



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 15, 2024 – 05:20 pm GMT

PDB ID : 6HTR  
Title : Yeast 20S proteasome with human beta2c (S171G) in complex with 13  
Authors : Huber, E.M.; Groll, M.  
Deposited on : 2018-10-04  
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

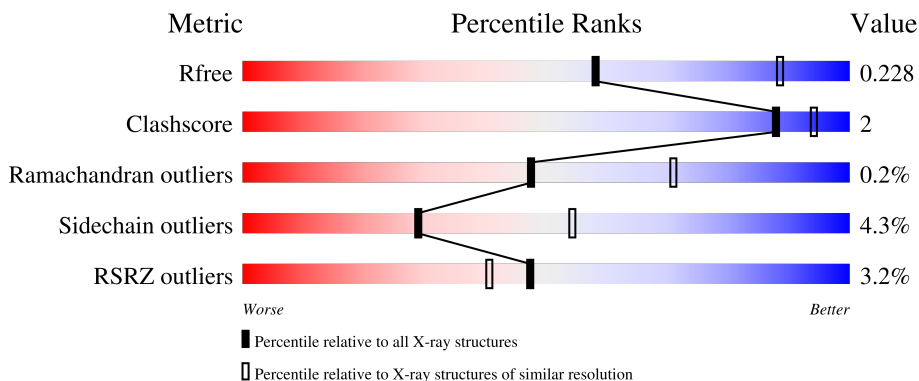
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	 4% 93%
1	O	250	 6% 93%
2	B	258	 5% 86% 9% 5%
2	P	258	 5% 88% 7% 5%
3	C	254	 6% 87% 6% 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	 9% 87% 6% • 6%
4	D	260	 2% 84% 6% 10%
4	R	260	 3% 82% 8% 10%
5	E	234	 3% 88% 10% ..
5	S	234	 3% 88% 10% ..
6	F	288	 3% 79% 5% • 16%
6	T	288	 3% 79% 5% • 16%
7	G	252	 3% 90% 5% •
7	U	252	 3% 90% 5% •
8	H	234	 2% 88% • • 6%
8	V	234	 4% 88% • 6%
9	I	205	 % 90% 9%
9	W	205	 % 90% 8% •
10	J	198	 2% 91% 6% ••
10	X	198	 2% 90% 7% ••
11	K	212	 % 91% 8% •
11	Y	212	 % 89% 10% •
12	L	222	 % 88% 9% •
12	Z	222	 2% 86% 11% •
13	M	246	 2% 90% • 7%
13	a	246	 % 90% • 7%
14	N	196	 % 95% 5%
14	b	196	 % 97% •

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 49883 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	C	N	O	S	0	0	0
			1842	1171	305	362	4			
1	O	240	Total	C	N	O	S	0	0	0
			1842	1171	305	362	4			

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

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

- Molecule 3 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-4.

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

- Molecule 4 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-5.

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

- Molecule 5 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-6.

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

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

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

- Molecule 7 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-1.

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

- Molecule 8 is a protein called Proteasome subunit beta type-7.

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

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
			Total	C	N	O	S			
9	I	204	Total 1581	C 1010	N 258	O 305	S 8	0	0	0
9	W	204	Total 1581	C 1010	N 258	O 305	S 8	0	0	0

- Molecule 10 is a protein called PROTEASOME SUBUNIT BETA TYPE-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	228	Total	C	N	O	S	0	0	0
			1786	1131	305	343	7			
13	a	228	Total	C	N	O	S	0	0	0
			1786	1131	305	343	7			

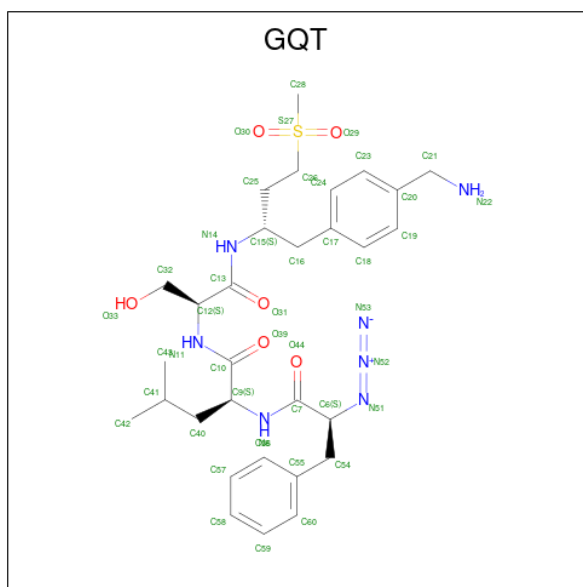
- Molecule 14 is a protein called PROTEASOME SUBUNIT BETA TYPE-1.

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 1 1	0	0
15	H	1	Total Mg 1 1	0	0
15	I	1	Total Mg 1 1	0	0
15	K	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	V	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 (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).



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

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

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
17	A	30	30	30	0	0
17	B	31	31	31	0	0
17	C	24	24	24	0	0
17	D	21	21	21	0	0
17	E	16	16	16	0	0
17	F	28	28	28	0	0
17	G	23	23	23	0	0
17	H	36	36	36	0	0
17	I	20	20	20	0	0
17	J	23	23	23	0	0
17	K	28	28	28	0	0
17	L	38	38	38	0	0
17	M	28	28	28	0	0
17	N	21	21	21	0	0
17	O	11	11	11	0	0
17	P	22	22	22	0	0
17	Q	21	21	21	0	0
17	R	11	11	11	0	0

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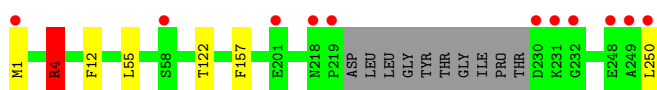
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
17	S	20	Total 20	O 20	0	0
17	T	23	Total 23	O 23	0	0
17	U	33	Total 33	O 33	0	0
17	V	21	Total 21	O 21	0	0
17	W	25	Total 25	O 25	0	0
17	X	21	Total 21	O 21	0	0
17	Y	32	Total 32	O 32	0	0
17	Z	22	Total 22	O 22	0	0
17	a	41	Total 41	O 41	0	0
17	b	27	Total 27	O 27	0	0

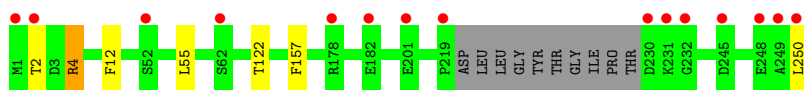
### 3 Residue-property plots [i](#)

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

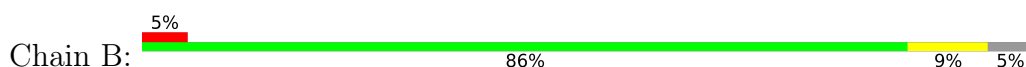
- Molecule 1: PROTEASOME SUBUNIT ALPHA TYPE-2



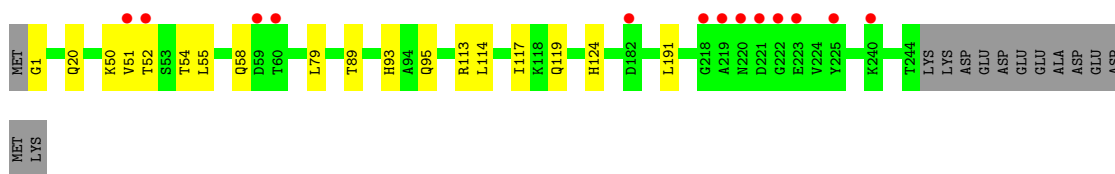
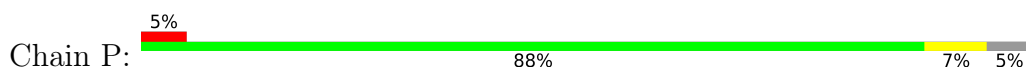
- Molecule 1: PROTEASOME SUBUNIT ALPHA TYPE-2



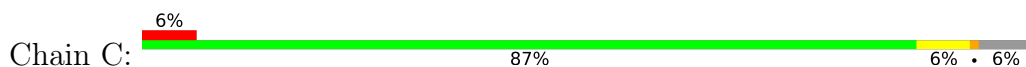
- Molecule 2: Proteasome subunit alpha type-3

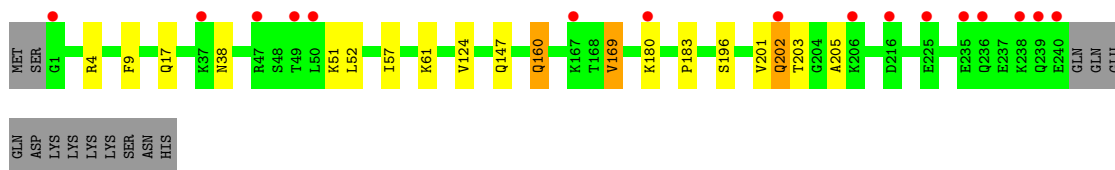


- Molecule 2: Proteasome subunit alpha type-3

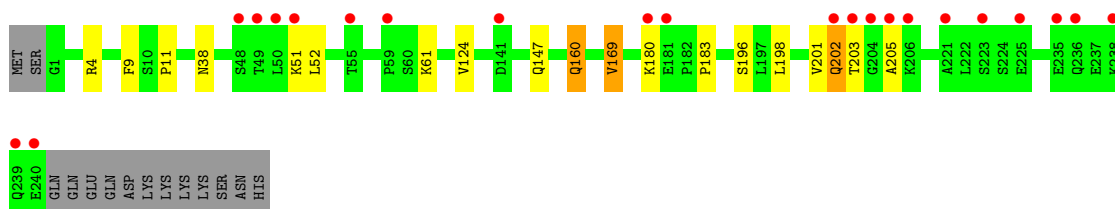
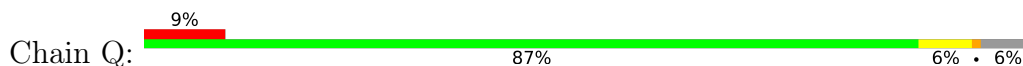


- Molecule 3: PROTEASOME SUBUNIT ALPHA TYPE-4

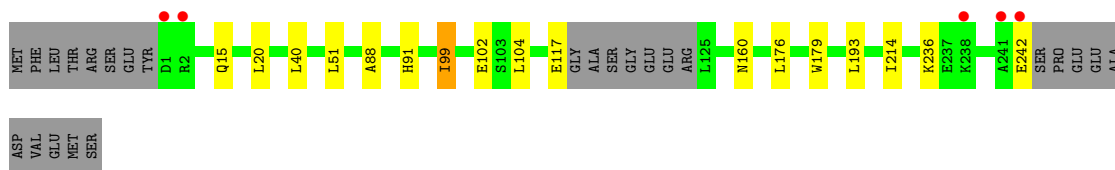
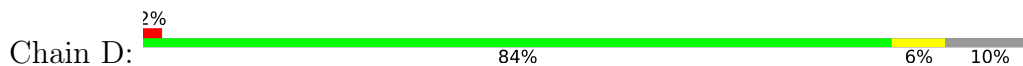




