



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 22, 2024 – 12:16 PM EDT

PDB ID : 4R67  
Title : Human constitutive 20S proteasome in complex with carfilzomib  
Authors : Sacchettini, J.C.; Harshbarger, W.H.  
Deposited on : 2014-08-22  
Resolution : 2.89 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

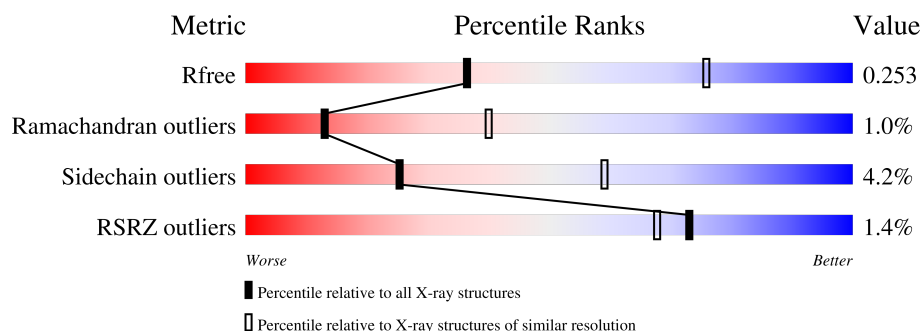
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.89 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.



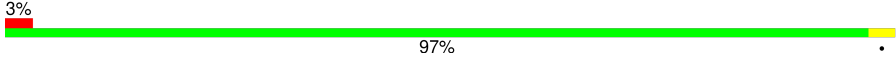
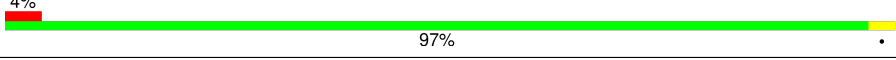
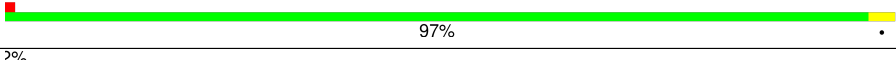
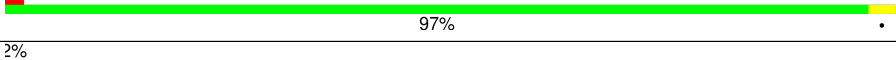
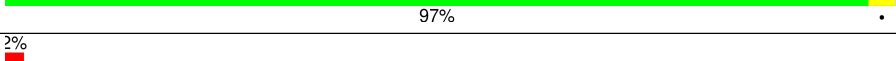
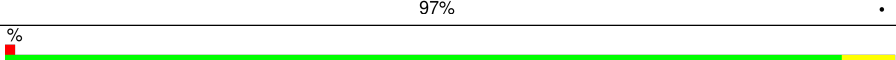
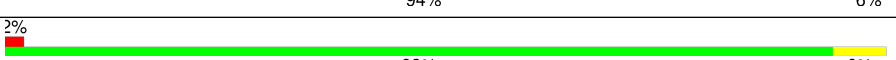
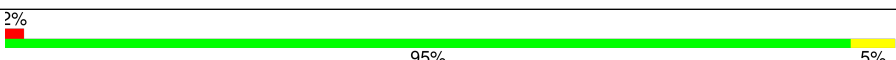
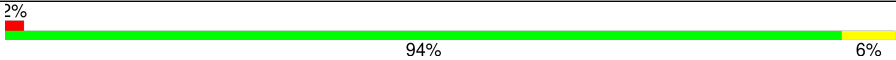
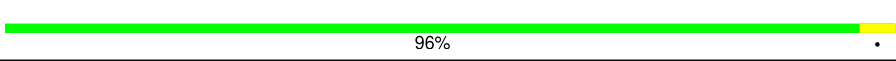
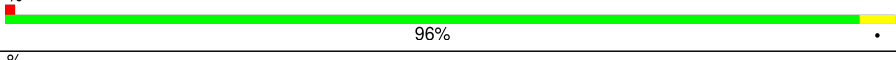
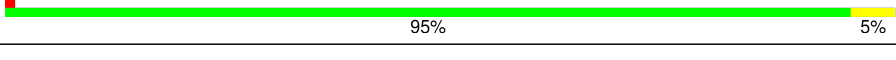
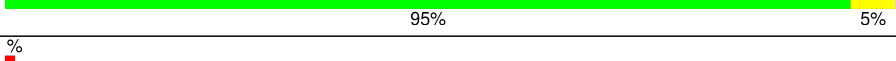
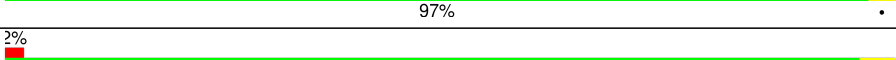
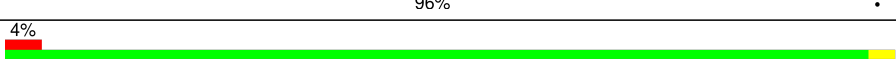
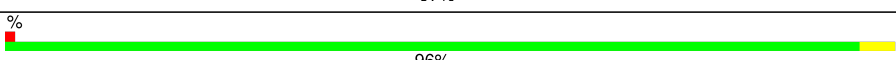
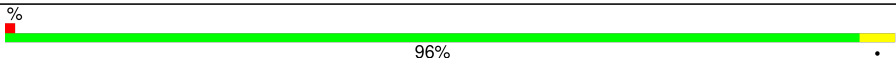
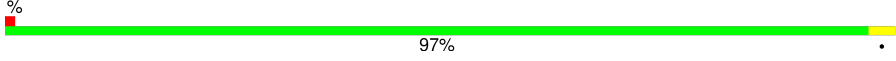
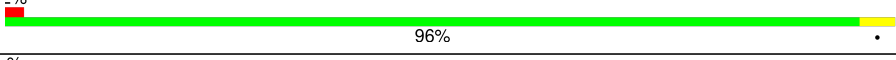
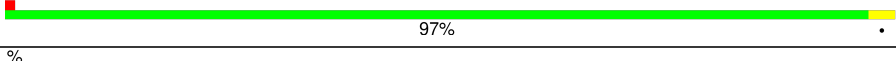
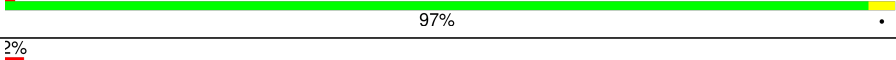
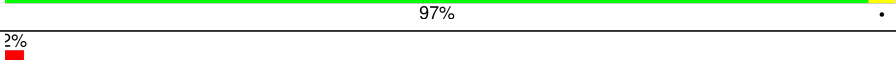
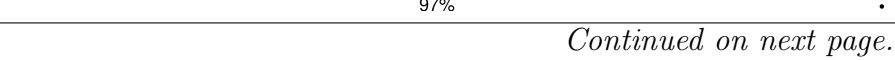


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	2335 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	244	<div> <div></div> <div>94%6%</div> </div>
1	O	244	<div> <div></div> <div>95%5%</div> </div>
1	c	244	<div> <div></div> <div>95%5%</div> </div>
1	q	244	<div> <div></div> <div>94%5%</div> </div>
2	B	233	<div> <div>3%</div> <div>97%.</div> </div>
2	P	233	<div> <div>3%</div> <div>97%.</div> </div>

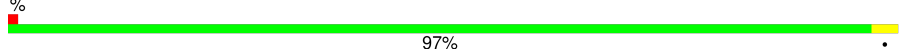
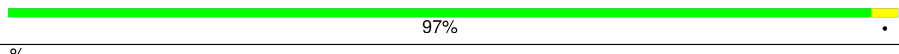
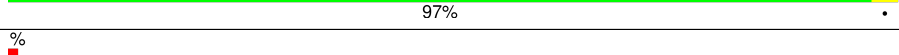
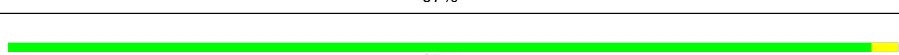
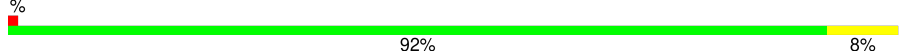
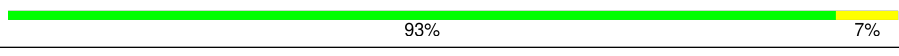
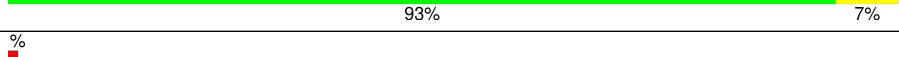
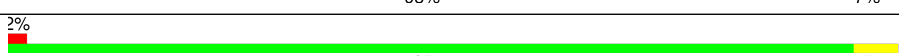
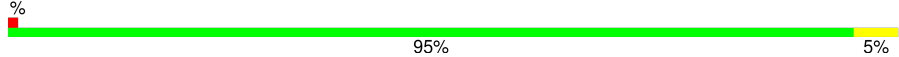
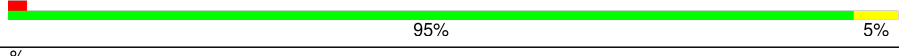
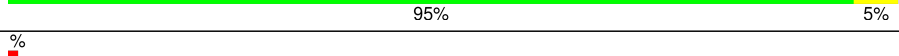
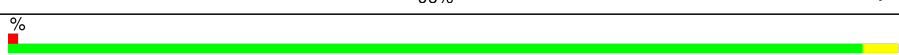
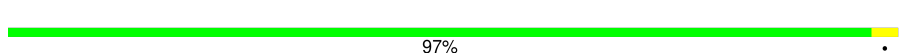
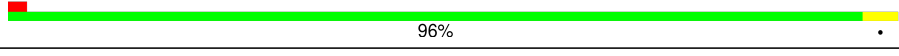
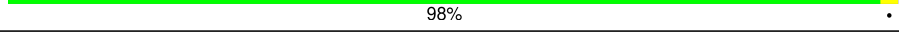
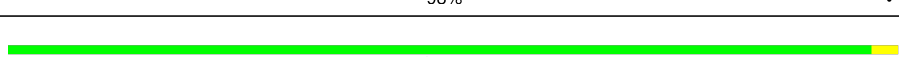
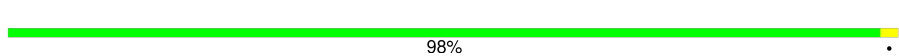
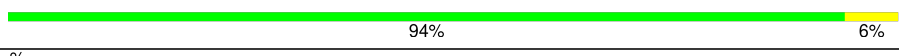
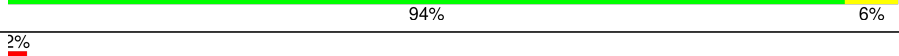
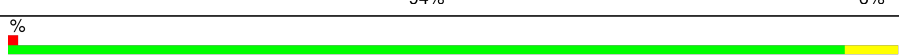



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Mol	Chain	Length	Quality of chain
2	d	233	
2	r	233	
3	C	250	
3	Q	250	
3	e	250	
3	s	250	
4	D	243	
4	R	243	
4	f	243	
4	t	243	
5	E	234	
5	S	234	
5	g	234	
5	u	234	
6	F	238	
6	T	238	
6	h	238	
6	v	238	
7	G	245	
7	U	245	
7	i	245	
7	w	245	
8	H	202	
8	V	202	
8	j	202	

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Mol	Chain	Length	Quality of chain	
8	x	202		.
9	I	220		.
9	W	220		.
9	k	220		.
9	y	220		.
10	J	204		.
10	X	204		.
10	l	204		.
10	z	204		.
11	0	199		.
11	K	199		.
11	Y	199		.
11	m	199		.
12	3	201		.
12	L	201		.
12	Z	201		.
12	n	201		.
13	1	213		.
13	M	213		.
13	a	213		.
13	o	213		.
14	2	217		.
14	N	217		.
14	b	217		.
14	p	217		.

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 96005 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-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1842	1170	309	350	13			
1	O	244	Total	C	N	O	S	0	0	0
			1845	1171	309	352	13			
1	c	244	Total	C	N	O	S	0	0	0
			1842	1170	309	350	13			
1	q	244	Total	C	N	O	S	0	0	0
			1842	1170	309	350	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	233	Total	C	N	O	S	0	0	0
			1713	1087	287	334	5			
2	P	233	Total	C	N	O	S	0	0	0
			1712	1085	287	334	6			
2	d	233	Total	C	N	O	S	0	0	0
			1710	1083	287	334	6			
2	r	233	Total	C	N	O	S	0	0	0
			1716	1090	287	334	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	250	Total	C	N	O	S	0	0	0
			1902	1195	329	370	8			
3	Q	250	Total	C	N	O	S	0	0	0
			1902	1195	329	370	8			
3	e	250	Total	C	N	O	S	0	0	0
			1902	1195	329	370	8			
3	s	250	Total	C	N	O	S	0	0	0
			1902	1195	329	370	8			

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	243	Total	C	N	O	S	0	0	0
			1684	1041	310	329	4			
4	R	243	Total	C	N	O	S	0	0	0
			1698	1053	312	329	4			
4	f	243	Total	C	N	O	S	0	0	0
			1668	1033	308	323	4			
4	t	243	Total	C	N	O	S	0	0	0
			1672	1035	309	324	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	234	Total	C	N	O	S	0	0	0
			1759	1102	290	356	11			
5	S	234	Total	C	N	O	S	0	0	0
			1759	1102	290	356	11			
5	g	234	Total	C	N	O	S	0	0	0
			1759	1102	290	356	11			
5	u	234	Total	C	N	O	S	0	0	0
			1763	1105	291	356	11			

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	238	Total	C	N	O	S	0	0	0
			1850	1159	334	346	11			
6	T	238	Total	C	N	O	S	0	0	0
			1850	1159	334	346	11			
6	h	238	Total	C	N	O	S	0	0	0
			1850	1159	334	346	11			
6	v	238	Total	C	N	O	S	0	0	0
			1850	1159	334	346	11			

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	245	Total	C	N	O	S	0	0	0
			1885	1195	319	360	11			
7	U	245	Total	C	N	O	S	0	0	0
			1885	1195	319	360	11			
7	i	245	Total	C	N	O	S	0	0	0
			1885	1195	319	360	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	w	245	Total	C	N	O	S	0	0	0
			1885	1195	319	360	11			

- Molecule 8 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	202	Total	C	N	O	S	0	0	0
			1509	945	258	294	12			
8	V	202	Total	C	N	O	S	0	0	0
			1509	945	258	294	12			
8	j	202	Total	C	N	O	S	0	0	0
			1509	945	258	294	12			
8	x	202	Total	C	N	O	S	0	0	0
			1509	945	258	294	12			

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	220	Total	C	N	O	S	0	0	0
			1643	1033	280	318	12			
9	W	220	Total	C	N	O	S	0	0	0
			1643	1033	280	318	12			
9	k	220	Total	C	N	O	S	0	0	0
			1643	1033	280	318	12			
9	y	220	Total	C	N	O	S	0	0	0
			1647	1035	280	320	12			

