



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 05:56 PM BST

PDB ID : 4INU  
Title : Yeast 20S proteasome in complex with the vinyl sulfone LU112  
Authors : Geurink, P.P.; van der Linden, W.A.; Mirabella, A.C.; Gallastegui, N.; de Bruin, G.; Blom, A.E.M.; Voges, M.J.; Mock, E.D.; Florea, B.I.; van der Marel, G.A.; Driessen, C.; van der Stelt, M.; Groll, M.; Overkleeft, H.S.; Kisselev, A.F.  
Deposited on : 2013-01-06  
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

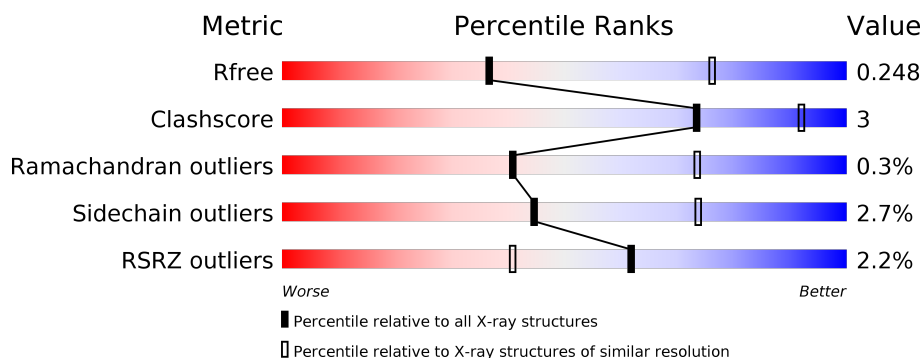
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	250	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
1	O	250	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
2	B	258	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>5%</div> </div> </div>
2	P	258	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>5%</div> </div> </div>
3	C	254	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>5%</div> </div> </div>
3	Q	254	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>5%</div> </div> </div>

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

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 51078 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome component Y7.

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

- Molecule 2 is a protein called Proteasome component Y13.

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

- Molecule 3 is a protein called Proteasome component PRE6.

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

- Molecule 4 is a protein called Proteasome component PUP2.

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

- Molecule 5 is a protein called Proteasome component PRE5.

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

- Molecule 6 is a protein called Proteasome component C1.

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

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

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

- Molecule 8 is a protein called Proteasome component PUP1.

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

- Molecule 9 is a protein called Proteasome component PUP3.

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

- Molecule 10 is a protein called Proteasome component C11.

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

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

- Molecule 11 is a protein called Proteasome component PRE2.

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

- Molecule 12 is a protein called Proteasome component C5.

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

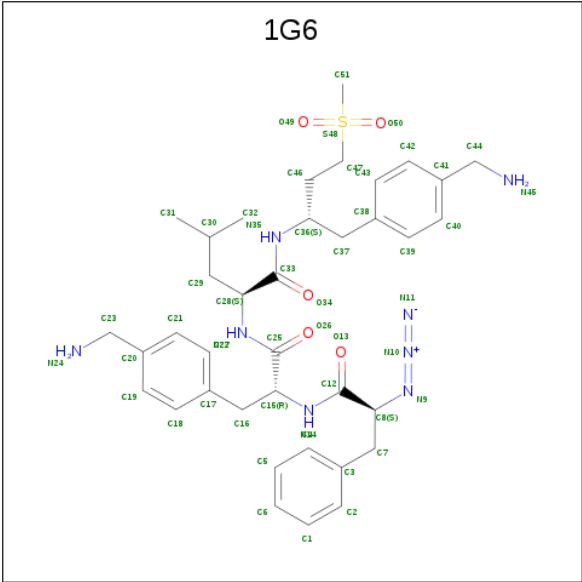
- Molecule 13 is a protein called Proteasome component PRE4.

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

- Molecule 14 is a protein called Proteasome component PRE3.

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

- Molecule 15 is N3Phe-Phe(4-NH<sub>2</sub>CH<sub>2</sub>)-Leu-Phe(4-NH<sub>2</sub>CH<sub>2</sub>)-methyl vinyl sulfone, bound form (three-letter code: 1G6) (formula: C<sub>37</sub>H<sub>50</sub>N<sub>8</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	H	1	Total	C	N	O	S	0	0
			51	37	8	5	1		
15	K	1	Total	C	N	O	S	0	0
			51	37	8	5	1		
15	V	1	Total	C	N	O	S	0	0
			51	37	8	5	1		
15	Y	1	Total	C	N	O	S	0	0
			51	37	8	5	1		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	60	Total	O	0	0
			60	60		
16	B	38	Total	O	0	0
			38	38		
16	C	42	Total	O	0	0
			42	42		
16	D	38	Total	O	0	0
			38	38		
16	E	20	Total	O	0	0
			20	20		
16	F	47	Total	O	0	0
			47	47		
16	G	61	Total	O	0	0
			61	61		
16	H	54	Total	O	0	0
			54	54		

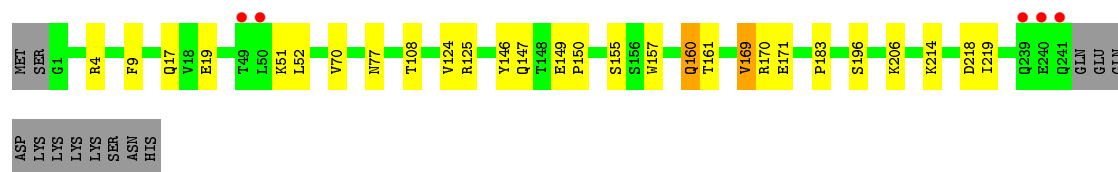
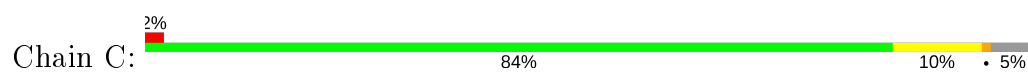
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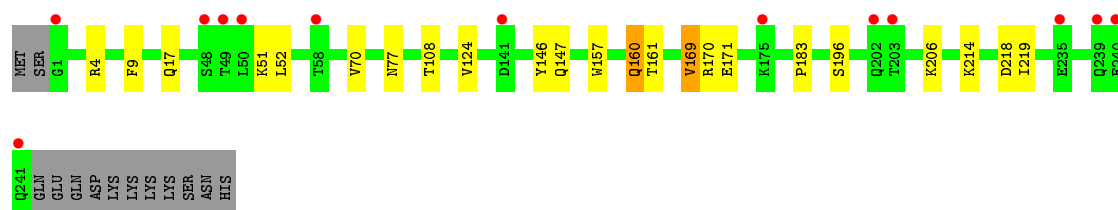
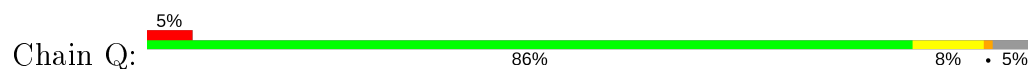
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	I	66	Total O 66 66	0	0
16	J	50	Total O 50 50	0	0
16	K	49	Total O 49 49	0	0
16	L	56	Total O 56 56	0	0
16	M	79	Total O 79 79	0	0
16	N	54	Total O 54 54	0	0
16	O	34	Total O 34 34	0	0
16	P	29	Total O 29 29	0	0
16	Q	29	Total O 29 29	0	0
16	R	29	Total O 29 29	0	0
16	S	18	Total O 18 18	0	0
16	T	43	Total O 43 43	0	0
16	U	59	Total O 59 59	0	0
16	V	50	Total O 50 50	0	0
16	W	54	Total O 54 54	0	0
16	X	44	Total O 44 44	0	0
16	Y	50	Total O 50 50	0	0
16	Z	47	Total O 47 47	0	0
16	a	74	Total O 74 74	0	0
16	b	62	Total O 62 62	0	0



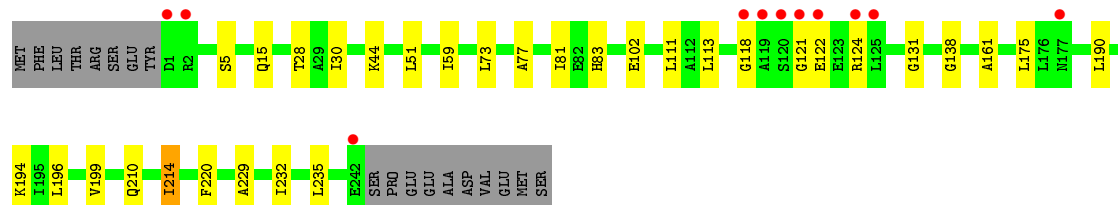
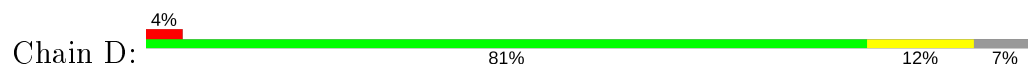




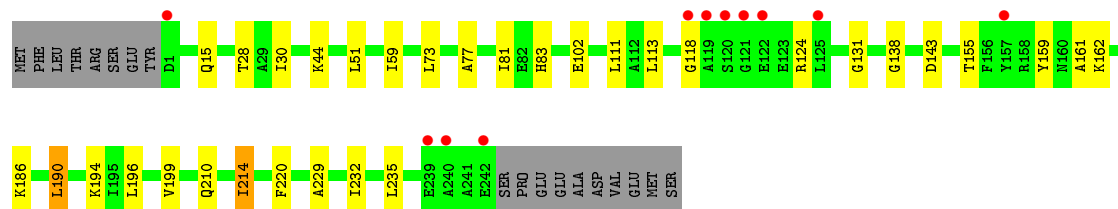
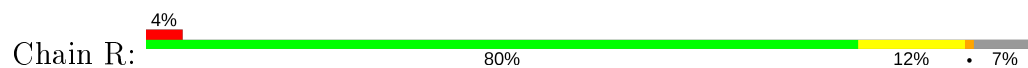
- Molecule 3: Proteasome component PRE6



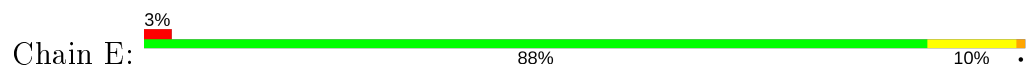
- Molecule 4: Proteasome component PUP2



- Molecule 4: Proteasome component PUP2

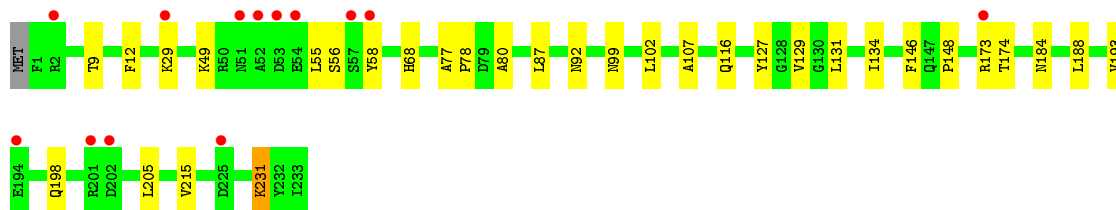
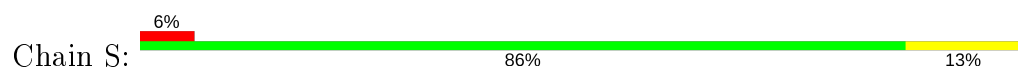


- Molecule 5: Proteasome component PRE5

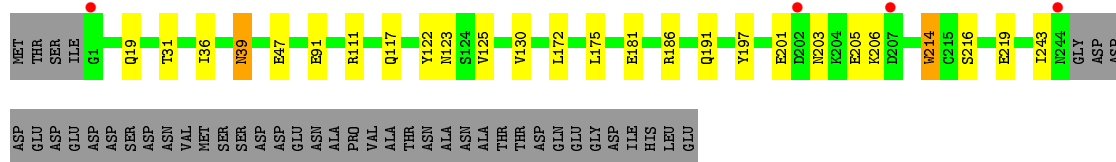
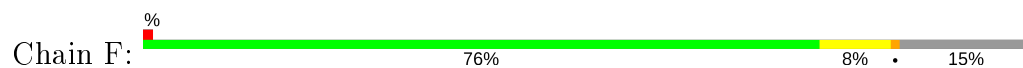




