



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 21, 2025 – 11:07 AM EDT

PDB ID : 9C98 / pdb\_00009c98  
Title : Yeast 20S proteasome soaked with isolated TMC-86A  
Authors : Meneghello, R.; Rustiguel, J.K.  
Deposited on : 2024-06-13  
Resolution : 3.04 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

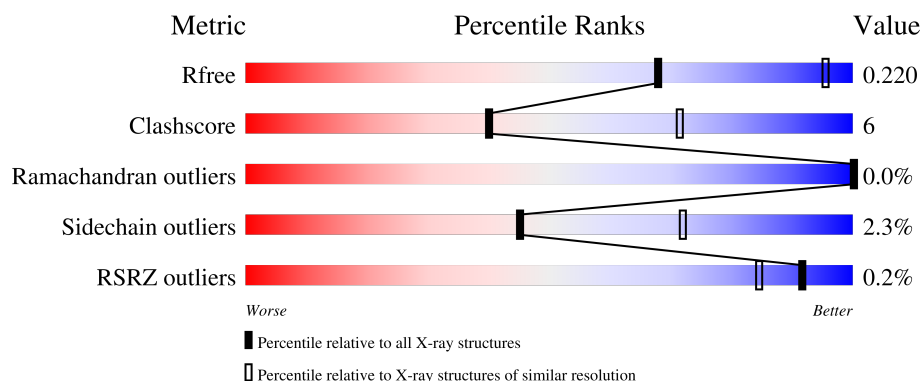
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*






The reported resolution of this entry is 3.04 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.

























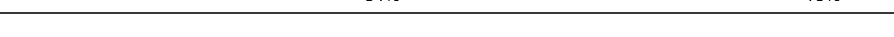
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	3418 (3.08-3.00)
Clashscore	180529	3811 (3.08-3.00)
Ramachandran outliers	177936	3656 (3.08-3.00)
Sidechain outliers	177891	3658 (3.08-3.00)
RSRZ outliers	164620	3430 (3.08-3.00)

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	 83% 16% .
1	O	250	 79% 19% .
2	B	258	 76% 18% 6%
2	P	258	 73% 21% . 5%
3	C	254	 78% 16% . 5%

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Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	287	
6	T	287	
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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	SO4	V	306	-	-	X	-

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 50225 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1907	1214	314	376	3			
1	O	249	Total	C	N	O	S	0	0	0
			1907	1214	314	376	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	243	Total	C	N	O	S	0	0	0
			1905	1204	321	377	3			
2	P	244	Total	C	N	O	S	0	0	0
			1909	1206	322	378	3			

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

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 subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	240	Total	C	N	O	S	0	0	0
			1854	1161	309	377	7			
4	R	240	Total	C	N	O	S	0	0	0
			1855	1161	312	375	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			
5	S	232	Total	C	N	O	S	0	0	0
			1777	1116	311	346	4			

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

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
			1891	1202	328	357	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			
7	U	242	Total	C	N	O	S	0	0	0
			1916	1218	321	369	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	221	Total	C	N	O	S	0	0	0
			1676	1057	292	320	7			
8	V	221	Total	C	N	O	S	0	0	0
			1676	1057	292	320	7			

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

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

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

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

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

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

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

- Molecule 12 is a protein called Proteasome subunit beta type-6.

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

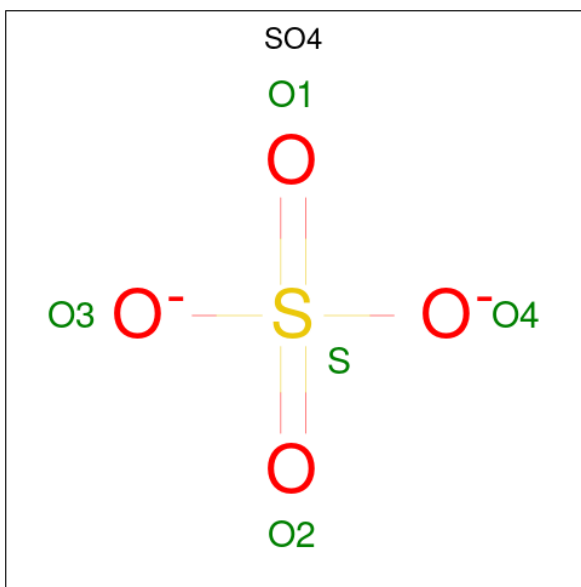
- Molecule 13 is a protein called Proteasome subunit beta type-7.

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

- Molecule 14 is a protein called Proteasome subunit beta type-1.

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

- Molecule 15 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	B	1	Total	O	S	0	0
			5	4	1		
15	B	1	Total	O	S	0	0
			5	4	1		
15	B	1	Total	O	S	0	0
			5	4	1		
15	C	1	Total	O	S	0	0
			5	4	1		
15	D	1	Total	O	S	0	0
			5	4	1		
15	E	1	Total	O	S	0	0
			5	4	1		
15	E	1	Total	O	S	0	0
			5	4	1		
15	E	1	Total	O	S	0	0
			5	4	1		
15	E	1	Total	O	S	0	0
			5	4	1		
15	F	1	Total	O	S	0	0
			5	4	1		
15	F	1	Total	O	S	0	0
			5	4	1		
15	G	1	Total	O	S	0	0
			5	4	1		
15	G	1	Total	O	S	0	0
			5	4	1		
15	P	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	P	1	Total	O	S	0	0
			5	4	1		
15	Q	1	Total	O	S	0	0
			5	4	1		
15	Q	1	Total	O	S	0	0
			5	4	1		
15	S	1	Total	O	S	0	0
			5	4	1		
15	S	1	Total	O	S	0	0
			5	4	1		
15	S	1	Total	O	S	0	0
			5	4	1		
15	S	1	Total	O	S	0	0
			5	4	1		
15	T	1	Total	O	S	0	0
			5	4	1		
15	T	1	Total	O	S	0	0
			5	4	1		
15	T	1	Total	O	S	0	0
			5	4	1		
15	U	1	Total	O	S	0	0
			5	4	1		
15	H	1	Total	O	S	0	0
			5	4	1		
15	H	1	Total	O	S	0	0
			5	4	1		
15	I	1	Total	O	S	0	0
			5	4	1		
15	J	1	Total	O	S	0	0
			5	4	1		
15	J	1	Total	O	S	0	0
			5	4	1		
15	J	1	Total	O	S	0	0
			5	4	1		
15	J	1	Total	O	S	0	0
			5	4	1		
15	K	1	Total	O	S	0	0
			5	4	1		
15	K	1	Total	O	S	0	0
			5	4	1		
15	K	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	K	1	Total	O	S	0	0
			5	4	1		
15	K	1	Total	O	S	0	0
			5	4	1		
15	L	1	Total	O	S	0	0
			5	4	1		
15	L	1	Total	O	S	0	0
			5	4	1		
15	M	1	Total	O	S	0	0
			5	4	1		
15	M	1	Total	O	S	0	0
			5	4	1		
15	M	1	Total	O	S	0	0
			5	4	1		
15	M	1	Total	O	S	0	0
			5	4	1		
15	M	1	Total	O	S	0	0
			5	4	1		
15	M	1	Total	O	S	0	0
			5	4	1		
15	N	1	Total	O	S	0	0
			5	4	1		
15	N	1	Total	O	S	0	0
			5	4	1		
15	V	1	Total	O	S	0	0
			5	4	1		
15	V	1	Total	O	S	0	0
			5	4	1		
15	V	1	Total	O	S	0	0
			5	4	1		
15	V	1	Total	O	S	0	0
			5	4	1		
15	W	1	Total	O	S	0	0
			5	4	1		
15	W	1	Total	O	S	0	0
			5	4	1		
15	X	1	Total	O	S	0	0
			5	4	1		
15	Y	1	Total	O	S	0	0
			5	4	1		
15	Y	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	Y	1	Total	O	S	0	0
			5	4	1		
15	Y	1	Total	O	S	0	0
			5	4	1		
15	Z	1	Total	O	S	0	0
			5	4	1		
15	Z	1	Total	O	S	0	0
			5	4	1		
15	Z	1	Total	O	S	0	0
			5	4	1		
15	Z	1	Total	O	S	0	0
			5	4	1		
15	a	1	Total	O	S	0	0
			5	4	1		
15	a	1	Total	O	S	0	0
			5	4	1		
15	a	1	Total	O	S	0	0
			5	4	1		
15	a	1	Total	O	S	0	0
			5	4	1		
15	a	1	Total	O	S	0	0
			5	4	1		
15	b	1	Total	O	S	0	0
			5	4	1		
15	b	1	Total	O	S	0	0
			5	4	1		

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

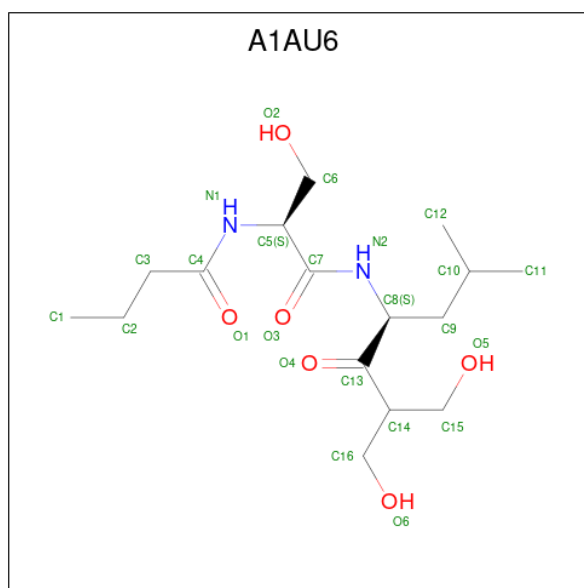
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total	Mg	0	0
			1	1		
16	U	1	Total	Mg	0	0
			1	1		
16	H	1	Total	Mg	0	0
			1	1		
16	I	1	Total	Mg	0	0
			1	1		
16	K	1	Total	Mg	0	0
			1	1		
16	L	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	N	1	Total	Mg	0	0
			1	1		
16	V	1	Total	Mg	0	0
			1	1		
16	W	1	Total	Mg	0	0
			1	1		
16	Y	1	Total	Mg	0	0
			1	1		
16	Z	1	Total	Mg	0	0
			1	1		
16	b	1	Total	Mg	0	0
			1	1		

- Molecule 17 is N-[(2S)-3-hydroxy-1-{[(4S)-1-hydroxy-2-(hydroxymethyl)-6-methyl-3-oxohexan-4-yl]amino}-1-oxopropan-2-yl]butanamide (CCD ID: A1AU6) (formula: C<sub>16</sub>H<sub>30</sub>N<sub>2</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	H	1	Total	C	N	O	0	0
			24	16	2	6		
17	K	1	Total	C	N	O	0	0
			24	16	2	6		
17	N	1	Total	C	N	O	0	0
			24	16	2	6		
17	V	1	Total	C	N	O	0	0
			24	16	2	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	Y	1	Total	C	N	O	0	0
			24	16	2	6		
17	b	1	Total	C	N	O	0	0
			24	16	2	6		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	15	Total	O	0	0
			15	15		
18	B	14	Total	O	0	0
			14	14		
18	C	4	Total	O	0	0
			4	4		
18	D	17	Total	O	0	0
			17	17		
18	E	15	Total	O	0	0
			15	15		
18	F	9	Total	O	0	0
			9	9		
18	G	16	Total	O	0	0
			16	16		
18	O	20	Total	O	0	0
			20	20		
18	P	12	Total	O	0	0
			12	12		
18	Q	13	Total	O	0	0
			13	13		
18	R	5	Total	O	0	0
			5	5		
18	S	6	Total	O	0	0
			6	6		
18	T	8	Total	O	0	0
			8	8		
18	U	10	Total	O	0	0
			10	10		
18	H	11	Total	O	0	0
			11	11		
18	I	6	Total	O	0	0
			6	6		
18	J	9	Total	O	0	0
			9	9		

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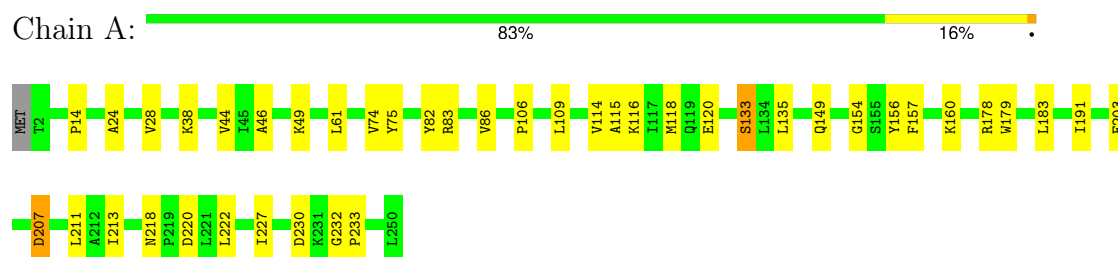
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	K	19	Total 19	O 19	0	0
18	L	9	Total 9	O 9	0	0
18	M	13	Total 13	O 13	0	0
18	N	11	Total 11	O 11	0	0
18	V	11	Total 11	O 11	0	0
18	W	9	Total 9	O 9	0	0
18	X	28	Total 28	O 28	0	0
18	Y	17	Total 17	O 17	0	0
18	Z	11	Total 11	O 11	0	0
18	a	13	Total 13	O 13	0	0
18	b	6	Total 6	O 6	0	0

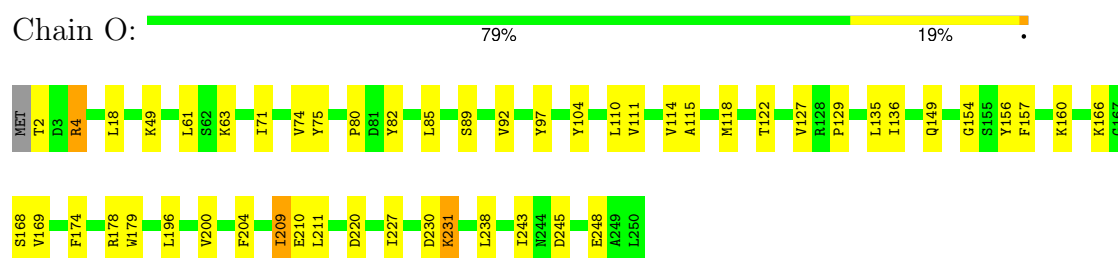
### 3 Residue-property plots

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.

