



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:27 AM UTC

PDB ID : 5TRY / pdb\_00005try  
Title : Structure of Mycobacterium tuberculosis proteasome in complex with N,C-capped dipeptide PKS2206  
Authors : Hsu, H.-C.; Fan, H.; Singh, P.K.; Wang, R.; Sukenick, G.; Nathan, C.; Lin, G.; Li, H.  
Deposited on : 2016-10-27  
Resolution : 3.00 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](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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

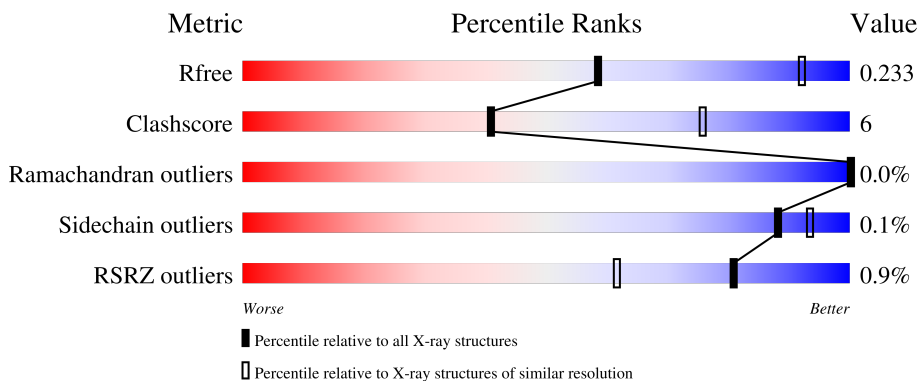
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.










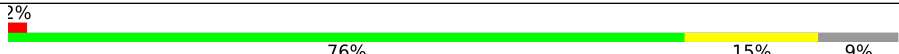








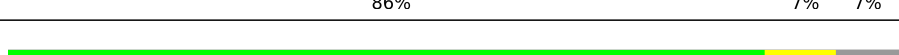




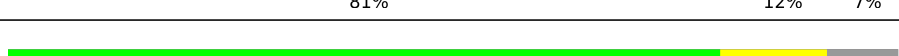

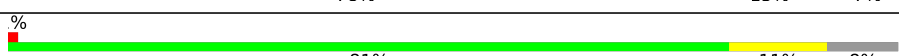
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	240	 72% 18% 9%
1	B	240	 73% 17% 10%
1	C	240	 76% 14% 10%
1	D	240	 80% 10% 10%

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Mol	Chain	Length	Quality of chain
1	E	240	 71% 19% 10%
1	F	240	 2% 67% 24% 9%
1	G	240	 73% 17% 10%
1	O	240	 3% 70% 20% 10%
1	P	240	 2% 67% 24% 10%
1	Q	240	 2% 69% 22% 9%
1	R	240	 75% 16% 10%
1	S	240	 2% 76% 15% 9%
1	T	240	 71% 19% 10%
1	U	240	 73% 17% 10%
2	H	240	 82% 11% 8%
2	I	240	 84% 9% 8%
2	J	240	 81% 12% 8%
2	K	240	 81% 12% 7%
2	L	240	 86% 7% 7%
2	M	240	 85% 8% 8%
2	N	240	 79% 14% 7%
2	V	240	 82% 11% 7%
2	W	240	 81% 12% 7%
2	X	240	 80% 12% 8%
2	Y	240	 78% 15% 7%
2	Z	240	 81% 11% 8%
2	a	240	 82% 11% 7%
2	b	240	 82% 11% 7%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 47136 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	218	Total 1677	C 1050	N 306	O 317	S 4	0	0	0
1	B	215	Total 1660	C 1041	N 303	O 312	S 4	0	0	0
1	C	216	Total 1664	C 1043	N 304	O 313	S 4	0	0	0
1	D	217	Total 1670	C 1046	N 305	O 315	S 4	0	0	0
1	E	217	Total 1671	C 1047	N 305	O 315	S 4	0	0	0
1	F	218	Total 1678	C 1050	N 306	O 318	S 4	0	0	0
1	G	216	Total 1662	C 1040	N 304	O 314	S 4	0	0	0
1	O	216	Total 1662	C 1040	N 304	O 314	S 4	0	0	0
1	P	217	Total 1674	C 1050	N 305	O 315	S 4	0	0	0
1	Q	218	Total 1679	C 1051	N 306	O 318	S 4	0	0	0
1	R	217	Total 1671	C 1047	N 305	O 315	S 4	0	0	0
1	S	219	Total 1683	C 1053	N 307	O 319	S 4	0	0	0
1	T	216	Total 1664	C 1043	N 304	O 313	S 4	0	0	0
1	U	216	Total 1664	C 1043	N 304	O 313	S 4	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	initiating methionine	UNP A5U4D5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	MET	-	initiating methionine	UNP A5U4D5
C	9	MET	-	initiating methionine	UNP A5U4D5
D	9	MET	-	initiating methionine	UNP A5U4D5
E	9	MET	-	initiating methionine	UNP A5U4D5
F	9	MET	-	initiating methionine	UNP A5U4D5
G	9	MET	-	initiating methionine	UNP A5U4D5
O	9	MET	-	initiating methionine	UNP A5U4D5
P	9	MET	-	initiating methionine	UNP A5U4D5
Q	9	MET	-	initiating methionine	UNP A5U4D5
R	9	MET	-	initiating methionine	UNP A5U4D5
S	9	MET	-	initiating methionine	UNP A5U4D5
T	9	MET	-	initiating methionine	UNP A5U4D5
U	9	MET	-	initiating methionine	UNP A5U4D5

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	222	1638	1027	282	324	5	0	0	0
2	I	222	1638	1027	282	324	5	0	0	0
2	J	222	1638	1027	282	324	5	0	0	0
2	K	223	1642	1029	283	325	5	0	0	0
2	L	223	1642	1029	283	325	5	0	0	0
2	M	222	1638	1027	282	324	5	0	0	0
2	N	223	1642	1029	283	325	5	0	0	0
2	V	223	1642	1029	283	325	5	0	0	0
2	W	223	1642	1029	283	325	5	0	0	0
2	X	222	1638	1027	282	324	5	0	0	0
2	Y	223	1642	1029	283	325	5	0	0	0
2	Z	222	1638	1027	282	324	5	0	0	0
2	a	223	1642	1029	283	325	5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	b	223	1642	1029	283	325	5	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	235	HIS	-	expression tag	UNP A5U4D6
H	236	HIS	-	expression tag	UNP A5U4D6
H	237	HIS	-	expression tag	UNP A5U4D6
H	238	HIS	-	expression tag	UNP A5U4D6
H	239	HIS	-	expression tag	UNP A5U4D6
H	240	HIS	-	expression tag	UNP A5U4D6
I	235	HIS	-	expression tag	UNP A5U4D6
I	236	HIS	-	expression tag	UNP A5U4D6
I	237	HIS	-	expression tag	UNP A5U4D6
I	238	HIS	-	expression tag	UNP A5U4D6
I	239	HIS	-	expression tag	UNP A5U4D6
I	240	HIS	-	expression tag	UNP A5U4D6
J	235	HIS	-	expression tag	UNP A5U4D6
J	236	HIS	-	expression tag	UNP A5U4D6
J	237	HIS	-	expression tag	UNP A5U4D6
J	238	HIS	-	expression tag	UNP A5U4D6
J	239	HIS	-	expression tag	UNP A5U4D6
J	240	HIS	-	expression tag	UNP A5U4D6
K	235	HIS	-	expression tag	UNP A5U4D6
K	236	HIS	-	expression tag	UNP A5U4D6
K	237	HIS	-	expression tag	UNP A5U4D6
K	238	HIS	-	expression tag	UNP A5U4D6
K	239	HIS	-	expression tag	UNP A5U4D6
K	240	HIS	-	expression tag	UNP A5U4D6
L	235	HIS	-	expression tag	UNP A5U4D6
L	236	HIS	-	expression tag	UNP A5U4D6
L	237	HIS	-	expression tag	UNP A5U4D6
L	238	HIS	-	expression tag	UNP A5U4D6
L	239	HIS	-	expression tag	UNP A5U4D6
L	240	HIS	-	expression tag	UNP A5U4D6
M	235	HIS	-	expression tag	UNP A5U4D6
M	236	HIS	-	expression tag	UNP A5U4D6
M	237	HIS	-	expression tag	UNP A5U4D6
M	238	HIS	-	expression tag	UNP A5U4D6
M	239	HIS	-	expression tag	UNP A5U4D6
M	240	HIS	-	expression tag	UNP A5U4D6

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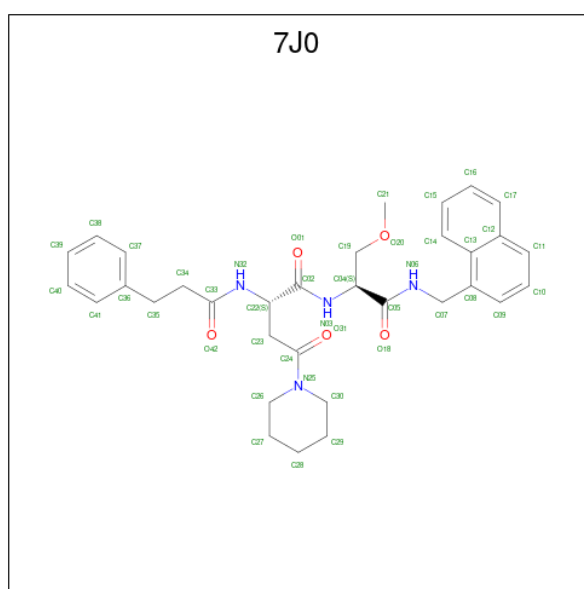
Chain	Residue	Modelled	Actual	Comment	Reference
N	235	HIS	-	expression tag	UNP A5U4D6
N	236	HIS	-	expression tag	UNP A5U4D6
N	237	HIS	-	expression tag	UNP A5U4D6
N	238	HIS	-	expression tag	UNP A5U4D6
N	239	HIS	-	expression tag	UNP A5U4D6
N	240	HIS	-	expression tag	UNP A5U4D6
V	235	HIS	-	expression tag	UNP A5U4D6
V	236	HIS	-	expression tag	UNP A5U4D6
V	237	HIS	-	expression tag	UNP A5U4D6
V	238	HIS	-	expression tag	UNP A5U4D6
V	239	HIS	-	expression tag	UNP A5U4D6
V	240	HIS	-	expression tag	UNP A5U4D6
W	235	HIS	-	expression tag	UNP A5U4D6
W	236	HIS	-	expression tag	UNP A5U4D6
W	237	HIS	-	expression tag	UNP A5U4D6
W	238	HIS	-	expression tag	UNP A5U4D6
W	239	HIS	-	expression tag	UNP A5U4D6
W	240	HIS	-	expression tag	UNP A5U4D6
X	235	HIS	-	expression tag	UNP A5U4D6
X	236	HIS	-	expression tag	UNP A5U4D6
X	237	HIS	-	expression tag	UNP A5U4D6
X	238	HIS	-	expression tag	UNP A5U4D6
X	239	HIS	-	expression tag	UNP A5U4D6
X	240	HIS	-	expression tag	UNP A5U4D6
Y	235	HIS	-	expression tag	UNP A5U4D6
Y	236	HIS	-	expression tag	UNP A5U4D6
Y	237	HIS	-	expression tag	UNP A5U4D6
Y	238	HIS	-	expression tag	UNP A5U4D6
Y	239	HIS	-	expression tag	UNP A5U4D6
Y	240	HIS	-	expression tag	UNP A5U4D6
Z	235	HIS	-	expression tag	UNP A5U4D6
Z	236	HIS	-	expression tag	UNP A5U4D6
Z	237	HIS	-	expression tag	UNP A5U4D6
Z	238	HIS	-	expression tag	UNP A5U4D6
Z	239	HIS	-	expression tag	UNP A5U4D6
Z	240	HIS	-	expression tag	UNP A5U4D6
a	235	HIS	-	expression tag	UNP A5U4D6
a	236	HIS	-	expression tag	UNP A5U4D6
a	237	HIS	-	expression tag	UNP A5U4D6
a	238	HIS	-	expression tag	UNP A5U4D6
a	239	HIS	-	expression tag	UNP A5U4D6
a	240	HIS	-	expression tag	UNP A5U4D6

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Chain	Residue	Modelled	Actual	Comment	Reference
b	235	HIS	-	expression tag	UNP A5U4D6
b	236	HIS	-	expression tag	UNP A5U4D6
b	237	HIS	-	expression tag	UNP A5U4D6
b	238	HIS	-	expression tag	UNP A5U4D6
b	239	HIS	-	expression tag	UNP A5U4D6
b	240	HIS	-	expression tag	UNP A5U4D6

- Molecule 3 is (2 {S})- {N}-[(2 {S})-3-methoxy-1-(naphthalen-1-ylmethylamino)-1-oxidanylidene-propan-2-yl]-4-oxidanylidene-2-(3-phenylpropanoylamino)-4-piperidin-1-yl-butanamide (CCD ID: 7J0) (formula: C<sub>33</sub>H<sub>40</sub>N<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	H	1	Total	C	N	O	0	0
			42	33	4	5		
3	I	1	Total	C	N	O	0	0
			42	33	4	5		
3	J	1	Total	C	N	O	0	0
			42	33	4	5		
3	K	1	Total	C	N	O	0	0
			42	33	4	5		
3	L	1	Total	C	N	O	0	0
			42	33	4	5		
3	M	1	Total	C	N	O	0	0
			42	33	4	5		
3	N	1	Total	C	N	O	0	0
			42	33	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	V	1	42	33	4	5	0	0
3	W	1	42	33	4	5	0	0
3	X	1	42	33	4	5	0	0
3	Y	1	42	33	4	5	0	0
3	Z	1	42	33	4	5	0	0
3	a	1	42	33	4	5	0	0
3	b	1	42	33	4	5	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		
4	B	2	Total	O	0	0
			2	2		
4	C	5	Total	O	0	0
			5	5		
4	D	3	Total	O	0	0
			3	3		
4	E	5	Total	O	0	0
			5	5		
4	F	8	Total	O	0	0
			8	8		
4	G	7	Total	O	0	0
			7	7		
4	H	7	Total	O	0	0
			7	7		
4	I	8	Total	O	0	0
			8	8		
4	J	7	Total	O	0	0
			7	7		
4	K	12	Total	O	0	0
			12	12		
4	L	5	Total	O	0	0
			5	5		

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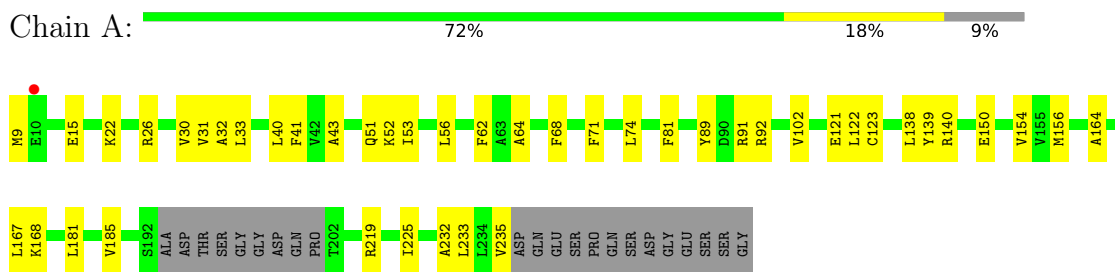
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	12	Total O 12 12	0	0
4	N	7	Total O 7 7	0	0
4	O	6	Total O 6 6	0	0
4	P	6	Total O 6 6	0	0
4	Q	5	Total O 5 5	0	0
4	R	8	Total O 8 8	0	0
4	S	9	Total O 9 9	0	0
4	T	6	Total O 6 6	0	0
4	U	7	Total O 7 7	0	0
4	V	9	Total O 9 9	0	0
4	W	8	Total O 8 8	0	0
4	X	8	Total O 8 8	0	0
4	Y	11	Total O 11 11	0	0
4	Z	11	Total O 11 11	0	0
4	a	6	Total O 6 6	0	0
4	b	8	Total O 8 8	0	0

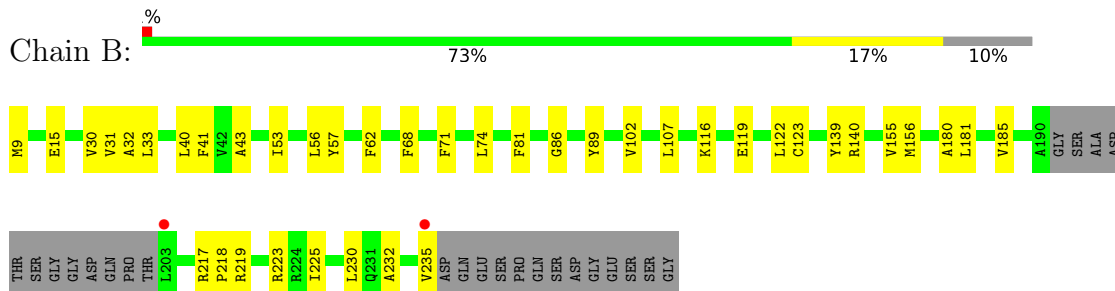
### 3 Residue-property plots i

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

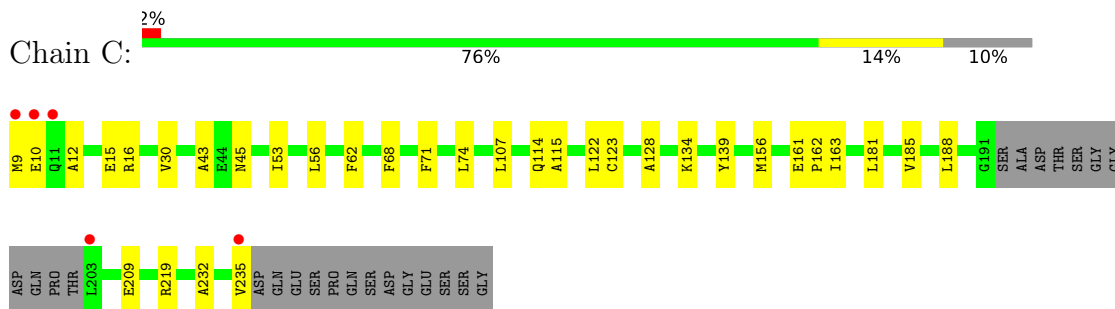
- Molecule 1: Proteasome subunit alpha



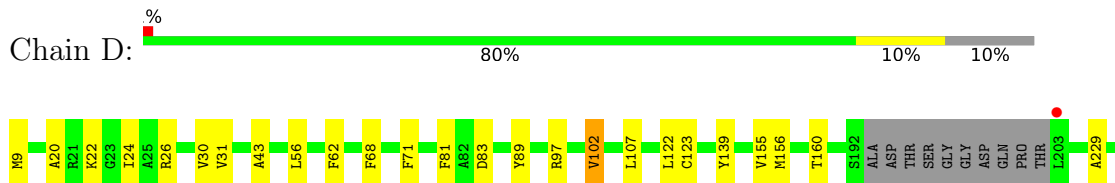
- Molecule 1: Proteasome subunit alpha

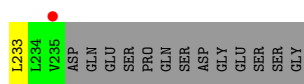


- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha

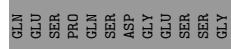
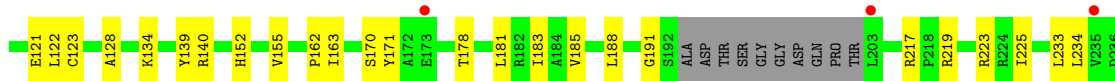
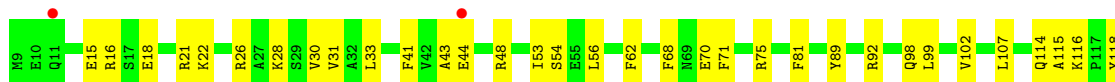




• Molecule 1: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha



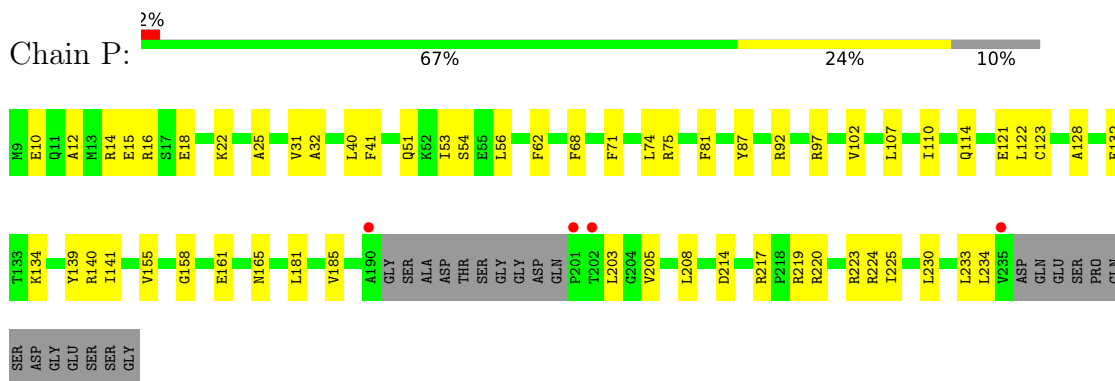
• Molecule 1: Proteasome subunit alpha



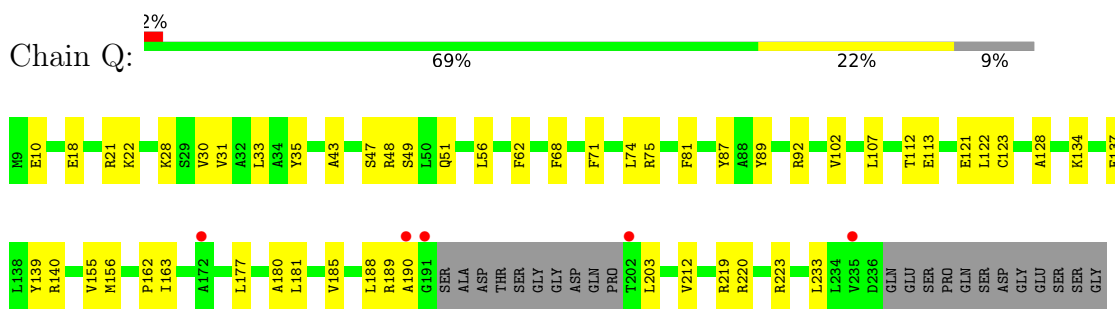
• Molecule 1: Proteasome subunit alpha



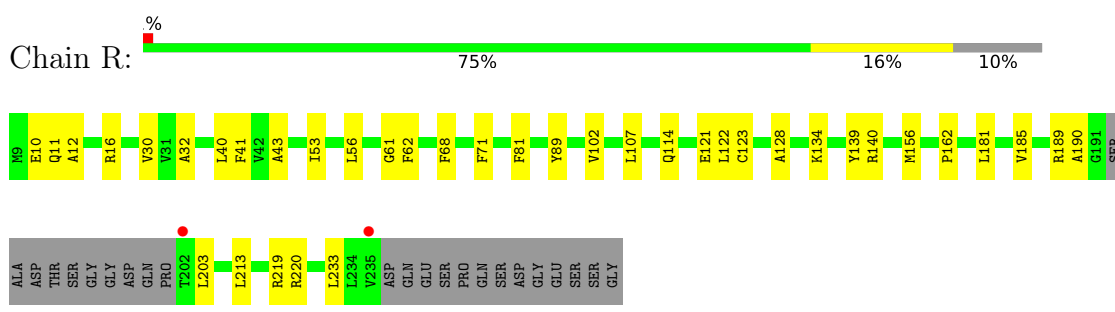
• Molecule 1: Proteasome subunit alpha



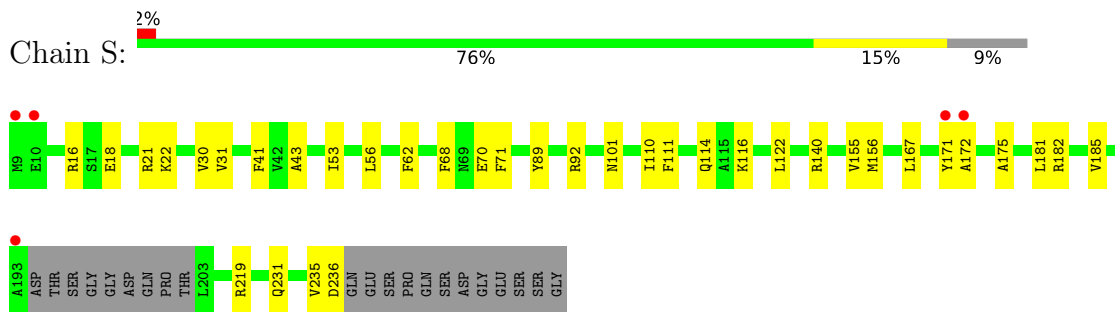
• Molecule 1: Proteasome subunit alpha



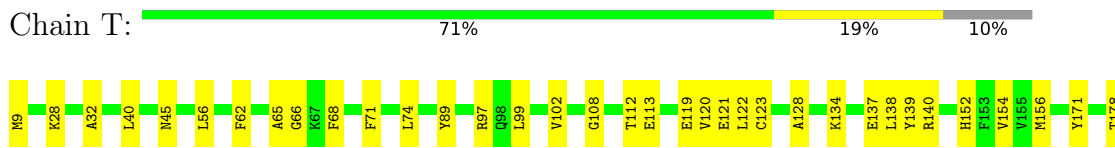
• Molecule 1: Proteasome subunit alpha



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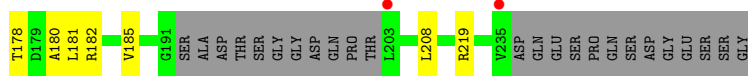
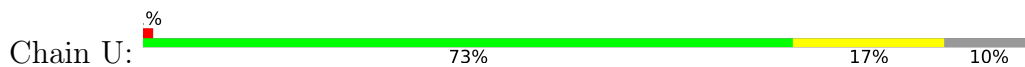


• Molecule 1: Proteasome subunit alpha

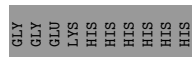
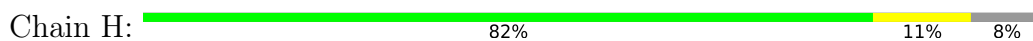




