



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2024 – 12:16 am GMT

PDB ID : 5L5Z
Title : Yeast 20S proteasome with human beta5c (1-138) and human beta6 (97-111; 118-133) in complex with bortezomib
Authors : Groll, M.; Huber, E.M.
Deposited on : 2016-05-28
Resolution : 2.70 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

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>.

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

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

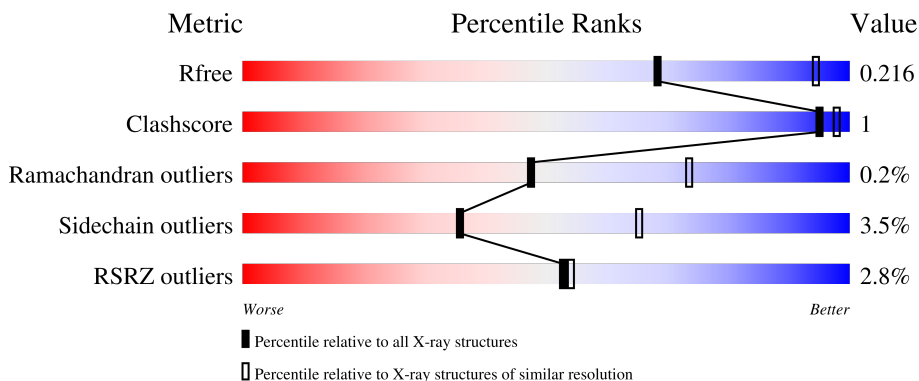
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	 4% 98%
1	O	250	 4% 98%
2	B	258	 3% 89% 5% 5%
2	P	258	 3% 90% 5% 5%
3	C	254	 7% 87% 6% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Q	254	8% 87% 6% • 6%
4	D	260	2% 87% • 10%
4	R	260	3% 86% • 10%
5	E	234	3% 95% • •
5	S	234	4% 95% • •
6	F	288	3% 82% • 16%
6	T	288	3% 81% • 16%
7	G	252	3% 91% 5% •
7	U	252	2% 90% 5% •
8	H	232	2% 92% • • •
8	V	232	3% 92% • • •
9	I	205	93% 6%
9	W	205	92% 7%
10	J	198	3% 91% 7% • •
10	X	198	3% 91% 7% • •
11	K	211	3% 88% 9% •
11	Y	211	% 87% 10% •
12	L	222	% 95% 5% •
12	Z	222	% 95% 5%
13	M	246	% 91% • 5%
13	a	246	92% • 5%
14	N	196	% 94% 5% •
14	b	196	% 97% •

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 50018 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	226	Total 1719	C 1082	N 298	O 332	S 7	0	0	0
8	V	226	Total 1719	C 1082	N 298	O 332	S 7	0	0	0

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	211	1632	1036	282	306	8	0	0	0
11	Y	211	1632	1036	282	306	8	0	0	0

- Molecule 12 is a protein called Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	222	1764	1119	305	336	4	0	0	0
12	Z	222	1764	1119	305	336	4	0	0	0

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

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

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

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

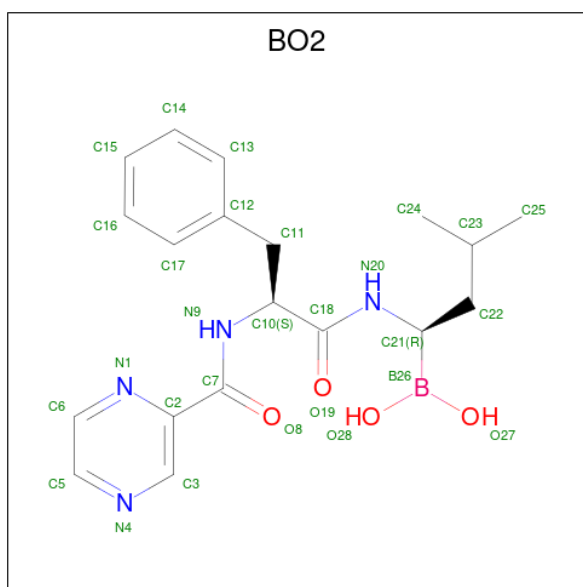
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total Mg 1 1	0	0
15	I	3	Total Mg 3 3	0	0
15	J	1	Total Mg 1 1	0	0
15	K	2	Total Mg 2 2	0	0
15	L	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	Z	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	N	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0
16	b	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: C₁₉H₂₅BN₄O₄).



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

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	22	Total 22	O 22	0	0
18	B	14	Total 14	O 14	0	0
18	C	13	Total 13	O 13	0	0
18	D	11	Total 11	O 11	0	0
18	E	7	Total 7	O 7	0	0
18	F	17	Total 17	O 17	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	G	15	Total O 15 15	0	0
18	H	22	Total O 22 22	0	0
18	I	17	Total O 17 17	0	0
18	J	23	Total O 23 23	0	0
18	K	16	Total O 16 16	0	0
18	L	29	Total O 29 29	0	0
18	M	27	Total O 27 27	0	0
18	N	19	Total O 19 19	0	0
18	O	12	Total O 12 12	0	0
18	P	11	Total O 11 11	0	0
18	Q	11	Total O 11 11	0	0
18	R	11	Total O 11 11	0	0
18	S	10	Total O 10 10	0	0
18	T	9	Total O 9 9	0	0
18	U	20	Total O 20 20	0	0
18	V	35	Total O 35 35	0	0
18	W	18	Total O 18 18	0	0
18	X	15	Total O 15 15	0	0
18	Y	12	Total O 12 12	0	0
18	Z	16	Total O 16 16	0	0
18	a	29	Total O 29 29	0	0

Continued on next page...

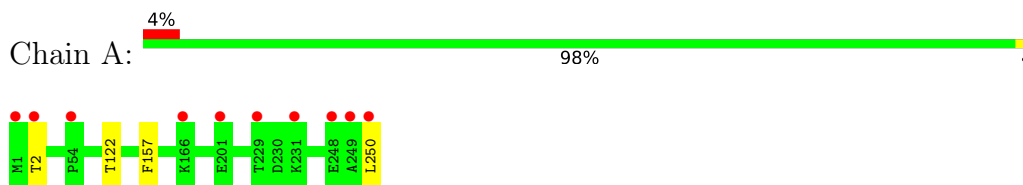
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	b	19	Total	O	0	0
			19	19		

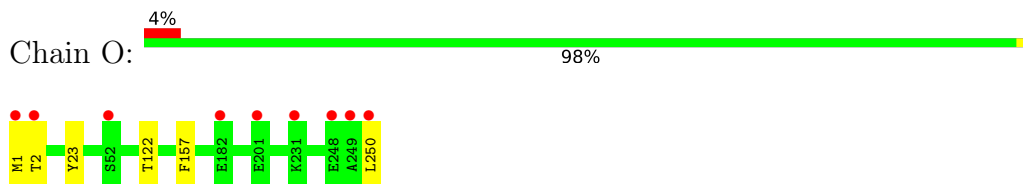
3 Residue-property plots [i](#)

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

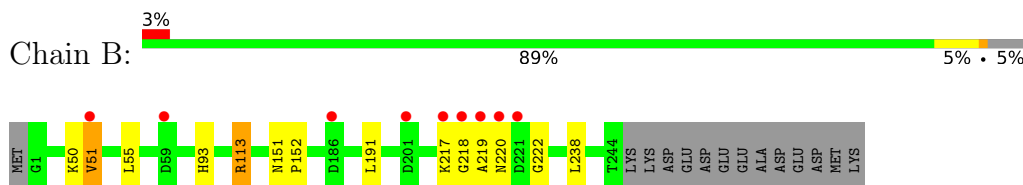
- Molecule 1: Proteasome subunit alpha type-2



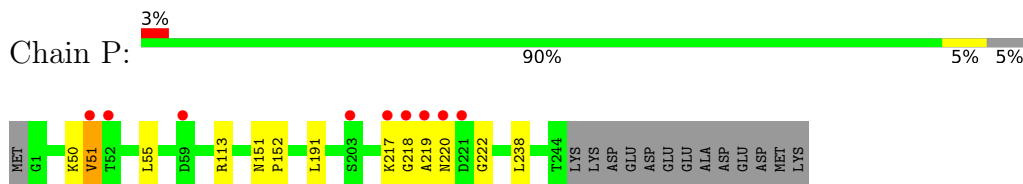
- Molecule 1: Proteasome subunit alpha type-2



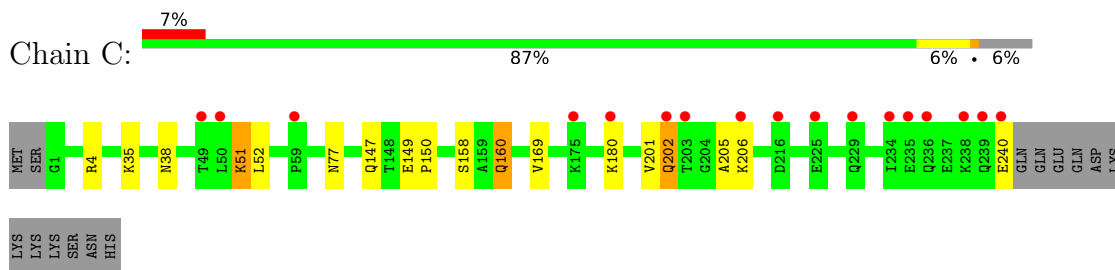
- Molecule 2: Proteasome subunit alpha type-3

