



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:40 PM UTC

PDB ID : 4QVV / pdb_00004qvv
Title : yCP beta5-A49V mutant in complex with bortezomib
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on : 2014-07-16
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

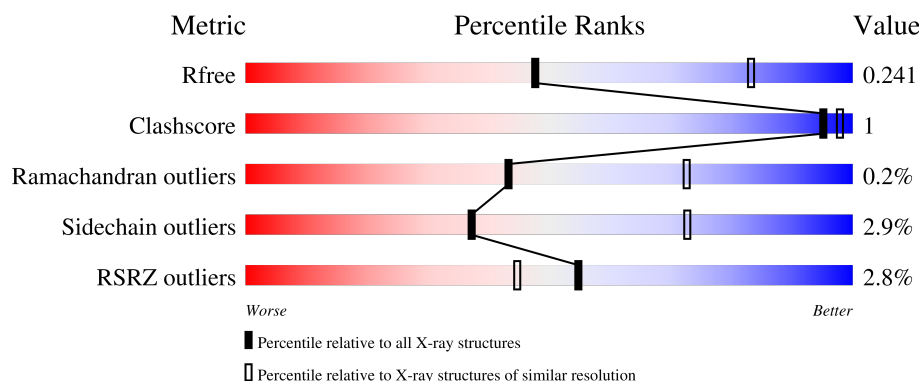
1 Overall quality at a glance

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	0% 98% •
1	O	250	2% 97% •
2	B	258	6% 87% 7% • 5%
2	P	258	2% 88% 6% 5%
3	C	254	4% 89% • • 6%

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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 49917 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			

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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
			1646	1047	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1646	1047	280	312	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	49	VAL	ALA	engineered mutation	UNP P30656
Y	49	VAL	ALA	engineered mutation	UNP P30656

- 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			

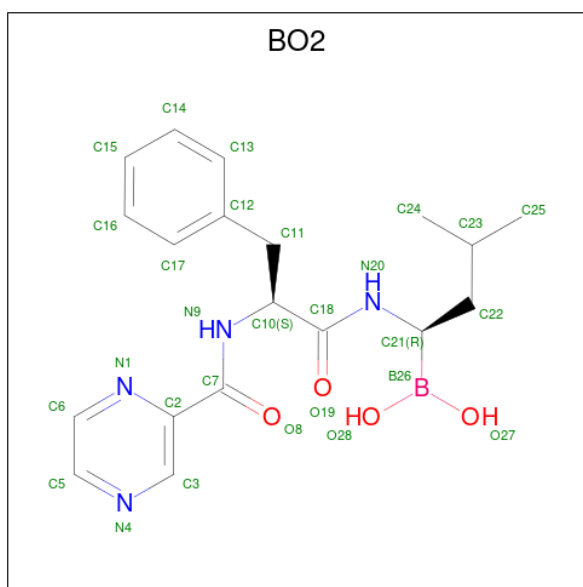
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total Mg 1 1	0	0
15	I	1	Total Mg 1 1	0	0
15	J	1	Total Mg 1 1	0	0
15	K	2	Total Mg 2 2	0	0
15	N	1	Total Mg 1 1	0	0
15	V	1	Total Mg 1 1	0	0
15	Y	1	Total Mg 1 1	0	0

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

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

- Molecule 17 is N-[(1R)-1-(DIHYDROXYBORYL)-3-METHYLBUTYL]-N-(PYRAZIN-2-YLCARBONYL)-L-PHENYLALANINAMIDE (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	10	Total	O	0	0
			10	10		
18	C	11	Total	O	0	0
			11	11		
18	D	13	Total	O	0	0
			13	13		
18	E	9	Total	O	0	0
			9	9		
18	F	14	Total	O	0	0
			14	14		

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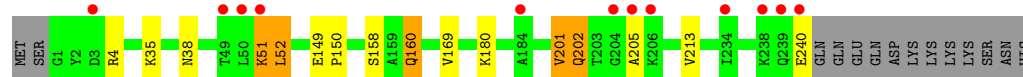
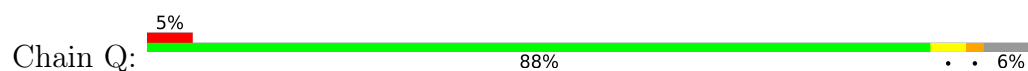
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	G	10	Total O 10 10	0	0
18	H	20	Total O 20 20	0	0
18	I	7	Total O 7 7	0	0
18	J	12	Total O 12 12	0	0
18	K	14	Total O 14 14	0	0
18	L	14	Total O 14 14	0	0
18	M	23	Total O 23 23	0	0
18	N	15	Total O 15 15	0	0
18	O	7	Total O 7 7	0	0
18	P	4	Total O 4 4	0	0
18	Q	7	Total O 7 7	0	0
18	R	17	Total O 17 17	0	0
18	S	6	Total O 6 6	0	0
18	T	11	Total O 11 11	0	0
18	U	16	Total O 16 16	0	0
18	V	13	Total O 13 13	0	0
18	W	10	Total O 10 10	0	0
18	X	18	Total O 18 18	0	0
18	Y	15	Total O 15 15	0	0
18	Z	17	Total O 17 17	0	0
18	a	28	Total O 28 28	0	0

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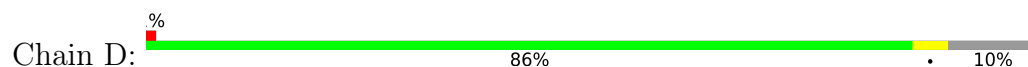
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	b	13	Total	O	0	0
			13	13		

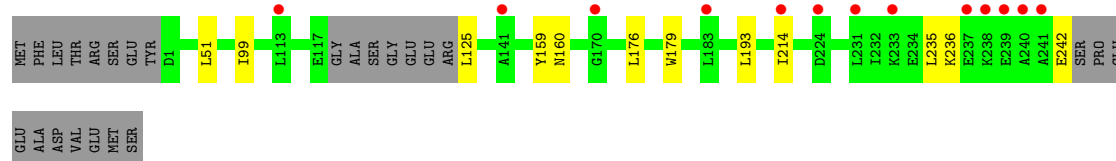
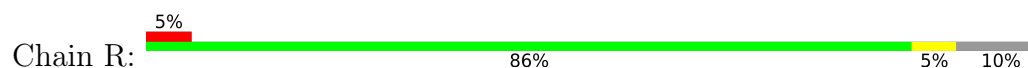
- Molecule 3: Proteasome subunit alpha type-4



- Molecule 4: Proteasome subunit alpha type-5



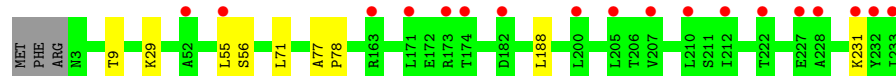
- Molecule 4: Proteasome subunit alpha type-5



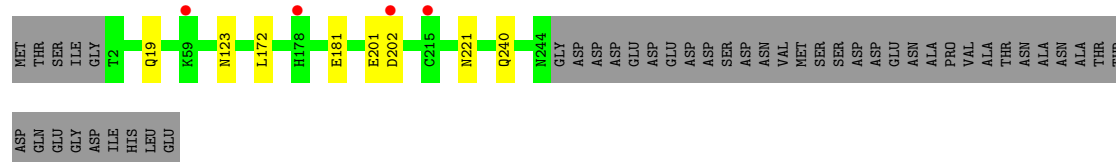
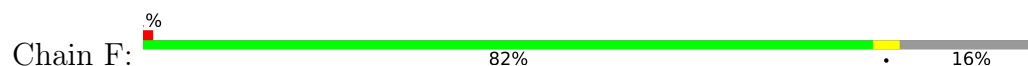
- Molecule 5: Proteasome subunit alpha type-6



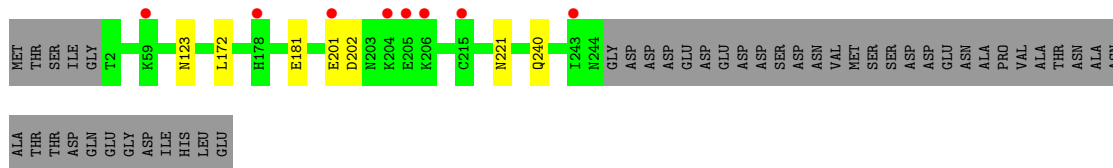
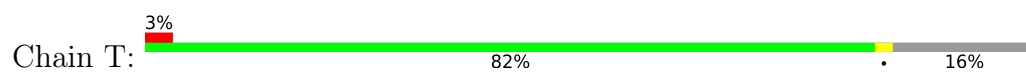
- Molecule 5: Proteasome subunit alpha type-6



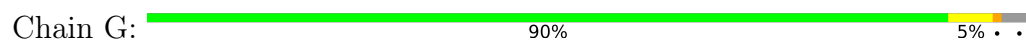
- Molecule 6: Probable proteasome subunit alpha type-7



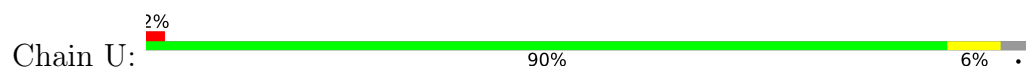
- Molecule 6: Probable proteasome subunit alpha type-7



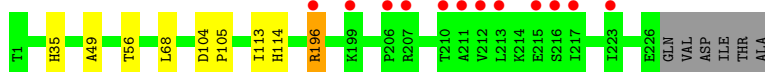
• Molecule 7: Proteasome subunit alpha type-1



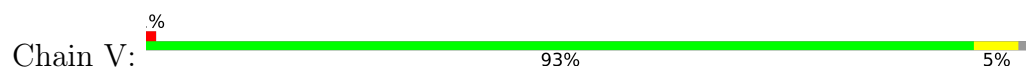
• Molecule 7: Proteasome subunit alpha type-1



• Molecule 8: Proteasome subunit beta type-2



• Molecule 8: Proteasome subunit beta type-2

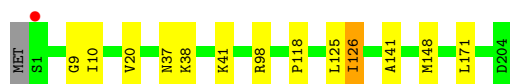


• Molecule 9: Proteasome subunit beta type-3

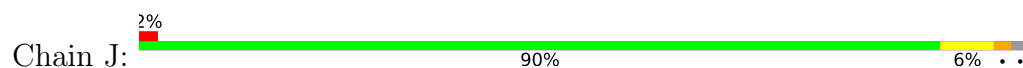


• Molecule 9: Proteasome subunit beta type-3

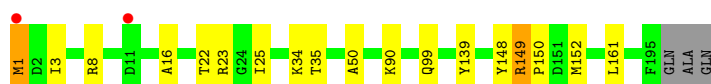
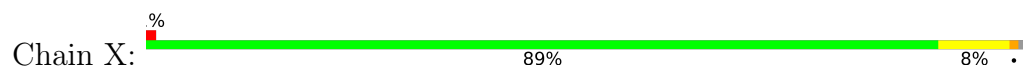




