



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 04:33 PM BST

PDB ID : 3UNB
Title : Mouse constitutive 20S proteasome in complex with PR-957
Authors : Huber, E.; Basler, M.; Schwab, R.; Heinemeyer, W.; Kirk, C.; Groettrup, M.; Groll, M.
Deposited on : 2011-11-15
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

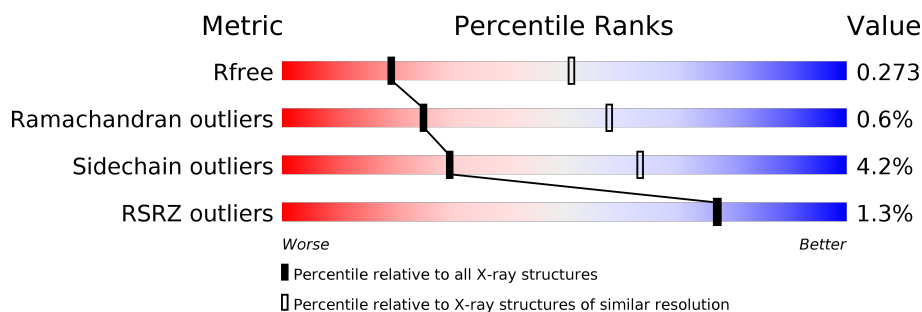
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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






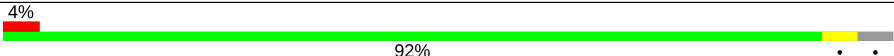


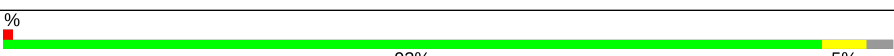
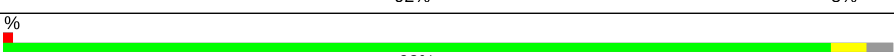
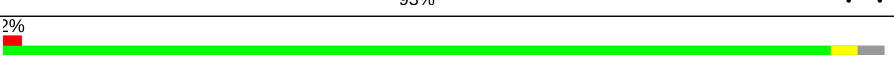
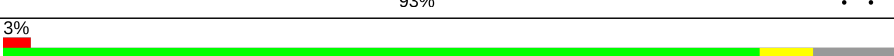
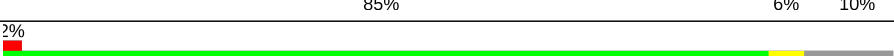
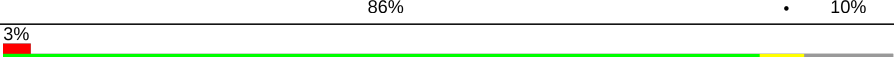

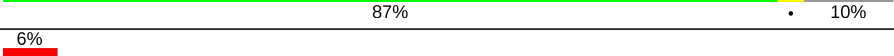
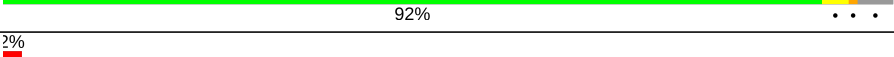
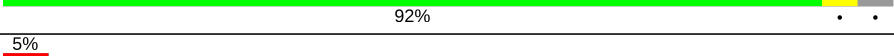
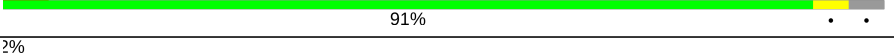

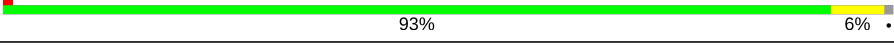
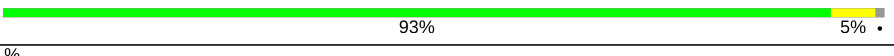
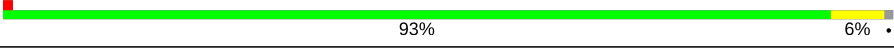
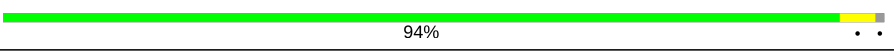
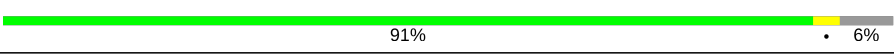
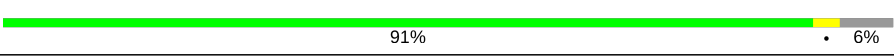

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	234	<div> <div>%</div> <div>94% 5% .</div> </div>
1	O	234	<div> <div>%</div> <div>94% . .</div> </div>
1	c	234	<div> <div>%</div> <div>95% . .</div> </div>
1	q	234	<div> <div>%</div> <div>94% . .</div> </div>
2	B	261	<div> <div>%</div> <div>89% 6% 5%</div> </div>
2	P	261	<div> <div>%</div> <div>90% 5% 5%</div> </div>
2	d	261	<div> <div>%</div> <div>90% 5% 5%</div> </div>

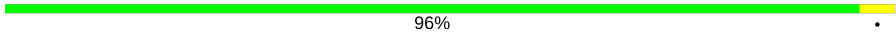
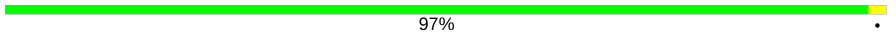
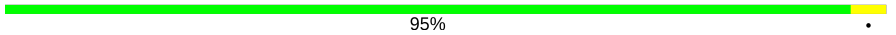
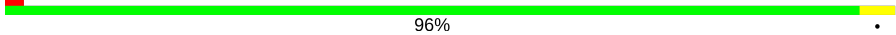
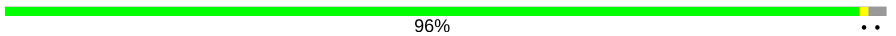

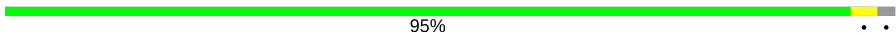
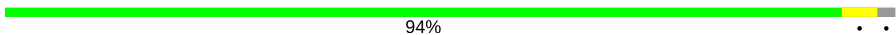

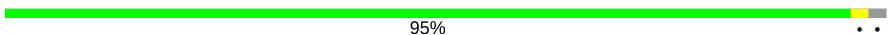


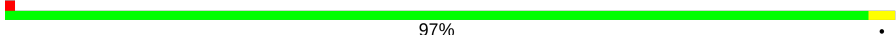

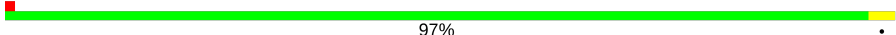
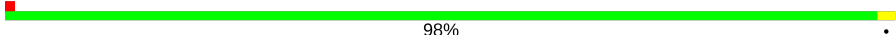
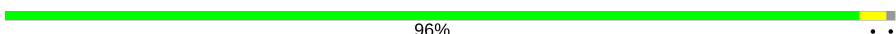



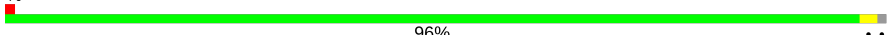
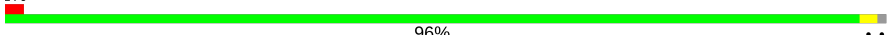

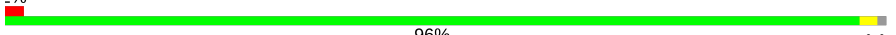
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Mol	Chain	Length	Quality of chain
2	r	261	 91% 5%
3	C	248	 91% 5%
3	Q	248	 93%
3	e	248	 92%
3	s	248	 92% 5%
4	D	241	 92% 5%
4	R	241	 92% 5%
4	f	241	 93%
4	t	241	 93%
5	E	263	 85% 6% 10%
5	S	263	 86% 10%
5	g	263	 85% 5% 10%
5	u	263	 87% 10%
6	F	255	 92%
6	T	255	 92%
6	h	255	 91%
6	v	255	 89% 6%
7	G	246	 93% 6%
7	U	246	 93% 5%
7	i	246	 93% 6%
7	w	246	 94%
8	H	234	 91% 6%
8	V	234	 91% 6%
8	j	234	 89% 5% 6%
8	x	234	 89% 5% 6%

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Mol	Chain	Length	Quality of chain
9	I	205	 96% .
9	W	205	 97% .
9	k	205	 95% .
9	y	205	 2% 96% .
10	J	201	 96% ..
10	X	201	 92% 5% .
10	l	201	 95% ..
10	z	201	 94% . .
11	1	205	 93% 5% .
11	K	205	 95% ..
11	Y	205	 92% 5% .
11	m	205	 95% . .
12	2	213	 % 97% .
12	L	213	 96% .
12	Z	213	 % 97% .
12	n	213	 % 98% .
13	3	219	 96% . .
13	M	219	 94% 5% .
13	a	219	 95% . .
13	o	219	 95% . .
14	4	205	 % 96% ..
14	N	205	 2% 96% ..
14	b	205	 % 95% . .
14	p	205	 2% 96% ..

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 99236 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1806	1153	309	338	6			
1	O	231	Total	C	N	O	S	0	0	0
			1806	1153	309	338	6			
1	c	231	Total	C	N	O	S	0	0	0
			1806	1153	309	338	6			
1	q	231	Total	C	N	O	S	0	0	0
			1806	1153	309	338	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	LYS	GLU	CONFLICT	UNP P49722
O	2	LYS	GLU	CONFLICT	UNP P49722
c	2	LYS	GLU	CONFLICT	UNP P49722
q	2	LYS	GLU	CONFLICT	UNP P49722

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	248	Total	C	N	O	S	0	0	0
			1950	1232	335	373	10			
2	P	248	Total	C	N	O	S	0	0	0
			1950	1232	335	373	10			
2	d	248	Total	C	N	O	S	0	0	0
			1950	1232	335	373	10			
2	r	248	Total	C	N	O	S	0	0	0
			1950	1232	335	373	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	239	Total 1881	C 1182	N 332	O 362	S 5	0	0	0
3	Q	239	Total 1881	C 1182	N 332	O 362	S 5	0	0	0
3	e	239	Total 1881	C 1182	N 332	O 362	S 5	0	0	0
3	s	239	Total 1881	C 1182	N 332	O 362	S 5	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	45	ALA	GLU	CONFLICT	UNP Q9Z2U0
Q	45	ALA	GLU	CONFLICT	UNP Q9Z2U0
e	45	ALA	GLU	CONFLICT	UNP Q9Z2U0
s	45	ALA	GLU	CONFLICT	UNP Q9Z2U0

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	233	Total 1778	C 1116	N 294	O 357	S 11	0	0	0
4	R	233	Total 1778	C 1116	N 294	O 357	S 11	0	0	0
4	f	233	Total 1778	C 1116	N 294	O 357	S 11	0	0	0
4	t	233	Total 1778	C 1116	N 294	O 357	S 11	0	0	0

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	238	Total 1872	C 1171	N 336	O 354	S 11	0	0	0
5	S	238	Total 1872	C 1171	N 336	O 354	S 11	0	0	0
5	g	238	Total 1872	C 1171	N 336	O 354	S 11	0	0	0
5	u	238	Total 1872	C 1171	N 336	O 354	S 11	0	0	0

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1903	1206	325	361	11			
6	T	244	Total	C	N	O	S	0	0	0
			1903	1206	325	361	11			
6	h	244	Total	C	N	O	S	0	0	0
			1903	1206	325	361	11			
6	v	244	Total	C	N	O	S	0	0	0
			1903	1206	325	361	11			

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1890	1199	315	363	13			
7	U	243	Total	C	N	O	S	0	0	0
			1890	1199	315	363	13			
7	i	243	Total	C	N	O	S	0	0	0
			1890	1199	315	363	13			
7	w	243	Total	C	N	O	S	0	0	0
			1890	1199	315	363	13			

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	220	Total	C	N	O	S	0	0	0
			1656	1044	282	318	12			
8	V	220	Total	C	N	O	S	0	0	0
			1656	1044	282	318	12			
8	j	220	Total	C	N	O	S	0	0	0
			1656	1044	282	318	12			
8	x	220	Total	C	N	O	S	0	0	0
			1656	1044	282	318	12			

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1592	1013	265	295	19			
9	W	204	Total	C	N	O	S	0	0	0
			1592	1013	265	295	19			
9	k	204	Total	C	N	O	S	0	0	0
			1592	1013	265	295	19			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	y	204	Total	C	N	O	S	0	0	0
			1592	1013	265	295	19			

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	196	Total	C	N	O	S	0	0	0
			1570	1006	267	288	9			
10	X	196	Total	C	N	O	S	0	0	0
			1570	1006	267	288	9			
10	l	196	Total	C	N	O	S	0	0	0
			1570	1006	267	288	9			
10	z	196	Total	C	N	O	S	0	0	0
			1570	1006	267	288	9			

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	201	Total	C	N	O	S	0	0	0
			1557	983	271	294	9			
11	Y	201	Total	C	N	O	S	0	0	0
			1557	983	271	294	9			
11	m	201	Total	C	N	O	S	0	0	0
			1557	983	271	294	9			
11	1	201	Total	C	N	O	S	0	0	0
			1557	983	271	294	9			

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	213	Total	C	N	O	S	0	0	0
			1654	1047	284	313	10			
12	Z	213	Total	C	N	O	S	0	0	0
			1654	1047	284	313	10			
12	n	213	Total	C	N	O	S	0	0	0
			1654	1047	284	313	10			
12	2	213	Total	C	N	O	S	0	0	0
			1654	1047	284	313	10			

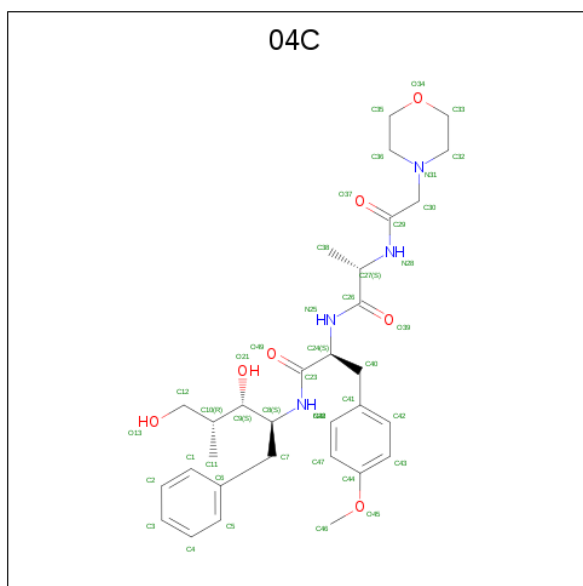
- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	216	Total	C	N	O	S	0	0	0
			1685	1063	291	319	12			
13	a	216	Total	C	N	O	S	0	0	0
			1685	1063	291	319	12			
13	o	216	Total	C	N	O	S	0	0	0
			1685	1063	291	319	12			
13	3	216	Total	C	N	O	S	0	0	0
			1685	1063	291	319	12			

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	202	Total	C	N	O	S	0	0	0
			1519	952	259	296	12			
14	b	202	Total	C	N	O	S	0	0	0
			1519	952	259	296	12			
14	p	202	Total	C	N	O	S	0	0	0
			1519	952	259	296	12			
14	4	202	Total	C	N	O	S	0	0	0
			1519	952	259	296	12			