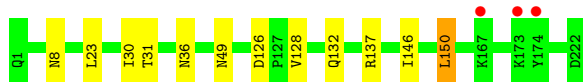
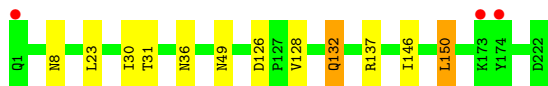
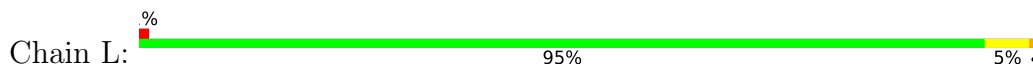
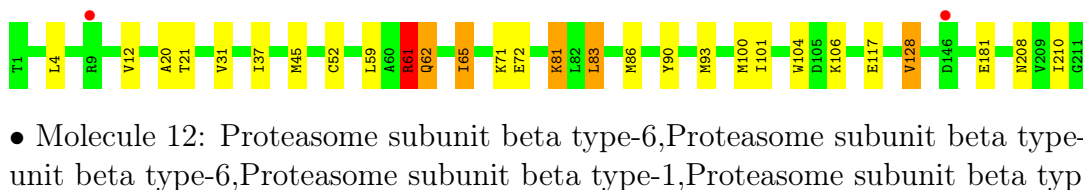
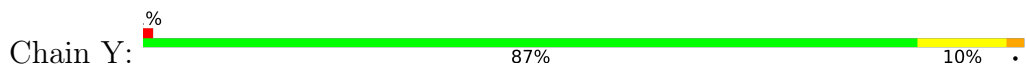
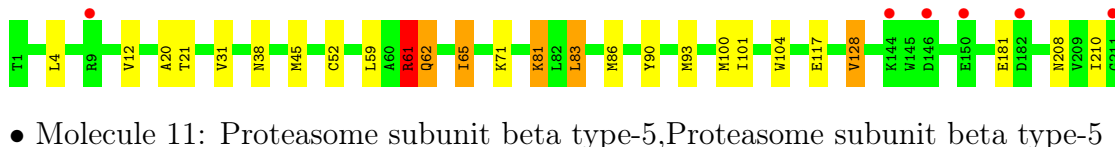
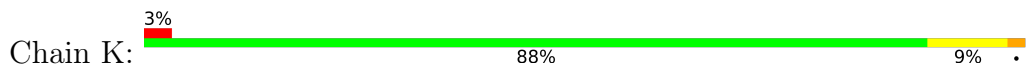
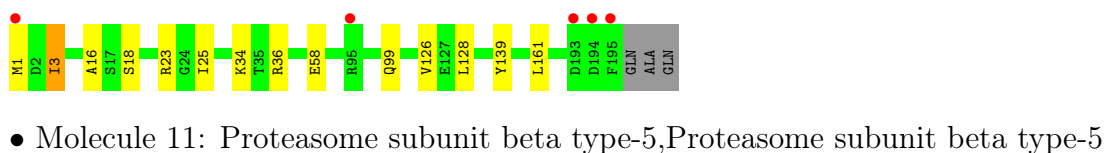
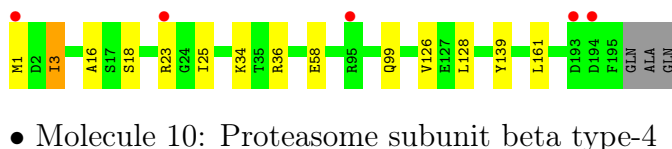
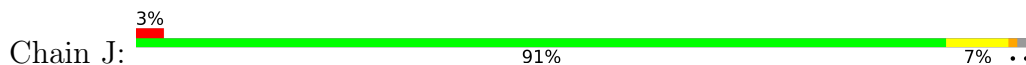
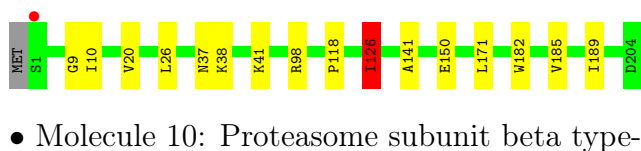


- Molecule 2: Proteasome subunit alpha type-3

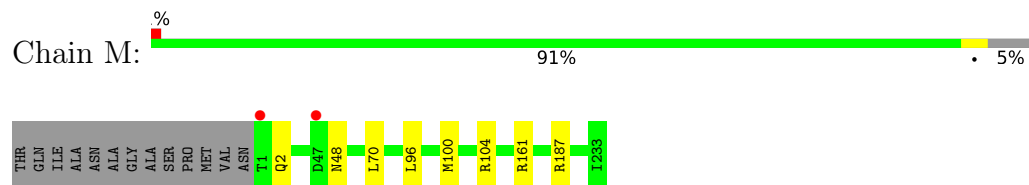


- Molecule 3: Proteasome subunit alpha type-4

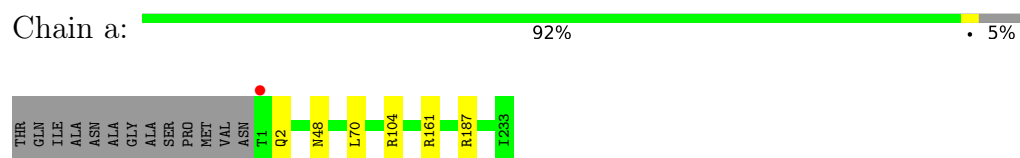




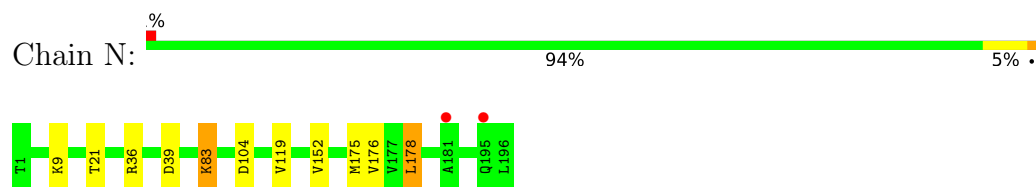
- Molecule 13: Proteasome subunit beta type-7



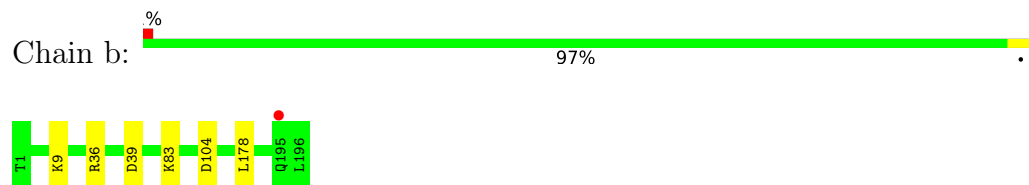
- Molecule 13: Proteasome subunit beta type-7



