Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2023 – 10:55 PM EDT

PDB ID	:	4QVV
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:

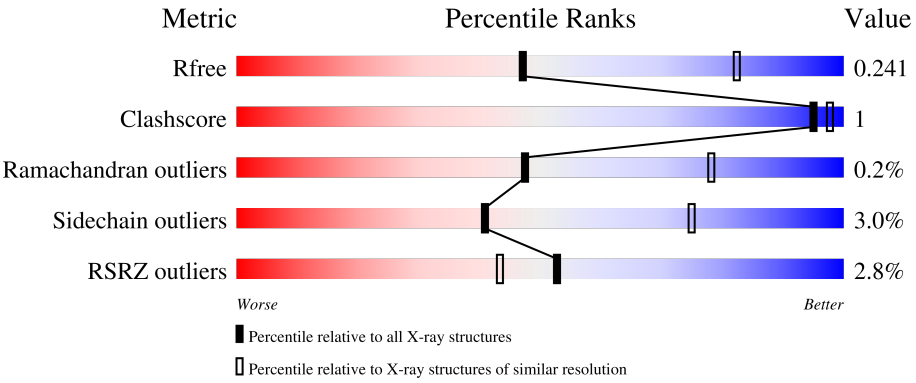
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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% 97% ·
2	B	258	5% 89% 5% · 5%
2	P	258	2% 90% · 5%
3	C	254	7% 88% 6% · 6%

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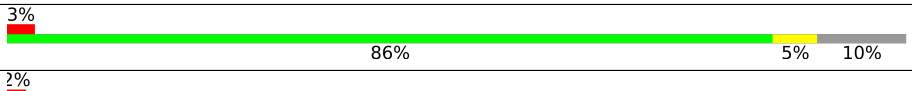
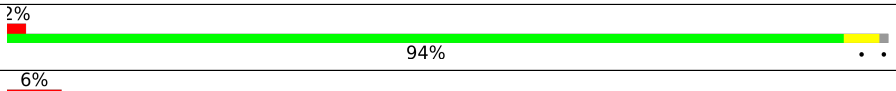
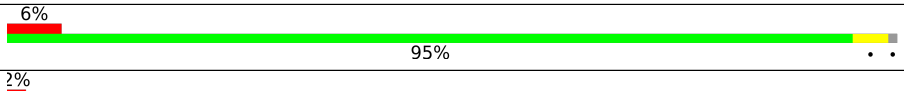
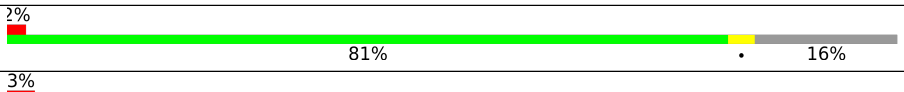
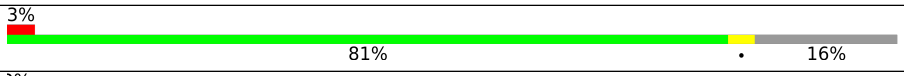
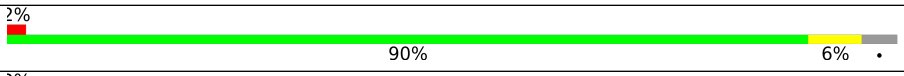
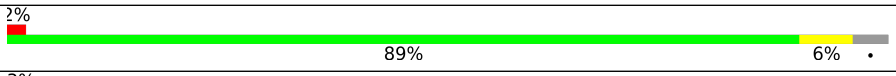
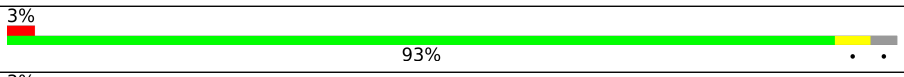
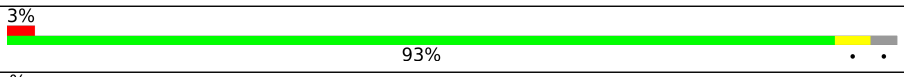
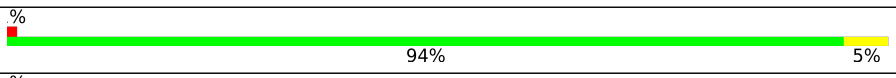
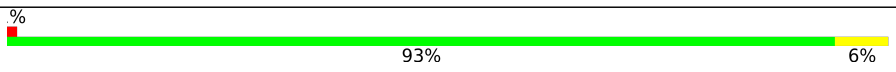
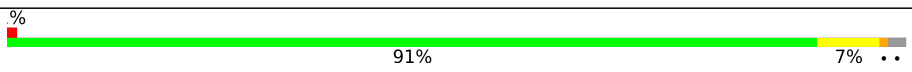
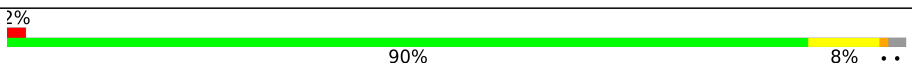
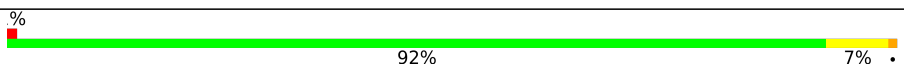
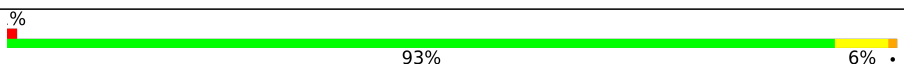
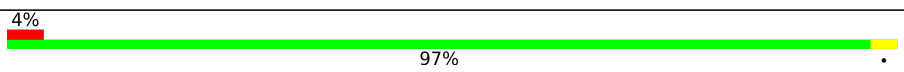
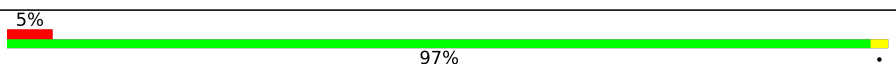
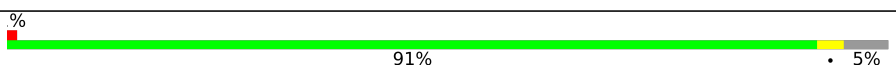
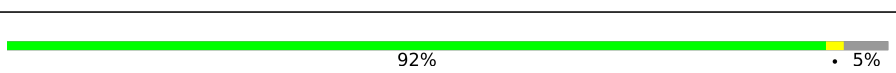
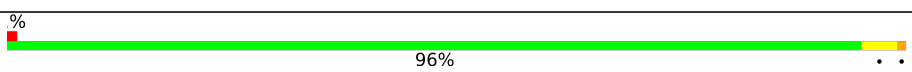
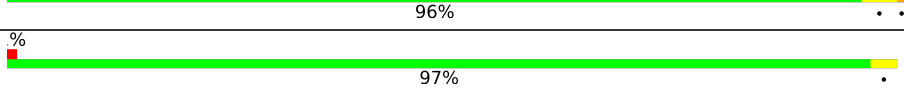
Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

2 Entry composition (i)

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			

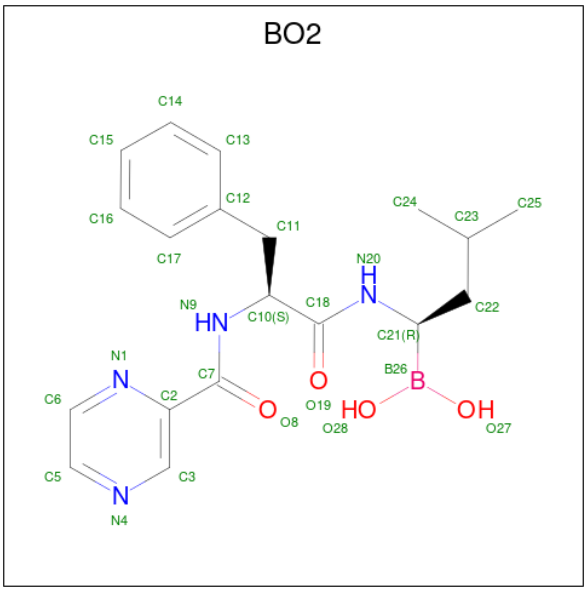
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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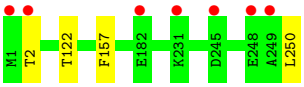
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	b	13	Total O 13 13	0	0

3 Residue-property plots (i)

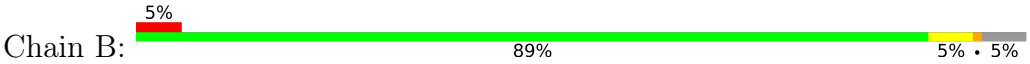
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

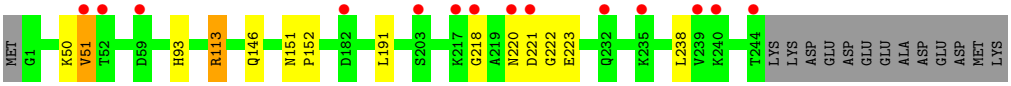
• Molecule 1: Proteasome subunit alpha type-2



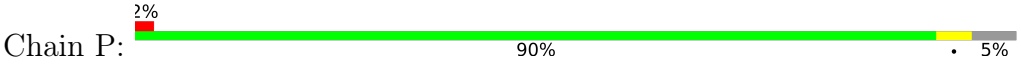
• Molecule 1: Proteasome subunit alpha type-2

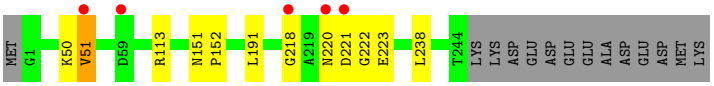
• Molecule 2: Proteasome subunit alpha type-3



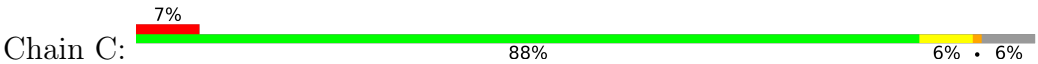


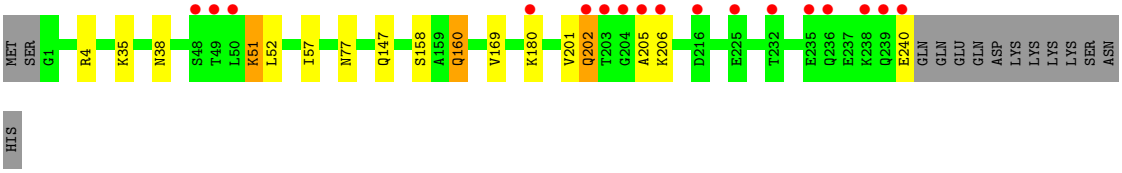
• Molecule 2: Proteasome subunit alpha type-3





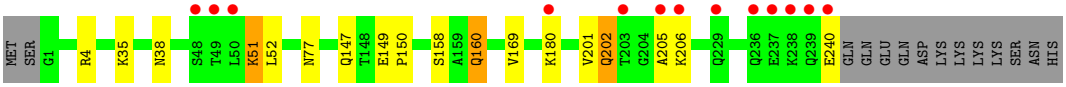
• Molecule 3: Proteasome subunit alpha type-4





