



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:36 AM UTC

PDB ID : 4QVL / pdb_00004qvl
Title : yCP in complex with bortezomib
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on : 2014-07-15
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (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

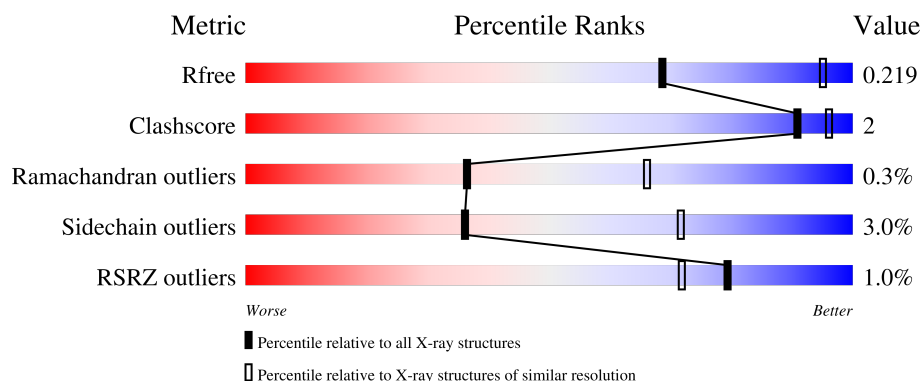
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

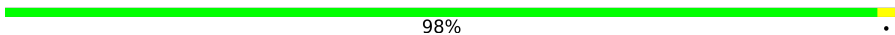
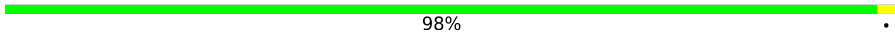
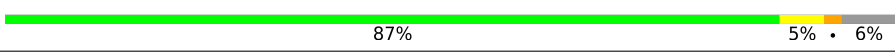
The reported resolution of this entry is 2.80 Å.

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))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 $\leq 5\%$. 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	 98% .
1	O	250	 98% .
2	B	258	 86% 7% . 5%
2	P	258	 86% 7% . 5%
3	C	254	 87% 5% . 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49903 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	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 subunit beta type-6.

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

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

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

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

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

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	I	1	Total	Mg	0	0
			1	1		

Continued on next page...

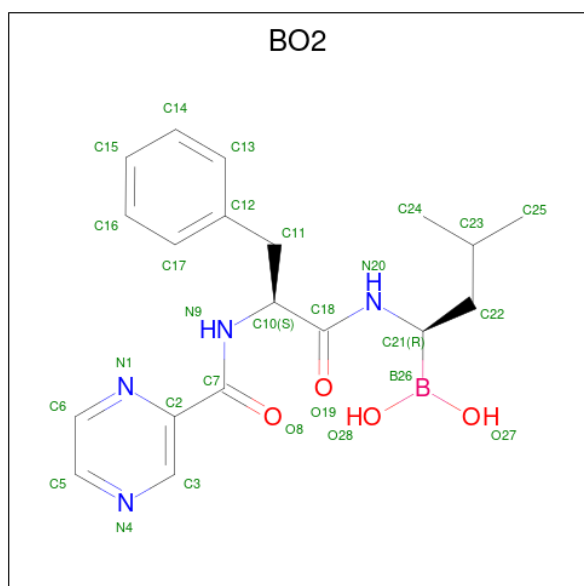
Continued from previous page...

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

- Molecule 16 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 17 is N-[(1R)-1-(DIHYDROXYBORYL)-3-METHYLBUTYL]-N-(PYRAZIN-2-YLCARBONYL)-L-PHENYLALANINAMIDE (CCD ID: BO2) (formula: C₁₉H₂₅BN₄O₄).



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

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	13	Total	O	0	0
			13	13		
18	B	14	Total	O	0	0
			14	14		
18	C	15	Total	O	0	0
			15	15		
18	D	12	Total	O	0	0
			12	12		
18	E	5	Total	O	0	0
			5	5		
18	F	13	Total	O	0	0
			13	13		
18	G	13	Total	O	0	0
			13	13		
18	H	13	Total	O	0	0
			13	13		
18	I	10	Total	O	0	0
			10	10		
18	J	13	Total	O	0	0
			13	13		
18	K	9	Total	O	0	0
			9	9		
18	L	25	Total	O	0	0
			25	25		
18	M	17	Total	O	0	0
			17	17		
18	N	16	Total	O	0	0
			16	16		

Continued on next page...

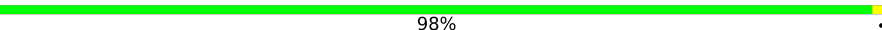
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	O	4	Total 4	O 4	0	0
18	P	11	Total 11	O 11	0	0
18	Q	9	Total 9	O 9	0	0
18	R	7	Total 7	O 7	0	0
18	S	6	Total 6	O 6	0	0
18	T	13	Total 13	O 13	0	0
18	U	8	Total 8	O 8	0	0
18	V	18	Total 18	O 18	0	0
18	W	11	Total 11	O 11	0	0
18	X	21	Total 21	O 21	0	0
18	Y	15	Total 15	O 15	0	0
18	Z	13	Total 13	O 13	0	0
18	a	23	Total 23	O 23	0	0
18	b	10	Total 10	O 10	0	0

3 Residue-property plots [i](#)

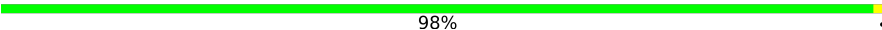
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Proteasome subunit alpha type-2

Chain A:  98% .



- Molecule 1: Proteasome subunit alpha type-2

Chain O:  98% .



- Molecule 2: Proteasome subunit alpha type-3

Chain B:  86% 7% . 5%



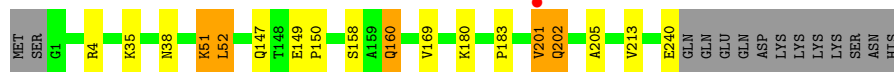
- Molecule 2: Proteasome subunit alpha type-3

Chain P:  86% 7% . 5%

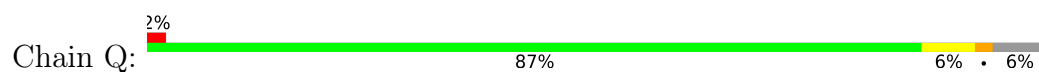


- Molecule 3: Proteasome subunit alpha type-4

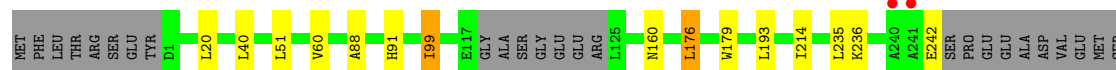
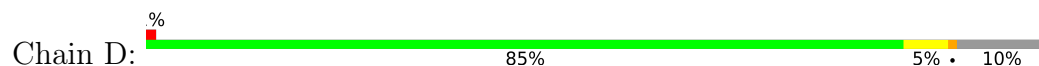
Chain C:  87% 5% . 6%



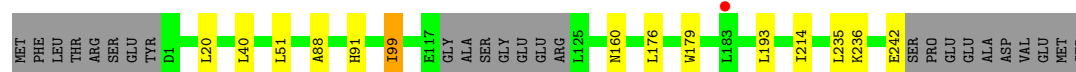
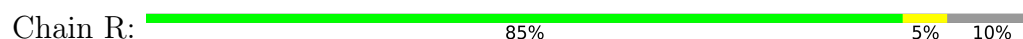
- Molecule 3: Proteasome subunit alpha type-4



- Molecule 4: Proteasome subunit alpha type-5



- Molecule 4: Proteasome subunit alpha type-5



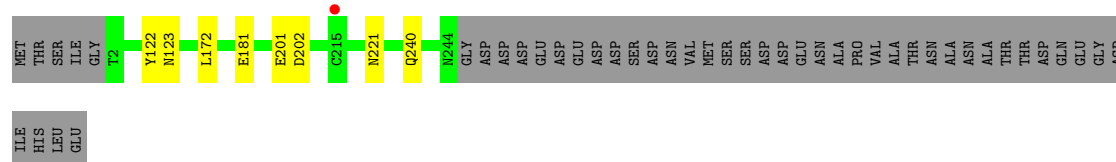
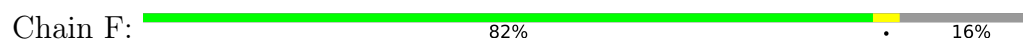
- Molecule 5: Proteasome subunit alpha type-6



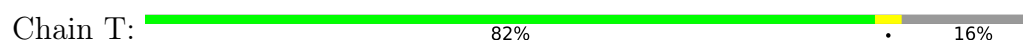
- Molecule 5: Proteasome subunit alpha type-6

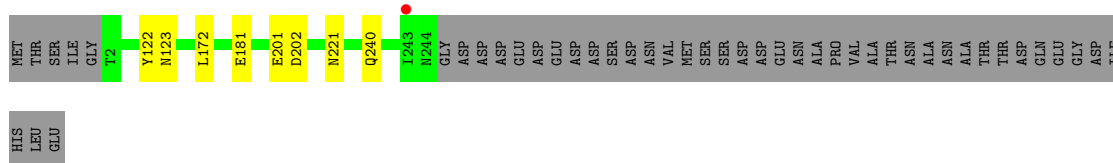


- Molecule 6: Probable proteasome subunit alpha type-7

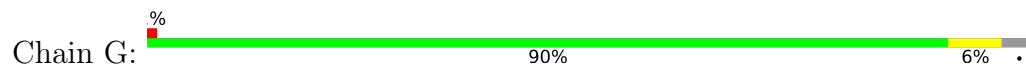


- Molecule 6: Probable proteasome subunit alpha type-7

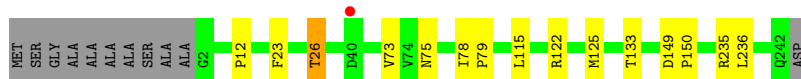




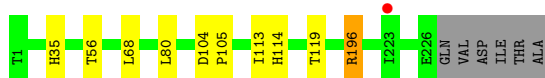
- Molecule 7: Proteasome subunit alpha type-1



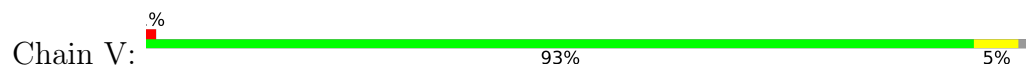
- Molecule 7: Proteasome subunit alpha type-1



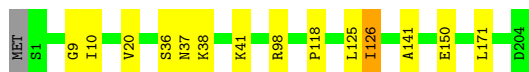
- Molecule 8: Proteasome subunit beta type-2



- Molecule 8: Proteasome subunit beta type-2



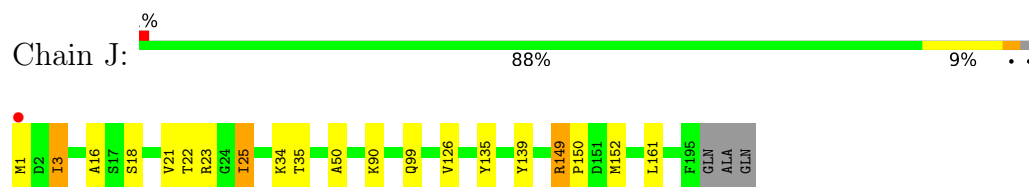
- Molecule 9: Proteasome subunit beta type-3