- 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, α , β , γ	135.80Å 300.28Å 145.75Å 90.00° 112.93° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.7 (15.00-2.70) 97.8 (15.00-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.190 , 0.212 0.195 , 0.216	Depositor DCC
R_{free} test set	14246 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtrriage
Anisotropy	0.079	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	50018	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.46	0/2642
1	O	0.27	0/1952	0.46	0/2642
2	B	0.27	0/1934	0.48	0/2618
2	P	0.27	0/1934	0.49	0/2618
3	C	0.27	0/1910	0.50	0/2586
3	Q	0.27	0/1910	0.50	0/2586
4	D	0.27	0/1837	0.47	0/2475
4	R	0.26	0/1837	0.46	0/2475
5	E	0.27	0/1800	0.47	0/2433
5	S	0.27	0/1800	0.46	0/2433
6	F	0.27	0/1932	0.44	0/2609
6	T	0.27	0/1932	0.45	0/2609
7	G	0.27	0/1945	0.46	0/2634
7	U	0.27	0/1945	0.46	0/2634
8	H	0.25	0/1750	0.51	0/2373
8	V	0.25	0/1750	0.52	1/2373 (0.0%)
9	I	0.31	1/1611 (0.1%)	0.67	2/2174 (0.1%)
9	W	0.29	0/1611	0.74	2/2174 (0.1%)
10	J	0.26	0/1589	0.48	0/2142
10	X	0.26	0/1589	0.48	0/2142
11	K	0.28	0/1668	0.72	6/2253 (0.3%)
11	Y	0.28	0/1668	0.75	4/2253 (0.2%)
12	L	0.27	0/1802	0.50	0/2430
12	Z	0.28	0/1802	0.49	0/2430
13	M	0.27	0/1855	0.50	0/2514
13	a	0.26	0/1855	0.51	0/2514
14	N	0.25	0/1541	0.48	0/2087
14	b	0.25	0/1541	0.48	0/2087
All	All	0.27	1/50252 (0.0%)	0.52	15/67940 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	K	0	1
11	Y	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	126	ILE	CB-CG2	-5.69	1.35	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	W	126	ILE	CG1-CB-CG2	-23.06	60.67	111.40
11	Y	61	ARG	NE-CZ-NH1	18.14	129.37	120.30
9	I	126	ILE	CG1-CB-CG2	-16.32	75.51	111.40
11	K	61	ARG	NE-CZ-NH2	15.43	128.02	120.30
11	Y	61	ARG	NE-CZ-NH2	-13.89	113.35	120.30
11	K	61	ARG	NE-CZ-NH1	-11.15	114.73	120.30
9	I	126	ILE	CA-CB-CG1	10.67	131.28	111.00
9	W	126	ILE	CA-CB-CG1	9.30	128.68	111.00
11	K	61	ARG	CD-NE-CZ	6.81	133.13	123.60
11	K	61	ARG	CB-CG-CD	6.63	128.84	111.60
11	Y	61	ARG	CD-NE-CZ	6.14	132.20	123.60
8	V	22	GLN	CB-CG-CD	6.03	127.27	111.60
11	Y	61	ARG	CA-CB-CG	5.78	126.11	113.40
11	K	61	ARG	CG-CD-NE	-5.50	100.24	111.80
11	K	61	ARG	CA-CB-CG	5.46	125.41	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	K	61	ARG	Sidechain
11	Y	61	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	0	0
1	O	1915	0	1929	2	0
2	B	1904	0	1904	5	0
2	P	1904	0	1904	4	0
3	C	1881	0	1895	6	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	1	0
4	R	1813	0	1797	3	0
5	E	1773	0	1775	2	0
5	S	1773	0	1775	2	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	3	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	4	0
8	H	1719	0	1718	7	0
8	V	1719	0	1718	7	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	10	0
10	J	1561	0	1569	9	0
10	X	1561	0	1569	9	0
11	K	1632	0	1592	12	0
11	Y	1632	0	1592	15	0
12	L	1764	0	1716	4	0
12	Z	1764	0	1716	3	0
13	M	1824	0	1832	1	0
13	a	1824	0	1832	0	0
14	N	1512	0	1480	4	0
14	b	1512	0	1480	0	0
15	G	1	0	0	0	0
15	I	3	0	0	0	0
15	J	1	0	0	0	0
15	K	2	0	0	0	0
15	L	1	0	0	0	0
15	N	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	U	1	0	0	0	0
16	b	1	0	0	0	0
17	H	28	0	25	0	0
17	K	28	0	25	0	0
17	N	28	0	25	1	0
17	V	28	0	25	0	0
17	Y	28	0	25	0	0
17	b	28	0	25	0	0
18	A	22	0	0	0	0
18	B	14	0	0	2	0
18	C	13	0	0	0	0
18	D	11	0	0	0	0
18	E	7	0	0	0	0
18	F	17	0	0	0	0
18	G	15	0	0	0	0
18	H	22	0	0	0	0
18	I	17	0	0	0	0
18	J	23	0	0	0	0
18	K	16	0	0	0	0
18	L	29	0	0	0	0
18	M	27	0	0	0	0
18	N	19	0	0	0	0
18	O	12	0	0	0	0
18	P	11	0	0	0	0
18	Q	11	0	0	0	0
18	R	11	0	0	0	0
18	S	10	0	0	0	0
18	T	9	0	0	1	0
18	U	20	0	0	0	0
18	V	35	0	0	0	0
18	W	18	0	0	0	0
18	X	15	0	0	0	0
18	Y	12	0	0	1	0
18	Z	16	0	0	0	0
18	a	29	0	0	0	0
18	b	19	0	0	0	0
All	All	50018	0	49280	115	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 (115) 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)
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.68	0.74
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.69	0.74
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.84	0.60
8:H:196:ARG:NH2	9:I:150:GLU:O	2.35	0.60
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.84	0.59
9:I:98:ARG:HD2	9:I:126:ILE:HD12	1.83	0.58
11:K:208:ASN:O	9:W:38:LYS:NZ	2.37	0.58
14:N:152:VAL:HA	14:N:175:MET:HE1	1.87	0.57
11:Y:61:ARG:HD2	11:Y:62:GLN:OE1	2.05	0.56
9:W:98:ARG:HD2	9:W:126:ILE:CD1	2.37	0.55
11:K:104:TRP:CE2	11:K:181:GLU:HB3	2.42	0.55
10:J:25:ILE:O	10:X:139:TYR:OH	2.21	0.55
10:J:139:TYR:OH	10:X:25:ILE:O	2.25	0.54
9:I:38:LYS:NZ	11:Y:208:ASN:O	2.40	0.54
11:Y:104:TRP:CE2	11:Y:181:GLU:HB3	2.42	0.54
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.90	0.54
8:V:196:ARG:NH2	9:W:150:GLU:O	2.40	0.54
8:V:53:GLU:HA	8:V:53:GLU:OE2	2.09	0.53
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.91	0.53
11:Y:61:ARG:HD3	11:Y:61:ARG:C	2.28	0.53
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.91	0.52
11:Y:72:GLU:OE1	11:Y:106:LYS:NZ	2.33	0.52
10:J:58:GLU:OE1	11:K:81:LYS:NZ	2.42	0.52
10:X:58:GLU:OE1	11:Y:81:LYS:NZ	2.43	0.52
8:H:53:GLU:OE2	8:H:53:GLU:HA	2.09	0.52
10:X:126:VAL:HG12	10:X:128:LEU:HG	1.90	0.51
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.76	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.51
2:B:93:HIS:HB3	18:B:301:HOH:O	2.11	0.50
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.76	0.50
9:W:98:ARG:CZ	9:W:126:ILE:HD11	2.42	0.49
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.94	0.49
10:X:1:MET:HB3	10:X:34:LYS:HE3	1.95	0.49
7:U:23:PHE:O	7:U:26:THR:HB	2.12	0.49
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.94	0.49
7:G:23:PHE:O	7:G:26:THR:HB	2.13	0.48
4:R:93:LEU:HD22	11:Y:61:ARG:HG3	1.94	0.48
10:J:1:MET:HB3	10:J:34:LYS:HE3	1.95	0.48
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.79	0.47
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.79	0.47
2:B:113:ARG:NE	18:B:301:HOH:O	2.35	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:98:ARG:HD2	9:W:126:ILE:HD12	1.97	0.47
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.97	0.47
3:C:51:LYS:O	3:C:52:LEU:HB2	2.14	0.47
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.97	0.46
4:R:89:VAL:HG12	11:Y:61:ARG:HG2	1.97	0.46
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.50	0.46
11:K:61:ARG:O	11:K:65:ILE:HG12	2.15	0.46
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.97	0.46
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.15	0.46
9:I:98:ARG:CD	9:I:126:ILE:HD12	2.45	0.46
14:N:21:THR:O	17:N:201:BO2:H3	2.16	0.46
11:K:31:VAL:HA	12:L:132:GLN:HE22	1.81	0.46
8:H:35:HIS:CB	8:H:56:THR:HG21	2.42	0.45
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.97	0.45
11:Y:61:ARG:O	11:Y:65:ILE:HG12	2.17	0.45
2:B:50:LYS:O	2:B:51:VAL:C	2.55	0.45
2:P:50:LYS:O	2:P:51:VAL:C	2.55	0.45
11:K:61:ARG:HD2	11:K:62:GLN:OE1	2.17	0.45
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.98	0.45
11:Y:208:ASN:ND2	18:Y:401:HOH:O	2.50	0.44
8:V:35:HIS:CB	8:V:56:THR:HG21	2.43	0.44
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.99	0.44
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.98	0.44
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.18	0.44
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.98	0.44
13:M:96:LEU:O	13:M:100:MET:HG2	2.18	0.44
3:C:35:LYS:HG2	3:C:158:SER:O	2.18	0.43
11:K:100:MET:SD	11:K:128:VAL:CG1	3.06	0.43
9:I:26:LEU:HD21	9:I:185:VAL:HG23	2.00	0.43
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.99	0.43
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.52	0.43
3:C:201:VAL:O	3:C:202:GLN:HB3	2.18	0.43
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.00	0.43
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.99	0.43
11:Y:100:MET:SD	11:Y:128:VAL:CG1	3.06	0.43
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.49	0.43
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.49	0.43
11:K:45:MET:HG2	11:K:52:CYS:HB3	2.01	0.43
11:Y:45:MET:HG2	11:Y:52:CYS:HB3	2.01	0.43
12:L:146:ILE:HG22	12:L:150:LEU:HD22	2.01	0.43
11:K:90:TYR:HA	11:K:93:MET:HG3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:50:LYS:HD3	2:P:50:LYS:HA	1.87	0.42
9:W:26:LEU:HD21	9:W:185:VAL:HG23	2.00	0.42
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	2.01	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.49	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.42
11:Y:90:TYR:HA	11:Y:93:MET:HG3	2.00	0.42
2:B:217:LYS:C	2:B:219:ALA:H	2.23	0.42
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.20	0.42
6:T:19:GLN:NE2	18:T:301:HOH:O	2.47	0.42
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.50	0.41
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.49	0.41
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.50	0.41
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.49	0.41
5:S:12:PHE:H	6:T:19:GLN:HE22	1.68	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.03	0.41
12:L:8:ASN:HA	12:L:30:ILE:O	2.21	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.41
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.02	0.41
10:J:36:ARG:NH1	10:J:58:GLU:OE2	2.54	0.41
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.03	0.41
5:E:12:PHE:H	6:F:19:GLN:HE22	1.69	0.41
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.51	0.41
2:P:217:LYS:C	2:P:219:ALA:H	2.23	0.41
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.02	0.41
10:X:36:ARG:NH1	10:X:58:GLU:OE2	2.54	0.41
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.51	0.41
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.21	0.41
11:K:38:ASN:OD1	11:K:38:ASN:C	2.59	0.40
11:K:83:LEU:HD12	11:K:101:ILE:HD11	2.04	0.40
11:Y:83:LEU:HD12	11:Y:101:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	34	60
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	34	60
2	B	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	9	23
2	P	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	9	23
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	19	43
3	Q	238/254 (94%)	232 (98%)	4 (2%)	2 (1%)	19	43
4	D	231/260 (89%)	230 (100%)	1 (0%)	0	100	100
4	R	231/260 (89%)	230 (100%)	1 (0%)	0	100	100
5	E	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
6	T	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
7	G	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
8	H	224/232 (97%)	219 (98%)	5 (2%)	0	100	100
8	V	224/232 (97%)	219 (98%)	5 (2%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
10	X	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
11	K	209/211 (99%)	205 (98%)	4 (2%)	0	100	100
11	Y	209/211 (99%)	205 (98%)	4 (2%)	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%)	221 (96%)	10 (4%)	0	100	100
13	a	231/246 (94%)	222 (96%)	9 (4%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6282/6612 (95%)	6134 (98%)	134 (2%)	14 (0%)	47	73

All (14) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	209/209 (100%)	206 (99%)	3 (1%)	67 86
1	O	209/209 (100%)	206 (99%)	3 (1%)	67 86
2	B	203/216 (94%)	199 (98%)	4 (2%)	55 81
2	P	203/216 (94%)	199 (98%)	4 (2%)	55 81
3	C	212/226 (94%)	202 (95%)	10 (5%)	26 54
3	Q	212/226 (94%)	202 (95%)	10 (5%)	26 54
4	D	194/215 (90%)	185 (95%)	9 (5%)	27 54
4	R	194/215 (90%)	185 (95%)	9 (5%)	27 54
5	E	190/193 (98%)	184 (97%)	6 (3%)	39 68
5	S	190/193 (98%)	184 (97%)	6 (3%)	39 68
6	F	201/239 (84%)	194 (96%)	7 (4%)	36 65
6	T	201/239 (84%)	194 (96%)	7 (4%)	36 65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	206/210 (98%)	200 (97%)	6 (3%)	42	71
7	U	206/210 (98%)	200 (97%)	6 (3%)	42	71
8	H	185/190 (97%)	177 (96%)	8 (4%)	29	57
8	V	185/190 (97%)	178 (96%)	7 (4%)	33	62
9	I	172/173 (99%)	168 (98%)	4 (2%)	50	78
9	W	172/173 (99%)	168 (98%)	4 (2%)	50	78
10	J	173/175 (99%)	170 (98%)	3 (2%)	60	84
10	X	173/175 (99%)	170 (98%)	3 (2%)	60	84
11	K	165/165 (100%)	151 (92%)	14 (8%)	10	24
11	Y	165/165 (100%)	150 (91%)	15 (9%)	9	21
12	L	186/186 (100%)	179 (96%)	7 (4%)	33	62
12	Z	186/186 (100%)	179 (96%)	7 (4%)	33	62
13	M	199/208 (96%)	193 (97%)	6 (3%)	41	70
13	a	199/208 (96%)	193 (97%)	6 (3%)	41	70
14	N	162/162 (100%)	156 (96%)	6 (4%)	34	63
14	b	162/162 (100%)	156 (96%)	6 (4%)	34	63
All	All	5314/5534 (96%)	5128 (96%)	186 (4%)	36	65

All (186) 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	55	LEU
2	B	113	ARG
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	206	LYS
3	C	240	GLU
4	D	99	ILE
4	D	125	LEU
4	D	143	ASP
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
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
5	E	202	ASP
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
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
7	G	236	LEU
8	H	22	GLN
8	H	30	ASN
8	H	35	HIS
8	H	43	CYS
8	H	53	GLU
8	H	68	LEU
8	H	113	ILE
8	H	196	ARG
9	I	37	ASN
9	I	126	ILE
9	I	171	LEU
9	I	182	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	3	ILE
10	J	23	ARG
10	J	99	GLN
11	K	4	LEU
11	K	12	VAL
11	K	21	THR
11	K	59	LEU
11	K	61	ARG
11	K	62	GLN
11	K	65	ILE
11	K	71	LYS
11	K	81	LYS
11	K	83	LEU
11	K	86	MET
11	K	117	GLU
11	K	128	VAL
11	K	210	ILE
12	L	23	LEU
12	L	49	ASN
12	L	126	ASP
12	L	128	VAL
12	L	132	GLN
12	L	137	ARG
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	39	ASP
14	N	83	LYS
14	N	104	ASP
14	N	178	LEU
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	55	LEU
2	P	113	ARG
2	P	191	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	206	LYS
3	Q	240	GLU
4	R	99	ILE
4	R	125	LEU
4	R	143	ASP
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
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
5	S	188	LEU
5	S	202	ASP
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
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
7	U	236	LEU
8	V	30	ASN
8	V	35	HIS
8	V	43	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	V	53	GLU
8	V	68	LEU
8	V	113	ILE
8	V	196	ARG
9	W	37	ASN
9	W	126	ILE
9	W	171	LEU
9	W	182	TRP
10	X	3	ILE
10	X	23	ARG
10	X	99	GLN
11	Y	4	LEU
11	Y	12	VAL
11	Y	21	THR
11	Y	37	ILE
11	Y	59	LEU
11	Y	61	ARG
11	Y	62	GLN
11	Y	65	ILE
11	Y	71	LYS
11	Y	81	LYS
11	Y	83	LEU
11	Y	86	MET
11	Y	117	GLU
11	Y	128	VAL
11	Y	210	ILE
12	Z	23	LEU
12	Z	49	ASN
12	Z	126	ASP
12	Z	128	VAL
12	Z	132	GLN
12	Z	137	ARG
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	39	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	b	83	LYS
14	b	104	ASP
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
3	C	17	GLN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	91	HIS
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
8	H	57	GLN
8	H	66	HIS
8	H	86	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	37	ASN
10	J	55	GLN
11	K	85	ASN
11	K	175	ASN
11	K	207	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	79	HIS
12	L	94	GLN
12	L	132	GLN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
2	P	20	GLN
2	P	58	GLN
2	P	119	GLN
2	P	123	GLN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	146	GLN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
7	U	83	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
8	V	57	GLN
8	V	86	HIS
9	W	37	ASN
10	X	55	GLN
11	Y	85	ASN
11	Y	175	ASN
11	Y	207	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	79	HIS
12	Z	94	GLN
12	Z	158	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN
14	b	161	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 14 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	V	301	8	25,29,29	1.60	5 (20%)	32,38,38	1.40	4 (12%)
17	BO2	K	301	11	25,29,29	1.62	5 (20%)	32,38,38	1.32	4 (12%)
17	BO2	H	301	8	25,29,29	1.61	5 (20%)	32,38,38	1.39	4 (12%)
17	BO2	N	201	14	25,29,29	1.58	5 (20%)	32,38,38	1.30	4 (12%)
17	BO2	b	201	14	25,29,29	1.59	5 (20%)	32,38,38	1.28	4 (12%)
17	BO2	Y	301	11	25,29,29	1.60	5 (20%)	32,38,38	1.30	3 (9%)