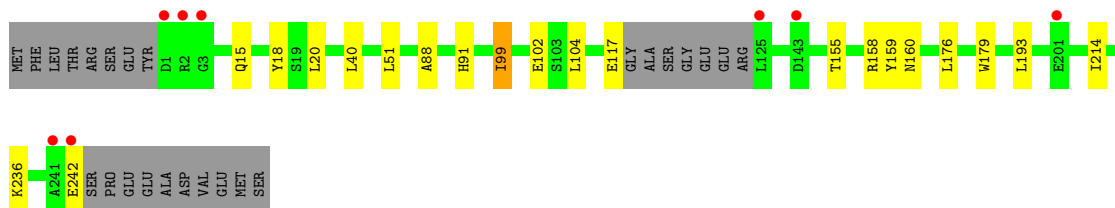
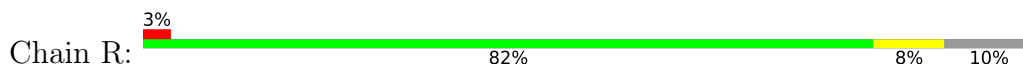
- Molecule 3: PROTEASOME SUBUNIT ALPHA TYPE-4



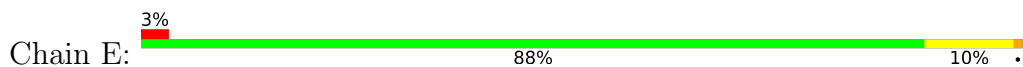
- Molecule 4: PROTEASOME SUBUNIT ALPHA TYPE-5



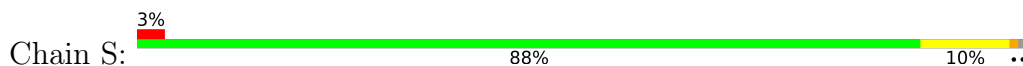
- Molecule 4: PROTEASOME SUBUNIT ALPHA TYPE-5

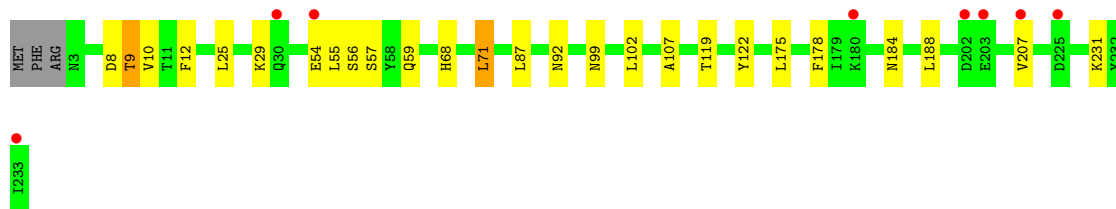


- Molecule 5: PROTEASOME SUBUNIT ALPHA TYPE-6

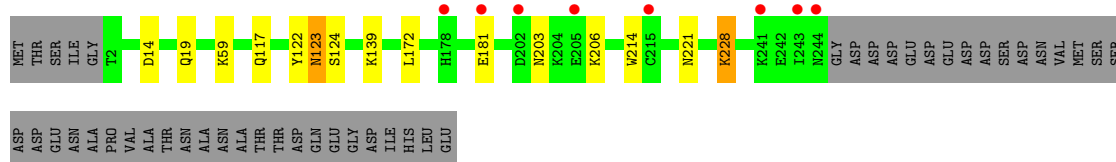
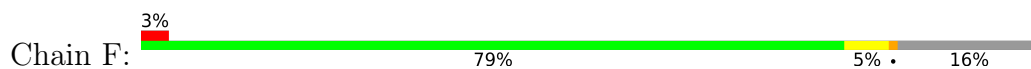


- Molecule 5: PROTEASOME SUBUNIT ALPHA TYPE-6

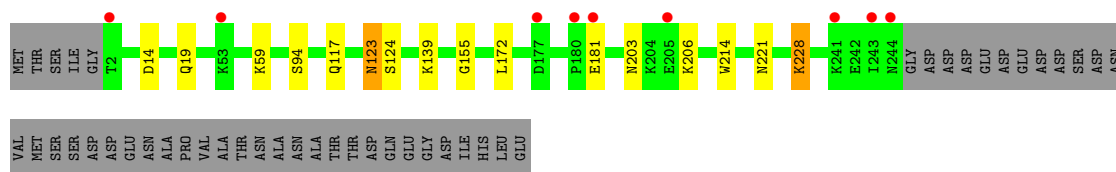
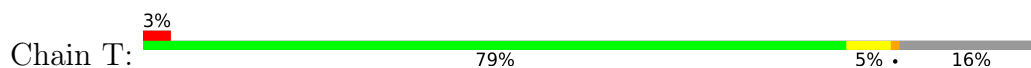




- Molecule 6: Probable proteasome subunit alpha type-7



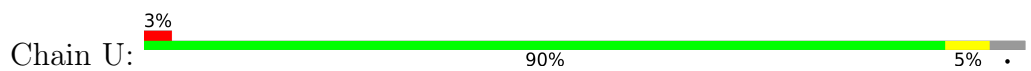
- Molecule 6: Probable proteasome subunit alpha type-7



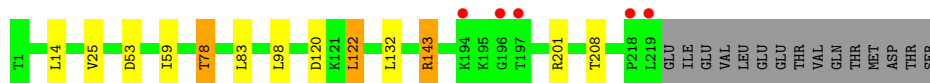
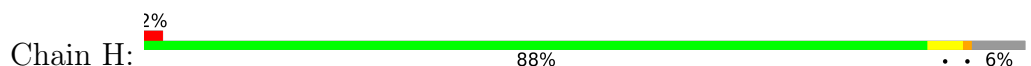
- Molecule 7: PROTEASOME SUBUNIT ALPHA TYPE-1



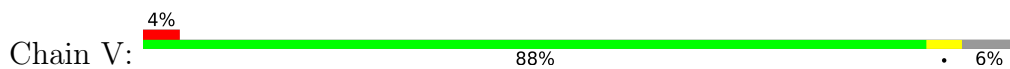
- Molecule 7: PROTEASOME SUBUNIT ALPHA TYPE-1



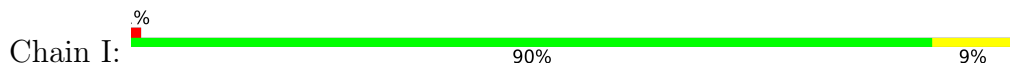
- Molecule 8: Proteasome subunit beta type-7



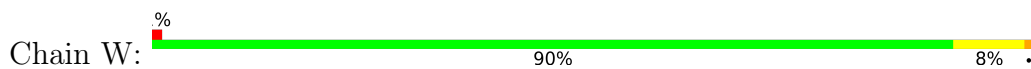
- Molecule 8: Proteasome subunit beta type-7



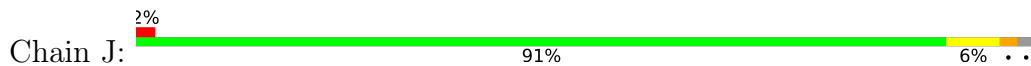
- Molecule 9: Proteasome subunit beta type-3



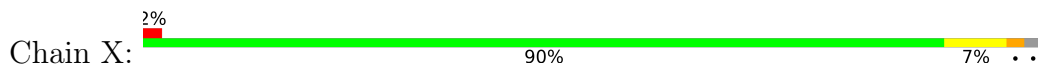
- Molecule 9: Proteasome subunit beta type-3



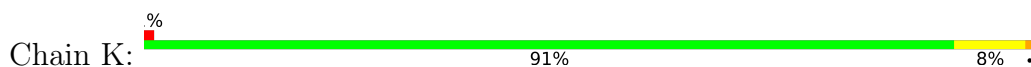
- Molecule 10: PROTEASOME SUBUNIT BETA TYPE-4



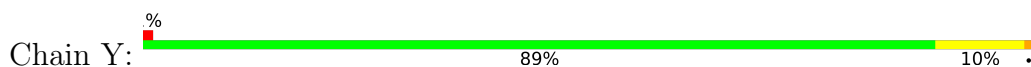
- Molecule 10: PROTEASOME SUBUNIT BETA TYPE-4



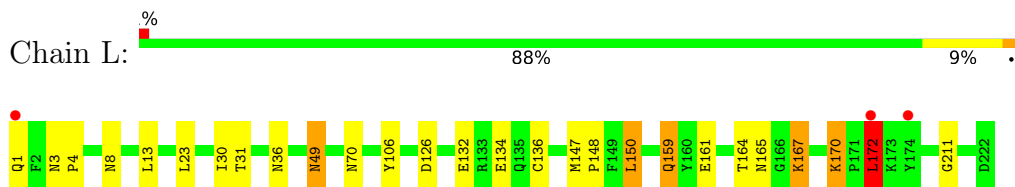
- Molecule 11: Proteasome subunit beta type-5



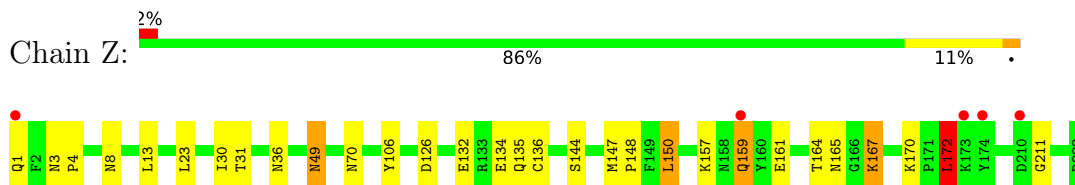
- Molecule 11: Proteasome subunit beta type-5



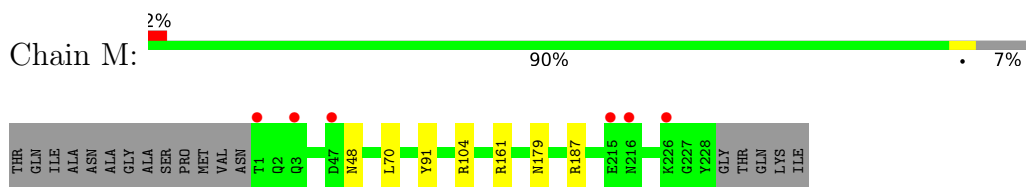
- Molecule 12: Proteasome subunit beta type-6



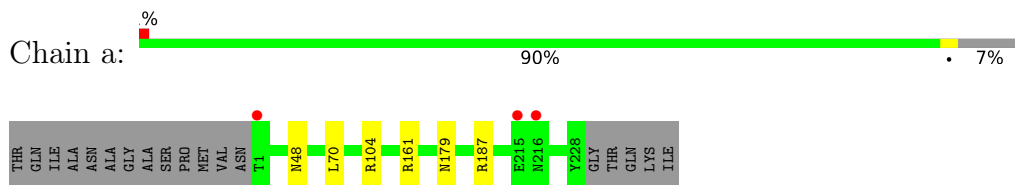
- Molecule 12: Proteasome subunit beta type-6



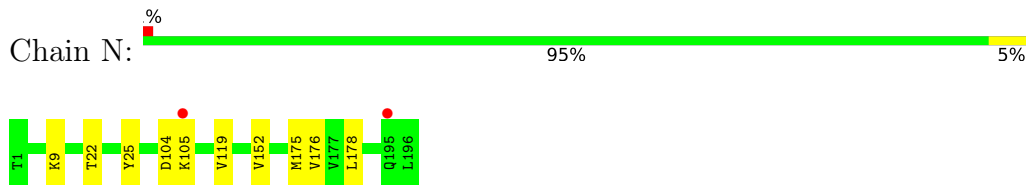
- Molecule 13: Proteasome subunit beta type-7



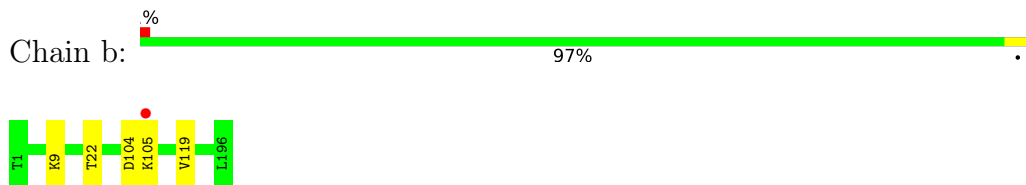
- Molecule 13: Proteasome subunit beta type-7



