



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:32 PM UTC

PDB ID : 6HTC / pdb\_00006htc  
Title : Yeast 20S proteasome with human beta2c (S171G) in complex with ONX 0914  
Authors : Huber, E.M.; Groll, M.  
Deposited on : 2018-10-03  
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

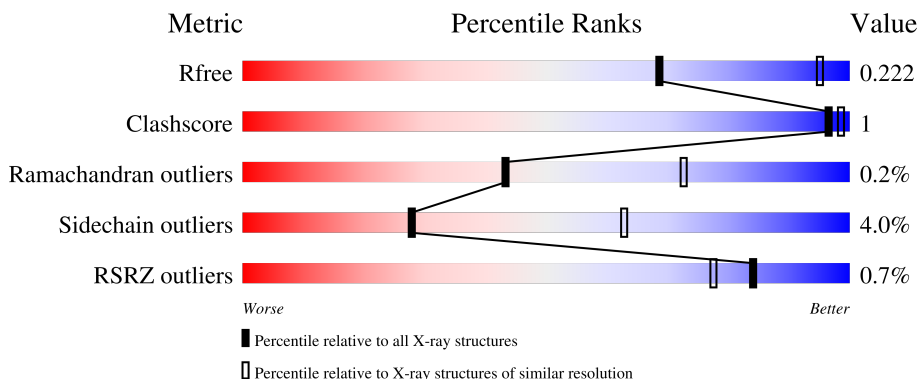
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	94% (0% poor fit, 0% 3+ outliers, 0% 2 outliers, 0% 1 outlier, 94% 0 outliers)
1	O	250	94% (0% poor fit, 0% 3+ outliers, 0% 2 outliers, 0% 1 outlier, 94% 0 outliers)
2	B	258	90% (0% poor fit, 0% 3+ outliers, 0% 2 outliers, 5% 1 outlier, 5% 0 outliers)
2	P	258	90% (0% poor fit, 0% 3+ outliers, 0% 2 outliers, 5% 1 outlier, 5% 0 outliers)
3	C	254	89% (0% poor fit, 0% 3+ outliers, 0% 2 outliers, 5% 1 outlier, 6% 0 outliers)

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Mol	Chain	Length	Quality of chain
3	Q	254	2% 89% 6% 6%
4	D	260	86% 10%
4	R	260	86% 10%
5	E	234	94% ..
5	S	234	94% ..
6	F	288	81% 16%
6	T	288	81% 16%
7	G	252	90% . . .
7	U	252	90% 5% . .
8	H	234	2% 88% . . 6%
8	V	234	2% 90% . . 6%
9	I	205	95% .
9	W	205	96% .
10	J	198	% 91% 7% ..
10	X	198	% 91% 7% ..
11	K	212	91% 9%
11	Y	212	90% 9% .
12	L	222	3% 94% 5% .
12	Z	222	4% 93% 6% .
13	M	246	87% . 9%
13	a	246	87% . 9%
14	N	196	93% 6% .
14	b	196	94% 6% .

## 2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 49687 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	240	Total 1842	C 1171	N 305	O 362	S 4	0	0	0
1	O	240	Total 1842	C 1171	N 305	O 362	S 4	0	0	0

- 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 1904	C 1201	N 321	O 379	S 3	0	0	0
2	P	244	Total 1904	C 1201	N 321	O 379	S 3	0	0	0

- 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 1881	C 1176	N 329	O 372	S 4	0	0	0
3	Q	240	Total 1881	C 1176	N 329	O 372	S 4	0	0	0

- 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 1813	C 1136	N 304	O 366	S 7	0	0	0
4	R	235	Total 1813	C 1136	N 304	O 366	S 7	0	0	0

- 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-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	219	Total	C	N	O	S	0	0	0
			1648	1038	282	316	12			
8	V	219	Total	C	N	O	S	0	0	0
			1648	1038	282	316	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	171	GLY	SER	engineered mutation	UNP Q99436
V	171	GLY	SER	engineered mutation	UNP Q99436

- 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			
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	224	Total	C	N	O	S	0	0	0
			1753	1108	300	338	7			
13	a	224	Total	C	N	O	S	0	0	0
			1753	1108	300	338	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			

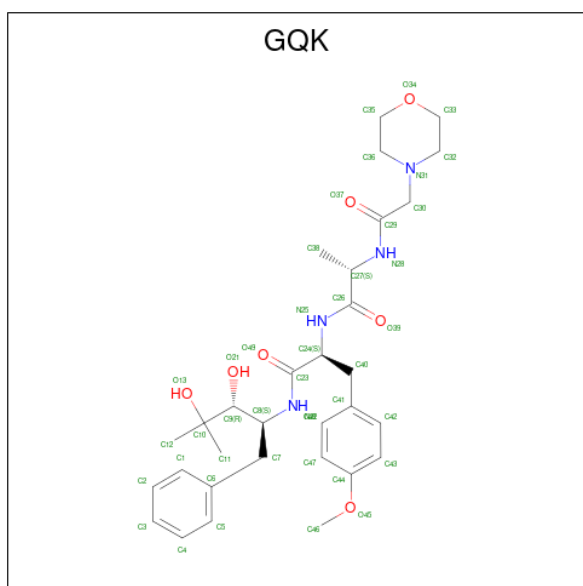
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 16 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

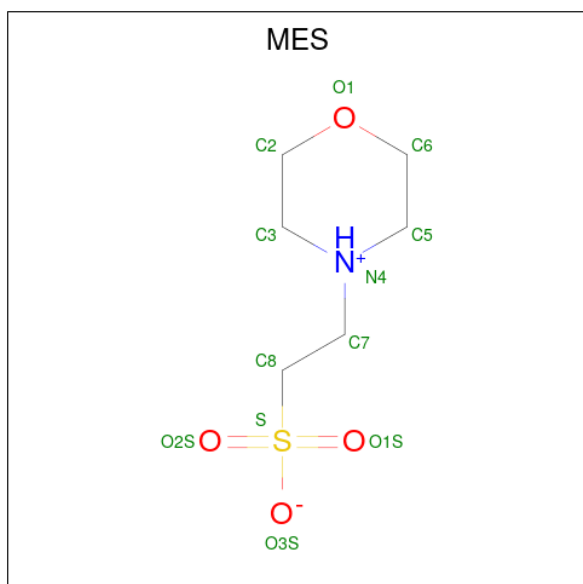
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

- Molecule 17 is (2 {S})-3-(4-methoxyphenyl)- {N}-[(2 {S},3 {R})-4-methyl-3,4-bis(oxidanyl)-1-phenyl-pentan-2-yl]-2-[[ (2 {S})-2-(2-morpholin-4-ylethanoylamino)propanoyl]amino]propanamide (CCD ID: GQK) (formula: C<sub>31</sub>H<sub>44</sub>N<sub>4</sub>O<sub>7</sub>).



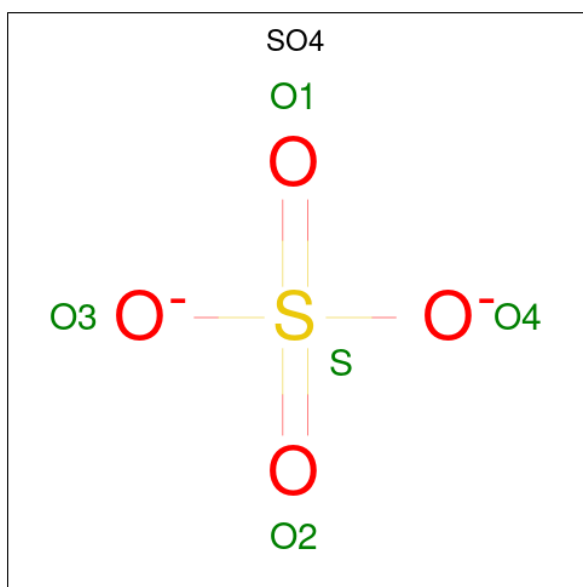
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	H	1	Total	C	N	O	0	0
			42	31	4	7		
17	K	1	Total	C	N	O	0	0
			42	31	4	7		
17	N	1	Total	C	N	O	0	0
			42	31	4	7		
17	V	1	Total	C	N	O	0	0
			42	31	4	7		
17	Y	1	Total	C	N	O	0	0
			42	31	4	7		
17	b	1	Total	C	N	O	0	0
			42	31	4	7		