- Molecule 10: Proteasome subunit beta type-4



- Molecule 10: Proteasome subunit beta type-4



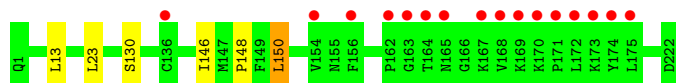
- Molecule 11: Proteasome subunit beta type-5



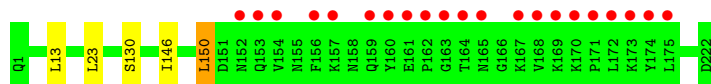
- Molecule 11: Proteasome subunit beta type-5



- Molecule 12: Proteasome subunit beta type-6

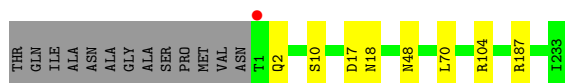


- Molecule 12: Proteasome subunit beta type-6

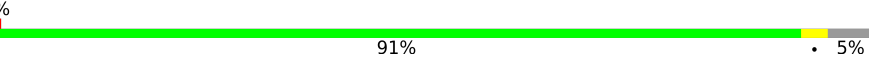


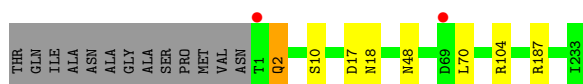
- Molecule 13: Proteasome subunit beta type-7

Chain M:  91% • 5%

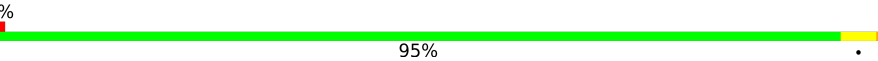


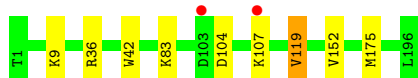
- Molecule 13: Proteasome subunit beta type-7

Chain a:  91% • 5%

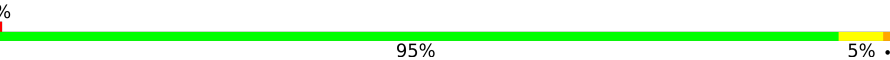


- Molecule 14: Proteasome subunit beta type-1

Chain N:  95% • •



- Molecule 14: Proteasome subunit beta type-1

Chain b:  95% 5% •



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.52Å 300.75Å 145.35Å 90.00° 113.24° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.8 (15.00-2.80) 97.2 (15.00-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.199 , 0.235 0.206 , 0.241	Depositor DCC
R_{free} test set	12806 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	55.5	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	49917	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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: CL, BO2, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.42	0/1952	0.69	0/2642
1	O	0.42	0/1952	0.69	0/2642
2	B	0.42	0/1934	0.68	0/2618
2	P	0.42	0/1934	0.68	0/2618
3	C	0.40	0/1910	0.69	1/2586 (0.0%)
3	Q	0.40	0/1910	0.69	1/2586 (0.0%)
4	D	0.40	0/1837	0.67	0/2475
4	R	0.41	0/1837	0.68	0/2475
5	E	0.42	0/1800	0.66	0/2433
5	S	0.41	0/1800	0.66	0/2433
6	F	0.42	0/1932	0.69	0/2609
6	T	0.41	0/1932	0.70	0/2609
7	G	0.40	0/1945	0.68	0/2634
7	U	0.41	0/1945	0.68	0/2634
8	H	0.40	0/1750	0.66	0/2373
8	V	0.39	0/1750	0.65	0/2373
9	I	0.41	0/1611	0.70	0/2174
9	W	0.41	0/1611	0.70	0/2174
10	J	0.50	0/1589	0.69	0/2142
10	X	0.51	0/1589	0.70	0/2142
11	K	0.38	0/1683	0.68	0/2277
11	Y	0.39	0/1683	0.69	0/2277
12	L	0.40	0/1795	0.69	0/2420
12	Z	0.41	0/1795	0.69	0/2420
13	M	0.41	0/1855	0.69	1/2514 (0.0%)
13	a	0.41	0/1855	0.69	1/2514 (0.0%)
14	N	0.38	0/1541	0.66	0/2087
14	b	0.38	0/1541	0.67	0/2087
All	All	0.41	0/50268	0.68	4/67968 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	201	VAL	N-CA-C	6.41	116.55	110.53
3	C	201	VAL	N-CA-C	6.33	116.48	110.53
13	a	10	SER	N-CA-C	5.37	117.81	110.24
13	M	10	SER	N-CA-C	5.34	117.77	110.24

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	0	0
1	O	1915	0	1929	2	0
2	B	1904	0	1904	7	0
2	P	1904	0	1904	5	0
3	C	1881	0	1895	5	0
3	Q	1881	0	1895	5	0
4	D	1813	0	1797	2	0
4	R	1813	0	1797	2	0
5	E	1773	0	1775	3	0
5	S	1773	0	1775	2	0
6	F	1892	0	1883	2	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	5	0
7	U	1907	0	1901	5	0
8	H	1719	0	1718	5	0
8	V	1719	0	1718	5	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	14	0
10	X	1561	0	1569	15	0
11	K	1646	0	1598	14	0
11	Y	1646	0	1598	11	0
12	L	1757	0	1711	4	0
12	Z	1757	0	1711	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	1824	0	1832	1	0
13	a	1824	0	1832	2	0
14	N	1512	0	1480	3	0
14	b	1512	0	1480	4	0
15	G	1	0	0	0	0
15	I	1	0	0	0	0
15	J	1	0	0	0	0
15	K	2	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
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	1	0
17	H	28	0	25	1	0
17	K	28	0	25	3	0
17	N	28	0	25	1	0
17	V	28	0	25	1	0
17	Y	28	0	25	3	0
17	b	28	0	25	1	0
18	A	13	0	0	1	0
18	B	10	0	0	2	0
18	C	11	0	0	0	0
18	D	13	0	0	0	0
18	E	9	0	0	0	0
18	F	14	0	0	0	0
18	G	10	0	0	0	0
18	H	20	0	0	0	0
18	I	7	0	0	0	0
18	J	12	0	0	1	0
18	K	14	0	0	0	0
18	L	14	0	0	0	0
18	M	23	0	0	0	0
18	N	15	0	0	0	0
18	O	7	0	0	0	0
18	P	4	0	0	0	0
18	Q	7	0	0	0	0
18	R	17	0	0	0	0
18	S	6	0	0	0	0
18	T	11	0	0	0	0
18	U	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	V	13	0	0	0	0
18	W	10	0	0	0	0
18	X	18	0	0	0	0
18	Y	15	0	0	0	0
18	Z	17	0	0	0	0
18	a	28	0	0	1	0
18	b	13	0	0	0	0
All	All	49917	0	49282	120	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (120) 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)
11:K:208:ASN:OD1	10:X:149:ARG:HD3	1.61	0.99
11:Y:49:VAL:HG23	17:Y:301:BO2:H251	1.47	0.97
11:K:49:VAL:HG23	17:K:301:BO2:H251	1.47	0.95
10:J:8:ARG:O	10:J:148:TYR:OH	2.05	0.70
10:J:149:ARG:HD3	18:J:304:HOH:O	1.93	0.67
11:Y:49:VAL:CG2	17:Y:301:BO2:H251	2.24	0.67
11:K:205:GLY:O	10:X:149:ARG:NE	2.29	0.66
11:K:49:VAL:HG23	17:K:301:BO2:C25	2.25	0.65
13:a:2:GLN:NE2	18:a:327:HOH:O	2.31	0.63
8:V:114:HIS:CD2	17:b:201:BO2:H5	2.34	0.62
11:K:49:VAL:CG2	17:K:301:BO2:H251	2.24	0.62
10:X:149:ARG:HH11	10:X:149:ARG:CG	2.12	0.62
8:H:49:ALA:HA	17:H:301:BO2:H241	1.82	0.61
8:V:49:ALA:HA	17:V:301:BO2:H241	1.82	0.61
11:Y:49:VAL:HG23	17:Y:301:BO2:C25	2.25	0.60
10:J:149:ARG:CG	10:J:149:ARG:HH21	2.14	0.60
10:X:22:THR:O	10:X:23:ARG:HD3	2.02	0.60
10:J:149:ARG:HG3	10:J:149:ARG:NH2	2.20	0.57
11:Y:49:VAL:HG13	12:Z:130:SER:CB	2.34	0.57
11:Y:45:MET:HG2	11:Y:52:CYS:HB3	1.86	0.56
9:W:125:LEU:HG	9:W:126:ILE:HG22	1.88	0.56
11:K:209:ASN:O	9:W:38:LYS:NZ	2.38	0.56
11:K:45:MET:HG2	11:K:52:CYS:HB3	1.87	0.55
14:b:152:VAL:HA	14:b:175:MET:HE1	1.89	0.55
9:I:125:LEU:HG	9:I:126:ILE:HG22	1.88	0.55
10:J:25:ILE:O	10:X:139:TYR:OH	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:116:ASP:C	11:Y:116:ASP:OD2	2.49	0.55
11:K:116:ASP:OD2	11:K:116:ASP:C	2.50	0.54
14:N:152:VAL:HA	14:N:175:MET:HE1	1.90	0.54
10:J:149:ARG:O	10:J:152:MET:HB2	2.08	0.53
9:I:38:LYS:NZ	11:Y:209:ASN:O	2.42	0.53
10:X:149:ARG:HH11	10:X:149:ARG:HG3	1.73	0.52
8:H:114:HIS:CD2	17:N:201:BO2:H5	2.45	0.52
7:G:23:PHE:O	7:G:26:THR:HB	2.10	0.52
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.42	0.51
10:J:23:ARG:NH1	11:K:120:THR:OG1	2.44	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.51
10:X:8:ARG:O	10:X:148:TYR:OH	2.25	0.50
7:U:23:PHE:O	7:U:26:THR:HB	2.11	0.50
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.50
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.94	0.50
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.94	0.49
10:J:149:ARG:HH21	10:J:149:ARG:HG3	1.77	0.49
11:K:49:VAL:HG13	12:L:130:SER:CB	2.43	0.49
2:B:93:HIS:HB3	18:B:301:HOH:O	2.12	0.49
10:X:149:ARG:CG	10:X:149:ARG:NH1	2.73	0.48
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.49	0.48
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.96	0.47
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.96	0.47
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.96	0.47
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.79	0.47
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.97	0.47
3:C:35:LYS:HG2	3:C:158:SER:O	2.14	0.47
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.80	0.47
2:B:50:LYS:O	2:B:51:VAL:C	2.58	0.46
10:X:149:ARG:O	10:X:152:MET:HG3	2.15	0.46
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.97	0.46
2:P:50:LYS:O	2:P:51:VAL:C	2.58	0.46
10:J:139:TYR:OH	10:X:25:ILE:O	2.33	0.46
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.96	0.46
10:J:149:ARG:CG	10:J:149:ARG:NH2	2.73	0.46
2:B:113:ARG:NE	18:B:301:HOH:O	2.41	0.45
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	1.99	0.45
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.52	0.45
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.17	0.45
11:Y:49:VAL:CG1	12:Z:130:SER:CB	2.95	0.45
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.52	0.44
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.99	0.44
8:H:196:ARG:NH2	9:I:150:GLU:O	2.50	0.44
12:L:148:PRO:HB2	9:W:148:MET:SD	2.58	0.44
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.01	0.43
2:P:50:LYS:HD3	2:P:50:LYS:HA	1.84	0.43
12:L:146:ILE:HG22	12:L:150:LEU:HD22	1.99	0.43
2:B:217:LYS:C	2:B:219:ALA:H	2.27	0.43
11:K:208:ASN:OD1	10:X:149:ARG:CD	2.49	0.43
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.00	0.43
2:P:217:LYS:C	2:P:219:ALA:H	2.27	0.42
14:b:45:ARG:NH2	16:b:202:CL:CL	2.77	0.42
18:A:304:HOH:O	7:G:122:ARG:HD2	2.19	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.42
13:M:17:ASP:OD1	13:M:18:ASN:N	2.53	0.42
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.02	0.42
6:T:202:ASP:OD1	6:T:202:ASP:N	2.53	0.42
5:E:12:PHE:H	6:F:19:GLN:HE22	1.67	0.42
9:W:98:ARG:HD2	9:W:126:ILE:HD12	2.02	0.42
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.49	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.42
11:K:55:TRP:HB2	11:K:97:MET:HE1	2.01	0.42
6:F:202:ASP:N	6:F:202:ASP:OD1	2.53	0.41
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.02	0.41
11:Y:49:VAL:HG13	12:Z:130:SER:HB2	2.01	0.41
9:I:98:ARG:HD2	9:I:126:ILE:HD12	2.02	0.41
11:K:208:ASN:HB3	10:X:150:PRO:HD3	2.02	0.41
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.54	0.41
2:P:221:ASP:O	2:P:223:GLU:N	2.54	0.41
11:Y:55:TRP:HB2	11:Y:97:MET:HE1	2.01	0.41
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.51	0.41
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.50	0.41
3:C:51:LYS:O	3:C:52:LEU:HB2	2.20	0.41
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.51	0.41
14:b:36:ARG:HG3	14:b:42:TRP:CE2	2.55	0.41
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.02	0.41
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.50	0.41
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.20	0.41
7:U:73:VAL:HG12	7:U:133:THR:HB	2.02	0.41
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.56	0.41
2:B:146:GLN:HG2	3:C:57:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:221:ASP:O	2:B:223:GLU:N	2.54	0.41
10:J:25:ILE:HD13	11:K:134:THR:HG21	2.03	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.03	0.41
13:a:17:ASP:OD1	13:a:18:ASN:N	2.54	0.41
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.51	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.40
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.04	0.40
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.52	0.40
7:G:73:VAL:HG12	7:G:133:THR:HB	2.02	0.40
1:O:49:LYS:HG3	1:O:210:GLU:HB2	2.04	0.40
8:V:84:LYS:HE2	8:V:119:THR:HG23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	240 (97%)	7 (3%)	1 (0%)	30	60
1	O	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	30	60
2	B	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	7	25
2	P	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	7	25
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	16	44
3	Q	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	16	44
4	D	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
4	R	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	221 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
6	T	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
7	G	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
8	H	224/232 (97%)	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%)	188 (97%)	5 (3%)	0	100	100
10	X	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
11	K	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
11	Y	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
12	L	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
13	M	231/246 (94%)	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%)	6132 (98%)	138 (2%)	14 (0%)	43	72

