



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 02:57 am BST

PDB ID : 3MG0
Title : Structure of yeast 20S proteasome with bortezomib
Authors : Sintchak, M.D.
Deposited on : 2010-04-05
Resolution : 2.68 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

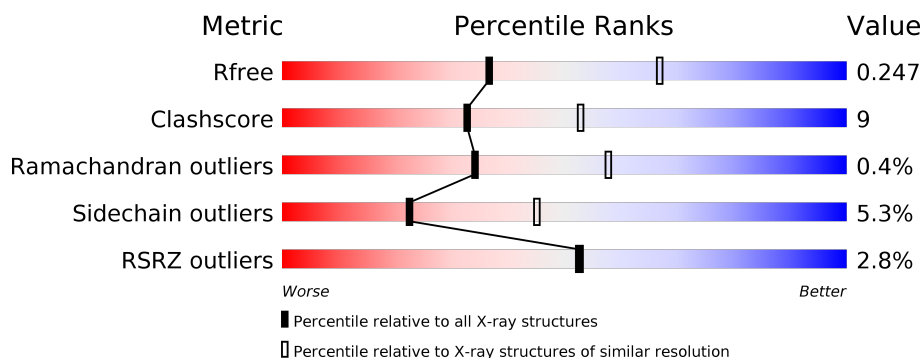
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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

Mol	Chain	Length	Quality of chain
1	A	250	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>11%</div> </div> <div></div> </div>
1	O	250	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>13%</div> </div> <div></div> </div>
2	B	244	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>24%</div> </div> <div></div> </div>
2	P	244	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>21%</div> </div> <div></div> </div>
3	C	241	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>21%</div> </div> <div></div> </div>
3	Q	241	<div> <div>11%</div> <div> <div></div> <div>76%</div> <div>22%</div> </div> <div></div> </div>

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Mol	Chain	Length	Quality of chain
4	D	242	
4	R	242	
5	E	233	
5	S	233	
6	F	244	
6	T	244	
7	G	243	
7	U	243	
8	H	222	
8	V	222	
9	I	204	
9	W	204	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	1	233	
13	M	233	
14	2	196	
14	N	196	

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
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
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
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
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
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
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
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
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
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 (three-letter code: BO2) (formula: C₁₉H₂₅BN₄O₄).



- Molecule 16 is water.

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	46	Total 46	O 46	0	0
16	H	41	Total 41	O 41	0	0
16	I	52	Total 52	O 52	0	0
16	J	45	Total 45	O 45	0	0
16	K	33	Total 33	O 33	0	0
16	L	42	Total 42	O 42	0	0
16	M	53	Total 53	O 53	0	0
16	N	46	Total 46	O 46	0	0
16	O	24	Total 24	O 24	0	0
16	P	23	Total 23	O 23	0	0
16	Q	19	Total 19	O 19	0	0
16	R	24	Total 24	O 24	0	0
16	S	17	Total 17	O 17	0	0
16	T	32	Total 32	O 32	0	0
16	U	53	Total 53	O 53	0	0
16	V	35	Total 35	O 35	0	0
16	W	44	Total 44	O 44	0	0
16	X	38	Total 38	O 38	0	0
16	Y	30	Total 30	O 30	0	0
16	Z	38	Total 38	O 38	0	0
16	1	63	Total 63	O 63	0	0

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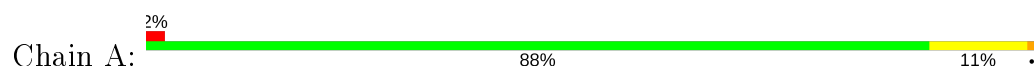
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	2	53	Total	O	0	0
			53	53		

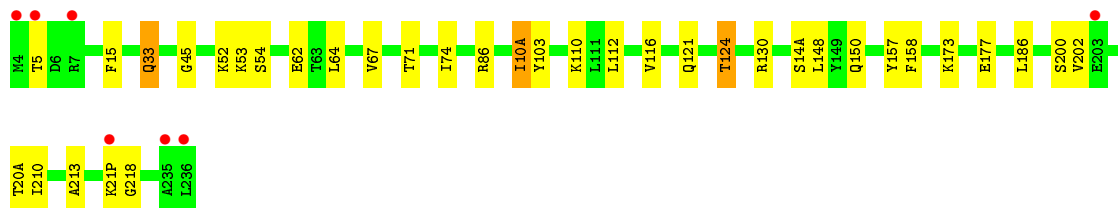
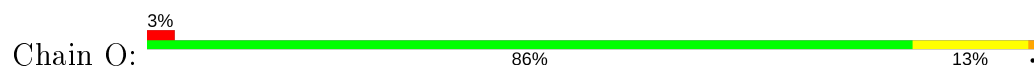
3 Residue-property plots [i](#)

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

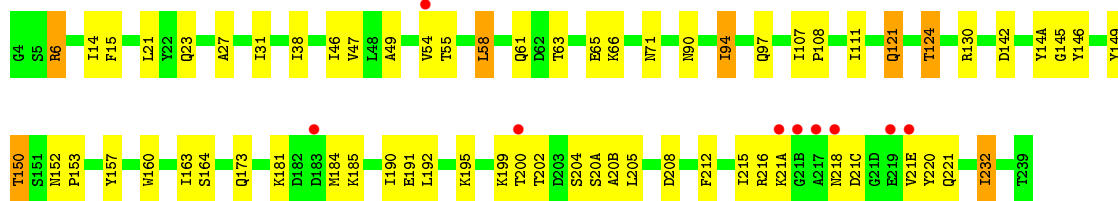
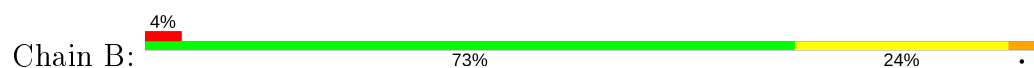
- Molecule 1: Proteasome component Y7



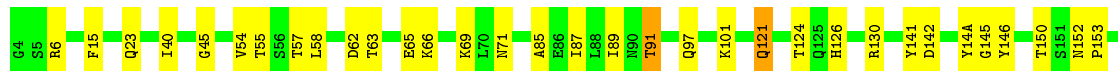
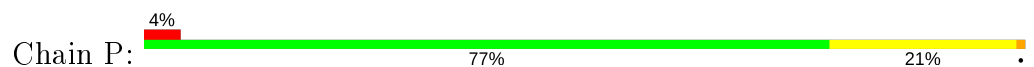
- Molecule 1: Proteasome component Y7



- Molecule 2: Proteasome component Y13

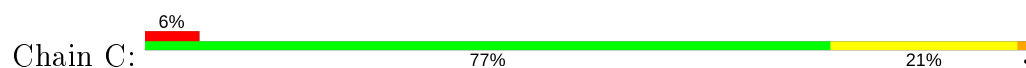


- Molecule 2: Proteasome component Y13

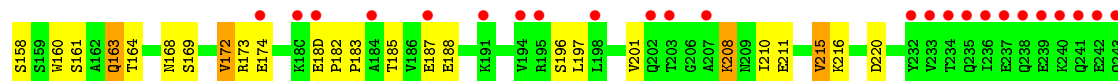
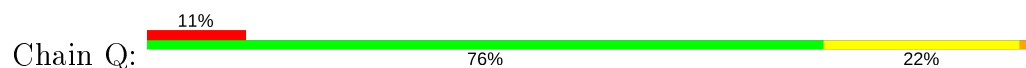




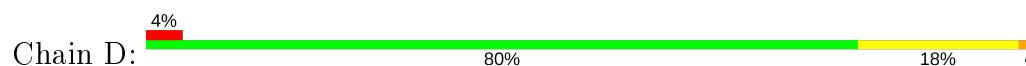
- Molecule 3: Proteasome component PRE6



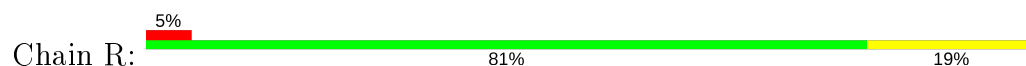
- Molecule 3: Proteasome component PRE6



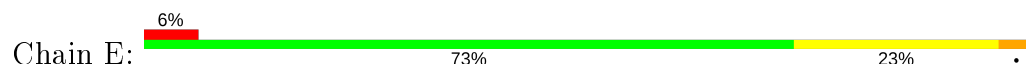
- Molecule 4: Proteasome component PUP2

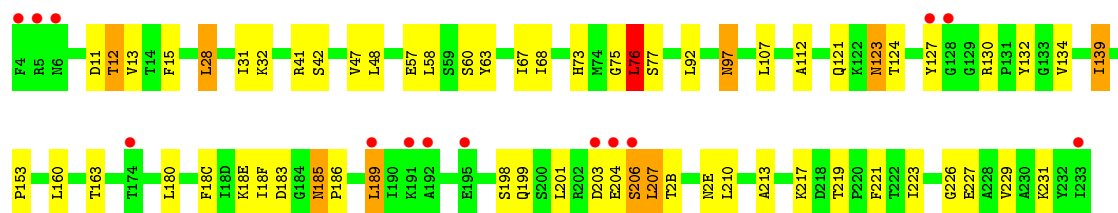


- Molecule 4: Proteasome component PUP2

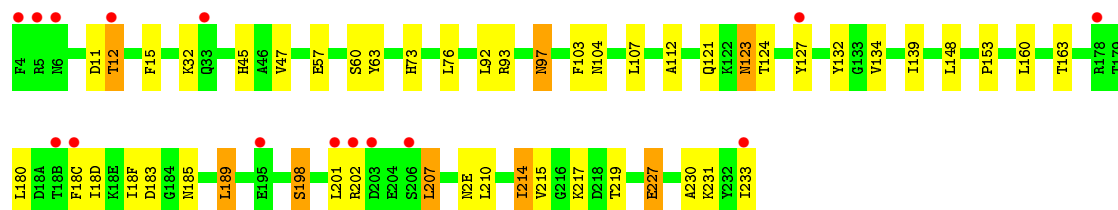
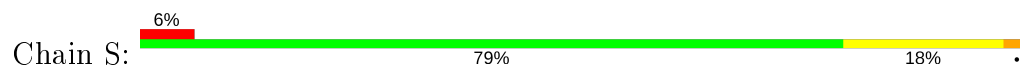


