240	ALA	3.0
11	K	212	GLY	3.0
2	P	52	THR	3.0
5	S	3	ASN	3.0
9	I	1	SER	3.0
3	C	225	GLU	3.0
11	Y	212	GLY	3.0
1	O	52	SER	2.9
6	T	2	THR	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	217	LYS	2.9
1	O	201	GLU	2.9
9	W	133	LYS	2.9
1	A	2	THR	2.8
1	A	228	PRO	2.8
4	R	125	LEU	2.8
5	S	225	ASP	2.7
1	O	2	THR	2.7
7	U	222	ASP	2.7
2	B	50	LYS	2.7
2	B	182	ASP	2.7
6	F	181	GLU	2.7
2	P	203	SER	2.7
6	T	241	LYS	2.7
5	S	173	ARG	2.6
6	F	243	ILE	2.6
7	U	2	GLY	2.6
6	T	244	ASN	2.6
6	F	178	HIS	2.6
3	Q	235	GLU	2.6
6	T	243	ILE	2.6
13	M	1	THR	2.6
9	I	133	LYS	2.6
7	G	2	GLY	2.6
6	F	2	THR	2.5
3	C	236	GLN	2.5
4	R	230	GLU	2.5
6	F	244	ASN	2.5
7	G	241	GLU	2.5
2	P	218	GLY	2.5
4	R	1	ASP	2.5
3	C	216	ASP	2.4
3	Q	205	ALA	2.4
12	Z	1	GLN	2.4
12	Z	210	ASP	2.4
14	b	105	LYS	2.4
13	M	82	ASP	2.4
5	S	52	ALA	2.4
2	P	182	ASP	2.4
6	F	230	ASP	2.4
2	P	60	THR	2.3
3	Q	225	GLU	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
12	Z	172	LEU	2.3
7	U	181	LYS	2.3
4	R	54	ASP	2.3
13	M	47	ASP	2.3
6	T	166	GLN	2.3
5	S	201	ARG	2.3
6	F	182	GLY	2.3
5	S	165	GLN	2.3
11	Y	147	ASP	2.3
2	P	223	GLU	2.3
2	B	242	GLY	2.3
1	A	201	GLU	2.3
10	X	193	ASP	2.2
5	E	54	GLU	2.2
7	U	241	GLU	2.2
1	O	230	ASP	2.2
2	B	222	GLY	2.2
3	Q	223	SER	2.2
6	F	180	PRO	2.2
14	N	105	LYS	2.2
4	D	201	GLU	2.2
3	C	47	ARG	2.2
6	T	178	HIS	2.2
12	L	172	LEU	2.2
12	Z	174	TYR	2.2
4	R	169	GLU	2.2
8	V	145	ASP	2.2
11	Y	106	ARG	2.2
3	C	181	GLU	2.2
1	A	230	ASP	2.2
2	P	225	TYR	2.1
5	E	121	SER	2.1
5	S	163	ARG	2.1
5	S	203	GLU	2.1
12	Z	165	ASN	2.1
1	A	248	GLU	2.1
1	A	249	ALA	2.1
3	C	175	LYS	2.1
7	G	230	GLU	2.1
1	O	227	ILE	2.1
3	C	180	LYS	2.1
6	T	181	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
6	T	230	ASP	2.1
7	G	242	GLN	2.0
4	R	142	ASP	2.0
5	S	210	LEU	2.0
6	T	205	GLU	2.0
6	F	203	ASN	2.0
14	N	195	GLN	2.0
3	C	37	LYS	2.0
3	Q	180	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