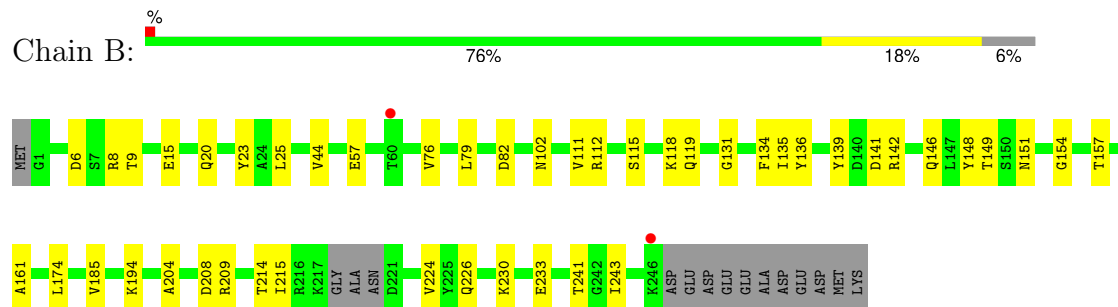
#### • Molecule 1: Proteasome subunit alpha type-2



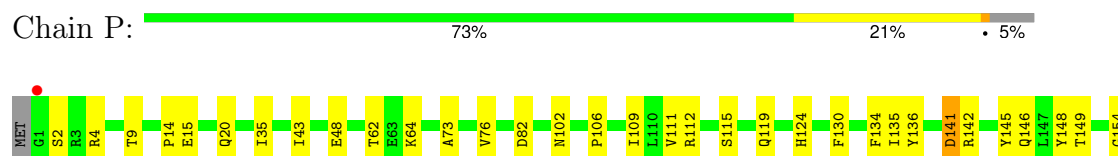
#### • Molecule 1: Proteasome subunit alpha type-2

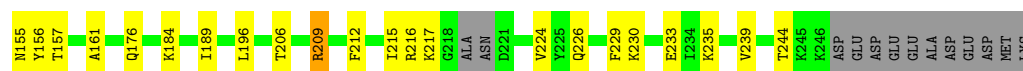


#### • Molecule 2: Proteasome subunit alpha type-3

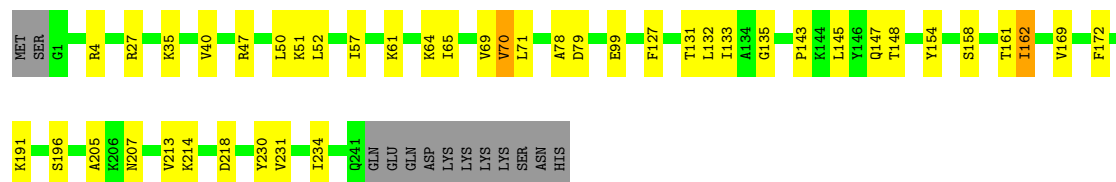
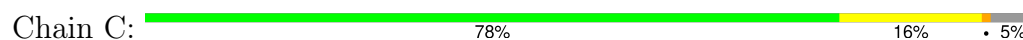


#### • Molecule 2: Proteasome subunit alpha type-3

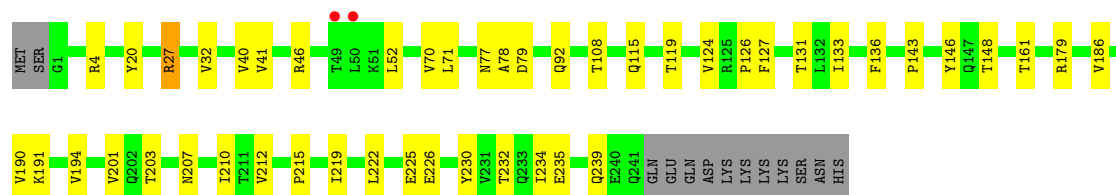
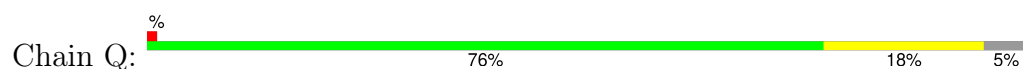




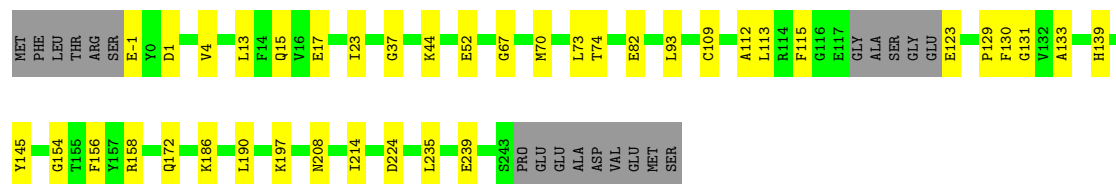
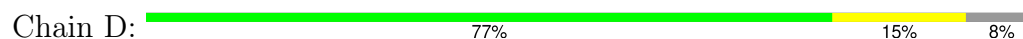
• Molecule 3: Proteasome subunit alpha type-4



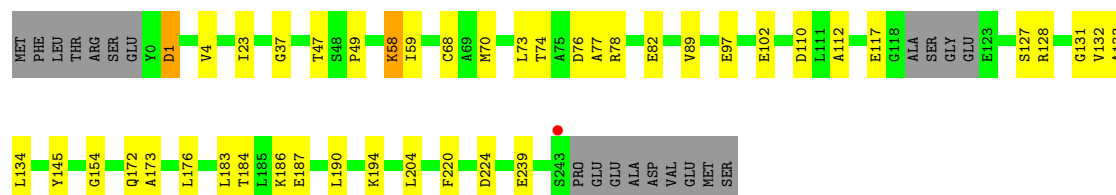
• Molecule 3: Proteasome subunit alpha type-4



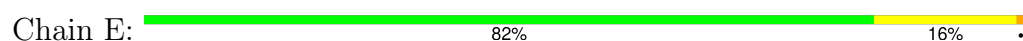
• Molecule 4: Proteasome subunit alpha type-5



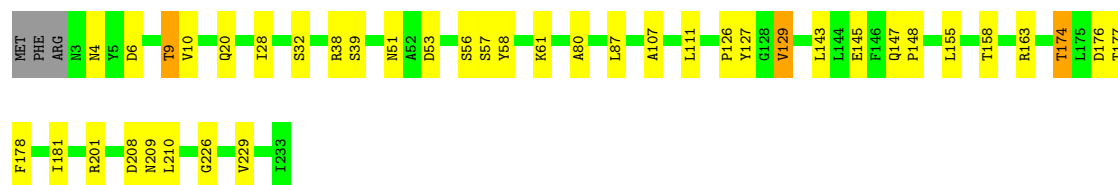
• Molecule 4: Proteasome subunit alpha type-5



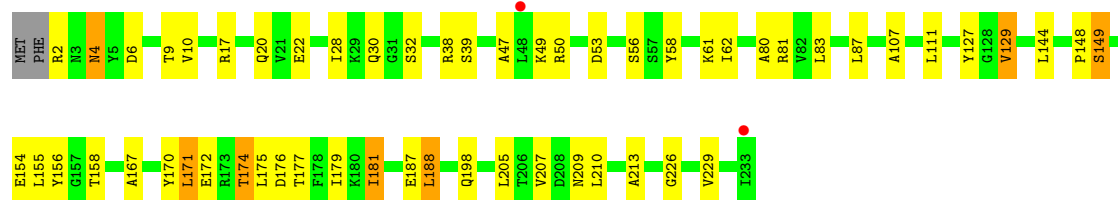
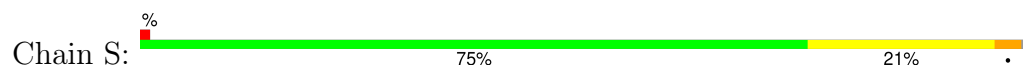
• Molecule 5: Proteasome subunit alpha type-6



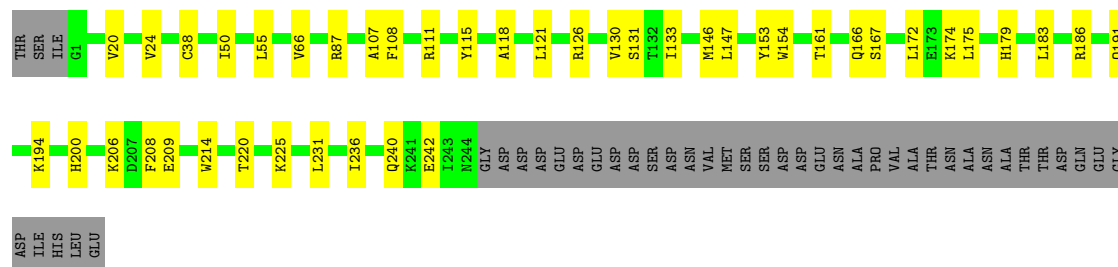




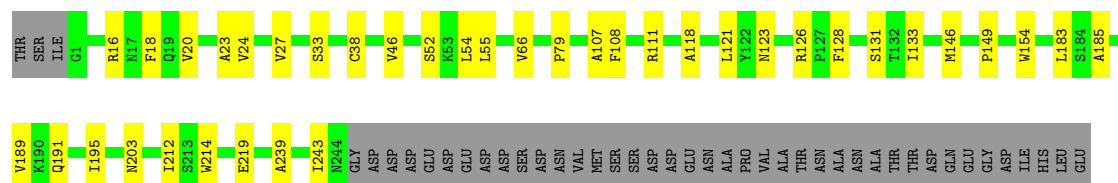
• Molecule 5: Proteasome subunit alpha type-6



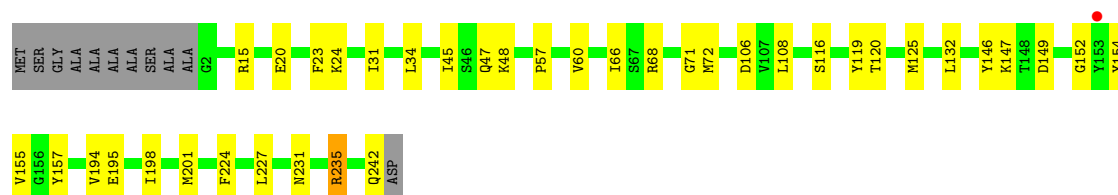
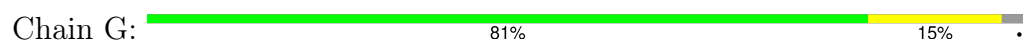
• Molecule 6: Probable proteasome subunit alpha type-7



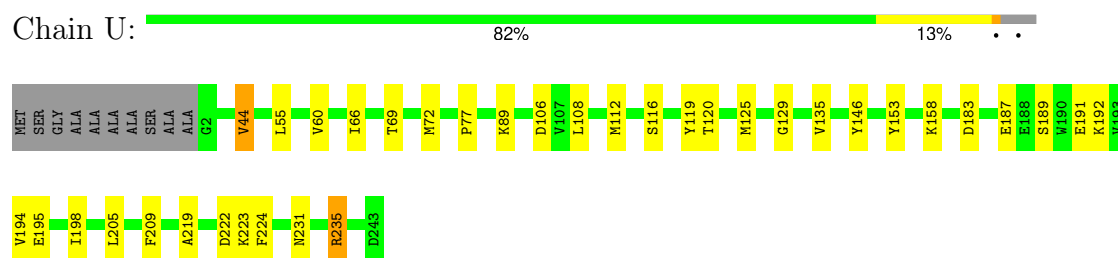
• Molecule 6: Probable proteasome subunit alpha type-7



