



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 19, 2026 – 12:16 AM UTC

PDB ID : 5LF3 / pdb\_00005lf3  
Title : Human 20S proteasome complex with Bortezomib at 2.1 Angstrom  
Authors : Schrader, J.; Henneberg, F.; Mata, R.; Tittmann, K.; Schneider, T.R.; Stark, H.; Bourenkov, G.; Chari, A.  
Deposited on : 2016-06-30  
Resolution : 2.10 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

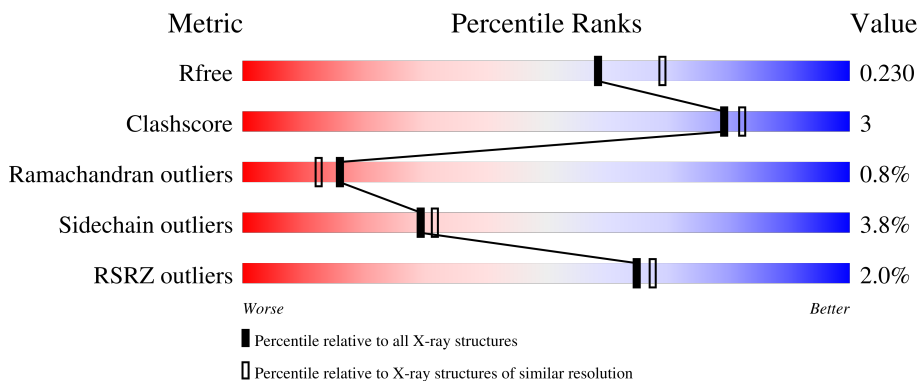
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



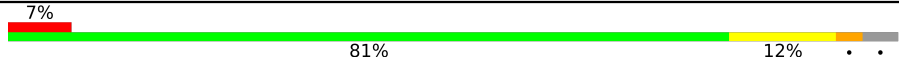

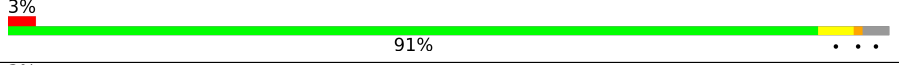



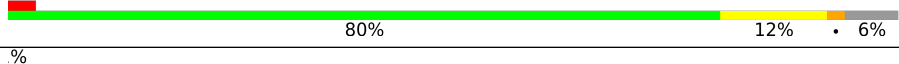
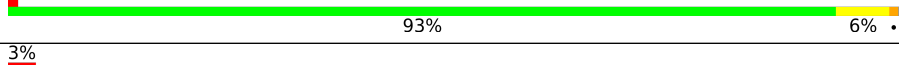
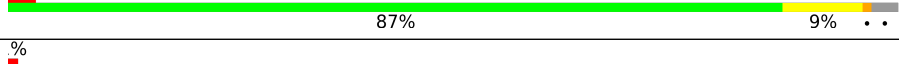
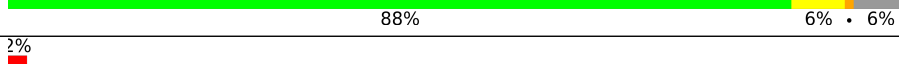

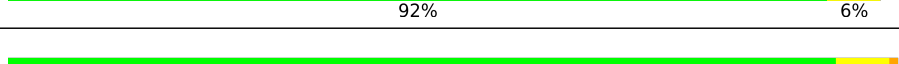
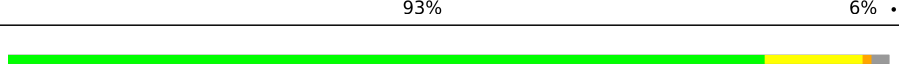
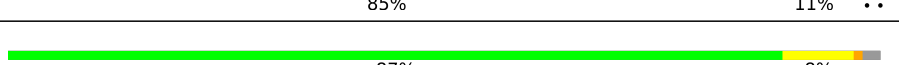

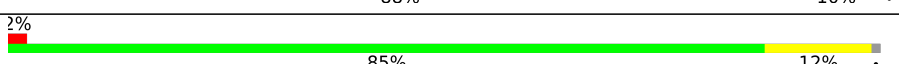
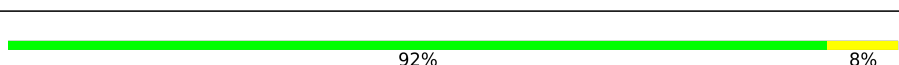
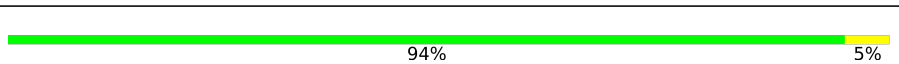
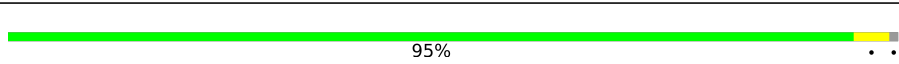
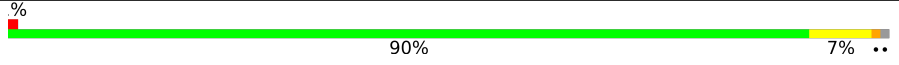
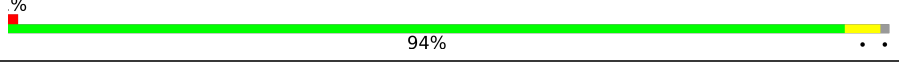
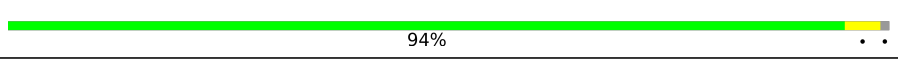

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	234	 2% 87% 9% . .
1	O	234	 6% 91% 6% . .
2	B	261	 2% 87% 7% . 5%
2	P	261	 3% 84% 9% . 5%
3	C	248	 2% 85% 8% . .

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Mol	Chain	Length	Quality of chain
3	Q	248	
4	D	241	
4	R	241	
5	E	263	
5	S	263	
6	F	255	
6	T	255	
7	G	246	
7	U	246	
8	H	234	
8	V	234	
9	I	205	
9	W	205	
10	J	201	
10	X	201	
11	K	204	
11	Y	204	
12	L	213	
12	Z	213	
13	M	219	
13	a	219	
14	N	205	
14	b	205	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	6V1	U	47	X	-	-	-

## 2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 52211 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	230	Total	C	N	O	S	0	3	0
			1788	1145	301	336	6			
1	O	230	Total	C	N	O	S	0	0	0
			1741	1111	293	331	6			

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	248	Total	C	N	O	S	0	2	0
			1926	1220	332	363	11			
2	P	248	Total	C	N	O	S	0	2	0
			1909	1206	325	367	11			

- Molecule 3 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	237	Total	C	N	O	S	0	2	0
			1798	1121	320	352	5			
3	Q	239	Total	C	N	O	S	0	0	0
			1820	1136	320	359	5			

- 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	233	Total	C	N	O	S	0	1	0
			1762	1105	290	356	11			
4	R	233	Total	C	N	O	S	0	1	0
			1753	1103	293	346	11			

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	234	Total	C	N	O	S	0	1	0
			1822	1144	325	342	11			
5	S	238	Total	C	N	O	S	0	3	0
			1875	1175	340	349	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	148	6V1	CYS	engineered mutation	UNP P25786
S	148	6V1	CYS	engineered mutation	UNP P25786

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	239	Total	C	N	O	S	0	4	0
			1888	1198	325	353	12			
6	T	240	Total	C	N	O	S	0	1	0
			1856	1178	315	351	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	244	Total	C	N	O	S	0	2	0
			1912	1214	321	364	13			
7	U	238	Total	C	N	O	S	0	1	0
			1815	1147	304	350	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	220	Total	C	N	O	S	0	2	0
			1664	1047	284	320	13			
8	V	220	Total	C	N	O	S	0	2	0
			1622	1023	269	318	12			

- 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	3	0
			1613	1028	270	295	20			
9	W	204	Total	C	N	O	S	0	2	0
			1599	1018	267	295	19			

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	196	Total	C	N	O	S	0	3	0
			1590	1021	271	288	10			
10	X	196	Total	C	N	O	S	0	2	0
			1574	1012	267	285	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	200	Total	C	N	O	S	0	1	0
			1550	978	269	293	10			
11	Y	201	Total	C	N	O	S	0	3	0
			1580	996	280	294	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	213	Total	C	N	O	S	0	2	0
			1636	1038	277	310	11			
12	Z	213	Total	C	N	O	S	0	1	0
			1642	1041	280	310	11			

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	216	Total	C	N	O	S	0	1	0
			1692	1067	291	322	12			
13	a	216	Total	C	N	O	S	0	2	0
			1688	1064	291	321	12			

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	202	Total	C	N	O	S	0	1	0
			1519	953	258	295	13			
14	b	203	Total	C	N	O	S	0	1	0
			1524	956	259	296	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	1	THR	-	expression tag	UNP P28072

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Chain	Residue	Modelled	Actual	Comment	Reference
b	1	THR	-	expression tag	UNP P28072

- Molecule 15 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	4	Total Cl 4 4	0	0
15	B	2	Total Cl 2 2	0	0
15	C	2	Total Cl 2 2	0	0
15	D	2	Total Cl 2 2	0	0
15	E	3	Total Cl 3 3	0	0
15	F	1	Total Cl 1 1	0	0
15	G	2	Total Cl 2 2	0	0
15	H	1	Total Cl 1 1	0	0
15	I	1	Total Cl 1 1	0	0
15	K	3	Total Cl 3 3	0	0
15	M	4	Total Cl 4 4	0	0
15	N	2	Total Cl 2 2	0	0
15	O	4	Total Cl 4 4	0	0
15	P	1	Total Cl 1 1	0	0
15	Q	2	Total Cl 2 2	0	0
15	R	2	Total Cl 2 2	0	0
15	S	3	Total Cl 3 3	0	0
15	U	1	Total Cl 1 1	0	0
15	V	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	W	1	Total 1	Cl 1	0	0
15	Y	4	Total 4	Cl 4	0	0
15	a	3	Total 3	Cl 3	0	0
15	b	2	Total 2	Cl 2	0	0

- Molecule 16 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total 1	K 1	0	0
16	L	1	Total 1	K 1	0	0
16	N	1	Total 1	K 1	0	0
16	U	1	Total 1	K 1	0	0
16	Z	1	Total 1	K 1	0	0
16	b	1	Total 1	K 1	0	0

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

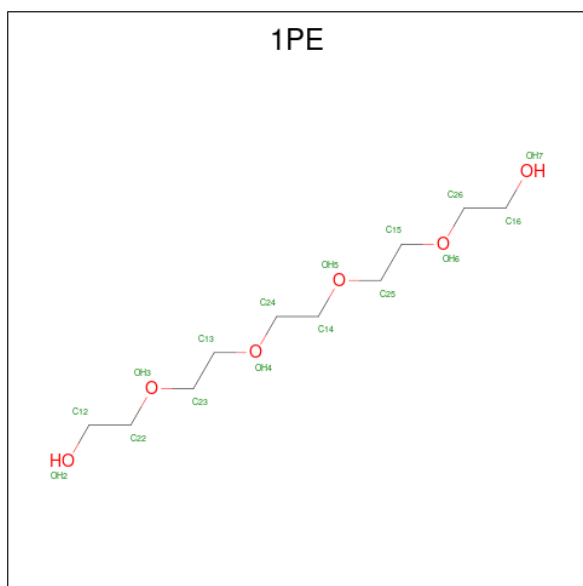
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	H	2	Total 2	Mg 2	0	0
17	I	2	Total 2	Mg 2	0	0
17	J	1	Total 1	Mg 1	0	0
17	K	1	Total 1	Mg 1	0	0
17	L	1	Total 1	Mg 1	0	0
17	V	1	Total 1	Mg 1	0	0
17	W	1	Total 1	Mg 1	0	0