- Molecule 5: Proteasome component PRE5

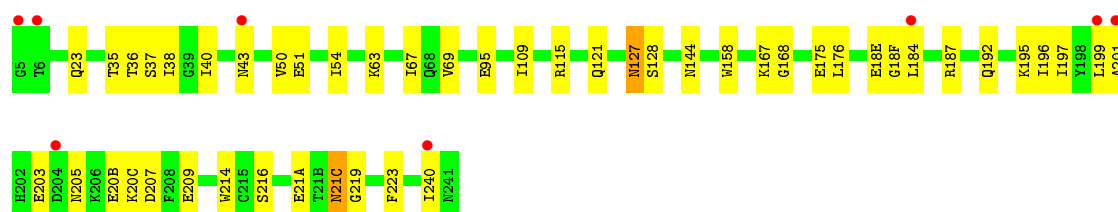
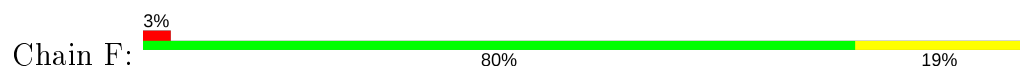




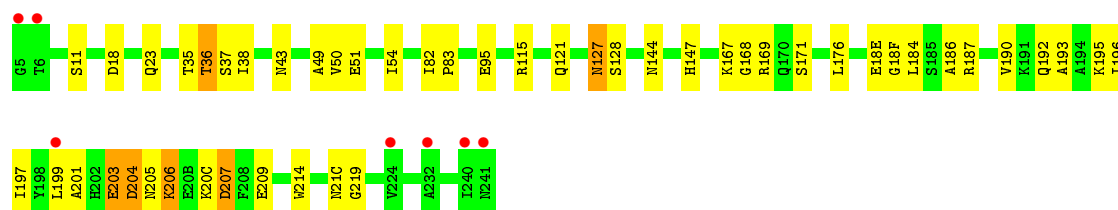
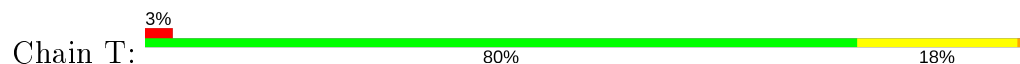
• Molecule 5: Proteasome component PRE5



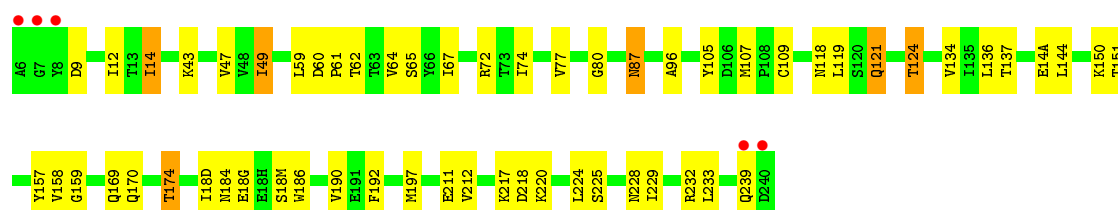
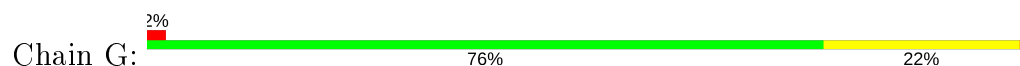
• Molecule 6: Proteasome component C1



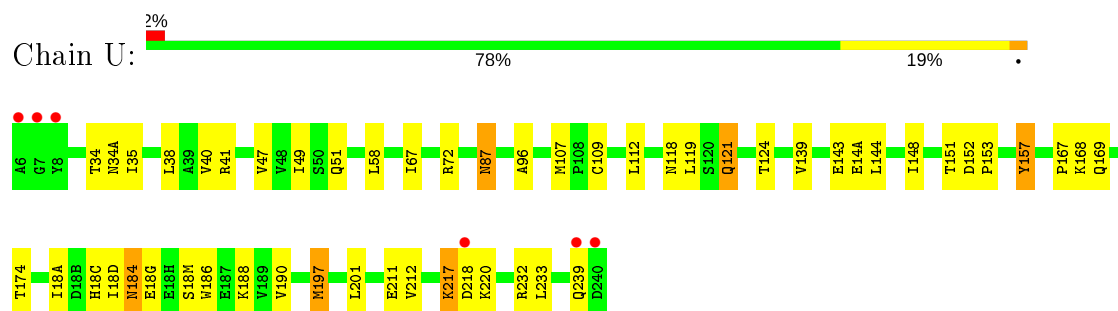
• Molecule 6: Proteasome component C1



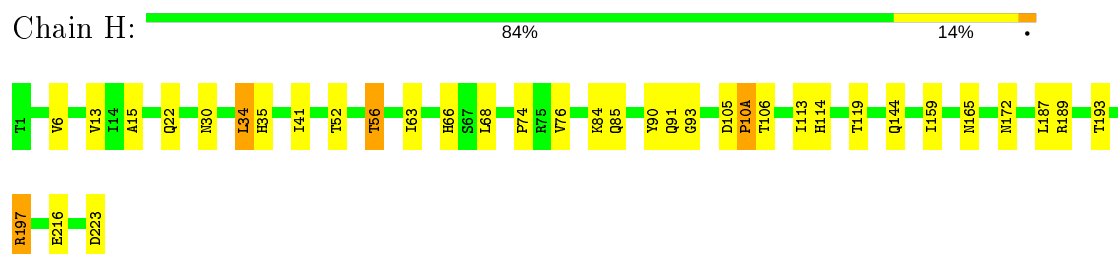
• Molecule 7: Proteasome component C7-alpha



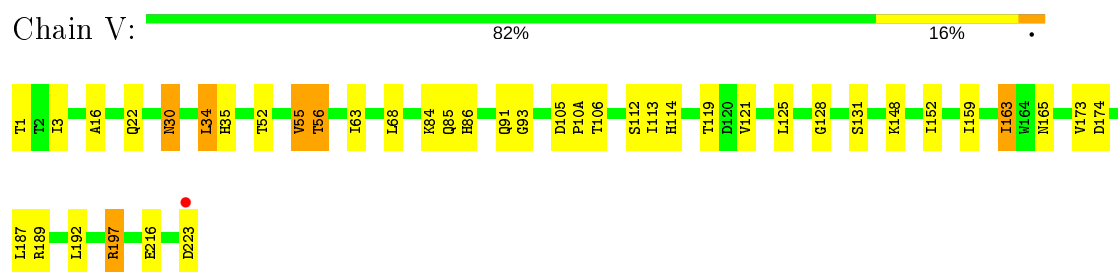
- Molecule 7: Proteasome component C7-alpha



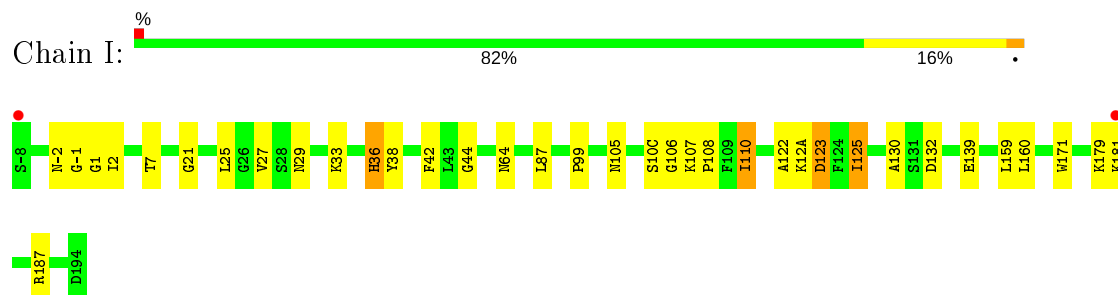
- Molecule 8: Proteasome component PUP1



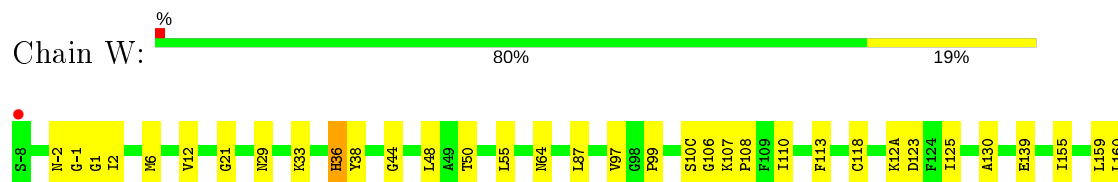
- Molecule 8: Proteasome component PUP1

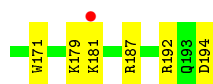


- Molecule 9: Proteasome component PUP3

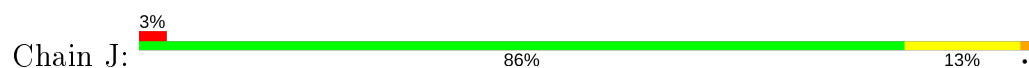


- Molecule 9: Proteasome component PUP3

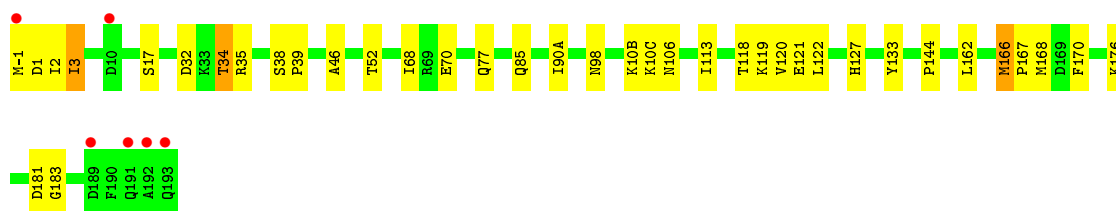
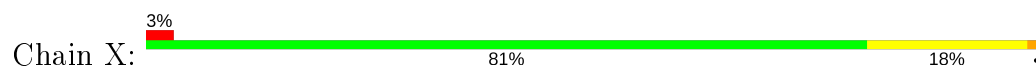