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	204	Total	C	N	O	S	0	0	0
			1585	1010	262	294	19			
10	X	204	Total	C	N	O	S	0	0	0
			1585	1010	262	294	19			
10	l	204	Total	C	N	O	S	0	0	0
			1585	1010	262	294	19			
10	z	204	Total	C	N	O	S	0	0	0
			1585	1010	262	294	19			

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	199	Total	C	N	O	S	0	0	0
			1570	1006	265	290	9			
11	Y	199	Total	C	N	O	S	0	0	0
			1570	1006	265	290	9			
11	m	199	Total	C	N	O	S	0	0	0
			1570	1006	265	290	9			
11	0	199	Total	C	N	O	S	0	0	0
			1570	1006	265	290	9			

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	201	Total	C	N	O	S	0	0	0
			1548	974	273	292	9			
12	Z	201	Total	C	N	O	S	0	0	0
			1551	977	273	292	9			
12	n	201	Total	C	N	O	S	0	0	0
			1548	974	273	292	9			
12	3	201	Total	C	N	O	S	0	0	0
			1551	977	273	292	9			

- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	213	Total	C	N	O	S	0	0	0
			1641	1036	282	313	10			
13	1	213	Total	C	N	O	S	0	0	0
			1639	1034	282	313	10			
13	o	213	Total	C	N	O	S	0	0	0
			1639	1034	282	313	10			
13	a	213	Total	C	N	O	S	0	0	0
			1639	1034	282	313	10			

- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	217	Total	C	N	O	S	0	0	0
			1676	1057	287	320	12			
14	2	217	Total	C	N	O	S	0	0	0
			1678	1058	290	318	12			
14	p	217	Total	C	N	O	S	0	0	0
			1672	1055	287	318	12			

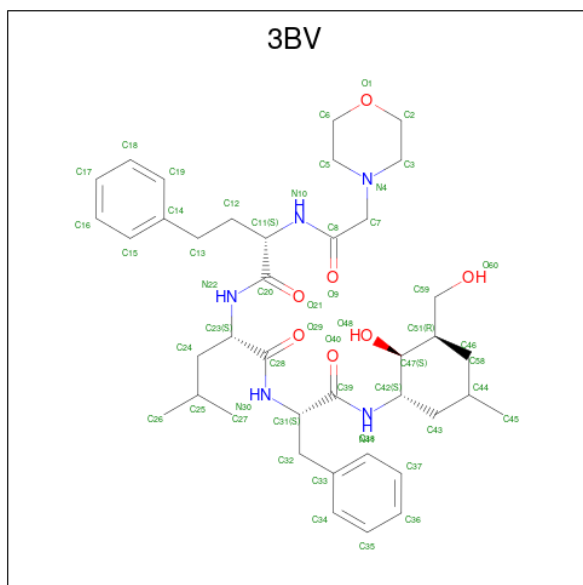
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	b	217	Total	C	N	O	S	0	0	0
			1669	1055	287	315	12			

- Molecule 15 is N-{(2S)-2-[(morpholin-4-ylacetyl)amino]-4-phenylbutanoyl}-L-leucyl-N-[(2R,3S,4S)-1,3-dihydroxy-2,6-dimethylheptan-4-yl]-L-phenylalaninamide (three-letter code: 3BV) (formula: C<sub>40</sub>H<sub>61</sub>N<sub>5</sub>O<sub>7</sub>).



*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	y	1	Total	C	N	O	0	0
			52	40	5	7		
15	3	1	Total	C	N	O	0	0
			52	40	5	7		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	O	0	0
			1	1		
16	B	4	Total	O	0	0
			4	4		
16	C	2	Total	O	0	0
			2	2		
16	D	1	Total	O	0	0
			1	1		
16	E	2	Total	O	0	0
			2	2		
16	F	4	Total	O	0	0
			4	4		
16	G	1	Total	O	0	0
			1	1		
16	H	1	Total	O	0	0
			1	1		
16	H	5	Total	O	0	0
			5	5		
16	I	1	Total	O	0	0
			1	1		
16	I	6	Total	O	0	0
			6	6		
16	J	2	Total	O	0	0
			2	2		
16	K	5	Total	O	0	0
			5	5		
16	L	1	Total	O	0	0
			1	1		
16	L	2	Total	O	0	0
			2	2		
16	M	8	Total	O	0	0
			8	8		
16	N	3	Total	O	0	0
			3	3		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	O	6	Total O 6 6	0	0
16	P	3	Total O 3 3	0	0
16	Q	9	Total O 9 9	0	0
16	R	2	Total O 2 2	0	0
16	S	1	Total O 1 1	0	0
16	U	2	Total O 2 2	0	0
16	V	1	Total O 1 1	0	0
16	V	3	Total O 3 3	0	0
16	W	1	Total O 1 1	0	0
16	W	4	Total O 4 4	0	0
16	X	9	Total O 9 9	0	0
16	Y	8	Total O 8 8	0	0
16	Z	1	Total O 1 1	0	0
16	Z	7	Total O 7 7	0	0
16	1	5	Total O 5 5	0	0
16	2	5	Total O 5 5	0	0
16	c	3	Total O 3 3	0	0
16	d	1	Total O 1 1	0	0
16	e	5	Total O 5 5	0	0
16	f	1	Total O 1 1	0	0
16	h	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	i	4	Total O 4 4	0	0
16	j	1	Total O 1 1	0	0
16	j	1	Total O 1 1	0	0
16	k	1	Total O 1 1	0	0
16	k	5	Total O 5 5	0	0
16	l	7	Total O 7 7	0	0
16	m	5	Total O 5 5	0	0
16	n	1	Total O 1 1	0	0
16	n	4	Total O 4 4	0	0
16	o	10	Total O 10 10	0	0
16	p	2	Total O 2 2	0	0
16	q	3	Total O 3 3	0	0
16	r	3	Total O 3 3	0	0
16	s	5	Total O 5 5	0	0
16	u	1	Total O 1 1	0	0
16	v	2	Total O 2 2	0	0
16	w	2	Total O 2 2	0	0
16	x	3	Total O 3 3	0	0
16	y	8	Total O 8 8	0	0
16	z	2	Total O 2 2	0	0
16	0	3	Total O 3 3	0	0

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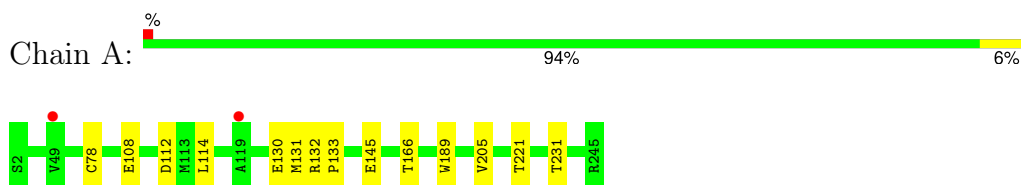
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	3	1	Total 1	O 1	0	0
16	3	6	Total 6	O 6	0	0
16	a	6	Total 6	O 6	0	0
16	b	5	Total 5	O 5	0	0

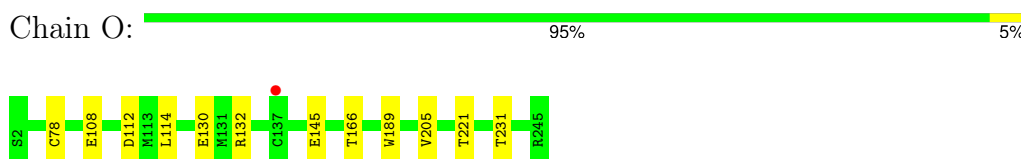
### 3 Residue-property plots [i](#)

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.

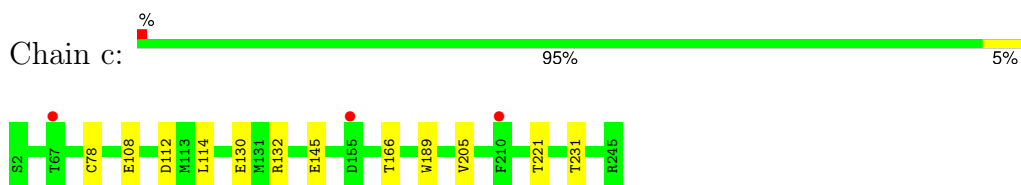
- Molecule 1: Proteasome subunit alpha type-6



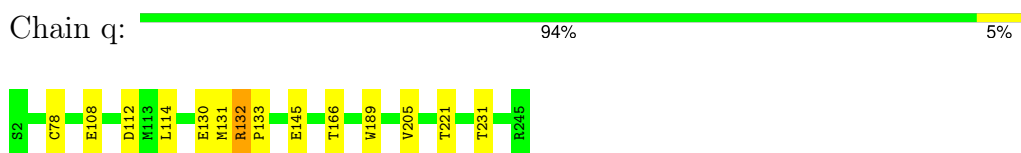
- Molecule 1: Proteasome subunit alpha type-6



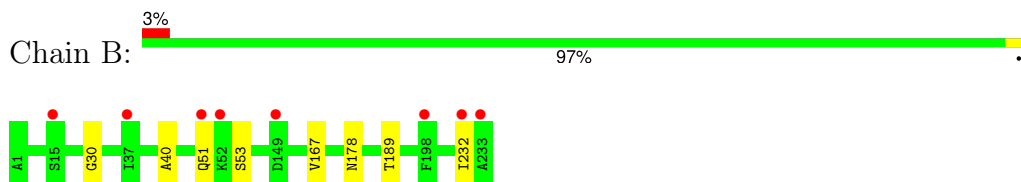
- Molecule 1: Proteasome subunit alpha type-6



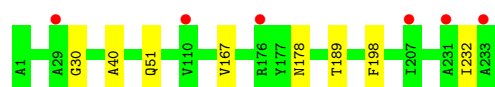
- Molecule 1: Proteasome subunit alpha type-6



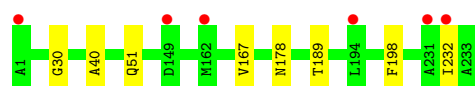
- Molecule 2: Proteasome subunit alpha type-2



- Molecule 2: Proteasome subunit alpha type-2



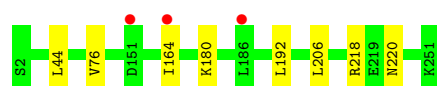
- Molecule 2: Proteasome subunit alpha type-2



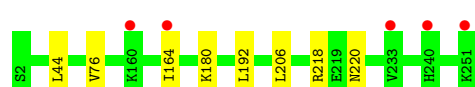
- Molecule 2: Proteasome subunit alpha type-2



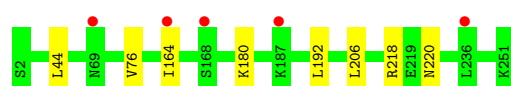
- Molecule 3: Proteasome subunit alpha type-4



- Molecule 3: Proteasome subunit alpha type-4



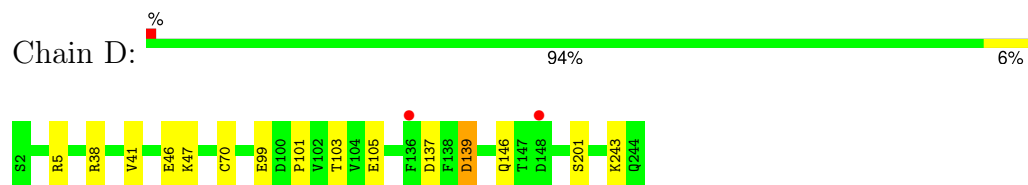
- Molecule 3: Proteasome subunit alpha type-4



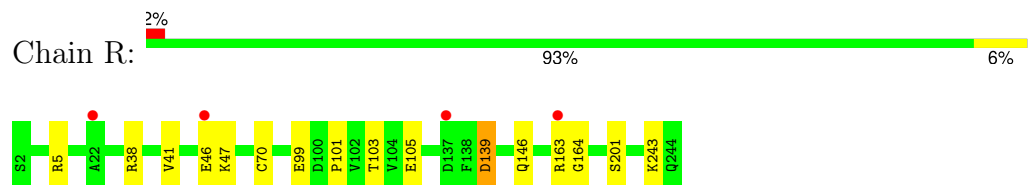
- Molecule 3: Proteasome subunit alpha type-4



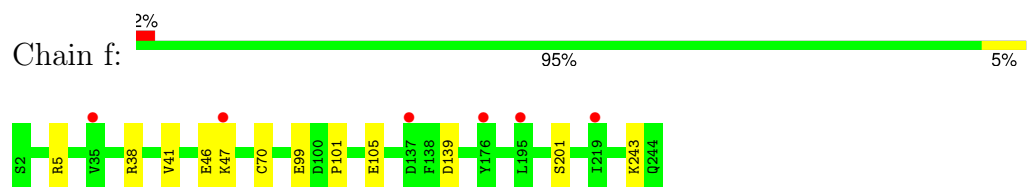
- Molecule 4: Proteasome subunit alpha type-7



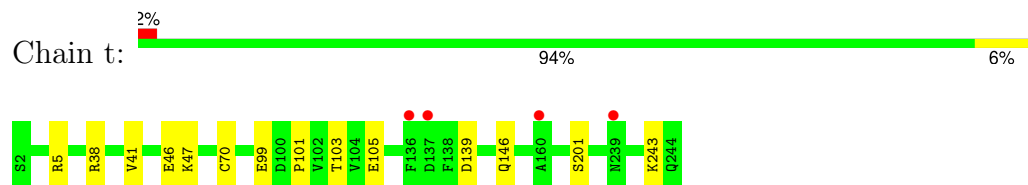
- Molecule 4: Proteasome subunit alpha type-7



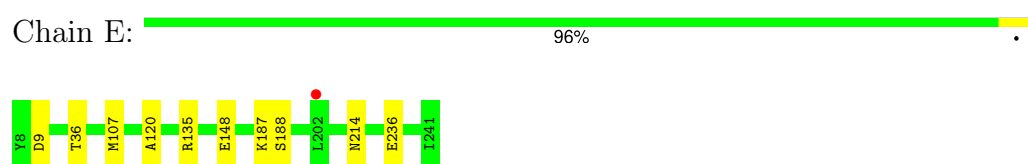
- Molecule 4: Proteasome subunit alpha type-7



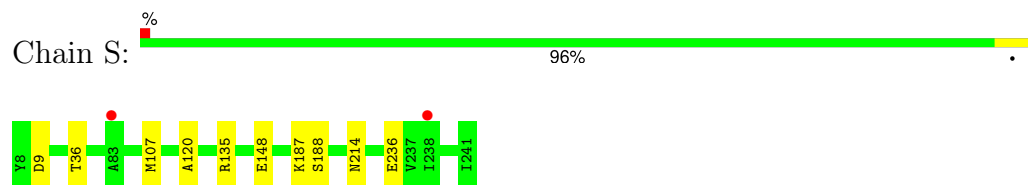
- Molecule 4: Proteasome subunit alpha type-7



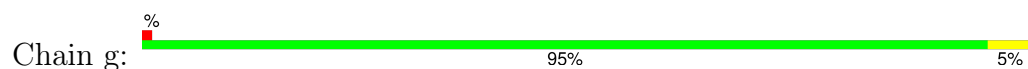
- Molecule 5: Proteasome subunit alpha type-5