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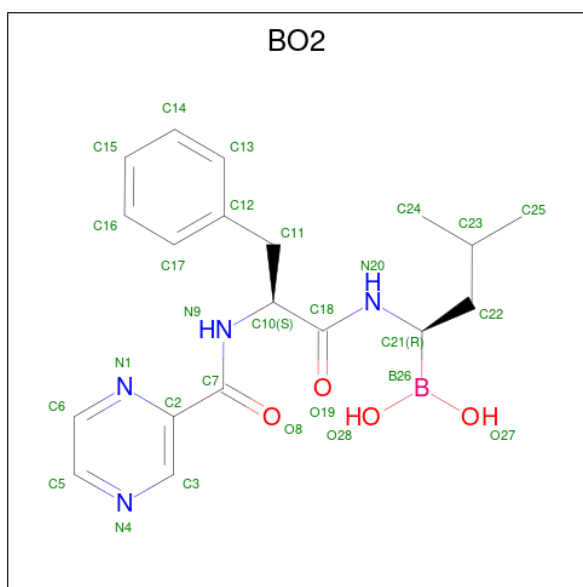
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	X	1	Total	Mg	0	0
			1	1		

- Molecule 18 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	H	1	Total	C	O	0	0
			16	10	6		
18	H	1	Total	C	O	0	0
			16	10	6		
18	I	1	Total	C	O	0	0
			16	10	6		
18	I	1	Total	C	O	0	0
			16	10	6		
18	L	1	Total	C	O	0	0
			16	10	6		
18	M	1	Total	C	O	0	0
			16	10	6		
18	W	1	Total	C	O	0	0
			16	10	6		
18	Z	1	Total	C	O	0	0
			16	10	6		
18	b	1	Total	C	O	0	0
			16	10	6		

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



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

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	115	Total 115	O 115	0	0
20	B	131	Total 131	O 131	0	0
20	C	75	Total 75	O 75	0	0
20	D	95	Total 95	O 95	0	0
20	E	147	Total 147	O 147	0	0
20	F	186	Total 186	O 186	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	G	196	Total 196	O 196	0	0
20	H	159	Total 159	O 159	0	0
20	I	157	Total 157	O 157	0	0
20	J	138	Total 138	O 138	0	0
20	K	105	Total 105	O 105	0	0
20	L	125	Total 125	O 125	0	0
20	M	147	Total 147	O 147	0	0
20	N	162	Total 162	O 162	0	0
20	O	95	Total 95	O 95	0	0
20	P	125	Total 125	O 125	0	0
20	Q	75	Total 75	O 75	0	0
20	R	132	Total 132	O 132	0	0
20	S	130	Total 130	O 130	0	0
20	T	100	Total 100	O 100	0	0
20	U	107	Total 107	O 107	0	0
20	V	120	Total 120	O 120	0	0
20	W	118	Total 118	O 118	0	0
20	X	125	Total 125	O 125	0	0
20	Y	142	Total 142	O 142	0	0
20	Z	169	Total 169	O 169	0	0
20	a	174	Total 174	O 174	0	0

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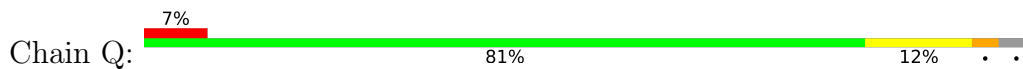
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
20	b	124	Total 124	O 124	0	0

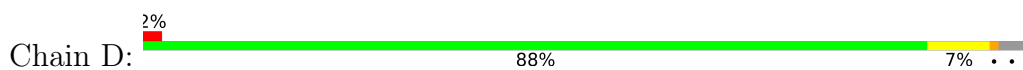


GLU  
LYS  
LYS  
LYS  
GLN  
LYS  
LYS  
ALA  
SER

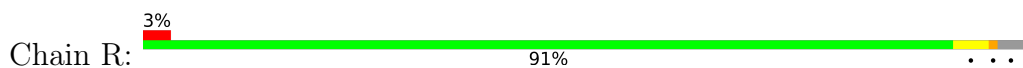
- Molecule 3: Proteasome subunit alpha type-7



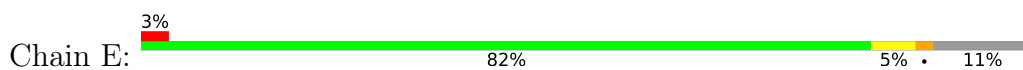
- Molecule 4: Proteasome subunit alpha type-5



- Molecule 4: Proteasome subunit alpha type-5

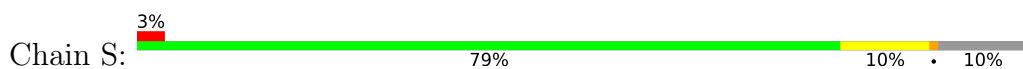


- Molecule 5: Proteasome subunit alpha type-1




GLU  
PRO  
ALA  
GLU  
LYS  
ALA  
ASP  
GLU  
PRO  
HIS

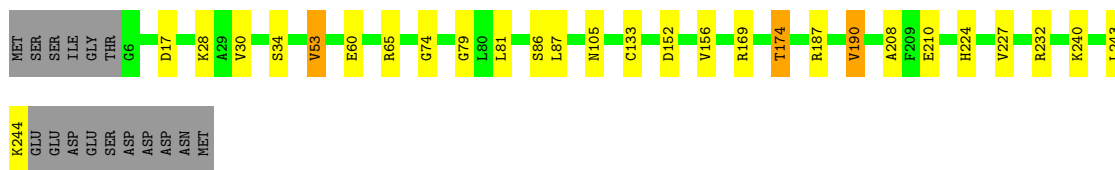
- Molecule 5: Proteasome subunit alpha type-1




GLN  
ARG  
LYS  
ALA  
GLN  
PRO  
ALA  
GLN  
PRO  
ALA  
PRO  
HIS

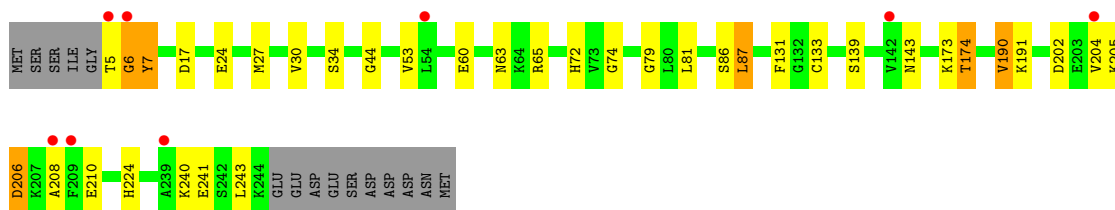
- Molecule 6: Proteasome subunit alpha type-3

Chain F:  83% 10% • 6%



• Molecule 6: Proteasome subunit alpha type-3

Chain T:  3% 80% 12% • 6%




• Molecule 7: Proteasome subunit alpha type-6

Chain G:  93% 6% ..




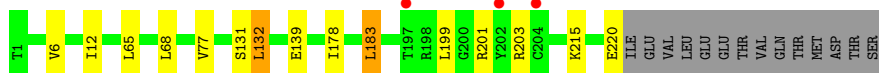
• Molecule 7: Proteasome subunit alpha type-6

Chain U:  3% 87% 9% ..




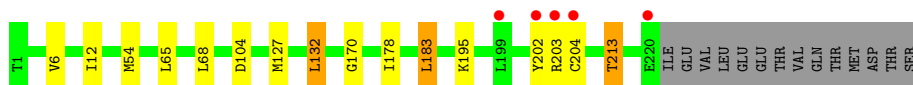
• Molecule 8: Proteasome subunit beta type-7

Chain H:  88% 6% • 6%



• Molecule 8: Proteasome subunit beta type-7

Chain V:  2% 87% 6% • 6%



• Molecule 9: Proteasome subunit beta type-3

Chain I:  92% 6%




- Molecule 9: Proteasome subunit beta type-3

Chain W:  93% 6%




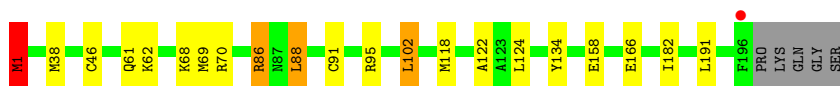
- Molecule 10: Proteasome subunit beta type-2

Chain J:  85% 11%




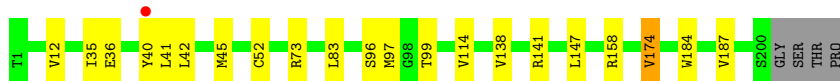
- Molecule 10: Proteasome subunit beta type-2

Chain X:  87% 8%




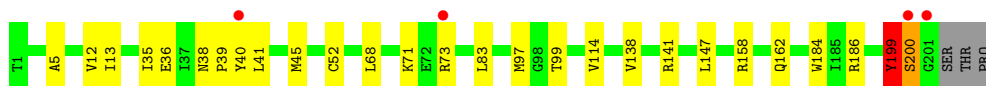
- Molecule 11: Proteasome subunit beta type-5

Chain K:  88% 10%



- Molecule 11: Proteasome subunit beta type-5

Chain Y:  2% 85% 12%



- Molecule 12: Proteasome subunit beta type-1

Chain L:  92% 8%



- Molecule 12: Proteasome subunit beta type-1

Chain Z:  94% 5%

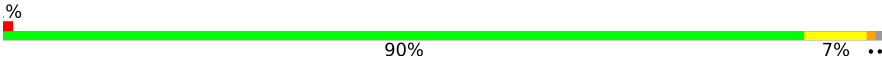


- Molecule 13: Proteasome subunit beta type-4

Chain M:  95%



- Molecule 13: Proteasome subunit beta type-4

Chain a:  90% 7%



- Molecule 14: Proteasome subunit beta type-6

Chain N:  94%



- Molecule 14: Proteasome subunit beta type-6

Chain b:  94%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.37Å 202.72Å 314.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	170.45 – 2.10 170.45 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.6 (170.45-2.10) 98.6 (170.45-2.10)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.15 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.184 , 0.226 0.191 , 0.230	Depositor DCC
$R_{free}$ test set	20644 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.7	Xtrriage
Anisotropy	0.168	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	52211	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, K, CL, BO2, YCM, 6V1, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.92	0/1833	0.99	1/2489 (0.0%)
1	O	0.84	0/1778	0.97	0/2419
2	B	0.91	0/1962	0.98	0/2649
2	P	0.90	0/1945	1.00	2/2631 (0.1%)
3	C	0.90	0/1818	1.08	1/2469 (0.0%)
3	Q	0.93	1/1834 (0.1%)	1.12	8/2490 (0.3%)
4	D	0.92	1/1789 (0.1%)	1.01	2/2424 (0.1%)
4	R	0.98	0/1780	1.04	3/2408 (0.1%)
5	E	0.97	0/1842	1.02	2/2493 (0.1%)
5	S	0.93	0/1901	1.03	3/2571 (0.1%)
6	F	1.02	1/1935 (0.1%)	1.05	3/2605 (0.1%)
6	T	0.91	2/1894 (0.1%)	1.07	10/2556 (0.4%)
7	G	0.99	0/1909	1.02	4/2579 (0.2%)
7	U	0.88	1/1804 (0.1%)	0.95	0/2441
8	H	1.08	0/1697	1.03	0/2299
8	V	0.91	0/1655	0.98	1/2251 (0.0%)
9	I	0.96	0/1648	1.10	7/2219 (0.3%)
9	W	0.86	0/1630	1.02	6/2197 (0.3%)
10	J	0.94	0/1613	0.96	2/2180 (0.1%)
10	X	0.95	0/1597	0.98	2/2160 (0.1%)
11	K	0.94	0/1584	0.98	1/2141 (0.0%)
11	Y	1.00	0/1620	1.02	3/2185 (0.1%)
12	L	0.94	1/1672 (0.1%)	1.00	1/2257 (0.0%)
12	Z	1.01	0/1675	1.01	0/2257
13	M	0.96	1/1728 (0.1%)	0.97	0/2339
13	a	0.98	0/1724	0.99	1/2336 (0.0%)
14	N	1.04	1/1548 (0.1%)	1.02	2/2095 (0.1%)
14	b	0.92	0/1554	1.01	2/2104 (0.1%)
All	All	0.95	9/48969 (0.0%)	1.02	67/66244 (0.1%)