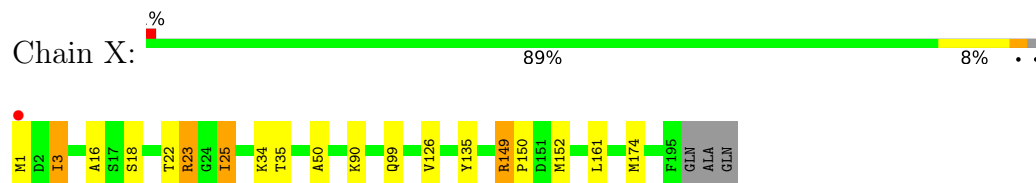
- Molecule 9: Proteasome subunit beta type-3



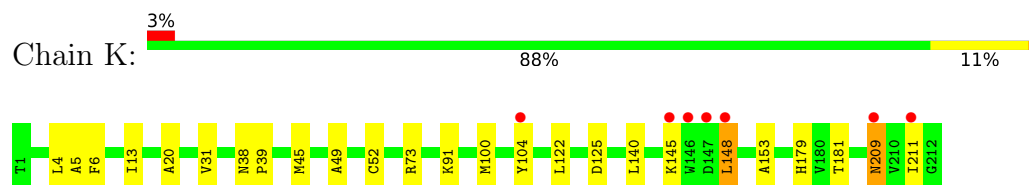
- Molecule 10: Proteasome subunit beta type-4



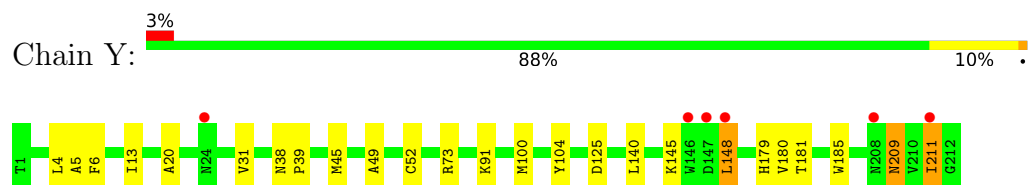
- Molecule 10: Proteasome subunit beta type-4



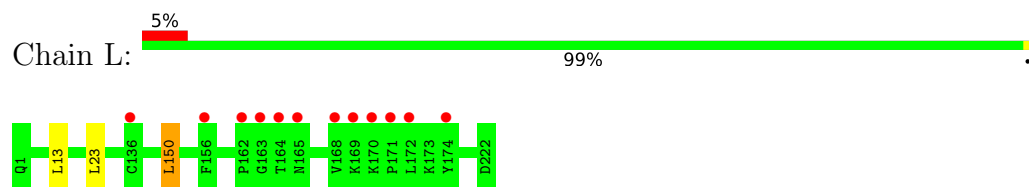
- Molecule 11: Proteasome subunit beta type-5



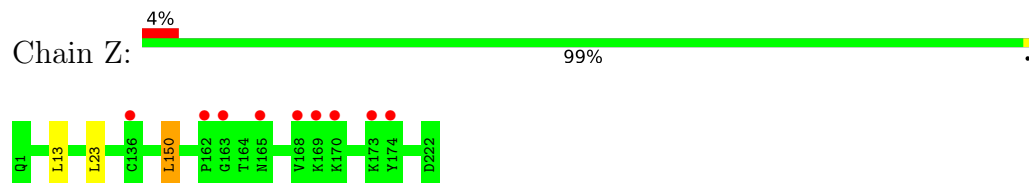
- Molecule 11: Proteasome subunit beta type-5



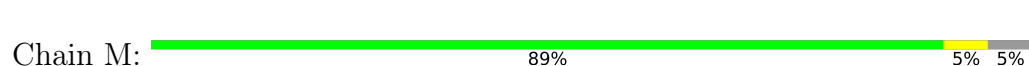
- Molecule 12: Proteasome subunit beta type-6



- Molecule 12: Proteasome subunit beta type-6

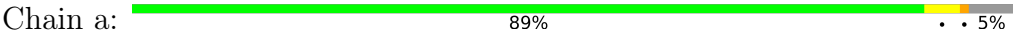


- Molecule 13: Proteasome subunit beta type-7

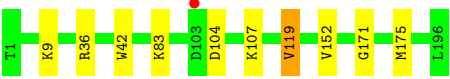
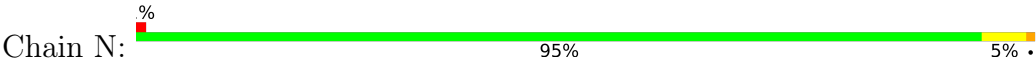




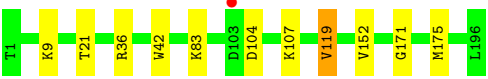
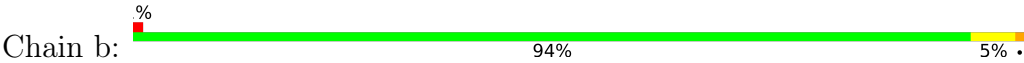
• Molecule 13: Proteasome subunit beta type-7



• Molecule 14: Proteasome subunit beta type-1



• Molecule 14: Proteasome subunit beta type-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.91Å 300.21Å 144.76Å 90.00° 112.85° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.9 (15.00-2.80) 92.4 (15.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.187 , 0.215 0.193 , 0.219	Depositor DCC
R_{free} test set	11992 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	60.3	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49903	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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: MG, BO2, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.39	0/1952	0.68	0/2642
1	O	0.39	0/1952	0.68	0/2642
2	B	0.40	0/1934	0.67	0/2618
2	P	0.40	0/1934	0.67	0/2618
3	C	0.39	0/1910	0.69	1/2586 (0.0%)
3	Q	0.39	0/1910	0.69	1/2586 (0.0%)
4	D	0.38	0/1837	0.66	0/2475
4	R	0.38	0/1837	0.65	0/2475
5	E	0.39	0/1800	0.65	0/2433
5	S	0.39	0/1800	0.65	0/2433
6	F	0.39	0/1932	0.68	0/2609
6	T	0.39	0/1932	0.69	0/2609
7	G	0.39	0/1945	0.67	0/2634
7	U	0.39	0/1945	0.67	0/2634
8	H	0.38	0/1750	0.65	0/2373
8	V	0.38	0/1750	0.64	0/2373
9	I	0.38	0/1611	0.67	0/2174
9	W	0.38	0/1611	0.66	0/2174
10	J	0.57	2/1589 (0.1%)	0.73	3/2142 (0.1%)
10	X	0.59	2/1589 (0.1%)	0.74	2/2142 (0.1%)
11	K	0.37	0/1681	0.67	0/2274
11	Y	0.37	0/1681	0.68	0/2274
12	L	0.38	0/1795	0.66	0/2420
12	Z	0.38	0/1795	0.66	0/2420
13	M	0.41	0/1855	0.67	0/2514
13	a	0.41	0/1855	0.67	0/2514
14	N	0.37	0/1541	0.66	0/2087
14	b	0.37	0/1541	0.67	0/2087
All	All	0.40	4/50264 (0.0%)	0.67	7/67962 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	149	ARG	C-N	7.60	1.40	1.33
10	X	149	ARG	C-N	6.95	1.40	1.33
10	X	150	PRO	N-CD	5.21	1.55	1.47
10	J	150	PRO	N-CD	5.11	1.54	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	149	ARG	N-CA-C	-6.77	99.74	110.10
10	J	149	ARG	CA-C-N	-6.49	113.04	120.89
10	J	149	ARG	C-N-CA	-6.49	113.04	120.89
10	X	149	ARG	CA-C-N	-6.28	113.48	120.45
10	X	149	ARG	C-N-CA	-6.28	113.48	120.45
3	Q	201	VAL	N-CA-C	6.25	116.42	110.42
3	C	201	VAL	N-CA-C	6.20	116.37	110.42

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	1929	1	0
1	O	1915	0	1929	2	0
2	B	1904	0	1904	10	0
2	P	1904	0	1904	9	0
3	C	1881	0	1895	6	0
3	Q	1881	0	1895	7	0
4	D	1813	0	1797	4	0
4	R	1813	0	1797	3	0
5	E	1773	0	1775	3	0
5	S	1773	0	1775	3	0
6	F	1892	0	1883	2	0
6	T	1892	0	1883	2	0
7	G	1907	0	1901	5	0
7	U	1907	0	1901	5	0
8	H	1719	0	1718	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	V	1719	0	1718	8	0
9	I	1581	0	1574	8	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	12	0
10	X	1561	0	1569	20	0
11	K	1644	0	1594	15	0
11	Y	1644	0	1594	16	0
12	L	1757	0	1711	1	0
12	Z	1757	0	1711	1	0
13	M	1824	0	1832	5	0
13	a	1824	0	1832	8	0
14	N	1512	0	1480	4	0
14	b	1512	0	1480	5	0
15	G	1	0	0	0	0
15	I	1	0	0	0	0
15	J	1	0	0	0	0
15	K	1	0	0	0	0
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	N	1	0	0	0	0
16	U	1	0	0	0	0
16	b	1	0	0	0	0
17	H	28	0	25	0	0
17	K	28	0	25	1	0
17	N	28	0	25	2	0
17	V	28	0	25	0	0
17	Y	28	0	25	1	0
17	b	28	0	25	3	0
18	A	13	0	0	0	0
18	B	14	0	0	2	0
18	C	15	0	0	0	0
18	D	12	0	0	0	0
18	E	5	0	0	0	0
18	F	13	0	0	0	0
18	G	13	0	0	0	0
18	H	13	0	0	0	0
18	I	10	0	0	0	0
18	J	13	0	0	0	0
18	K	9	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	L	25	0	0	0	0
18	M	17	0	0	0	0
18	N	16	0	0	0	0
18	O	4	0	0	0	0
18	P	11	0	0	0	0
18	Q	9	0	0	0	0
18	R	7	0	0	0	0
18	S	6	0	0	0	0
18	T	13	0	0	0	0
18	U	8	0	0	0	0
18	V	18	0	0	0	0
18	W	11	0	0	0	0
18	X	21	0	0	2	0
18	Y	15	0	0	1	0
18	Z	13	0	0	0	0
18	a	23	0	0	3	0
18	b	10	0	0	0	0
All	All	49903	0	49274	163	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 2.