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: 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 SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	N	1	Total	O	S	0	0
			5	4	1		
19	b	1	Total	O	S	0	0
			5	4	1		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	13	Total	O	0	0
			13	13		
20	B	19	Total	O	0	0
			19	19		
20	C	18	Total	O	0	0
			18	18		
20	D	12	Total	O	0	0
			12	12		
20	E	7	Total	O	0	0
			7	7		
20	F	8	Total	O	0	0
			8	8		
20	G	14	Total	O	0	0
			14	14		
20	H	13	Total	O	0	0
			13	13		
20	I	15	Total	O	0	0
			15	15		
20	J	23	Total	O	0	0
			23	23		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	K	22	Total O 22 22	0	0
20	L	15	Total O 15 15	0	0
20	M	21	Total O 21 21	0	0
20	N	17	Total O 17 17	0	0
20	O	7	Total O 7 7	0	0
20	P	13	Total O 13 13	0	0
20	Q	9	Total O 9 9	0	0
20	R	8	Total O 8 8	0	0
20	S	9	Total O 9 9	0	0
20	T	10	Total O 10 10	0	0
20	U	17	Total O 17 17	0	0
20	V	10	Total O 10 10	0	0
20	W	11	Total O 11 11	0	0
20	X	28	Total O 28 28	0	0
20	Y	26	Total O 26 26	0	0
20	Z	19	Total O 19 19	0	0
20	a	28	Total O 28 28	0	0
20	b	17	Total O 17 17	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

Chain A:  94%



- Molecule 1: Proteasome subunit alpha type-2

Chain O:  94%



- Molecule 2: Proteasome subunit alpha type-3

Chain B:  90% 5% 5%




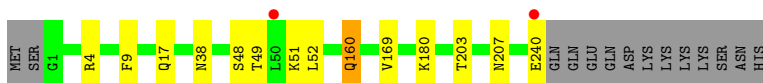
- Molecule 2: Proteasome subunit alpha type-3

Chain P:  90% 5%

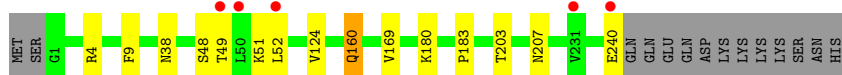
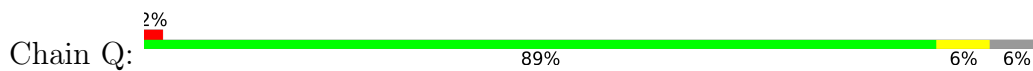


- Molecule 3: Proteasome subunit alpha type-4

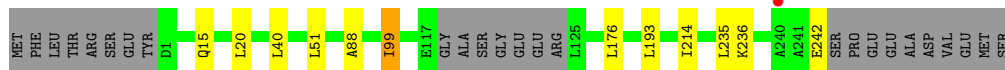
Chain C:  89% 5% 6%



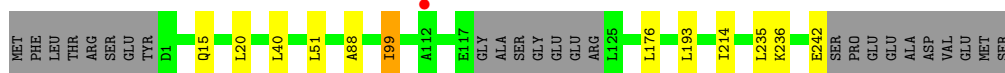
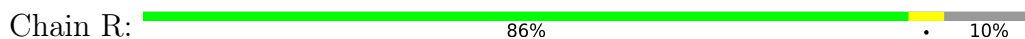
- Molecule 3: Proteasome subunit alpha type-4



• Molecule 4: Proteasome subunit alpha type-5



• Molecule 4: Proteasome subunit alpha type-5



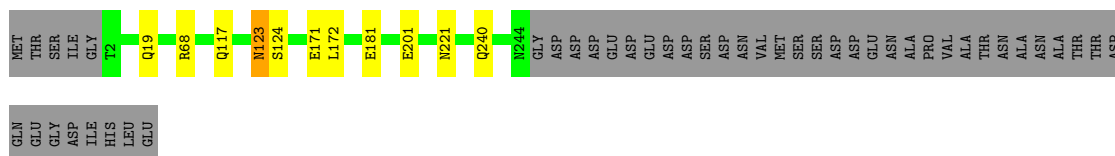
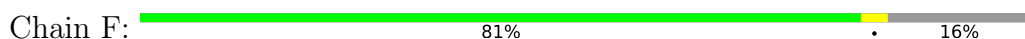
• Molecule 5: Proteasome subunit alpha type-6



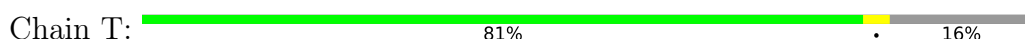
• Molecule 5: Proteasome subunit alpha type-6

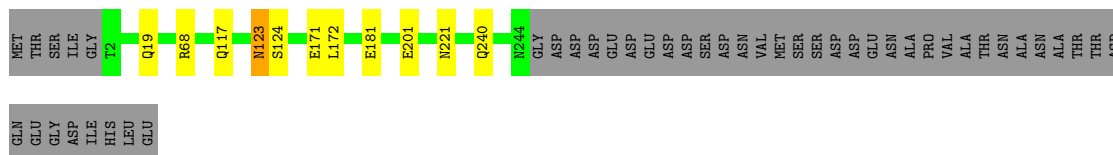


• Molecule 6: Probable proteasome subunit alpha type-7

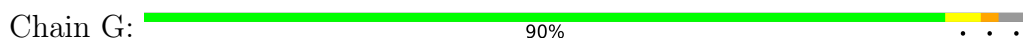


• Molecule 6: Probable proteasome subunit alpha type-7

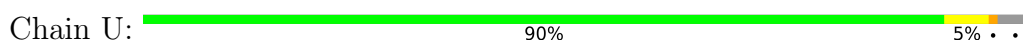




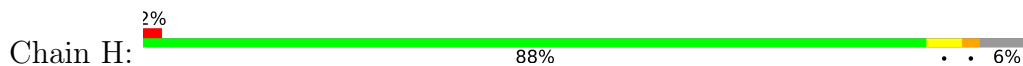
- Molecule 7: Proteasome subunit alpha type-1



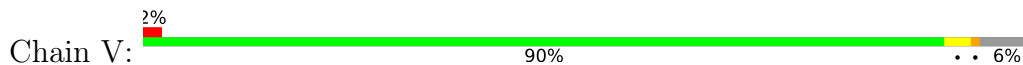
- Molecule 7: Proteasome subunit alpha type-1



- Molecule 8: Proteasome subunit beta type-7



- Molecule 8: Proteasome subunit beta type-7



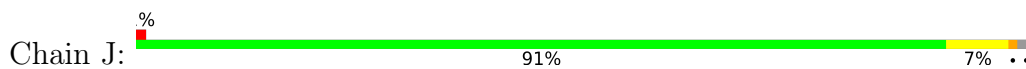
- Molecule 9: Proteasome subunit beta type-3



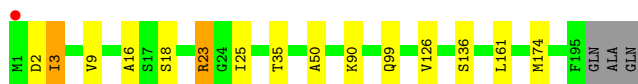
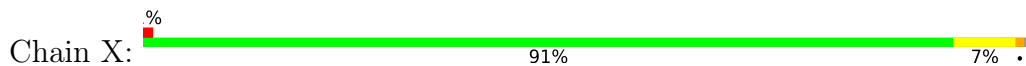
- Molecule 9: Proteasome subunit beta type-3



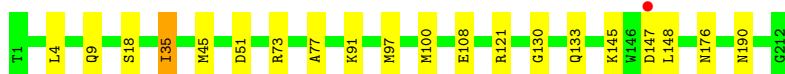
- Molecule 10: Proteasome subunit beta type-4



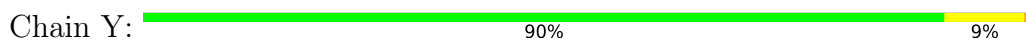
- Molecule 10: Proteasome subunit beta type-4



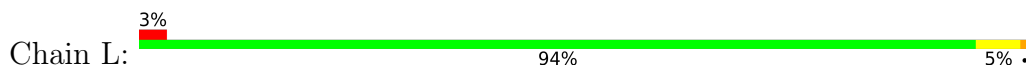
- Molecule 11: Proteasome subunit beta type-5



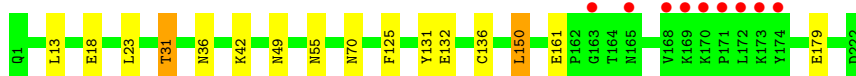
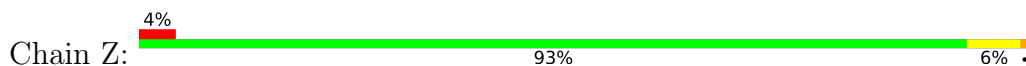
- Molecule 11: Proteasome subunit beta type-5



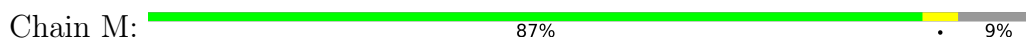
- Molecule 12: Proteasome subunit beta type-6




- Molecule 12: Proteasome subunit beta type-6

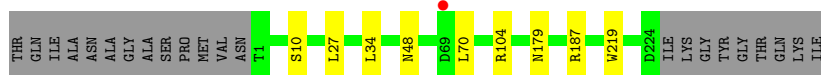


- Molecule 13: Proteasome subunit beta type-7



- Molecule 13: Proteasome subunit beta type-7

Chain a:  87% 9%



- Molecule 14: Proteasome subunit beta type-1

Chain N:  93% 6%



- Molecule 14: Proteasome subunit beta type-1

Chain b:  94% 6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.63Å 300.76Å 144.64Å 90.00° 112.88° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (15.00-2.80) 97.5 (15.00-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.180 , 0.218 0.185 , 0.222	Depositor DCC
$R_{free}$ test set	12731 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.5	Xtrriage
Anisotropy	0.585	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 56.1	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	0.96	EDS
Total number of atoms	49687	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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, GQK, CL, SO4, MES