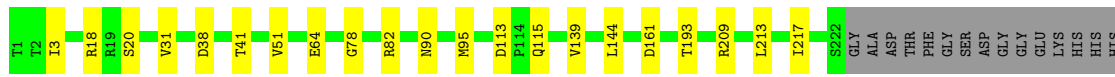
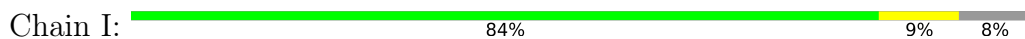
• Molecule 1: Proteasome subunit alpha



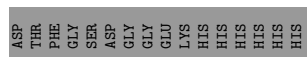
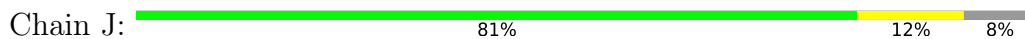
• Molecule 2: Proteasome subunit beta



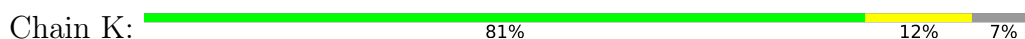
• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta




• Molecule 2: Proteasome subunit beta




SER  
ASP  
GLY  
GLU  
LYS  
HIS  
HIS  
HIS  
HIS  
HIS

- Molecule 2: Proteasome subunit beta

Chain L:  86% 7% 7%




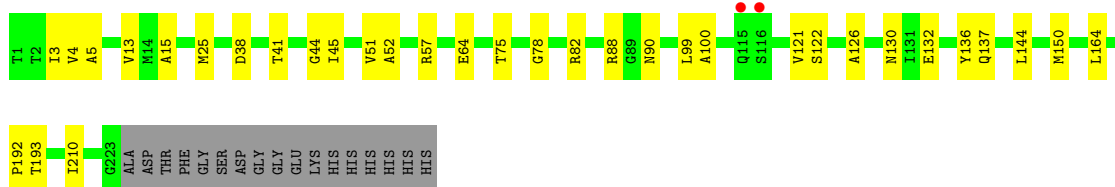
- Molecule 2: Proteasome subunit beta

Chain M:  85% 8% 8%




- Molecule 2: Proteasome subunit beta

Chain N:  79% 14% 7%




- Molecule 2: Proteasome subunit beta

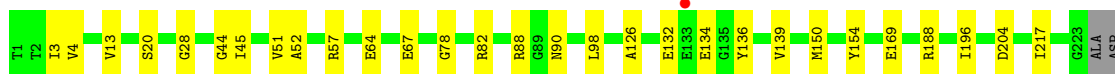
Chain V:  82% 11% 7%



SER  
ASP  
GLY  
GLU  
LYS  
HIS  
HIS  
HIS  
HIS  
HIS


- Molecule 2: Proteasome subunit beta

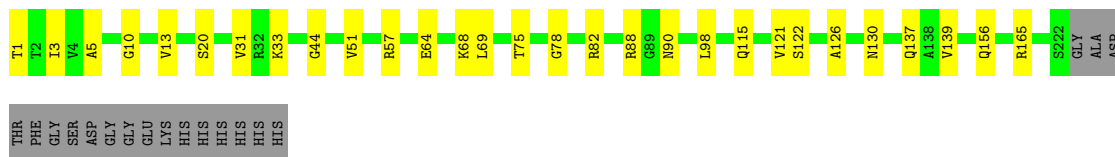
Chain W:  81% 12% 7%



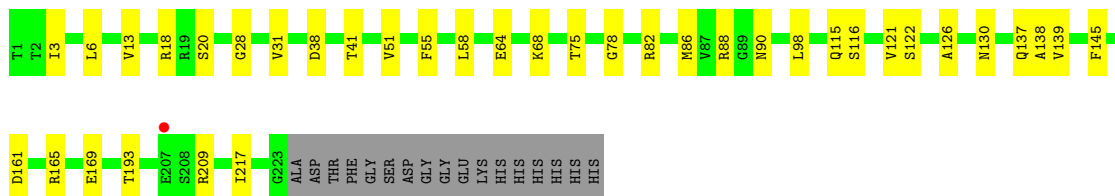
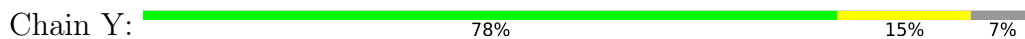
THR  
PHE  
GLY  
SER  
ASP  
GLY  
GLU  
LYS  
HIS  
HIS  
HIS  
HIS  
HIS

- Molecule 2: Proteasome subunit beta

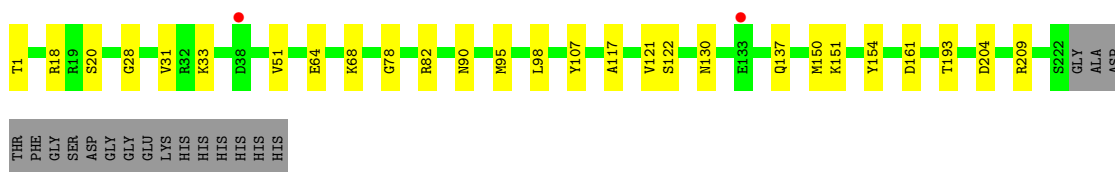
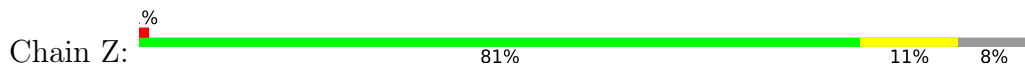
Chain X:  80% 12% 8%



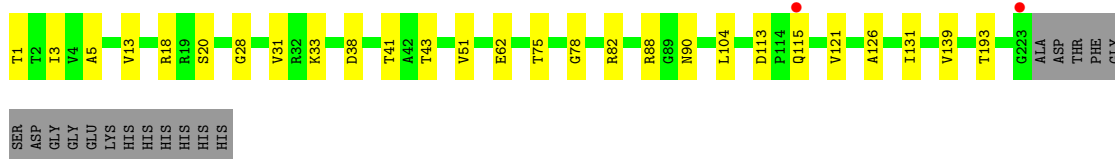
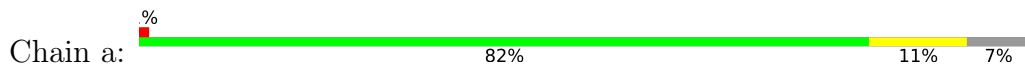
• Molecule 2: Proteasome subunit beta



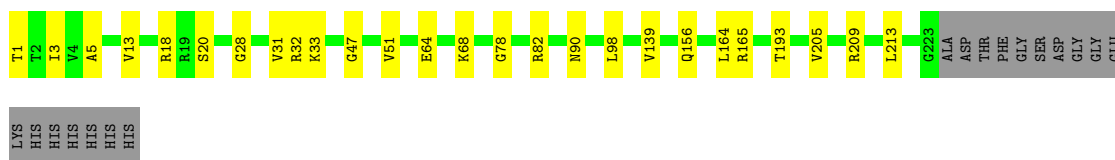
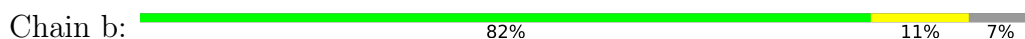
• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.65Å 197.48Å 164.81Å 90.00° 103.05° 90.00°	Depositor
Resolution (Å)	51.09 – 3.00 51.09 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (51.09-3.00) 92.7 (51.09-3.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.182 , 0.234 0.186 , 0.233	Depositor DCC
$R_{free}$ test set	7376 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.2	Xtrriage
Anisotropy	0.204	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 45.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	47136	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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: 7J0

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	0.16	0/1701	0.43	0/2297
1	B	0.15	0/1684	0.41	0/2274
1	C	0.14	0/1688	0.42	0/2279
1	D	0.15	0/1694	0.42	0/2287
1	E	0.16	0/1695	0.44	0/2289
1	F	0.15	0/1702	0.43	0/2298
1	G	0.16	0/1686	0.41	0/2276
1	O	0.14	0/1686	0.42	0/2276
1	P	0.17	0/1699	0.41	0/2295
1	Q	0.15	0/1703	0.42	1/2300 (0.0%)
1	R	0.16	0/1695	0.40	0/2289
1	S	0.15	0/1707	0.40	0/2305
1	T	0.15	0/1688	0.41	0/2279
1	U	0.16	0/1688	0.42	0/2279
2	H	0.15	0/1662	0.38	0/2254
2	I	0.15	0/1662	0.36	0/2254
2	J	0.16	0/1662	0.39	0/2254
2	K	0.15	0/1666	0.39	0/2259
2	L	0.16	0/1666	0.40	0/2259
2	M	0.15	0/1662	0.38	0/2254
2	N	0.16	0/1666	0.39	0/2259
2	V	0.16	0/1666	0.40	0/2259
2	W	0.18	0/1666	0.40	0/2259
2	X	0.15	0/1662	0.37	0/2254
2	Y	0.16	0/1666	0.39	0/2259
2	Z	0.15	0/1662	0.38	0/2254
2	a	0.15	0/1666	0.37	0/2259
2	b	0.15	0/1666	0.37	0/2259
All	All	0.15	0/47016	0.40	1/63619 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	203	LEU	CB-CA-C	-5.79	109.91	116.63

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	1677	0	1680	30	0
1	B	1660	0	1665	29	0
1	C	1664	0	1668	24	0
1	D	1670	0	1673	17	0
1	E	1671	0	1675	34	0
1	F	1678	0	1677	40	0
1	G	1662	0	1662	25	0
1	O	1662	0	1662	29	0
1	P	1674	0	1680	39	0
1	Q	1679	0	1679	38	0
1	R	1671	0	1675	22	0
1	S	1683	0	1682	25	0
1	T	1664	0	1668	28	0
1	U	1664	0	1668	27	0
2	H	1638	0	1633	19	0
2	I	1638	0	1633	14	0
2	J	1638	0	1633	21	0
2	K	1642	0	1636	17	0
2	L	1642	0	1636	12	0
2	M	1638	0	1633	12	0
2	N	1642	0	1636	22	0
2	V	1642	0	1636	17	0
2	W	1642	0	1636	21	0
2	X	1638	0	1633	20	0
2	Y	1642	0	1636	24	0
2	Z	1638	0	1633	19	0
2	a	1642	0	1636	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	1642	0	1636	18	0
3	H	42	0	0	0	0
3	I	42	0	0	1	0
3	J	42	0	0	1	0
3	K	42	0	0	0	0
3	L	42	0	0	0	0
3	M	42	0	0	0	0
3	N	42	0	0	0	0
3	V	42	0	0	0	0
3	W	42	0	0	0	0
3	X	42	0	0	0	0
3	Y	42	0	0	0	0
3	Z	42	0	0	0	0
3	a	42	0	0	0	0
3	b	42	0	0	1	0
4	A	9	0	0	0	0
4	B	2	0	0	0	0
4	C	5	0	0	0	0
4	D	3	0	0	0	0
4	E	5	0	0	0	0
4	F	8	0	0	0	0
4	G	7	0	0	0	0
4	H	7	0	0	0	0
4	I	8	0	0	0	0
4	J	7	0	0	0	0
4	K	12	0	0	0	0
4	L	5	0	0	0	0
4	M	12	0	0	0	0
4	N	7	0	0	0	0
4	O	6	0	0	0	0
4	P	6	0	0	0	0
4	Q	5	0	0	0	0
4	R	8	0	0	1	0
4	S	9	0	0	0	0
4	T	6	0	0	0	0
4	U	7	0	0	0	0
4	V	9	0	0	0	0
4	W	8	0	0	1	0
4	X	8	0	0	1	0
4	Y	11	0	0	0	0
4	Z	11	0	0	0	0
4	a	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	b	8	0	0	0	0
All	All	47136	0	46300	604	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 6.