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
2	P	0	3
3	C	0	1
3	Q	0	2
4	D	0	4
4	R	0	2
5	E	0	1
6	T	0	1
7	U	1	0
9	I	0	1
9	W	0	1
10	J	0	2
10	X	0	1
11	Y	0	1
13	a	0	1
All	All	1	21

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	104	ASP	N-CA	6.17	1.51	1.45
6	F	79	GLY	C-O	-5.50	1.20	1.24
6	T	7	TYR	N-CA	5.49	1.56	1.46
13	M	3	ASN	C-O	-5.42	1.20	1.25
3	Q	206	ILE	CA-C	5.32	1.59	1.52

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	16[A]	LYS	CA-C-N	9.43	135.94	122.08
9	I	16[A]	LYS	C-N-CA	9.43	135.94	122.08
9	I	16[B]	LYS	CA-C-N	9.43	135.94	122.08
9	I	16[B]	LYS	C-N-CA	9.43	135.94	122.08
7	G	183	VAL	CB-CA-C	-8.79	100.28	112.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	237	GLU	Peptide
4	D	127	ASP	Peptide
4	D	175[A]	GLU	Peptide
4	D	175[B]	GLU	Peptide
4	D	223	GLY	Peptide

## 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	1788	0	1761	11	0
1	O	1741	0	1683	6	0
2	B	1926	0	1924	8	0
2	P	1909	0	1874	14	0
3	C	1798	0	1718	14	0
3	Q	1820	0	1749	15	0
4	D	1762	0	1709	7	0
4	R	1753	0	1726	6	0
5	E	1822	0	1779	9	0
5	S	1875	0	1818	19	0
6	F	1888	0	1882	10	0
6	T	1856	0	1816	11	0
7	G	1912	0	1882	3	0
7	U	1815	0	1748	8	0
8	H	1664	0	1680	12	0
8	V	1622	0	1594	7	0
9	I	1613	0	1646	9	0
9	W	1599	0	1621	8	0
10	J	1590	0	1581	18	0
10	X	1574	0	1561	13	0
11	K	1550	0	1506	11	0
11	Y	1580	0	1557	19	0
12	L	1636	0	1625	5	0
12	Z	1642	0	1635	4	0
13	M	1692	0	1670	5	0
13	a	1688	0	1658	11	0
14	N	1519	0	1495	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	b	1524	0	1495	6	0
15	A	4	0	0	0	0
15	B	2	0	0	1	0
15	C	2	0	0	0	0
15	D	2	0	0	0	0
15	E	3	0	0	0	0
15	F	1	0	0	0	0
15	G	2	0	0	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0
15	K	3	0	0	0	0
15	M	4	0	0	1	0
15	N	2	0	0	0	0
15	O	4	0	0	0	0
15	P	1	0	0	0	0
15	Q	2	0	0	0	0
15	R	2	0	0	0	0
15	S	3	0	0	0	0
15	U	1	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	Y	4	0	0	0	0
15	a	3	0	0	1	0
15	b	2	0	0	1	0
16	G	1	0	0	0	0
16	L	1	0	0	0	0
16	N	1	0	0	0	0
16	U	1	0	0	0	0
16	Z	1	0	0	0	0
16	b	1	0	0	0	0
17	H	2	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	K	1	0	0	0	0
17	L	1	0	0	0	0
17	V	1	0	0	0	0
17	W	1	0	0	0	0
17	X	1	0	0	0	0
18	H	32	0	44	0	0
18	I	32	0	44	0	0
18	L	16	0	22	0	0
18	M	16	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	W	16	0	22	0	0
18	Z	16	0	22	0	0
18	b	16	0	22	0	0
19	H	28	0	25	1	0
19	K	28	0	25	0	0
19	N	28	0	25	1	0
19	V	28	0	25	0	0
19	Y	28	0	25	0	0
19	b	28	0	25	1	0
20	A	115	0	0	2	0
20	B	131	0	0	2	0
20	C	75	0	0	0	0
20	D	95	0	0	1	0
20	E	147	0	0	2	0
20	F	186	0	0	3	0
20	G	196	0	0	0	0
20	H	159	0	0	7	0
20	I	157	0	0	1	0
20	J	138	0	0	4	0
20	K	105	0	0	0	0
20	L	125	0	0	1	0
20	M	147	0	0	0	0
20	N	162	0	0	0	0
20	O	95	0	0	1	0
20	P	125	0	0	0	0
20	Q	75	0	0	2	0
20	R	132	0	0	0	0
20	S	130	0	0	3	0
20	T	100	0	0	1	0
20	U	107	0	0	1	0
20	V	120	0	0	1	0
20	W	118	0	0	2	0
20	X	125	0	0	0	0
20	Y	142	0	0	0	0
20	Z	169	0	0	1	0
20	a	174	0	0	3	0
20	b	124	0	0	0	0
All	All	52211	0	47741	257	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 257 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)
6:F:169[A]:ARG:NH1	20:F:401:HOH:O	2.02	0.92
2:P:25[B]:MET:HE3	2:P:25[B]:MET:HA	1.51	0.92
12:L:144:MET:HE1	12:L:185:ARG:HB2	1.53	0.88
10:X:1:MET:HE1	10:X:134:TYR:H	1.45	0.81
2:P:155:ASN:OD1	3:Q:77:THR:OG1	2.01	0.79

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	231/234 (99%)	222 (96%)	4 (2%)	5 (2%)	5 2
1	O	228/234 (97%)	218 (96%)	4 (2%)	6 (3%)	4 1
2	B	248/261 (95%)	239 (96%)	7 (3%)	2 (1%)	16 12
2	P	248/261 (95%)	232 (94%)	13 (5%)	3 (1%)	10 7
3	C	236/248 (95%)	224 (95%)	6 (2%)	6 (2%)	4 1
3	Q	236/248 (95%)	218 (92%)	8 (3%)	10 (4%)	2 0
4	D	232/241 (96%)	224 (97%)	4 (2%)	4 (2%)	7 3
4	R	232/241 (96%)	222 (96%)	7 (3%)	3 (1%)	9 6
5	E	232/263 (88%)	226 (97%)	5 (2%)	1 (0%)	30 28
5	S	238/263 (90%)	230 (97%)	6 (2%)	2 (1%)	16 12
6	F	241/255 (94%)	240 (100%)	1 (0%)	0	100 100
6	T	239/255 (94%)	233 (98%)	2 (1%)	4 (2%)	7 3
7	G	241/246 (98%)	235 (98%)	5 (2%)	1 (0%)	30 28
7	U	232/246 (94%)	228 (98%)	4 (2%)	0	100 100
8	H	220/234 (94%)	217 (99%)	3 (1%)	0	100 100
8	V	220/234 (94%)	217 (99%)	2 (1%)	1 (0%)	24 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	205/205 (100%)	200 (98%)	5 (2%)	0	100	100
9	W	204/205 (100%)	199 (98%)	5 (2%)	0	100	100
10	J	195/201 (97%)	192 (98%)	3 (2%)	0	100	100
10	X	195/201 (97%)	193 (99%)	2 (1%)	0	100	100
11	K	199/204 (98%)	196 (98%)	3 (2%)	0	100	100
11	Y	202/204 (99%)	198 (98%)	3 (2%)	1 (0%)	24	22
12	L	213/213 (100%)	211 (99%)	2 (1%)	0	100	100
12	Z	212/213 (100%)	210 (99%)	2 (1%)	0	100	100
13	M	215/219 (98%)	208 (97%)	7 (3%)	0	100	100
13	a	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
14	N	201/205 (98%)	199 (99%)	2 (1%)	0	100	100
14	b	202/205 (98%)	200 (99%)	2 (1%)	0	100	100
All	All	6213/6458 (96%)	6040 (97%)	124 (2%)	49 (1%)	16	12

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	52	LYS
1	A	53	SER
4	D	176	GLY
5	E	59	HIS

### 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	185/191 (97%)	172 (93%)	13 (7%)	14	11
1	O	176/191 (92%)	167 (95%)	9 (5%)	21	21
2	B	200/221 (90%)	193 (96%)	7 (4%)	32	35
2	P	197/221 (89%)	186 (94%)	11 (6%)	19	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	179/210 (85%)	169 (94%)	10 (6%)	19	18
3	Q	184/210 (88%)	172 (94%)	12 (6%)	15	13
4	D	189/203 (93%)	183 (97%)	6 (3%)	34	38
4	R	187/203 (92%)	185 (99%)	2 (1%)	65	74
5	E	192/223 (86%)	185 (96%)	7 (4%)	31	34
5	S	197/223 (88%)	191 (97%)	6 (3%)	36	41
6	F	199/212 (94%)	187 (94%)	12 (6%)	17	15
6	T	192/212 (91%)	182 (95%)	10 (5%)	21	20
7	G	202/207 (98%)	194 (96%)	8 (4%)	28	29
7	U	186/207 (90%)	178 (96%)	8 (4%)	26	27
8	H	181/195 (93%)	172 (95%)	9 (5%)	22	22
8	V	172/195 (88%)	163 (95%)	9 (5%)	21	20
9	I	176/174 (101%)	174 (99%)	2 (1%)	65	74
9	W	173/174 (99%)	170 (98%)	3 (2%)	53	62
10	J	166/170 (98%)	159 (96%)	7 (4%)	26	28
10	X	164/170 (96%)	158 (96%)	6 (4%)	30	33
11	K	155/159 (98%)	147 (95%)	8 (5%)	21	20
11	Y	159/159 (100%)	155 (98%)	4 (2%)	42	48
12	L	175/178 (98%)	167 (95%)	8 (5%)	24	25
12	Z	175/178 (98%)	169 (97%)	6 (3%)	32	35
13	M	180/181 (99%)	178 (99%)	2 (1%)	65	74
13	a	178/181 (98%)	174 (98%)	4 (2%)	45	53
14	N	158/159 (99%)	155 (98%)	3 (2%)	50	58
14	b	158/159 (99%)	154 (98%)	4 (2%)	42	48
All	All	5035/5366 (94%)	4839 (96%)	196 (4%)	29	31