- Molecule 5: Proteasome subunit alpha type-5



- Molecule 5: Proteasome subunit alpha type-5







- Molecule 5: Proteasome subunit alpha type-5



- Molecule 6: Proteasome subunit alpha type-1



- Molecule 6: Proteasome subunit alpha type-1



- Molecule 6: Proteasome subunit alpha type-1



- Molecule 6: Proteasome subunit alpha type-1



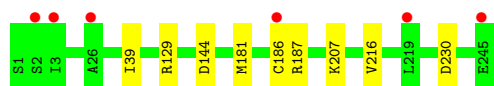
- Molecule 7: Proteasome subunit alpha type-3



- Molecule 7: Proteasome subunit alpha type-3



- Molecule 7: Proteasome subunit alpha type-3



- Molecule 7: Proteasome subunit alpha type-3



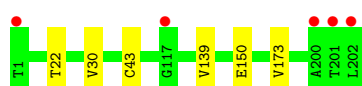
- Molecule 8: Proteasome subunit beta type-6



- Molecule 8: Proteasome subunit beta type-6



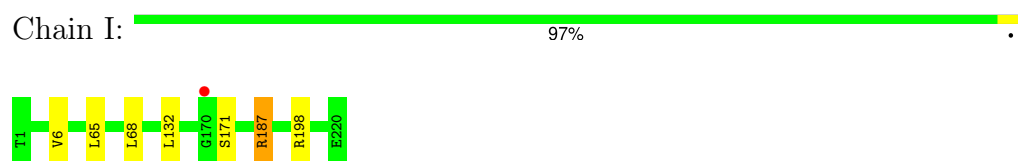
- Molecule 8: Proteasome subunit beta type-6



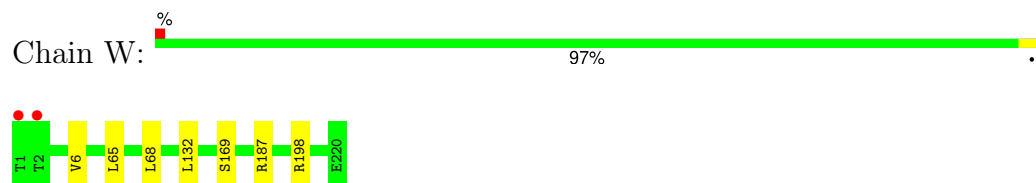
- Molecule 8: Proteasome subunit beta type-6



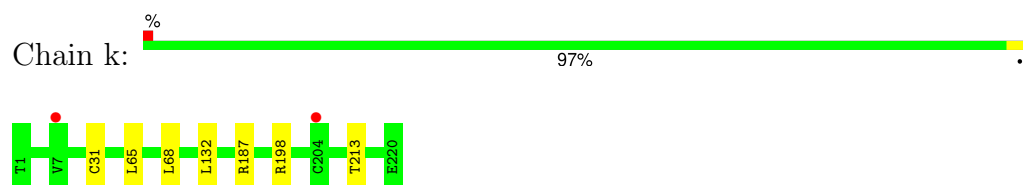
- Molecule 9: Proteasome subunit beta type-7



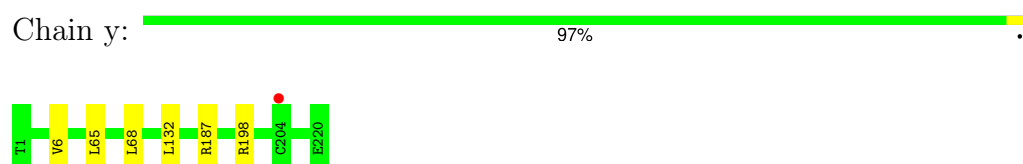
- Molecule 9: Proteasome subunit beta type-7



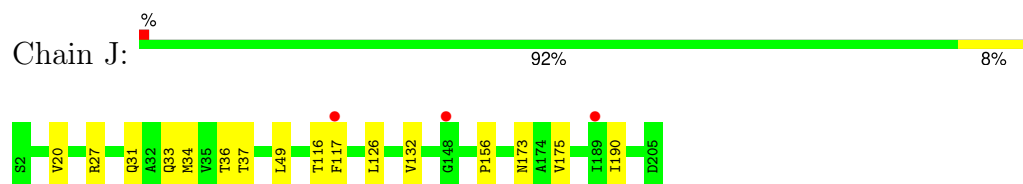
- Molecule 9: Proteasome subunit beta type-7



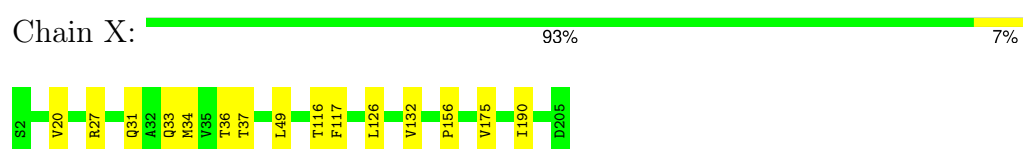
- Molecule 9: Proteasome subunit beta type-7



- Molecule 10: Proteasome subunit beta type-3



- Molecule 10: Proteasome subunit beta type-3

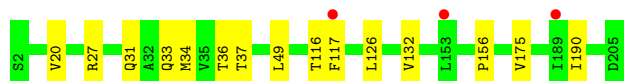
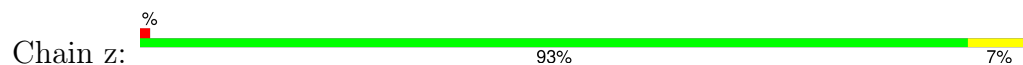


- Molecule 10: Proteasome subunit beta type-3





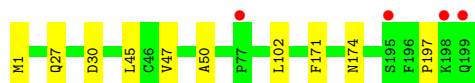
- Molecule 10: Proteasome subunit beta type-3



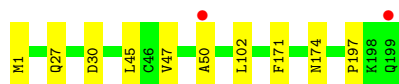
- Molecule 11: Proteasome subunit beta type-2



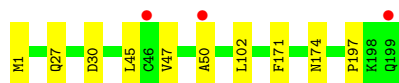
- Molecule 11: Proteasome subunit beta type-2



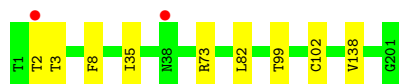
- Molecule 11: Proteasome subunit beta type-2



- Molecule 11: Proteasome subunit beta type-2



- Molecule 12: Proteasome subunit beta type-5



- Molecule 12: Proteasome subunit beta type-5

Chain Z:  97% .



- Molecule 12: Proteasome subunit beta type-5

Chain n:  96% .



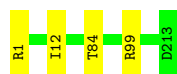
- Molecule 12: Proteasome subunit beta type-5

Chain 3:  96% .



- Molecule 13: Proteasome subunit beta type-1

Chain M:  98% .



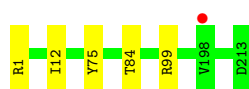
- Molecule 13: Proteasome subunit beta type-1

Chain 1:  98% .



- Molecule 13: Proteasome subunit beta type-1

Chain o:  98% .



- Molecule 13: Proteasome subunit beta type-1

Chain a:  97% .



- Molecule 14: Proteasome subunit beta type-4



- Molecule 14: Proteasome subunit beta type-4



- Molecule 14: Proteasome subunit beta type-4



- Molecule 14: Proteasome subunit beta type-4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	171.99Å 201.03Å 225.59Å 90.00° 107.93° 90.00°	Depositor
Resolution (Å)	33.51 – 2.89 33.51 – 2.89	Depositor EDS
% Data completeness (in resolution range)	98.6 (33.51-2.89) 98.7 (33.51-2.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.215 , 0.245 0.223 , 0.253	Depositor DCC
$R_{free}$ test set	16212 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.6	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	96005	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3BV

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	0.26	1/1875 (0.1%)	0.43	0/2545
1	O	0.23	0/1878	0.41	0/2549
1	c	0.23	0/1875	0.41	0/2545
1	q	0.27	1/1875 (0.1%)	0.44	1/2545 (0.0%)
2	B	0.23	0/1749	0.41	0/2381
2	P	0.23	0/1747	0.41	0/2378
2	d	0.24	0/1745	0.41	0/2375
2	r	0.25	0/1752	0.41	0/2385
3	C	0.23	0/1931	0.41	0/2613
3	Q	0.23	0/1931	0.41	0/2613
3	e	0.23	0/1931	0.41	0/2613
3	s	0.23	0/1931	0.41	0/2613
4	D	0.22	0/1707	0.41	0/2335
4	R	0.23	0/1723	0.43	0/2355
4	f	0.22	0/1691	0.41	0/2314
4	t	0.21	0/1695	0.41	0/2319
5	E	0.22	0/1786	0.41	0/2419
5	S	0.22	0/1786	0.41	0/2419
5	g	0.23	0/1786	0.42	0/2419
5	u	0.22	0/1790	0.41	0/2423
6	F	0.24	0/1885	0.42	0/2552
6	T	0.26	1/1885 (0.1%)	0.43	0/2552
6	h	0.23	0/1885	0.43	0/2552
6	v	0.23	0/1885	0.43	0/2552
7	G	0.32	0/1920	0.42	0/2591
7	U	0.22	0/1920	0.39	0/2591
7	i	0.22	0/1920	0.39	0/2591
7	w	0.22	0/1920	0.39	0/2591
8	H	0.27	0/1535	0.43	0/2078
8	V	0.23	0/1535	0.42	0/2078
8	j	0.23	0/1535	0.42	0/2078
8	x	0.23	0/1535	0.42	0/2078



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
9	I	0.28	0/1670	0.43	0/2265
9	W	0.24	0/1670	0.43	0/2265
9	k	0.23	0/1670	0.43	0/2265
9	y	0.23	0/1674	0.43	0/2270
10	J	0.28	1/1614 (0.1%)	0.42	0/2177
10	X	0.25	0/1614	0.43	0/2177
10	l	0.25	0/1614	0.42	0/2177
10	z	0.32	0/1614	0.44	0/2177
11	0	0.22	0/1603	0.42	0/2174
11	K	0.22	0/1603	0.42	0/2174
11	Y	0.22	0/1603	0.42	0/2174
11	m	0.23	0/1603	0.41	0/2174
12	3	0.23	0/1582	0.44	2/2138 (0.1%)
12	L	0.27	1/1579 (0.1%)	0.44	2/2134 (0.1%)
12	Z	0.23	0/1582	0.40	0/2138
12	n	0.28	0/1579	0.45	2/2134 (0.1%)
13	1	0.24	0/1669	0.43	0/2250
13	M	0.24	0/1671	0.43	0/2253
13	a	0.27	0/1669	0.45	0/2250
13	o	0.32	1/1669 (0.1%)	0.45	0/2250
14	2	0.23	0/1711	0.42	0/2319
14	N	0.23	0/1709	0.42	0/2317
14	b	0.23	0/1702	0.42	0/2306
14	p	0.23	0/1705	0.42	0/2312
All	All	0.24	6/96923 (0.0%)	0.42	7/131312 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	3	THR	C-N	-5.74	1.20	1.34
1	q	133	PRO	N-CD	5.28	1.55	1.47
1	A	133	PRO	N-CD	5.28	1.55	1.47
6	T	240	PRO	N-CD	5.25	1.55	1.47
10	J	173	ASN	CG-ND2	-5.05	1.20	1.32

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	n	73	ARG	NE-CZ-NH2	-5.93	117.34	120.30
12	3	73	ARG	NE-CZ-NH2	-5.89	117.35	120.30
12	L	73	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	q	132	ARG	C-N-CD	5.59	140.15	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	73	ARG	NE-CZ-NH1	5.58	123.09	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	242/244 (99%)	229 (95%)	12 (5%)	1 (0%)	30	60
1	O	242/244 (99%)	228 (94%)	13 (5%)	1 (0%)	30	60
1	c	242/244 (99%)	229 (95%)	12 (5%)	1 (0%)	30	60
1	q	242/244 (99%)	229 (95%)	12 (5%)	1 (0%)	30	60
2	B	231/233 (99%)	209 (90%)	17 (7%)	5 (2%)	5	21
2	P	231/233 (99%)	208 (90%)	18 (8%)	5 (2%)	5	21
2	d	231/233 (99%)	209 (90%)	17 (7%)	5 (2%)	5	21
2	r	231/233 (99%)	208 (90%)	19 (8%)	4 (2%)	7	27
3	C	248/250 (99%)	236 (95%)	11 (4%)	1 (0%)	30	60
3	Q	248/250 (99%)	236 (95%)	11 (4%)	1 (0%)	30	60
3	e	248/250 (99%)	236 (95%)	11 (4%)	1 (0%)	30	60
3	s	248/250 (99%)	236 (95%)	11 (4%)	1 (0%)	30	60
4	D	241/243 (99%)	225 (93%)	10 (4%)	6 (2%)	4	18
4	R	241/243 (99%)	222 (92%)	13 (5%)	6 (2%)	4	18
4	f	241/243 (99%)	225 (93%)	10 (4%)	6 (2%)	4	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	t	241/243 (99%)	225 (93%)	10 (4%)	6 (2%)	4	18
5	E	232/234 (99%)	220 (95%)	9 (4%)	3 (1%)	10	33
5	S	232/234 (99%)	220 (95%)	9 (4%)	3 (1%)	10	33
5	g	232/234 (99%)	219 (94%)	10 (4%)	3 (1%)	10	33
5	u	232/234 (99%)	220 (95%)	9 (4%)	3 (1%)	10	33
6	F	236/238 (99%)	227 (96%)	9 (4%)	0	100	100
6	T	236/238 (99%)	228 (97%)	6 (2%)	2 (1%)	16	45
6	h	236/238 (99%)	229 (97%)	6 (2%)	1 (0%)	30	60
6	v	236/238 (99%)	227 (96%)	6 (2%)	3 (1%)	10	33
7	G	243/245 (99%)	229 (94%)	12 (5%)	2 (1%)	16	45
7	U	243/245 (99%)	230 (95%)	11 (4%)	2 (1%)	16	45
7	i	243/245 (99%)	229 (94%)	12 (5%)	2 (1%)	16	45
7	w	243/245 (99%)	231 (95%)	9 (4%)	3 (1%)	11	35
8	H	200/202 (99%)	194 (97%)	5 (2%)	1 (0%)	25	56
8	V	200/202 (99%)	194 (97%)	5 (2%)	1 (0%)	25	56
8	j	200/202 (99%)	192 (96%)	7 (4%)	1 (0%)	25	56
8	x	200/202 (99%)	194 (97%)	5 (2%)	1 (0%)	25	56
9	I	218/220 (99%)	205 (94%)	11 (5%)	2 (1%)	14	43
9	W	218/220 (99%)	204 (94%)	13 (6%)	1 (0%)	25	56
9	k	218/220 (99%)	206 (94%)	11 (5%)	1 (0%)	25	56
9	y	218/220 (99%)	206 (94%)	11 (5%)	1 (0%)	25	56
10	J	202/204 (99%)	191 (95%)	7 (4%)	4 (2%)	6	23
10	X	202/204 (99%)	191 (95%)	7 (4%)	4 (2%)	6	23
10	l	202/204 (99%)	191 (95%)	7 (4%)	4 (2%)	6	23
10	z	202/204 (99%)	190 (94%)	8 (4%)	4 (2%)	6	23
11	0	197/199 (99%)	187 (95%)	7 (4%)	3 (2%)	8	29
11	K	197/199 (99%)	187 (95%)	7 (4%)	3 (2%)	8	29
11	Y	197/199 (99%)	187 (95%)	7 (4%)	3 (2%)	8	29
11	m	197/199 (99%)	187 (95%)	7 (4%)	3 (2%)	8	29
12	3	199/201 (99%)	185 (93%)	14 (7%)	0	100	100
12	L	199/201 (99%)	186 (94%)	12 (6%)	1 (0%)	25	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	Z	199/201 (99%)	186 (94%)	13 (6%)	0	100	100
12	n	199/201 (99%)	184 (92%)	15 (8%)	0	100	100
13	1	211/213 (99%)	207 (98%)	4 (2%)	0	100	100
13	M	211/213 (99%)	206 (98%)	5 (2%)	0	100	100
13	a	211/213 (99%)	207 (98%)	4 (2%)	0	100	100
13	o	211/213 (99%)	206 (98%)	5 (2%)	0	100	100
14	2	215/217 (99%)	199 (93%)	13 (6%)	3 (1%)	9	31
14	N	215/217 (99%)	199 (93%)	14 (6%)	2 (1%)	14	43
14	b	215/217 (99%)	199 (93%)	13 (6%)	3 (1%)	9	31
14	p	215/217 (99%)	199 (93%)	14 (6%)	2 (1%)	14	43
All	All	12460/12572 (99%)	11768 (94%)	566 (4%)	126 (1%)	13	40