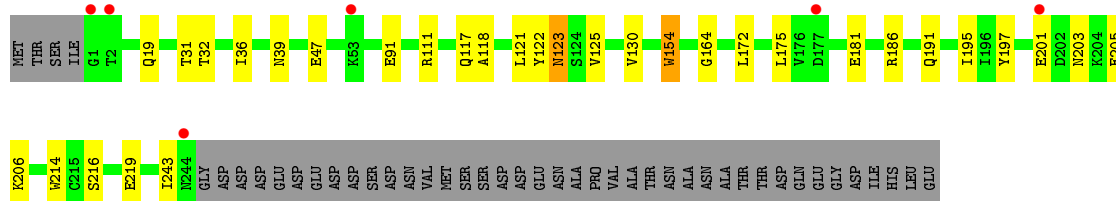
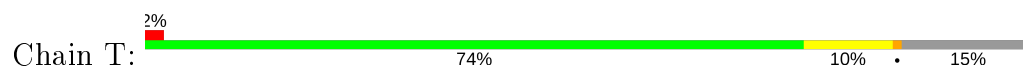
- Molecule 5: Proteasome component PRE5



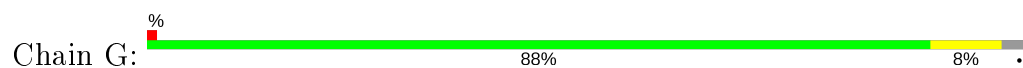
- Molecule 6: Proteasome component C1



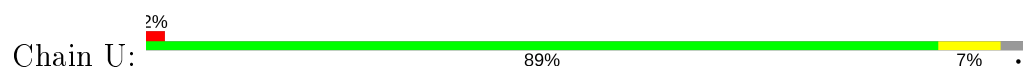
- Molecule 6: Proteasome component C1



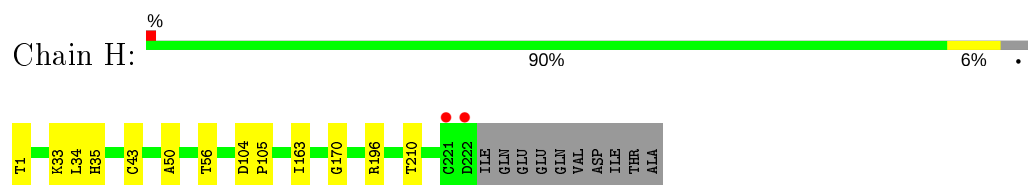
- Molecule 7: Proteasome component C7-alpha



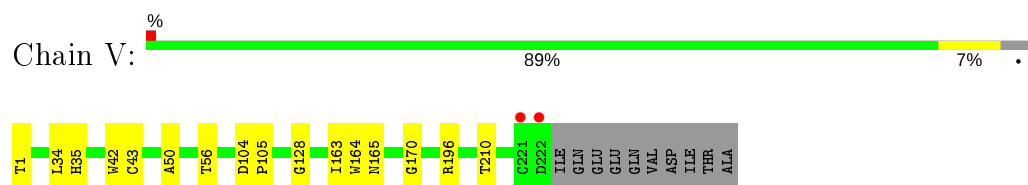
- Molecule 7: Proteasome component C7-alpha



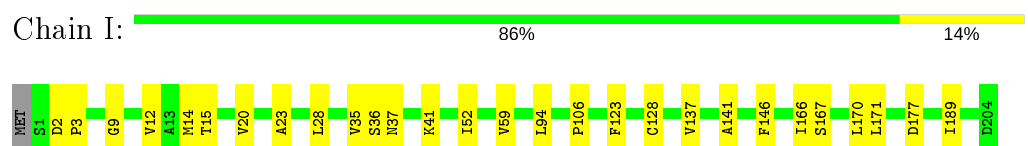
- Molecule 8: Proteasome component PUP1



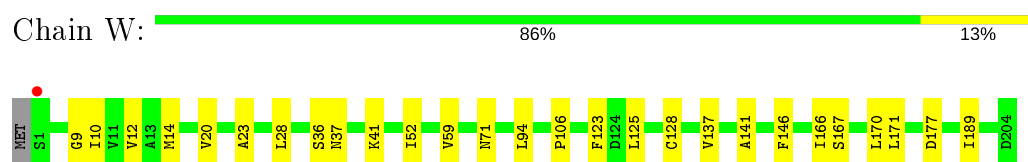
- Molecule 8: Proteasome component PUP1



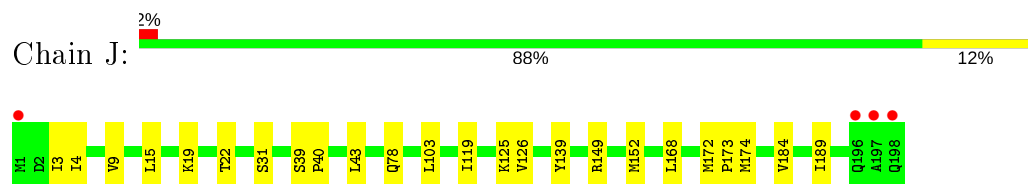
- Molecule 9: Proteasome component PUP3



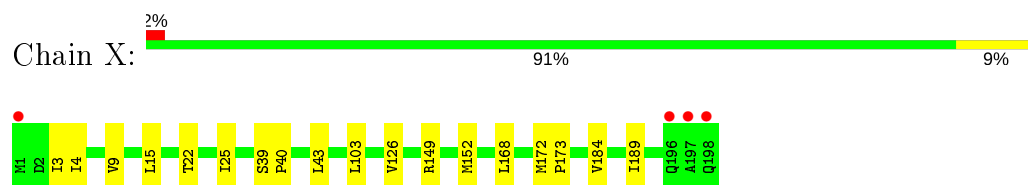
- Molecule 9: Proteasome component PUP3



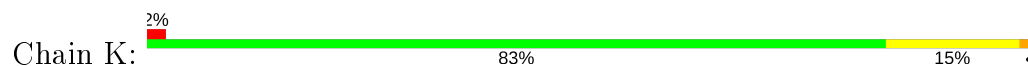
- Molecule 10: Proteasome component C11

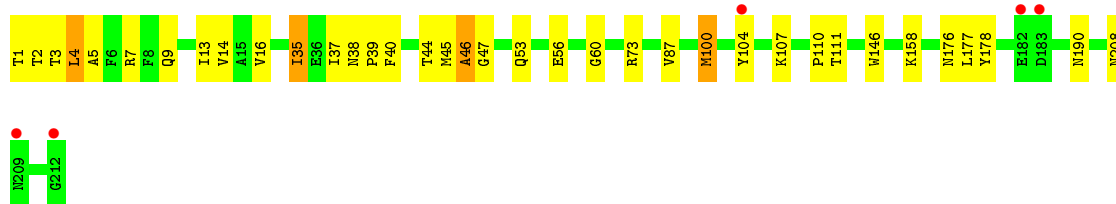


- Molecule 10: Proteasome component C11

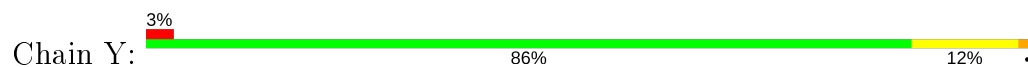


- Molecule 11: Proteasome component PRE2

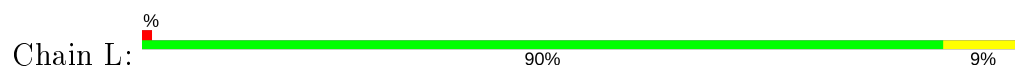




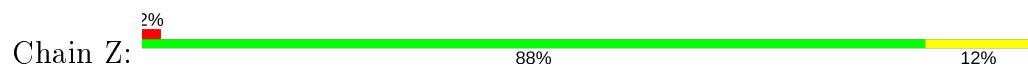
• Molecule 11: Proteasome component PRE2



• Molecule 12: Proteasome component C5



• Molecule 12: Proteasome component C5



• Molecule 13: Proteasome component PRE4



• Molecule 13: Proteasome component PRE4



• Molecule 14: Proteasome component PRE3



- Molecule 14: Proteasome component PRE3

Chain b:

100%

There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.91Å 300.90Å 143.62Å 90.00° 112.53° 90.00°	Depositor
Resolution (Å)	15.00 – 3.10 14.99 – 3.10	Depositor EDS
% Data completeness (in resolution range)	92.3 (15.00-3.10) 92.5 (14.99-3.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.08 (at 3.12Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.218 , 0.238 0.226 , 0.248	Depositor DCC
$R_{free}$ test set	8746 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.3	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 64.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	51078	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: 1G6

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	1/1952 (0.1%)	0.46	0/2642
1	O	0.37	0/1952	0.46	0/2642
2	B	0.34	0/1934	0.46	0/2618
2	P	0.34	0/1934	0.46	0/2618
3	C	0.34	0/1919	0.47	0/2598
3	Q	0.34	0/1919	0.47	0/2598
4	D	0.36	0/1886	0.47	0/2541
4	R	0.36	0/1886	0.47	0/2541
5	E	0.31	0/1823	0.45	0/2463
5	S	0.31	0/1823	0.45	0/2463
6	F	0.41	1/1936 (0.1%)	0.44	0/2614
6	T	0.41	1/1936 (0.1%)	0.44	0/2614
7	G	0.35	0/1959	0.46	0/2652
7	U	0.35	0/1959	0.46	0/2652
8	H	0.44	0/1715	0.47	0/2326
8	V	0.44	2/1715 (0.1%)	0.46	0/2326
9	I	0.34	0/1611	0.46	0/2174
9	W	0.34	0/1611	0.46	0/2174
10	J	0.31	0/1613	0.45	0/2173
10	X	0.31	0/1613	0.45	0/2173
11	K	0.51	1/1681 (0.1%)	0.49	1/2274 (0.0%)
11	Y	0.51	2/1681 (0.1%)	0.49	1/2274 (0.0%)
12	L	0.36	0/1795	0.45	0/2420
12	Z	0.36	0/1795	0.45	0/2420
13	M	0.36	0/1855	0.48	0/2514
13	a	0.36	0/1855	0.48	0/2514
14	N	0.39	0/1541	0.44	0/2087
14	b	0.39	0/1541	0.44	0/2087
All	All	0.37	8/50440 (0.0%)	0.46	2/68192 (0.0%)

All (8) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	146	TRP	CD2-CE2	5.11	1.47	1.41
11	Y	146	TRP	CD2-CE2	5.03	1.47	1.41
8	V	42	TRP	CD2-CE2	5.03	1.47	1.41
6	F	214	TRP	CD2-CE2	5.02	1.47	1.41
6	T	154	TRP	CD2-CE2	5.01	1.47	1.41
1	A	179	TRP	CD2-CE2	5.01	1.47	1.41
8	V	164	TRP	CD2-CE2	5.01	1.47	1.41
11	Y	58	TRP	CD2-CE2	5.00	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	4	LEU	CA-CB-CG	5.22	127.31	115.30
11	Y	4	LEU	CA-CB-CG	5.21	127.29	115.30

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	11	0
1	O	1915	0	1929	9	0
2	B	1904	0	1904	17	0
2	P	1904	0	1904	16	0
3	C	1890	0	1903	15	0
3	Q	1890	0	1903	11	0
4	D	1861	0	1839	17	0
4	R	1861	0	1839	18	0
5	E	1795	0	1800	14	0
5	S	1795	0	1800	14	0
6	F	1896	0	1889	14	0
6	T	1896	0	1889	17	0
7	G	1921	0	1913	9	0
7	U	1921	0	1913	8	0
8	H	1684	0	1687	6	0
8	V	1684	0	1687	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	1581	0	1574	16	0
9	W	1581	0	1574	16	0
10	J	1585	0	1590	14	0
10	X	1585	0	1590	12	0
11	K	1644	0	1594	17	0
11	Y	1644	0	1594	20	0
12	L	1757	0	1711	11	0
12	Z	1757	0	1711	13	0
13	M	1824	0	1832	13	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	6	0
14	b	1512	0	1481	0	0
15	H	51	0	49	0	0
15	K	51	0	49	1	0
15	V	51	0	49	2	0
15	Y	51	0	49	10	0
16	A	60	0	0	0	0
16	B	38	0	0	0	0
16	C	42	0	0	0	0
16	D	38	0	0	0	0
16	E	20	0	0	0	0
16	F	47	0	0	0	0
16	G	61	0	0	0	0
16	H	54	0	0	0	0
16	I	66	0	0	0	0
16	J	50	0	0	1	0
16	K	49	0	0	0	0
16	L	56	0	0	0	0
16	M	79	0	0	0	0
16	N	54	0	0	0	0
16	O	34	0	0	0	0
16	P	29	0	0	0	0
16	Q	29	0	0	0	0
16	R	29	0	0	0	0
16	S	18	0	0	0	0
16	T	43	0	0	0	0
16	U	59	0	0	0	0
16	V	50	0	0	0	0
16	W	54	0	0	0	0
16	X	44	0	0	0	0
16	Y	50	0	0	0	0
16	Z	47	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	a	74	0	0	0	0
16	b	62	0	0	0	0
All	All	51078	0	49488	309	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 3.

