Full wwPDB X-ray Structure Validation Report (i)

Oct 8, 2023 – 07:31 AM EDT

PDB ID	:	4QVM
Title	:	yCP beta5-M45A mutant 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 (i) 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 (i)) were used in the production of this report:

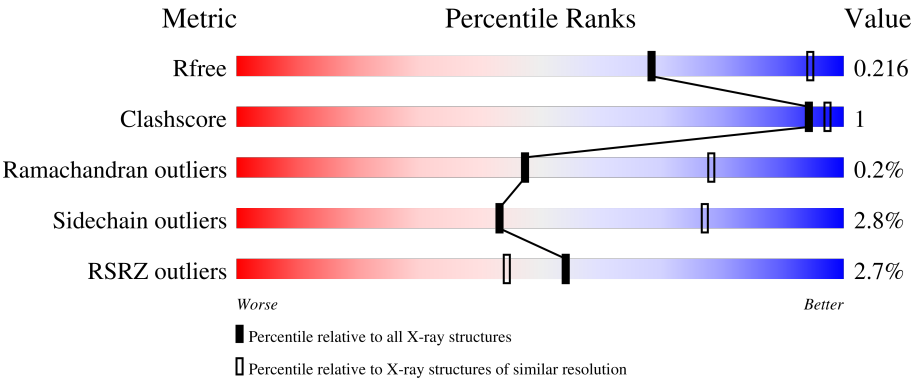
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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.



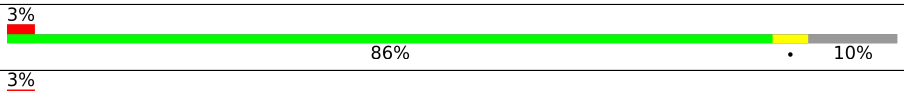
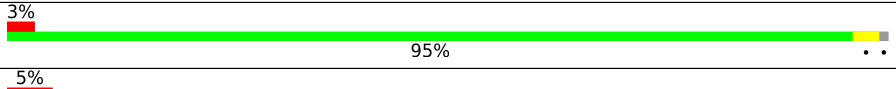
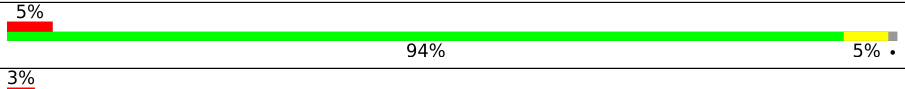
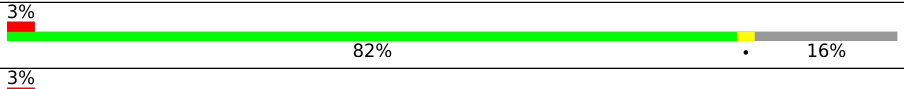
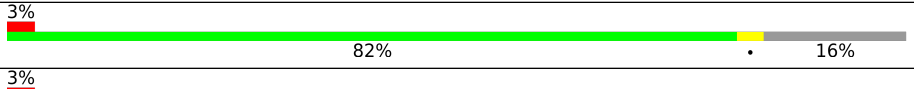
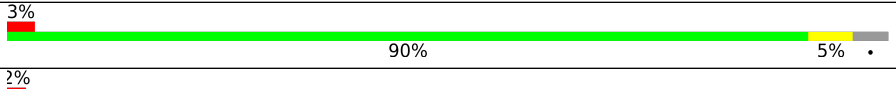
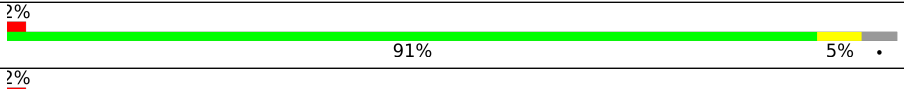
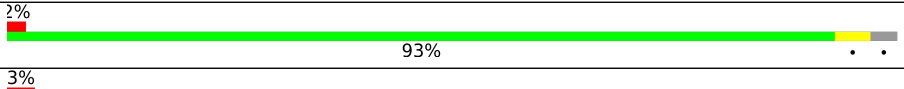
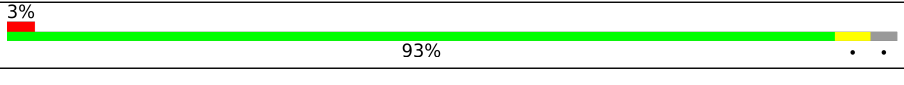
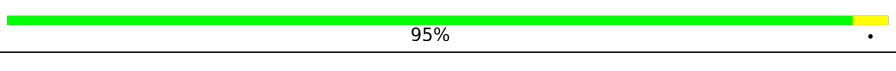
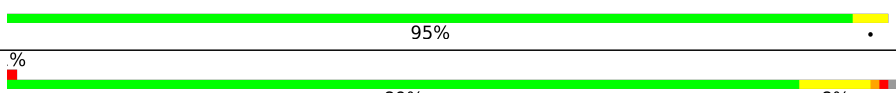
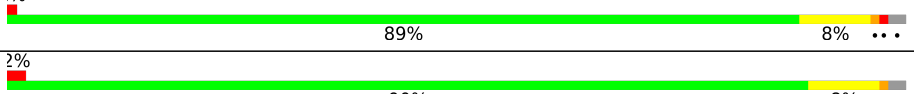
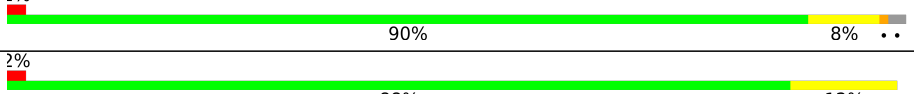
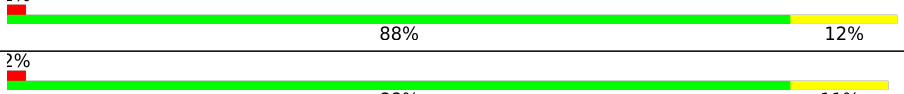
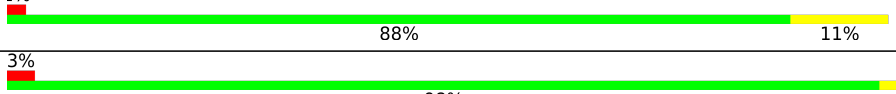
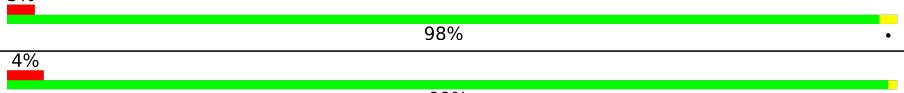
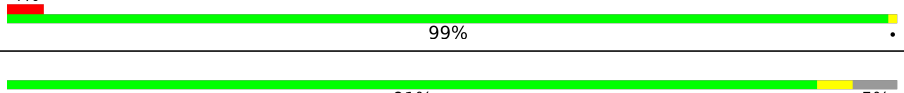
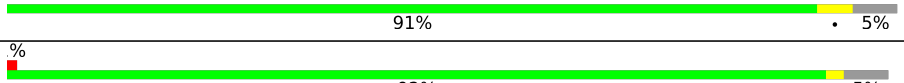
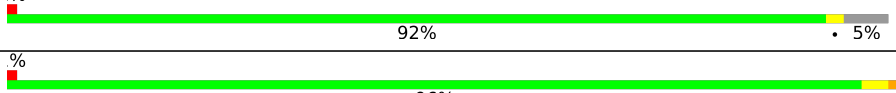
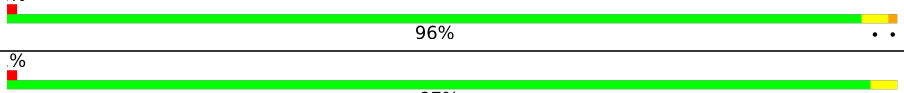
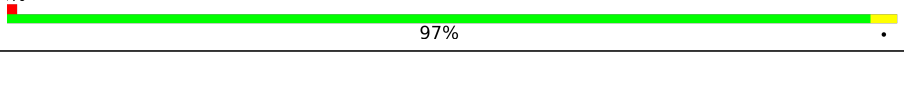
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	3% 98% ·
1	O	250	4% 98% ·
2	B	258	4% 90% · 5%
2	P	258	3% 90% 5% 5%
3	C	254	6% 87% 6% · 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 (i)

There are 18 unique types of molecules in this entry. The entry contains 49872 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
			1641	1043	280	312	6			
11	Y	212	Total	C	N	O	S	0	0	0
			1641	1043	280	312	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	45	ALA	MET	engineered mutation	UNP P30656
Y	45	ALA	MET	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			

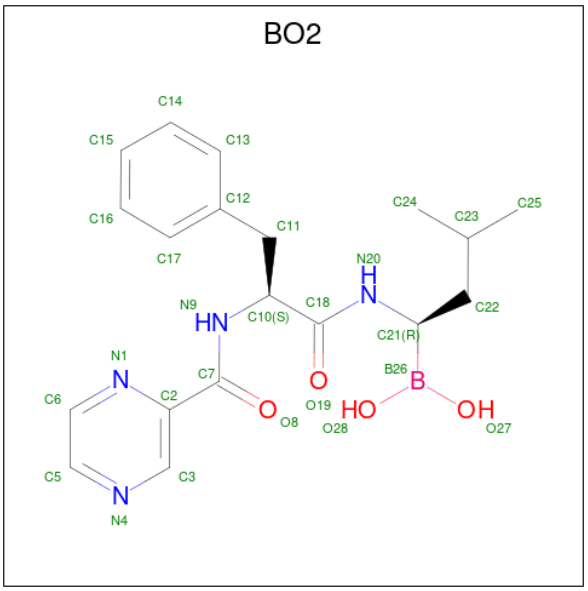
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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
15	Z	1	Total Mg 1 1	0	0

- Molecule 16 is CHLORIDE ION (three-letter code: 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 (three-letter code: BO2) (formula: $C_{19}H_{25}BN_4O_4$).



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	9	Total	O	0	0
			9	9		
18	B	16	Total	O	0	0
			16	16		
18	C	8	Total	O	0	0
			8	8		
18	D	2	Total	O	0	0
			2	2		
18	E	3	Total	O	0	0
			3	3		
18	F	13	Total	O	0	0
			13	13		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	G	12	Total O 12 12	0	0
18	H	19	Total O 19 19	0	0
18	I	12	Total O 12 12	0	0
18	J	13	Total O 13 13	0	0
18	K	14	Total O 14 14	0	0
18	L	17	Total O 17 17	0	0
18	M	21	Total O 21 21	0	0
18	N	7	Total O 7 7	0	0
18	O	7	Total O 7 7	0	0
18	P	8	Total O 8 8	0	0
18	Q	12	Total O 12 12	0	0
18	R	8	Total O 8 8	0	0
18	S	7	Total O 7 7	0	0
18	T	6	Total O 6 6	0	0
18	U	16	Total O 16 16	0	0
18	V	19	Total O 19 19	0	0
18	W	8	Total O 8 8	0	0
18	X	12	Total O 12 12	0	0
18	Y	18	Total O 18 18	0	0
18	Z	17	Total O 17 17	0	0
18	a	19	Total O 19 19	0	0

Continued on next page...

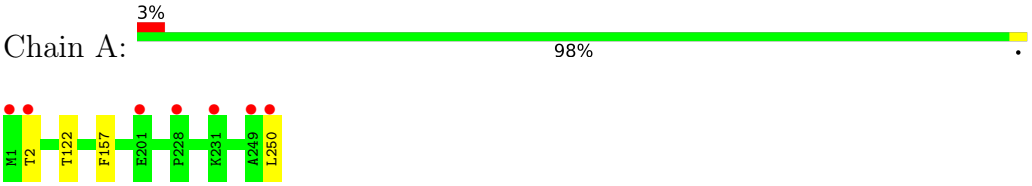
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	b	8	Total O 8 8	0	0

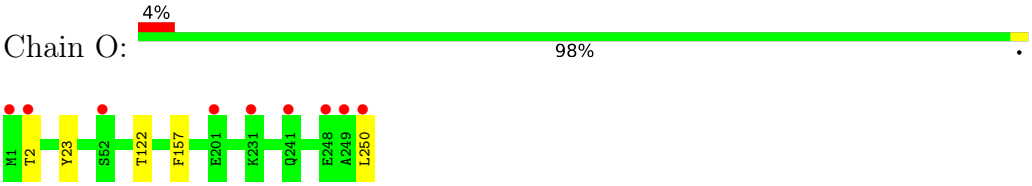
3 Residue-property plots (i)

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.