All (163) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:22:THR:O	10:X:23:ARG:NH2	2.16	0.78
11:Y:209:ASN:ND2	18:Y:402:HOH:O	2.21	0.73
11:K:73:ARG:NH2	11:K:104:TYR:O	2.21	0.72
11:K:209:ASN:O	9:W:38:LYS:NZ	2.23	0.71
13:M:32:SER:HA	13:M:190:ARG:HH21	1.53	0.71
13:a:32:SER:HA	13:a:190:ARG:HH21	1.55	0.70
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.22	0.67
10:X:23:ARG:CG	10:X:23:ARG:HH21	2.07	0.67
10:J:22:THR:O	10:J:23:ARG:HD3	1.96	0.65
8:V:114:HIS:CD2	17:b:201:BO2:H5	2.33	0.64
9:W:125:LEU:HG	9:W:126:ILE:HG22	1.81	0.62
8:H:114:HIS:CD2	17:N:201:BO2:H5	2.35	0.61
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.81	0.61
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.81	0.61
9:I:125:LEU:HG	9:I:126:ILE:HG22	1.82	0.61
10:J:149:ARG:O	10:J:152:MET:HG3	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:38:LYS:NZ	11:Y:209:ASN:O	2.33	0.60
10:X:149:ARG:O	10:X:152:MET:HG3	2.01	0.60
14:N:152:VAL:HA	14:N:175:MET:HE1	1.86	0.58
10:X:23:ARG:HH21	10:X:23:ARG:HG3	1.68	0.58
14:b:152:VAL:HA	14:b:175:MET:HE1	1.85	0.58
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.87	0.56
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.87	0.56
10:X:23:ARG:HH21	10:X:23:ARG:CB	2.19	0.56
2:B:113:ARG:NE	18:B:301:HOH:O	2.34	0.55
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.89	0.54
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.90	0.54
10:X:23:ARG:HH21	10:X:23:ARG:CA	2.22	0.53
10:X:23:ARG:NH2	10:X:23:ARG:HG3	2.23	0.52
13:a:31:GLY:C	13:a:190:ARG:NH2	2.68	0.52
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.51
2:B:217:LYS:C	2:B:219:ALA:H	2.18	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.57	0.51
2:P:217:LYS:C	2:P:219:ALA:H	2.18	0.51
11:Y:45:MET:HG2	11:Y:52:CYS:HB3	1.93	0.51
7:G:23:PHE:O	7:G:26:THR:HB	2.11	0.50
2:B:93:HIS:HB3	18:B:301:HOH:O	2.11	0.50
7:U:23:PHE:O	7:U:26:THR:HB	2.11	0.50
13:M:31:GLY:C	13:M:190:ARG:NH2	2.71	0.49
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.11	0.49
11:Y:49:ALA:HB3	17:Y:301:BO2:H3	1.94	0.49
10:J:25:ILE:HD11	10:X:135:TYR:HB3	1.94	0.49
11:K:45:MET:HG2	11:K:52:CYS:HB3	1.95	0.49
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.94	0.49
11:K:49:ALA:HB3	17:K:301:BO2:H3	1.95	0.49
3:C:51:LYS:O	3:C:52:LEU:HB2	2.12	0.48
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.78	0.48
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.78	0.48
2:P:50:LYS:O	2:P:51:VAL:C	2.56	0.48
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.96	0.47
14:b:36:ARG:HG3	14:b:42:TRP:CE2	2.49	0.47
2:B:50:LYS:O	2:B:51:VAL:C	2.56	0.47
10:J:135:TYR:HB3	10:X:25:ILE:HD11	1.96	0.47
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.95	0.47
10:J:50:ALA:O	11:K:91:LYS:NZ	2.48	0.47
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.49	0.47
3:C:35:LYS:HG2	3:C:158:SER:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.96	0.47
2:P:50:LYS:HD3	2:P:50:LYS:HA	1.82	0.47
11:Y:179:HIS:CE1	11:Y:181:THR:HG23	2.50	0.46
11:K:179:HIS:CE1	11:K:181:THR:HG23	2.51	0.46
10:J:139:TYR:OH	10:X:25:ILE:O	2.33	0.46
10:X:22:THR:C	10:X:23:ARG:NH2	2.74	0.46
10:X:23:ARG:NH1	18:X:209:HOH:O	2.45	0.46
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.97	0.46
9:I:98:ARG:HD2	9:I:126:ILE:HD12	1.98	0.46
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.97	0.46
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.46	0.45
11:K:104:TYR:CD1	11:K:104:TYR:C	2.94	0.45
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.16	0.45
9:W:98:ARG:HD2	9:W:126:ILE:HD12	1.98	0.45
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.98	0.45
2:B:221:ASP:O	2:B:223:GLU:N	2.50	0.45
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.98	0.45
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.46	0.45
8:H:114:HIS:HD2	17:N:201:BO2:H5	1.82	0.45
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.99	0.45
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.99	0.45
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.99	0.45
11:Y:104:TYR:C	11:Y:104:TYR:CD1	2.95	0.45
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	1.99	0.45
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.52	0.45
2:P:221:ASP:O	2:P:223:GLU:N	2.50	0.45
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.51	0.45
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.99	0.44
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.53	0.44
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.99	0.44
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.50	0.44
11:K:209:ASN:OD1	11:K:209:ASN:C	2.61	0.44
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.99	0.44
8:H:196:ARG:NH2	9:I:150:GLU:O	2.50	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.81	0.43
10:X:174:MET:HB2	18:X:204:HOH:O	2.18	0.43
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.53	0.43
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.00	0.43
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.00	0.43
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.19	0.43
11:Y:209:ASN:OD1	11:Y:209:ASN:C	2.61	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:TYR:OH	2:B:217:LYS:N	2.52	0.43
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.49	0.43
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.43
8:V:114:HIS:HD2	17:b:201:BO2:H5	1.81	0.43
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.00	0.43
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.49	0.43
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.49	0.43
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.49	0.42
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.54	0.42
2:P:145:TYR:OH	2:P:217:LYS:N	2.51	0.42
7:U:73:VAL:HG12	7:U:133:THR:HB	2.00	0.42
13:a:2:GLN:NE2	18:a:322:HOH:O	2.52	0.42
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.49	0.42
7:G:73:VAL:HG12	7:G:133:THR:HB	2.00	0.42
13:a:127:LEU:HG	13:a:142:LEU:HD12	2.01	0.42
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.02	0.42
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.49	0.42
13:a:190:ARG:CZ	18:a:305:HOH:O	2.66	0.42
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.02	0.42
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.50	0.42
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.02	0.42
8:V:84:LYS:HE2	8:V:119:THR:HG23	2.02	0.42
10:X:23:ARG:NH2	10:X:23:ARG:CG	2.73	0.42
2:B:217:LYS:C	2:B:219:ALA:N	2.78	0.42
3:C:201:VAL:O	3:C:202:GLN:HB3	2.19	0.42
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.50	0.42
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.02	0.41
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.55	0.41
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.02	0.41
11:K:6:PHE:HA	11:K:125:ASP:O	2.20	0.41
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.50	0.41
10:J:23:ARG:HD3	10:J:23:ARG:HA	1.81	0.41
11:K:5:ALA:HA	11:K:13:ILE:O	2.20	0.41
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.20	0.41
13:a:165:ILE:HB	13:a:166:PRO:HD3	2.02	0.41
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.50	0.41
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.50	0.41
6:F:202:ASP:OD1	6:F:202:ASP:N	2.53	0.41
13:M:219:TRP:CH2	14:b:171:GLY:HA2	2.56	0.41
11:Y:211:ILE:H	11:Y:211:ILE:HG13	1.72	0.41
8:H:35:HIS:CB	8:H:56:THR:HG21	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:21:VAL:HG11	11:K:122:LEU:HD11	2.02	0.41
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.56	0.41
2:P:47:ALA:HB1	2:P:64:LYS:HD2	2.03	0.41
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.03	0.41
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.03	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.55	0.41
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.20	0.41
13:a:190:ARG:NE	18:a:305:HOH:O	2.54	0.41
2:B:47:ALA:HB1	2:B:64:LYS:HD2	2.03	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.41
10:X:23:ARG:HH21	10:X:23:ARG:HA	1.86	0.41
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.03	0.40
10:J:3:ILE:HG23	10:J:18:SER:HB3	2.03	0.40
5:S:87:LEU:HD21	5:S:107:ALA:HB1	2.03	0.40
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.03	0.40
14:b:21:THR:O	17:b:201:BO2:H3	2.20	0.40
7:G:34:LEU:C	7:G:34:LEU:HD23	2.47	0.40
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.04	0.40
11:K:13:ILE:HG13	11:K:153:ALA:HB1	2.04	0.40
11:Y:180:VAL:HA	11:Y:185:TRP:HA	2.04	0.40
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.03	0.40
6:T:202:ASP:N	6:T:202:ASP:OD1	2.54	0.40
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	30 60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	30	60
2	B	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	7	25
2	P	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	7	25
3	C	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	9	31
3	Q	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	9	31
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
4	R	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	220 (96%)	9 (4%)	0	100	100
5	S	229/234 (98%)	220 (96%)	9 (4%)	0	100	100
6	F	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
6	T	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
7	G	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
7	U	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
8	H	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
10	X	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
13	a	231/246 (94%)	224 (97%)	7 (3%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6284/6614 (95%)	6124 (98%)	144 (2%)	16 (0%)	36	66

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	222	GLY
3	C	202	GLN
2	P	51	VAL
2	P	222	GLY
3	Q	202	GLN
1	A	2	THR
2	B	218	GLY
1	O	2	THR
2	P	218	GLY
2	B	220	ASN
3	C	205	ALA
2	P	220	ASN
3	Q	205	ALA
3	C	183	PRO
3	Q	183	PRO

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%)	205 (98%)	4 (2%)	50	81
1	O	209/209 (100%)	205 (98%)	4 (2%)	50	81
2	B	203/216 (94%)	196 (97%)	7 (3%)	32	68
2	P	203/216 (94%)	196 (97%)	7 (3%)	32	68
3	C	212/226 (94%)	202 (95%)	10 (5%)	23	57
3	Q	212/226 (94%)	202 (95%)	10 (5%)	23	57
4	D	194/215 (90%)	183 (94%)	11 (6%)	18	49
4	R	194/215 (90%)	184 (95%)	10 (5%)	21	53
5	E	190/193 (98%)	184 (97%)	6 (3%)	34	70
5	S	190/193 (98%)	184 (97%)	6 (3%)	34	70
6	F	201/239 (84%)	195 (97%)	6 (3%)	36	72
6	T	201/239 (84%)	195 (97%)	6 (3%)	36	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	206/210 (98%)	199 (97%)	7 (3%)	32	68
7	U	206/210 (98%)	199 (97%)	7 (3%)	32	68
8	H	185/190 (97%)	183 (99%)	2 (1%)	65	87
8	V	185/190 (97%)	183 (99%)	2 (1%)	65	87
9	I	172/173 (99%)	169 (98%)	3 (2%)	53	83
9	W	172/173 (99%)	169 (98%)	3 (2%)	53	83
10	J	173/175 (99%)	168 (97%)	5 (3%)	37	73
10	X	173/175 (99%)	167 (96%)	6 (4%)	32	67
11	K	169/169 (100%)	163 (96%)	6 (4%)	31	66
11	Y	169/169 (100%)	163 (96%)	6 (4%)	31	66
12	L	185/185 (100%)	183 (99%)	2 (1%)	65	87
12	Z	185/185 (100%)	183 (99%)	2 (1%)	65	87
13	M	199/208 (96%)	193 (97%)	6 (3%)	36	72
13	a	199/208 (96%)	193 (97%)	6 (3%)	36	72
14	N	162/162 (100%)	158 (98%)	4 (2%)	42	76
14	b	162/162 (100%)	158 (98%)	4 (2%)	42	76
All	All	5320/5540 (96%)	5162 (97%)	158 (3%)	36	72