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
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

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Mol	Chain	Res	Type
3	Q	205	ALA

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%)	197 (97%)	6 (3%)	36	72
2	P	203/216 (94%)	197 (97%)	6 (3%)	36	72
3	C	212/226 (94%)	203 (96%)	9 (4%)	26	61
3	Q	212/226 (94%)	203 (96%)	9 (4%)	26	61
4	D	194/215 (90%)	185 (95%)	9 (5%)	24	58
4	R	194/215 (90%)	185 (95%)	9 (5%)	24	58
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
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%)	182 (98%)	3 (2%)	55	83
8	V	185/190 (97%)	182 (98%)	3 (2%)	55	83
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%)	165 (95%)	8 (5%)	24	58
10	X	173/175 (99%)	167 (96%)	6 (4%)	32	67
11	K	170/170 (100%)	163 (96%)	7 (4%)	27	62
11	Y	170/170 (100%)	163 (96%)	7 (4%)	27	62
12	L	185/185 (100%)	183 (99%)	2 (1%)	65	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	Z	185/185 (100%)	183 (99%)	2 (1%)	65	87
13	M	199/208 (96%)	194 (98%)	5 (2%)	42	76
13	a	199/208 (96%)	194 (98%)	5 (2%)	42	76
14	N	162/162 (100%)	158 (98%)	4 (2%)	42	76
14	b	162/162 (100%)	158 (98%)	4 (2%)	42	76
All	All	5322/5542 (96%)	5166 (97%)	156 (3%)	37	73

All (156) 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	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
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	213	VAL
3	C	240	GLU
4	D	51	LEU
4	D	99	ILE
4	D	125	LEU
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

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Mol	Chain	Res	Type
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	113	ILE
8	H	196	ARG
9	I	37	ASN
9	I	126	ILE
9	I	171	LEU
10	J	1	MET
10	J	3	ILE
10	J	23	ARG
10	J	35	THR
10	J	90	LYS
10	J	99	GLN
10	J	149	ARG
10	J	152	MET
11	K	4	LEU
11	K	49	VAL
11	K	100	MET
11	K	116	ASP
11	K	140	LEU
11	K	148	LEU
11	K	211	ILE
12	L	23	LEU
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN

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Mol	Chain	Res	Type
13	M	70	LEU
13	M	104	ARG
13	M	187	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	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	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	213	VAL
3	Q	240	GLU
4	R	51	LEU
4	R	99	ILE
4	R	125	LEU
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

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Mol	Chain	Res	Type
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	113	ILE
8	V	196	ARG
9	W	37	ASN
9	W	126	ILE
9	W	171	LEU
10	X	1	MET
10	X	3	ILE
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
10	X	149	ARG
11	Y	4	LEU
11	Y	49	VAL
11	Y	100	MET
11	Y	116	ASP
11	Y	140	LEU
11	Y	148	LEU
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
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 (109) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	124	HIS
2	B	155	ASN
2	B	176	GLN
2	B	232	GLN
3	C	17	GLN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	100	ASN
4	D	106	GLN
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	123	ASN
6	F	143	HIS
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	175	ASN
7	G	176	HIS
7	G	212	ASN
8	H	22	GLN
8	H	30	ASN
8	H	66	HIS
8	H	189	ASN
9	I	88	GLN
9	I	203	GLN
10	J	55	GLN
10	J	63	ASN
11	K	9	GLN
11	K	85	ASN
11	K	143	ASN

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Mol	Chain	Res	Type
11	K	176	ASN
12	L	70	ASN
12	L	79	HIS
12	L	158	ASN
12	L	197	GLN
13	M	26	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	194	ASN
13	M	213	GLN
14	N	38	HIS
14	N	141	ASN
2	P	119	GLN
2	P	123	GLN
2	P	124	HIS
2	P	232	GLN
3	Q	17	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	106	GLN
4	R	146	GLN
4	R	225	ASN
5	S	68	HIS
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	117	GLN
6	T	123	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	175	ASN
7	U	176	HIS

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Mol	Chain	Res	Type
8	V	22	GLN
8	V	30	ASN
8	V	66	HIS
8	V	189	ASN
9	W	203	GLN
10	X	55	GLN
10	X	63	ASN
11	Y	9	GLN
11	Y	85	ASN
11	Y	143	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	79	HIS
12	Z	135	GLN
12	Z	155	ASN
12	Z	158	ASN
12	Z	159	GLN
12	Z	197	GLN
13	a	102	GLN
13	a	108	ASN
13	a	149	HIS
13	a	194	ASN
13	a	213	GLN
14	b	38	HIS
14	b	141	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	Y	301	11	25,29,29	1.58	5 (20%)	33,38,38	1.50	5 (15%)
17	BO2	N	201	14	25,29,29	1.55	4 (16%)	33,38,38	1.38	5 (15%)
17	BO2	H	301	8	25,29,29	1.62	5 (20%)	33,38,38	1.32	4 (12%)
17	BO2	V	301	8	25,29,29	1.63	5 (20%)	33,38,38	1.34	5 (15%)
17	BO2	K	301	11	25,29,29	1.60	5 (20%)	33,38,38	1.49	6 (18%)
17	BO2	b	201	14	25,29,29	1.56	5 (20%)	33,38,38	1.38	6 (18%)

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	Y	301	11	-	0/23/28/28	0/2/2/2
17	BO2	N	201	14	-	4/23/28/28	0/2/2/2
17	BO2	H	301	8	-	7/23/28/28	0/2/2/2
17	BO2	V	301	8	-	7/23/28/28	0/2/2/2
17	BO2	K	301	11	-	0/23/28/28	0/2/2/2
17	BO2	b	201	14	-	4/23/28/28	0/2/2/2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	301	BO2	C11-C12	-4.53	1.40	1.51
17	b	201	BO2	C11-C12	-4.52	1.40	1.51
17	N	201	BO2	C11-C12	-4.51	1.40	1.51
17	Y	301	BO2	C11-C12	-4.50	1.40	1.51
17	H	301	BO2	C11-C12	-4.38	1.41	1.51
17	b	201	BO2	C2-C7	-4.28	1.38	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	V	301	BO2	C11-C12	-4.22	1.41	1.51
17	K	301	BO2	C2-C7	-4.16	1.39	1.50
17	N	201	BO2	C2-C7	-4.06	1.39	1.50
17	Y	301	BO2	C2-C7	-4.03	1.39	1.50
17	V	301	BO2	C2-C7	-3.99	1.39	1.50
17	H	301	BO2	C2-C7	-3.89	1.39	1.50
17	V	301	BO2	C3-N4	3.14	1.40	1.34
17	H	301	BO2	C3-N4	3.09	1.40	1.34
17	V	301	BO2	C6-N1	3.05	1.41	1.34
17	H	301	BO2	C6-N1	2.99	1.40	1.34
17	Y	301	BO2	C3-N4	2.96	1.40	1.34
17	K	301	BO2	C3-N4	2.94	1.40	1.34
17	N	201	BO2	C6-N1	2.73	1.40	1.34
17	b	201	BO2	C6-N1	2.71	1.40	1.34
17	K	301	BO2	C6-N1	2.70	1.40	1.34
17	Y	301	BO2	C6-N1	2.69	1.40	1.34
17	N	201	BO2	C3-N4	2.54	1.39	1.34
17	V	301	BO2	C5-N4	2.49	1.40	1.33
17	K	301	BO2	C5-N4	2.48	1.40	1.33
17	Y	301	BO2	C5-N4	2.44	1.40	1.33
17	H	301	BO2	C5-N4	2.43	1.40	1.33
17	b	201	BO2	C3-N4	2.32	1.39	1.34
17	b	201	BO2	C5-N4	2.01	1.39	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Y	301	BO2	C21-C22-C23	-4.84	109.14	115.32
17	K	301	BO2	C21-C22-C23	-4.71	109.31	115.32
17	b	201	BO2	C21-C22-C23	-4.20	109.96	115.32
17	N	201	BO2	C21-C22-C23	-4.09	110.09	115.32
17	V	301	BO2	C21-C22-C23	-3.55	110.80	115.32
17	V	301	BO2	C6-N1-C2	3.47	121.40	116.93
17	H	301	BO2	C21-C22-C23	-3.46	110.90	115.32
17	H	301	BO2	C6-N1-C2	3.46	121.39	116.93
17	K	301	BO2	C6-N1-C2	3.43	121.36	116.93
17	Y	301	BO2	C6-N1-C2	3.37	121.27	116.93
17	N	201	BO2	C6-N1-C2	2.79	120.53	116.93
17	Y	301	BO2	B26-C21-C22	-2.77	107.07	112.31
17	K	301	BO2	B26-C21-C22	-2.74	107.13	112.31
17	b	201	BO2	C11-C10-N9	-2.69	105.25	110.83
17	N	201	BO2	C11-C10-N9	-2.66	105.33	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	V	301	BO2	B26-C21-C22	-2.64	107.33	112.31
17	K	301	BO2	C11-C10-N9	-2.62	105.40	110.83
17	Y	301	BO2	C11-C10-N9	-2.62	105.40	110.83
17	H	301	BO2	B26-C21-C22	-2.57	107.46	112.31
17	b	201	BO2	C6-N1-C2	2.57	120.24	116.93
17	b	201	BO2	B26-C21-C22	-2.22	108.13	112.31
17	N	201	BO2	B26-C21-C22	-2.20	108.16	112.31
17	b	201	BO2	C18-C10-N9	-2.08	105.48	111.11
17	K	301	BO2	C5-C6-N1	-2.05	119.30	122.19
17	N	201	BO2	C18-C10-N9	-2.05	105.57	111.11
17	K	301	BO2	C2-C3-N4	-2.03	119.31	121.97
17	V	301	BO2	C12-C11-C10	-2.02	107.97	113.36
17	V	301	BO2	C6-C5-N4	-2.02	119.45	121.96
17	H	301	BO2	C12-C11-C10	-2.02	107.99	113.36
17	Y	301	BO2	C6-C5-N4	-2.01	119.46	121.96
17	b	201	BO2	C5-C6-N1	-2.00	119.37	122.19