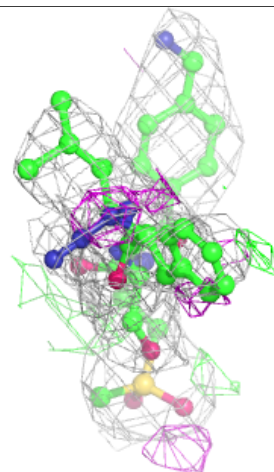
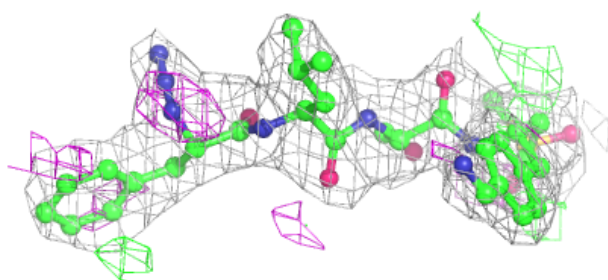
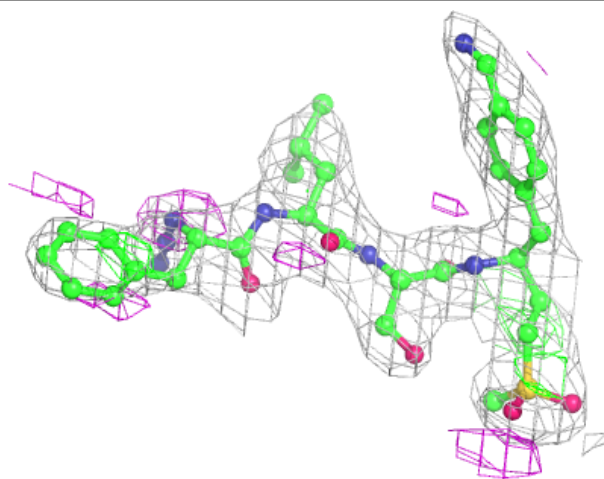
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
17	GQT	K	301	44/44	0.89	0.19	46,59,81,92	0
17	GQT	Y	301	44/44	0.89	0.21	44,60,76,95	0
17	GQT	H	301	44/44	0.90	0.22	40,55,80,111	0
17	GQT	V	301	44/44	0.90	0.22	47,61,81,99	0
15	MG	G	301	1/1	0.93	0.08	52,52,52,52	0
15	MG	I	301	1/1	0.96	0.24	67,67,67,67	0
15	MG	X	201	1/1	0.97	0.32	46,46,46,46	0
15	MG	Z	301	1/1	0.98	0.16	54,54,54,54	0
15	MG	N	201	1/1	0.98	0.12	45,45,45,45	0
16	CL	G	302	1/1	0.99	0.07	49,49,49,49	0
15	MG	I	302	1/1	0.99	0.07	56,56,56,56	0
15	MG	L	301	1/1	0.99	0.08	72,72,72,72	0
16	CL	U	301	1/1	0.99	0.12	50,50,50,50	0
15	MG	K	302	1/1	0.99	0.10	71,71,71,71	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.

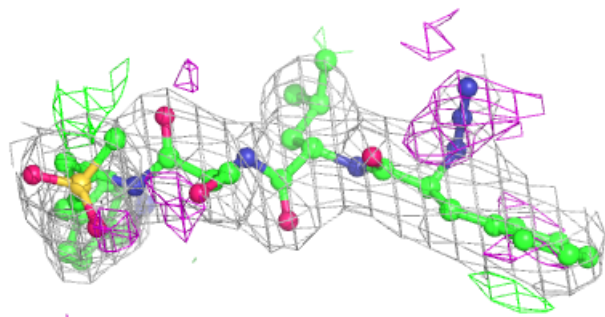
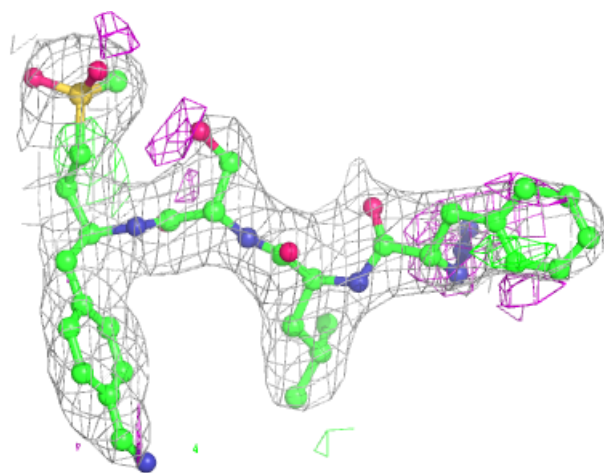
**Electron density around GQT K 301:**

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



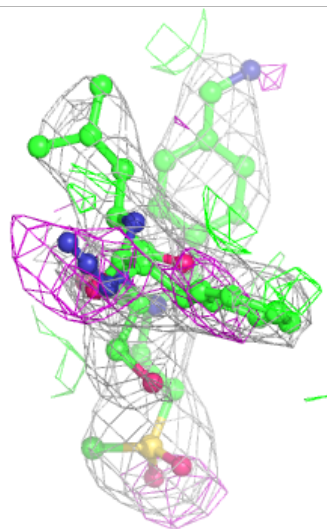
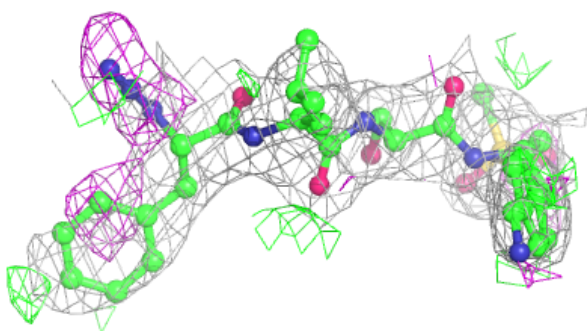
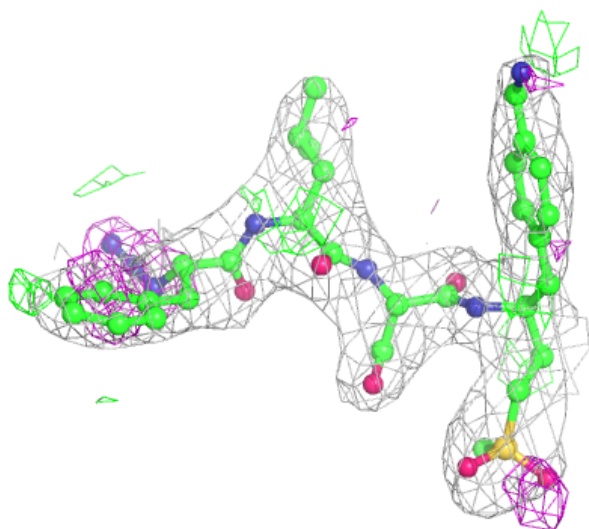
**Electron density around GQT Y 301:**