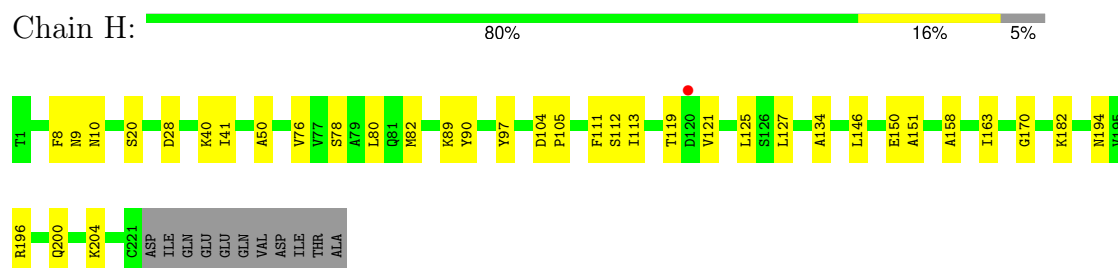
• Molecule 7: Proteasome subunit alpha type-1



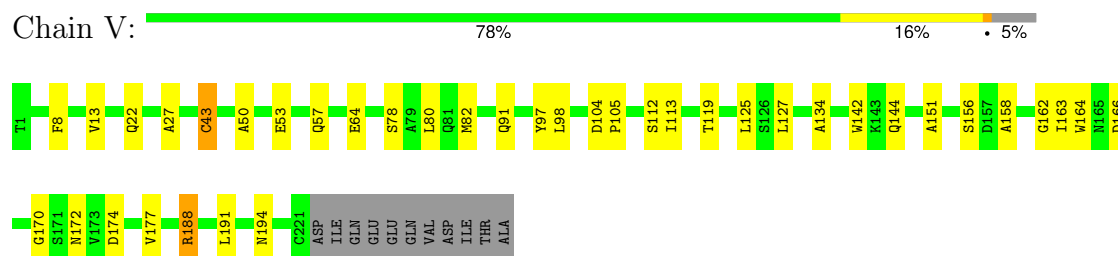
- Molecule 7: Proteasome subunit alpha type-1



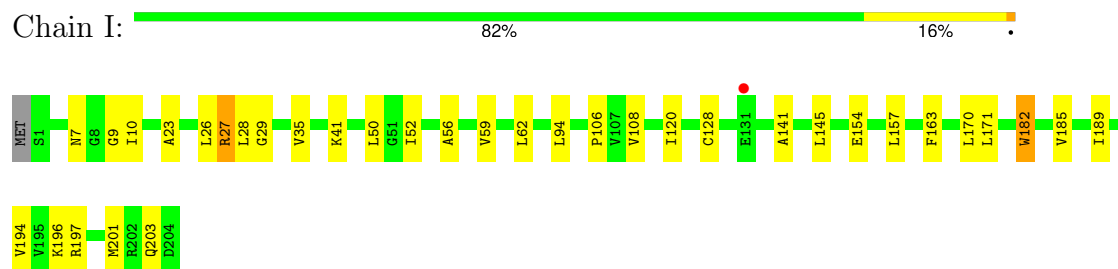
- Molecule 8: Proteasome subunit beta type-2



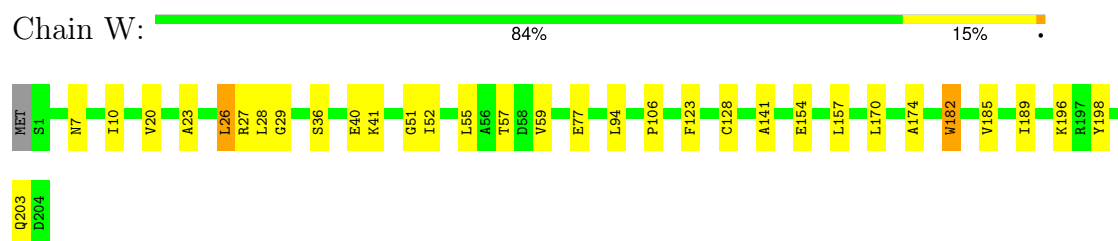
- Molecule 8: Proteasome subunit beta type-2



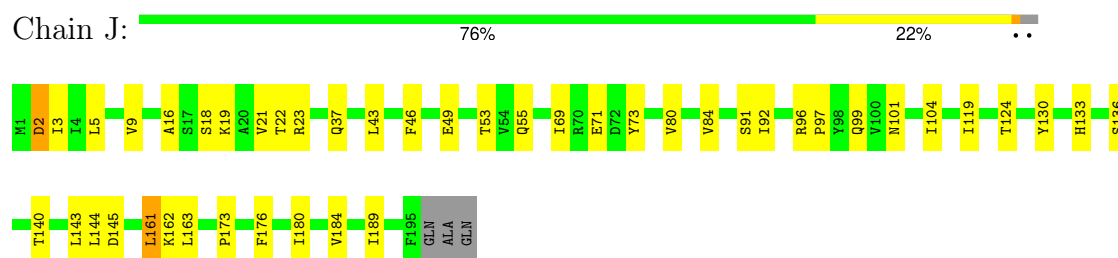
- Molecule 9: Proteasome subunit beta type-3



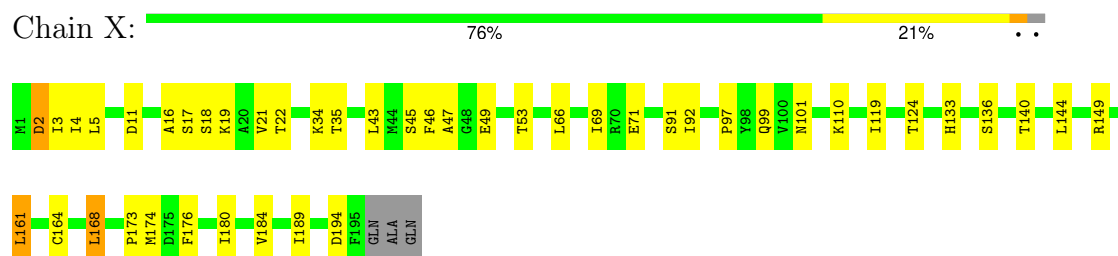
- Molecule 9: Proteasome subunit beta type-3



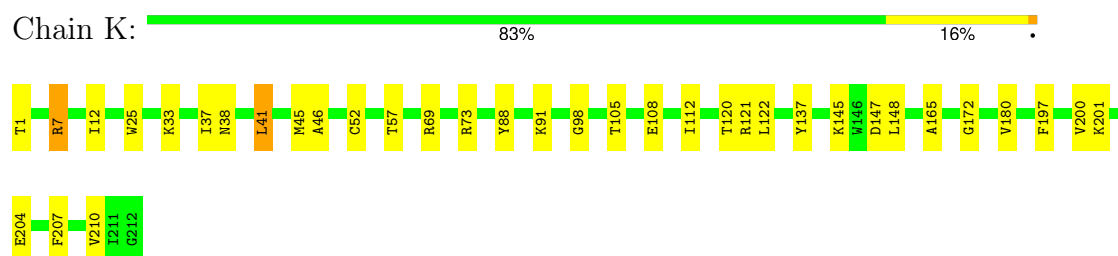
- Molecule 10: Proteasome subunit beta type-4



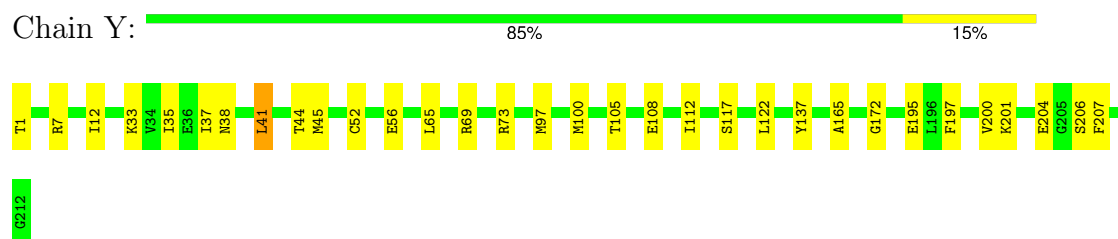
- Molecule 10: Proteasome subunit beta type-4



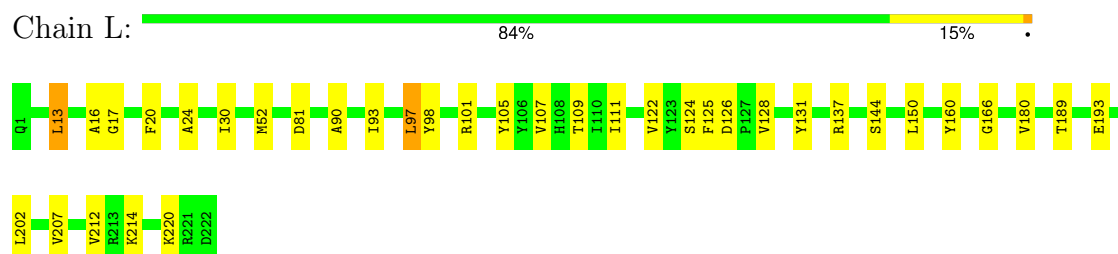
- Molecule 11: Proteasome subunit beta type-5



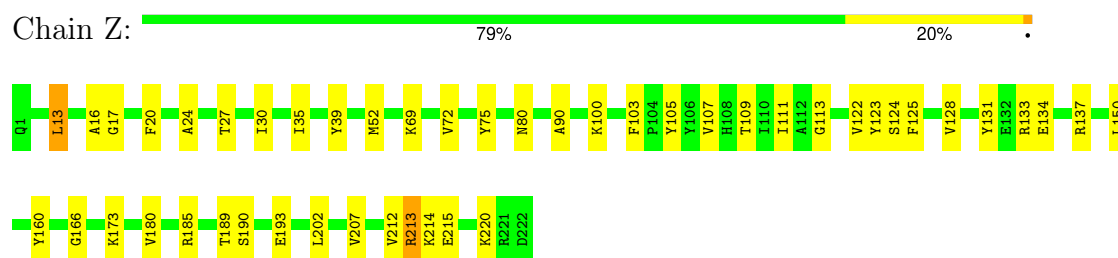
- Molecule 11: Proteasome subunit beta type-5



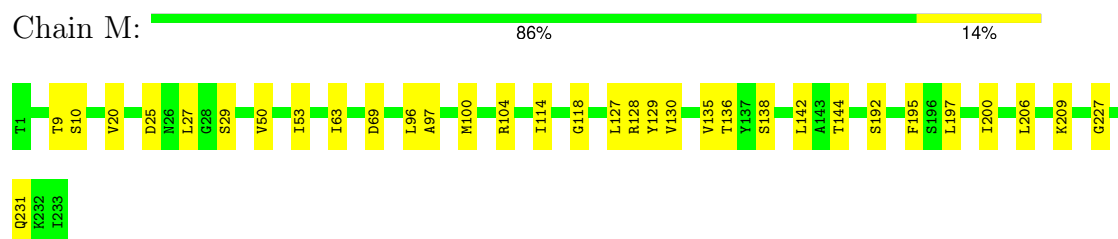
- Molecule 12: Proteasome subunit beta type-6



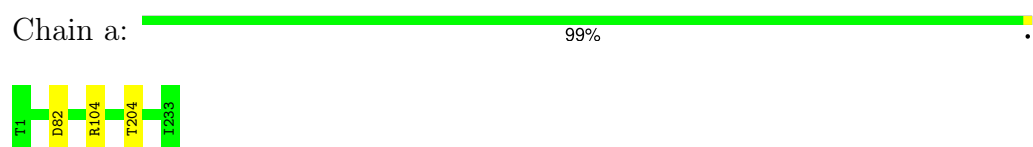
- Molecule 12: Proteasome subunit beta type-6



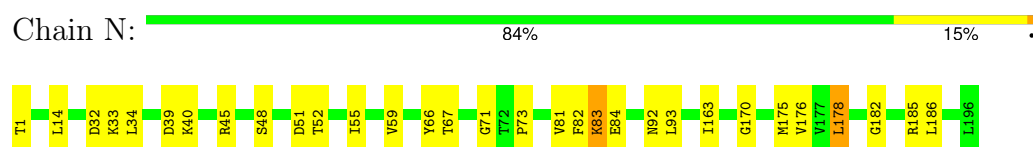
- Molecule 13: Proteasome subunit beta type-7