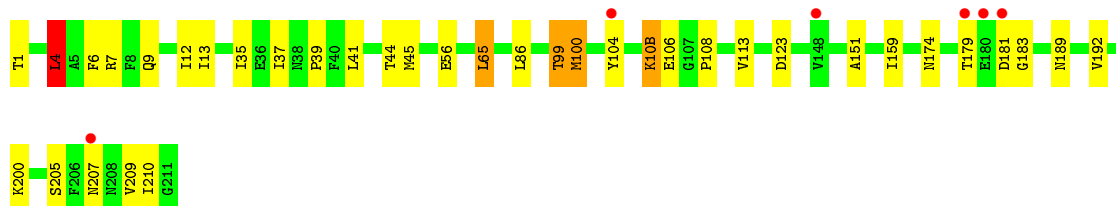
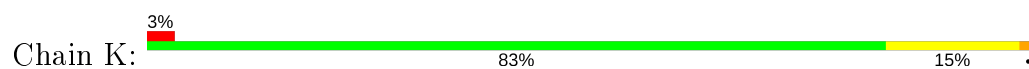
• Molecule 10: Proteasome component C11



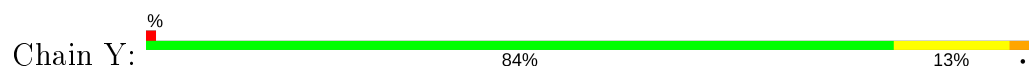
• Molecule 10: Proteasome component C11



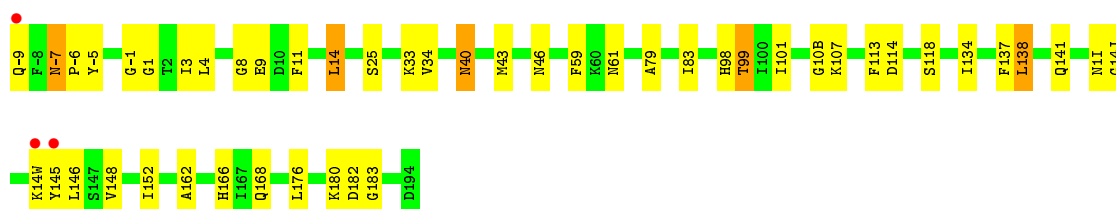
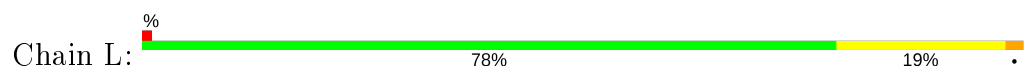
• Molecule 11: Proteasome component PRE2



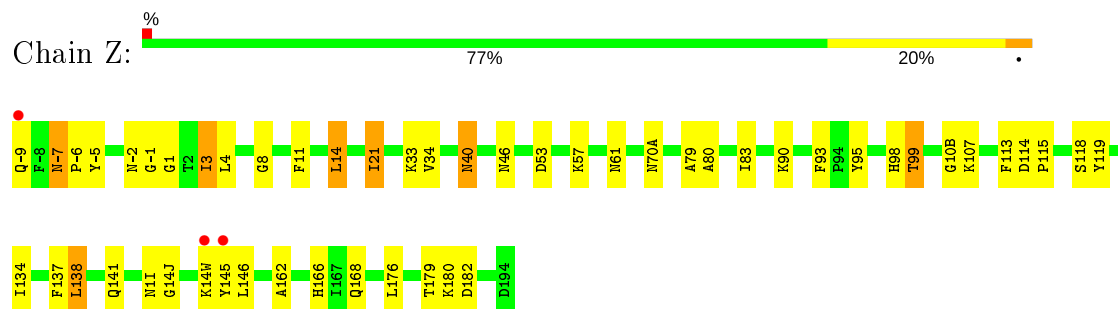
• Molecule 11: Proteasome component PRE2



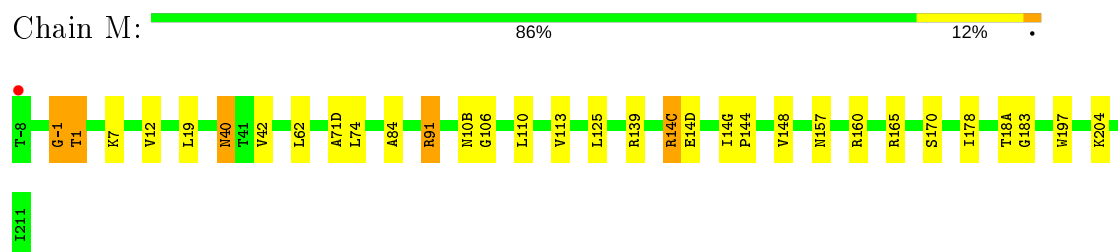
• Molecule 12: Proteasome component C5



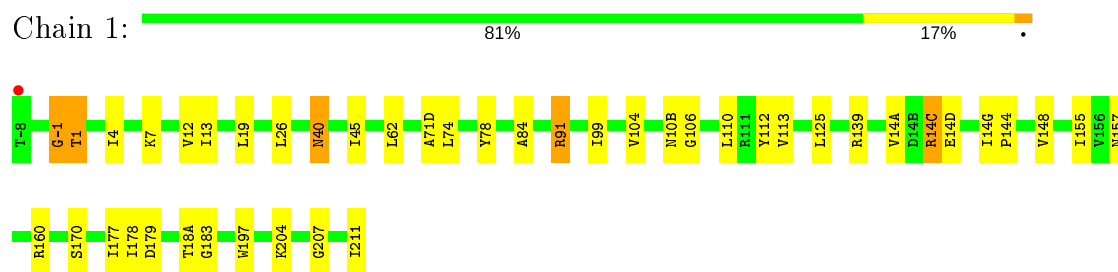
- Molecule 12: Proteasome component C5



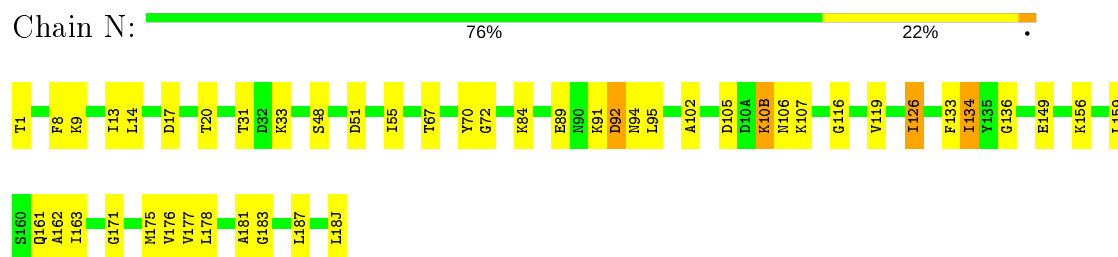
- Molecule 13: Proteasome component PRE4



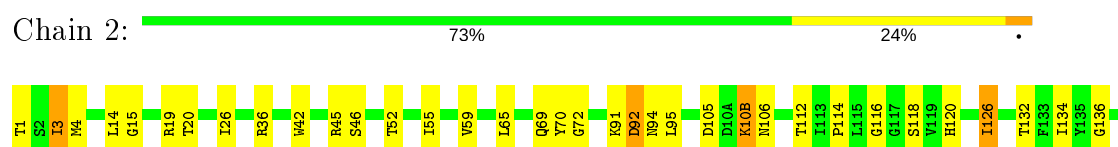
- Molecule 13: Proteasome component PRE4



- Molecule 14: Proteasome component PRE3



- Molecule 14: Proteasome component PRE3





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.12Å 300.53Å 145.83Å 90.00° 113.16° 90.00°	Depositor
Resolution (Å)	50.00 – 2.68 49.04 – 2.68	Depositor EDS
% Data completeness (in resolution range)	92.0 (50.00-2.68) 92.1 (49.04-2.68)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.226 , 0.253 0.224 , 0.247	Depositor DCC
R_{free} test set	2818 reflections (1.02%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	50753	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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

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	0.68	1/1948 (0.1%)	0.55	0/2630
1	O	0.68	1/1948 (0.1%)	0.55	0/2630
2	B	0.41	0/1929	0.58	0/2600
2	P	0.43	0/1929	0.58	0/2600
3	C	0.41	0/1916	0.56	0/2585
3	Q	0.40	0/1916	0.56	0/2585
4	D	0.42	0/1881	0.58	0/2523
4	R	0.41	0/1881	0.58	0/2523
5	E	0.40	0/1819	0.57	1/2451 (0.0%)
5	S	0.41	0/1819	0.55	0/2451
6	F	0.42	0/1933	0.54	0/2602
6	T	0.43	0/1933	0.55	0/2602
7	G	0.45	0/1955	0.55	0/2640
7	U	0.44	0/1955	0.55	0/2640
8	H	0.74	1/1714 (0.1%)	0.55	1/2320 (0.0%)
8	V	0.38	0/1713	0.55	0/2317
9	I	0.72	1/1607 (0.1%)	0.60	2/2162 (0.1%)
9	W	0.65	1/1607 (0.1%)	0.58	1/2162 (0.0%)
10	J	0.41	0/1610	0.56	0/2164
10	X	0.41	0/1610	0.56	0/2164
11	K	0.42	0/1679	0.56	1/2268 (0.0%)
11	Y	0.41	0/1679	0.58	1/2268 (0.0%)
12	L	0.42	0/1790	0.56	0/2405
12	Z	0.42	0/1790	0.58	0/2405
13	1	0.73	1/1851 (0.1%)	0.63	1/2501 (0.0%)
13	M	0.60	1/1851 (0.1%)	0.58	0/2501
14	2	0.66	1/1538 (0.1%)	0.55	0/2078
14	N	0.76	1/1538 (0.1%)	0.56	0/2078
All	All	0.52	9/50339 (0.0%)	0.57	8/67855 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	1	-1	GLY	C-N	25.93	1.93	1.34
8	H	10(A)	PRO	C-N	25.92	1.93	1.34
14	N	92	ASP	C-N	24.57	1.90	1.34
9	I	36	HIS	C-N	23.90	1.89	1.34
1	O	10(A)	ILE	C-N	23.90	1.89	1.34