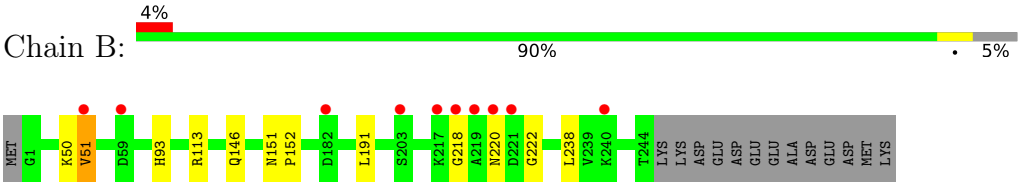
• Molecule 1: Proteasome subunit alpha type-2



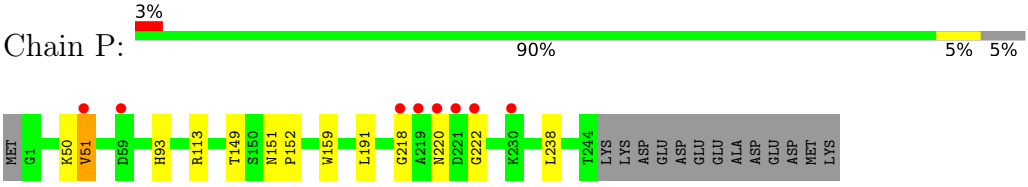
• Molecule 1: Proteasome subunit alpha type-2



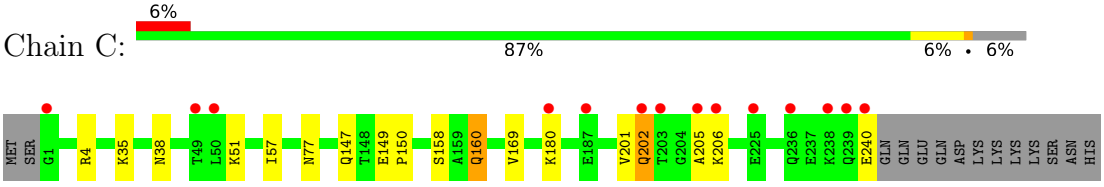
• Molecule 2: Proteasome subunit alpha type-3



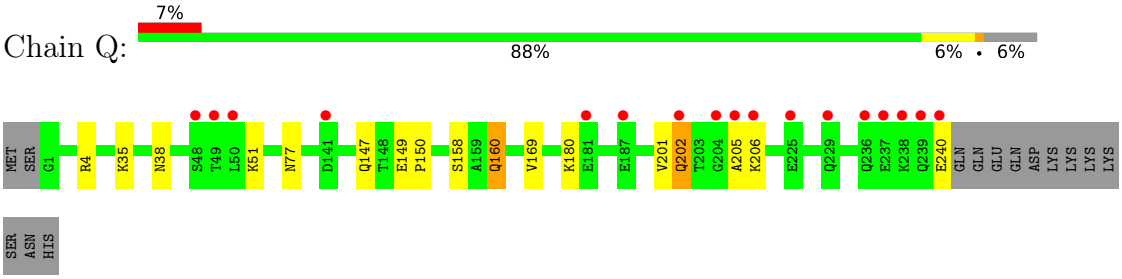
• Molecule 2: Proteasome subunit alpha type-3



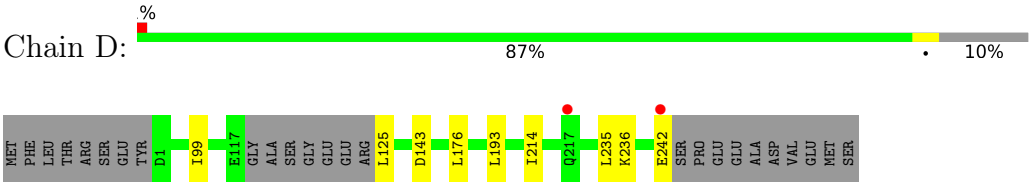
• Molecule 3: Proteasome subunit alpha type-4



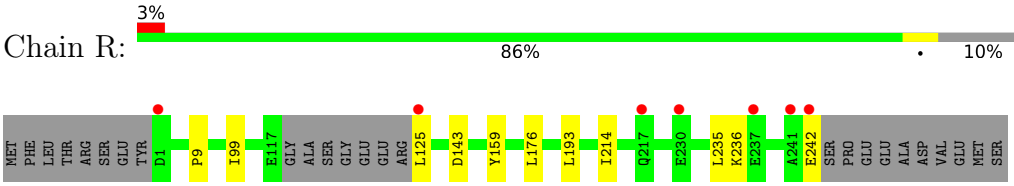
• Molecule 3: Proteasome subunit alpha type-4



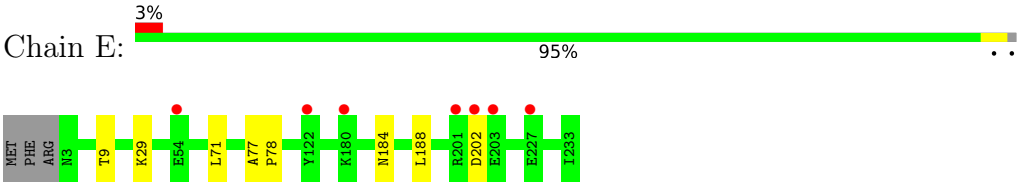
• Molecule 4: Proteasome subunit alpha type-5



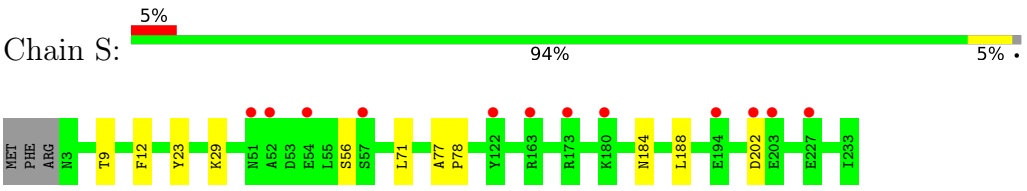
• Molecule 4: Proteasome subunit alpha type-5



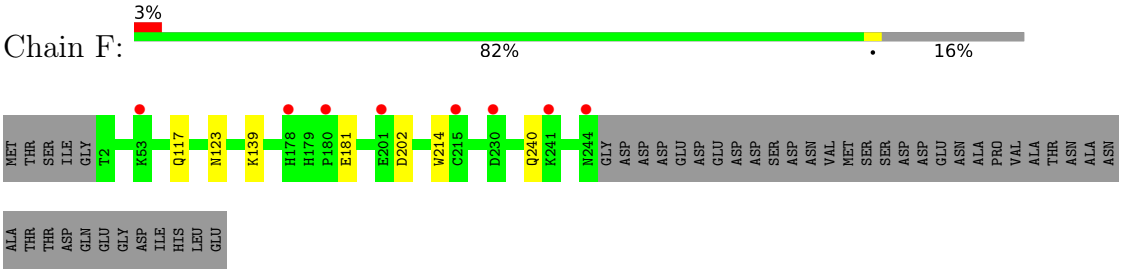
• Molecule 5: Proteasome subunit alpha type-6



• Molecule 5: Proteasome subunit alpha type-6

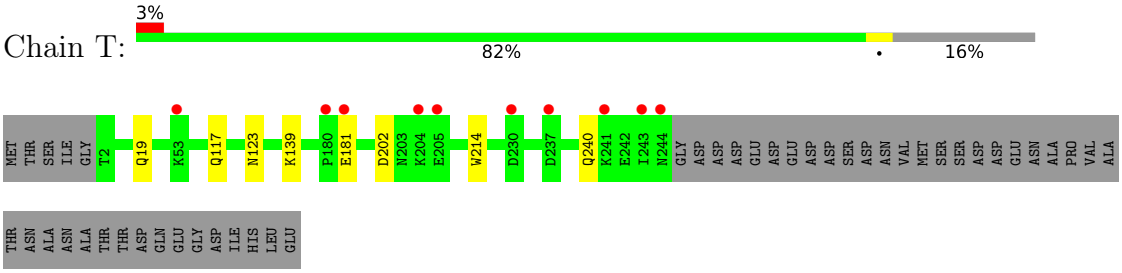


• Molecule 6: Probable proteasome subunit alpha type-7



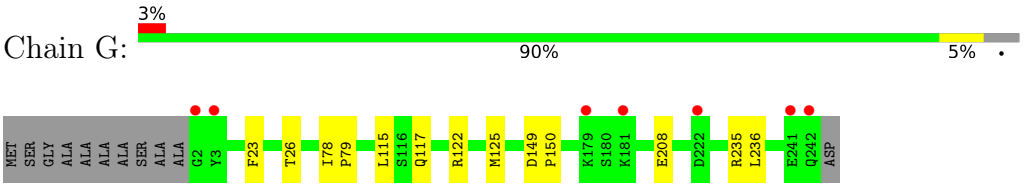
• Molecule 6: Probable proteasome subunit alpha type-7

Chain T:



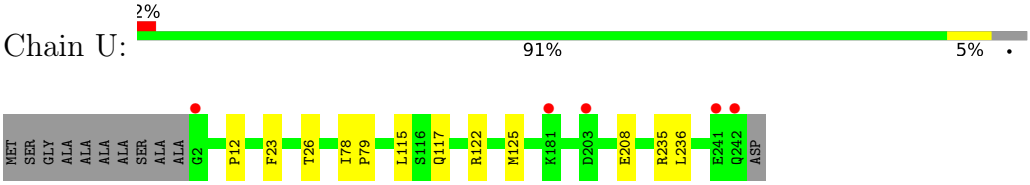
• Molecule 7: Proteasome subunit alpha type-1

Chain G:



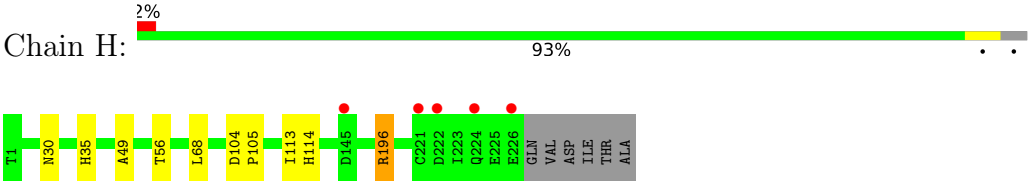
• Molecule 7: Proteasome subunit alpha type-1

Chain U:



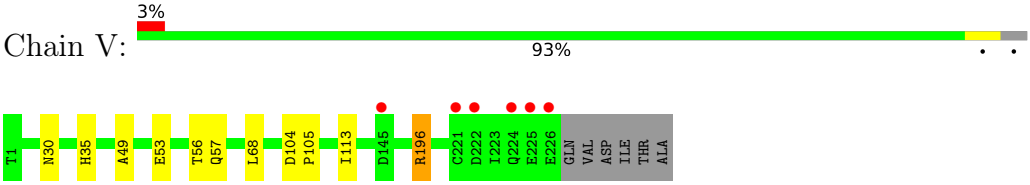
• Molecule 8: Proteasome subunit beta type-2

Chain H:



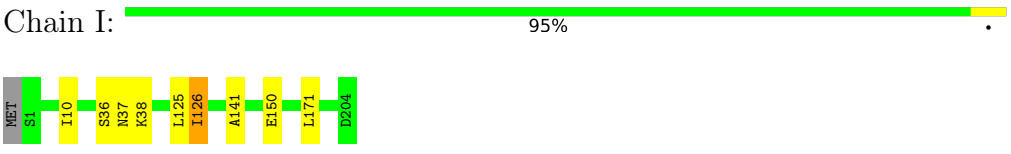
• Molecule 8: Proteasome subunit beta type-2

Chain V:



• Molecule 9: Proteasome subunit beta type-3

Chain I:

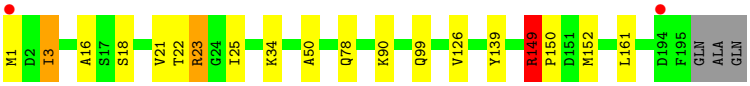


• Molecule 9: Proteasome subunit beta type-3

Chain W:

• Molecule 10: Proteasome subunit beta type-4

Chain J:

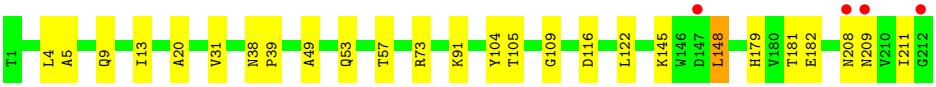


• Molecule 10: Proteasome subunit beta type-4

Chain X:

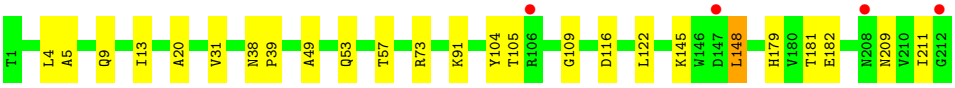
• Molecule 11: Proteasome subunit beta type-5

Chain K:



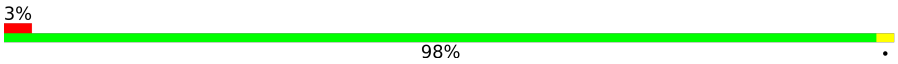
• Molecule 11: Proteasome subunit beta type-5

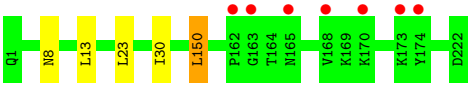
Chain Y:



• Molecule 12: Proteasome subunit beta type-6

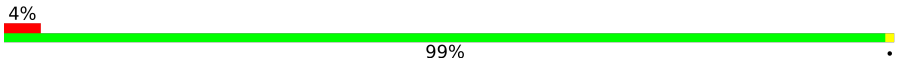
Chain L:

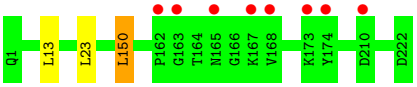




• Molecule 12: Proteasome subunit beta type-6

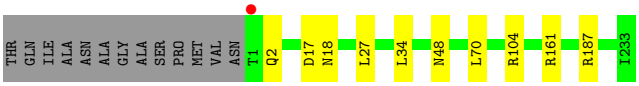
Chain Z:





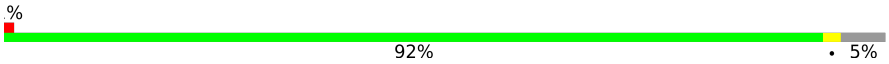
• Molecule 13: Proteasome subunit beta type-7

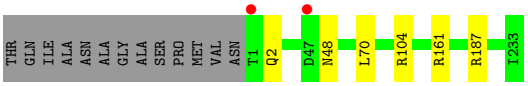
Chain M:



• Molecule 13: Proteasome subunit beta type-7

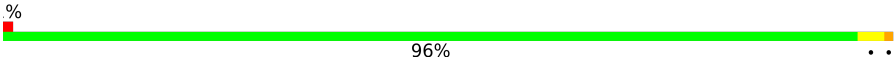
Chain a:

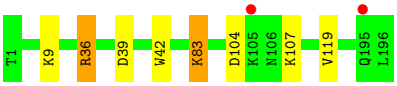




• Molecule 14: Proteasome subunit beta type-1

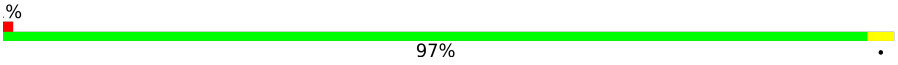
Chain N:

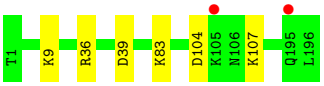




• Molecule 14: Proteasome subunit beta type-1

Chain b:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	136.89Å 299.88Å 145.90Å 90.00° 112.96° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (15.00-2.80) 97.0 (15.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.81 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.187 , 0.215 0.192 , 0.216	Depositor DCC
R_{free} test set	12767 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	61.9	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 38.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	49872	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, CL, BO2

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.27	0/1952	0.46	0/2642
1	O	0.27	0/1952	0.46	0/2642
2	B	0.27	0/1934	0.49	0/2618
2	P	0.27	0/1934	0.49	0/2618
3	C	0.27	0/1910	0.50	0/2586
3	Q	0.27	0/1910	0.50	0/2586
4	D	0.26	0/1837	0.47	0/2475
4	R	0.26	0/1837	0.46	0/2475
5	E	0.27	0/1800	0.46	0/2433
5	S	0.27	0/1800	0.46	0/2433
6	F	0.27	0/1932	0.44	0/2609
6	T	0.27	0/1932	0.44	0/2609
7	G	0.27	0/1945	0.46	0/2634
7	U	0.27	0/1945	0.46	0/2634
8	H	0.25	0/1750	0.46	0/2373
8	V	0.25	0/1750	0.46	0/2373
9	I	0.27	0/1611	0.47	0/2174
9	W	0.27	0/1611	0.48	0/2174
10	J	0.39	1/1589 (0.1%)	0.52	1/2142 (0.0%)
10	X	0.36	0/1589	0.48	0/2142
11	K	0.29	0/1678	0.50	0/2271
11	Y	0.29	0/1678	0.50	0/2271
12	L	0.27	0/1795	0.47	0/2420
12	Z	0.27	0/1795	0.47	0/2420
13	M	0.27	0/1855	0.50	0/2514
13	a	0.27	0/1855	0.50	0/2514
14	N	0.25	0/1541	0.46	0/2087
14	b	0.25	0/1541	0.46	0/2087
All	All	0.28	1/50258 (0.0%)	0.47	1/67956 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	150	PRO	N-CD	5.12	1.55	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	149	ARG	C-N-CD	5.74	140.45	128.40

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	1	0
2	B	1904	0	1904	5	0
2	P	1904	0	1904	6	0
3	C	1881	0	1895	6	0
3	Q	1881	0	1895	5	0
4	D	1813	0	1797	0	0
4	R	1813	0	1797	2	0
5	E	1773	0	1775	1	0
5	S	1773	0	1775	4	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	2	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	3	0
8	H	1719	0	1718	7	0
8	V	1719	0	1718	7	0
9	I	1581	0	1574	5	0
9	W	1581	0	1574	5	0
10	J	1561	0	1569	15	0
10	X	1561	0	1569	15	0
11	K	1641	0	1590	24	0
11	Y	1641	0	1590	22	0
12	L	1757	0	1711	2	0
12	Z	1757	0	1711	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	1824	0	1832	2	0
13	a	1824	0	1832	0	0
14	N	1512	0	1480	2	0
14	b	1512	0	1480	0	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
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	1	0
17	K	28	0	25	1	0
17	N	28	0	25	1	0
17	V	28	0	25	1	0
17	Y	28	0	25	2	0
17	b	28	0	25	0	0
18	A	9	0	0	0	0
18	B	16	0	0	1	0
18	C	8	0	0	0	0
18	D	2	0	0	0	0
18	E	3	0	0	0	0
18	F	13	0	0	0	0
18	G	12	0	0	0	0
18	H	19	0	0	0	0
18	I	12	0	0	0	0
18	J	13	0	0	0	0
18	K	14	0	0	0	0
18	L	17	0	0	0	0
18	M	21	0	0	0	0
18	N	7	0	0	0	0
18	O	7	0	0	0	0
18	P	8	0	0	1	0
18	Q	12	0	0	0	0
18	R	8	0	0	0	0
18	S	7	0	0	0	0
18	T	6	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	U	16	0	0	0	0
18	V	19	0	0	0	0
18	W	8	0	0	0	0
18	X	12	0	0	0	0
18	Y	18	0	0	1	0
18	Z	17	0	0	0	0
18	a	19	0	0	0	0
18	b	8	0	0	0	0
All	All	49872	0	49266	127	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 (127) 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:104:TYR:CE2	11:K:182:GLU:HA	2.03	0.94
10:X:152:MET:HE3	10:X:156:GLU:HB3	1.50	0.91
11:Y:104:TYR:CE2	11:Y:182:GLU:HA	2.04	0.91
11:K:104:TYR:CD2	11:K:182:GLU:HA	2.05	0.89
11:Y:104:TYR:CD2	11:Y:182:GLU:HA	2.07	0.89
10:J:149:ARG:O	10:J:152:MET:HG3	1.74	0.87
11:K:104:TYR:HE2	11:K:182:GLU:HG3	1.38	0.86
11:Y:104:TYR:HE2	11:Y:182:GLU:HG3	1.49	0.77
11:K:104:TYR:CE2	11:K:182:GLU:HG3	2.19	0.76
11:Y:104:TYR:CE2	11:Y:182:GLU:HG3	2.24	0.72
11:K:73:ARG:NH2	11:K:104:TYR:O	2.23	0.72
11:K:104:TYR:HE2	11:K:182:GLU:HA	1.56	0.69
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.23	0.69
11:Y:53:GLN:O	11:Y:57:THR:HG23	1.96	0.66
11:K:53:GLN:O	11:K:57:THR:HG23	1.98	0.64
10:X:152:MET:HE3	10:X:156:GLU:CB	2.27	0.64
11:Y:104:TYR:HE2	11:Y:182:GLU:HA	1.60	0.63
10:X:149:ARG:O	10:X:152:MET:HG3	2.00	0.61
10:J:22:THR:O	10:J:23:ARG:HD3	2.01	0.60
11:K:104:TYR:CE1	11:K:109:GLY:HA2	2.36	0.60
10:J:149:ARG:HD3	18:Y:403:HOH:O	2.02	0.60
11:K:104:TYR:HE2	11:K:182:GLU:CG	2.15	0.58
11:K:104:TYR:HD2	11:K:182:GLU:HA	1.63	0.58
11:Y:104:TYR:CE1	11:Y:109:GLY:HA2	2.39	0.58
10:J:139:TYR:OH	10:X:25:ILE:O	2.24	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:104:TYR:HD2	11:Y:182:GLU:HA	1.65	0.55
10:J:25:ILE:O	10:X:139:TYR:OH	2.24	0.55
11:K:209:ASN:O	9:W:38:LYS:NZ	2.40	0.54
8:H:196:ARG:NH2	9:I:150:GLU:O	2.41	0.52
9:I:38:LYS:NZ	11:Y:209:ASN:O	2.42	0.52
9:I:125:LEU:HG	9:I:126:ILE:HG22	1.92	0.52
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.92	0.51
9:W:125:LEU:HG	9:W:126:ILE:HG22	1.92	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.51
8:V:196:ARG:NH2	9:W:150:GLU:O	2.43	0.51
8:V:49:ALA:HA	17:V:301:BO2:H241	1.93	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.50
8:H:49:ALA:HA	17:H:301:BO2:H241	1.94	0.50
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.92	0.50
2:P:93:HIS:HB3	18:P:301:HOH:O	2.11	0.50
11:K:104:TYR:HE1	11:K:109:GLY:HA2	1.77	0.50
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.93	0.50
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.94	0.49
10:J:50:ALA:O	11:K:91:LYS:NZ	2.45	0.49
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.45	0.49
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.96	0.48
11:Y:104:TYR:CD1	11:Y:105:THR:N	2.82	0.48
11:Y:104:TYR:HE2	11:Y:182:GLU:CG	2.20	0.48
11:K:208:ASN:HB3	10:X:150:PRO:HD3	1.95	0.48
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.48	0.48
7:G:23:PHE:O	7:G:26:THR:HB	2.14	0.47
10:J:149:ARG:CG	10:J:149:ARG:HH21	2.27	0.47
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.96	0.47
2:B:93:HIS:HB3	18:B:313:HOH:O	2.14	0.47
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.96	0.47
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.50	0.47
11:K:104:TYR:HE2	11:K:182:GLU:CA	2.27	0.46
7:U:23:PHE:O	7:U:26:THR:HB	2.15	0.46
10:J:149:ARG:HG3	10:J:149:ARG:NH2	2.30	0.46
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.99	0.45
10:X:152:MET:HE3	10:X:152:MET:HB3	1.92	0.45
3:C:35:LYS:HG2	3:C:158:SER:O	2.16	0.45
2:P:50:LYS:O	2:P:51:VAL:C	2.55	0.45
2:P:149:THR:HG1	2:P:159:TRP:HE1	1.64	0.45
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.97	0.45
11:Y:104:TYR:HE2	11:Y:182:GLU:CA	2.27	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:LYS:O	2:B:51:VAL:C	2.56	0.44
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.17	0.44
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.83	0.44
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.00	0.44
10:J:25:ILE:O	10:J:25:ILE:HG12	2.18	0.44
8:V:53:GLU:OE2	8:V:57:GLN:NE2	2.43	0.44
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.83	0.43
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.00	0.43
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.99	0.43
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.00	0.43
8:H:35:HIS:CB	8:H:56:THR:HG21	2.48	0.43
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.48	0.43
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.19	0.43
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.99	0.43
11:Y:49:ALA:HB3	17:Y:301:BO2:H3	2.01	0.43
11:K:104:TYR:CD1	11:K:105:THR:N	2.87	0.42
8:V:35:HIS:CB	8:V:56:THR:HG21	2.49	0.42
11:K:208:ASN:CB	10:X:150:PRO:HD3	2.49	0.42
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.49	0.42
2:B:146:GLN:HG2	3:C:57:ILE:HG21	2.01	0.42
2:P:50:LYS:HD3	2:P:50:LYS:HA	1.89	0.42
10:X:25:ILE:O	10:X:25:ILE:HG12	2.18	0.42
11:K:49:ALA:HB3	17:K:301:BO2:H3	2.02	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	2.01	0.42
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.02	0.41
8:H:114:HIS:CD2	17:N:201:BO2:H5	2.55	0.41
11:K:5:ALA:HA	11:K:13:ILE:O	2.20	0.41
4:R:9:PRO:HA	5:S:23:TYR:CD1	2.55	0.41
10:J:3:ILE:HG23	10:J:18:SER:HB3	2.02	0.41
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.55	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	2.02	0.41
11:Y:49:ALA:HA	17:Y:301:BO2:H241	2.02	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.41
11:K:179:HIS:CE1	11:K:181:THR:HG23	2.55	0.41
5:S:12:PHE:H	6:T:19:GLN:HE22	1.68	0.41
11:K:145:LYS:HB2	11:K:148:LEU:HD13	2.02	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:17:ASP:OD1	13:M:18:ASN:N	2.53	0.41
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	2.02	0.41
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.02	0.41
11:Y:179:HIS:CE1	11:Y:181:THR:HG23	2.55	0.41
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.02	0.41
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.51	0.41
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.21	0.41
3:C:201:VAL:O	3:C:202:GLN:HB3	2.19	0.41
10:J:149:ARG:CG	10:J:149:ARG:NH2	2.84	0.41
12:L:8:ASN:HA	12:L:30:ILE:O	2.21	0.41
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.02	0.41
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.51	0.41
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.51	0.41
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.02	0.41
12:L:13:LEU:HD11	12:L:150:LEU:HD21	2.02	0.41
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.51	0.41
6:F:202:ASP:OD1	6:F:202:ASP:N	2.54	0.40
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.51	0.40
6:T:202:ASP:OD1	6:T:202:ASP:N	2.55	0.40
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.52	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%)	241 (97%)	6 (2%)	1 (0%)	34 66
1	O	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	34 66
2	B	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	9 29
2	P	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	9 29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	19 49
3	Q	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	19 49
4	D	231/260 (89%)	229 (99%)	2 (1%)	0	100 100
4	R	231/260 (89%)	229 (99%)	2 (1%)	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%)	238 (99%)	3 (1%)	0	100 100
6	T	241/288 (84%)	237 (98%)	4 (2%)	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%)	195 (96%)	7 (4%)	0	100 100
9	W	202/205 (98%)	195 (96%)	7 (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%)	207 (99%)	3 (1%)	0	100 100
11	Y	210/212 (99%)	207 (99%)	3 (1%)	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%)	224 (97%)	7 (3%)	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%)	6136 (98%)	134 (2%)	14 (0%)	47 78