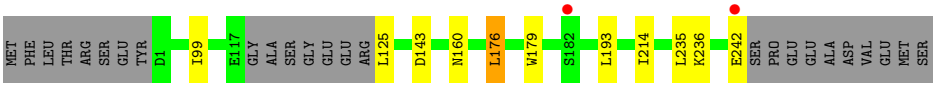
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



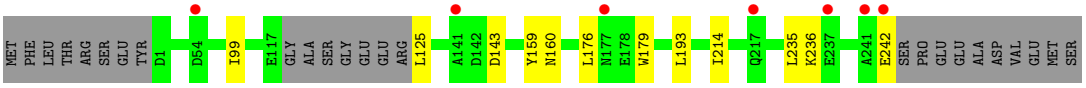
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



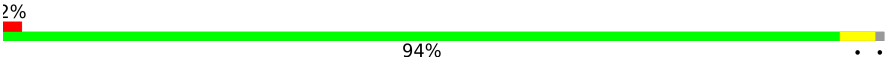
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



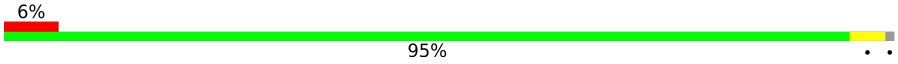
• Molecule 5: Proteasome subunit alpha type-6

Chain E:



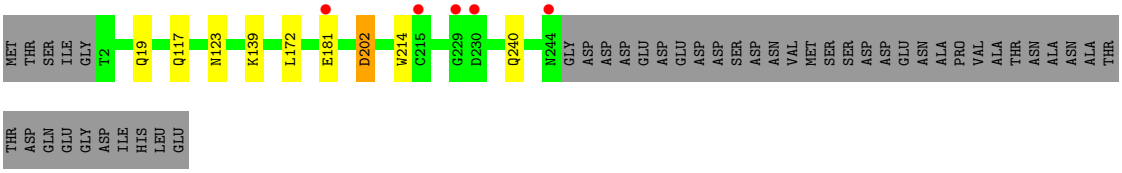
• Molecule 5: Proteasome subunit alpha type-6

Chain S:



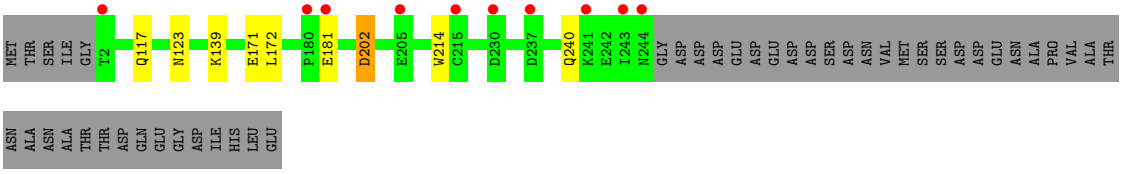
• Molecule 6: Probable proteasome subunit alpha type-7

Chain F:

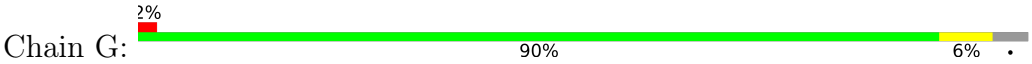


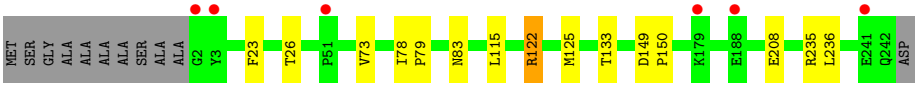
• Molecule 6: Probable proteasome subunit alpha type-7

Chain T:

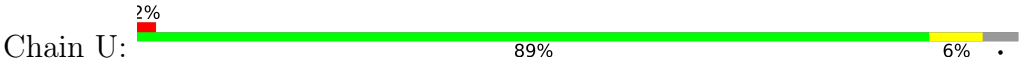


• Molecule 7: Proteasome subunit alpha type-1

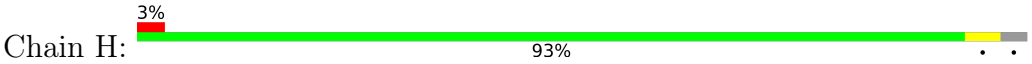


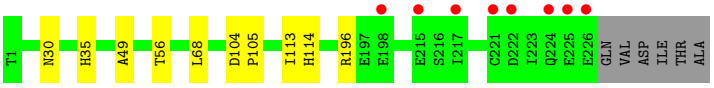


• Molecule 7: Proteasome subunit alpha type-1

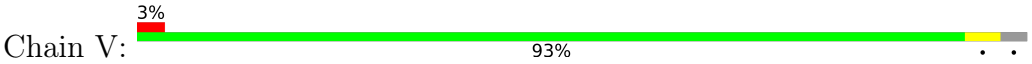


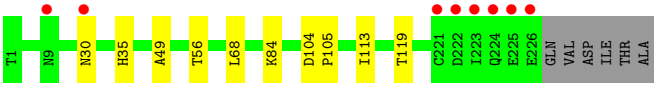
• Molecule 8: Proteasome subunit beta type-2



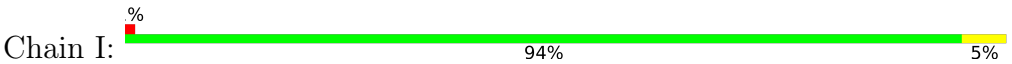


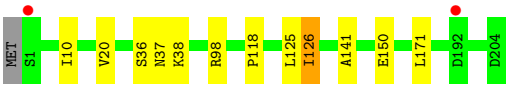
• Molecule 8: Proteasome subunit beta type-2



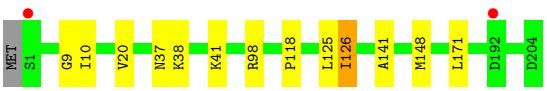


• Molecule 9: Proteasome subunit beta type-3



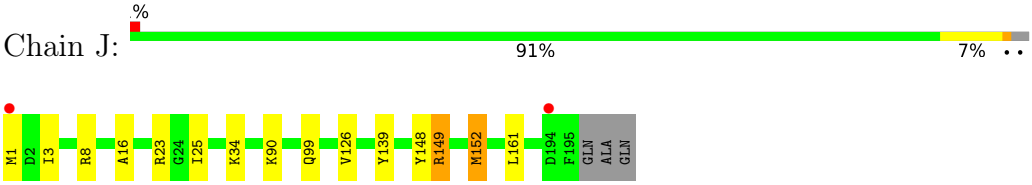


• Molecule 9: Proteasome subunit beta type-3



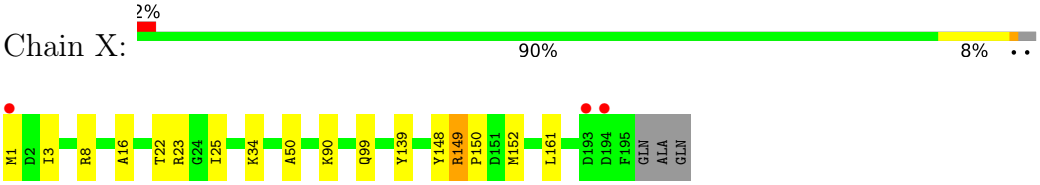
• Molecule 10: Proteasome subunit beta type-4

Chain J:



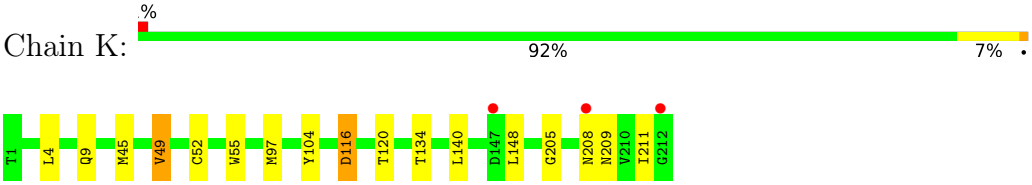
• Molecule 10: Proteasome subunit beta type-4

Chain X:



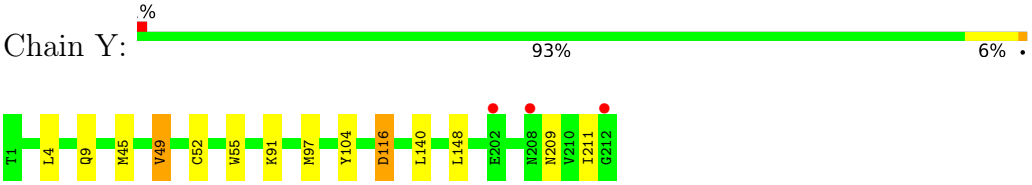
• Molecule 11: Proteasome subunit beta type-5

Chain K:



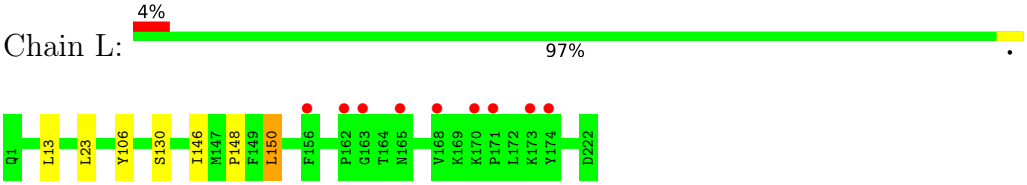
• Molecule 11: Proteasome subunit beta type-5

Chain Y:



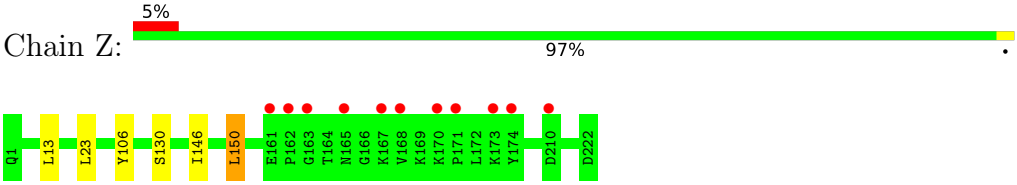
• Molecule 12: Proteasome subunit beta type-6

Chain L:



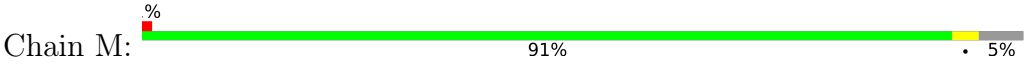
• Molecule 12: Proteasome subunit beta type-6

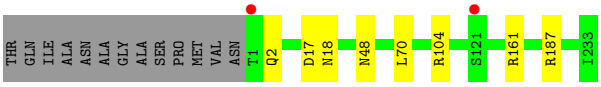
Chain Z:



• Molecule 13: Proteasome subunit beta type-7

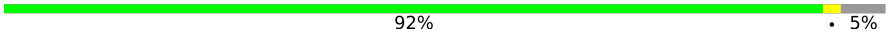
Chain M:

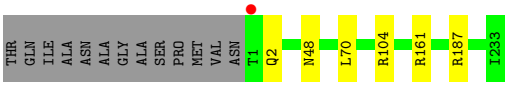




• Molecule 13: Proteasome subunit beta type-7

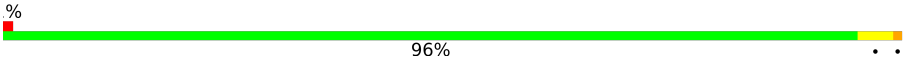
Chain a:

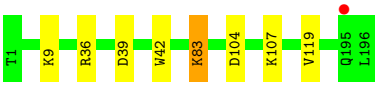




• Molecule 14: Proteasome subunit beta type-1

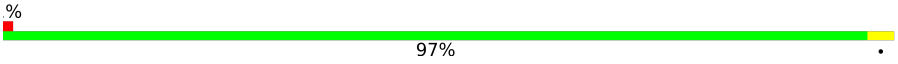
Chain N:

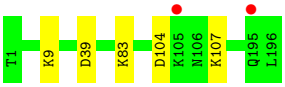




• Molecule 14: Proteasome subunit beta type-1

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	136.52Å 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) 97.9 (15.00-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.31 , 37.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[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

5.1 Standard geometry

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	0.28	0/1952	0.47	0/2642
1	O	0.28	0/1952	0.47	0/2642
2	B	0.28	0/1934	0.50	0/2618
2	P	0.28	0/1934	0.49	0/2618
3	C	0.28	0/1910	0.50	0/2586
3	Q	0.27	0/1910	0.50	0/2586
4	D	0.27	0/1837	0.47	0/2475
4	R	0.27	0/1837	0.47	0/2475
5	E	0.28	0/1800	0.47	0/2433
5	S	0.28	0/1800	0.47	0/2433
6	F	0.28	0/1932	0.45	0/2609
6	T	0.28	0/1932	0.45	0/2609
7	G	0.28	0/1945	0.47	0/2634
7	U	0.28	0/1945	0.47	0/2634
8	H	0.26	0/1750	0.47	0/2373
8	V	0.26	0/1750	0.46	0/2373
9	I	0.28	0/1611	0.49	0/2174
9	W	0.28	0/1611	0.48	0/2174
10	J	0.35	0/1589	0.49	0/2142
10	X	0.36	0/1589	0.50	0/2142
11	K	0.27	0/1683	0.50	0/2277
11	Y	0.27	0/1683	0.50	0/2277
12	L	0.28	0/1795	0.48	0/2420
12	Z	0.28	0/1795	0.48	0/2420
13	M	0.28	0/1855	0.50	0/2514
13	a	0.28	0/1855	0.51	0/2514
14	N	0.26	0/1541	0.47	0/2087
14	b	0.26	0/1541	0.47	0/2087
All	All	0.28	0/50268	0.48	0/67968

There are no bond length outliers.

There are no bond angle outliers.

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	6	0
2	P	1904	0	1904	4	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	4	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
13	M	1824	0	1832	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	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	0	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
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	0	0
18	b	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	49917	0	49282	110	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 (110) 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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.50
11:Y:116:ASP:C	11:Y:116:ASP:OD2	2.49	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
11:K:116:ASP:OD2	11:K:116:ASP:C	2.50	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
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
10:J:139:TYR:OH	10:X:25:ILE:O	2.33	0.46
11:K:55:TRP:HB2	11:K:97:MET:HE1	1.98	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
11:Y:55:TRP:HB2	11:Y:97:MET:HE1	1.98	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:50:LYS:O	2:B:51:VAL:C	2.58	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:50:LYS:O	2:P:51:VAL:C	2.58	0.41
2:P:221:ASP:O	2:P:223:GLU:N	2.54	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
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
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
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 (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%)	240 (97%)	7 (3%)	1 (0%)	34	66
1	O	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	34	66
2	B	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	9	29
2	P	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	9	29
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%)	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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%)	47 78

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	193 (96%)	8 (4%)	31	65
6	T	201/239 (84%)	192 (96%)	9 (4%)	27	60
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%)	182 (98%)	3 (2%)	62	88
8	V	185/190 (97%)	182 (98%)	3 (2%)	62	88
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	87
9	W	172/173 (99%)	169 (98%)	3 (2%)	60	87
10	J	173/175 (99%)	168 (97%)	5 (3%)	42	76
10	X	173/175 (99%)	169 (98%)	4 (2%)	50	82
11	K	170/170 (100%)	162 (95%)	8 (5%)	26	59
11	Y	170/170 (100%)	162 (95%)	8 (5%)	26	59
12	L	185/185 (100%)	182 (98%)	3 (2%)	62	88
12	Z	185/185 (100%)	182 (98%)	3 (2%)	62	88
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%)	157 (97%)	5 (3%)	40	74
14	b	162/162 (100%)	157 (97%)	5 (3%)	40	74
All	All	5322/5542 (96%)	5164 (97%)	158 (3%)	41	75

All (158) 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

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Mol	Chain	Res	Type
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
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	172	LEU
6	F	181	GLU
6	F	202	ASP
6	F	214	TRP
6	F	240	GLN
7	G	83	ASN
7	G	115	LEU
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

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Mol	Chain	Res	Type
9	I	37	ASN
9	I	126	ILE
9	I	171	LEU
10	J	3	ILE
10	J	90	LYS
10	J	99	GLN
10	J	149	ARG
10	J	152	MET
11	K	4	LEU
11	K	9	GLN
11	K	49	VAL
11	K	104	TYR
11	K	116	ASP
11	K	140	LEU
11	K	148	LEU
11	K	211	ILE
12	L	23	LEU
12	L	106	TYR
12	L	150	LEU
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	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

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Mol	Chain	Res	Type
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
5	S	202	ASP
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	171	GLU
6	T	172	LEU
6	T	181	GLU
6	T	202	ASP
6	T	214	TRP
6	T	240	GLN
7	U	83	ASN
7	U	115	LEU
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
9	W	37	ASN
9	W	126	ILE
9	W	171	LEU
10	X	3	ILE

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Mol	Chain	Res	Type
10	X	90	LYS
10	X	99	GLN
10	X	149	ARG
11	Y	4	LEU
11	Y	9	GLN
11	Y	49	VAL
11	Y	104	TYR
11	Y	116	ASP
11	Y	140	LEU
11	Y	148	LEU
11	Y	211	ILE
12	Z	23	LEU
12	Z	106	TYR
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	39	ASP
14	b	83	LYS
14	b	104	ASP
14	b	107	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
3	C	17	GLN
3	C	77	ASN
3	C	92	GLN
3	C	147	GLN
3	C	160	GLN
4	D	91	HIS

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Mol	Chain	Res	Type
4	D	146	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	123	ASN
6	F	191	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
8	H	66	HIS
9	I	203	GLN
10	J	55	GLN
11	K	9	GLN
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
13	M	48	ASN
13	M	102	GLN
1	O	94	HIS
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	146	GLN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN

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Mol	Chain	Res	Type
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
11	Y	9	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	79	HIS
13	a	48	ASN
13	a	102	GLN

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 monosaccharides 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	K	301	11	25,29,29	1.64	5 (20%)	32,38,38	1.46	4 (12%)
17	BO2	V	301	8	25,29,29	1.65	5 (20%)	32,38,38	1.29	3 (9%)
17	BO2	N	201	14	25,29,29	1.59	4 (16%)	32,38,38	1.35	4 (12%)
17	BO2	b	201	14	25,29,29	1.61	4 (16%)	32,38,38	1.35	4 (12%)
17	BO2	H	301	8	25,29,29	1.65	5 (20%)	32,38,38	1.28	2 (6%)
17	BO2	Y	301	11	25,29,29	1.61	5 (20%)	32,38,38	1.46	4 (12%)

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	K	301	11	-	0/22/28/28	0/2/2/2
17	BO2	V	301	8	-	7/22/28/28	0/2/2/2
17	BO2	N	201	14	-	4/22/28/28	0/2/2/2
17	BO2	b	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	Y	301	11	-	0/22/28/28	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	-4.86	1.38	1.50
17	K	301	BO2	C2-C7	-4.72	1.39	1.50
17	N	201	BO2	C2-C7	-4.62	1.39	1.50
17	Y	301	BO2	C2-C7	-4.58	1.39	1.50
17	V	301	BO2	C2-C7	-4.54	1.39	1.50
17	K	301	BO2	C11-C12	-4.44	1.40	1.51
17	b	201	BO2	C11-C12	-4.43	1.40	1.51
17	H	301	BO2	C2-C7	-4.43	1.39	1.50
17	N	201	BO2	C11-C12	-4.41	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	301	BO2	C11-C12	-4.40	1.40	1.51
17	H	301	BO2	C11-C12	-4.29	1.41	1.51
17	V	301	BO2	C11-C12	-4.13	1.41	1.51
17	V	301	BO2	C3-N4	3.08	1.40	1.34
17	H	301	BO2	C3-N4	3.03	1.40	1.34
17	V	301	BO2	C6-N1	3.03	1.41	1.34
17	H	301	BO2	C6-N1	2.97	1.40	1.34
17	Y	301	BO2	C3-N4	2.90	1.40	1.34
17	K	301	BO2	C3-N4	2.88	1.40	1.34
17	N	201	BO2	C6-N1	2.72	1.40	1.34
17	b	201	BO2	C6-N1	2.70	1.40	1.34
17	K	301	BO2	C6-N1	2.68	1.40	1.34
17	Y	301	BO2	C6-N1	2.67	1.40	1.34
17	N	201	BO2	C3-N4	2.48	1.39	1.34
17	V	301	BO2	C5-N4	2.39	1.40	1.33
17	K	301	BO2	C5-N4	2.38	1.40	1.33
17	Y	301	BO2	C5-N4	2.34	1.40	1.33
17	H	301	BO2	C5-N4	2.33	1.40	1.33
17	b	201	BO2	C3-N4	2.27	1.39	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Y	301	BO2	C21-C22-C23	-4.98	109.14	115.39
17	K	301	BO2	C21-C22-C23	-4.84	109.31	115.39
17	b	201	BO2	C21-C22-C23	-4.33	109.96	115.39
17	N	201	BO2	C21-C22-C23	-4.22	110.09	115.39
17	V	301	BO2	C21-C22-C23	-3.66	110.80	115.39
17	H	301	BO2	C21-C22-C23	-3.58	110.90	115.39
17	V	301	BO2	C6-N1-C2	3.44	121.40	116.93
17	H	301	BO2	C6-N1-C2	3.43	121.39	116.93
17	K	301	BO2	C6-N1-C2	3.41	121.36	116.93
17	Y	301	BO2	C6-N1-C2	3.35	121.27	116.93
17	N	201	BO2	C6-N1-C2	2.78	120.53	116.93
17	b	201	BO2	C11-C10-N9	-2.63	105.25	110.79
17	N	201	BO2	C11-C10-N9	-2.59	105.33	110.79
17	K	301	BO2	C11-C10-N9	-2.56	105.40	110.79
17	Y	301	BO2	C11-C10-N9	-2.56	105.40	110.79
17	b	201	BO2	C6-N1-C2	2.55	120.24	116.93
17	K	301	BO2	C2-C3-N4	-2.20	119.31	122.05
17	Y	301	BO2	C2-C3-N4	-2.10	119.43	122.05
17	b	201	BO2	C18-C10-N9	-2.09	105.48	111.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	N	201	BO2	C18-C10-N9	-2.05	105.57	111.16
17	V	301	BO2	C6-C5-N4	-2.00	119.45	121.95

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	N	201	BO2	N1-C2-C7-N9
17	b	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
17	b	201	BO2	C3-C2-C7-N9

There are no ring outliers.

