



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:26 am BST

PDB ID : 4QVQ  
Title : yCP beta5-M45I mutant in complex with bortezomib  
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.  
Deposited on : 2014-07-15  
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

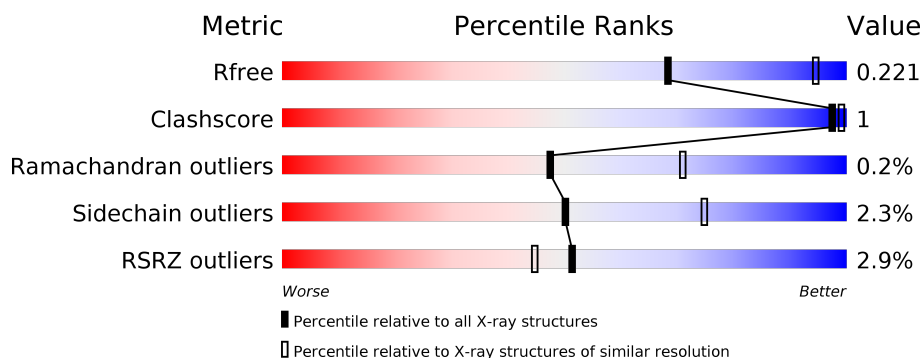
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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






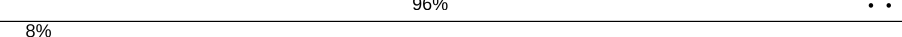
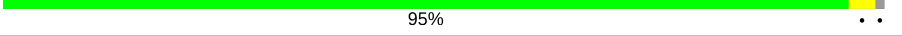

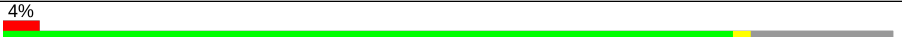
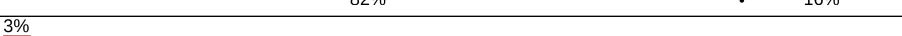



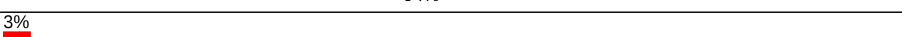
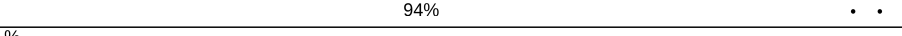
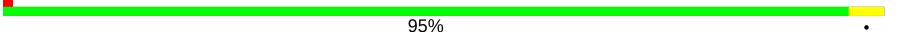
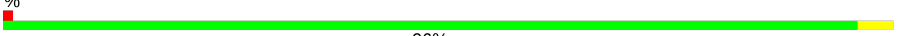





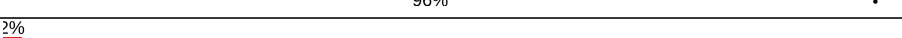
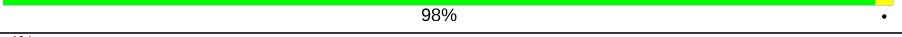
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	250	<div> <div>2%</div> <div> <div></div> <div>98%</div> <div></div> </div> <div></div> </div>
1	O	250	<div> <div>3%</div> <div> <div></div> <div>98%</div> <div></div> </div> <div></div> </div>
2	B	258	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div></div> </div> <div>5%</div> </div>
2	P	258	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div></div> </div> <div>5%</div> </div>
3	C	254	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div></div> </div> <div>5% • 6%</div> </div>
3	Q	254	<div> <div>10%</div> <div> <div></div> <div>88%</div> <div></div> </div> <div>6% • 6%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 50050 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			
8	V	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	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	1046	280	312	6			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1046	280	312	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	45	ILE	MET	ENGINEERED MUTATION	UNP P30656
Y	45	ILE	MET	ENGINEERED MUTATION	UNP P30656

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

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

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

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

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

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

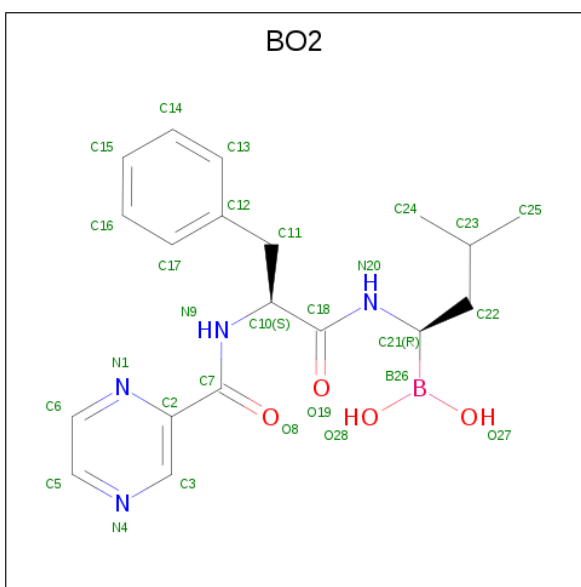
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 17 is N-[(1R)-1-(DIHYDROXYBORYL)-3-METHYLBUTYL]-N-(PYRAZIN-2-YLCARBONYL)-L-PHENYLALANINAMIDE (three-letter code: BO2) (formula: C<sub>19</sub>H<sub>25</sub>BN<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	H	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
17	K	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
17	N	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
17	V	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
17	Y	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
17	b	1	Total	B	C	N	O	0	0
			28	1	19	4	4		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	20	Total	O	0	0
			20	20		
18	B	15	Total	O	0	0
			15	15		
18	C	20	Total	O	0	0
			20	20		
18	D	7	Total	O	0	0
			7	7		
18	E	6	Total	O	0	0
			6	6		
18	F	18	Total	O	0	0
			18	18		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	G	24	Total O 24 24	0	0
18	H	38	Total O 38 38	0	0
18	I	17	Total O 17 17	0	0
18	J	17	Total O 17 17	0	0
18	K	25	Total O 25 25	0	0
18	L	29	Total O 29 29	0	0
18	M	29	Total O 29 29	0	0
18	N	15	Total O 15 15	0	0
18	O	9	Total O 9 9	0	0
18	P	12	Total O 12 12	0	0
18	Q	10	Total O 10 10	0	0
18	R	7	Total O 7 7	0	0
18	S	6	Total O 6 6	0	0
18	T	11	Total O 11 11	0	0
18	U	18	Total O 18 18	0	0
18	V	18	Total O 18 18	0	0
18	W	18	Total O 18 18	0	0
18	X	17	Total O 17 17	0	0
18	Y	18	Total O 18 18	0	0
18	Z	24	Total O 24 24	0	0
18	a	34	Total O 34 34	0	0

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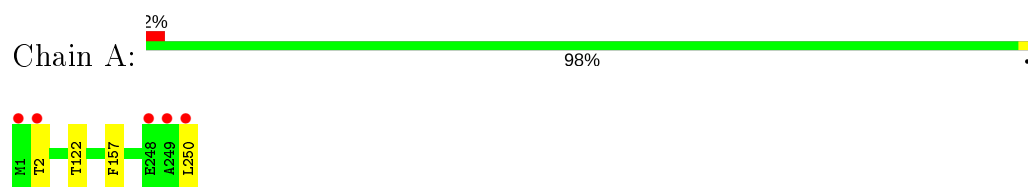
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	b	21	Total	O	0	0
			21	21		

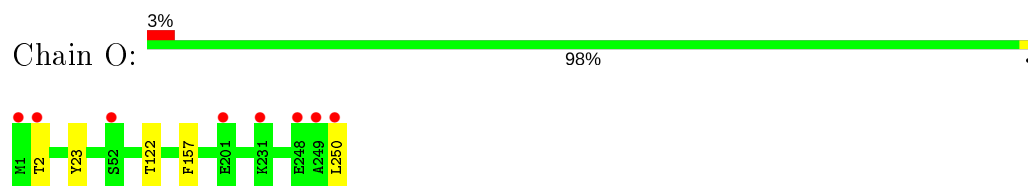
### 3 Residue-property plots [i](#)

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

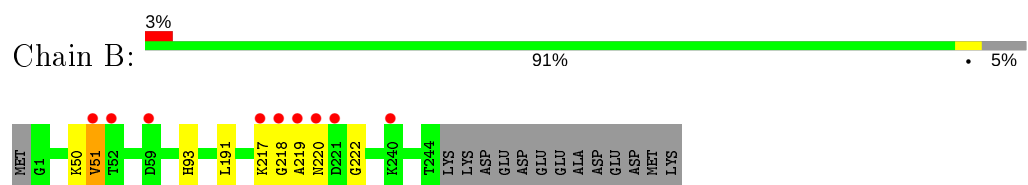
- Molecule 1: Proteasome subunit alpha type-2



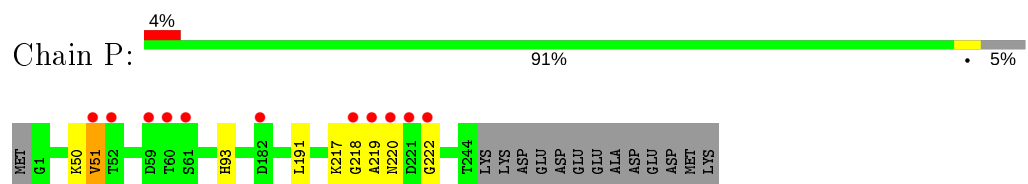
- Molecule 1: Proteasome subunit alpha type-2



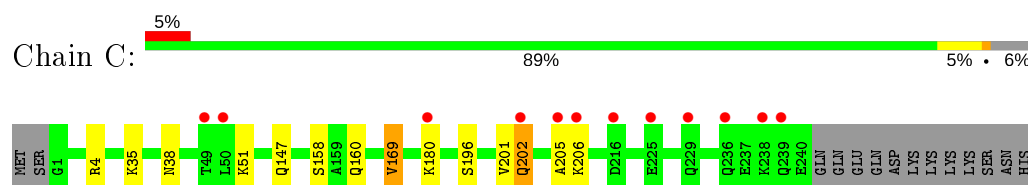
- Molecule 2: Proteasome subunit alpha type-3