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	V	301	8	-	4/22/28/28	0/2/2/2
17	BO2	K	301	11	-	0/22/28/28	0/2/2/2
17	BO2	H	301	8	-	4/22/28/28	0/2/2/2
17	BO2	N	201	14	-	6/22/28/28	0/2/2/2
17	BO2	b	201	14	-	6/22/28/28	0/2/2/2
17	BO2	Y	301	11	-	0/22/28/28	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	-4.50	1.39	1.50
17	V	301	BO2	C2-C7	-4.46	1.39	1.50
17	Y	301	BO2	C2-C7	-4.40	1.39	1.50
17	K	301	BO2	C2-C7	-4.32	1.40	1.50
17	b	201	BO2	C2-C7	-4.32	1.40	1.50
17	N	201	BO2	C2-C7	-4.29	1.40	1.50
17	b	201	BO2	C11-C12	-4.14	1.41	1.51
17	V	301	BO2	C11-C12	-4.14	1.41	1.51
17	H	301	BO2	C11-C12	-4.12	1.41	1.51
17	N	201	BO2	C11-C12	-4.09	1.41	1.51
17	K	301	BO2	C11-C12	-4.01	1.41	1.51
17	Y	301	BO2	C11-C12	-4.00	1.41	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	301	BO2	C3-N4	3.17	1.41	1.34
17	Y	301	BO2	C3-N4	3.10	1.41	1.34
17	b	201	BO2	C6-N1	3.01	1.40	1.34
17	N	201	BO2	C6-N1	2.99	1.40	1.34
17	V	301	BO2	C6-N1	2.97	1.40	1.34
17	K	301	BO2	C6-N1	2.92	1.40	1.34
17	H	301	BO2	C6-N1	2.90	1.40	1.34
17	H	301	BO2	C3-N4	2.88	1.40	1.34
17	V	301	BO2	C3-N4	2.88	1.40	1.34
17	Y	301	BO2	C6-N1	2.86	1.40	1.34
17	b	201	BO2	C3-N4	2.75	1.40	1.34
17	N	201	BO2	C3-N4	2.74	1.40	1.34
17	K	301	BO2	C5-N4	2.44	1.41	1.33
17	H	301	BO2	C5-N4	2.34	1.40	1.33
17	Y	301	BO2	C5-N4	2.31	1.40	1.33
17	V	301	BO2	C5-N4	2.30	1.40	1.33
17	b	201	BO2	C5-N4	2.12	1.40	1.33
17	N	201	BO2	C5-N4	2.07	1.39	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	V	301	BO2	C21-C22-C23	-4.86	109.29	115.39
17	H	301	BO2	C21-C22-C23	-4.82	109.34	115.39
17	K	301	BO2	C21-C22-C23	-3.62	110.85	115.39
17	Y	301	BO2	C21-C22-C23	-3.55	110.94	115.39
17	K	301	BO2	C6-N1-C2	3.51	121.48	116.93
17	Y	301	BO2	C6-N1-C2	3.38	121.31	116.93
17	b	201	BO2	C21-C22-C23	-3.29	111.26	115.39
17	V	301	BO2	C6-N1-C2	3.28	121.19	116.93
17	H	301	BO2	C6-N1-C2	3.25	121.15	116.93
17	N	201	BO2	C21-C22-C23	-3.25	111.32	115.39
17	N	201	BO2	C6-N1-C2	3.23	121.12	116.93
17	b	201	BO2	C6-N1-C2	3.16	121.03	116.93
17	V	301	BO2	C12-C11-C10	-2.26	107.14	113.39
17	H	301	BO2	C12-C11-C10	-2.26	107.16	113.39
17	b	201	BO2	C11-C10-N9	-2.22	106.11	110.79
17	N	201	BO2	C6-C5-N4	-2.20	119.20	121.95
17	Y	301	BO2	C6-C5-N4	-2.19	119.21	121.95
17	N	201	BO2	C11-C10-N9	-2.17	106.21	110.79
17	K	301	BO2	C6-C5-N4	-2.13	119.29	121.95
17	V	301	BO2	C6-C5-N4	-2.05	119.39	121.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	201	BO2	C6-C5-N4	-2.04	119.41	121.95
17	K	301	BO2	C18-C10-N9	-2.03	105.63	111.16
17	H	301	BO2	C6-C5-N4	-2.00	119.45	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	V	301	BO2	C3-C2-C7-O8
17	V	301	BO2	C3-C2-C7-N9
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	N	201	BO2	N1-C2-C7-O8
17	b	201	BO2	N1-C2-C7-O8
17	N	201	BO2	N1-C2-C7-N9
17	b	201	BO2	N1-C2-C7-N9
17	N	201	BO2	C3-C2-C7-O8
17	b	201	BO2	C3-C2-C7-O8
17	N	201	BO2	C3-C2-C7-N9
17	b	201	BO2	C3-C2-C7-N9
17	N	201	BO2	C21-C22-C23-C25
17	b	201	BO2	C21-C22-C23-C25
17	N	201	BO2	C21-C22-C23-C24
17	b	201	BO2	C21-C22-C23-C24

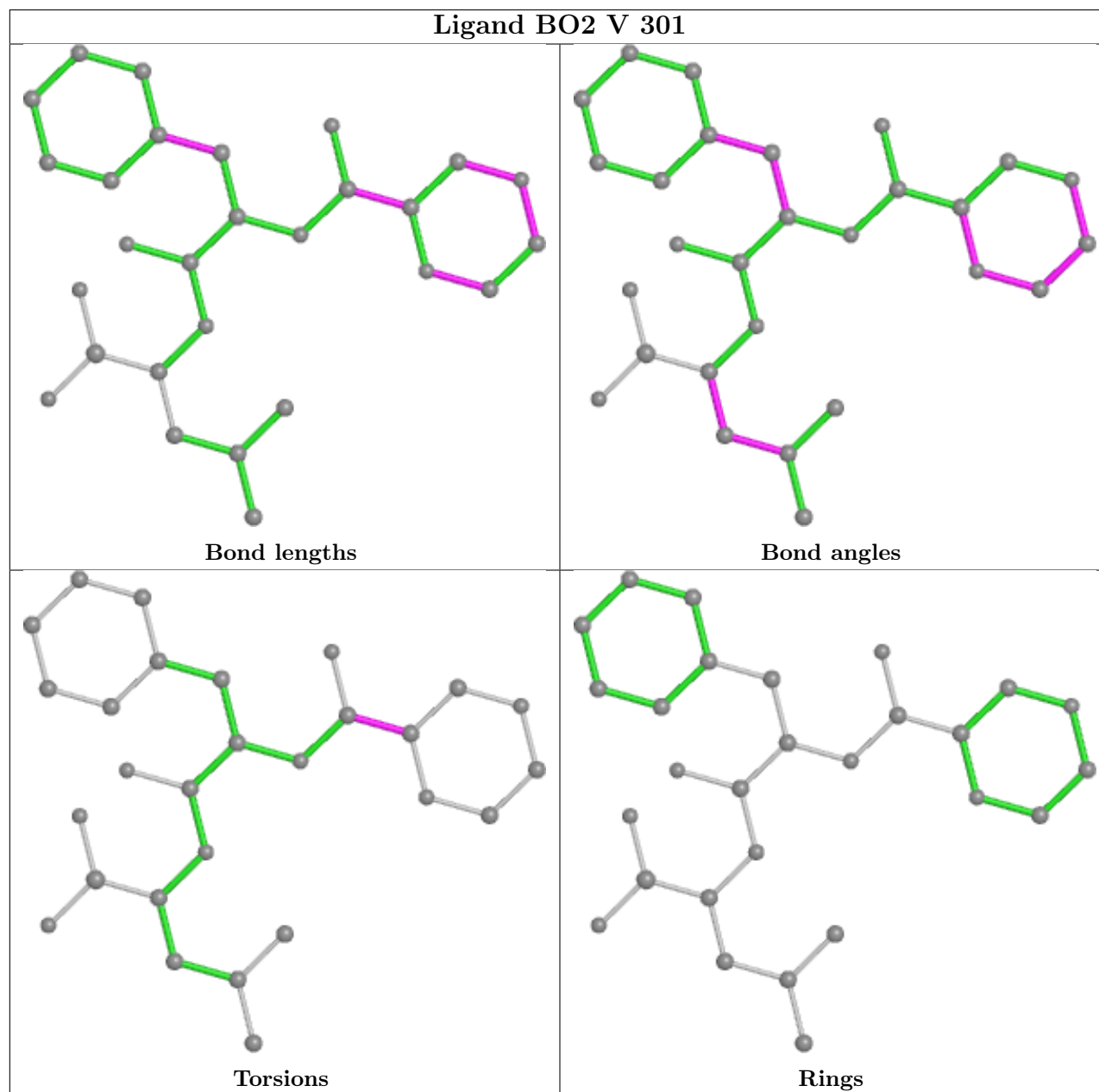
There are no ring outliers.