- Molecule 14: PROTEASOME SUBUNIT BETA TYPE-1



- Molecule 14: PROTEASOME SUBUNIT BETA TYPE-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.36Å 300.53Å 144.81Å 90.00° 113.41° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 15.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.6 (15.00-2.60) 97.1 (15.00-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.194 , 0.225 0.197 , 0.228	Depositor DCC
$R_{free}$ test set	15777 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.3	Xtrriage
Anisotropy	0.652	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 32.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	49883	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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: GQT, MG

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	0.37	0/1876	0.81	3/2535 (0.1%)
1	O	0.37	0/1876	0.80	4/2535 (0.2%)
2	B	0.38	0/1934	0.63	0/2618
2	P	0.38	0/1934	0.63	0/2618
3	C	0.39	0/1910	0.66	0/2586
3	Q	0.39	0/1910	0.66	0/2586
4	D	0.38	0/1837	0.61	0/2475
4	R	0.38	0/1837	0.61	0/2475
5	E	0.38	0/1800	0.61	1/2433 (0.0%)
5	S	0.37	0/1800	0.61	1/2433 (0.0%)
6	F	0.38	0/1932	0.59	0/2609
6	T	0.38	0/1932	0.58	0/2609
7	G	0.39	0/1945	0.60	0/2634
7	U	0.39	0/1945	0.60	0/2634
8	H	0.37	0/1675	0.86	3/2267 (0.1%)
8	V	0.36	0/1675	0.87	3/2267 (0.1%)
9	I	0.38	0/1611	0.60	0/2174
9	W	0.37	0/1611	0.60	0/2174
10	J	0.37	0/1589	0.62	0/2142
10	X	0.37	0/1589	0.62	0/2142
11	K	0.37	0/1681	0.61	1/2274 (0.0%)
11	Y	0.37	0/1681	0.61	1/2274 (0.0%)
12	L	0.42	0/1795	0.74	2/2420 (0.1%)
12	Z	0.42	0/1795	0.72	2/2420 (0.1%)
13	M	0.38	0/1817	0.64	0/2465
13	a	0.38	0/1817	0.65	0/2465
14	N	0.36	0/1541	0.60	0/2087
14	b	0.36	0/1541	0.60	0/2087
All	All	0.38	0/49886	0.66	21/67438 (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
8	V	0	1
All	All	0	3

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	ARG	NE-CZ-NH2	-21.46	109.57	120.30
8	V	143	ARG	NE-CZ-NH2	-20.52	110.04	120.30
1	O	4	ARG	NE-CZ-NH1	-19.96	110.32	120.30
8	H	143	ARG	NE-CZ-NH1	-18.52	111.04	120.30
8	H	143	ARG	NE-CZ-NH2	16.52	128.56	120.30
1	O	4	ARG	NE-CZ-NH2	15.92	128.26	120.30
1	A	4	ARG	NE-CZ-NH1	15.28	127.94	120.30
8	V	143	ARG	NE-CZ-NH1	14.50	127.55	120.30
12	L	172	LEU	CB-CG-CD2	-10.34	93.43	111.00
1	A	4	ARG	CD-NE-CZ	10.20	137.88	123.60
8	V	143	ARG	CD-NE-CZ	10.12	137.77	123.60
1	O	4	ARG	CD-NE-CZ	9.58	137.01	123.60
12	Z	172	LEU	CB-CG-CD2	-9.29	95.21	111.00
12	L	172	LEU	CB-CG-CD1	9.01	126.31	111.00
8	H	143	ARG	CD-NE-CZ	8.12	134.97	123.60
12	Z	172	LEU	CB-CG-CD1	7.48	123.72	111.00
1	O	4	ARG	CG-CD-NE	5.73	123.84	111.80
11	Y	4	LEU	CA-CB-CG	5.61	128.21	115.30
5	E	71	LEU	CA-CB-CG	5.43	127.80	115.30
11	K	4	LEU	CA-CB-CG	5.38	127.67	115.30
5	S	71	LEU	CA-CB-CG	5.20	127.27	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4	ARG	Sidechain
1	O	4	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	5	0
1	O	1842	0	1855	2	0
2	B	1904	0	1904	11	0
2	P	1904	0	1904	8	0
3	C	1881	0	1895	8	0
3	Q	1881	0	1895	8	0
4	D	1813	0	1797	5	0
4	R	1813	0	1797	9	0
5	E	1773	0	1775	12	0
5	S	1773	0	1775	12	0
6	F	1892	0	1883	5	0
6	T	1892	0	1883	5	0
7	G	1907	0	1901	6	0
7	U	1907	0	1901	6	0
8	H	1648	0	1672	16	0
8	V	1648	0	1672	16	0
9	I	1581	0	1574	11	0
9	W	1581	0	1574	12	0
10	J	1561	0	1569	8	0
10	X	1561	0	1569	10	0
11	K	1644	0	1594	8	0
11	Y	1644	0	1594	12	0
12	L	1757	0	1711	26	0
12	Z	1757	0	1711	27	0
13	M	1786	0	1790	1	0
13	a	1786	0	1790	0	0
14	N	1512	0	1481	3	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0
15	K	1	0	0	0	0
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	H	44	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	K	44	0	0	0	0
16	V	44	0	0	1	0
16	Y	44	0	0	0	0
17	A	30	0	0	0	0
17	B	31	0	0	1	0
17	C	24	0	0	0	0
17	D	21	0	0	0	0
17	E	16	0	0	0	0
17	F	28	0	0	0	0
17	G	23	0	0	0	0
17	H	36	0	0	1	0
17	I	20	0	0	0	0
17	J	23	0	0	0	0
17	K	28	0	0	0	0
17	L	38	0	0	0	0
17	M	28	0	0	0	0
17	N	21	0	0	0	0
17	O	11	0	0	0	0
17	P	22	0	0	1	0
17	Q	21	0	0	0	0
17	R	11	0	0	0	0
17	S	20	0	0	0	0
17	T	23	0	0	0	0
17	U	33	0	0	1	0
17	V	21	0	0	0	0
17	W	25	0	0	0	0
17	X	21	0	0	0	0
17	Y	32	0	0	0	0
17	Z	22	0	0	0	0
17	a	41	0	0	0	0
17	b	27	0	0	0	0
All	All	49883	0	48802	183	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 2.