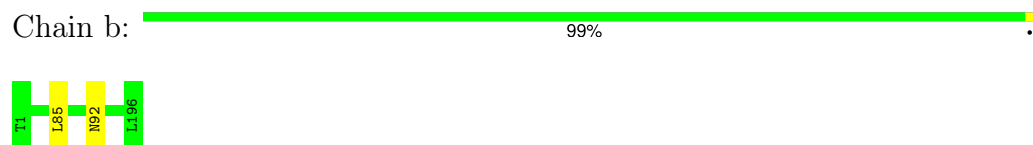
- Molecule 13: Proteasome subunit beta type-7



- 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, $\alpha$ , $\beta$ , $\gamma$	117.31Å 298.28Å 144.57Å 90.00° 108.80° 90.00°	Depositor
Resolution (Å)	48.54 – 3.04 48.54 – 3.04	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.54-3.04) 93.3 (48.54-3.04)	Depositor EDS
$R_{merge}$	0.33	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, $R_{free}$	0.174 , 0.221 0.174 , 0.220	Depositor DCC
$R_{free}$ test set	8953 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.6	Xtriage
Anisotropy	0.818	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 43.4	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	0.94	EDS
Total number of atoms	50225	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, A1AU6, SO4

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	0.26	0/1944	0.49	0/2632
1	O	0.26	0/1944	0.49	0/2632
2	B	0.25	0/1934	0.50	0/2614
2	P	0.25	0/1938	0.51	0/2619
3	C	0.25	0/1919	0.52	0/2598
3	Q	0.25	0/1919	0.52	0/2598
4	D	0.26	0/1879	0.49	0/2532
4	R	0.25	0/1880	0.49	0/2532
5	E	0.26	0/1800	0.52	0/2433
5	S	0.26	0/1804	0.53	0/2439
6	F	0.27	0/1936	0.49	0/2614
6	T	0.26	0/1930	0.48	0/2606
7	G	0.27	0/1945	0.49	0/2634
7	U	0.27	0/1954	0.49	0/2645
8	H	0.26	0/1707	0.51	0/2315
8	V	0.27	0/1707	0.51	0/2315
9	I	0.27	0/1611	0.50	0/2174
9	W	0.27	0/1611	0.51	0/2174
10	J	0.27	0/1589	0.50	0/2142
10	X	0.27	0/1589	0.51	0/2142
11	K	0.26	0/1681	0.51	0/2274
11	Y	0.26	0/1681	0.51	0/2274
12	L	0.28	0/1795	0.53	0/2420
12	Z	0.27	0/1795	0.52	0/2420
13	M	0.26	0/1855	0.52	0/2514
13	a	0.26	0/1855	0.51	0/2514
14	N	0.26	0/1541	0.49	0/2087
14	b	0.26	0/1541	0.49	0/2087
All	All	0.26	0/50284	0.50	0/67980

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	1907	0	1917	26	0
1	O	1907	0	1917	30	0
2	B	1905	0	1915	29	0
2	P	1909	0	1918	33	0
3	C	1890	0	1903	29	0
3	Q	1890	0	1903	32	0
4	D	1854	0	1825	22	0
4	R	1855	0	1833	30	0
5	E	1773	0	1775	25	0
5	S	1777	0	1777	36	0
6	F	1896	0	1889	24	0
6	T	1891	0	1884	22	0
7	G	1907	0	1901	21	0
7	U	1916	0	1905	21	0
8	H	1676	0	1681	24	0
8	V	1676	0	1681	24	0
9	I	1581	0	1574	22	0
9	W	1581	0	1574	18	0
10	J	1561	0	1569	32	0
10	X	1561	0	1569	30	0
11	K	1644	0	1592	24	0
11	Y	1644	0	1592	21	0
12	L	1757	0	1711	22	0
12	Z	1757	0	1711	29	0
13	M	1824	0	1832	18	0
13	a	1824	0	1832	0	0
14	N	1512	0	1478	20	0
14	b	1512	0	1478	0	0
15	B	15	0	0	0	0
15	C	5	0	0	0	0
15	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	E	20	0	0	0	0
15	F	10	0	0	0	0
15	G	10	0	0	0	0
15	H	10	0	0	0	0
15	I	5	0	0	0	0
15	J	20	0	0	0	0
15	K	25	0	0	0	0
15	L	10	0	0	0	0
15	M	30	0	0	0	0
15	N	10	0	0	0	0
15	P	10	0	0	0	0
15	Q	10	0	0	0	0
15	S	20	0	0	0	0
15	T	15	0	0	0	0
15	U	5	0	0	0	0
15	V	20	0	0	3	0
15	W	10	0	0	0	0
15	X	5	0	0	0	0
15	Y	20	0	0	0	0
15	Z	20	0	0	0	0
15	a	25	0	0	0	0
15	b	10	0	0	0	0
16	G	1	0	0	0	0
16	H	1	0	0	0	0
16	I	1	0	0	0	0
16	K	1	0	0	0	0
16	L	1	0	0	0	0
16	N	1	0	0	0	0
16	U	1	0	0	0	0
16	V	1	0	0	0	0
16	W	1	0	0	0	0
16	Y	1	0	0	0	0
16	Z	1	0	0	0	0
16	b	1	0	0	0	0
17	H	24	0	0	0	0
17	K	24	0	0	0	0
17	N	24	0	0	0	0
17	V	24	0	0	0	0
17	Y	24	0	0	0	0
17	b	24	0	0	0	0
18	A	15	0	0	0	0
18	B	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	C	4	0	0	0	0
18	D	17	0	0	0	0
18	E	15	0	0	0	0
18	F	9	0	0	0	0
18	G	16	0	0	0	0
18	H	11	0	0	0	0
18	I	6	0	0	0	0
18	J	9	0	0	0	0
18	K	19	0	0	0	0
18	L	9	0	0	0	0
18	M	13	0	0	0	0
18	N	11	0	0	0	0
18	O	20	0	0	0	0
18	P	12	0	0	0	0
18	Q	13	0	0	0	0
18	R	5	0	0	0	0
18	S	6	0	0	1	0
18	T	8	0	0	0	0
18	U	10	0	0	0	0
18	V	11	0	0	0	0
18	W	9	0	0	0	0
18	X	28	0	0	0	0
18	Y	17	0	0	0	0
18	Z	11	0	0	0	0
18	a	13	0	0	0	0
18	b	6	0	0	0	0
All	All	50225	0	49136	595	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 6.

The worst 5 of 595 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:220:LYS:HE3	8:V:194:ASN:HB3	1.49	0.94
1:A:46:ALA:HB2	1:A:211:LEU:HD13	1.63	0.80
8:H:194:ASN:HB3	12:Z:220:LYS:HE3	1.66	0.75
1:A:49:LYS:NZ	1:A:61:LEU:O	2.20	0.74
4:D:4:VAL:HG13	4:D:15:GLN:HG3	1.68	0.74

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	247/250 (99%)	243 (98%)	4 (2%)	0	100	100
1	O	247/250 (99%)	242 (98%)	5 (2%)	0	100	100
2	B	239/258 (93%)	235 (98%)	4 (2%)	0	100	100
2	P	240/258 (93%)	236 (98%)	4 (2%)	0	100	100
3	C	239/254 (94%)	230 (96%)	9 (4%)	0	100	100
3	Q	239/254 (94%)	232 (97%)	7 (3%)	0	100	100
4	D	236/260 (91%)	229 (97%)	7 (3%)	0	100	100
4	R	236/260 (91%)	225 (95%)	11 (5%)	0	100	100
5	E	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
5	S	230/234 (98%)	225 (98%)	5 (2%)	0	100	100
6	F	242/287 (84%)	234 (97%)	8 (3%)	0	100	100
6	T	242/287 (84%)	233 (96%)	9 (4%)	0	100	100
7	G	239/252 (95%)	233 (98%)	6 (2%)	0	100	100
7	U	240/252 (95%)	235 (98%)	5 (2%)	0	100	100
8	H	219/232 (94%)	212 (97%)	7 (3%)	0	100	100
8	V	219/232 (94%)	212 (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	193/198 (98%)	190 (98%)	2 (1%)	1 (0%)	25	58
10	X	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
11	K	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
11	Y	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
12	L	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
12	Z	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
13	M	231/233 (99%)	221 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	231/233 (99%)	223 (96%)	8 (4%)	0	100	100
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
All	All	6283/6586 (95%)	6097 (97%)	185 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	9	VAL

### 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	208/209 (100%)	204 (98%)	4 (2%)	52	76
1	O	208/209 (100%)	199 (96%)	9 (4%)	25	55
2	B	204/216 (94%)	199 (98%)	5 (2%)	42	70
2	P	204/216 (94%)	196 (96%)	8 (4%)	27	59
3	C	213/226 (94%)	208 (98%)	5 (2%)	45	72
3	Q	213/226 (94%)	211 (99%)	2 (1%)	75	88
4	D	198/215 (92%)	195 (98%)	3 (2%)	60	80
4	R	198/215 (92%)	194 (98%)	4 (2%)	50	75
5	E	190/193 (98%)	184 (97%)	6 (3%)	34	64
5	S	189/193 (98%)	178 (94%)	11 (6%)	17	45
6	F	201/238 (84%)	198 (98%)	3 (2%)	60	80
6	T	200/238 (84%)	198 (99%)	2 (1%)	73	87
7	G	206/210 (98%)	204 (99%)	2 (1%)	73	87
7	U	207/210 (99%)	203 (98%)	4 (2%)	52	76
8	H	180/190 (95%)	180 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	V	180/190 (95%)	177 (98%)	3 (2%)	56	78
9	I	172/173 (99%)	169 (98%)	3 (2%)	56	78
9	W	172/173 (99%)	169 (98%)	3 (2%)	56	78
10	J	173/175 (99%)	168 (97%)	5 (3%)	37	67
10	X	173/175 (99%)	166 (96%)	7 (4%)	27	58
11	K	169/169 (100%)	164 (97%)	5 (3%)	36	66
11	Y	169/169 (100%)	165 (98%)	4 (2%)	44	71
12	L	185/185 (100%)	179 (97%)	6 (3%)	34	64
12	Z	185/185 (100%)	181 (98%)	4 (2%)	47	73
13	M	199/199 (100%)	195 (98%)	4 (2%)	50	75
13	a	199/199 (100%)	196 (98%)	3 (2%)	60	80
14	N	162/162 (100%)	159 (98%)	3 (2%)	52	76
14	b	162/162 (100%)	160 (99%)	2 (1%)	67	84
All	All	5319/5520 (96%)	5199 (98%)	120 (2%)	45	72