- Molecule 15 is 1,2,4-trideoxy-4-methyl-2-{[N-(morpholin-4-ylacetyl)-L-alanyl-O-methyl-L-tyrosyl]amino}-1-phenyl-D-xylitol (three-letter code: 04C) (formula: C₃₁H₄₄N₄O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	H	1	Total	C	N	O	0	0
			42	31	4	7		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	K	1	Total	C	N	O	0	0
			42	31	4	7		
15	N	1	Total	C	N	O	0	0
			42	31	4	7		
15	V	1	Total	C	N	O	0	0
			42	31	4	7		
15	Y	1	Total	C	N	O	0	0
			42	31	4	7		
15	b	1	Total	C	N	O	0	0
			42	31	4	7		
15	j	1	Total	C	N	O	0	0
			42	31	4	7		
15	m	1	Total	C	N	O	0	0
			42	31	4	7		
15	p	1	Total	C	N	O	0	0
			42	31	4	7		
15	x	1	Total	C	N	O	0	0
			42	31	4	7		
15	1	1	Total	C	N	O	0	0
			42	31	4	7		
15	4	1	Total	C	N	O	0	0
			42	31	4	7		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	19	Total	O	0	0
			19	19		
16	B	24	Total	O	0	0
			24	24		
16	C	13	Total	O	0	0
			13	13		
16	D	16	Total	O	0	0
			16	16		
16	E	21	Total	O	0	0
			21	21		
16	F	20	Total	O	0	0
			20	20		
16	G	22	Total	O	0	0
			22	22		
16	H	31	Total	O	0	0
			31	31		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	I	32	Total O 32 32	0	0
16	J	25	Total O 25 25	0	0
16	K	28	Total O 28 28	0	0
16	L	23	Total O 23 23	0	0
16	M	27	Total O 27 27	0	0
16	N	33	Total O 33 33	0	0
16	O	33	Total O 33 33	0	0
16	P	38	Total O 38 38	0	0
16	Q	16	Total O 16 16	0	0
16	R	19	Total O 19 19	0	0
16	S	25	Total O 25 25	0	0
16	T	25	Total O 25 25	0	0
16	U	37	Total O 37 37	0	0
16	V	35	Total O 35 35	0	0
16	W	37	Total O 37 37	0	0
16	X	33	Total O 33 33	0	0
16	Y	16	Total O 16 16	0	0
16	Z	32	Total O 32 32	0	0
16	a	33	Total O 33 33	0	0
16	b	40	Total O 40 40	0	0
16	c	21	Total O 21 21	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	d	19	Total 19	O 19	0	0
16	e	14	Total 14	O 14	0	0
16	f	13	Total 13	O 13	0	0
16	g	15	Total 15	O 15	0	0
16	h	19	Total 19	O 19	0	0
16	i	29	Total 29	O 29	0	0
16	j	25	Total 25	O 25	0	0
16	k	30	Total 30	O 30	0	0
16	l	22	Total 22	O 22	0	0
16	m	20	Total 20	O 20	0	0
16	n	29	Total 29	O 29	0	0
16	o	27	Total 27	O 27	0	0
16	p	32	Total 32	O 32	0	0
16	q	26	Total 26	O 26	0	0
16	r	34	Total 34	O 34	0	0
16	s	19	Total 19	O 19	0	0
16	t	17	Total 17	O 17	0	0
16	u	27	Total 27	O 27	0	0
16	v	31	Total 31	O 31	0	0
16	w	27	Total 27	O 27	0	0
16	x	34	Total 34	O 34	0	0

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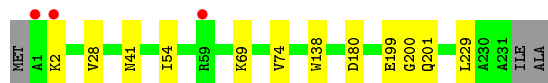
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	y	32	Total 32	O 32	0	0
16	z	38	Total 38	O 38	0	0
16	1	27	Total 27	O 27	0	0
16	2	33	Total 33	O 33	0	0
16	3	37	Total 37	O 37	0	0
16	4	30	Total 30	O 30	0	0

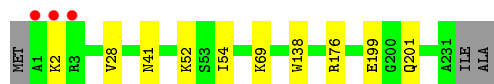
3 Residue-property plots [i](#)

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

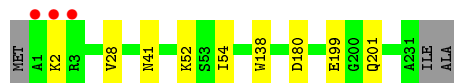
- Molecule 1: Proteasome subunit alpha type-2



- Molecule 1: Proteasome subunit alpha type-2



- Molecule 1: Proteasome subunit alpha type-2



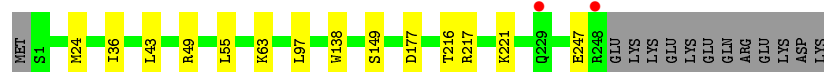
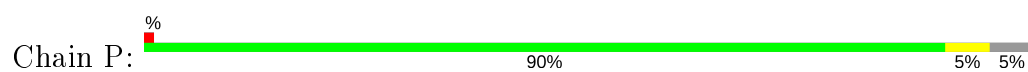
- Molecule 1: Proteasome subunit alpha type-2



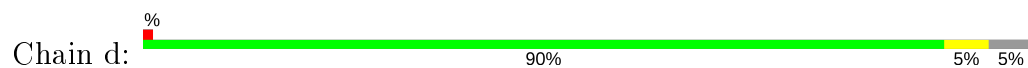
- Molecule 2: Proteasome subunit alpha type-4



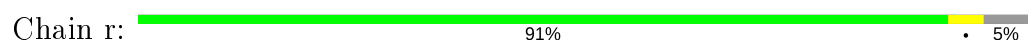
- Molecule 2: Proteasome subunit alpha type-4



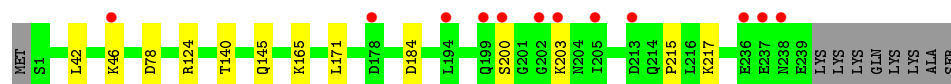
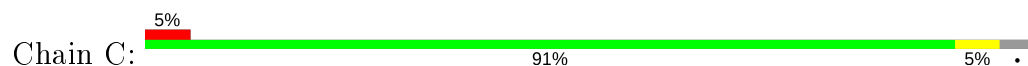
- Molecule 2: Proteasome subunit alpha type-4



- Molecule 2: Proteasome subunit alpha type-4



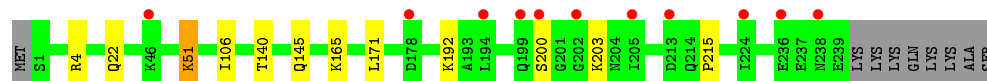
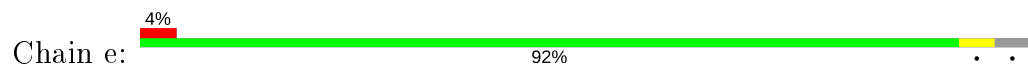
- Molecule 3: Proteasome subunit alpha type-7



- Molecule 3: Proteasome subunit alpha type-7




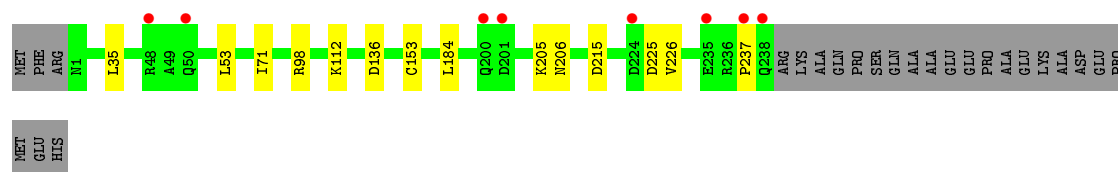
- Molecule 3: Proteasome subunit alpha type-7



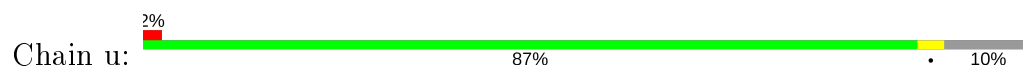
- Molecule 3: Proteasome subunit alpha type-7



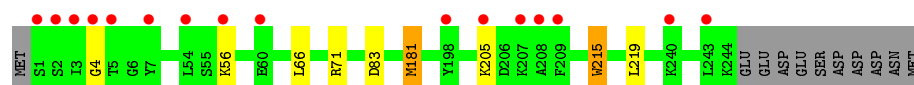
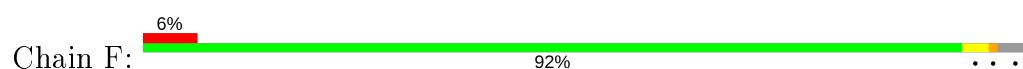
- Chain g: 



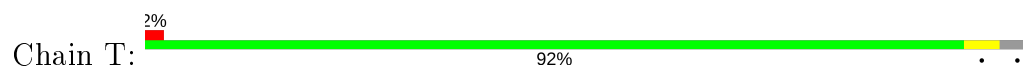
- Molecule 5: Proteasome subunit alpha type-1



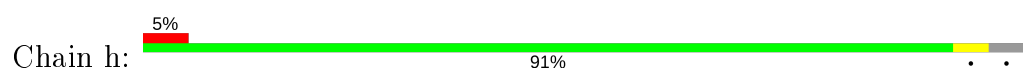
- Molecule 6: Proteasome subunit alpha type-3



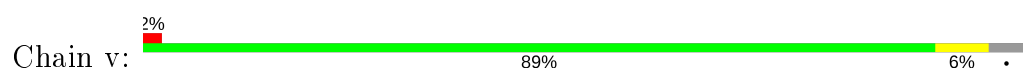
- Molecule 6: Proteasome subunit alpha type-3



- Molecule 6: Proteasome subunit alpha type-3



- Molecule 6: Proteasome subunit alpha type-3



- Molecule 7: Proteasome subunit alpha type-6

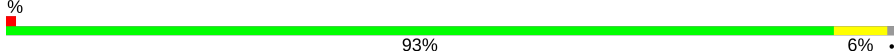


- Molecule 7: Proteasome subunit alpha type-6

Chain U:  93% 5%



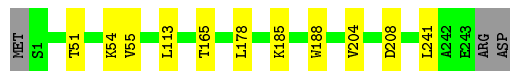
- Molecule 7: Proteasome subunit alpha type-6

Chain i:  93% 6%



- Molecule 7: Proteasome subunit alpha type-6

Chain w:  94%



- Molecule 8: Proteasome subunit beta type-7

Chain H:  91% 6%




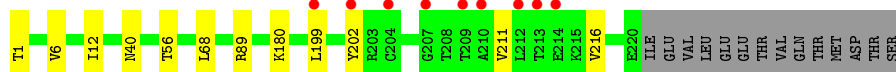
- Molecule 8: Proteasome subunit beta type-7

Chain V:  91% 6%




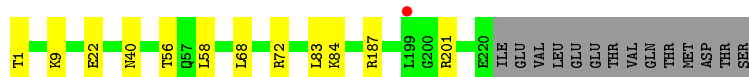
- Molecule 8: Proteasome subunit beta type-7

Chain j:  89% 5% 6% 4%



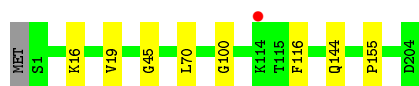
- Molecule 8: Proteasome subunit beta type-7

Chain x:  89% 5% 6%



- Molecule 9: Proteasome subunit beta type-3

Chain I:  96% .



- Molecule 9: Proteasome subunit beta type-3

Chain W:  97% .



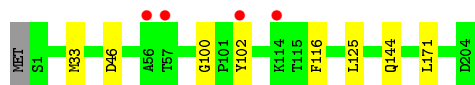
- Molecule 9: Proteasome subunit beta type-3

Chain k:  95% .



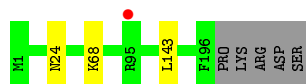
- Molecule 9: Proteasome subunit beta type-3

Chain y:  96% .



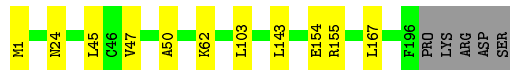
- Molecule 10: Proteasome subunit beta type-2

Chain J:  96% ..



- Molecule 10: Proteasome subunit beta type-2

Chain X:  92% 5% .



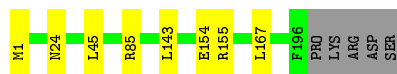
- Molecule 10: Proteasome subunit beta type-2

Chain l:  95% ..



- Molecule 10: Proteasome subunit beta type-2

Chain z:  94% 



- Molecule 11: Proteasome subunit beta type-5

Chain K:  95% 



- Molecule 11: Proteasome subunit beta type-5

Chain Y:  92% 5% 



- Molecule 11: Proteasome subunit beta type-5

Chain m:  95% 



- Molecule 11: Proteasome subunit beta type-5

Chain 1:  93% 5% 



- Molecule 12: Proteasome subunit beta type-1

Chain L:  96% 



- Molecule 12: Proteasome subunit beta type-1

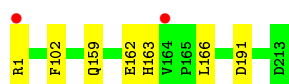
Chain Z:  97% 



• Molecule 12: Proteasome subunit beta type-1



• Molecule 12: Proteasome subunit beta type-1



• Molecule 13: Proteasome subunit beta type-4



• Molecule 13: Proteasome subunit beta type-4



• Molecule 13: Proteasome subunit beta type-4

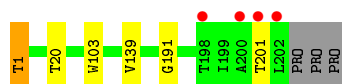


• Molecule 13: Proteasome subunit beta type-4



• Molecule 14: Proteasome subunit beta type-6

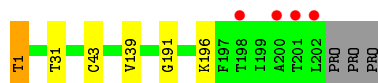




- Molecule 14: Proteasome subunit beta type-6



- Molecule 14: Proteasome subunit beta type-6



- Molecule 14: Proteasome subunit beta type-6



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	171.72Å 198.59Å 226.75Å 90.00° 106.59° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 49.19 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.0 (15.00-2.90) 96.0 (49.19-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, R_{free}	0.230 , 0.273 0.230 , 0.273	Depositor DCC
R_{free} test set	15447 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	99236	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 98.11 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3244e-11. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 04C