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS
2	B	55	LEU
2	B	79	LEU
2	B	102	ASN
2	B	113	ARG
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	52	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	213	VAL
3	C	240	GLU
4	D	20	LEU
4	D	40	LEU
4	D	51	LEU
4	D	60	VAL
4	D	99	ILE
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	188	LEU
5	E	231	LYS
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	221	ASN
6	F	240	GLN
7	G	26	THR
7	G	75	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	235	ARG
7	G	236	LEU
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	126	ILE
9	I	171	LEU
10	J	3	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	25	ILE
10	J	35	THR
10	J	90	LYS
10	J	99	GLN
11	K	4	LEU
11	K	100	MET
11	K	140	LEU
11	K	148	LEU
11	K	209	ASN
11	K	211	ILE
12	L	23	LEU
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	187	ARG
13	M	190	ARG
14	N	9	LYS
14	N	104	ASP
14	N	107	LYS
14	N	119	VAL
1	O	1	MET
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	55	LEU
2	P	79	LEU
2	P	102	ASN
2	P	113	ARG
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	52	LEU
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	213	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Q	240	GLU
4	R	20	LEU
4	R	40	LEU
4	R	51	LEU
4	R	99	ILE
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	188	LEU
5	S	231	LYS
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	221	ASN
6	T	240	GLN
7	U	26	THR
7	U	75	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	235	ARG
7	U	236	LEU
8	V	68	LEU
8	V	196	ARG
9	W	37	ASN
9	W	126	ILE
9	W	171	LEU
10	X	3	ILE
10	X	23	ARG
10	X	25	ILE
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
11	Y	4	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	Y	100	MET
11	Y	140	LEU
11	Y	148	LEU
11	Y	209	ASN
11	Y	211	ILE
12	Z	23	LEU
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	187	ARG
13	a	190	ARG
14	b	9	LYS
14	b	104	ASP
14	b	107	LYS
14	b	119	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	93	HIS
2	B	119	GLN
2	B	123	GLN
2	B	124	HIS
3	C	17	GLN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	86	ASN
6	F	123	ASN
7	G	30	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	175	ASN
8	H	22	GLN
8	H	86	HIS
8	H	114	HIS
8	H	194	ASN
9	I	63	ASN
9	I	88	GLN
9	I	168	GLN
9	I	203	GLN
10	J	55	GLN
10	J	61	GLN
10	J	63	ASN
10	J	146	HIS
11	K	9	GLN
11	K	85	ASN
11	K	143	ASN
11	K	176	ASN
11	K	208	ASN
12	L	49	ASN
12	L	70	ASN
12	L	79	HIS
12	L	135	GLN
12	L	152	ASN
12	L	153	GLN
12	L	155	ASN
12	L	158	ASN
12	L	197	GLN
13	M	26	ASN
13	M	48	ASN
13	M	149	HIS
13	M	194	ASN
13	M	213	GLN
14	N	38	HIS
14	N	141	ASN
2	P	119	GLN
2	P	123	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	124	HIS
2	P	176	GLN
2	P	220	ASN
3	Q	17	GLN
3	Q	115	GLN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	123	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	175	ASN
8	V	22	GLN
8	V	30	ASN
8	V	114	HIS
8	V	189	ASN
8	V	194	ASN
9	W	44	HIS
9	W	63	ASN
9	W	88	GLN
9	W	168	GLN
9	W	203	GLN
10	X	37	GLN
10	X	55	GLN
10	X	63	ASN
10	X	78	GLN
10	X	146	HIS
11	Y	9	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	Y	85	ASN
11	Y	143	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	135	GLN
12	Z	152	ASN
12	Z	153	GLN
12	Z	155	ASN
12	Z	158	ASN
12	Z	197	GLN
13	a	26	ASN
13	a	48	ASN
13	a	102	GLN
13	a	149	HIS
13	a	194	ASN
13	a	213	GLN
14	b	38	HIS
14	b	141	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](#)

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](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BO2	H	301	8	25,29,29	1.58	5 (20%)	33,38,38	1.45	4 (12%)
17	BO2	Y	301	11	25,29,29	1.59	5 (20%)	33,38,38	1.38	4 (12%)
17	BO2	b	201	14	25,29,29	1.53	4 (16%)	33,38,38	1.29	4 (12%)
17	BO2	V	301	8	25,29,29	1.57	5 (20%)	33,38,38	1.48	4 (12%)
17	BO2	N	201	14	25,29,29	1.53	4 (16%)	33,38,38	1.28	5 (15%)
17	BO2	K	301	11	25,29,29	1.58	5 (20%)	33,38,38	1.37	3 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BO2	H	301	8	-	4/23/28/28	0/2/2/2
17	BO2	Y	301	11	-	4/23/28/28	0/2/2/2
17	BO2	b	201	14	-	4/23/28/28	0/2/2/2
17	BO2	V	301	8	-	4/23/28/28	0/2/2/2
17	BO2	N	201	14	-	4/23/28/28	0/2/2/2
17	BO2	K	301	11	-	4/23/28/28	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	201	BO2	C11-C12	-4.47	1.40	1.51
17	b	201	BO2	C11-C12	-4.44	1.40	1.51
17	K	301	BO2	C11-C12	-4.40	1.40	1.51
17	Y	301	BO2	C11-C12	-4.37	1.41	1.51
17	H	301	BO2	C11-C12	-4.37	1.41	1.51
17	N	201	BO2	C2-C7	-4.32	1.38	1.50
17	V	301	BO2	C11-C12	-4.29	1.41	1.51
17	b	201	BO2	C2-C7	-4.29	1.38	1.50
17	Y	301	BO2	C2-C7	-4.14	1.39	1.50
17	K	301	BO2	C2-C7	-4.10	1.39	1.50
17	H	301	BO2	C2-C7	-4.07	1.39	1.50
17	V	301	BO2	C2-C7	-4.00	1.39	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	301	BO2	C3-N4	2.94	1.40	1.34
17	Y	301	BO2	C6-N1	2.92	1.40	1.34
17	V	301	BO2	C6-N1	2.90	1.40	1.34
17	H	301	BO2	C6-N1	2.88	1.40	1.34
17	H	301	BO2	C3-N4	2.85	1.40	1.34
17	K	301	BO2	C3-N4	2.83	1.40	1.34
17	K	301	BO2	C6-N1	2.80	1.40	1.34
17	V	301	BO2	C3-N4	2.80	1.40	1.34
17	N	201	BO2	C6-N1	2.38	1.39	1.34
17	b	201	BO2	C6-N1	2.35	1.39	1.34
17	K	301	BO2	C5-N4	2.34	1.40	1.33
17	Y	301	BO2	C5-N4	2.32	1.40	1.33
17	V	301	BO2	C5-N4	2.32	1.40	1.33
17	b	201	BO2	C3-N4	2.31	1.39	1.34
17	H	301	BO2	C5-N4	2.27	1.40	1.33
17	N	201	BO2	C3-N4	2.22	1.39	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	V	301	BO2	C21-C22-C23	-5.22	108.66	115.32
17	H	301	BO2	C21-C22-C23	-5.03	108.90	115.32
17	Y	301	BO2	C21-C22-C23	-4.30	109.84	115.32
17	K	301	BO2	C21-C22-C23	-4.23	109.92	115.32
17	N	201	BO2	C21-C22-C23	-3.97	110.25	115.32
17	b	201	BO2	C21-C22-C23	-3.94	110.30	115.32
17	Y	301	BO2	C6-N1-C2	3.21	121.06	116.93
17	V	301	BO2	C6-N1-C2	3.18	121.03	116.93
17	H	301	BO2	C6-N1-C2	3.14	120.98	116.93
17	K	301	BO2	C6-N1-C2	3.11	120.94	116.93
17	b	201	BO2	C11-C10-N9	-2.70	105.24	110.83
17	N	201	BO2	C11-C10-N9	-2.57	105.51	110.83
17	H	301	BO2	C12-C11-C10	-2.49	106.74	113.36
17	V	301	BO2	C12-C11-C10	-2.48	106.77	113.36
17	V	301	BO2	B26-C21-C22	-2.45	107.68	112.31
17	b	201	BO2	C6-N1-C2	2.41	120.04	116.93
17	N	201	BO2	C6-N1-C2	2.34	119.94	116.93
17	H	301	BO2	B26-C21-C22	-2.28	108.00	112.31
17	K	301	BO2	C6-C5-N4	-2.18	119.25	121.96
17	Y	301	BO2	C6-C5-N4	-2.11	119.33	121.96
17	b	201	BO2	B26-C21-C22	-2.09	108.36	112.31
17	Y	301	BO2	C18-C10-N9	-2.06	105.53	111.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	201	BO2	B26-C21-C22	-2.06	108.43	112.31
17	N	201	BO2	C18-C10-N9	-2.01	105.67	111.11

There are no chirality outliers.

All (24) torsion outliers are listed below:

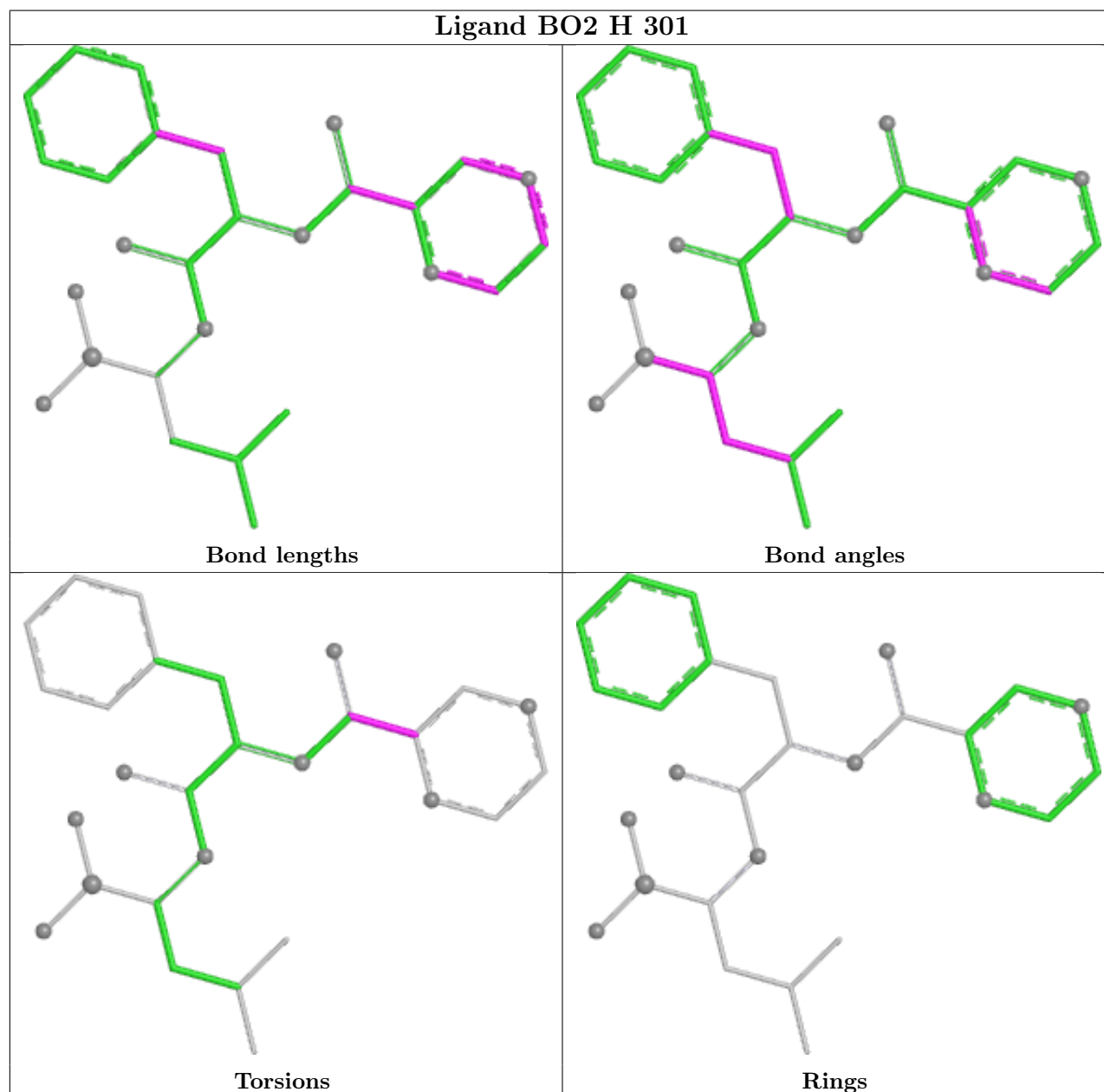
Mol	Chain	Res	Type	Atoms
17	H	301	BO2	C3-C2-C7-O8
17	H	301	BO2	C3-C2-C7-N9
17	V	301	BO2	C3-C2-C7-O8
17	V	301	BO2	C3-C2-C7-N9
17	V	301	BO2	N1-C2-C7-O8
17	H	301	BO2	N1-C2-C7-O8
17	H	301	BO2	N1-C2-C7-N9
17	V	301	BO2	N1-C2-C7-N9
17	b	201	BO2	N1-C2-C7-O8
17	N	201	BO2	N1-C2-C7-N9
17	b	201	BO2	N1-C2-C7-N9
17	N	201	BO2	N1-C2-C7-O8
17	N	201	BO2	C3-C2-C7-O8
17	b	201	BO2	C3-C2-C7-O8
17	N	201	BO2	C3-C2-C7-N9
17	b	201	BO2	C3-C2-C7-N9
17	K	301	BO2	C3-C2-C7-O8
17	Y	301	BO2	C3-C2-C7-O8
17	K	301	BO2	C3-C2-C7-N9
17	Y	301	BO2	C3-C2-C7-N9
17	Y	301	BO2	N1-C2-C7-O8
17	K	301	BO2	N1-C2-C7-O8
17	K	301	BO2	N1-C2-C7-N9
17	Y	301	BO2	N1-C2-C7-N9

There are no ring outliers.

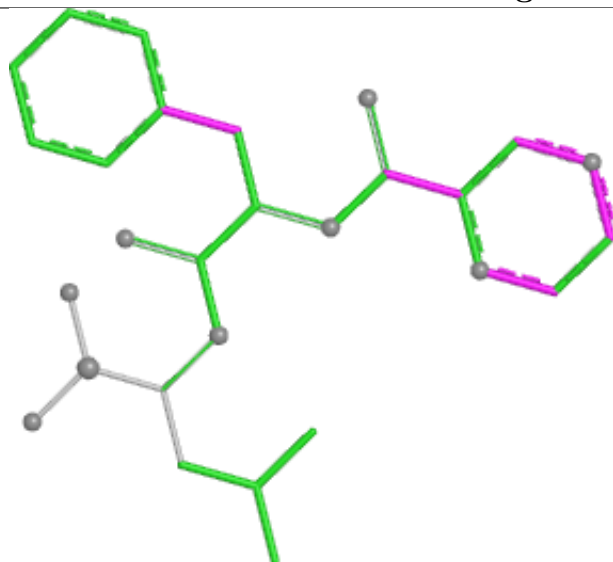
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	Y	301	BO2	1	0
17	b	201	BO2	3	0
17	N	201	BO2	2	0
17	K	301	BO2	1	0

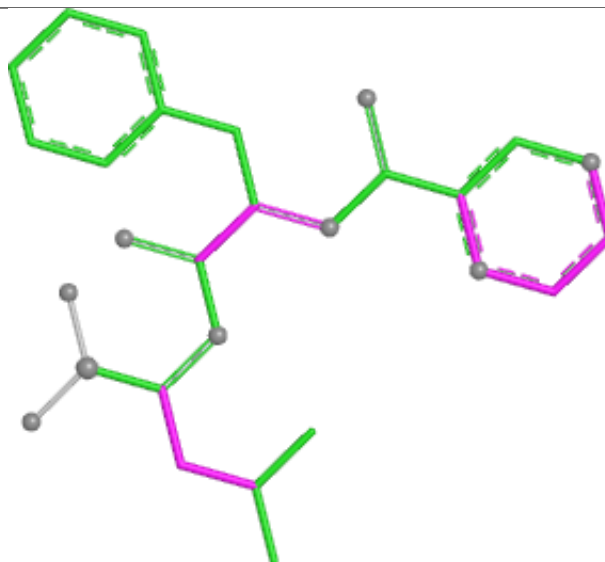
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