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	S	176	ASP
11	Y	195	GLU
10	J	2	ASP
11	Y	137	TYR
14	b	85	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
8	H	165	ASN
8	V	91	GLN
14	b	161	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 87 ligands modelled in this entry, 12 are monoatomic - leaving 75 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$
15	SO4	a	304	-	4,4,4	0.68	0	6,6,6	0.07	0
17	A1AU6	V	301	-	23,23,23	1.85	4 (17%)	22,29,29	1.09	1 (4%)
15	SO4	T	302	-	4,4,4	0.67	0	6,6,6	0.10	0
15	SO4	W	303	-	4,4,4	0.69	0	6,6,6	0.17	0
15	SO4	b	204	-	4,4,4	0.70	0	6,6,6	0.08	0
17	A1AU6	K	301	-	23,23,23	1.76	4 (17%)	22,29,29	1.23	1 (4%)
17	A1AU6	H	301	-	23,23,23	1.84	4 (17%)	22,29,29	1.21	3 (13%)
15	SO4	N	203	-	4,4,4	0.70	0	6,6,6	0.10	0
15	SO4	H	304	-	4,4,4	0.68	0	6,6,6	0.10	0
15	SO4	K	305	-	4,4,4	0.71	0	6,6,6	0.10	0
15	SO4	S	304	-	4,4,4	0.69	0	6,6,6	0.09	0
15	SO4	Z	302	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	Z	303	-	4,4,4	0.68	0	6,6,6	0.11	0
17	A1AU6	Y	301	-	23,23,23	1.80	4 (17%)	22,29,29	1.19	3 (13%)
15	SO4	D	301	-	4,4,4	0.69	0	6,6,6	0.10	0
15	SO4	E	303	-	4,4,4	0.69	0	6,6,6	0.09	0
15	SO4	E	304	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	G	302	-	4,4,4	0.69	0	6,6,6	0.12	0
15	SO4	J	203	-	4,4,4	0.68	0	6,6,6	0.08	0
15	SO4	M	301	-	4,4,4	0.69	0	6,6,6	0.07	0
15	SO4	B	303	-	4,4,4	0.68	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	SO4	Z	305	-	4,4,4	0.68	0	6,6,6	0.08	0
15	SO4	T	301	-	4,4,4	0.69	0	6,6,6	0.07	0
15	SO4	S	302	-	4,4,4	0.70	0	6,6,6	0.05	0
15	SO4	Y	304	-	4,4,4	0.69	0	6,6,6	0.11	0
15	SO4	Y	305	-	4,4,4	0.70	0	6,6,6	0.06	0
15	SO4	K	307	-	4,4,4	0.68	0	6,6,6	0.06	0
15	SO4	J	204	-	4,4,4	0.68	0	6,6,6	0.07	0
15	SO4	a	305	-	4,4,4	0.69	0	6,6,6	0.09	0
15	SO4	S	301	-	4,4,4	0.68	0	6,6,6	0.08	0
15	SO4	L	302	-	4,4,4	0.69	0	6,6,6	0.08	0
15	SO4	M	302	-	4,4,4	0.67	0	6,6,6	0.10	0
15	SO4	a	302	-	4,4,4	0.69	0	6,6,6	0.10	0
15	SO4	T	303	-	4,4,4	0.69	0	6,6,6	0.11	0
15	SO4	E	301	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	J	201	-	4,4,4	0.69	0	6,6,6	0.08	0
15	SO4	C	301	-	4,4,4	0.68	0	6,6,6	0.08	0
15	SO4	Y	306	-	4,4,4	0.68	0	6,6,6	0.10	0
15	SO4	P	302	-	4,4,4	0.68	0	6,6,6	0.10	0
15	SO4	W	302	-	4,4,4	0.67	0	6,6,6	0.07	0
15	SO4	V	306	-	4,4,4	0.72	0	6,6,6	0.14	0
15	SO4	b	203	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	Q	301	-	4,4,4	0.68	0	6,6,6	0.08	0
15	SO4	M	306	-	4,4,4	0.68	0	6,6,6	0.08	0
15	SO4	L	303	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	K	303	-	4,4,4	0.69	0	6,6,6	0.10	0
15	SO4	P	301	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	K	304	-	4,4,4	0.68	0	6,6,6	0.11	0
17	A1AU6	N	201	-	23,23,23	1.81	4 (17%)	22,29,29	1.26	4 (18%)
15	SO4	F	301	-	4,4,4	0.69	0	6,6,6	0.14	0
17	A1AU6	b	201	-	23,23,23	1.81	4 (17%)	22,29,29	1.11	2 (9%)
15	SO4	H	303	-	4,4,4	0.67	0	6,6,6	0.11	0
15	SO4	B	301	-	4,4,4	0.68	0	6,6,6	0.10	0
15	SO4	I	302	-	4,4,4	0.69	0	6,6,6	0.11	0
15	SO4	a	301	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	U	302	-	4,4,4	0.69	0	6,6,6	0.11	0
15	SO4	B	302	-	4,4,4	0.69	0	6,6,6	0.07	0
15	SO4	X	201	-	4,4,4	0.68	0	6,6,6	0.07	0
15	SO4	E	302	-	4,4,4	0.68	0	6,6,6	0.08	0
15	SO4	Q	302	-	4,4,4	0.69	0	6,6,6	0.12	0
15	SO4	a	303	-	4,4,4	0.68	0	6,6,6	0.07	0
15	SO4	M	304	-	4,4,4	0.69	0	6,6,6	0.12	0
15	SO4	G	303	-	4,4,4	0.71	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	SO4	N	204	-	4,4,4	0.70	0	6,6,6	0.07	0
15	SO4	K	306	-	4,4,4	0.68	0	6,6,6	0.08	0
15	SO4	V	303	-	4,4,4	0.69	0	6,6,6	0.07	0
15	SO4	F	302	-	4,4,4	0.68	0	6,6,6	0.08	0
15	SO4	V	305	-	4,4,4	0.68	0	6,6,6	0.07	0
15	SO4	Y	303	-	4,4,4	0.69	0	6,6,6	0.10	0
15	SO4	J	202	-	4,4,4	0.68	0	6,6,6	0.08	0
15	SO4	V	304	-	4,4,4	0.68	0	6,6,6	0.08	0
15	SO4	M	303	-	4,4,4	0.69	0	6,6,6	0.09	0
15	SO4	M	305	-	4,4,4	0.70	0	6,6,6	0.10	0
15	SO4	Z	304	-	4,4,4	0.69	0	6,6,6	0.09	0
15	SO4	S	303	-	4,4,4	0.68	0	6,6,6	0.07	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	A1AU6	V	301	-	-	16/33/33/33	-
17	A1AU6	H	301	-	-	17/33/33/33	-
17	A1AU6	Y	301	-	-	17/33/33/33	-
17	A1AU6	b	201	-	-	16/33/33/33	-
17	A1AU6	N	201	-	-	13/33/33/33	-
17	A1AU6	K	301	-	-	17/33/33/33	-

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	V	301	A1AU6	C4-N1	5.57	1.45	1.34
17	H	301	A1AU6	C4-N1	5.49	1.45	1.34
17	b	201	A1AU6	C4-N1	5.47	1.45	1.34
17	Y	301	A1AU6	C4-N1	5.44	1.45	1.34
17	H	301	A1AU6	C7-N2	5.41	1.45	1.34

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	201	A1AU6	C9-C8-N2	-2.87	104.11	110.58
17	H	301	A1AU6	C3-C4-N1	2.81	120.82	115.86
17	b	201	A1AU6	C9-C8-N2	-2.75	104.38	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	201	A1AU6	C3-C4-N1	2.61	120.46	115.86
17	V	301	A1AU6	C3-C4-N1	2.49	120.25	115.86

There are no chirality outliers.

5 of 96 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	301	A1AU6	N1-C5-C6-O2
17	H	301	A1AU6	C7-C5-C6-O2
17	H	301	A1AU6	O4-C13-C8-N2
17	H	301	A1AU6	C8-C13-C14-C16
17	H	301	A1AU6	O4-C13-C14-C16

There are no ring outliers.

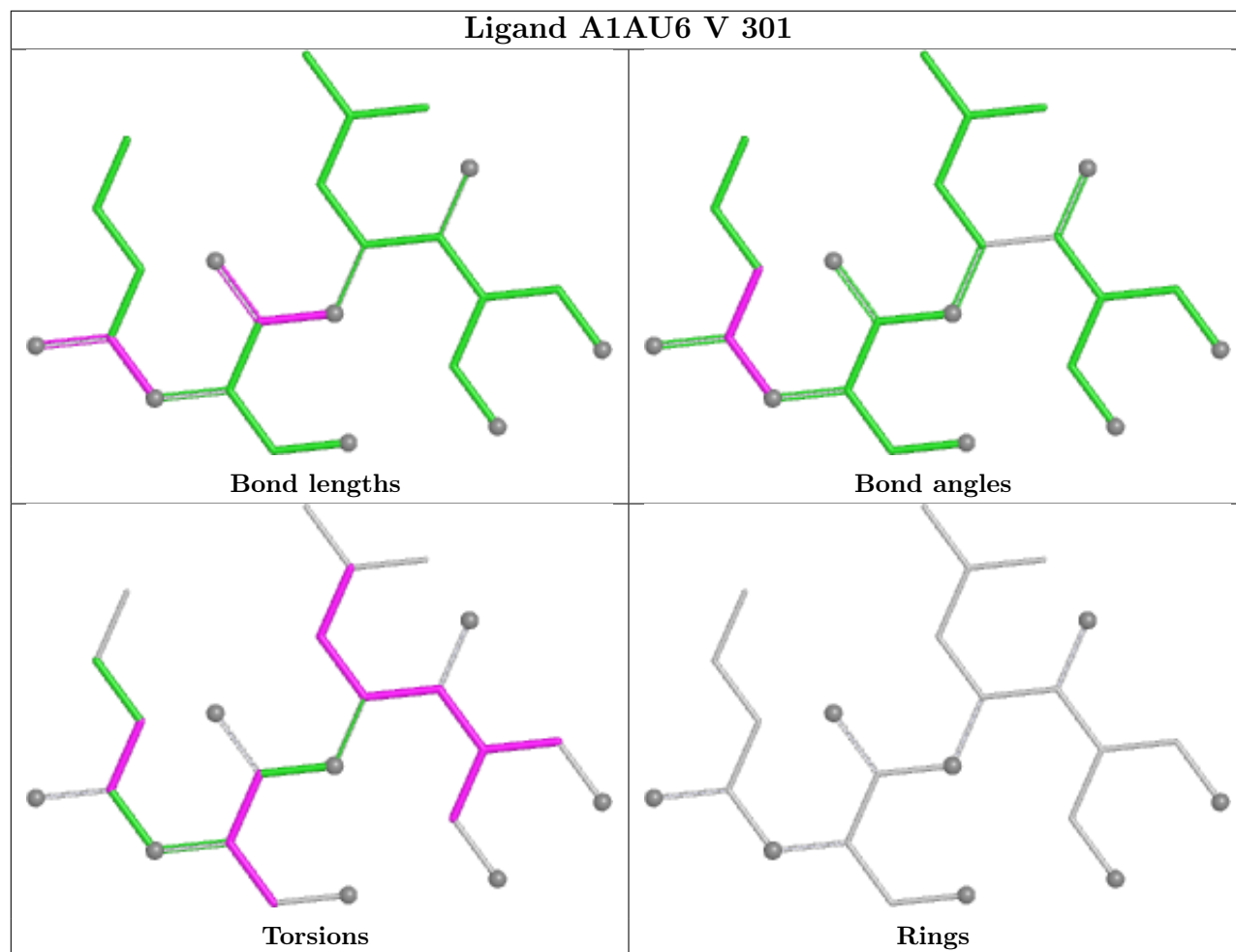
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	V	306	SO4	3	0

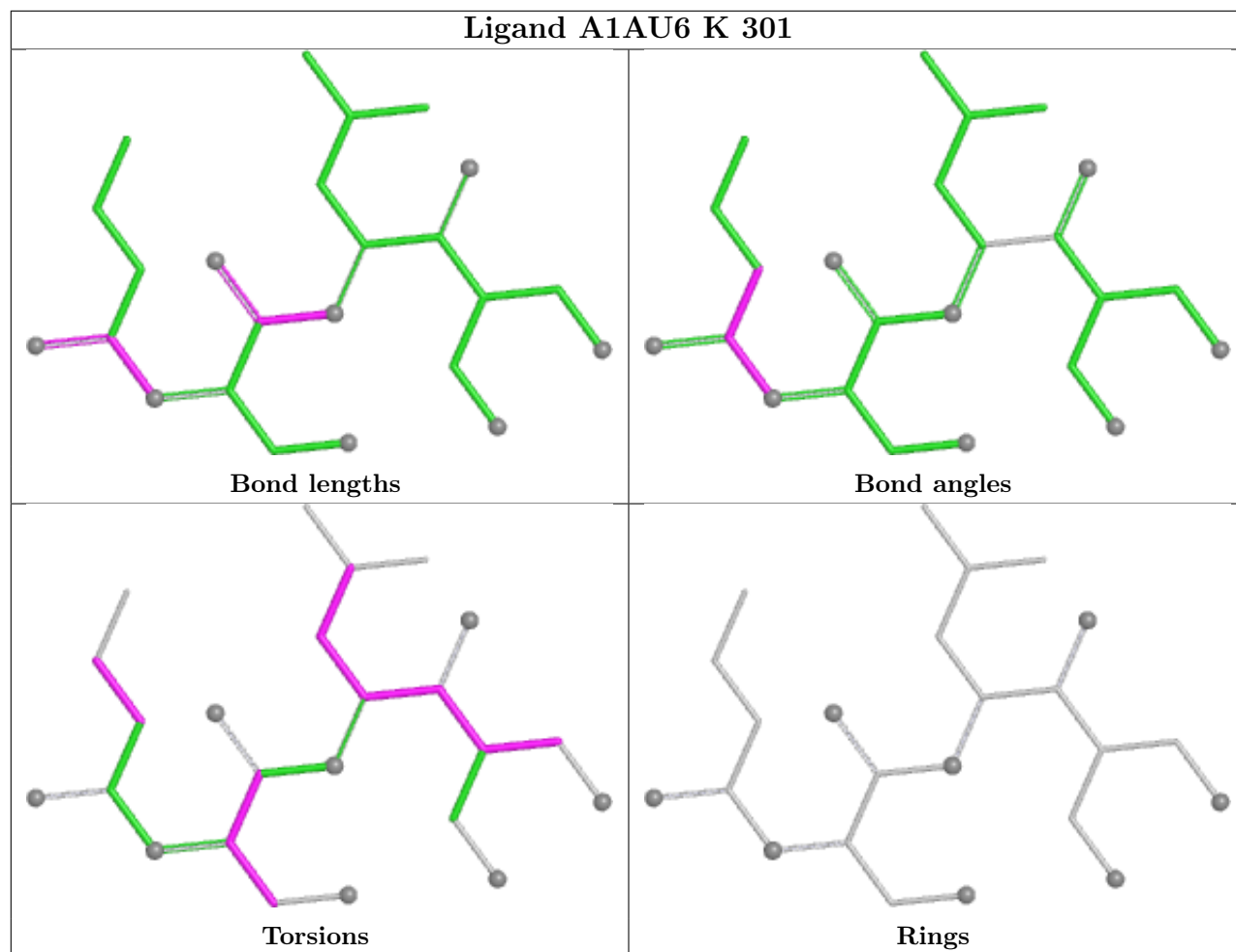
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