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	0.39	1/1845 (0.1%)	0.49	0/2498
1	O	0.39	1/1845 (0.1%)	0.48	0/2498
1	c	0.39	1/1845 (0.1%)	0.48	0/2498
1	q	0.39	0/1845	0.47	0/2498
2	B	0.37	1/1980 (0.1%)	0.48	0/2667
2	P	0.37	1/1980 (0.1%)	0.48	0/2667
2	d	0.37	0/1980	0.48	0/2667
2	r	0.37	0/1980	0.48	0/2667
3	C	0.33	0/1908	0.47	0/2576
3	Q	0.34	0/1908	0.48	0/2576
3	e	0.33	0/1908	0.47	0/2576
3	s	0.34	1/1908 (0.1%)	0.47	0/2576
4	D	0.36	1/1805 (0.1%)	0.47	0/2437
4	R	0.36	1/1805 (0.1%)	0.46	0/2437
4	f	0.36	1/1805 (0.1%)	0.47	0/2437
4	t	0.37	0/1805	0.47	0/2437
5	E	0.37	0/1907	0.49	0/2578
5	S	0.38	1/1907 (0.1%)	0.51	0/2578
5	g	0.37	0/1907	0.48	0/2578
5	u	0.38	1/1907 (0.1%)	0.50	0/2578
6	F	0.39	1/1938 (0.1%)	0.48	0/2608
6	T	0.38	1/1938 (0.1%)	0.48	0/2608
6	h	0.38	1/1938 (0.1%)	0.48	0/2608
6	v	0.39	2/1938 (0.1%)	0.48	0/2608
7	G	0.37	1/1924 (0.1%)	0.48	0/2600
7	U	0.38	1/1924 (0.1%)	0.49	0/2600
7	i	0.37	1/1924 (0.1%)	0.48	0/2600
7	w	0.38	1/1924 (0.1%)	0.48	0/2600
8	H	0.35	0/1683	0.51	1/2276 (0.0%)
8	V	0.37	1/1683 (0.1%)	0.51	0/2276
8	j	0.33	0/1683	0.52	0/2276
8	x	0.36	1/1683 (0.1%)	0.52	1/2276 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	I	0.34	0/1621	0.49	0/2185
9	W	0.35	0/1621	0.49	0/2185
9	k	0.34	0/1621	0.48	0/2185
9	y	0.35	0/1621	0.50	0/2185
10	J	0.33	0/1602	0.49	0/2167
10	X	0.33	0/1602	0.49	0/2167
10	l	0.33	0/1602	0.49	0/2167
10	z	0.33	0/1602	0.49	0/2167
11	1	0.44	1/1588 (0.1%)	0.50	0/2145
11	K	0.44	1/1588 (0.1%)	0.50	0/2145
11	Y	0.46	2/1588 (0.1%)	0.48	0/2145
11	m	0.45	1/1588 (0.1%)	0.50	0/2145
12	2	0.32	0/1685	0.48	0/2271
12	L	0.33	0/1685	0.48	0/2271
12	Z	0.33	0/1685	0.48	0/2271
12	n	0.33	0/1685	0.47	0/2271
13	3	0.40	0/1718	0.50	0/2325
13	M	0.41	3/1718 (0.2%)	0.50	0/2325
13	a	0.41	1/1718 (0.1%)	0.51	0/2325
13	o	0.40	1/1718 (0.1%)	0.48	0/2325
14	4	0.39	1/1546 (0.1%)	0.48	0/2094
14	N	0.39	2/1546 (0.1%)	0.48	0/2094
14	b	0.39	1/1546 (0.1%)	0.49	0/2094
14	p	0.39	1/1546 (0.1%)	0.48	0/2094
All	All	0.37	37/99000 (0.0%)	0.49	2/133708 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	1
8	V	0	1
8	j	0	1
11	1	0	1
11	K	0	1
11	Y	0	1
11	m	0	1
14	4	0	1
14	N	0	1
14	b	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
14	p	0	1
All	All	0	11

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Y	1	THR	C-N	7.39	1.51	1.34
11	m	1	THR	C-N	7.02	1.50	1.34
11	K	1	THR	C-N	6.13	1.48	1.34
8	V	1	THR	C-N	6.04	1.48	1.34
8	x	1	THR	C-N	6.00	1.47	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	1	THR	C-N-CA	6.26	137.36	121.70
8	x	1	THR	C-N-CA	5.11	134.48	121.70

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	1	THR	Peptide
11	K	1	THR	Peptide
14	N	1	THR	Peptide
8	V	1	THR	Mainchain
11	Y	1	THR	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	229/234 (98%)	214 (93%)	9 (4%)	6 (3%)	5	20
1	O	229/234 (98%)	215 (94%)	9 (4%)	5 (2%)	6	24
1	c	229/234 (98%)	217 (95%)	7 (3%)	5 (2%)	6	24
1	q	229/234 (98%)	216 (94%)	9 (4%)	4 (2%)	9	31
2	B	246/261 (94%)	239 (97%)	7 (3%)	0	100	100
2	P	246/261 (94%)	238 (97%)	8 (3%)	0	100	100
2	d	246/261 (94%)	237 (96%)	9 (4%)	0	100	100
2	r	246/261 (94%)	239 (97%)	6 (2%)	1 (0%)	34	66
3	C	237/248 (96%)	220 (93%)	15 (6%)	2 (1%)	19	51
3	Q	237/248 (96%)	227 (96%)	8 (3%)	2 (1%)	19	51
3	e	237/248 (96%)	224 (94%)	10 (4%)	3 (1%)	12	37
3	s	237/248 (96%)	225 (95%)	11 (5%)	1 (0%)	34	66
4	D	231/241 (96%)	222 (96%)	9 (4%)	0	100	100
4	R	231/241 (96%)	220 (95%)	10 (4%)	1 (0%)	34	66
4	f	231/241 (96%)	217 (94%)	14 (6%)	0	100	100
4	t	231/241 (96%)	219 (95%)	12 (5%)	0	100	100
5	E	236/263 (90%)	223 (94%)	10 (4%)	3 (1%)	12	37
5	S	236/263 (90%)	219 (93%)	15 (6%)	2 (1%)	19	51
5	g	236/263 (90%)	220 (93%)	15 (6%)	1 (0%)	34	66
5	u	236/263 (90%)	221 (94%)	14 (6%)	1 (0%)	34	66
6	F	242/255 (95%)	232 (96%)	8 (3%)	2 (1%)	19	51
6	T	242/255 (95%)	234 (97%)	8 (3%)	0	100	100
6	h	242/255 (95%)	235 (97%)	5 (2%)	2 (1%)	19	51
6	v	242/255 (95%)	233 (96%)	7 (3%)	2 (1%)	19	51
7	G	241/246 (98%)	235 (98%)	3 (1%)	3 (1%)	13	40
7	U	241/246 (98%)	235 (98%)	6 (2%)	0	100	100
7	i	241/246 (98%)	234 (97%)	5 (2%)	2 (1%)	19	51
7	w	241/246 (98%)	234 (97%)	6 (2%)	1 (0%)	34	66
8	H	218/234 (93%)	213 (98%)	5 (2%)	0	100	100
8	V	218/234 (93%)	210 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	j	218/234 (93%)	212 (97%)	6 (3%)	0	100	100
8	x	218/234 (93%)	210 (96%)	7 (3%)	1 (0%)	29	61
9	I	202/205 (98%)	188 (93%)	9 (4%)	5 (2%)	5	21
9	W	202/205 (98%)	189 (94%)	12 (6%)	1 (0%)	29	61
9	k	202/205 (98%)	187 (93%)	12 (6%)	3 (2%)	10	34
9	y	202/205 (98%)	183 (91%)	16 (8%)	3 (2%)	10	34
10	J	194/201 (96%)	187 (96%)	6 (3%)	1 (0%)	29	61
10	X	194/201 (96%)	188 (97%)	4 (2%)	2 (1%)	15	45
10	l	194/201 (96%)	186 (96%)	7 (4%)	1 (0%)	29	61
10	z	194/201 (96%)	186 (96%)	7 (4%)	1 (0%)	29	61
11	1	199/205 (97%)	192 (96%)	7 (4%)	0	100	100
11	K	199/205 (97%)	193 (97%)	6 (3%)	0	100	100
11	Y	199/205 (97%)	196 (98%)	3 (2%)	0	100	100
11	m	199/205 (97%)	192 (96%)	7 (4%)	0	100	100
12	2	211/213 (99%)	204 (97%)	5 (2%)	2 (1%)	17	48
12	L	211/213 (99%)	204 (97%)	6 (3%)	1 (0%)	29	61
12	Z	211/213 (99%)	200 (95%)	11 (5%)	0	100	100
12	n	211/213 (99%)	205 (97%)	6 (3%)	0	100	100
13	3	214/219 (98%)	200 (94%)	13 (6%)	1 (0%)	29	61
13	M	214/219 (98%)	203 (95%)	10 (5%)	1 (0%)	29	61
13	a	214/219 (98%)	202 (94%)	11 (5%)	1 (0%)	29	61
13	o	214/219 (98%)	206 (96%)	7 (3%)	1 (0%)	29	61
14	4	200/205 (98%)	193 (96%)	7 (4%)	0	100	100
14	N	200/205 (98%)	191 (96%)	8 (4%)	1 (0%)	29	61
14	b	200/205 (98%)	189 (94%)	10 (5%)	1 (0%)	29	61
14	p	200/205 (98%)	188 (94%)	11 (6%)	1 (0%)	29	61
All	All	12400/12920 (96%)	11841 (96%)	482 (4%)	77 (1%)	25	58

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	181	MET
14	N	191	GLY

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Mol	Chain	Res	Type
1	O	54	ILE
5	S	52	GLU
10	X	24	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/191 (99%)	184 (97%)	5 (3%)	46	77
1	O	189/191 (99%)	185 (98%)	4 (2%)	53	81
1	c	189/191 (99%)	186 (98%)	3 (2%)	62	86
1	q	189/191 (99%)	183 (97%)	6 (3%)	39	73
2	B	208/221 (94%)	194 (93%)	14 (7%)	16	43
2	P	208/221 (94%)	195 (94%)	13 (6%)	18	46
2	d	208/221 (94%)	196 (94%)	12 (6%)	20	50
2	r	208/221 (94%)	198 (95%)	10 (5%)	25	58
3	C	202/210 (96%)	191 (95%)	11 (5%)	22	54
3	Q	202/210 (96%)	195 (96%)	7 (4%)	36	70
3	e	202/210 (96%)	192 (95%)	10 (5%)	24	57
3	s	202/210 (96%)	192 (95%)	10 (5%)	24	57
4	D	195/203 (96%)	185 (95%)	10 (5%)	24	56
4	R	195/203 (96%)	185 (95%)	10 (5%)	24	56
4	f	195/203 (96%)	186 (95%)	9 (5%)	27	60
4	t	195/203 (96%)	187 (96%)	8 (4%)	30	64
5	E	204/224 (91%)	192 (94%)	12 (6%)	19	49
5	S	204/224 (91%)	195 (96%)	9 (4%)	28	61
5	g	204/224 (91%)	191 (94%)	13 (6%)	17	45
5	u	204/224 (91%)	197 (97%)	7 (3%)	37	71
6	F	200/211 (95%)	192 (96%)	8 (4%)	31	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	T	200/211 (95%)	190 (95%)	10 (5%)	24	57
6	h	200/211 (95%)	191 (96%)	9 (4%)	27	61
6	v	200/211 (95%)	187 (94%)	13 (6%)	17	45
7	G	207/210 (99%)	196 (95%)	11 (5%)	22	54
7	U	207/210 (99%)	195 (94%)	12 (6%)	20	50
7	i	207/210 (99%)	195 (94%)	12 (6%)	20	50
7	w	207/210 (99%)	198 (96%)	9 (4%)	29	62
8	H	181/195 (93%)	174 (96%)	7 (4%)	32	66
8	V	181/195 (93%)	174 (96%)	7 (4%)	32	66
8	j	181/195 (93%)	170 (94%)	11 (6%)	18	48
8	x	181/195 (93%)	171 (94%)	10 (6%)	21	53
9	I	174/175 (99%)	171 (98%)	3 (2%)	60	86
9	W	174/175 (99%)	170 (98%)	4 (2%)	50	80
9	k	174/175 (99%)	168 (97%)	6 (3%)	37	71
9	y	174/175 (99%)	169 (97%)	5 (3%)	42	76
10	J	166/171 (97%)	164 (99%)	2 (1%)	71	91
10	X	166/171 (97%)	157 (95%)	9 (5%)	22	54
10	l	166/171 (97%)	161 (97%)	5 (3%)	41	75
10	z	166/171 (97%)	159 (96%)	7 (4%)	30	63
11	1	157/161 (98%)	147 (94%)	10 (6%)	17	45
11	K	157/161 (98%)	152 (97%)	5 (3%)	39	73
11	Y	157/161 (98%)	147 (94%)	10 (6%)	17	45
11	m	157/161 (98%)	151 (96%)	6 (4%)	33	67
12	2	178/178 (100%)	173 (97%)	5 (3%)	43	76
12	L	178/178 (100%)	170 (96%)	8 (4%)	27	61
12	Z	178/178 (100%)	171 (96%)	7 (4%)	32	66
12	n	178/178 (100%)	173 (97%)	5 (3%)	43	76
13	3	178/180 (99%)	173 (97%)	5 (3%)	43	76
13	M	178/180 (99%)	172 (97%)	6 (3%)	37	71
13	a	178/180 (99%)	172 (97%)	6 (3%)	37	71
13	o	178/180 (99%)	172 (97%)	6 (3%)	37	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	4	159/162 (98%)	156 (98%)	3 (2%)	57 84
14	N	159/162 (98%)	156 (98%)	3 (2%)	57 84
14	b	159/162 (98%)	153 (96%)	6 (4%)	33 67
14	p	159/162 (98%)	155 (98%)	4 (2%)	47 78
All	All	10392/10768 (96%)	9954 (96%)	438 (4%)	30 63

5 of 438 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	Y	186	ARG
4	f	81	ILE
9	y	102	TYR
12	Z	160	ASN
2	d	24	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 160 such sidechains are listed below:

Mol	Chain	Res	Type
13	a	46	ASN
5	g	143	GLN
10	z	71	ASN
13	a	157	GLN
3	e	91	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	04C	Y	301	11	44,44,44	1.38	5 (11%)	56,58,58	1.09	3 (5%)
15	04C	x	301	8	44,44,44	1.24	3 (6%)	56,58,58	0.91	2 (3%)
15	04C	b	301	14	44,44,44	1.19	2 (4%)	56,58,58	1.01	3 (5%)
15	04C	N	301	14	44,44,44	1.24	3 (6%)	56,58,58	1.07	2 (3%)
15	04C	j	301	8	44,44,44	1.28	5 (11%)	56,58,58	0.84	0
15	04C	m	301	11	44,44,44	1.26	3 (6%)	56,58,58	1.12	2 (3%)
15	04C	V	301	8	44,44,44	1.28	4 (9%)	56,58,58	0.88	2 (3%)
15	04C	H	301	8	44,44,44	1.35	6 (13%)	56,58,58	0.87	1 (1%)
15	04C	K	301	11	44,44,44	1.27	4 (9%)	56,58,58	1.22	2 (3%)
15	04C	4	301	14	44,44,44	1.25	2 (4%)	56,58,58	1.00	3 (5%)
15	04C	1	301	11	44,44,44	1.88	8 (18%)	56,58,58	0.98	3 (5%)
15	04C	p	301	14	44,44,44	1.28	4 (9%)	56,58,58	1.11	4 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	04C	Y	301	11	-	13/44/52/52	0/3/3/3
15	04C	x	301	8	-	10/44/52/52	0/3/3/3
15	04C	b	301	14	-	15/44/52/52	0/3/3/3
15	04C	N	301	14	-	15/44/52/52	0/3/3/3
15	04C	j	301	8	-	15/44/52/52	0/3/3/3
15	04C	m	301	11	-	14/44/52/52	0/3/3/3
15	04C	V	301	8	-	13/44/52/52	0/3/3/3
15	04C	H	301	8	-	14/44/52/52	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	04C	K	301	11	-	12/44/52/52	0/3/3/3
15	04C	4	301	14	-	16/44/52/52	0/3/3/3
15	04C	1	301	11	-	14/44/52/52	0/3/3/3
15	04C	p	301	14	-	14/44/52/52	0/3/3/3

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	301	04C	O45-C44	-8.84	1.19	1.37
15	H	301	04C	C12-C10	3.47	1.56	1.52
15	j	301	04C	C12-C10	3.36	1.56	1.52
15	H	301	04C	C10-C9	3.35	1.59	1.53
15	K	301	04C	C10-C9	3.33	1.59	1.53

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	K	301	04C	C11-C10-C12	-5.42	102.76	109.88
15	p	301	04C	C11-C10-C12	-4.90	103.44	109.88
15	m	301	04C	C11-C10-C12	-4.76	103.62	109.88
15	N	301	04C	C11-C10-C12	-4.75	103.63	109.88
15	Y	301	04C	C6-C7-C8	4.55	121.23	113.33

There are no chirality outliers.