There are no chirality outliers.

All (22) 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	H	301	BO2	C21-C22-C23-C24
17	H	301	BO2	C21-C22-C23-C25
17	V	301	BO2	C3-C2-C7-O8
17	V	301	BO2	C3-C2-C7-N9
17	V	301	BO2	C21-C22-C23-C24
17	V	301	BO2	C21-C22-C23-C25
17	H	301	BO2	N1-C2-C7-N9
17	V	301	BO2	N1-C2-C7-N9
17	H	301	BO2	N1-C2-C7-O8
17	V	301	BO2	N1-C2-C7-O8
17	N	201	BO2	N1-C2-C7-O8
17	b	201	BO2	N1-C2-C7-O8
17	b	201	BO2	N1-C2-C7-N9
17	N	201	BO2	N1-C2-C7-N9
17	H	301	BO2	N20-C21-C22-C23
17	V	301	BO2	N20-C21-C22-C23
17	N	201	BO2	C3-C2-C7-O8
17	b	201	BO2	C3-C2-C7-O8
17	N	201	BO2	C3-C2-C7-N9

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Mol	Chain	Res	Type	Atoms
17	b	201	BO2	C3-C2-C7-N9

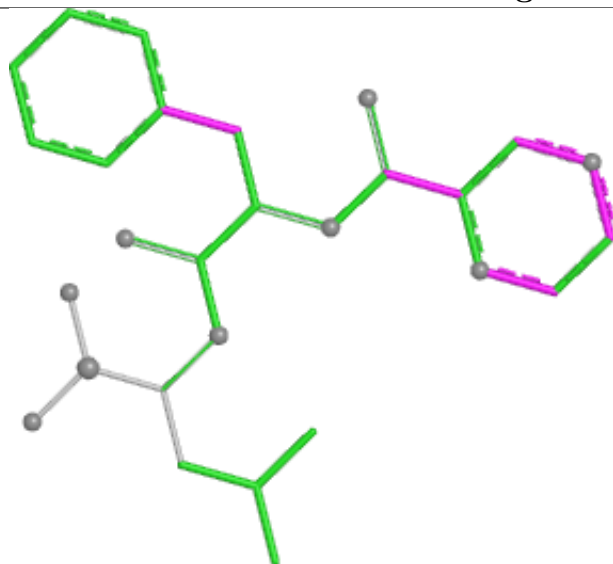
There are no ring outliers.

6 monomers are involved in 10 short contacts:

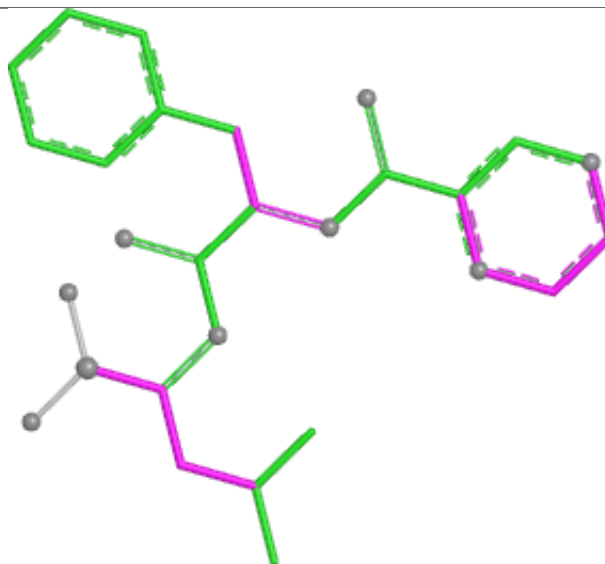
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	Y	301	BO2	3	0
17	N	201	BO2	1	0
17	H	301	BO2	1	0
17	V	301	BO2	1	0
17	K	301	BO2	3	0
17	b	201	BO2	1	0