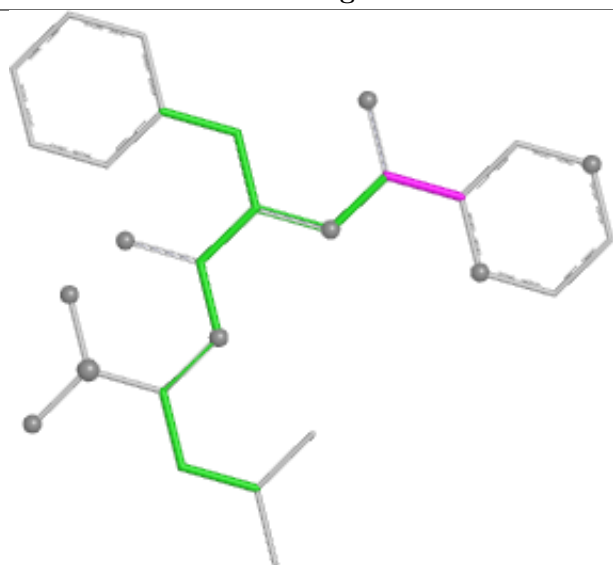
Ligand BO2 Y 301



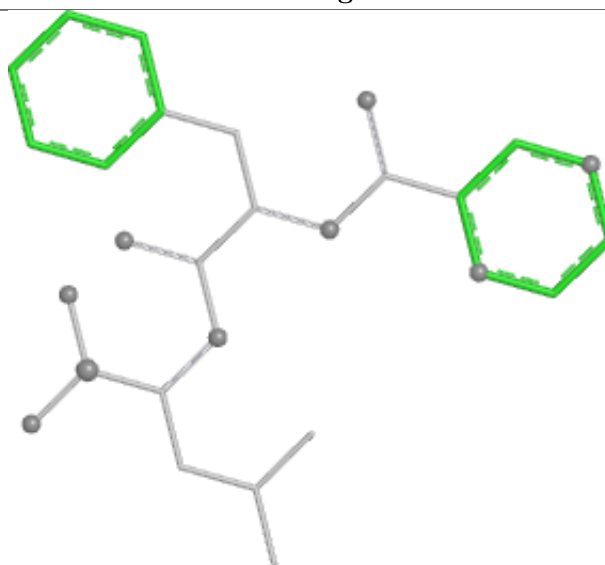
Bond lengths



Bond angles

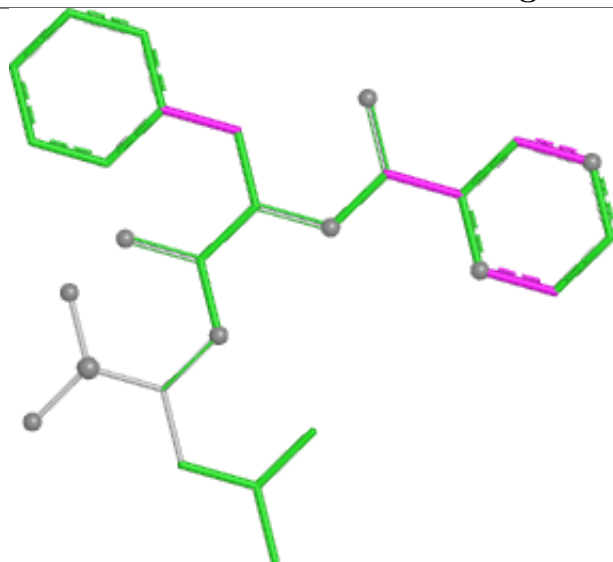


Torsions

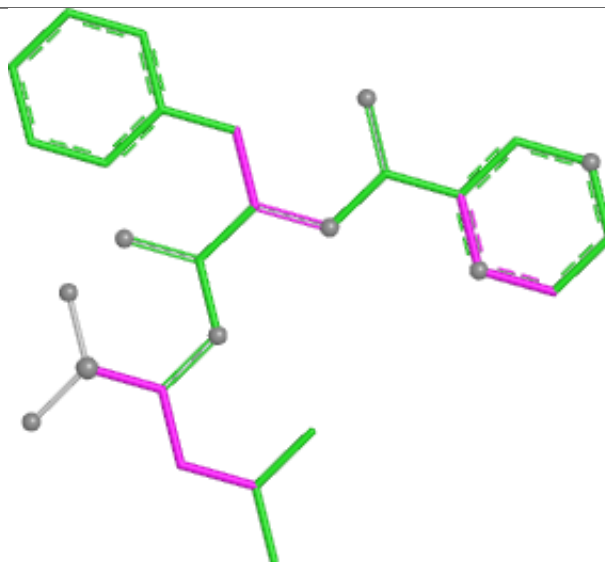


Rings

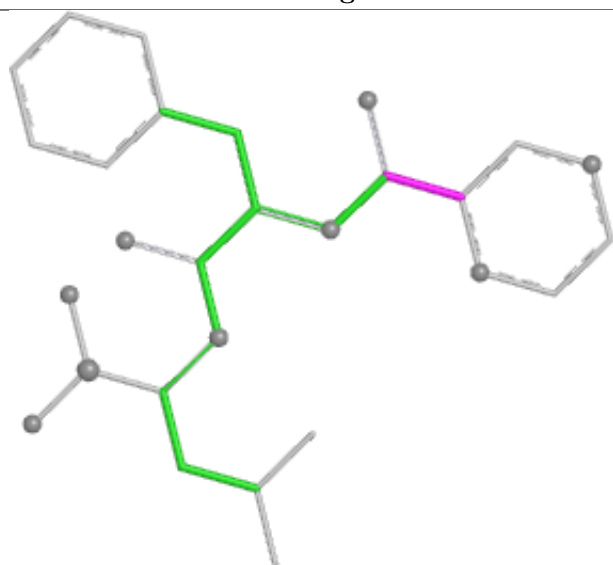
Ligand BO2 b 201



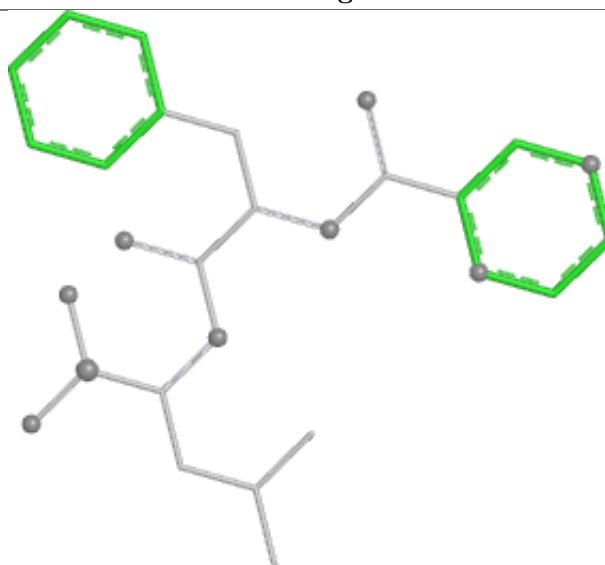
Bond lengths



Bond angles

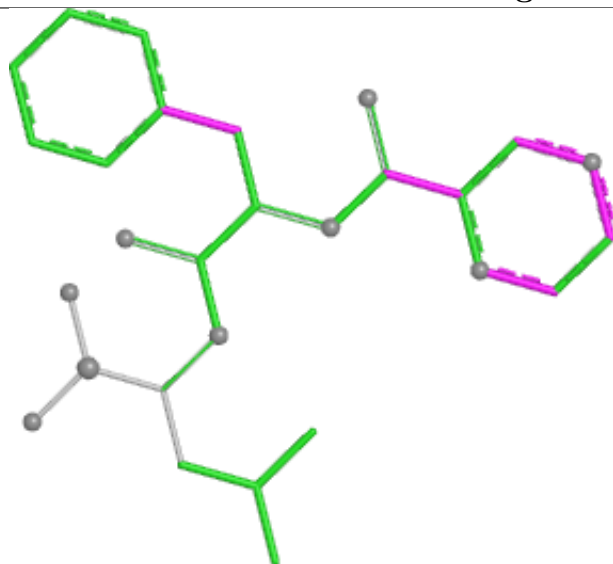


Torsions

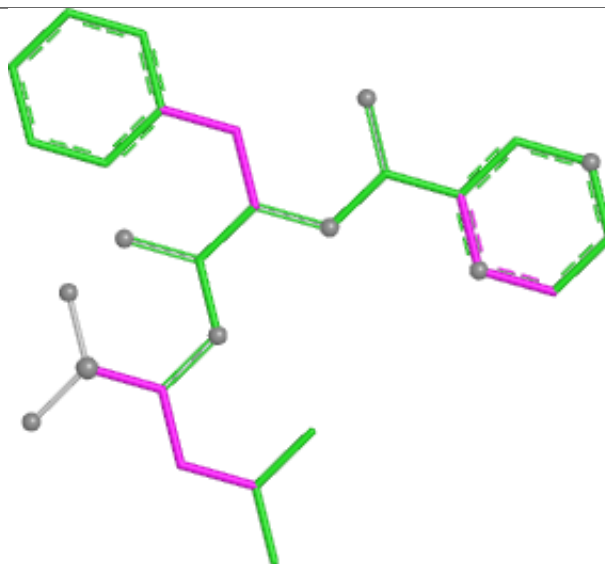


Rings

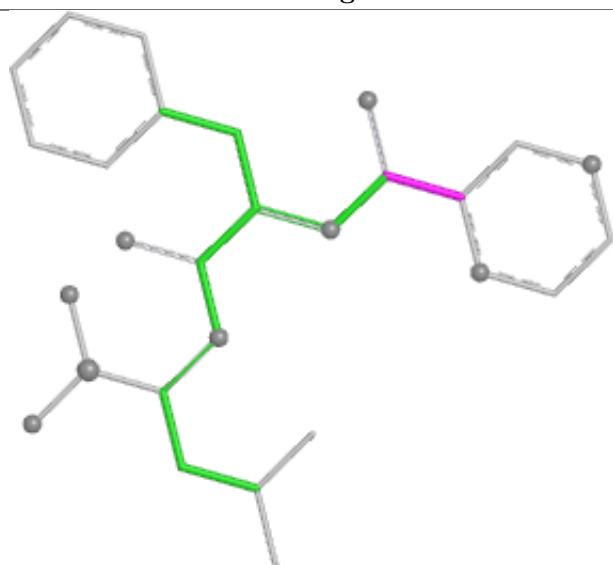
Ligand BO2 V 301



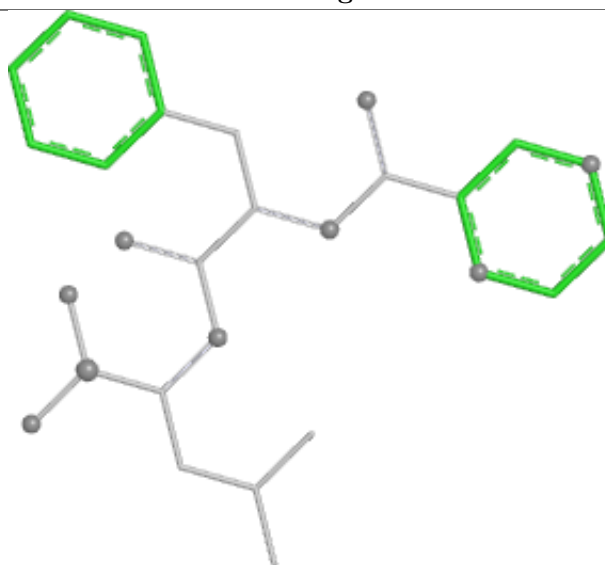
Bond lengths



Bond angles

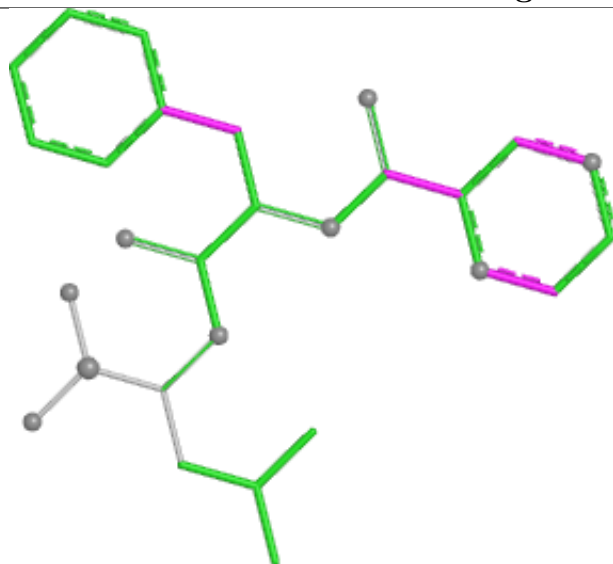


Torsions

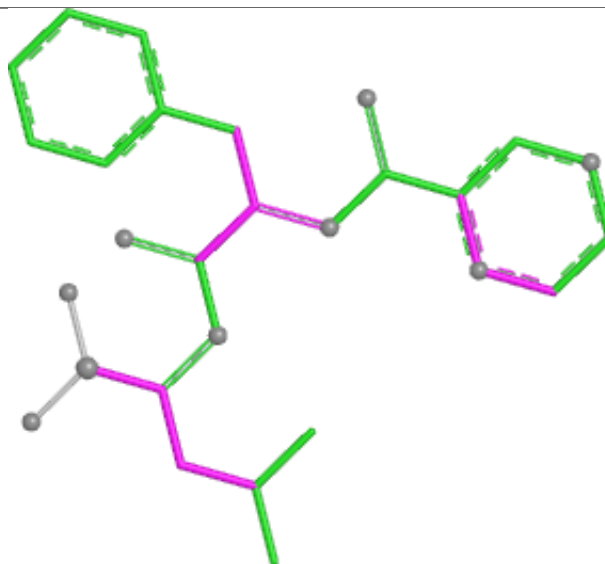


Rings

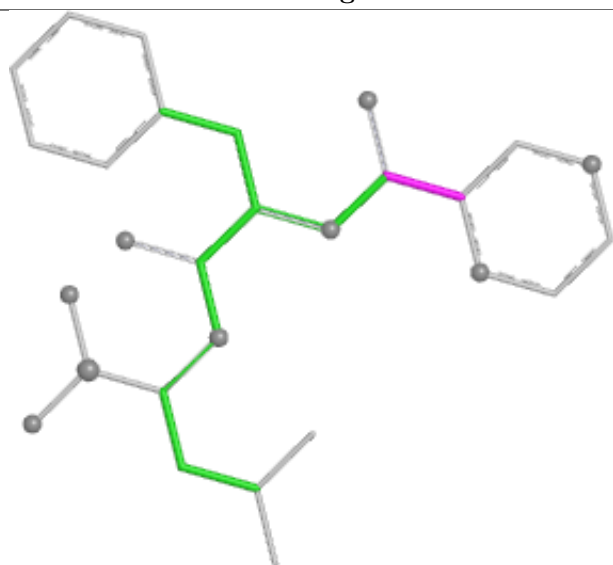
Ligand BO2 N 201



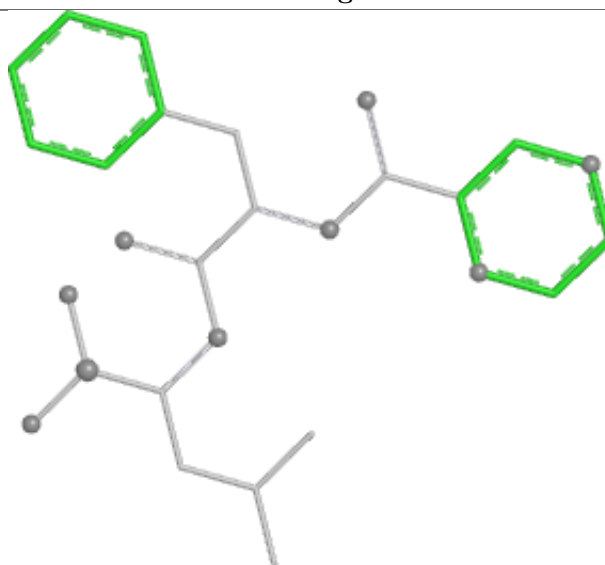
Bond lengths



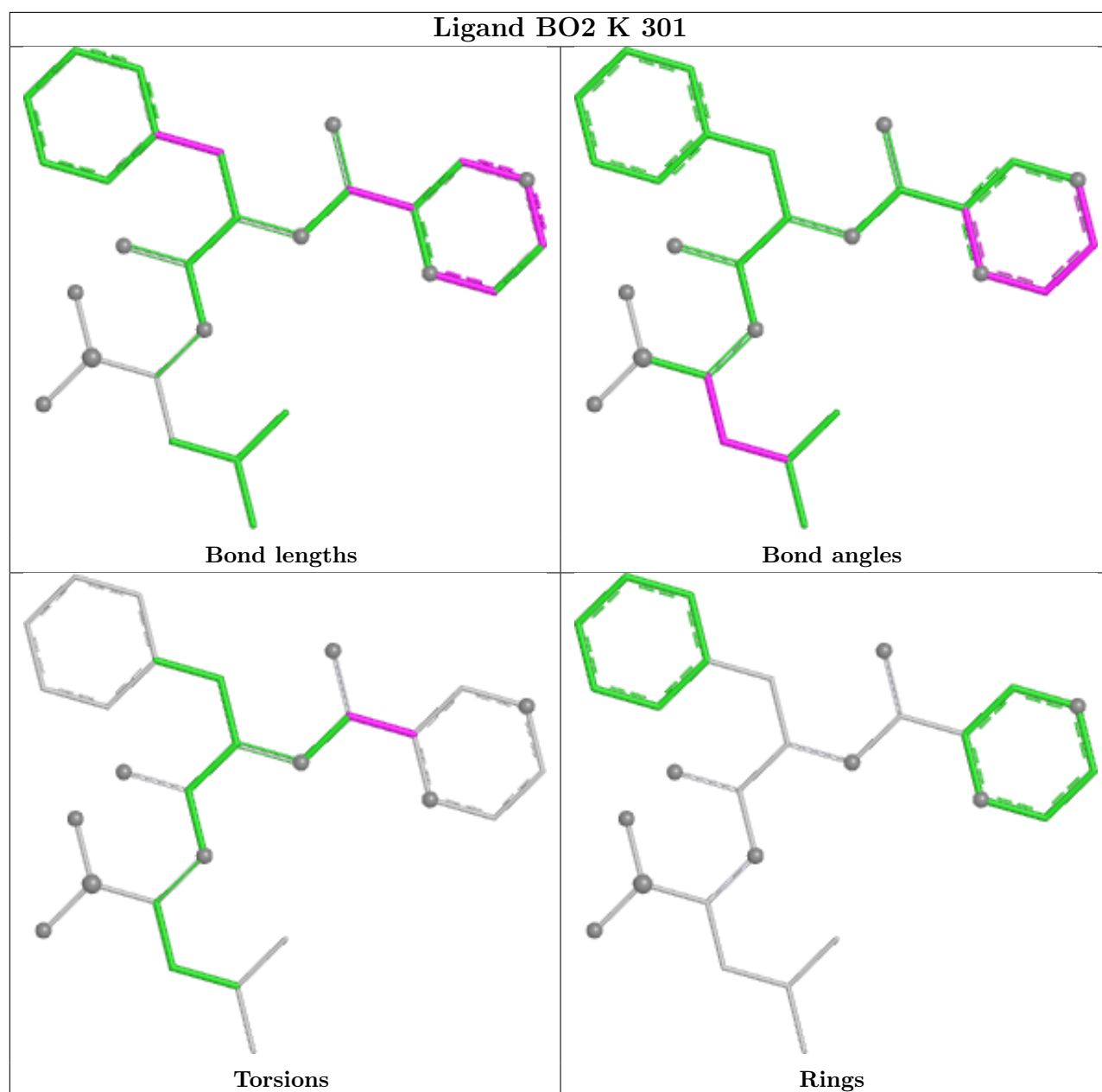
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.42	0 100 100	43, 57, 95, 135	0
1	O	250/250 (100%)	-0.38	1 (0%) 88 84	44, 64, 109, 142	0
2	B	244/258 (94%)	-0.27	2 (0%) 82 75	42, 63, 108, 162	0
2	P	244/258 (94%)	-0.28	3 (1%) 76 68	48, 66, 108, 152	0
3	C	240/254 (94%)	-0.25	1 (0%) 88 84	41, 65, 125, 156	0
3	Q	240/254 (94%)	-0.08	6 (2%) 58 48	49, 81, 162, 186	0
4	D	235/260 (90%)	-0.41	2 (0%) 81 74	46, 66, 96, 141	0
4	R	235/260 (90%)	-0.22	1 (0%) 88 84	54, 74, 112, 152	0
5	E	231/234 (98%)	-0.26	0 100 100	47, 70, 107, 152	0
5	S	231/234 (98%)	-0.10	0 100 100	52, 78, 123, 158	0
6	F	243/288 (84%)	-0.33	1 (0%) 88 84	42, 65, 112, 141	0
6	T	243/288 (84%)	-0.24	1 (0%) 88 84	44, 72, 130, 161	0
7	G	241/252 (95%)	-0.40	2 (0%) 82 75	42, 60, 98, 147	0
7	U	241/252 (95%)	-0.36	1 (0%) 88 84	45, 61, 96, 144	0
8	H	226/232 (97%)	-0.32	1 (0%) 88 84	40, 56, 95, 153	0
8	V	226/232 (97%)	-0.35	2 (0%) 81 74	41, 57, 93, 169	0
9	I	204/205 (99%)	-0.48	0 100 100	38, 54, 86, 108	0
9	W	204/205 (99%)	-0.48	0 100 100	40, 56, 86, 106	0
10	J	195/198 (98%)	-0.40	1 (0%) 87 82	40, 56, 86, 126	0
10	X	195/198 (98%)	-0.35	1 (0%) 87 82	42, 59, 87, 140	0
11	K	212/212 (100%)	-0.16	7 (3%) 49 39	38, 57, 94, 110	0
11	Y	212/212 (100%)	-0.09	6 (2%) 55 45	40, 57, 98, 116	0
12	L	222/222 (100%)	-0.21	12 (5%) 31 24	40, 57, 106, 139	0
12	Z	222/222 (100%)	-0.27	9 (4%) 41 33	34, 58, 108, 141	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.52	1 (0%) 88 84	38, 55, 77, 96	0
13	a	233/246 (94%)	-0.53	1 (0%) 88 84	38, 55, 77, 97	0