5 of 126 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	232	ILE
4	D	47	LYS
9	I	187	ARG
10	J	117	PHE
10	J	156	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	192/208 (92%)	180 (94%)	12 (6%)	15	42
1	O	193/208 (93%)	182 (94%)	11 (6%)	17	47
1	c	192/208 (92%)	181 (94%)	11 (6%)	17	47
1	q	192/208 (92%)	180 (94%)	12 (6%)	15	42
2	B	164/190 (86%)	161 (98%)	3 (2%)	54	82
2	P	165/190 (87%)	162 (98%)	3 (2%)	54	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	d	164/190 (86%)	161 (98%)	3 (2%)	54	82
2	r	165/190 (87%)	162 (98%)	3 (2%)	54	82
3	C	191/210 (91%)	184 (96%)	7 (4%)	29	64
3	Q	191/210 (91%)	184 (96%)	7 (4%)	29	64
3	e	191/210 (91%)	184 (96%)	7 (4%)	29	64
3	s	191/210 (91%)	184 (96%)	7 (4%)	29	64
4	D	142/207 (69%)	132 (93%)	10 (7%)	12	36
4	R	143/207 (69%)	132 (92%)	11 (8%)	10	31
4	f	137/207 (66%)	131 (96%)	6 (4%)	24	57
4	t	138/207 (67%)	130 (94%)	8 (6%)	17	46
5	E	189/196 (96%)	182 (96%)	7 (4%)	29	64
5	S	189/196 (96%)	182 (96%)	7 (4%)	29	64
5	g	189/196 (96%)	181 (96%)	8 (4%)	25	59
5	u	190/196 (97%)	182 (96%)	8 (4%)	25	59
6	F	198/204 (97%)	190 (96%)	8 (4%)	27	61
6	T	198/204 (97%)	190 (96%)	8 (4%)	27	61
6	h	198/204 (97%)	191 (96%)	7 (4%)	31	66
6	v	198/204 (97%)	190 (96%)	8 (4%)	27	61
7	G	195/202 (96%)	186 (95%)	9 (5%)	23	55
7	U	195/202 (96%)	190 (97%)	5 (3%)	41	74
7	i	195/202 (96%)	188 (96%)	7 (4%)	30	65
7	w	195/202 (96%)	190 (97%)	5 (3%)	41	74
8	H	155/157 (99%)	150 (97%)	5 (3%)	34	69
8	V	155/157 (99%)	150 (97%)	5 (3%)	34	69
8	j	155/157 (99%)	150 (97%)	5 (3%)	34	69
8	x	155/157 (99%)	150 (97%)	5 (3%)	34	69
9	I	177/181 (98%)	171 (97%)	6 (3%)	32	67
9	W	177/181 (98%)	171 (97%)	6 (3%)	32	67
9	k	177/181 (98%)	171 (97%)	6 (3%)	32	67
9	y	178/181 (98%)	173 (97%)	5 (3%)	38	73
10	J	172/173 (99%)	161 (94%)	11 (6%)	14	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	X	172/173 (99%)	161 (94%)	11 (6%)	14	41
10	l	172/173 (99%)	161 (94%)	11 (6%)	14	41
10	z	172/173 (99%)	161 (94%)	11 (6%)	14	41
11	0	164/170 (96%)	157 (96%)	7 (4%)	25	57
11	K	164/170 (96%)	157 (96%)	7 (4%)	25	57
11	Y	164/170 (96%)	157 (96%)	7 (4%)	25	57
11	m	164/170 (96%)	157 (96%)	7 (4%)	25	57
12	3	154/156 (99%)	146 (95%)	8 (5%)	19	50
12	L	153/156 (98%)	147 (96%)	6 (4%)	27	62
12	Z	154/156 (99%)	147 (96%)	7 (4%)	23	56
12	n	153/156 (98%)	145 (95%)	8 (5%)	19	50
13	1	173/178 (97%)	169 (98%)	4 (2%)	45	77
13	M	174/178 (98%)	170 (98%)	4 (2%)	45	77
13	a	173/178 (97%)	167 (96%)	6 (4%)	31	66
13	o	173/178 (97%)	169 (98%)	4 (2%)	45	77
14	2	175/179 (98%)	165 (94%)	10 (6%)	17	47
14	N	175/179 (98%)	165 (94%)	10 (6%)	17	47
14	b	174/179 (97%)	164 (94%)	10 (6%)	17	47
14	p	174/179 (97%)	164 (94%)	10 (6%)	17	47
All	All	9758/10444 (93%)	9348 (96%)	410 (4%)	25	59

5 of 410 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	f	70	CYS
12	n	8	PHE
13	a	109	ILE
5	g	148	GLU
8	j	173	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
10	l	173	ASN

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Mol	Chain	Res	Type
13	o	146	GLN
13	a	146	GLN
5	u	152	GLN
10	z	173	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
15	3BV	H	301	8	54,54,54	2.66	11 (20%)	68,71,71	1.59	10 (14%)
15	3BV	3	301	12	54,54,54	2.44	12 (22%)	68,71,71	1.64	10 (14%)
15	3BV	L	301	-	54,54,54	2.45	13 (24%)	68,71,71	1.95	18 (26%)
15	3BV	n	301	12	54,54,54	2.66	13 (24%)	68,71,71	2.25	23 (33%)
15	3BV	I	301	-	54,54,54	2.69	15 (27%)	68,71,71	2.07	16 (23%)
15	3BV	j	301	8	54,54,54	2.45	10 (18%)	68,71,71	2.37	20 (29%)
15	3BV	y	301	9	54,54,54	2.77	13 (24%)	68,71,71	1.90	9 (13%)
15	3BV	W	301	-	54,54,54	2.44	12 (22%)	68,71,71	2.00	21 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	3BV	Z	301	12	54,54,54	3.02	16 (29%)	68,71,71	3.18	22 (32%)
15	3BV	k	301	9	54,54,54	2.56	13 (24%)	68,71,71	1.83	17 (25%)
15	3BV	V	301	8	54,54,54	2.43	11 (20%)	68,71,71	1.58	8 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	3BV	H	301	8	-	22/59/67/67	0/3/3/3
15	3BV	3	301	12	-	19/59/67/67	0/3/3/3
15	3BV	L	301	-	-	16/59/67/67	0/3/3/3
15	3BV	n	301	12	-	18/59/67/67	0/3/3/3
15	3BV	I	301	-	-	18/59/67/67	0/3/3/3
15	3BV	j	301	8	-	29/59/67/67	0/3/3/3
15	3BV	y	301	9	-	22/59/67/67	0/3/3/3
15	3BV	W	301	-	-	22/59/67/67	0/3/3/3
15	3BV	Z	301	12	-	22/59/67/67	0/3/3/3
15	3BV	k	301	9	-	14/59/67/67	0/3/3/3
15	3BV	V	301	8	-	26/59/67/67	0/3/3/3

The worst 5 of 139 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	I	301	3BV	O48-C47	-12.33	1.12	1.43
15	n	301	3BV	O48-C47	-11.42	1.14	1.43
15	Z	301	3BV	C43-C42	-10.98	1.37	1.53
15	Z	301	3BV	O48-C47	-10.43	1.17	1.43
15	k	301	3BV	O48-C47	-10.07	1.18	1.43

The worst 5 of 174 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Z	301	3BV	C44-C43-C42	10.35	136.42	115.54
15	j	301	3BV	O48-C47-C51	-9.90	90.93	109.79
15	Z	301	3BV	C58-C51-C59	-9.77	97.33	109.76
15	y	301	3BV	O48-C47-C51	9.14	127.20	109.79
15	Z	301	3BV	O48-C47-C42	8.58	129.84	109.28



There are no chirality outliers.

5 of 228 torsion outliers are listed below:

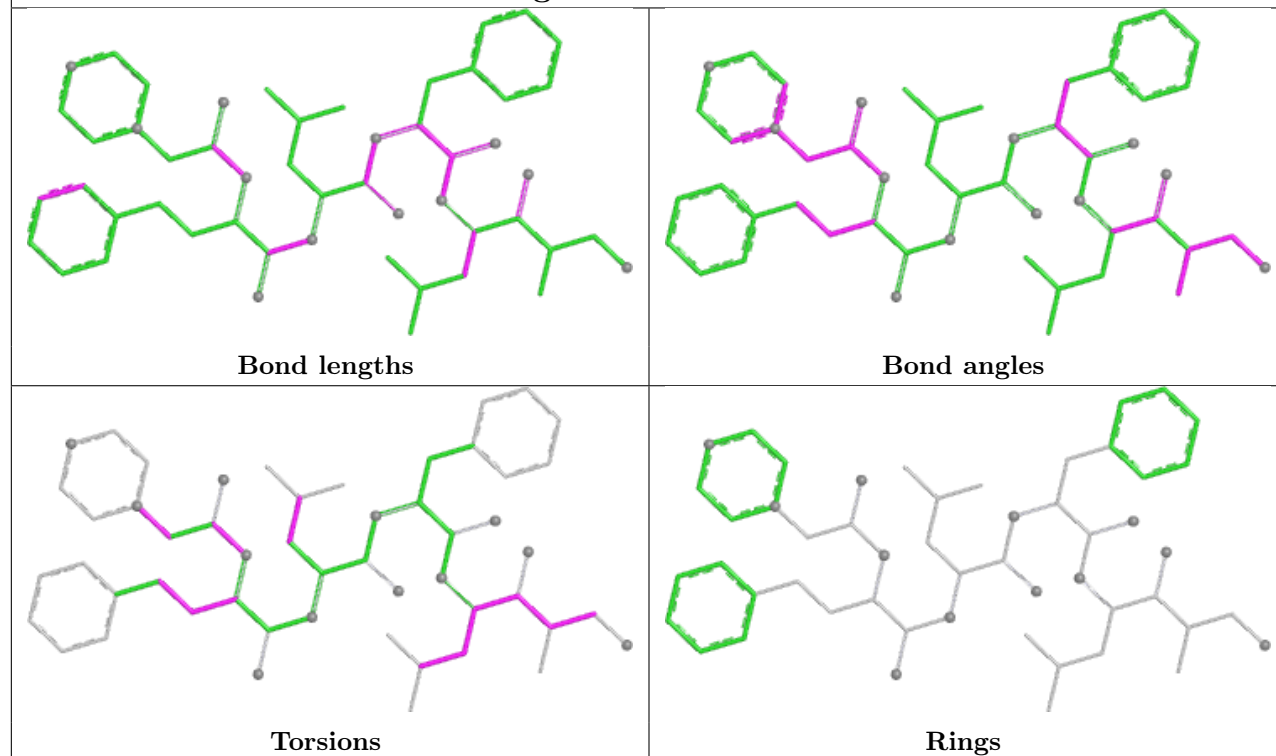
Mol	Chain	Res	Type	Atoms
15	H	301	3BV	C11-C12-C13-C14
15	H	301	3BV	N41-C42-C43-C44
15	H	301	3BV	C47-C42-C43-C44
15	H	301	3BV	N41-C42-C47-C51
15	H	301	3BV	N41-C42-C47-O48

There are no ring outliers.

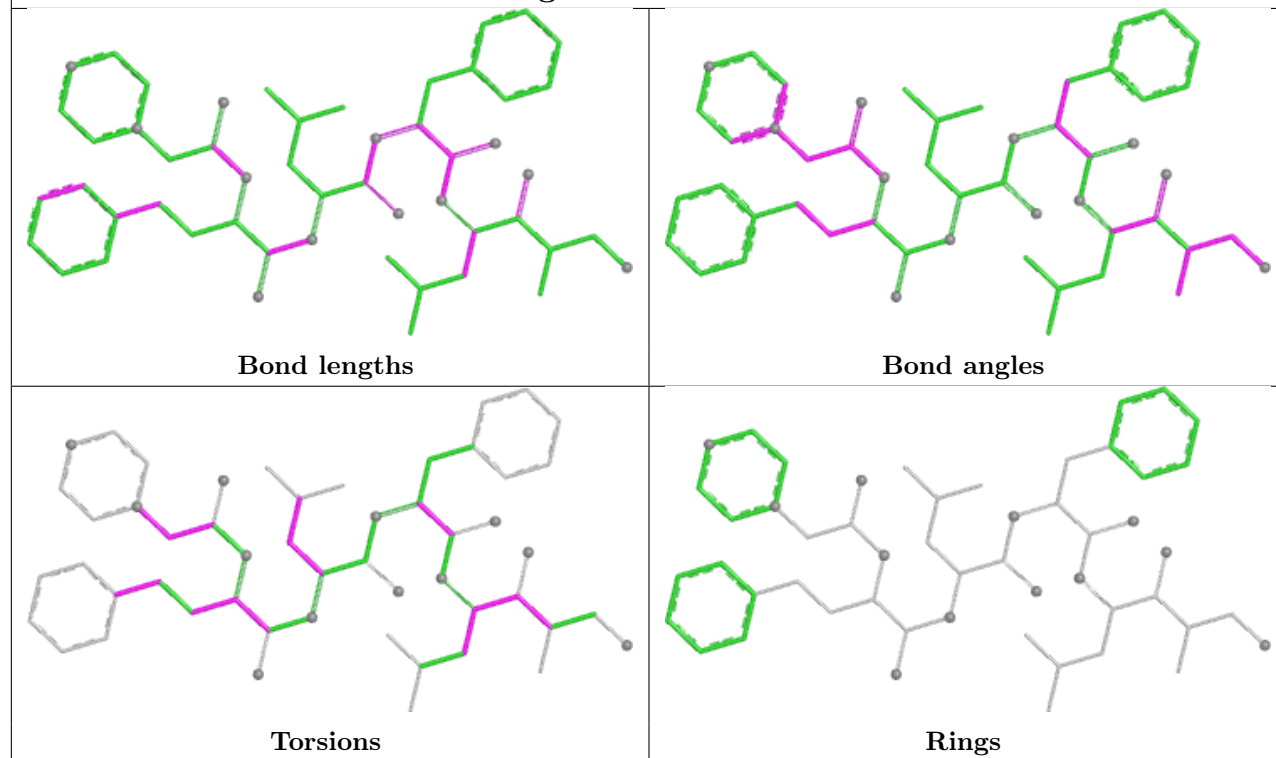
No monomer is involved in short contacts.