5 of 196 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	P	59	VAL
6	T	53	VAL
2	P	235	GLN
3	Q	206	ILE
6	T	241	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
10	X	65	GLN
11	Y	119	ASN
13	a	188	GLN
10	J	61	GLN
9	I	172	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	6V1	S	148	5	13,15,16	2.17	4 (30%)	10,20,22	3.23	6 (60%)
7	6V1	G	161	7	13,15,16	1.60	2 (15%)	10,20,22	2.15	5 (50%)
3	YCM	C	63	3	7,9,10	0.87	0	5,10,12	1.04	0
3	YCM	Q	63	3	7,9,10	1.30	1 (14%)	5,10,12	3.08	4 (80%)
7	YCM	G	137	7	7,9,10	1.71	1 (14%)	5,10,12	2.04	2 (40%)
7	6V1	G	47	7	13,15,16	2.23	3 (23%)	10,20,22	1.69	2 (20%)
7	6V1	U	47	7	13,15,16	2.04	4 (30%)	10,20,22	2.49	4 (40%)
7	6V1	U	161	7	13,15,16	1.56	2 (15%)	10,20,22	2.31	4 (40%)
10	6V1	X	91	10	13,15,16	1.70	2 (15%)	10,20,22	4.47	6 (60%)
5	6V1	E	148	5	13,15,16	2.06	3 (23%)	10,20,22	2.95	5 (50%)
10	6V1	J	91	10	13,15,16	2.21	3 (23%)	10,20,22	3.91	6 (60%)
7	YCM	U	137	7	7,9,10	1.12	1 (14%)	5,10,12	1.20	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	6V1	S	148	5	-	0/6/25/27	0/1/1/1
7	6V1	G	161	7	-	1/6/25/27	0/1/1/1
3	YCM	C	63	3	-	0/6/8/10	-
3	YCM	Q	63	3	-	4/6/8/10	-
7	YCM	G	137	7	-	2/6/8/10	-
7	6V1	G	47	7	-	1/6/25/27	0/1/1/1
7	6V1	U	47	7	1/1/5/6	0/6/25/27	0/1/1/1
7	6V1	U	161	7	-	1/6/25/27	0/1/1/1
10	6V1	X	91	10	-	2/6/25/27	0/1/1/1
5	6V1	E	148	5	-	2/6/25/27	0/1/1/1
10	6V1	J	91	10	-	2/6/25/27	0/1/1/1
7	YCM	U	137	7	-	2/6/8/10	-

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	91	6V1	C1-SG	-6.57	1.76	1.83
7	G	47	6V1	CB-SG	-6.44	1.75	1.82
5	S	148	6V1	CB-SG	-6.05	1.76	1.82
5	E	148	6V1	CB-SG	-5.48	1.76	1.82
7	U	47	6V1	CB-SG	-5.00	1.77	1.82

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	X	91	6V1	C5-C4-N3	8.12	113.18	108.07
10	J	91	6V1	C5-C4-N3	7.42	112.74	108.07
10	X	91	6V1	C2-N3-C4	-6.82	109.08	113.07
5	E	148	6V1	C5-C4-N3	6.78	112.34	108.07
5	S	148	6V1	C2-N3-C4	-6.11	109.49	113.07

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	137	YCM	SG-CD-CE-NZ2
10	J	91	6V1	C3-C6-N3-C2
10	J	91	6V1	C3-C6-N3-C4
3	Q	63	YCM	CE-CD-SG-CB
3	Q	63	YCM	SG-CD-CE-OZ1

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	63	YCM	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 82 ligands modelled in this entry, 67 are monoatomic - leaving 15 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	$\# Z  > 2$
18	1PE	L	301	-	15,15,15	0.56	0	14,14,14	0.67	0
18	1PE	W	303	-	15,15,15	0.58	0	14,14,14	0.38	0
19	BO2	V	303	8	25,29,29	0.80	0	33,38,38	1.50	2 (6%)
19	BO2	K	305	11	25,29,29	0.70	0	33,38,38	1.26	4 (12%)
19	BO2	N	304	14	25,29,29	0.96	0	33,38,38	1.78	9 (27%)
18	1PE	Z	301	-	15,15,15	0.58	0	14,14,14	0.45	0
18	1PE	H	304	-	15,15,15	0.51	0	14,14,14	0.52	0
18	1PE	b	303	-	15,15,15	0.61	0	14,14,14	0.65	0
18	1PE	H	305	-	15,15,15	0.56	0	14,14,14	0.38	0
19	BO2	H	306	8	25,29,29	1.11	1 (4%)	33,38,38	1.22	1 (3%)
18	1PE	I	304	-	15,15,15	0.52	0	14,14,14	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	1PE	I	303	-	15,15,15	0.55	0	14,14,14	0.85	1 (7%)
19	BO2	b	305	14	25,29,29	0.93	1 (4%)	33,38,38	1.35	5 (15%)
19	BO2	Y	305	11	25,29,29	0.73	1 (4%)	33,38,38	1.15	1 (3%)
18	1PE	M	305	-	15,15,15	0.53	0	14,14,14	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	1PE	L	301	-	-	6/13/13/13	-
18	1PE	W	303	-	-	9/13/13/13	-
19	BO2	V	303	8	-	5/23/28/28	0/2/2/2
19	BO2	K	305	11	-	3/23/28/28	0/2/2/2
19	BO2	N	304	14	-	0/23/28/28	0/2/2/2
18	1PE	Z	301	-	-	6/13/13/13	-
18	1PE	H	304	-	-	7/13/13/13	-
18	1PE	b	303	-	-	5/13/13/13	-
18	1PE	H	305	-	-	4/13/13/13	-
19	BO2	H	306	8	-	5/23/28/28	0/2/2/2
18	1PE	I	304	-	-	10/13/13/13	-
18	1PE	I	303	-	-	6/13/13/13	-
19	BO2	b	305	14	-	0/23/28/28	0/2/2/2
19	BO2	Y	305	11	-	3/23/28/28	0/2/2/2
18	1PE	M	305	-	-	6/13/13/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	H	306	BO2	C11-C10	-2.28	1.48	1.54
19	Y	305	BO2	C16-C17	2.17	1.42	1.38
19	b	305	BO2	C15-C14	2.04	1.42	1.38

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	V	303	BO2	C7-C2-N1	5.02	123.29	117.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	N	304	BO2	C6-N1-C2	4.66	122.94	116.93
19	H	306	BO2	C7-C2-N1	4.26	122.39	117.42
19	N	304	BO2	C3-C2-N1	-3.55	117.42	121.60
19	K	305	BO2	C7-C2-N1	3.38	121.37	117.42

There are no chirality outliers.

5 of 75 torsion outliers are listed below:

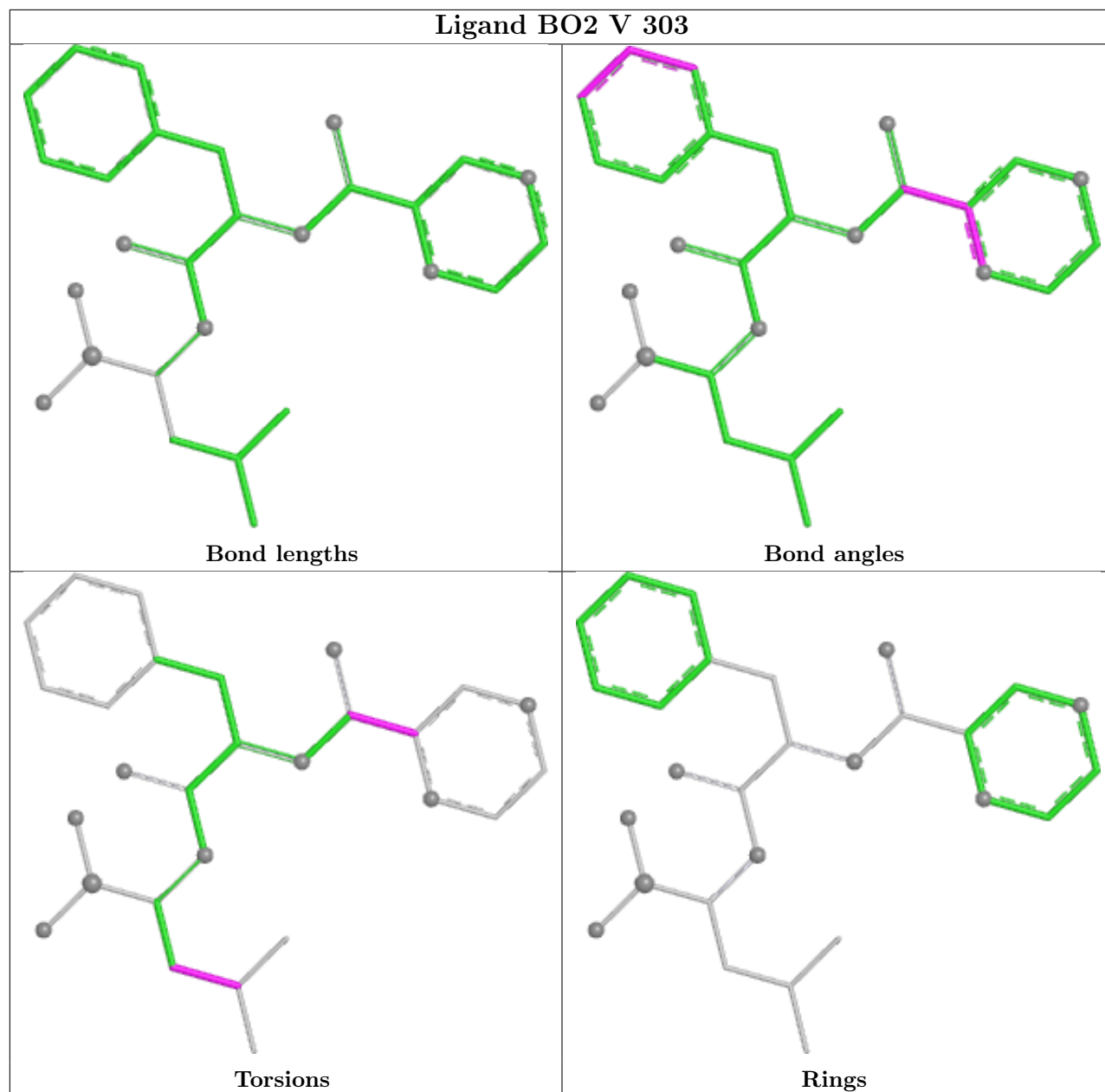
Mol	Chain	Res	Type	Atoms
19	H	306	BO2	N1-C2-C7-N9
19	H	306	BO2	C3-C2-C7-O8
19	H	306	BO2	C3-C2-C7-N9
19	V	303	BO2	C3-C2-C7-O8
19	V	303	BO2	C3-C2-C7-N9