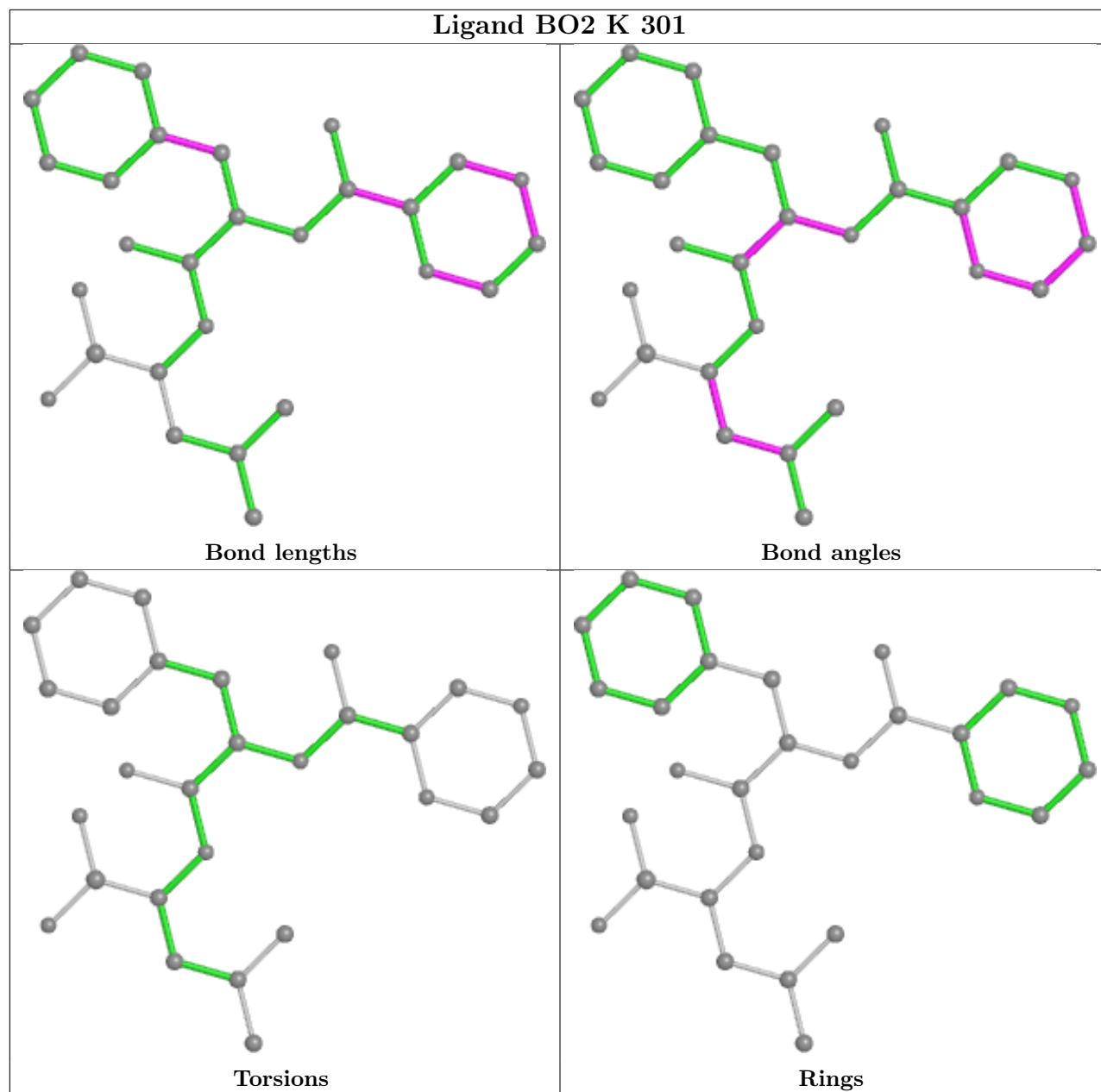
1 monomer is involved in 1 short contact:

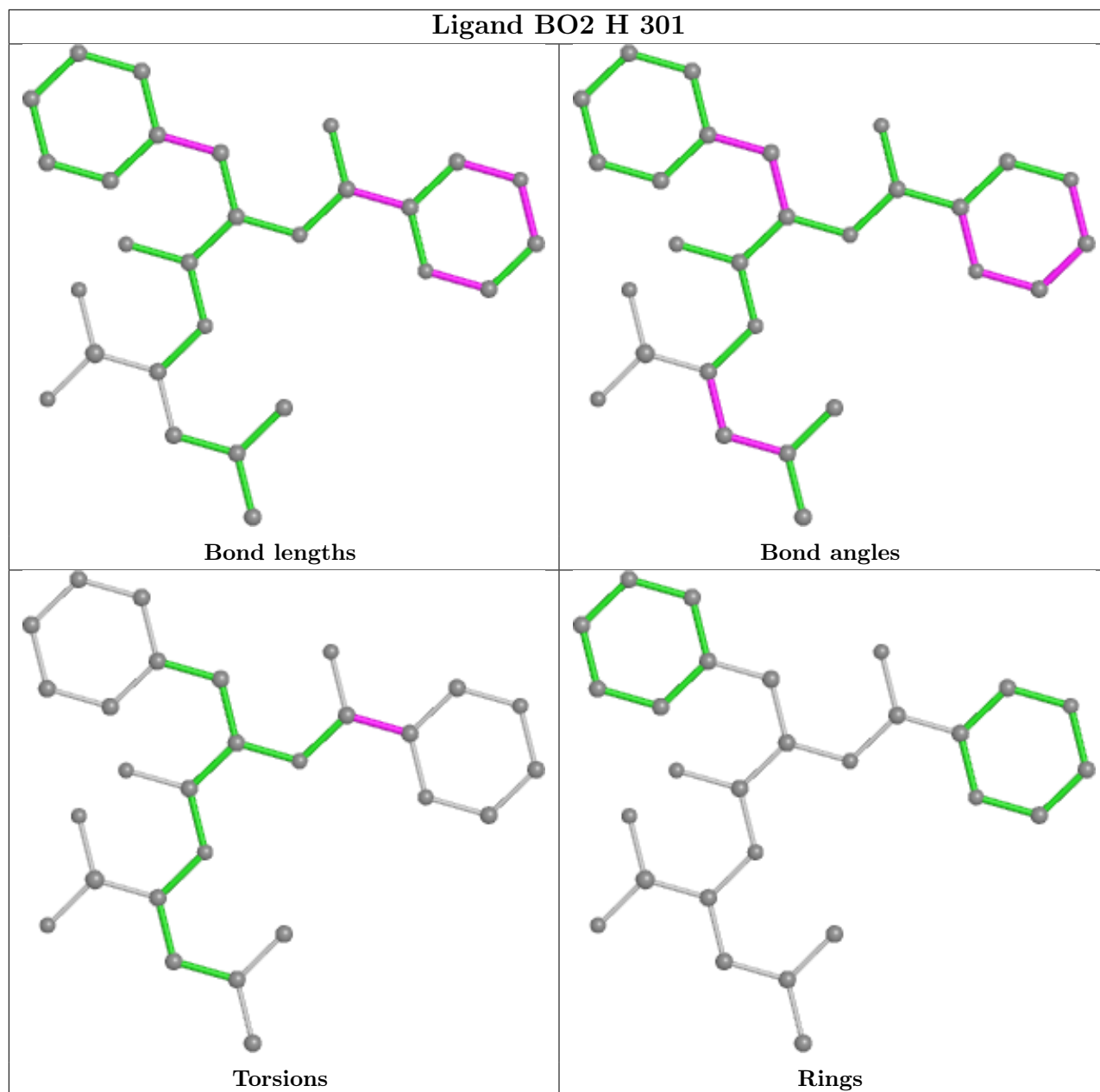
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	N	201	BO2	1	0

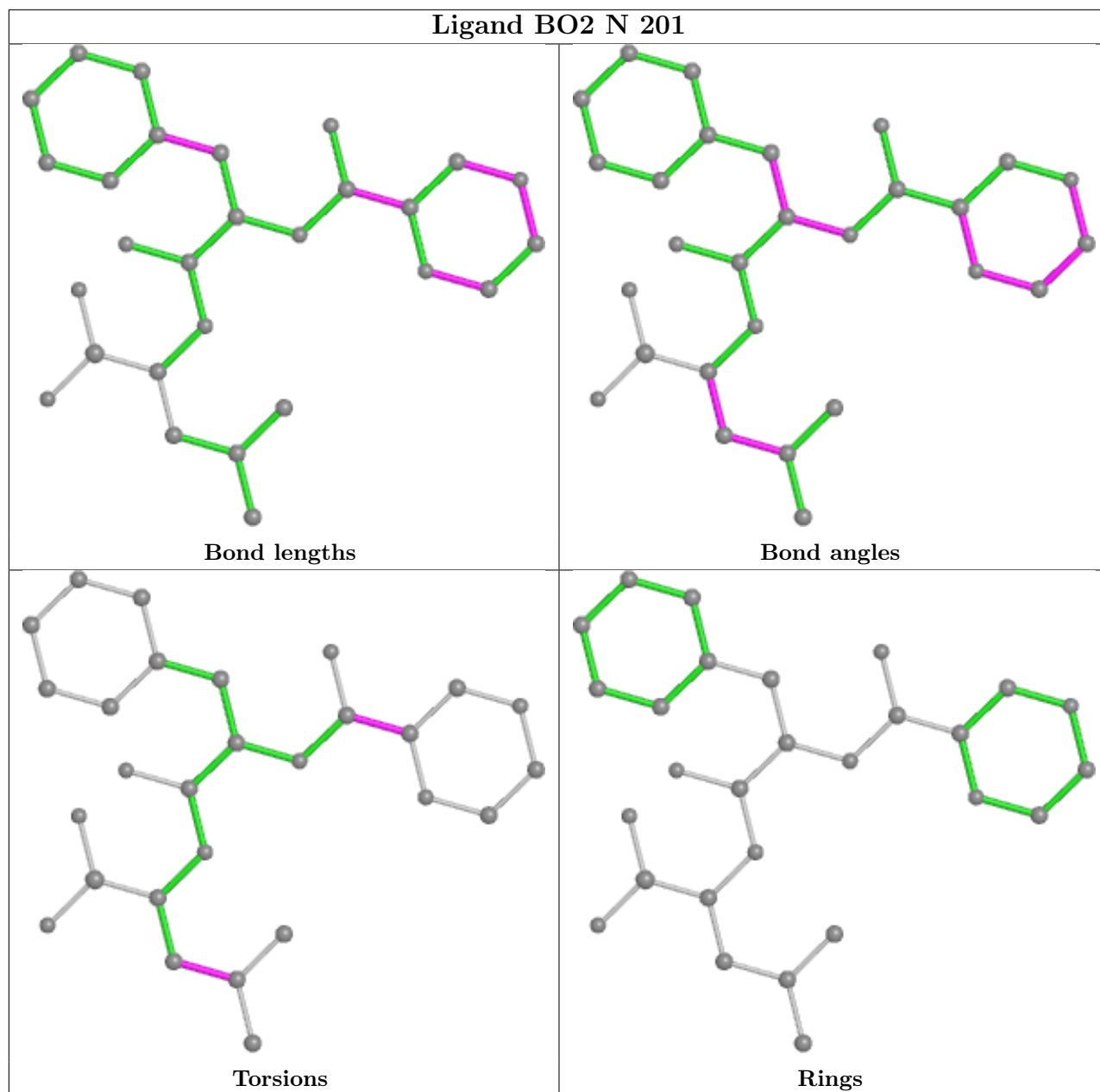
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