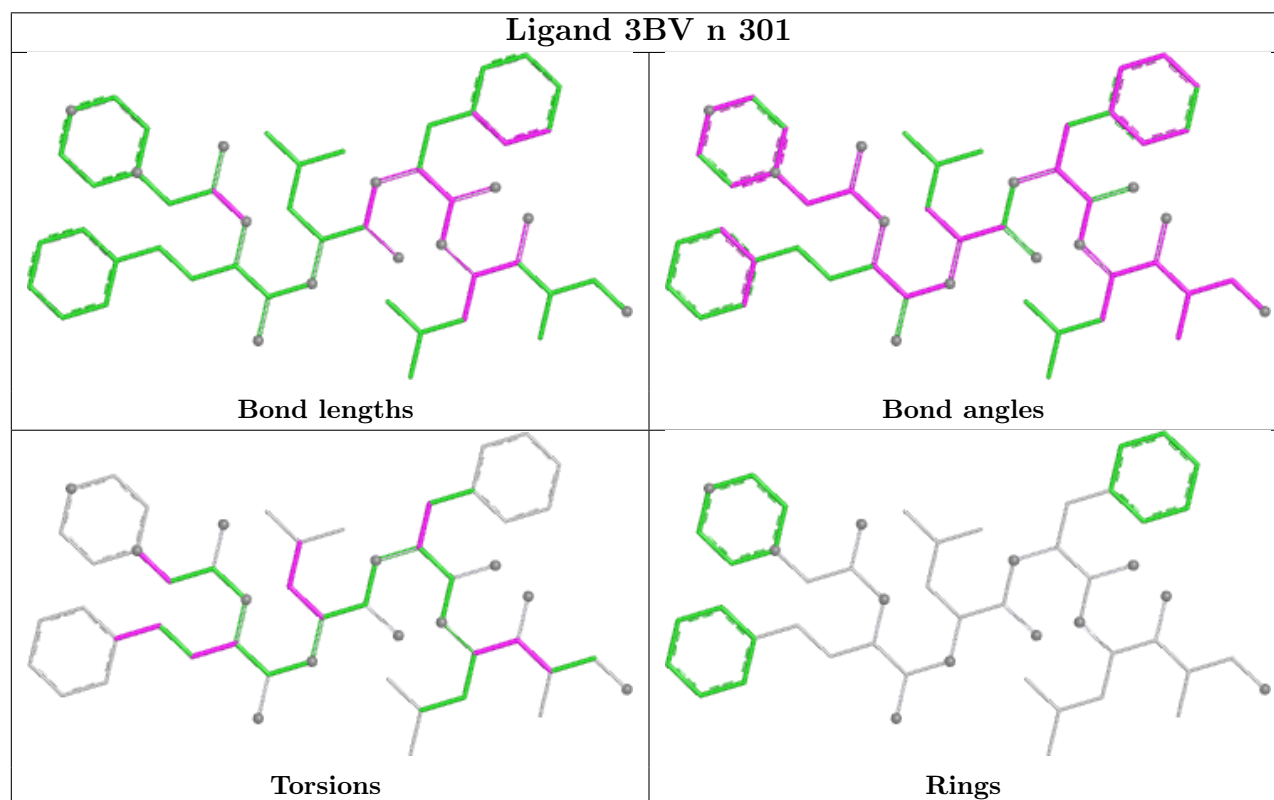
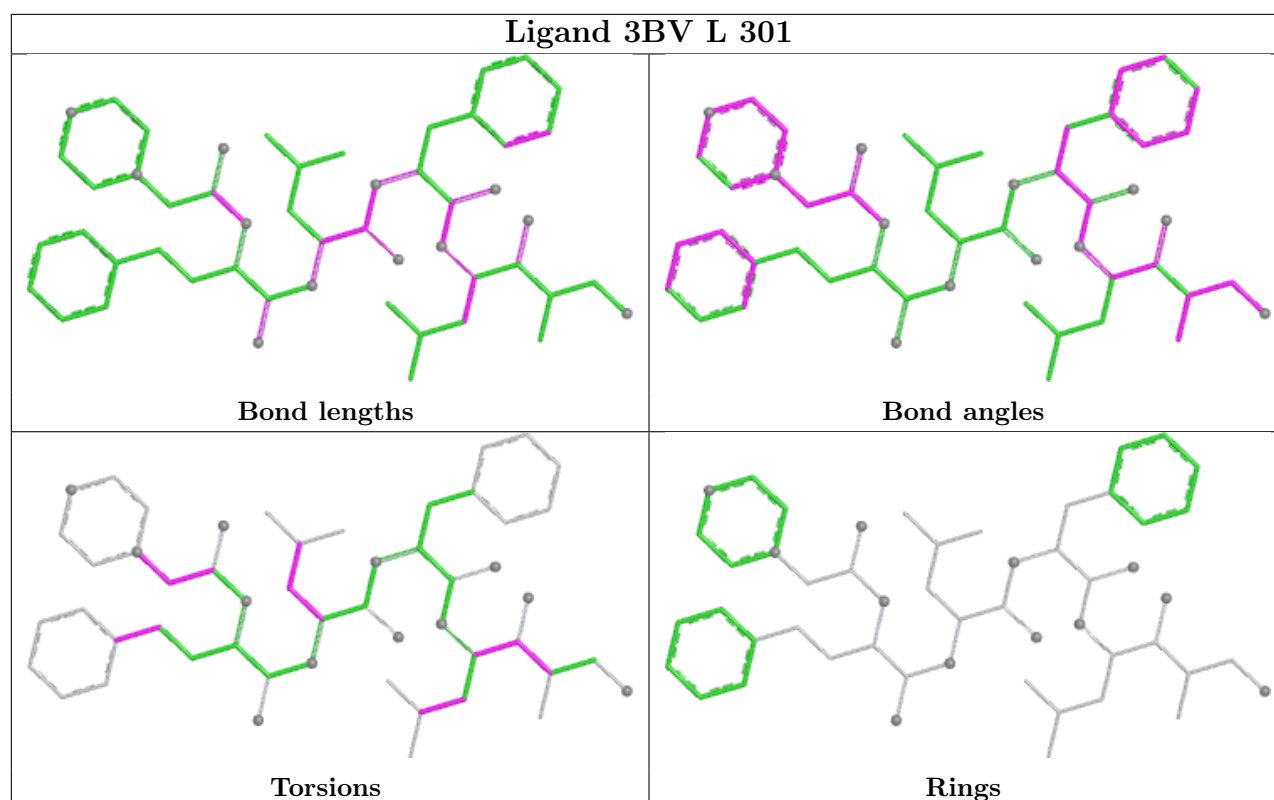
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

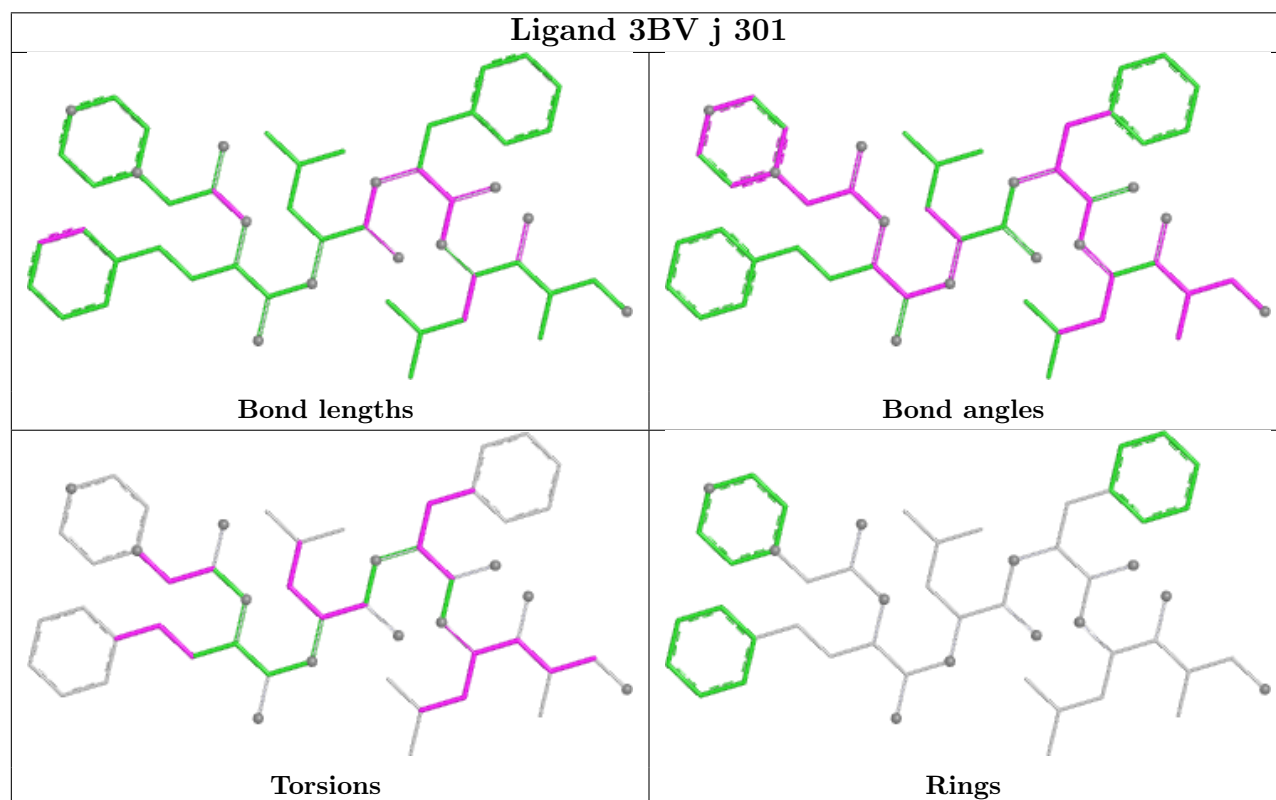
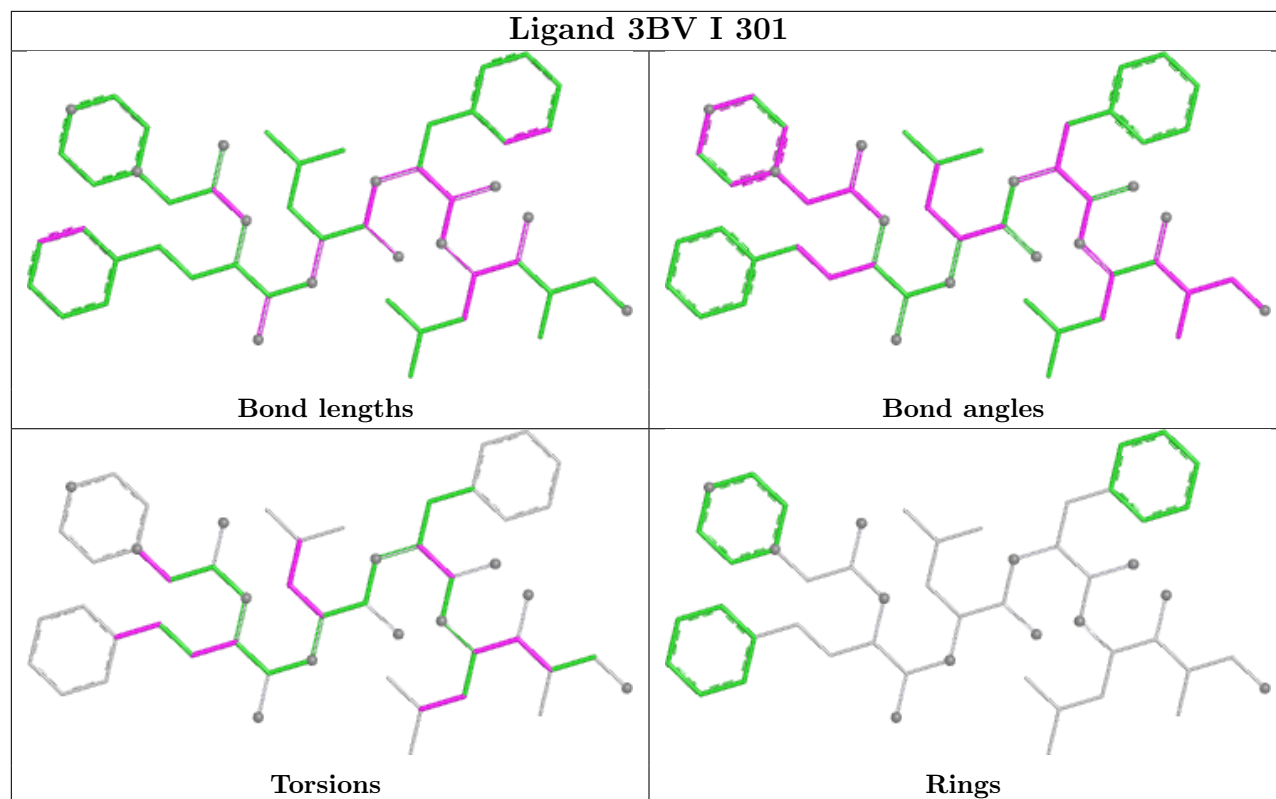
## Ligand 3BV H 301