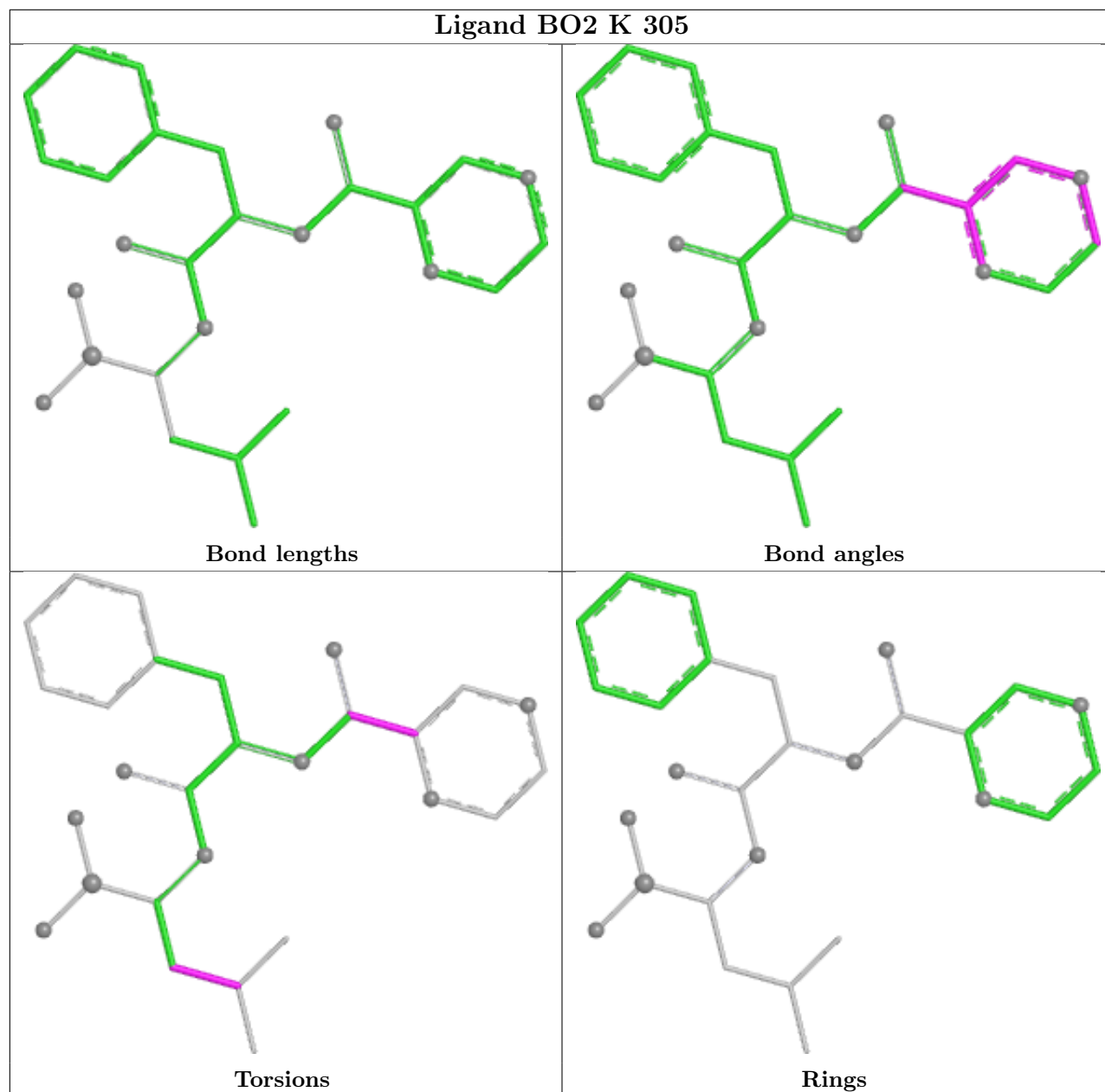
There are no ring outliers.

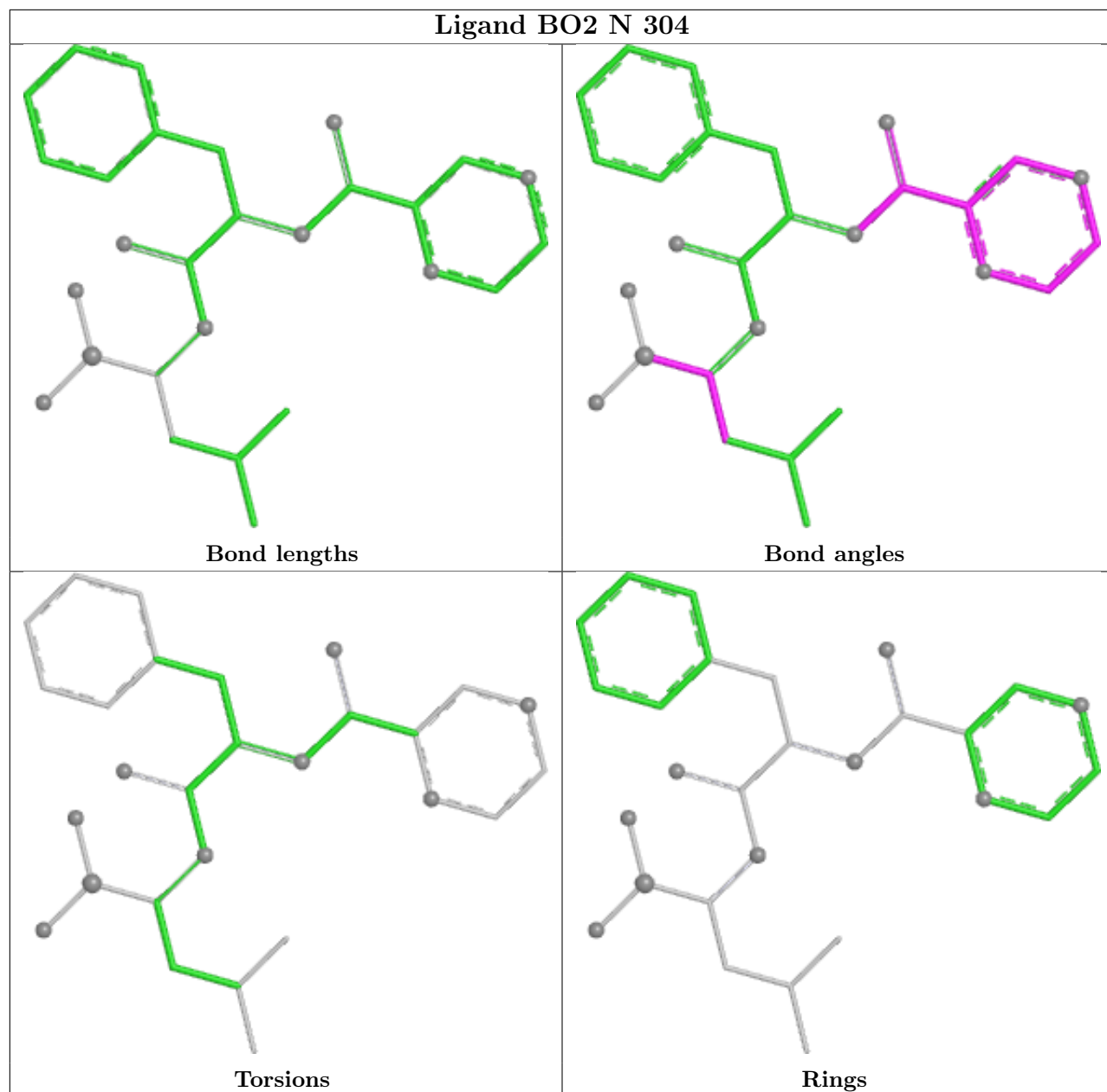
3 monomers are involved in 3 short contacts:

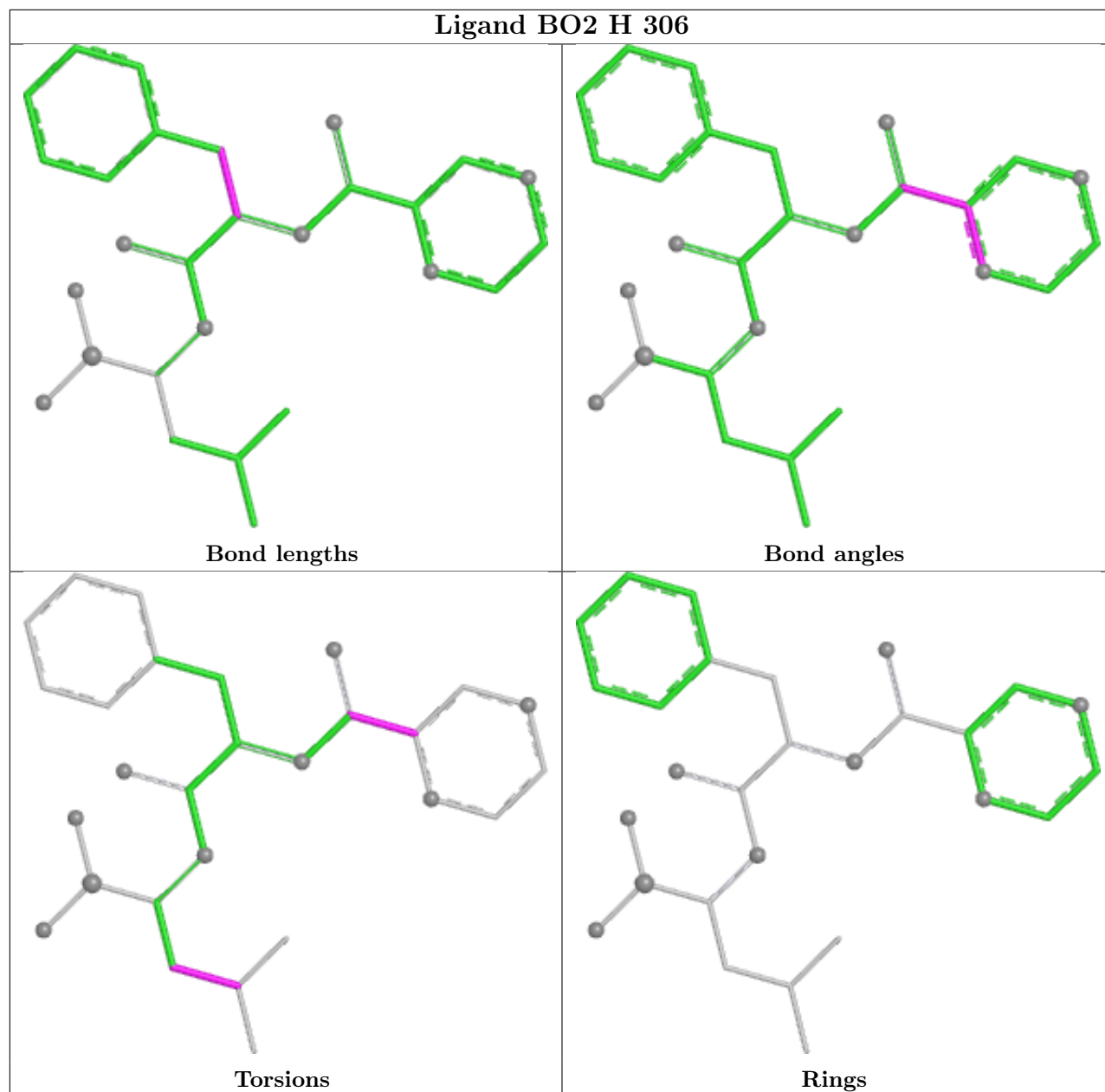
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	N	304	BO2	1	0
19	H	306	BO2	1	0
19	b	305	BO2	1	0

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.