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

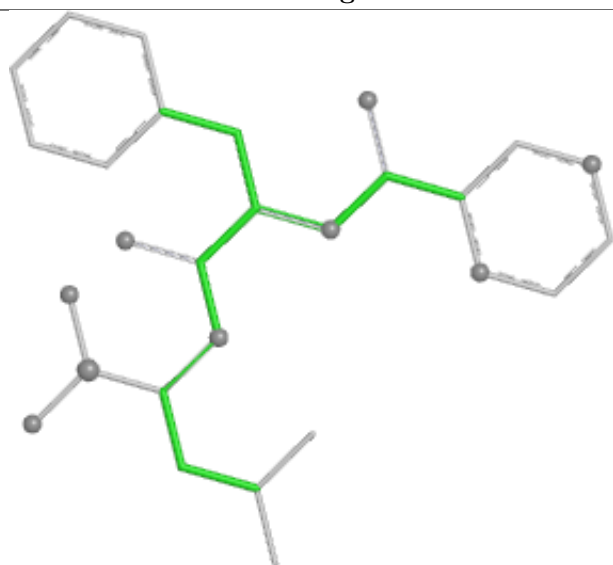
Ligand BO2 Y 301



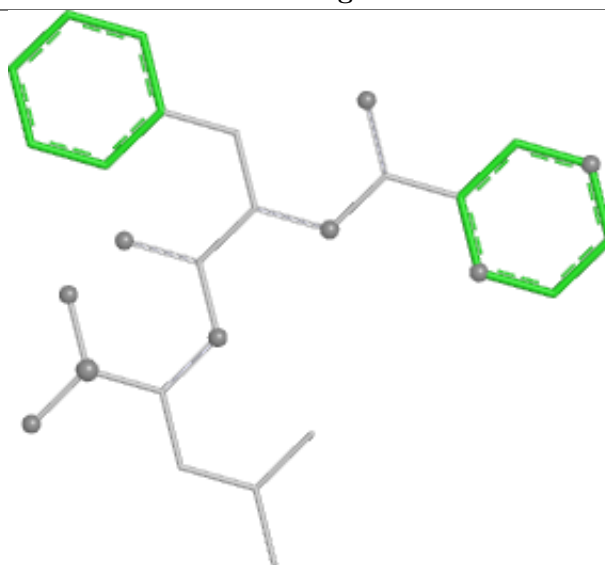
Bond lengths



Bond angles

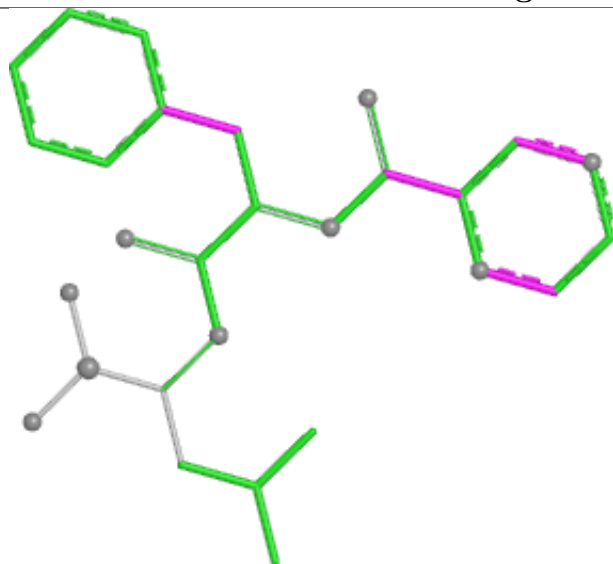


Torsions

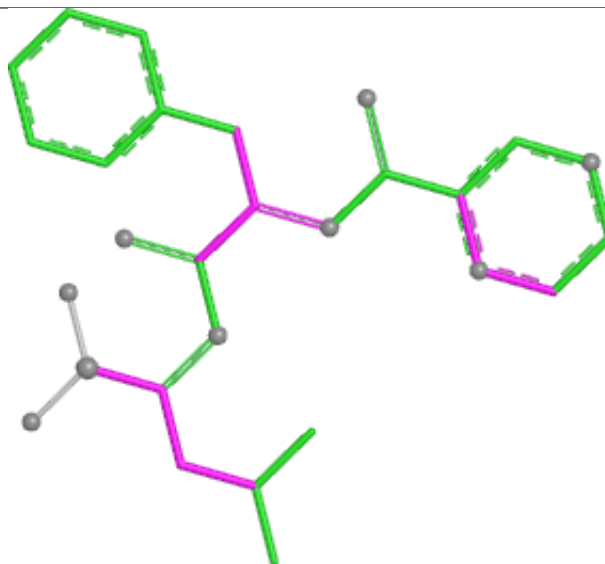


Rings

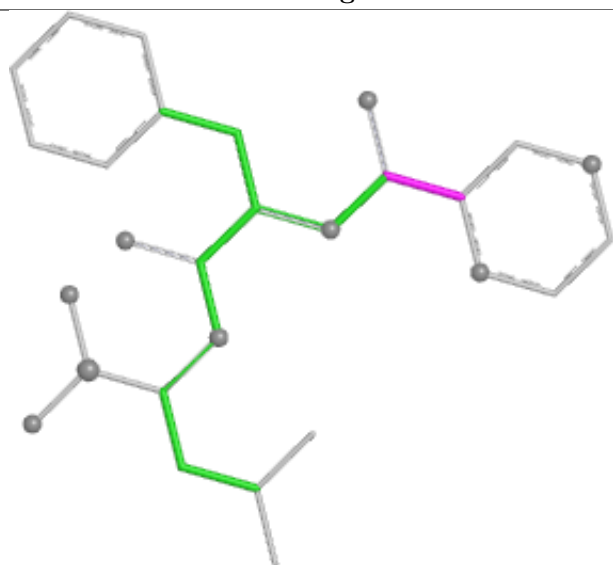
Ligand BO2 N 201



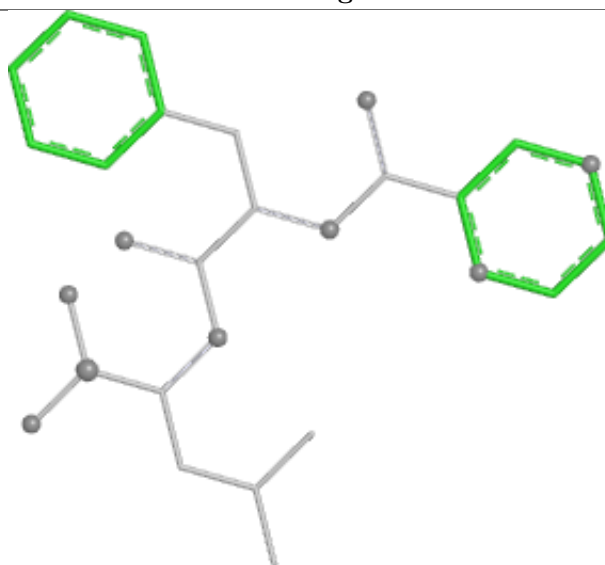
Bond lengths



Bond angles

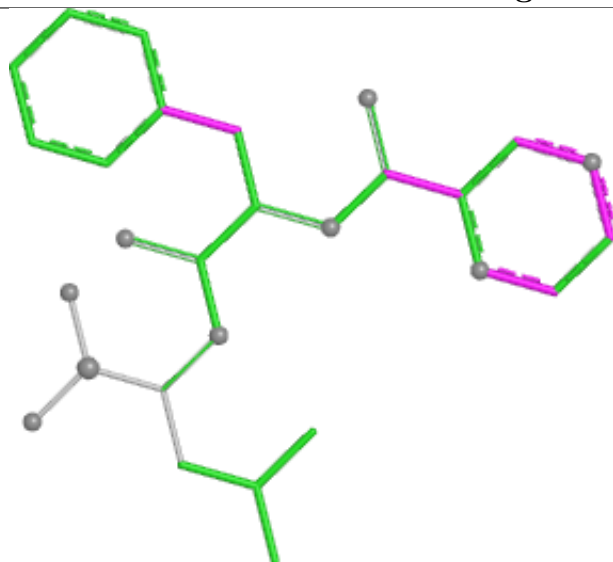


Torsions

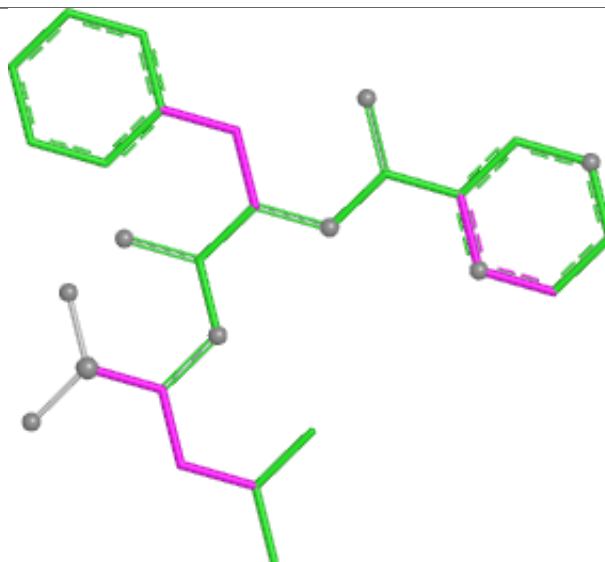


Rings

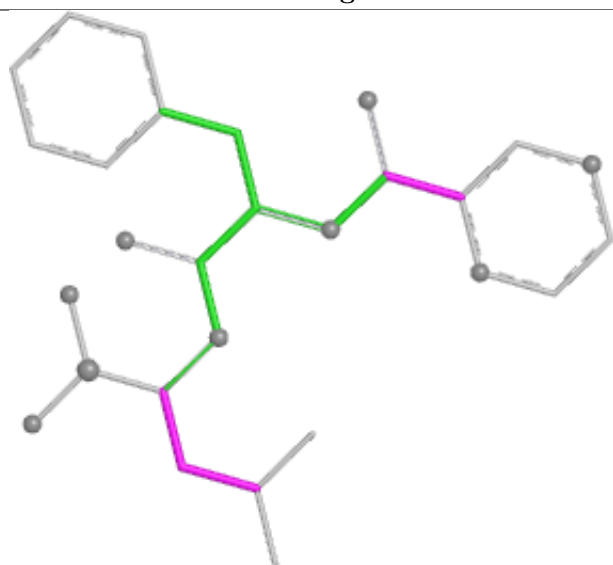
Ligand BO2 H 301



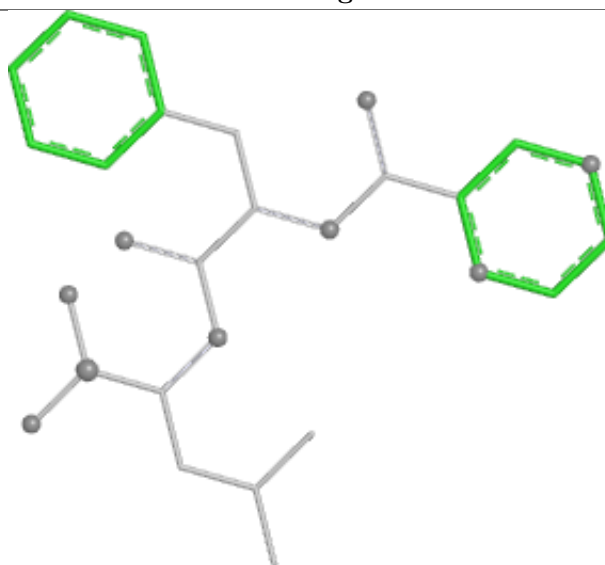
Bond lengths



Bond angles

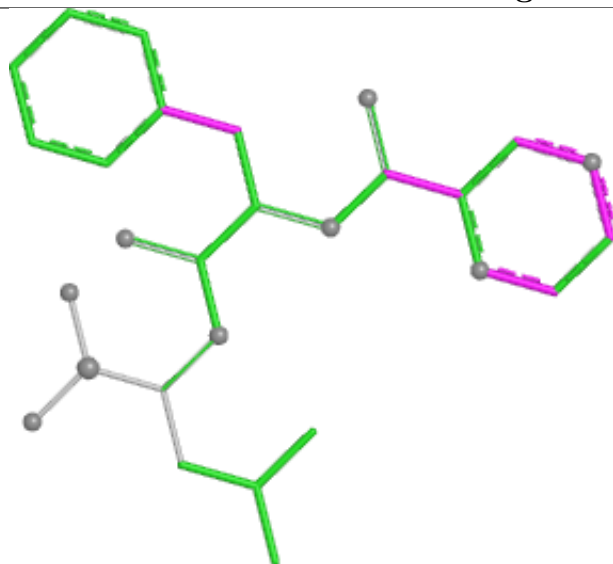


Torsions

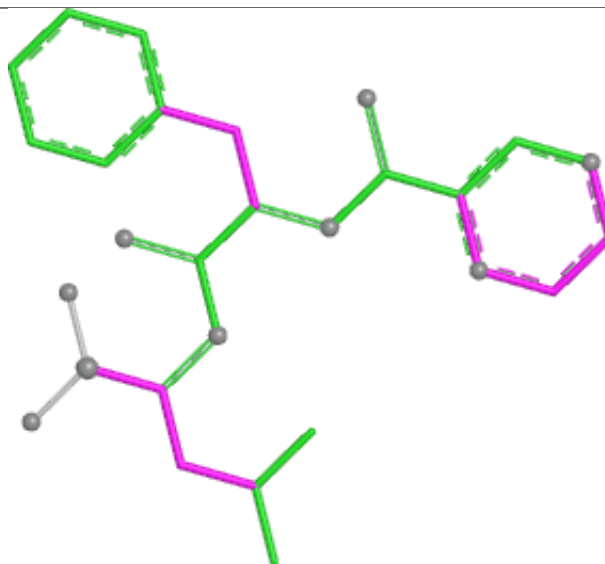


Rings

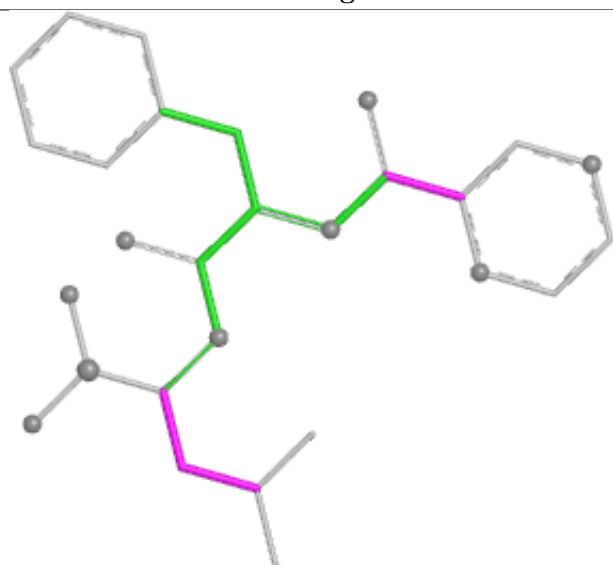
Ligand BO2 V 301



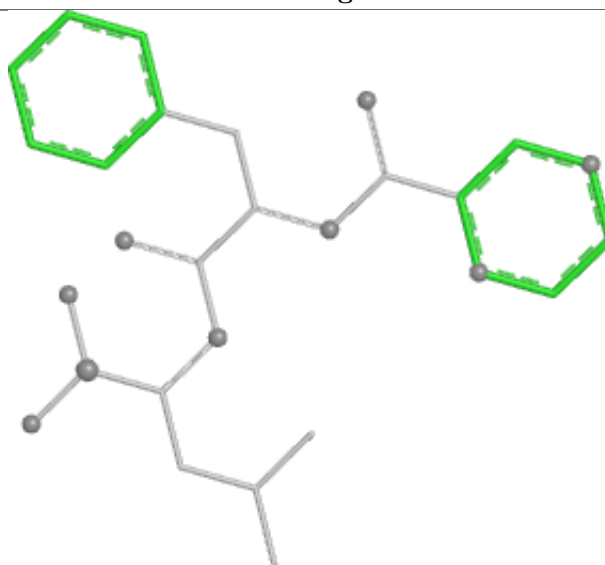
Bond lengths



Bond angles

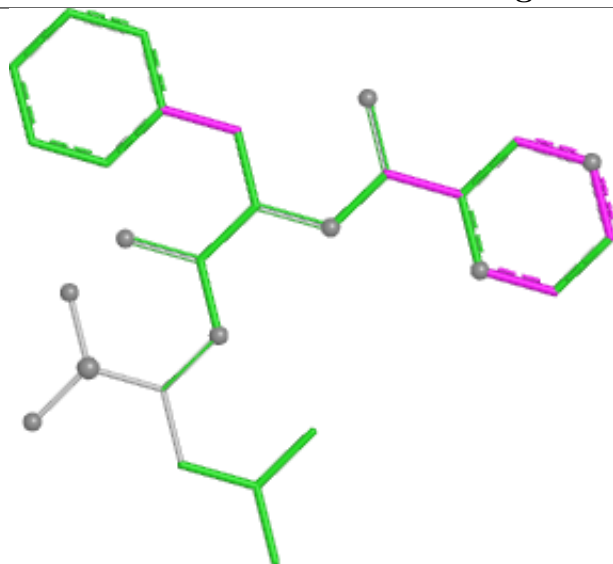


Torsions

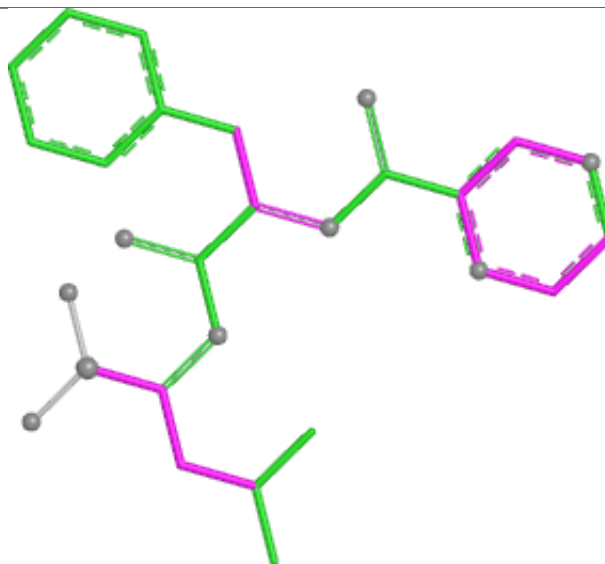


Rings

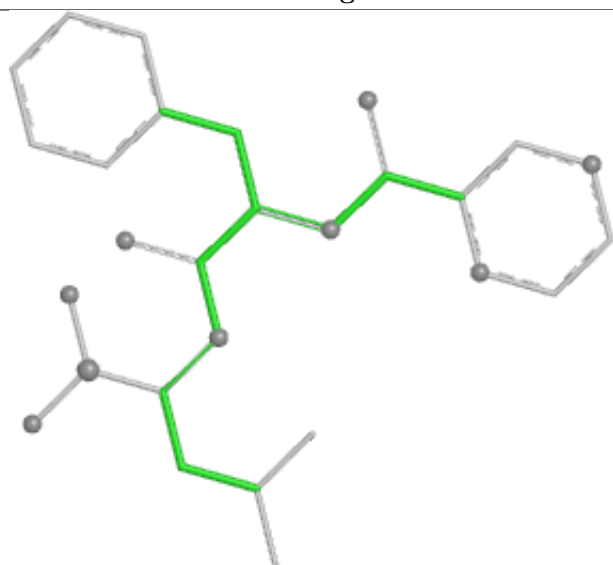
Ligand BO2 K 301



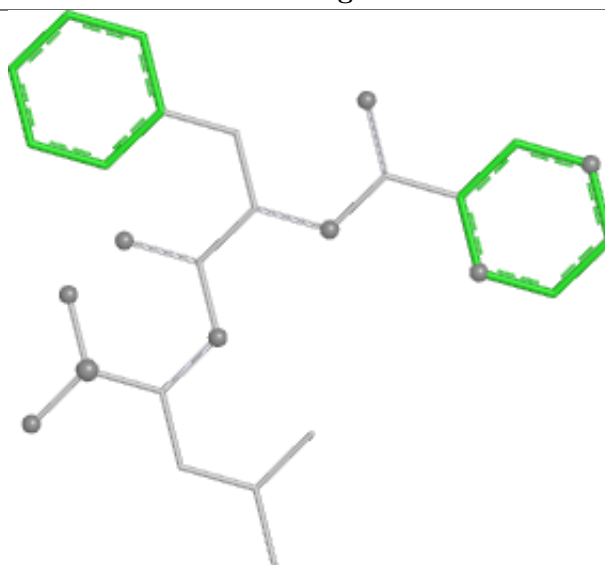
Bond lengths



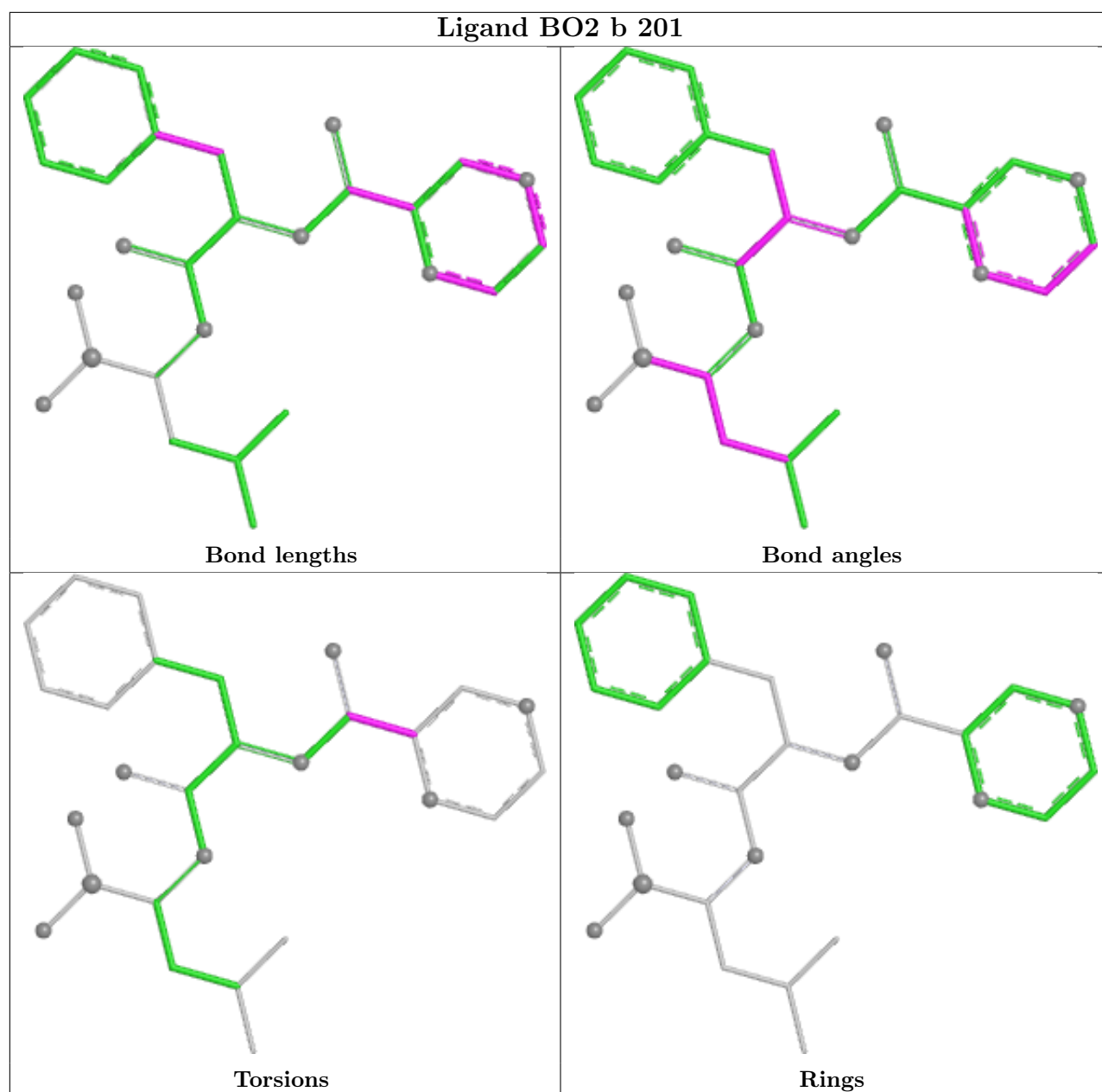
Bond angles



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%)	-0.00	3 (1%) 76 68	39, 54, 91, 133	0
1	O	250/250 (100%)	-0.16	4 (1%) 70 61	39, 58, 102, 141	0
2	B	244/258 (94%)	0.25	15 (6%) 27 20	40, 60, 102, 153	0
2	P	244/258 (94%)	-0.12	4 (1%) 70 61	43, 62, 101, 144	0
3	C	240/254 (94%)	0.02	10 (4%) 40 32	39, 61, 121, 151	0
3	Q	240/254 (94%)	0.33	12 (5%) 34 26	47, 75, 153, 172	0
4	D	235/260 (90%)	-0.22	3 (1%) 75 66	44, 64, 95, 133	0
4	R	235/260 (90%)	0.57	13 (5%) 30 23	51, 70, 108, 143	0
5	E	231/234 (98%)	0.05	4 (1%) 69 60	45, 66, 106, 147	0