5 of 165 torsion outliers are listed below:

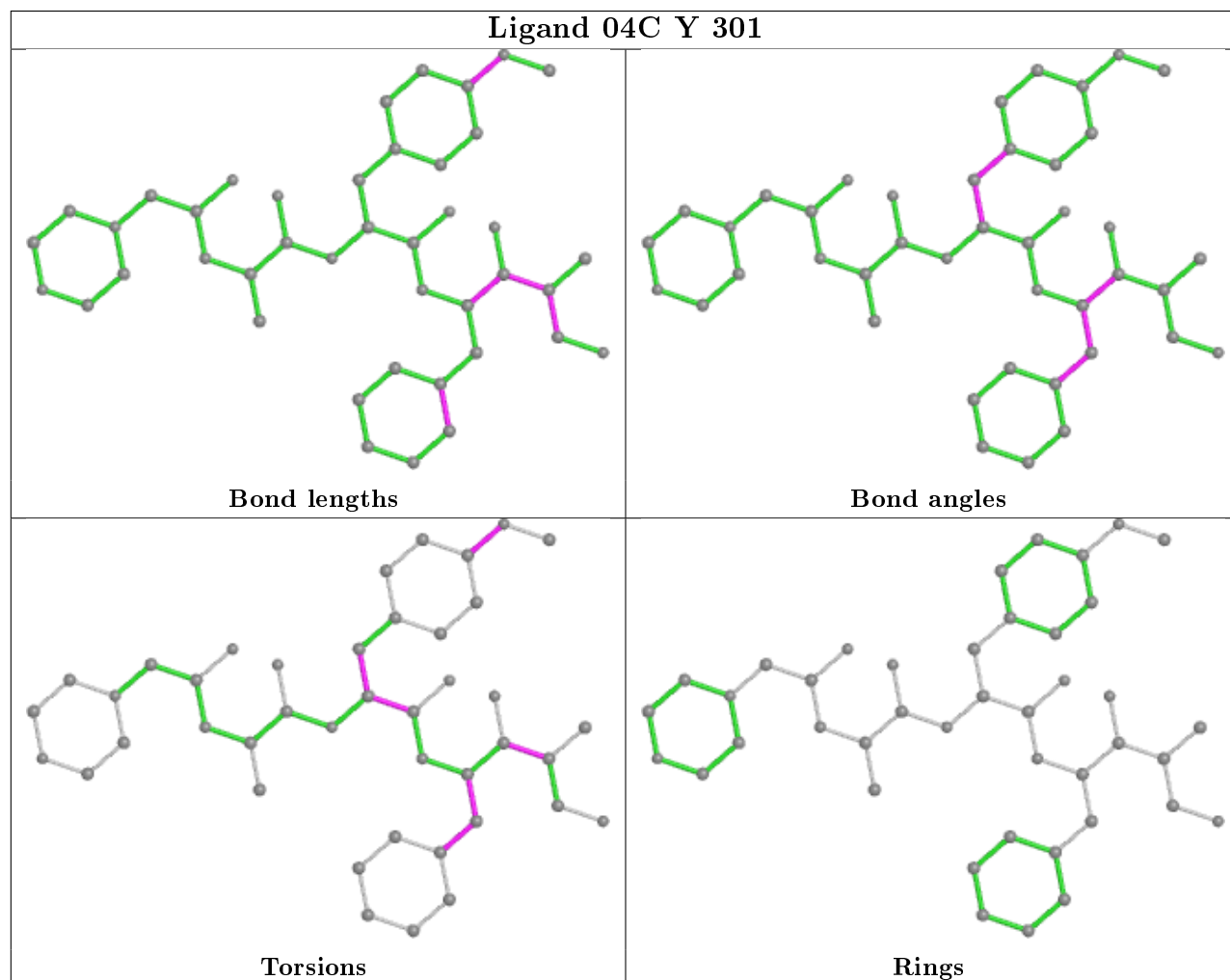
Mol	Chain	Res	Type	Atoms
15	Y	301	04C	C11-C10-C9-C8
15	Y	301	04C	C12-C10-C9-C8
15	x	301	04C	C6-C7-C8-N22
15	x	301	04C	C6-C7-C8-C9
15	x	301	04C	C11-C10-C9-O21

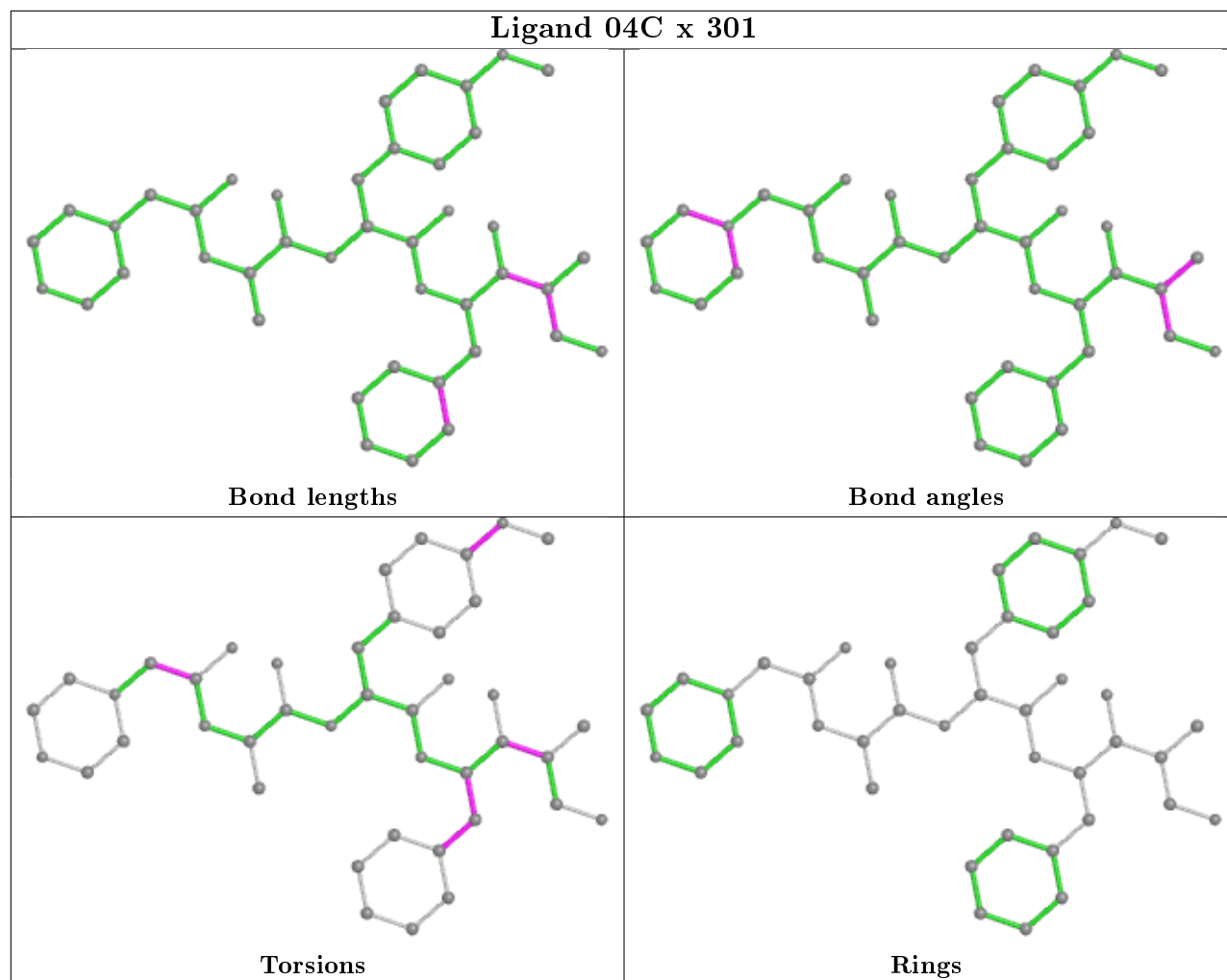
There are no ring outliers.

No monomer is involved in short contacts.

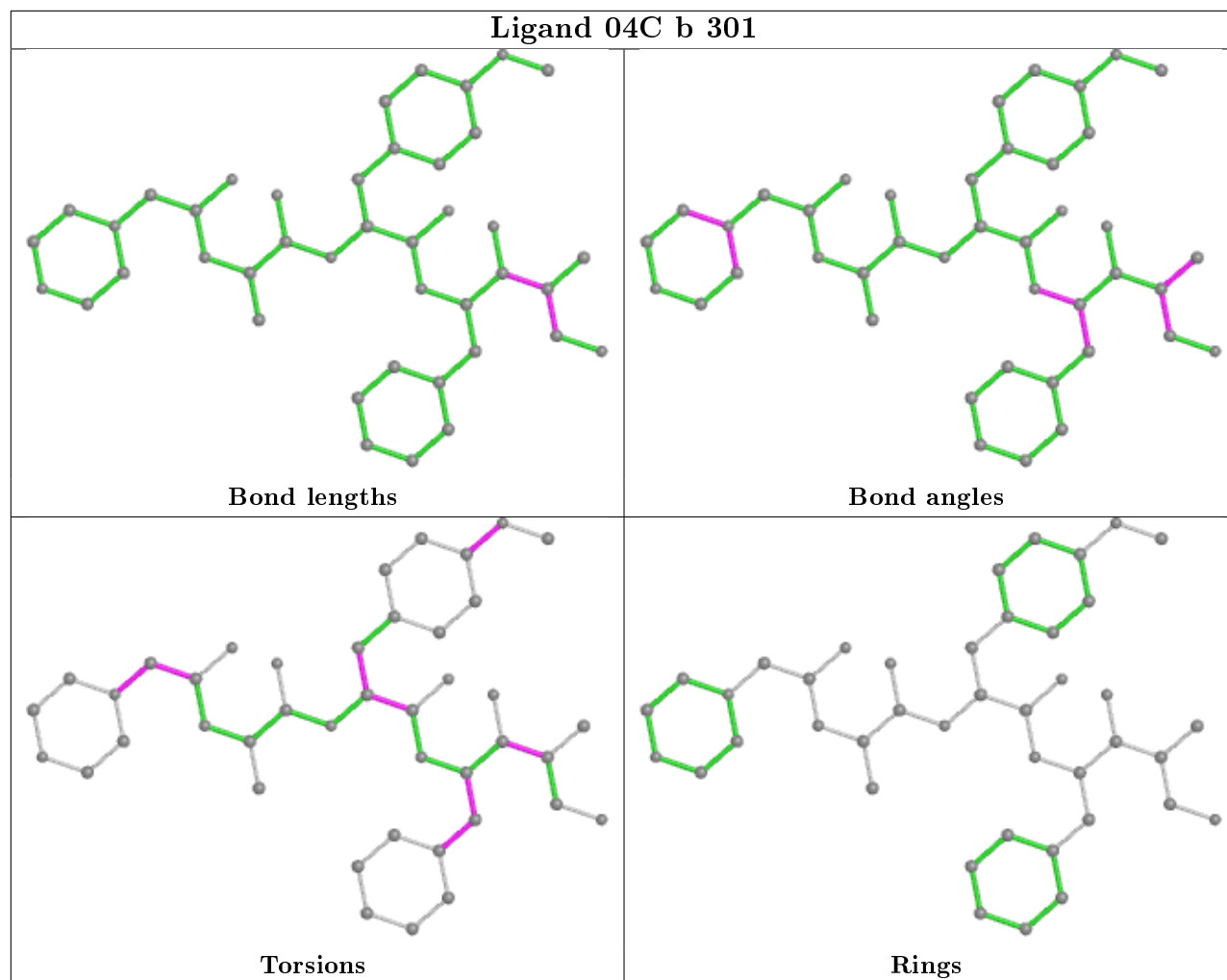
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

