



wwPDB X-ray Structure Validation Summary Report

Mar 6, 2026 – 11:30 PM UTC

PDB ID : 2F16 / pdb_00002f16
Title : Crystal structure of the yeast 20S proteasome in complex with bortezomib
Authors : Groll, M.
Deposited on : 2005-11-14
Resolution : 2.80 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

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

<https://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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

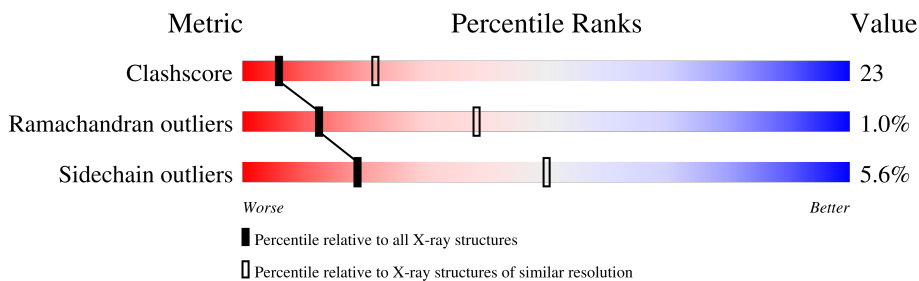
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	250	72% 24% .
1	O	250	73% 24% .
2	B	244	50% 45% 6%
2	P	244	52% 44% .
3	C	241	56% 39% 5%
3	Q	241	54% 41% 5%
4	D	242	68% 29% .
4	R	242	63% 33% .

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Mol	Chain	Length	Quality of chain
5	E	233	54% 40% 5%
5	S	233	52% 43% 5%
6	F	244	61% 33% 6%
6	T	244	59% 34% 6% .
7	G	243	58% 37% 5%
7	U	243	58% 37% 5%
8	H	222	72% 25% .
8	V	222	68% 28% .
9	I	204	67% 29% .
9	W	204	69% 27% .
10	J	198	68% 29% . .
10	X	198	65% 32% . .
11	K	212	66% 32% .
11	Y	212	67% 31% .
12	L	222	58% 34% 8%
12	Z	222	58% 33% 8%
13	1	233	65% 30% 5%
13	M	233	61% 35% 5%
14	2	196	58% 39% .
14	N	196	65% 32% .

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50753 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome component Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			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 component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			
2	P	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			

- Molecule 3 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			
4	R	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			

- Molecule 5 is a protein called Proteasome component PRE5.

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

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			
6	T	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			

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

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

- Molecule 8 is a protein called Proteasome component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			
8	V	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			

- Molecule 9 is a protein called Proteasome component PUP3.

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

- Molecule 10 is a protein called Proteasome component C11.

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

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

- Molecule 11 is a protein called Proteasome component PRE2.

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

- Molecule 12 is a protein called Proteasome component C5.

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

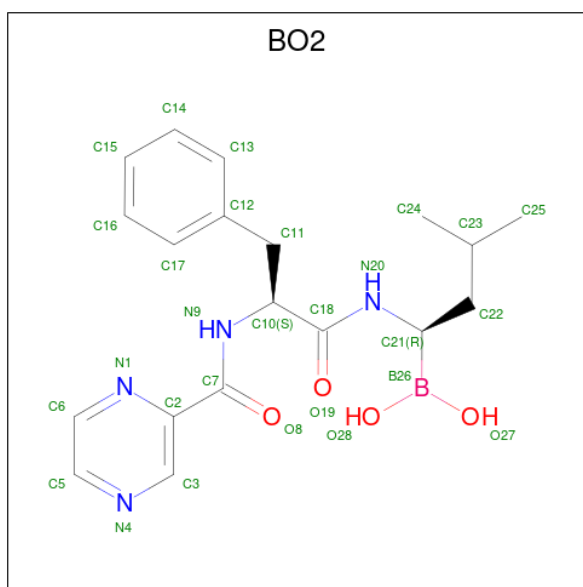
- Molecule 13 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	1	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome component PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	2	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is N-[(1R)-1-(DIHYDROXYBORYL)-3-METHYLBUTYL]-N-(PYRAZIN-2-YLCARBONYL)-L-PHENYLALANINAMIDE (CCD ID: BO2) (formula: C₁₉H₂₅BN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	B	C	N	O		
15	H	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
15	K	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
15	N	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
15	V	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
15	Y	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
15	2	1	Total	B	C	N	O	0	0
			28	1	19	4	4		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	46	Total	O	0	0
			46	46		
16	B	31	Total	O	0	0
			31	31		
16	C	33	Total	O	0	0
			33	33		
16	D	26	Total	O	0	0
			26	26		
16	E	14	Total	O	0	0
			14	14		
16	F	36	Total	O	0	0
			36	36		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	48	Total O 48 48	0	0
16	H	42	Total O 42 42	0	0
16	I	50	Total O 50 50	0	0
16	J	45	Total O 45 45	0	0
16	K	33	Total O 33 33	0	0
16	L	42	Total O 42 42	0	0
16	M	52	Total O 52 52	0	0
16	N	43	Total O 43 43	0	0
16	O	23	Total O 23 23	0	0
16	P	21	Total O 21 21	0	0
16	Q	21	Total O 21 21	0	0
16	R	20	Total O 20 20	0	0
16	S	16	Total O 16 16	0	0
16	T	32	Total O 32 32	0	0
16	U	56	Total O 56 56	0	0
16	V	34	Total O 34 34	0	0
16	W	46	Total O 46 46	0	0
16	X	39	Total O 39 39	0	0
16	Y	32	Total O 32 32	0	0
16	Z	42	Total O 42 42	0	0
16	1	63	Total O 63 63	0	0

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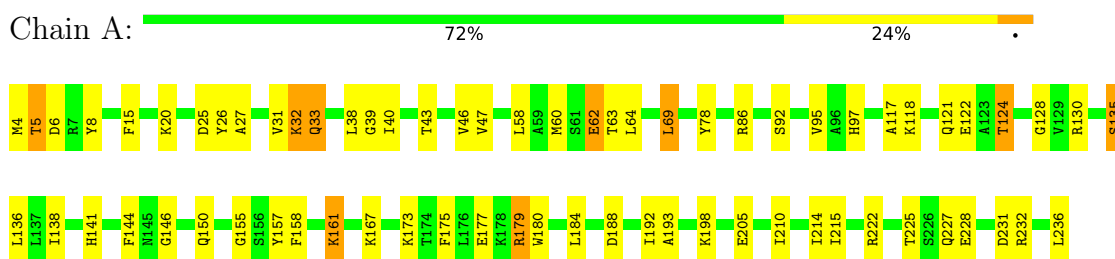
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	2	51	Total	O	0	0
			51	51		

3 Residue-property plots [i](#)

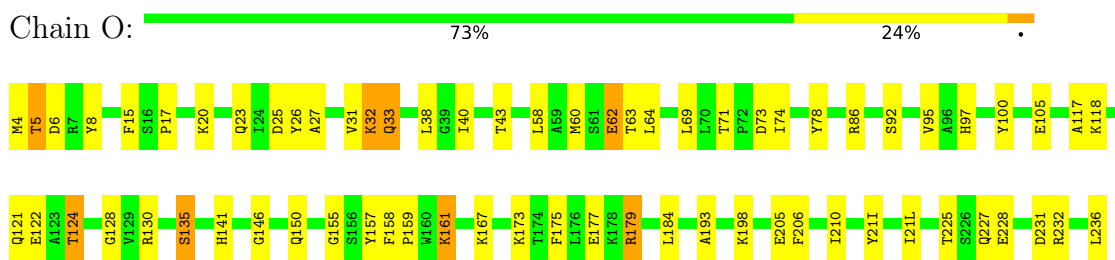
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