- Molecule 2: Proteasome subunit alpha type-3

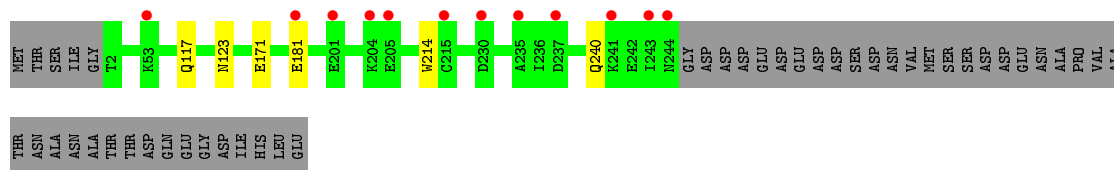
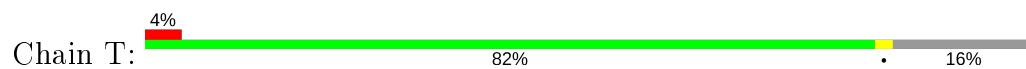


- Molecule 3: Proteasome subunit alpha type-4

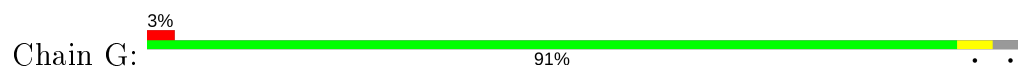


- Molecule 3: Proteasome subunit alpha type-4

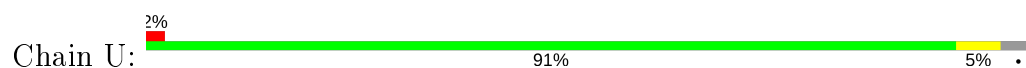




- Molecule 7: Proteasome subunit alpha type-1



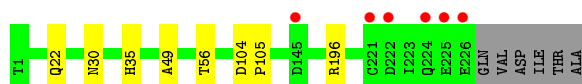
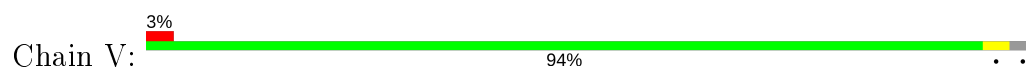
- Molecule 7: Proteasome subunit alpha type-1



- Molecule 8: Proteasome subunit beta type-2



- Molecule 8: Proteasome subunit beta type-2



- Molecule 9: Proteasome subunit beta type-3

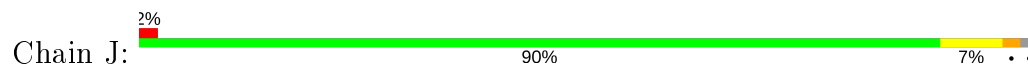


- Molecule 9: Proteasome subunit beta type-3

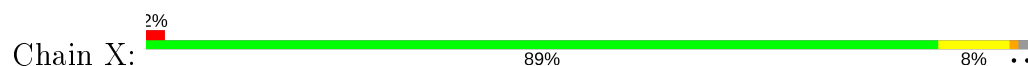




- Molecule 10: Proteasome subunit beta type-4



- Molecule 10: Proteasome subunit beta type-4



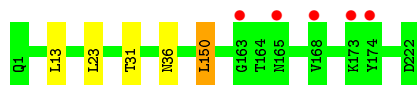
- Molecule 11: Proteasome subunit beta type-5



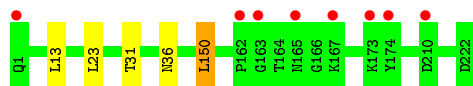
- Molecule 11: Proteasome subunit beta type-5



- Molecule 12: Proteasome subunit beta type-6



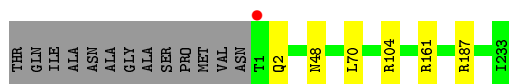
- Molecule 12: Proteasome subunit beta type-6



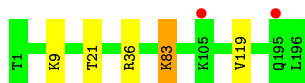
- Molecule 13: Proteasome subunit beta type-7



- 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, $\alpha$ , $\beta$ , $\gamma$	136.67Å 300.62Å 145.52Å 90.00° 113.19° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 15.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (15.00-2.60) 99.1 (15.00-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.195 , 0.219 0.200 , 0.221	Depositor DCC
$R_{free}$ test set	16249 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.5	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 31.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	50050	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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: BO2, MG, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.27	0/1952	0.45	0/2642
1	O	0.27	0/1952	0.45	0/2642
2	B	0.27	0/1934	0.47	0/2618
2	P	0.27	0/1934	0.47	0/2618
3	C	0.27	0/1910	0.49	0/2586
3	Q	0.27	0/1910	0.48	0/2586
4	D	0.27	0/1837	0.45	0/2475
4	R	0.26	0/1837	0.45	0/2475
5	E	0.27	0/1800	0.45	0/2433
5	S	0.27	0/1800	0.45	0/2433
6	F	0.27	0/1932	0.44	0/2609
6	T	0.27	0/1932	0.44	0/2609
7	G	0.27	0/1945	0.46	0/2634
7	U	0.27	0/1945	0.45	0/2634
8	H	0.25	0/1750	0.45	0/2373
8	V	0.25	0/1750	0.46	0/2373
9	I	0.27	0/1611	0.47	0/2174
9	W	0.27	0/1611	0.47	0/2174
10	J	0.35	0/1589	0.48	0/2142
10	X	0.37	0/1589	0.48	0/2142
11	K	0.26	0/1681	0.48	0/2275
11	Y	0.26	0/1681	0.51	2/2275 (0.1%)
12	L	0.27	0/1795	0.46	0/2420
12	Z	0.27	0/1795	0.46	0/2420
13	M	0.27	0/1855	0.49	0/2514
13	a	0.27	0/1855	0.49	0/2514
14	N	0.26	0/1541	0.46	0/2087
14	b	0.26	0/1541	0.45	0/2087
All	All	0.27	0/50264	0.47	2/67964 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	116	ASP	CB-CG-OD1	-5.33	113.50	118.30
11	Y	116	ASP	CB-CG-OD2	5.25	123.02	118.30

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	1915	0	1929	0	0
1	O	1915	0	1929	1	0
2	B	1904	0	1904	3	0
2	P	1904	0	1904	3	0
3	C	1881	0	1895	4	0
3	Q	1881	0	1895	5	0
4	D	1813	0	1797	0	0
4	R	1813	0	1797	1	0
5	E	1773	0	1775	1	0
5	S	1773	0	1775	2	0
6	F	1892	0	1883	0	0
6	T	1892	0	1883	0	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	4	0
8	H	1719	0	1718	5	0
8	V	1719	0	1718	4	0
9	I	1581	0	1574	5	0
9	W	1581	0	1574	4	0
10	J	1561	0	1569	14	0
10	X	1561	0	1569	11	0
11	K	1644	0	1596	5	0
11	Y	1644	0	1596	4	0
12	L	1757	0	1711	2	0
12	Z	1757	0	1711	2	0
13	M	1824	0	1832	2	0
13	a	1824	0	1832	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	N	1512	0	1480	2	0
14	b	1512	0	1480	0	0
15	G	1	0	0	0	0
15	I	1	0	0	0	0
15	J	1	0	0	0	0
15	K	2	0	0	0	0
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	N	1	0	0	0	0
16	U	1	0	0	0	0
16	b	1	0	0	0	0
17	H	28	0	25	1	0
17	K	28	0	25	1	0
17	N	28	0	25	1	0
17	V	28	0	25	1	0
17	Y	28	0	25	0	0
17	b	28	0	25	0	0
18	A	20	0	0	0	0
18	B	15	0	0	1	0
18	C	20	0	0	0	0
18	D	7	0	0	0	0
18	E	6	0	0	0	0
18	F	18	0	0	0	0
18	G	24	0	0	0	0
18	H	38	0	0	0	0
18	I	17	0	0	0	0
18	J	17	0	0	0	0
18	K	25	0	0	0	0
18	L	29	0	0	0	0
18	M	29	0	0	1	0
18	N	15	0	0	0	0
18	O	9	0	0	0	0
18	P	12	0	0	1	0
18	Q	10	0	0	0	0
18	R	7	0	0	0	0
18	S	6	0	0	0	0
18	T	11	0	0	0	0
18	U	18	0	0	0	0
18	V	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	W	18	0	0	0	0
18	X	17	0	0	1	0
18	Y	18	0	0	0	0
18	Z	24	0	0	0	0
18	a	34	0	0	0	0
18	b	21	0	0	0	0
All	All	50050	0	49278	74	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (74) 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)
10:J:152:MET:HE3	10:J:156:GLU:HB3	1.55	0.85
10:J:149:ARG:HG3	10:J:149:ARG:HH21	1.41	0.84
10:X:149:ARG:O	10:X:152:MET:HG3	1.77	0.83
10:J:149:ARG:HG3	10:J:149:ARG:NH2	1.98	0.75
10:J:149:ARG:O	10:J:152:MET:HG3	1.91	0.70
10:X:152:MET:HE3	10:X:156:GLU:HB3	1.72	0.70
10:J:149:ARG:CG	10:J:149:ARG:HH21	2.12	0.60
8:V:49:ALA:HA	17:V:301:BO2:H241	1.84	0.59
8:H:49:ALA:HA	17:H:301:BO2:H241	1.84	0.58
10:J:152:MET:HE3	10:J:156:GLU:CB	2.29	0.58
10:J:139:TYR:OH	10:X:25:ILE:O	2.25	0.54
10:J:25:ILE:O	10:X:139:TYR:OH	2.26	0.53
11:K:209:ASN:O	9:W:38:LYS:NZ	2.41	0.53
10:X:25:ILE:HD11	11:Y:134:THR:HG21	1.93	0.51
3:C:201:VAL:O	3:C:202:GLN:HB3	2.10	0.51
9:I:38:LYS:NZ	11:Y:209:ASN:O	2.43	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.59	0.51
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.10	0.51
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.93	0.50
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.94	0.50
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.94	0.49
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.59	0.49
10:J:50:ALA:O	11:K:91:LYS:NZ	2.46	0.49
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.94	0.49
2:B:217:LYS:O	2:B:219:ALA:N	2.45	0.48
10:J:25:ILE:HD11	11:K:134:THR:HG21	1.95	0.48
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.80	0.47
10:X:174:MET:HB2	18:X:208:HOH:O	2.15	0.47
2:P:93:HIS:HB3	18:P:301:HOH:O	2.14	0.47
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.95	0.46
2:B:93:HIS:HB3	18:B:301:HOH:O	2.16	0.46
2:P:217:LYS:O	2:P:219:ALA:N	2.46	0.46
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.79	0.46
13:M:2:GLN:NE2	18:M:329:HOH:O	2.48	0.45
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.52	0.45
11:K:45:ILE:HB	11:K:52:CYS:HB3	1.98	0.45
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.99	0.45
7:G:23:PHE:O	7:G:26:THR:HB	2.17	0.44
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.00	0.44
8:H:35:HIS:CB	8:H:56:THR:HG21	2.47	0.44
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.47	0.44
11:Y:45:ILE:HB	11:Y:52:CYS:HB3	1.99	0.44
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.49	0.44
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	2.00	0.44
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.00	0.44
7:U:23:PHE:O	7:U:26:THR:HB	2.18	0.44
3:C:35:LYS:HG2	3:C:158:SER:O	2.17	0.43
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.99	0.43
8:V:35:HIS:CB	8:V:56:THR:HG21	2.47	0.43
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.47	0.43
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.00	0.43
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.18	0.43
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.00	0.43
9:W:36:SER:HB2	10:X:126:VAL:HG11	2.00	0.43
3:C:169:VAL:HG23	3:C:196:SER:HB2	2.00	0.43
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.00	0.43
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.00	0.43
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.00	0.43
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.49	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.42
2:P:50:LYS:O	2:P:51:VAL:C	2.57	0.42
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.50	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.50	0.42
5:S:77:ALA:N	5:S:78:PRO:CD	2.83	0.42
5:E:77:ALA:N	5:E:78:PRO:CD	2.83	0.41
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:LYS:O	2:B:51:VAL:C	2.58	0.41
11:K:1:THR:OG1	17:K:301:BO2:C22	2.69	0.41
14:N:21:THR:O	17:N:201:BO2:H3	2.21	0.41
8:H:196:ARG:NH2	9:I:150:GLU:O	2.54	0.41
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.03	0.41
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	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%)	239 (96%)	8 (3%)	1 (0%)	34	57
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	34	57
2	B	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	9	18
2	P	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	9	18
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	19	39
3	Q	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	19	39
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
4	R	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
6	F	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
6	T	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
7	G	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
7	U	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
8	H	224/232 (97%)	219 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	V	224/232 (97%)	219 (98%)	5 (2%)	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%)	189 (98%)	4 (2%)	0	100	100
10	X	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
11	K	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
11	Y	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
12	L	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
13	M	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
13	a	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6284/6614 (95%)	6127 (98%)	143 (2%)	14 (0%)	47	71