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

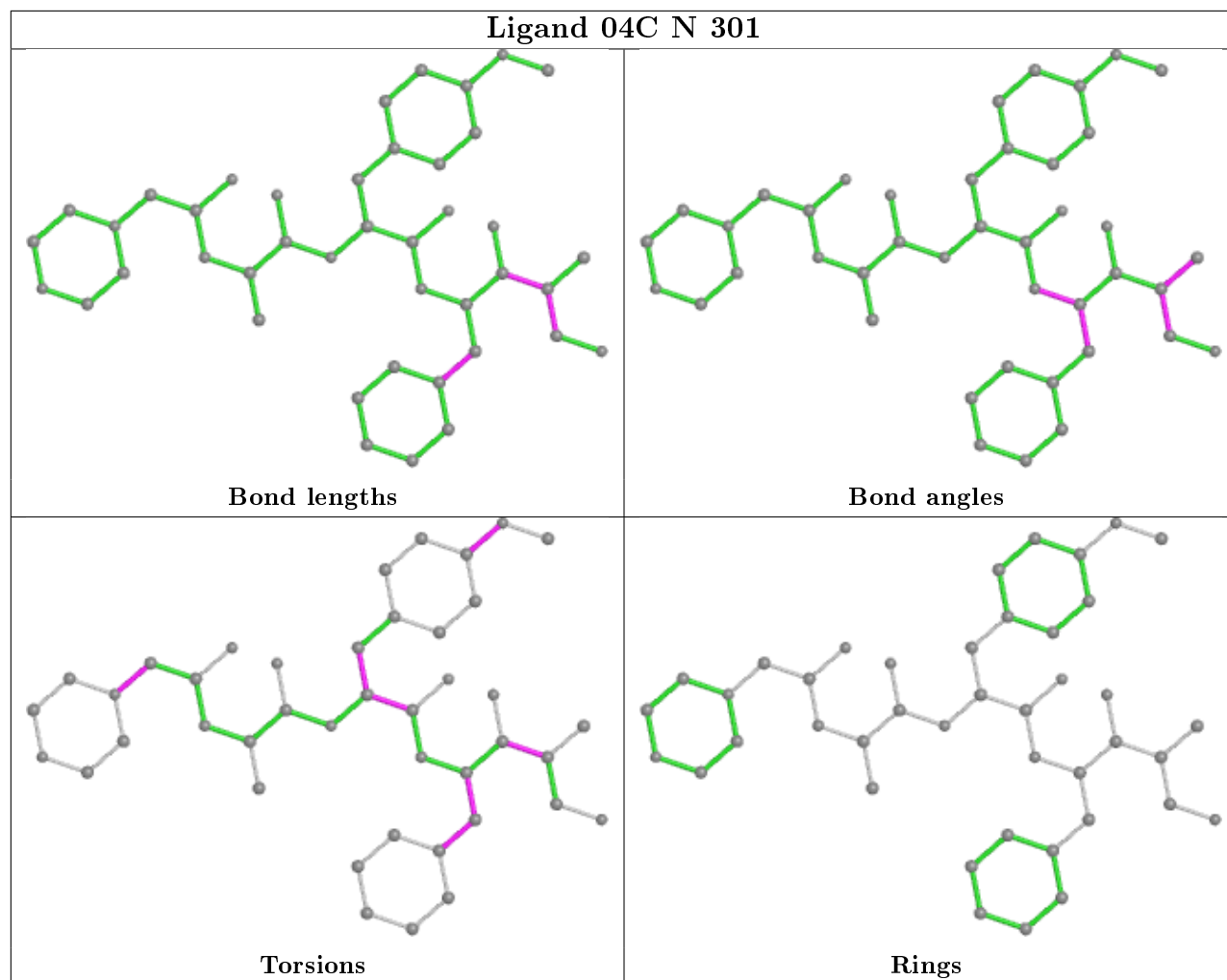


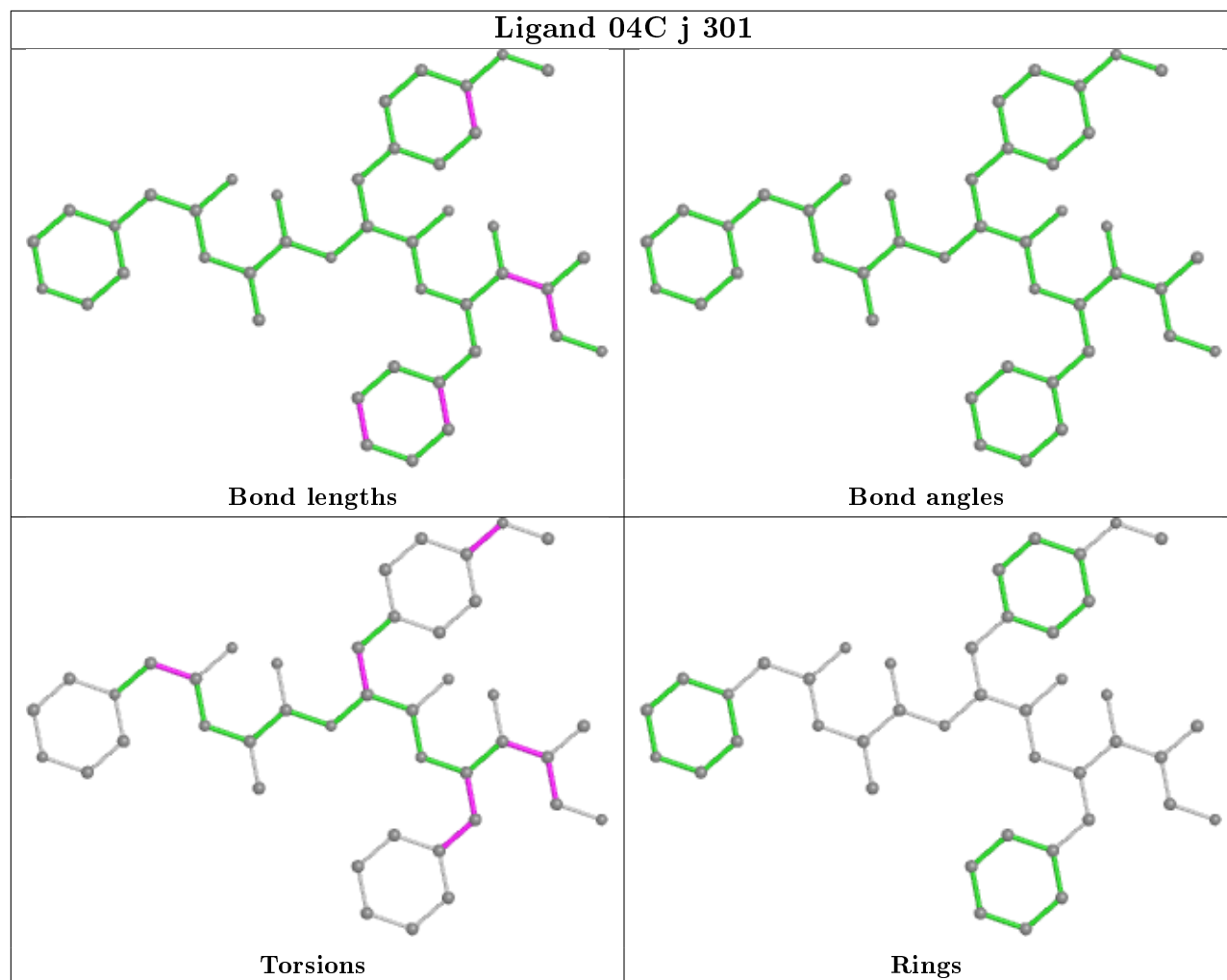


Ligand 04C b 301

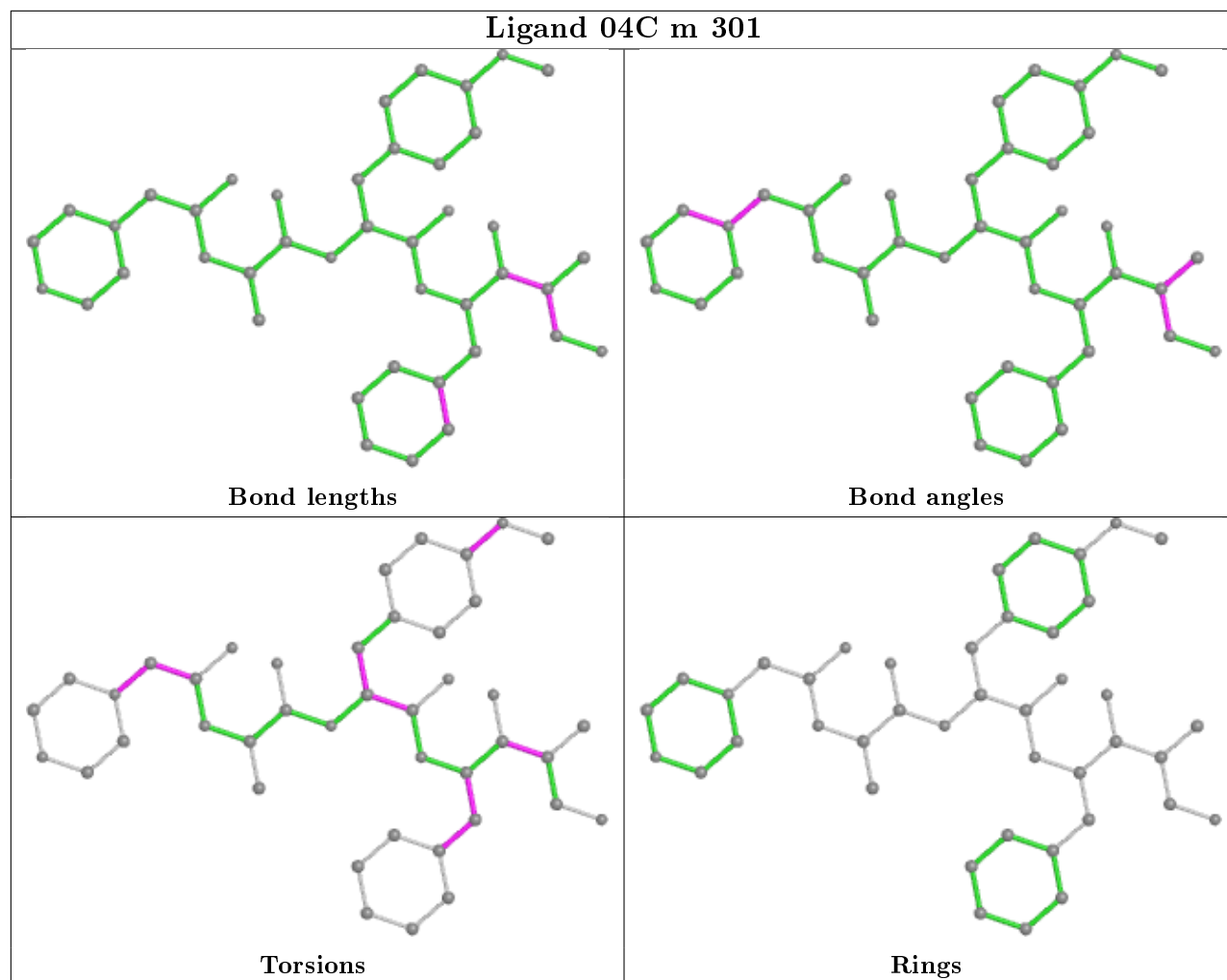


Ligand 04C N 301

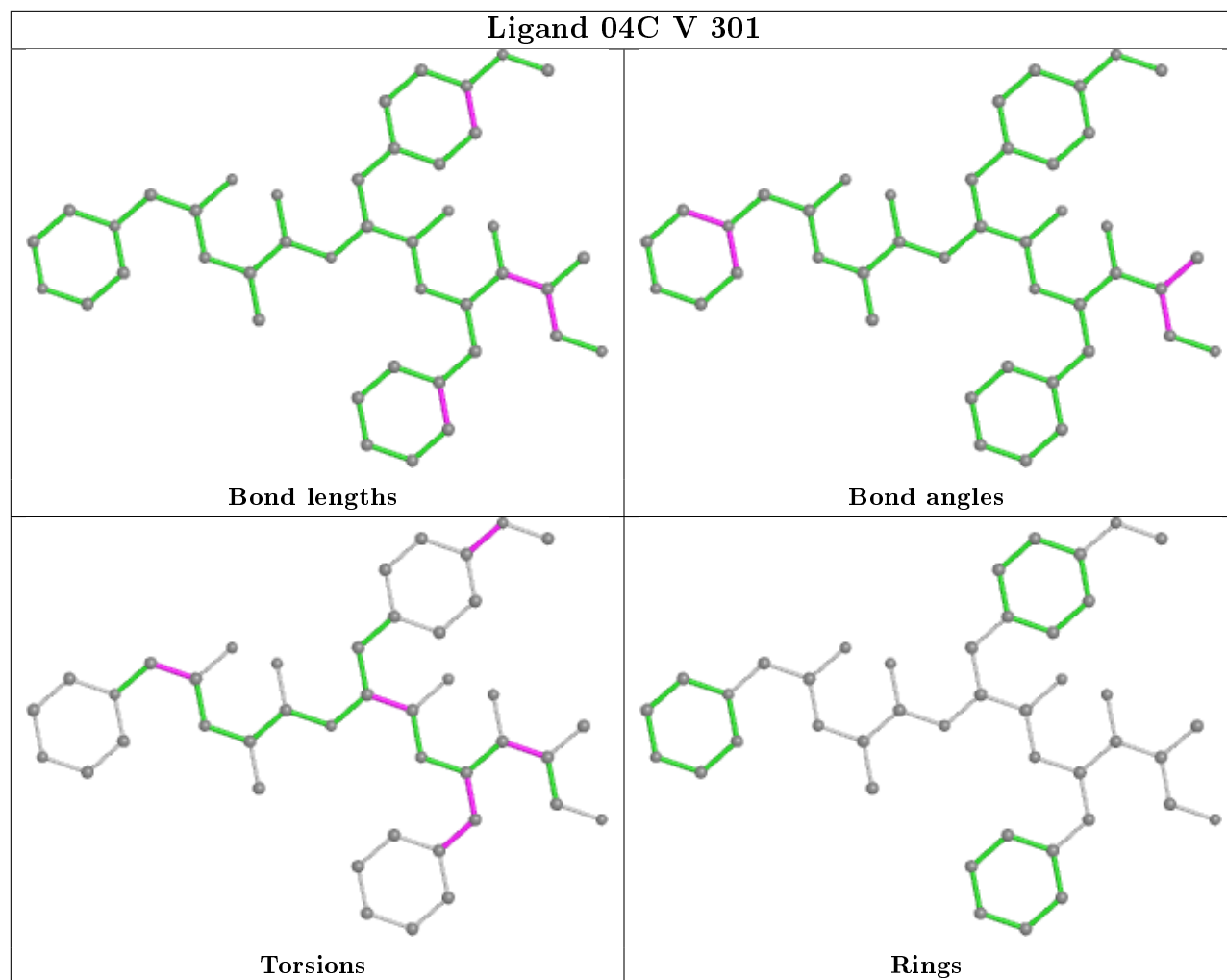


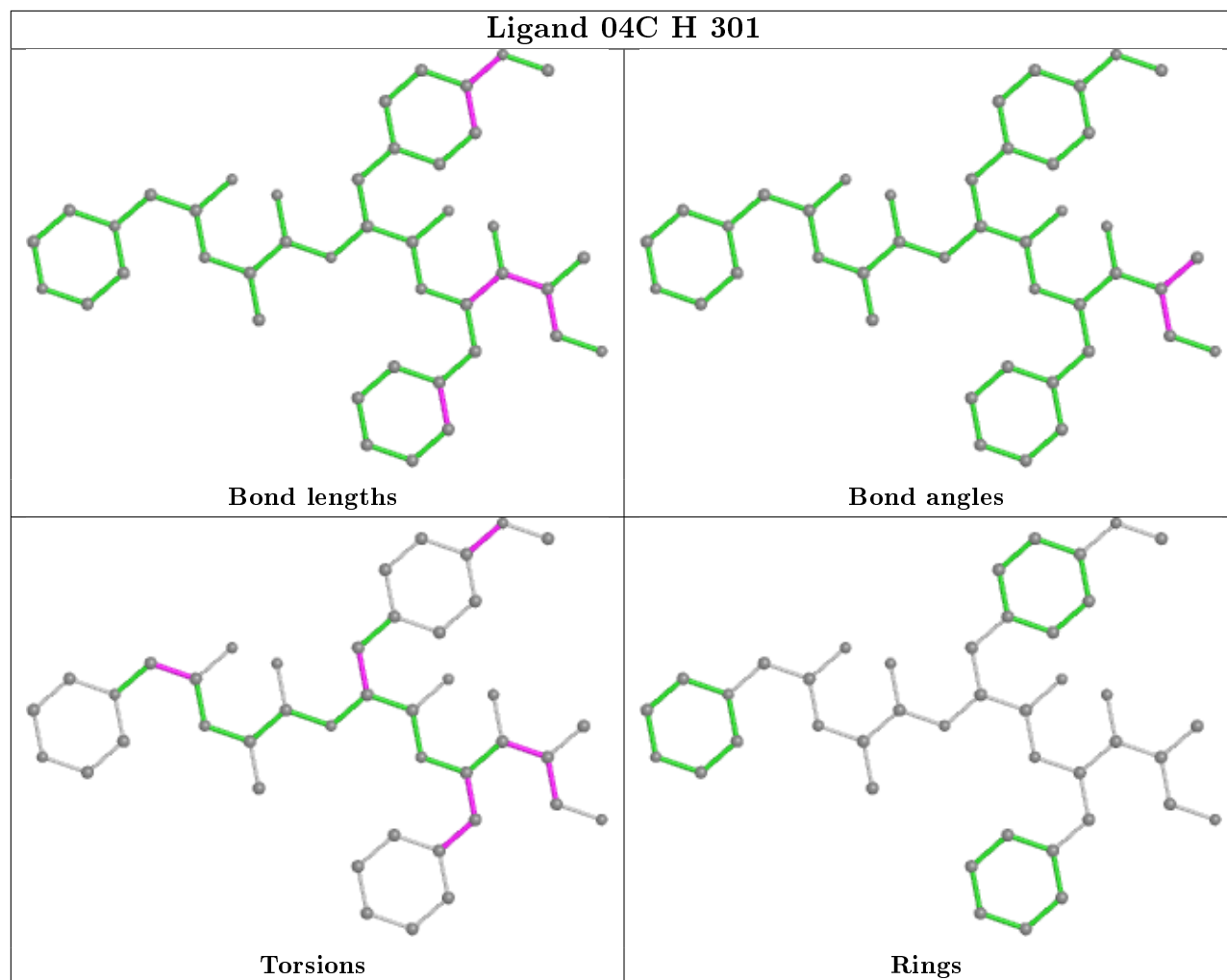


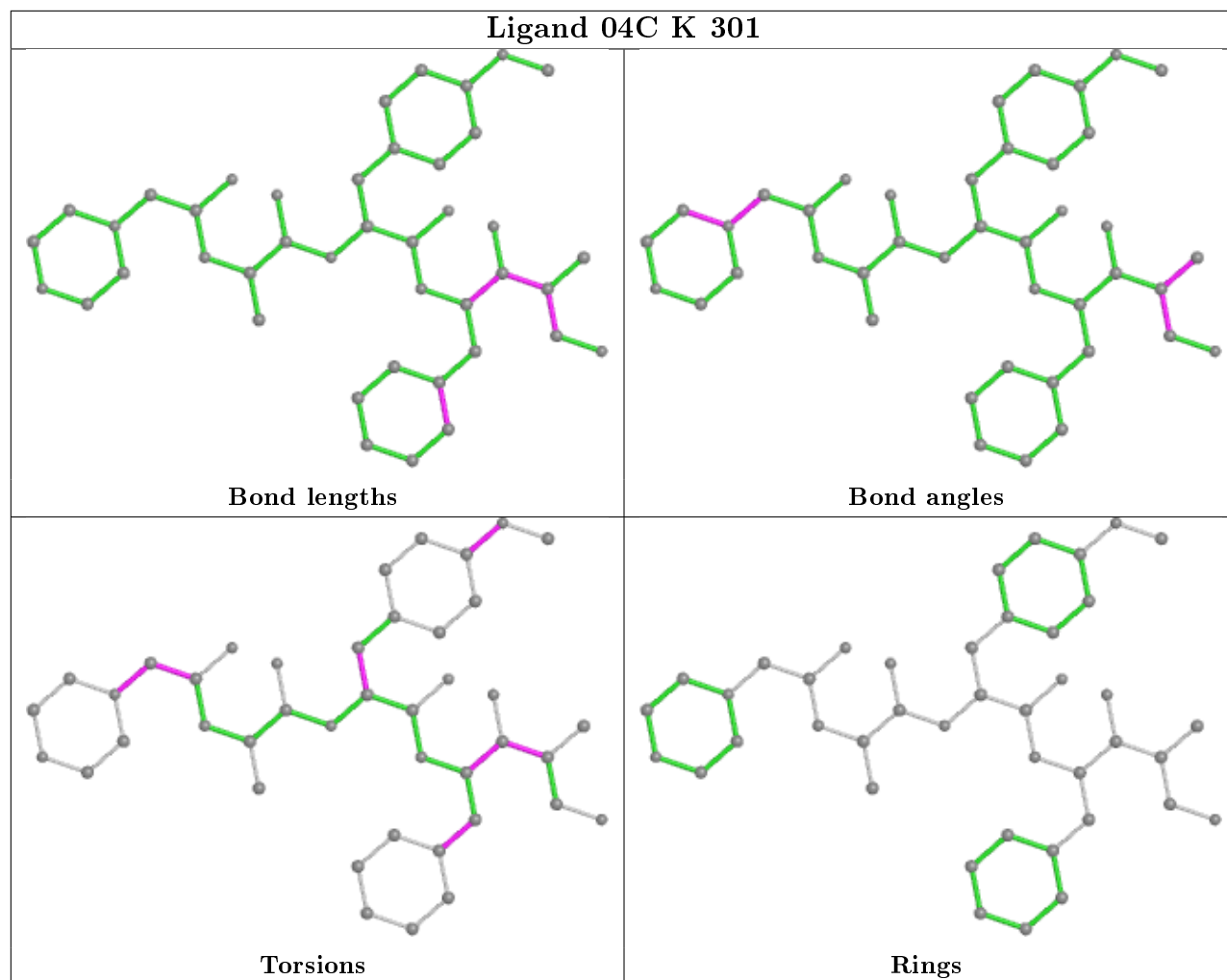
Ligand 04C m 301

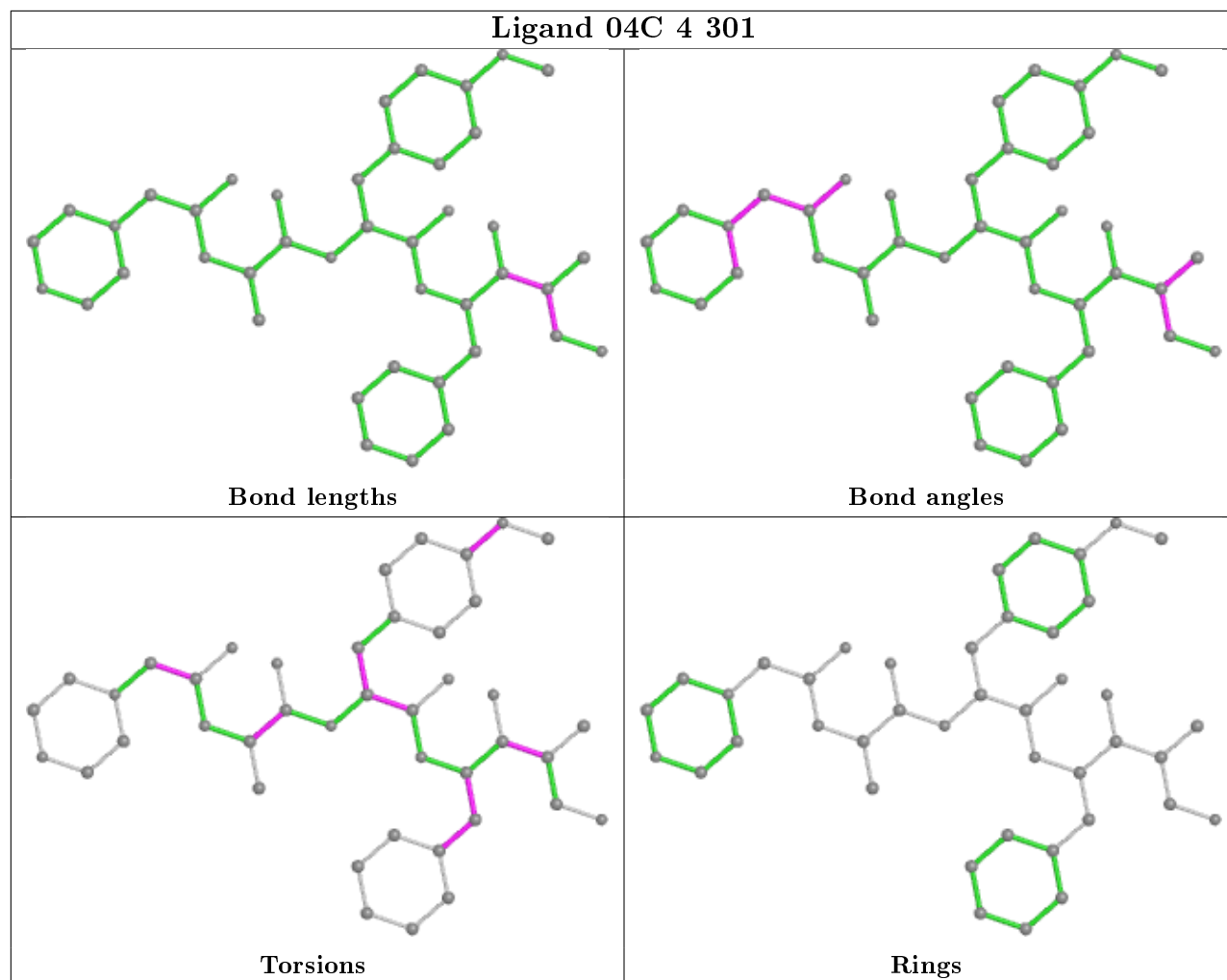


Ligand 04C V 301

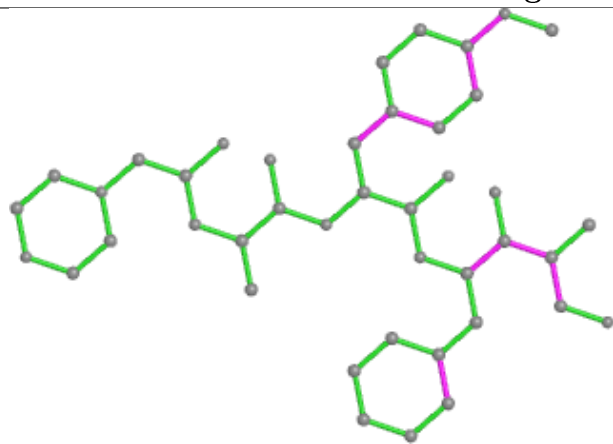




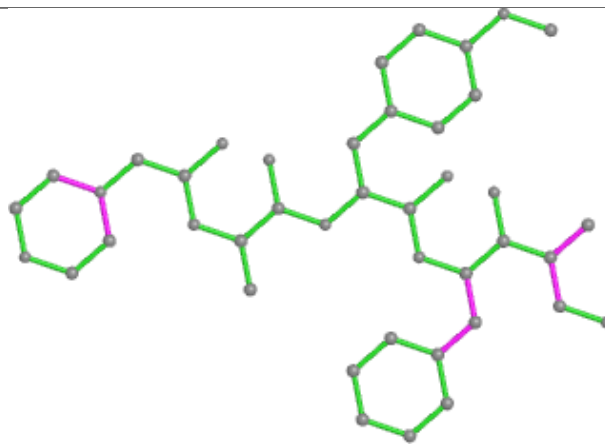




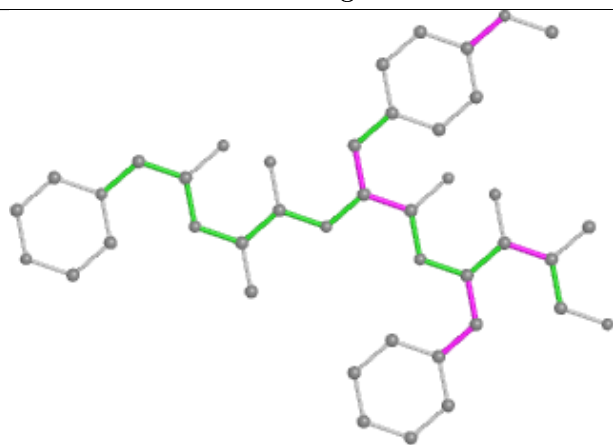
Ligand 04C 1 301



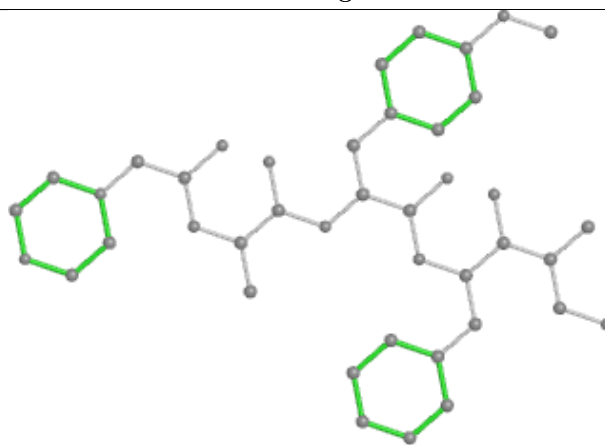
Bond lengths



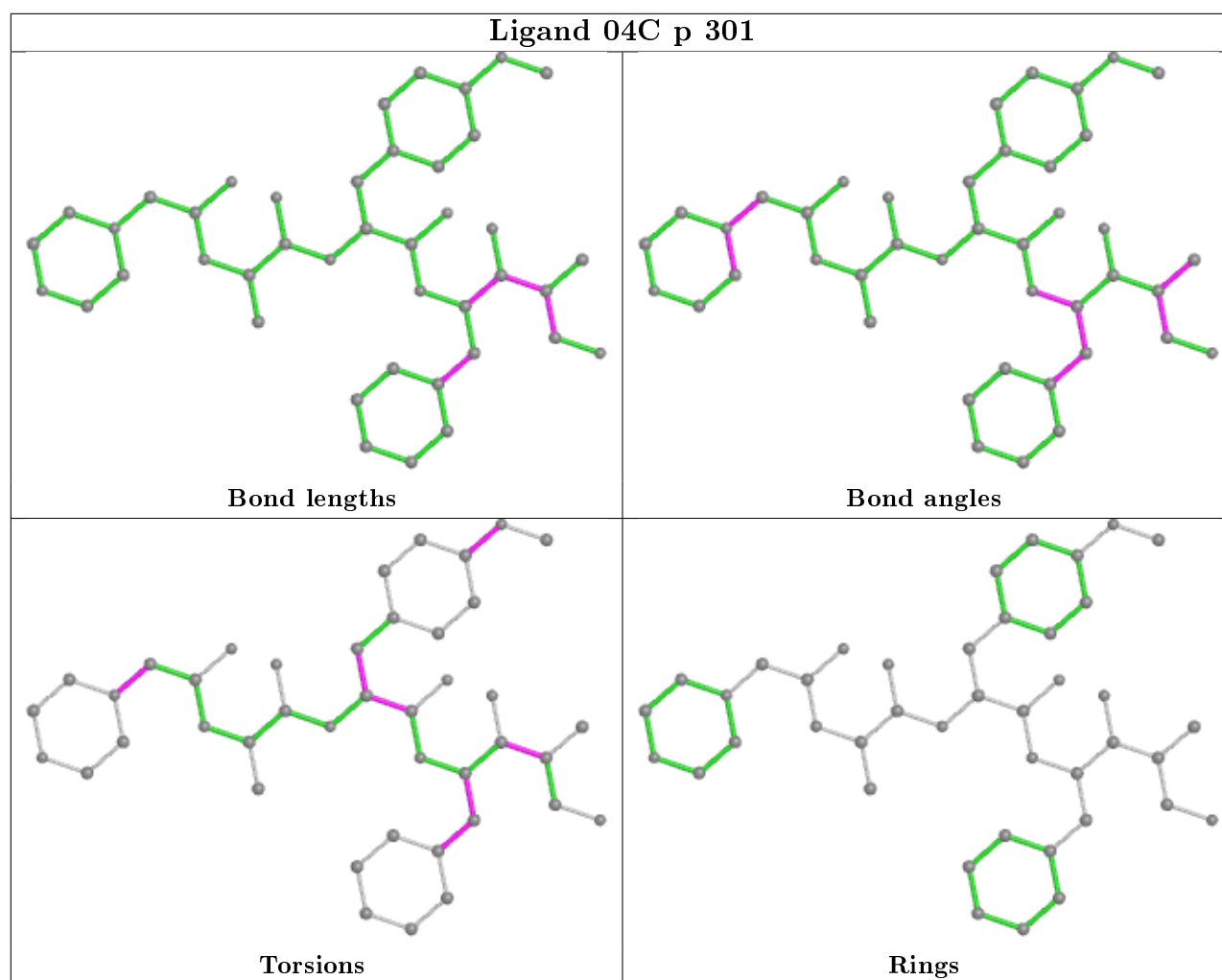
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data (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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	231/234 (98%)	-0.35	3 (1%) 77 77	42, 62, 99, 145	0
1	O	231/234 (98%)	-0.34	3 (1%) 77 77	40, 59, 95, 145	0
1	c	231/234 (98%)	-0.34	3 (1%) 77 77	44, 64, 99, 143	0
1	q	231/234 (98%)	-0.34	3 (1%) 77 77	39, 61, 97, 140	0
2	B	248/261 (95%)	-0.31	2 (0%) 86 86	42, 69, 115, 156	0
2	P	248/261 (95%)	-0.30	2 (0%) 86 86	34, 62, 108, 155	0
2	d	248/261 (95%)	-0.27	2 (0%) 86 86	42, 71, 112, 161	0
2	r	248/261 (95%)	-0.28	1 (0%) 92 93	40, 63, 109, 143	0
3	C	239/248 (96%)	0.16	12 (5%) 28 25	47, 83, 153, 182	0
3	Q	239/248 (96%)	-0.07	0 100 100	42, 74, 129, 163	0
3	e	239/248 (96%)	0.16	11 (4%) 32 29	51, 85, 148, 175	0
3	s	239/248 (96%)	-0.06	0 100 100	45, 75, 129, 164	0
4	D	233/241 (96%)	-0.29	2 (0%) 84 84	50, 74, 104, 149	0
4	R	233/241 (96%)	-0.26	3 (1%) 77 77	43, 72, 108, 163	0
4	f	233/241 (96%)	-0.30	2 (0%) 84 84	47, 75, 108, 158	0
4	t	233/241 (96%)	-0.23	5 (2%) 63 61	47, 73, 111, 171	0
5	E	238/263 (90%)	0.00	7 (2%) 51 47	45, 81, 135, 180	0
5	S	238/263 (90%)	-0.09	5 (2%) 63 61	39, 65, 125, 160	0
5	g	238/263 (90%)	0.04	8 (3%) 45 40	48, 81, 136, 172	0