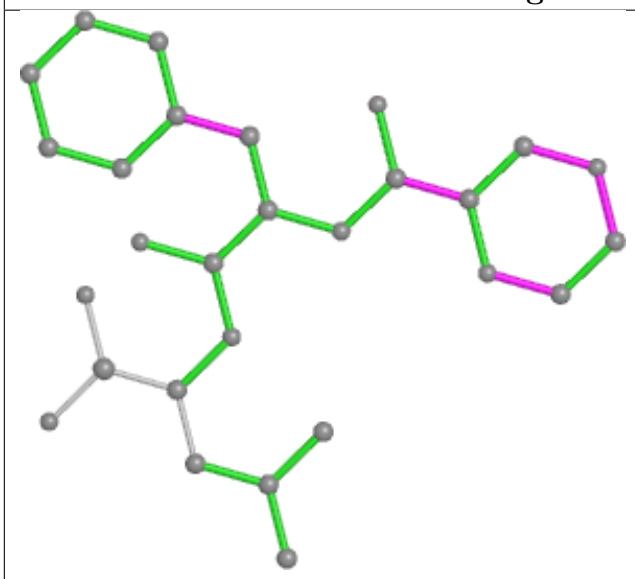
5 monomers are involved in 9 short contacts:

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

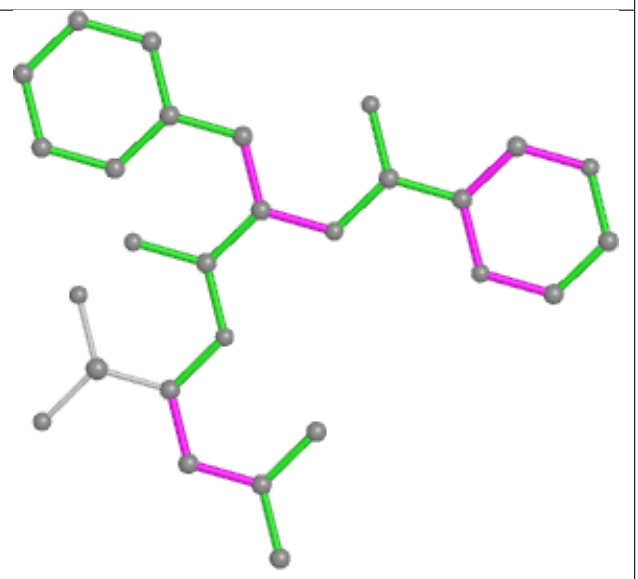
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