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	218	GLY
3	C	202	GLN
2	P	51	VAL
2	P	218	GLY
3	Q	202	GLN
2	B	222	GLY
2	P	222	GLY
1	A	2	THR
1	O	2	THR
2	B	220	ASN
2	P	220	ASN
3	C	205	ALA
3	Q	205	ALA

### 5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	206 (99%)	3 (1%)	67	85
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	85
2	B	203/216 (94%)	202 (100%)	1 (0%)	88	96
2	P	203/216 (94%)	202 (100%)	1 (0%)	88	96
3	C	212/226 (94%)	204 (96%)	8 (4%)	33	59
3	Q	212/226 (94%)	204 (96%)	8 (4%)	33	59
4	D	194/215 (90%)	187 (96%)	7 (4%)	35	61
4	R	194/215 (90%)	187 (96%)	7 (4%)	35	61
5	E	190/193 (98%)	185 (97%)	5 (3%)	46	72
5	S	190/193 (98%)	185 (97%)	5 (3%)	46	72
6	F	201/239 (84%)	195 (97%)	6 (3%)	41	67
6	T	201/239 (84%)	195 (97%)	6 (3%)	41	67
7	G	206/210 (98%)	201 (98%)	5 (2%)	49	74
7	U	206/210 (98%)	201 (98%)	5 (2%)	49	74
8	H	185/190 (97%)	182 (98%)	3 (2%)	62	82
8	V	185/190 (97%)	182 (98%)	3 (2%)	62	82
9	I	172/173 (99%)	170 (99%)	2 (1%)	71	87
9	W	172/173 (99%)	170 (99%)	2 (1%)	71	87
10	J	173/175 (99%)	167 (96%)	6 (4%)	36	62
10	X	173/175 (99%)	167 (96%)	6 (4%)	36	62
11	K	169/169 (100%)	165 (98%)	4 (2%)	49	74
11	Y	169/169 (100%)	165 (98%)	4 (2%)	49	74
12	L	185/185 (100%)	183 (99%)	2 (1%)	73	88
12	Z	185/185 (100%)	183 (99%)	2 (1%)	73	88
13	M	199/208 (96%)	193 (97%)	6 (3%)	41	67
13	a	199/208 (96%)	193 (97%)	6 (3%)	41	67
14	N	162/162 (100%)	159 (98%)	3 (2%)	57	79
14	b	162/162 (100%)	159 (98%)	3 (2%)	57	79
All	All	5320/5540 (96%)	5198 (98%)	122 (2%)	50	75



All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	191	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	206	LYS
4	D	99	ILE
4	D	125	LEU
4	D	176	LEU
4	D	193	LEU
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
6	F	117	GLN
6	F	123	ASN
6	F	171	GLU
6	F	181	GLU
6	F	214	TRP
6	F	240	GLN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
8	H	22	GLN
8	H	30	ASN
8	H	196	ARG
9	I	37	ASN
9	I	182	TRP
10	J	3	ILE
10	J	25	ILE

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Mol	Chain	Res	Type
10	J	78	GLN
10	J	90	LYS
10	J	99	GLN
10	J	149	ARG
11	K	4	LEU
11	K	9	GLN
11	K	99	THR
11	K	116	ASP
12	L	23	LEU
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	9	LYS
14	N	36	ARG
14	N	83	LYS
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	206	LYS
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	71	LEU
5	S	184	ASN

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Mol	Chain	Res	Type
5	S	188	LEU
6	T	117	GLN
6	T	123	ASN
6	T	171	GLU
6	T	181	GLU
6	T	214	TRP
6	T	240	GLN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
8	V	22	GLN
8	V	30	ASN
8	V	196	ARG
9	W	37	ASN
9	W	182	TRP
10	X	3	ILE
10	X	23	ARG
10	X	25	ILE
10	X	78	GLN
10	X	90	LYS
10	X	99	GLN
11	Y	4	LEU
11	Y	9	GLN
11	Y	99	THR
11	Y	116	ASP
12	Z	23	LEU
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	9	LYS
14	b	36	ARG
14	b	83	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
3	C	92	GLN
3	C	147	GLN
3	C	160	GLN
4	D	91	HIS
4	D	146	GLN
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
9	I	203	GLN
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	70	ASN
12	L	79	HIS
13	M	48	ASN
13	M	102	GLN
2	P	20	GLN
2	P	58	GLN
2	P	119	GLN
2	P	123	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	91	HIS
4	R	146	GLN
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN

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Mol	Chain	Res	Type
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
10	X	55	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	70	ASN
12	Z	79	HIS
13	a	48	ASN
13	a	102	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 13 are monoatomic - leaving 6 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
17	BO2	N	201	14	25,29,29	1.60	5 (20%)	32,38,38	1.43	4 (12%)
17	BO2	Y	301	11	25,29,29	1.60	5 (20%)	32,38,38	1.37	4 (12%)
17	BO2	H	301	8	25,29,29	1.63	5 (20%)	32,38,38	1.34	3 (9%)
17	BO2	b	201	14	25,29,29	1.58	5 (20%)	32,38,38	1.45	4 (12%)
17	BO2	K	301	11	25,29,29	1.61	5 (20%)	32,38,38	1.35	4 (12%)
17	BO2	V	301	8	25,29,29	1.61	5 (20%)	32,38,38	1.35	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BO2	N	201	14	-	4/22/28/28	0/2/2/2
17	BO2	Y	301	11	-	0/22/28/28	0/2/2/2
17	BO2	H	301	8	-	6/22/28/28	0/2/2/2
17	BO2	b	201	14	-	4/22/28/28	0/2/2/2
17	BO2	K	301	11	-	0/22/28/28	0/2/2/2
17	BO2	V	301	8	-	6/22/28/28	0/2/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	301	BO2	C2-C7	-4.56	1.39	1.50
17	K	301	BO2	C2-C7	-4.55	1.39	1.50
17	V	301	BO2	C2-C7	-4.51	1.39	1.50
17	Y	301	BO2	C2-C7	-4.51	1.39	1.50
17	N	201	BO2	C2-C7	-4.49	1.39	1.50
17	b	201	BO2	C2-C7	-4.39	1.39	1.50
17	H	301	BO2	C11-C12	-4.38	1.40	1.51
17	K	301	BO2	C11-C12	-4.34	1.40	1.51
17	Y	301	BO2	C11-C12	-4.29	1.41	1.51
17	b	201	BO2	C11-C12	-4.27	1.41	1.51
17	V	301	BO2	C11-C12	-4.26	1.41	1.51
17	N	201	BO2	C11-C12	-4.24	1.41	1.51
17	Y	301	BO2	C3-N4	2.95	1.40	1.34
17	K	301	BO2	C3-N4	2.93	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	V	301	BO2	C3-N4	2.88	1.40	1.34
17	H	301	BO2	C3-N4	2.85	1.40	1.34
17	N	201	BO2	C3-N4	2.84	1.40	1.34
17	V	301	BO2	C6-N1	2.81	1.40	1.34
17	N	201	BO2	C6-N1	2.80	1.40	1.34
17	H	301	BO2	C6-N1	2.77	1.40	1.34
17	K	301	BO2	C6-N1	2.75	1.40	1.34
17	Y	301	BO2	C6-N1	2.74	1.40	1.34
17	b	201	BO2	C6-N1	2.72	1.40	1.34
17	b	201	BO2	C3-N4	2.71	1.40	1.34
17	H	301	BO2	C5-N4	2.35	1.40	1.33
17	K	301	BO2	C5-N4	2.33	1.40	1.33
17	V	301	BO2	C5-N4	2.33	1.40	1.33
17	Y	301	BO2	C5-N4	2.33	1.40	1.33
17	b	201	BO2	C5-N4	2.20	1.40	1.33
17	N	201	BO2	C5-N4	2.10	1.40	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	201	BO2	C21-C22-C23	-4.98	109.13	115.39
17	N	201	BO2	C21-C22-C23	-4.92	109.22	115.39
17	V	301	BO2	C21-C22-C23	-4.07	110.29	115.39
17	H	301	BO2	C21-C22-C23	-3.93	110.46	115.39
17	Y	301	BO2	C21-C22-C23	-3.87	110.53	115.39
17	K	301	BO2	C21-C22-C23	-3.79	110.63	115.39
17	Y	301	BO2	C6-N1-C2	3.49	121.46	116.93
17	H	301	BO2	C6-N1-C2	3.46	121.42	116.93
17	K	301	BO2	C6-N1-C2	3.45	121.41	116.93
17	V	301	BO2	C6-N1-C2	3.38	121.32	116.93
17	b	201	BO2	C6-N1-C2	3.19	121.07	116.93
17	N	201	BO2	C6-N1-C2	3.15	121.02	116.93
17	V	301	BO2	C12-C11-C10	-2.27	107.13	113.39
17	N	201	BO2	C18-C10-N9	-2.26	105.01	111.16
17	H	301	BO2	C12-C11-C10	-2.25	107.17	113.39
17	b	201	BO2	C18-C10-N9	-2.21	105.14	111.16
17	Y	301	BO2	C18-C10-N9	-2.21	105.15	111.16
17	b	201	BO2	C11-C10-N9	-2.18	106.20	110.79
17	K	301	BO2	C18-C10-N9	-2.12	105.39	111.16
17	Y	301	BO2	C6-C5-N4	-2.11	119.32	121.95
17	N	201	BO2	C11-C10-N9	-2.07	106.42	110.79
17	V	301	BO2	C6-C5-N4	-2.04	119.41	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	301	BO2	C6-C5-N4	-2.01	119.44	121.95