5	u	238/263 (90%)	-0.06	5 (2%) 63 61	41, 65, 126, 156	0
6	F	244/255 (95%)	-0.01	16 (6%) 18 14	44, 76, 134, 167	0
6	T	244/255 (95%)	-0.21	5 (2%) 65 63	40, 64, 106, 159	0
6	h	244/255 (95%)	0.02	13 (5%) 26 22	47, 77, 135, 156	0
6	v	244/255 (95%)	-0.21	5 (2%) 65 63	39, 65, 110, 158	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
7	G	243/246 (98%)	-0.15	3 (1%) 79 79	42, 68, 108, 161	0
7	U	243/246 (98%)	-0.37	0 100 100	39, 59, 87, 121	0
7	i	243/246 (98%)	-0.13	3 (1%) 79 79	44, 70, 108, 138	0
7	w	243/246 (98%)	-0.40	0 100 100	39, 59, 88, 122	0
8	H	220/234 (94%)	-0.30	0 100 100	24, 52, 91, 127	0
8	V	220/234 (94%)	-0.36	1 (0%) 91 91	23, 49, 89, 126	0
8	j	220/234 (94%)	-0.11	9 (4%) 37 32	27, 54, 113, 146	0
8	x	220/234 (94%)	-0.29	1 (0%) 91 91	33, 54, 91, 127	0
9	I	204/205 (99%)	-0.33	1 (0%) 91 91	40, 55, 87, 119	0
9	W	204/205 (99%)	-0.36	0 100 100	35, 54, 89, 122	0
9	k	204/205 (99%)	-0.31	0 100 100	40, 56, 88, 122	0
9	y	204/205 (99%)	-0.17	4 (1%) 65 63	41, 60, 89, 126	0
10	J	196/201 (97%)	-0.36	1 (0%) 91 91	44, 59, 87, 114	0
10	X	196/201 (97%)	-0.42	0 100 100	40, 58, 85, 107	0
10	l	196/201 (97%)	-0.37	0 100 100	42, 59, 88, 112	0
10	z	196/201 (97%)	-0.37	0 100 100	40, 59, 86, 106	0
11	1	201/205 (98%)	-0.33	1 (0%) 91 91	36, 57, 88, 111	0
11	K	201/205 (98%)	-0.39	1 (0%) 91 91	38, 58, 92, 113	0
11	Y	201/205 (98%)	-0.34	1 (0%) 91 91	35, 56, 86, 109	0
11	m	201/205 (98%)	-0.34	1 (0%) 91 91	40, 59, 92, 117	0
12	2	213/213 (100%)	-0.30	2 (0%) 84 84	36, 57, 84, 135	0
12	L	213/213 (100%)	-0.25	1 (0%) 91 91	40, 56, 90, 123	0
12	Z	213/213 (100%)	-0.35	2 (0%) 84 84	37, 54, 86, 135	0
12	n	213/213 (100%)	-0.22	2 (0%) 84 84	42, 57, 91, 132	0
13	3	216/219 (98%)	-0.30	0 100 100	34, 52, 79, 101	0
13	M	216/219 (98%)	-0.37	0 100 100	36, 53, 82, 115	0
13	a	216/219 (98%)	-0.37	0 100 100	33, 49, 79, 105	0
13	o	216/219 (98%)	-0.32	0 100 100	40, 56, 84, 123	0