- Molecule 1: Proteasome component Y7



- Molecule 1: Proteasome component Y7

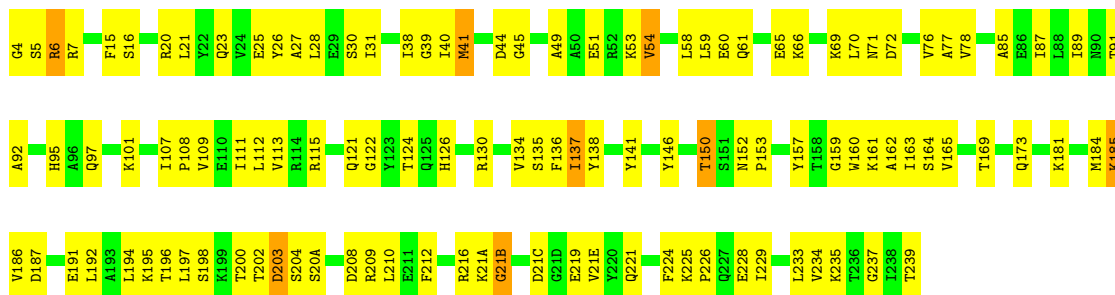


- Molecule 2: Proteasome component Y13

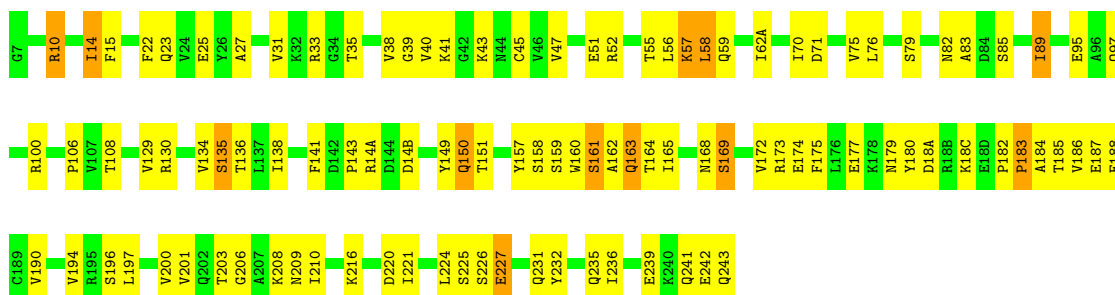


- Molecule 2: Proteasome component Y13

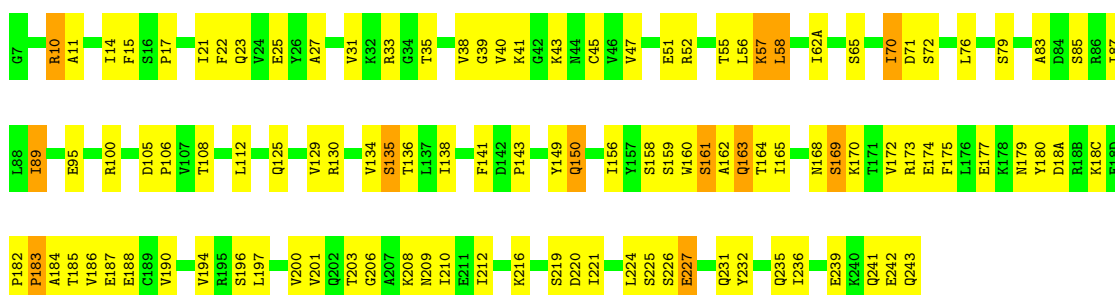




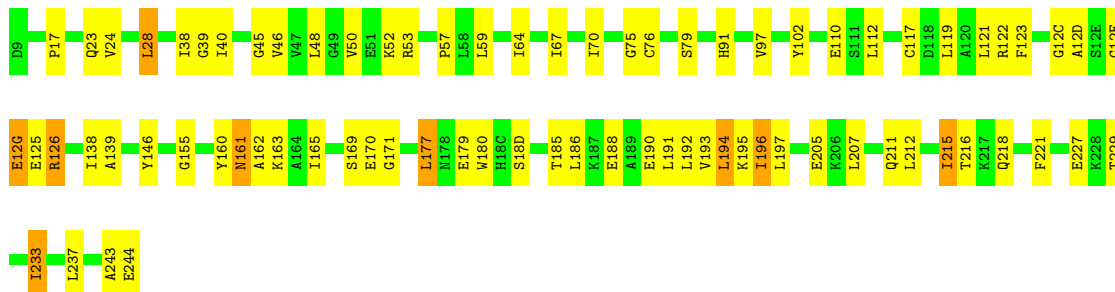
- Molecule 3: Proteasome component PRE6



- Molecule 3: Proteasome component PRE6

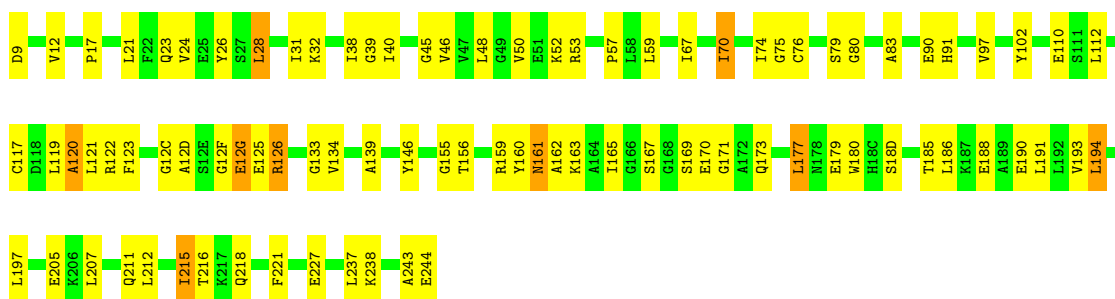


- Molecule 4: Proteasome component PUP2



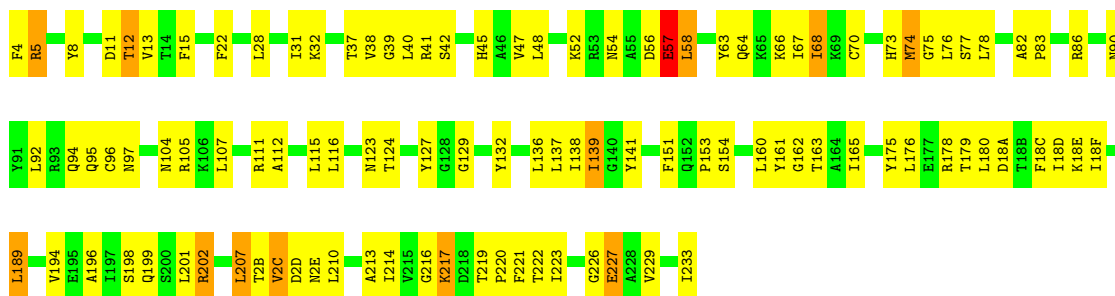
- Molecule 4: Proteasome component PUP2

Chain R:  63% 33%



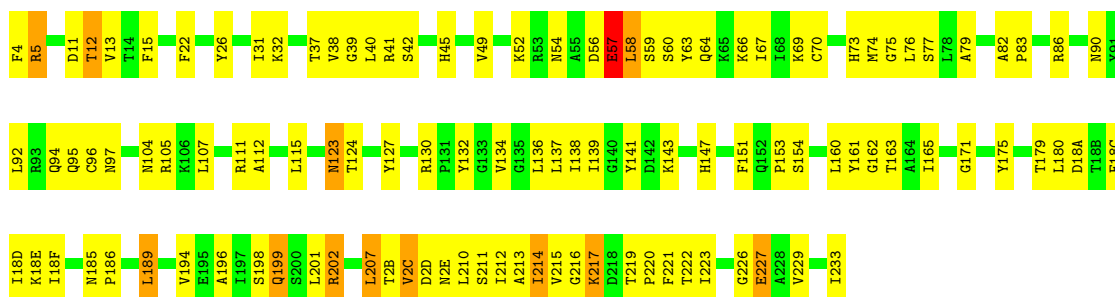
• Molecule 5: Proteasome component PRE5

Chain E:  54% 40% 5%



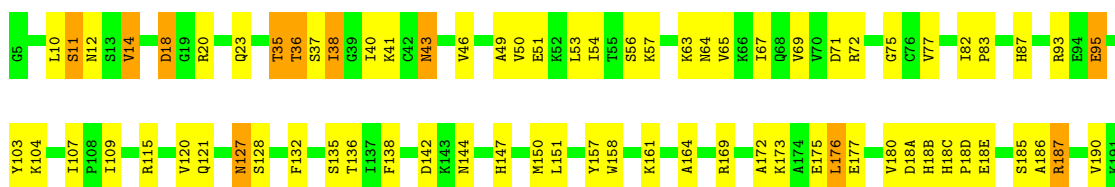
• Molecule 5: Proteasome component PRE5

Chain S:  52% 43% 5%



• Molecule 6: Proteasome component C1

Chain F:  61% 33% 6%





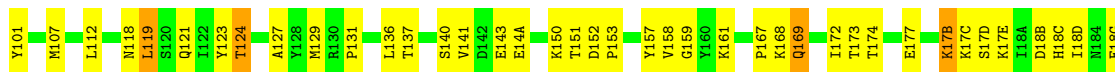
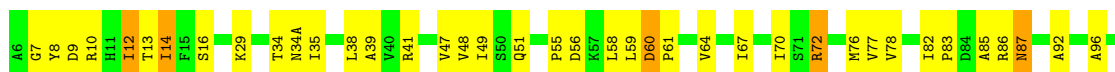
- Molecule 6: Proteasome component C1