All (183) 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)
12:L:159:GLN:NE2	8:V:208:THR:HG22	1.25	1.46
12:L:159:GLN:NE2	8:V:208:THR:CG2	1.86	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:208:THR:CG2	12:Z:159:GLN:NE2	1.88	1.37
12:L:159:GLN:CD	8:V:208:THR:HG22	1.53	1.28
8:H:208:THR:HG23	12:Z:159:GLN:NE2	1.45	1.17
12:L:159:GLN:CD	8:V:208:THR:CG2	2.11	1.13
12:Z:172:LEU:H	12:Z:172:LEU:HD23	1.16	1.06
12:L:159:GLN:HE22	8:V:208:THR:CG2	1.60	1.04
12:L:172:LEU:H	12:L:172:LEU:HD23	1.26	0.98
12:L:159:GLN:HE22	8:V:208:THR:HG23	1.26	0.94
8:H:208:THR:HG23	12:Z:159:GLN:HE21	1.24	0.92
8:H:208:THR:CG2	12:Z:159:GLN:HE21	1.68	0.91
12:L:159:GLN:OE1	8:V:208:THR:CG2	2.21	0.89
12:Z:172:LEU:HD23	12:Z:172:LEU:N	1.81	0.87
12:L:159:GLN:NE2	8:V:208:THR:HG23	1.82	0.85
8:H:208:THR:HG23	12:Z:159:GLN:HE22	1.43	0.82
8:H:208:THR:HG21	12:Z:159:GLN:NE2	1.93	0.81
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.30	0.79
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.30	0.78
12:L:172:LEU:HD23	12:L:172:LEU:N	1.90	0.78
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.34	0.76
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.34	0.75
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.54	0.73
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.54	0.72
5:E:12:PHE:H	6:F:19:GLN:HE22	1.38	0.72
12:Z:172:LEU:H	12:Z:172:LEU:CD2	1.98	0.71
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.55	0.71
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.56	0.70
8:H:208:THR:HG22	12:Z:159:GLN:NE2	2.04	0.69
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.41	0.68
5:S:12:PHE:H	6:T:19:GLN:HE22	1.41	0.67
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.79	0.64
11:K:31:VAL:HA	12:L:132:GLU:OE2	1.97	0.64
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	1.95	0.64
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.79	0.63
1:O:12:PHE:H	2:P:20:GLN:HE22	1.47	0.62
2:P:95:GLN:NE2	9:W:71:ASN:HD22	1.98	0.61
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.83	0.60
3:C:9:PHE:H	4:D:15:GLN:HE22	1.47	0.60
2:B:95:GLN:NE2	9:I:71:ASN:HD22	2.00	0.60
5:E:92:ASN:ND2	12:L:70:ASN:HD21	2.00	0.60
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	1.97	0.60
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:208:THR:HG22	12:Z:159:GLN:HE21	1.59	0.60
8:V:219:LEU:HD21	9:W:194:VAL:HG23	1.83	0.59
5:E:92:ASN:HD21	12:L:70:ASN:ND2	1.97	0.59
2:B:12:PHE:H	3:C:17:GLN:HE22	1.50	0.59
11:K:209:ASN:O	9:W:37:ASN:ND2	2.36	0.58
11:Y:31:VAL:HA	12:Z:132:GLU:OE2	2.04	0.57
10:J:1:MET:O	10:J:2:ASP:HB2	2.05	0.57
1:A:12:PHE:H	2:B:20:GLN:HE22	1.53	0.56
12:L:164:THR:O	12:L:165:ASN:HB3	2.05	0.56
7:G:23:PHE:O	7:G:26:THR:HB	2.05	0.56
7:U:23:PHE:O	7:U:26:THR:HB	2.06	0.55
12:L:159:GLN:OE1	8:V:208:THR:HG21	2.06	0.55
12:Z:164:THR:O	12:Z:165:ASN:HB3	2.05	0.55
12:L:164:THR:O	12:L:167:LYS:HB2	2.07	0.54
12:Z:164:THR:O	12:Z:167:LYS:HB2	2.08	0.54
1:A:55:LEU:HD12	7:G:170:THR:HG23	1.89	0.54
8:H:78:THR:HG21	17:H:413:HOH:O	2.08	0.53
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.73	0.53
10:X:1:MET:O	10:X:2:ASP:HB2	2.08	0.53
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.91	0.53
9:I:37:ASN:ND2	11:Y:209:ASN:O	2.43	0.52
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.74	0.52
12:Z:172:LEU:N	12:Z:172:LEU:CD2	2.63	0.52
1:A:4:ARG:HD3	5:E:122:TYR:CD2	2.45	0.52
12:L:159:GLN:OE1	8:V:208:THR:HG23	2.09	0.51
8:H:208:THR:CG2	12:Z:159:GLN:CD	2.73	0.51
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.92	0.51
14:N:152:VAL:HA	14:N:175:MET:HE1	1.92	0.51
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.93	0.51
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.92	0.51
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.93	0.50
2:P:113:ARG:NH1	17:P:301:HOH:O	2.42	0.50
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.93	0.50
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.76	0.50
7:U:99:TYR:O	8:V:78:THR:HB	2.12	0.50
2:B:113:ARG:NH1	17:B:301:HOH:O	2.40	0.50
10:J:174:MET:HA	10:X:174:MET:HA	1.93	0.50
7:G:99:TYR:O	8:H:78:THR:HB	2.13	0.49
3:C:51:LYS:O	3:C:52:LEU:HB2	2.13	0.49
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.93	0.49
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.13	0.49
11:Y:35:ILE:HB	11:Y:45:MET:CE	2.43	0.49
6:F:123:ASN:HD22	6:F:124:SER:N	2.10	0.48
12:L:161:GLU:O	12:L:164:THR:OG1	2.21	0.48
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.95	0.48
11:K:176:ASN:ND2	11:K:190:ASN:HD22	2.11	0.48
6:T:123:ASN:HD22	6:T:124:SER:N	2.10	0.48
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.78	0.48
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.94	0.48
10:J:1:MET:HA	10:J:34:LYS:HE3	1.96	0.48
11:K:35:ILE:HB	11:K:45:MET:CE	2.44	0.48
6:T:123:ASN:HD22	6:T:123:ASN:C	2.18	0.47
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.97	0.47
7:U:203:ASP:HB3	17:U:327:HOH:O	2.15	0.47
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.46	0.47
11:Y:176:ASN:ND2	11:Y:190:ASN:HD22	2.13	0.47
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.97	0.47
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.95	0.47
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.95	0.47
10:X:1:MET:HA	10:X:34:LYS:HE3	1.96	0.47
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.50	0.47
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.97	0.46
4:R:155:THR:HG23	5:S:59:GLN:HE22	1.81	0.46
5:E:9:THR:HG21	5:E:119:THR:HA	1.98	0.46
5:S:9:THR:HG21	5:S:119:THR:HA	1.98	0.46
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.98	0.46
10:J:1:MET:HA	10:J:34:LYS:CE	2.46	0.45
10:J:139:TYR:CZ	11:Y:134:THR:HG22	2.51	0.45
7:U:83:ASN:C	7:U:83:ASN:HD22	2.20	0.45
8:V:53:ASP:OD2	16:V:301:GQT:N22	2.49	0.45
11:Y:25:TRP:CH2	12:Z:144:SER:HA	2.51	0.45
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.97	0.45
11:K:77:ALA:O	11:K:121:ARG:NH1	2.49	0.45
11:K:45:MET:HG2	11:K:52:CYS:HB3	1.99	0.45
5:S:68:HIS:HE1	5:S:102:LEU:O	2.00	0.45
2:P:93:HIS:HB3	2:P:113:ARG:HH21	1.81	0.45
8:H:25:VAL:HG11	9:I:146:PHE:CD2	2.52	0.45
9:W:98:ARG:O	9:W:126:ILE:HD11	2.17	0.45
11:Y:77:ALA:O	11:Y:121:ARG:NH1	2.50	0.45
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.47	0.44
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:1:MET:HA	10:X:34:LYS:CE	2.46	0.44
5:E:98:PHE:O	13:M:91:TYR:HA	2.18	0.44
6:F:123:ASN:HD22	6:F:123:ASN:C	2.20	0.44
8:H:53:ASP:OD2	16:H:301:GQT:N22	2.50	0.44
8:H:132:LEU:HD22	14:N:25:TYR:CE1	2.53	0.44
9:I:98:ARG:O	9:I:126:ILE:HD11	2.17	0.44
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.53	0.44
12:L:170:LYS:HA	12:L:170:LYS:HD2	1.82	0.44
5:E:68:HIS:HE1	5:E:102:LEU:O	2.01	0.44
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.53	0.43
6:F:228:LYS:HE3	6:F:228:LYS:HB2	1.84	0.43
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.99	0.43
3:Q:11:PRO:HA	4:R:18:TYR:CD1	2.53	0.43
4:R:158:ARG:HB3	5:S:57:SER:HB3	2.00	0.43
1:A:1:MET:HG3	6:F:122:TYR:CE1	2.54	0.43
9:I:101:PRO:HB3	9:I:126:ILE:HD12	2.01	0.43
2:B:93:HIS:HB3	2:B:113:ARG:HH21	1.82	0.43
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	2.00	0.43
11:Y:45:MET:HG2	11:Y:52:CYS:HB3	1.99	0.43
8:H:120:ASP:HB3	8:H:122:LEU:HD22	2.01	0.43
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.53	0.43
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.19	0.43
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.54	0.43
9:W:101:PRO:HB3	9:W:126:ILE:HD12	2.01	0.43
5:E:118:ASN:HD22	5:E:118:ASN:N	2.16	0.43
1:O:55:LEU:HB3	7:U:159:ALA:O	2.18	0.43
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.48	0.42
12:L:8:ASN:HA	12:L:30:ILE:O	2.18	0.42
12:Z:161:GLU:O	12:Z:164:THR:OG1	2.22	0.42
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	2.01	0.42
8:V:59:ILE:HG13	8:V:83:LEU:HD23	2.02	0.42
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.34	0.42
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.55	0.42
8:V:50:ALA:HB2	9:W:128:CYS:HB2	2.02	0.42
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.55	0.42
2:B:89:THR:HG21	2:B:117:ILE:HD13	2.02	0.42
3:C:169:VAL:HG23	3:C:196:SER:HB2	2.01	0.41
7:G:114:ASN:HD22	7:G:114:ASN:HA	1.72	0.41
11:Y:44:THR:OG1	11:Y:100:MET:HB2	2.19	0.41
8:V:203:ARG:HH11	9:W:154:GLU:CD	2.24	0.41
1:A:4:ARG:CD	5:E:122:TYR:HD2	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:44:THR:OG1	11:K:100:MET:HB2	2.20	0.41
2:B:47:ALA:HB1	2:B:64:LYS:HD2	2.03	0.41
12:L:147:MET:N	12:L:148:PRO:HD2	2.35	0.41
8:H:59:ILE:HG13	8:H:83:LEU:HD23	2.01	0.41
3:C:201:VAL:O	3:C:202:GLN:CB	2.69	0.41
2:P:1:GLY:HA3	5:S:122:TYR:CD1	2.56	0.41
6:T:228:LYS:HB2	6:T:228:LYS:HE3	1.85	0.41
2:B:180:LYS:O	2:B:183:MET:HB2	2.21	0.40
2:P:89:THR:HG21	2:P:117:ILE:HD13	2.02	0.40
10:X:36:ARG:NH1	10:X:58:GLU:OE2	2.53	0.40
3:Q:198:LEU:HA	3:Q:201:VAL:HG12	2.04	0.40
9:I:120:ILE:HD12	9:I:136:ILE:HG12	2.04	0.40
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.04	0.40
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.69	0.40
7:G:83:ASN:HD22	7:G:83:ASN:C	2.25	0.40
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.87	0.40
6:T:155:GLY:HA3	7:U:59:THR:HG21	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	236/250 (94%)	227 (96%)	9 (4%)	0	100	100
1	O	236/250 (94%)	228 (97%)	8 (3%)	0	100	100
2	B	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	34	57
2	P	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	34	57
3	C	238/254 (94%)	230 (97%)	5 (2%)	3 (1%)	12	24
3	Q	238/254 (94%)	231 (97%)	4 (2%)	3 (1%)	12	24
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
5	E	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	235 (98%)	6 (2%)	0	100	100
6	T	241/288 (84%)	235 (98%)	6 (2%)	0	100	100
7	G	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
7	U	239/252 (95%)	236 (99%)	3 (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%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	188 (97%)	4 (2%)	1 (0%)	29	52
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	52
11	K	210/212 (99%)	203 (97%)	5 (2%)	2 (1%)	15	32
11	Y	210/212 (99%)	203 (97%)	5 (2%)	2 (1%)	15	32
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
13	M	226/246 (92%)	217 (96%)	9 (4%)	0	100	100
13	a	226/246 (92%)	217 (96%)	9 (4%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6236/6618 (94%)	6066 (97%)	156 (2%)	14 (0%)	47	71

All (14) 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
11	Y	148	LEU

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Mol	Chain	Res	Type
11	K	39	PRO
11	K	148	LEU
11	Y	39	PRO
3	C	183	PRO
3	Q	183	PRO

### 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%)	198 (98%)	3 (2%)	65 83
1	O	201/209 (96%)	197 (98%)	4 (2%)	55 78
2	B	203/216 (94%)	194 (96%)	9 (4%)	28 53
2	P	203/216 (94%)	194 (96%)	9 (4%)	28 53
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%)	183 (94%)	11 (6%)	20 41
4	R	194/215 (90%)	183 (94%)	11 (6%)	20 41
5	E	190/193 (98%)	176 (93%)	14 (7%)	13 28
5	S	190/193 (98%)	177 (93%)	13 (7%)	16 32
6	F	201/239 (84%)	189 (94%)	12 (6%)	19 39
6	T	201/239 (84%)	188 (94%)	13 (6%)	17 34
7	G	206/210 (98%)	199 (97%)	7 (3%)	37 63
7	U	206/210 (98%)	199 (97%)	7 (3%)	37 63
8	H	179/194 (92%)	173 (97%)	6 (3%)	37 63
8	V	179/194 (92%)	174 (97%)	5 (3%)	43 69
9	I	172/173 (99%)	167 (97%)	5 (3%)	42 68
9	W	172/173 (99%)	166 (96%)	6 (4%)	36 62
10	J	173/175 (99%)	167 (96%)	6 (4%)	36 62
10	X	173/175 (99%)	167 (96%)	6 (4%)	36 62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	169/169 (100%)	162 (96%)	7 (4%)	30	56
11	Y	169/169 (100%)	162 (96%)	7 (4%)	30	56
12	L	185/185 (100%)	173 (94%)	12 (6%)	17	34
12	Z	185/185 (100%)	171 (92%)	14 (8%)	13	26
13	M	195/208 (94%)	189 (97%)	6 (3%)	40	66
13	a	195/208 (94%)	189 (97%)	6 (3%)	40	66
14	N	162/162 (100%)	157 (97%)	5 (3%)	40	66
14	b	162/162 (100%)	157 (97%)	5 (3%)	40	66
All	All	5284/5548 (95%)	5059 (96%)	225 (4%)	29	54