14	4	202/205 (98%)	-0.38	3 (1%) 73 73	31, 50, 99, 152	0
14	N	202/205 (98%)	-0.25	4 (1%) 65 63	30, 52, 91, 148	0
14	b	202/205 (98%)	-0.38	3 (1%) 73 73	30, 49, 95, 161	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
14	p	202/205 (98%)	-0.24	4 (1%) 65 63	32, 53, 92, 147	0
All	All	12512/12920 (96%)	-0.24	166 (1%) 77 77	23, 62, 111, 182	0

The worst 5 of 166 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	t	233	ILE	9.0
6	T	1	SER	8.6
6	v	1	SER	8.4
8	j	212	LEU	7.2
14	N	201	THR	6.4

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

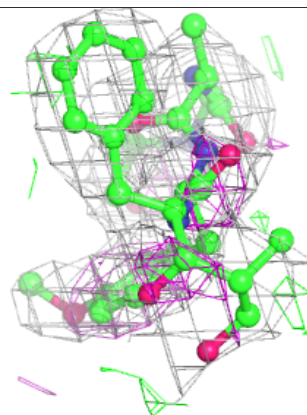
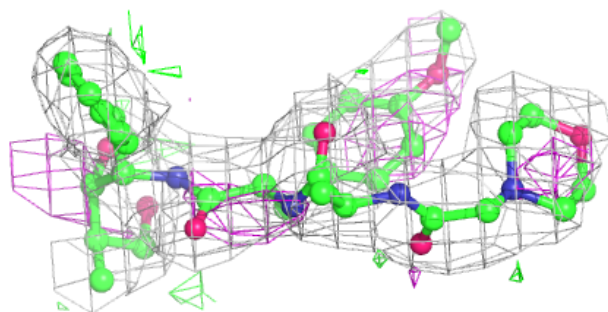
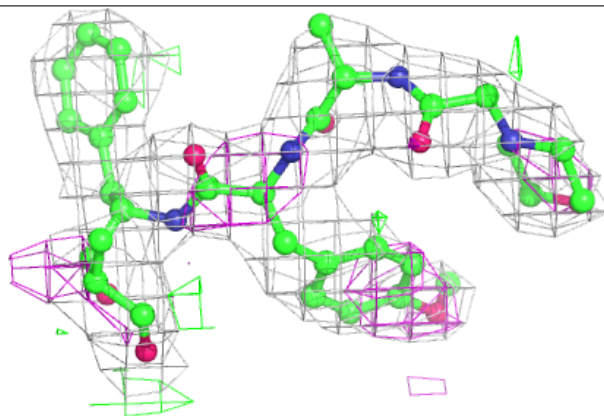
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	04C	4	301	42/42	0.92	0.17	30,39,54,64	0
15	04C	p	301	42/42	0.93	0.18	25,37,63,75	0
15	04C	N	301	42/42	0.94	0.18	24,34,58,70	0
15	04C	m	301	42/42	0.94	0.17	27,42,84,90	0
15	04C	H	301	42/42	0.94	0.14	30,37,50,51	0
15	04C	Y	301	42/42	0.94	0.19	24,41,70,74	0
15	04C	l	301	42/42	0.94	0.19	24,39,71,77	0
15	04C	b	301	42/42	0.94	0.17	28,36,55,65	0
15	04C	V	301	42/42	0.95	0.16	28,40,52,54	0
15	04C	j	301	42/42	0.95	0.15	33,37,50,53	0
15	04C	K	301	42/42	0.95	0.17	24,41,79,87	0
15	04C	x	301	42/42	0.96	0.17	31,40,52,58	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.

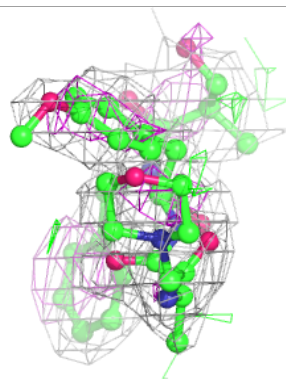
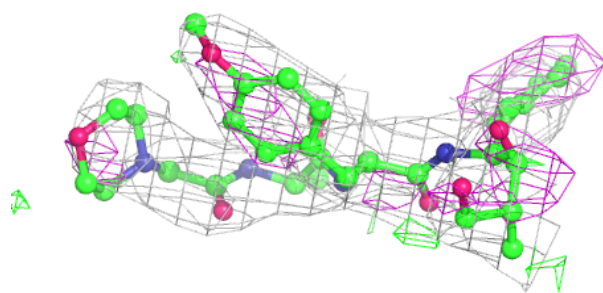
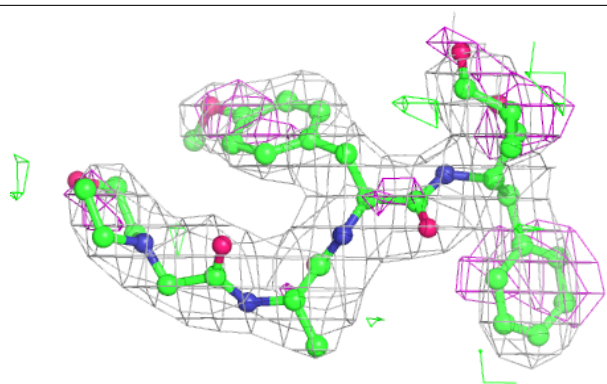
Electron density around 04C 4 301:

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

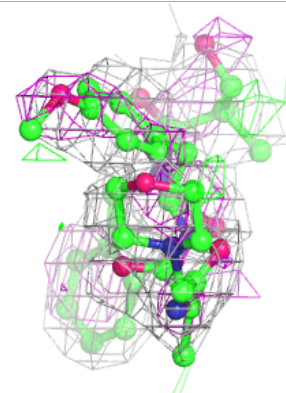
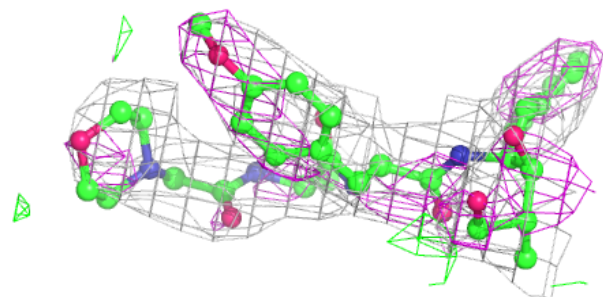
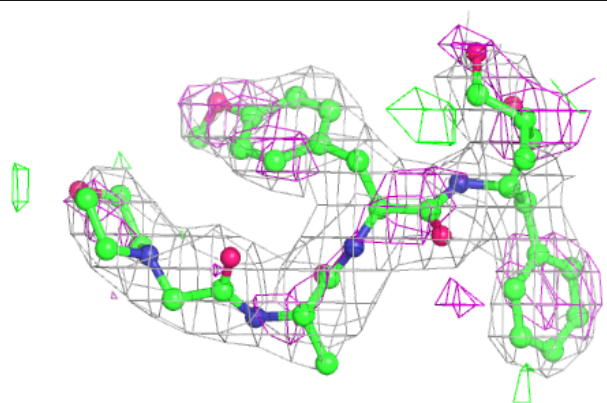


Electron density around 04C p 301:

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

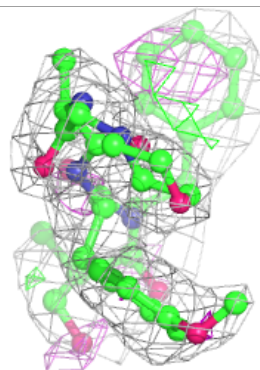
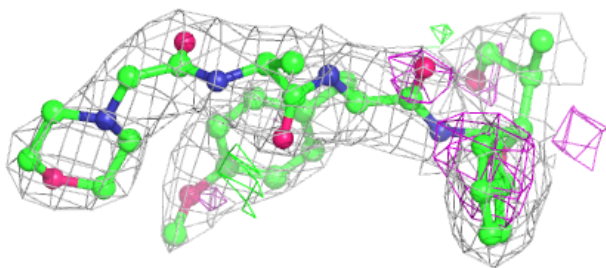
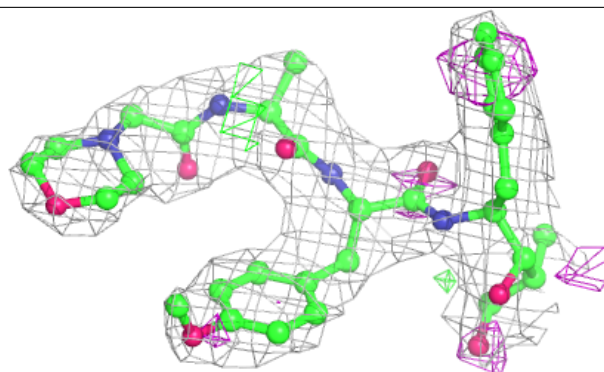
**Electron density around 04C N 301:**