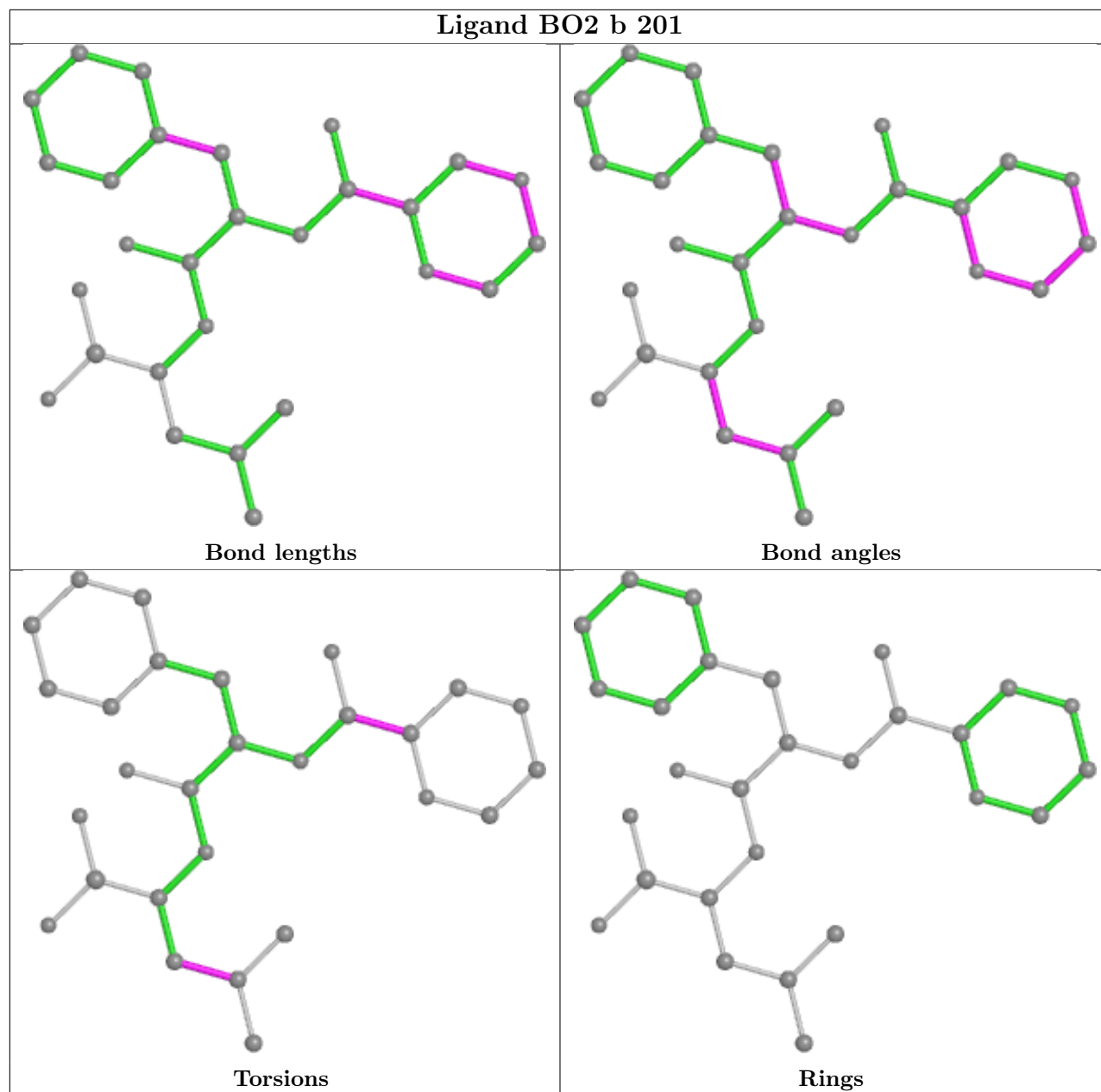
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

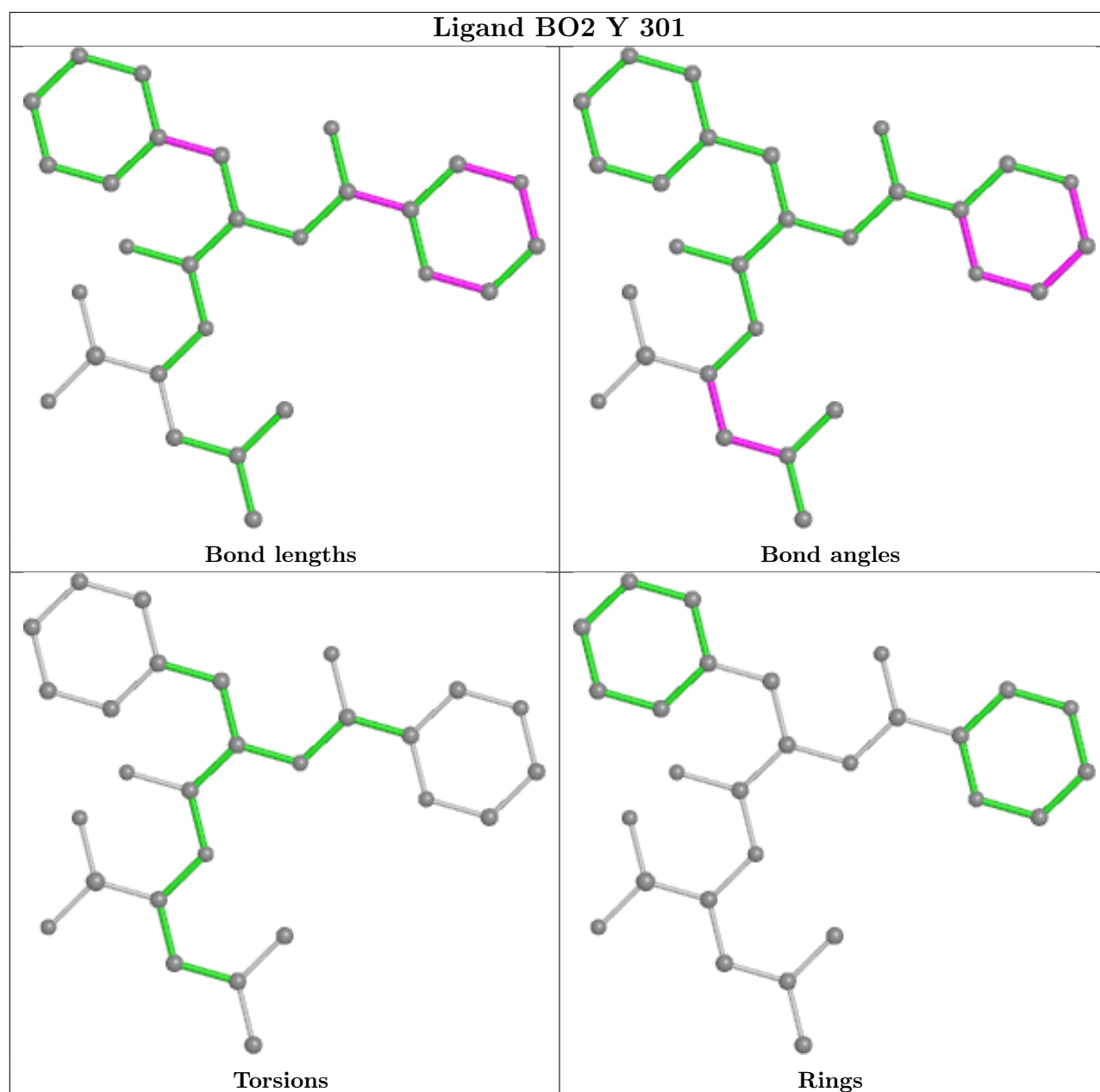












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	250/250 (100%)	-0.29	10 (4%) 38 37	32, 49, 86, 126	0
1	O	250/250 (100%)	-0.22	9 (3%) 42 42	35, 52, 99, 133	0
2	B	244/258 (94%)	-0.22	9 (3%) 41 41	35, 53, 98, 151	0
2	P	244/258 (94%)	-0.16	9 (3%) 41 41	38, 55, 99, 149	0
3	C	240/254 (94%)	0.02	17 (7%) 16 14	33, 61, 133, 172	0
3	Q	240/254 (94%)	0.10	21 (8%) 10 8	30, 67, 144, 187	0
4	D	235/260 (90%)	-0.31	4 (1%) 70 72	39, 56, 86, 127	0
4	R	235/260 (90%)	-0.16	7 (2%) 50 51	46, 64, 103, 135	0
5	E	231/234 (98%)	-0.17	7 (3%) 50 51	39, 59, 100, 146	0
5	S	231/234 (98%)	-0.16	10 (4%) 35 33	42, 64, 101, 138	0
6	F	243/288 (84%)	-0.37	8 (3%) 46 46	33, 53, 102, 128	0
6	T	243/288 (84%)	-0.22	10 (4%) 37 36	35, 61, 114, 147	0
7	G	241/252 (95%)	-0.35	7 (2%) 51 52	32, 50, 91, 150	0
7	U	241/252 (95%)	-0.33	6 (2%) 57 59	33, 50, 87, 129	0
8	H	226/232 (97%)	-0.45	4 (1%) 68 70	29, 45, 83, 149	0
8	V	226/232 (97%)	-0.37	7 (3%) 49 49	31, 45, 81, 155	0
9	I	204/205 (99%)	-0.60	1 (0%) 91 92	29, 45, 72, 97	0
9	W	204/205 (99%)	-0.57	1 (0%) 91 92	31, 47, 76, 98	0
10	J	195/198 (98%)	-0.37	5 (2%) 56 57	32, 51, 83, 126	0
10	X	195/198 (98%)	-0.34	5 (2%) 56 57	36, 54, 82, 128	0
11	K	211/211 (100%)	-0.24	6 (2%) 53 54	37, 56, 87, 116	0
11	Y	211/211 (100%)	-0.29	2 (0%) 84 85	37, 57, 90, 115	0
12	L	222/222 (100%)	-0.28	3 (1%) 75 77	40, 53, 100, 128	0
12	Z	222/222 (100%)	-0.26	3 (1%) 75 77	39, 55, 101, 132	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.52	2 (0%) 84 85	30, 47, 70, 88	0
13	a	233/246 (94%)	-0.51	1 (0%) 92 93	31, 48, 71, 90	0
14	N	196/196 (100%)	-0.55	2 (1%) 82 83	28, 43, 73, 100	0
14	b	196/196 (100%)	-0.58	1 (0%) 91 92	30, 43, 73, 102	0
All	All	6342/6612 (95%)	-0.31	177 (2%) 53 54	28, 53, 98, 187	0