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	W	36	HIS	CA-C-N	-6.43	103.05	117.20
11	K	4	LEU	CA-CB-CG	5.82	128.69	115.30
8	H	10(A)	PRO	O-C-N	-5.80	113.41	122.70
9	I	36	HIS	CA-C-N	-5.50	105.11	117.20
5	E	76	LEU	CA-CB-CG	5.43	127.79	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1921	27	0
1	O	1915	0	1921	30	0
2	B	1905	0	1895	47	0
2	P	1905	0	1895	45	0
3	C	1891	0	1897	35	0
3	Q	1891	0	1897	42	0
4	D	1862	0	1830	25	0
4	R	1862	0	1830	26	0
5	E	1795	0	1793	50	0
5	S	1795	0	1793	32	0
6	F	1897	0	1882	34	0
6	T	1897	0	1882	33	0
7	G	1921	0	1906	37	0
7	U	1921	0	1906	36	0
8	H	1685	0	1685	32	0
8	V	1685	0	1685	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	1581	0	1572	31	0
9	W	1581	0	1572	27	0
10	J	1585	0	1590	26	0
10	X	1585	0	1590	34	0
11	K	1644	0	1593	31	0
11	Y	1644	0	1593	22	0
12	L	1757	0	1709	39	0
12	Z	1757	0	1709	41	0
13	1	1824	0	1831	36	0
13	M	1824	0	1831	29	0
14	2	1512	0	1477	46	0
14	N	1512	0	1477	40	0
15	2	28	0	25	7	0
15	H	28	0	25	0	0
15	K	28	0	25	2	0
15	N	28	0	25	3	0
15	V	28	0	25	2	0
15	Y	28	0	25	3	0
16	1	63	0	0	0	0
16	2	53	0	0	3	0
16	A	49	0	0	1	0
16	B	31	0	0	1	0
16	C	32	0	0	0	0
16	D	25	0	0	0	0
16	E	14	0	0	0	0
16	F	35	0	0	1	0
16	G	46	0	0	0	0
16	H	41	0	0	1	0
16	I	52	0	0	1	0
16	J	45	0	0	2	0
16	K	33	0	0	0	0
16	L	42	0	0	3	0
16	M	53	0	0	0	0
16	N	46	0	0	1	0
16	O	24	0	0	2	0
16	P	23	0	0	0	0
16	Q	19	0	0	0	0
16	R	24	0	0	3	0
16	S	17	0	0	0	0
16	T	32	0	0	1	0
16	U	53	0	0	1	0
16	V	35	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	W	44	0	0	0	0
16	X	38	0	0	1	0
16	Y	30	0	0	3	0
16	Z	38	0	0	3	0
All	All	50753	0	49312	858	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 9.

The worst 5 of 858 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)
13:M:-1:GLY:C	13:M:1:THR:N	1.77	1.36
9:W:36:HIS:C	9:W:38:TYR:N	1.80	1.35
14:2:92:ASP:C	14:2:94:ASN:N	1.80	1.33
13:M:-1:GLY:C	13:M:1:THR:H2	1.34	1.30
1:O:10(A):ILE:C	1:O:103:TYR:N	1.89	1.26

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	240/250 (96%)	233 (97%)	6 (2%)	1 (0%)	34	58
1	O	240/250 (96%)	231 (96%)	7 (3%)	2 (1%)	19	40
2	B	230/244 (94%)	222 (96%)	4 (2%)	4 (2%)	9	20
2	P	230/244 (94%)	217 (94%)	10 (4%)	3 (1%)	12	27
3	C	231/241 (96%)	226 (98%)	4 (2%)	1 (0%)	34	58
3	Q	231/241 (96%)	226 (98%)	3 (1%)	2 (1%)	17	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	228/242 (94%)	221 (97%)	6 (3%)	1 (0%)	34	58
4	R	228/242 (94%)	218 (96%)	9 (4%)	1 (0%)	34	58
5	E	223/233 (96%)	210 (94%)	11 (5%)	2 (1%)	17	37
5	S	223/233 (96%)	214 (96%)	7 (3%)	2 (1%)	17	37
6	F	234/244 (96%)	220 (94%)	14 (6%)	0	100	100
6	T	234/244 (96%)	224 (96%)	9 (4%)	1 (0%)	34	58
7	G	233/243 (96%)	222 (95%)	10 (4%)	1 (0%)	34	58
7	U	233/243 (96%)	225 (97%)	7 (3%)	1 (0%)	34	58
8	H	216/222 (97%)	211 (98%)	5 (2%)	0	100	100
8	V	214/222 (96%)	210 (98%)	4 (2%)	0	100	100
9	I	194/204 (95%)	189 (97%)	5 (3%)	0	100	100
9	W	194/204 (95%)	189 (97%)	5 (3%)	0	100	100
10	J	191/198 (96%)	184 (96%)	6 (3%)	1 (0%)	29	52
10	X	191/198 (96%)	183 (96%)	8 (4%)	0	100	100
11	K	206/212 (97%)	200 (97%)	6 (3%)	0	100	100
11	Y	206/212 (97%)	200 (97%)	5 (2%)	1 (0%)	29	52
12	L	210/222 (95%)	204 (97%)	6 (3%)	0	100	100
12	Z	210/222 (95%)	204 (97%)	6 (3%)	0	100	100
13	1	223/233 (96%)	216 (97%)	5 (2%)	2 (1%)	17	37
13	M	223/233 (96%)	214 (96%)	8 (4%)	1 (0%)	34	58
14	2	188/196 (96%)	182 (97%)	6 (3%)	0	100	100
14	N	188/196 (96%)	183 (97%)	5 (3%)	0	100	100
All	All	6092/6368 (96%)	5878 (96%)	187 (3%)	27 (0%)	34	58

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	58	LEU
2	P	20(A)	SER
3	Q	58	LEU
2	B	54	VAL
5	E	217	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	206 (99%)	3 (1%)	67	85
1	O	209/209 (100%)	203 (97%)	6 (3%)	42	69
2	B	203/203 (100%)	189 (93%)	14 (7%)	15	33
2	P	203/203 (100%)	191 (94%)	12 (6%)	19	40
3	C	213/213 (100%)	199 (93%)	14 (7%)	16	35
3	Q	213/213 (100%)	201 (94%)	12 (6%)	21	42
4	D	198/198 (100%)	184 (93%)	14 (7%)	14	31
4	R	198/198 (100%)	188 (95%)	10 (5%)	24	46
5	E	192/192 (100%)	173 (90%)	19 (10%)	8	16
5	S	192/192 (100%)	174 (91%)	18 (9%)	8	18
6	F	201/201 (100%)	187 (93%)	14 (7%)	15	32
6	T	201/201 (100%)	184 (92%)	17 (8%)	10	22
7	G	207/207 (100%)	193 (93%)	14 (7%)	16	33
7	U	207/207 (100%)	195 (94%)	12 (6%)	20	41
8	H	181/181 (100%)	173 (96%)	8 (4%)	28	53
8	V	181/181 (100%)	170 (94%)	11 (6%)	18	38
9	I	172/172 (100%)	165 (96%)	7 (4%)	30	56
9	W	172/172 (100%)	168 (98%)	4 (2%)	50	76
10	J	175/175 (100%)	167 (95%)	8 (5%)	27	51
10	X	175/175 (100%)	167 (95%)	8 (5%)	27	51
11	K	169/169 (100%)	162 (96%)	7 (4%)	30	56
11	Y	169/169 (100%)	160 (95%)	9 (5%)	22	45
12	L	185/185 (100%)	177 (96%)	8 (4%)	29	54
12	Z	185/185 (100%)	175 (95%)	10 (5%)	22	44
13	1	199/199 (100%)	192 (96%)	7 (4%)	36	62
13	M	199/199 (100%)	193 (97%)	6 (3%)	41	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	2	162/162 (100%)	158 (98%)	4 (2%)	47	74
14	N	162/162 (100%)	155 (96%)	7 (4%)	29	54
All	All	5332/5332 (100%)	5049 (95%)	283 (5%)	22	45

5 of 283 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	99	THR
2	P	192	LEU
11	Y	210	ILE
13	M	62	LEU
1	O	33	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 177 such sidechains are listed below:

Mol	Chain	Res	Type
12	L	166	HIS
2	P	177	GLN
12	Z	14(B)	ASN
13	M	40	ASN
14	N	69	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 carbohydrates 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	-	25,29,29	0.67	0	32,38,38	1.49	5 (15%)
15	BO2	V	1401	-	25,29,29	0.56	0	32,38,38	1.37	5 (15%)
15	BO2	Y	1403	-	25,29,29	0.55	0	32,38,38	1.19	3 (9%)
15	BO2	2	1405	-	25,29,29	0.69	0	32,38,38	1.36	6 (18%)
15	BO2	K	1402	-	25,29,29	0.57	0	32,38,38	1.44	7 (21%)
15	BO2	H	1400	-	25,29,29	0.53	0	32,38,38	1.28	5 (15%)

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	-	-	7/22/28/28	0/2/2/2
15	BO2	V	1401	-	-	7/22/28/28	0/2/2/2
15	BO2	Y	1403	-	-	3/22/28/28	0/2/2/2
15	BO2	2	1405	-	-	7/22/28/28	0/2/2/2
15	BO2	K	1402	-	-	3/22/28/28	0/2/2/2
15	BO2	H	1400	-	-	5/22/28/28	0/2/2/2

There are no bond length outliers.