All (309) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:1:THR:N	15:Y:301:1G6:H5	1.59	1.17
11:Y:1:THR:CA	15:Y:301:1G6:H5	2.04	0.87
11:Y:1:THR:H1	15:Y:301:1G6:H5	1.31	0.85
11:Y:1:THR:N	15:Y:301:1G6:C47	2.40	0.85
10:J:4:ILE:HG22	10:J:103:LEU:HD12	1.65	0.76
11:Y:45:MET:HG3	11:Y:52:CYS:HB3	1.68	0.75
5:S:12:PHE:H	6:T:19:GLN:HE22	1.36	0.74
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.54	0.73
12:L:109:THR:HG23	12:L:125:PHE:HB2	1.70	0.73
10:X:4:ILE:HG22	10:X:103:LEU:HD12	1.69	0.73
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.53	0.72
6:F:91:GLU:HG2	6:F:111:ARG:HB3	1.71	0.72
5:E:12:PHE:H	6:F:19:GLN:HE22	1.38	0.72
4:R:44:LYS:HE3	4:R:210:GLN:HB2	1.72	0.71
6:T:91:GLU:HG2	6:T:111:ARG:HB3	1.73	0.70
4:R:161:ALA:HB3	5:S:55:LEU:HD23	1.74	0.68
3:C:9:PHE:H	4:D:15:GLN:HE22	1.40	0.68
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.43	0.67
4:D:44:LYS:HE3	4:D:210:GLN:HB2	1.76	0.67
1:A:12:PHE:H	2:B:20:GLN:HE22	1.44	0.64
11:Y:1:THR:H3	15:Y:301:1G6:C47	2.07	0.64
1:O:12:PHE:H	2:P:20:GLN:HE22	1.44	0.64
13:M:48:ASN:H	13:M:48:ASN:HD22	1.46	0.63
11:Y:1:THR:HB	15:Y:301:1G6:O49	1.99	0.63
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.82	0.61
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.82	0.61
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.82	0.60
2:B:86:LEU:HB3	2:B:114:LEU:HD21	1.84	0.60
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.84	0.59
2:P:86:LEU:HB3	2:P:114:LEU:HD21	1.83	0.59
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:168:LEU:O	10:J:172:MET:HB2	2.02	0.59
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.84	0.59
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.85	0.58
11:Y:35:ILE:HG21	11:Y:56:GLU:HB3	1.85	0.58
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.87	0.57
8:V:1:THR:O	8:V:128:GLY:HA3	2.03	0.57
10:X:39:SER:HB2	10:X:40:PRO:HD2	1.86	0.57
13:M:129:TYR:HE1	13:M:144:THR:HG22	1.70	0.57
10:J:149:ARG:HB2	10:J:152:MET:HG3	1.87	0.57
11:K:35:ILE:HG21	11:K:56:GLU:HB3	1.87	0.57
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.85	0.57
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.52	0.57
9:I:28:LEU:HB3	9:I:36:SER:HB3	1.86	0.56
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	1.86	0.56
2:B:151:ASN:HB2	2:B:152:PRO:HD2	1.86	0.56
4:D:73:LEU:HD12	4:D:131:GLY:HA3	1.88	0.56
11:Y:45:MET:HB3	15:Y:301:1G6:H11	1.88	0.56
12:Z:109:THR:HG23	12:Z:125:PHE:HB2	1.88	0.55
11:K:107:LYS:H	11:K:107:LYS:HD2	1.72	0.55
6:T:91:GLU:HG3	6:T:111:ARG:HH11	1.71	0.55
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.86	0.55
6:F:39:ASN:HD22	6:F:39:ASN:N	2.05	0.54
2:P:35:ILE:HD12	2:P:196:LEU:HG	1.88	0.54
2:B:35:ILE:HD12	2:B:196:LEU:HG	1.90	0.54
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.90	0.54
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.89	0.54
2:P:200:THR:HG22	2:P:202:SER:H	1.73	0.54
15:Y:301:1G6:H22	15:Y:301:1G6:H2	1.89	0.54
10:X:168:LEU:O	10:X:172:MET:HB2	2.08	0.54
8:H:50:ALA:HB2	9:I:128:CYS:HB2	1.89	0.54
2:B:63:GLU:HG3	2:B:64:LYS:HG3	1.90	0.53
1:O:21:ILE:HD11	1:O:122:THR:HG21	1.91	0.53
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.91	0.53
10:J:39:SER:HB2	10:J:40:PRO:HD2	1.90	0.53
2:P:136:TYR:HB2	2:P:148:TYR:HB2	1.91	0.53
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.91	0.53
2:B:215:ILE:HG12	2:B:226:GLN:HG2	1.90	0.53
11:K:47:GLY:H	15:K:301:1G6:H5	1.72	0.53
6:T:31:THR:HG23	6:T:47:GLU:HB3	1.90	0.53
6:F:91:GLU:HG3	6:F:111:ARG:HH11	1.75	0.53
11:Y:107:LYS:H	11:Y:107:LYS:HD2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:36:ILE:HG12	6:T:172:LEU:HD11	1.91	0.52
3:C:161:THR:HG21	3:C:169:VAL:HG13	1.91	0.52
2:B:12:PHE:H	3:C:17:GLN:HE22	1.56	0.52
11:K:45:MET:O	11:K:46:ALA:CB	2.57	0.52
8:V:210:THR:HG21	9:W:167:SER:HB3	1.92	0.52
4:R:77:ALA:O	4:R:81:ILE:HG12	2.11	0.51
15:V:301:1G6:H4	15:V:301:1G6:C33	2.37	0.51
8:V:50:ALA:HB2	9:W:128:CYS:HB2	1.91	0.51
7:G:78:ILE:N	7:G:79:PRO:HD2	2.25	0.51
8:H:210:THR:HG21	9:I:167:SER:HB3	1.92	0.51
2:P:63:GLU:HG3	2:P:64:LYS:HG3	1.92	0.51
3:Q:161:THR:HG21	3:Q:169:VAL:HG13	1.91	0.51
2:B:136:TYR:HB2	2:B:148:TYR:HB2	1.91	0.51
11:K:53:GLN:HE22	12:L:131:TYR:H	1.55	0.51
1:A:21:ILE:HD11	1:A:122:THR:HG21	1.91	0.51
1:O:211:LEU:HD22	1:O:238:LEU:HD12	1.92	0.51
4:D:77:ALA:O	4:D:81:ILE:HG12	2.11	0.51
14:N:83:LYS:HG3	14:N:119:VAL:HG22	1.93	0.51
14:N:175:MET:HB2	14:N:186:LEU:HB2	1.91	0.51
4:R:73:LEU:HD12	4:R:131:GLY:HA3	1.92	0.51
3:Q:214:LYS:HB2	3:Q:218:ASP:HB3	1.93	0.51
11:K:45:MET:O	11:K:46:ALA:HB2	2.10	0.50
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.92	0.50
9:W:28:LEU:HB3	9:W:36:SER:HB3	1.93	0.50
15:Y:301:1G6:C51	15:Y:301:1G6:H22	2.40	0.50
9:I:23:ALA:HB1	9:I:170:LEU:HD22	1.93	0.50
2:P:215:ILE:HG12	2:P:226:GLN:HG2	1.93	0.50
6:T:122:TYR:HB2	6:T:125:VAL:HG22	1.94	0.50
9:I:94:LEU:HD11	9:I:106:PRO:HG2	1.92	0.50
10:J:15:LEU:HD12	10:J:43:LEU:HD23	1.92	0.50
11:K:14:VAL:HB	11:K:178:TYR:HB2	1.94	0.50
1:A:211:LEU:HD22	1:A:238:LEU:HD12	1.94	0.49
4:D:113:LEU:HD12	5:E:78:PRO:HB2	1.94	0.49
6:F:39:ASN:HD22	6:F:39:ASN:H	1.60	0.49
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.42	0.49
7:U:78:ILE:N	7:U:79:PRO:HD2	2.26	0.49
10:X:149:ARG:HB2	10:X:152:MET:HG3	1.93	0.49
1:A:30:GLN:HE21	1:A:30:GLN:HA	1.78	0.49
7:U:63:ILE:HD12	7:U:215:GLU:HG2	1.94	0.49
2:B:75:ALA:HB3	2:B:135:ILE:HB	1.94	0.49
5:E:80:ALA:HB2	5:E:129:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:106:PRO:HD2	9:I:123:PHE:HB2	1.95	0.49
9:I:14:MET:HB2	9:I:166:ILE:HD12	1.95	0.49
12:Z:16:ALA:HB2	12:Z:122:VAL:HG23	1.95	0.49
5:E:193:VAL:HG13	5:E:205:LEU:HD11	1.94	0.49
4:R:155:THR:HG22	5:S:77:ALA:HB3	1.95	0.49
10:X:15:LEU:HD12	10:X:43:LEU:HD23	1.95	0.49
12:L:195:HIS:HD2	12:L:197:GLN:H	1.59	0.49
3:Q:157:TRP:CE2	4:R:51:LEU:HD23	2.48	0.49
9:W:94:LEU:HD11	9:W:106:PRO:HG2	1.94	0.49
11:Y:53:GLN:HE22	12:Z:131:TYR:H	1.60	0.49
12:L:126:ASP:HB2	12:L:130:SER:HB3	1.95	0.48
2:P:75:ALA:HB3	2:P:135:ILE:HB	1.95	0.48
3:C:214:LYS:HB2	3:C:218:ASP:HB3	1.94	0.48
9:I:36:SER:HB2	10:J:126:VAL:HG21	1.95	0.48
2:B:200:THR:HG22	2:B:202:SER:H	1.78	0.48
1:O:42:GLY:HA3	1:O:185:LEU:HD13	1.96	0.48
12:Z:24:ALA:HB1	12:Z:202:LEU:HD11	1.95	0.48
4:R:28:THR:HG21	4:R:199:VAL:HG21	1.95	0.48
2:B:122:THR:HG22	3:C:125:ARG:HH21	1.78	0.48
4:D:59:ILE:HG22	4:D:220:PHE:HZ	1.79	0.48
5:S:193:VAL:HG13	5:S:205:LEU:HD11	1.95	0.48
6:F:36:ILE:HG12	6:F:172:LEU:HD11	1.95	0.48
13:M:27:LEU:HD11	13:M:34:LEU:HB3	1.96	0.48
12:Z:17:GLY:HA2	12:Z:174:TYR:HE1	1.79	0.48
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.61	0.47
7:U:195:GLU:HG3	7:U:235:ARG:HG3	1.94	0.47
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.95	0.47
6:T:31:THR:HG21	6:T:47:GLU:O	2.14	0.47
6:T:123:ASN:HD22	6:T:123:ASN:H	1.62	0.47
11:Y:158:LYS:HB2	11:Y:177:LEU:HD11	1.96	0.47
3:C:157:TRP:CE2	4:D:51:LEU:HD23	2.49	0.47
13:M:48:ASN:HD22	13:M:48:ASN:N	2.09	0.47
9:W:106:PRO:HD2	9:W:123:PHE:HB2	1.97	0.47
9:W:12:VAL:HG23	9:W:137:VAL:HG12	1.97	0.47
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.96	0.47
10:J:174:MET:HE1	10:X:173:PRO:HB2	1.96	0.47
9:I:141:ALA:HB2	9:I:177:ASP:HB2	1.96	0.46
1:O:222:LEU:HD13	1:O:232:GLY:HA2	1.97	0.46
15:Y:301:1G6:N35	15:Y:301:1G6:H3	2.29	0.46
7:G:63:ILE:HD12	7:G:215:GLU:HG2	1.97	0.46
10:J:139:TYR:OH	10:X:25:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:31:THR:HG23	6:F:47:GLU:HB3	1.97	0.46
12:L:16:ALA:HB2	12:L:122:VAL:HG23	1.97	0.46
4:R:30:ILE:HD12	4:R:196:LEU:HG	1.97	0.46
10:J:184:VAL:HG22	10:J:189:ILE:HG12	1.98	0.46
13:M:129:TYR:CE1	13:M:144:THR:HG22	2.51	0.46
4:R:59:ILE:HG22	4:R:220:PHE:HZ	1.79	0.46
9:W:52:ILE:HB	9:W:59:VAL:HG13	1.98	0.46
14:N:172:VAL:HG12	14:N:190:PRO:HD3	1.98	0.46
4:D:30:ILE:HD12	4:D:196:LEU:HG	1.98	0.46
6:F:31:THR:HG21	6:F:47:GLU:O	2.16	0.46
1:A:42:GLY:HA3	1:A:185:LEU:HD13	1.98	0.46
1:A:222:LEU:HD13	1:A:232:GLY:HA2	1.97	0.46
12:L:24:ALA:HB1	12:L:202:LEU:HD11	1.96	0.46
6:T:205:GLU:HG3	6:T:206:LYS:HG3	1.98	0.46
1:O:68:THR:HB	1:O:69:PRO:HD2	1.97	0.46
5:S:80:ALA:HB2	5:S:129:VAL:HG21	1.96	0.46
9:W:14:MET:HB2	9:W:166:ILE:HD12	1.97	0.46
10:J:173:PRO:HB3	10:X:22:THR:HG21	1.98	0.45
4:R:113:LEU:HD12	5:S:78:PRO:HB2	1.99	0.45
9:W:125:LEU:H	9:W:125:LEU:HD23	1.81	0.45
10:X:3:ILE:HD13	10:X:168:LEU:HD13	1.98	0.45
12:Z:126:ASP:HB2	12:Z:130:SER:HB3	1.97	0.45
4:D:229:ALA:HA	4:D:232:ILE:HD12	1.97	0.45
9:W:36:SER:HB2	10:X:126:VAL:HG21	1.98	0.45
10:X:184:VAL:HG22	10:X:189:ILE:HG12	1.97	0.45
4:D:5:SER:HB2	5:E:125:ARG:HD3	1.98	0.45
11:K:158:LYS:HB2	11:K:177:LEU:HD11	1.97	0.45
5:E:99:ASN:HB2	13:M:94:GLU:HG2	1.99	0.45
6:F:197:TYR:HB3	6:F:243:ILE:HD12	1.98	0.45
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.45
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.47	0.45
5:E:131:LEU:HB2	5:E:146:PHE:HB3	1.98	0.45
5:E:231:LYS:H	5:E:231:LYS:HD2	1.81	0.45
13:M:193:ARG:HG3	13:M:214:VAL:HB	1.98	0.45
6:T:197:TYR:HB3	6:T:243:ILE:HD12	1.99	0.45
5:S:68:HIS:HE1	5:S:102:LEU:O	2.00	0.45
11:Y:14:VAL:HB	11:Y:178:TYR:HB2	1.99	0.45
12:Z:30:ILE:HG22	12:Z:35:ILE:HA	1.99	0.45
12:Z:93:ILE:HA	12:Z:96:LEU:HD12	1.99	0.45
2:B:149:THR:HG22	2:B:159:TRP:HE1	1.82	0.45
2:P:236:ASP:O	2:P:240:LYS:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:TYR:CD1	2:B:224:VAL:HG21	2.51	0.44
2:B:236:ASP:O	2:B:240:LYS:HG2	2.16	0.44
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.64	0.44
10:J:22:THR:HG21	10:X:173:PRO:HB3	1.99	0.44
9:W:23:ALA:HB1	9:W:170:LEU:HD22	1.98	0.44
9:I:12:VAL:HG23	9:I:137:VAL:HG12	1.99	0.44
6:T:123:ASN:N	6:T:123:ASN:HD22	2.16	0.44
6:F:175:LEU:HD21	6:F:191:GLN:HG2	1.99	0.44
2:P:139:TYR:CD1	2:P:224:VAL:HG21	2.53	0.44
6:F:216:SER:HB3	6:F:219:GLU:HB2	1.98	0.44
4:R:229:ALA:HA	4:R:232:ILE:HD12	1.98	0.44
5:E:127:TYR:O	5:E:148:PRO:HB3	2.17	0.44
12:L:111:ILE:HG12	12:L:125:PHE:HE1	1.83	0.44
13:M:15:LYS:HB3	13:M:20:VAL:HG12	1.98	0.44
5:S:87:LEU:HD11	5:S:107:ALA:HB1	2.00	0.44
12:Z:111:ILE:HG12	12:Z:125:PHE:HE1	1.81	0.44
1:A:26:THR:O	1:A:30:GLN:HG2	2.18	0.44
10:J:19:LYS:HD2	10:J:31:SER:HA	2.00	0.44
12:L:93:ILE:HA	12:L:96:LEU:HD12	1.99	0.44
5:S:127:TYR:O	5:S:148:PRO:HB3	2.18	0.44
3:C:70:VAL:HG13	3:C:219:ILE:HD13	2.00	0.43
7:G:43:VAL:HG11	7:G:194:VAL:HG22	2.00	0.43
11:K:38:ASN:C	11:K:40:PHE:H	2.22	0.43
14:N:34:LEU:HD13	14:N:176:VAL:HG23	2.00	0.43
6:F:122:TYR:HB2	6:F:125:VAL:HG22	1.99	0.43
6:F:205:GLU:HG3	6:F:206:LYS:HG3	2.00	0.43
9:I:52:ILE:HB	9:I:59:VAL:HG13	2.01	0.43
1:A:110:LEU:O	1:A:114:VAL:HG23	2.18	0.43
12:L:161:GLU:HA	12:L:162:PRO:HD3	1.93	0.43
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	1.99	0.43
4:D:161:ALA:HB1	4:D:175:LEU:HD22	2.00	0.43
7:G:195:GLU:HG3	7:G:235:ARG:HG3	2.00	0.43
4:R:159:TYR:CE2	4:R:162:LYS:HD3	2.54	0.43
4:R:194:LYS:HB2	4:R:235:LEU:HD21	2.00	0.43
6:T:216:SER:HB3	6:T:219:GLU:HB2	2.00	0.43
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.66	0.43
9:I:35:VAL:HG13	16:J:238:HOH:O	2.18	0.43
11:K:44:THR:OG1	11:K:100:MET:HB2	2.18	0.43
11:Y:38:ASN:C	11:Y:40:PHE:H	2.22	0.43
3:C:160:GLN:HE21	3:C:160:GLN:CA	2.26	0.43
1:O:110:LEU:O	1:O:114:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:231:LYS:HD2	5:S:231:LYS:H	1.83	0.43
4:R:138:GLY:HA2	4:R:214:ILE:HG12	2.01	0.43
10:J:3:ILE:HD13	10:J:168:LEU:HD13	2.01	0.42
5:S:131:LEU:HB2	5:S:146:PHE:HB3	2.01	0.42
1:A:68:THR:HB	1:A:69:PRO:HD2	2.00	0.42
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.67	0.42
6:T:154:TRP:CZ3	7:U:60:VAL:HA	2.54	0.42
8:H:1:THR:HG23	8:H:33:LYS:HD3	2.01	0.42
9:I:2:ASP:HA	9:I:3:PRO:HD3	1.93	0.42
8:H:35:HIS:HB2	8:H:56:THR:HG21	2.02	0.42
2:P:149:THR:HG22	2:P:159:TRP:HE1	1.83	0.42
12:L:124:SER:HB3	12:L:137:ARG:HG2	2.01	0.42
7:G:106:ASP:HB3	7:G:146:TYR:CZ	2.55	0.42
11:K:7:ARG:HD2	11:K:110:PRO:HB2	2.01	0.42
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.67	0.42
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.02	0.42
11:K:3:THR:HG22	11:K:16:VAL:HG12	2.02	0.42
1:O:38:LYS:HG3	1:O:43:VAL:HG22	2.02	0.42
6:T:172:LEU:HD22	6:T:195:ILE:HD13	2.02	0.42
9:W:141:ALA:HB2	9:W:177:ASP:HB2	2.02	0.42
7:G:115:LEU:HA	7:G:118:ILE:HD12	2.01	0.41
10:J:119:ILE:HG12	10:J:125:LYS:HG3	2.01	0.41
11:K:37:ILE:HG23	11:K:60:GLY:HA2	2.02	0.41
13:M:97:ALA:HA	13:M:130:VAL:HG21	2.02	0.41
4:R:83:HIS:CG	4:R:111:LEU:HD11	2.54	0.41
8:V:35:HIS:HB2	8:V:56:THR:HG21	2.01	0.41
7:U:70:ILE:HD11	7:U:103:MET:O	2.21	0.41
1:A:38:LYS:HG3	1:A:43:VAL:HG22	2.02	0.41
4:D:83:HIS:CG	4:D:111:LEU:HD11	2.55	0.41
7:G:7:ILE:HG13	7:G:9:ILE:HG12	2.03	0.41
11:K:1:THR:CG2	11:K:2:THR:N	2.83	0.41
3:Q:108:THR:HG21	3:Q:146:TYR:HB3	2.01	0.41
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.55	0.41
11:Y:7:ARG:HD2	11:Y:110:PRO:HB2	2.03	0.41
11:Y:1:THR:CG2	11:Y:2:THR:N	2.83	0.41
11:Y:46:ALA:HB3	11:Y:98:GLY:O	2.20	0.41
5:E:134:ILE:HD12	5:E:215:VAL:HG12	2.02	0.41
6:T:175:LEU:HD21	6:T:191:GLN:HG2	2.01	0.41
7:U:149:ASP:HB2	7:U:150:PRO:HD2	2.02	0.41
4:D:161:ALA:HB3	5:E:55:LEU:HD23	2.01	0.41
6:T:32:THR:HB	6:T:164:GLY:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:301:1G6:H11	15:V:301:1G6:H8	1.82	0.41
6:T:118:ALA:HA	6:T:121:LEU:HD12	2.03	0.41
7:U:43:VAL:HG11	7:U:194:VAL:HG22	2.03	0.41
6:F:175:LEU:HD11	6:F:191:GLN:HG2	2.02	0.41
11:K:5:ALA:HA	11:K:13:ILE:O	2.21	0.41
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.55	0.41
12:Z:124:SER:HB3	12:Z:137:ARG:HG2	2.02	0.41
4:D:138:GLY:HA2	4:D:214:ILE:HG12	2.03	0.41
11:K:40:PHE:HB3	11:K:73:ARG:NH2	2.35	0.41
5:S:134:ILE:HD12	5:S:215:VAL:HG12	2.02	0.41
5:S:49:LYS:HB2	5:S:58:TYR:HB3	2.02	0.41
4:D:28:THR:HG21	4:D:199:VAL:HG21	2.03	0.41
5:E:184:ASN:HA	5:E:185:PRO:HD2	1.99	0.41
3:C:155:SER:HB2	4:D:51:LEU:HD21	2.02	0.41
5:E:87:LEU:HD11	5:E:107:ALA:HB1	2.02	0.41
11:K:176:ASN:HD21	11:K:190:ASN:HD22	1.68	0.41
13:M:96:LEU:O	13:M:100:MET:HG2	2.21	0.41
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.02	0.41
1:A:75:TYR:HB3	1:A:82:TYR:CD1	2.56	0.40
5:E:205:LEU:HA	5:E:209:ASN:HD22	1.86	0.40
7:G:70:ILE:HD11	7:G:103:MET:O	2.22	0.40
3:Q:70:VAL:HG13	3:Q:219:ILE:HD13	2.02	0.40
11:Y:158:LYS:HD3	11:Y:196:LEU:HD11	2.03	0.40
12:Z:161:GLU:HA	12:Z:162:PRO:HD3	1.94	0.40
2:B:184:LYS:HD3	2:B:186:ASP:H	1.86	0.40
9:I:15:THR:HG22	9:I:20:VAL:HG12	2.03	0.40
1:O:26:THR:O	1:O:30:GLN:HG2	2.21	0.40
3:C:108:THR:HG21	3:C:146:TYR:HB3	2.04	0.40
14:N:163:ILE:HG23	14:N:170:GLY:HA2	2.03	0.40
4:R:186:LYS:O	4:R:190:LEU:HD22	2.22	0.40
11:Y:40:PHE:HB3	11:Y:73:ARG:NH2	2.36	0.40
4:D:194:LYS:HB2	4:D:235:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	34	69
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	34	69
2	B	242/258 (94%)	236 (98%)	5 (2%)	1 (0%)	34	69
2	P	242/258 (94%)	236 (98%)	5 (2%)	1 (0%)	34	69
3	C	239/254 (94%)	232 (97%)	5 (2%)	2 (1%)	19	54
3	Q	239/254 (94%)	232 (97%)	5 (2%)	2 (1%)	19	54
4	D	240/260 (92%)	233 (97%)	4 (2%)	3 (1%)	12	42
4	R	240/260 (92%)	233 (97%)	6 (2%)	1 (0%)	34	69
5	E	231/234 (99%)	223 (96%)	8 (4%)	0	100	100
5	S	231/234 (99%)	223 (96%)	8 (4%)	0	100	100
6	F	242/288 (84%)	232 (96%)	10 (4%)	0	100	100
6	T	242/288 (84%)	232 (96%)	10 (4%)	0	100	100
7	G	241/252 (96%)	235 (98%)	6 (2%)	0	100	100
7	U	241/252 (96%)	236 (98%)	5 (2%)	0	100	100
8	H	220/232 (95%)	214 (97%)	6 (3%)	0	100	100
8	V	220/232 (95%)	213 (97%)	7 (3%)	0	100	100
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	J	196/198 (99%)	189 (96%)	6 (3%)	1 (0%)	29	64
10	X	196/198 (99%)	188 (96%)	7 (4%)	1 (0%)	29	64
11	K	210/212 (99%)	200 (95%)	8 (4%)	2 (1%)	15	49
11	Y	210/212 (99%)	201 (96%)	8 (4%)	1 (0%)	29	64
12	L	220/222 (99%)	212 (96%)	8 (4%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	231/233 (99%)	220 (95%)	10 (4%)	1 (0%)	34	69
13	a	231/233 (99%)	217 (94%)	13 (6%)	1 (0%)	34	69
14	N	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
14	b	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
All	All	6312/6588 (96%)	6088 (96%)	205 (3%)	19 (0%)	41	73