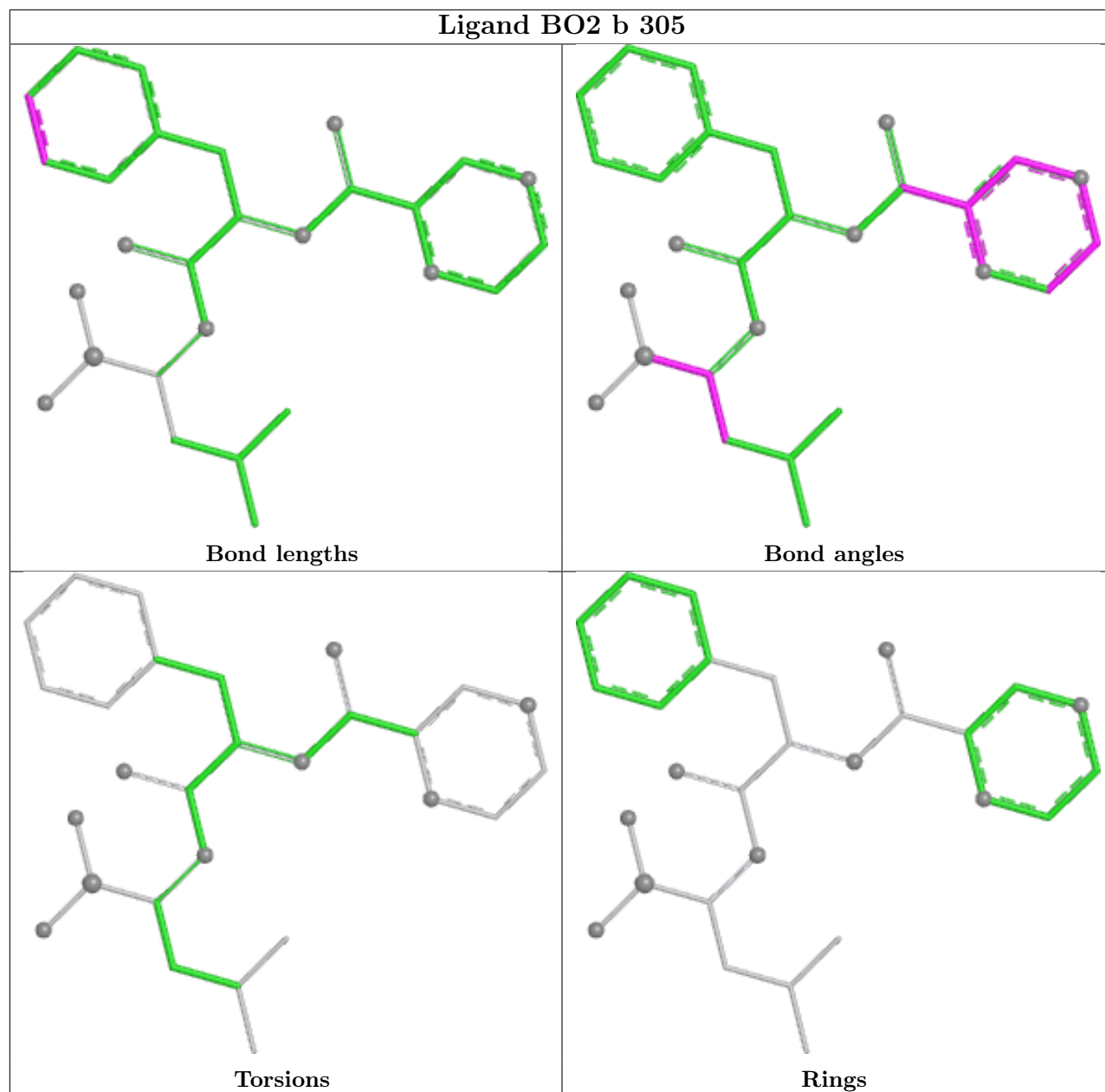


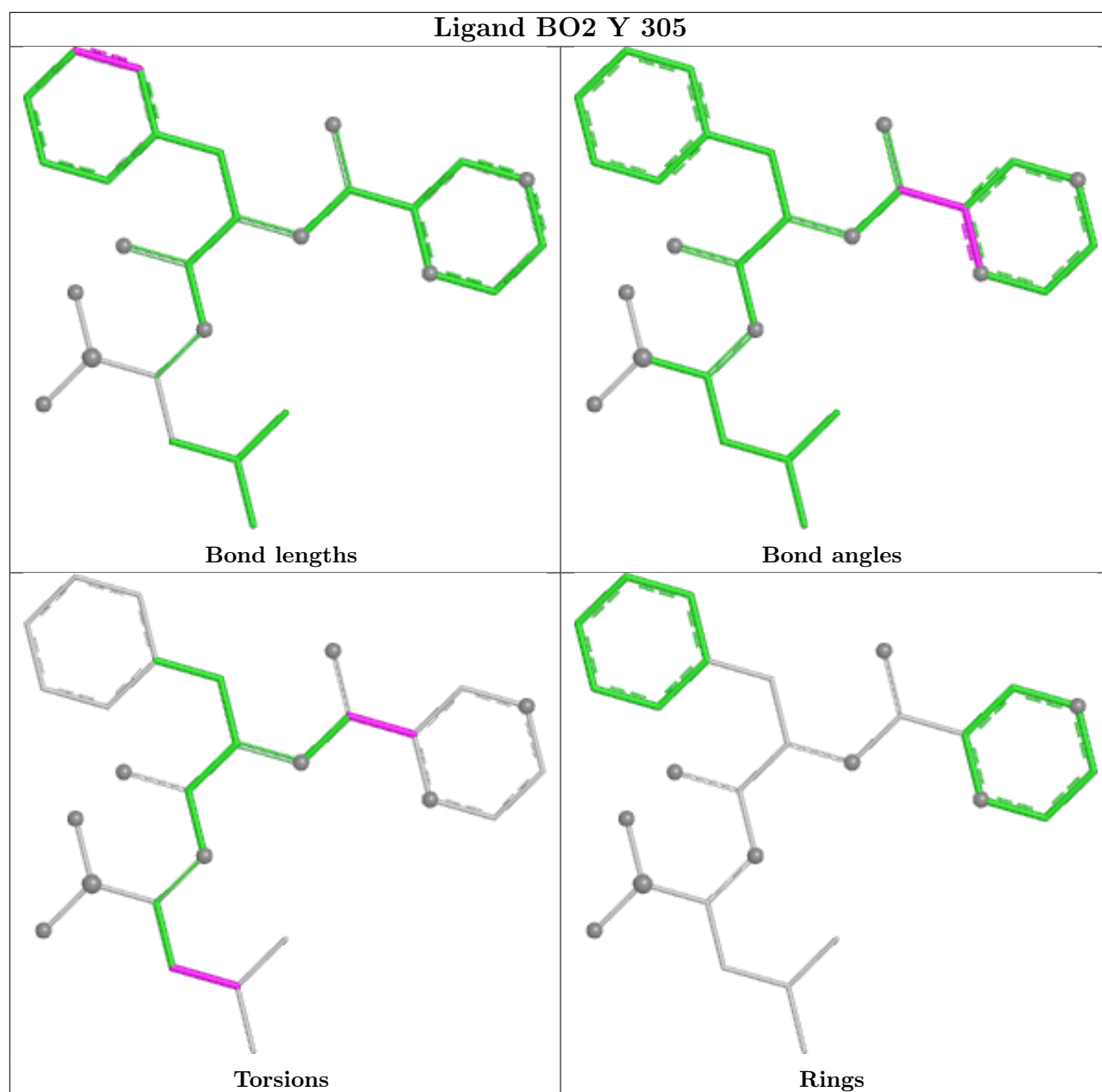






## Ligand BO2 b 305





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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	230/234 (98%)	-0.08	4 (1%) 69 71	24, 46, 82, 94	3 (1%)
1	O	230/234 (98%)	0.56	15 (6%) 25 26	43, 63, 103, 122	0
2	B	248/261 (95%)	0.11	5 (2%) 65 67	21, 52, 94, 132	2 (0%)
2	P	248/261 (95%)	0.27	7 (2%) 55 57	34, 57, 100, 142	2 (0%)
3	C	236/248 (95%)	0.38	6 (2%) 58 61	27, 62, 101, 125	2 (0%)
3	Q	238/248 (95%)	0.56	17 (7%) 22 23	38, 66, 116, 153	0
4	D	233/241 (96%)	0.31	5 (2%) 63 66	31, 57, 85, 118	1 (0%)
4	R	233/241 (96%)	0.13	8 (3%) 48 50	22, 47, 75, 97	1 (0%)
5	E	233/263 (88%)	-0.02	9 (3%) 43 45	26, 43, 89, 116	1 (0%)
5	S	237/263 (90%)	0.15	9 (3%) 44 46	24, 51, 89, 114	3 (1%)
6	F	239/255 (93%)	-0.33	0 100 100	20, 37, 59, 74	4 (1%)
6	T	240/255 (94%)	0.46	8 (3%) 49 51	32, 60, 90, 114	1 (0%)
7	G	241/246 (97%)	-0.16	2 (0%) 82 84	21, 42, 74, 108	2 (0%)
7	U	235/246 (95%)	0.45	7 (2%) 52 55	33, 68, 100, 131	1 (0%)
8	H	220/234 (94%)	-0.25	3 (1%) 73 75	21, 38, 69, 109	2 (0%)
8	V	220/234 (94%)	0.07	5 (2%) 61 64	25, 49, 79, 105	2 (0%)
9	I	204/205 (99%)	-0.38	0 100 100	21, 38, 58, 76	3 (1%)
9	W	204/205 (99%)	-0.05	0 100 100	26, 47, 70, 77	2 (0%)
10	J	195/201 (97%)	-0.25	1 (0%) 87 88	17, 43, 60, 75	3 (1%)
10	X	195/201 (97%)	-0.17	1 (0%) 87 88	20, 43, 58, 73	2 (1%)
11	K	200/204 (98%)	-0.16	1 (0%) 87 88	24, 44, 69, 81	1 (0%)
11	Y	201/204 (98%)	-0.27	4 (1%) 65 67	21, 39, 63, 80	3 (1%)
12	L	213/213 (100%)	-0.18	0 100 100	25, 45, 68, 82	2 (0%)
12	Z	213/213 (100%)	-0.38	0 100 100	28, 39, 61, 73	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	216/219 (98%)	-0.32	1 (0%) 87 88	28, 41, 64, 90	1 (0%)
13	a	216/219 (98%)	-0.20	2 (0%) 81 83	27, 42, 64, 83	2 (0%)
14	N	202/205 (98%)	-0.39	2 (0%) 79 81	21, 38, 57, 87	1 (0%)
14	b	203/205 (99%)	-0.15	1 (0%) 87 88	34, 46, 72, 101	1 (0%)
All	All	6223/6458 (96%)	0.00	123 (1%) 65 67	17, 47, 87, 153	49 (0%)

The worst 5 of 123 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	40	TYR	5.1
11	Y	201	GLY	4.6
5	S	57	ALA	4.4
8	V	204	CYS	4.3
11	Y	40	TYR	4.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	6V1	U	47	15/16	0.84	0.16	82,108,112,115	0
7	YCM	G	137	10/11	0.89	0.13	35,43,60,61	0
7	YCM	U	137	10/11	0.89	0.12	57,65,83,84	0
3	YCM	C	63	10/11	0.90	0.11	55,60,68,69	0
7	6V1	U	161	15/16	0.92	0.12	58,72,79,80	0
7	6V1	G	47	15/16	0.93	0.10	42,58,60,61	0
5	6V1	E	148	15/16	0.93	0.11	32,51,59,59	0
5	6V1	S	148	15/16	0.93	0.12	39,63,69,69	0
10	6V1	X	91	15/16	0.94	0.12	38,59,64,70	0
7	6V1	G	161	15/16	0.95	0.11	33,54,60,63	0
10	6V1	J	91	15/16	0.95	0.11	36,55,59,59	0
3	YCM	Q	63	10/11	0.96	0.07	54,57,66,68	0