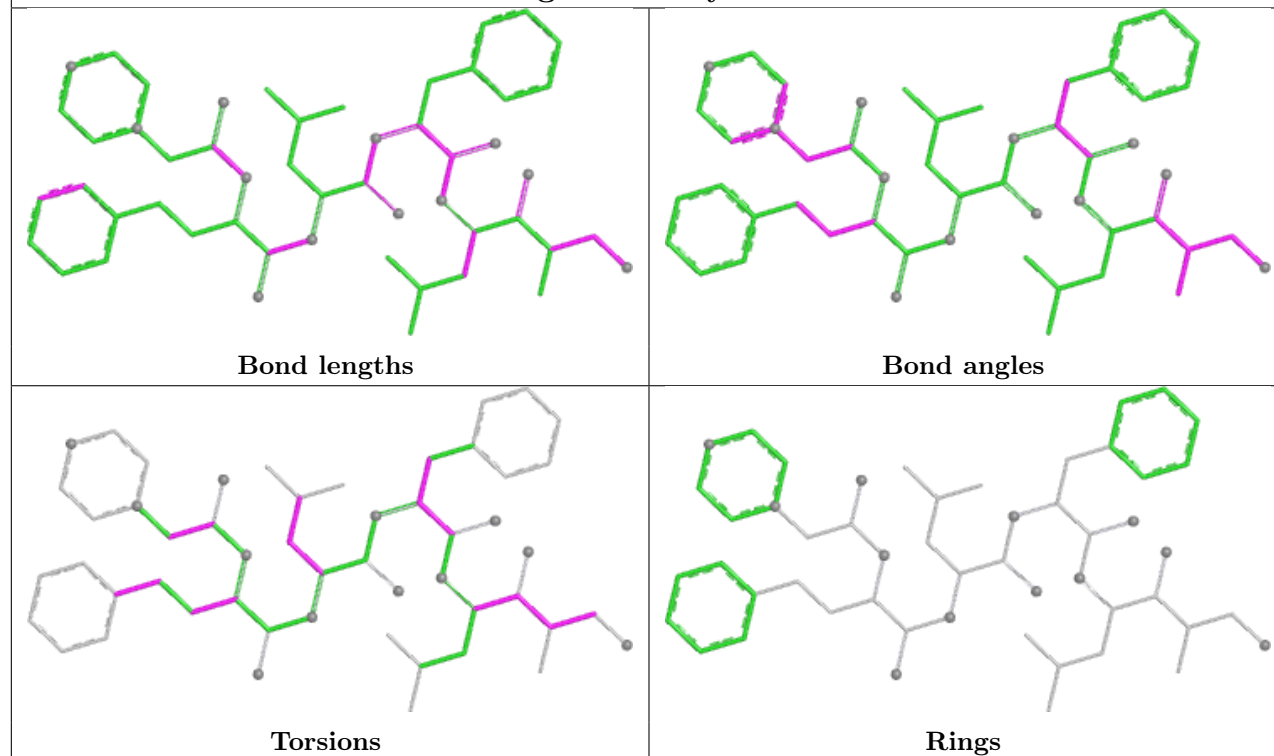
## Ligand 3BV 3 301



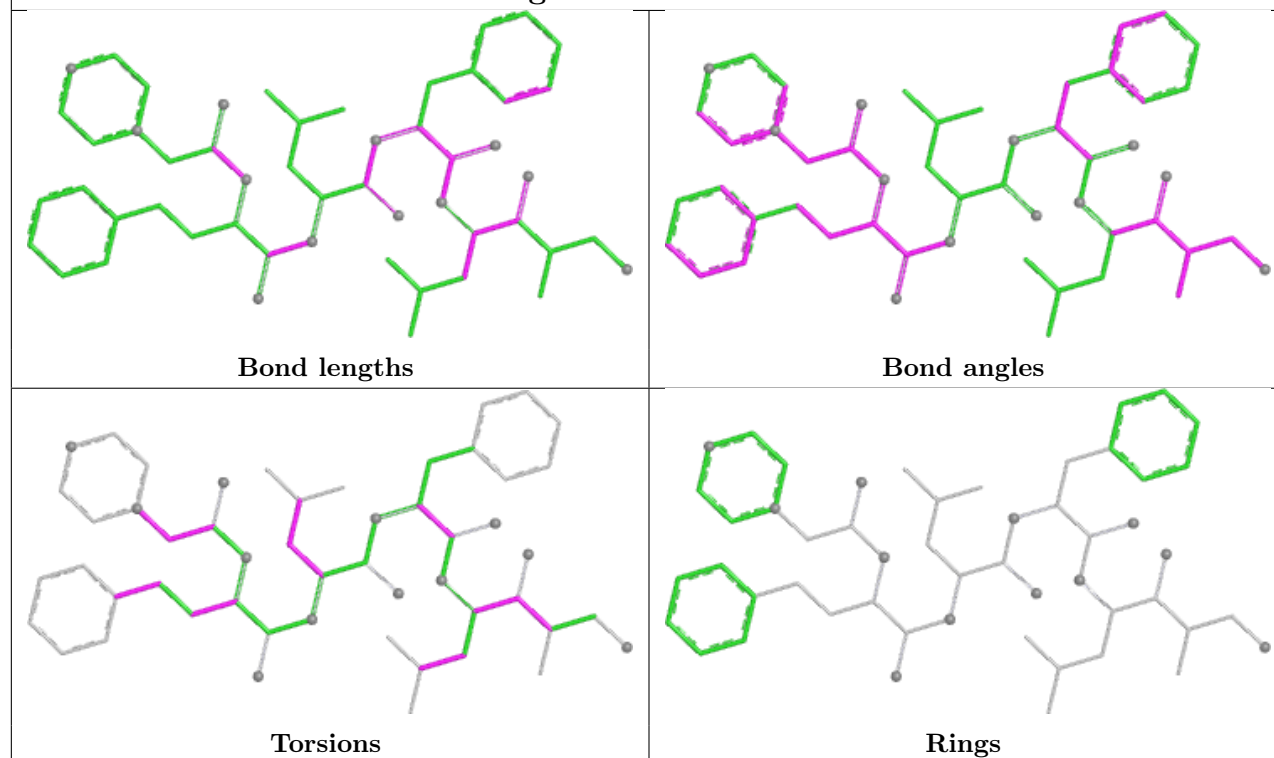


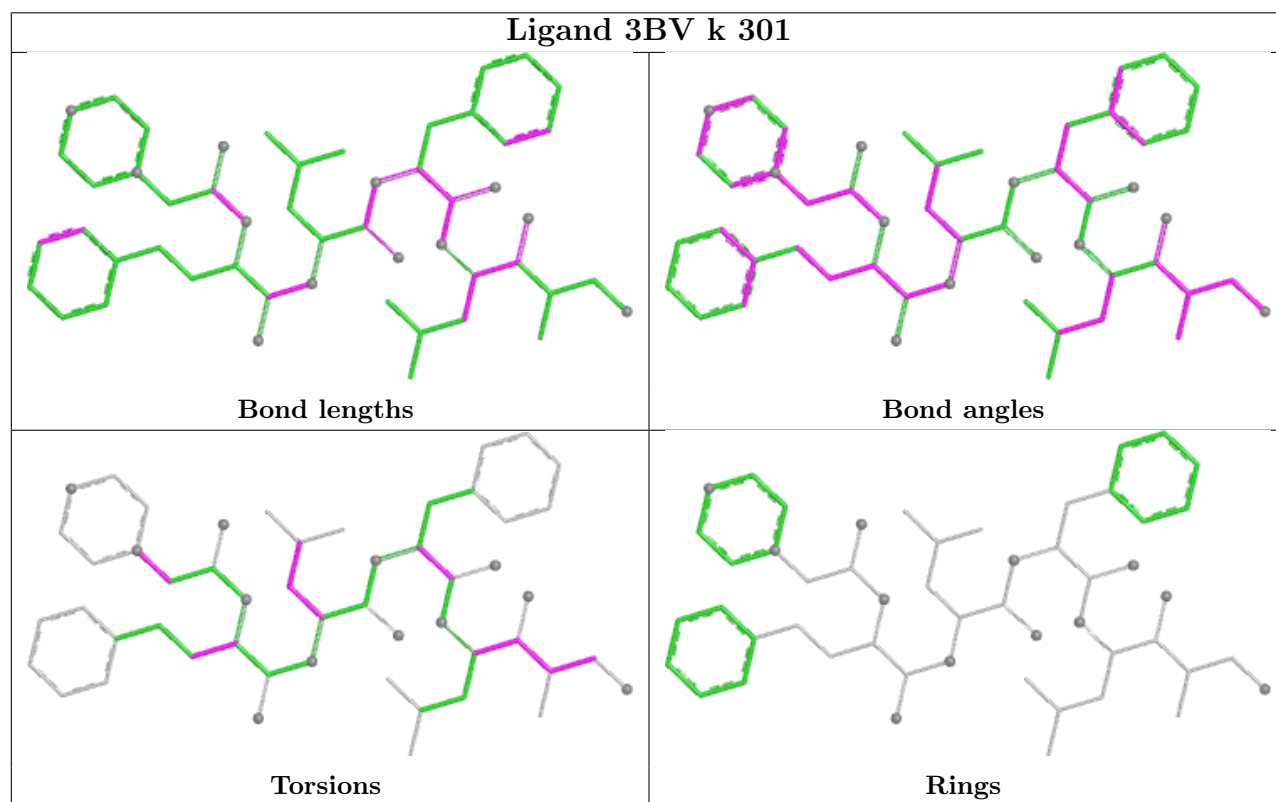
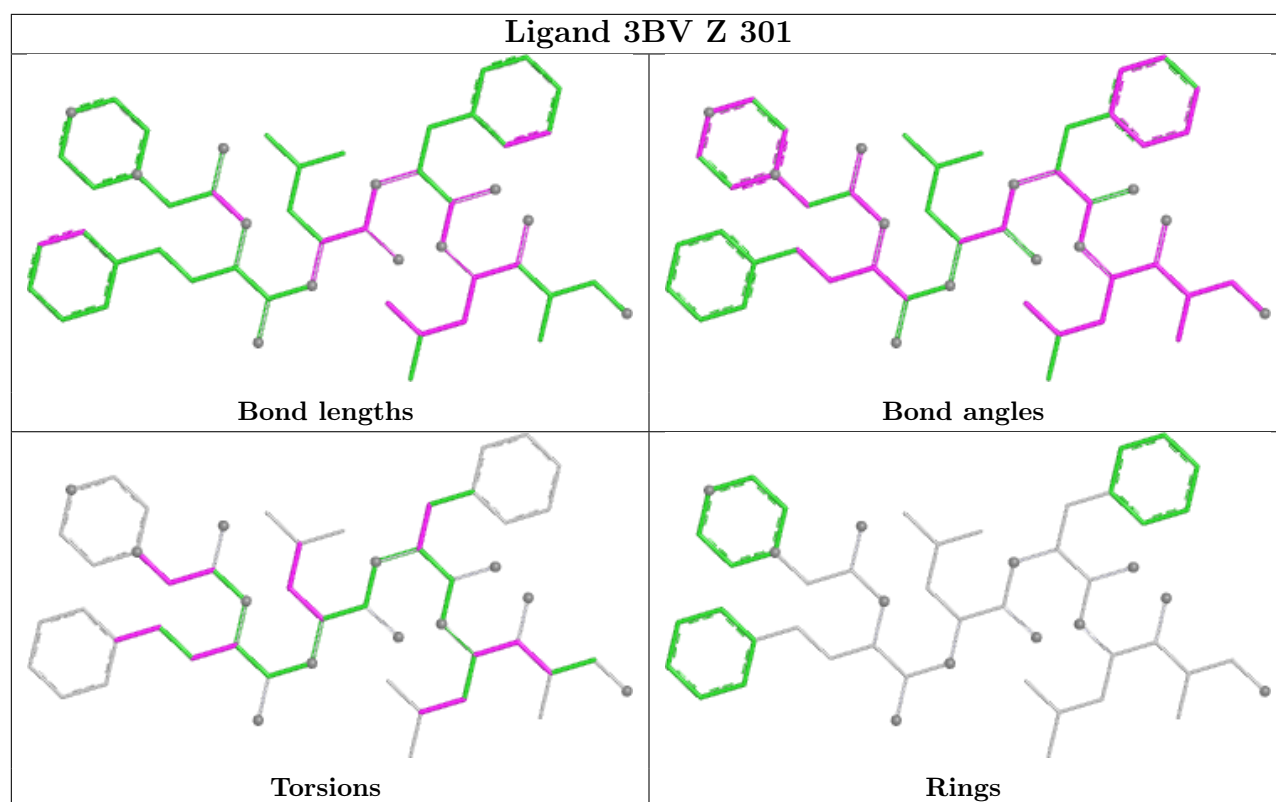