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	K	46	ALA
11	K	39	PRO
3	Q	52	LEU
11	Y	39	PRO
1	A	2	THR
3	C	52	LEU
3	Q	183	PRO
2	B	51	VAL
3	C	183	PRO
1	O	2	THR
2	P	51	VAL
4	D	122	GLU
10	J	9	VAL
10	X	9	VAL
13	M	229	GLY
13	a	229	GLY
4	D	118	GLY
4	D	121	GLY
4	R	118	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	206 (99%)	3 (1%)	67	86
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	86
2	B	203/216 (94%)	196 (97%)	7 (3%)	37	69
2	P	203/216 (94%)	195 (96%)	8 (4%)	32	65
3	C	213/226 (94%)	204 (96%)	9 (4%)	30	62
3	Q	213/226 (94%)	205 (96%)	8 (4%)	33	66
4	D	198/215 (92%)	194 (98%)	4 (2%)	55	80
4	R	198/215 (92%)	193 (98%)	5 (2%)	47	75
5	E	192/193 (100%)	183 (95%)	9 (5%)	26	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	S	192/193 (100%)	181 (94%)	11 (6%)	20	52
6	F	201/239 (84%)	192 (96%)	9 (4%)	27	60
6	T	201/239 (84%)	192 (96%)	9 (4%)	27	60
7	G	207/210 (99%)	203 (98%)	4 (2%)	57	81
7	U	207/210 (99%)	203 (98%)	4 (2%)	57	81
8	H	181/190 (95%)	178 (98%)	3 (2%)	60	83
8	V	181/190 (95%)	178 (98%)	3 (2%)	60	83
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	83
9	W	172/173 (99%)	169 (98%)	3 (2%)	60	83
10	J	175/175 (100%)	174 (99%)	1 (1%)	86	94
10	X	175/175 (100%)	175 (100%)	0	100	100
11	K	169/169 (100%)	161 (95%)	8 (5%)	26	59
11	Y	169/169 (100%)	161 (95%)	8 (5%)	26	59
12	L	185/185 (100%)	182 (98%)	3 (2%)	62	84
12	Z	185/185 (100%)	183 (99%)	2 (1%)	73	89
13	M	199/199 (100%)	192 (96%)	7 (4%)	36	68
13	a	199/199 (100%)	192 (96%)	7 (4%)	36	68
14	N	162/162 (100%)	161 (99%)	1 (1%)	86	94
14	b	162/162 (100%)	162 (100%)	0	100	100
All	All	5332/5522 (97%)	5190 (97%)	142 (3%)	44	74