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	0.56	0/1876	0.87	3/2535 (0.1%)
1	O	0.56	0/1876	0.89	4/2535 (0.2%)
2	B	0.58	0/1934	0.83	0/2618
2	P	0.58	0/1934	0.83	0/2618
3	C	0.58	0/1910	0.82	0/2586
3	Q	0.58	0/1910	0.82	0/2586
4	D	0.55	0/1837	0.81	0/2475
4	R	0.56	0/1837	0.80	0/2475
5	E	0.56	0/1800	0.79	0/2433
5	S	0.56	0/1800	0.80	0/2433
6	F	0.58	0/1932	0.82	0/2609
6	T	0.57	0/1932	0.82	0/2609
7	G	0.55	0/1945	0.86	3/2634 (0.1%)
7	U	0.57	0/1945	0.87	3/2634 (0.1%)
8	H	0.60	0/1675	0.92	3/2267 (0.1%)
8	V	0.57	0/1675	0.89	3/2267 (0.1%)
9	I	0.56	0/1611	0.81	0/2174
9	W	0.56	0/1611	0.81	0/2174
10	J	0.55	0/1589	0.81	1/2142 (0.0%)
10	X	0.55	0/1589	0.81	1/2142 (0.0%)
11	K	0.51	0/1681	0.82	0/2274
11	Y	0.51	0/1681	0.82	0/2274
12	L	0.55	0/1795	0.79	0/2420
12	Z	0.55	0/1795	0.78	0/2420
13	M	0.56	0/1783	0.81	0/2420
13	a	0.57	0/1783	0.81	0/2420
14	N	0.53	0/1541	0.80	0/2087
14	b	0.53	0/1541	0.79	0/2087
All	All	0.56	0/49818	0.83	21/67348 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	O	0	1
7	U	0	1
8	V	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	4	ARG	NE-CZ-NH1	-11.28	110.22	121.50
7	U	68	ARG	NE-CZ-NH2	-11.18	109.14	119.20
7	U	68	ARG	CD-NE-CZ	10.78	139.50	124.40
8	H	143	ARG	NE-CZ-NH1	-10.68	110.82	121.50
1	A	4	ARG	NE-CZ-NH2	-10.60	109.66	119.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4	ARG	Sidechain
1	O	4	ARG	Sidechain
7	U	68	ARG	Sidechain
8	V	143	ARG	Sidechain

## 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	1842	0	1855	1	0
1	O	1842	0	1855	1	0
2	B	1904	0	1904	4	0
2	P	1904	0	1904	4	0
3	C	1881	0	1895	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	1881	0	1895	5	0
4	D	1813	0	1797	2	0
4	R	1813	0	1797	2	0
5	E	1773	0	1775	6	0
5	S	1773	0	1775	6	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	3	0
7	G	1907	0	1901	7	0
7	U	1907	0	1901	5	0
8	H	1648	0	1671	4	0
8	V	1648	0	1671	2	0
9	I	1581	0	1574	5	0
9	W	1581	0	1574	4	0
10	J	1561	0	1569	5	0
10	X	1561	0	1569	5	0
11	K	1644	0	1593	7	0
11	Y	1644	0	1593	7	0
12	L	1757	0	1711	7	0
12	Z	1757	0	1711	8	0
13	M	1753	0	1754	3	0
13	a	1753	0	1754	2	0
14	N	1512	0	1479	8	0
14	b	1512	0	1479	7	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0
15	K	1	0	0	0	0
15	N	1	0	0	0	0
15	V	2	0	0	0	0
15	W	1	0	0	0	0
15	Y	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	42	0	0	0	0
17	K	42	0	0	0	0
17	N	42	0	0	0	0
17	V	42	0	0	0	0
17	Y	42	0	0	0	0
17	b	42	0	0	0	0
18	H	12	0	13	0	0
18	K	12	0	13	0	0
18	V	12	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	Y	12	0	13	0	0
19	N	5	0	0	0	0
19	b	5	0	0	0	0
20	A	13	0	0	0	0
20	B	19	0	0	0	0
20	C	18	0	0	0	0
20	D	12	0	0	0	0
20	E	7	0	0	0	0
20	F	8	0	0	0	0
20	G	14	0	0	1	0
20	H	13	0	0	0	0
20	I	15	0	0	0	0
20	J	23	0	0	1	0
20	K	22	0	0	0	0
20	L	15	0	0	0	0
20	M	21	0	0	1	0
20	N	17	0	0	0	0
20	O	7	0	0	0	0
20	P	13	0	0	0	0
20	Q	9	0	0	0	0
20	R	8	0	0	0	0
20	S	9	0	0	0	0
20	T	10	0	0	0	0
20	U	17	0	0	1	0
20	V	10	0	0	0	0
20	W	11	0	0	0	0
20	X	28	0	0	1	0
20	Y	26	0	0	0	0
20	Z	19	0	0	0	0
20	a	28	0	0	0	0
20	b	17	0	0	0	0
All	All	49687	0	48774	96	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.

The worst 5 of 96 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.20	0.89
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.24	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.59	0.68
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.61	0.65
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	1.94	0.64

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	236/250 (94%)	229 (97%)	7 (3%)	0	100	100
1	O	236/250 (94%)	228 (97%)	8 (3%)	0	100	100
2	B	242/258 (94%)	237 (98%)	3 (1%)	2 (1%)	16	44
2	P	242/258 (94%)	236 (98%)	4 (2%)	2 (1%)	16	44
3	C	238/254 (94%)	235 (99%)	3 (1%)	0	100	100
3	Q	238/254 (94%)	236 (99%)	1 (0%)	1 (0%)	30	60
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%)	220 (96%)	9 (4%)	0	100	100
5	S	229/234 (98%)	220 (96%)	9 (4%)	0	100	100
6	F	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
6	T	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
7	G	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
8	H	217/234 (93%)	215 (99%)	2 (1%)	0	100	100
8	V	217/234 (93%)	215 (99%)	2 (1%)	0	100	100
9	I	202/205 (98%)	193 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	W	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	24	55
10	X	193/198 (98%)	190 (98%)	2 (1%)	1 (0%)	24	55
11	K	210/212 (99%)	203 (97%)	6 (3%)	1 (0%)	24	55
11	Y	210/212 (99%)	203 (97%)	5 (2%)	2 (1%)	12	38
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	222/246 (90%)	213 (96%)	9 (4%)	0	100	100
13	a	222/246 (90%)	213 (96%)	9 (4%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6228/6618 (94%)	6079 (98%)	139 (2%)	10 (0%)	43	72

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	52	THR
2	B	218	GLY
2	P	52	THR
2	P	218	GLY
11	K	147	ASP

### 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	201/209 (96%)	197 (98%)	4 (2%)	48	80
1	O	201/209 (96%)	197 (98%)	4 (2%)	48	80
2	B	203/216 (94%)	194 (96%)	9 (4%)	25	59
2	P	203/216 (94%)	195 (96%)	8 (4%)	28	64
3	C	212/226 (94%)	202 (95%)	10 (5%)	23	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	212/226 (94%)	202 (95%)	10 (5%)	23	57
4	D	194/215 (90%)	184 (95%)	10 (5%)	21	53
4	R	194/215 (90%)	184 (95%)	10 (5%)	21	53
5	E	190/193 (98%)	184 (97%)	6 (3%)	34	70
5	S	190/193 (98%)	184 (97%)	6 (3%)	34	70
6	F	201/239 (84%)	192 (96%)	9 (4%)	24	58
6	T	201/239 (84%)	192 (96%)	9 (4%)	24	58
7	G	206/210 (98%)	198 (96%)	8 (4%)	28	64
7	U	206/210 (98%)	198 (96%)	8 (4%)	28	64
8	H	179/194 (92%)	168 (94%)	11 (6%)	17	46
8	V	179/194 (92%)	170 (95%)	9 (5%)	22	54
9	I	172/173 (99%)	167 (97%)	5 (3%)	37	73
9	W	172/173 (99%)	167 (97%)	5 (3%)	37	73
10	J	173/175 (99%)	165 (95%)	8 (5%)	24	58
10	X	173/175 (99%)	165 (95%)	8 (5%)	24	58
11	K	169/169 (100%)	162 (96%)	7 (4%)	27	62
11	Y	169/169 (100%)	161 (95%)	8 (5%)	23	57
12	L	185/185 (100%)	176 (95%)	9 (5%)	22	55
12	Z	185/185 (100%)	176 (95%)	9 (5%)	22	55
13	M	192/208 (92%)	186 (97%)	6 (3%)	35	70
13	a	192/208 (92%)	186 (97%)	6 (3%)	35	70
14	N	162/162 (100%)	158 (98%)	4 (2%)	42	76
14	b	162/162 (100%)	158 (98%)	4 (2%)	42	76
All	All	5278/5548 (95%)	5068 (96%)	210 (4%)	28	63