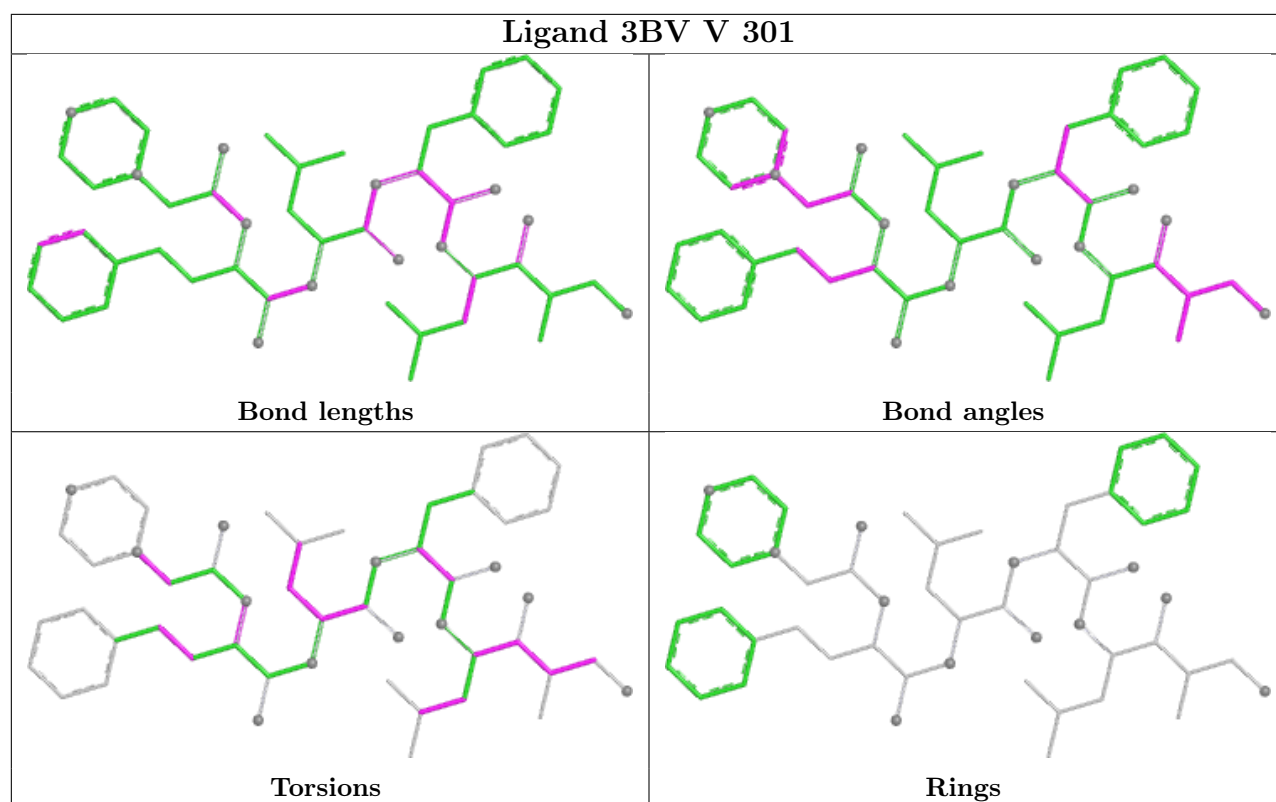
## Ligand 3BV y 301



## Ligand 3BV W 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	244/244 (100%)	0.20	2 (0%)	82 78	48, 84, 133, 170	0
1	O	244/244 (100%)	0.17	1 (0%)	89 86	48, 80, 118, 153	0
1	c	244/244 (100%)	0.12	3 (1%)	76 71	52, 89, 131, 180	0
1	q	244/244 (100%)	0.20	0	100 100	55, 87, 130, 178	0
2	B	233/233 (100%)	0.25	8 (3%)	48 42	48, 72, 123, 252	0
2	P	233/233 (100%)	0.28	6 (2%)	57 51	47, 77, 121, 237	0
2	d	233/233 (100%)	0.15	6 (2%)	57 51	46, 77, 120, 234	0
2	r	233/233 (100%)	0.24	9 (3%)	44 37	50, 76, 119, 248	0
3	C	250/250 (100%)	0.05	3 (1%)	76 71	50, 79, 135, 232	0
3	Q	250/250 (100%)	0.25	5 (2%)	64 58	48, 77, 127, 221	0
3	e	250/250 (100%)	0.11	5 (2%)	64 58	32, 77, 124, 193	0
3	s	250/250 (100%)	0.22	4 (1%)	70 64	55, 86, 152, 251	0
4	D	243/243 (100%)	0.28	2 (0%)	82 78	53, 94, 180, 223	0
4	R	243/243 (100%)	0.36	4 (1%)	70 64	42, 86, 174, 239	0
4	f	243/243 (100%)	0.36	6 (2%)	58 52	51, 91, 162, 233	0
4	t	243/243 (100%)	0.36	4 (1%)	70 64	54, 95, 184, 221	0
5	E	234/234 (100%)	0.03	1 (0%)	89 86	49, 83, 118, 173	0
5	S	234/234 (100%)	0.21	2 (0%)	81 76	50, 86, 127, 169	0
5	g	234/234 (100%)	0.31	2 (0%)	81 76	49, 88, 127, 163	0
5	u	234/234 (100%)	0.07	1 (0%)	89 86	59, 87, 126, 164	0
6	F	238/238 (100%)	0.02	3 (1%)	74 69	46, 73, 125, 231	0
6	T	238/238 (100%)	0.33	5 (2%)	63 57	46, 81, 135, 205	0
6	h	238/238 (100%)	0.36	9 (3%)	44 38	48, 83, 135, 225	0
6	v	238/238 (100%)	0.17	2 (0%)	82 78	53, 80, 135, 208	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
7	G	245/245 (100%)	0.14	3 (1%) 76 71	48, 82, 133, 254	0
7	U	245/245 (100%)	0.11	3 (1%) 76 71	44, 83, 139, 261	0
7	i	245/245 (100%)	0.20	6 (2%) 59 53	57, 87, 133, 235	0
7	w	245/245 (100%)	0.22	3 (1%) 76 71	57, 87, 131, 274	0
8	H	202/202 (100%)	-0.01	3 (1%) 71 66	43, 65, 114, 206	0
8	V	202/202 (100%)	-0.02	5 (2%) 58 52	46, 69, 110, 177	0
8	j	202/202 (100%)	0.01	5 (2%) 58 52	48, 74, 116, 186	0
8	x	202/202 (100%)	0.10	2 (0%) 79 74	43, 72, 115, 193	0
9	I	220/220 (100%)	-0.12	1 (0%) 87 84	44, 61, 92, 139	0
9	W	220/220 (100%)	-0.06	2 (0%) 81 76	40, 63, 98, 134	0
9	k	220/220 (100%)	-0.05	2 (0%) 81 76	45, 65, 98, 126	0
9	y	220/220 (100%)	0.04	1 (0%) 87 84	45, 68, 99, 139	0
10	J	204/204 (100%)	0.01	3 (1%) 71 66	42, 64, 93, 156	0
10	X	204/204 (100%)	0.06	0 100 100	41, 64, 99, 150	0
10	l	204/204 (100%)	-0.08	1 (0%) 87 84	42, 66, 90, 143	0
10	z	204/204 (100%)	0.11	3 (1%) 71 66	42, 68, 93, 148	0
11	0	199/199 (100%)	0.01	3 (1%) 71 66	50, 71, 111, 201	0
11	K	199/199 (100%)	0.03	2 (1%) 79 74	50, 70, 106, 194	0
11	Y	199/199 (100%)	0.08	4 (2%) 64 58	40, 70, 102, 218	0
11	m	199/199 (100%)	-0.01	2 (1%) 79 74	40, 71, 100, 184	0
12	3	201/201 (100%)	0.04	3 (1%) 71 66	38, 68, 103, 134	0
12	L	201/201 (100%)	0.02	2 (0%) 79 74	45, 67, 106, 158	0
12	Z	201/201 (100%)	0.06	0 100 100	45, 68, 98, 164	0
12	n	201/201 (100%)	0.07	4 (1%) 64 58	44, 69, 97, 158	0
13	1	213/213 (100%)	-0.05	1 (0%) 87 84	38, 60, 94, 181	0
13	M	213/213 (100%)	-0.22	0 100 100	37, 58, 91, 180	0
13	a	213/213 (100%)	-0.02	1 (0%) 87 84	40, 63, 98, 161	0
13	o	213/213 (100%)	0.11	1 (0%) 87 84	37, 67, 98, 145	0
14	2	217/217 (100%)	-0.07	1 (0%) 87 84	36, 63, 100, 177	0
14	N	217/217 (100%)	-0.18	3 (1%) 73 68	39, 62, 102, 159	0
14	b	217/217 (100%)	0.02	5 (2%) 61 54	45, 68, 104, 189	0

*Continued on next page...*

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
14	p	217/217 (100%)	0.02	3 (1%) 73 68	45, 70, 99, 172	0
All	All	12572/12572 (100%)	0.11	171 (1%) 73 68	32, 75, 126, 274	0

The worst 5 of 171 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	Y	199	GLN	5.8
2	B	232	ILE	4.4
9	I	170	GLY	4.2
4	R	46	GLU	3.9
3	Q	251	LYS	3.8

## 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](#)

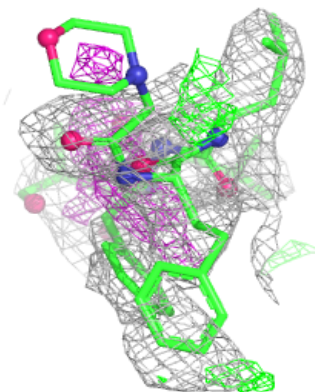
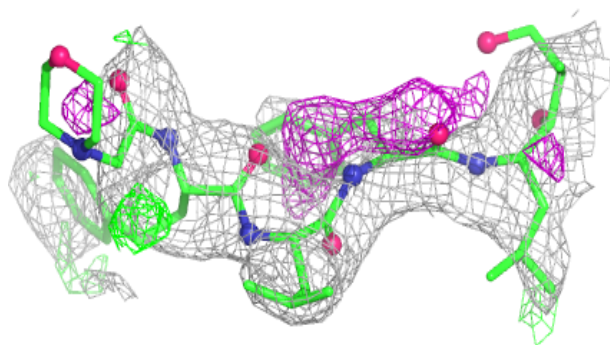
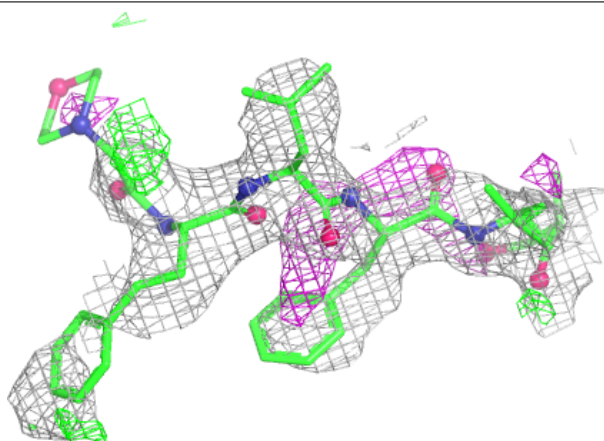
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
15	3BV	H	301	52/52	0.70	0.19	55,115,155,162	0
15	3BV	V	301	52/52	0.78	0.17	67,120,158,160	0
15	3BV	j	301	52/52	0.79	0.17	43,141,173,181	0
15	3BV	I	301	52/52	0.87	0.13	51,80,119,132	0
15	3BV	k	301	52/52	0.87	0.13	39,88,123,130	0
15	3BV	y	301	52/52	0.87	0.13	55,81,141,146	0
15	3BV	W	301	52/52	0.88	0.12	44,78,127,140	0
15	3BV	n	301	52/52	0.89	0.14	41,72,103,124	0
15	3BV	3	301	52/52	0.89	0.15	42,72,95,102	0
15	3BV	Z	301	52/52	0.92	0.12	45,62,91,103	0
15	3BV	L	301	52/52	0.92	0.11	33,63,97,106	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.

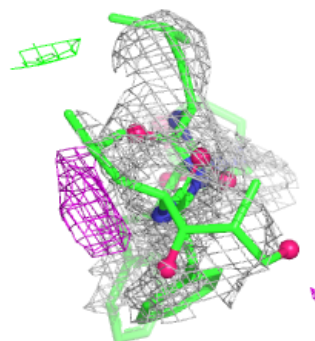
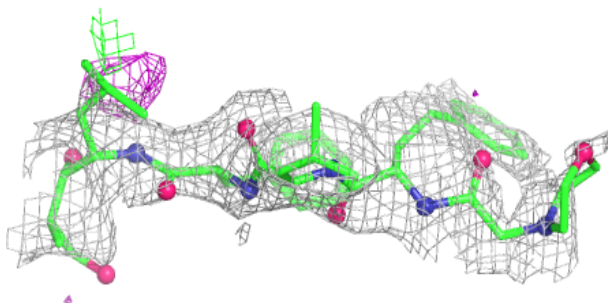
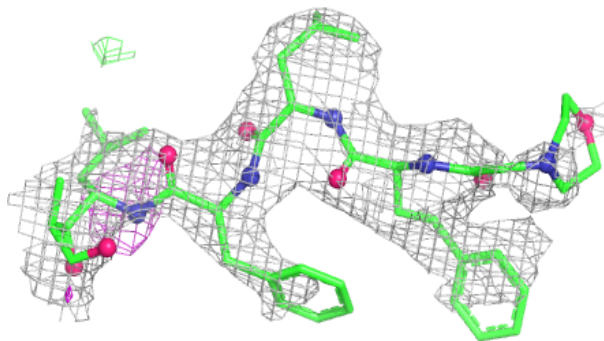
**Electron density around 3BV H 301:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



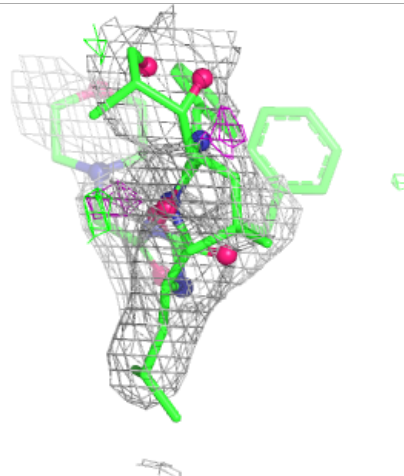
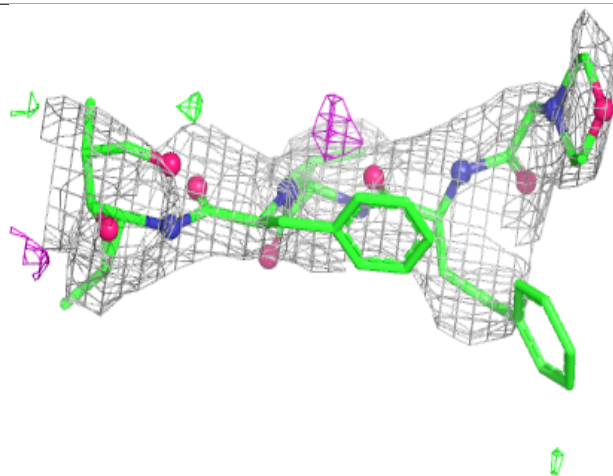
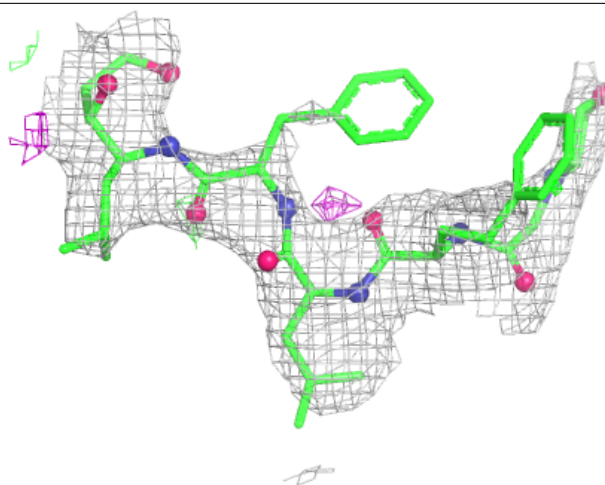
**Electron density around 3BV V 301:**

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



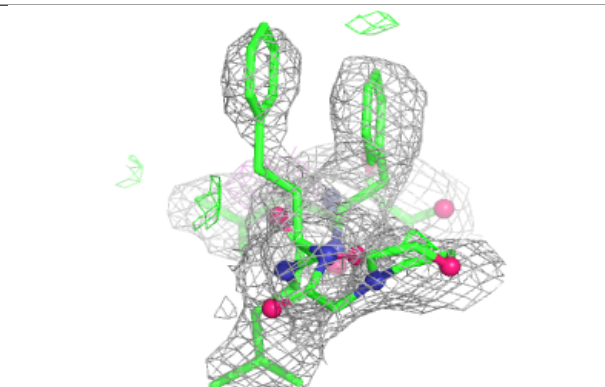
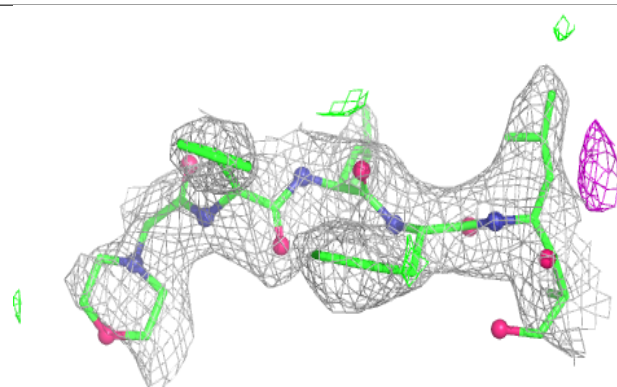
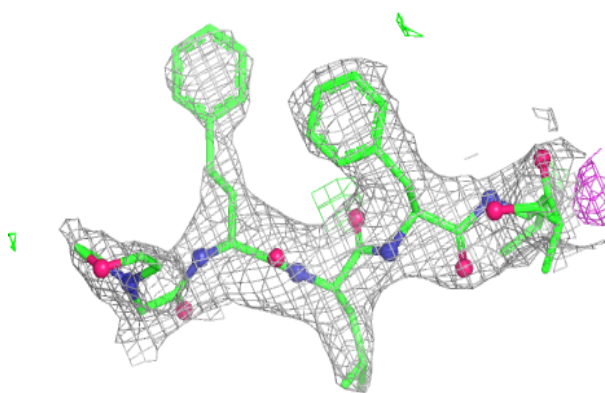
**Electron density around 3BV j 301:**