Chain T: 59% 34% 6%



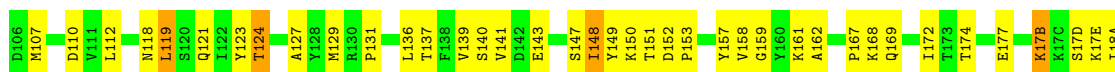
- Molecule 7: Proteasome component C7-alpha

Chain G: 58% 37% 5%



- Molecule 7: Proteasome component C7-alpha

Chain U: 58% 37% 5%



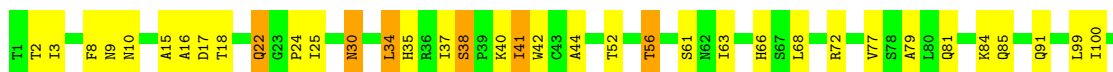
- Molecule 8: Proteasome component PUP1

Chain H: 72% 25% 3%





- Molecule 8: Proteasome component PUP1



- Molecule 9: Proteasome component PUP3



- Molecule 9: Proteasome component PUP3



- Molecule 10: Proteasome component C11



- Molecule 10: Proteasome component C11





- Molecule 11: Proteasome component PRE2



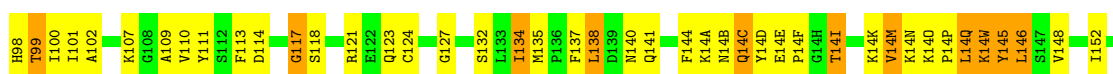
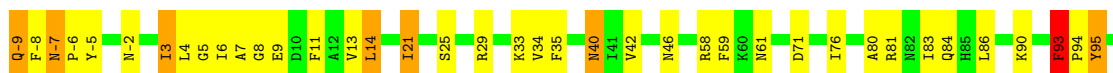
- Molecule 11: Proteasome component PRE2



- Molecule 12: Proteasome component C5

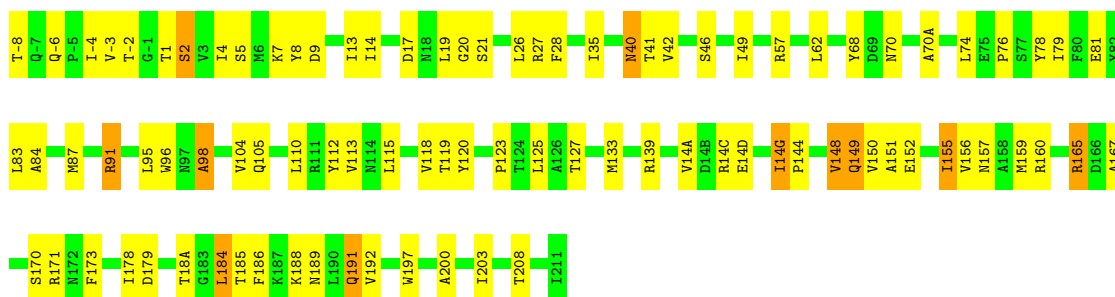


- Molecule 12: Proteasome component C5



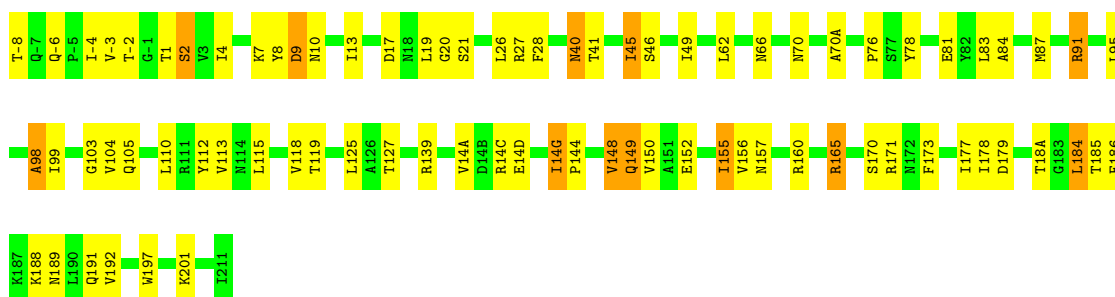
- Molecule 13: Proteasome component PRE4

Chain M:  61% 35% 5%



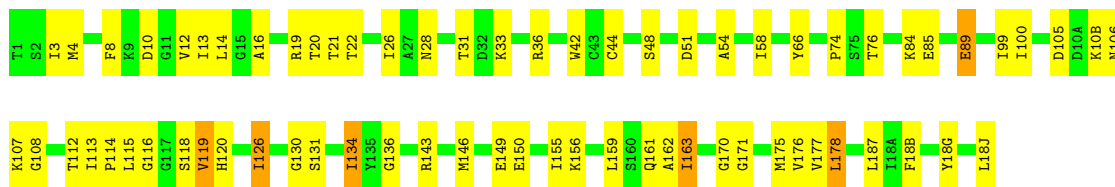
- Molecule 13: Proteasome component PRE4