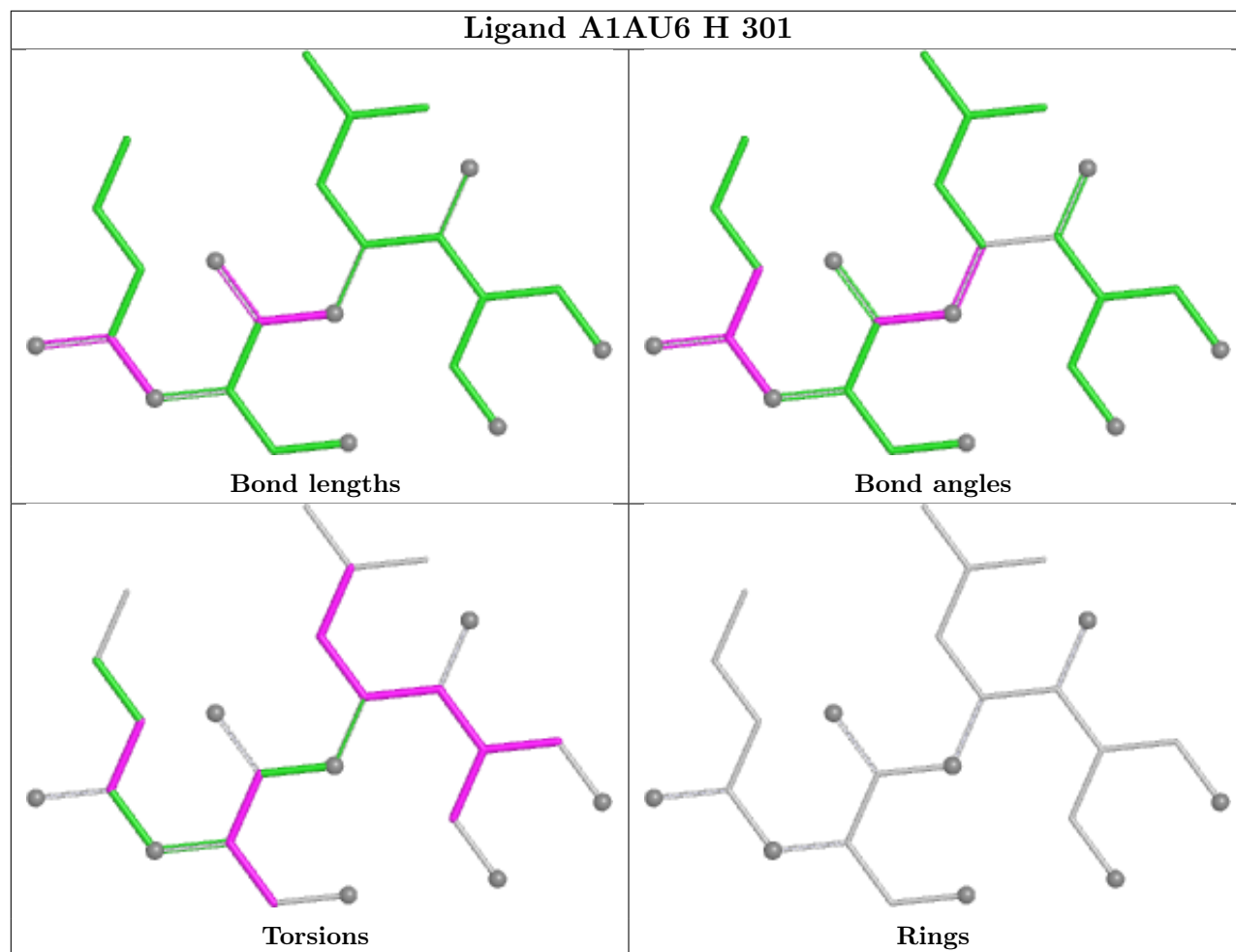
## Ligand A1AU6 V 301



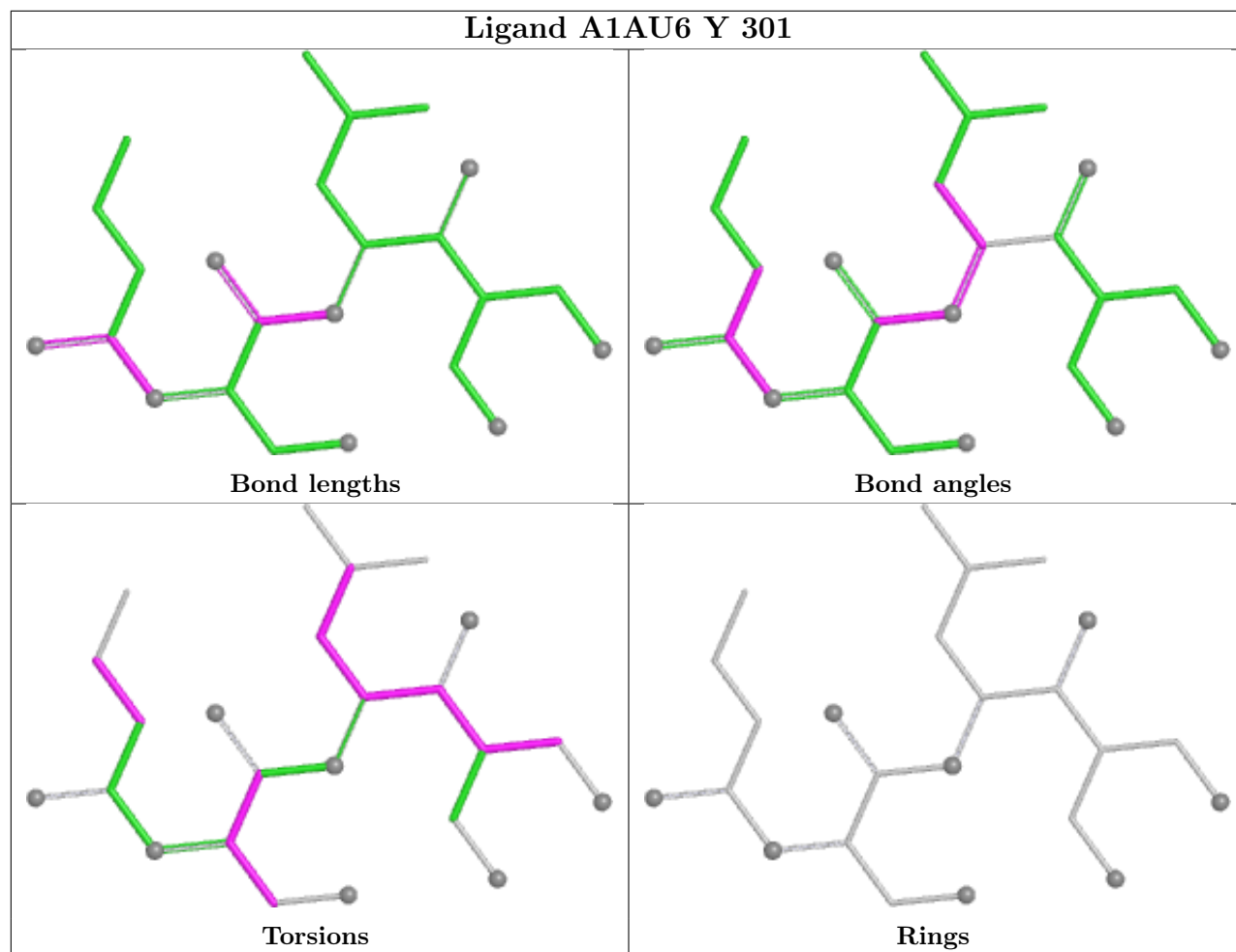
## Ligand A1AU6 K 301



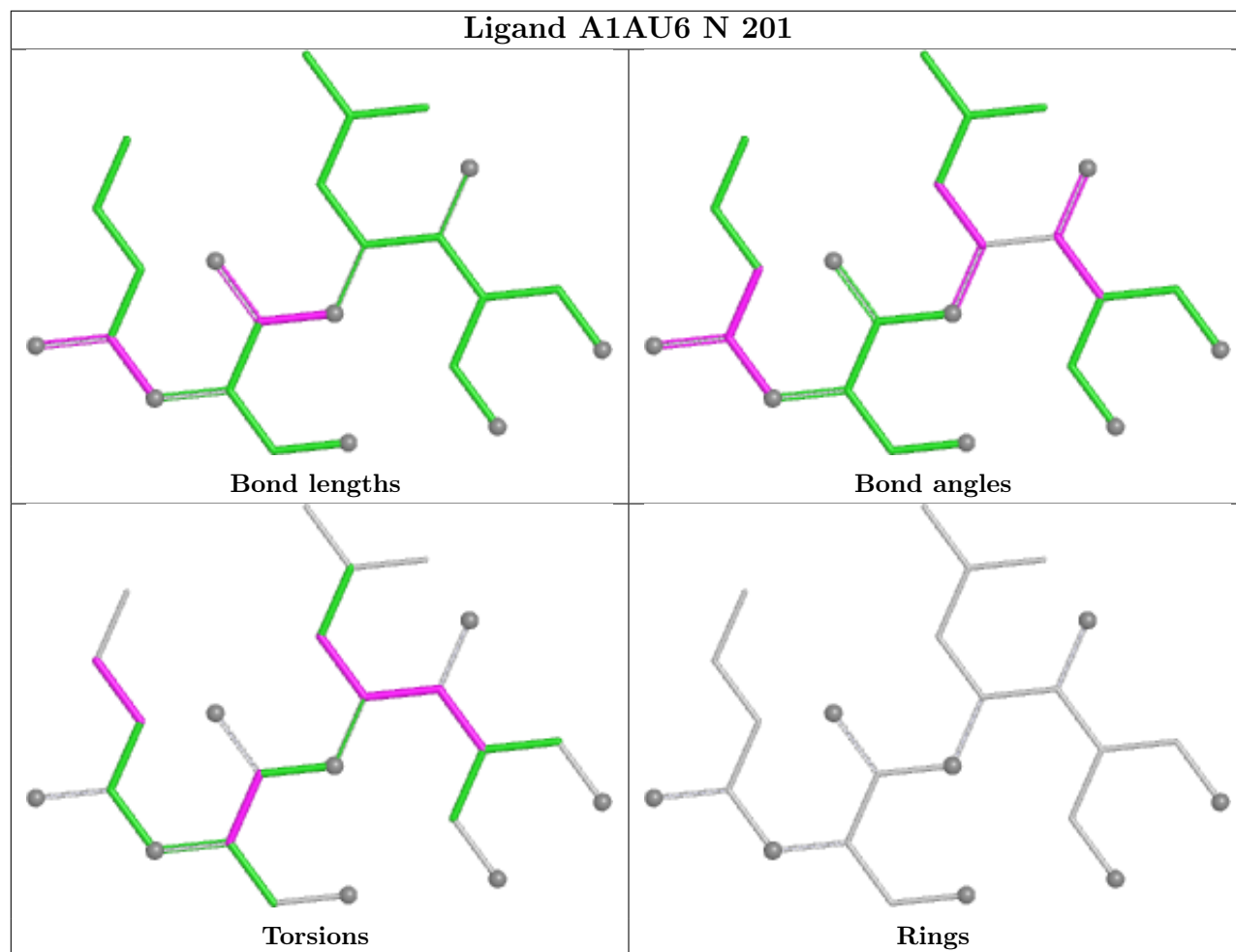
## Ligand A1AU6 H 301

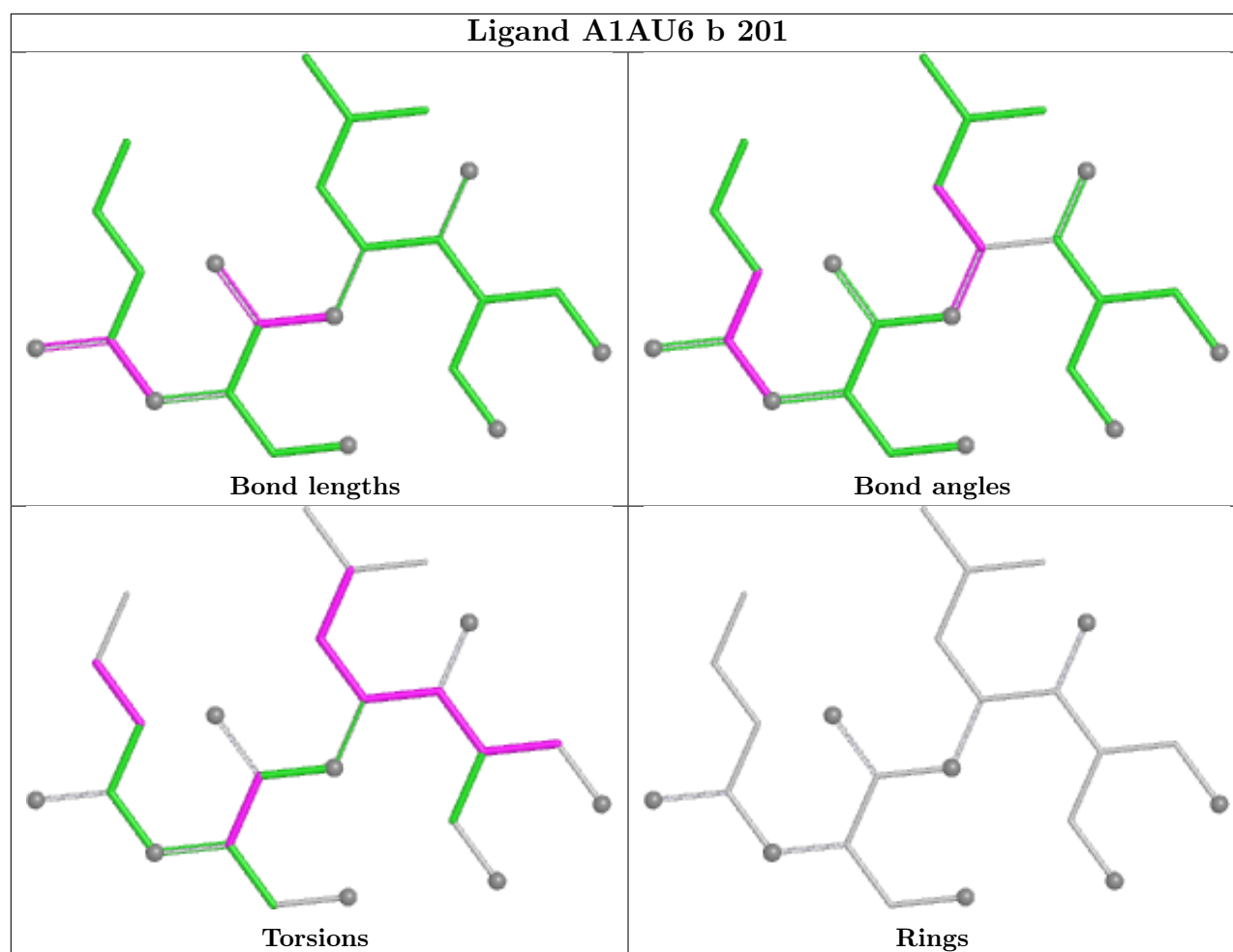


## Ligand A1AU6 Y 301



## Ligand A1AU6 N 201





## 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	249/250 (99%)	-0.41	0 100 100	38, 59, 96, 115	0
1	O	249/250 (99%)	-0.53	0 100 100	37, 55, 90, 126	0
2	B	243/258 (94%)	-0.40	2 (0%) 82 66	34, 63, 98, 116	0
2	P	244/258 (94%)	-0.46	1 (0%) 89 77	36, 58, 96, 116	0
3	C	241/254 (94%)	-0.26	0 100 100	38, 68, 120, 150	0
3	Q	241/254 (94%)	-0.33	2 (0%) 82 66	40, 68, 116, 131	0
4	D	240/260 (92%)	-0.35	0 100 100	34, 64, 93, 129	0
4	R	240/260 (92%)	-0.16	1 (0%) 89 77	42, 73, 105, 121	0
5	E	231/234 (98%)	-0.33	0 100 100	39, 65, 93, 117	0
5	S	232/234 (99%)	-0.17	2 (0%) 81 63	46, 69, 101, 123	0
6	F	244/287 (85%)	-0.40	0 100 100	38, 60, 96, 118	0
6	T	244/287 (85%)	-0.36	0 100 100	42, 62, 103, 126	0
7	G	241/252 (95%)	-0.55	1 (0%) 89 77	39, 57, 87, 113	0
7	U	242/252 (96%)	-0.52	0 100 100	37, 58, 87, 110	0
8	H	221/232 (95%)	-0.54	1 (0%) 87 74	36, 53, 74, 110	0
8	V	221/232 (95%)	-0.67	0 100 100	35, 48, 68, 108	0
9	I	204/205 (99%)	-0.60	1 (0%) 87 74	36, 50, 76, 108	0
9	W	204/205 (99%)	-0.68	0 100 100	33, 46, 72, 108	0
10	J	195/198 (98%)	-0.63	0 100 100	36, 51, 71, 112	0
10	X	195/198 (98%)	-0.66	0 100 100	33, 50, 70, 116	0
11	K	212/212 (100%)	-0.69	0 100 100	36, 48, 70, 97	0
11	Y	212/212 (100%)	-0.60	0 100 100	38, 51, 72, 104	0
12	L	222/222 (100%)	-0.68	0 100 100	32, 44, 67, 89	0
12	Z	222/222 (100%)	-0.57	0 100 100	39, 54, 73, 89	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/233 (100%)	-0.65	0 100 100	31, 48, 71, 84	0
13	a	233/233 (100%)	-0.60	0 100 100	38, 52, 77, 92	0
14	N	196/196 (100%)	-0.66	0 100 100	35, 50, 76, 103	0
14	b	196/196 (100%)	-0.68	0 100 100	38, 49, 75, 94	0
All	All	6347/6586 (96%)	-0.50	11 (0%) 92 84	31, 56, 93, 150	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	S	233	ILE	3.0
4	R	243	SER	2.8
3	Q	50	LEU	2.6
8	H	120	ASP	2.6
2	B	246	LYS	2.5

## 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	SO4	Q	302	5/5	0.68	0.15	74,77,112,133	5
15	SO4	B	301	5/5	0.69	0.16	118,120,136,160	0
15	SO4	Z	303	5/5	0.73	0.17	98,100,136,140	0
15	SO4	Y	303	5/5	0.76	0.19	67,91,95,131	0
15	SO4	Z	302	5/5	0.78	0.19	108,109,143,153	0
15	SO4	S	302	5/5	0.80	0.19	54,61,71,93	5
15	SO4	J	202	5/5	0.82	0.15	80,87,100,121	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	SO4	B	302	5/5	0.82	0.14	78,83,111,122	5
15	SO4	G	303	5/5	0.82	0.15	69,76,102,124	5
15	SO4	T	303	5/5	0.82	0.28	97,117,131,148	0
15	SO4	P	301	5/5	0.83	0.17	67,76,110,121	5
15	SO4	a	305	5/5	0.83	0.13	57,75,103,123	0
15	SO4	a	301	5/5	0.84	0.18	81,86,97,106	5
15	SO4	b	204	5/5	0.84	0.17	59,66,79,102	5
15	SO4	V	304	5/5	0.85	0.18	50,55,68,86	5
15	SO4	V	306	5/5	0.85	0.22	76,87,92,141	0
15	SO4	K	304	5/5	0.85	0.19	108,112,127,130	0
15	SO4	M	304	5/5	0.85	0.10	68,71,95,124	0
15	SO4	M	301	5/5	0.86	0.15	49,65,78,88	5
15	SO4	D	301	5/5	0.86	0.21	95,99,118,141	0