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
2	P	51	VAL
3	Q	202	GLN
1	A	2	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	218	GLY
2	B	222	GLY
1	O	2	THR
2	P	218	GLY
2	P	222	GLY
2	B	220	ASN
3	C	205	ALA
2	P	220	ASN
3	Q	205	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	206 (99%)	3 (1%)	67	90
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	90
2	B	203/216 (94%)	200 (98%)	3 (2%)	65	89
2	P	203/216 (94%)	200 (98%)	3 (2%)	65	89
3	C	212/226 (94%)	202 (95%)	10 (5%)	26	59
3	Q	212/226 (94%)	202 (95%)	10 (5%)	26	59
4	D	194/215 (90%)	185 (95%)	9 (5%)	27	60
4	R	194/215 (90%)	185 (95%)	9 (5%)	27	60
5	E	190/193 (98%)	184 (97%)	6 (3%)	39	73
5	S	190/193 (98%)	184 (97%)	6 (3%)	39	73
6	F	201/239 (84%)	195 (97%)	6 (3%)	41	75
6	T	201/239 (84%)	195 (97%)	6 (3%)	41	75
7	G	206/210 (98%)	199 (97%)	7 (3%)	37	71
7	U	206/210 (98%)	199 (97%)	7 (3%)	37	71
8	H	185/190 (97%)	181 (98%)	4 (2%)	52	83
8	V	185/190 (97%)	181 (98%)	4 (2%)	52	83
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	87

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	W	172/173 (99%)	169 (98%)	3 (2%)	60 87
10	J	173/175 (99%)	167 (96%)	6 (4%)	36 70
10	X	173/175 (99%)	169 (98%)	4 (2%)	50 82
11	K	168/168 (100%)	163 (97%)	5 (3%)	41 75
11	Y	168/168 (100%)	163 (97%)	5 (3%)	41 75
12	L	185/185 (100%)	183 (99%)	2 (1%)	73 92
12	Z	185/185 (100%)	183 (99%)	2 (1%)	73 92
13	M	199/208 (96%)	193 (97%)	6 (3%)	41 75
13	a	199/208 (96%)	193 (97%)	6 (3%)	41 75
14	N	162/162 (100%)	156 (96%)	6 (4%)	34 68
14	b	162/162 (100%)	156 (96%)	6 (4%)	34 68
All	All	5318/5538 (96%)	5168 (97%)	150 (3%)	43 77

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
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	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	206	LYS
3	C	240	GLU
4	D	99	ILE
4	D	125	LEU
4	D	143	ASP
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	181	GLU
6	F	214	TRP
6	F	240	GLN
7	G	115	LEU
7	G	117	GLN
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
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	3	ILE
10	J	23	ARG
10	J	78	GLN
10	J	90	LYS
10	J	99	GLN
10	J	149	ARG
11	K	4	LEU
11	K	9	GLN
11	K	116	ASP
11	K	148	LEU
11	K	211	ILE
12	L	23	LEU
12	L	150	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	9	LYS
14	N	36	ARG
14	N	39	ASP
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
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	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	206	LYS
3	Q	240	GLU
4	R	99	ILE
4	R	125	LEU
4	R	143	ASP
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	71	LEU
5	S	184	ASN
5	S	188	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	S	202	ASP
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	181	GLU
6	T	214	TRP
6	T	240	GLN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
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	3	ILE
10	X	90	LYS
10	X	99	GLN
10	X	152	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	116	ASP
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	161	ARG
13	a	187	ARG
14	b	9	LYS
14	b	36	ARG
14	b	39	ASP
14	b	83	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	b	104	ASP
14	b	107	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	146	GLN
4	D	210	GLN
4	D	225	ASN
5	E	68	HIS
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
6	F	86	ASN
6	F	117	GLN
6	F	191	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
10	J	55	GLN
11	K	9	GLN
11	K	62	GLN
11	K	85	ASN
11	K	176	ASN
11	K	188	HIS
12	L	3	ASN
12	L	79	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	48	ASN
13	M	102	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	91	HIS
4	R	146	GLN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
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
6	T	191	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
10	X	55	GLN
10	X	146	HIS
11	Y	9	GLN
11	Y	85	ASN
11	Y	176	ASN
11	Y	188	HIS
12	Z	3	ASN
13	a	48	ASN
13	a	102	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 13 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	V	301	8	25,29,29	1.59	5 (20%)	32,38,38	1.44	4 (12%)
17	BO2	K	301	11	25,29,29	1.63	5 (20%)	32,38,38	1.41	3 (9%)
17	BO2	N	201	14	25,29,29	1.58	4 (16%)	32,38,38	1.41	3 (9%)
17	BO2	H	301	8	25,29,29	1.61	5 (20%)	32,38,38	1.44	4 (12%)
17	BO2	b	201	14	25,29,29	1.59	4 (16%)	32,38,38	1.38	3 (9%)
17	BO2	Y	301	11	25,29,29	1.62	5 (20%)	32,38,38	1.41	5 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BO2	V	301	8	-	7/22/28/28	0/2/2/2
17	BO2	K	301	11	-	2/22/28/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BO2	N	201	14	-	4/22/28/28	0/2/2/2
17	BO2	H	301	8	-	7/22/28/28	0/2/2/2
17	BO2	b	201	14	-	4/22/28/28	0/2/2/2
17	BO2	Y	301	11	-	3/22/28/28	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	201	BO2	C2-C7	-4.80	1.38	1.50
17	N	201	BO2	C2-C7	-4.79	1.39	1.50
17	Y	301	BO2	C2-C7	-4.70	1.39	1.50
17	K	301	BO2	C2-C7	-4.66	1.39	1.50
17	H	301	BO2	C2-C7	-4.54	1.39	1.50
17	V	301	BO2	C2-C7	-4.44	1.39	1.50
17	K	301	BO2	C11-C12	-4.43	1.40	1.51
17	b	201	BO2	C11-C12	-4.38	1.40	1.51
17	H	301	BO2	C11-C12	-4.36	1.40	1.51
17	Y	301	BO2	C11-C12	-4.32	1.40	1.51
17	N	201	BO2	C11-C12	-4.27	1.41	1.51
17	V	301	BO2	C11-C12	-4.25	1.41	1.51
17	K	301	BO2	C3-N4	2.86	1.40	1.34
17	Y	301	BO2	C3-N4	2.84	1.40	1.34
17	V	301	BO2	C6-N1	2.82	1.40	1.34
17	H	301	BO2	C6-N1	2.78	1.40	1.34
17	V	301	BO2	C3-N4	2.78	1.40	1.34
17	K	301	BO2	C6-N1	2.77	1.40	1.34
17	H	301	BO2	C3-N4	2.74	1.40	1.34
17	Y	301	BO2	C6-N1	2.72	1.40	1.34
17	N	201	BO2	C3-N4	2.64	1.40	1.34
17	b	201	BO2	C3-N4	2.44	1.39	1.34
17	Y	301	BO2	C5-N4	2.29	1.40	1.33
17	K	301	BO2	C5-N4	2.28	1.40	1.33
17	b	201	BO2	C6-N1	2.28	1.39	1.34
17	N	201	BO2	C6-N1	2.28	1.39	1.34
17	H	301	BO2	C5-N4	2.17	1.40	1.33
17	V	301	BO2	C5-N4	2.17	1.40	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	V	301	BO2	C21-C22-C23	-4.90	109.23	115.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	N	201	BO2	C21-C22-C23	-4.90	109.24	115.39
17	b	201	BO2	C21-C22-C23	-4.85	109.30	115.39
17	H	301	BO2	C21-C22-C23	-4.75	109.43	115.39
17	K	301	BO2	C21-C22-C23	-4.44	109.82	115.39
17	Y	301	BO2	C21-C22-C23	-4.42	109.84	115.39
17	H	301	BO2	C6-N1-C2	3.46	121.42	116.93
17	V	301	BO2	C6-N1-C2	3.42	121.37	116.93
17	Y	301	BO2	C6-N1-C2	3.21	121.09	116.93
17	K	301	BO2	C6-N1-C2	3.20	121.08	116.93
17	N	201	BO2	C6-N1-C2	2.90	120.69	116.93
17	b	201	BO2	C11-C10-N9	-2.76	104.97	110.79
17	N	201	BO2	C11-C10-N9	-2.76	104.98	110.79
17	b	201	BO2	C6-N1-C2	2.62	120.33	116.93
17	Y	301	BO2	C18-C10-N9	-2.48	104.42	111.16
17	K	301	BO2	C18-C10-N9	-2.42	104.57	111.16
17	H	301	BO2	C12-C11-C10	-2.29	107.06	113.39
17	V	301	BO2	C12-C11-C10	-2.25	107.18	113.39
17	V	301	BO2	C6-C5-N4	-2.08	119.35	121.95
17	H	301	BO2	C6-C5-N4	-2.07	119.37	121.95
17	Y	301	BO2	C2-C3-N4	-2.00	119.56	122.05
17	Y	301	BO2	C6-C5-N4	-2.00	119.45	121.95

There are no chirality outliers.

All (27) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	H	301	BO2	C21-C22-C23-C25
17	V	301	BO2	C21-C22-C23-C25
17	K	301	BO2	C3-C2-C7-N9
17	Y	301	BO2	C3-C2-C7-N9
17	V	301	BO2	N9-C10-C18-O19
17	K	301	BO2	C3-C2-C7-O8
17	Y	301	BO2	C3-C2-C7-O8
17	H	301	BO2	N9-C10-C18-O19
17	H	301	BO2	C21-C22-C23-C24
17	V	301	BO2	C21-C22-C23-C24
17	Y	301	BO2	N20-C21-C22-C23

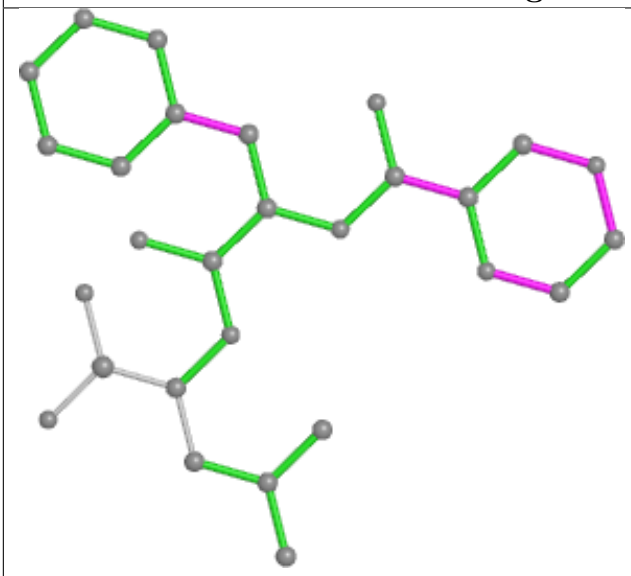
There are no ring outliers.

5 monomers are involved in 6 short contacts:

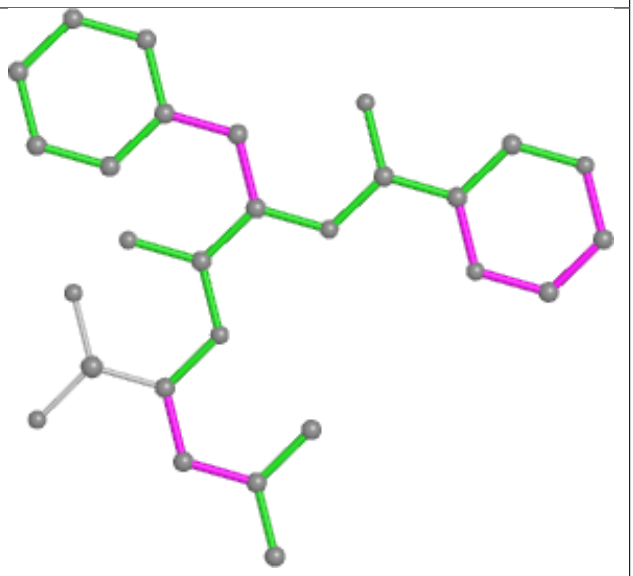
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	V	301	BO2	1	0
17	K	301	BO2	1	0
17	N	201	BO2	1	0
17	H	301	BO2	1	0
17	Y	301	BO2	2	0