Chain 1:  65% 30% 5%



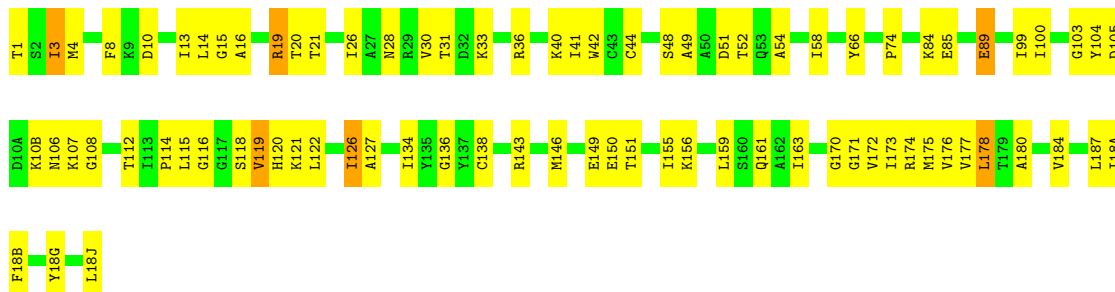
- Molecule 14: Proteasome component PRE3

Chain N:  65% 32% 3%



- Molecule 14: Proteasome component PRE3

Chain 2:  58% 39% 3%



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.18Å 300.72Å 144.66Å 90.00° 113.28° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80	Depositor
% Data completeness (in resolution range)	96.4 (15.00-2.80)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	50753	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

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

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	0.44	0/1952	0.91	3/2642 (0.1%)
1	O	0.44	0/1952	0.91	3/2642 (0.1%)
2	B	0.43	0/1935	0.94	8/2618 (0.3%)
2	P	0.43	0/1935	0.94	8/2618 (0.3%)
3	C	0.42	0/1920	0.94	6/2598 (0.2%)
3	Q	0.41	0/1920	0.94	6/2598 (0.2%)
4	D	0.42	0/1887	0.93	5/2541 (0.2%)
4	R	0.42	0/1887	0.91	5/2541 (0.2%)
5	E	0.42	1/1823 (0.1%)	0.92	5/2463 (0.2%)
5	S	0.42	0/1823	0.93	5/2463 (0.2%)
6	F	0.43	0/1937	0.96	8/2614 (0.3%)
6	T	0.44	0/1937	0.97	8/2614 (0.3%)
7	G	0.47	0/1959	0.98	8/2652 (0.3%)
7	U	0.48	0/1959	0.98	7/2652 (0.3%)
8	H	0.48	0/1716	0.98	7/2326 (0.3%)
8	V	0.44	0/1716	0.98	6/2326 (0.3%)
9	I	0.45	0/1611	0.98	6/2174 (0.3%)
9	W	0.47	0/1611	0.99	5/2174 (0.2%)
10	J	0.47	0/1613	0.99	9/2173 (0.4%)
10	X	0.46	0/1613	0.99	10/2173 (0.5%)
11	K	0.47	0/1681	0.93	6/2274 (0.3%)
11	Y	0.45	0/1681	0.92	3/2274 (0.1%)
12	L	0.43	0/1795	1.00	10/2420 (0.4%)
12	Z	0.42	0/1795	1.01	9/2420 (0.4%)
13	1	0.49	0/1855	0.97	10/2514 (0.4%)
13	M	0.46	0/1855	0.97	10/2514 (0.4%)
14	2	0.49	0/1541	0.97	2/2087 (0.1%)
14	N	0.49	0/1541	0.97	3/2087 (0.1%)
All	All	0.45	1/50450 (0.0%)	0.96	181/68192 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	74	MET	SD-CE	5.41	1.93	1.79

The worst 5 of 181 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	27	ARG	N-CA-C	10.25	122.04	111.07
13	1	27	ARG	N-CA-C	10.15	121.93	111.07
6	F	107	ILE	N-CA-C	9.19	118.97	108.96
6	T	12	ASN	N-CA-C	9.08	120.79	111.07
6	T	107	ILE	N-CA-C	9.06	118.84	108.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1926	61	0
1	O	1915	0	1926	62	0
2	B	1905	0	1901	146	0
2	P	1905	0	1901	123	0
3	C	1891	0	1900	120	0
3	Q	1891	0	1900	126	0
4	D	1862	0	1836	72	0
4	R	1862	0	1836	84	0
5	E	1795	0	1797	123	0
5	S	1795	0	1797	132	0
6	F	1897	0	1886	93	0
6	T	1897	0	1886	91	0
7	G	1921	0	1910	96	0
7	U	1921	0	1910	110	0
8	H	1685	0	1687	59	0
8	V	1685	0	1687	62	0
9	I	1581	0	1574	77	0
9	W	1581	0	1574	68	0
10	J	1585	0	1590	73	0
10	X	1585	0	1590	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	1644	0	1594	76	0
11	Y	1644	0	1594	70	0
12	L	1757	0	1711	77	0
12	Z	1757	0	1711	80	0
13	1	1824	0	1832	85	0
13	M	1824	0	1832	83	0
14	2	1512	0	1480	97	0
14	N	1512	0	1480	74	0
15	2	28	0	25	8	0
15	H	28	0	25	2	0
15	K	28	0	25	0	0
15	N	28	0	25	5	0
15	V	28	0	25	2	0
15	Y	28	0	25	1	0
16	1	63	0	0	4	0
16	2	51	0	0	6	0
16	A	46	0	0	1	0
16	B	31	0	0	5	0
16	C	33	0	0	1	0
16	D	26	0	0	1	0
16	E	14	0	0	0	0
16	F	36	0	0	2	0
16	G	48	0	0	2	0
16	H	42	0	0	1	0
16	I	50	0	0	0	0
16	J	45	0	0	5	0
16	K	33	0	0	3	0
16	L	42	0	0	4	0
16	M	52	0	0	4	0
16	N	43	0	0	1	0
16	O	23	0	0	0	0
16	P	21	0	0	1	0
16	Q	21	0	0	5	0
16	R	20	0	0	2	0
16	S	16	0	0	3	0
16	T	32	0	0	2	0
16	U	56	0	0	5	0
16	V	34	0	0	2	0
16	W	46	0	0	2	0
16	X	39	0	0	4	0
16	Y	32	0	0	7	0
16	Z	42	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	50753	0	49398	2257	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 23.

The worst 5 of 2257 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)
14:N:13:ILE:CD1	14:N:177:VAL:HG13	1.58	1.31
3:Q:197:LEU:HD13	3:Q:210:ILE:HD12	1.22	1.20
5:S:49:VAL:HG13	5:S:212:ILE:CD1	1.72	1.19
3:C:197:LEU:HD13	3:C:210:ILE:HD12	1.20	1.16
1:A:177:GLU:HG2	2:B:58:LEU:HD21	1.20	1.16