All (225) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS
2	B	52	THR
2	B	54	THR
2	B	55	LEU
2	B	58	GLN
2	B	79	LEU
2	B	114	LEU
2	B	119	GLN
2	B	191	LEU
3	C	4	ARG
3	C	38	ASN
3	C	61	LYS
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	40	LEU
4	D	51	LEU
4	D	99	ILE
4	D	102	GLU
4	D	117	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	236	LYS
4	D	242	GLU
5	E	8	ASP
5	E	9	THR
5	E	10	VAL
5	E	25	LEU
5	E	29	LYS
5	E	54	GLU
5	E	55	LEU
5	E	71	LEU
5	E	99	ASN
5	E	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	207	VAL
5	E	231	LYS
6	F	14	ASP
6	F	59	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	172	LEU
6	F	181	GLU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
6	F	228	LYS
7	G	83	ASN
7	G	115	LEU
7	G	125	MET
7	G	166	GLN
7	G	181	LYS
7	G	235	ARG
7	G	236	LEU
8	H	14	LEU
8	H	78	THR
8	H	98	LEU
8	H	122	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	H	143	ARG
8	H	201	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
9	I	191	LYS
9	I	192	ASP
10	J	23	ARG
10	J	35	THR
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	18	SER
11	K	35	ILE
11	K	73	ARG
11	K	100	MET
11	K	108	GLU
12	L	1	GLN
12	L	23	LEU
12	L	49	ASN
12	L	106	TYR
12	L	126	ASP
12	L	134	GLU
12	L	136	CYS
12	L	150	LEU
12	L	159	GLN
12	L	167	LYS
12	L	170	LYS
12	L	172	LEU
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	179	ASN
13	M	187	ARG
14	N	9	LYS
14	N	22	THR
14	N	104	ASP
14	N	105	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
14	N	119	VAL
1	O	2	THR
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	52	THR
2	P	54	THR
2	P	55	LEU
2	P	58	GLN
2	P	79	LEU
2	P	114	LEU
2	P	119	GLN
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	61	LYS
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	40	LEU
4	R	51	LEU
4	R	99	ILE
4	R	102	GLU
4	R	117	GLU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	236	LYS
4	R	242	GLU
5	S	8	ASP
5	S	9	THR
5	S	10	VAL
5	S	25	LEU
5	S	29	LYS
5	S	54	GLU
5	S	55	LEU
5	S	71	LEU
5	S	99	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	S	184	ASN
5	S	188	LEU
5	S	207	VAL
5	S	231	LYS
6	T	14	ASP
6	T	59	LYS
6	T	94	SER
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	172	LEU
6	T	181	GLU
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN
6	T	228	LYS
7	U	83	ASN
7	U	115	LEU
7	U	125	MET
7	U	166	GLN
7	U	181	LYS
7	U	235	ARG
7	U	236	LEU
8	V	14	LEU
8	V	78	THR
8	V	98	LEU
8	V	143	ARG
8	V	201	ARG
9	W	20	VAL
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
9	W	191	LYS
9	W	192	ASP
10	X	23	ARG
10	X	35	THR
10	X	75	LEU
10	X	78	GLN
10	X	144	LEU
10	X	174	MET
11	Y	4	LEU

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Mol	Chain	Res	Type
11	Y	9	GLN
11	Y	18	SER
11	Y	35	ILE
11	Y	73	ARG
11	Y	100	MET
11	Y	108	GLU
12	Z	1	GLN
12	Z	23	LEU
12	Z	49	ASN
12	Z	106	TYR
12	Z	126	ASP
12	Z	134	GLU
12	Z	135	GLN
12	Z	136	CYS
12	Z	150	LEU
12	Z	157	LYS
12	Z	159	GLN
12	Z	167	LYS
12	Z	170	LYS
12	Z	172	LEU
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	179	ASN
13	a	187	ARG
14	b	9	LYS
14	b	22	THR
14	b	104	ASP
14	b	105	LYS
14	b	119	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (130) 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	17	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	100	ASN
4	D	146	GLN
4	D	160	ASN
4	D	198	GLN
4	D	210	GLN
4	D	225	ASN
5	E	59	GLN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	147	GLN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	6	HIS
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	167	GLN
7	G	175	ASN
8	H	153	ASN
9	I	37	ASN
10	J	55	GLN
10	J	118	GLN
10	J	191	GLN
11	K	9	GLN
11	K	85	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	K	176	ASN
12	L	1	GLN
12	L	3	ASN
12	L	36	ASN
12	L	49	ASN
12	L	55	ASN
12	L	70	ASN
12	L	80	ASN
12	L	158	ASN
12	L	159	GLN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
2	P	20	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
3	Q	17	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	100	ASN
4	R	146	GLN
4	R	160	ASN
4	R	198	GLN
4	R	210	GLN
4	R	225	ASN
5	S	59	GLN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	S	147	GLN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	167	GLN
7	U	175	ASN
8	V	153	ASN
9	W	37	ASN
10	X	55	GLN
10	X	86	GLN
10	X	118	GLN
10	X	191	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	55	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	158	ASN
12	Z	159	GLN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	194	ASN
13	a	213	GLN
14	b	161	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 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
16	GQT	V	301	8	44,45,45	1.80	8 (18%)	56,60,60	1.36	8 (14%)
16	GQT	K	301	11	44,45,45	1.56	6 (13%)	56,60,60	1.33	7 (12%)
16	GQT	Y	301	11	44,45,45	1.61	6 (13%)	56,60,60	1.34	7 (12%)
16	GQT	H	301	8	44,45,45	1.84	8 (18%)	56,60,60	1.35	7 (12%)

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
16	GQT	V	301	8	-	15/49/49/49	0/2/2/2
16	GQT	K	301	11	-	9/49/49/49	0/2/2/2
16	GQT	Y	301	11	-	10/49/49/49	0/2/2/2
16	GQT	H	301	8	-	13/49/49/49	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	K	301	GQT	C16-C17	-5.68	1.37	1.51
16	Y	301	GQT	C16-C17	-5.68	1.37	1.51
16	H	301	GQT	N52-N51	-5.50	1.08	1.23
16	H	301	GQT	C16-C17	-5.12	1.39	1.51
16	V	301	GQT	C16-C17	-4.98	1.39	1.51
16	V	301	GQT	N52-N51	-4.94	1.10	1.23
16	Y	301	GQT	C54-C55	-4.70	1.40	1.51
16	K	301	GQT	C54-C55	-4.56	1.40	1.51
16	H	301	GQT	C54-C55	-4.07	1.41	1.51
16	V	301	GQT	O30-S27	4.05	1.53	1.44
16	V	301	GQT	C54-C55	-4.01	1.41	1.51
16	H	301	GQT	O29-S27	4.01	1.53	1.44
16	V	301	GQT	O29-S27	3.88	1.52	1.44
16	H	301	GQT	O30-S27	3.82	1.52	1.44
16	V	301	GQT	C26-S27	3.75	1.83	1.78
16	Y	301	GQT	O29-S27	3.75	1.52	1.44
16	Y	301	GQT	O30-S27	3.68	1.52	1.44
16	H	301	GQT	C26-S27	3.67	1.83	1.78
16	K	301	GQT	O30-S27	3.65	1.52	1.44
16	K	301	GQT	O29-S27	3.56	1.52	1.44
16	H	301	GQT	C21-C20	-3.51	1.39	1.51
16	Y	301	GQT	C21-C20	-3.47	1.39	1.51
16	V	301	GQT	C21-C20	-3.43	1.39	1.51
16	K	301	GQT	C21-C20	-3.39	1.39	1.51
16	Y	301	GQT	C26-S27	2.58	1.81	1.78
16	V	301	GQT	C25-C26	2.34	1.55	1.52
16	K	301	GQT	C26-S27	2.33	1.81	1.78
16	H	301	GQT	C25-C26	2.20	1.54	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	V	301	GQT	C41-C40-C9	-4.12	104.09	115.43
16	H	301	GQT	C41-C40-C9	-3.97	104.50	115.43
16	Y	301	GQT	O30-S27-O29	-3.88	108.81	117.09
16	V	301	GQT	O30-S27-O29	-3.76	109.05	117.09
16	H	301	GQT	O30-S27-O29	-3.74	109.09	117.09
16	K	301	GQT	O30-S27-O29	-3.61	109.38	117.09
16	Y	301	GQT	C16-C17-C18	-3.37	114.22	120.91
16	K	301	GQT	C16-C17-C18	-3.35	114.26	120.91
16	H	301	GQT	C43-C41-C42	-3.33	95.14	110.51
16	V	301	GQT	C43-C41-C42	-3.22	95.65	110.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	301	GQT	C6-N51-N52	3.22	118.63	115.24
16	Y	301	GQT	C16-C17-C24	3.09	127.05	120.91
16	K	301	GQT	C16-C17-C24	3.07	127.00	120.91
16	K	301	GQT	C6-N51-N52	3.01	118.40	115.24
16	K	301	GQT	C28-S27-C26	2.78	115.93	105.21
16	Y	301	GQT	C28-S27-C26	2.73	115.73	105.21
16	H	301	GQT	C16-C17-C18	-2.43	116.08	120.91
16	H	301	GQT	C16-C17-C24	2.41	125.68	120.91
16	V	301	GQT	C28-S27-C26	2.39	114.43	105.21
16	V	301	GQT	C16-C17-C24	2.36	125.60	120.91
16	H	301	GQT	C28-S27-C26	2.31	114.12	105.21
16	V	301	GQT	C16-C17-C18	-2.30	116.34	120.91
16	Y	301	GQT	C9-C10-N11	-2.29	111.67	116.70
16	H	301	GQT	C54-C6-N51	2.21	112.94	109.30
16	K	301	GQT	C54-C6-N51	2.20	112.94	109.30
16	Y	301	GQT	C54-C6-N51	2.20	112.93	109.30
16	K	301	GQT	C9-C10-N11	-2.18	111.92	116.70
16	V	301	GQT	C54-C6-N51	2.10	112.77	109.30
16	V	301	GQT	C42-C41-C40	2.01	118.51	111.11

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	H	301	GQT	C25-C26-S27-O29
16	H	301	GQT	C25-C26-S27-O30
16	H	301	GQT	C13-C12-C32-O33
16	K	301	GQT	N51-C6-C7-N8
16	K	301	GQT	C25-C26-S27-C28
16	K	301	GQT	C25-C26-S27-O29
16	K	301	GQT	C25-C26-S27-O30
16	K	301	GQT	C13-C12-C32-O33
16	V	301	GQT	C25-C26-S27-C28
16	V	301	GQT	C25-C26-S27-O29
16	V	301	GQT	C25-C26-S27-O30
16	V	301	GQT	C13-C12-C32-O33
16	V	301	GQT	C6-N51-N52-N53
16	Y	301	GQT	N51-C6-C7-N8
16	Y	301	GQT	C25-C26-S27-C28
16	Y	301	GQT	C25-C26-S27-O29
16	Y	301	GQT	C25-C26-S27-O30
16	Y	301	GQT	C13-C12-C32-O33

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Mol	Chain	Res	Type	Atoms
16	H	301	GQT	C41-C40-C9-N8
16	H	301	GQT	C9-C40-C41-C42
16	V	301	GQT	C9-C40-C41-C42
16	V	301	GQT	C9-C40-C41-C43
16	H	301	GQT	N11-C12-C32-O33
16	K	301	GQT	N11-C12-C32-O33
16	V	301	GQT	N11-C12-C32-O33
16	Y	301	GQT	N11-C12-C32-O33
16	K	301	GQT	C15-C25-C26-S27
16	V	301	GQT	C15-C25-C26-S27
16	Y	301	GQT	C15-C25-C26-S27
16	H	301	GQT	C41-C40-C9-C10
16	H	301	GQT	C9-C40-C41-C43
16	H	301	GQT	C15-C25-C26-S27
16	V	301	GQT	C41-C40-C9-N8
16	K	301	GQT	C15-C16-C17-C24
16	Y	301	GQT	C15-C16-C17-C24
16	K	301	GQT	C15-C16-C17-C18
16	Y	301	GQT	C15-C16-C17-C18
16	V	301	GQT	C41-C40-C9-C10
16	H	301	GQT	C15-C16-C17-C18
16	V	301	GQT	C15-C16-C17-C18
16	H	301	GQT	C15-C16-C17-C24
16	V	301	GQT	C15-C16-C17-C24
16	H	301	GQT	C25-C26-S27-C28
16	V	301	GQT	C7-C6-N51-N52
16	Y	301	GQT	C6-N51-N52-N53
16	H	301	GQT	C54-C6-N51-N52
16	V	301	GQT	C54-C6-N51-N52