16	MG	I	301	1/1	0.86	0.19	63,63,63,63	0
17	A1AU6	V	301	24/24	0.86	0.15	55,67,75,84	0
15	SO4	S	303	5/5	0.87	0.14	97,100,107,128	5
15	SO4	E	303	5/5	0.87	0.17	59,84,91,117	5
15	SO4	F	302	5/5	0.87	0.20	95,103,123,139	0
17	A1AU6	H	301	24/24	0.87	0.16	44,67,84,87	0
15	SO4	E	302	5/5	0.87	0.19	60,62,68,83	5
15	SO4	H	304	5/5	0.88	0.13	69,70,81,99	5
15	SO4	Z	304	5/5	0.88	0.17	95,96,111,140	0
15	SO4	S	304	5/5	0.88	0.15	70,76,80,90	5
15	SO4	N	204	5/5	0.88	0.17	63,63,88,111	5
15	SO4	K	303	5/5	0.88	0.14	53,57,71,94	5
15	SO4	E	301	5/5	0.88	0.14	81,82,84,107	5
15	SO4	L	302	5/5	0.88	0.20	57,66,81,101	5
15	SO4	L	303	5/5	0.88	0.14	71,87,95,108	5
15	SO4	a	303	5/5	0.89	0.17	89,91,117,122	0
15	SO4	Y	304	5/5	0.89	0.18	91,95,109,128	0
15	SO4	Y	306	5/5	0.89	0.22	113,119,139,155	0
15	SO4	T	302	5/5	0.90	0.21	55,78,94,101	5
15	SO4	M	303	5/5	0.90	0.17	68,73,118,123	0
15	SO4	U	302	5/5	0.90	0.16	83,87,106,135	0
15	SO4	M	305	5/5	0.90	0.23	81,90,98,122	0
15	SO4	a	302	5/5	0.91	0.14	79,87,103,129	0
15	SO4	V	303	5/5	0.91	0.13	51,51,77,84	5
15	SO4	F	301	5/5	0.91	0.20	58,88,118,136	0
15	SO4	K	307	5/5	0.91	0.12	74,75,95,113	5
15	SO4	M	306	5/5	0.91	0.17	68,72,100,102	5
15	SO4	Z	305	5/5	0.91	0.18	102,118,128,148	0
17	A1AU6	N	201	24/24	0.91	0.12	35,49,61,68	0

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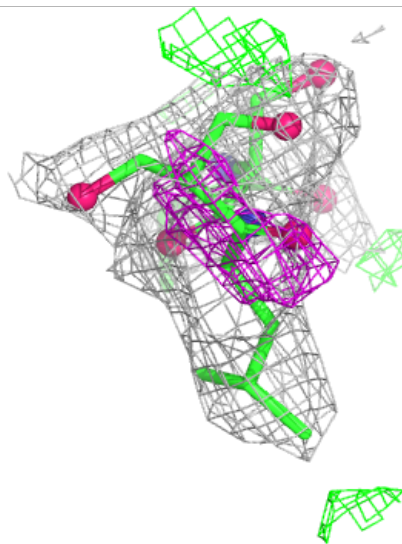
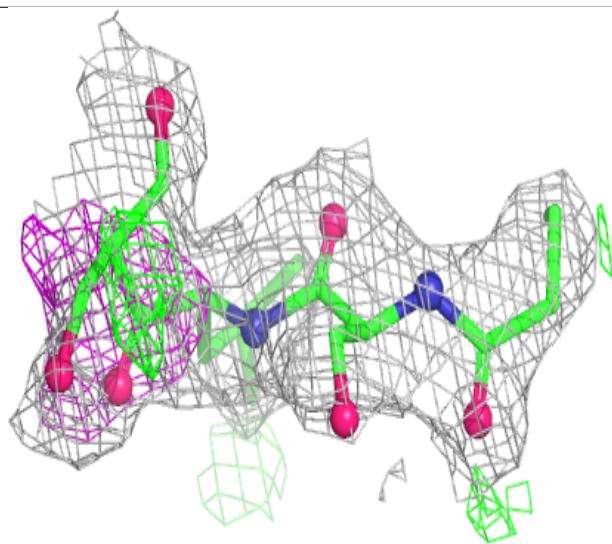
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	SO4	C	301	5/5	0.91	0.10	71,77,105,113	5
15	SO4	J	204	5/5	0.92	0.10	51,63,72,91	5
15	SO4	Y	305	5/5	0.92	0.15	68,80,95,126	0
15	SO4	G	302	5/5	0.92	0.13	60,61,87,112	5
15	SO4	b	203	5/5	0.92	0.12	45,47,63,76	5
15	SO4	I	302	5/5	0.92	0.14	59,61,85,105	5
15	SO4	K	305	5/5	0.92	0.12	59,71,95,119	0
15	SO4	V	305	5/5	0.92	0.09	62,66,73,94	5
15	SO4	K	306	5/5	0.92	0.14	78,94,115,137	0
15	SO4	H	303	5/5	0.92	0.20	56,59,66,68	5
17	A1AU6	b	201	24/24	0.92	0.13	42,50,65,68	0
15	SO4	N	203	5/5	0.93	0.10	48,50,58,81	5
15	SO4	E	304	5/5	0.93	0.10	68,72,76,88	5
17	A1AU6	K	301	24/24	0.93	0.12	33,44,65,74	0
15	SO4	P	302	5/5	0.94	0.10	42,49,67,72	5
15	SO4	J	201	5/5	0.94	0.14	48,66,73,94	5
15	SO4	W	303	5/5	0.94	0.11	44,47,96,120	5
15	SO4	X	201	5/5	0.94	0.11	39,47,72,78	5
15	SO4	S	301	5/5	0.94	0.22	63,63,79,83	5
17	A1AU6	Y	301	24/24	0.94	0.11	39,56,68,72	0
15	SO4	M	302	5/5	0.94	0.11	57,61,69,84	5
15	SO4	a	304	5/5	0.95	0.14	54,55,75,77	5
15	SO4	Q	301	5/5	0.95	0.10	64,66,70,90	5
15	SO4	T	301	5/5	0.95	0.12	55,58,81,102	5
15	SO4	W	302	5/5	0.95	0.10	44,55,64,67	5
15	SO4	J	203	5/5	0.95	0.11	44,55,59,67	5
16	MG	L	301	1/1	0.95	0.06	43,43,43,43	0
16	MG	G	301	1/1	0.96	0.07	54,54,54,54	0
16	MG	Y	302	1/1	0.96	0.04	52,52,52,52	1
16	MG	Z	301	1/1	0.96	0.12	62,62,62,62	0
16	MG	b	202	1/1	0.96	0.08	49,49,49,49	0
15	SO4	B	303	5/5	0.96	0.11	45,46,60,70	5
16	MG	U	301	1/1	0.97	0.08	64,64,64,64	0
16	MG	N	202	1/1	0.97	0.10	50,50,50,50	0
16	MG	W	301	1/1	0.97	0.05	44,44,44,44	0
16	MG	K	302	1/1	0.97	0.08	63,63,63,63	0
16	MG	H	302	1/1	0.98	0.07	73,73,73,73	0
16	MG	V	302	1/1	0.98	0.05	49,49,49,49	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.