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%)	236 (95%)	10 (4%)	2 (1%)	16	44
1	O	248/250 (99%)	235 (95%)	11 (4%)	2 (1%)	16	44
2	B	242/244 (99%)	221 (91%)	16 (7%)	5 (2%)	5	20
2	P	242/244 (99%)	220 (91%)	17 (7%)	5 (2%)	5	20
3	C	239/241 (99%)	219 (92%)	16 (7%)	4 (2%)	7	25
3	Q	239/241 (99%)	218 (91%)	17 (7%)	4 (2%)	7	25
4	D	240/242 (99%)	225 (94%)	11 (5%)	4 (2%)	7	25
4	R	240/242 (99%)	223 (93%)	12 (5%)	5 (2%)	5	20
5	E	231/233 (99%)	210 (91%)	15 (6%)	6 (3%)	4	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	S	231/233 (99%)	210 (91%)	15 (6%)	6 (3%)	4	15
6	F	242/244 (99%)	222 (92%)	17 (7%)	3 (1%)	10	34
6	T	242/244 (99%)	222 (92%)	17 (7%)	3 (1%)	10	34
7	G	241/243 (99%)	226 (94%)	12 (5%)	3 (1%)	10	34
7	U	241/243 (99%)	224 (93%)	15 (6%)	2 (1%)	16	44
8	H	220/222 (99%)	208 (94%)	11 (5%)	1 (0%)	24	55
8	V	220/222 (99%)	211 (96%)	8 (4%)	1 (0%)	24	55
9	I	202/204 (99%)	195 (96%)	6 (3%)	1 (0%)	24	55
9	W	202/204 (99%)	195 (96%)	6 (3%)	1 (0%)	24	55
10	J	196/198 (99%)	184 (94%)	11 (6%)	1 (0%)	24	55
10	X	196/198 (99%)	186 (95%)	9 (5%)	1 (0%)	24	55
11	K	210/212 (99%)	201 (96%)	9 (4%)	0	100	100
11	Y	210/212 (99%)	202 (96%)	8 (4%)	0	100	100
12	L	220/222 (99%)	205 (93%)	14 (6%)	1 (0%)	24	55
12	Z	220/222 (99%)	206 (94%)	12 (6%)	2 (1%)	14	41
13	1	231/233 (99%)	218 (94%)	13 (6%)	0	100	100
13	M	231/233 (99%)	218 (94%)	11 (5%)	2 (1%)	14	41
14	2	194/196 (99%)	184 (95%)	10 (5%)	0	100	100
14	N	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
All	All	6312/6368 (99%)	5909 (94%)	338 (5%)	65 (1%)	12	38

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	20(A)	SER
3	C	58	LEU
4	D	12(G)	GLU
5	E	217	LYS
2	P	20(A)	SER

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%)	199 (95%)	10 (5%)	23	56
1	O	209/209 (100%)	201 (96%)	8 (4%)	29	64
2	B	203/203 (100%)	191 (94%)	12 (6%)	18	48
2	P	203/203 (100%)	198 (98%)	5 (2%)	42	76
3	C	213/213 (100%)	201 (94%)	12 (6%)	19	50
3	Q	213/213 (100%)	204 (96%)	9 (4%)	26	61
4	D	198/198 (100%)	185 (93%)	13 (7%)	15	43
4	R	198/198 (100%)	187 (94%)	11 (6%)	19	50
5	E	192/192 (100%)	182 (95%)	10 (5%)	21	53
5	S	192/192 (100%)	182 (95%)	10 (5%)	21	53
6	F	201/201 (100%)	181 (90%)	20 (10%)	7	24
6	T	201/201 (100%)	182 (90%)	19 (10%)	8	26
7	G	207/207 (100%)	194 (94%)	13 (6%)	16	45
7	U	207/207 (100%)	196 (95%)	11 (5%)	20	52
8	H	181/181 (100%)	173 (96%)	8 (4%)	25	59
8	V	181/181 (100%)	173 (96%)	8 (4%)	25	59
9	I	172/172 (100%)	166 (96%)	6 (4%)	32	67
9	W	172/172 (100%)	166 (96%)	6 (4%)	32	67
10	J	175/175 (100%)	170 (97%)	5 (3%)	37	73
10	X	175/175 (100%)	170 (97%)	5 (3%)	37	73
11	K	169/169 (100%)	160 (95%)	9 (5%)	20	52
11	Y	169/169 (100%)	160 (95%)	9 (5%)	20	52
12	L	185/185 (100%)	160 (86%)	25 (14%)	4	13
12	Z	185/185 (100%)	161 (87%)	24 (13%)	4	14
13	1	199/199 (100%)	191 (96%)	8 (4%)	28	63
13	M	199/199 (100%)	191 (96%)	8 (4%)	28	63
14	2	162/162 (100%)	156 (96%)	6 (4%)	30	65
14	N	162/162 (100%)	155 (96%)	7 (4%)	26	60
All	All	5332/5332 (100%)	5035 (94%)	297 (6%)	19	50

5 of 297 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	V	22	GLN
13	1	148	VAL
8	V	197	ARG
12	Z	-7	ASN
8	H	197	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 231 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	161	GLN
13	1	149	GLN
4	R	161	ASN
13	1	93	ASN
11	Y	131	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	BO2	N	1404	14	25,29,29	1.76	8 (32%)	33,38,38	2.26	12 (36%)
15	BO2	Y	1403	11	25,29,29	1.39	6 (24%)	33,38,38	2.02	11 (33%)
15	BO2	V	1401	8	25,29,29	1.54	6 (24%)	33,38,38	2.00	9 (27%)
15	BO2	H	1400	8	25,29,29	1.59	6 (24%)	33,38,38	1.94	8 (24%)
15	BO2	K	1402	11	25,29,29	1.32	3 (12%)	33,38,38	2.08	11 (33%)
15	BO2	2	1405	14	25,29,29	1.66	7 (28%)	33,38,38	2.24	12 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BO2	N	1404	14	-	8/23/28/28	0/2/2/2
15	BO2	Y	1403	11	-	5/23/28/28	0/2/2/2
15	BO2	V	1401	8	-	6/23/28/28	0/2/2/2
15	BO2	H	1400	8	-	5/23/28/28	0/2/2/2
15	BO2	K	1402	11	-	5/23/28/28	0/2/2/2
15	BO2	2	1405	14	-	8/23/28/28	0/2/2/2

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	1404	BO2	C14-C13	3.27	1.44	1.38
15	2	1405	BO2	C17-C12	3.12	1.45	1.38
15	N	1404	BO2	C17-C12	3.11	1.45	1.38
15	H	1400	BO2	C16-C17	3.05	1.44	1.38
15	N	1404	BO2	C13-C12	2.94	1.44	1.38

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	1404	BO2	C21-C22-C23	6.42	123.51	115.32
15	K	1402	BO2	C21-C22-C23	5.93	122.90	115.32
15	2	1405	BO2	C21-C22-C23	5.93	122.89	115.32
15	Y	1403	BO2	C21-C22-C23	5.78	122.70	115.32
15	V	1401	BO2	C21-C22-C23	5.16	121.91	115.32