5 of 210 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	P	113	ARG
5	S	188	LEU
12	Z	179	GLU
3	Q	38	ASN
4	R	51	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 162 such sidechains are listed below:

Mol	Chain	Res	Type
6	T	117	GLN
12	Z	3	ASN
7	U	28	GLN
8	V	153	ASN
12	Z	158	ASN

### 5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 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	GQK	K	301	11	44,44,44	1.33	3 (6%)	60,60,60	1.68	8 (13%)
17	GQK	b	201	14	44,44,44	1.57	6 (13%)	60,60,60	1.32	7 (11%)
17	GQK	H	301	8	44,44,44	1.67	6 (13%)	60,60,60	1.40	8 (13%)
18	MES	V	304	-	12,12,12	2.35	1 (8%)	15,16,16	1.35	2 (13%)
17	GQK	N	201	14	44,44,44	1.55	5 (11%)	60,60,60	1.32	8 (13%)
19	SO4	b	202	-	4,4,4	0.41	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	GQK	V	301	8	44,44,44	1.62	6 (13%)	60,60,60	1.40	8 (13%)
18	MES	Y	303	-	12,12,12	2.46	1 (8%)	15,16,16	1.47	3 (20%)
17	GQK	Y	301	11	44,44,44	1.26	3 (6%)	60,60,60	1.62	8 (13%)
19	SO4	N	203	-	4,4,4	0.45	0	6,6,6	0.14	0
18	MES	K	303	-	12,12,12	2.49	1 (8%)	15,16,16	1.57	3 (20%)
18	MES	H	302	-	12,12,12	2.13	1 (8%)	15,16,16	1.48	3 (20%)

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	GQK	K	301	11	-	9/44/52/52	0/3/3/3
17	GQK	b	201	14	-	6/44/52/52	0/3/3/3
17	GQK	H	301	8	-	5/44/52/52	0/3/3/3
18	MES	V	304	-	-	2/6/14/14	0/1/1/1
17	GQK	N	201	14	-	6/44/52/52	0/3/3/3
17	GQK	V	301	8	-	6/44/52/52	0/3/3/3
18	MES	Y	303	-	-	0/6/14/14	0/1/1/1
17	GQK	Y	301	11	-	9/44/52/52	0/3/3/3
18	MES	K	303	-	-	3/6/14/14	0/1/1/1
18	MES	H	302	-	-	3/6/14/14	0/1/1/1

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	K	303	MES	C8-S	-8.53	1.65	1.77
18	Y	303	MES	C8-S	-8.38	1.65	1.77
18	V	304	MES	C8-S	-7.95	1.66	1.77
18	H	302	MES	C8-S	-7.17	1.67	1.77
17	H	301	GQK	C11-C10	6.40	1.63	1.52

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	301	GQK	C12-C10-C11	-7.45	99.65	110.52
17	Y	301	GQK	C12-C10-C11	-7.12	100.12	110.52
17	H	301	GQK	C11-C10-C9	4.20	119.19	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	V	301	GQK	C11-C10-C9	4.17	119.12	111.27
17	K	301	GQK	C46-O45-C44	3.76	125.56	117.50

There are no chirality outliers.

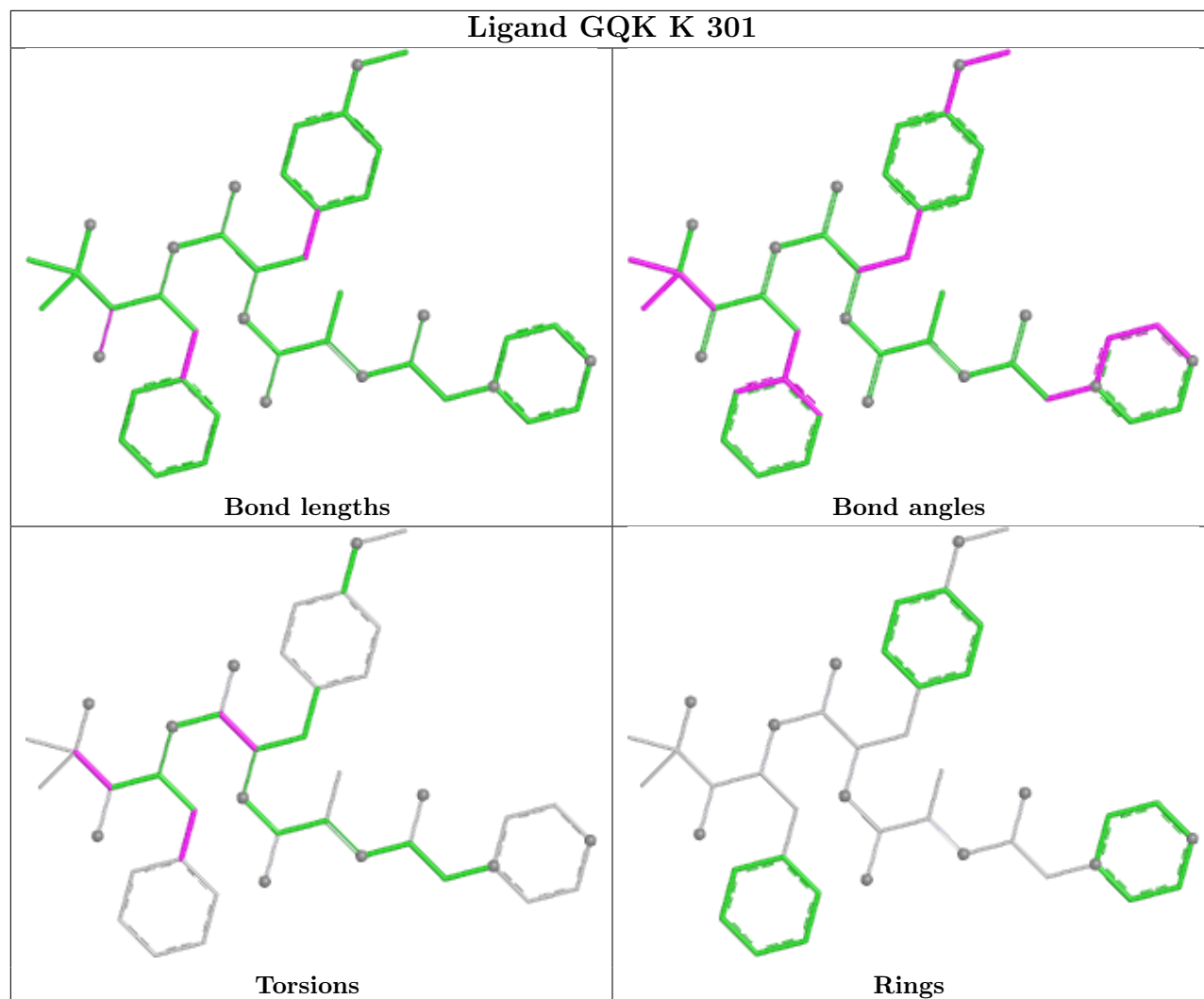
5 of 49 torsion outliers are listed below:

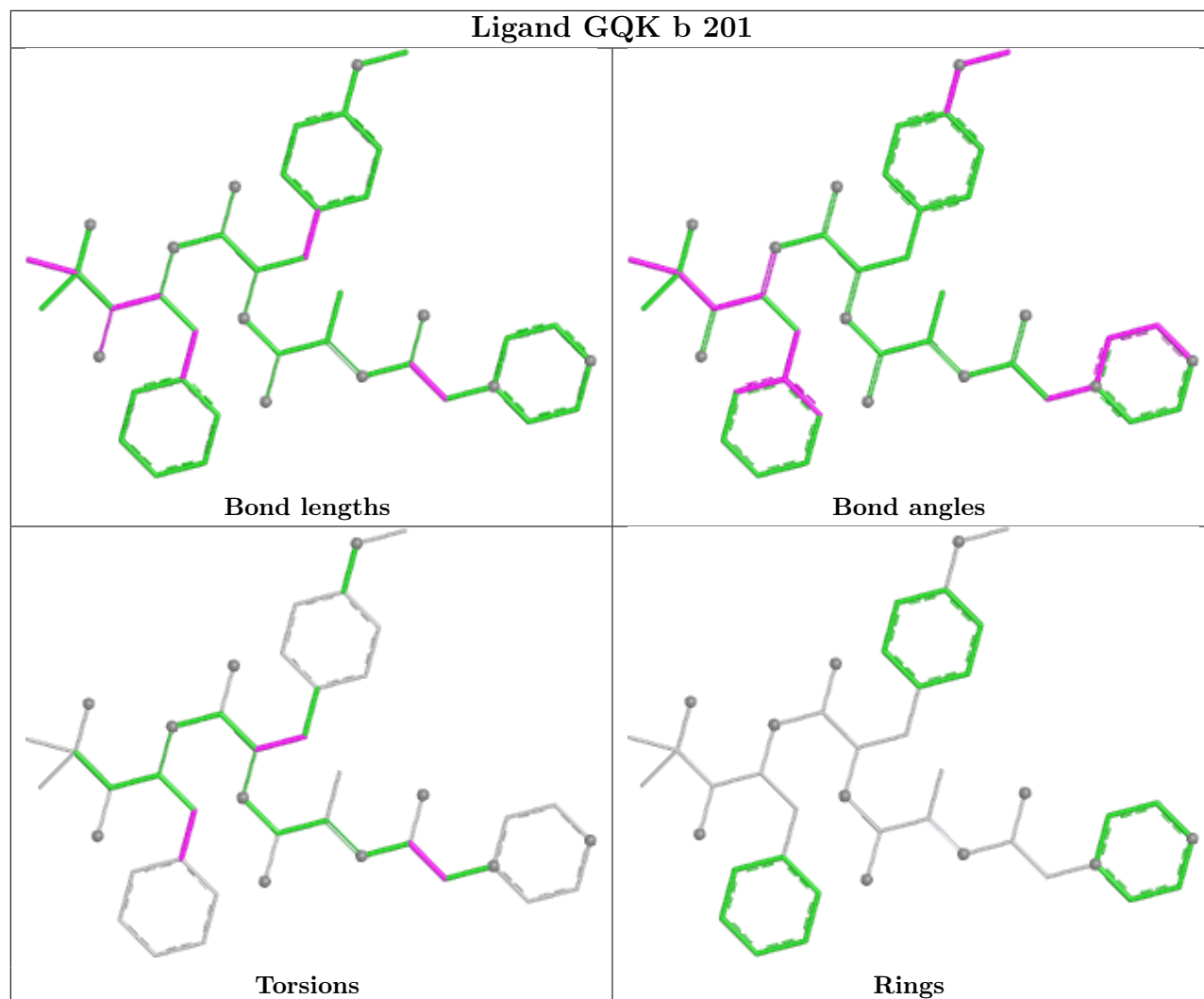
Mol	Chain	Res	Type	Atoms
17	K	301	GQK	C11-C10-C9-C8
17	K	301	GQK	C11-C10-C9-O21
17	K	301	GQK	C12-C10-C9-C8
17	K	301	GQK	C12-C10-C9-O21
17	K	301	GQK	O13-C10-C9-C8

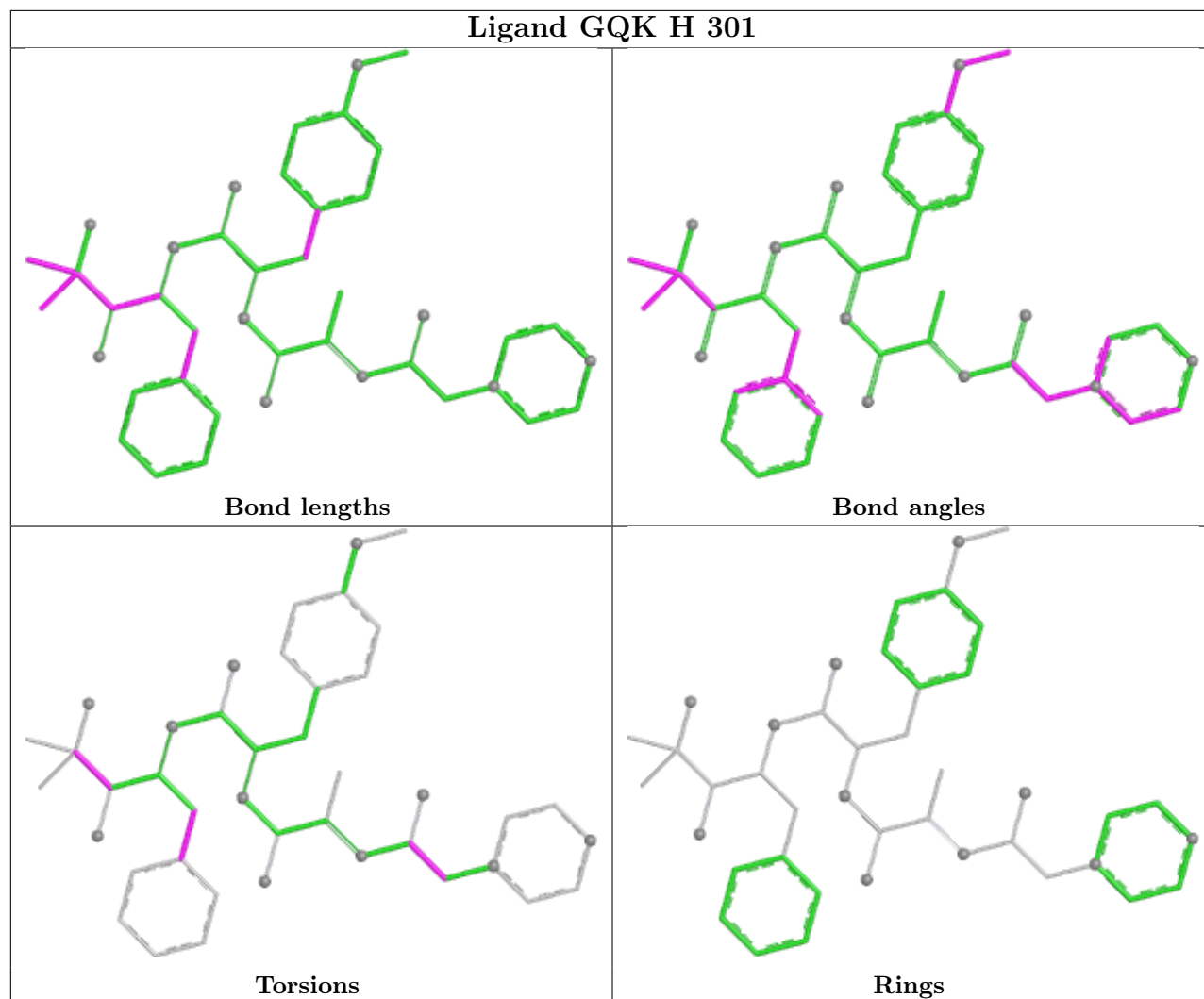
There are no ring outliers.

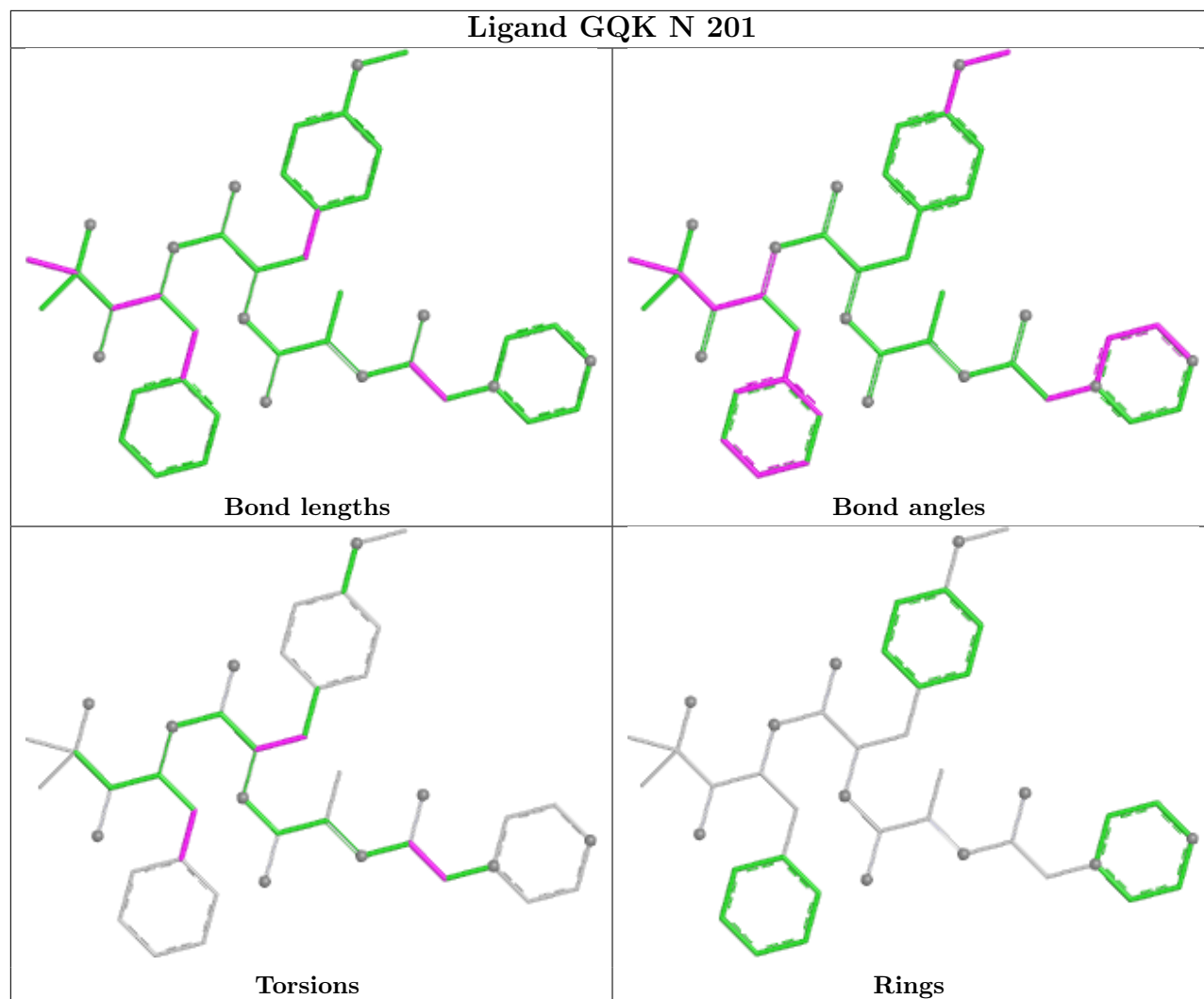
No monomer is involved in short contacts.