All (604) 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)
1:D:9:MET:N	1:E:15:GLU:OE1	2.14	0.81
1:R:16:ARG:NH2	1:R:114:GLN:O	2.13	0.80
2:V:29:ARG:NH1	2:W:134:GLU:OE2	2.15	0.80
1:P:219:ARG:NH2	2:W:64:GLU:OE1	2.14	0.79
1:Q:140:ARG:NH2	1:Q:155:VAL:O	2.13	0.78
1:F:18:GLU:HG3	1:F:22:LYS:HE3	1.65	0.78
1:G:87:TYR:O	2:N:57:ARG:NH2	2.16	0.78
1:P:31:VAL:HG12	1:P:155:VAL:HG22	1.65	0.77
1:B:31:VAL:HG12	1:B:155:VAL:HG22	1.68	0.76
1:S:182:ARG:HH22	1:S:236:ASP:HB2	1.50	0.75
1:O:16:ARG:NH2	1:O:114:GLN:O	2.17	0.75
1:F:16:ARG:NH2	1:F:114:GLN:O	2.19	0.75
1:Q:31:VAL:HG12	1:Q:155:VAL:HG22	1.67	0.75
1:P:87:TYR:O	2:W:57:ARG:NH2	2.21	0.74
1:R:189:ARG:HG2	1:R:203:LEU:HD22	1.69	0.73
1:F:31:VAL:HG12	1:F:155:VAL:HG22	1.70	0.73
1:U:18:GLU:HG3	1:U:22:LYS:HE3	1.70	0.72
1:F:140:ARG:NH1	1:F:155:VAL:O	2.22	0.72
2:M:95:MET:HA	2:M:95:MET:HE2	1.71	0.72
1:C:16:ARG:NH2	1:C:114:GLN:O	2.23	0.71
1:P:97:ARG:NH2	1:Q:51:GLN:OE1	2.24	0.71
1:O:31:VAL:HG12	1:O:155:VAL:HG12	1.71	0.71
1:Q:219:ARG:NH2	2:X:64:GLU:OE1	2.24	0.70
2:V:156:GLN:OE1	2:V:165:ARG:NH1	2.24	0.70
1:U:56:LEU:HD13	1:U:99:LEU:HD23	1.73	0.70
1:E:10:GLU:HG3	1:F:15:GLU:HG2	1.73	0.70
2:J:64:GLU:HG2	2:J:68:LYS:HE2	1.72	0.70
1:F:219:ARG:NH2	2:M:64:GLU:OE2	2.24	0.69
1:A:121:GLU:OE2	1:A:140:ARG:NH1	2.25	0.69
1:P:92:ARG:NH2	1:P:132:GLU:OE2	2.26	0.69
1:D:97:ARG:NH2	2:L:70:GLU:O	2.26	0.69
1:A:52:LYS:NZ	1:A:64:ALA:O	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:155:VAL:HG21	1:O:164:ALA:HB2	1.75	0.68
2:I:95:MET:HE2	2:I:95:MET:HA	1.75	0.67
2:W:13:VAL:HG23	2:W:196:ILE:HG22	1.76	0.67
1:R:41:PHE:HB3	1:R:53:ILE:HD13	1.75	0.67
1:Q:112:THR:HG22	1:Q:113:GLU:HG3	1.77	0.67
1:U:140:ARG:NH1	1:U:155:VAL:O	2.28	0.66
2:L:161:ASP:OD1	2:L:209:ARG:NH2	2.29	0.66
1:C:219:ARG:NH2	2:J:64:GLU:OE2	2.23	0.66
1:A:138:LEU:HB2	1:A:150:GLU:O	1.96	0.65
1:F:41:PHE:HB3	1:F:53:ILE:HD13	1.77	0.65
2:J:4:VAL:HB	2:J:150:MET:HE1	1.79	0.65
2:W:4:VAL:HB	2:W:150:MET:HE1	1.79	0.65
2:N:121:VAL:HA	2:N:130:ASN:O	1.97	0.64
1:P:161:GLU:O	1:P:165:ASN:ND2	2.29	0.64
2:H:164:LEU:HD12	2:H:213:LEU:HD12	1.80	0.63
1:O:28:LYS:HB3	1:O:44:GLU:HG3	1.80	0.63
2:V:95:MET:HA	2:V:95:MET:HE2	1.79	0.63
1:F:92:ARG:HB2	2:N:75:THR:HG21	1.81	0.63
1:G:214:ASP:OD2	1:G:223:ARG:NH2	2.31	0.63
1:O:150:GLU:HG3	1:O:154:VAL:HG12	1.81	0.63
2:L:51:VAL:HG21	2:L:98:LEU:HB3	1.82	0.62
1:C:45:ASN:ND2	1:C:209:GLU:OE1	2.32	0.62
1:G:121:GLU:OE2	1:G:140:ARG:NH1	2.32	0.62
1:O:121:GLU:OE2	1:O:140:ARG:NH2	2.32	0.62
1:R:123:CYS:HA	1:R:139:TYR:O	2.00	0.62
1:D:31:VAL:HG22	1:D:155:VAL:HG22	1.81	0.62
1:E:41:PHE:HB3	1:E:53:ILE:HD13	1.81	0.62
1:P:92:ARG:HB3	2:X:75:THR:HG21	1.80	0.62
1:C:161:GLU:HG2	1:C:162:PRO:HD3	1.82	0.62
1:F:121:GLU:OE2	1:F:140:ARG:NH2	2.33	0.62
1:S:70:GLU:OE2	1:S:116:LYS:NZ	2.32	0.62
1:P:97:ARG:NH1	1:Q:49:SER:O	2.33	0.61
2:L:62:GLU:OE2	2:L:82:ARG:HD3	2.00	0.61
2:Y:58:LEU:HD23	2:Y:86:MET:HE3	1.82	0.61
2:N:122:SER:HB3	2:N:137:GLN:HG2	1.81	0.61
2:X:156:GLN:OE1	2:X:165:ARG:NH2	2.30	0.61
2:Y:58:LEU:HB3	2:Y:86:MET:HE1	1.82	0.61
2:b:32:ARG:HD2	2:b:193:THR:HG21	1.82	0.61
1:P:51:GLN:OE1	1:P:224:ARG:NH2	2.34	0.61
2:J:37:THR:HB	2:J:41:THR:HG23	1.83	0.61
1:B:219:ARG:NH1	2:I:64:GLU:OE2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:VAL:HG11	1:E:215:ALA:HB2	1.82	0.61
1:G:35:TYR:CZ	1:G:177:LEU:HD23	2.36	0.61
2:Z:95:MET:HE2	2:Z:95:MET:HA	1.83	0.61
2:L:113:ASP:OD2	2:L:115:GLN:HG2	2.00	0.60
1:P:205:VAL:HG13	1:P:230:LEU:HD23	1.82	0.60
2:V:165:ARG:HG3	2:V:213:LEU:HD22	1.83	0.60
2:a:43:THR:HG22	2:a:104:LEU:HD13	1.81	0.60
1:A:91:ARG:HH11	1:A:91:ARG:HG2	1.66	0.60
1:O:163:ILE:HD13	1:O:188:LEU:HD12	1.82	0.60
1:B:217:ARG:HG3	1:B:218:PRO:HD2	1.83	0.59
1:T:128:ALA:HB2	1:T:134:LYS:HB3	1.84	0.59
1:U:165:ASN:OD1	1:U:166:ALA:N	2.35	0.59
1:Q:74:LEU:HD13	1:Q:122:LEU:HD11	1.84	0.59
1:B:41:PHE:HB3	1:B:53:ILE:HD13	1.85	0.59
2:I:161:ASP:OD1	2:I:209:ARG:NH1	2.35	0.59
1:O:165:ASN:OD1	1:O:166:ALA:N	2.36	0.59
1:T:179:ASP:OD1	1:T:179:ASP:N	2.33	0.59
2:V:121:VAL:HA	2:V:130:ASN:O	2.03	0.59
1:E:205:VAL:HG23	1:E:230:LEU:HD23	1.85	0.59
1:Q:87:TYR:O	2:X:57:ARG:NH1	2.36	0.58
1:R:233:LEU:O	4:R:301:HOH:O	2.17	0.58
1:C:74:LEU:HD13	1:C:122:LEU:HD11	1.84	0.58
1:Q:18:GLU:HG3	1:Q:22:LYS:HE2	1.84	0.58
1:Q:181:LEU:O	1:Q:185:VAL:HG23	2.03	0.58
1:U:123:CYS:HA	1:U:139:TYR:O	2.04	0.58
1:O:85:ARG:NH2	1:O:98:GLN:OE1	2.36	0.58
1:U:30:VAL:HG13	1:U:43:ALA:HB2	1.86	0.58
1:A:15:GLU:OE1	1:G:9:MET:N	2.37	0.58
1:C:123:CYS:HA	1:C:139:TYR:O	2.04	0.58
1:G:31:VAL:HG22	1:G:155:VAL:HG22	1.85	0.58
1:S:68:PHE:HA	1:S:71:PHE:CE2	2.39	0.58
1:P:203:LEU:HD12	1:P:208:LEU:HD21	1.86	0.58
1:O:123:CYS:HA	1:O:139:TYR:O	2.04	0.57
1:P:68:PHE:HA	1:P:71:PHE:CE2	2.39	0.57
2:H:10:GLY:HA2	2:H:115:GLN:HA	1.86	0.57
1:F:181:LEU:O	1:F:185:VAL:HG23	2.04	0.57
1:B:217:ARG:HH12	1:B:223:ARG:HD3	1.68	0.57
1:D:89:TYR:CE2	2:L:82:ARG:HD2	2.39	0.57
1:U:28:LYS:HB3	1:U:44:GLU:HG3	1.87	0.57
2:K:95:MET:HE2	2:K:95:MET:HA	1.86	0.57
1:U:68:PHE:HA	1:U:71:PHE:CE2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:PHE:HA	1:B:71:PHE:CE2	2.40	0.56
1:E:107:LEU:HD11	1:E:122:LEU:HD13	1.88	0.56
1:Q:134:LYS:NZ	1:Q:137:GLU:OE2	2.39	0.56
1:F:107:LEU:HD11	1:F:122:LEU:HD13	1.88	0.56
1:T:219:ARG:HD2	1:T:220:ARG:HG3	1.86	0.56
1:G:219:ARG:NH2	2:N:64:GLU:OE2	2.39	0.56
2:Y:51:VAL:HG21	2:Y:98:LEU:HB3	1.88	0.56
1:T:181:LEU:O	1:T:185:VAL:HG23	2.05	0.56
1:G:56:LEU:HG	1:G:62:PHE:HB2	1.88	0.55
1:O:74:LEU:HD13	1:O:122:LEU:HD11	1.87	0.55
2:J:176:ASP:OD1	2:W:188:ARG:NH1	2.39	0.55
1:F:123:CYS:HA	1:F:139:TYR:O	2.07	0.55
1:R:68:PHE:HA	1:R:71:PHE:CE2	2.41	0.55
2:Y:122:SER:HB3	2:Y:137:GLN:HG2	1.88	0.55
1:C:128:ALA:HB2	1:C:134:LYS:HB3	1.89	0.55
1:B:232:ALA:O	1:B:235:VAL:HG23	2.05	0.55
2:J:10:GLY:HA2	2:J:115:GLN:HA	1.88	0.55
1:Q:10:GLU:N	1:Q:10:GLU:OE1	2.39	0.55
1:E:181:LEU:O	1:E:185:VAL:HG23	2.07	0.55
2:W:51:VAL:HG21	2:W:98:LEU:HB3	1.89	0.55
1:S:182:ARG:NH2	1:S:236:ASP:HB2	2.20	0.54
1:T:74:LEU:HD13	1:T:122:LEU:HD11	1.89	0.54
1:T:97:ARG:HE	1:U:49:SER:HB2	1.73	0.54
2:a:113:ASP:OD1	2:a:115:GLN:NE2	2.40	0.54
2:b:20:SER:HB2	2:b:31:VAL:HG21	1.89	0.54
2:b:156:GLN:OE1	2:b:165:ARG:NH2	2.29	0.54
1:S:181:LEU:O	1:S:185:VAL:HG23	2.07	0.54
3:I:301:7J0:C39	2:J:91:LEU:HD11	2.37	0.54
1:T:112:THR:HG23	1:T:113:GLU:HG3	1.89	0.54
2:X:51:VAL:HG11	2:X:90:ASN:HD21	1.73	0.54
1:C:53:ILE:HG12	1:C:209:GLU:OE2	2.07	0.54
1:C:181:LEU:O	1:C:185:VAL:HG23	2.08	0.54
1:F:28:LYS:HB3	1:F:44:GLU:HB2	1.89	0.54
1:Q:56:LEU:HG	1:Q:62:PHE:HB2	1.89	0.54
1:Q:163:ILE:HD13	1:Q:188:LEU:HD23	1.90	0.54
1:S:30:VAL:HG13	1:S:43:ALA:HB2	1.90	0.54
1:F:89:TYR:CD2	2:N:82:ARG:HD3	2.43	0.54
1:G:181:LEU:O	1:G:185:VAL:HG23	2.07	0.54
1:P:217:ARG:NH1	1:P:223:ARG:HD3	2.23	0.54
1:C:161:GLU:H	1:C:161:GLU:CD	2.16	0.53
2:N:130:ASN:ND2	2:N:132:GLU:OE1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:68:PHE:HA	1:O:71:PHE:CE2	2.44	0.53
1:C:56:LEU:HG	1:C:62:PHE:HB2	1.89	0.53
1:T:68:PHE:HA	1:T:71:PHE:CE2	2.44	0.53
1:E:68:PHE:HA	1:E:71:PHE:CE2	2.44	0.53
1:A:22:LYS:O	1:A:26:ARG:HG3	2.08	0.53
1:Q:92:ARG:HB3	2:Y:75:THR:HG21	1.90	0.53
2:b:209:ARG:HH11	2:b:213:LEU:HD21	1.73	0.53
1:A:9:MET:N	1:B:15:GLU:OE1	2.41	0.53
1:T:32:ALA:HA	1:T:40:LEU:O	2.09	0.53
2:Z:64:GLU:HG2	2:Z:68:LYS:HE2	1.91	0.53
1:D:22:LYS:O	1:D:26:ARG:HG2	2.08	0.52
1:F:33:LEU:HD11	1:F:171:TYR:CE1	2.44	0.52
2:K:169:GLU:OE2	2:K:221:ARG:NH2	2.41	0.52
1:R:107:LEU:HD11	1:R:122:LEU:HD13	1.91	0.52
1:T:178:THR:HG22	1:T:233:LEU:HD13	1.91	0.52
2:a:104:LEU:HB3	2:a:121:VAL:CG2	2.40	0.52
1:A:51:GLN:N	1:A:51:GLN:OE1	2.40	0.52
1:A:138:LEU:HD13	1:A:154:VAL:HG23	1.89	0.52
1:P:110:ILE:HG23	1:P:114:GLN:HG3	1.92	0.52
1:C:30:VAL:HG13	1:C:43:ALA:HB2	1.91	0.52
1:D:123:CYS:HA	1:D:139:TYR:O	2.09	0.52
1:O:56:LEU:HG	1:O:62:PHE:HB2	1.90	0.52
1:P:217:ARG:HH11	1:P:223:ARG:HD3	1.75	0.52
1:O:123:CYS:SG	1:O:154:VAL:HG21	2.50	0.52
1:F:225:ILE:HG21	1:F:233:LEU:HD12	1.92	0.52
1:G:107:LEU:HD11	1:G:122:LEU:HD23	1.91	0.52
2:N:13:VAL:HG21	2:N:164:LEU:HD12	1.92	0.52
1:P:81:PHE:CZ	1:P:102:VAL:HG21	2.44	0.52
1:Q:68:PHE:HA	1:Q:71:PHE:CE2	2.45	0.52
1:U:181:LEU:O	1:U:185:VAL:HG23	2.08	0.52
2:K:3:ILE:HG21	2:K:44:GLY:HA3	1.92	0.52
1:F:152:HIS:HB3	1:F:171:TYR:CE2	2.45	0.52
2:M:51:VAL:HG21	2:M:98:LEU:HB3	1.92	0.52
2:M:64:GLU:HG2	2:M:68:LYS:HE2	1.91	0.52
1:S:18:GLU:O	1:S:22:LYS:HG3	2.10	0.52
1:U:219:ARG:NH2	2:b:64:GLU:OE1	2.35	0.52
1:Q:121:GLU:OE2	1:Q:140:ARG:NH1	2.43	0.51
2:N:3:ILE:HG21	2:N:44:GLY:HA3	1.92	0.51
2:W:132:GLU:OE2	4:W:401:HOH:O	2.18	0.51
2:X:51:VAL:HG21	2:X:98:LEU:HB3	1.91	0.51
1:O:137:GLU:OE1	1:O:139:TYR:OH	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:20:SER:HB2	2:a:31:VAL:HG21	1.92	0.51
2:a:38:ASP:OD1	2:a:41:THR:N	2.44	0.51
1:B:217:ARG:NH1	1:B:223:ARG:HD3	2.25	0.51
1:U:56:LEU:HG	1:U:62:PHE:HB2	1.92	0.51
1:T:123:CYS:HA	1:T:139:TYR:O	2.10	0.51
1:T:137:GLU:HG2	1:U:48:ARG:HH12	1.76	0.51
1:E:56:LEU:HG	1:E:62:PHE:HB2	1.93	0.51
1:Q:123:CYS:HA	1:Q:139:TYR:O	2.11	0.51
1:D:68:PHE:HA	1:D:71:PHE:CE2	2.45	0.51
1:S:219:ARG:NH2	2:Z:64:GLU:OE2	2.44	0.51
1:E:112:THR:HG22	1:F:115:ALA:HB3	1.93	0.51
2:b:51:VAL:HG21	2:b:98:LEU:HB3	1.93	0.51
2:H:176:ASP:OD2	2:Z:151:LYS:NZ	2.43	0.50
1:R:89:TYR:CD1	2:Z:82:ARG:HD3	2.45	0.50
2:I:78:GLY:O	2:I:82:ARG:HG2	2.12	0.50
1:T:89:TYR:CD2	2:b:82:ARG:HD3	2.46	0.50
1:U:74:LEU:HD13	1:U:122:LEU:HD11	1.93	0.50
1:A:91:ARG:HG2	1:A:91:ARG:NH1	2.26	0.50
1:B:140:ARG:NH2	1:B:155:VAL:O	2.45	0.50
1:E:135:ARG:HH21	1:F:48:ARG:HH22	1.58	0.50
1:F:70:GLU:OE2	1:F:116:LYS:NZ	2.44	0.50
1:Q:33:LEU:HD11	1:Q:180:ALA:HB1	1.94	0.50
2:V:122:SER:HB3	2:V:137:GLN:HG2	1.93	0.50
1:G:68:PHE:HA	1:G:71:PHE:CE2	2.47	0.50
2:K:121:VAL:HA	2:K:130:ASN:O	2.12	0.50
2:Z:51:VAL:HG21	2:Z:98:LEU:HB3	1.93	0.50
1:D:107:LEU:HD11	1:D:122:LEU:HD13	1.93	0.50
2:H:78:GLY:O	2:H:82:ARG:HG2	2.11	0.50
1:T:108:GLY:O	1:T:112:THR:HG22	2.11	0.50
1:T:229:ALA:O	1:T:233:LEU:HD23	2.11	0.50
2:Z:20:SER:HB2	2:Z:31:VAL:HG21	1.94	0.50
2:b:1:THR:HG23	2:b:33:LYS:HD3	1.93	0.50
1:A:225:ILE:HG21	1:A:233:LEU:HD12	1.94	0.50
1:S:18:GLU:HB3	1:S:22:LYS:HE3	1.93	0.50
1:F:152:HIS:HB3	1:F:171:TYR:HE2	1.76	0.50
2:X:90:ASN:ND2	4:X:402:HOH:O	2.44	0.50
1:A:32:ALA:HA	1:A:40:LEU:O	2.11	0.50
1:F:22:LYS:O	1:F:26:ARG:HG3	2.12	0.50
2:W:20:SER:HB3	2:W:28:GLY:HA3	1.94	0.50
2:L:62:GLU:OE2	2:L:82:ARG:NH1	2.35	0.49
1:Q:62:PHE:CE2	1:Q:122:LEU:HD22	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:121:VAL:HG12	2:a:131:ILE:HG12	1.94	0.49
1:A:181:LEU:O	1:A:185:VAL:HG23	2.11	0.49
1:U:178:THR:O	1:U:182:ARG:HG3	2.12	0.49
1:B:123:CYS:HA	1:B:139:TYR:O	2.12	0.49
2:M:25:MET:HE1	2:N:144:LEU:HD21	1.94	0.49
1:P:25:ALA:O	1:P:158:GLY:HA2	2.13	0.49
1:P:140:ARG:NH1	1:P:155:VAL:O	2.33	0.49
1:P:107:LEU:HD11	1:P:122:LEU:CD1	2.42	0.49
1:C:68:PHE:HA	1:C:71:PHE:CE2	2.48	0.49
1:G:92:ARG:HB2	2:H:75:THR:HG21	1.94	0.49
2:X:121:VAL:HA	2:X:130:ASN:O	2.12	0.49
2:Y:51:VAL:HG11	2:Y:90:ASN:HD21	1.78	0.49
1:A:41:PHE:HB3	1:A:53:ILE:HD13	1.95	0.49
1:C:163:ILE:HD13	1:C:188:LEU:HD23	1.93	0.49
2:N:4:VAL:HB	2:N:150:MET:HE1	1.95	0.49
2:K:164:LEU:HD21	2:K:205:VAL:HG11	1.93	0.49
1:R:162:PRO:HB2	1:R:190:ALA:O	2.13	0.49
2:M:51:VAL:HG11	2:M:90:ASN:ND2	2.27	0.49
2:N:136:TYR:HB2	2:N:150:MET:SD	2.53	0.49
1:U:81:PHE:CE2	1:U:102:VAL:HG21	2.48	0.49
2:Y:121:VAL:HA	2:Y:130:ASN:O	2.12	0.49
1:E:161:GLU:HB3	1:E:162:PRO:HD3	1.95	0.48
2:N:78:GLY:O	2:N:82:ARG:HG2	2.13	0.48
1:R:81:PHE:CE2	1:R:102:VAL:HG21	2.48	0.48
1:T:56:LEU:HG	1:T:62:PHE:HB2	1.94	0.48
2:a:20:SER:HB3	2:a:28:GLY:HA3	1.95	0.48
1:B:56:LEU:HG	1:B:62:PHE:HB2	1.94	0.48
2:J:38:ASP:CG	2:J:41:THR:HG22	2.37	0.48
2:Z:122:SER:HB3	2:Z:137:GLN:HG2	1.95	0.48
1:S:18:GLU:OE2	1:S:21:ARG:NH2	2.45	0.48
1:A:56:LEU:HG	1:A:62:PHE:HB2	1.96	0.48
1:E:127:VAL:CG1	1:E:215:ALA:HB2	2.43	0.48
1:E:212:VAL:HG12	1:E:223:ARG:HG2	1.94	0.48
2:X:122:SER:HB3	2:X:137:GLN:HG2	1.96	0.48
1:G:123:CYS:HA	1:G:139:TYR:O	2.13	0.48
2:L:150:MET:O	2:L:154:TYR:HB2	2.13	0.48
1:O:83:ASP:OD2	2:V:65:HIS:ND1	2.34	0.48
1:A:164:ALA:O	1:A:168:LYS:HB2	2.13	0.48
1:E:18:GLU:O	1:E:22:LYS:HG3	2.13	0.48
1:E:121:GLU:OE2	1:E:140:ARG:NH1	2.46	0.48
1:P:56:LEU:HG	1:P:62:PHE:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:104:LEU:HB3	2:a:121:VAL:HG22	1.95	0.48
2:J:51:VAL:HG21	2:J:98:LEU:HB3	1.96	0.48
1:O:225:ILE:HG21	1:O:233:LEU:HD21	1.95	0.48
1:Q:162:PRO:HB2	1:Q:190:ALA:O	2.13	0.48
1:S:92:ARG:HB3	2:a:75:THR:HG21	1.94	0.48
2:X:1:THR:HG23	2:X:33:LYS:HD3	1.95	0.48
2:b:164:LEU:HD21	2:b:205:VAL:HG11	1.95	0.48
1:D:56:LEU:HG	1:D:62:PHE:HB2	1.95	0.48
1:R:181:LEU:O	1:R:185:VAL:HG23	2.14	0.48
2:W:204:ASP:OD1	2:W:204:ASP:N	2.47	0.48
1:R:121:GLU:OE2	1:R:140:ARG:NH2	2.46	0.48
2:a:3:ILE:HB	2:a:139:VAL:HG12	1.96	0.47
2:K:37:THR:HG21	2:K:59:TYR:HD2	1.79	0.47
1:U:138:LEU:HB2	1:U:150:GLU:O	2.13	0.47
2:Z:150:MET:O	2:Z:154:TYR:HB2	2.15	0.47
2:b:51:VAL:HG11	2:b:90:ASN:ND2	2.28	0.47
1:F:81:PHE:CZ	1:F:102:VAL:HG21	2.49	0.47
2:J:78:GLY:O	2:J:82:ARG:HG2	2.14	0.47
2:M:3:ILE:HB	2:M:139:VAL:HG12	1.97	0.47
2:W:3:ILE:HG21	2:W:44:GLY:HA3	1.96	0.47
2:Z:121:VAL:HA	2:Z:130:ASN:O	2.15	0.47
1:G:33:LEU:HD11	1:G:180:ALA:HB1	1.95	0.47
1:G:225:ILE:HG21	1:G:233:LEU:HD22	1.96	0.47
2:Y:18:ARG:HD3	2:Y:193:THR:HG23	1.97	0.47
2:Y:38:ASP:OD1	2:Y:41:THR:N	2.47	0.47
2:b:78:GLY:O	2:b:82:ARG:HG2	2.14	0.47
2:K:20:SER:HB2	2:K:31:VAL:HG21	1.96	0.47
2:Y:78:GLY:O	2:Y:82:ARG:HG2	2.14	0.47
1:A:89:TYR:CD1	2:I:82:ARG:HD3	2.50	0.47
2:H:8:TYR:CZ	2:H:11:GLY:HA3	2.50	0.47
2:K:3:ILE:HB	2:K:139:VAL:HG12	1.96	0.47
1:Q:18:GLU:O	1:Q:22:LYS:HG3	2.14	0.47
1:Q:89:TYR:CD2	2:Y:82:ARG:HD3	2.48	0.47
2:V:18:ARG:HD3	2:V:193:THR:HG23	1.96	0.47
2:Z:204:ASP:N	2:Z:204:ASP:OD1	2.41	0.47
2:a:78:GLY:O	2:a:82:ARG:HG2	2.15	0.47
1:F:18:GLU:OE2	1:F:21:ARG:NH1	2.47	0.47
2:K:122:SER:HB3	2:K:137:GLN:HG2	1.96	0.47
2:L:1:THR:HG23	2:L:33:LYS:HD3	1.96	0.47
1:Q:212:VAL:HG13	1:Q:223:ARG:HG3	1.97	0.47
1:S:172:ALA:HB3	1:S:175:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:88:ARG:HD3	2:Y:126:ALA:O	2.15	0.47
2:L:144:LEU:HD21	2:V:144:LEU:HB3	1.97	0.47
2:M:18:ARG:HD3	2:M:193:THR:HG23	1.96	0.47
1:P:74:LEU:HD23	1:P:122:LEU:HD11	1.96	0.47
2:V:20:SER:HB2	2:V:31:VAL:HG21	1.97	0.47
2:a:121:VAL:HG12	2:a:131:ILE:HA	1.96	0.47
1:A:62:PHE:CE2	1:A:122:LEU:HD22	2.50	0.46
1:O:89:TYR:CD2	2:W:82:ARG:HD3	2.51	0.46
1:Q:128:ALA:HB2	1:Q:134:LYS:HB3	1.97	0.46
1:O:9:MET:HB3	1:P:15:GLU:HB3	1.97	0.46
1:R:56:LEU:HG	1:R:62:PHE:HB2	1.97	0.46
2:H:64:GLU:HG2	2:H:68:LYS:HE2	1.98	0.46
1:O:140:ARG:NH1	1:O:155:VAL:O	2.46	0.46
1:P:181:LEU:O	1:P:185:VAL:HG23	2.15	0.46
1:S:16:ARG:NH1	1:S:111:PHE:O	2.49	0.46
1:A:219:ARG:NH2	2:H:64:GLU:OE2	2.48	0.46
2:K:213:LEU:O	2:K:217:ILE:HG12	2.15	0.46
1:S:89:TYR:CD2	2:a:82:ARG:HD3	2.50	0.46
1:P:107:LEU:HD12	1:P:141:ILE:HG22	1.98	0.46
2:I:3:ILE:HB	2:I:139:VAL:HG12	1.98	0.46
1:S:110:ILE:HG23	1:S:114:GLN:HG3	1.98	0.46
2:X:51:VAL:HG11	2:X:90:ASN:ND2	2.30	0.46
2:Y:3:ILE:HB	2:Y:139:VAL:HG12	1.97	0.46
2:Y:64:GLU:HG2	2:Y:68:LYS:HE2	1.98	0.46
1:O:30:VAL:HG13	1:O:43:ALA:HB2	1.98	0.46
2:W:51:VAL:HG11	2:W:90:ASN:HD21	1.81	0.46
1:Q:81:PHE:CZ	1:Q:102:VAL:HG21	2.50	0.46
1:A:68:PHE:HA	1:A:71:PHE:CE2	2.51	0.46
1:F:30:VAL:HG13	1:F:43:ALA:HB2	1.97	0.46
1:P:214:ASP:HB3	1:P:217:ARG:HG2	1.98	0.46
1:Q:35:TYR:CZ	1:Q:177:LEU:HD13	2.51	0.46
2:Y:20:SER:HB2	2:Y:31:VAL:HG21	1.97	0.46
1:C:232:ALA:O	1:C:235:VAL:HG12	2.15	0.45
1:R:89:TYR:CE1	2:Z:82:ARG:HD3	2.52	0.45
1:U:33:LEU:HD11	1:U:180:ALA:HB1	1.98	0.45
1:E:127:VAL:HG12	1:E:128:ALA:H	1.82	0.45
1:O:62:PHE:CE2	1:O:122:LEU:HD22	2.51	0.45
1:P:18:GLU:O	1:P:22:LYS:HG3	2.15	0.45
1:P:32:ALA:HA	1:P:40:LEU:O	2.14	0.45
1:P:225:ILE:HG21	1:P:233:LEU:HD12	1.97	0.45
2:W:136:TYR:HB2	2:W:150:MET:SD	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:20:SER:HB2	2:I:31:VAL:HG21	1.97	0.45
2:K:78:GLY:O	2:K:82:ARG:HG2	2.16	0.45
1:Q:185:VAL:O	1:Q:189:ARG:HG3	2.16	0.45
1:A:123:CYS:HA	1:A:139:TYR:O	2.16	0.45
1:B:181:LEU:O	1:B:185:VAL:HG23	2.16	0.45
1:B:225:ILE:HG22	1:B:230:LEU:HB2	1.98	0.45
1:D:81:PHE:CE2	1:D:102:VAL:HG21	2.52	0.45
1:B:30:VAL:HG13	1:B:43:ALA:HB2	1.98	0.45
1:G:156:MET:HE3	1:G:156:MET:HB2	1.89	0.45
1:O:53:ILE:HD12	1:O:209:GLU:HG2	1.98	0.45
1:P:10:GLU:O	1:P:14:ARG:HG2	2.17	0.45
2:W:150:MET:O	2:W:154:TYR:HB2	2.16	0.45
2:a:43:THR:HG22	2:a:104:LEU:CD1	2.47	0.45
1:C:10:GLU:OE1	1:D:22:LYS:NZ	2.36	0.45
1:C:156:MET:HE3	1:C:156:MET:HB2	1.91	0.45
2:K:179:SER:HB2	2:V:179:SER:HB2	1.97	0.45
1:U:152:HIS:CD2	1:U:171:TYR:HE2	2.34	0.45
2:a:18:ARG:HD3	2:a:193:THR:HG23	1.98	0.45
1:F:68:PHE:HA	1:F:71:PHE:CE2	2.52	0.45
2:K:204:ASP:OD1	2:K:204:ASP:N	2.45	0.45
1:R:30:VAL:HG13	1:R:43:ALA:HB2	1.99	0.45
1:D:20:ALA:O	1:D:24:ILE:HG13	2.17	0.45
2:J:37:THR:HG21	2:J:59:TYR:CD2	2.51	0.45
2:J:38:ASP:OD2	2:J:41:THR:N	2.49	0.45
2:Z:1:THR:HG23	2:Z:33:LYS:HD3	1.98	0.45
1:B:116:LYS:NZ	1:B:119:GLU:OE2	2.47	0.45
1:E:89:TYR:CD2	2:M:82:ARG:HD3	2.52	0.45
1:F:56:LEU:HD13	1:F:99:LEU:HD13	1.99	0.45
1:P:41:PHE:HB3	1:P:53:ILE:HD13	1.99	0.45
1:E:128:ALA:HB2	1:E:134:LYS:HG3	1.99	0.45
1:F:162:PRO:HB2	1:F:191:GLY:HA3	1.99	0.45
2:I:18:ARG:HD3	2:I:193:THR:HG23	1.97	0.45
2:N:192:PRO:O	2:N:210:ILE:HG21	2.17	0.45
1:Q:30:VAL:HG13	1:Q:43:ALA:HB2	1.99	0.45
1:B:9:MET:HE1	1:C:115:ALA:O	2.17	0.44
1:T:121:GLU:OE2	1:T:140:ARG:NH2	2.50	0.44
1:S:140:ARG:NH1	1:S:155:VAL:O	2.32	0.44
2:Z:161:ASP:OD2	2:Z:209:ARG:NH2	2.51	0.44
1:C:62:PHE:CE2	1:C:122:LEU:HD22	2.53	0.44
1:P:54:SER:CB	1:P:75:ARG:HD2	2.48	0.44
1:A:74:LEU:HD13	1:A:122:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:LEU:HD11	1:E:184:ALA:HB2	2.00	0.44
2:H:164:LEU:HD12	2:H:213:LEU:CD1	2.45	0.44
1:O:41:PHE:HB3	1:O:53:ILE:HD13	2.00	0.44
1:S:56:LEU:HG	1:S:62:PHE:HB2	1.99	0.44
1:T:45:ASN:ND2	1:T:209:GLU:OE1	2.51	0.44
1:T:138:LEU:HD13	1:T:154:VAL:HG23	2.00	0.44
2:Z:51:VAL:HG11	2:Z:90:ASN:HD21	1.83	0.44
2:Z:107:TYR:CE1	2:Z:117:ALA:HB3	2.52	0.44
1:B:32:ALA:HA	1:B:40:LEU:O	2.18	0.44
1:E:168:LYS:HA	1:E:168:LYS:HD3	1.83	0.44
1:G:205:VAL:HG13	1:G:230:LEU:HD23	2.00	0.44
2:L:64:GLU:HG2	2:L:68:LYS:HE2	1.99	0.44
1:C:9:MET:HA	1:C:12:ALA:HB3	2.00	0.44
1:F:217:ARG:HH21	1:F:223:ARG:HD2	1.83	0.44
2:H:144:LEU:HD21	2:N:25:MET:HE1	1.99	0.44
2:M:51:VAL:HG11	2:M:90:ASN:HD21	1.82	0.44
1:S:31:VAL:HG22	1:S:155:VAL:HG22	1.99	0.44
2:X:3:ILE:HB	2:X:139:VAL:HG12	2.00	0.44
2:Z:18:ARG:HD3	2:Z:193:THR:HG23	2.00	0.44
1:A:81:PHE:CZ	1:A:102:VAL:HG21	2.53	0.44
1:B:9:MET:N	1:C:15:GLU:HB3	2.32	0.44
1:E:9:MET:HB3	1:F:15:GLU:CD	2.42	0.44
1:P:62:PHE:CE2	1:P:122:LEU:HD23	2.53	0.44
1:R:128:ALA:HB2	1:R:134:LYS:HB3	1.99	0.44
2:W:78:GLY:O	2:W:82:ARG:HG2	2.18	0.44
2:a:5:ALA:HA	2:a:13:VAL:O	2.18	0.44
1:E:142:THR:OG1	1:E:146:SER:HB2	2.18	0.44
1:F:56:LEU:HG	1:F:62:PHE:HB2	1.98	0.44
1:T:62:PHE:CE2	1:T:122:LEU:HD22	2.53	0.44
2:J:3:ILE:HB	2:J:139:VAL:HG12	2.00	0.43
1:S:101:ASN:C	1:S:101:ASN:HD22	2.26	0.43
1:S:156:MET:HE3	1:S:156:MET:HB2	1.90	0.43
2:I:213:LEU:O	2:I:217:ILE:HG12	2.18	0.43
2:b:5:ALA:HA	2:b:13:VAL:O	2.18	0.43
2:b:18:ARG:HD3	2:b:193:THR:HG23	1.98	0.43
1:G:32:ALA:HA	1:G:40:LEU:O	2.18	0.43
2:H:45:ILE:HG21	2:H:52:ALA:HA	2.00	0.43
1:Q:219:ARG:NH2	1:Q:220:ARG:HD2	2.33	0.43
2:a:62:GLU:OE2	2:a:82:ARG:NE	2.43	0.43
1:A:33:LEU:HD11	1:A:40:LEU:HD23	1.99	0.43
1:A:156:MET:HE3	1:A:156:MET:HB2	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:161:GLU:HB2	1:G:162:PRO:HD3	2.00	0.43
1:S:62:PHE:HE2	1:S:122:LEU:HD13	1.82	0.43
1:B:57:TYR:OH	1:B:86:GLY:HA3	2.18	0.43
2:J:38:ASP:OD2	2:J:41:THR:HG22	2.19	0.43
1:Q:75:ARG:NH1	2:X:69:LEU:O	2.48	0.43
2:b:51:VAL:HG11	2:b:90:ASN:HD21	1.84	0.43
2:H:62:GLU:OE2	2:H:82:ARG:NE	2.46	0.43
2:J:122:SER:HB3	2:J:137:GLN:HG2	2.00	0.43
2:J:164:LEU:HD21	2:J:205:VAL:HG11	1.99	0.43
2:N:45:ILE:HG21	2:N:52:ALA:HA	2.00	0.43
1:C:74:LEU:HD11	1:C:107:LEU:HD21	1.99	0.43
1:Q:47:SER:C	1:Q:48:ARG:HD2	2.44	0.43
2:W:45:ILE:HG21	2:W:52:ALA:HA	2.01	0.43
2:X:88:ARG:HD3	2:X:126:ALA:O	2.19	0.43
1:A:81:PHE:CE1	1:A:102:VAL:HG21	2.54	0.43
1:B:81:PHE:CZ	1:B:102:VAL:HG21	2.53	0.43
1:G:81:PHE:CZ	1:G:102:VAL:HG21	2.54	0.43
1:T:156:MET:HE3	1:T:156:MET:HB2	1.90	0.43
2:V:78:GLY:O	2:V:82:ARG:HG2	2.19	0.43
2:b:20:SER:HB3	2:b:28:GLY:HA3	1.99	0.43
1:A:30:VAL:HG13	1:A:43:ALA:HB2	1.99	0.43
1:B:74:LEU:HD11	1:B:107:LEU:HD21	2.00	0.43
1:B:89:TYR:CD1	2:J:82:ARG:HD3	2.53	0.43
1:D:30:VAL:HG13	1:D:43:ALA:HB2	2.01	0.43
2:H:51:VAL:HG21	2:H:98:LEU:HB3	2.01	0.43
1:U:44:GLU:HA	1:U:208:LEU:HD23	2.01	0.43
1:B:74:LEU:HD13	1:B:122:LEU:HD11	2.01	0.42
1:G:89:TYR:CD2	2:H:82:ARG:HD3	2.53	0.42
1:G:163:ILE:HD13	1:G:188:LEU:HD23	2.01	0.42
1:S:167:LEU:O	1:S:171:TYR:HB2	2.19	0.42
1:U:161:GLU:HB2	1:U:162:PRO:HD3	2.01	0.42
2:W:3:ILE:HB	2:W:139:VAL:HG12	1.99	0.42
2:Y:6:LEU:HG	2:Y:13:VAL:HG12	2.00	0.42
2:Z:20:SER:HB3	2:Z:28:GLY:HA3	2.01	0.42
1:B:33:LEU:HD11	1:B:180:ALA:HB1	2.00	0.42
1:D:9:MET:HE3	1:E:19:LEU:HD13	2.01	0.42
2:H:123:PHE:HA	2:H:128:GLY:O	2.19	0.42
1:O:219:ARG:NH2	1:O:220:ARG:HD2	2.34	0.42
1:P:81:PHE:CE2	1:P:102:VAL:HG21	2.54	0.42
2:Y:115:GLN:O	2:Y:116:SER:OG	2.29	0.42
2:Z:78:GLY:O	2:Z:82:ARG:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:178:THR:HG22	1:F:233:LEU:HD22	2.01	0.42
1:R:10:GLU:HG3	1:R:11:GLN:N	2.35	0.42
1:T:28:LYS:HE2	1:T:28:LYS:HB2	1.88	0.42
1:E:56:LEU:HD23	1:E:56:LEU:HA	1.89	0.42
1:S:231:GLN:O	1:S:235:VAL:HG12	2.19	0.42
2:Y:3:ILE:O	2:Y:138:ALA:HA	2.20	0.42
2:H:150:MET:O	2:H:154:TYR:HB2	2.19	0.42
1:O:45:ASN:ND2	1:O:52:LYS:HG3	2.35	0.42
1:P:230:LEU:O	1:P:234:LEU:HD22	2.19	0.42
1:R:61:GLY:N	1:R:213:LEU:HD11	2.34	0.42
1:U:62:PHE:CE2	1:U:122:LEU:HD22	2.55	0.42
2:M:38:ASP:OD1	2:M:41:THR:N	2.52	0.42
2:X:3:ILE:HG21	2:X:44:GLY:HA3	2.01	0.42
2:X:64:GLU:HG2	2:X:68:LYS:HE2	2.00	0.42
1:E:162:PRO:HB2	1:E:190:ALA:O	2.20	0.42
1:E:225:ILE:HG22	1:E:230:LEU:HB2	2.02	0.42
2:I:113:ASP:OD2	2:I:115:GLN:HB2	2.19	0.42
2:N:15:ALA:HA	2:N:193:THR:O	2.20	0.42
2:N:38:ASP:OD1	2:N:41:THR:N	2.53	0.42
2:N:51:VAL:HG11	2:N:90:ASN:HD21	1.85	0.42
2:N:88:ARG:HD3	2:N:126:ALA:O	2.20	0.42
1:P:121:GLU:OE2	1:P:140:ARG:NH2	2.52	0.42
1:E:30:VAL:HG13	1:E:43:ALA:HB2	2.02	0.42
1:E:123:CYS:HA	1:E:139:TYR:O	2.20	0.42
2:J:132:GLU:OE1	2:J:134:GLU:HB2	2.20	0.42
2:N:5:ALA:HA	2:N:13:VAL:O	2.20	0.42
1:Q:74:LEU:HD11	1:Q:107:LEU:HD21	2.02	0.42
1:Q:156:MET:HE3	1:Q:156:MET:HB2	1.84	0.42
1:T:99:LEU:O	1:T:102:VAL:HG12	2.19	0.42
1:T:152:HIS:HB3	1:T:171:TYR:CE2	2.55	0.42
1:U:32:ALA:HA	1:U:40:LEU:O	2.19	0.42
2:Y:20:SER:HB3	2:Y:28:GLY:HA3	2.02	0.42
2:I:38:ASP:OD1	2:I:41:THR:OG1	2.35	0.41
2:L:101:LEU:HD23	2:L:101:LEU:HA	1.84	0.41
1:U:18:GLU:O	1:U:22:LYS:HG3	2.20	0.41
2:Y:165:ARG:NH1	2:Y:169:GLU:OE1	2.53	0.41
2:a:51:VAL:HG11	2:a:90:ASN:ND2	2.35	0.41
1:F:163:ILE:HD13	1:F:188:LEU:HD23	2.02	0.41
1:G:89:TYR:CE2	2:H:82:ARG:HD3	2.55	0.41
2:I:144:LEU:HD22	2:Y:145:PHE:HE1	1.85	0.41
1:O:96:GLY:H	1:O:126:GLU:CD	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:181:LEU:HD23	1:Q:233:LEU:HB3	2.03	0.41
2:V:14:MET:HE3	2:V:105:ALA:HB2	2.03	0.41
2:W:88:ARG:HD3	2:W:126:ALA:O	2.19	0.41
1:B:123:CYS:HB2	1:B:156:MET:SD	2.60	0.41
1:D:123:CYS:HB2	1:D:156:MET:SD	2.59	0.41
1:E:28:LYS:HE2	1:E:28:LYS:HB2	1.78	0.41
1:F:185:VAL:HG21	1:F:234:LEU:HD11	2.02	0.41
2:K:1:THR:HG23	2:K:33:LYS:HD3	2.03	0.41
1:Q:81:PHE:CE1	1:Q:102:VAL:HG21	2.55	0.41
1:R:32:ALA:HA	1:R:40:LEU:O	2.19	0.41
2:V:3:ILE:HG21	2:V:44:GLY:HA3	2.03	0.41
2:Y:161:ASP:CG	2:Y:209:ARG:HH21	2.28	0.41
2:a:121:VAL:CG1	2:a:131:ILE:HG12	2.51	0.41
1:F:170:SER:O	1:F:183:ILE:HD12	2.19	0.41
1:G:155:VAL:HG12	1:G:160:THR:HG22	2.01	0.41
2:W:169:GLU:HA	2:W:217:ILE:HD13	2.03	0.41
1:A:232:ALA:O	1:A:235:VAL:HG12	2.20	0.41
1:E:127:VAL:HG12	1:E:128:ALA:N	2.35	0.41
1:F:70:GLU:HB3	1:F:118:TYR:CD2	2.56	0.41
1:G:229:ALA:O	1:G:233:LEU:HD13	2.20	0.41
2:H:3:ILE:HG21	2:H:44:GLY:HA3	2.02	0.41
2:J:22:GLN:HG3	3:J:301:7J0:O31	2.21	0.41
2:X:10:GLY:HA2	2:X:115:GLN:HA	2.02	0.41
1:R:219:ARG:NH1	1:R:220:ARG:HD2	2.35	0.41
1:T:65:ALA:O	1:T:120:VAL:HA	2.21	0.41
2:V:5:ALA:HA	2:V:13:VAL:O	2.21	0.41
2:Y:55:PHE:CD1	2:Y:86:MET:HE2	2.55	0.41
2:a:51:VAL:HG11	2:a:90:ASN:HD21	1.85	0.41
2:b:3:ILE:HB	2:b:139:VAL:HG12	2.02	0.41
1:D:83:ASP:OD2	2:K:65:HIS:ND1	2.43	0.41
1:S:56:LEU:HD23	1:S:56:LEU:HA	1.91	0.41
1:U:56:LEU:HD23	1:U:56:LEU:HA	1.85	0.41
2:X:20:SER:HB2	2:X:31:VAL:HG21	2.02	0.41
1:C:188:LEU:HD23	1:C:188:LEU:HA	1.95	0.41
1:F:33:LEU:HD11	1:F:171:TYR:CD1	2.56	0.41
1:F:54:SER:CB	1:F:75:ARG:HD2	2.51	0.41
2:J:3:ILE:HG21	2:J:44:GLY:HA3	2.03	0.41
2:K:139:VAL:C	2:K:143:SER:HB3	2.46	0.41
2:M:20:SER:HB3	2:M:28:GLY:HA3	2.03	0.41
1:O:32:ALA:HA	1:O:40:LEU:O	2.21	0.41
1:O:127:VAL:CG2	1:O:215:ALA:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:128:ALA:HB2	1:P:134:LYS:HB3	2.03	0.41
1:T:214:ASP:OD2	1:T:223:ARG:NH2	2.54	0.41
1:U:150:GLU:HA	1:U:151:PRO:HD3	1.94	0.41
2:V:38:ASP:OD1	2:V:41:THR:N	2.54	0.41
2:a:1:THR:HG23	2:a:33:LYS:HD3	2.02	0.41
2:a:88:ARG:HD3	2:a:126:ALA:O	2.21	0.41
1:A:92:ARG:HA	1:A:92:ARG:HD2	1.92	0.41
1:D:229:ALA:O	1:D:233:LEU:HD23	2.21	0.41
1:E:54:SER:CB	1:E:75:ARG:HD2	2.50	0.41
1:F:128:ALA:HB2	1:F:134:LYS:HG2	2.03	0.41
2:I:144:LEU:HD23	2:I:144:LEU:HA	1.84	0.41
1:P:220:ARG:HH12	2:W:67:GLU:CD	2.29	0.41
1:T:9:MET:HB2	1:T:9:MET:HE2	1.83	0.41
1:A:31:VAL:HG21	1:A:167:LEU:HD11	2.04	0.40
1:E:212:VAL:CG1	1:E:223:ARG:HG2	2.51	0.40
1:F:98:GLN:O	1:F:102:VAL:HG23	2.21	0.40
1:Q:18:GLU:OE1	1:Q:21:ARG:NH1	2.43	0.40
2:X:5:ALA:HA	2:X:13:VAL:O	2.21	0.40
2:b:47:GLY:O	3:b:301:7J0:N06	2.54	0.40
1:B:9:MET:N	1:C:15:GLU:OE1	2.54	0.40
1:E:21:ARG:HH21	1:E:22:LYS:HG2	1.86	0.40
1:R:156:MET:HE3	1:R:156:MET:HB2	1.83	0.40
2:J:20:SER:HB2	2:J:31:VAL:HG21	2.02	0.40
1:P:123:CYS:HA	1:P:139:TYR:O	2.21	0.40
1:S:41:PHE:HB3	1:S:53:ILE:HD13	2.02	0.40
1:U:92:ARG:HB2	2:V:75:THR:HG21	2.04	0.40
1:B:56:LEU:HD23	1:B:56:LEU:HA	1.84	0.40
2:N:99:LEU:HD22	2:N:100:ALA:N	2.36	0.40
1:T:66:GLY:HA3	1:T:119:GLU:O	2.21	0.40
2:X:78:GLY:O	2:X:82:ARG:HG2	2.22	0.40
2:Y:169:GLU:HA	2:Y:217:ILE:HD13	2.04	0.40
1:B:33:LEU:CD1	1:B:180:ALA:HB1	2.52	0.40
2:H:122:SER:O	2:H:129:TRP:HA	2.21	0.40
2:I:51:VAL:HG11	2:I:90:ASN:HD21	1.87	0.40
2:K:7:LYS:HD3	2:K:135:GLY:HA2	2.04	0.40
1:P:12:ALA:O	1:P:16:ARG:HG3	2.22	0.40
1:Q:28:LYS:HE2	1:Q:28:LYS:HB2	1.95	0.40
1:R:12:ALA:O	1:R:16:ARG:HG3	2.21	0.40
2:b:64:GLU:HG2	2:b:68:LYS:HE2	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	214/240 (89%)	207 (97%)	7 (3%)	0	100	100
1	B	211/240 (88%)	206 (98%)	5 (2%)	0	100	100
1	C	212/240 (88%)	206 (97%)	6 (3%)	0	100	100
1	D	213/240 (89%)	206 (97%)	7 (3%)	0	100	100
1	E	213/240 (89%)	206 (97%)	7 (3%)	0	100	100
1	F	214/240 (89%)	206 (96%)	8 (4%)	0	100	100
1	G	212/240 (88%)	207 (98%)	5 (2%)	0	100	100
1	O	212/240 (88%)	205 (97%)	6 (3%)	1 (0%)	24	60
1	P	213/240 (89%)	205 (96%)	8 (4%)	0	100	100
1	Q	214/240 (89%)	207 (97%)	7 (3%)	0	100	100
1	R	213/240 (89%)	205 (96%)	8 (4%)	0	100	100
1	S	215/240 (90%)	205 (95%)	10 (5%)	0	100	100
1	T	212/240 (88%)	204 (96%)	8 (4%)	0	100	100
1	U	212/240 (88%)	206 (97%)	6 (3%)	0	100	100
2	H	220/240 (92%)	216 (98%)	4 (2%)	0	100	100
2	I	220/240 (92%)	214 (97%)	6 (3%)	0	100	100
2	J	220/240 (92%)	216 (98%)	4 (2%)	0	100	100
2	K	221/240 (92%)	216 (98%)	5 (2%)	0	100	100
2	L	221/240 (92%)	217 (98%)	4 (2%)	0	100	100
2	M	220/240 (92%)	215 (98%)	4 (2%)	1 (0%)	24	60
2	N	221/240 (92%)	217 (98%)	4 (2%)	0	100	100
2	V	221/240 (92%)	217 (98%)	4 (2%)	0	100	100
2	W	221/240 (92%)	216 (98%)	5 (2%)	0	100	100
2	X	220/240 (92%)	216 (98%)	4 (2%)	0	100	100
2	Y	221/240 (92%)	215 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Z	220/240 (92%)	213 (97%)	7 (3%)	0	100	100
2	a	221/240 (92%)	217 (98%)	4 (2%)	0	100	100
2	b	221/240 (92%)	217 (98%)	4 (2%)	0	100	100
All	All	6068/6720 (90%)	5903 (97%)	163 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	205	VAL
2	M	114	PRO

