



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:37 PM UTC

PDB ID : 4UM3 / pdb_00004um3
Title : Engineered Ls-AChBP with alpha4-alpha4 binding pocket in complex with NS3920
Authors : Shahsavar, A.; Kastrup, J.S.; Balle, T.; Gajhede, M.
Deposited on : 2014-05-14
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (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

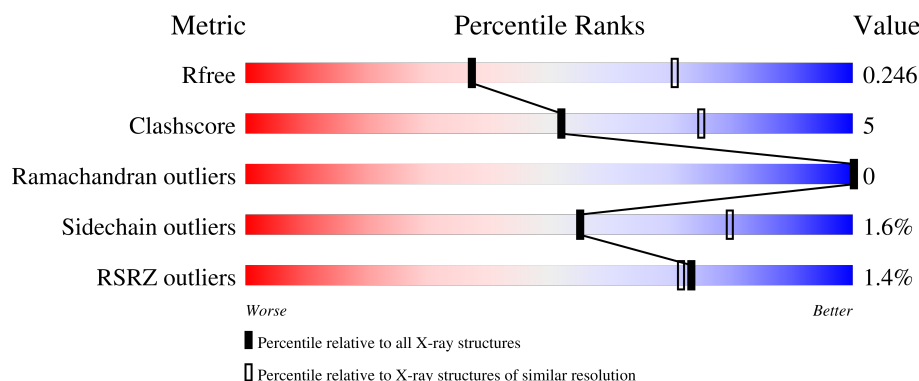
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.



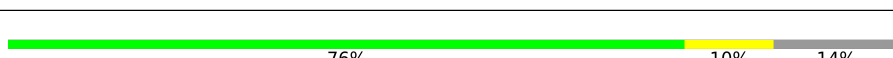
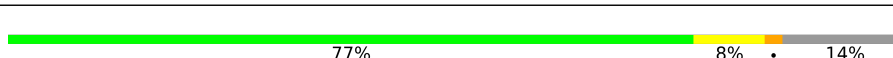
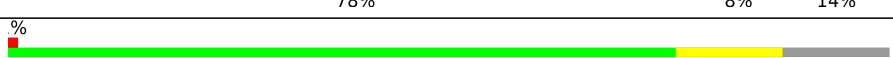
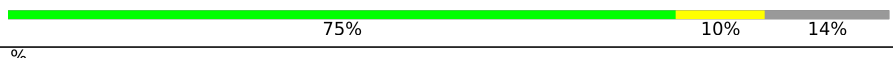
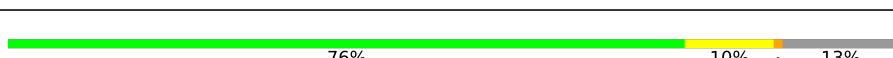
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	229	0% 75% 11% 12%
1	B	229	80% 6% 14%
1	C	229	0% 78% 9% 12%
1	D	229	3% 77% 10% 12%
1	E	229	2% 73% 11% 15%

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Mol	Chain	Length	Quality of chain
1	F	229	
1	G	229	
1	H	229	
1	I	229	
1	J	229	
1	K	229	
1	L	229	
1	M	229	
1	N	229	
1	O	229	
1	Q	229	
1	R	229	
1	T	229	
1	U	229	
1	V	229	
1	W	229	
1	X	229	
1	Y	229	
1	Z	229	
1	a	229	
1	b	229	
1	c	229	
1	d	229	
1	e	229	
1	f	229	