5	S	231/234 (98%)	0.46	18 (7%) 19 14	46, 69, 111, 143	0
6	F	243/288 (84%)	-0.07	4 (1%) 70 61	38, 60, 111, 135	0
6	T	243/288 (84%)	-0.08	8 (3%) 49 39	35, 62, 118, 146	0
7	G	241/252 (95%)	-0.32	0 100 100	37, 55, 94, 151	0
7	U	241/252 (95%)	-0.24	4 (1%) 69 60	37, 53, 88, 135	0
8	H	226/232 (97%)	0.14	12 (5%) 32 24	35, 51, 99, 151	0
8	V	226/232 (97%)	-0.14	2 (0%) 81 74	34, 51, 84, 160	0
9	I	204/205 (99%)	0.04	2 (0%) 79 72	35, 50, 85, 110	0
9	W	204/205 (99%)	-0.41	1 (0%) 87 82	35, 51, 80, 107	0
10	J	195/198 (98%)	0.01	4 (2%) 63 54	37, 53, 82, 127	0
10	X	195/198 (98%)	-0.22	2 (1%) 79 72	39, 55, 83, 127	0
11	K	212/212 (100%)	-0.16	2 (0%) 81 74	35, 53, 89, 107	0
11	Y	212/212 (100%)	0.39	9 (4%) 40 32	38, 55, 93, 111	0
12	L	222/222 (100%)	0.04	16 (7%) 21 16	37, 54, 110, 143	0
12	Z	222/222 (100%)	0.48	21 (9%) 14 10	31, 53, 112, 145	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.33	1 (0%) 88 84	34, 52, 74, 91	0
13	a	233/246 (94%)	-0.32	2 (0%) 81 74	32, 49, 72, 88	0
14	N	196/196 (100%)	-0.49	2 (1%) 79 72	34, 46, 75, 97	0
14	b	196/196 (100%)	-0.51	1 (0%) 87 82	33, 46, 77, 108	0
All	All	6344/6614 (95%)	-0.03	179 (2%) 55 45	31, 57, 101, 172	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	L	174	TYR	7.8
12	Z	174	TYR	7.2
10	X	1	MET	6.2
12	Z	169	LYS	5.3
12	L	156	PHE	5.3
12	Z	168	VAL	5.0
12	Z	162	PRO	5.0
10	J	1	MET	5.0
3	Q	205	ALA	5.0
12	Z	170	LYS	4.9
11	Y	208	ASN	4.8
12	L	170	LYS	4.7
12	L	165	ASN	4.7
12	L	169	LYS	4.7
2	B	218	GLY	4.7
12	Z	163	GLY	4.5
3	Q	50	LEU	4.3
12	Z	165	ASN	4.2
12	Z	175	LEU	4.2
12	Z	172	LEU	4.1
12	Z	171	PRO	4.0
6	F	215	CYS	3.9
6	T	243	ILE	3.9
12	L	168	VAL	3.9
12	L	171	PRO	3.7
11	K	208	ASN	3.6
12	Z	156	PHE	3.5
12	L	172	LEU	3.5
12	Z	154	VAL	3.5
4	R	214	ILE	3.4
6	T	205	GLU	3.4
3	Q	49	THR	3.4