### 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	167/184 (91%)	167 (100%)	0	100	100
1	B	165/184 (90%)	165 (100%)	0	100	100
1	C	165/184 (90%)	165 (100%)	0	100	100
1	D	166/184 (90%)	164 (99%)	2 (1%)	63	82
1	E	166/184 (90%)	165 (99%)	1 (1%)	78	88
1	F	167/184 (91%)	167 (100%)	0	100	100
1	G	165/184 (90%)	165 (100%)	0	100	100
1	O	165/184 (90%)	165 (100%)	0	100	100
1	P	167/184 (91%)	167 (100%)	0	100	100
1	Q	167/184 (91%)	167 (100%)	0	100	100
1	R	166/184 (90%)	166 (100%)	0	100	100
1	S	167/184 (91%)	167 (100%)	0	100	100
1	T	165/184 (90%)	165 (100%)	0	100	100
1	U	165/184 (90%)	165 (100%)	0	100	100
2	H	165/178 (93%)	165 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	165/178 (93%)	165 (100%)	0	100	100
2	J	165/178 (93%)	165 (100%)	0	100	100
2	K	165/178 (93%)	165 (100%)	0	100	100
2	L	165/178 (93%)	165 (100%)	0	100	100
2	M	165/178 (93%)	164 (99%)	1 (1%)	78	88
2	N	165/178 (93%)	165 (100%)	0	100	100
2	V	165/178 (93%)	165 (100%)	0	100	100
2	W	165/178 (93%)	165 (100%)	0	100	100
2	X	165/178 (93%)	165 (100%)	0	100	100
2	Y	165/178 (93%)	165 (100%)	0	100	100
2	Z	165/178 (93%)	165 (100%)	0	100	100
2	a	165/178 (93%)	165 (100%)	0	100	100
2	b	165/178 (93%)	165 (100%)	0	100	100
All	All	4633/5068 (91%)	4629 (100%)	4 (0%)	88	93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	102	VAL
1	D	160	THR
1	E	33	LEU
2	M	158	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	174	ASN
1	D	101	ASN
1	D	129	HIS
1	E	152	HIS
1	F	165	ASN
1	F	231	GLN
1	G	101	ASN
2	I	137	GLN
2	J	130	ASN

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Mol	Chain	Res	Type
1	O	98	GLN
1	P	101	ASN
1	S	98	GLN
1	T	129	HIS
1	U	129	HIS
1	U	174	ASN
2	V	115	GLN
2	V	137	GLN
2	W	115	GLN
2	X	137	GLN
2	Z	96	GLN
2	a	115	GLN
2	b	130	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](#)

14 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	$\# Z  > 2$
3	7J0	J	301	-	45,45,45	1.90	12 (26%)	59,59,59	1.57	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	7J0	W	301	-	45,45,45	1.91	12 (26%)	59,59,59	1.50	9 (15%)
3	7J0	b	301	-	45,45,45	1.88	12 (26%)	59,59,59	1.52	9 (15%)
3	7J0	a	301	-	45,45,45	1.90	12 (26%)	59,59,59	1.51	9 (15%)
3	7J0	Y	301	-	45,45,45	1.89	12 (26%)	59,59,59	1.50	9 (15%)
3	7J0	I	301	-	45,45,45	1.90	12 (26%)	59,59,59	1.50	9 (15%)
3	7J0	H	301	-	45,45,45	1.90	12 (26%)	59,59,59	1.51	10 (16%)
3	7J0	X	301	-	45,45,45	1.89	12 (26%)	59,59,59	1.50	9 (15%)
3	7J0	N	301	-	45,45,45	1.89	12 (26%)	59,59,59	1.51	10 (16%)
3	7J0	M	301	-	45,45,45	1.90	12 (26%)	59,59,59	1.51	9 (15%)
3	7J0	L	301	-	45,45,45	1.88	12 (26%)	59,59,59	1.50	9 (15%)
3	7J0	Z	301	-	45,45,45	1.89	12 (26%)	59,59,59	1.50	9 (15%)
3	7J0	V	301	-	45,45,45	1.88	12 (26%)	59,59,59	1.50	9 (15%)
3	7J0	K	301	-	45,45,45	1.91	12 (26%)	59,59,59	1.52	9 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	7J0	J	301	-	-	6/37/45/45	0/4/4/4
3	7J0	W	301	-	-	2/37/45/45	0/4/4/4
3	7J0	b	301	-	-	4/37/45/45	0/4/4/4
3	7J0	a	301	-	-	6/37/45/45	0/4/4/4
3	7J0	Y	301	-	-	3/37/45/45	0/4/4/4
3	7J0	I	301	-	-	2/37/45/45	0/4/4/4
3	7J0	H	301	-	-	8/37/45/45	0/4/4/4
3	7J0	X	301	-	-	3/37/45/45	0/4/4/4
3	7J0	N	301	-	-	5/37/45/45	0/4/4/4
3	7J0	M	301	-	-	5/37/45/45	0/4/4/4
3	7J0	L	301	-	-	3/37/45/45	0/4/4/4
3	7J0	Z	301	-	-	5/37/45/45	0/4/4/4
3	7J0	V	301	-	-	6/37/45/45	0/4/4/4
3	7J0	K	301	-	-	7/37/45/45	0/4/4/4

All (168) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	301	7J0	C33-N32	6.28	1.47	1.34
3	K	301	7J0	C33-N32	6.26	1.47	1.34
3	W	301	7J0	C33-N32	6.24	1.47	1.34
3	M	301	7J0	C33-N32	6.24	1.47	1.34
3	N	301	7J0	C33-N32	6.24	1.47	1.34
3	H	301	7J0	C33-N32	6.24	1.47	1.34
3	I	301	7J0	C33-N32	6.24	1.47	1.34
3	Y	301	7J0	C33-N32	6.22	1.47	1.34
3	a	301	7J0	C33-N32	6.22	1.47	1.34
3	X	301	7J0	C33-N32	6.22	1.47	1.34
3	V	301	7J0	C33-N32	6.21	1.47	1.34
3	Z	301	7J0	C33-N32	6.20	1.47	1.34
3	b	301	7J0	C33-N32	6.20	1.47	1.34
3	L	301	7J0	C33-N32	6.18	1.47	1.34
3	W	301	7J0	C24-N25	4.67	1.44	1.35
3	I	301	7J0	C24-N25	4.66	1.44	1.35
3	M	301	7J0	C24-N25	4.65	1.44	1.35
3	Y	301	7J0	C24-N25	4.64	1.44	1.35
3	K	301	7J0	C24-N25	4.64	1.44	1.35
3	a	301	7J0	C24-N25	4.64	1.44	1.35
3	L	301	7J0	C24-N25	4.64	1.44	1.35
3	Z	301	7J0	C24-N25	4.63	1.44	1.35
3	N	301	7J0	C24-N25	4.63	1.44	1.35
3	b	301	7J0	C24-N25	4.62	1.44	1.35
3	H	301	7J0	C24-N25	4.61	1.44	1.35
3	V	301	7J0	C24-N25	4.60	1.44	1.35
3	X	301	7J0	C24-N25	4.59	1.44	1.35
3	J	301	7J0	C24-N25	4.54	1.43	1.35
3	Y	301	7J0	C23-C24	3.70	1.58	1.51
3	W	301	7J0	C23-C24	3.70	1.58	1.51
3	X	301	7J0	C05-N06	3.69	1.42	1.33
3	K	301	7J0	C23-C24	3.68	1.58	1.51
3	X	301	7J0	C23-C24	3.68	1.58	1.51
3	W	301	7J0	C05-N06	3.67	1.42	1.33
3	K	301	7J0	C05-N06	3.67	1.42	1.33
3	Z	301	7J0	C23-C24	3.66	1.58	1.51
3	a	301	7J0	C23-C24	3.65	1.57	1.51
3	H	301	7J0	C23-C24	3.65	1.57	1.51
3	a	301	7J0	C05-N06	3.64	1.42	1.33
3	M	301	7J0	C05-N06	3.64	1.42	1.33
3	b	301	7J0	C23-C24	3.64	1.57	1.51
3	H	301	7J0	C05-N06	3.64	1.42	1.33
3	N	301	7J0	C23-C24	3.63	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	301	7J0	C05-N06	3.63	1.42	1.33
3	Z	301	7J0	C05-N06	3.63	1.42	1.33
3	J	301	7J0	C23-C24	3.63	1.57	1.51
3	I	301	7J0	C23-C24	3.63	1.57	1.51
3	L	301	7J0	C05-N06	3.63	1.42	1.33
3	I	301	7J0	C05-N06	3.62	1.42	1.33
3	b	301	7J0	C05-N06	3.62	1.42	1.33
3	L	301	7J0	C23-C24	3.61	1.57	1.51
3	V	301	7J0	C05-N06	3.60	1.42	1.33
3	M	301	7J0	C23-C24	3.59	1.57	1.51
3	J	301	7J0	C05-N06	3.58	1.42	1.33
3	V	301	7J0	C23-C24	3.58	1.57	1.51
3	Y	301	7J0	C05-N06	3.58	1.42	1.33
3	J	301	7J0	C23-C22	3.15	1.60	1.53
3	W	301	7J0	C23-C22	3.14	1.60	1.53
3	H	301	7J0	C23-C22	3.12	1.60	1.53
3	Y	301	7J0	C23-C22	3.11	1.60	1.53
3	M	301	7J0	C23-C22	3.09	1.60	1.53
3	a	301	7J0	C23-C22	3.09	1.60	1.53
3	I	301	7J0	C23-C22	3.09	1.60	1.53
3	K	301	7J0	C23-C22	3.09	1.60	1.53
3	Z	301	7J0	C23-C22	3.08	1.60	1.53
3	N	301	7J0	C23-C22	3.08	1.60	1.53
3	b	301	7J0	C23-C22	3.07	1.60	1.53
3	X	301	7J0	C23-C22	3.06	1.60	1.53
3	L	301	7J0	C23-C22	3.04	1.60	1.53
3	V	301	7J0	C23-C22	3.00	1.60	1.53
3	J	301	7J0	C34-C33	3.00	1.57	1.51
3	K	301	7J0	C34-C33	2.96	1.57	1.51
3	M	301	7J0	C34-C33	2.96	1.57	1.51
3	W	301	7J0	C34-C33	2.95	1.57	1.51
3	a	301	7J0	C34-C33	2.94	1.57	1.51
3	V	301	7J0	C34-C33	2.94	1.57	1.51
3	I	301	7J0	C34-C33	2.93	1.57	1.51
3	Y	301	7J0	C34-C33	2.92	1.57	1.51
3	N	301	7J0	C34-C33	2.92	1.57	1.51
3	Z	301	7J0	C34-C33	2.91	1.57	1.51
3	H	301	7J0	C34-C33	2.90	1.57	1.51
3	X	301	7J0	C34-C33	2.89	1.57	1.51
3	b	301	7J0	C34-C33	2.89	1.57	1.51
3	L	301	7J0	C34-C33	2.84	1.57	1.51
3	K	301	7J0	C02-N03	2.79	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	b	301	7J0	C04-C05	2.77	1.59	1.52
3	L	301	7J0	C02-N03	2.74	1.39	1.34
3	W	301	7J0	C02-N03	2.74	1.39	1.34
3	K	301	7J0	C04-C05	2.74	1.59	1.52
3	N	301	7J0	C02-N03	2.73	1.39	1.34
3	a	301	7J0	C02-N03	2.73	1.39	1.34
3	V	301	7J0	C04-C05	2.72	1.59	1.52
3	I	301	7J0	C04-C05	2.72	1.59	1.52
3	M	301	7J0	C02-N03	2.72	1.39	1.34
3	X	301	7J0	C04-C05	2.72	1.59	1.52
3	a	301	7J0	C04-C05	2.72	1.59	1.52
3	J	301	7J0	C02-N03	2.71	1.39	1.34
3	H	301	7J0	C02-N03	2.71	1.39	1.34
3	Y	301	7J0	C02-N03	2.71	1.39	1.34
3	J	301	7J0	C04-C05	2.70	1.59	1.52
3	I	301	7J0	C02-N03	2.70	1.39	1.34
3	W	301	7J0	C04-C05	2.70	1.59	1.52
3	H	301	7J0	C04-C05	2.70	1.59	1.52
3	X	301	7J0	C02-N03	2.69	1.39	1.34
3	Y	301	7J0	C04-C05	2.69	1.59	1.52
3	L	301	7J0	C04-C05	2.69	1.59	1.52
3	Z	301	7J0	C02-N03	2.69	1.39	1.34
3	V	301	7J0	C02-N03	2.68	1.39	1.34
3	M	301	7J0	C04-C05	2.68	1.59	1.52
3	Z	301	7J0	C04-C05	2.67	1.59	1.52
3	N	301	7J0	C04-C05	2.66	1.59	1.52
3	b	301	7J0	C02-N03	2.63	1.39	1.34
3	Z	301	7J0	C10-C09	2.43	1.43	1.38
3	K	301	7J0	C10-C09	2.43	1.43	1.38
3	W	301	7J0	C10-C09	2.43	1.43	1.38
3	M	301	7J0	C10-C09	2.42	1.43	1.38
3	H	301	7J0	C10-C09	2.42	1.43	1.38
3	I	301	7J0	C10-C09	2.42	1.43	1.38
3	a	301	7J0	C10-C09	2.42	1.43	1.38
3	J	301	7J0	C10-C09	2.42	1.43	1.38
3	b	301	7J0	C10-C09	2.41	1.43	1.38
3	V	301	7J0	C10-C09	2.41	1.43	1.38
3	X	301	7J0	C10-C09	2.41	1.43	1.38
3	N	301	7J0	C10-C09	2.41	1.43	1.38
3	L	301	7J0	C10-C09	2.40	1.43	1.38
3	Y	301	7J0	C10-C09	2.38	1.43	1.38
3	J	301	7J0	C22-N32	2.30	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	301	7J0	C22-N32	2.30	1.50	1.45
3	M	301	7J0	C22-N32	2.27	1.50	1.45
3	W	301	7J0	C22-N32	2.25	1.50	1.45
3	I	301	7J0	C22-N32	2.24	1.50	1.45
3	Y	301	7J0	C22-N32	2.24	1.50	1.45
3	V	301	7J0	C22-N32	2.24	1.50	1.45
3	a	301	7J0	C22-N32	2.23	1.50	1.45
3	N	301	7J0	C22-N32	2.22	1.50	1.45
3	H	301	7J0	C22-N32	2.22	1.50	1.45
3	b	301	7J0	C22-N32	2.21	1.50	1.45
3	X	301	7J0	C22-N32	2.20	1.50	1.45
3	L	301	7J0	C22-N32	2.20	1.50	1.45
3	b	301	7J0	C19-C04	2.19	1.58	1.52
3	H	301	7J0	C19-C04	2.18	1.58	1.52
3	Y	301	7J0	C19-C04	2.17	1.58	1.52
3	X	301	7J0	C19-C04	2.17	1.58	1.52
3	I	301	7J0	C19-C04	2.17	1.58	1.52
3	Z	301	7J0	C22-N32	2.17	1.50	1.45
3	K	301	7J0	C19-C04	2.17	1.58	1.52
3	V	301	7J0	C19-C04	2.16	1.58	1.52
3	W	301	7J0	C19-C04	2.16	1.58	1.52
3	a	301	7J0	C19-C04	2.16	1.58	1.52
3	N	301	7J0	C19-C04	2.15	1.58	1.52
3	Z	301	7J0	C19-C04	2.15	1.58	1.52
3	L	301	7J0	C19-C04	2.14	1.58	1.52
3	J	301	7J0	C19-C04	2.14	1.58	1.52
3	M	301	7J0	C19-C04	2.12	1.58	1.52
3	H	301	7J0	C07-N06	2.11	1.50	1.46
3	W	301	7J0	C07-N06	2.11	1.50	1.46
3	X	301	7J0	C07-N06	2.11	1.50	1.46
3	V	301	7J0	C07-N06	2.10	1.50	1.46
3	b	301	7J0	C07-N06	2.09	1.50	1.46
3	Z	301	7J0	C07-N06	2.09	1.50	1.46
3	K	301	7J0	C07-N06	2.08	1.50	1.46
3	a	301	7J0	C07-N06	2.08	1.50	1.46
3	M	301	7J0	C07-N06	2.07	1.50	1.46
3	J	301	7J0	C07-N06	2.07	1.50	1.46
3	Y	301	7J0	C07-N06	2.06	1.50	1.46
3	N	301	7J0	C07-N06	2.05	1.50	1.46
3	I	301	7J0	C07-N06	2.05	1.50	1.46
3	L	301	7J0	C07-N06	2.04	1.50	1.46