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

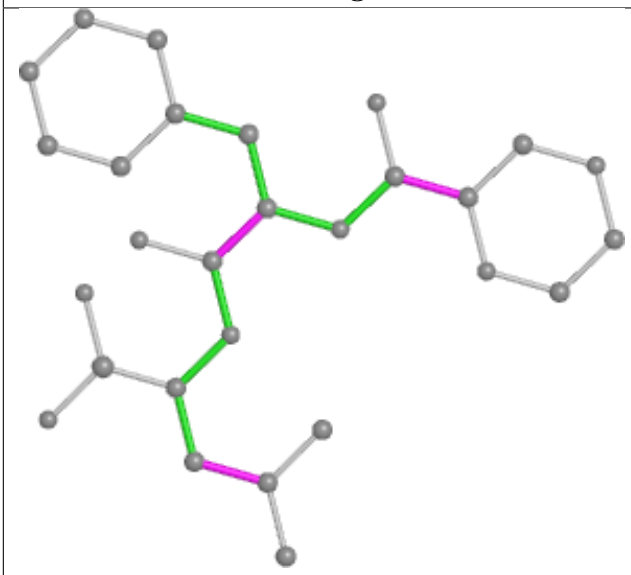
Ligand BO2 V 301



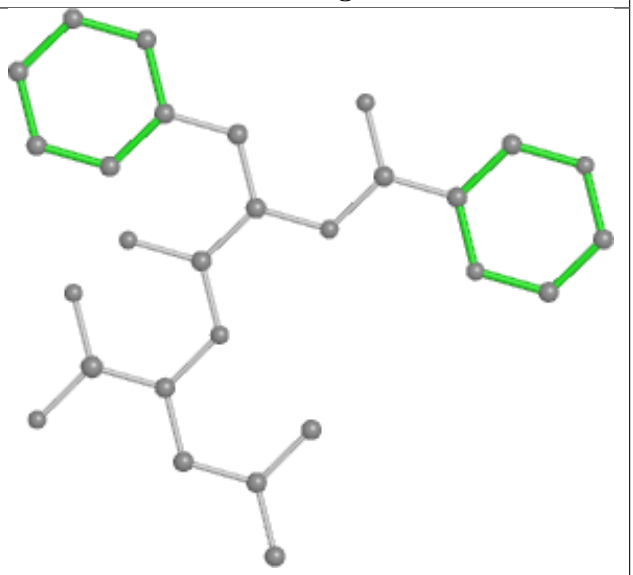
Bond lengths



Bond angles

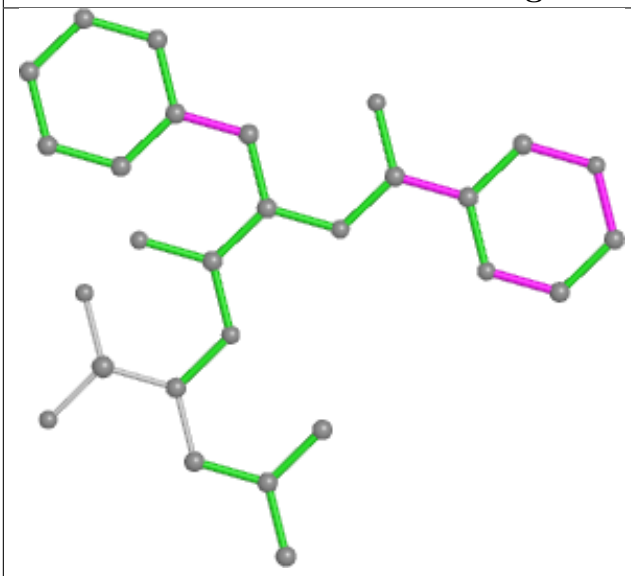


Torsions

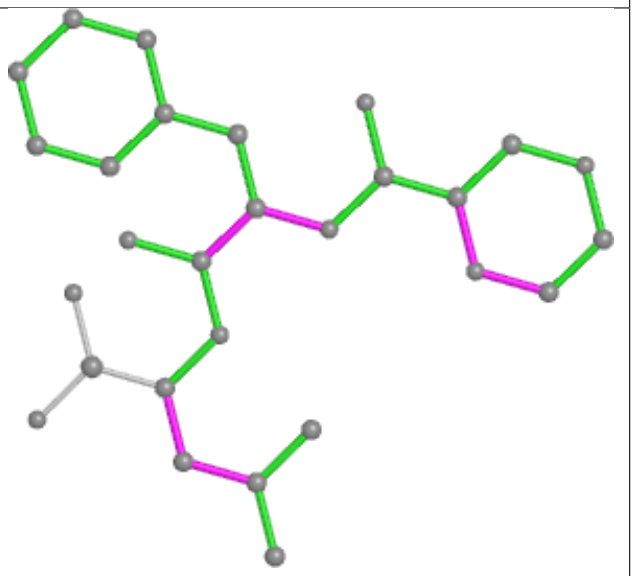


Rings

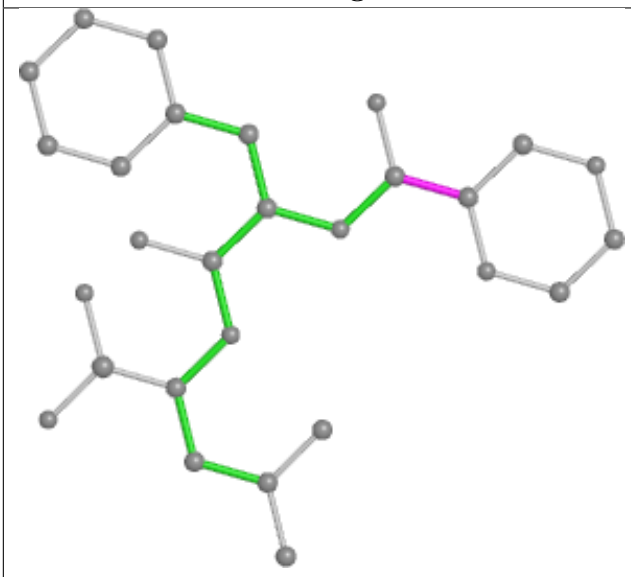
Ligand BO2 K 301



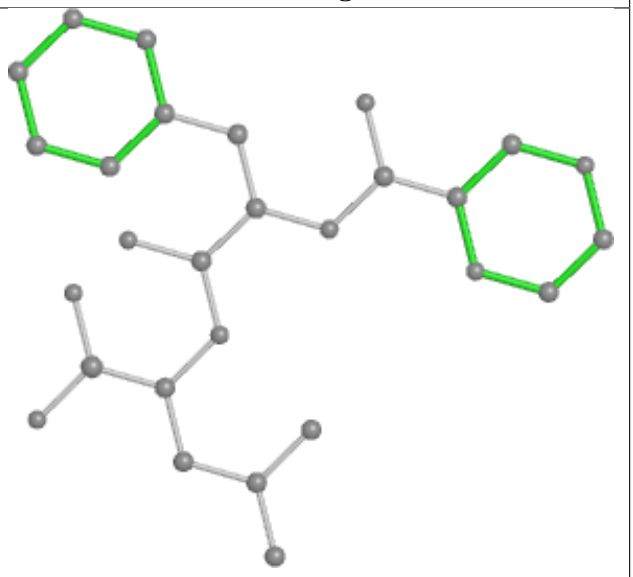
Bond lengths



Bond angles

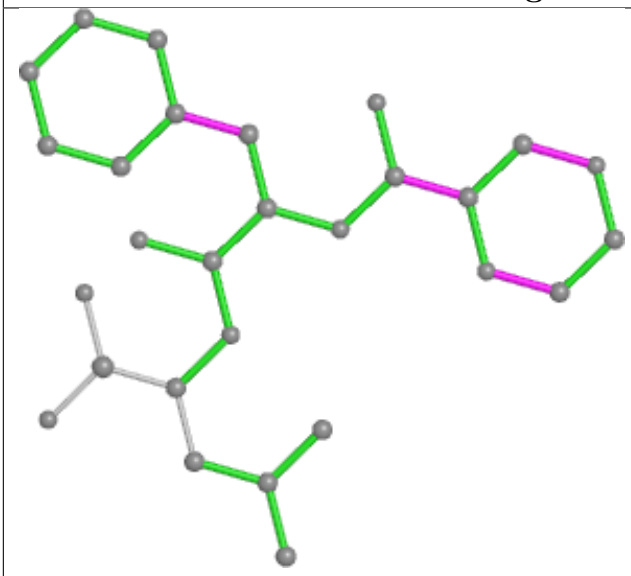


Torsions

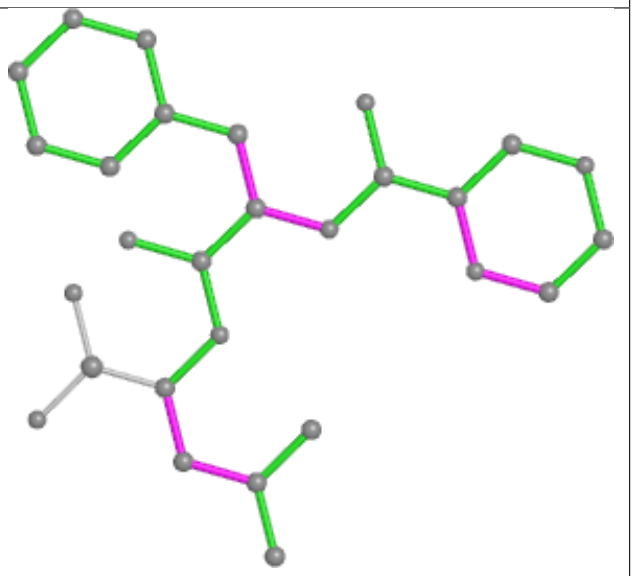


Rings

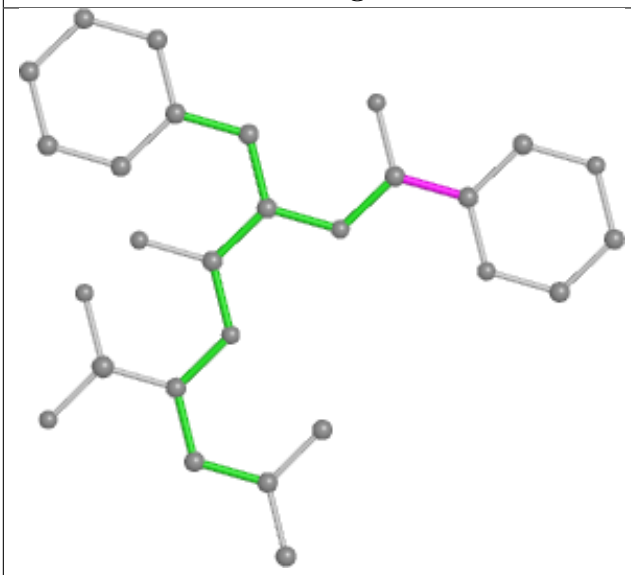
Ligand BO2 N 201



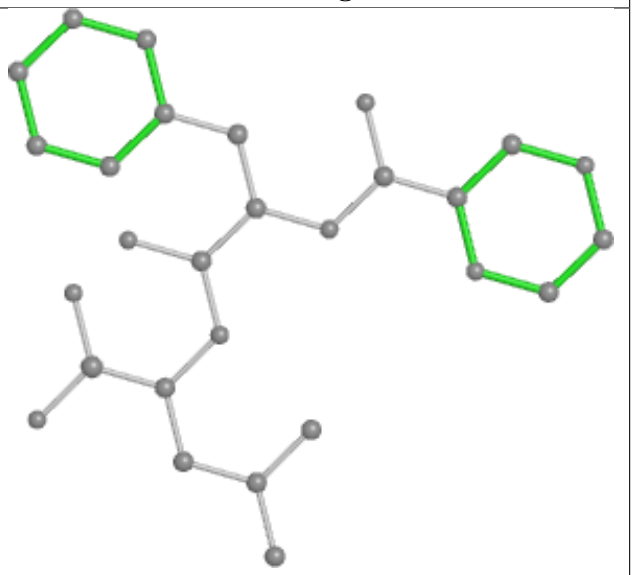
Bond lengths



Bond angles

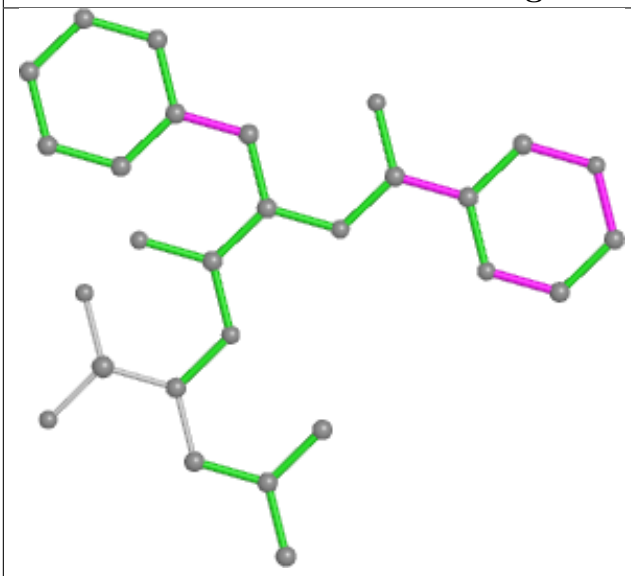


Torsions

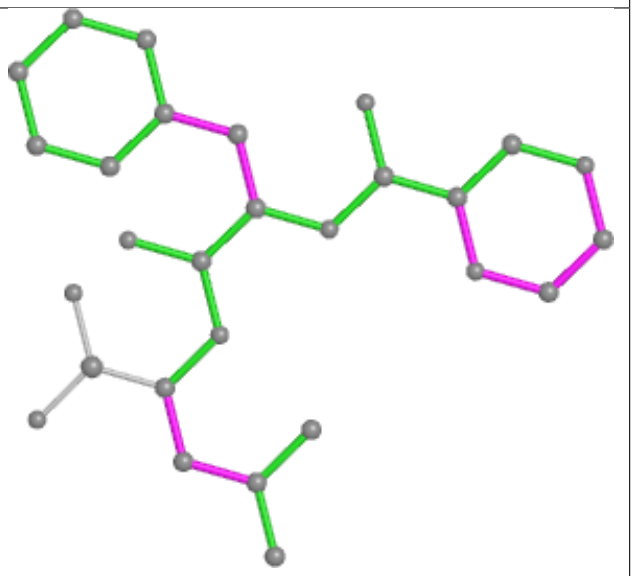


Rings

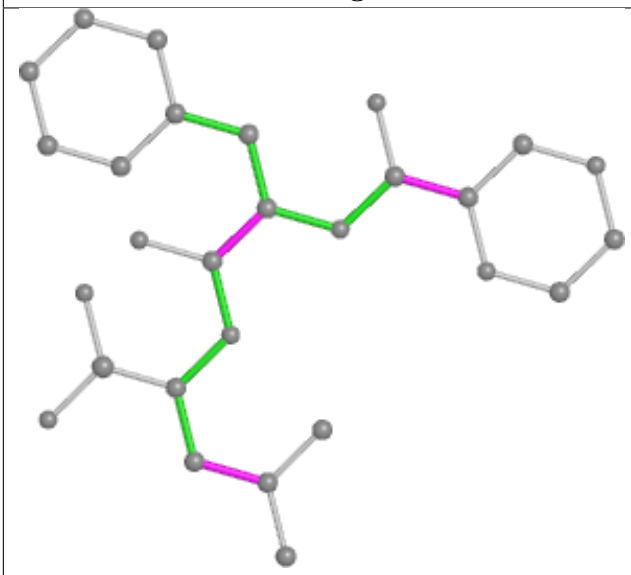
Ligand BO2 H 301



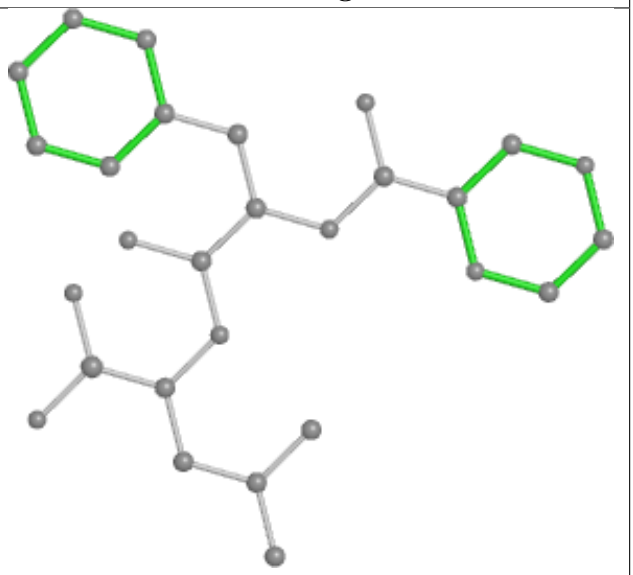
Bond lengths



Bond angles

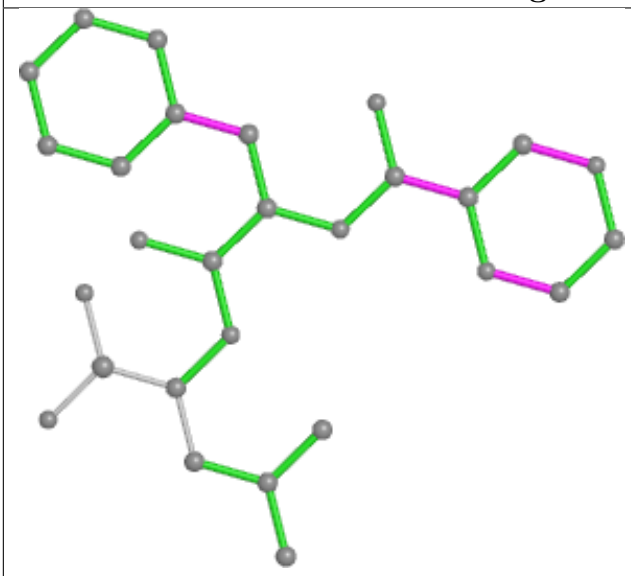


Torsions

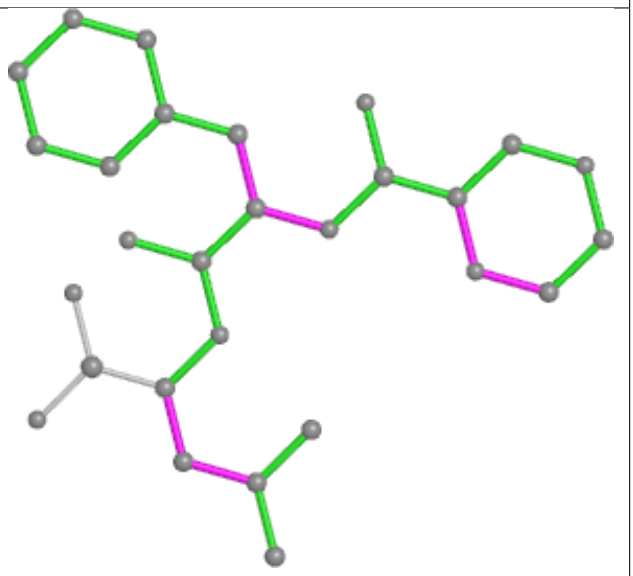


Rings

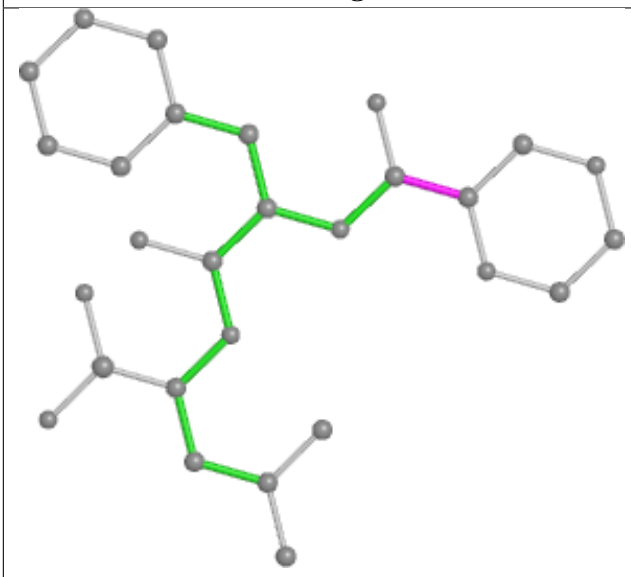
Ligand BO2 b 201



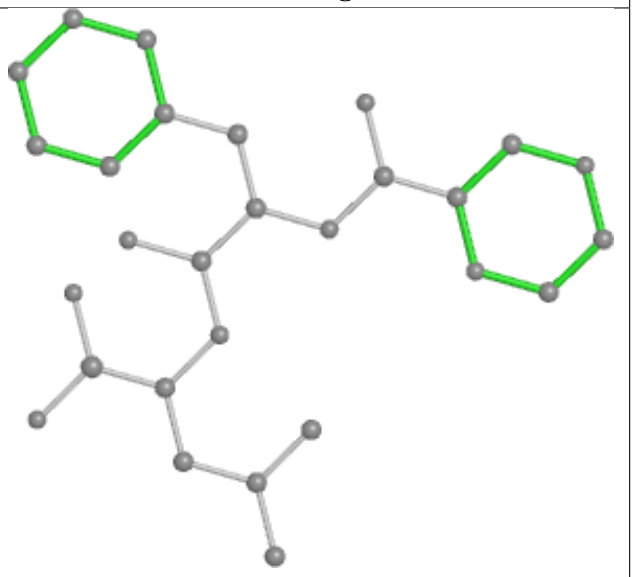
Bond lengths



Bond angles

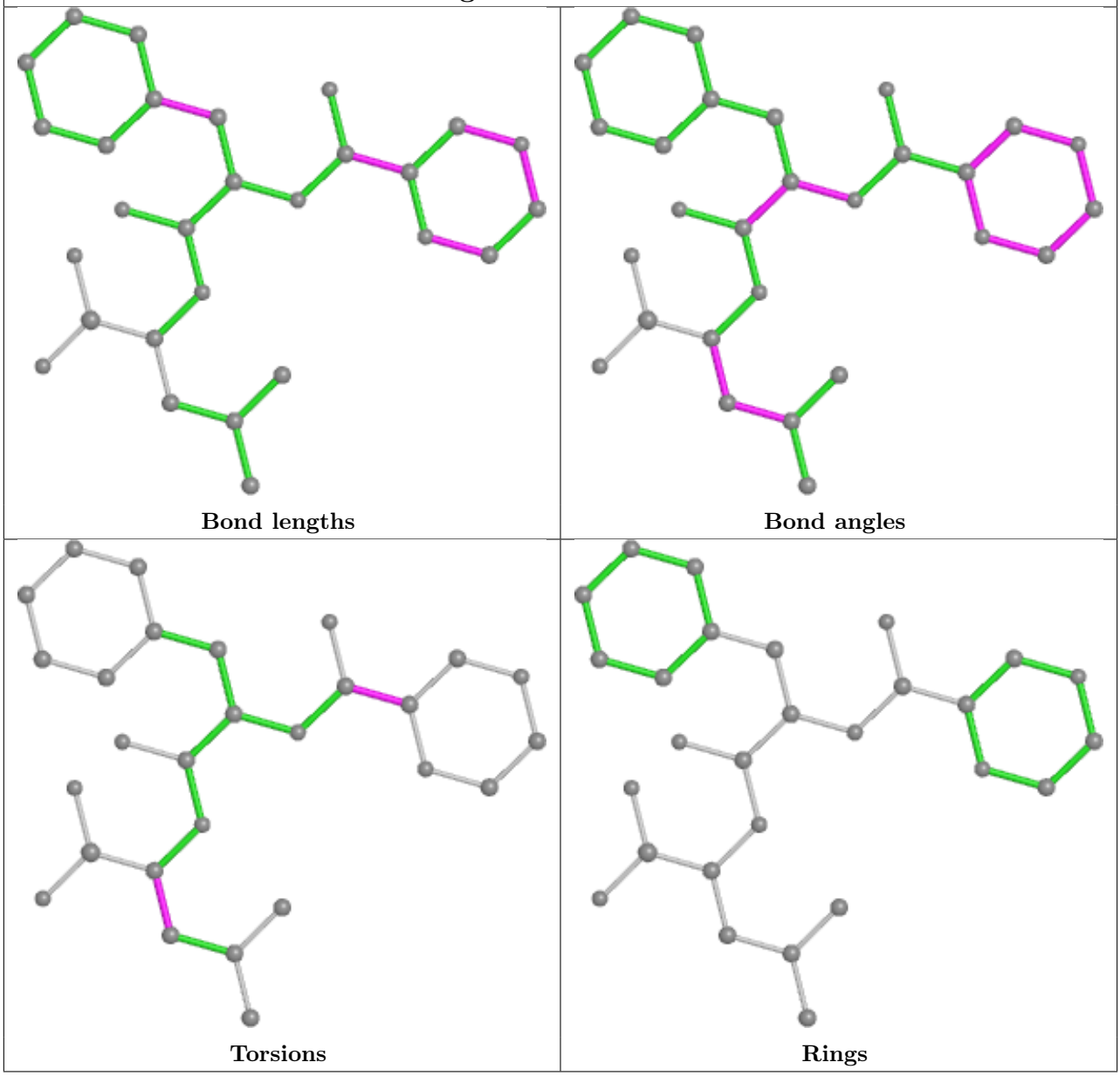


Torsions



Rings

Ligand BO2 Y 301



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, 95^{th} 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%)	-0.36	7 (2%) 53 43	42, 58, 97, 136	0
1	O	250/250 (100%)	-0.34	9 (3%) 42 32	45, 65, 112, 151	0
2	B	244/258 (94%)	-0.29	10 (4%) 37 27	42, 63, 110, 160	0
2	P	244/258 (94%)	-0.28	8 (3%) 46 36	48, 68, 106, 160	0
3	C	240/254 (94%)	-0.19	14 (5%) 23 15	40, 67, 131, 160	0
3	Q	240/254 (94%)	0.08	17 (7%) 16 9	54, 85, 168, 197	0
4	D	235/260 (90%)	-0.41	2 (0%) 84 80	47, 68, 101, 144	0
4	R	235/260 (90%)	-0.23	7 (2%) 50 40	55, 75, 118, 154	0
5	E	231/234 (98%)	-0.22	7 (3%) 50 40	50, 73, 111, 156	0
5	S	231/234 (98%)	-0.12	12 (5%) 27 18	51, 79, 128, 167	0
6	F	243/288 (84%)	-0.38	8 (3%) 46 36	43, 66, 118, 141	0
6	T	243/288 (84%)	-0.28	10 (4%) 37 27	44, 74, 134, 166	0
7	G	241/252 (95%)	-0.42	7 (2%) 51 41	43, 63, 103, 153	0
7	U	241/252 (95%)	-0.40	5 (2%) 63 54	45, 62, 99, 143	0
8	H	226/232 (97%)	-0.42	5 (2%) 62 52	38, 55, 94, 144	0
8	V	226/232 (97%)	-0.40	6 (2%) 54 44	40, 59, 94, 169	0
9	I	204/205 (99%)	-0.64	0 100 100	37, 54, 84, 112	0
9	W	204/205 (99%)	-0.64	1 (0%) 91 88	36, 55, 88, 111	0
10	J	195/198 (98%)	-0.52	2 (1%) 82 77	40, 57, 89, 131	0