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	301	BO2	C3-C2-C7-O8
17	H	301	BO2	C3-C2-C7-N9
17	H	301	BO2	C21-C22-C23-C24
17	H	301	BO2	C21-C22-C23-C25
17	V	301	BO2	C3-C2-C7-O8
17	V	301	BO2	C3-C2-C7-N9
17	V	301	BO2	C21-C22-C23-C24
17	V	301	BO2	C21-C22-C23-C25
17	H	301	BO2	N1-C2-C7-O8
17	V	301	BO2	N1-C2-C7-O8
17	H	301	BO2	N1-C2-C7-N9
17	V	301	BO2	N1-C2-C7-N9
17	b	201	BO2	N1-C2-C7-O8
17	N	201	BO2	N1-C2-C7-O8
17	b	201	BO2	N1-C2-C7-N9
17	N	201	BO2	N1-C2-C7-N9
17	N	201	BO2	C3-C2-C7-O8
17	b	201	BO2	C3-C2-C7-N9
17	N	201	BO2	C3-C2-C7-N9
17	b	201	BO2	C3-C2-C7-O8

There are no ring outliers.

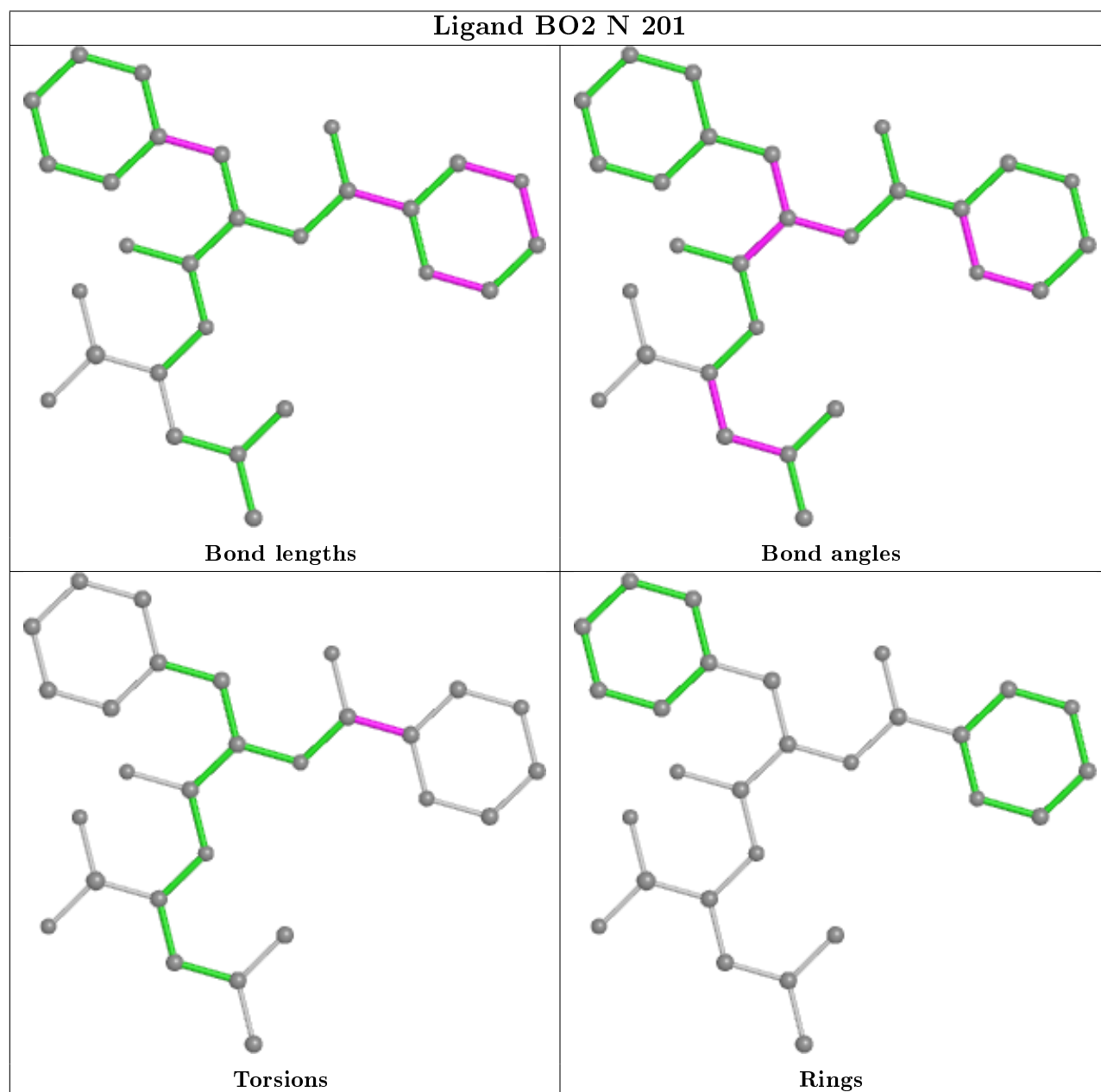
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	N	201	BO2	1	0
17	H	301	BO2	1	0
17	K	301	BO2	1	0
17	V	301	BO2	1	0

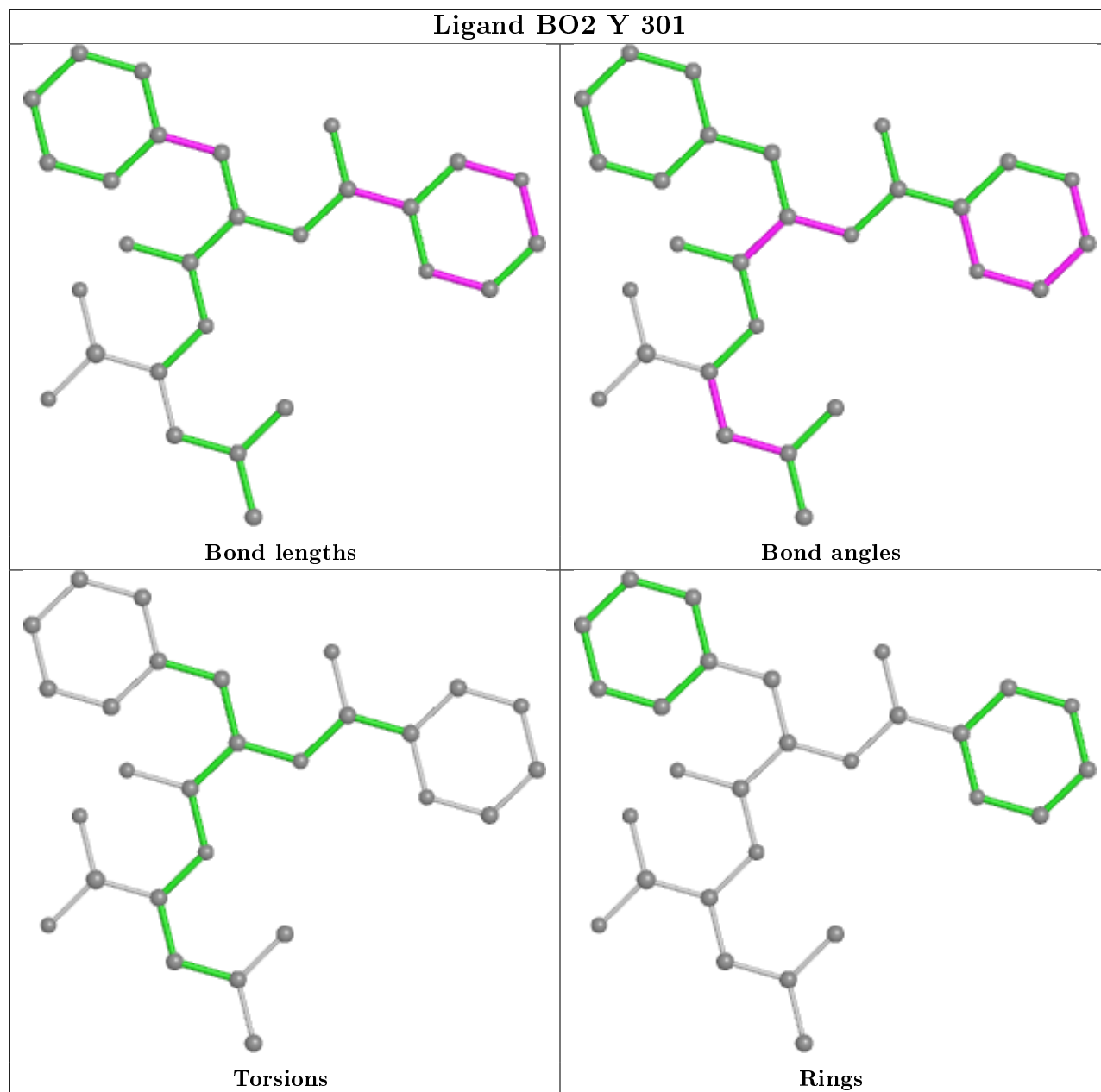
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