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	301	7J0	C34-C33-N32	4.48	123.76	115.86
3	K	301	7J0	C34-C33-N32	4.44	123.68	115.86
3	I	301	7J0	C34-C33-N32	4.43	123.66	115.86
3	a	301	7J0	C34-C33-N32	4.42	123.65	115.86
3	L	301	7J0	C34-C33-N32	4.42	123.65	115.86
3	Y	301	7J0	C34-C33-N32	4.41	123.64	115.86
3	M	301	7J0	C34-C33-N32	4.41	123.64	115.86
3	N	301	7J0	C34-C33-N32	4.40	123.61	115.86
3	X	301	7J0	C34-C33-N32	4.39	123.60	115.86
3	W	301	7J0	C34-C33-N32	4.38	123.58	115.86
3	b	301	7J0	C34-C33-N32	4.37	123.56	115.86
3	H	301	7J0	C34-C33-N32	4.35	123.52	115.86
3	Z	301	7J0	C34-C33-N32	4.33	123.50	115.86
3	V	301	7J0	C34-C33-N32	4.33	123.50	115.86
3	Y	301	7J0	C22-C23-C24	4.18	120.57	112.22
3	W	301	7J0	C22-C23-C24	4.13	120.47	112.22
3	Z	301	7J0	C22-C23-C24	4.13	120.47	112.22
3	M	301	7J0	C22-C23-C24	4.11	120.44	112.22
3	b	301	7J0	C22-C23-C24	4.10	120.42	112.22
3	J	301	7J0	C22-C23-C24	4.07	120.36	112.22
3	I	301	7J0	C22-C23-C24	4.02	120.25	112.22
3	a	301	7J0	C22-C23-C24	4.01	120.24	112.22
3	V	301	7J0	C22-C23-C24	3.99	120.20	112.22
3	L	301	7J0	C22-C23-C24	3.95	120.12	112.22
3	K	301	7J0	C22-C23-C24	3.94	120.09	112.22
3	X	301	7J0	C22-C23-C24	3.94	120.09	112.22
3	N	301	7J0	C22-C23-C24	3.93	120.07	112.22
3	H	301	7J0	C22-C23-C24	3.89	119.99	112.22
3	J	301	7J0	C23-C22-N32	3.48	117.28	110.64
3	J	301	7J0	O42-C33-C34	-2.82	116.91	122.02
3	L	301	7J0	O42-C33-C34	-2.82	116.91	122.02
3	I	301	7J0	O42-C33-C34	-2.81	116.92	122.02
3	X	301	7J0	C19-C04-N03	-2.81	105.11	111.31
3	K	301	7J0	O42-C33-C34	-2.81	116.94	122.02
3	M	301	7J0	O42-C33-C34	-2.79	116.96	122.02
3	b	301	7J0	C19-C04-N03	-2.79	105.14	111.31
3	X	301	7J0	O42-C33-C34	-2.79	116.97	122.02
3	N	301	7J0	O42-C33-C34	-2.79	116.97	122.02
3	H	301	7J0	O42-C33-C34	-2.78	116.97	122.02
3	a	301	7J0	O42-C33-C34	-2.78	116.98	122.02
3	Y	301	7J0	O42-C33-C34	-2.78	116.98	122.02
3	H	301	7J0	C19-C04-N03	-2.78	105.17	111.31
3	W	301	7J0	O42-C33-C34	-2.78	116.99	122.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	b	301	7J0	C23-C22-N32	2.78	115.94	110.64
3	V	301	7J0	C19-C04-N03	-2.76	105.21	111.31
3	b	301	7J0	O42-C33-C34	-2.76	117.02	122.02
3	V	301	7J0	O42-C33-C34	-2.75	117.04	122.02
3	L	301	7J0	C19-C04-N03	-2.75	105.24	111.31
3	Z	301	7J0	O42-C33-C34	-2.75	117.05	122.02
3	K	301	7J0	C19-C04-N03	-2.74	105.25	111.31
3	J	301	7J0	C19-C04-N03	-2.72	105.30	111.31
3	a	301	7J0	C19-C04-N03	-2.71	105.33	111.31
3	Z	301	7J0	C19-C04-N03	-2.70	105.35	111.31
3	N	301	7J0	C19-C04-N03	-2.67	105.41	111.31
3	I	301	7J0	C19-C04-N03	-2.65	105.45	111.31
3	W	301	7J0	C19-C04-N03	-2.65	105.47	111.31
3	M	301	7J0	C19-C04-N03	-2.62	105.52	111.31
3	M	301	7J0	C23-C22-C02	-2.62	104.39	110.57
3	Y	301	7J0	C23-C22-C02	-2.58	104.47	110.57
3	J	301	7J0	C23-C22-C02	-2.56	104.54	110.57
3	b	301	7J0	C23-C22-C02	-2.56	104.54	110.57
3	Y	301	7J0	C19-C04-N03	-2.53	105.72	111.31
3	a	301	7J0	C23-C22-N32	2.53	115.47	110.64
3	V	301	7J0	C23-C22-C02	-2.53	104.60	110.57
3	Z	301	7J0	C23-C22-C02	-2.53	104.60	110.57
3	V	301	7J0	C35-C34-C33	2.53	118.50	112.83
3	I	301	7J0	C23-C22-C02	-2.50	104.67	110.57
3	M	301	7J0	C35-C34-C33	2.48	118.40	112.83
3	W	301	7J0	C23-C22-C02	-2.47	104.73	110.57
3	K	301	7J0	C35-C34-C33	2.47	118.38	112.83
3	a	301	7J0	C23-C22-C02	-2.45	104.78	110.57
3	J	301	7J0	C41-C36-C37	-2.43	114.62	118.23
3	L	301	7J0	C23-C22-C02	-2.42	104.85	110.57
3	H	301	7J0	C23-C22-C02	-2.42	104.86	110.57
3	K	301	7J0	C23-C22-N32	2.42	115.25	110.64
3	M	301	7J0	C41-C36-C37	-2.41	114.65	118.23
3	N	301	7J0	C23-C22-C02	-2.40	104.90	110.57
3	a	301	7J0	C41-C36-C37	-2.40	114.67	118.23
3	N	301	7J0	C41-C36-C37	-2.39	114.68	118.23
3	K	301	7J0	C41-C36-C37	-2.39	114.68	118.23
3	W	301	7J0	C41-C36-C37	-2.39	114.69	118.23
3	X	301	7J0	C41-C36-C37	-2.38	114.70	118.23
3	I	301	7J0	C41-C36-C37	-2.38	114.70	118.23
3	a	301	7J0	C35-C34-C33	2.37	118.15	112.83
3	Y	301	7J0	C41-C36-C37	-2.37	114.72	118.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	301	7J0	C41-C36-C37	-2.36	114.73	118.23
3	b	301	7J0	C35-C34-C33	2.35	118.11	112.83
3	Z	301	7J0	C41-C36-C37	-2.35	114.74	118.23
3	b	301	7J0	C41-C36-C37	-2.35	114.75	118.23
3	J	301	7J0	C35-C34-C33	2.33	118.06	112.83
3	H	301	7J0	C41-C36-C37	-2.32	114.78	118.23
3	X	301	7J0	C23-C22-C02	-2.32	105.10	110.57
3	N	301	7J0	C35-C34-C33	2.31	118.02	112.83
3	L	301	7J0	C41-C36-C37	-2.31	114.80	118.23
3	K	301	7J0	C23-C22-C02	-2.29	105.16	110.57
3	H	301	7J0	C35-C34-C33	2.28	117.95	112.83
3	X	301	7J0	C35-C34-C33	2.26	117.90	112.83
3	Z	301	7J0	C35-C34-C33	2.26	117.89	112.83
3	Y	301	7J0	C35-C34-C33	2.25	117.89	112.83
3	N	301	7J0	C23-C22-N32	2.24	114.92	110.64
3	I	301	7J0	C23-C22-N32	2.22	114.88	110.64
3	W	301	7J0	C23-C22-N32	2.19	114.82	110.64
3	I	301	7J0	C35-C34-C33	2.17	117.71	112.83
3	W	301	7J0	C35-C34-C33	2.17	117.70	112.83
3	N	301	7J0	C29-C30-N25	2.15	115.04	110.67
3	L	301	7J0	C35-C34-C33	2.15	117.65	112.83
3	J	301	7J0	O42-C33-N32	-2.14	119.32	122.95
3	H	301	7J0	C29-C30-N25	2.13	115.00	110.67
3	X	301	7J0	C23-C22-N32	2.13	114.70	110.64
3	a	301	7J0	O42-C33-N32	-2.11	119.37	122.95
3	V	301	7J0	C23-C22-N32	2.11	114.67	110.64
3	L	301	7J0	C23-C22-N32	2.11	114.67	110.64
3	Y	301	7J0	O42-C33-N32	-2.11	119.38	122.95
3	K	301	7J0	O42-C33-N32	-2.11	119.38	122.95
3	M	301	7J0	O42-C33-N32	-2.10	119.40	122.95
3	I	301	7J0	O42-C33-N32	-2.09	119.41	122.95
3	N	301	7J0	O42-C33-N32	-2.09	119.42	122.95
3	b	301	7J0	O42-C33-N32	-2.09	119.42	122.95
3	W	301	7J0	O42-C33-N32	-2.08	119.42	122.95
3	L	301	7J0	O42-C33-N32	-2.08	119.44	122.95
3	X	301	7J0	O42-C33-N32	-2.08	119.44	122.95
3	H	301	7J0	C23-C22-N32	2.07	114.59	110.64
3	Z	301	7J0	O42-C33-N32	-2.07	119.45	122.95
3	V	301	7J0	O42-C33-N32	-2.06	119.46	122.95
3	M	301	7J0	C23-C22-N32	2.05	114.54	110.64
3	H	301	7J0	O42-C33-N32	-2.04	119.50	122.95
3	Y	301	7J0	C23-C22-N32	2.01	114.48	110.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Z	301	7J0	C23-C22-N32	2.00	114.46	110.64

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	301	7J0	C33-C34-C35-C36
3	H	301	7J0	N03-C04-C19-O20
3	H	301	7J0	C05-C04-C19-O20
3	I	301	7J0	C04-C19-O20-C21
3	J	301	7J0	C33-C34-C35-C36
3	J	301	7J0	N03-C04-C19-O20
3	J	301	7J0	C05-C04-C19-O20
3	K	301	7J0	N03-C04-C19-O20
3	K	301	7J0	C05-C04-C19-O20
3	L	301	7J0	N03-C04-C19-O20
3	L	301	7J0	C05-C04-C19-O20
3	M	301	7J0	C04-C19-O20-C21
3	V	301	7J0	C33-C34-C35-C36
3	V	301	7J0	C05-C04-C19-O20
3	W	301	7J0	N03-C04-C19-O20
3	W	301	7J0	C05-C04-C19-O20
3	X	301	7J0	N03-C04-C19-O20
3	X	301	7J0	C05-C04-C19-O20
3	a	301	7J0	N03-C04-C19-O20
3	a	301	7J0	C05-C04-C19-O20
3	b	301	7J0	C04-C19-O20-C21
3	V	301	7J0	N03-C04-C19-O20
3	H	301	7J0	C04-C19-O20-C21
3	J	301	7J0	C04-C19-O20-C21
3	X	301	7J0	C04-C19-O20-C21
3	Z	301	7J0	C04-C19-O20-C21
3	Z	301	7J0	C05-C04-C19-O20
3	I	301	7J0	N03-C04-C19-O20
3	Z	301	7J0	N03-C04-C19-O20
3	V	301	7J0	C04-C19-O20-C21
3	a	301	7J0	O42-C33-C34-C35
3	N	301	7J0	C33-C34-C35-C36
3	Y	301	7J0	C04-C19-O20-C21
3	a	301	7J0	N32-C33-C34-C35
3	H	301	7J0	C22-C23-C24-N25
3	N	301	7J0	C22-C23-C24-N25

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Mol	Chain	Res	Type	Atoms
3	K	301	7J0	C02-C22-C23-C24
3	M	301	7J0	C05-C04-C19-O20
3	M	301	7J0	N03-C04-C19-O20
3	K	301	7J0	O42-C33-C34-C35
3	a	301	7J0	C34-C35-C36-C41
3	N	301	7J0	N03-C04-C19-O20
3	J	301	7J0	C34-C35-C36-C41
3	J	301	7J0	C34-C35-C36-C37
3	K	301	7J0	C34-C35-C36-C37
3	a	301	7J0	C34-C35-C36-C37
3	K	301	7J0	C34-C35-C36-C41
3	b	301	7J0	C34-C35-C36-C41
3	Z	301	7J0	C34-C35-C36-C41
3	b	301	7J0	C34-C35-C36-C37
3	L	301	7J0	C04-C19-O20-C21
3	K	301	7J0	N32-C33-C34-C35
3	Z	301	7J0	C34-C35-C36-C37
3	H	301	7J0	C22-C23-C24-O31
3	N	301	7J0	C22-C23-C24-O31
3	V	301	7J0	O42-C33-C34-C35
3	N	301	7J0	C05-C04-C19-O20
3	Y	301	7J0	C34-C35-C36-C41
3	H	301	7J0	C34-C35-C36-C37
3	M	301	7J0	C34-C35-C36-C41
3	Y	301	7J0	C34-C35-C36-C37
3	H	301	7J0	C34-C35-C36-C41
3	V	301	7J0	N32-C33-C34-C35
3	M	301	7J0	C34-C35-C36-C37
3	b	301	7J0	O42-C33-C34-C35

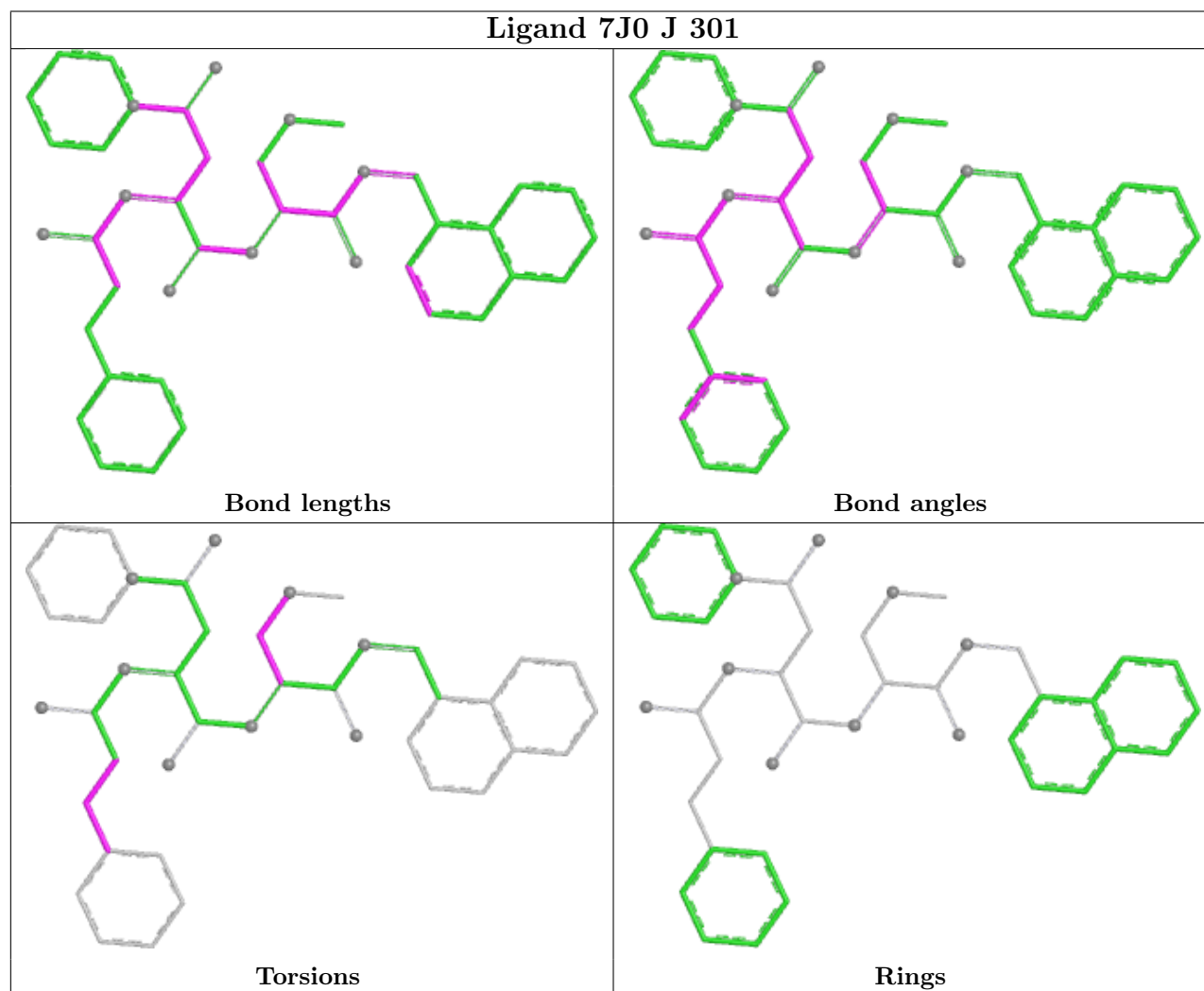
There are no ring outliers.

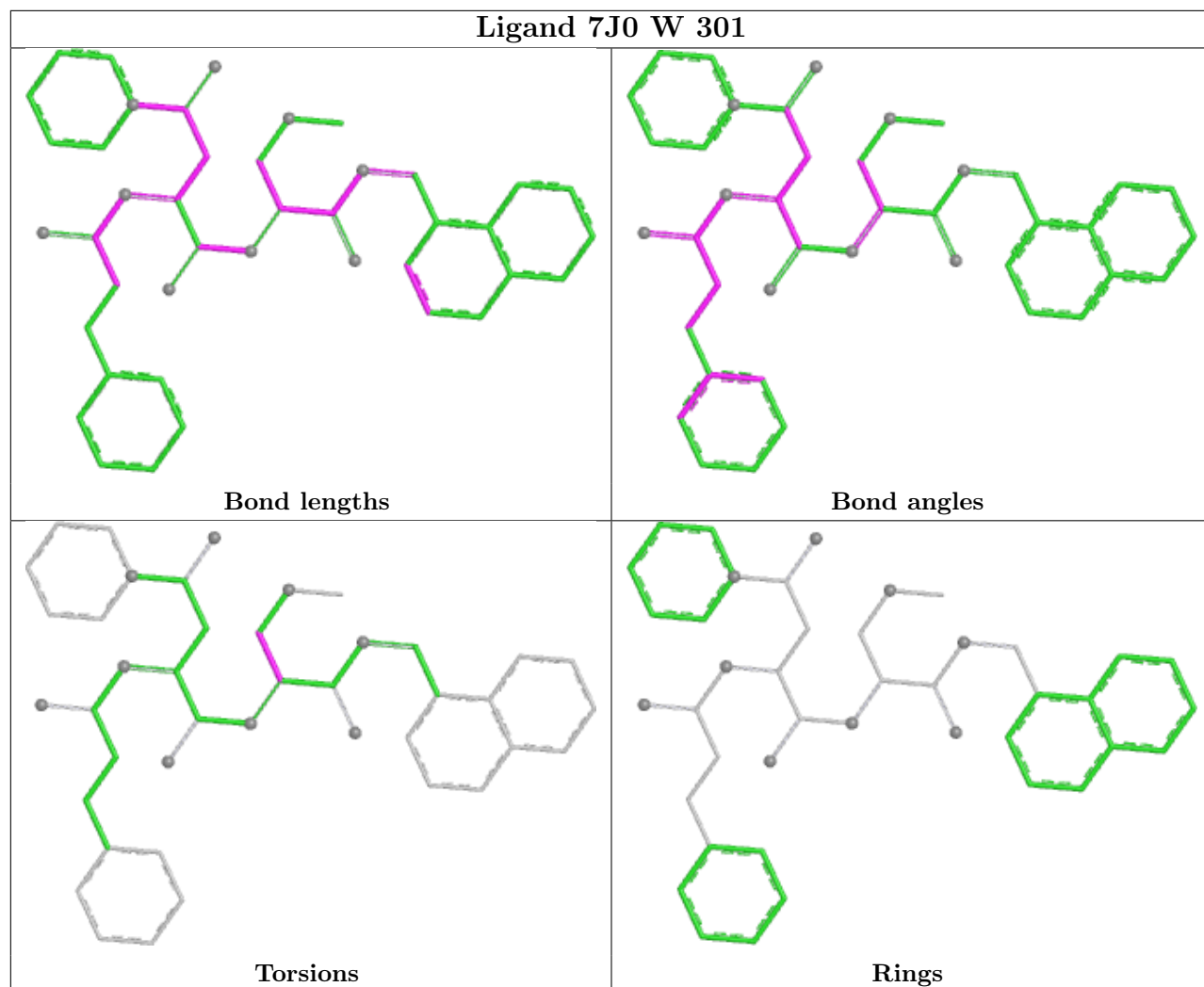
3 monomers are involved in 3 short contacts:

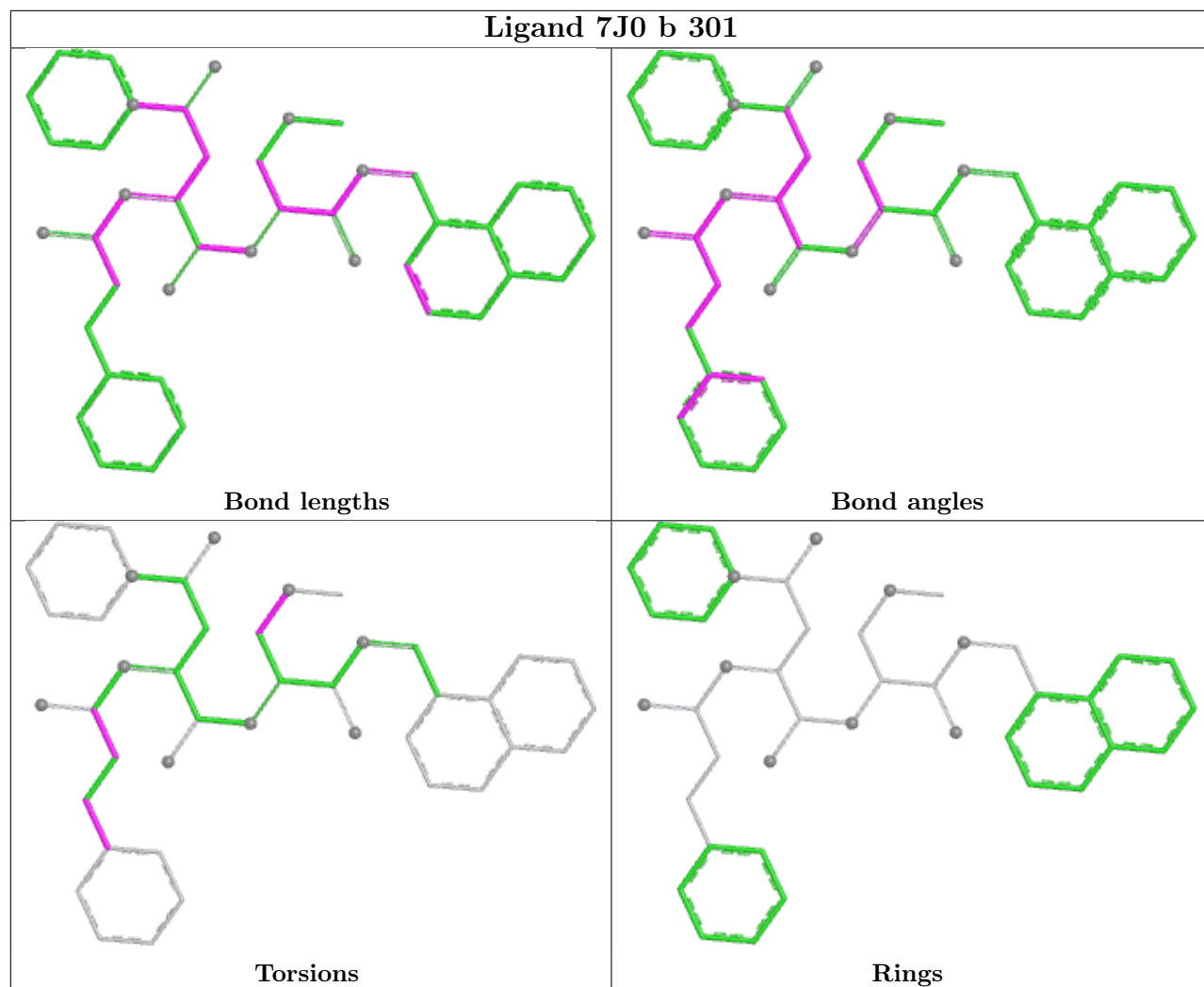
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	301	7J0	1	0
3	b	301	7J0	1	0
3	I	301	7J0	1	0