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



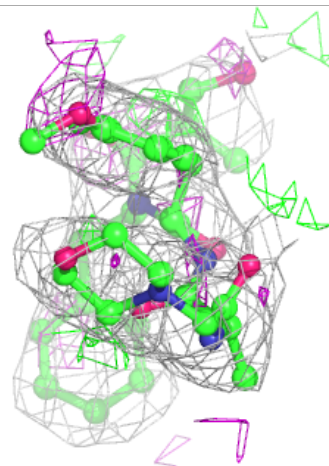
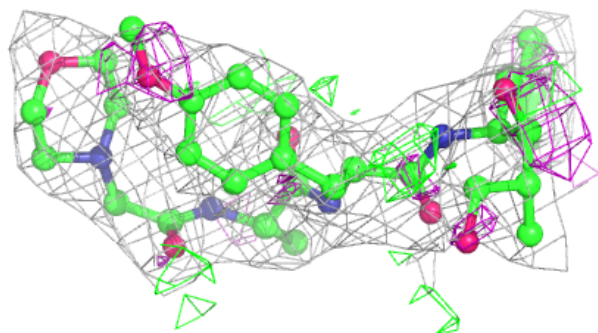
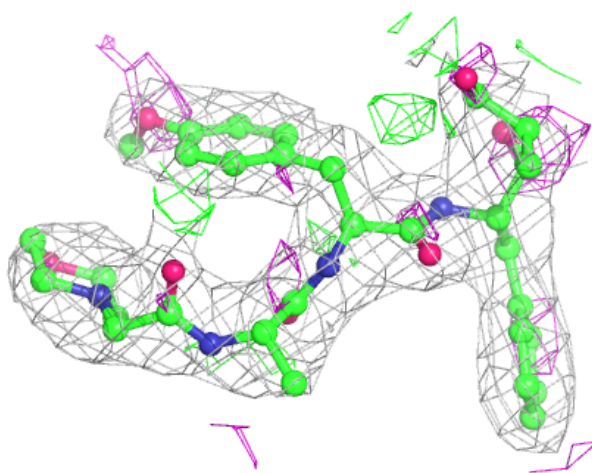
Electron density around 04C m 301:

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



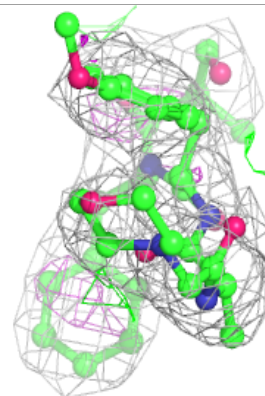
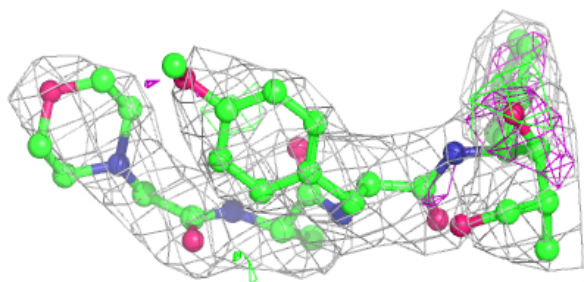
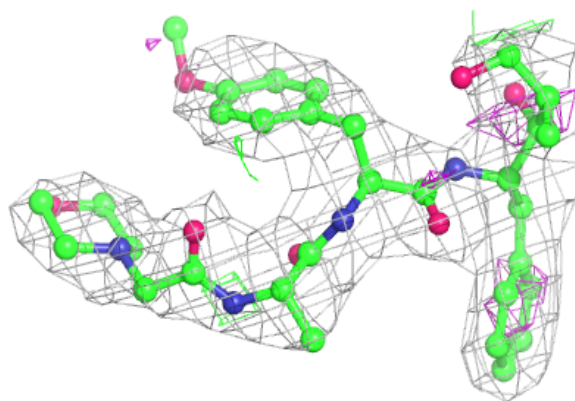
Electron density around 04C H 301:

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

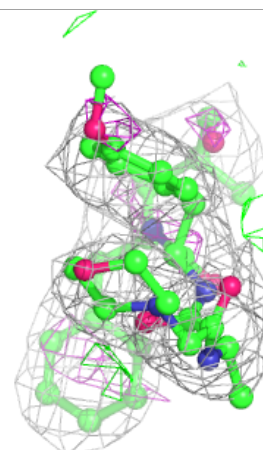
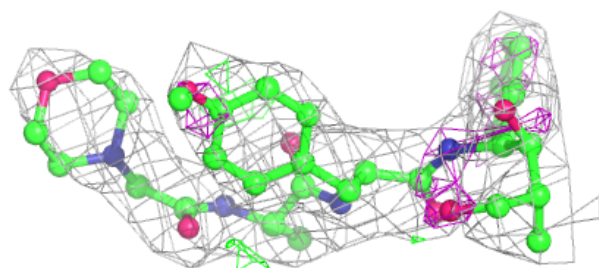
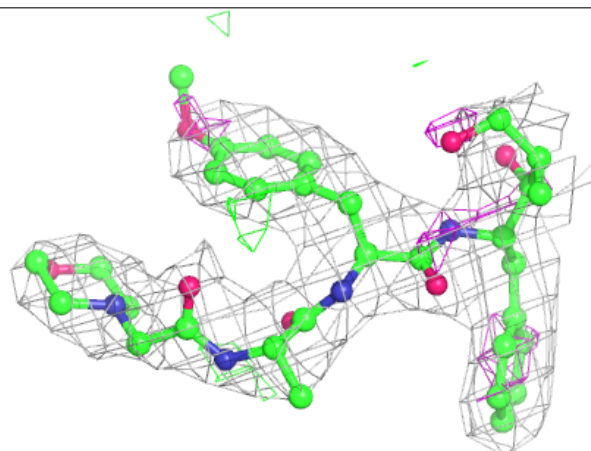


Electron density around 04C Y 301:

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and green (positive)

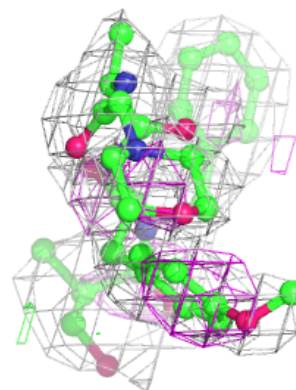
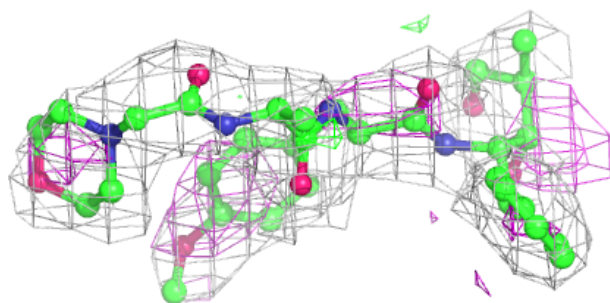
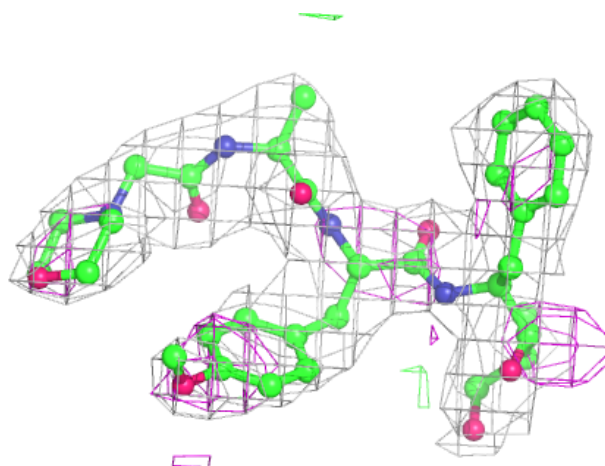
**Electron density around 04C 1 301:**

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



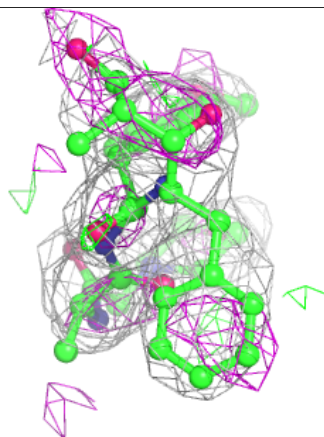
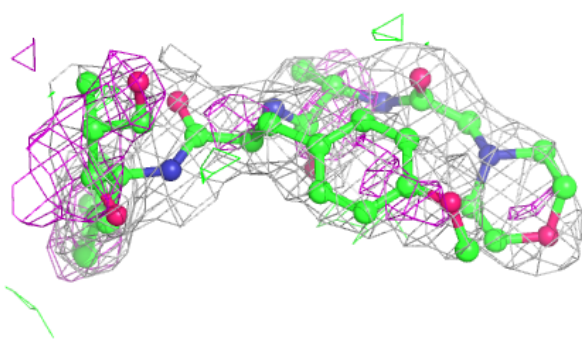
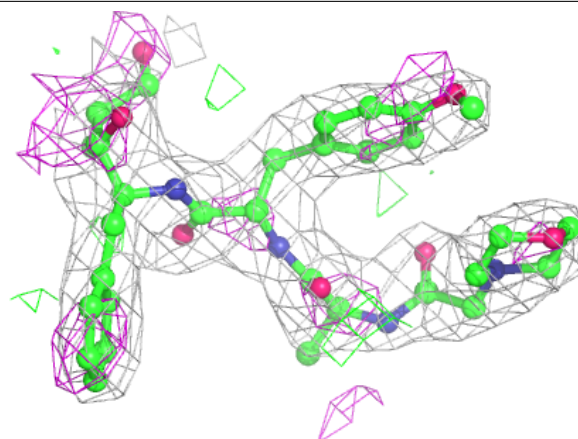
Electron density around 04C b 301:

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



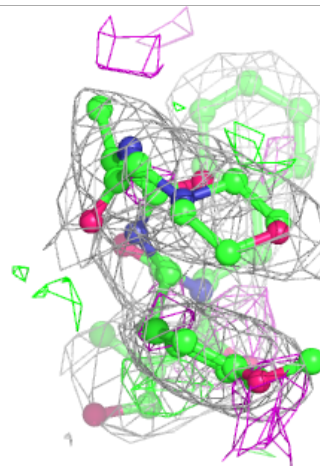
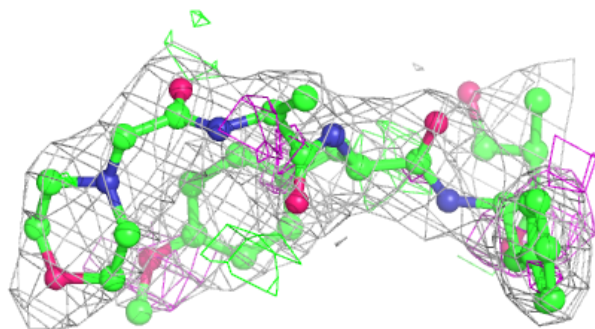
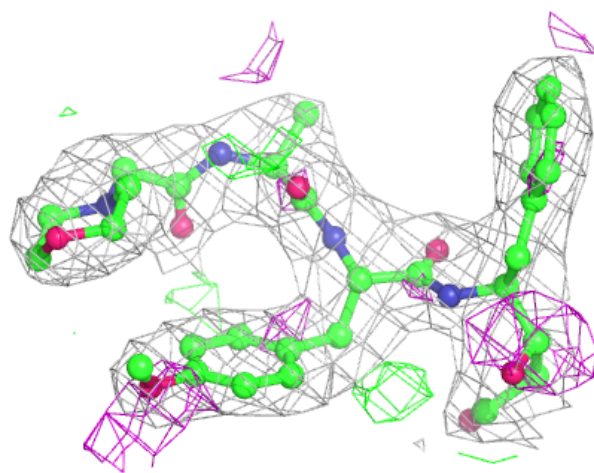
Electron density around 04C V 301:

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



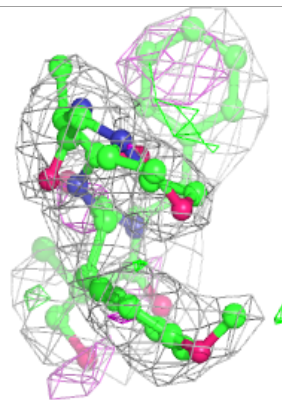
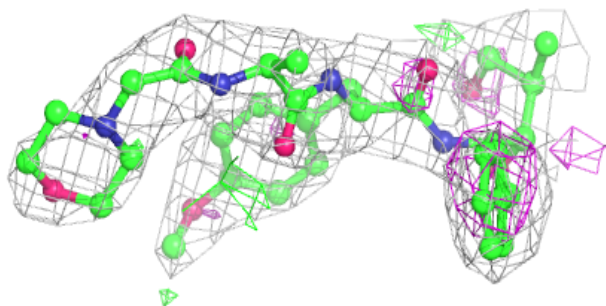
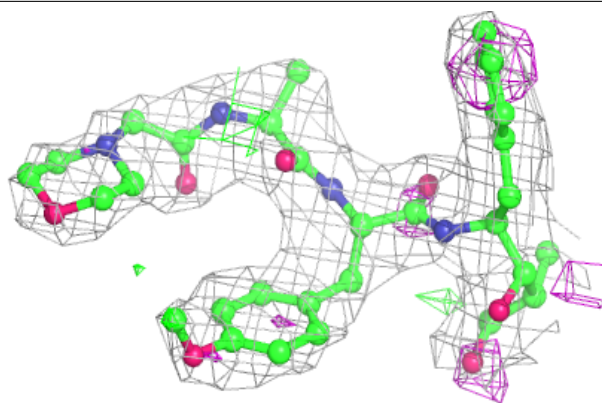
Electron density around 04C j 301:

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

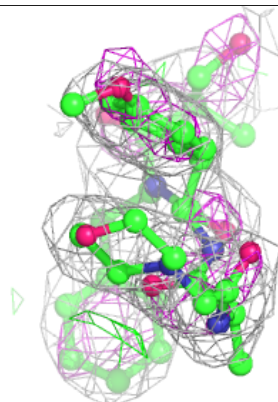
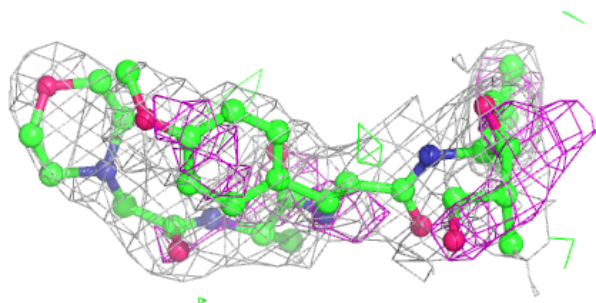
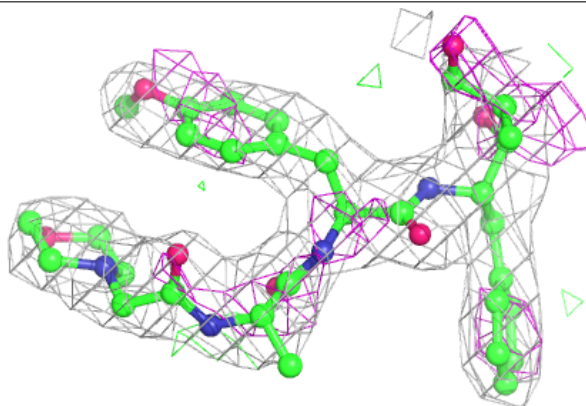


Electron density around 04C K 301:

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

**Electron density around 04C x 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.