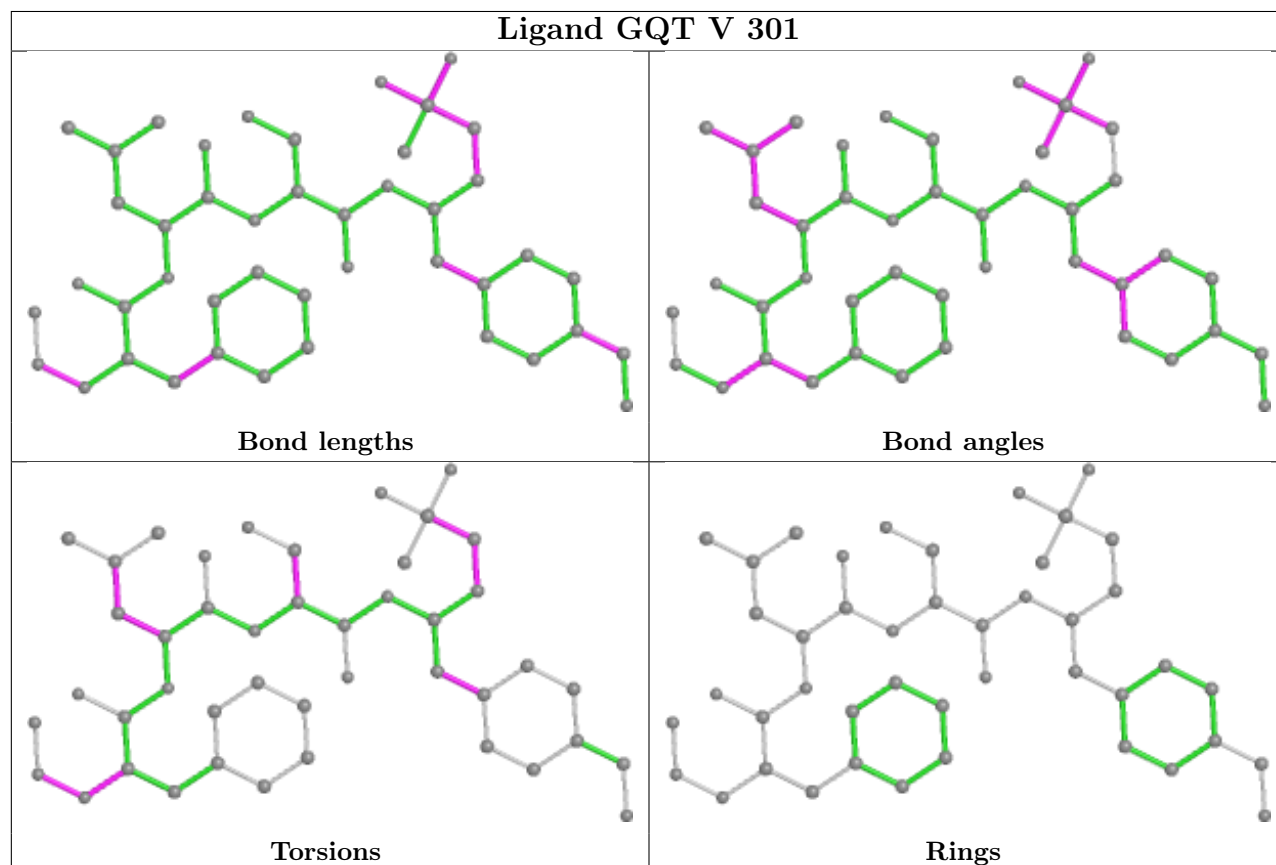
There are no ring outliers.

2 monomers are involved in 2 short contacts:

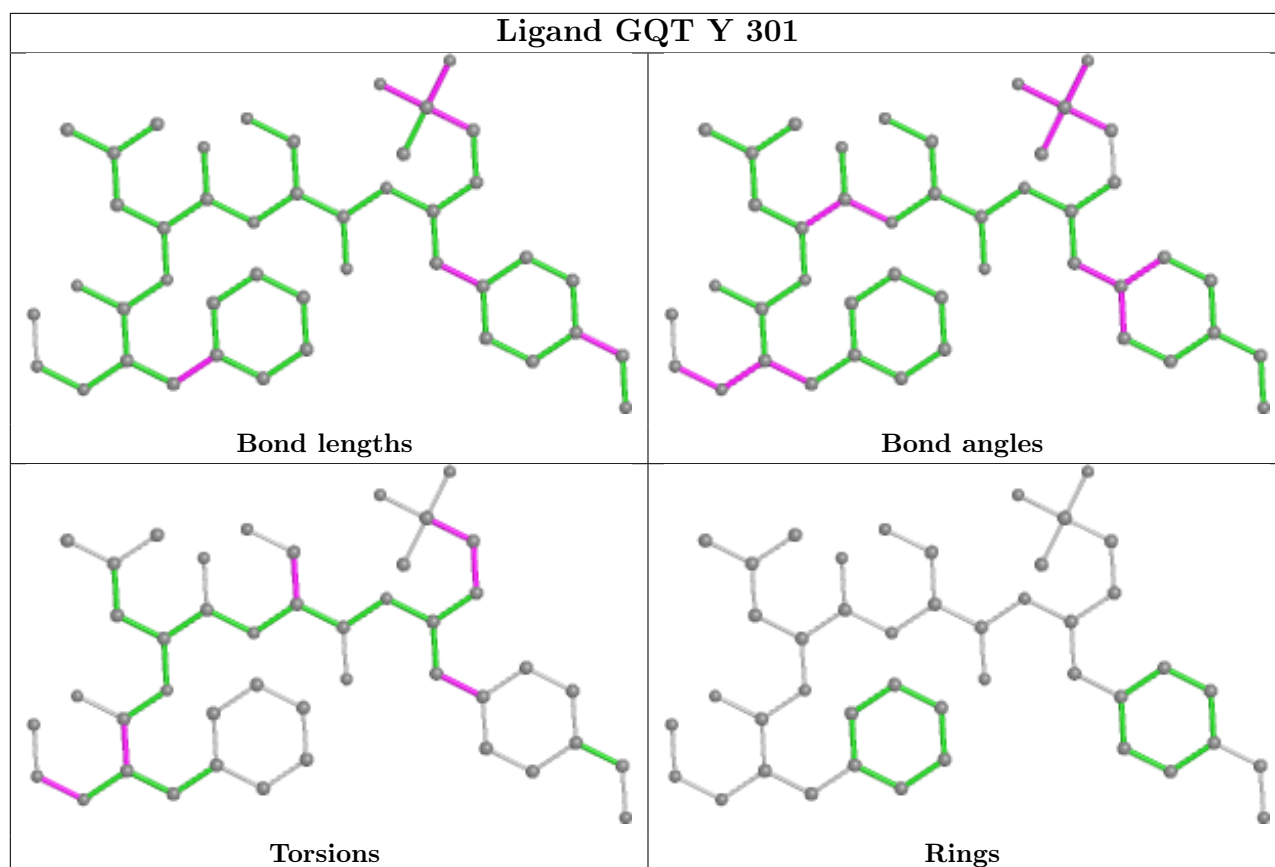
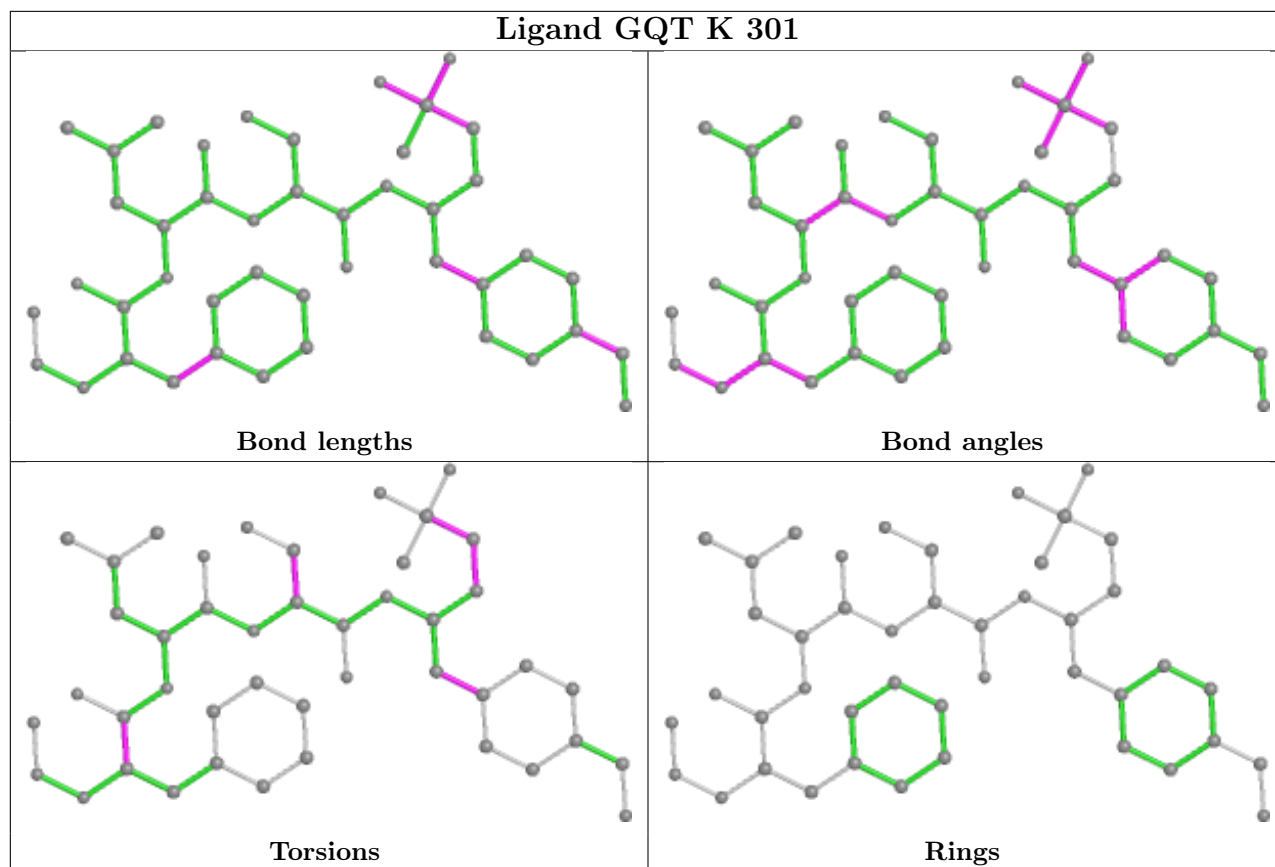
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	V	301	GQT	1	0
16	H	301	GQT	1	0