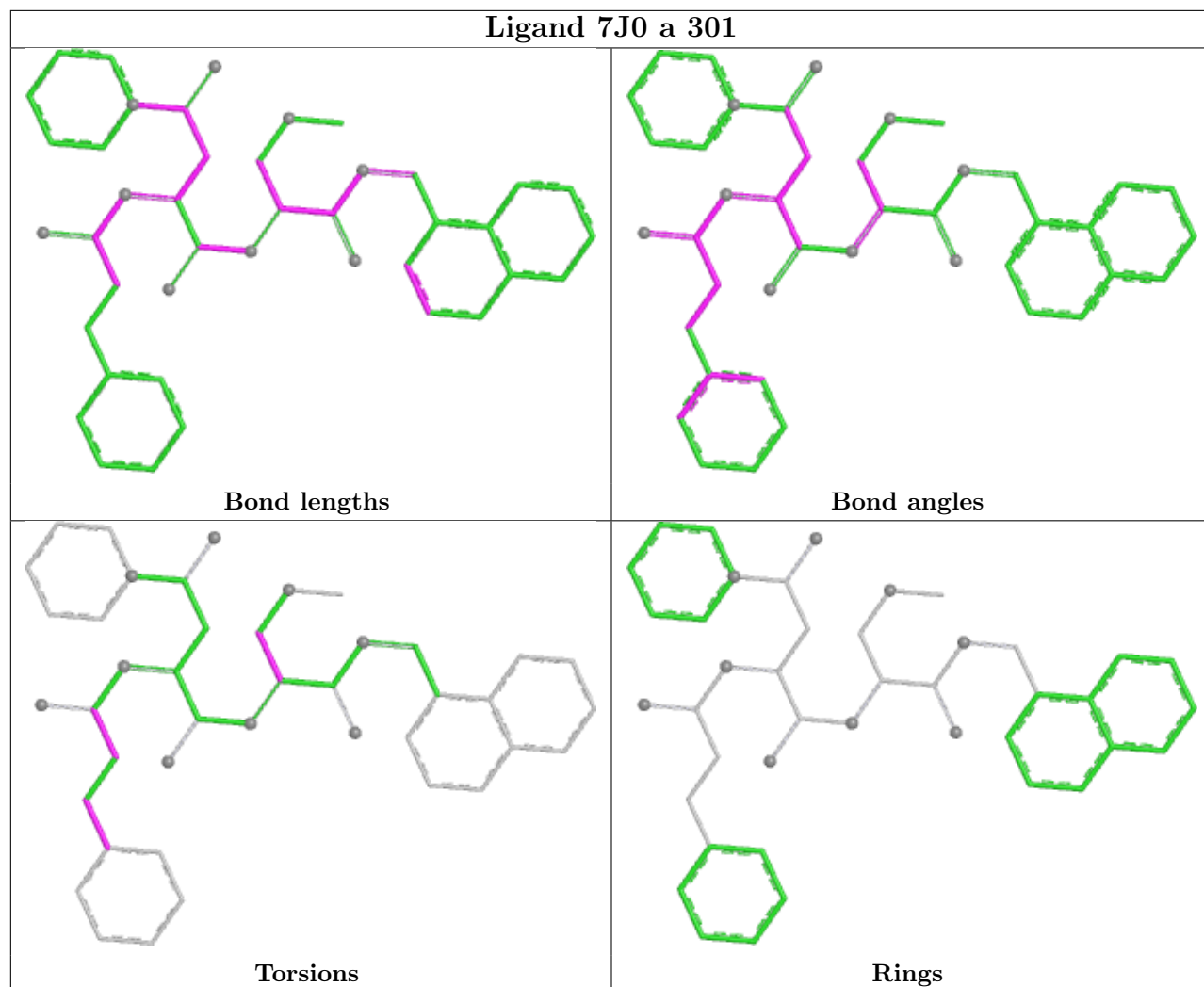
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

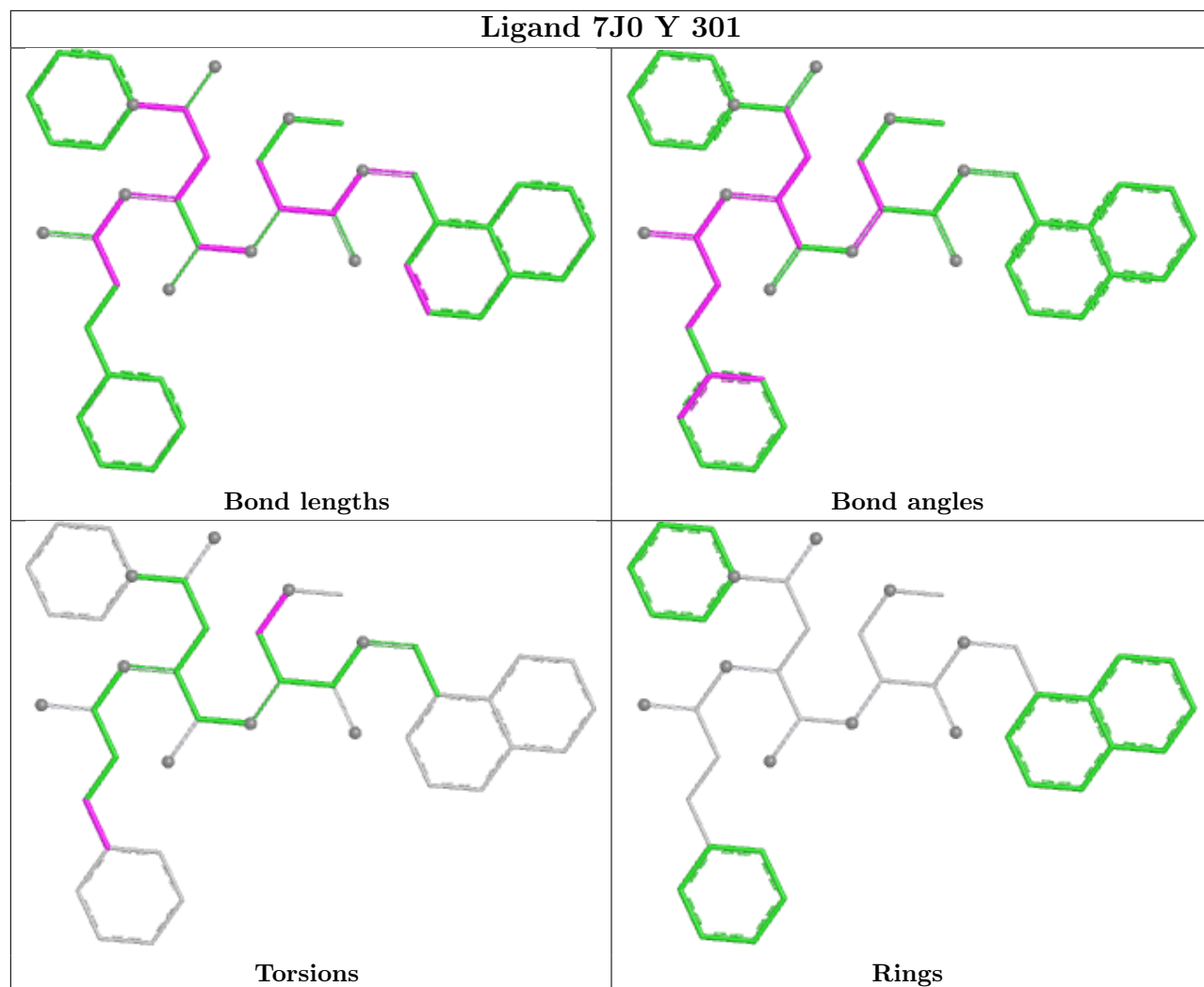
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