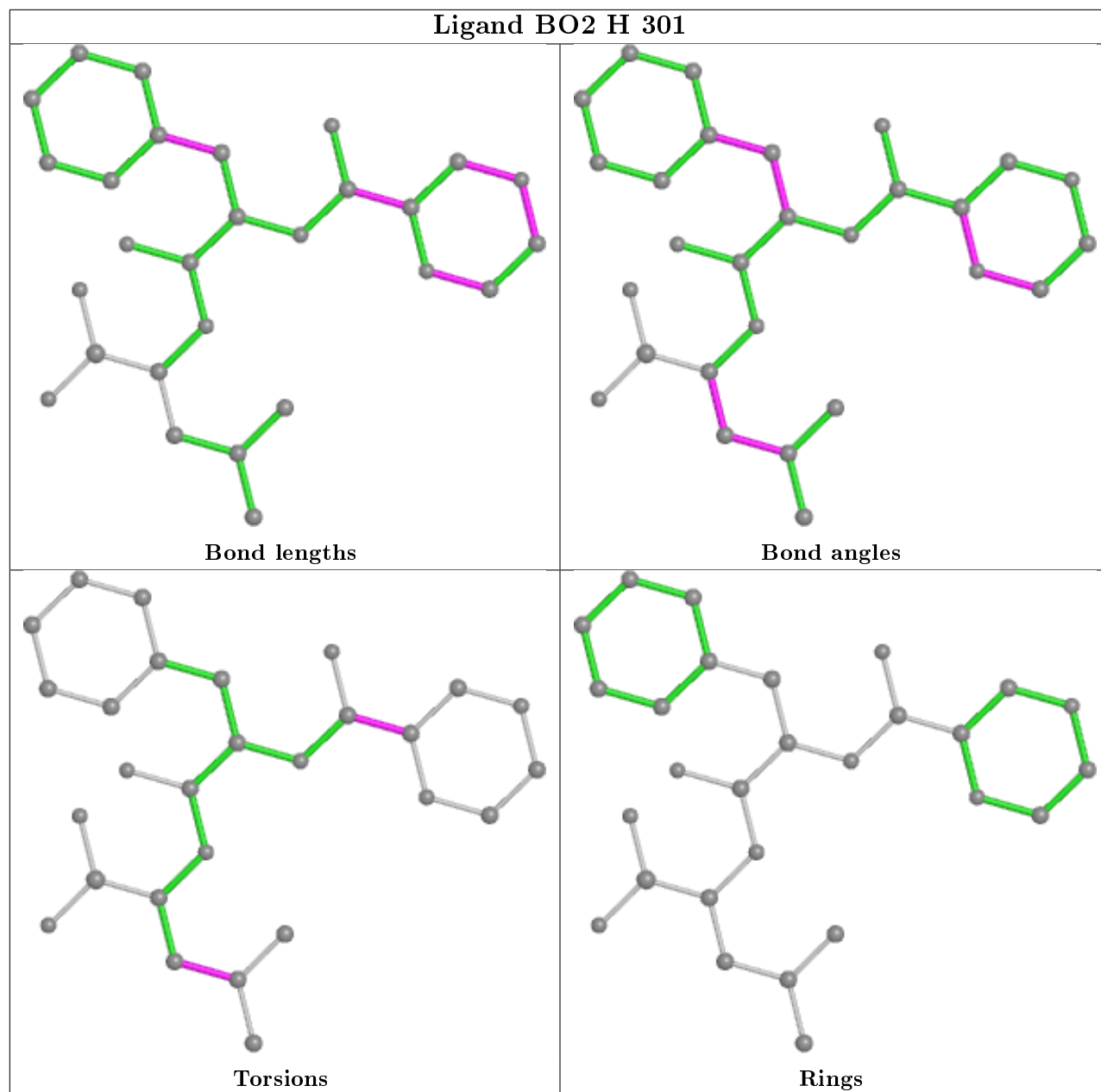
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