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	132	VAL
1	A	157	PHE
2	B	59	ASP
2	B	60	THR
2	B	114	LEU
2	B	119	GLN
2	B	184	LYS
2	B	191	LEU
2	B	212	PHE
3	C	4	ARG

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Mol	Chain	Res	Type
3	C	19	GLU
3	C	51	LYS
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	171	GLU
3	C	206	LYS
4	D	102	GLU
4	D	124	ARG
4	D	190	LEU
4	D	214	ILE
5	E	9	THR
5	E	29	LYS
5	E	99	ASN
5	E	116	GLN
5	E	174	THR
5	E	184	ASN
5	E	188	LEU
5	E	198	GLN
5	E	231	LYS
6	F	39	ASN
6	F	117	GLN
6	F	123	ASN
6	F	130	VAL
6	F	181	GLU
6	F	186	ARG
6	F	201	GLU
6	F	203	ASN
6	F	214	TRP
7	G	117	GLN
7	G	166	GLN
7	G	221	LYS
7	G	235	ARG
8	H	34	LEU
8	H	43	CYS
8	H	196	ARG
9	I	37	ASN
9	I	146	PHE
9	I	171	LEU
10	J	78	GLN
11	K	4	LEU

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Mol	Chain	Res	Type
11	K	9	GLN
11	K	35	ILE
11	K	87	VAL
11	K	100	MET
11	K	104	TYR
11	K	111	THR
11	K	208	ASN
12	L	49	ASN
12	L	109	THR
12	L	128	VAL
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	146	PHE
13	M	159	VAL
13	M	161	ARG
13	M	226	LYS
14	N	119	VAL
1	O	30	GLN
1	O	132	VAL
1	O	157	PHE
2	P	59	ASP
2	P	60	THR
2	P	114	LEU
2	P	119	GLN
2	P	184	LYS
2	P	191	LEU
2	P	212	PHE
2	P	220	ASN
3	Q	4	ARG
3	Q	51	LYS
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	171	GLU
3	Q	206	LYS
4	R	102	GLU
4	R	124	ARG
4	R	143	ASP
4	R	190	LEU
4	R	214	ILE

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Mol	Chain	Res	Type
5	S	9	THR
5	S	29	LYS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	173	ARG
5	S	174	THR
5	S	184	ASN
5	S	188	LEU
5	S	198	GLN
5	S	231	LYS
6	T	39	ASN
6	T	117	GLN
6	T	123	ASN
6	T	130	VAL
6	T	181	GLU
6	T	186	ARG
6	T	201	GLU
6	T	203	ASN
6	T	214	TRP
7	U	117	GLN
7	U	166	GLN
7	U	221	LYS
7	U	235	ARG
8	V	34	LEU
8	V	43	CYS
8	V	196	ARG
9	W	37	ASN
9	W	146	PHE
9	W	171	LEU
11	Y	1	THR
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	45	MET
11	Y	100	MET
11	Y	104	TYR
11	Y	208	ASN
12	Z	49	ASN
12	Z	128	VAL
13	a	48	ASN
13	a	70	LEU

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Mol	Chain	Res	Type
13	a	104	ARG
13	a	146	PHE
13	a	159	VAL
13	a	161	ARG
13	a	226	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (135) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	143	ASN
2	B	20	GLN
2	B	69	ASN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
2	B	220	ASN
3	C	17	GLN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	241	GLN
4	D	15	GLN
4	D	100	ASN
4	D	210	GLN
4	D	225	ASN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
5	E	198	GLN
5	E	209	ASN
6	F	19	GLN
6	F	39	ASN
6	F	86	ASN
6	F	117	GLN

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Mol	Chain	Res	Type
6	F	123	ASN
7	G	75	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	175	ASN
7	G	186	ASN
8	H	30	ASN
8	H	141	HIS
8	H	165	ASN
8	H	172	ASN
9	I	88	GLN
10	J	55	GLN
10	J	118	GLN
11	K	9	GLN
11	K	53	GLN
11	K	85	ASN
11	K	176	ASN
11	K	208	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	80	ASN
12	L	152	ASN
12	L	153	GLN
12	L	165	ASN
12	L	195	HIS
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	171	GLN
13	M	179	ASN
13	M	213	GLN
14	N	161	GLN
1	O	30	GLN
1	O	143	ASN
2	P	20	GLN
2	P	69	ASN
2	P	95	GLN
2	P	119	GLN

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Mol	Chain	Res	Type
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
2	P	220	ASN
3	Q	17	GLN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	241	GLN
4	R	15	GLN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
5	S	198	GLN
5	S	209	ASN
6	T	19	GLN
6	T	39	ASN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
7	U	75	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	175	ASN
7	U	186	ASN
8	V	30	ASN
8	V	141	HIS
8	V	165	ASN
8	V	172	ASN
9	W	168	GLN
10	X	55	GLN
10	X	86	GLN
10	X	118	GLN

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Mol	Chain	Res	Type
10	X	191	GLN
11	Y	53	GLN
11	Y	85	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	195	HIS
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	171	GLN
13	a	179	ASN
13	a	213	GLN
14	b	69	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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
15	1G6	Y	301	11	52,53,53	1.15	2 (3%)	67,71,71	1.74	14 (20%)
15	1G6	H	301	8	52,53,53	1.21	4 (7%)	67,71,71	1.42	7 (10%)
15	1G6	V	301	8	52,53,53	1.19	2 (3%)	67,71,71	1.68	9 (13%)
15	1G6	K	301	11	52,53,53	1.16	3 (5%)	67,71,71	1.53	7 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	1G6	Y	301	11	-	12/53/53/53	0/3/3/3
15	1G6	H	301	8	-	16/53/53/53	0/3/3/3
15	1G6	V	301	8	-	21/53/53/53	0/3/3/3
15	1G6	K	301	11	-	16/53/53/53	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	V	301	1G6	C46-C47	4.30	1.57	1.52
15	H	301	1G6	C46-C47	4.19	1.57	1.52
15	K	301	1G6	C46-C47	3.88	1.56	1.52
15	Y	301	1G6	C47-S48	3.65	1.83	1.78
15	Y	301	1G6	C46-C47	3.04	1.55	1.52
15	H	301	1G6	C47-S48	2.37	1.81	1.78
15	H	301	1G6	C8-N9	-2.34	1.45	1.48
15	K	301	1G6	C8-N9	-2.34	1.45	1.48
15	K	301	1G6	C47-S48	2.27	1.81	1.78
15	H	301	1G6	C46-C36	2.14	1.57	1.53
15	V	301	1G6	C46-C36	2.12	1.57	1.53