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

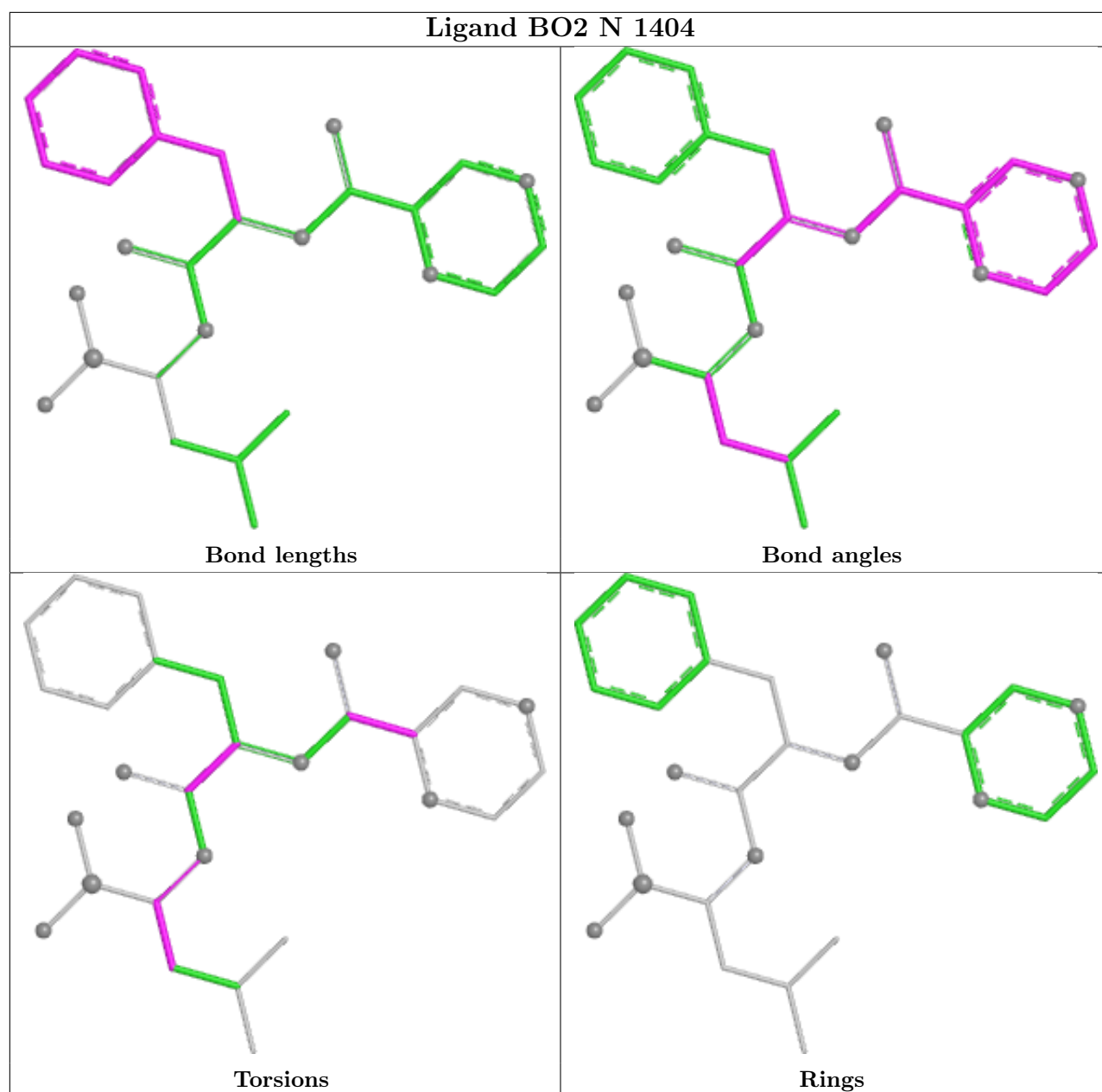
Mol	Chain	Res	Type	Atoms
15	H	1400	BO2	N20-C21-C22-C23
15	H	1400	BO2	B26-C21-C22-C23
15	K	1402	BO2	N20-C21-C22-C23
15	K	1402	BO2	B26-C21-C22-C23
15	V	1401	BO2	N20-C21-C22-C23

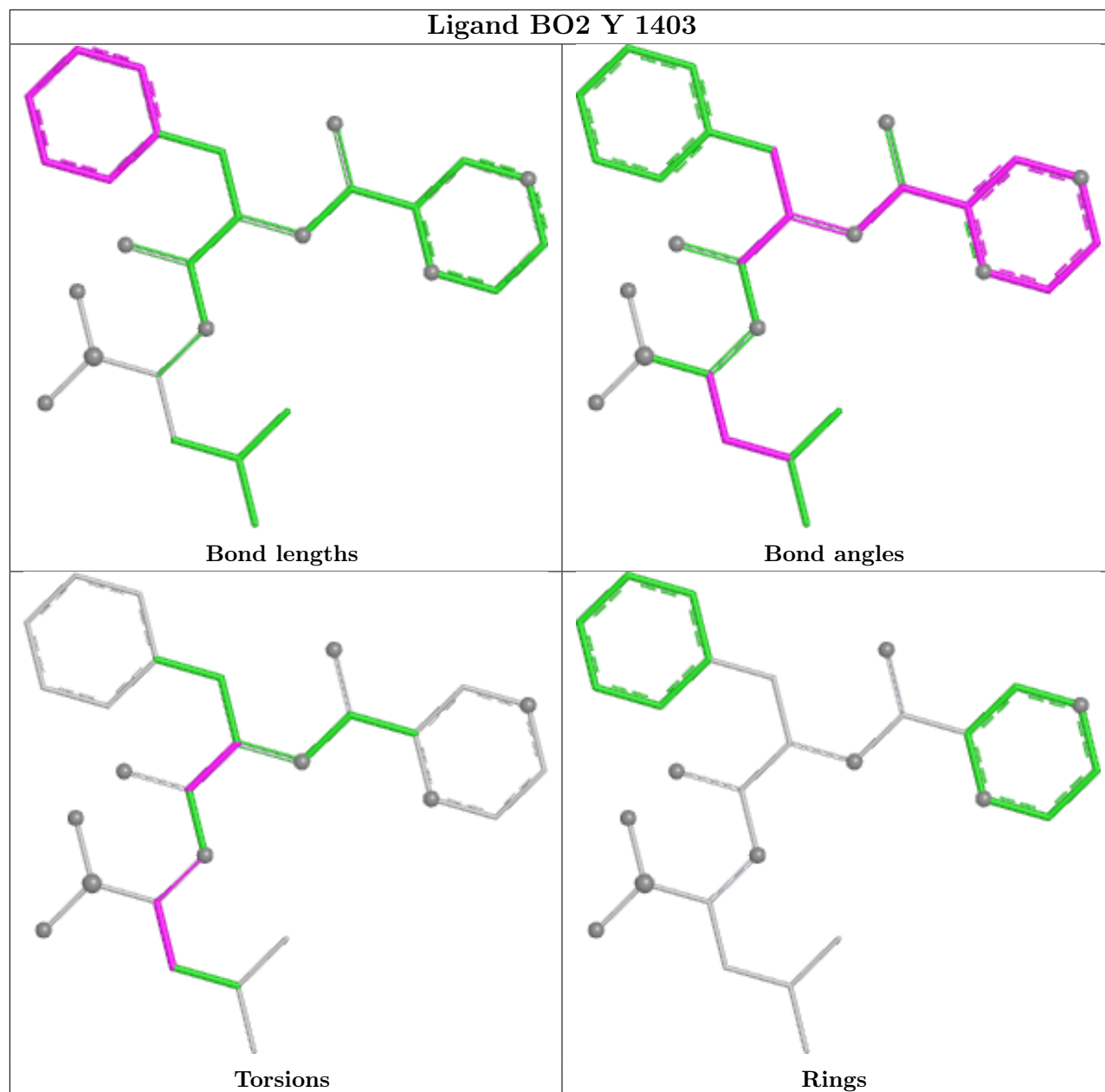
There are no ring outliers.