10	X	195/198 (98%)	-0.51	3 (1%) 73 68	42, 60, 89, 140	0
11	K	212/212 (100%)	-0.39	4 (1%) 66 59	39, 57, 98, 116	0
11	Y	212/212 (100%)	-0.41	4 (1%) 66 59	39, 57, 101, 120	0
12	L	222/222 (100%)	-0.38	7 (3%) 47 37	39, 57, 112, 145	0
12	Z	222/222 (100%)	-0.40	8 (3%) 42 32	31, 57, 110, 139	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%)	-0.57	1 (0%)	92 91	38, 57, 81, 103	0
13	a	233/246 (94%)	-0.57	2 (0%)	84 80	37, 56, 81, 98	0
14	N	196/196 (100%)	-0.63	2 (1%)	82 77	38, 52, 85, 113	0
14	b	196/196 (100%)	-0.61	2 (1%)	82 77	40, 53, 86, 114	0
All	All	6344/6614 (95%)	-0.38	170 (2%)	54 44	31, 63, 112, 197	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	206	LYS	8.2
3	Q	236	GLN	7.5
3	Q	49	THR	6.5
2	P	221	ASP	5.8
3	C	49	THR	5.7
2	B	221	ASP	5.6
3	Q	239	GLN	5.6
12	L	174	TYR	5.4
12	Z	174	TYR	5.3
2	P	51	VAL	5.0
10	X	1	MET	5.0
3	Q	48	SER	4.9
2	B	218	GLY	4.9
3	C	206	LYS	4.8
3	Q	50	LEU	4.8
5	E	202	ASP	4.7
9	W	1	SER	4.7
8	H	224	GLN	4.6
10	J	1	MET	4.5
2	P	59	ASP	4.5
3	Q	240	GLU	4.3
12	Z	163	GLY	4.2
8	V	222	ASP	4.2
8	V	224	GLN	4.2
3	C	236	GLN	4.0
14	b	195	GLN	4.0
5	S	202	ASP	4.0
8	V	226	GLU	4.0
2	B	51	VAL	3.9
7	U	242	GLN	3.8
12	L	165	ASN	3.8
12	L	163	GLY	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	X	194	ASP	3.7
12	Z	167	LYS	3.7
3	Q	205	ALA	3.7
14	N	105	LYS	3.6
2	P	220	ASN	3.6
12	Z	173	LYS	3.6
3	C	225	GLU	3.5
6	T	181	GLU	3.5
1	O	249	ALA	3.4
11	Y	212	GLY	3.4
3	Q	237	GLU	3.4
2	P	219	ALA	3.3
12	L	173	LYS	3.3
10	J	194	ASP	3.3
1	A	1	MET	3.3
11	K	208	ASN	3.2
6	T	241	LYS	3.2
11	Y	147	ASP	3.2
1	O	52	SER	3.2
3	C	239	GLN	3.2
1	A	201	GLU	3.2
5	S	173	ARG	3.2
1	O	248	GLU	3.1
6	F	244	ASN	3.1
3	C	205	ALA	3.1
11	K	212	GLY	3.1
2	B	219	ALA	3.0
1	O	2	THR	3.0
8	H	222	ASP	3.0
7	G	241	GLU	3.0
12	Z	168	VAL	3.0
5	S	52	ALA	2.9
12	L	162	PRO	2.9
14	N	195	GLN	2.9
6	T	244	ASN	2.9
7	G	2	GLY	2.9
1	A	249	ALA	2.9
2	B	220	ASN	2.9
3	C	240	GLU	2.9
6	T	237	ASP	2.9
5	S	194	GLU	2.8
5	E	122	TYR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	S	54	GLU	2.8
6	T	230	ASP	2.8
13	M	1	THR	2.8
12	Z	162	PRO	2.8
3	Q	187	GLU	2.8
4	R	217	GLN	2.8
1	A	2	THR	2.7
12	L	170	LYS	2.7
2	B	203	SER	2.7
5	E	180	LYS	2.7
14	b	105	LYS	2.7
3	C	50	LEU	2.7
4	R	125	LEU	2.7
8	V	145	ASP	2.7
2	P	218	GLY	2.7
2	B	217	LYS	2.7
3	C	202	GLN	2.7
3	Q	229	GLN	2.7
4	R	242	GLU	2.7
1	A	250	LEU	2.6
3	C	203	THR	2.6
11	Y	208	ASN	2.6
5	S	51	ASN	2.6
13	a	1	THR	2.6
4	R	241	ALA	2.6
1	O	201	GLU	2.6
8	V	225	GLU	2.6
11	Y	106	ARG	2.6
3	C	238	LYS	2.6