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	V	301	1G6	C8-N9-N10	7.31	122.93	115.24
15	Y	301	1G6	C8-N9-N10	6.18	121.74	115.24
15	V	301	1G6	C15-C25-N27	6.12	130.13	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	K	301	1G6	C15-C25-N27	5.96	129.76	116.70
15	H	301	1G6	C15-C25-N27	5.74	129.30	116.70
15	Y	301	1G6	C15-C25-N27	5.47	128.70	116.70
15	K	301	1G6	C8-N9-N10	4.65	120.13	115.24
15	Y	301	1G6	C38-C37-C36	4.54	124.08	113.78
15	H	301	1G6	C8-N9-N10	4.05	119.50	115.24
15	K	301	1G6	C38-C37-C36	3.89	122.60	113.78
15	V	301	1G6	O26-C25-C15	-3.79	112.48	120.45
15	K	301	1G6	O26-C25-C15	-3.73	112.61	120.45
15	H	301	1G6	C46-C36-C37	3.64	117.07	111.14
15	H	301	1G6	O26-C25-C15	-3.47	113.16	120.45
15	Y	301	1G6	O26-C25-C15	-3.38	113.34	120.45
15	Y	301	1G6	O49-S48-C47	3.34	110.69	108.34
15	Y	301	1G6	C28-N27-C25	3.29	128.72	121.67
15	V	301	1G6	C37-C36-N35	3.26	116.65	110.39
15	Y	301	1G6	C46-C36-C37	-3.18	105.97	111.14
15	K	301	1G6	C37-C36-N35	3.06	116.26	110.39
15	V	301	1G6	C7-C8-N9	3.03	114.29	109.30
15	V	301	1G6	O26-C25-N27	-2.99	117.39	122.93
15	Y	301	1G6	O49-S48-C51	-2.96	105.93	108.91
15	H	301	1G6	O26-C25-N27	-2.91	117.54	122.93
15	K	301	1G6	O26-C25-N27	-2.87	117.62	122.93
15	Y	301	1G6	C7-C8-C12	2.76	115.41	109.55
15	Y	301	1G6	O26-C25-N27	-2.69	117.95	122.93
15	K	301	1G6	C28-N27-C25	2.57	127.18	121.67
15	V	301	1G6	C46-C36-C37	2.55	115.29	111.14
15	H	301	1G6	C28-N27-C25	2.53	127.09	121.67
15	V	301	1G6	C28-N27-C25	2.51	127.04	121.67
15	H	301	1G6	C7-C8-C12	2.49	114.84	109.55
15	Y	301	1G6	C37-C36-N35	2.40	115.01	110.39
15	Y	301	1G6	C15-N14-C12	2.23	126.44	121.67
15	Y	301	1G6	C25-C15-N14	2.16	117.05	111.16
15	Y	301	1G6	C30-C29-C28	2.09	121.18	115.43
15	V	301	1G6	O49-S48-C47	2.07	109.79	108.34

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	Y	301	1G6	O13-C12-C8-N9
15	Y	301	1G6	N14-C12-C8-N9
15	Y	301	1G6	C3-C7-C8-N9

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Mol	Chain	Res	Type	Atoms
15	Y	301	1G6	C25-C15-N14-C12
15	H	301	1G6	O13-C12-N14-C15
15	H	301	1G6	C8-C12-N14-C15
15	H	301	1G6	C12-C8-N9-N10
15	H	301	1G6	C25-C15-N14-C12
15	H	301	1G6	C37-C36-C46-C47
15	H	301	1G6	N35-C36-C46-C47
15	V	301	1G6	C7-C8-N9-N10
15	V	301	1G6	C46-C47-S48-O50
15	V	301	1G6	C46-C47-S48-O49
15	V	301	1G6	N35-C36-C46-C47
15	K	301	1G6	C46-C47-S48-O50
15	K	301	1G6	C46-C47-S48-O49
15	K	301	1G6	C46-C47-S48-C51
15	K	301	1G6	C46-C36-C37-C38
15	Y	301	1G6	O13-C12-N14-C15
15	Y	301	1G6	C8-C12-N14-C15
15	V	301	1G6	O13-C12-N14-C15
15	Y	301	1G6	C36-C46-C47-S48
15	V	301	1G6	C36-C46-C47-S48
15	V	301	1G6	C8-C12-N14-C15
15	Y	301	1G6	C16-C15-C25-N27
15	K	301	1G6	C16-C15-C25-N27
15	Y	301	1G6	C16-C15-C25-O26
15	K	301	1G6	C16-C15-C25-O26
15	V	301	1G6	C16-C15-C25-O26
15	V	301	1G6	C16-C15-C25-N27
15	H	301	1G6	C16-C15-C25-N27
15	V	301	1G6	C37-C36-C46-C47
15	H	301	1G6	C16-C15-C25-O26
15	H	301	1G6	C36-C46-C47-S48
15	V	301	1G6	C36-C37-C38-C43
15	K	301	1G6	C36-C37-C38-C43
15	V	301	1G6	C46-C36-C37-C38
15	V	301	1G6	C36-C37-C38-C39
15	K	301	1G6	C36-C37-C38-C39
15	K	301	1G6	N35-C36-C37-C38
15	V	301	1G6	C25-C15-N14-C12
15	Y	301	1G6	C36-C37-C38-C43
15	H	301	1G6	C36-C37-C38-C43
15	Y	301	1G6	C36-C37-C38-C39
15	H	301	1G6	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
15	H	301	1G6	N14-C15-C25-N27
15	V	301	1G6	C46-C47-S48-C51
15	H	301	1G6	N14-C15-C25-O26
15	K	301	1G6	C36-C46-C47-S48
15	V	301	1G6	C4-C3-C7-C8
15	V	301	1G6	C2-C3-C7-C8
15	H	301	1G6	C28-C29-C30-C32
15	K	301	1G6	C12-C8-N9-N10
15	H	301	1G6	N14-C15-C16-C17
15	K	301	1G6	C25-C15-N14-C12
15	V	301	1G6	C33-C28-C29-C30
15	V	301	1G6	N27-C28-C29-C30
15	K	301	1G6	N27-C28-C33-O34
15	V	301	1G6	C42-C41-C44-N45
15	V	301	1G6	C40-C41-C44-N45
15	Y	301	1G6	C3-C7-C8-C12
15	K	301	1G6	O26-C25-N27-C28
15	K	301	1G6	N27-C28-C33-N35
15	H	301	1G6	C28-C29-C30-C31
15	K	301	1G6	C7-C8-N9-N10

There are no ring outliers.

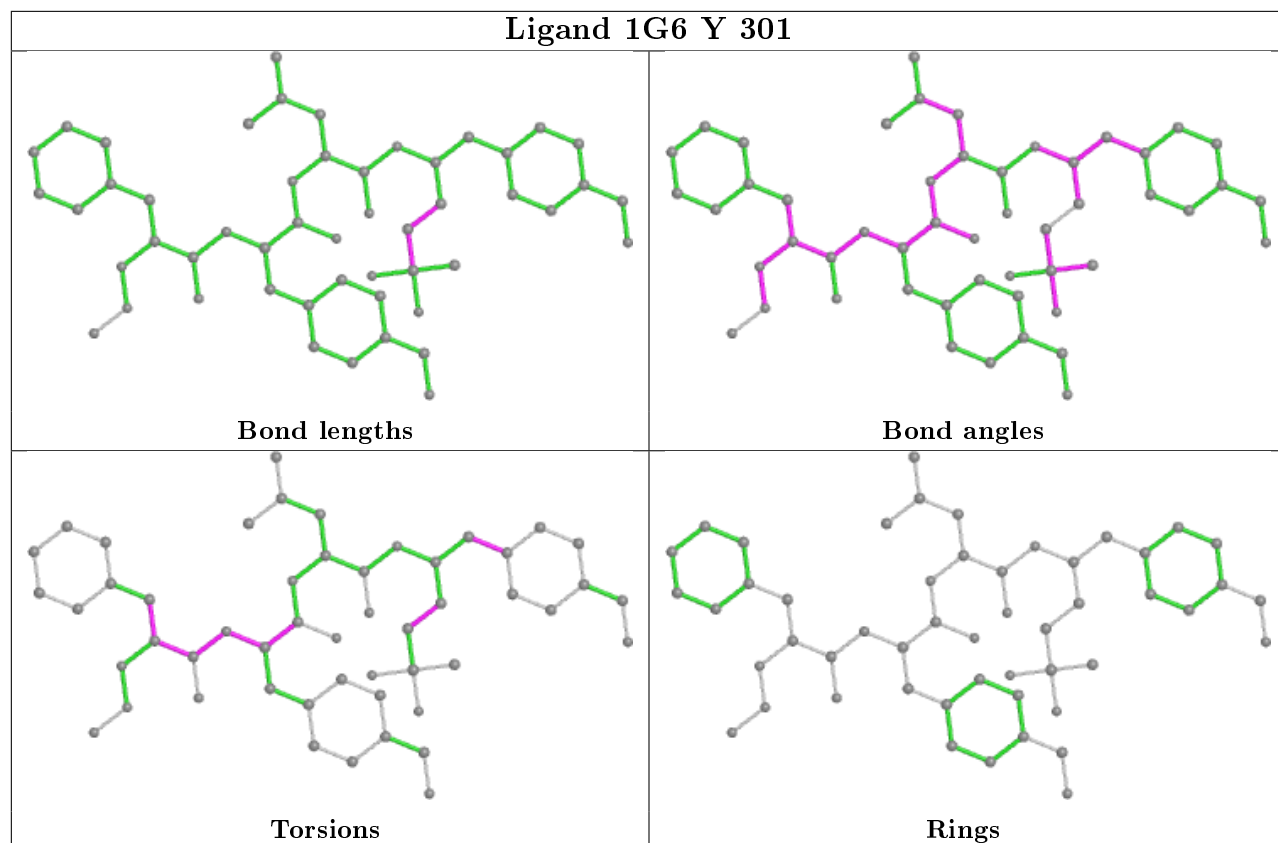
3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	Y	301	1G6	10	0
15	V	301	1G6	2	0
15	K	301	1G6	1	0

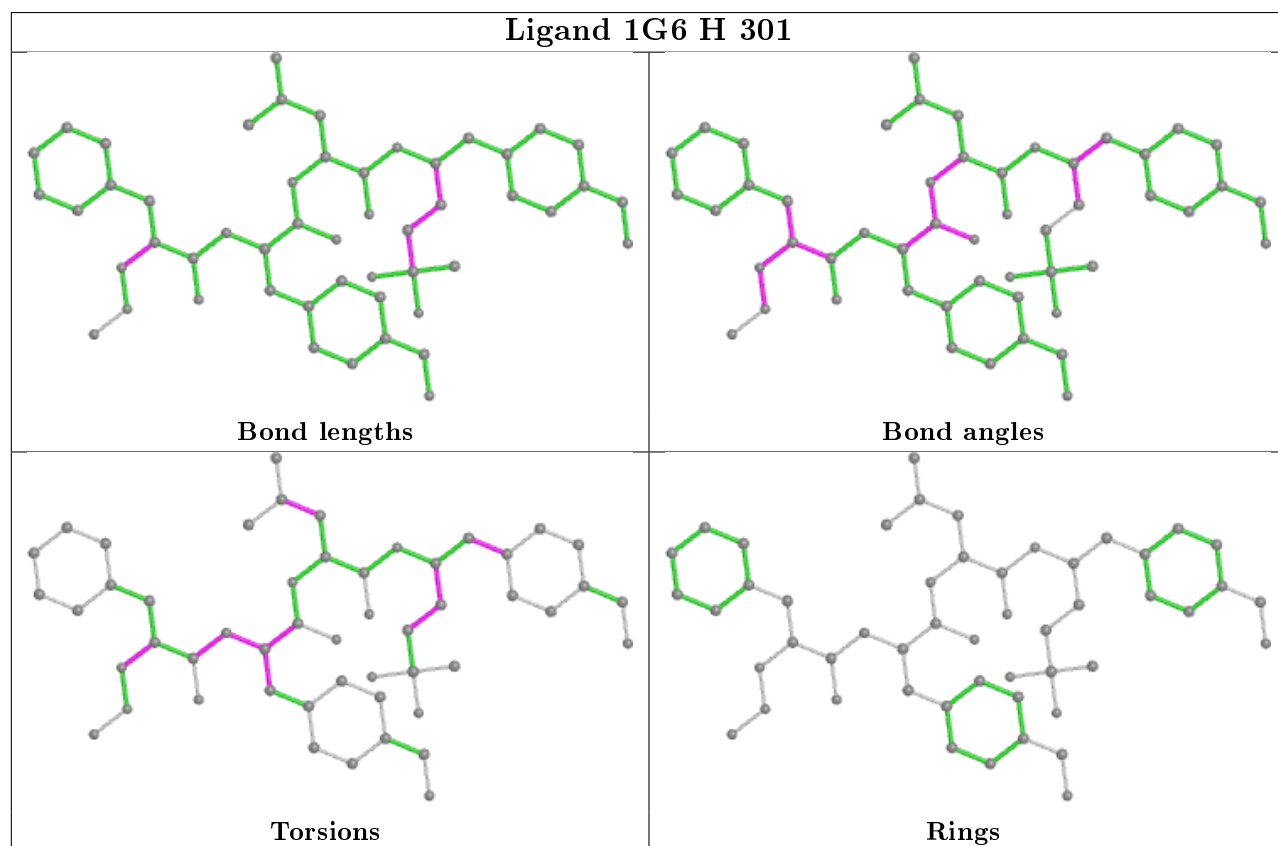
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