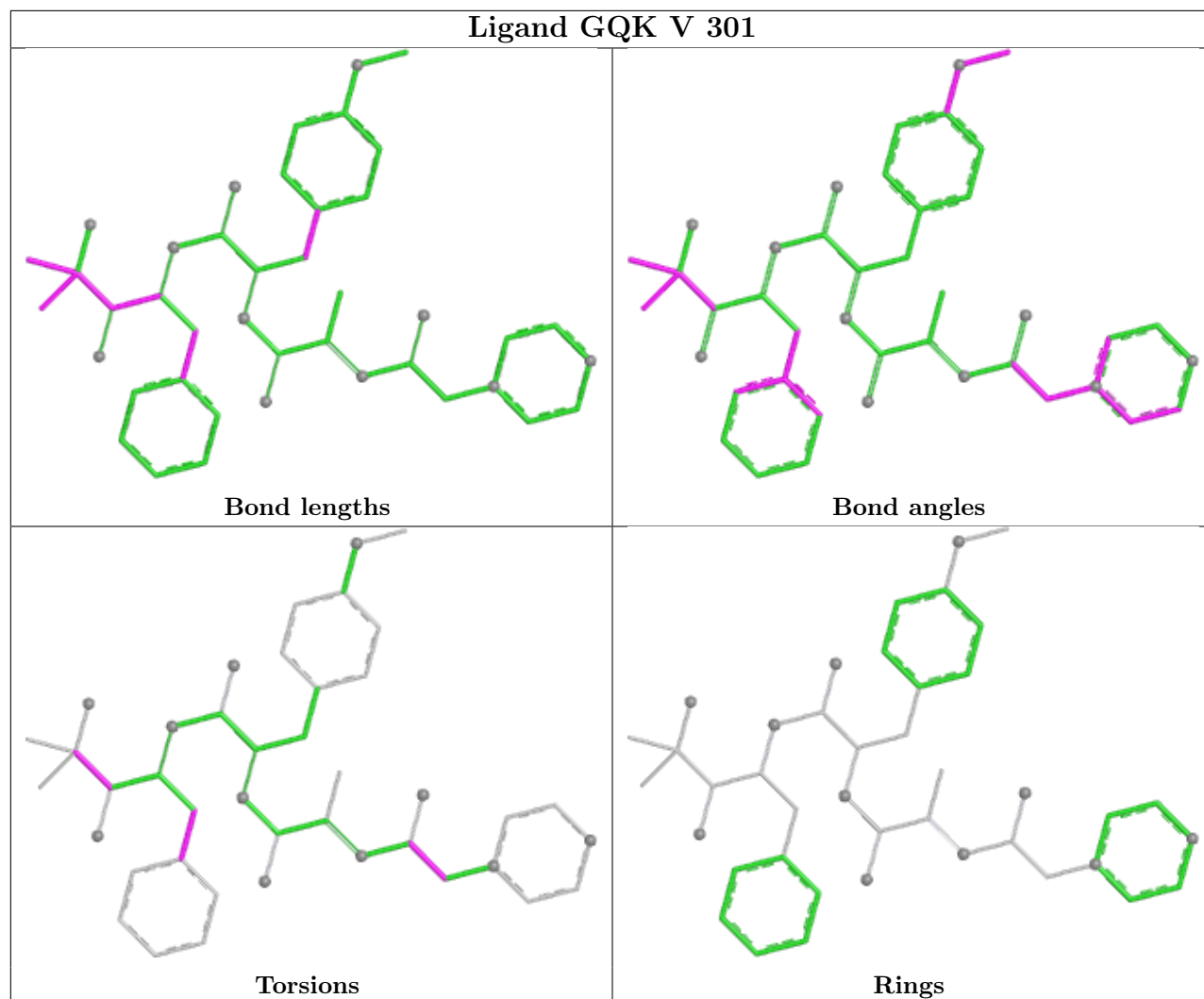
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