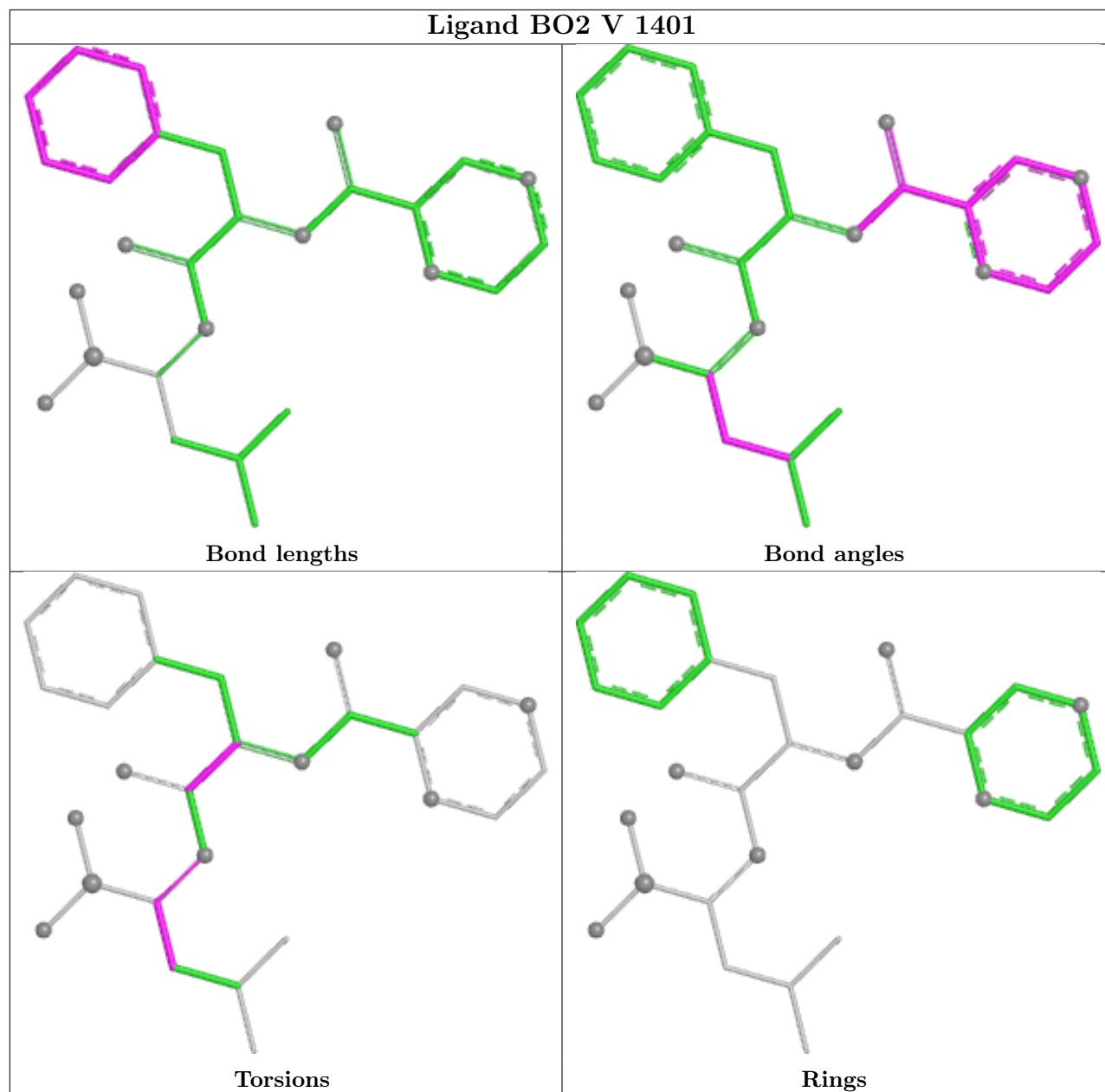
5 monomers are involved in 18 short contacts:

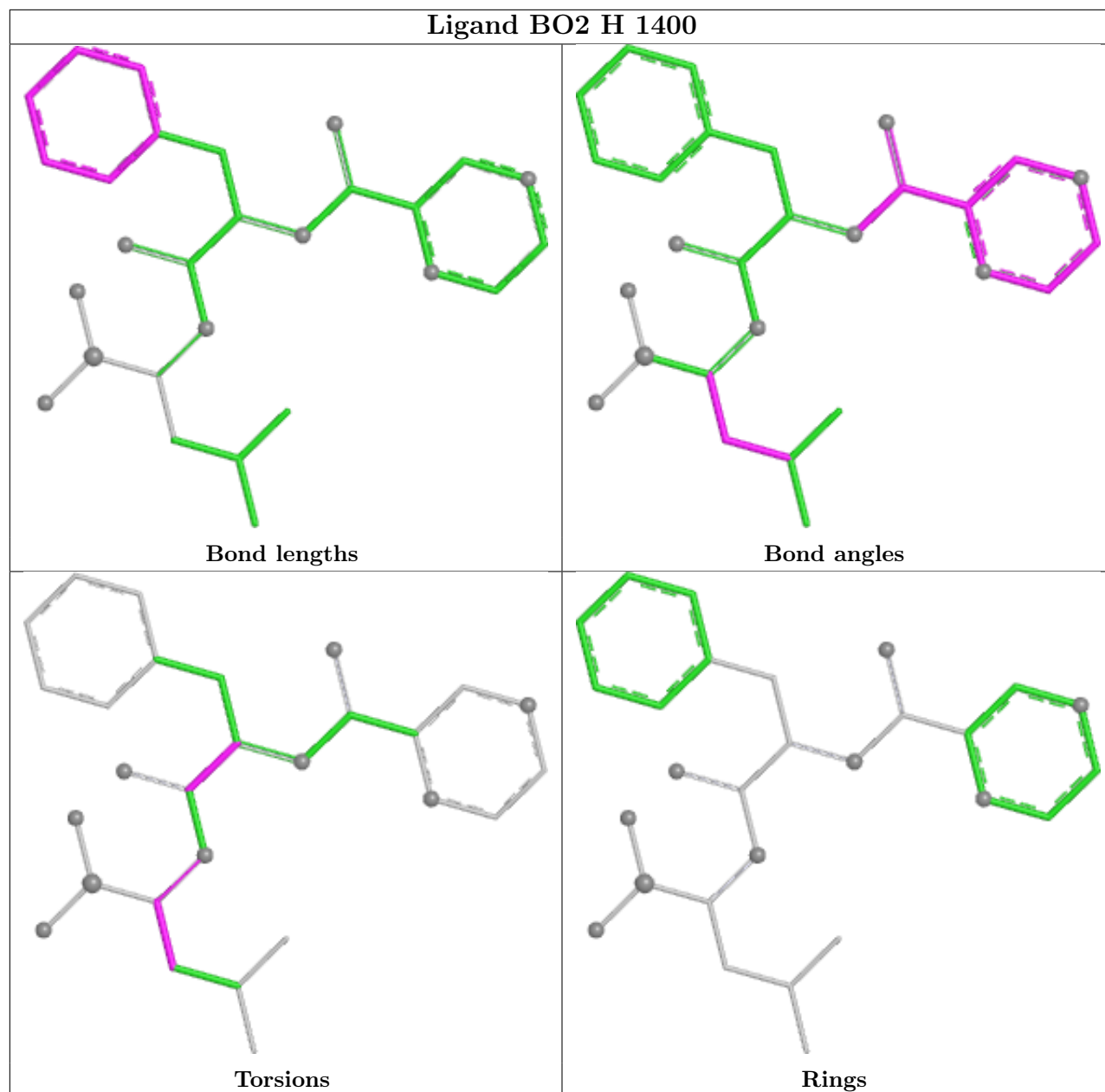
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	N	1404	BO2	5	0
15	Y	1403	BO2	1	0
15	V	1401	BO2	2	0
15	H	1400	BO2	2	0
15	2	1405	BO2	8	0