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	V	1401	BO2	C21-C22-C23	4.06	120.50	115.39
15	N	1404	BO2	C21-C22-C23	3.97	120.38	115.39
15	K	1402	BO2	C6-N1-C2	3.27	121.18	116.93
15	K	1402	BO2	C21-C22-C23	3.27	119.50	115.39
15	H	1400	BO2	C21-C22-C23	3.01	119.18	115.39

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

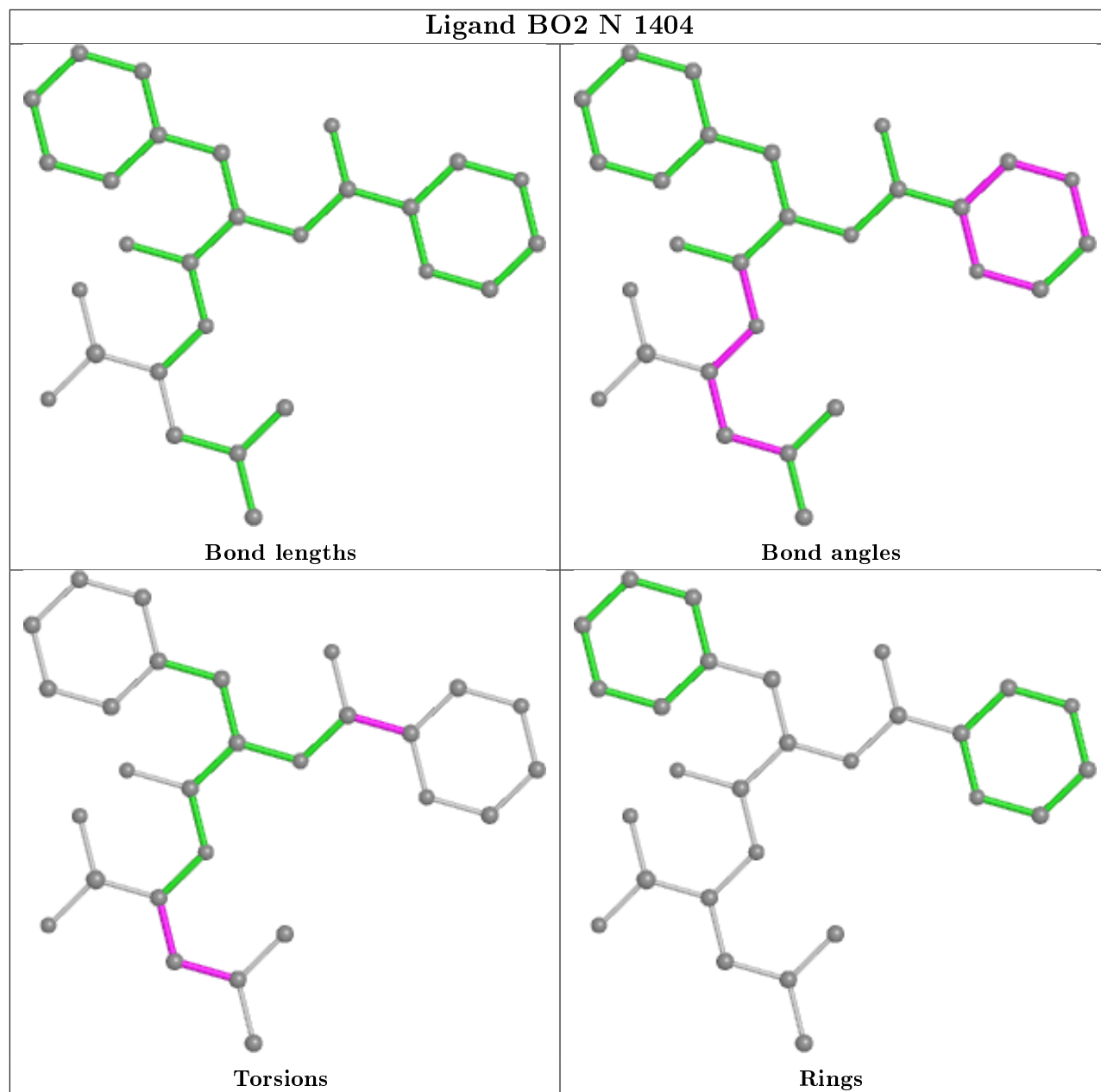
Mol	Chain	Res	Type	Atoms
15	N	1404	BO2	N20-C21-C22-C23
15	N	1404	BO2	C21-C22-C23-C24
15	N	1404	BO2	C21-C22-C23-C25
15	V	1401	BO2	C3-C2-C7-O8
15	V	1401	BO2	C3-C2-C7-N9

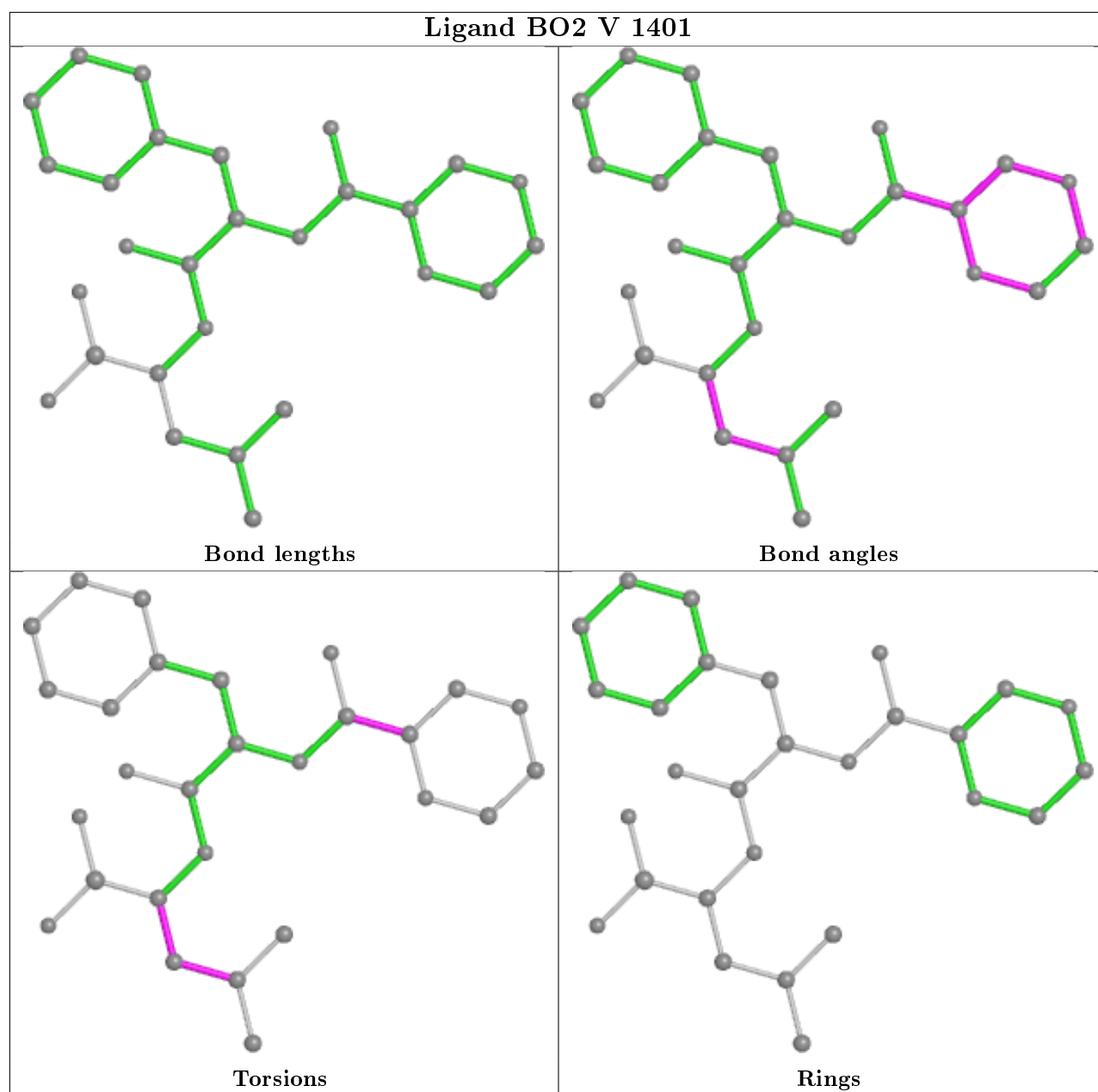
There are no ring outliers.

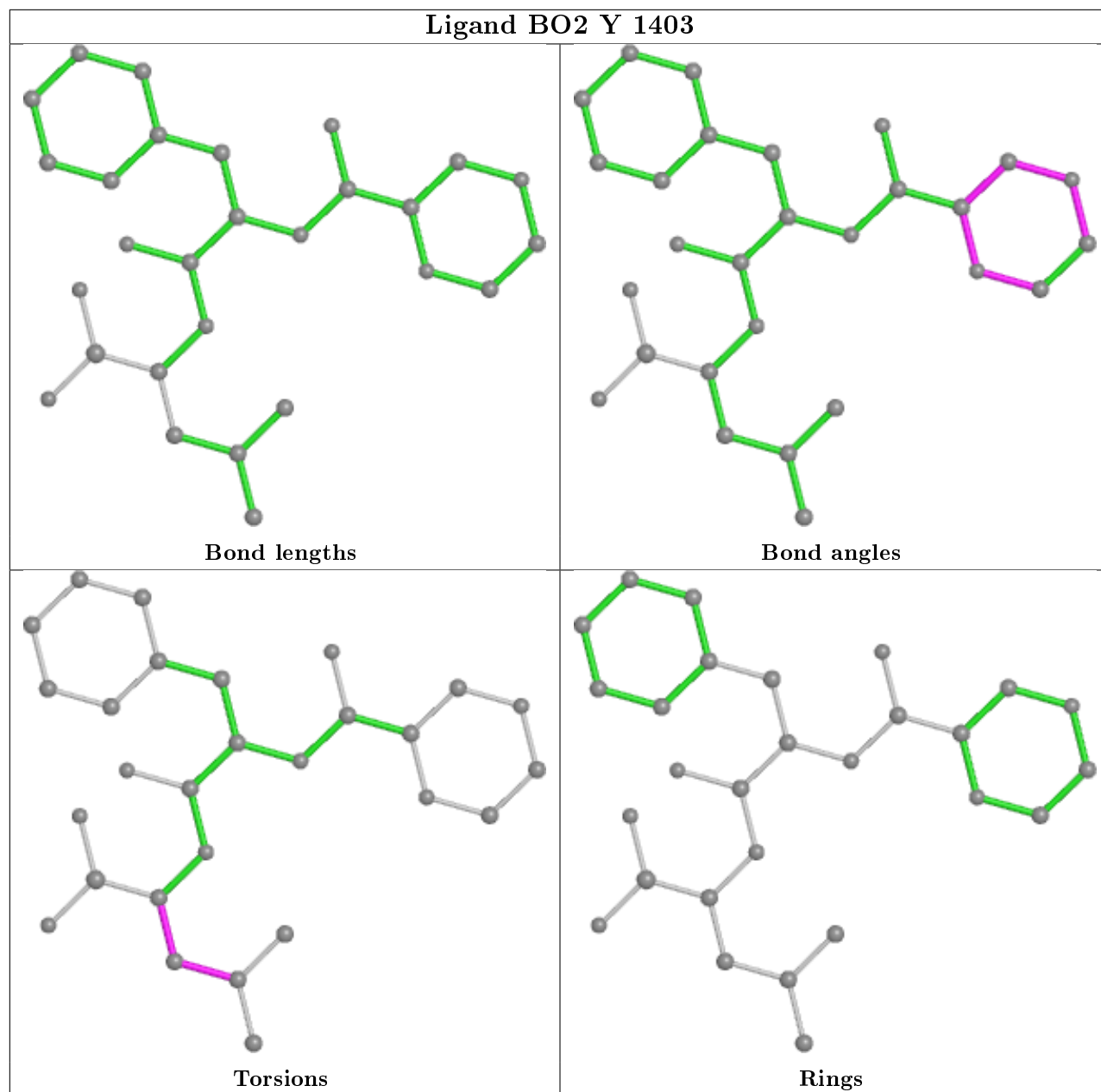
5 monomers are involved in 17 short contacts:

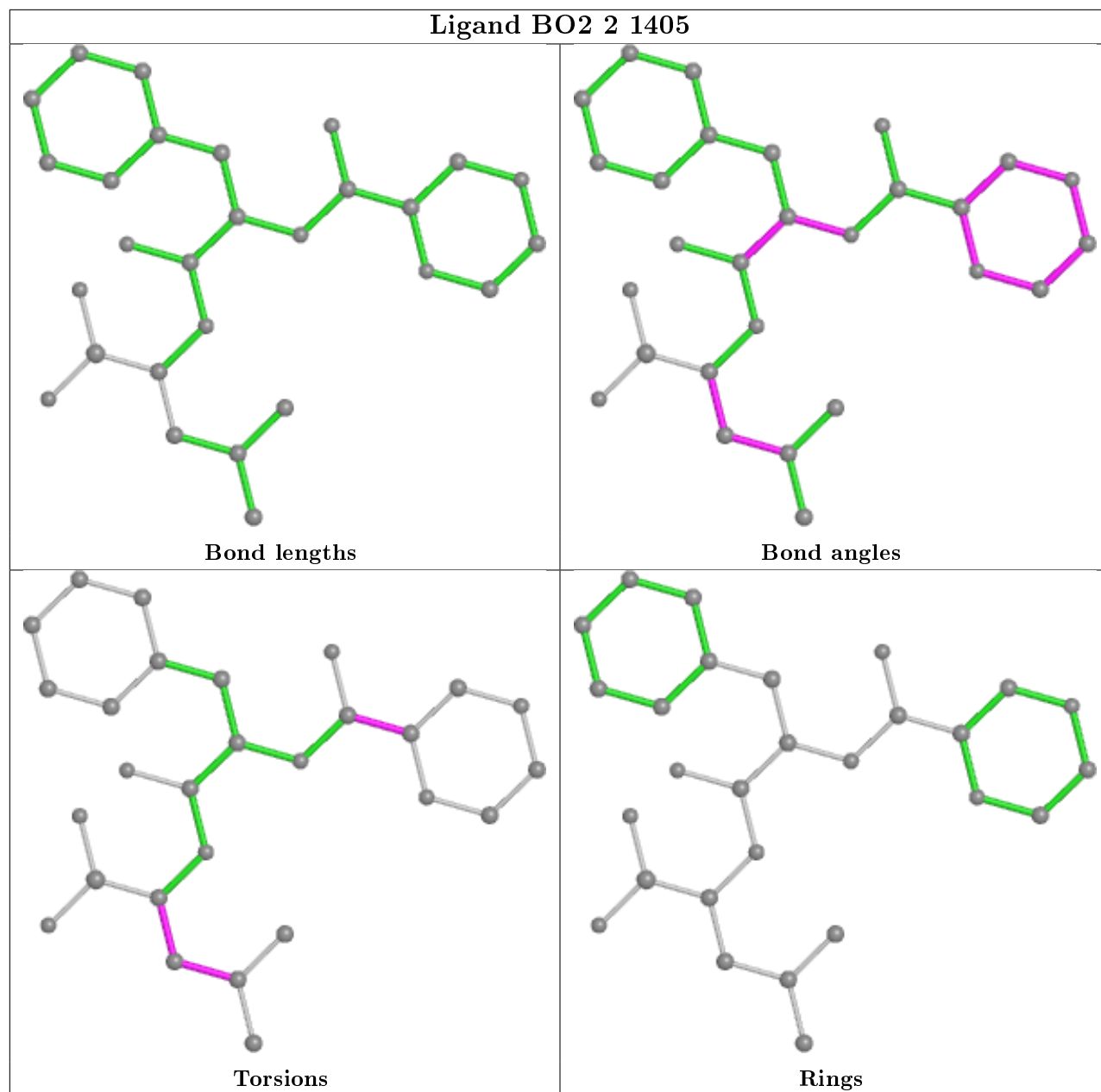
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	N	1404	BO2	3	0
15	V	1401	BO2	2	0
15	Y	1403	BO2	3	0
15	2	1405	BO2	7	0
15	K	1402	BO2	2	0

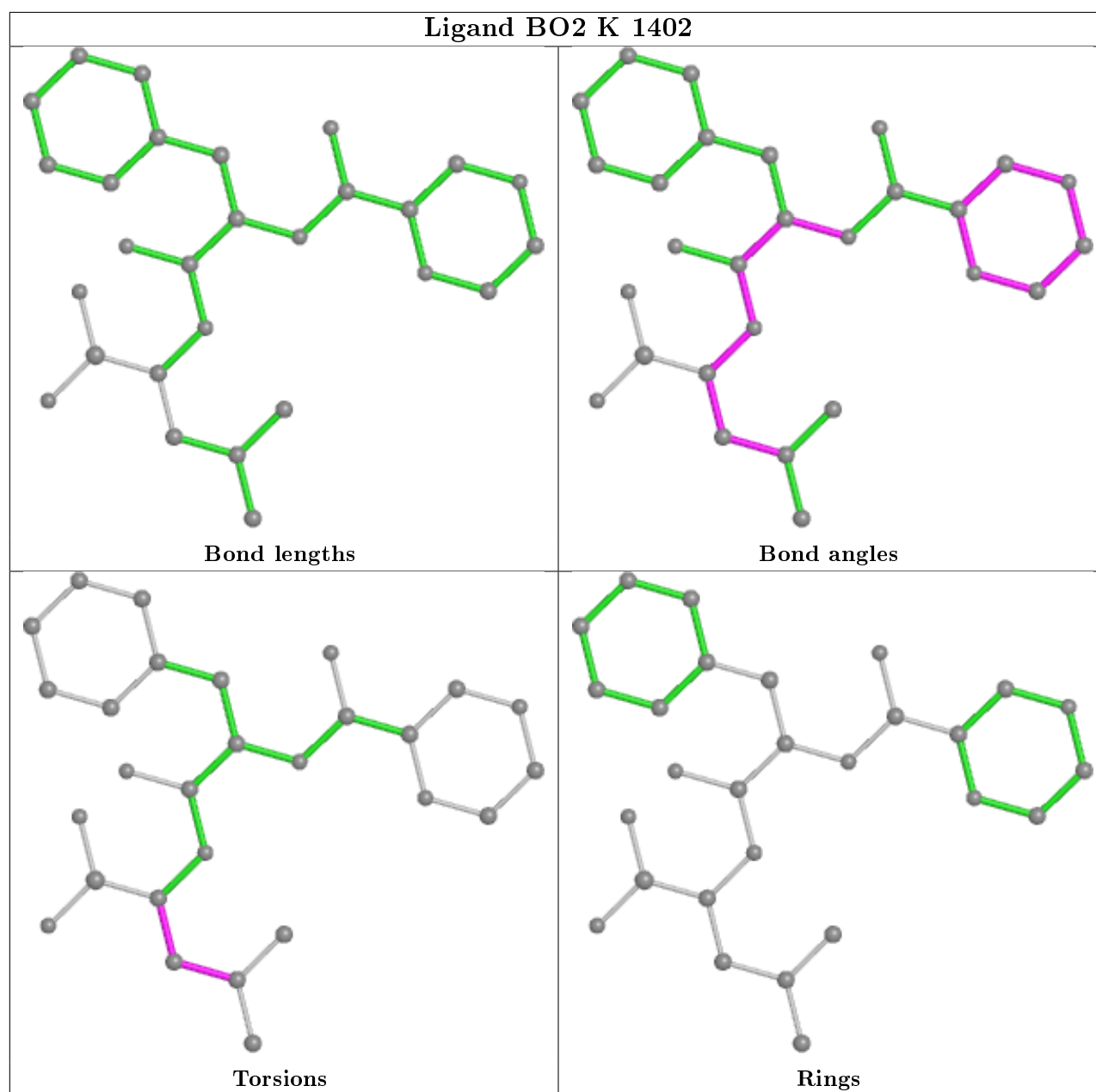
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