5	S	180	LYS	2.6
11	K	209	ASN	2.6
6	F	241	LYS	2.5
7	G	181	LYS	2.5
4	D	242	GLU	2.5
3	C	187	GLU	2.5
7	U	181	LYS	2.5
11	K	147	ASP	2.5
7	G	242	GLN	2.5
6	T	243	ILE	2.5
5	E	227	GLU	2.4
2	P	222	GLY	2.4
3	Q	181	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	F	201	GLU	2.4
5	S	227	GLU	2.4
3	Q	141	ASP	2.4
1	O	231	LYS	2.4
2	P	230	LYS	2.4
3	Q	238	LYS	2.4
1	A	228	PRO	2.4
5	E	203	GLU	2.3
1	O	1	MET	2.3
12	Z	165	ASN	2.3
8	H	226	GLU	2.3
6	F	53	LYS	2.3
2	B	182	ASP	2.3
4	D	217	GLN	2.3
3	Q	225	GLU	2.3
4	R	230	GLU	2.3
13	a	47	ASP	2.3
8	H	145	ASP	2.2
1	A	231	LYS	2.2
3	C	180	LYS	2.2
3	Q	204	GLY	2.2
6	T	180	PRO	2.2
2	B	59	ASP	2.2
8	H	221	CYS	2.2
7	G	179	LYS	2.2
8	V	221	CYS	2.2
1	O	250	LEU	2.2
5	S	203	GLU	2.2
7	U	203	ASP	2.2
5	S	122	TYR	2.2
12	Z	210	ASP	2.2
6	F	180	PRO	2.2
1	O	241	GLN	2.1
5	S	57	SER	2.1
7	U	2	GLY	2.1
5	S	163	ARG	2.1
7	G	222	ASP	2.1
2	B	240	LYS	2.1
6	T	53	LYS	2.1
7	U	241	GLU	2.1
6	F	178	HIS	2.1
6	F	215	CYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	R	1	ASP	2.1
6	T	204	LYS	2.1
7	G	3	TYR	2.1
5	E	201	ARG	2.1
6	T	205	GLU	2.1
12	L	168	VAL	2.1
10	X	193	ASP	2.0
3	C	1	GLY	2.0
5	E	54	GLU	2.0
6	F	230	ASP	2.0
4	R	237	GLU	2.0
3	Q	202	GLN	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	b	201	28/28	0.88	0.21	43,51,61,63	0
17	BO2	N	201	28/28	0.90	0.23	37,50,63,63	0
17	BO2	V	301	28/28	0.91	0.20	52,56,66,67	0
15	MG	G	301	1/1	0.91	0.19	64,64,64,64	0
17	BO2	H	301	28/28	0.93	0.17	48,52,71,74	0
15	MG	Z	301	1/1	0.93	0.19	68,68,68,68	0
17	BO2	Y	301	28/28	0.94	0.17	47,59,66,71	0
15	MG	K	303	1/1	0.95	0.27	55,55,55,55	0
17	BO2	K	301	28/28	0.96	0.14	42,53,63,64	0
15	MG	I	301	1/1	0.97	0.24	62,62,62,62	0
15	MG	K	302	1/1	0.97	0.09	60,60,60,60	0

Continued on next page...

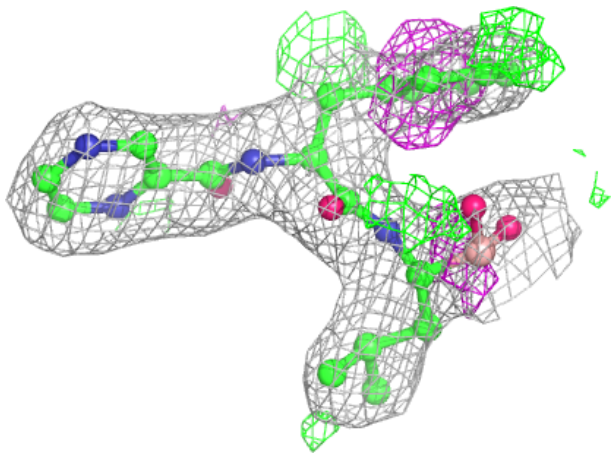
Continued from previous page...

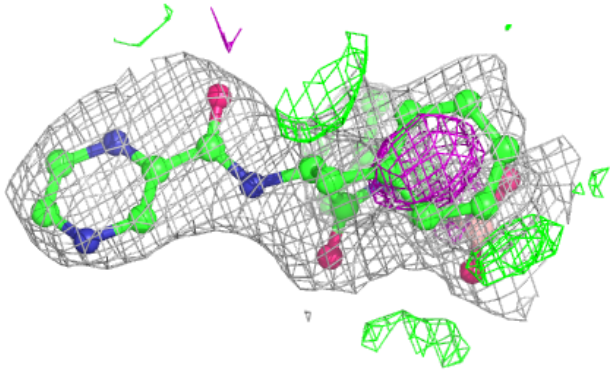
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	CL	N	203	1/1	0.97	0.09	46,46,46,46	0
15	MG	N	202	1/1	0.98	0.11	49,49,49,49	0
15	MG	Y	302	1/1	0.98	0.12	57,57,57,57	0
16	CL	U	301	1/1	0.98	0.18	47,47,47,47	0
15	MG	V	302	1/1	0.99	0.05	64,64,64,64	0
16	CL	b	202	1/1	0.99	0.09	46,46,46,46	0
16	CL	G	302	1/1	0.99	0.17	46,46,46,46	0
15	MG	J	201	1/1	0.99	0.25	44,44,44,44	0

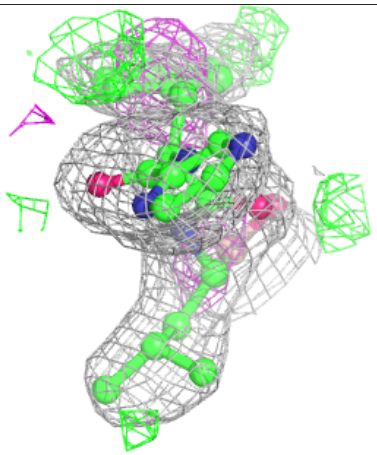
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

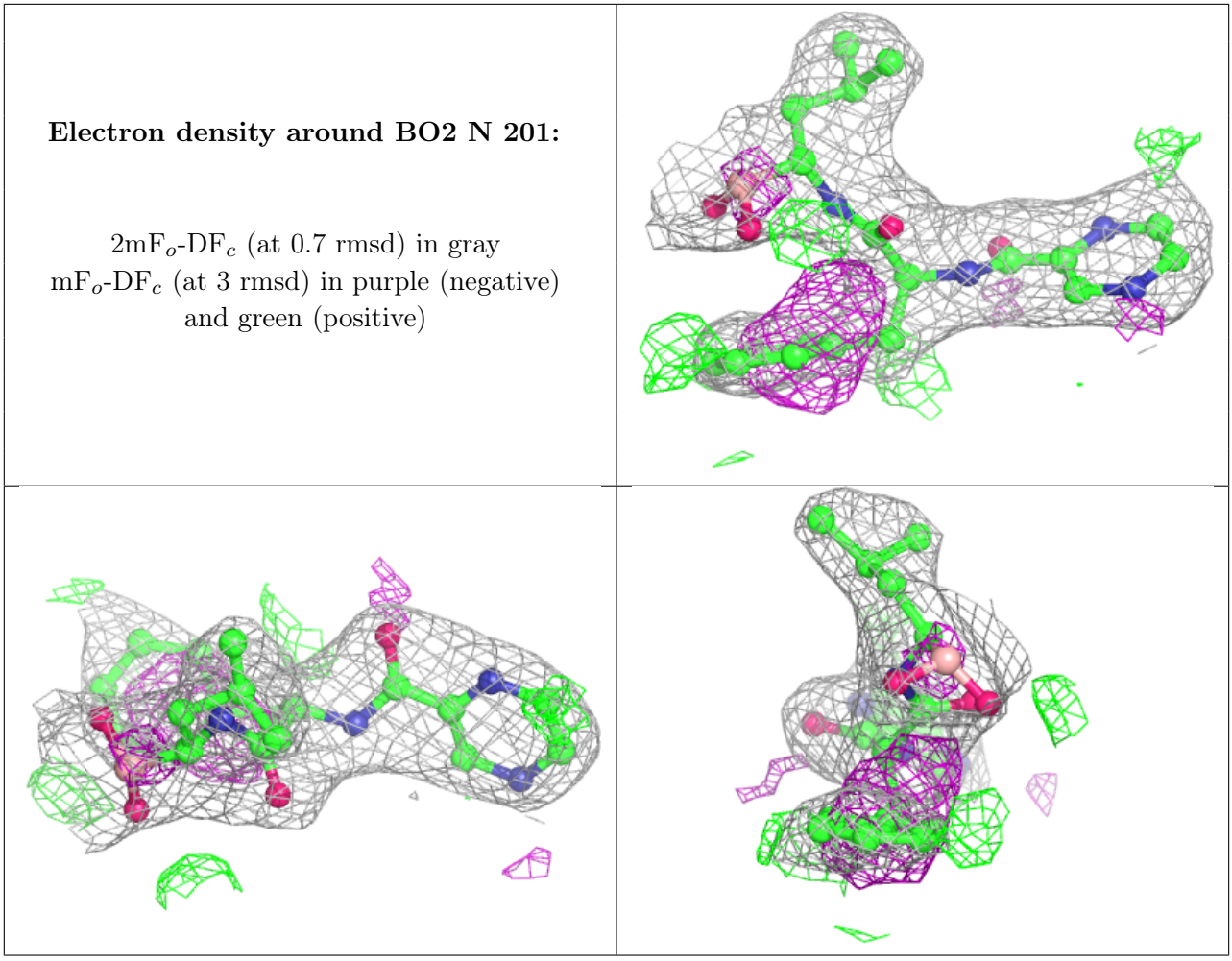






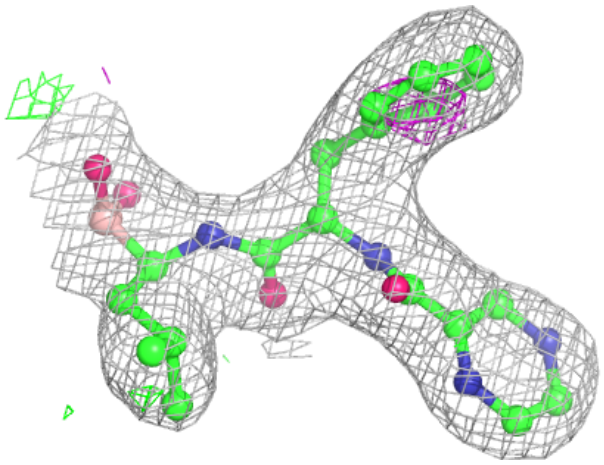
Electron density around BO2 N 201:

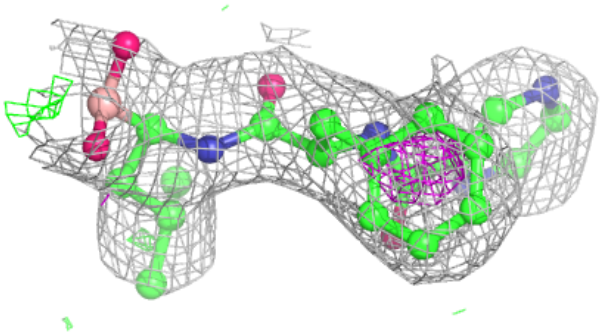
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

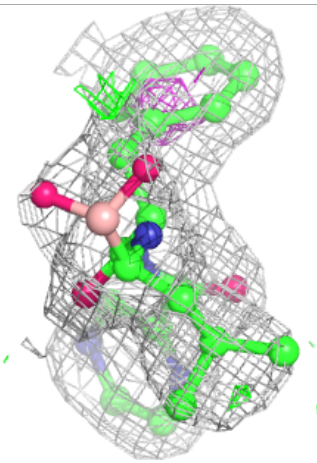


Electron density around BO2 V 301:

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

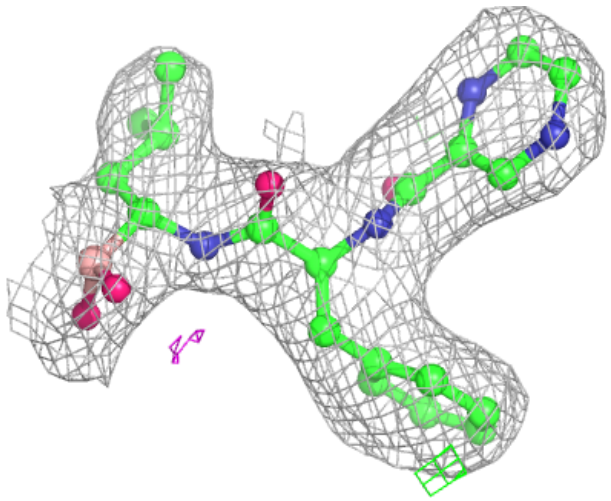


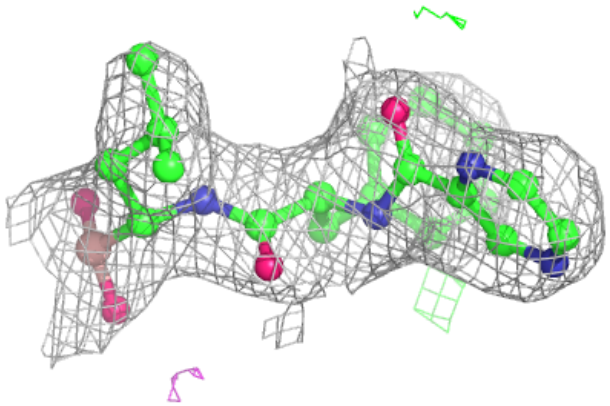


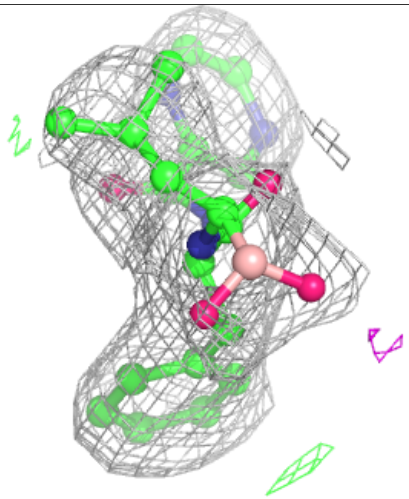


Electron density around BO2 H 301:

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

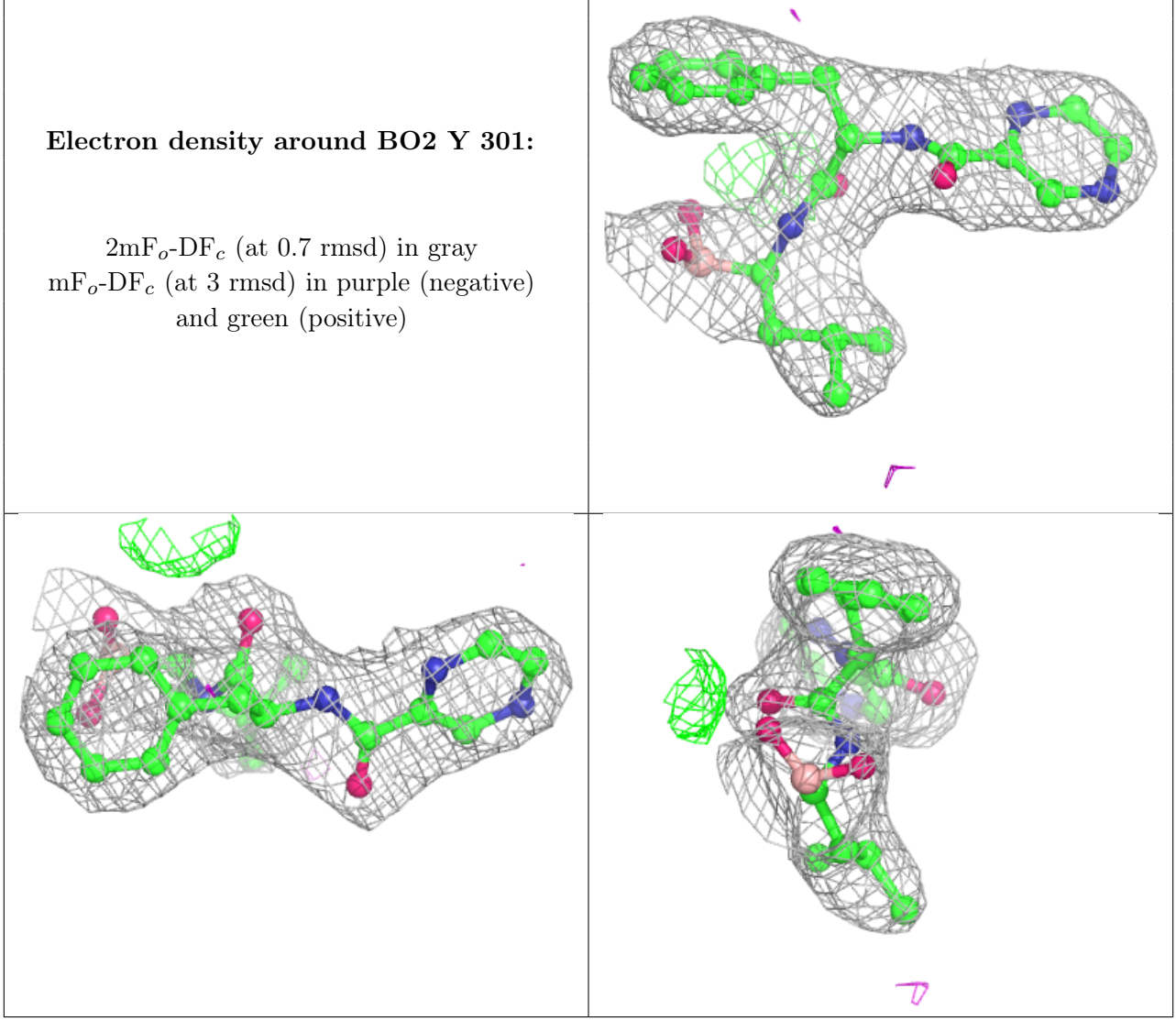






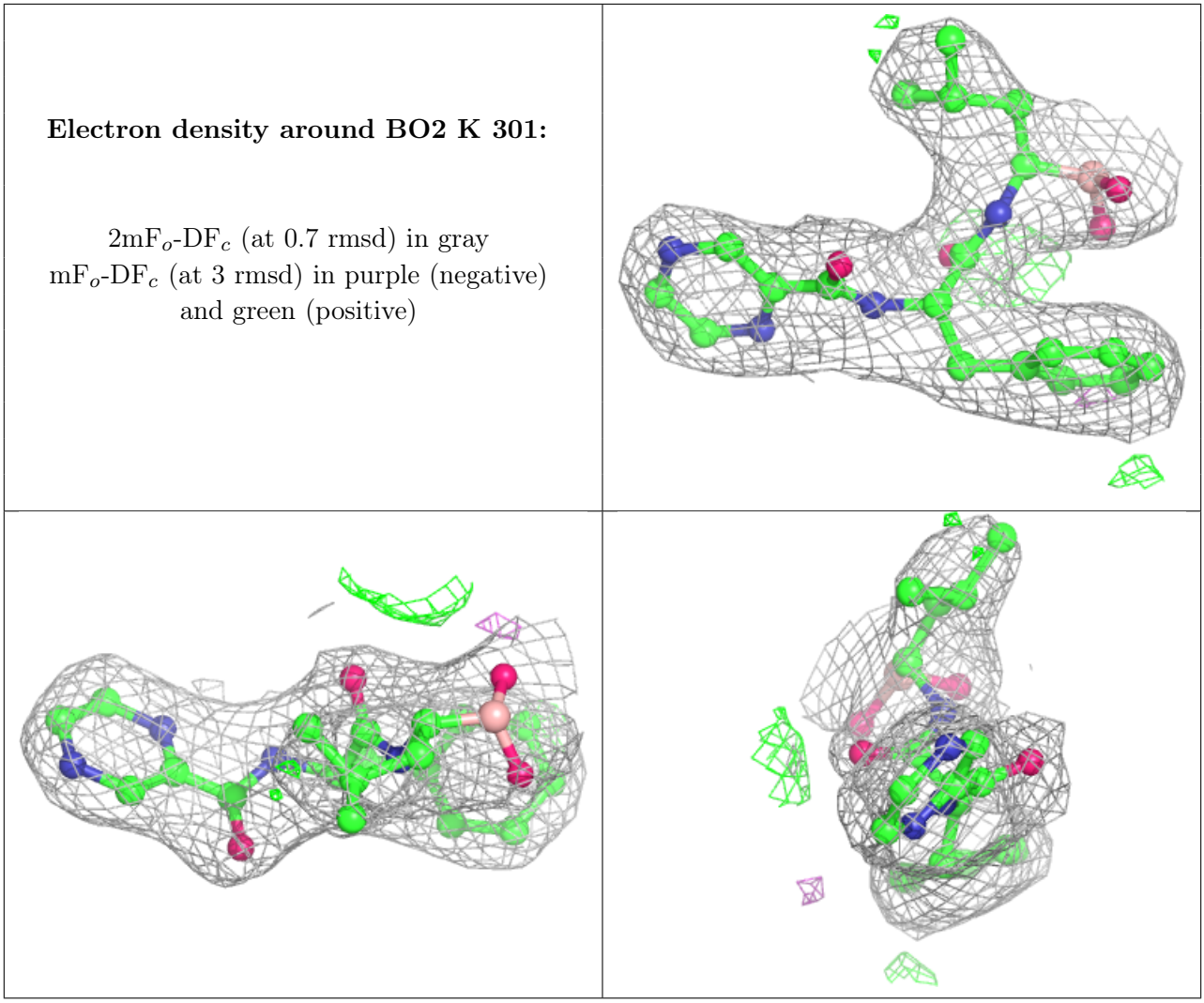
Electron density around BO2 Y 301:

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



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 (i)

There are no such residues in this entry.