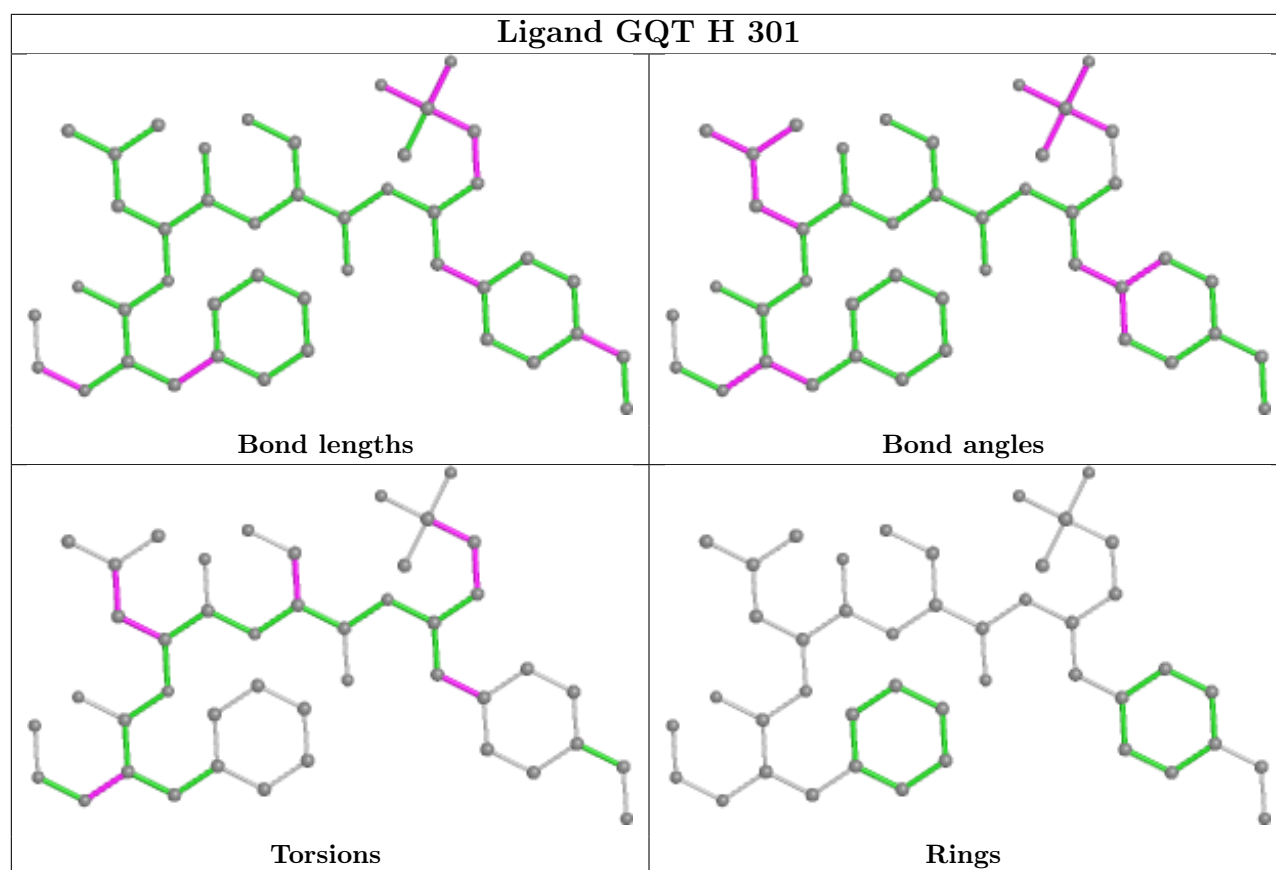
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	240/250 (96%)	-0.23	11 (4%) 32 26	45, 64, 106, 141	0
1	O	240/250 (96%)	-0.03	15 (6%) 20 15	52, 74, 120, 158	0
2	B	244/258 (94%)	-0.09	14 (5%) 23 18	46, 64, 114, 181	0
2	P	244/258 (94%)	-0.10	13 (5%) 26 20	50, 68, 121, 178	0
3	C	240/254 (94%)	-0.10	16 (6%) 17 13	46, 67, 132, 168	0
3	Q	240/254 (94%)	0.11	22 (9%) 9 6	51, 78, 158, 200	0
4	D	235/260 (90%)	-0.32	5 (2%) 63 58	49, 68, 100, 143	0
4	R	235/260 (90%)	-0.31	8 (3%) 45 38	48, 69, 107, 150	0
5	E	231/234 (98%)	-0.19	7 (3%) 50 43	52, 71, 104, 147	0
5	S	231/234 (98%)	-0.14	8 (3%) 44 36	50, 73, 109, 150	0
6	F	243/288 (84%)	-0.34	8 (3%) 46 39	45, 62, 111, 138	0
6	T	243/288 (84%)	-0.31	9 (3%) 41 34	44, 67, 111, 146	0
7	G	241/252 (95%)	-0.40	8 (3%) 46 39	43, 60, 98, 149	0
7	U	241/252 (95%)	-0.36	7 (2%) 51 45	48, 61, 94, 134	0
8	H	219/234 (93%)	-0.25	5 (2%) 60 54	45, 61, 116, 138	0
8	V	219/234 (93%)	-0.17	10 (4%) 32 26	46, 64, 120, 155	0
9	I	204/205 (99%)	-0.58	2 (0%) 82 80	43, 56, 83, 105	0
9	W	204/205 (99%)	-0.54	2 (0%) 82 80	43, 58, 88, 108	0
10	J	195/198 (98%)	-0.48	4 (2%) 63 58	43, 57, 84, 129	0
10	X	195/198 (98%)	-0.52	3 (1%) 73 70	46, 59, 84, 141	0
11	K	212/212 (100%)	-0.43	3 (1%) 75 71	46, 62, 95, 121	0
11	Y	212/212 (100%)	-0.33	2 (0%) 84 82	47, 63, 97, 128	0
12	L	222/222 (100%)	-0.39	3 (1%) 75 71	46, 60, 93, 125	0
12	Z	222/222 (100%)	-0.32	5 (2%) 60 54	46, 59, 98, 130	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	228/246 (92%)	-0.37	6 (2%) 56 50	42, 62, 92, 128	0
13	a	228/246 (92%)	-0.43	3 (1%) 77 73	41, 61, 87, 121	0
14	N	196/196 (100%)	-0.52	2 (1%) 82 80	43, 53, 78, 106	0
14	b	196/196 (100%)	-0.50	1 (0%) 91 89	43, 54, 78, 100	0
All	All	6300/6618 (95%)	-0.30	202 (3%) 47 40	41, 63, 108, 200	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	219	ALA	11.8
2	B	219	ALA	11.2
2	B	220	ASN	9.1
2	B	222	GLY	8.7
3	Q	49	THR	7.7
5	S	202	ASP	7.0
1	O	249	ALA	7.0
2	P	221	ASP	6.9
2	P	222	GLY	6.9
2	B	221	ASP	6.9
3	Q	206	LYS	6.9
8	V	219	LEU	6.7
1	O	230	ASP	6.7
3	C	206	LYS	6.2
3	Q	50	LEU	6.2
1	A	230	ASP	5.8
2	P	220	ASN	5.5
1	O	1	MET	5.5
11	Y	147	ASP	5.4
5	E	202	ASP	5.4
3	Q	238	LYS	5.4
1	A	1	MET	5.3
2	P	218	GLY	5.2
1	O	231	LYS	5.0
2	B	51	VAL	4.9
10	X	194	ASP	4.9
8	H	219	LEU	4.9
1	O	219	PRO	4.7
8	V	194	LYS	4.6
3	Q	204	GLY	4.6
10	X	1	MET	4.5
3	Q	51	LYS	4.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	Q	48	SER	4.5
13	M	216	ASN	4.5
12	Z	174	TYR	4.5
10	J	1	MET	4.4
2	B	218	GLY	4.4
2	P	51	VAL	4.3
3	Q	240	GLU	4.2
3	Q	205	ALA	4.2
13	a	1	THR	4.1
3	C	238	LYS	4.1
13	M	1	THR	4.0
1	A	249	ALA	4.0
6	T	244	ASN	3.9
11	K	147	ASP	3.9
8	H	194	LYS	3.9
3	C	239	GLN	3.9
8	V	218	PRO	3.9
8	V	196	GLY	3.7
3	Q	239	GLN	3.6
6	T	205	GLU	3.6
6	F	243	ILE	3.6
13	a	216	ASN	3.6
9	W	1	SER	3.6
7	U	242	GLN	3.6
6	F	202	ASP	3.5
5	S	54	GLU	3.5
3	C	202	GLN	3.5
6	F	241	LYS	3.5
8	H	196	GLY	3.4
4	D	242	GLU	3.4
1	A	219	PRO	3.4
7	U	222	ASP	3.4
3	C	1	GLY	3.4
3	C	49	THR	3.3
12	L	172	LEU	3.3
12	L	174	TYR	3.3
2	B	225	TYR	3.3
4	R	125	LEU	3.2
2	P	59	ASP	3.2
10	J	194	ASP	3.2
1	O	201	GLU	3.2
5	E	54	GLU	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
6	F	205	GLU	3.1
2	B	217	LYS	3.1
14	b	105	LYS	3.1
5	S	180	LYS	3.1
9	I	1	SER	3.1
9	I	133	LYS	3.1
3	Q	202	GLN	3.1
3	Q	55	THR	3.0
4	R	241	ALA	3.0
5	S	225	ASP	3.0
2	P	60	THR	3.0
6	T	53	LYS	3.0
1	A	218	ASN	3.0
10	X	193	ASP	3.0
3	Q	221	ALA	3.0
5	E	123	GLY	2.9
4	R	1	ASP	2.9
7	G	241	GLU	2.9
2	P	52	THR	2.9
5	E	3	ASN	2.9
1	O	232	GLY	2.9
7	G	3	TYR	2.9
5	E	121	SER	2.9
7	G	222	ASP	2.9
3	C	225	GLU	2.8
6	T	181	GLU	2.8
3	Q	235	GLU	2.8
3	Q	223	SER	2.8
4	D	241	ALA	2.8
14	N	195	GLN	2.8
1	O	62	SER	2.8
1	A	231	LYS	2.8
2	P	225	TYR	2.7
6	F	244	ASN	2.7
13	M	215	GLU	2.7
2	P	240	LYS	2.7
3	Q	236	GLN	2.7
11	Y	202	GLU	2.7
8	V	195	LYS	2.7
8	V	216	ILE	2.7
6	T	2	THR	2.7
1	A	248	GLU	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	C	235	GLU	2.7
5	S	233	ILE	2.7
4	D	2	ARG	2.6
7	G	181	LYS	2.6
2	B	203	SER	2.6
6	T	241	LYS	2.6
8	H	218	PRO	2.6
5	E	233	ILE	2.6
2	P	223	GLU	2.6
2	B	52	THR	2.6
12	Z	1	GLN	2.6
1	O	250	LEU	2.6
11	K	212	GLY	2.6
3	C	167	LYS	2.6
6	F	181	GLU	2.6
7	G	188	GLU	2.6
8	V	197	THR	2.5
3	Q	225	GLU	2.5
9	W	133	LYS	2.5
7	G	2	GLY	2.5
1	O	248	GLU	2.5
2	B	223	GLU	2.5
6	T	243	ILE	2.5
4	R	2	ARG	2.5
4	R	3	GLY	2.5
14	N	105	LYS	2.5
3	Q	59	PRO	2.5
7	U	241	GLU	2.5
12	L	1	GLN	2.5
7	U	51	PRO	2.5
4	D	238	LYS	2.4
3	Q	181	GLU	2.4
5	S	203	GLU	2.4
3	C	240	GLU	2.4
4	R	242	GLU	2.4
11	K	151	GLU	2.4
7	U	2	GLY	2.4
8	V	205	GLU	2.4
3	C	236	GLN	2.4
1	O	182	GLU	2.4
2	B	3	ARG	2.4
7	G	178	LYS	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	201	GLU	2.4
5	E	201	ARG	2.4
6	F	178	HIS	2.3
3	C	50	LEU	2.3
4	D	1	ASP	2.3
8	V	201	ARG	2.3
3	Q	180	LYS	2.3
7	U	181	LYS	2.3
3	C	216	ASP	2.2
13	M	3	GLN	2.2
3	Q	203	THR	2.2
2	B	240	LYS	2.2
2	B	230	LYS	2.2
10	J	193	ASP	2.2
1	O	2	THR	2.2
8	H	197	THR	2.2
13	M	47	ASP	2.1
3	C	180	LYS	2.1
13	a	215	GLU	2.1
5	S	30	GLN	2.1
6	T	177	ASP	2.1
7	G	68	ARG	2.1
1	O	52	SER	2.1
13	M	226	LYS	2.1
8	V	217	THR	2.1
3	Q	141	ASP	2.1
4	R	143	ASP	2.1
1	A	250	LEU	2.1
6	F	215	CYS	2.1
12	Z	173	LYS	2.1
1	O	178	ARG	2.1
7	U	183	ASP	2.1
12	Z	210	ASP	2.1
5	S	207	VAL	2.1
6	T	180	PRO	2.1
1	A	58	SER	2.1
2	P	182	ASP	2.0
10	J	95	ARG	2.0
1	O	245	ASP	2.0
3	C	47	ARG	2.0
1	A	232	GLY	2.0
12	Z	159	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
4	R	201	GLU	2.0
3	C	37	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