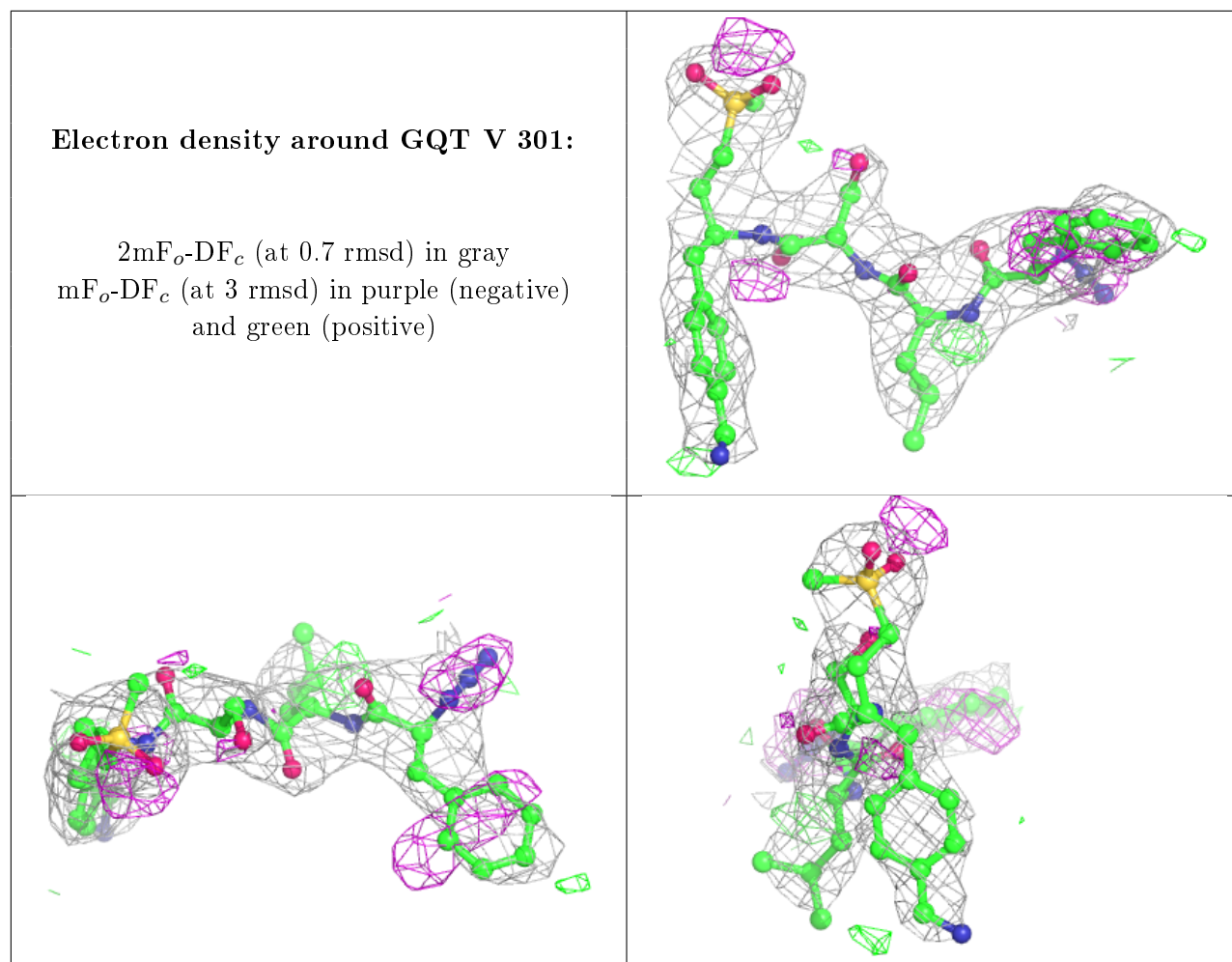
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around GQT 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.