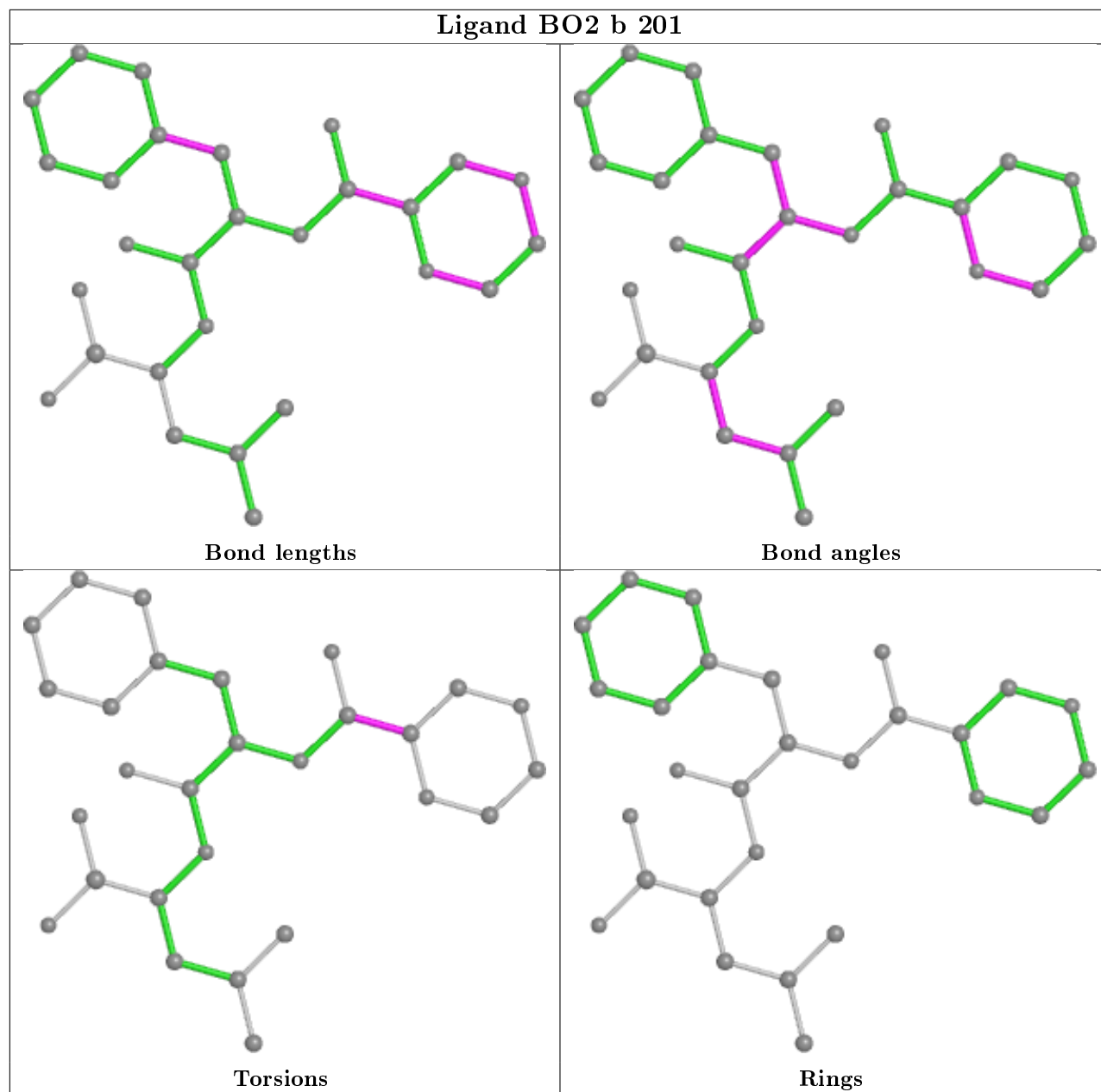
## Ligand BO2 Y 301



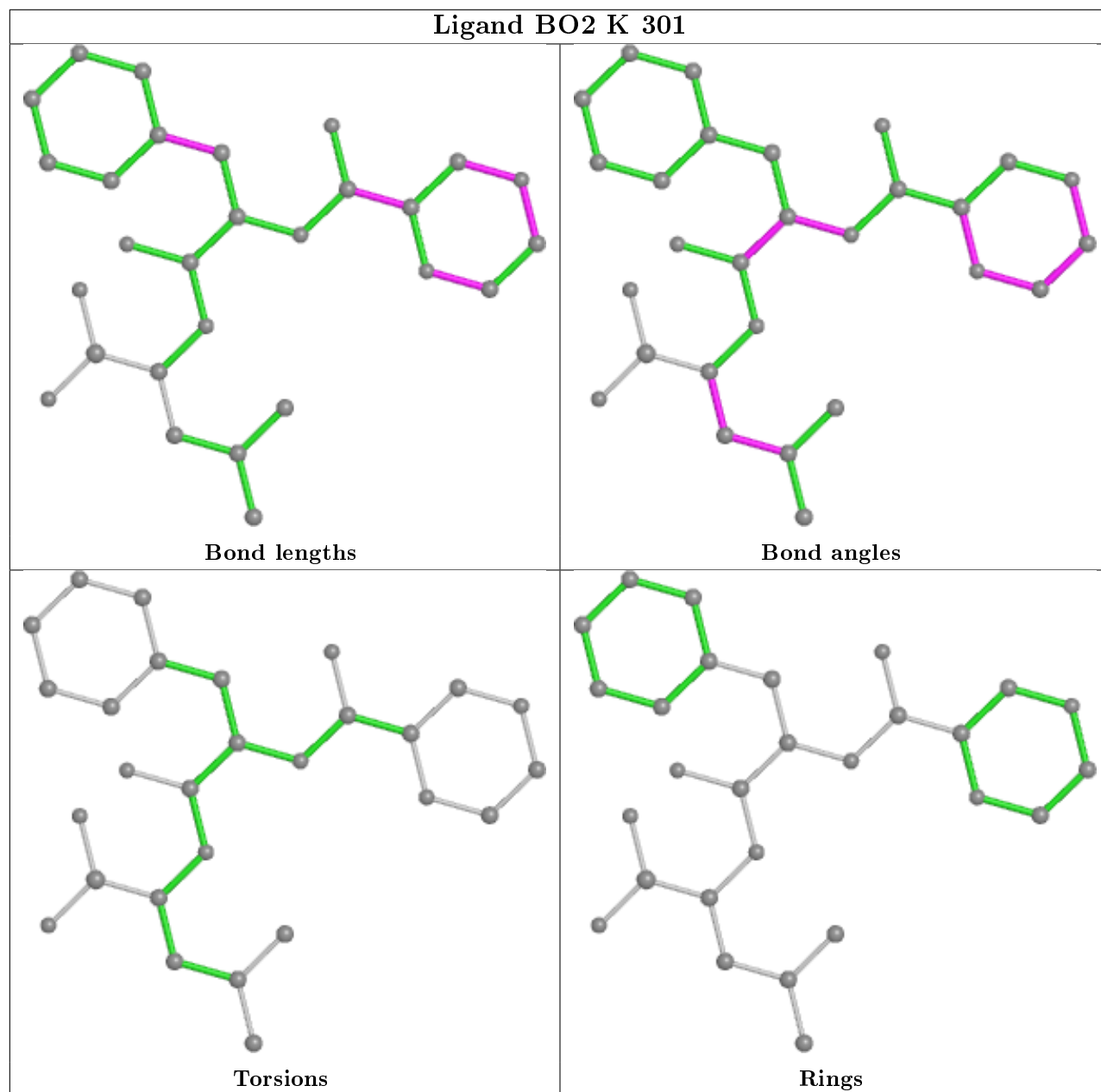
## Ligand BO2 H 301

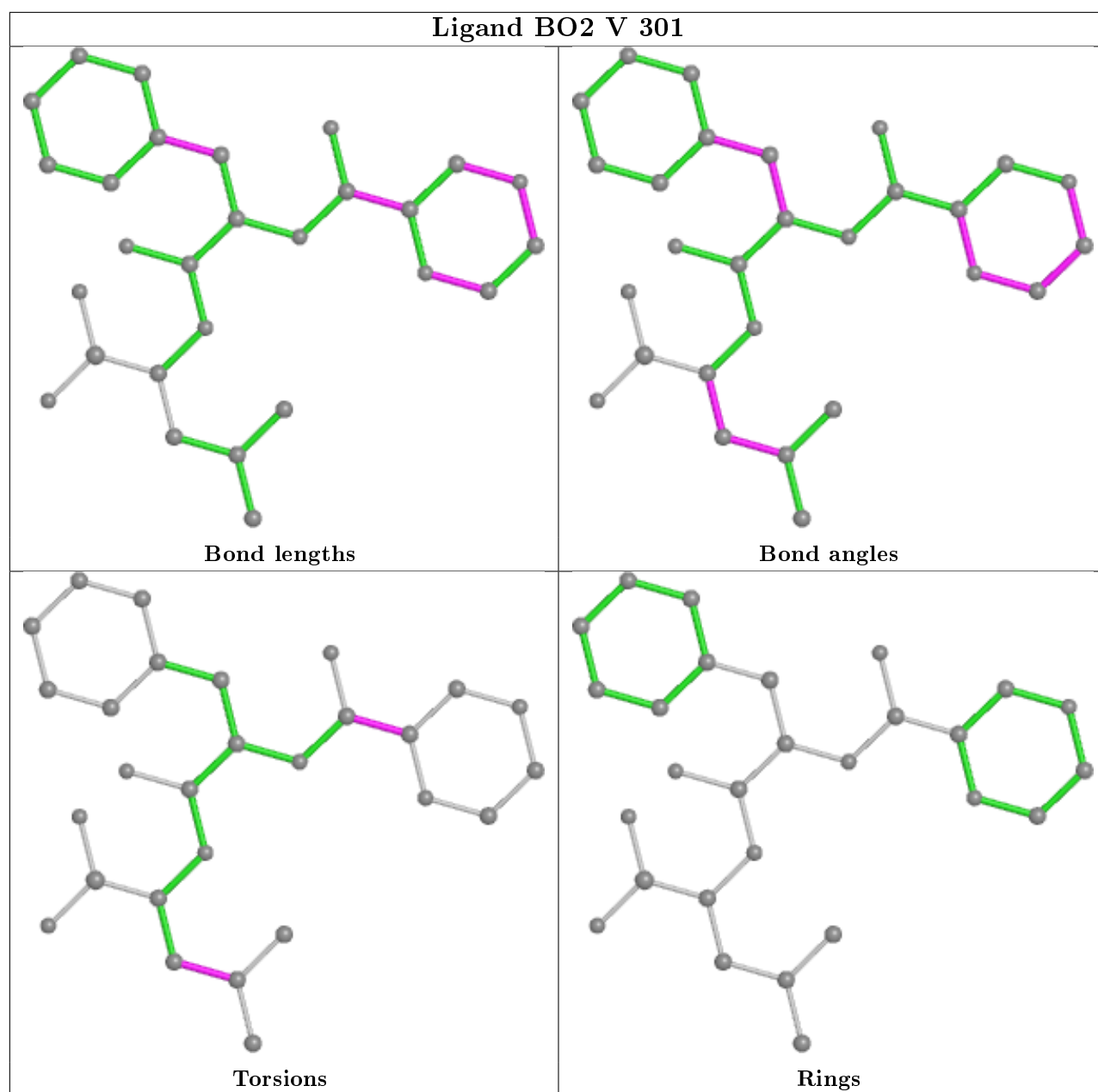


## Ligand BO2 b 201



## Ligand BO2 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%)	-0.35	5 (2%) 65 60	38, 54, 92, 130	0
1	O	250/250 (100%)	-0.26	8 (3%) 47 40	42, 63, 108, 145	0
2	B	244/258 (94%)	-0.18	9 (3%) 41 34	40, 61, 107, 156	0
2	P	244/258 (94%)	-0.14	11 (4%) 33 26	44, 65, 107, 157	0
3	C	240/254 (94%)	-0.01	12 (5%) 28 23	39, 65, 132, 160	0
3	Q	240/254 (94%)	0.24	25 (10%) 6 4	49, 78, 167, 189	0
4	D	235/260 (90%)	-0.29	1 (0%) 92 91	45, 66, 101, 145	0
4	R	235/260 (90%)	-0.15	8 (3%) 45 38	51, 70, 114, 152	0
5	E	231/234 (98%)	-0.15	6 (2%) 56 50	46, 70, 108, 145	0
5	S	231/234 (98%)	0.02	18 (7%) 13 9	50, 78, 129, 163	0
6	F	243/288 (84%)	-0.35	6 (2%) 57 51	40, 62, 114, 138	0
6	T	243/288 (84%)	-0.18	12 (4%) 29 23	42, 71, 132, 173	0
7	G	241/252 (95%)	-0.38	7 (2%) 51 45	39, 58, 101, 156	0
7	U	241/252 (95%)	-0.34	5 (2%) 63 58	42, 59, 98, 143	0
8	H	226/232 (97%)	-0.43	3 (1%) 77 73	34, 51, 86, 140	0
8	V	226/232 (97%)	-0.37	6 (2%) 54 48	36, 55, 90, 162	0
9	I	204/205 (99%)	-0.63	2 (0%) 82 80	31, 50, 79, 113	0
9	W	204/205 (99%)	-0.59	2 (0%) 82 80	35, 53, 83, 111	0
10	J	195/198 (98%)	-0.46	3 (1%) 73 70	36, 54, 85, 117	0
10	X	195/198 (98%)	-0.45	3 (1%) 73 70	39, 57, 86, 132	0
11	K	212/212 (100%)	-0.38	5 (2%) 59 53	37, 55, 92, 112	0
11	Y	212/212 (100%)	-0.36	4 (1%) 66 62	38, 53, 97, 113	0
12	L	222/222 (100%)	-0.37	5 (2%) 60 54	32, 55, 109, 141	0
12	Z	222/222 (100%)	-0.33	8 (3%) 42 35	37, 54, 110, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/246 (94%)	-0.57	3 (1%)	77 73	35, 54, 78, 97	0
13	a	233/246 (94%)	-0.55	1 (0%)	92 91	33, 52, 75, 94	0
14	N	196/196 (100%)	-0.61	2 (1%)	82 80	32, 49, 78, 109	0
14	b	196/196 (100%)	-0.54	2 (1%)	82 80	35, 50, 81, 109	0
All	All	6344/6614 (95%)	-0.32	182 (2%)	51 45	31, 59, 110, 189	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	49	THR	10.7
3	Q	206	LYS	8.4
3	Q	50	LEU	7.8
1	O	1	MET	7.2
10	J	1	MET	6.9
2	P	51	VAL	6.2
10	X	1	MET	6.2
3	C	50	LEU	5.9
12	L	174	TYR	5.8
12	Z	174	TYR	5.8
5	S	202	ASP	5.7
2	B	221	ASP	5.7
12	L	163	GLY	5.6
1	A	1	MET	5.6
3	C	238	LYS	5.4
12	L	165	ASN	5.3
2	P	220	ASN	5.2
3	Q	239	GLN	5.1
11	Y	212	GLY	5.0
3	C	206	LYS	5.0
3	C	49	THR	5.0
2	B	218	GLY	4.8
12	Z	163	GLY	4.8
2	B	51	VAL	4.5
2	P	219	ALA	4.5
9	W	1	SER	4.4
3	Q	236	GLN	4.4
12	Z	173	LYS	4.3
5	E	202	ASP	4.3
12	Z	165	ASN	4.3
3	C	202	GLN	4.2
1	O	249	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
2	P	59	ASP	4.2
3	Q	205	ALA	4.2
2	P	221	ASP	4.1
8	V	226	GLU	4.1
2	P	218	GLY	4.0
4	R	241	ALA	3.8
10	X	194	ASP	3.8
6	T	241	LYS	3.8
7	U	242	GLN	3.8
1	A	2	THR	3.8
6	T	243	ILE	3.8
11	K	212	GLY	3.7
3	C	225	GLU	3.7
6	T	181	GLU	3.6
3	Q	240	GLU	3.6
2	B	220	ASN	3.6
2	B	219	ALA	3.5
1	O	2	THR	3.5
3	Q	48	SER	3.5
3	Q	55	THR	3.5
6	F	215	CYS	3.4
11	K	147	ASP	3.4
3	Q	225	GLU	3.4
8	H	224	GLN	3.4
4	D	242	GLU	3.4
3	C	236	GLN	3.3
8	H	222	ASP	3.3
10	J	194	ASP	3.3
3	Q	181	GLU	3.2
3	Q	202	GLN	3.2
5	E	54	GLU	3.2
2	B	217	LYS	3.2
14	N	195	GLN	3.1
6	T	244	ASN	3.1
8	V	224	GLN	3.1
5	E	122	TYR	3.1
10	X	193	ASP	3.1
14	b	195	GLN	3.1
5	S	204	SER	3.1
2	B	59	ASP	3.0
7	G	2	GLY	3.0
9	I	1	SER	3.0