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Mol	Chain	Res	Type	RSRZ
5	S	228	ALA	3.4
8	H	223	ILE	3.4
12	L	175	LEU	3.2
8	H	206	PRO	3.2
12	Z	157	LYS	3.2
11	Y	132	GLY	3.2
5	S	52	ALA	3.2
13	a	1	THR	3.2
12	L	163	GLY	3.1
4	R	233	LYS	3.1
3	Q	204	GLY	3.1
12	L	162	PRO	3.1
11	Y	206	SER	3.1
1	O	1	MET	3.0
12	Z	167	LYS	3.0
5	S	222	THR	3.0
13	M	1	THR	3.0
4	R	141	ALA	2.9
9	W	1	SER	2.9
12	Z	173	LYS	2.9
6	F	178	HIS	2.9
4	R	240	ALA	2.9
12	Z	164	THR	2.9
2	P	222	GLY	2.8
8	H	215	GLU	2.8
8	H	210	THR	2.8
5	S	231	LYS	2.7
14	N	103	ASP	2.7
5	S	173	ARG	2.7
8	V	223	ILE	2.7
8	H	207	ARG	2.7
1	A	183	LEU	2.7
2	B	222	GLY	2.7
2	B	51	VAL	2.7
4	R	231	LEU	2.7
11	Y	177	LEU	2.7
6	T	204	LYS	2.7
6	T	178	HIS	2.6
11	Y	104	TYR	2.6
3	C	204	GLY	2.6
5	S	55	LEU	2.6
1	O	249	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	205	ALA	2.6
2	B	239	VAL	2.6
3	Q	234	ILE	2.6
5	E	233	ILE	2.6
12	Z	159	GLN	2.6
5	S	212	ILE	2.6
12	Z	153	GLN	2.6
12	Z	161	GLU	2.6
2	B	198	LYS	2.5
7	U	179	LYS	2.5
2	B	231	PRO	2.5
4	R	170	GLY	2.5
10	J	163	LEU	2.5
6	T	201	GLU	2.5
2	B	220	ASN	2.5
8	H	217	ILE	2.5
4	R	239	GLU	2.5
2	B	244	THR	2.5
6	F	202	ASP	2.4
3	C	240	GLU	2.4
3	Q	240	GLU	2.4
1	A	249	ALA	2.4
2	B	54	THR	2.4
5	S	171	LEU	2.4
9	I	192	ASP	2.4
2	B	242	GLY	2.4
6	F	59	LYS	2.4
5	S	174	THR	2.4
12	L	167	LYS	2.4
1	O	2	THR	2.4
5	S	210	LEU	2.4
11	Y	148	LEU	2.4
2	B	243	ILE	2.4
12	Z	152	ASN	2.4
6	T	206	LYS	2.4
12	L	173	LYS	2.4
3	Q	184	ALA	2.4
5	S	207	VAL	2.3
12	L	136	CYS	2.3
11	Y	209	ASN	2.3
5	S	163	ARG	2.3
12	L	154	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
5	S	227	GLU	2.3
4	R	224	ASP	2.3
5	S	205	LEU	2.3
8	H	212	VAL	2.3
4	D	241	ALA	2.3
2	B	205	LEU	2.3
4	R	183	LEU	2.2
1	O	53	SER	2.2
8	H	216	SER	2.2
12	Z	160	TYR	2.2
3	Q	238	LYS	2.2
2	P	58	GLN	2.2
5	S	182	ASP	2.2
7	U	183	ASP	2.2
2	P	51	VAL	2.2
3	C	224	SER	2.2
3	Q	51	LYS	2.2
4	D	240	ALA	2.2
5	S	233	ILE	2.2
10	X	11	ASP	2.2
2	B	52	THR	2.2
3	C	52	LEU	2.2
4	D	242	GLU	2.2
4	R	237	GLU	2.2
8	H	211	ALA	2.2
8	H	196	ARG	2.2
1	A	54	PRO	2.2
3	C	51	LYS	2.2
3	Q	206	LYS	2.2
5	S	232	TYR	2.2
13	a	69	ASP	2.1
14	N	107	LYS	2.1
14	b	107	LYS	2.1
5	S	200	LEU	2.1
6	T	215	CYS	2.1
5	E	228	ALA	2.1
7	U	182	ILE	2.1
3	C	58	THR	2.1
4	R	238	LYS	2.1
8	V	9	ASN	2.1
8	H	213	LEU	2.1
5	E	181	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
5	E	207	VAL	2.1
3	C	207	ASN	2.1
10	J	143	LEU	2.1
2	P	218	GLY	2.1
11	Y	189	GLY	2.1
2	B	241	THR	2.1
11	K	147	ASP	2.1
12	L	164	THR	2.1
3	Q	239	GLN	2.0
4	R	113	LEU	2.0
9	I	152	LEU	2.0
4	R	241	ALA	2.0
2	B	235	LYS	2.0
6	T	59	LYS	2.0
7	U	184	HIS	2.0
10	J	146	HIS	2.0
11	Y	139	VAL	2.0
3	C	203	THR	2.0
3	Q	3	ASP	2.0
8	H	199	LYS	2.0
3	C	231	VAL	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 [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($\text{\AA}^2$)	Q<0.9
17	BO2	b	201	28/28	0.91	0.11	38,46,54,55	0
15	MG	V	302	1/1	0.92	0.11	62,62,62,62	0

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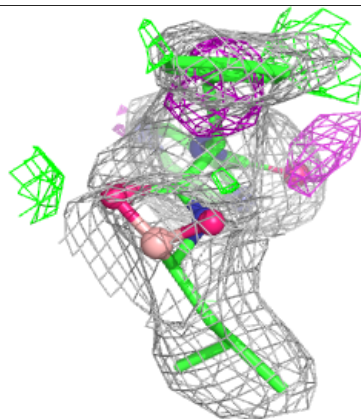
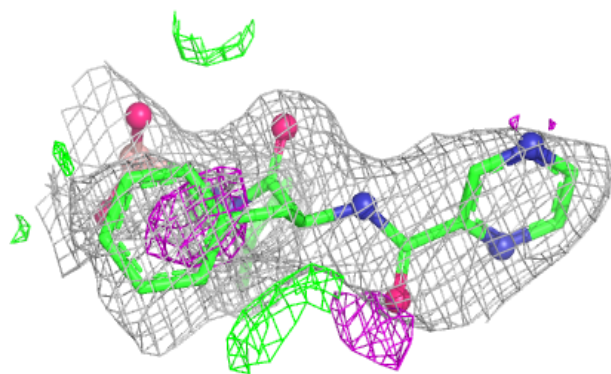
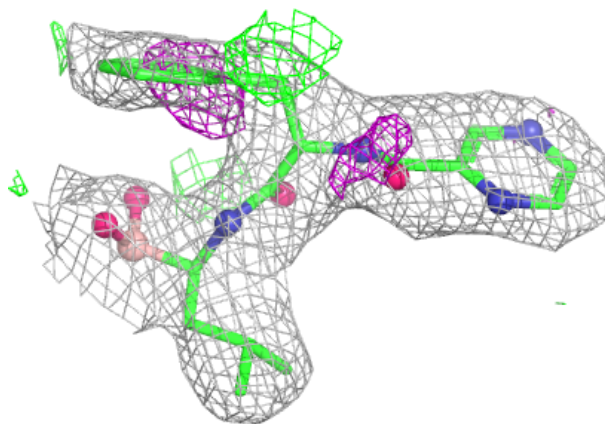
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	BO2	H	301	28/28	0.92	0.11	45,52,74,76	0
17	BO2	N	201	28/28	0.92	0.10	32,41,51,52	0
17	BO2	Y	301	28/28	0.92	0.10	42,52,67,68	0
15	MG	I	301	1/1	0.92	0.12	63,63,63,63	0
17	BO2	V	301	28/28	0.93	0.10	44,49,73,77	0
15	MG	K	302	1/1	0.94	0.07	55,55,55,55	0
17	BO2	K	301	28/28	0.94	0.08	38,47,61,63	0
15	MG	K	303	1/1	0.95	0.08	45,45,45,45	0
15	MG	Y	302	1/1	0.97	0.07	52,52,52,52	0
16	CL	G	302	1/1	0.97	0.05	43,43,43,43	0
15	MG	J	201	1/1	0.98	0.11	42,42,42,42	0
15	MG	G	301	1/1	0.99	0.02	51,51,51,51	0
16	CL	N	203	1/1	0.99	0.07	41,41,41,41	0
16	CL	U	301	1/1	0.99	0.07	38,38,38,38	0
16	CL	b	202	1/1	0.99	0.09	43,43,43,43	0
15	MG	N	202	1/1	0.99	0.02	39,39,39,39	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.