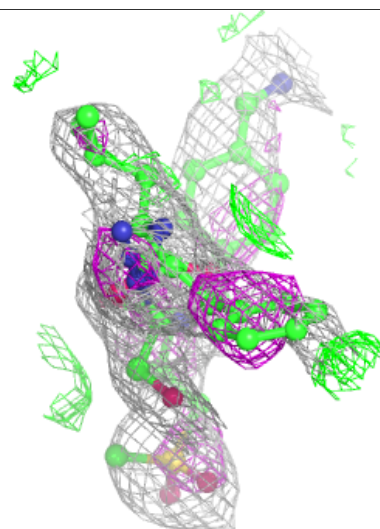
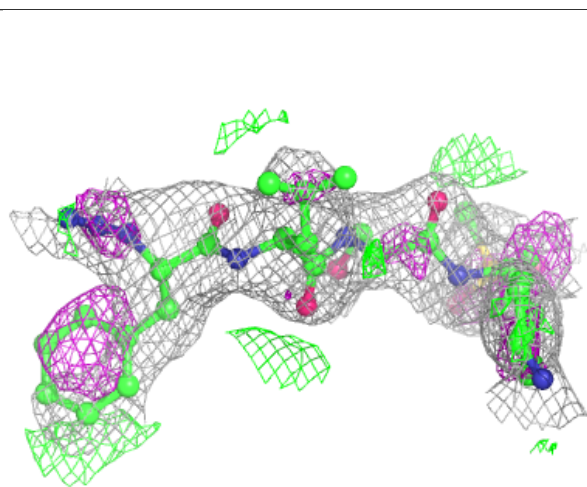
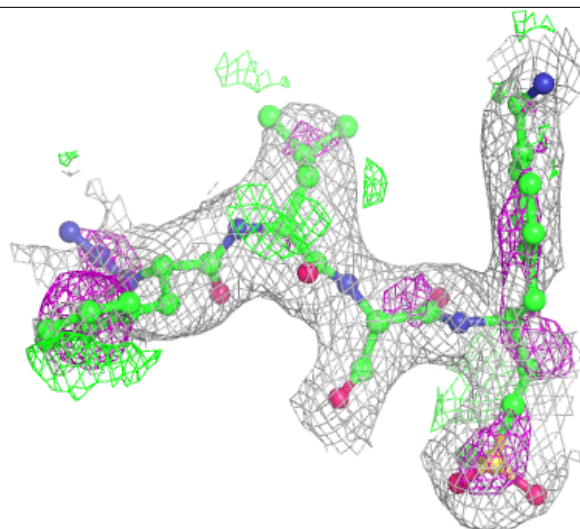
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
15	MG	H	302	1/1	0.76	0.23	76,76,76,76	0
16	GQT	H	301	44/44	0.88	0.26	52,66,90,100	0
16	GQT	V	301	44/44	0.88	0.28	55,69,88,103	0
16	GQT	Y	301	44/44	0.92	0.18	48,61,79,93	0
15	MG	I	301	1/1	0.93	0.58	83,83,83,83	0
16	GQT	K	301	44/44	0.93	0.18	51,62,83,91	0
15	MG	Z	301	1/1	0.95	0.28	72,72,72,72	0
15	MG	N	201	1/1	0.96	0.14	63,63,63,63	0
15	MG	Y	302	1/1	0.97	0.17	95,95,95,95	0
15	MG	K	302	1/1	0.99	0.07	72,72,72,72	0
15	MG	G	301	1/1	0.99	0.06	78,78,78,78	0
15	MG	V	302	1/1	0.99	0.03	78,78,78,78	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.

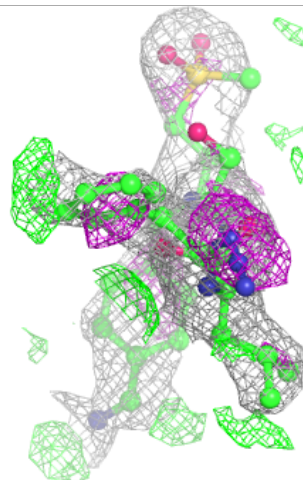
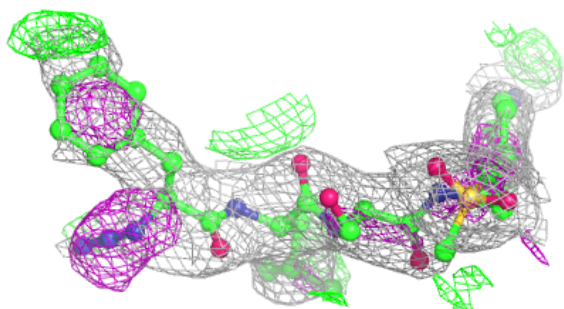
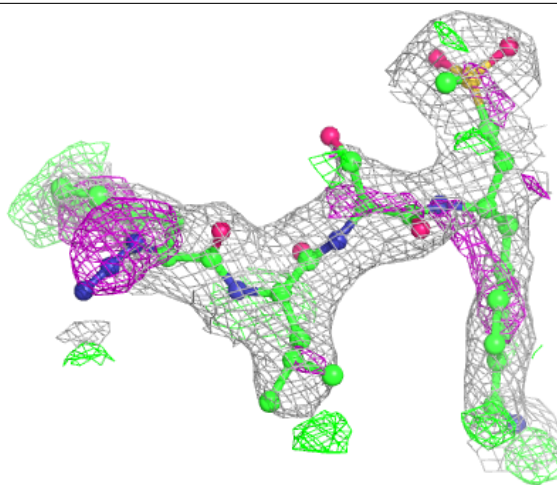
**Electron density around GQT H 301:**

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



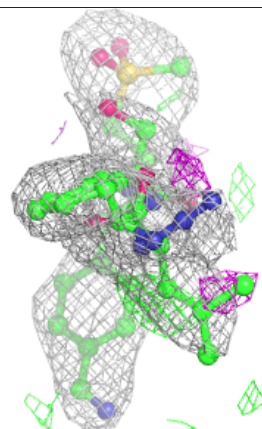
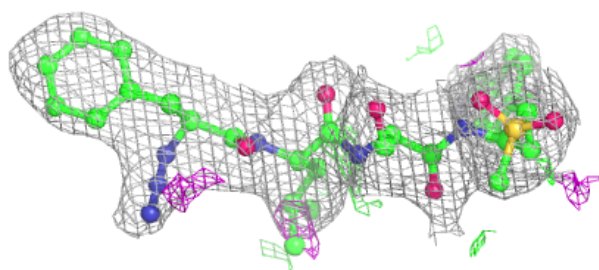
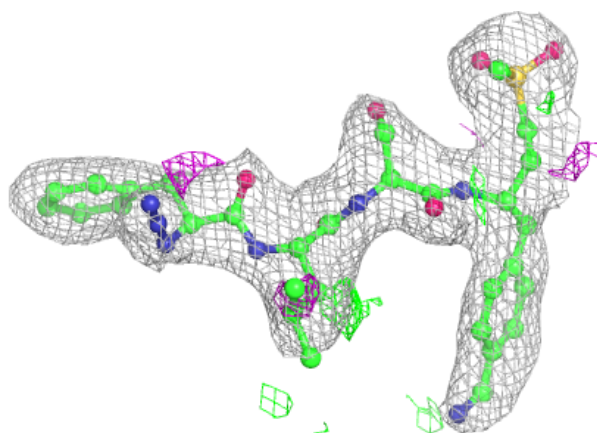
**Electron density around GQT V 301:**

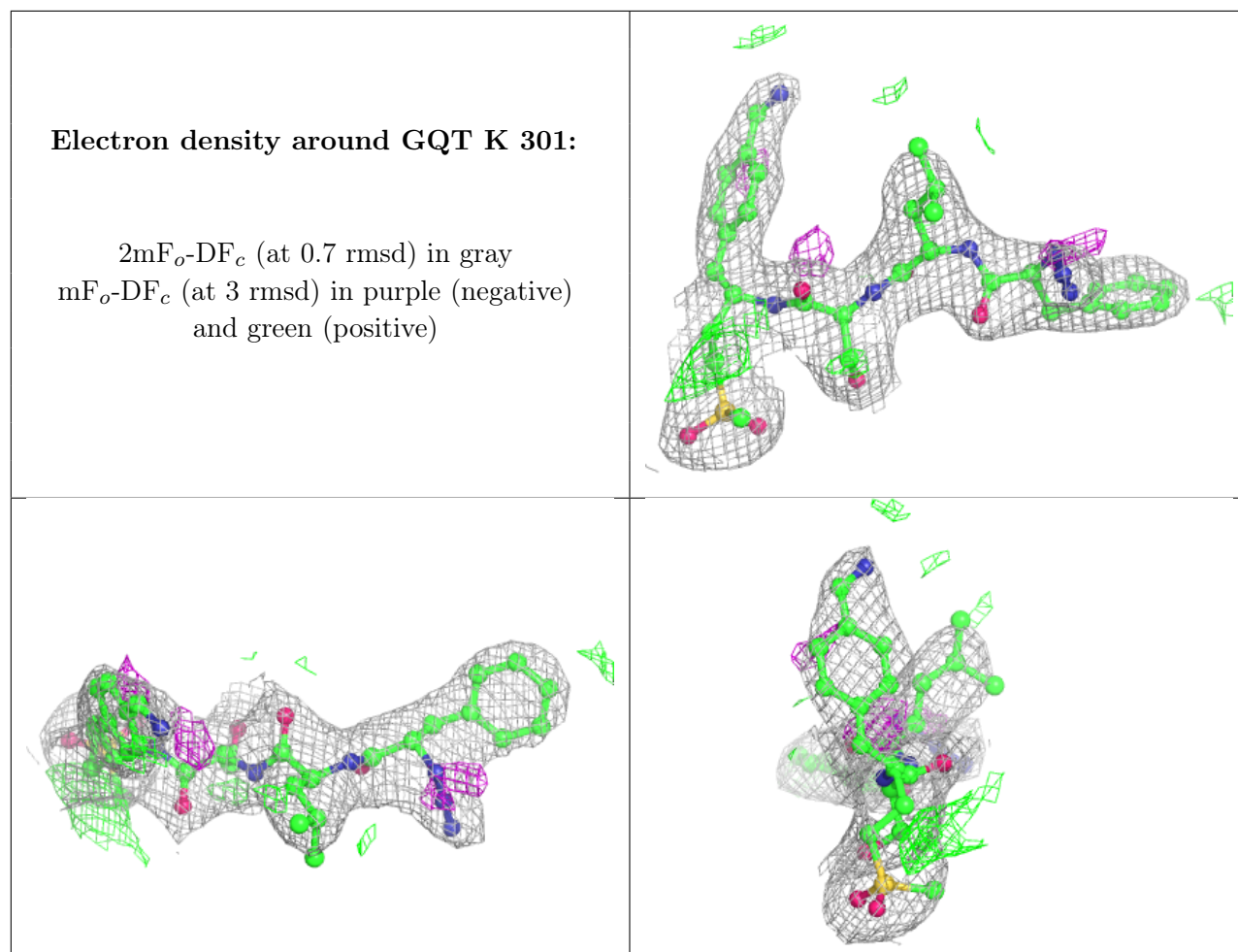
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.