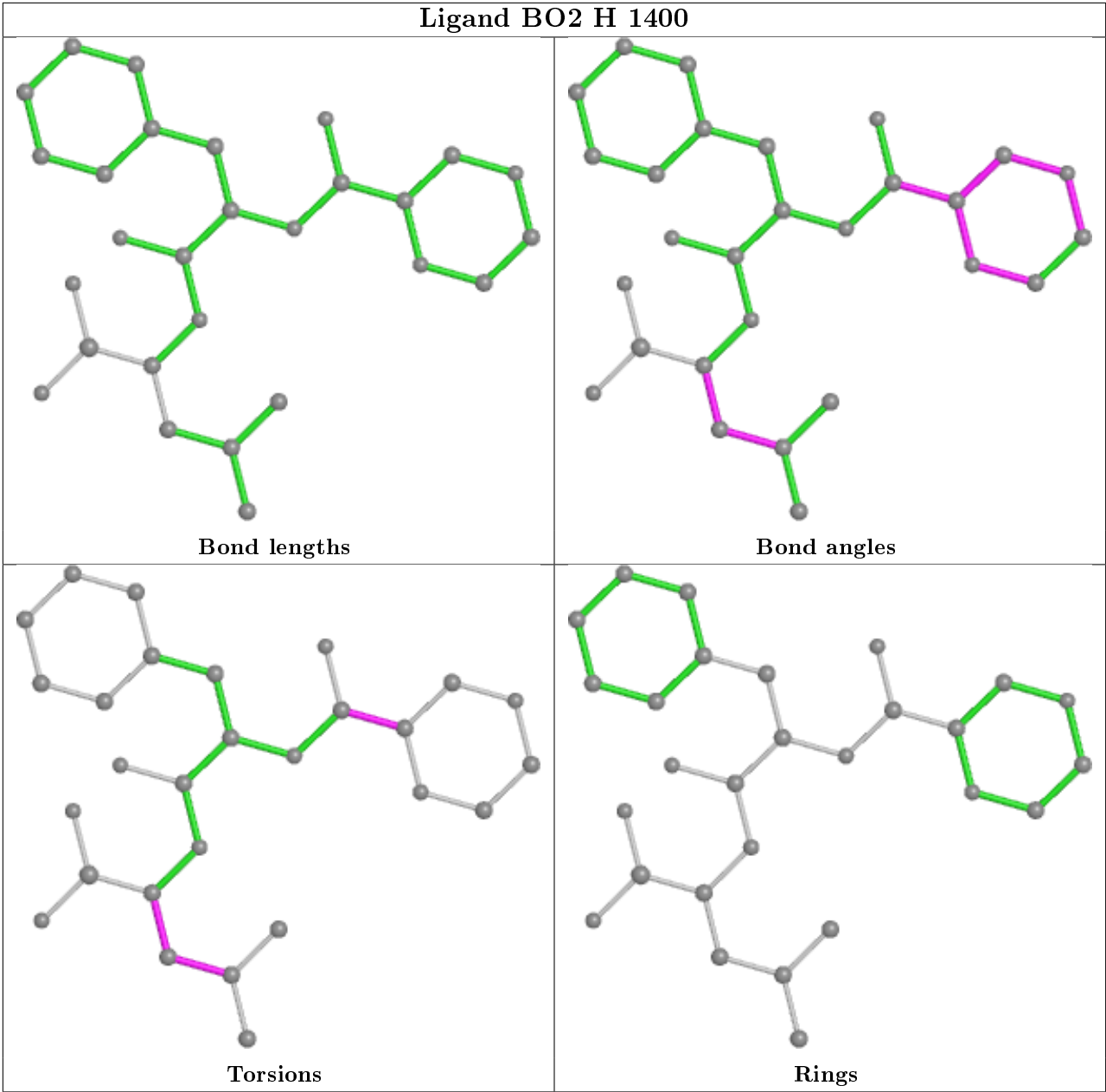












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	P	6

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Mol	Chain	Number of breaks
2	B	6
4	R	6
4	D	6
9	W	5
1	A	5
13	M	5
13	1	5
9	I	5
12	Z	5
12	L	5
1	O	5
14	N	4
14	2	4
5	S	4
5	E	4
7	U	4
7	G	4
3	Q	4
3	C	4
6	T	4
6	F	4
10	X	3
10	J	3
8	V	3
8	H	3
11	K	2
11	Y	2

The worst 5 of 120 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	21(B):GLY	C	217:ALA	N	3.40
1	P	21(B):GLY	C	217:ALA	N	3.34
1	Z	14(W):LYS	C	145:TYR	N	3.32
1	L	14(W):LYS	C	145:TYR	N	3.28
1	C	203:THR	C	206:GLY	N	3.22

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.19	5 (2%) 65 65	27, 40, 64, 79	0
1	O	250/250 (100%)	-0.08	7 (2%) 53 52	29, 44, 75, 86	0
2	B	244/244 (100%)	0.02	9 (3%) 41 40	27, 43, 79, 121	0
2	P	244/244 (100%)	0.08	9 (3%) 41 40	27, 44, 75, 123	0
3	C	241/241 (100%)	0.08	14 (5%) 23 21	28, 44, 86, 109	0
3	Q	241/241 (100%)	0.37	26 (10%) 5 4	33, 48, 95, 119	0
4	D	242/242 (100%)	0.05	10 (4%) 37 35	28, 45, 73, 94	0
4	R	242/242 (100%)	0.18	11 (4%) 33 31	30, 49, 73, 101	0
5	E	233/233 (100%)	0.19	14 (6%) 21 20	34, 51, 75, 91	0
5	S	233/233 (100%)	0.21	15 (6%) 19 17	35, 55, 79, 91	0
6	F	244/244 (100%)	-0.04	8 (3%) 46 45	28, 44, 76, 97	0
6	T	244/244 (100%)	0.05	7 (2%) 51 51	26, 45, 80, 89	0
7	G	243/243 (100%)	-0.07	5 (2%) 63 63	26, 40, 70, 91	0
7	U	243/243 (100%)	-0.18	6 (2%) 57 57	26, 39, 64, 83	0
8	H	222/222 (100%)	-0.32	0 100 100	25, 36, 53, 76	0
8	V	222/222 (100%)	-0.37	1 (0%) 91 92	28, 36, 53, 78	0
9	I	204/204 (100%)	-0.35	2 (0%) 82 82	26, 37, 51, 62	0
9	W	204/204 (100%)	-0.23	2 (0%) 82 82	25, 36, 51, 66	0
10	J	198/198 (100%)	-0.19	6 (3%) 50 49	26, 39, 53, 103	0
10	X	198/198 (100%)	-0.12	6 (3%) 50 49	28, 39, 52, 104	0
11	K	212/212 (100%)	-0.19	6 (2%) 53 52	26, 37, 59, 70	0
11	Y	212/212 (100%)	-0.25	3 (1%) 75 76	28, 39, 63, 71	0
12	L	222/222 (100%)	-0.26	3 (1%) 75 76	25, 37, 58, 70	0
12	Z	222/222 (100%)	-0.20	3 (1%) 75 76	28, 38, 60, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1	233/233 (100%)	-0.30	1 (0%) 92 93	26, 36, 49, 52	0
13	M	233/233 (100%)	-0.35	1 (0%) 92 93	27, 37, 49, 52	0
14	2	196/196 (100%)	-0.35	0 100 100	23, 34, 51, 63	0
14	N	196/196 (100%)	-0.31	0 100 100	26, 34, 49, 62	0
All	All	6368/6368 (100%)	-0.10	180 (2%) 53 52	23, 41, 73, 123	0

The worst 5 of 180 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	217	ALA	12.8
4	R	12(F)	GLY	12.2
4	R	12(E)	SER	11.2
4	R	12(C)	GLY	9.4
4	R	12(D)	ALA	9.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

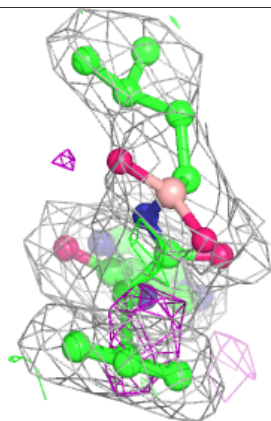
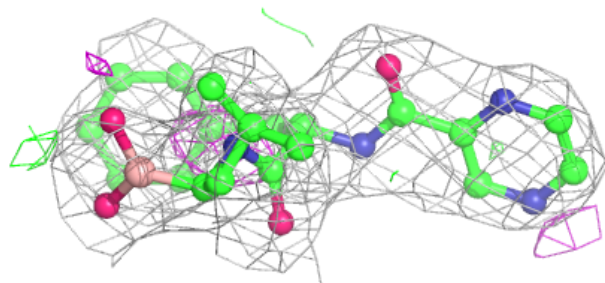
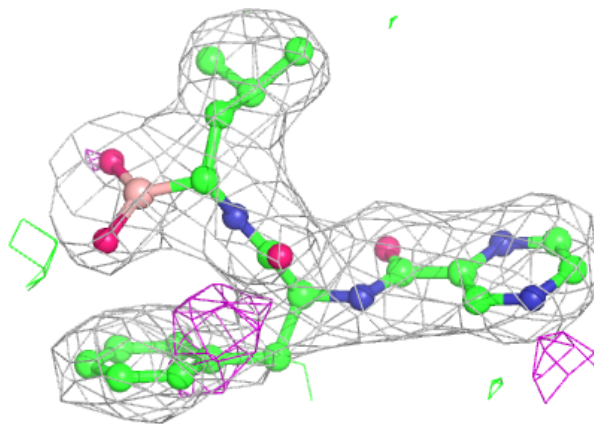
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	BO2	N	1404	28/28	0.93	0.19	30,33,37,37	0
15	BO2	V	1401	28/28	0.94	0.17	40,45,49,49	0
15	BO2	Y	1403	28/28	0.94	0.20	29,38,42,42	0
15	BO2	K	1402	28/28	0.94	0.19	22,35,37,38	0
15	BO2	H	1400	28/28	0.94	0.18	38,41,43,43	0
15	BO2	2	1405	28/28	0.95	0.16	28,33,35,35	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.

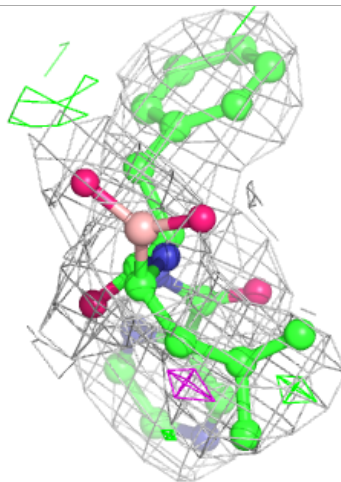
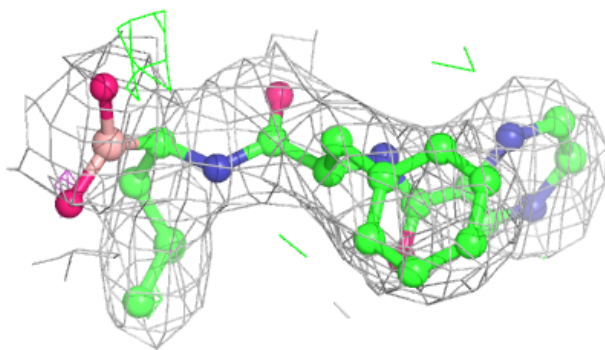
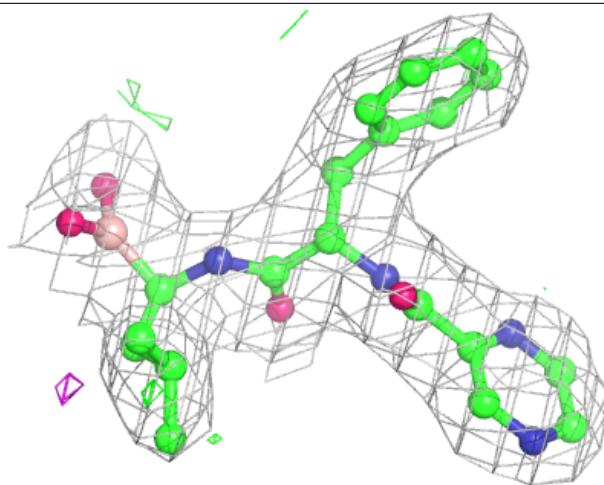
Electron density around BO2 N 1404:

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



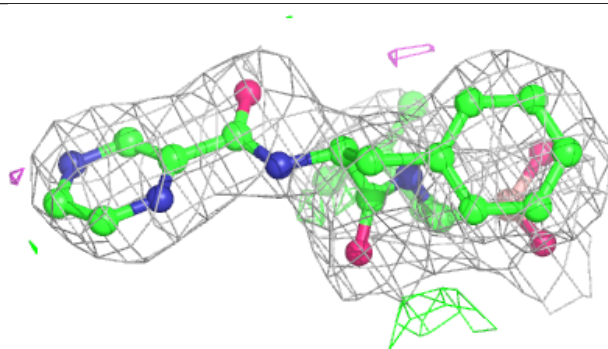
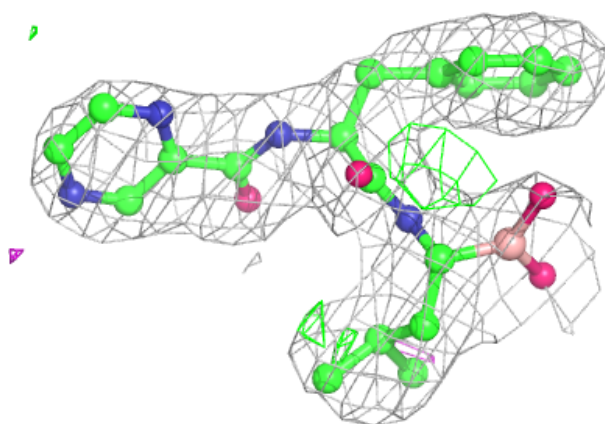
Electron density around BO2 V 1401:

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



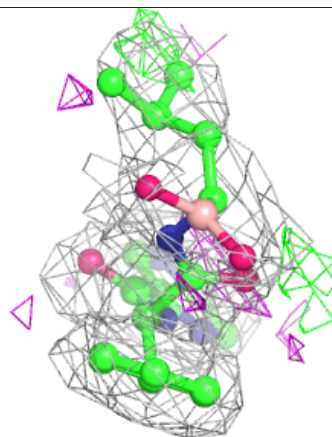
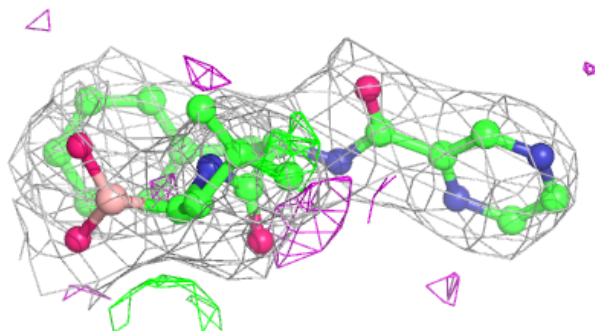
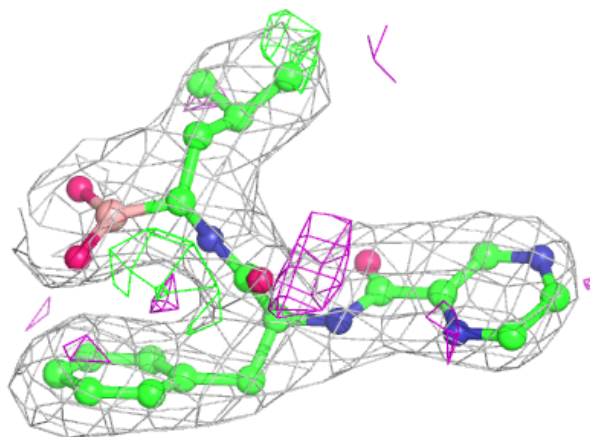
Electron density around BO2 Y 1403:

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



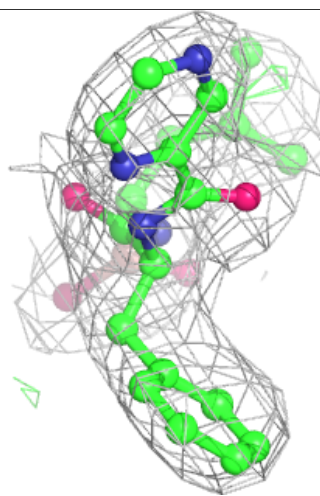
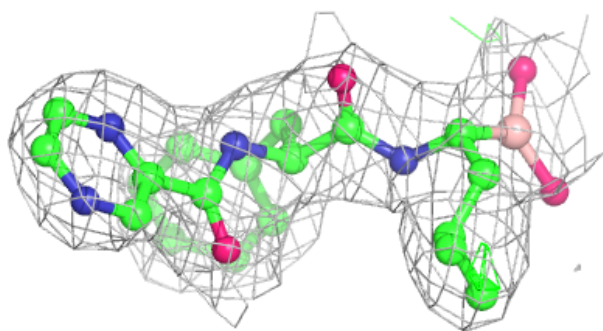
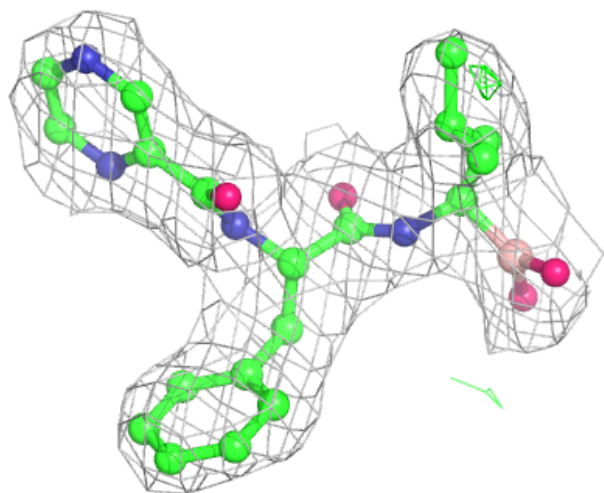
Electron density around BO2 K 1402:

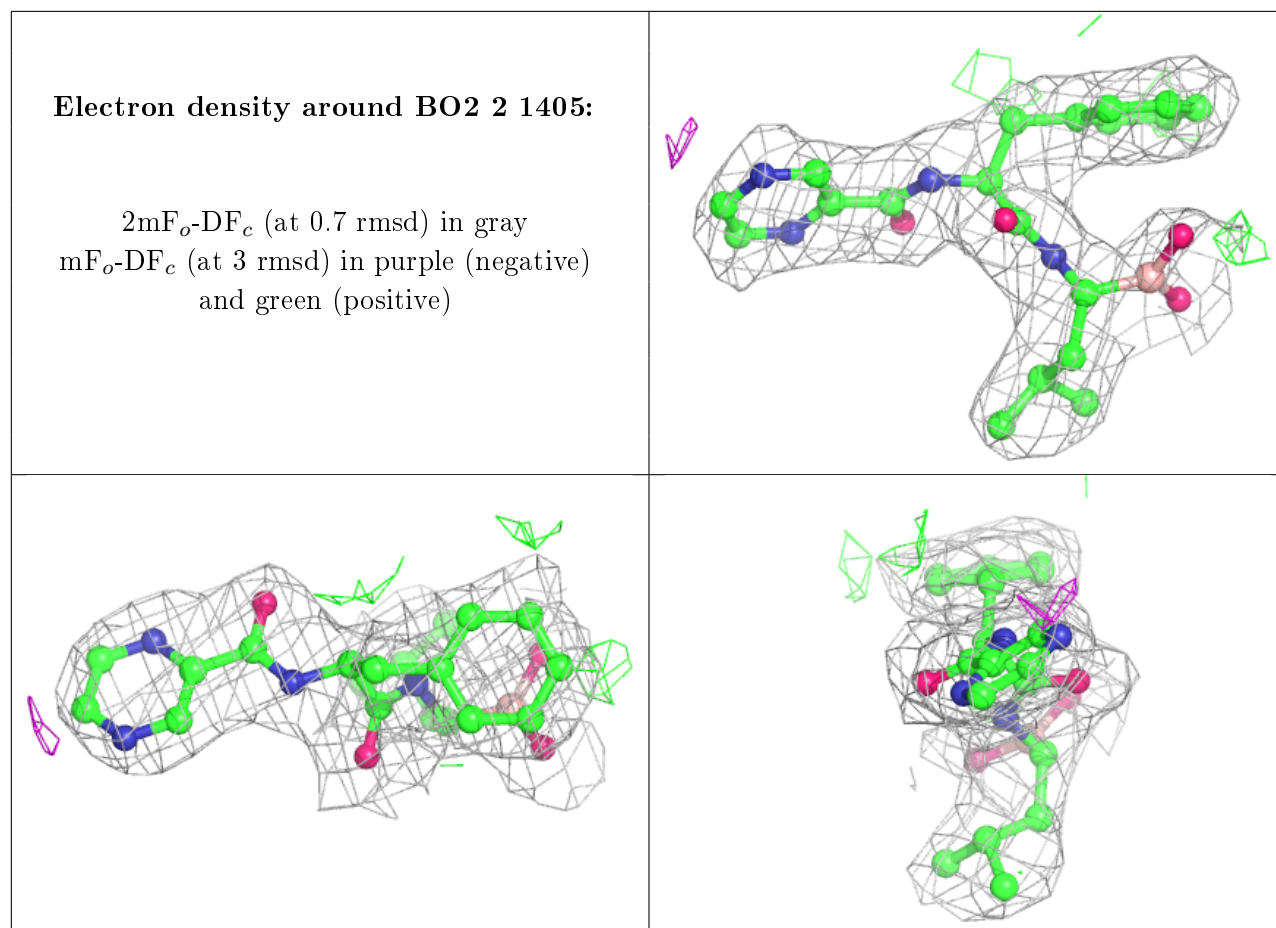
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BO2 H 1400:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.