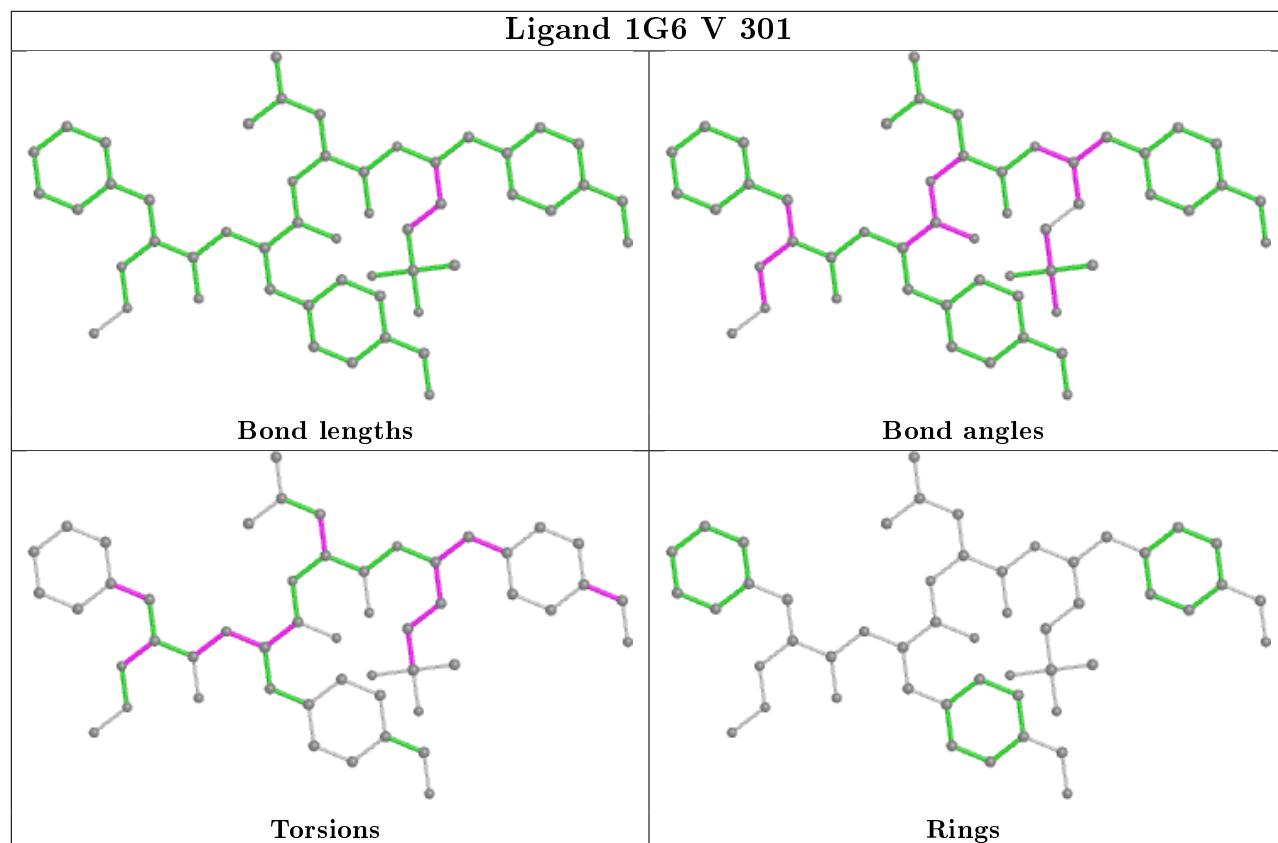
## Ligand 1G6 Y 301



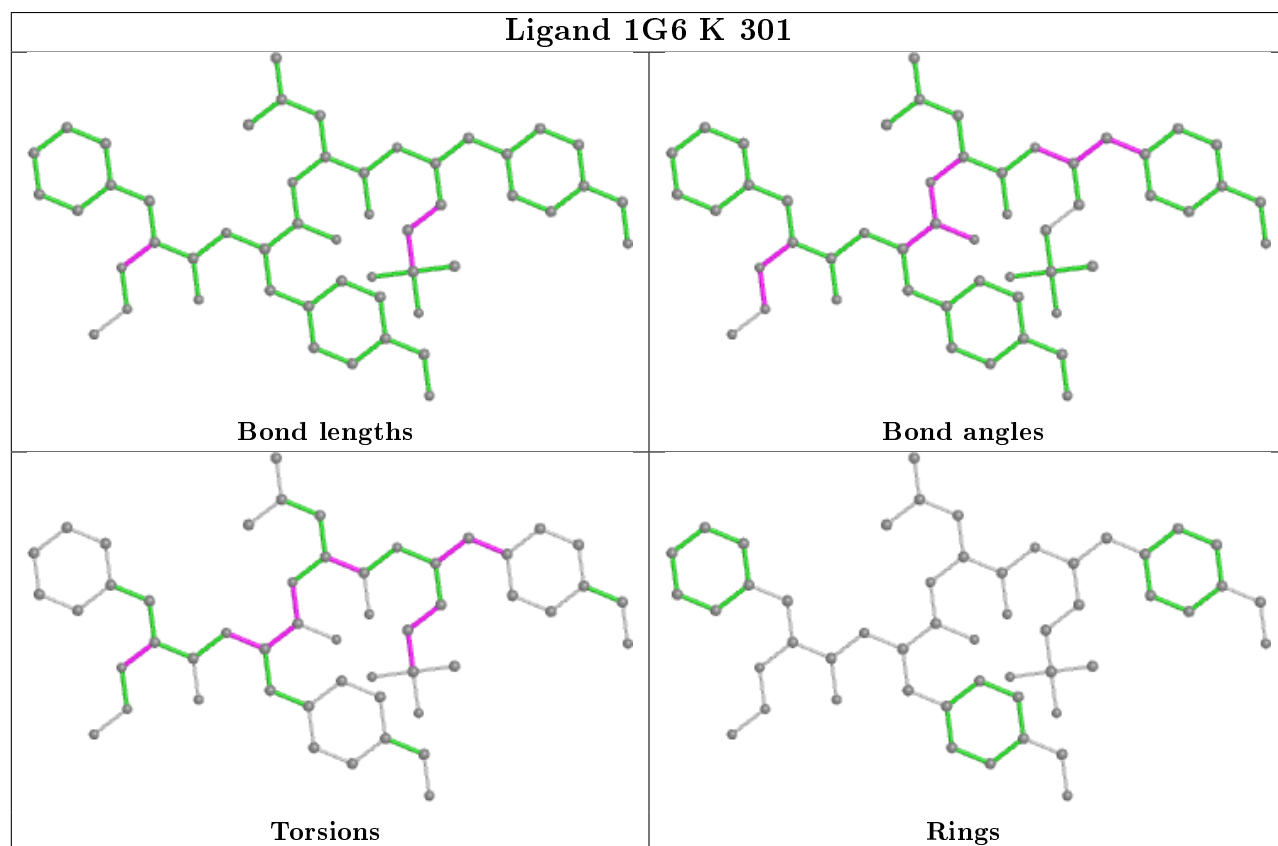
## Ligand 1G6 H 301



## Ligand 1G6 V 301



## Ligand 1G6 K 301



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	250/250 (100%)	-0.29	6 (2%) 59 37	72, 91, 117, 134	0
1	O	250/250 (100%)	-0.30	3 (1%) 79 61	74, 92, 120, 135	0
2	B	244/258 (94%)	-0.15	9 (3%) 41 21	69, 93, 134, 152	0
2	P	244/258 (94%)	-0.15	9 (3%) 41 21	76, 96, 127, 145	0
3	C	241/254 (94%)	-0.16	5 (2%) 63 43	70, 94, 134, 170	0
3	Q	241/254 (94%)	0.08	13 (5%) 25 12	83, 114, 158, 196	0
4	D	242/260 (93%)	-0.17	11 (4%) 33 16	73, 95, 125, 142	0
4	R	242/260 (93%)	-0.06	11 (4%) 33 16	81, 105, 137, 169	0
5	E	233/234 (99%)	-0.14	7 (3%) 50 27	77, 106, 138, 149	0
5	S	233/234 (99%)	-0.03	13 (5%) 24 11	76, 106, 146, 160	0
6	F	244/288 (84%)	-0.24	4 (1%) 72 51	77, 100, 132, 154	0
6	T	244/288 (84%)	-0.27	6 (2%) 57 34	69, 90, 130, 158	0
7	G	243/252 (96%)	-0.28	3 (1%) 79 61	72, 95, 119, 149	0
7	U	243/252 (96%)	-0.32	5 (2%) 63 43	67, 84, 107, 138	0
8	H	222/232 (95%)	-0.41	2 (0%) 84 69	66, 79, 102, 120	0
8	V	222/232 (95%)	-0.45	2 (0%) 84 69	61, 76, 95, 126	0
9	I	204/205 (99%)	-0.58	0 100 100	60, 76, 96, 104	0
9	W	204/205 (99%)	-0.51	1 (0%) 91 81	66, 76, 97, 110	0
10	J	198/198 (100%)	-0.41	4 (2%) 65 44	61, 77, 99, 138	0
10	X	198/198 (100%)	-0.35	4 (2%) 65 44	67, 82, 99, 144	0
11	K	212/212 (100%)	-0.32	5 (2%) 59 37	65, 80, 100, 107	0
11	Y	212/212 (100%)	-0.32	6 (2%) 53 30	67, 81, 108, 114	0
12	L	222/222 (100%)	-0.41	2 (0%) 84 69	60, 80, 111, 120	0
12	Z	222/222 (100%)	-0.37	4 (1%) 68 47	64, 83, 111, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/233 (100%)	-0.47	1 (0%) 92 84	62, 81, 96, 102	0
13	a	233/233 (100%)	-0.49	1 (0%) 92 84	64, 78, 95, 98	0
14	N	196/196 (100%)	-0.49	0 100 100	65, 74, 95, 103	0
14	b	196/196 (100%)	-0.51	0 100 100	63, 72, 91, 101	0
All	All	6368/6588 (96%)	-0.30	137 (2%) 62 41	60, 87, 130, 196	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	198	GLN	7.8
3	Q	241	GLN	6.7
2	P	220	ASN	6.3
4	D	120	SER	6.2
2	B	220	ASN	6.1
4	R	120	SER	5.6
10	J	197	ALA	5.6
3	Q	48	SER	5.6
10	X	197	ALA	5.5
7	G	243	ASP	5.5
3	C	49	THR	5.4
4	D	119	ALA	5.0
4	R	119	ALA	4.9
2	B	221	ASP	4.9
7	U	243	ASP	4.8
5	S	52	ALA	4.8
4	D	118	GLY	4.7
4	R	121	GLY	4.6
8	H	222	ASP	4.5
8	V	222	ASP	4.4
6	T	1	GLY	4.3
3	C	50	LEU	4.2
3	Q	50	LEU	4.2
5	E	202	ASP	4.1
4	D	121	GLY	4.1
7	G	1	ALA	4.1
2	P	219	ALA	4.1
2	B	219	ALA	4.0
3	Q	240	GLU	4.0
11	Y	212	GLY	4.0
10	J	198	GLN	3.9
6	F	1	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
4	R	118	GLY	3.8
5	S	54	GLU	3.8
9	W	1	SER	3.8
3	Q	203	THR	3.7
2	B	51	VAL	3.7
5	S	57	SER	3.6
4	D	122	GLU	3.6
7	G	242	GLN	3.6
3	C	241	GLN	3.6
5	S	2	ARG	3.6
4	R	122	GLU	3.5
12	L	163	GLY	3.5
6	T	244	ASN	3.5
7	U	242	GLN	3.5
2	P	50	LYS	3.4
7	U	1	ALA	3.4
8	V	221	CYS	3.4
2	P	221	ASP	3.4
2	B	223	GLU	3.4
5	S	202	ASP	3.4
1	O	2	THR	3.4
11	Y	104	TYR	3.3
2	P	51	VAL	3.3
5	S	51	ASN	3.3
3	Q	202	GLN	3.3
3	C	240	GLU	3.2
8	H	221	CYS	3.2
3	Q	49	THR	3.1
4	R	239	GLU	3.0
1	O	249	ALA	3.0
5	E	3	ASN	3.0
6	T	53	LYS	3.0
4	R	125	LEU	2.9
1	A	250	LEU	2.9
11	K	104	TYR	2.9
11	K	183	ASP	2.9
11	Y	182	GLU	2.9
11	Y	183	ASP	2.8
10	J	196	GLN	2.8
11	K	182	GLU	2.8
11	K	209	ASN	2.8
1	A	2	THR	2.8