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands i

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
18	1PE	I	304	16/16	0.82	0.16	62,76,88,88	0
15	CL	Q	301	1/1	0.83	0.16	78,78,78,78	0
18	1PE	M	305	16/16	0.85	0.14	75,80,95,96	0
15	CL	O	304	1/1	0.87	0.18	70,70,70,70	0
15	CL	D	301	1/1	0.88	0.18	73,73,73,73	0
18	1PE	H	305	16/16	0.88	0.14	65,69,89,90	0
18	1PE	W	303	16/16	0.88	0.13	56,63,79,79	0
18	1PE	b	303	16/16	0.89	0.13	52,59,77,78	0
19	BO2	V	303	28/28	0.89	0.12	49,54,66,67	0
18	1PE	Z	301	16/16	0.90	0.14	57,71,80,80	0
15	CL	O	303	1/1	0.90	0.10	87,87,87,87	0
19	BO2	H	306	28/28	0.90	0.11	38,45,67,67	0
15	CL	Q	302	1/1	0.90	0.23	70,70,70,70	0
15	CL	C	302	1/1	0.91	0.16	69,69,69,69	0
18	1PE	I	303	16/16	0.91	0.11	56,60,68,72	0
15	CL	S	301	1/1	0.91	0.24	75,75,75,75	0
18	1PE	L	301	16/16	0.91	0.13	55,70,75,76	0
15	CL	S	302	1/1	0.91	0.15	69,69,69,69	0
15	CL	O	302	1/1	0.92	0.17	60,60,60,60	0
15	CL	Y	304	1/1	0.92	0.21	70,70,70,70	0
15	CL	K	304	1/1	0.92	0.18	71,71,71,71	0
15	CL	R	302	1/1	0.93	0.28	58,58,58,58	0
15	CL	C	301	1/1	0.93	0.12	66,66,66,66	0
15	CL	D	302	1/1	0.93	0.12	65,65,65,65	0
15	CL	V	302	1/1	0.93	0.16	60,60,60,60	0
15	CL	K	303	1/1	0.93	0.17	68,68,68,68	0
15	CL	G	302	1/1	0.94	0.09	62,62,62,62	0
15	CL	a	303	1/1	0.94	0.10	66,66,66,66	0
17	MG	I	301	1/1	0.94	0.11	37,37,37,37	0
18	1PE	H	304	16/16	0.94	0.09	46,51,64,67	0
15	CL	A	302	1/1	0.94	0.09	69,69,69,69	0
15	CL	S	303	1/1	0.94	0.15	61,61,61,61	0
19	BO2	N	304	28/28	0.94	0.08	35,37,44,47	0
15	CL	B	302	1/1	0.94	0.21	62,62,62,62	0
19	BO2	b	305	28/28	0.94	0.09	37,43,53,55	0
15	CL	b	302	1/1	0.95	0.20	64,64,64,64	0
15	CL	K	302	1/1	0.95	0.13	74,74,74,74	0

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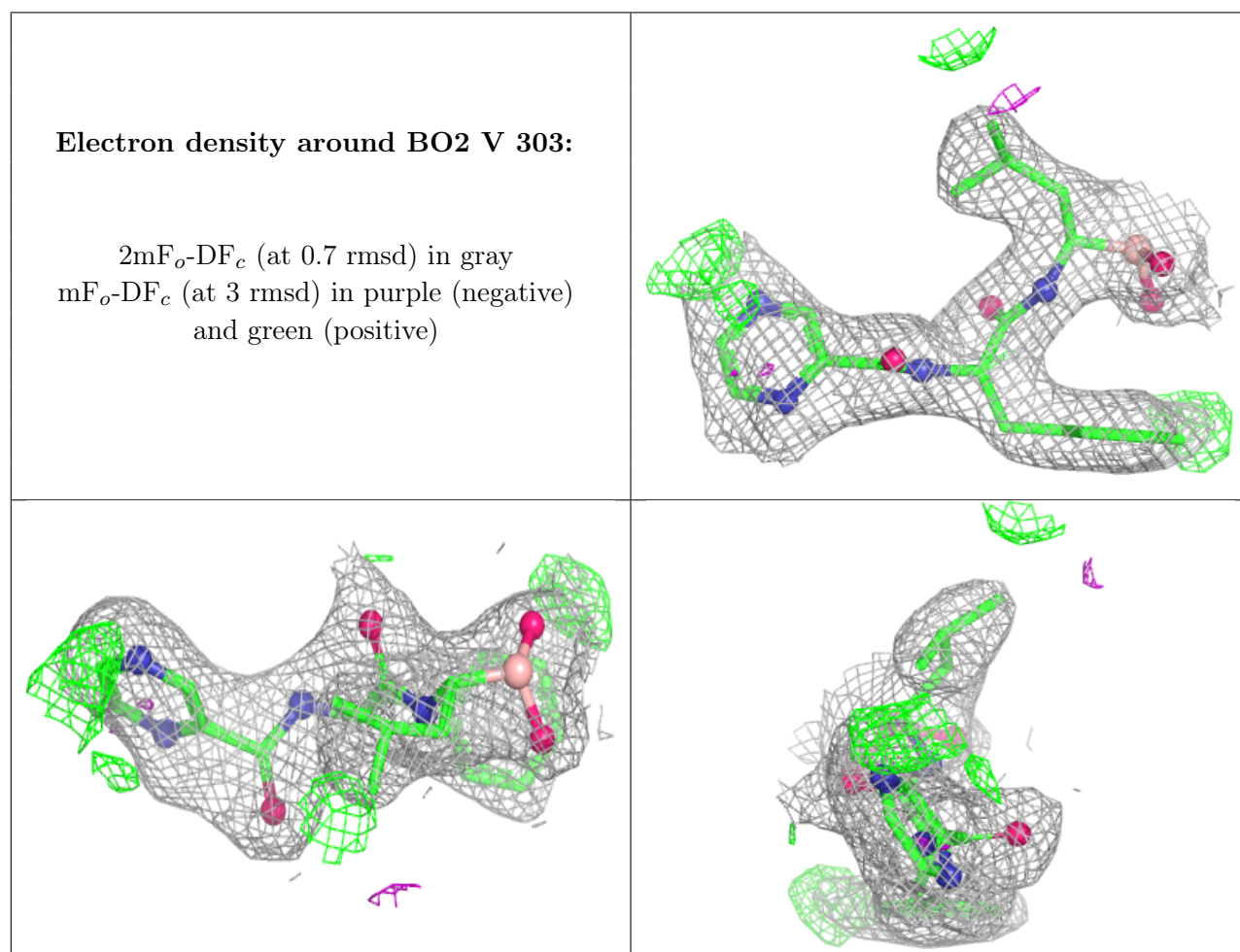
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	CL	M	301	1/1	0.95	0.31	68,68,68,68	0
15	CL	a	302	1/1	0.95	0.13	49,49,49,49	0
15	CL	M	304	1/1	0.95	0.14	58,58,58,58	0
15	CL	Y	302	1/1	0.96	0.09	68,68,68,68	0
15	CL	Y	303	1/1	0.96	0.10	64,64,64,64	0
15	CL	E	301	1/1	0.96	0.12	65,65,65,65	0
15	CL	a	301	1/1	0.96	0.14	67,67,67,67	0
15	CL	M	302	1/1	0.96	0.23	65,65,65,65	0
15	CL	E	303	1/1	0.96	0.14	60,60,60,60	0
15	CL	b	301	1/1	0.96	0.20	68,68,68,68	0
15	CL	A	304	1/1	0.96	0.17	59,59,59,59	0
16	K	L	302	1/1	0.96	0.11	49,49,49,49	0
16	K	b	304	1/1	0.96	0.15	46,46,46,46	0
15	CL	U	301	1/1	0.96	0.15	64,64,64,64	0
15	CL	R	301	1/1	0.96	0.12	61,61,61,61	0
17	MG	K	301	1/1	0.97	0.07	34,34,34,34	0
15	CL	I	302	1/1	0.97	0.07	44,44,44,44	0
15	CL	N	302	1/1	0.97	0.20	59,59,59,59	0
15	CL	E	302	1/1	0.97	0.11	53,53,53,53	0
15	CL	A	301	1/1	0.97	0.10	48,48,48,48	0
15	CL	F	301	1/1	0.97	0.13	56,56,56,56	0
15	CL	P	301	1/1	0.97	0.10	51,51,51,51	0
15	CL	B	301	1/1	0.97	0.09	45,45,45,45	0
15	CL	W	302	1/1	0.97	0.09	52,52,52,52	0
16	K	N	303	1/1	0.97	0.14	45,45,45,45	0
16	K	Z	302	1/1	0.97	0.08	42,42,42,42	0
19	BO2	K	305	28/28	0.97	0.06	32,37,41,42	0
15	CL	Y	301	1/1	0.97	0.15	67,67,67,67	0
15	CL	H	303	1/1	0.97	0.11	47,47,47,47	0
19	BO2	Y	305	28/28	0.97	0.05	29,32,37,38	0
17	MG	I	305	1/1	0.97	0.12	31,31,31,31	0
17	MG	L	303	1/1	0.98	0.13	37,37,37,37	0
17	MG	V	301	1/1	0.98	0.07	57,57,57,57	0
17	MG	W	301	1/1	0.98	0.08	36,36,36,36	0
15	CL	N	301	1/1	0.98	0.05	37,37,37,37	0
15	CL	M	303	1/1	0.98	0.12	47,47,47,47	0
17	MG	H	302	1/1	0.98	0.16	34,34,34,34	0
15	CL	O	301	1/1	0.98	0.08	59,59,59,59	0
15	CL	A	303	1/1	0.98	0.12	52,52,52,52	0
16	K	U	302	1/1	0.98	0.10	46,46,46,46	0
17	MG	X	301	1/1	0.99	0.03	49,49,49,49	0
15	CL	G	301	1/1	0.99	0.19	50,50,50,50	0

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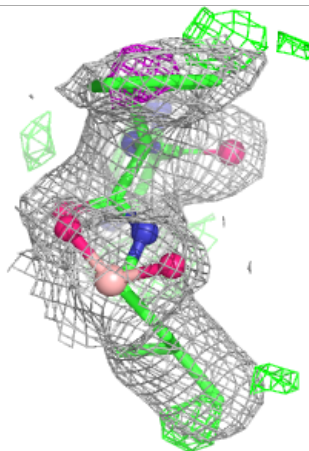
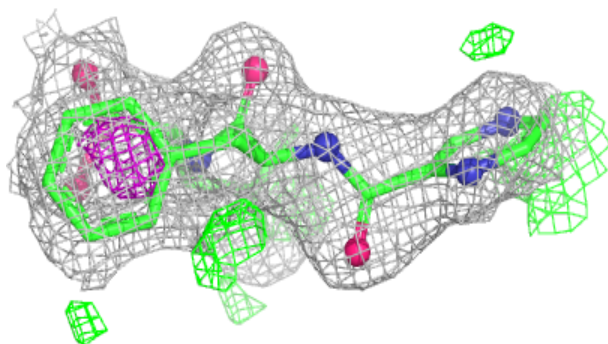
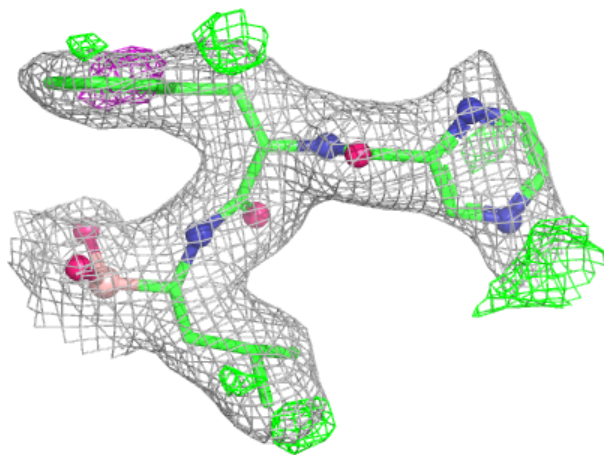
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
17	MG	H	301	1/1	0.99	0.03	53,53,53,53	0
16	K	G	303	1/1	0.99	0.07	37,37,37,37	0
17	MG	J	301	1/1	1.00	0.02	48,48,48,48	0

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.