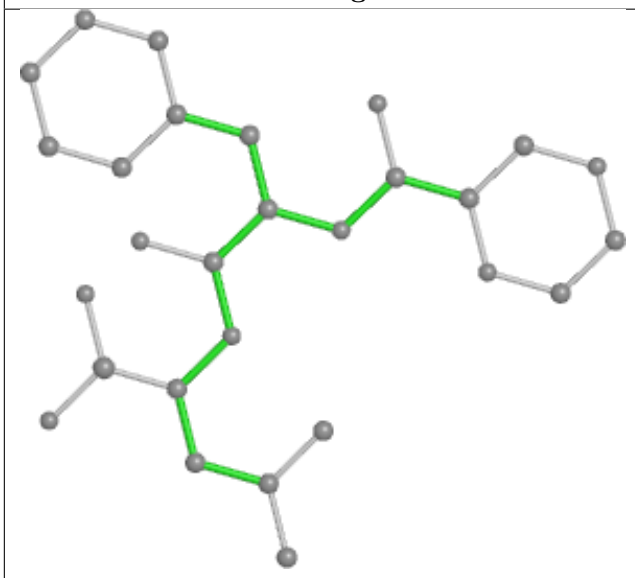
Ligand BO2 K 301



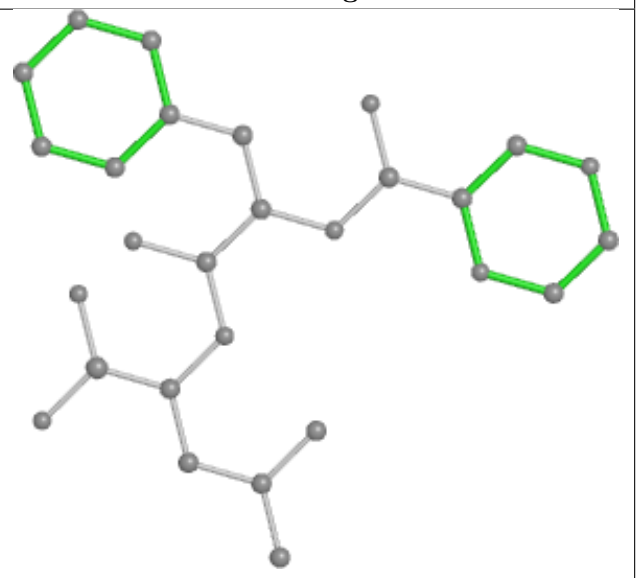
Bond lengths



Bond angles

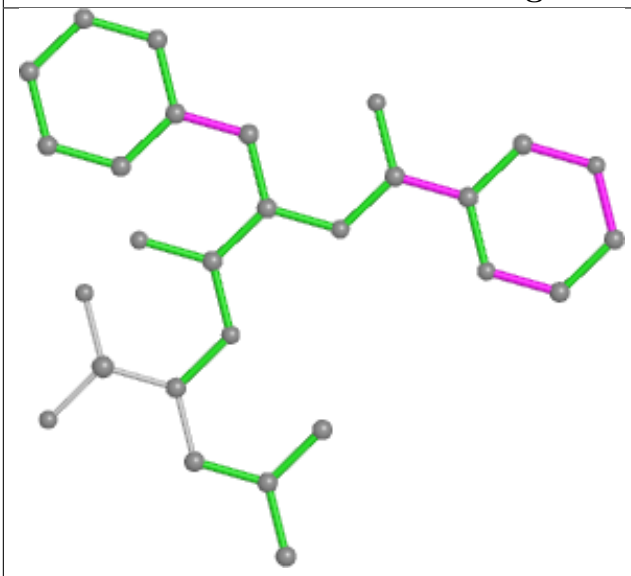


Torsions

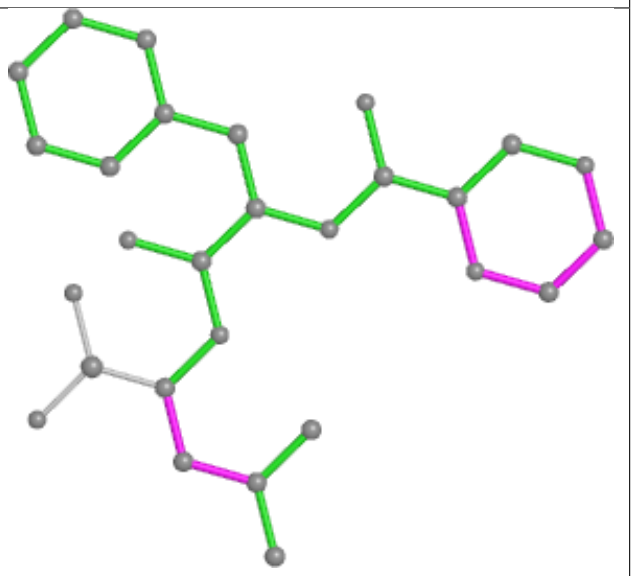


Rings

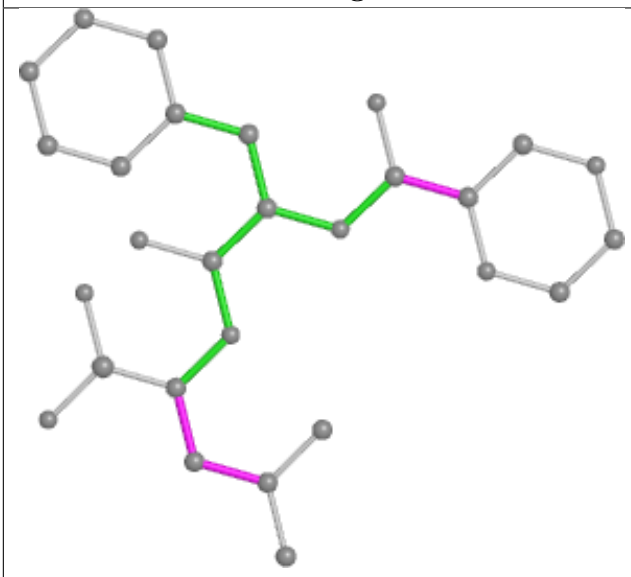
Ligand BO2 V 301



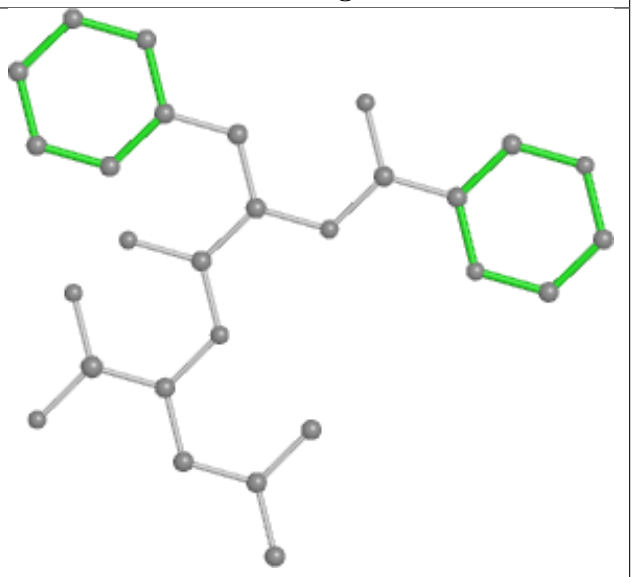
Bond lengths



Bond angles

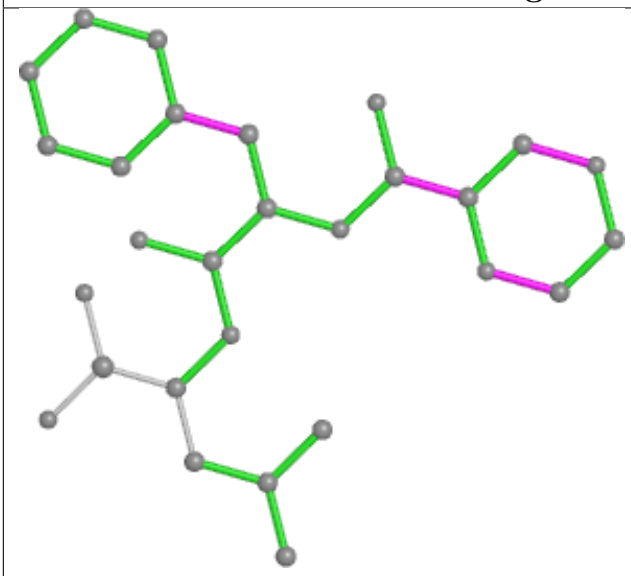


Torsions

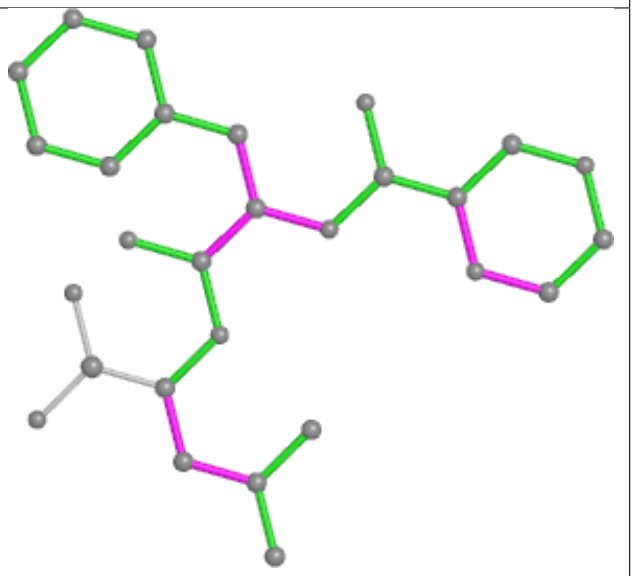


Rings

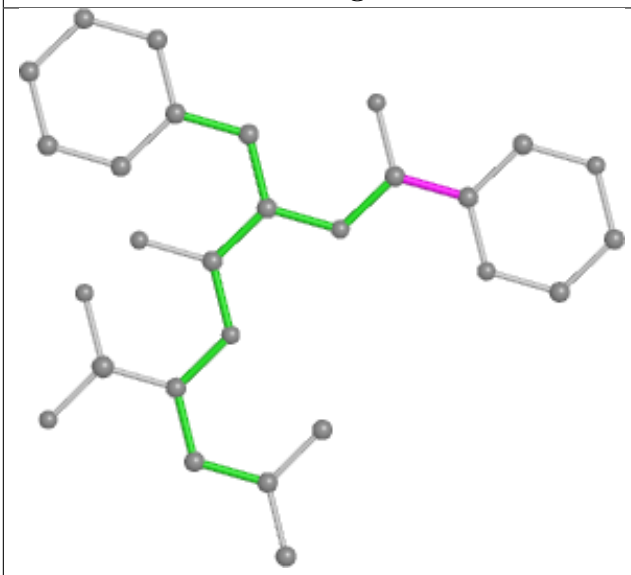
Ligand BO2 N 201



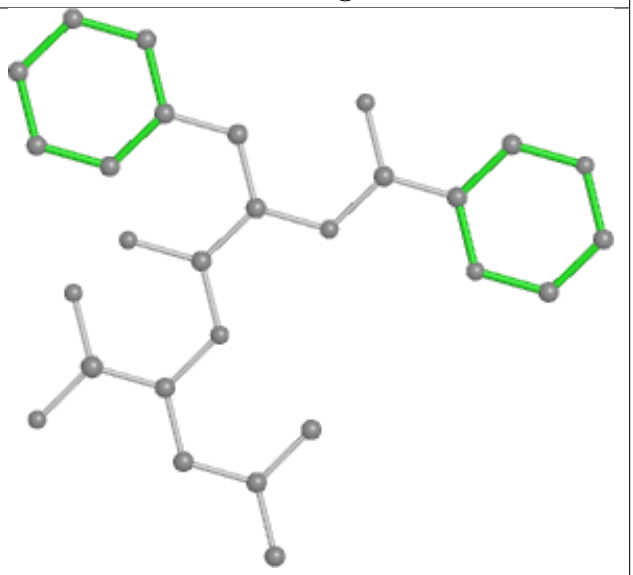
Bond lengths



Bond angles

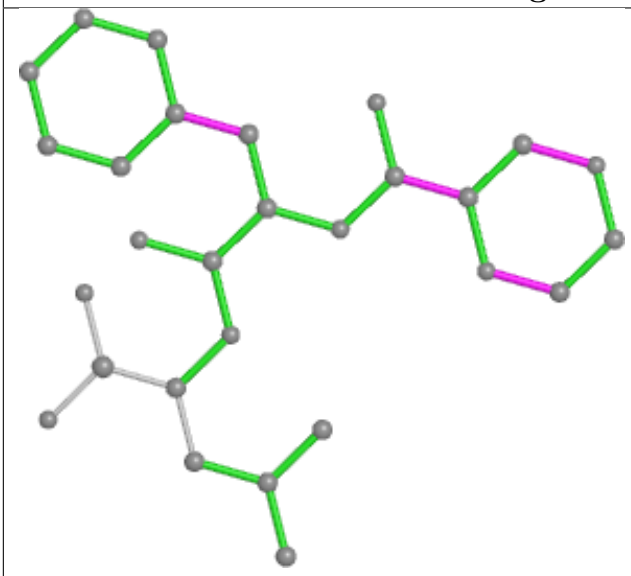


Torsions

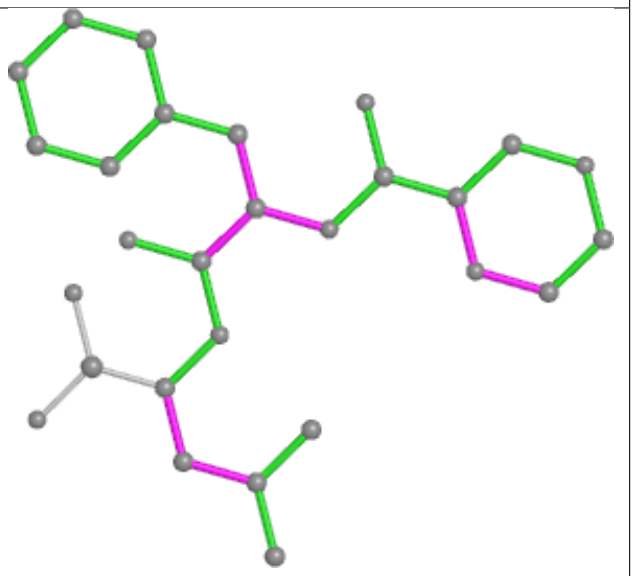


Rings

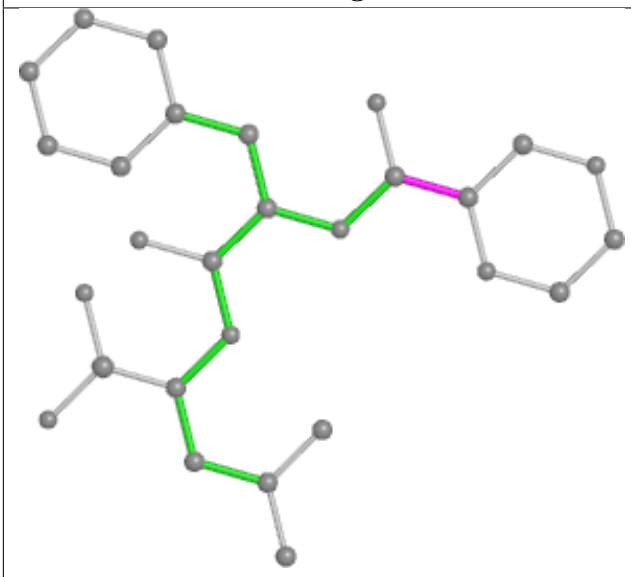
Ligand BO2 b 201



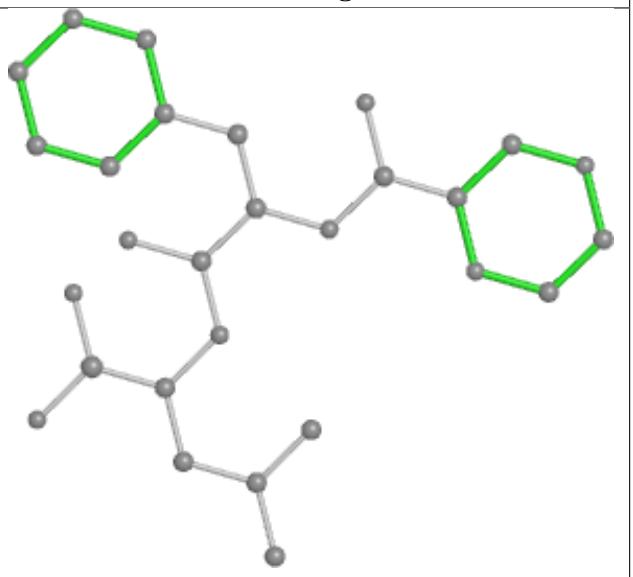
Bond lengths



Bond angles

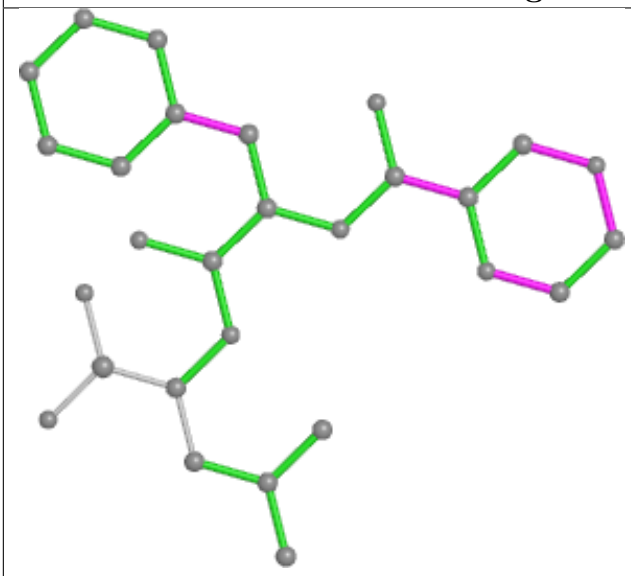


Torsions

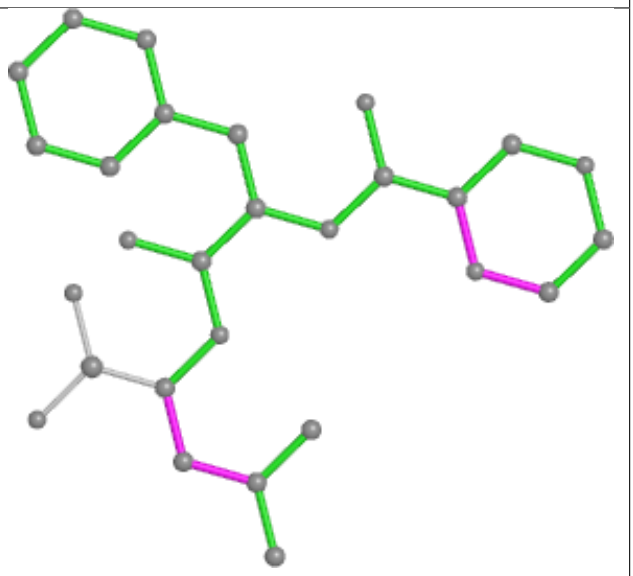


Rings

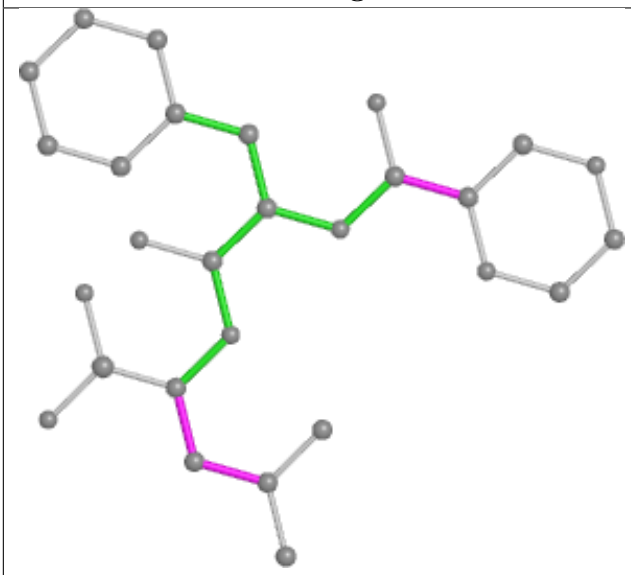
Ligand BO2 H 301



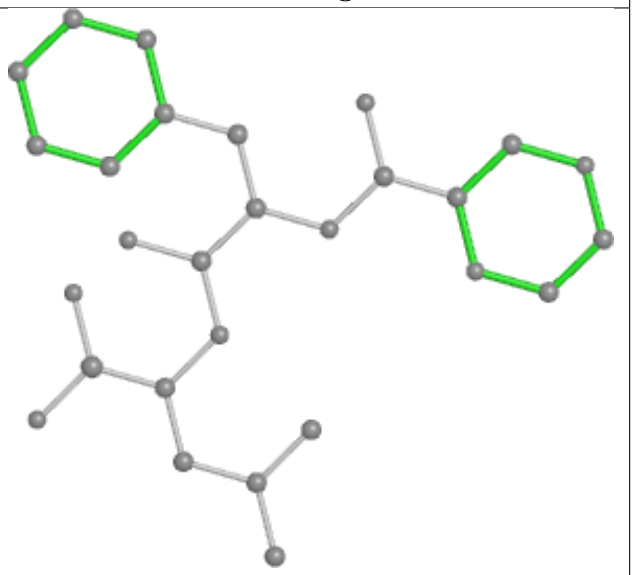
Bond lengths



Bond angles

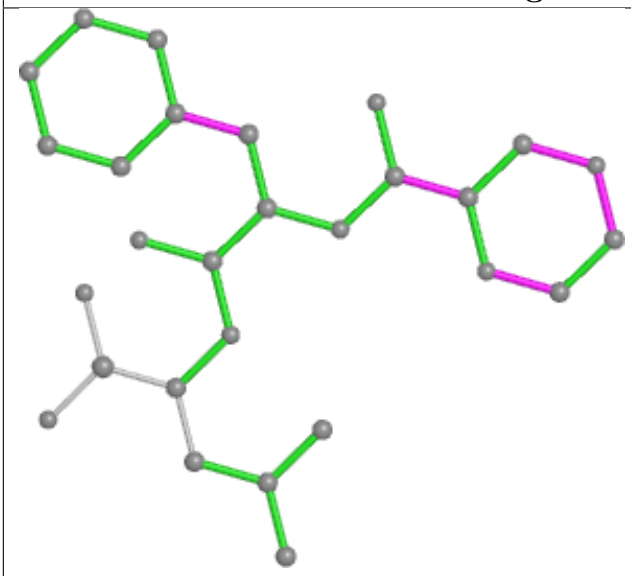


Torsions

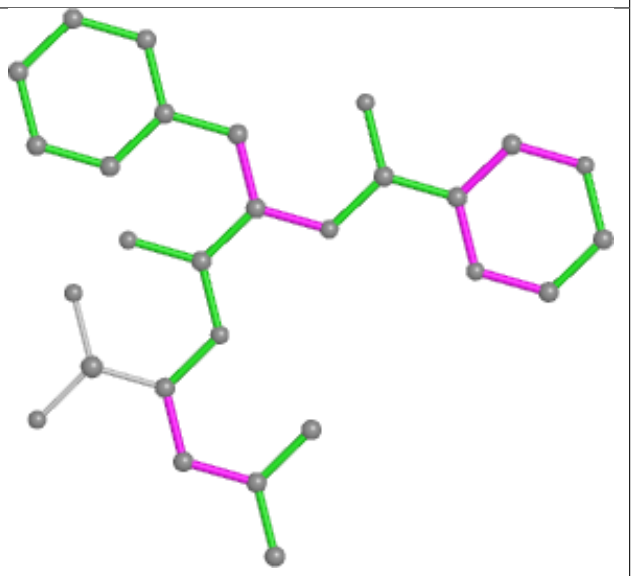


Rings

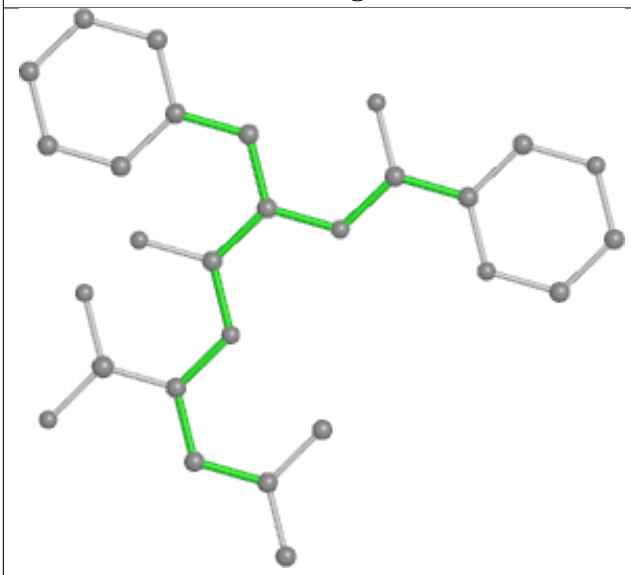
Ligand BO2 Y 301



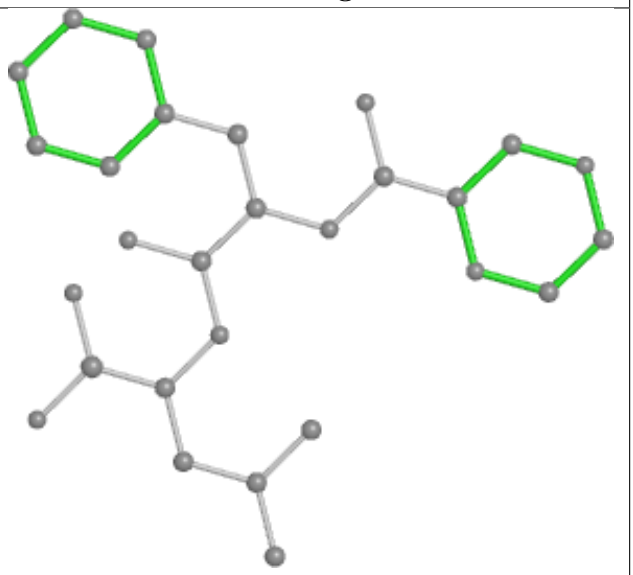
Bond lengths



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, 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%)	-0.24	7 (2%) 53 43	39, 54, 91, 133	0
1	O	250/250 (100%)	-0.31	10 (4%) 38 28	39, 58, 102, 141	0
2	B	244/258 (94%)	-0.11	14 (5%) 23 15	40, 60, 102, 153	0
2	P	244/258 (94%)	-0.30	5 (2%) 65 56	43, 62, 101, 144	0
3	C	240/254 (94%)	-0.14	17 (7%) 16 9	39, 61, 121, 151	0
3	Q	240/254 (94%)	0.09	13 (5%) 25 17	47, 75, 153, 172	0
4	D	235/260 (90%)	-0.42	2 (0%) 84 80	44, 64, 95, 133	0
4	R	235/260 (90%)	0.04	7 (2%) 50 40	51, 70, 108, 143	0
5	E	231/234 (98%)	-0.16	5 (2%) 62 52	45, 66, 106, 147	0
5	S	231/234 (98%)	0.04	13 (5%) 24 16	46, 69, 111, 143	0
6	F	243/288 (84%)	-0.37	5 (2%) 63 54	38, 60, 111, 135	0
6	T	243/288 (84%)	-0.33	10 (4%) 37 27	35, 62, 118, 146	0
7	G	241/252 (95%)	-0.48	6 (2%) 57 47	37, 55, 94, 151	0
7	U	241/252 (95%)	-0.43	5 (2%) 63 54	37, 53, 88, 135	0
8	H	226/232 (97%)	-0.25	8 (3%) 44 34	35, 51, 99, 151	0
8	V	226/232 (97%)	-0.36	8 (3%) 44 34	34, 51, 84, 160	0
9	I	204/205 (99%)	-0.36	2 (0%) 82 77	35, 50, 85, 110	0
9	W	204/205 (99%)	-0.58	2 (0%) 82 77	35, 51, 80, 107	0
10	J	195/198 (98%)	-0.35	2 (1%) 82 77	37, 53, 82, 127	0