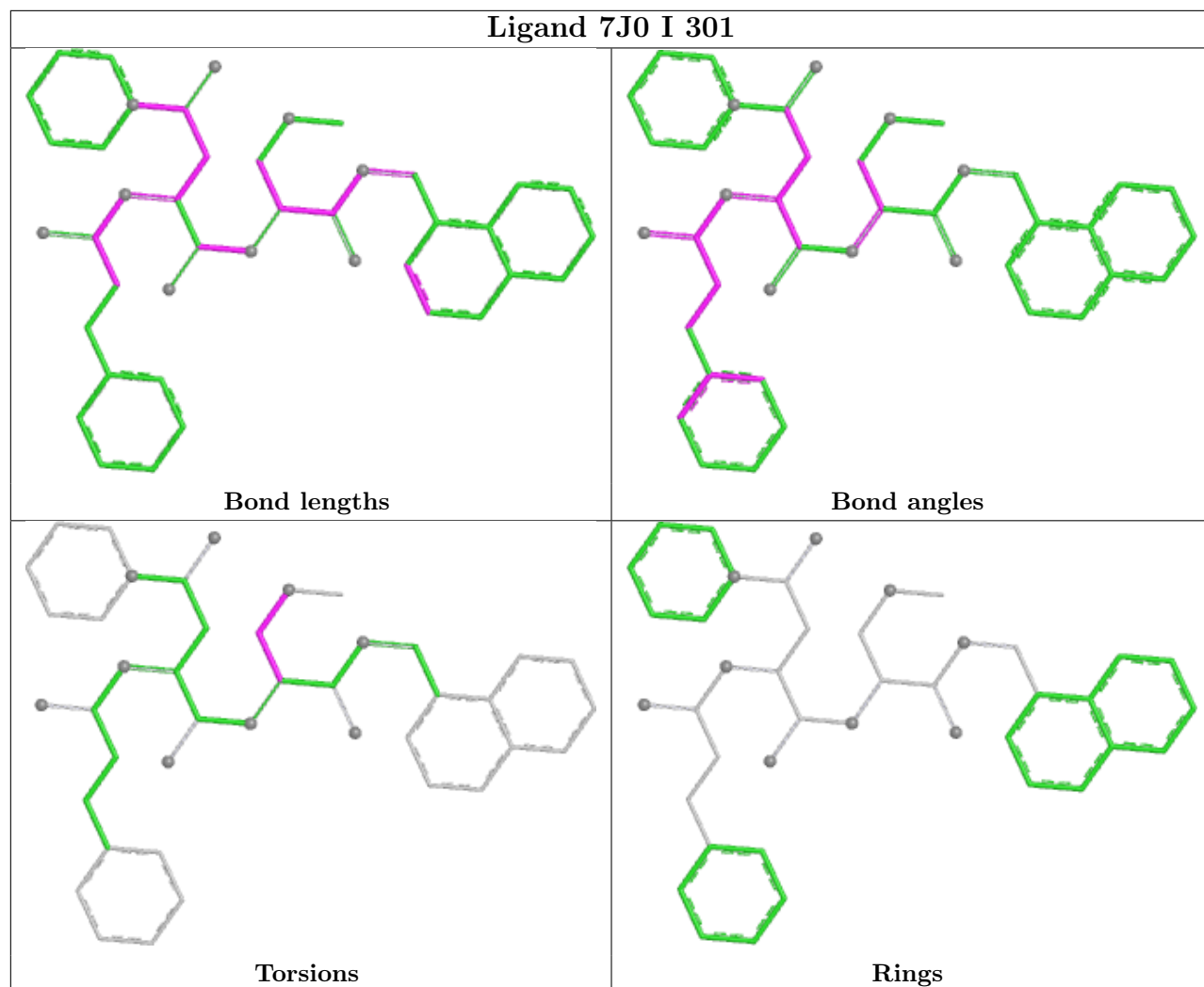


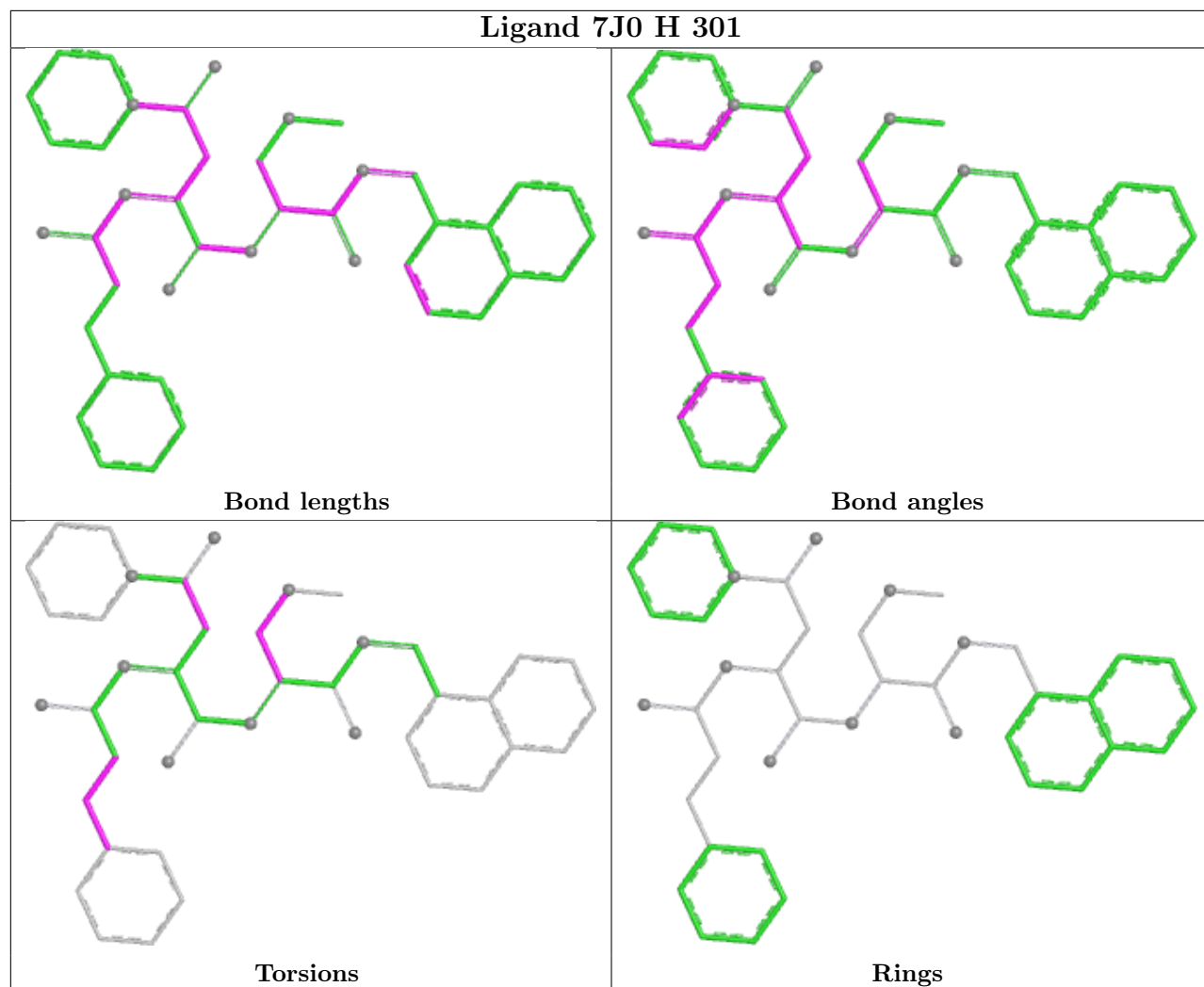


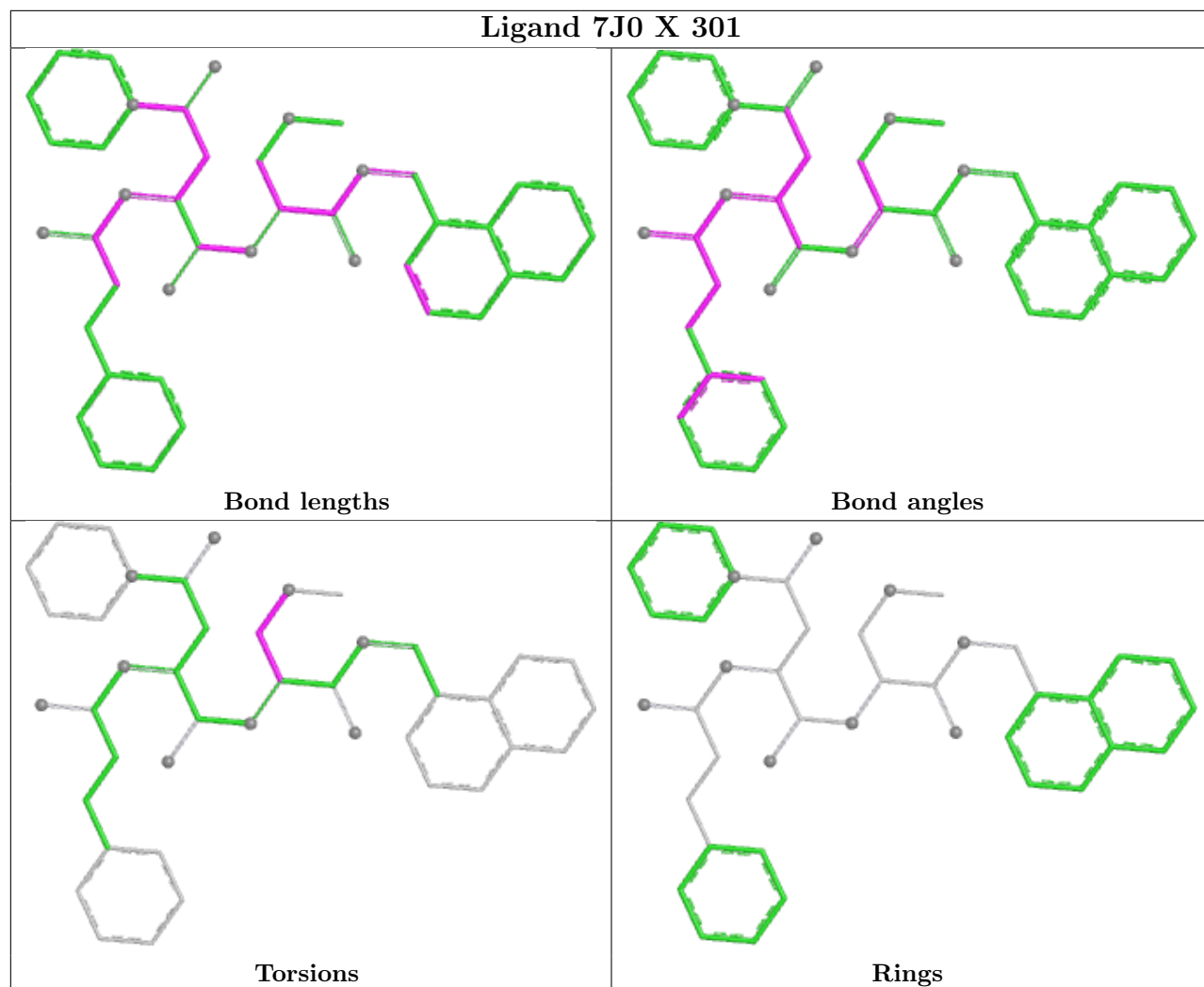


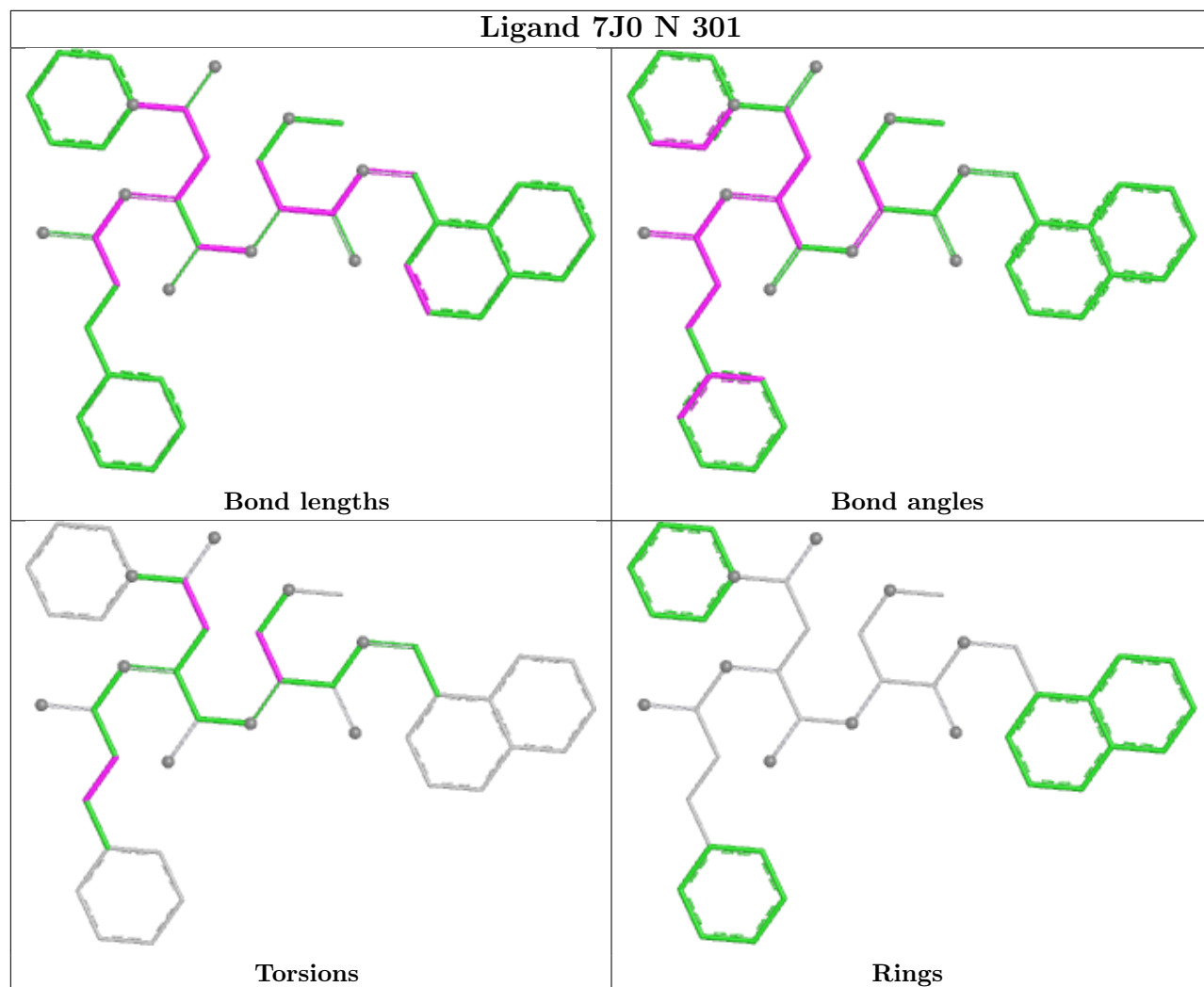


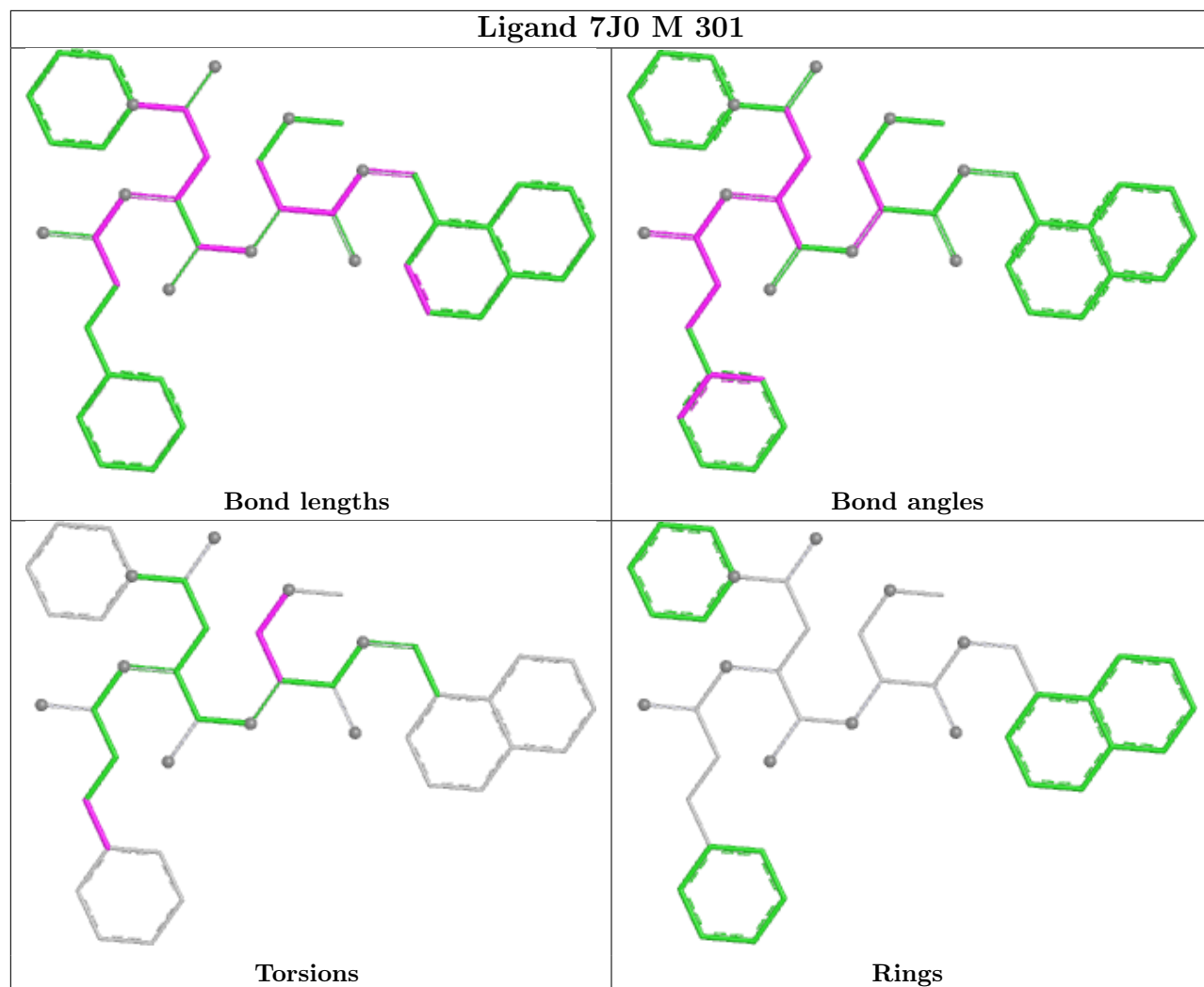


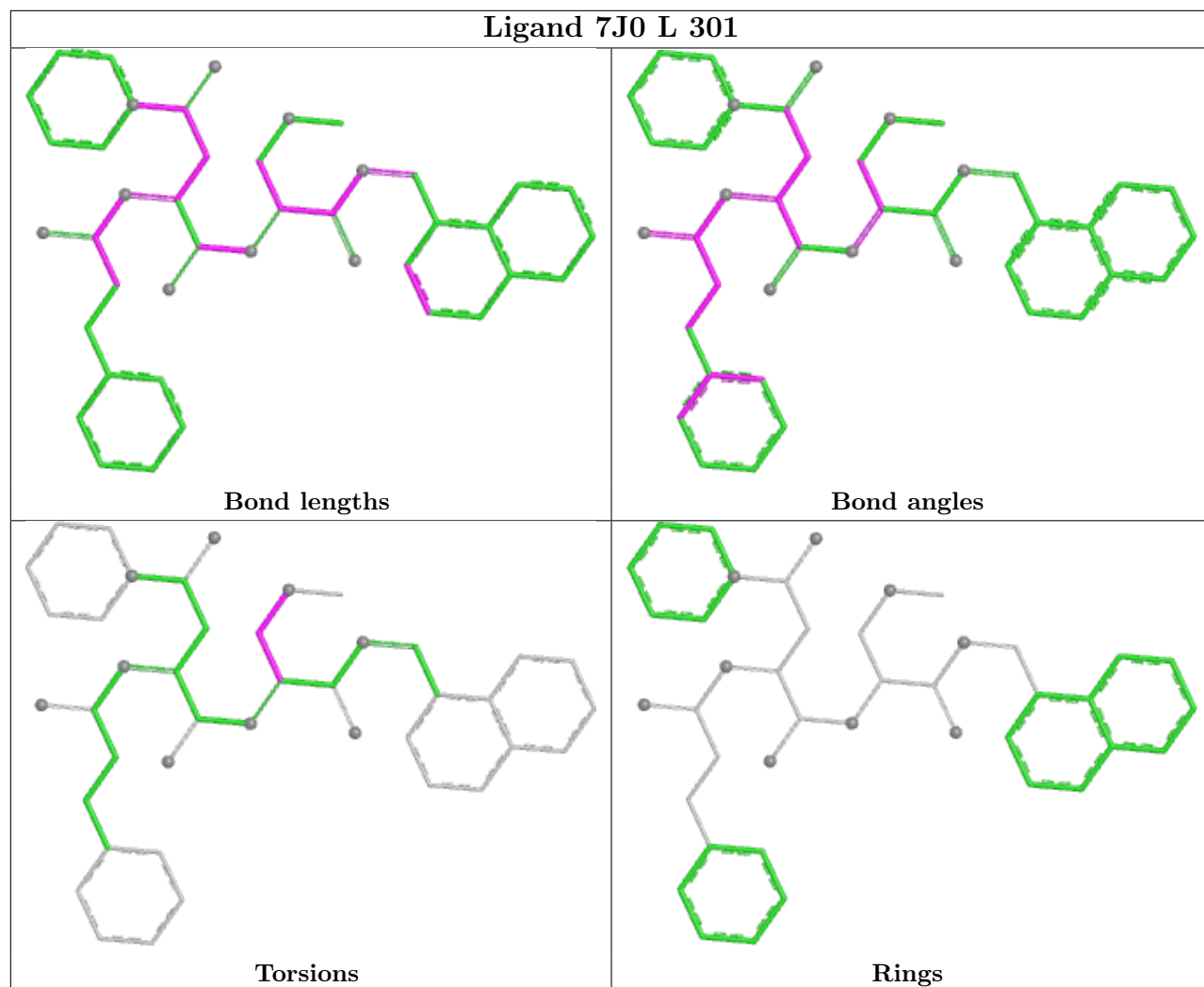


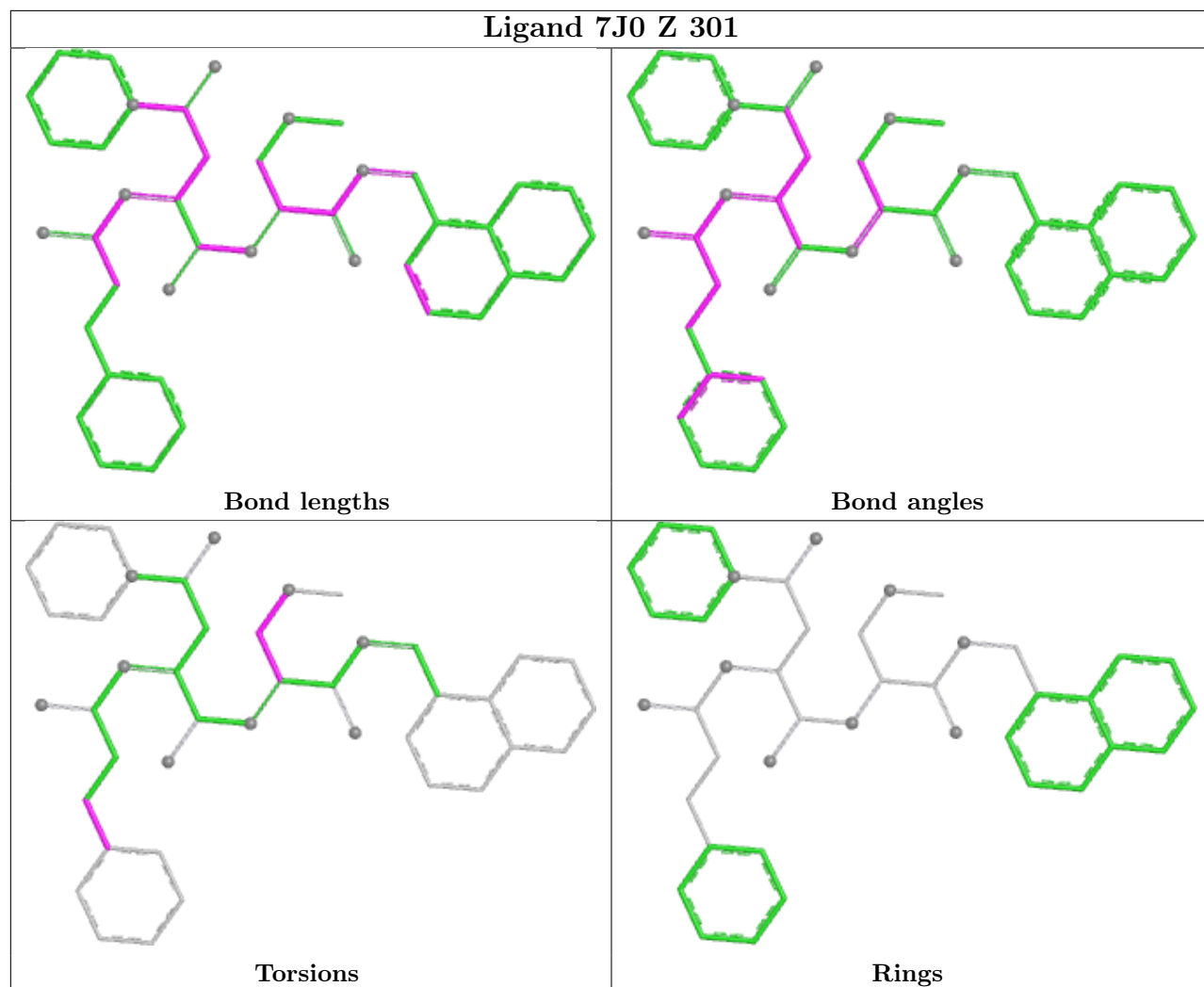


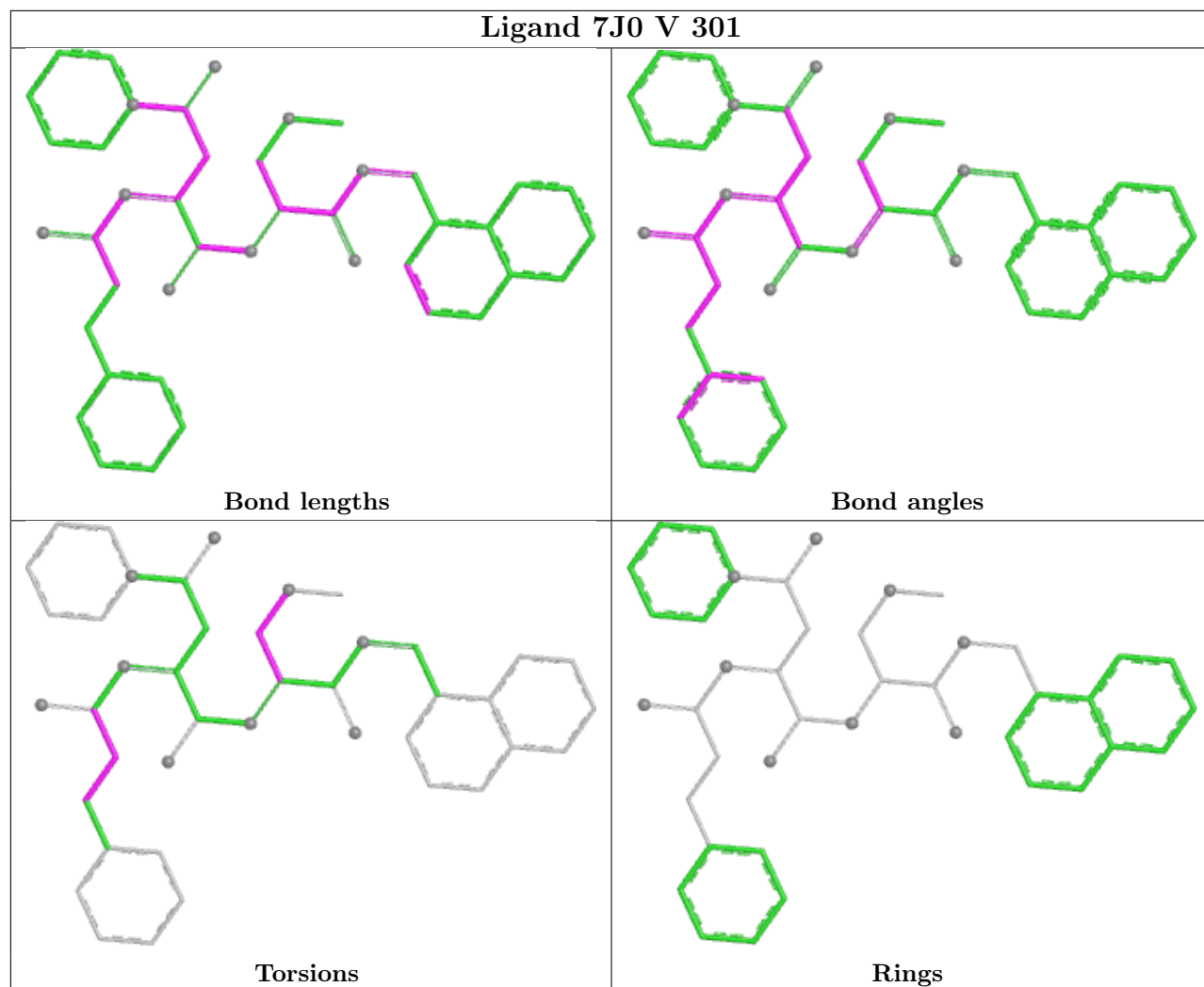


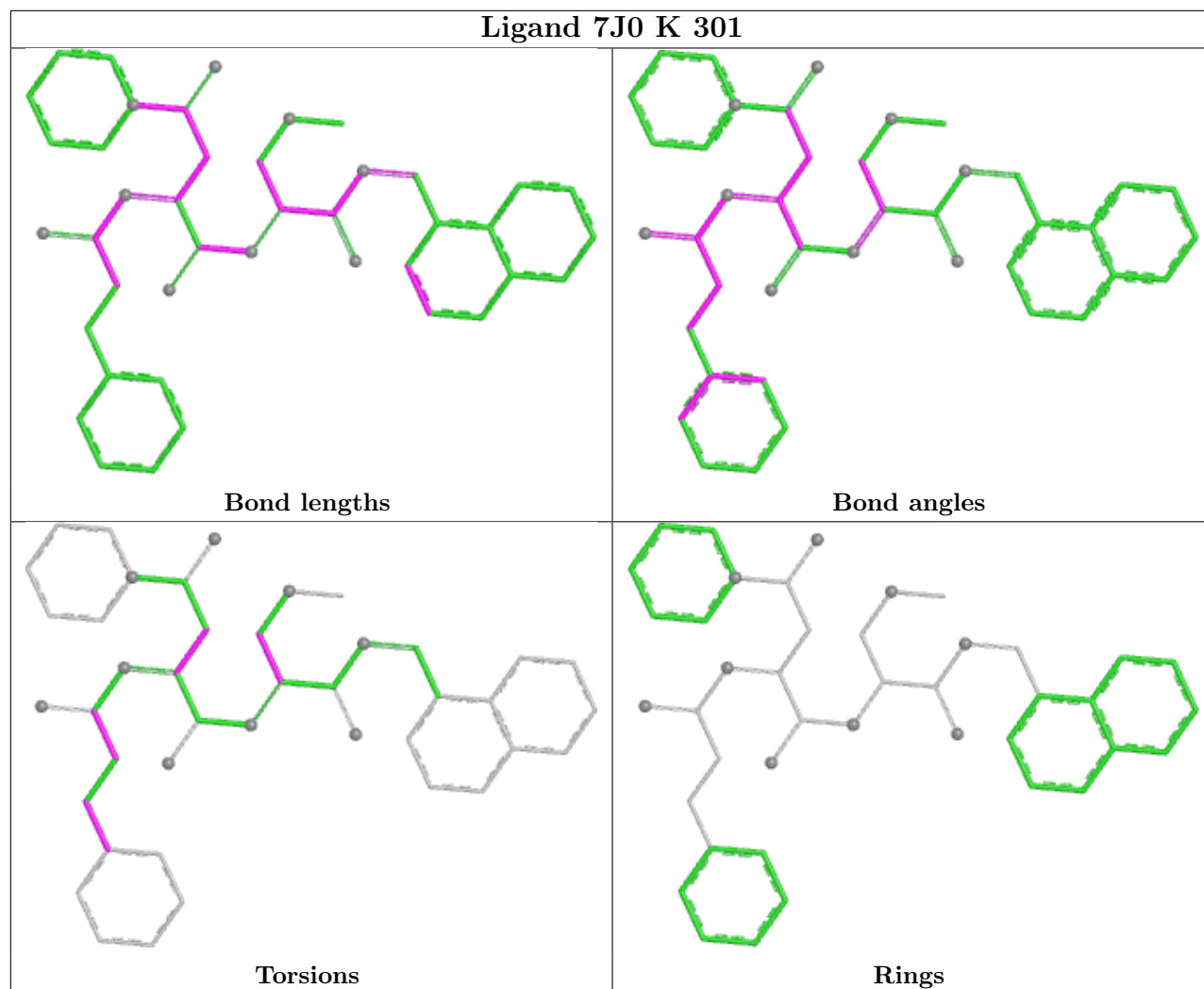












## 5.7 Other polymers [\(i\)](#)

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 i

### 6.1 Protein, DNA and RNA chains i

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	218/240 (90%)	-0.15	1 (0%) 87 72	17, 36, 59, 80	0
1	B	215/240 (89%)	0.11	2 (0%) 81 61	21, 45, 77, 92	0
1	C	216/240 (90%)	0.24	5 (2%) 61 38	19, 49, 81, 101	0
1	D	217/240 (90%)	0.08	2 (0%) 81 61	21, 45, 75, 83	0
1	E	217/240 (90%)	0.01	1 (0%) 87 72	16, 42, 65, 95	0
1	F	218/240 (90%)	0.23	5 (2%) 61 38	19, 47, 81, 113	0
1	G	216/240 (90%)	-0.13	1 (0%) 87 72	15, 37, 66, 82	0
1	O	216/240 (90%)	0.32	7 (3%) 50 29	20, 51, 87, 102	0
1	P	217/240 (90%)	0.22	4 (1%) 67 44	20, 47, 77, 111	0
1	Q	218/240 (90%)	0.06	5 (2%) 61 38	23, 44, 75, 115	0
1	R	217/240 (90%)	0.13	2 (0%) 81 61	17, 45, 71, 92	0
1	S	219/240 (91%)	0.02	5 (2%) 61 38	19, 38, 76, 101	0
1	T	216/240 (90%)	0.16	1 (0%) 87 72	21, 46, 76, 85	0
1	U	216/240 (90%)	0.07	3 (1%) 73 51	20, 41, 73, 101	0
2	H	222/240 (92%)	-0.26	1 (0%) 87 72	19, 29, 50, 81	0
2	I	222/240 (92%)	-0.39	0 100 100	16, 27, 47, 65	0
2	J	222/240 (92%)	-0.25	1 (0%) 87 72	19, 30, 54, 86	0
2	K	223/240 (92%)	-0.27	0 100 100	18, 30, 53, 70	0
2	L	223/240 (92%)	-0.26	1 (0%) 88 76	17, 27, 51, 72	0
2	M	222/240 (92%)	-0.27	0 100 100	18, 30, 53, 82	0
2	N	223/240 (92%)	-0.19	2 (0%) 81 61	18, 32, 59, 85	0
2	V	223/240 (92%)	-0.35	0 100 100	19, 28, 48, 64	0
2	W	223/240 (92%)	-0.21	1 (0%) 88 76	18, 30, 57, 73	0
2	X	222/240 (92%)	-0.28	0 100 100	19, 30, 54, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
2	Y	223/240 (92%)	-0.21	1 (0%) 88 76	17, 29, 55, 87	0
2	Z	222/240 (92%)	-0.27	2 (0%) 81 61	16, 28, 53, 76	0
2	a	223/240 (92%)	-0.18	2 (0%) 81 61	19, 32, 58, 77	0
2	b	223/240 (92%)	-0.27	0 100 100	18, 30, 56, 77	0
All	All	6152/6720 (91%)	-0.08	55 (0%) 81 61	15, 35, 71, 115	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	203	LEU	4.2
1	O	235	VAL	4.0
1	D	203	LEU	3.5
1	S	172	ALA	3.4
1	C	11	GLN	3.3
1	B	235	VAL	3.1
1	S	171	TYR	3.1
1	B	203	LEU	3.0
1	P	201	PRO	3.0
1	C	235	VAL	3.0
1	F	173	GLU	3.0
2	N	116	SER	2.9
1	S	193	ALA	2.8
1	S	10	GLU	2.8
1	E	202	THR	2.8
2	L	38	ASP	2.7
2	Z	38	ASP	2.7
1	O	10	GLU	2.6
1	D	235	VAL	2.6
1	U	203	LEU	2.5
1	F	11	GLN	2.5
2	N	115	GLN	2.5
2	a	115	GLN	2.5
1	F	235	VAL	2.5
1	S	9	MET	2.5
2	a	223	GLY	2.5
1	U	235	VAL	2.5
1	O	231	GLN	2.4
2	Z	133	GLU	2.4
1	R	202	THR	2.4
1	F	44	GLU	2.4
1	F	203	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	O	234	LEU	2.4
2	J	114	PRO	2.4
1	Q	190	ALA	2.3
1	C	10	GLU	2.3
2	H	38	ASP	2.3
1	O	206	ALA	2.3
1	Q	235	VAL	2.3
1	G	204	GLY	2.2
1	U	9	MET	2.2
1	P	190	ALA	2.2
1	C	9	MET	2.2
1	R	235	VAL	2.1
2	Y	207	GLU	2.1
1	Q	172	ALA	2.1
1	O	204	GLY	2.1
1	T	191	GLY	2.1
1	Q	191	GLY	2.1
1	O	192	SER	2.0
1	P	202	THR	2.0
1	Q	202	THR	2.0
1	A	10	GLU	2.0
2	W	133	GLU	2.0
1	P	235	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

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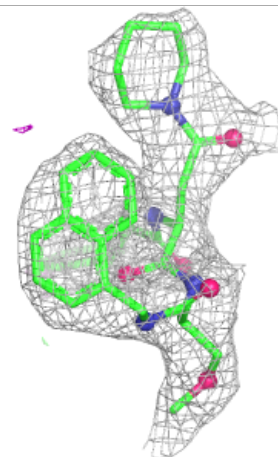
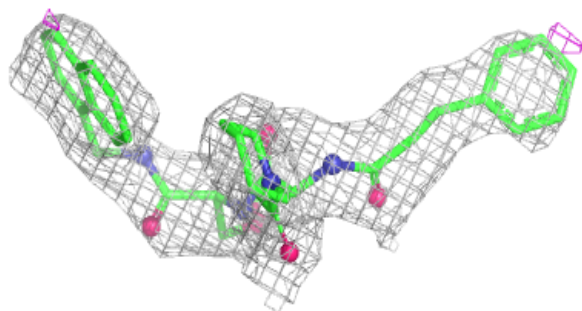
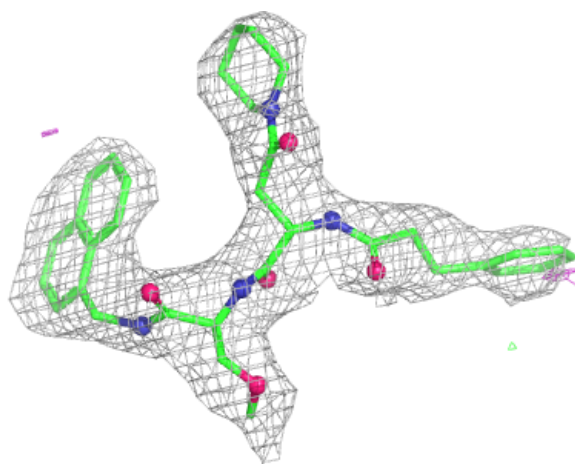
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	7J0	N	301	42/42	0.92	0.12	20,29,53,59	0
3	7J0	H	301	42/42	0.93	0.12	15,25,45,66	0
3	7J0	K	301	42/42	0.94	0.11	21,31,52,64	0
3	7J0	M	301	42/42	0.94	0.11	14,24,49,63	0
3	7J0	J	301	42/42	0.94	0.12	19,26,60,81	0
3	7J0	V	301	42/42	0.94	0.11	21,30,51,62	0
3	7J0	b	301	42/42	0.94	0.11	16,24,38,41	0
3	7J0	I	301	42/42	0.95	0.10	16,26,46,64	0
3	7J0	W	301	42/42	0.95	0.10	14,24,43,55	0
3	7J0	X	301	42/42	0.95	0.10	15,25,41,47	0
3	7J0	Y	301	42/42	0.95	0.11	14,24,53,75	0
3	7J0	Z	301	42/42	0.95	0.10	19,25,38,50	0
3	7J0	a	301	42/42	0.95	0.10	21,27,48,62	0
3	7J0	L	301	42/42	0.95	0.10	14,24,39,52	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.