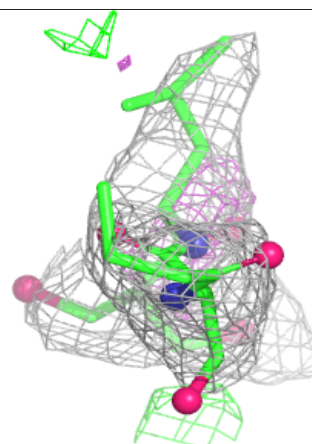
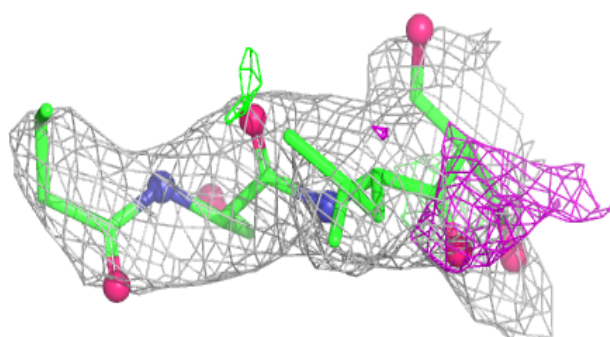
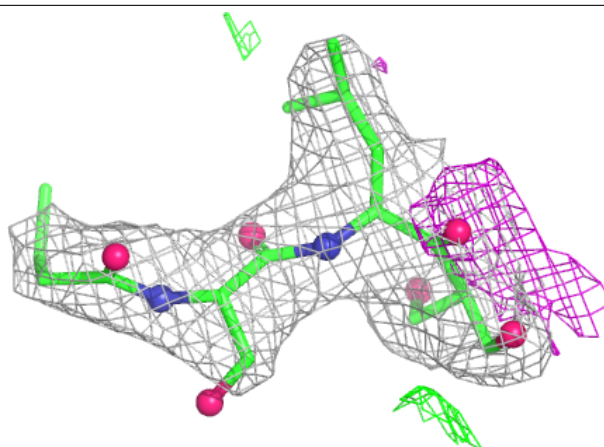
**Electron density around A1AU6 V 301:**

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

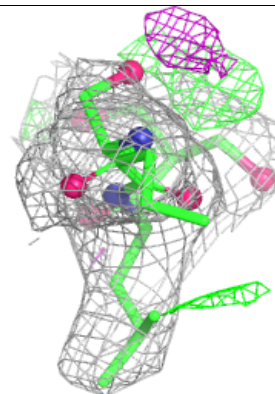
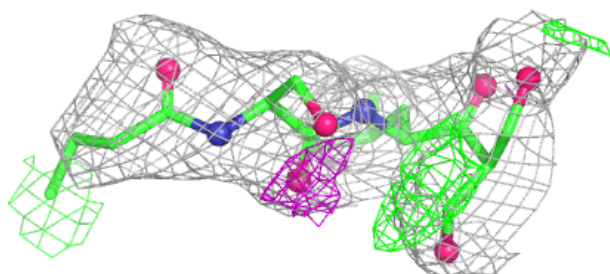
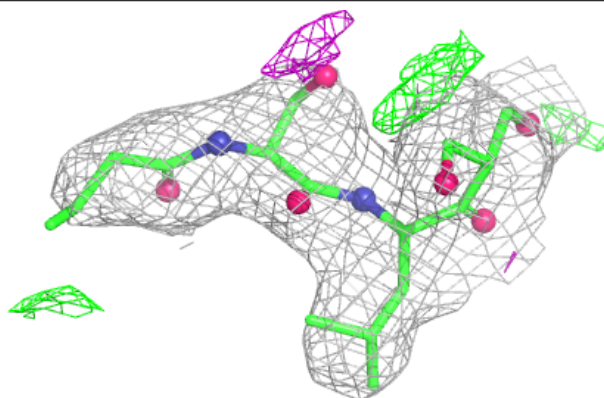


**Electron density around A1AU6 H 301:**

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

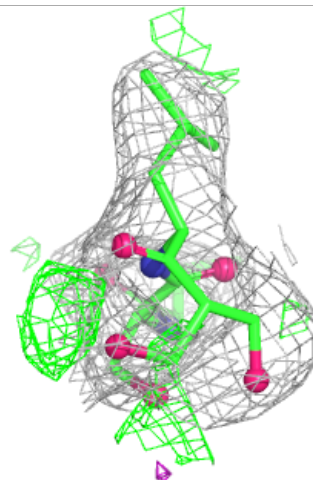
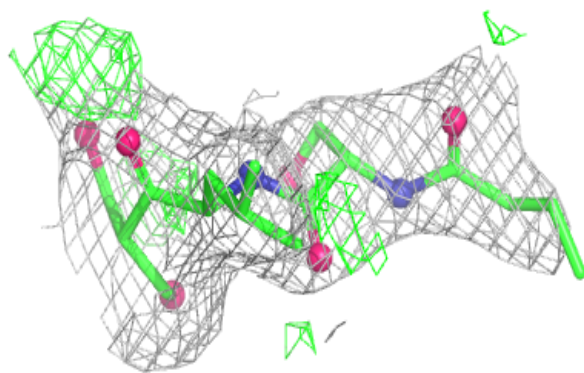
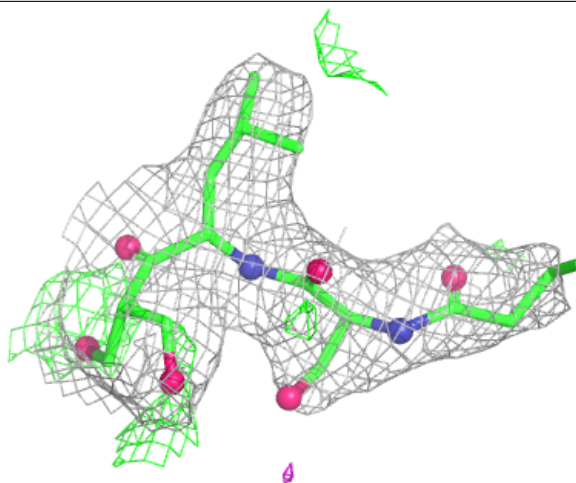
**Electron density around A1AU6 N 201:**

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



**Electron density around A1AU6 b 201:**

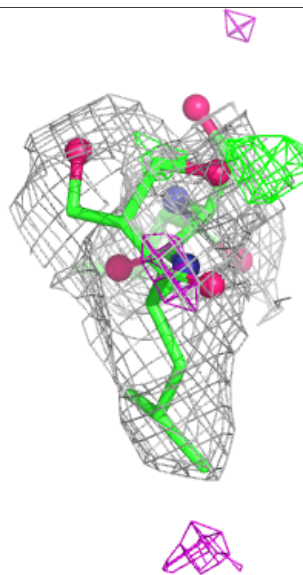
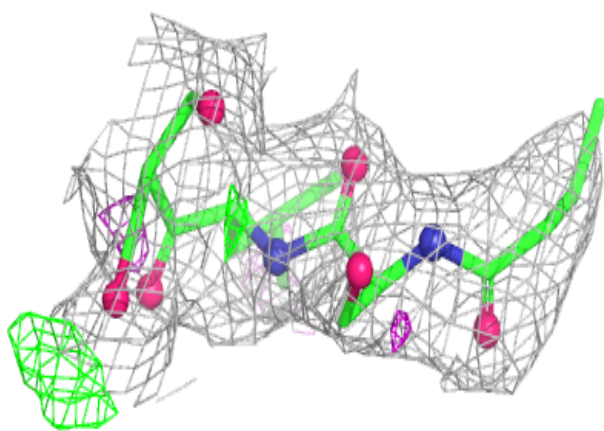
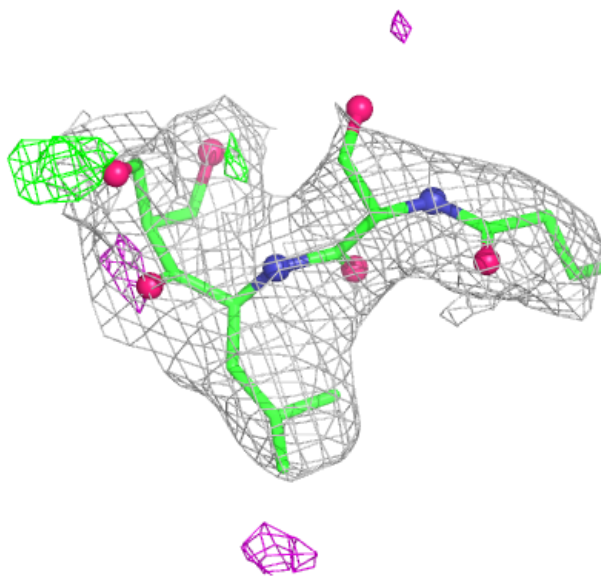
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





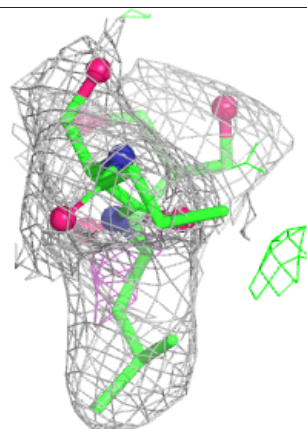
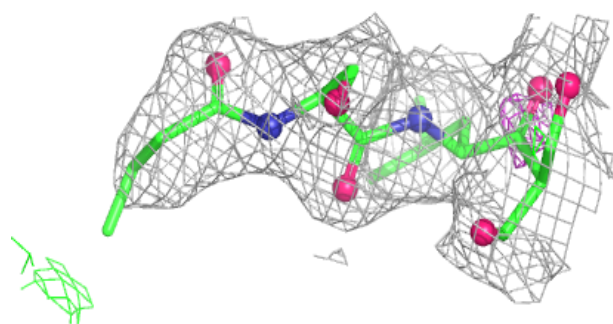
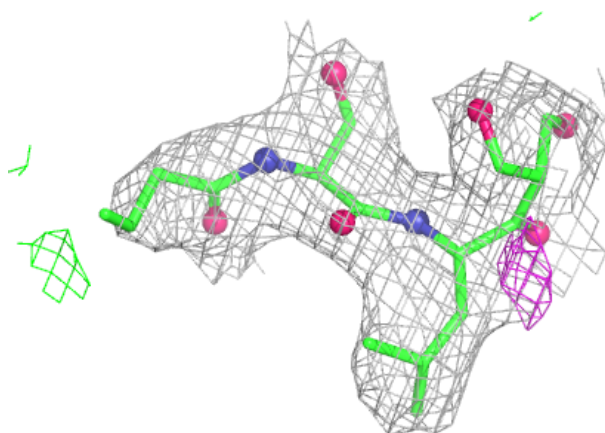
**Electron density around A1AU6 K 301:**

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



**Electron density around A1AU6 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.