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Mol	Chain	Res	Type	RSRZ
5	S	173	ARG	2.8
2	P	223	GLU	2.7
11	K	212	GLY	2.7
4	D	125	LEU	2.7
5	E	2	ARG	2.6
6	F	244	ASN	2.6
12	Z	173	LYS	2.6
2	B	218	GLY	2.6
2	P	218	GLY	2.6
3	C	239	GLN	2.6
11	Y	209	ASN	2.6
10	X	1	MET	2.5
1	A	1	MET	2.5
3	Q	239	GLN	2.5
3	Q	141	ASP	2.5
13	a	1	THR	2.5
2	B	61	SER	2.5
10	J	1	MET	2.5
5	S	225	ASP	2.5
5	E	233	ILE	2.5
7	U	203	ASP	2.5
1	A	201	GLU	2.4
6	F	202	ASP	2.4
5	S	58	TYR	2.4
4	R	1	ASP	2.4
2	P	225	TYR	2.4
12	L	173	LYS	2.4
3	Q	235	GLU	2.4
4	D	242	GLU	2.4
5	E	30	GLN	2.4
10	X	196	GLN	2.4
11	Y	208	ASN	2.4
5	S	29	LYS	2.3
4	R	242	GLU	2.3
3	Q	175	LYS	2.3
5	S	201	ARG	2.3
6	T	2	THR	2.2
5	E	1	PHE	2.2
1	A	245	ASP	2.2
5	S	53	ASP	2.2
2	B	240	LYS	2.2
7	U	222	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
6	T	177	ASP	2.2
5	S	194	GLU	2.2
6	T	201	GLU	2.2
4	D	124	ARG	2.1
12	Z	165	ASN	2.1
1	O	1	MET	2.1
2	P	59	ASP	2.1
4	D	177	ASN	2.1
4	R	157	TYR	2.1
6	F	207	ASP	2.1
3	Q	58	THR	2.1
13	M	1	THR	2.1
5	E	54	GLU	2.1
4	R	240	ALA	2.1
1	A	202	GLY	2.1
2	B	50	LYS	2.0
12	Z	174	TYR	2.0
12	Z	163	GLY	2.0
4	D	1	ASP	2.0
4	D	2	ARG	2.0
3	Q	1	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	1G6	V	301	51/51	0.84	0.32	62,68,75,78	0
15	1G6	K	301	51/51	0.86	0.30	58,65,76,79	0

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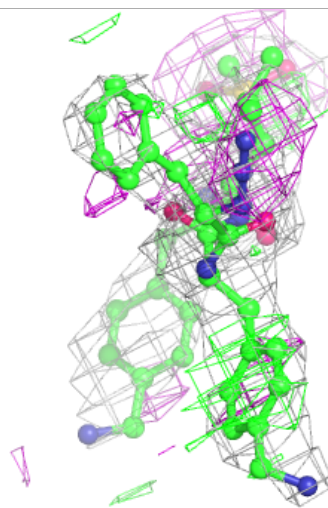
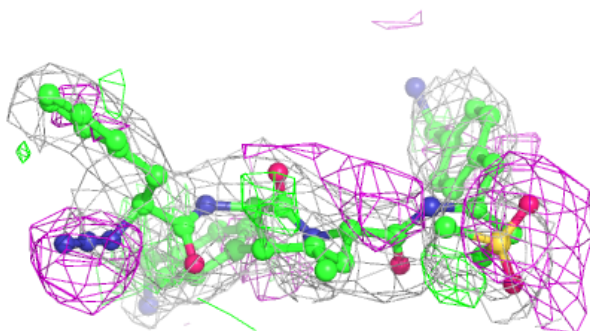
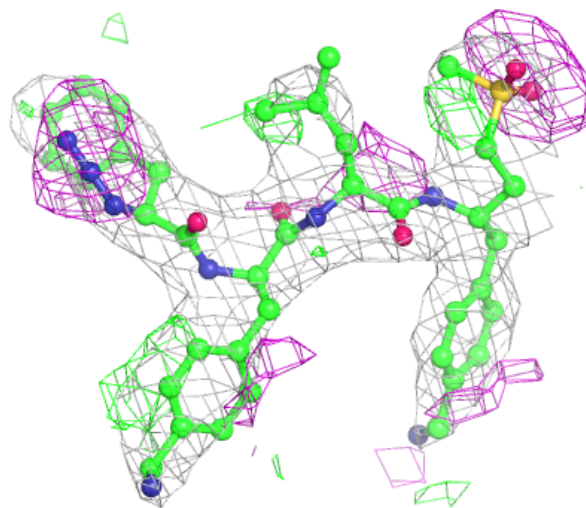
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	1G6	Y	301	51/51	0.90	0.28	57,65,70,71	0
15	1G6	H	301	51/51	0.90	0.25	59,62,67,69	0

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.

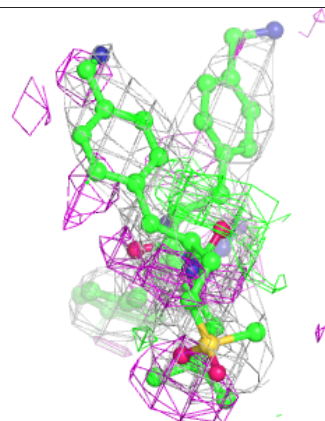
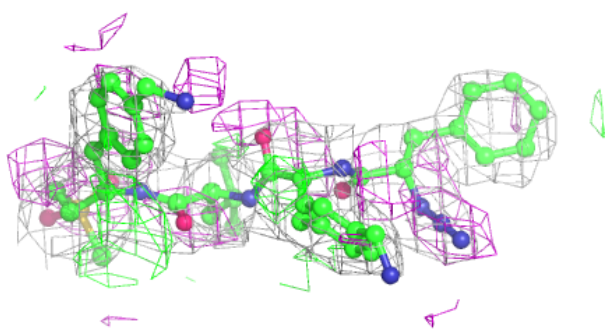
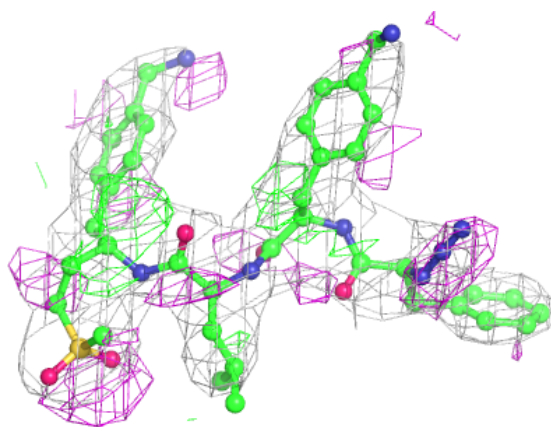
**Electron density around 1G6 V 301:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

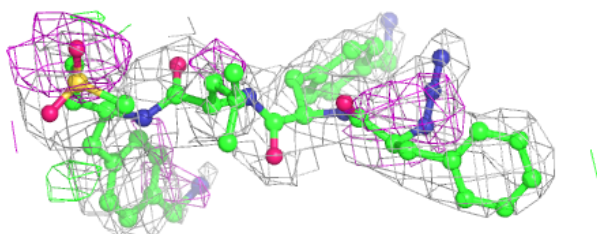
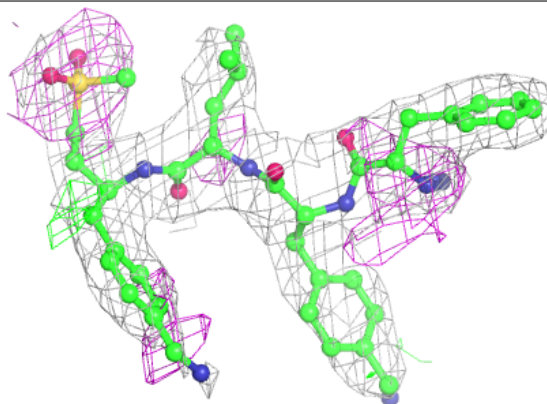


**Electron density around 1G6 K 301:**

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

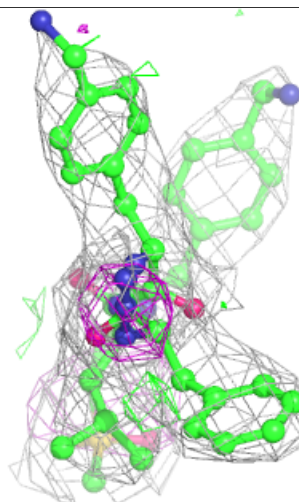
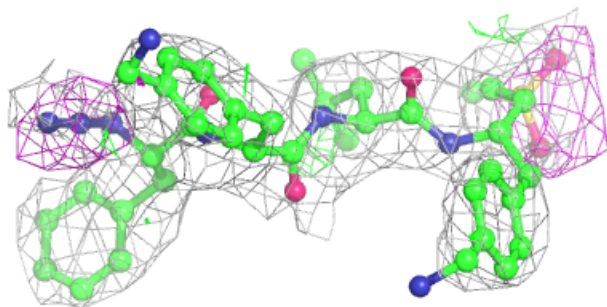
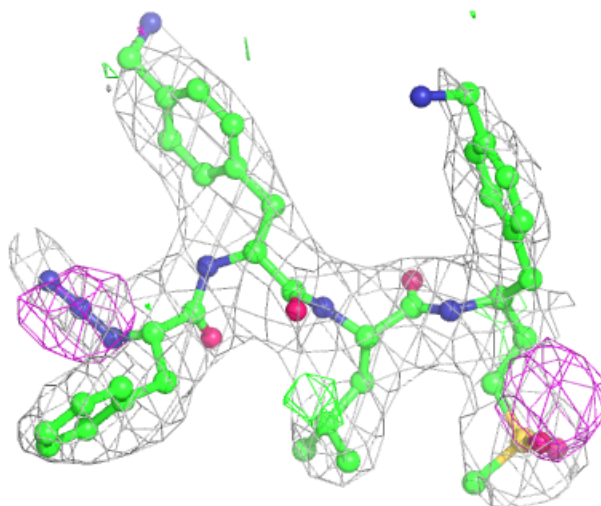
**Electron density around 1G6 Y 301:**

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



**Electron density around 1G6 H 301:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.