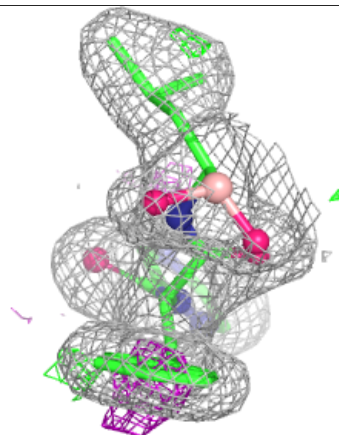
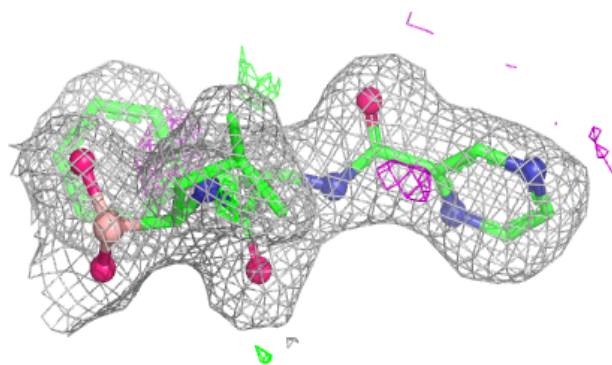
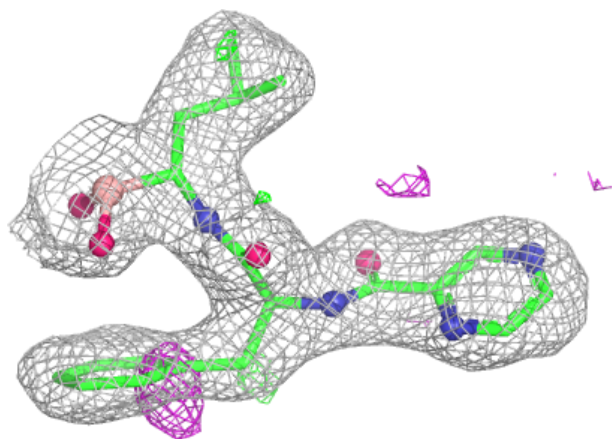
**Electron density around BO2 H 306:**

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



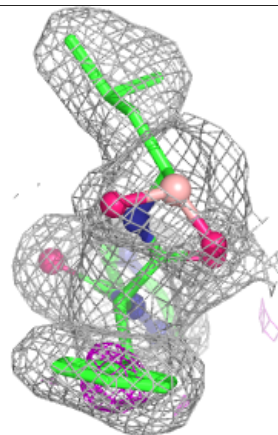
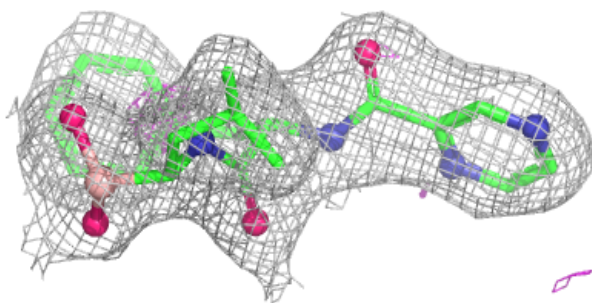
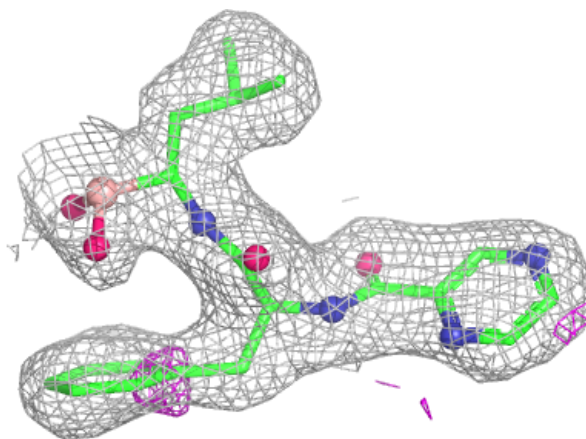
**Electron density around BO2 N 304:**

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



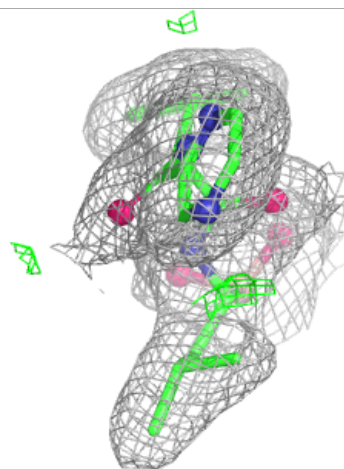
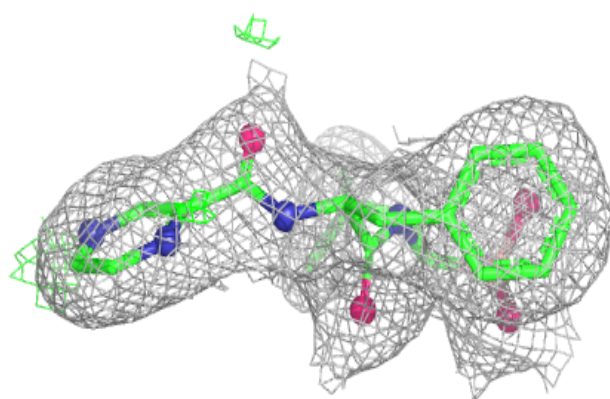
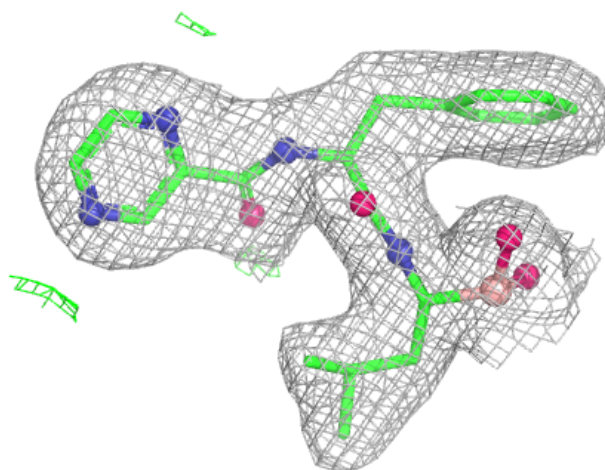
**Electron density around BO2 b 305:**

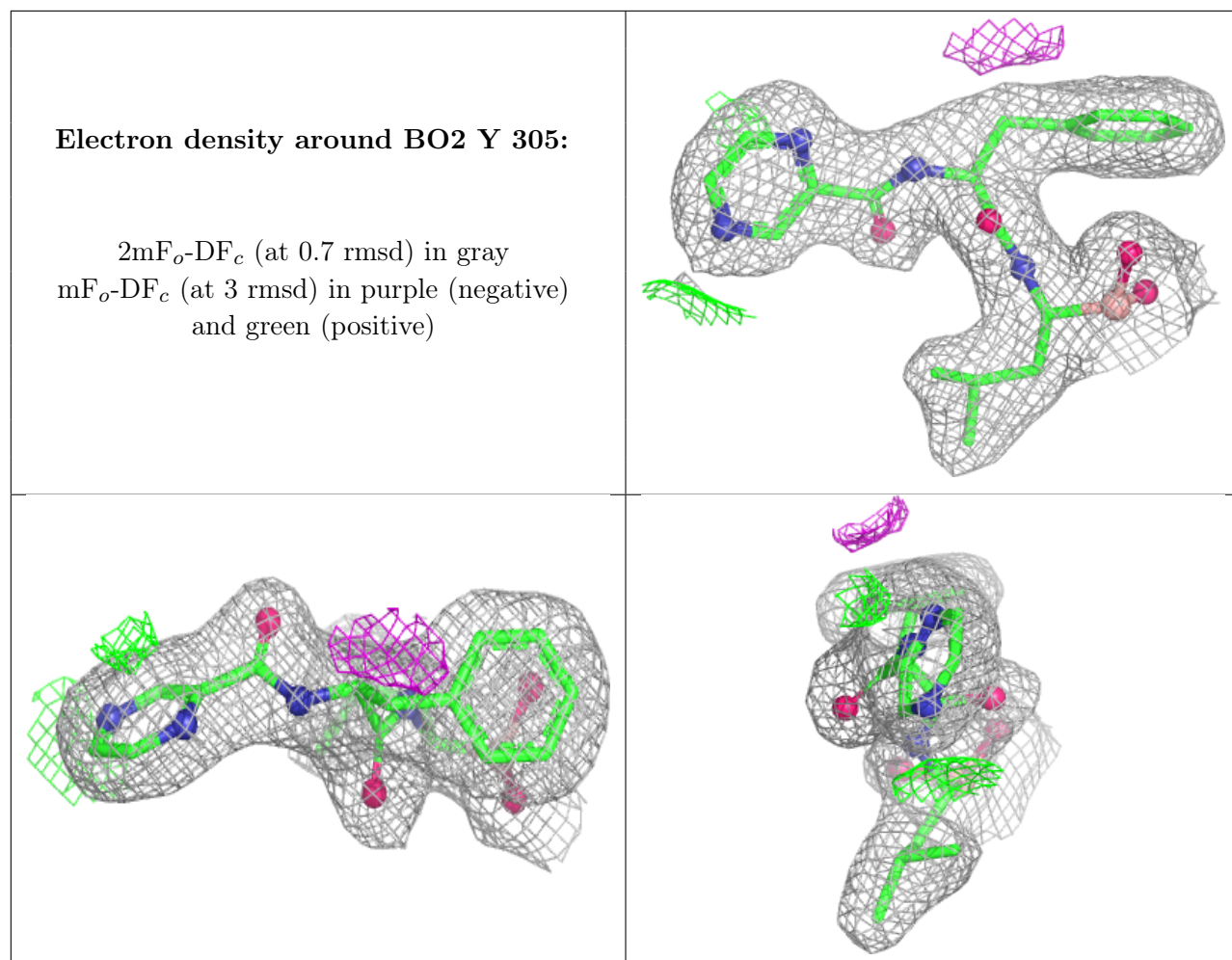
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around BO2 K 305:**

$2mF_o-DF_c$  (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.