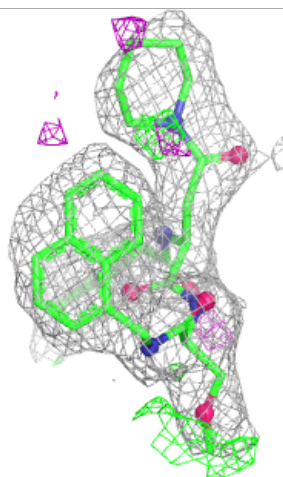
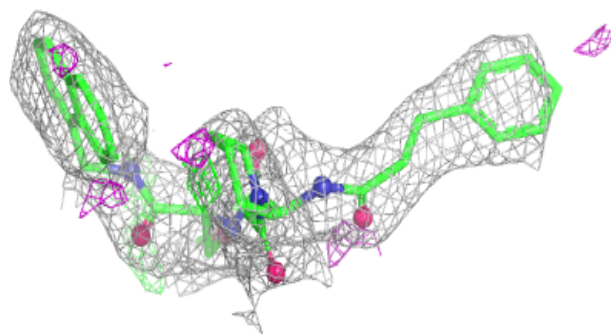
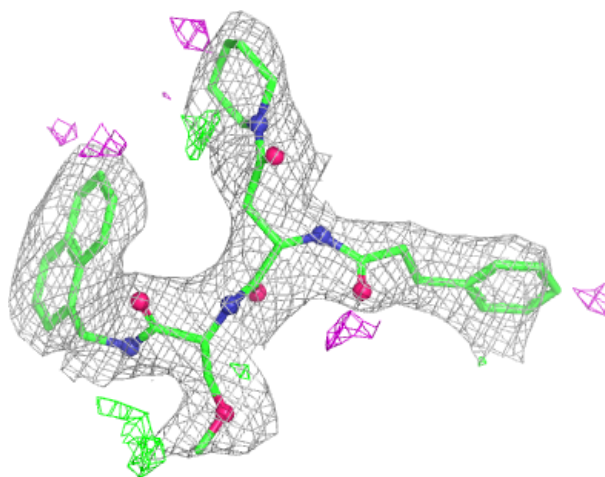
**Electron density around 7J0 N 301:**

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



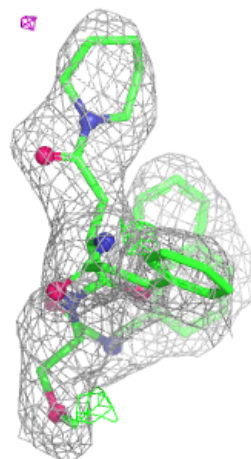
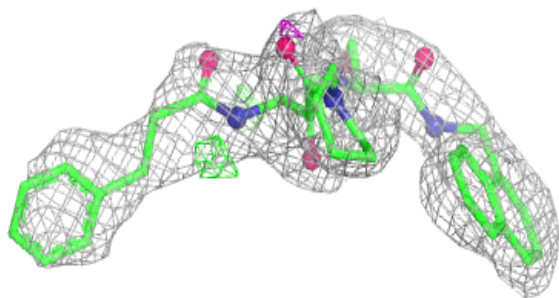
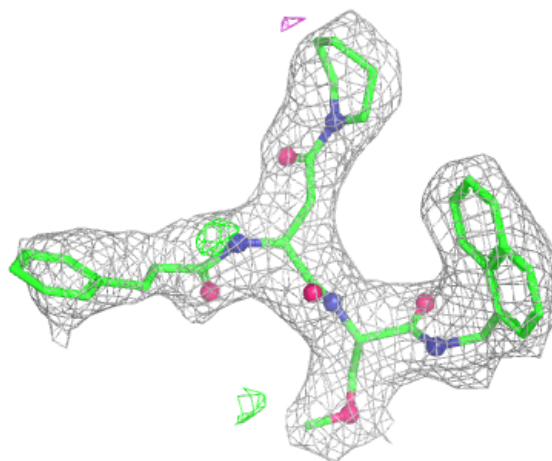
**Electron density around 7J0 H 301:**

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and green (positive)



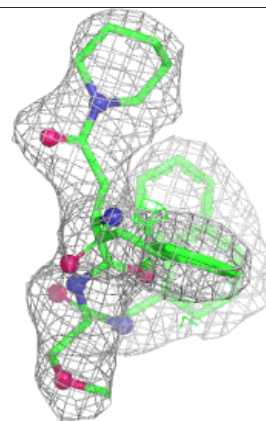
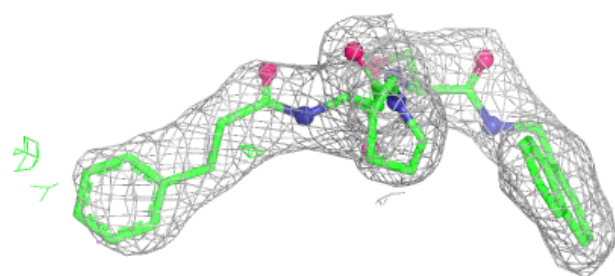
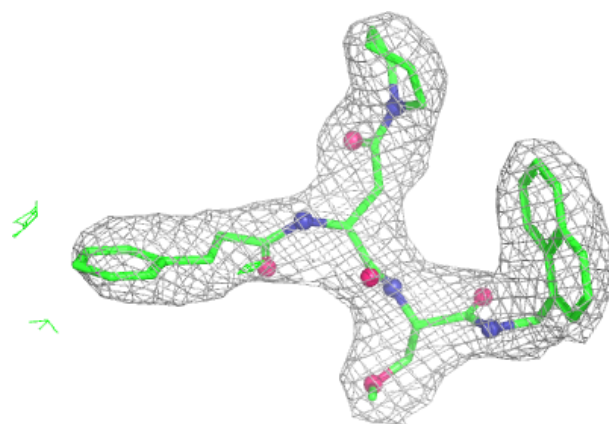
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and green (positive)



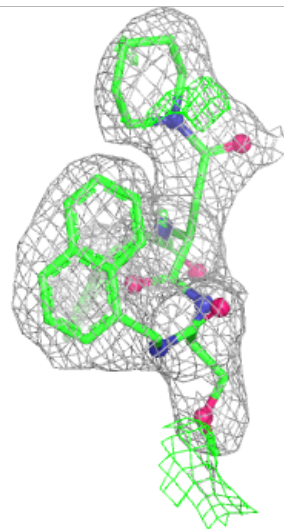
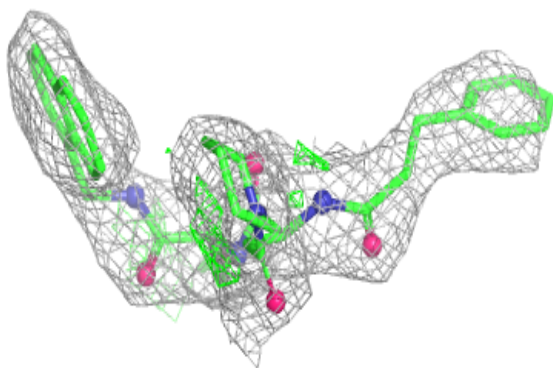
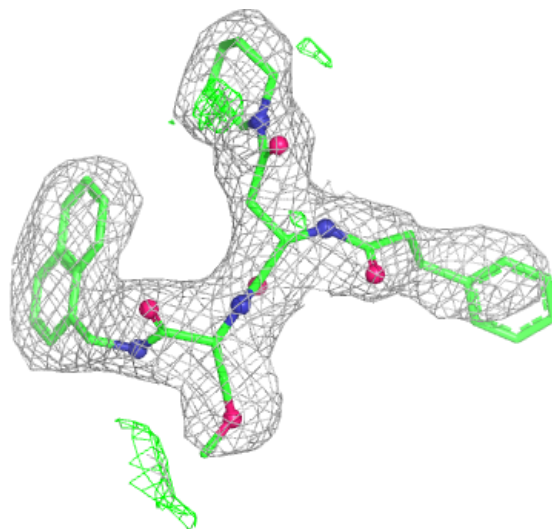
**Electron density around 7J0 M 301:**

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and green (positive)



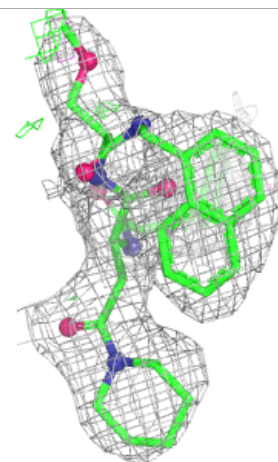
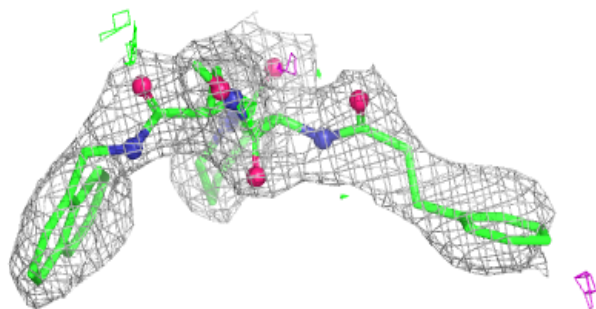
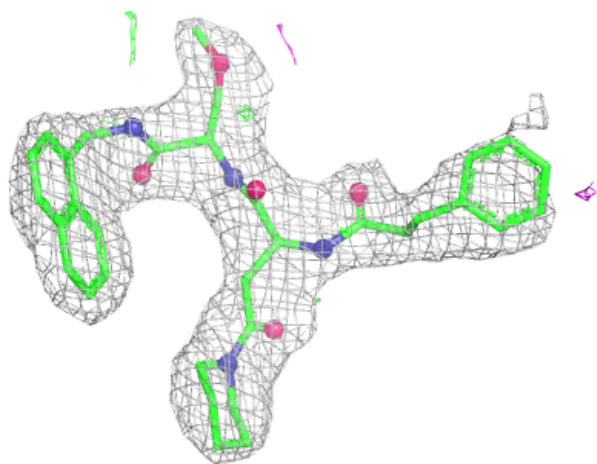
**Electron density around 7J0 J 301:**

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and green (positive)



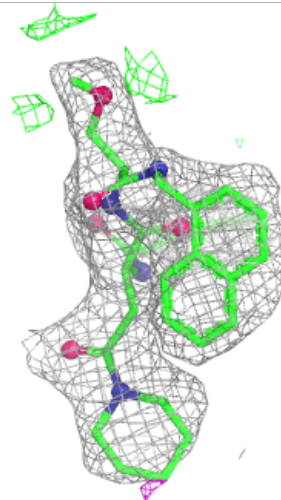
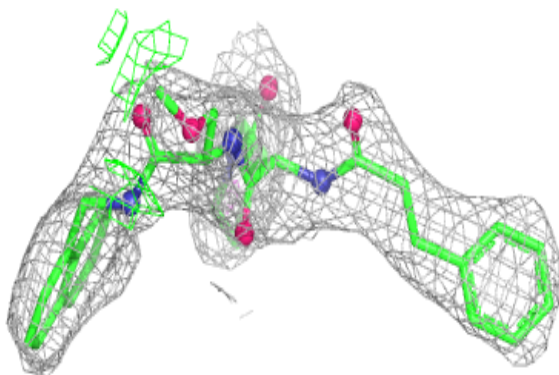
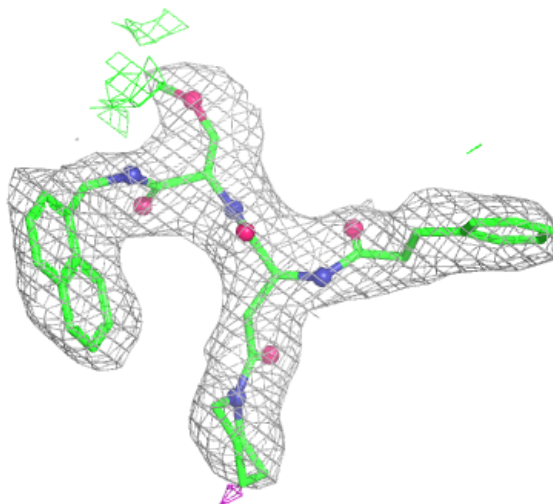
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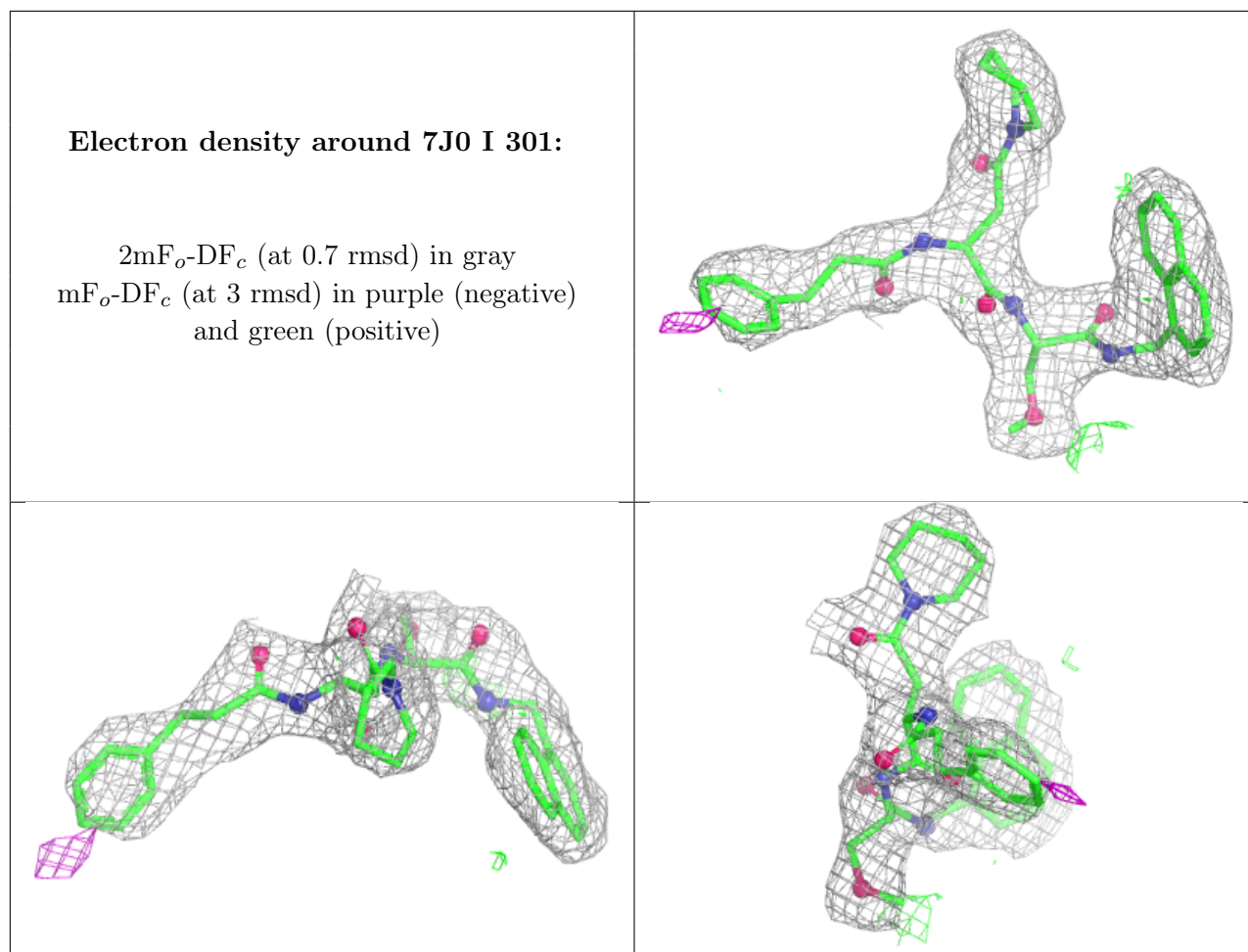
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and green (positive)



**Electron density around 7J0 b 301:**

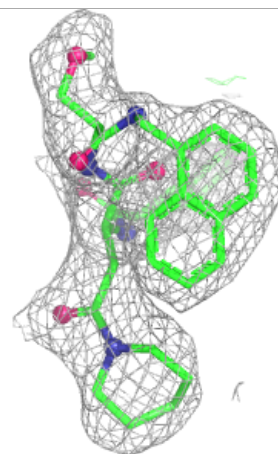
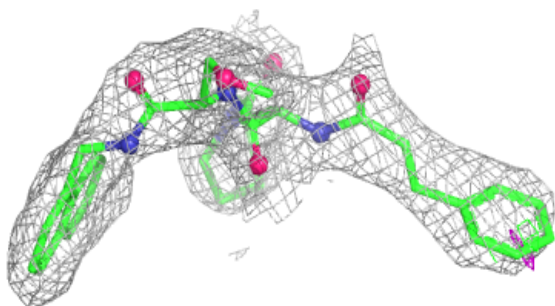
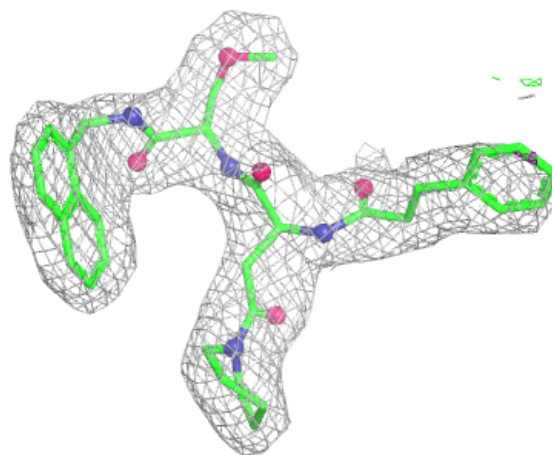
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





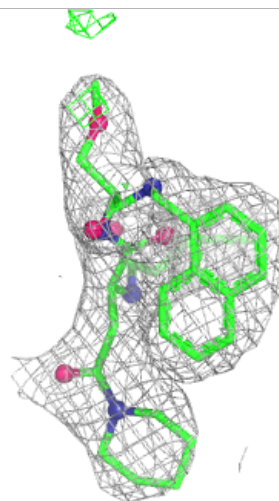
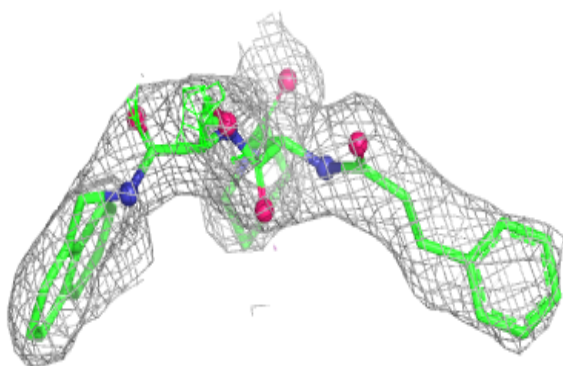
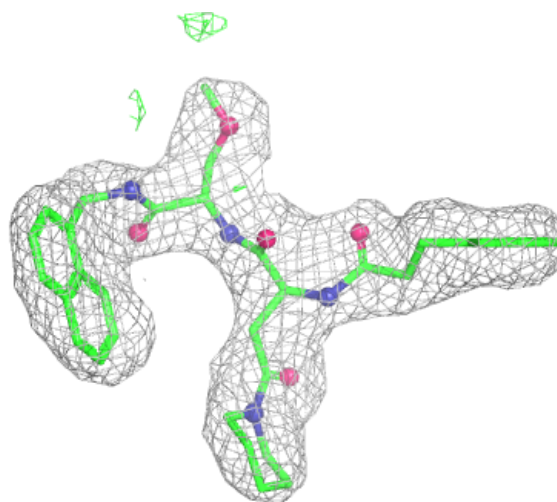
**Electron density around 7J0 W 301:**

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and green (positive)



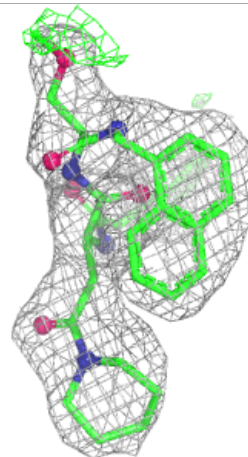
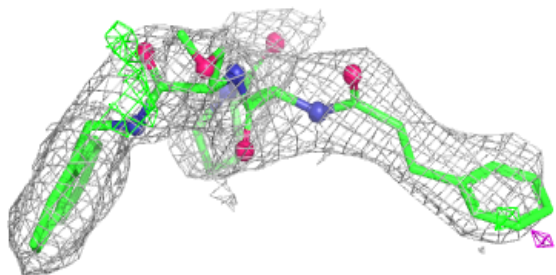
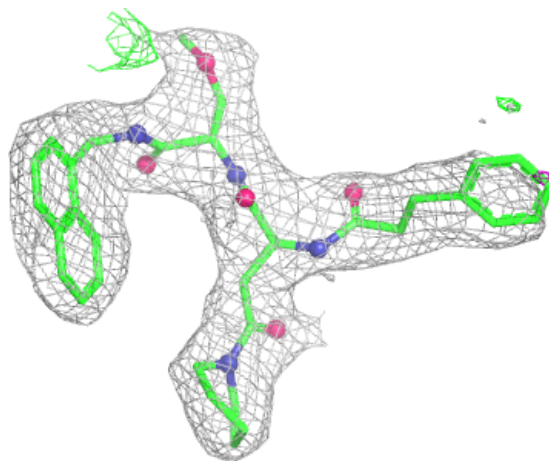
**Electron density around 7J0 X 301:**

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and green (positive)



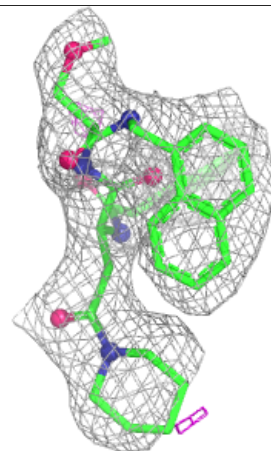
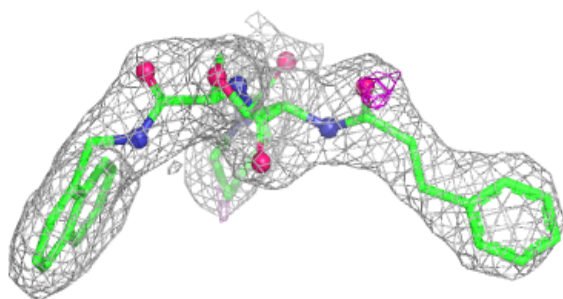
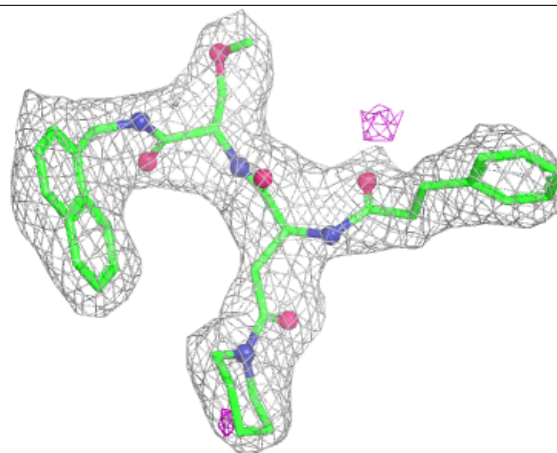
**Electron density around 7J0 Y 301:**

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and green (positive)



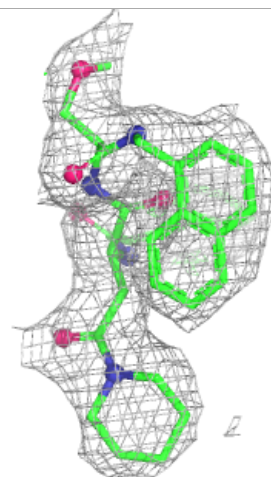
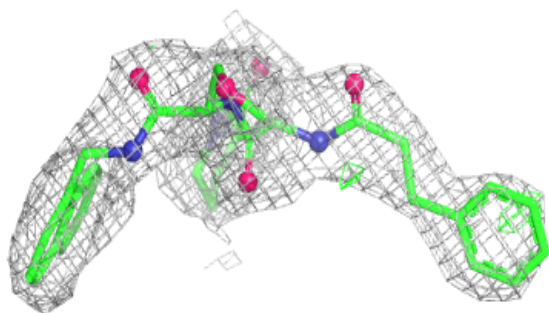
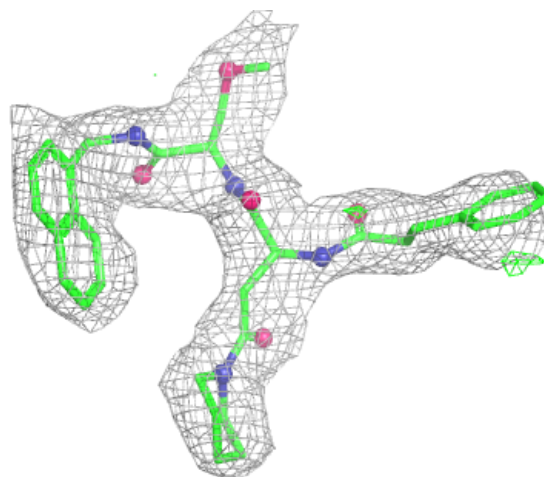
**Electron density around 7J0 Z 301:**

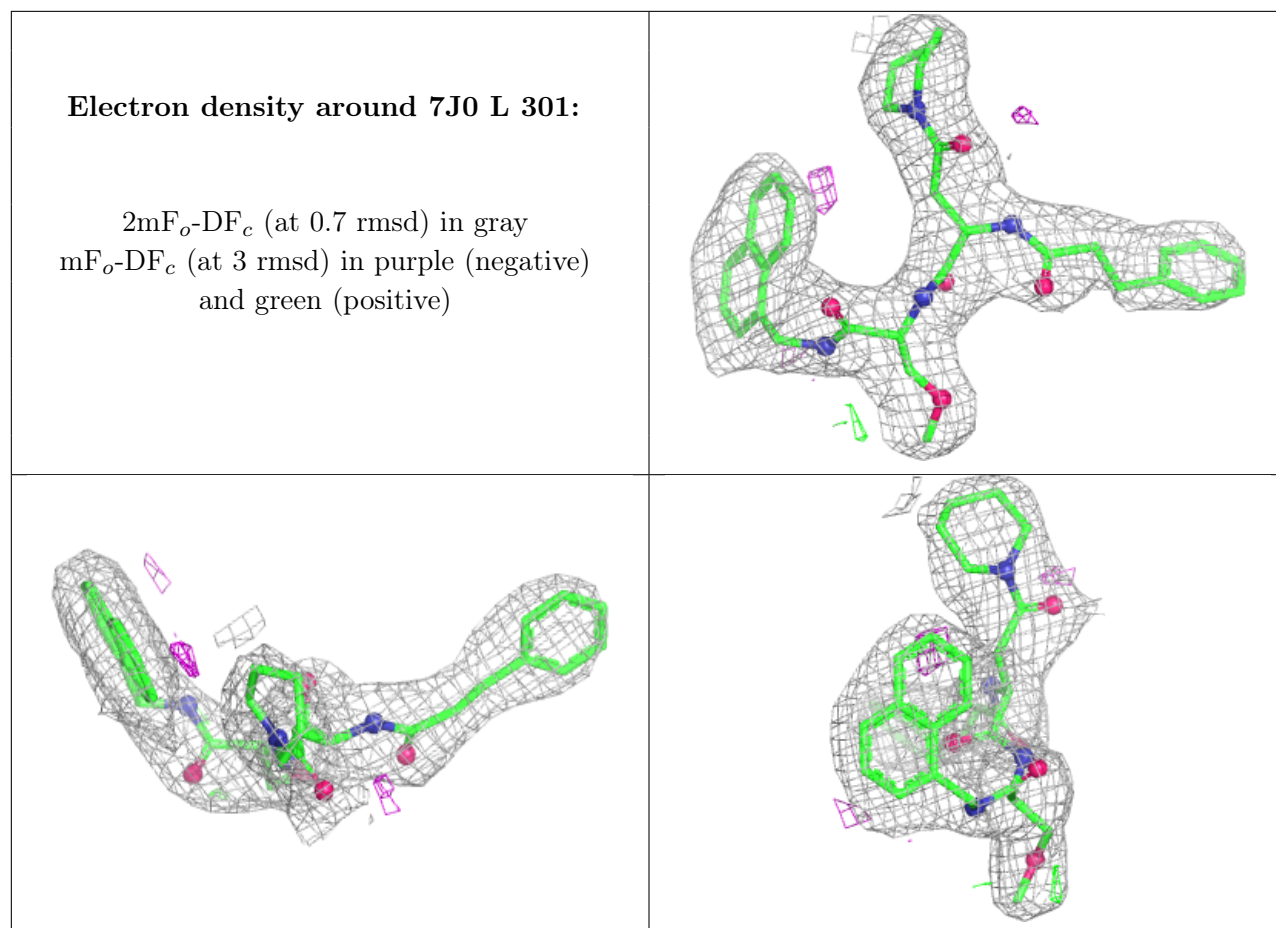
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 7J0 a 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.