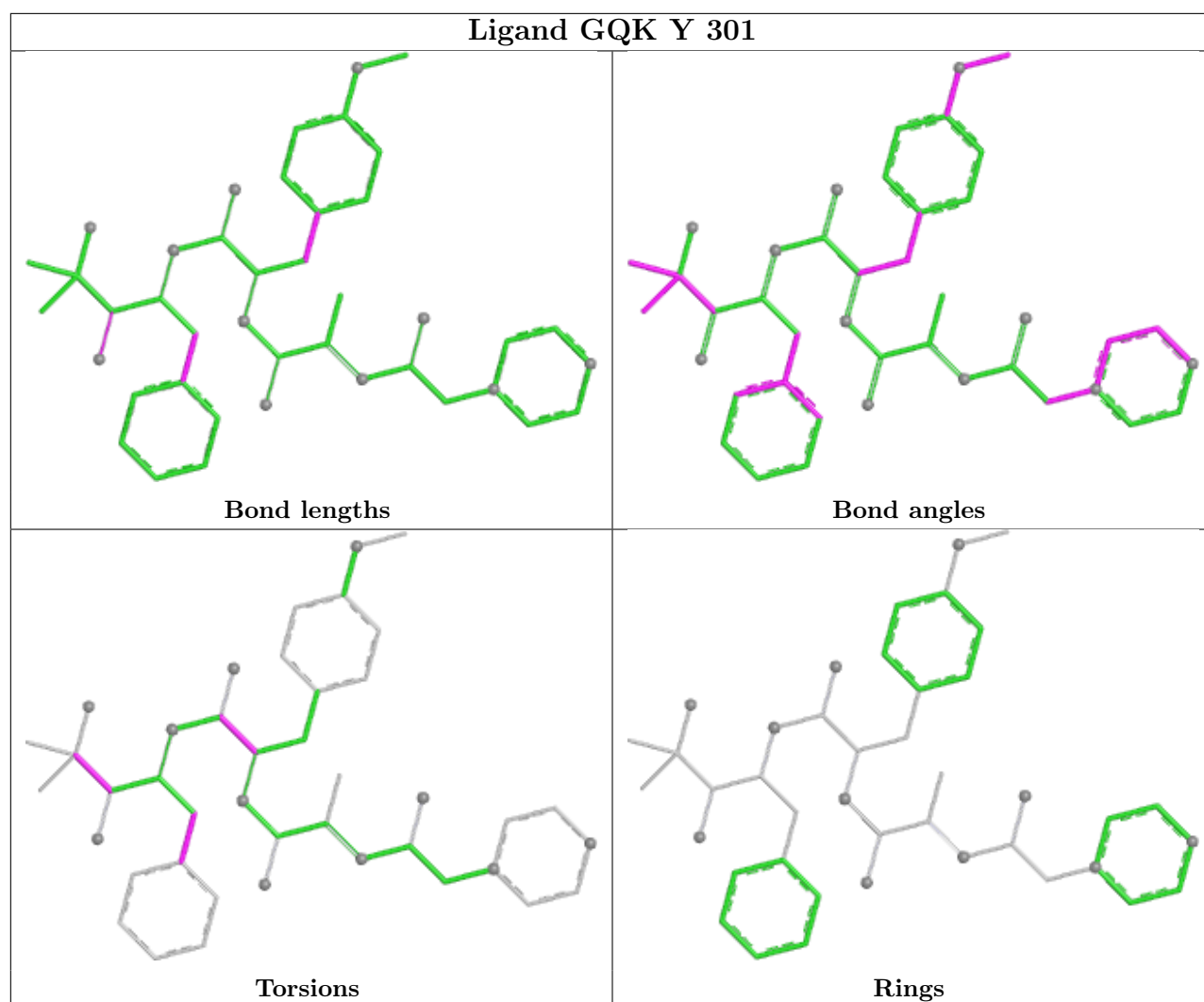












### 5.7 Other polymers [i](#)

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	240/250 (96%)	-0.54	1 (0%) 88 84	47, 68, 108, 146	0
1	O	240/250 (96%)	-0.45	2 (0%) 82 75	55, 76, 121, 154	0
2	B	244/258 (94%)	-0.44	1 (0%) 88 84	48, 70, 121, 176	0
2	P	244/258 (94%)	-0.42	1 (0%) 88 84	53, 72, 117, 170	0
3	C	240/254 (94%)	-0.50	2 (0%) 82 75	49, 73, 133, 160	0
3	Q	240/254 (94%)	-0.22	5 (2%) 63 54	57, 91, 171, 190	0
4	D	235/260 (90%)	-0.54	1 (0%) 88 84	47, 72, 103, 140	0
4	R	235/260 (90%)	-0.44	1 (0%) 88 84	56, 78, 121, 151	0
5	E	231/234 (98%)	-0.48	0 100 100	52, 74, 111, 153	0
5	S	231/234 (98%)	-0.26	1 (0%) 88 84	54, 86, 134, 170	0
6	F	243/288 (84%)	-0.54	0 100 100	46, 67, 117, 147	0
6	T	243/288 (84%)	-0.39	0 100 100	50, 79, 131, 165	0
7	G	241/252 (95%)	-0.60	0 100 100	45, 64, 103, 156	0
7	U	241/252 (95%)	-0.51	0 100 100	51, 67, 102, 140	0
8	H	219/234 (93%)	-0.38	4 (1%) 67 58	45, 63, 115, 133	0
8	V	219/234 (93%)	-0.33	4 (1%) 67 58	45, 66, 118, 155	0
9	I	204/205 (99%)	-0.71	0 100 100	42, 58, 86, 114	0
9	W	204/205 (99%)	-0.74	0 100 100	41, 59, 87, 106	0
10	J	195/198 (98%)	-0.58	1 (0%) 87 82	44, 61, 89, 128	0
10	X	195/198 (98%)	-0.62	1 (0%) 87 82	44, 63, 88, 149	0
11	K	212/212 (100%)	-0.60	1 (0%) 87 82	32, 61, 89, 110	0
11	Y	212/212 (100%)	-0.48	1 (0%) 87 82	31, 66, 96, 122	0
12	L	222/222 (100%)	-0.41	7 (3%) 50 40	46, 62, 108, 137	0
12	Z	222/222 (100%)	-0.38	9 (4%) 41 33	44, 63, 114, 145	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	224/246 (91%)	-0.61	1 (0%) 88 84	44, 63, 90, 123	0
13	a	224/246 (91%)	-0.67	1 (0%) 88 84	42, 62, 91, 125	0
14	N	196/196 (100%)	-0.67	0 100 100	40, 57, 88, 115	0
14	b	196/196 (100%)	-0.67	0 100 100	39, 59, 90, 116	0
All	All	6292/6618 (95%)	-0.50	45 (0%) 84 77	31, 67, 118, 190	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	50	LEU	5.9
12	L	174	TYR	5.5
12	Z	174	TYR	5.2
10	X	1	MET	5.2
8	H	196	GLY	4.4

## 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 oligosaccharides 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
18	MES	V	304	12/12	0.90	0.24	38,39,45,46	12
18	MES	H	302	12/12	0.91	0.22	35,39,41,43	12
19	SO4	N	203	5/5	0.91	0.23	69,78,81,91	5
17	GQK	N	201	42/42	0.92	0.09	42,57,75,80	0
17	GQK	H	301	42/42	0.93	0.09	44,54,81,84	0
18	MES	K	303	12/12	0.93	0.26	30,37,39,39	12
17	GQK	V	301	42/42	0.93	0.10	43,50,83,87	0

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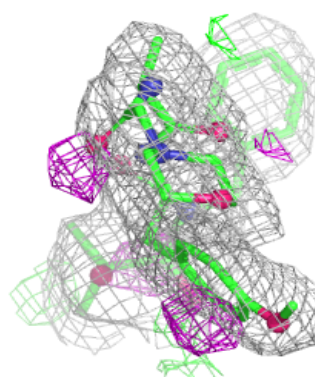
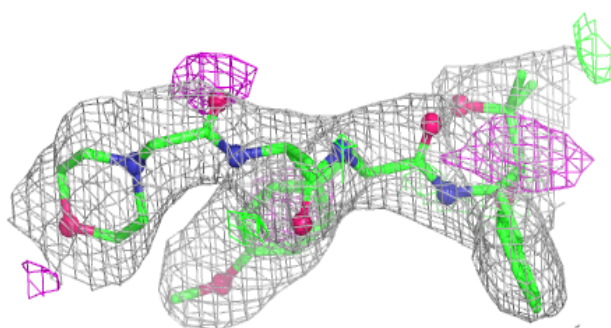
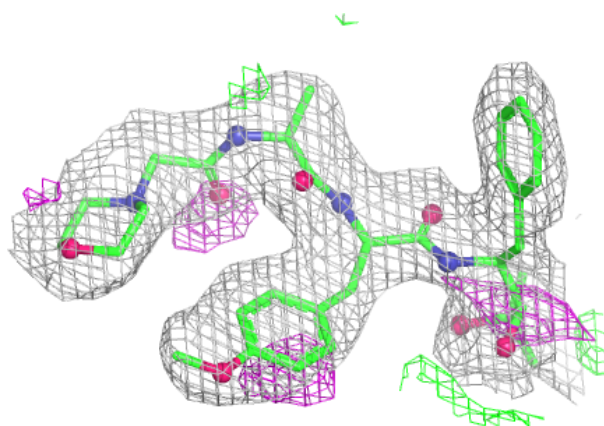
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
17	GQK	b	201	42/42	0.93	0.09	41,58,82,85	0
15	MG	V	303	1/1	0.94	0.15	61,61,61,61	0
18	MES	Y	303	12/12	0.94	0.27	27,38,38,39	12
16	CL	U	301	1/1	0.94	0.16	88,88,88,88	0
17	GQK	K	301	42/42	0.95	0.07	28,43,59,60	0
15	MG	K	302	1/1	0.95	0.10	92,92,92,92	0
15	MG	Z	301	1/1	0.95	0.12	79,79,79,79	0
15	MG	I	302	1/1	0.96	0.14	61,61,61,61	0
17	GQK	Y	301	42/42	0.96	0.07	27,44,63,64	0
19	SO4	b	202	5/5	0.96	0.20	75,77,86,99	5
15	MG	W	301	1/1	0.97	0.05	60,60,60,60	0
15	MG	Y	302	1/1	0.98	0.03	67,67,67,67	0
15	MG	G	301	1/1	0.98	0.04	71,71,71,71	0
16	CL	G	302	1/1	0.98	0.09	77,77,77,77	0
15	MG	I	301	1/1	0.98	0.10	81,81,81,81	0
15	MG	N	202	1/1	0.99	0.06	60,60,60,60	0
15	MG	V	302	1/1	0.99	0.06	85,85,85,85	0

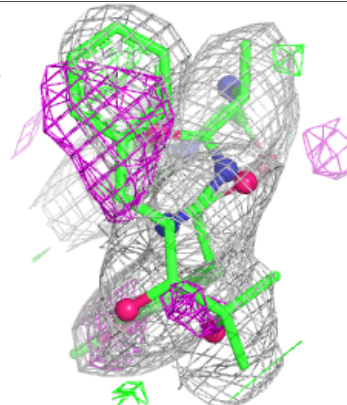
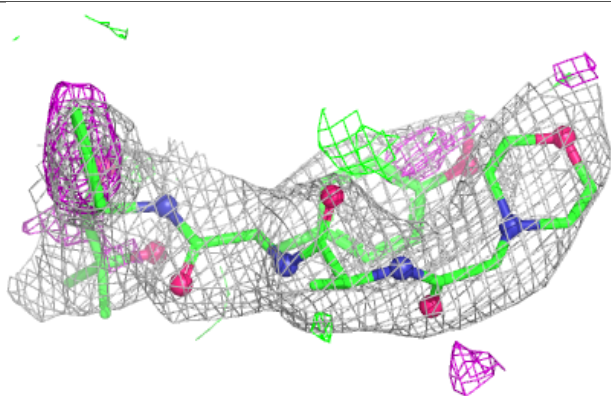
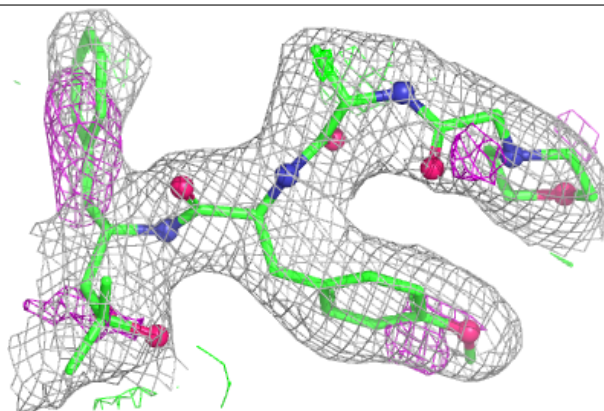
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around GQK N 201:**