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	1	MET	7.8
10	J	1	MET	7.7
9	W	1	SER	6.4
10	X	1	MET	6.3
3	Q	240	GLU	6.2
2	P	218	GLY	6.0
1	O	249	ALA	5.9
5	E	202	ASP	5.7
2	B	221	ASP	5.5
12	Z	174	TYR	5.5
3	Q	238	LYS	5.5
2	P	51	VAL	5.4
2	P	219	ALA	5.1
7	G	2	GLY	4.9
1	A	1	MET	4.9
3	Q	206	LYS	4.8
3	C	206	LYS	4.8
2	B	218	GLY	4.7
12	L	174	TYR	4.5
3	Q	50	LEU	4.5
3	C	202	GLN	4.4
2	B	220	ASN	4.4
8	V	224	GLN	4.4
2	B	51	VAL	4.3
3	C	238	LYS	4.3
14	N	195	GLN	4.2
3	Q	202	GLN	4.2
10	X	194	ASP	4.1
3	C	239	GLN	4.1
9	I	1	SER	4.1
8	V	222	ASP	4.0
3	Q	205	ALA	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	Q	236	GLN	4.0
7	U	2	GLY	3.9
2	P	221	ASP	3.9
5	S	202	ASP	3.9
1	O	2	THR	3.9
10	J	194	ASP	3.9
1	A	231	LYS	3.9
6	F	181	GLU	3.9
1	A	249	ALA	3.7
3	Q	225	GLU	3.7
3	Q	239	GLN	3.7
6	T	243	ILE	3.6
4	R	1	ASP	3.6
6	F	202	ASP	3.6
3	C	50	LEU	3.5
3	Q	49	THR	3.4
5	S	3	ASN	3.3
11	K	146	ASP	3.3
11	Y	146	ASP	3.3
4	R	241	ALA	3.3
4	R	125	LEU	3.3
3	C	225	GLU	3.3
8	H	226	GLU	3.2
1	A	2	THR	3.2
8	V	226	GLU	3.2
1	O	201	GLU	3.1
6	T	244	ASN	3.1
6	T	181	GLU	3.1
8	H	224	GLN	3.1
7	U	242	GLN	3.1
7	G	3	TYR	3.1
13	a	1	THR	3.1
6	T	2	THR	3.0
4	D	242	GLU	3.0
2	P	203	SER	3.0
11	K	211	GLY	2.9
12	Z	173	LYS	2.9
3	C	240	GLU	2.9
6	T	201	GLU	2.9
10	X	193	ASP	2.9
11	K	144	LYS	2.9
2	P	220	ASN	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	59	PRO	2.9
3	C	180	LYS	2.9
2	B	217	LYS	2.9
1	O	250	LEU	2.9
5	E	201	ARG	2.9
3	C	49	THR	2.8
7	G	242	GLN	2.8
4	D	117	GLU	2.8
3	C	236	GLN	2.8
1	A	201	GLU	2.8
7	G	241	GLU	2.8
5	S	173	ARG	2.8
3	Q	141	ASP	2.8
8	V	145	ASP	2.7
2	B	59	ASP	2.7
1	O	248	GLU	2.7
4	R	217	GLN	2.7
5	E	233	ILE	2.7
3	Q	237	GLU	2.7
2	B	186	ASP	2.7
7	G	188	GLU	2.7
5	S	203	GLU	2.7
6	F	244	ASN	2.7
3	C	235	GLU	2.6
10	J	193	ASP	2.6
12	L	1	GLN	2.6
6	F	205	GLU	2.6
1	A	248	GLU	2.5
3	Q	180	LYS	2.5
4	R	242	GLU	2.5
11	K	9	ARG	2.5
14	b	195	GLN	2.5
1	A	166	LYS	2.5
1	O	231	LYS	2.5
6	F	2	THR	2.5
5	S	123	GLY	2.5
3	Q	187	GLU	2.5
6	T	241	LYS	2.5
7	U	222	ASP	2.5
6	T	205	GLU	2.4
7	G	179	LYS	2.4
1	O	52	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	P	59	ASP	2.4
5	E	54	GLU	2.4
7	U	181	LYS	2.4
3	Q	181	GLU	2.4
11	Y	9	ARG	2.4
3	C	216	ASP	2.4
8	V	221	CYS	2.4
3	Q	234	ILE	2.4
6	F	215	CYS	2.3
2	B	201	ASP	2.3
2	B	219	ALA	2.3
13	M	1	THR	2.3
10	J	95	ARG	2.3
5	S	180	LYS	2.3
8	V	9	ASN	2.3
3	C	234	ILE	2.3
6	F	243	ILE	2.3
14	N	181	ALA	2.3
1	A	229	THR	2.3
6	T	215	CYS	2.3
5	S	233	ILE	2.3
5	E	180	LYS	2.2
5	S	207	VAL	2.2
8	V	223	ILE	2.2
1	A	250	LEU	2.2
3	C	175	LYS	2.2
5	E	173	ARG	2.2
7	U	241	GLU	2.2
10	J	23	ARG	2.2
13	M	47	ASP	2.2
7	U	3	TYR	2.2
8	H	222	ASP	2.2
2	P	52	THR	2.2
3	Q	203	THR	2.2
10	X	95	ARG	2.2
12	L	173	LYS	2.1
1	O	182	GLU	2.1
4	D	125	LEU	2.1
5	E	217	LYS	2.1
5	S	217	LYS	2.1
2	P	217	LYS	2.1
12	Z	167	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	R	230	GLU	2.1
3	Q	3	ASP	2.1
7	G	222	ASP	2.1
8	H	145	ASP	2.1
6	F	228	LYS	2.1
3	Q	216	ASP	2.1
4	R	117	GLU	2.1
11	K	182	ASP	2.1
6	T	180	PRO	2.1
6	T	230	ASP	2.1
3	C	203	THR	2.0
3	Q	223	SER	2.0
5	S	225	ASP	2.0
3	C	229	GLN	2.0
4	D	217	GLN	2.0
3	Q	233	GLN	2.0
10	X	195	PHE	2.0
11	K	150	GLU	2.0
1	A	54	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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 ²)	Q<0.9
15	MG	Z	301	1/1	0.86	0.22	74,74,74,74	0
17	BO2	N	201	28/28	0.88	0.21	28,40,49,50	0
15	MG	K	303	1/1	0.89	0.33	67,67,67,67	0
17	BO2	V	301	28/28	0.89	0.20	50,57,69,69	0

Continued on next page...

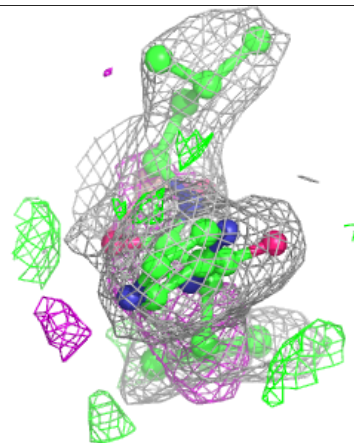
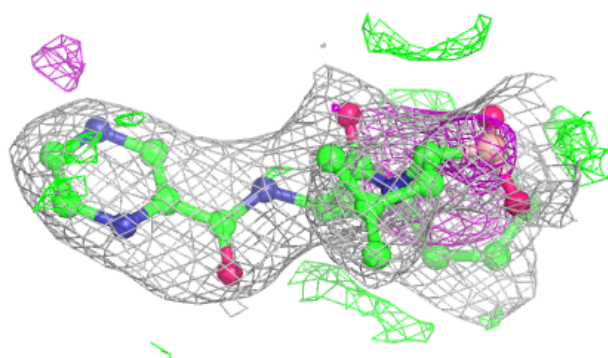
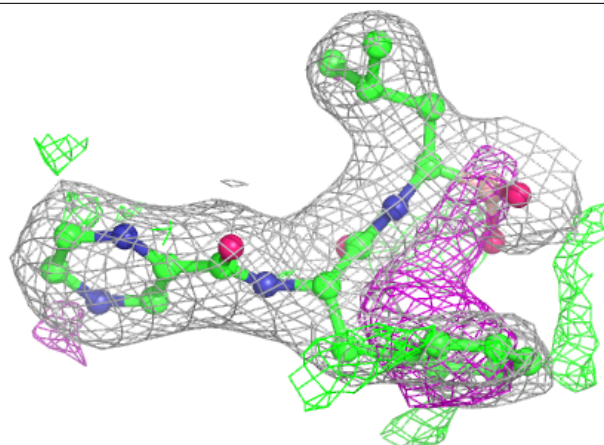
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
17	BO2	H	301	28/28	0.91	0.19	52,56,65,67	0
17	BO2	Y	301	28/28	0.92	0.22	40,44,59,61	0
17	BO2	b	201	28/28	0.92	0.19	31,41,51,52	0
15	MG	I	302	1/1	0.93	0.24	79,79,79,79	0
17	BO2	K	301	28/28	0.93	0.21	38,43,57,60	0
15	MG	G	301	1/1	0.94	0.07	44,44,44,44	0
15	MG	I	301	1/1	0.95	0.13	56,56,56,56	0
15	MG	L	301	1/1	0.98	0.06	51,51,51,51	0
15	MG	N	202	1/1	0.98	0.07	46,46,46,46	0
15	MG	J	201	1/1	0.98	0.24	47,47,47,47	0
16	CL	U	301	1/1	0.99	0.14	38,38,38,38	0
16	CL	b	202	1/1	0.99	0.06	47,47,47,47	0
15	MG	K	302	1/1	0.99	0.09	52,52,52,52	0
16	CL	N	203	1/1	0.99	0.03	43,43,43,43	0
16	CL	G	302	1/1	1.00	0.15	36,36,36,36	0
15	MG	I	303	1/1	1.00	0.05	48,48,48,48	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.