14	N	196/196 (100%)	-0.51	1 (0%) 87 82	39, 51, 78, 106	0
14	b	196/196 (100%)	-0.55	1 (0%) 87 82	39, 52, 80, 112	0
All	All	6344/6614 (95%)	-0.33	64 (1%) 79 72	34, 61, 108, 186	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	L	174	TYR	4.7
3	Q	50	LEU	4.3
3	Q	49	THR	4.1
10	X	1	MET	4.1
12	Z	174	TYR	3.8
12	L	162	PRO	3.6
11	Y	148	LEU	3.6
12	L	170	LYS	3.5
8	V	223	ILE	3.4
2	P	219	ALA	3.4
3	Q	205	ALA	3.4
12	Z	162	PRO	3.3
12	Z	165	ASN	3.2
11	K	148	LEU	3.2
8	H	223	ILE	3.1
11	Y	211	ILE	2.9
10	J	1	MET	2.8
11	K	211	ILE	2.7
12	L	165	ASN	2.7
7	G	68	ARG	2.7
11	Y	146	TRP	2.7
12	L	136	CYS	2.7
12	Z	169	LYS	2.6
11	K	146	TRP	2.6
12	L	171	PRO	2.6
2	B	51	VAL	2.6
1	O	1	MET	2.6
12	Z	168	VAL	2.6
11	K	147	ASP	2.5
11	Y	147	ASP	2.4
12	L	169	LYS	2.4
14	b	103	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	219	ALA	2.4
3	C	201	VAL	2.4
12	L	156	PHE	2.4
4	D	240	ALA	2.4
13	a	1	THR	2.3
7	G	2	GLY	2.3
4	D	241	ALA	2.3
11	Y	208	ASN	2.2
6	F	215	CYS	2.2
12	L	172	LEU	2.2
3	Q	51	LYS	2.2
3	Q	238	LYS	2.2
4	R	183	LEU	2.2
2	P	51	VAL	2.1
12	Z	163	GLY	2.1
12	Z	136	CYS	2.1
12	L	168	VAL	2.1
14	N	103	ASP	2.1
8	V	224	GLN	2.1
11	K	145	LYS	2.1
11	Y	24	ASN	2.1
6	T	243	ILE	2.1
11	K	104	TYR	2.1
11	K	209	ASN	2.1
3	Q	3	ASP	2.1
12	Z	170	LYS	2.0
12	Z	173	LYS	2.0
2	P	218	GLY	2.0
12	L	164	THR	2.0
13	M	1	THR	2.0
7	U	40	ASP	2.0
12	L	163	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

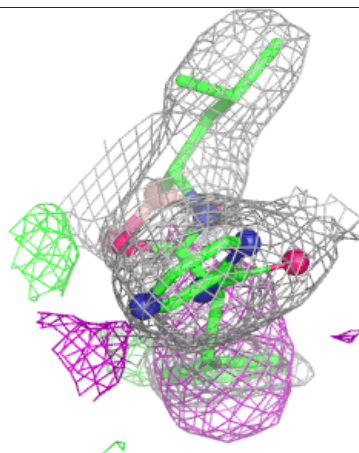
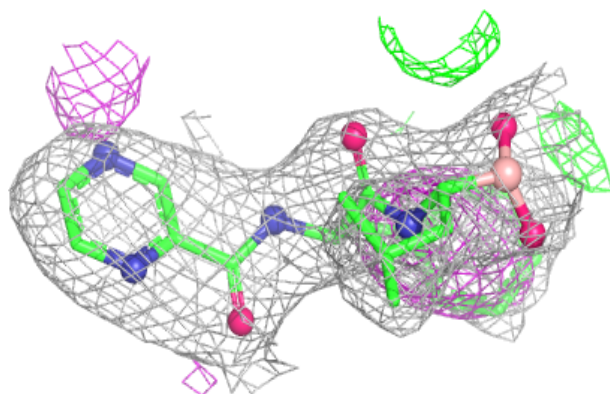
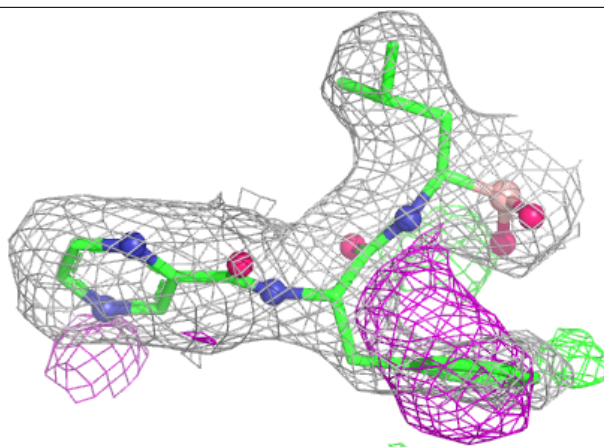
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	BO2	N	201	28/28	0.90	0.12	37,49,58,58	0
17	BO2	b	201	28/28	0.90	0.11	43,49,59,60	0
17	BO2	V	301	28/28	0.92	0.10	54,57,79,82	0
17	BO2	H	301	28/28	0.93	0.09	50,55,79,80	0
17	BO2	K	301	28/28	0.94	0.08	40,54,61,61	0
17	BO2	Y	301	28/28	0.95	0.09	45,57,65,67	0
15	MG	Z	301	1/1	0.96	0.10	74,74,74,74	0
16	CL	b	202	1/1	0.96	0.10	45,45,45,45	0
15	MG	I	301	1/1	0.97	0.09	72,72,72,72	0
15	MG	V	302	1/1	0.97	0.04	70,70,70,70	0
16	CL	U	301	1/1	0.98	0.13	48,48,48,48	0
15	MG	Y	302	1/1	0.98	0.07	46,46,46,46	0
15	MG	N	202	1/1	0.98	0.04	55,55,55,55	0
16	CL	G	302	1/1	0.98	0.08	44,44,44,44	0
15	MG	K	302	1/1	0.99	0.05	57,57,57,57	0
15	MG	G	301	1/1	0.99	0.03	58,58,58,58	0
15	MG	J	201	1/1	0.99	0.14	39,39,39,39	0
16	CL	N	203	1/1	0.99	0.07	45,45,45,45	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