10	X	195/198 (98%)	-0.47	3 (1%) 73 68	39, 55, 83, 127	0
11	K	212/212 (100%)	-0.41	3 (1%) 75 70	35, 53, 89, 107	0
11	Y	212/212 (100%)	-0.10	3 (1%) 75 70	38, 55, 93, 111	0
12	L	222/222 (100%)	-0.30	9 (4%) 37 27	37, 54, 110, 143	0
12	Z	222/222 (100%)	-0.01	11 (4%) 28 19	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%)	-0.54	2 (0%) 84 80	34, 52, 74, 91	0
13	a	233/246 (94%)	-0.56	1 (0%) 92 91	32, 49, 72, 88	0
14	N	196/196 (100%)	-0.68	1 (0%) 91 88	34, 46, 75, 97	0
14	b	196/196 (100%)	-0.66	2 (1%) 82 77	33, 46, 77, 108	0
All	All	6344/6614 (95%)	-0.31	176 (2%) 53 43	31, 57, 101, 172	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	L	174	TYR	8.1
12	Z	174	TYR	8.0
12	Z	162	PRO	7.0
3	Q	49	THR	7.0
3	Q	50	LEU	6.4
9	W	1	SER	6.3
12	Z	173	LYS	5.9
1	O	249	ALA	5.6
12	L	163	GLY	5.5
12	Z	163	GLY	5.2
10	X	1	MET	5.2
12	Z	165	ASN	5.2
3	Q	240	GLU	5.1
1	O	2	THR	5.1
12	Z	168	VAL	5.0
12	L	165	ASN	4.9
5	E	202	ASP	4.9
3	Q	206	LYS	4.8
1	A	2	THR	4.7
12	L	162	PRO	4.6
2	B	220	ASN	4.5
8	V	224	GLN	4.5
3	C	202	GLN	4.4
5	S	202	ASP	4.3
2	P	59	ASP	4.3
12	Z	171	PRO	4.3
3	C	206	LYS	4.2
4	R	241	ALA	4.1
8	V	221	CYS	4.1
1	O	1	MET	4.1
2	B	218	GLY	4.1
10	J	1	MET	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	221	ASP	4.1
3	Q	238	LYS	4.0
14	b	195	GLN	4.0
11	Y	212	GLY	3.9
4	R	242	GLU	3.9
11	Y	208	ASN	3.9
6	T	244	ASN	3.8
8	V	222	ASP	3.7
4	R	217	GLN	3.6
2	P	218	GLY	3.5
8	H	222	ASP	3.5
5	E	233	ILE	3.5
6	F	244	ASN	3.4
10	J	194	ASP	3.4
2	P	221	ASP	3.4
12	L	173	LYS	3.3
2	B	182	ASP	3.3
3	Q	236	GLN	3.3
1	A	1	MET	3.3
3	C	238	LYS	3.3
6	F	229	GLY	3.3
5	S	187	GLU	3.2
8	H	221	CYS	3.2
2	P	51	VAL	3.2
5	E	231	LYS	3.2
3	C	49	THR	3.2
8	V	226	GLU	3.2
4	R	54	ASP	3.1
6	T	205	GLU	3.1
3	C	205	ALA	3.1
5	S	173	ARG	3.1
6	T	243	ILE	3.1
5	S	233	ILE	3.0
2	B	244	THR	3.0
12	L	168	VAL	3.0
8	H	226	GLU	3.0
1	O	250	LEU	3.0
8	V	225	GLU	3.0
3	C	239	GLN	3.0
1	A	249	ALA	3.0
12	L	170	LYS	3.0
5	S	207	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
7	U	183	ASP	2.9
11	K	208	ASN	2.9
7	U	181	LYS	2.9
12	Z	170	LYS	2.9
8	H	224	GLN	2.9
7	G	2	GLY	2.9
1	O	231	LYS	2.9
7	U	242	GLN	2.9
7	G	188	GLU	2.8
3	Q	48	SER	2.8
1	O	248	GLU	2.8
3	Q	239	GLN	2.8
11	Y	202	GLU	2.8
3	Q	180	LYS	2.8
14	N	195	GLN	2.8
3	Q	205	ALA	2.8
5	S	227	GLU	2.7
9	I	1	SER	2.7
3	C	203	THR	2.7
3	C	225	GLU	2.7
5	S	203	GLU	2.7
4	R	237	GLU	2.7
3	C	50	LEU	2.7
4	R	177	ASN	2.7
5	E	201	ARG	2.7
10	X	193	ASP	2.6
11	K	212	GLY	2.6
3	C	235	GLU	2.6
1	A	248	GLU	2.6
2	P	220	ASN	2.6
12	Z	167	LYS	2.6
14	b	105	LYS	2.5
3	C	236	GLN	2.5
12	L	156	PHE	2.5
8	V	9	ASN	2.5