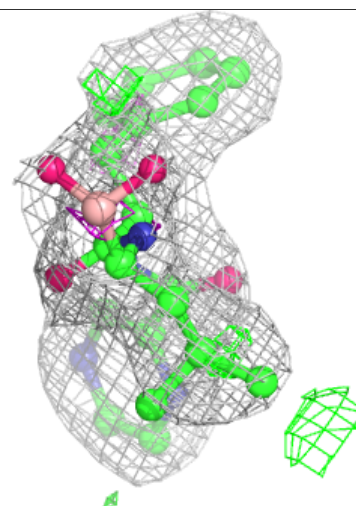
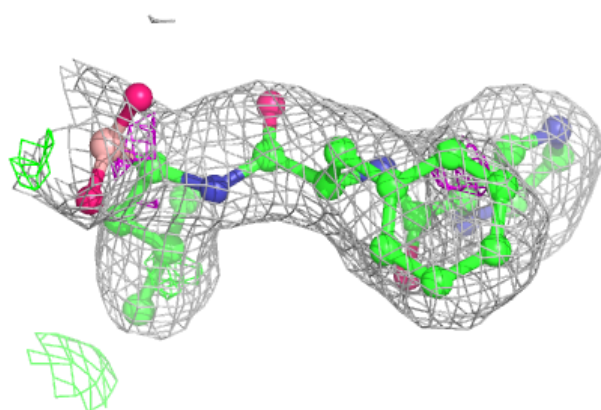
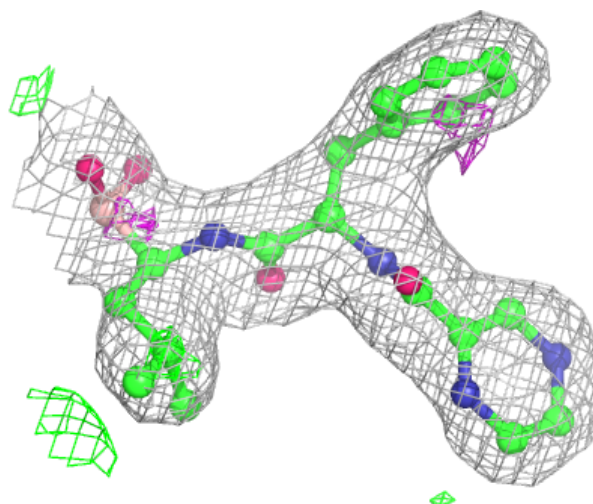
Electron density around BO2 N 201:

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



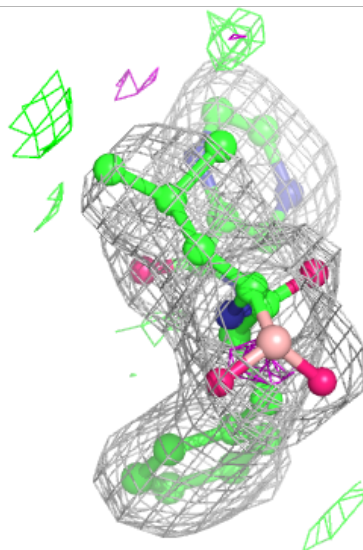
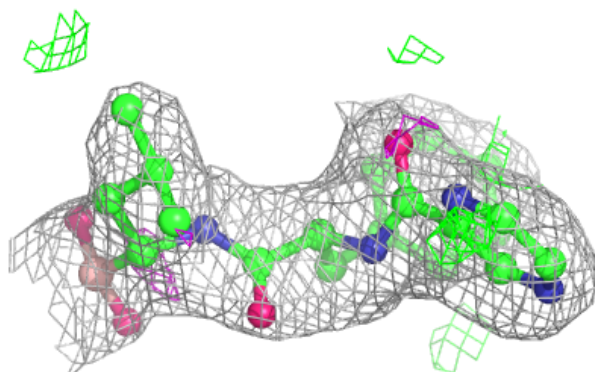
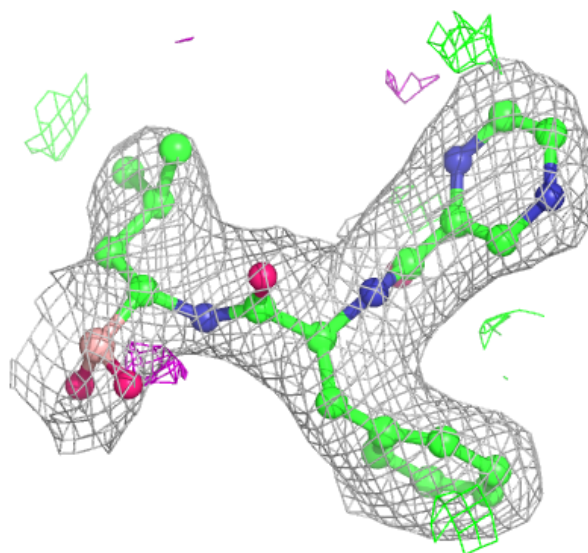
Electron density around BO2 V 301:

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



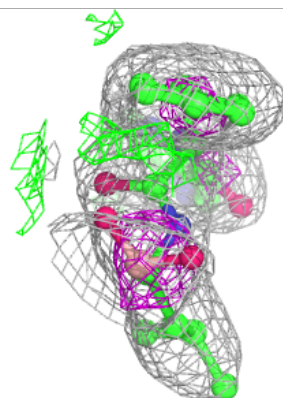
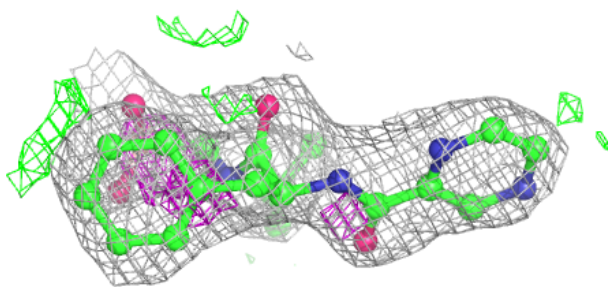
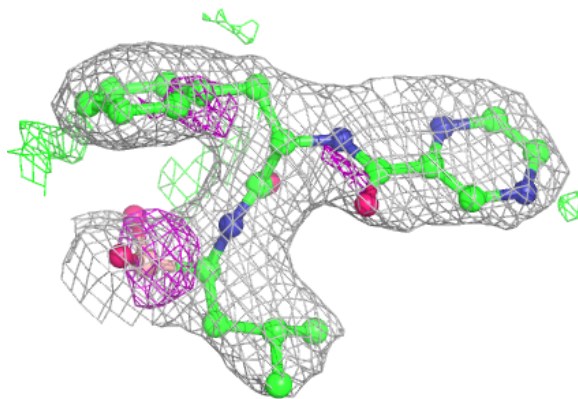
Electron density around BO2 H 301:

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



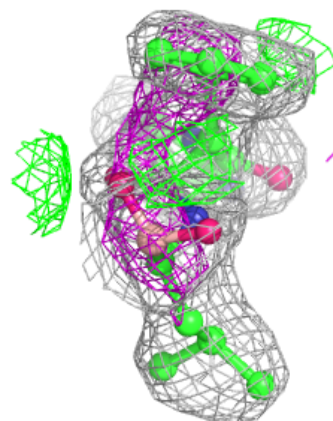
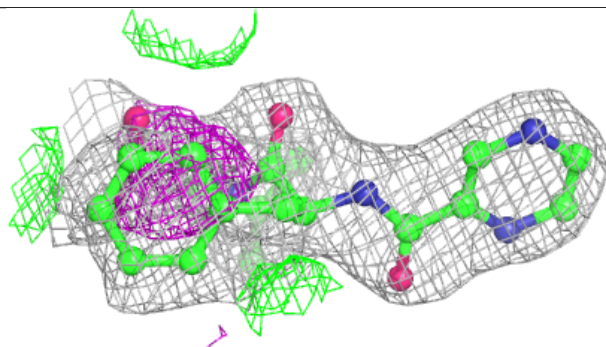
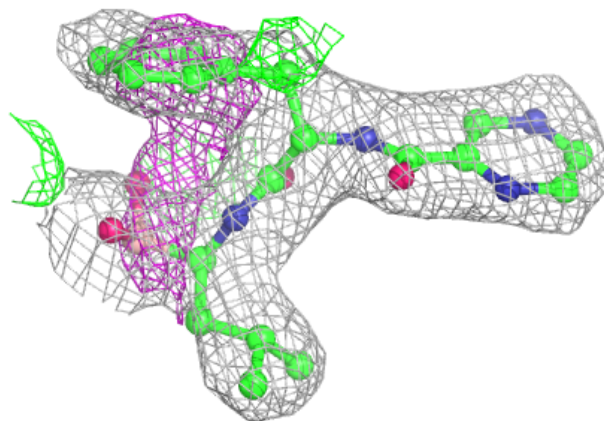
Electron density around BO2 Y 301:

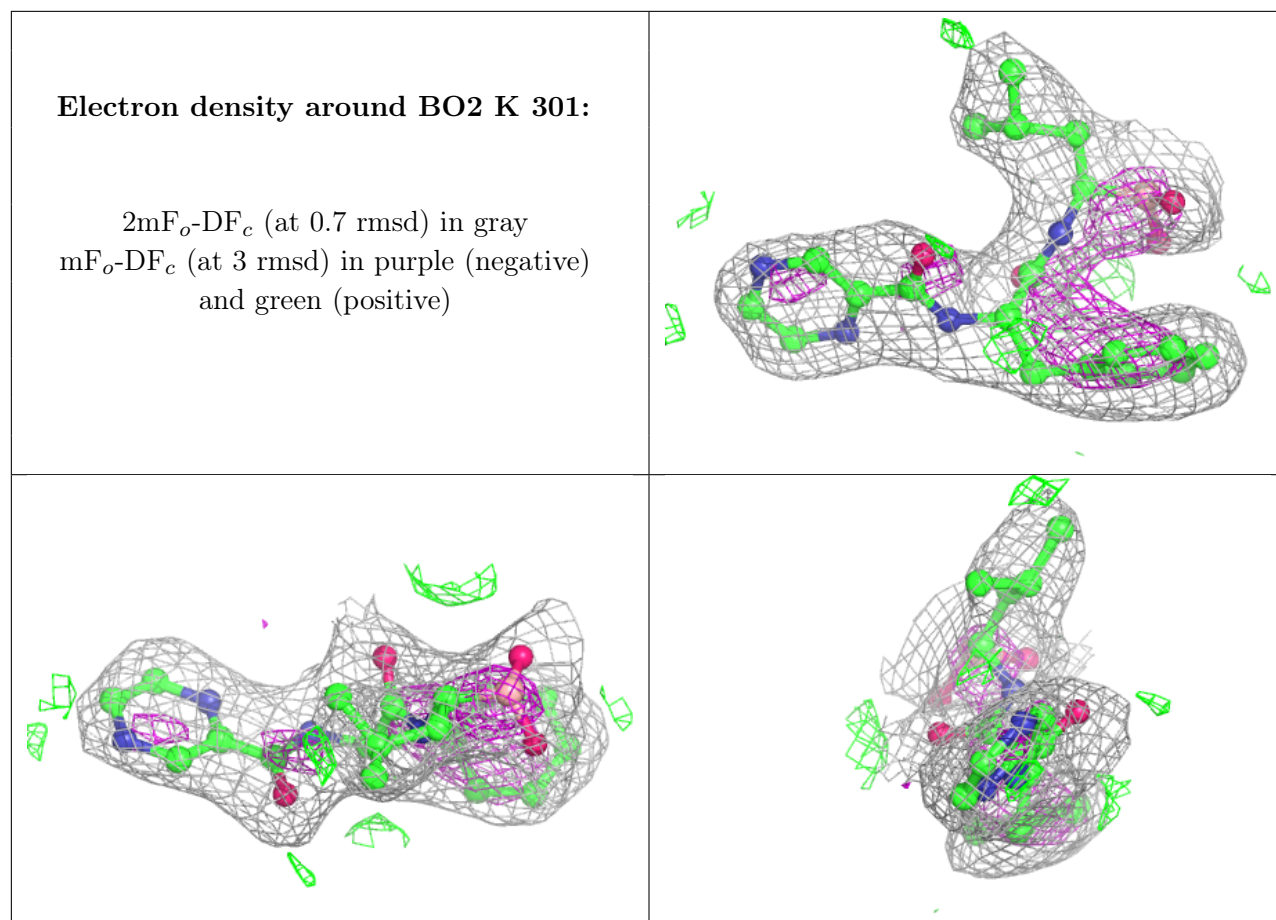
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BO2 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)





6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.