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Mol	Chain	Res	Type	RSRZ
12	Z	162	PRO	3.0
5	S	173	ARG	3.0
5	S	194	GLU	3.0
5	S	54	GLU	2.9
11	Y	208	ASN	2.9
7	G	242	GLN	2.9
2	P	52	THR	2.9
8	V	145	ASP	2.9
1	O	248	GLU	2.8
1	O	231	LYS	2.8
5	S	180	LYS	2.8
3	C	180	LYS	2.8
8	H	226	GLU	2.8
1	A	249	ALA	2.8
11	K	208	ASN	2.8
11	Y	106	ARG	2.8
1	O	201	GLU	2.8
12	L	173	LYS	2.8
5	S	163	ARG	2.8
12	L	168	VAL	2.7
4	R	217	GLN	2.7
2	B	240	LYS	2.7
11	K	211	ILE	2.7
13	a	1	THR	2.7
8	V	221	CYS	2.7
5	S	210	LEU	2.7
6	T	237	ASP	2.6
13	M	47	ASP	2.6
5	S	203	GLU	2.6
3	Q	141	ASP	2.6
5	E	233	ILE	2.6
11	Y	209	ASN	2.6
6	T	230	ASP	2.6
11	K	209	ASN	2.6
8	V	222	ASP	2.6
2	P	61	SER	2.6
1	O	52	SER	2.5
3	C	205	ALA	2.5
3	Q	171	GLU	2.5
1	O	250	LEU	2.5
7	G	179	LYS	2.5
2	P	60	THR	2.5

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Mol	Chain	Res	Type	RSRZ
3	Q	187	GLU	2.4
2	B	52	THR	2.4
7	U	222	ASP	2.4
3	Q	238	LYS	2.4
3	Q	180	LYS	2.4
3	C	229	GLN	2.4
6	T	204	LYS	2.4
2	P	222	GLY	2.4
8	V	225	GLU	2.4
1	A	250	LEU	2.4
3	Q	204	GLY	2.4
4	R	242	GLU	2.3
3	C	216	ASP	2.3
4	R	226	GLU	2.3
5	E	123	GLY	2.3
6	F	241	LYS	2.3
3	Q	60	SER	2.3
4	R	230	GLU	2.3
5	S	58	TYR	2.3
12	Z	167	LYS	2.3
6	F	181	GLU	2.3
6	F	202	ASP	2.3
3	Q	52	LEU	2.3
6	F	244	ASN	2.3
7	G	241	GLU	2.3
13	M	216	ASN	2.2
6	F	205	GLU	2.2
5	S	201	ARG	2.2
6	T	215	CYS	2.2
5	S	227	GLU	2.2
5	S	207	VAL	2.2
4	R	125	LEU	2.2
1	A	248	GLU	2.2
3	Q	216	ASP	2.2
7	G	3	TYR	2.1
6	T	201	GLU	2.1
3	Q	51	LYS	2.1
12	Z	1	GLN	2.1
10	J	193	ASP	2.1
3	Q	203	THR	2.1
13	M	1	THR	2.1
5	S	187	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	239	GLN	2.1
3	Q	223	SER	2.1
6	T	53	LYS	2.1
7	G	68	ARG	2.1
7	U	3	TYR	2.1
9	I	192	ASP	2.1
7	U	241	GLU	2.1
4	R	237	GLU	2.1
6	T	205	GLU	2.1
5	S	51	ASN	2.1
4	R	1	ASP	2.1
7	G	230	GLU	2.1
9	W	192	ASP	2.1
7	U	2	GLY	2.1
5	E	217	LYS	2.0
5	S	233	ILE	2.0
5	S	52	ALA	2.0
6	T	235	ALA	2.0
14	b	105	LYS	2.0
3	Q	234	ILE	2.0
5	S	3	ASN	2.0
2	P	182	ASP	2.0
12	Z	210	ASP	2.0
14	N	105	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

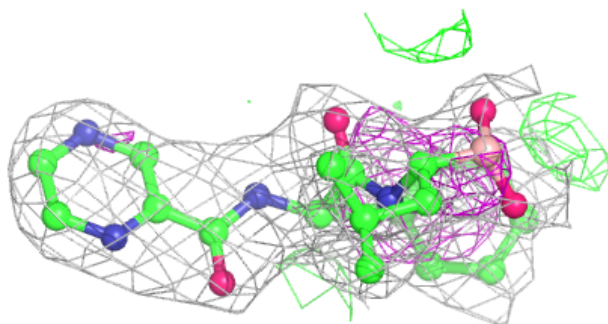
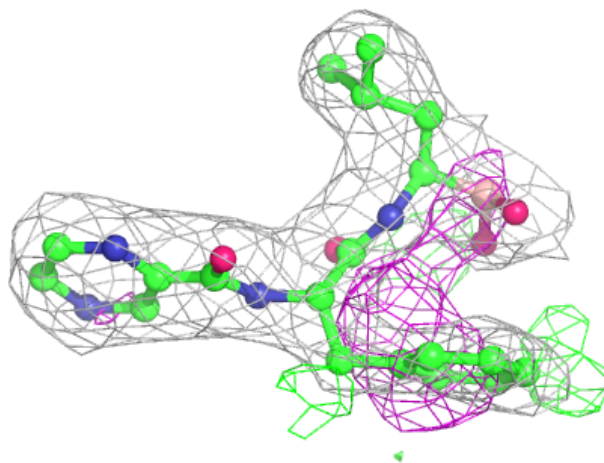
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
17	BO2	N	201	28/28	0.88	0.21	36,47,66,68	0
17	BO2	b	201	28/28	0.90	0.20	41,52,66,68	0
17	BO2	Y	301	28/28	0.93	0.16	44,53,58,61	0
17	BO2	H	301	28/28	0.93	0.17	47,50,61,65	0
17	BO2	V	301	28/28	0.93	0.17	51,54,65,67	0
15	MG	V	302	1/1	0.94	0.17	64,64,64,64	0
17	BO2	K	301	28/28	0.94	0.13	42,51,58,60	0
15	MG	G	301	1/1	0.94	0.17	58,58,58,58	0
15	MG	K	303	1/1	0.94	0.20	52,52,52,52	0
15	MG	Z	301	1/1	0.96	0.17	59,59,59,59	0
15	MG	I	301	1/1	0.97	0.21	60,60,60,60	0
15	MG	K	302	1/1	0.98	0.07	59,59,59,59	0
16	CL	b	202	1/1	0.98	0.05	47,47,47,47	0
15	MG	J	201	1/1	0.98	0.43	53,53,53,53	0
16	CL	G	302	1/1	0.99	0.05	46,46,46,46	0
16	CL	U	301	1/1	0.99	0.15	47,47,47,47	0
15	MG	N	202	1/1	0.99	0.06	45,45,45,45	0
15	MG	Y	302	1/1	0.99	0.06	53,53,53,53	0
16	CL	N	203	1/1	1.00	0.05	44,44,44,44	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.