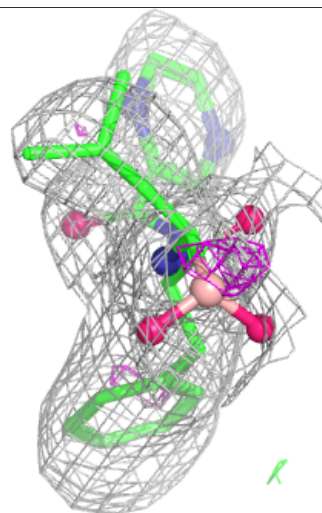
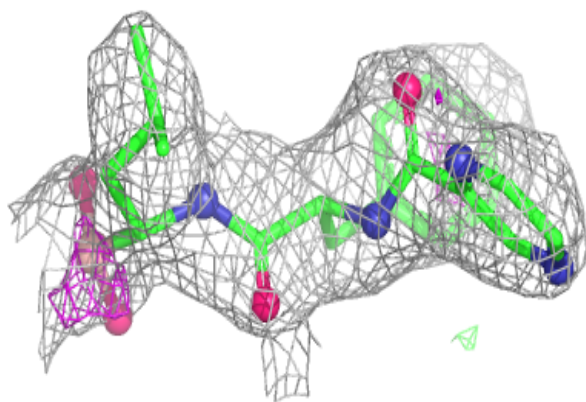
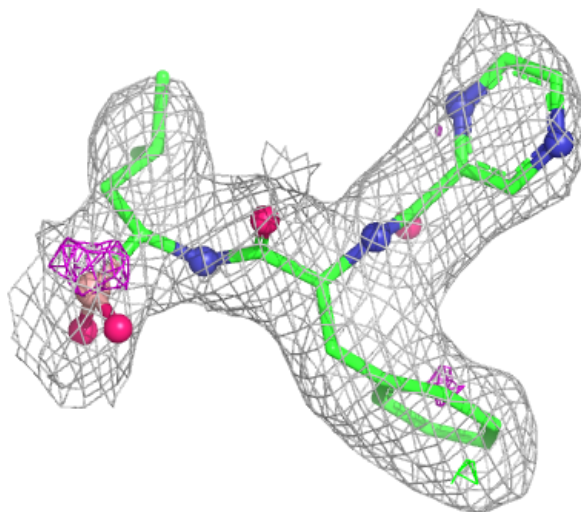
Electron density around BO2 b 201:

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



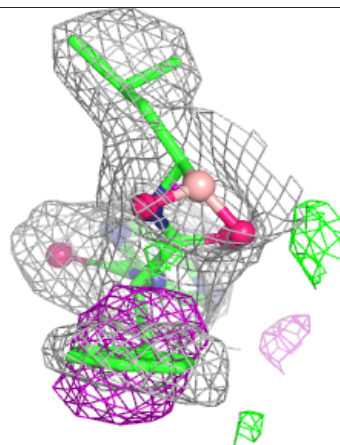
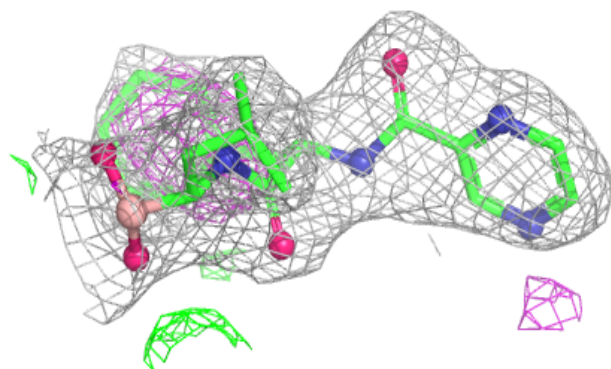
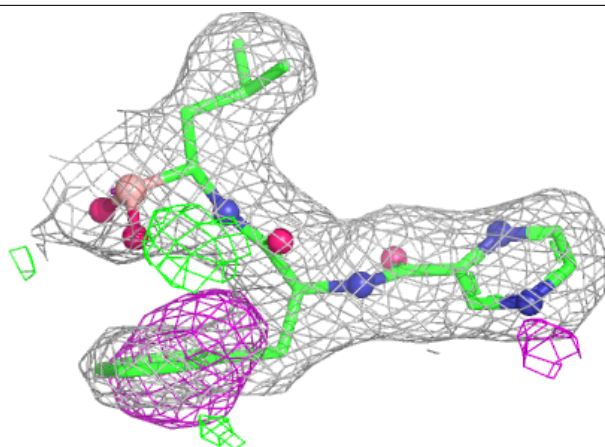
Electron density around BO2 H 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



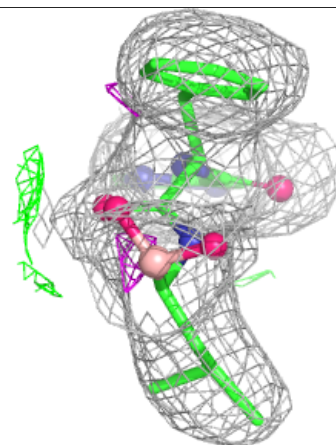
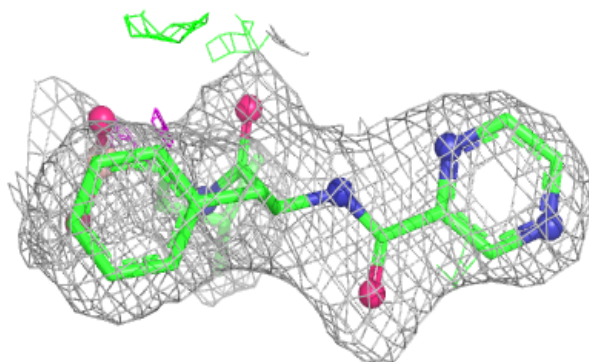
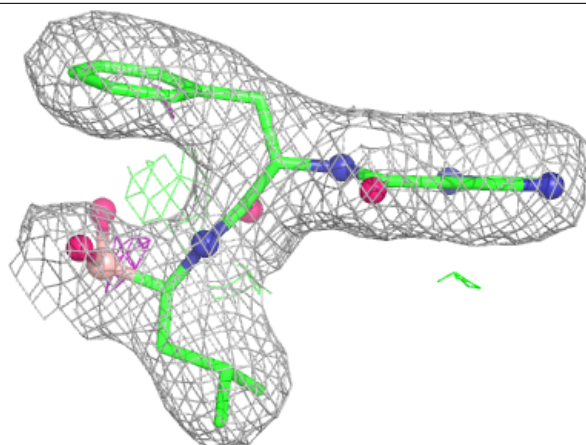
Electron density around BO2 N 201:

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



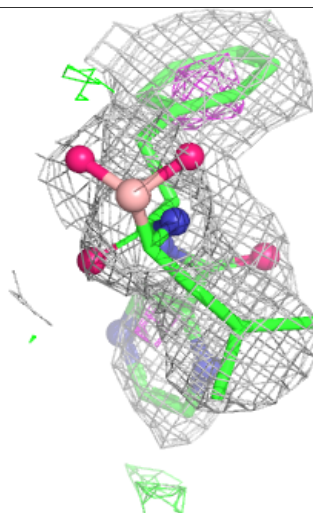
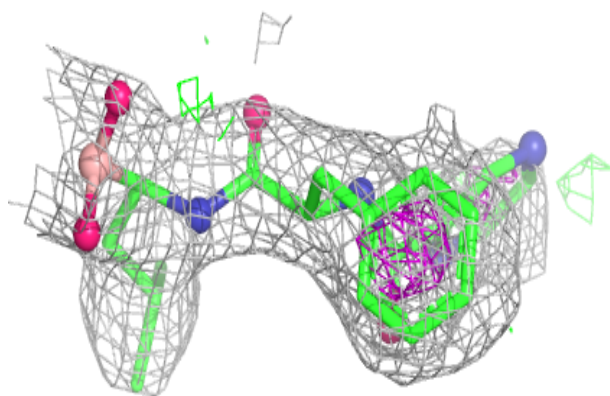
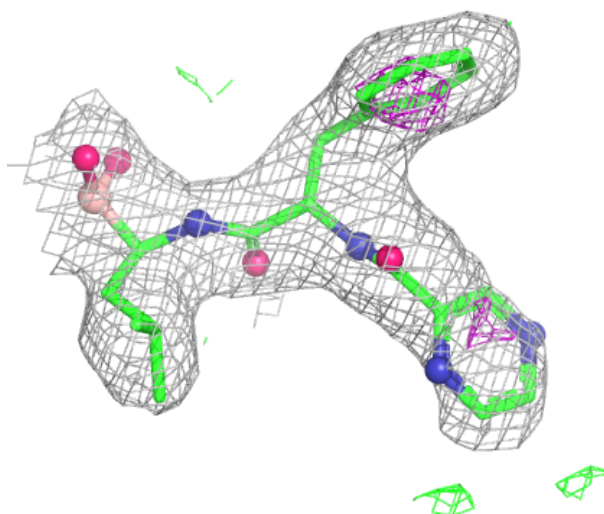
Electron density around BO2 Y 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



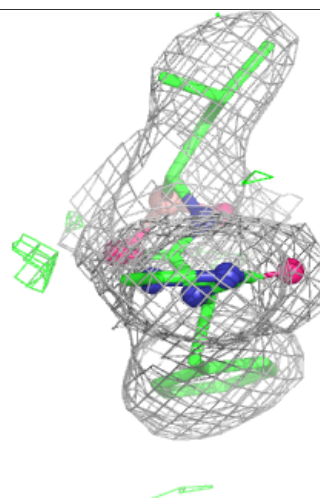
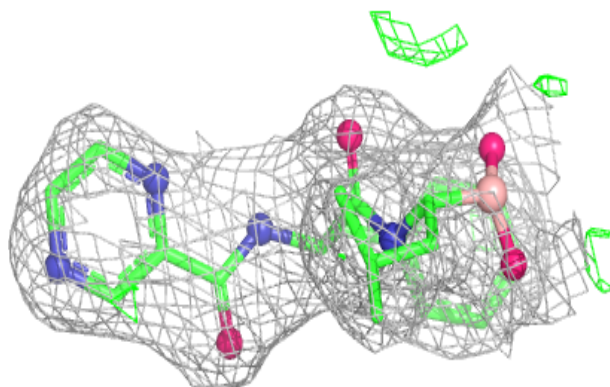
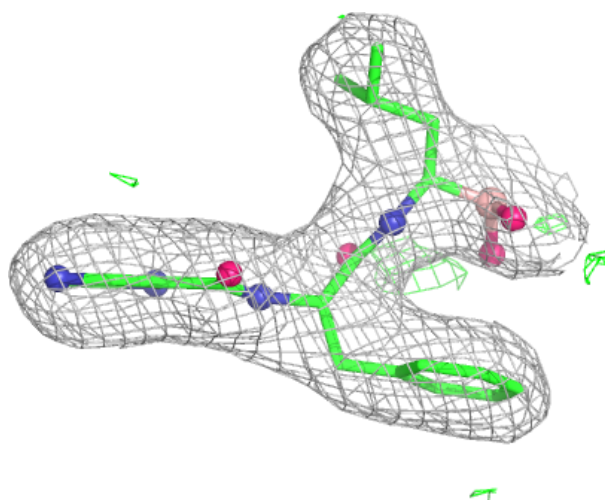
Electron density around BO2 V 301:

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



Electron density around BO2 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.