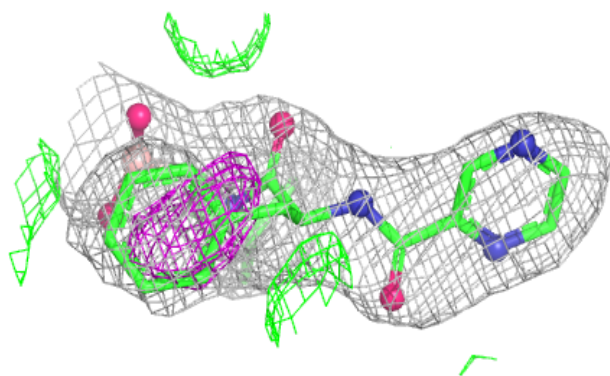
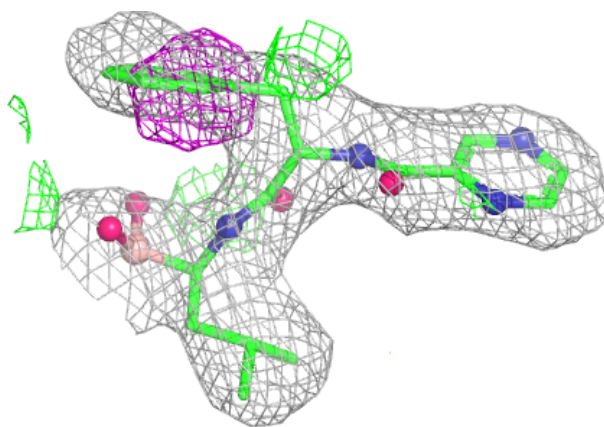
Electron density around BO2 N 201:

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



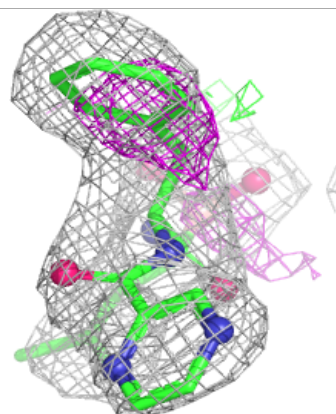
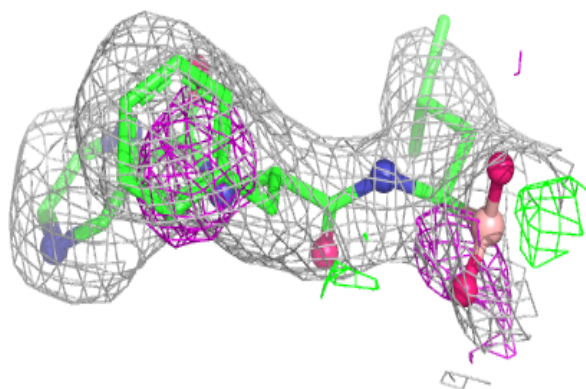
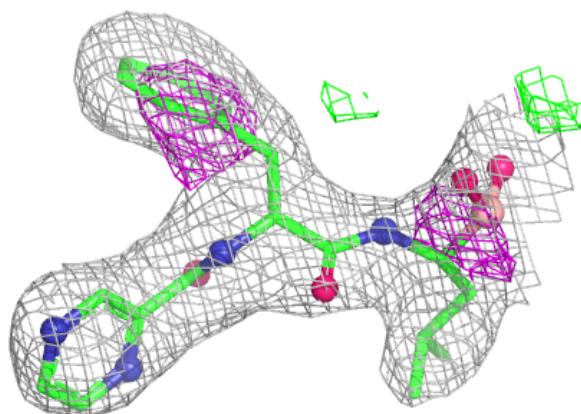
Electron density around BO2 b 201:

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



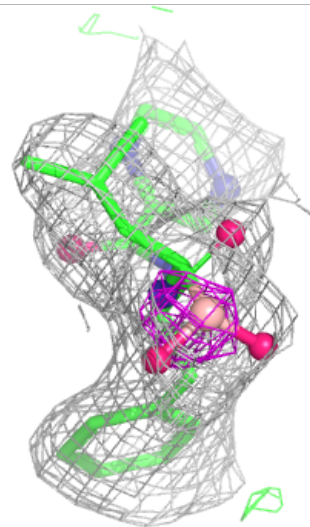
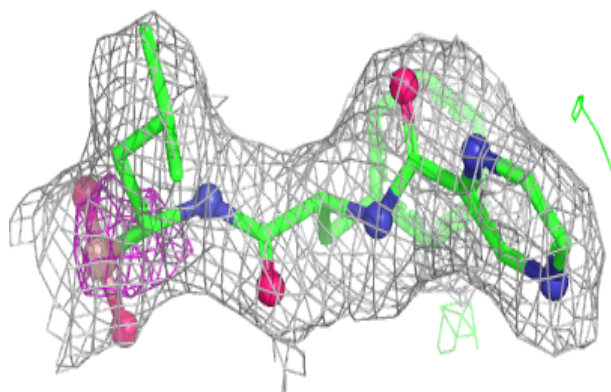
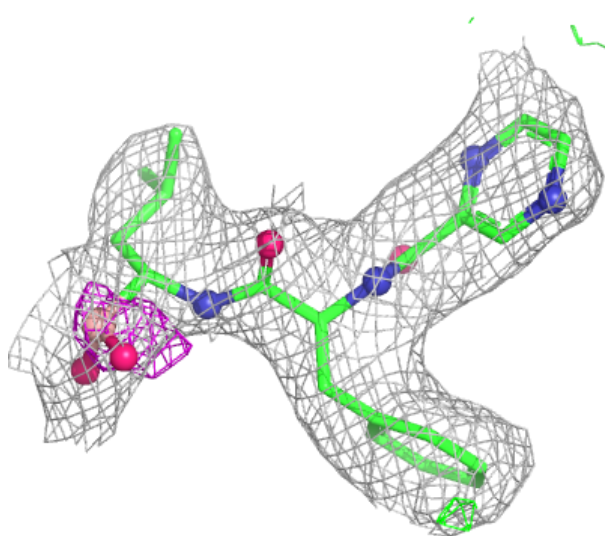
Electron density around BO2 V 301:

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



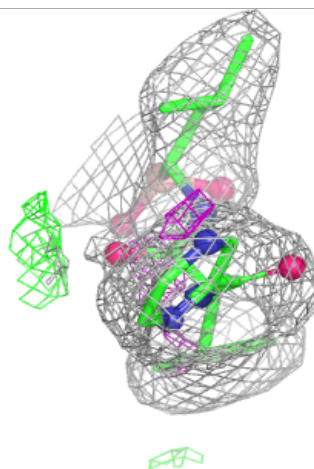
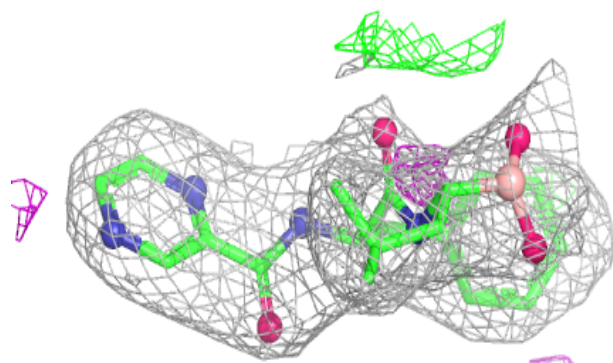
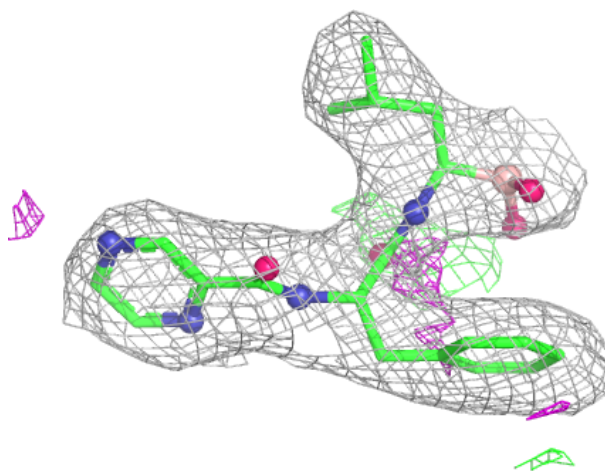
Electron density around BO2 H 301:

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



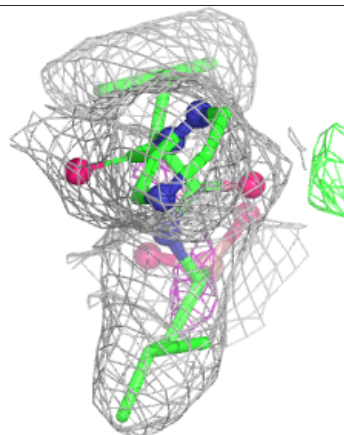
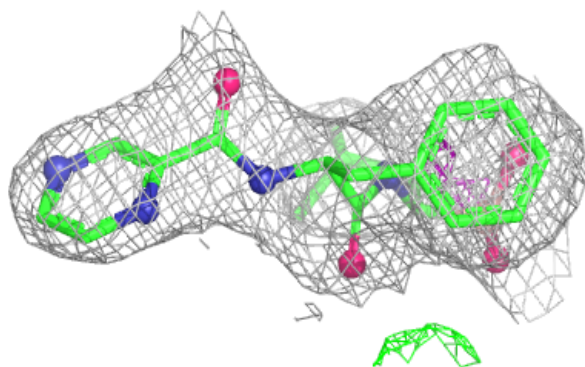
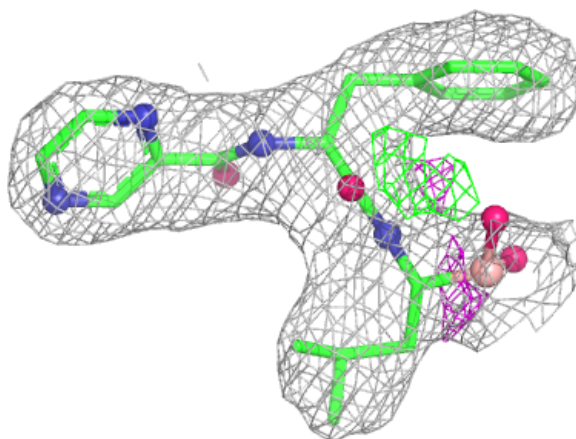
Electron density around BO2 K 301:

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



Electron density around BO2 Y 301:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.