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

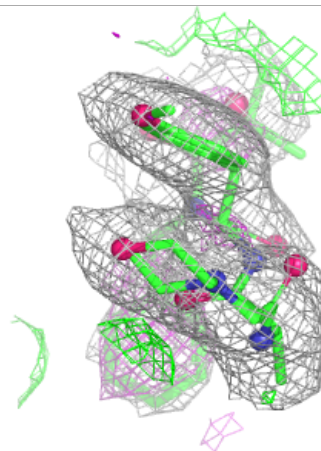
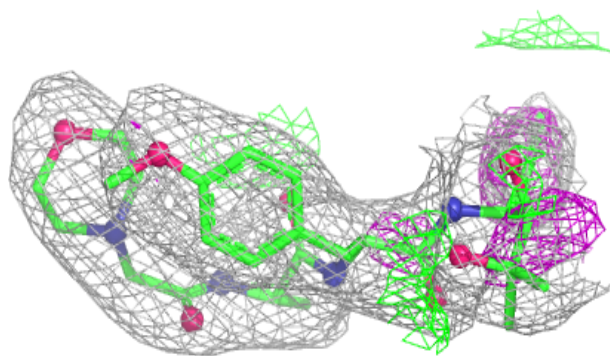
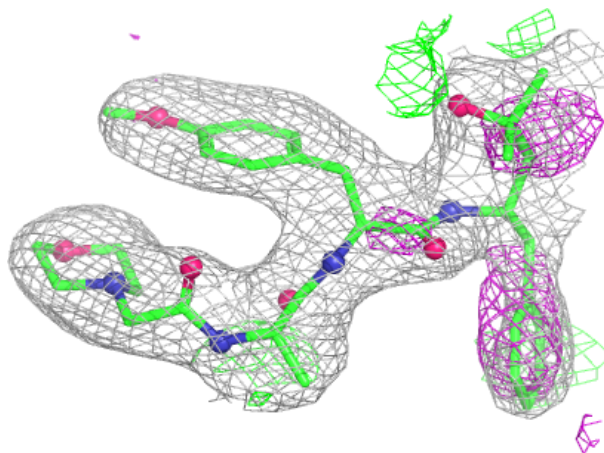
**Electron density around GQK H 301:**

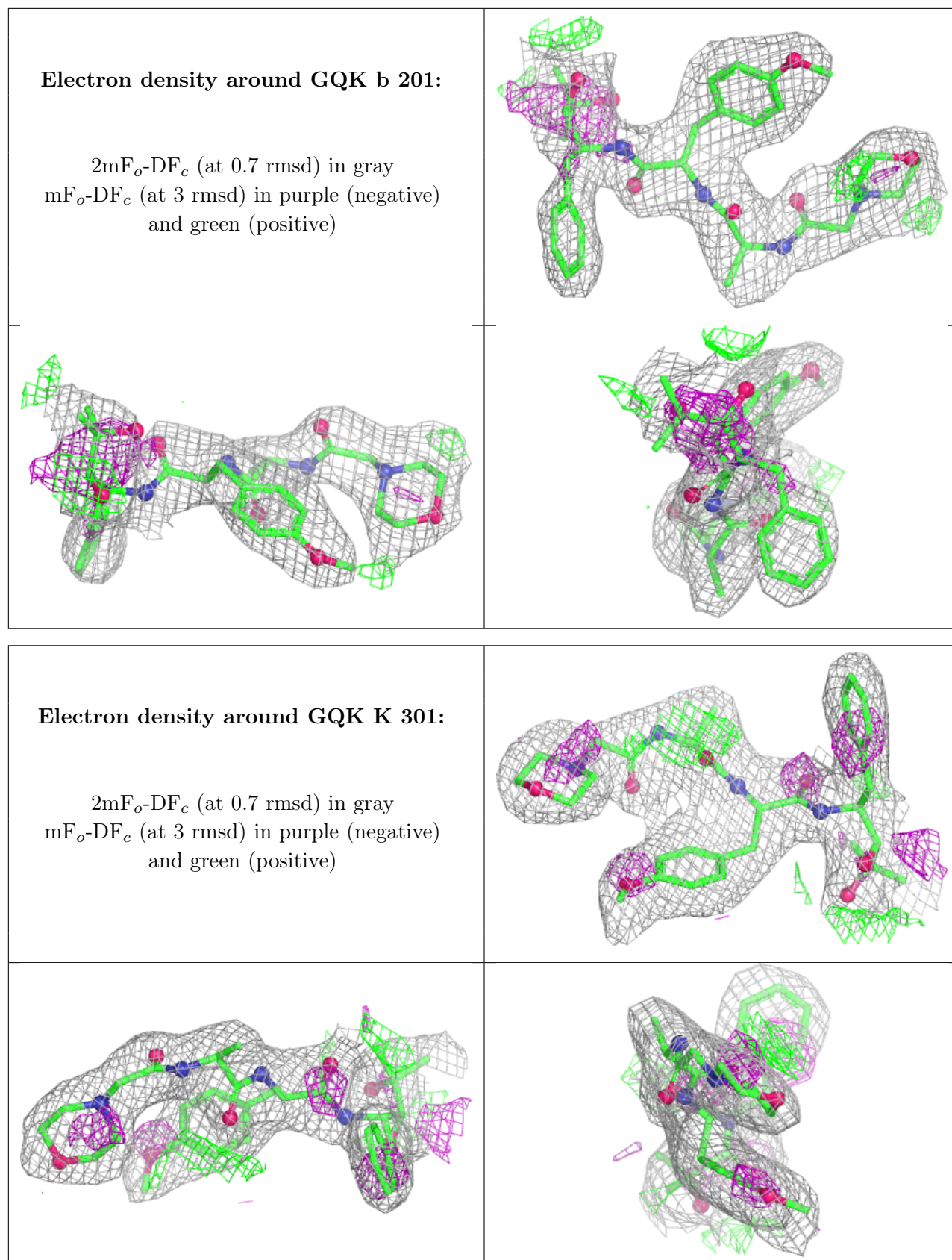
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

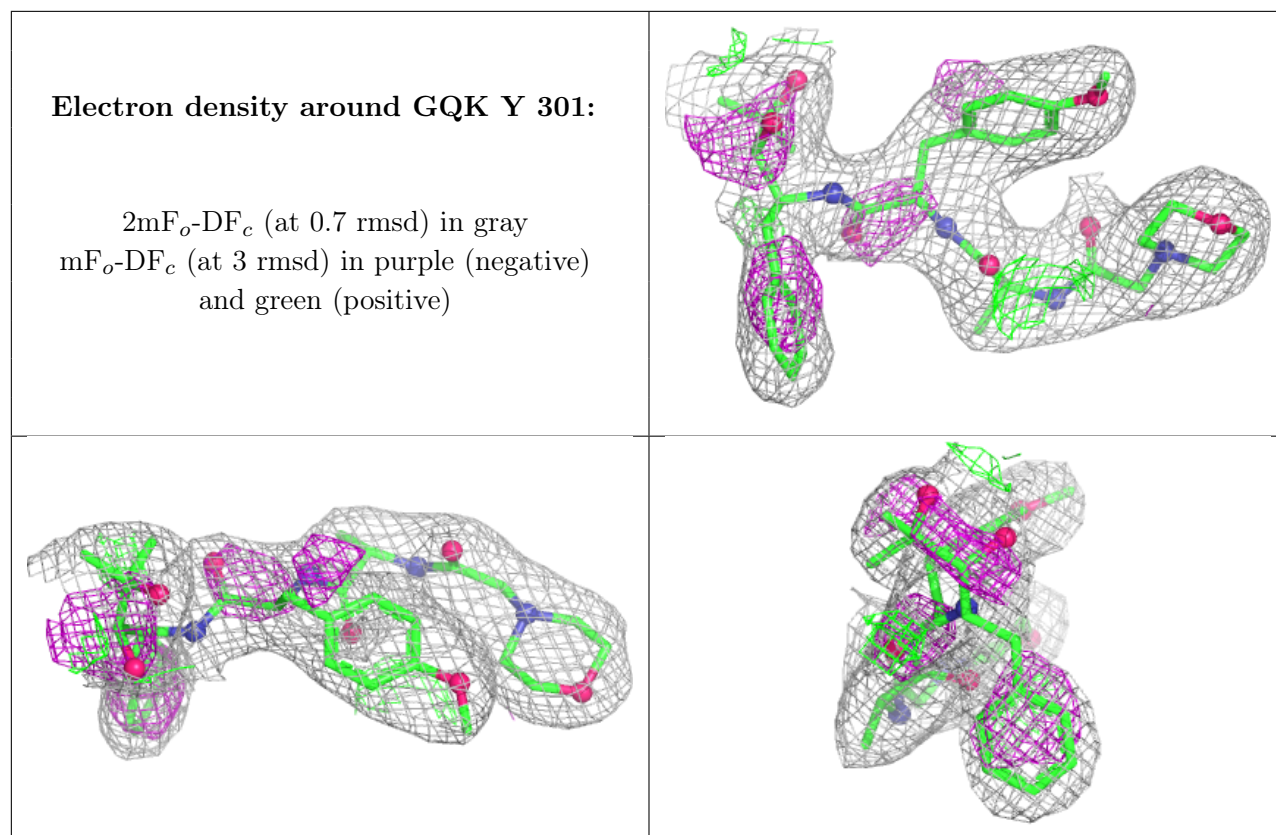


**Electron density around GQK V 301:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.