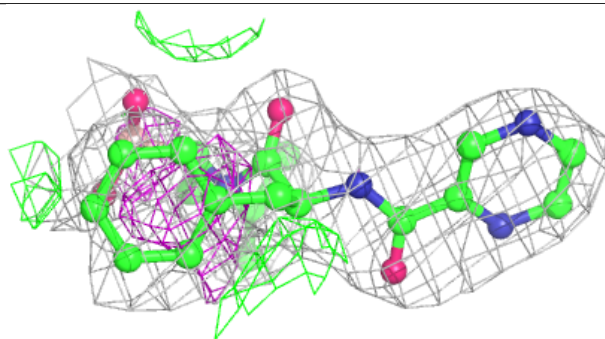
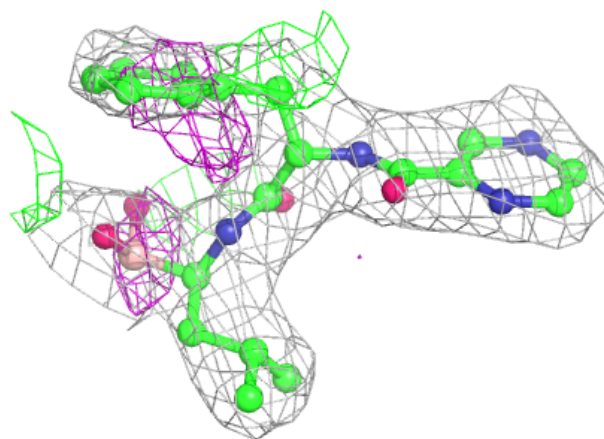
**Electron density around BO2 N 201:**

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



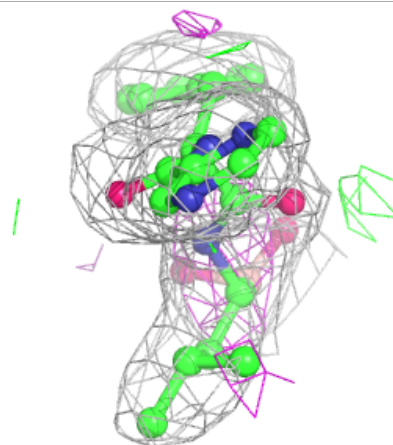
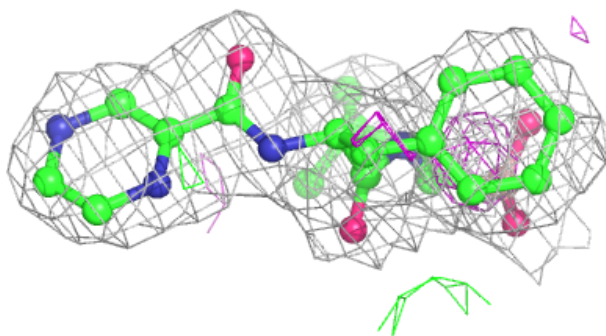
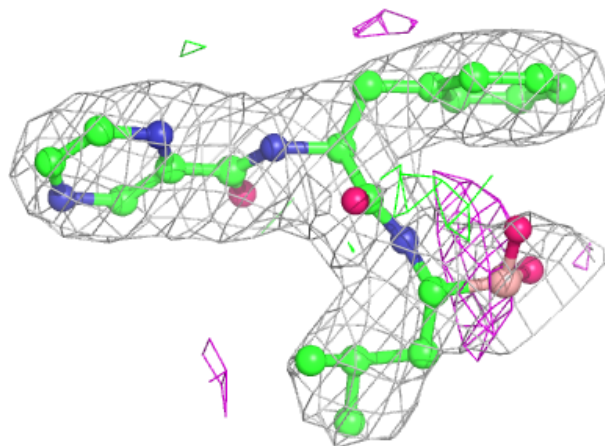
**Electron density around BO2 b 201:**

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



**Electron density around BO2 Y 301:**

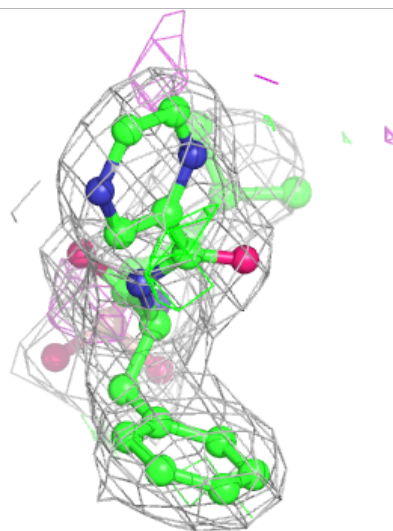
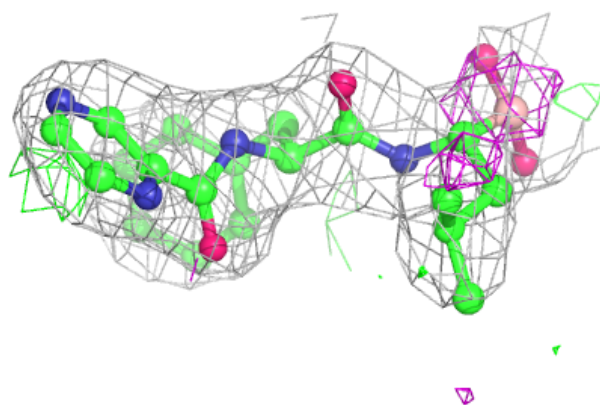
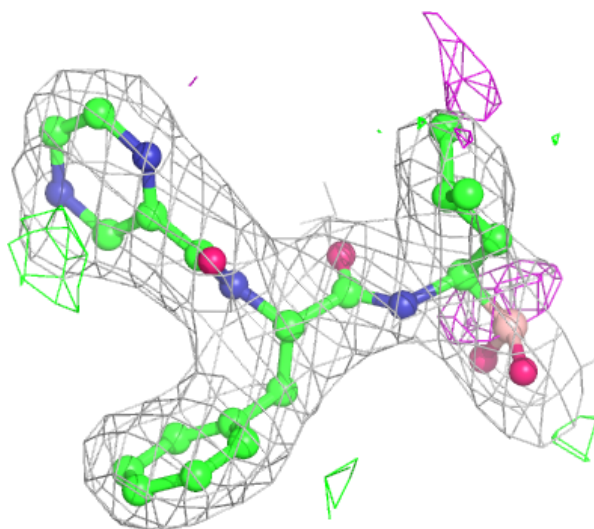
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





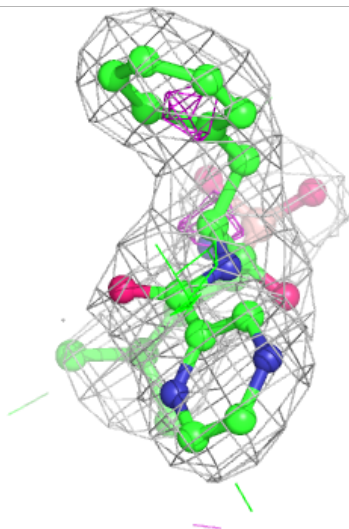
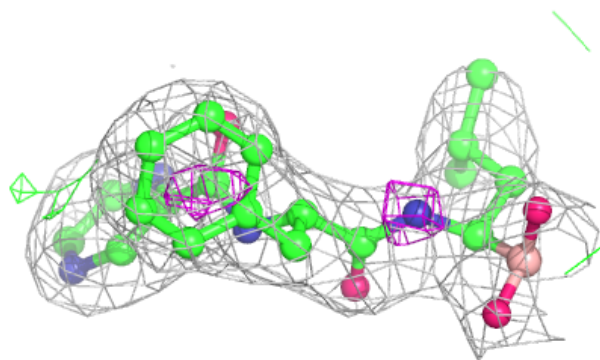
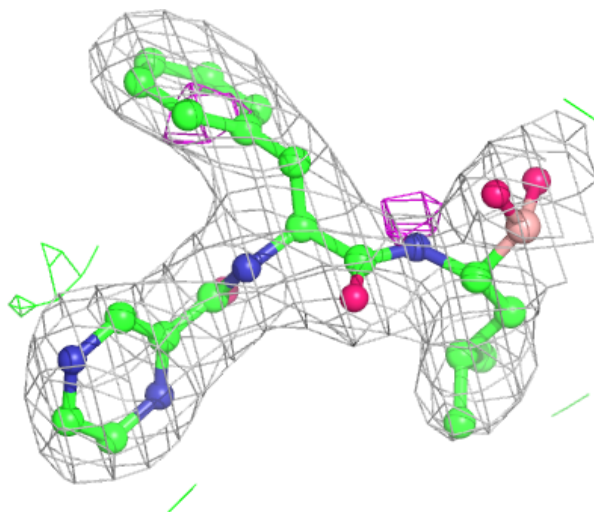
**Electron density around BO2 H 301:**

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



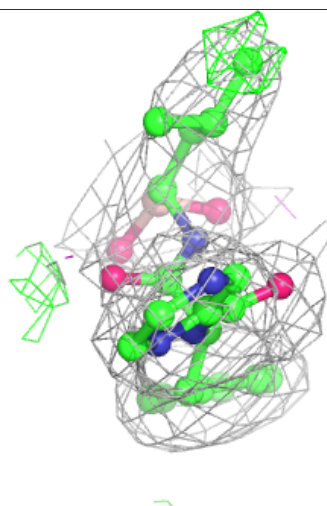
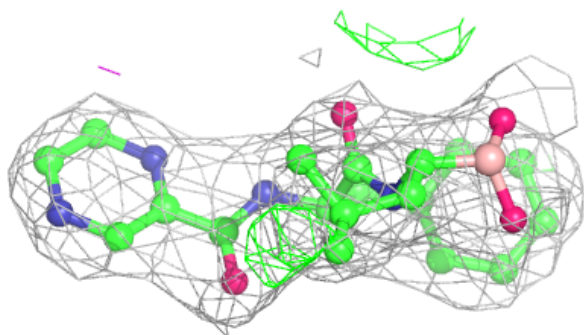
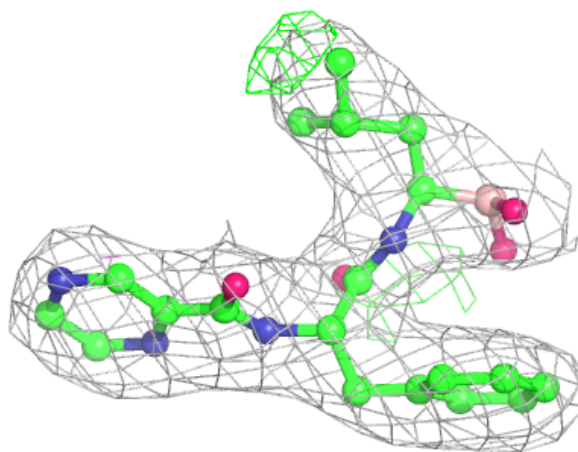
**Electron density around BO2 V 301:**

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



**Electron density around BO2 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.