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

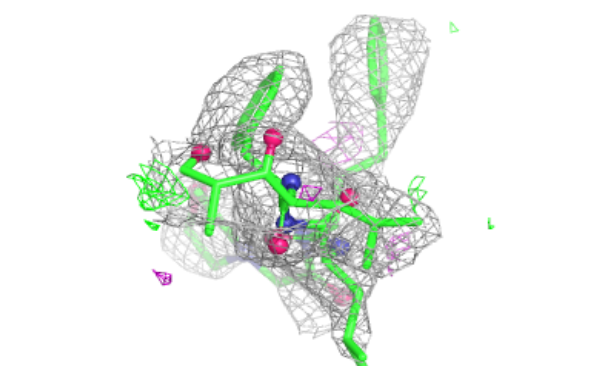
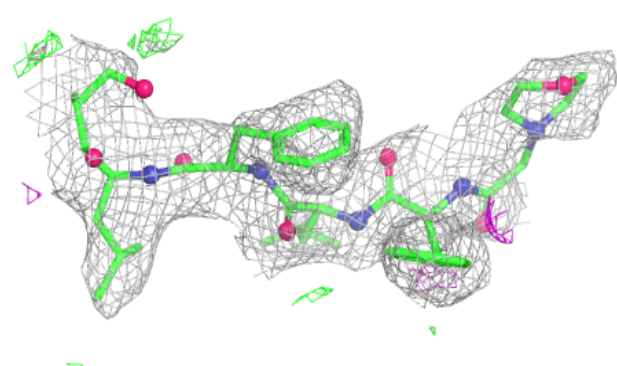
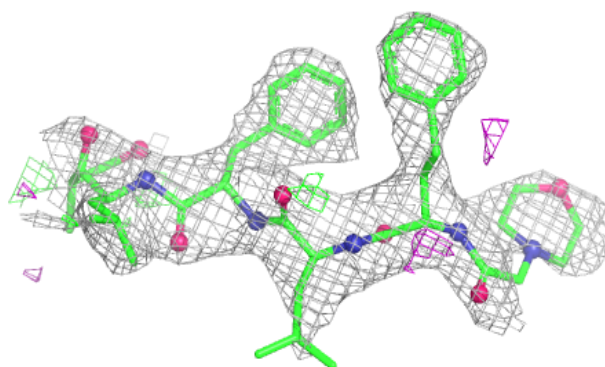


**Electron density around 3BV I 301:**

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

**Electron density around 3BV k 301:**

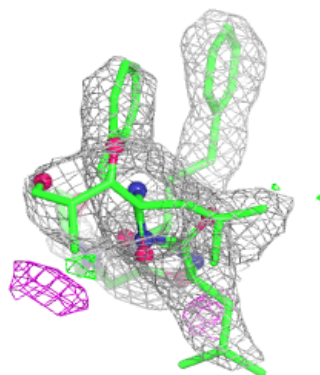
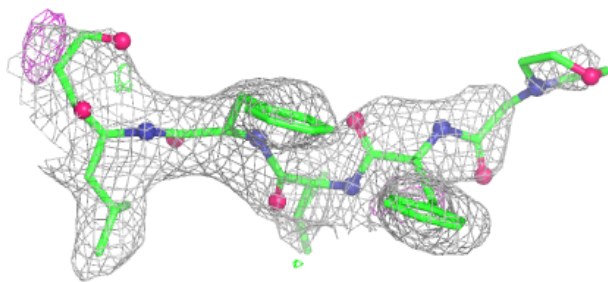
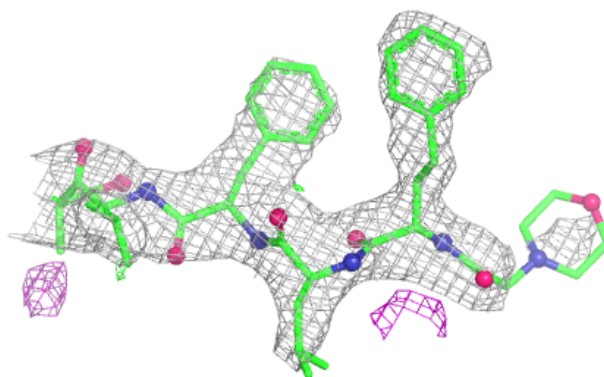
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



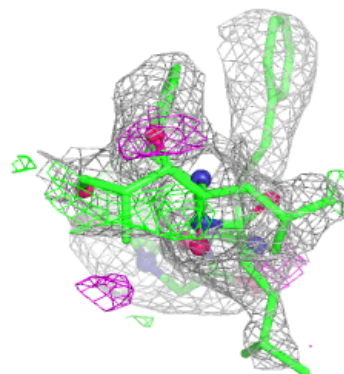
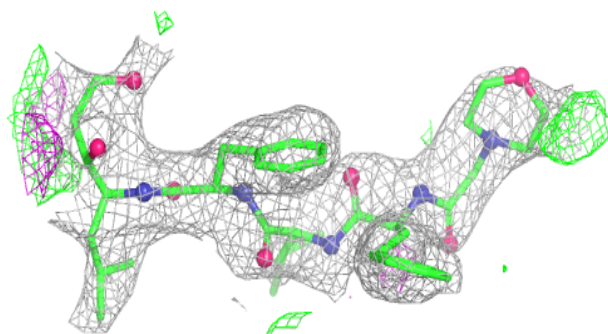
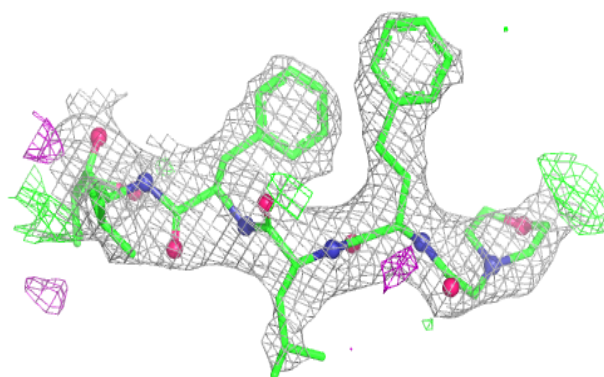


**Electron density around 3BV y 301:**

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

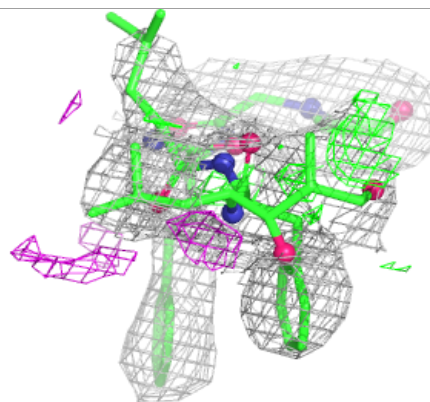
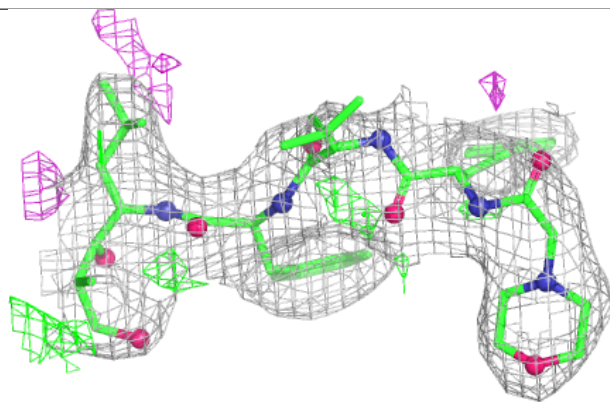
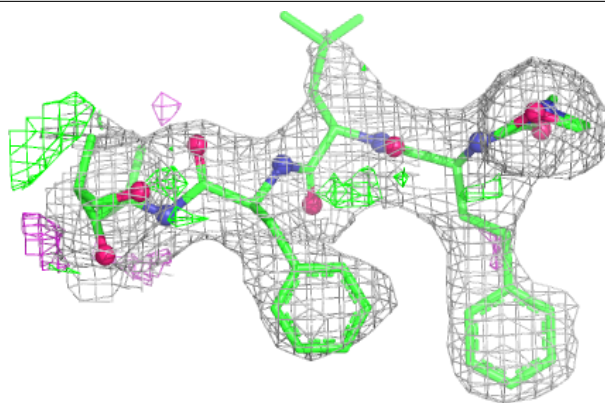
**Electron density around 3BV W 301:**

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

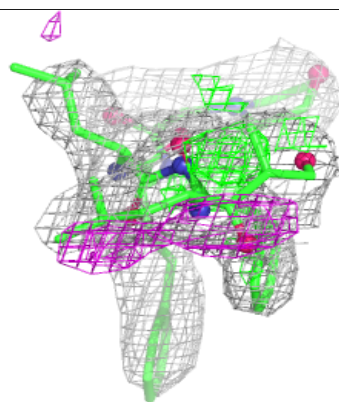
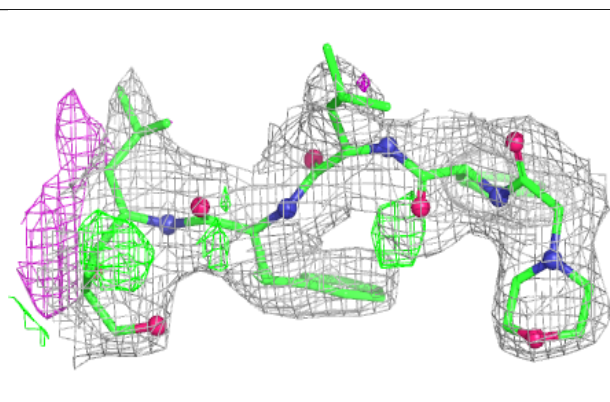
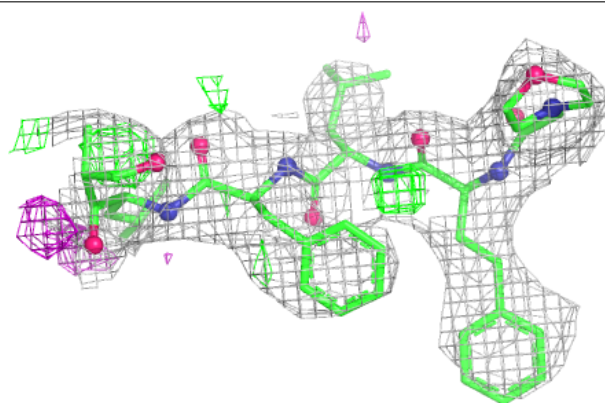


**Electron density around 3BV n 301:**

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

**Electron density around 3BV 3 301:**

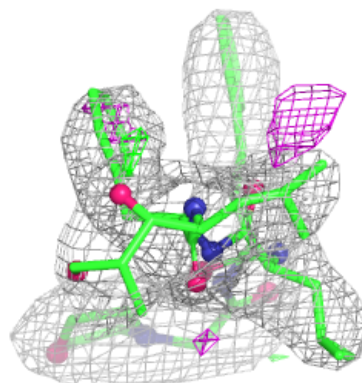
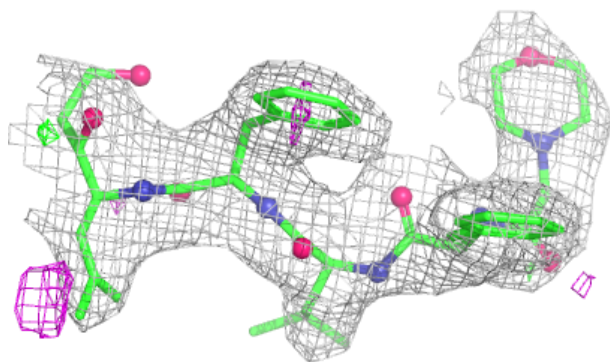
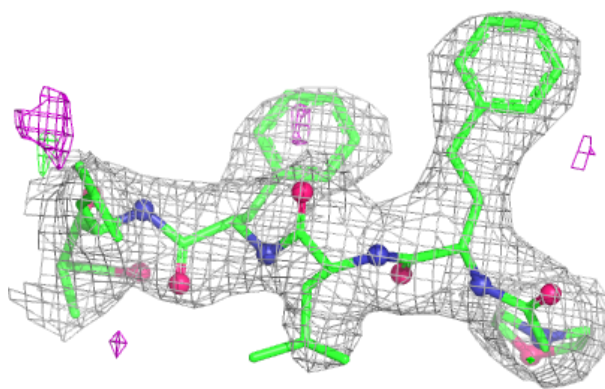
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





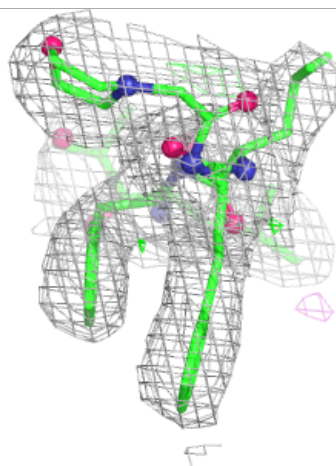
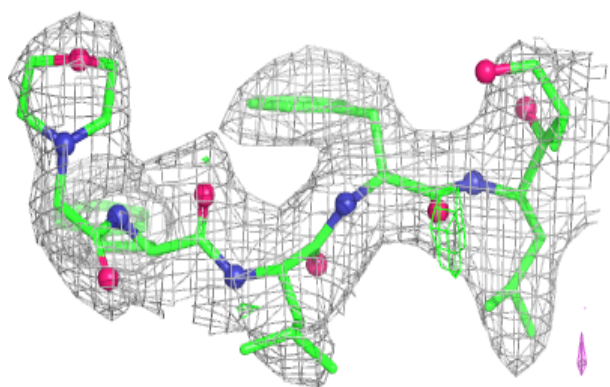
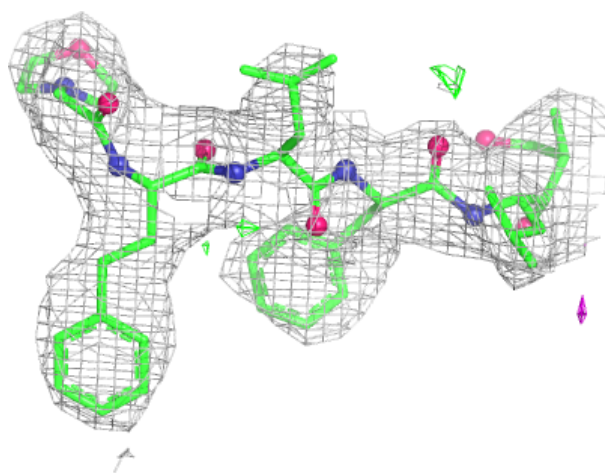
**Electron density around 3BV Z 301:**

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



**Electron density around 3BV L 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.