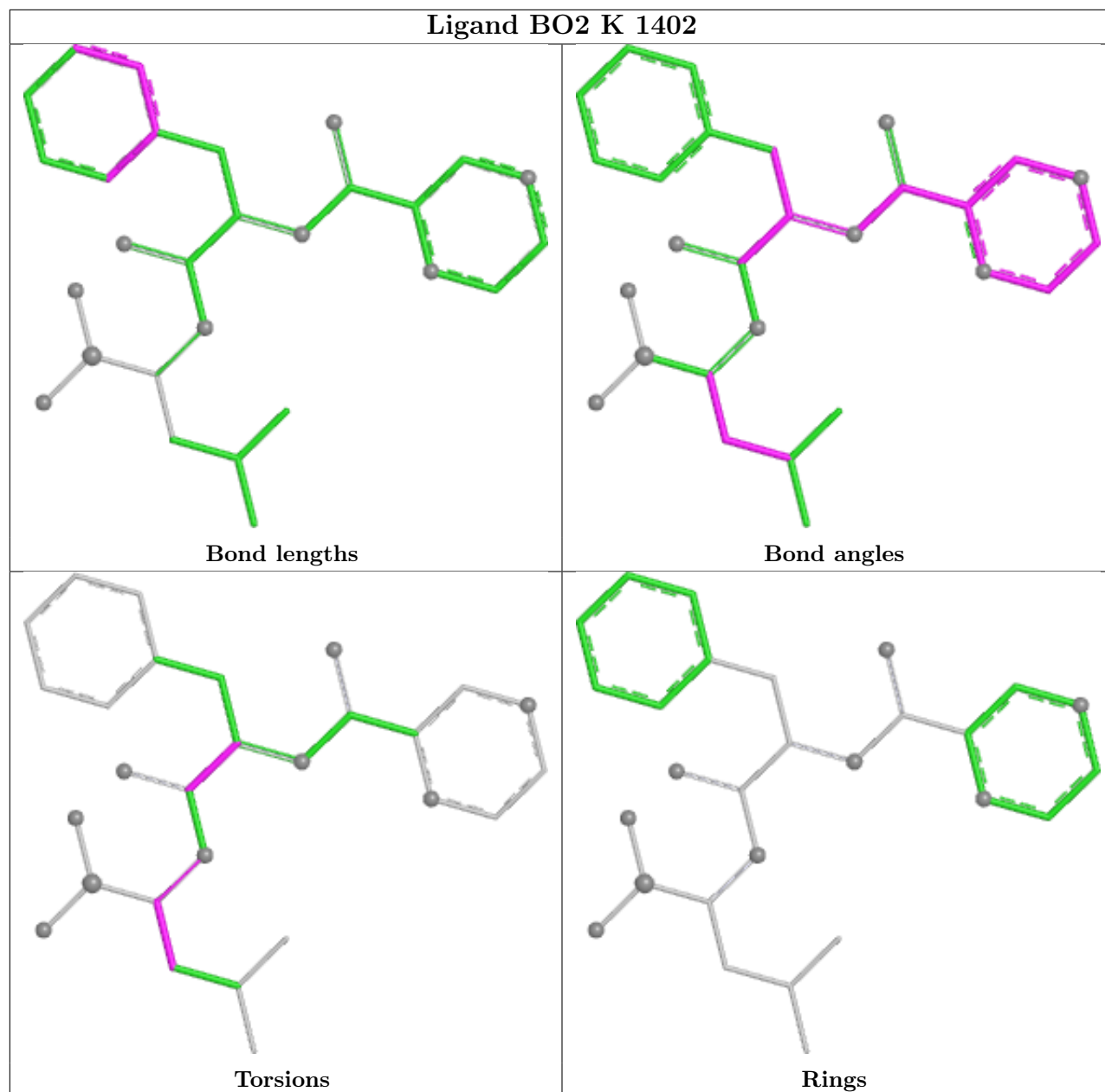
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

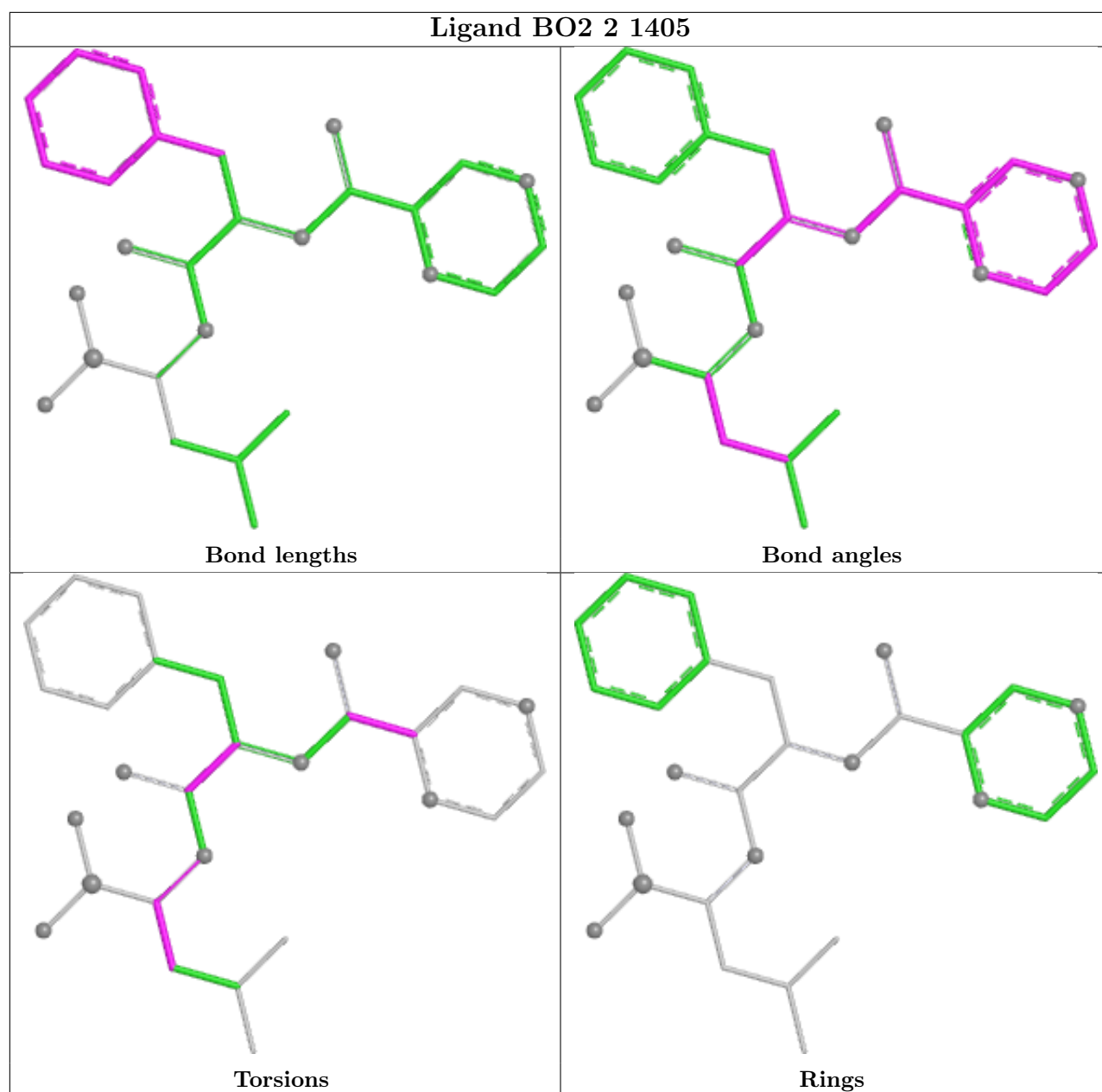












5.7 Other polymers [i](#)

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.