7	U	222	ASP	2.5
7	G	179	LYS	2.5
12	Z	161	GLU	2.5
2	B	232	GLN	2.5
13	a	1	THR	2.5
2	B	51	VAL	2.5
5	S	194	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
13	M	1	THR	2.5
3	C	216	ASP	2.4
12	Z	210	ASP	2.4
10	X	194	ASP	2.4
5	S	177	THR	2.4
2	B	239	VAL	2.4
6	F	215	CYS	2.4
2	B	59	ASP	2.4
6	T	230	ASP	2.4
6	T	241	LYS	2.4
7	U	2	GLY	2.4
2	B	217	LYS	2.4
1	A	245	ASP	2.3
2	B	240	LYS	2.3
3	C	204	GLY	2.3
6	T	181	GLU	2.3
7	G	241	GLU	2.3
1	O	182	GLU	2.3
6	F	230	ASP	2.3
9	I	192	ASP	2.3
3	Q	237	GLU	2.3
6	T	215	CYS	2.3
5	S	231	LYS	2.3
3	Q	229	GLN	2.3
1	O	201	GLU	2.2
2	B	203	SER	2.2
3	C	48	SER	2.2
2	B	52	THR	2.2
4	D	242	GLU	2.2
12	L	171	PRO	2.2
2	B	235	LYS	2.2
3	Q	203	THR	2.2
6	T	237	ASP	2.2
9	W	192	ASP	2.2
4	R	141	ALA	2.2
5	S	58	TYR	2.2
8	H	198	GLU	2.2
11	K	147	ASP	2.2
6	T	2	THR	2.2
3	C	180	LYS	2.1
4	D	182	SER	2.1
1	A	231	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	O	4	ARG	2.1
8	H	225	GLU	2.1
3	C	240	GLU	2.1
8	V	30	ASN	2.1
5	S	180	LYS	2.1
1	O	228	PRO	2.1
8	H	217	ILE	2.1
8	H	215	GLU	2.1
7	G	3	TYR	2.1
6	F	181	GLU	2.1
13	M	121	SER	2.0
5	E	206	THR	2.0
6	T	180	PRO	2.0
5	S	163	ARG	2.0
8	V	223	ILE	2.0
1	A	182	GLU	2.0
3	C	232	THR	2.0
7	G	51	PRO	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
15	MG	K	302	1/1	0.82	0.12	55,55,55,55	0
15	MG	K	303	1/1	0.89	0.29	45,45,45,45	0
17	BO2	N	201	28/28	0.91	0.20	32,41,51,52	0
17	BO2	b	201	28/28	0.91	0.20	38,46,54,55	0
17	BO2	H	301	28/28	0.92	0.21	45,52,74,76	0

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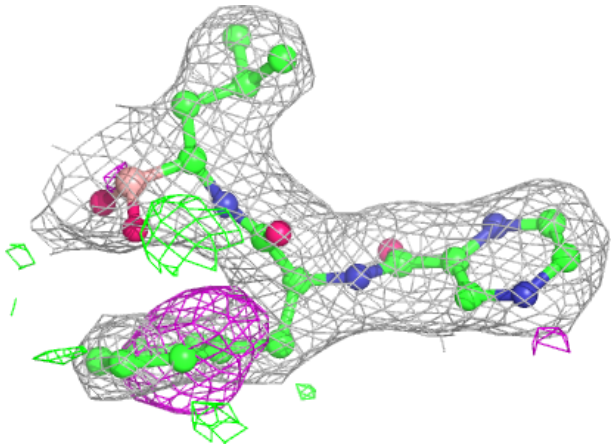
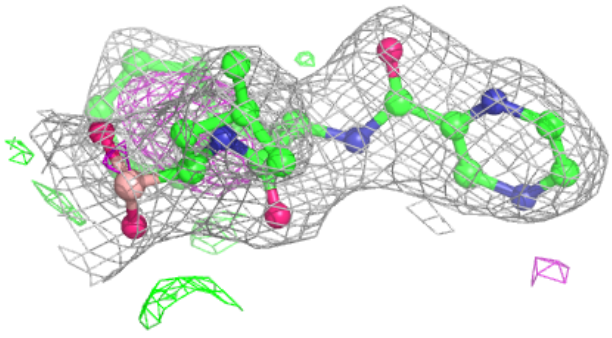
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	BO2	Y	301	28/28	0.93	0.17	42,52,67,68	0
17	BO2	K	301	28/28	0.93	0.19	38,47,61,63	0
15	MG	Y	302	1/1	0.94	0.08	52,52,52,52	0
17	BO2	V	301	28/28	0.94	0.20	44,49,73,77	0
15	MG	V	302	1/1	0.95	0.12	62,62,62,62	0
15	MG	I	301	1/1	0.95	0.24	63,63,63,63	0
15	MG	G	301	1/1	0.96	0.08	51,51,51,51	0
15	MG	J	201	1/1	0.97	0.17	42,42,42,42	0
16	CL	b	202	1/1	0.97	0.09	43,43,43,43	0
16	CL	N	203	1/1	0.98	0.07	41,41,41,41	0
15	MG	N	202	1/1	0.98	0.05	39,39,39,39	0
16	CL	U	301	1/1	0.99	0.14	38,38,38,38	0
16	CL	G	302	1/1	0.99	0.13	43,43,43,43	0

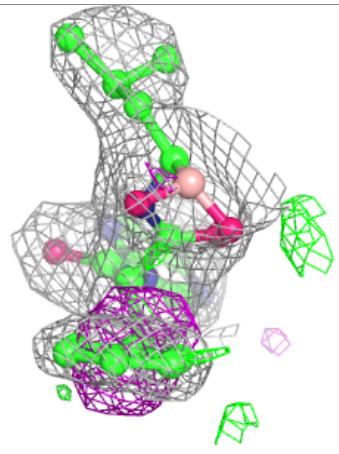
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BO2 N 201:

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

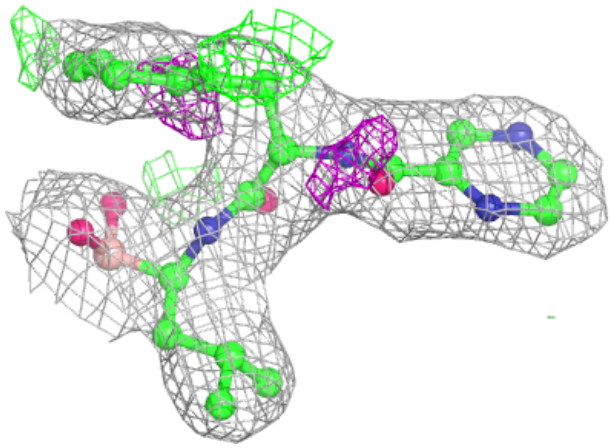


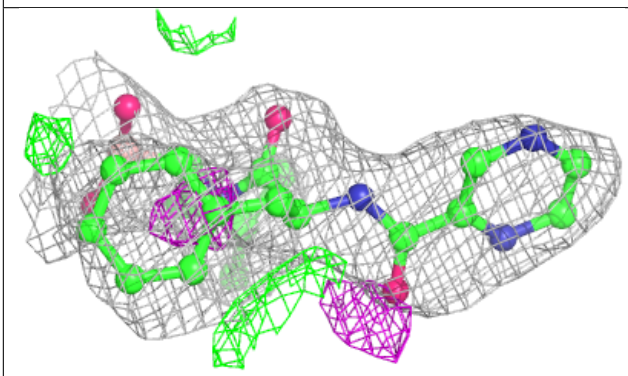


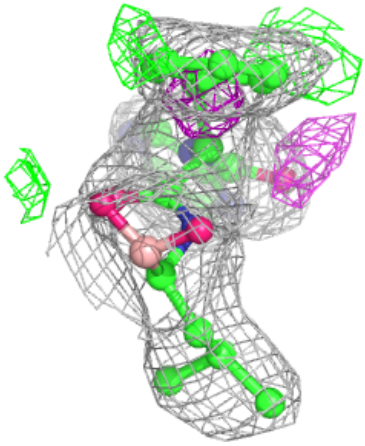


Electron density around BO2 b 201:

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

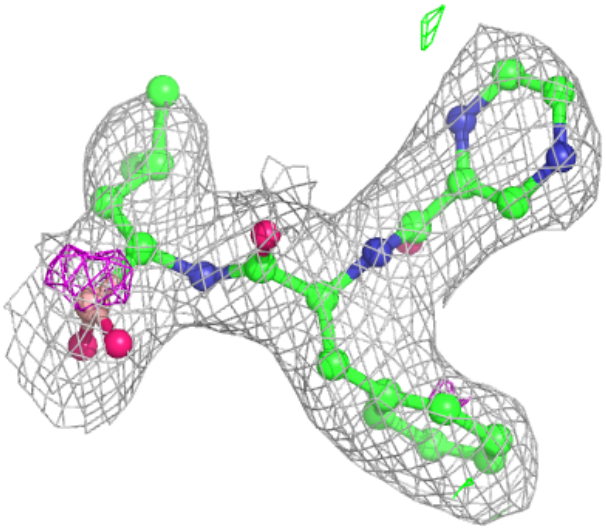


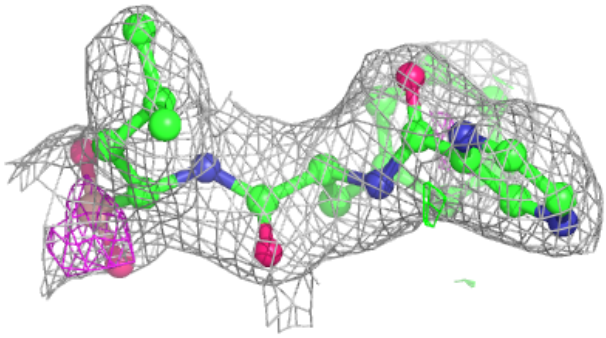


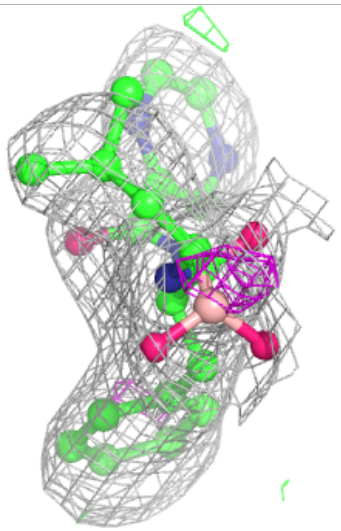


Electron density around BO2 H 301:

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

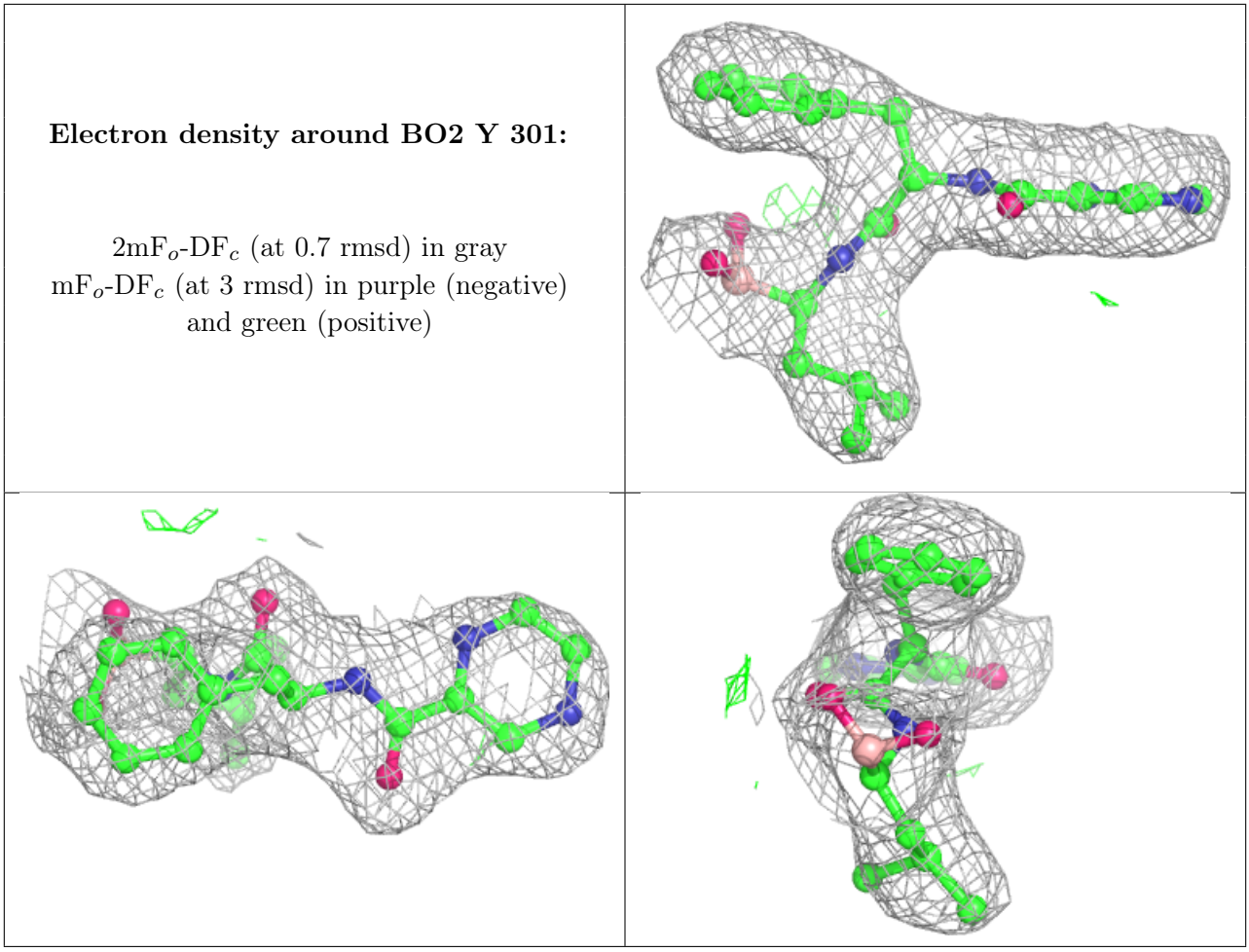






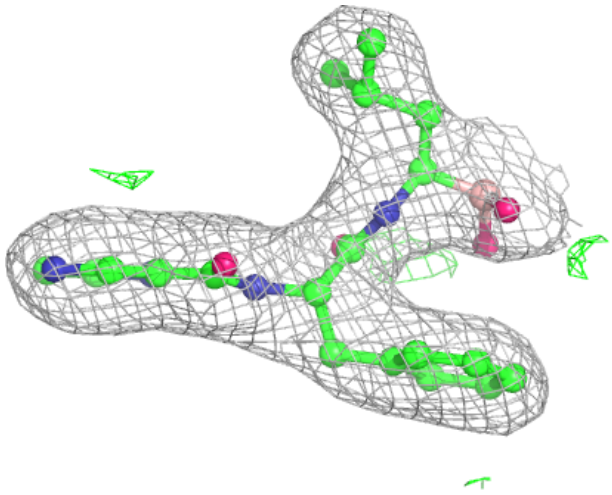
Electron density around BO2 Y 301:

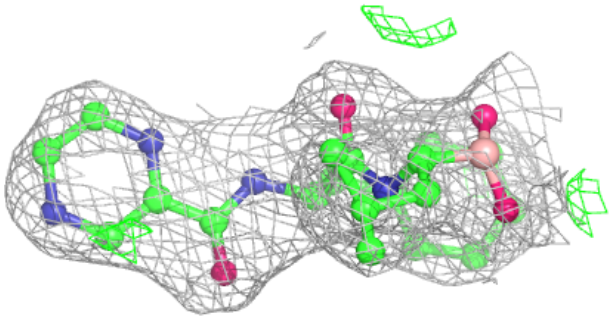
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

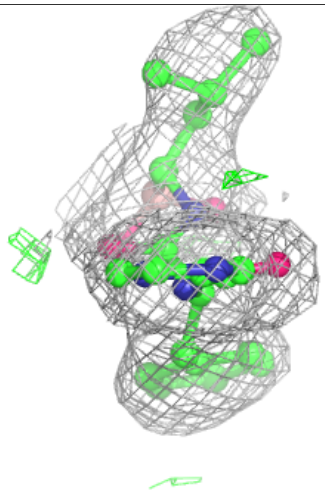


Electron density around BO2 K 301:

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

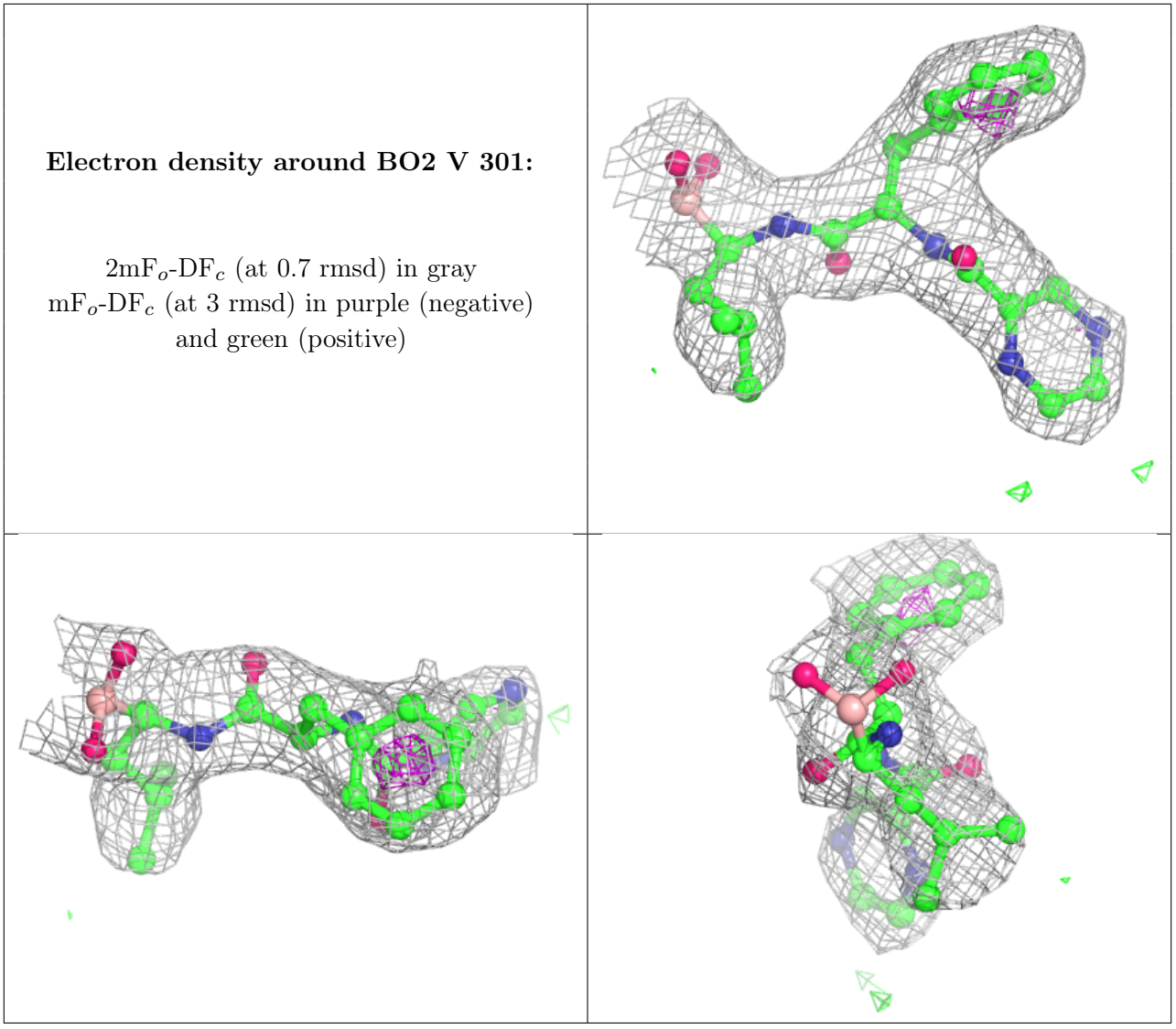






Electron density around BO2 V 301:

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



6.5 Other polymers (i)

There are no such residues in this entry.