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Mol	Chain	Length	Quality of chain
1	g	229	
1	h	229	
1	i	229	
1	j	229	
1	k	229	
1	l	229	
1	m	229	
1	n	229	
2	P	228	
3	S	229	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	09R	m	301	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 64774 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 ACETYLCHOLINE BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	2	0
			1619	1015	280	320	4			
1	B	198	Total	C	N	O	S	0	0	0
			1578	991	269	314	4			
1	C	201	Total	C	N	O	S	0	0	0
			1608	1007	278	319	4			
1	D	201	Total	C	N	O	S	0	0	0
			1605	1005	275	321	4			
1	E	195	Total	C	N	O	S	0	1	0
			1560	983	265	308	4			
1	F	196	Total	C	N	O	S	0	1	0
			1572	989	270	309	4			
1	G	200	Total	C	N	O	S	0	0	0
			1597	1001	274	318	4			
1	H	197	Total	C	N	O	S	0	0	0
			1567	985	265	313	4			
1	I	200	Total	C	N	O	S	0	1	0
			1603	1005	274	320	4			
1	J	200	Total	C	N	O	S	0	1	0
			1605	1006	277	318	4			
1	K	197	Total	C	N	O	S	0	1	0
			1575	990	268	313	4			
1	L	195	Total	C	N	O	S	0	1	0
			1565	985	268	308	4			
1	M	198	Total	C	N	O	S	0	1	0
			1590	998	272	316	4			
1	N	196	Total	C	N	O	S	0	1	0
			1564	984	264	312	4			
1	O	196	Total	C	N	O	S	0	0	0
			1563	983	264	312	4			
1	Q	196	Total	C	N	O	S	0	2	0
			1574	991	269	310	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	198	Total	C	N	O	S	0	0	0
			1585	995	272	314	4			
1	T	194	Total	C	N	O	S	0	0	0
			1552	978	265	305	4			
1	U	197	Total	C	N	O	S	0	0	0
			1575	990	271	310	4			
1	V	199	Total	C	N	O	S	0	0	0
			1589	997	273	315	4			
1	W	197	Total	C	N	O	S	0	0	0
			1570	987	268	311	4			
1	X	202	Total	C	N	O	S	0	0	0
			1611	1008	276	323	4			
1	Y	197	Total	C	N	O	S	0	0	0
			1567	985	265	313	4			
1	Z	196	Total	C	N	O	S	0	0	0
			1564	984	267	309	4			
1	a	197	Total	C	N	O	S	0	1	0
			1575	990	268	313	4			
1	b	198	Total	C	N	O	S	0	1	0
			1590	999	274	313	4			
1	c	200	Total	C	N	O	S	0	2	0
			1604	1005	273	322	4			
1	d	198	Total	C	N	O	S	0	0	0
			1578	991	269	314	4			
1	e	198	Total	C	N	O	S	0	0	0
			1583	994	272	313	4			
1	f	195	Total	C	N	O	S	0	0	0
			1560	982	266	308	4			
1	g	198	Total	C	N	O	S	0	0	0
			1585	995	272	314	4			
1	h	199	Total	C	N	O	S	0	1	0
			1596	1001	273	318	4			
1	i	197	Total	C	N	O	S	0	0	0
			1567	985	265	313	4			
1	j	198	Total	C	N	O	S	0	0	0
			1585	995	272	314	4			
1	k	198	Total	C	N	O	S	0	0	0
			1578	991	269	314	4			
1	l	200	Total	C	N	O	S	0	0	0
			1597	1001	274	318	4			
1	m	201	Total	C	N	O	S	0	0	0
			1605	1005	275	321	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	n	196	Total	C	N	O	S	0	0	0
			1559	981	264	310	4			

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	HIS	ARG	engineered mutation	UNP P58154
A	112	GLN	LEU	engineered mutation	UNP P58154
A	114	THR	MET	engineered mutation	UNP P58154
B	104	HIS	ARG	engineered mutation	UNP P58154
B	112	GLN	LEU	engineered mutation	UNP P58154
B	114	THR	MET	engineered mutation	UNP P58154
C	104	HIS	ARG	engineered mutation	UNP P58154
C	112	GLN	LEU	engineered mutation	UNP P58154
C	114	THR	MET	engineered mutation	UNP P58154
D	104	HIS	ARG	engineered mutation	UNP P58154
D	112	GLN	LEU	engineered mutation	UNP P58154
D	114	THR	MET	engineered mutation	UNP P58154
E	104	HIS	ARG	engineered mutation	UNP P58154
E	112	GLN	LEU	engineered mutation	UNP P58154
E	114	THR	MET	engineered mutation	UNP P58154
F	104	HIS	ARG	engineered mutation	UNP P58154
F	112	GLN	LEU	engineered mutation	UNP P58154
F	114	THR	MET	engineered mutation	UNP P58154
G	104	HIS	ARG	engineered mutation	UNP P58154
G	112	GLN	LEU	engineered mutation	UNP P58154
G	114	THR	MET	engineered mutation	UNP P58154
H	104	HIS	ARG	engineered mutation	UNP P58154
H	112	GLN	LEU	engineered mutation	UNP P58154
H	114	THR	MET	engineered mutation	UNP P58154
I	104	HIS	ARG	engineered mutation	UNP P58154
I	112	GLN	LEU	engineered mutation	UNP P58154
I	114	THR	MET	engineered mutation	UNP P58154
J	104	HIS	ARG	engineered mutation	UNP P58154
J	112	GLN	LEU	engineered mutation	UNP P58154
J	114	THR	MET	engineered mutation	UNP P58154
K	104	HIS	ARG	engineered mutation	UNP P58154
K	112	GLN	LEU	engineered mutation	UNP P58154
K	114	THR	MET	engineered mutation	UNP P58154
L	104	HIS	ARG	engineered mutation	UNP P58154
L	112	GLN	LEU	engineered mutation	UNP P58154
L	114	THR	MET	engineered mutation	UNP P58154

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Chain	Residue	Modelled	Actual	Comment	Reference
M	104	HIS	ARG	engineered mutation	UNP P58154
M	112	GLN	LEU	engineered mutation	UNP P58154
M	114	THR	MET	engineered mutation	UNP P58154
N	104	HIS	ARG	engineered mutation	UNP P58154
N	112	GLN	LEU	engineered mutation	UNP P58154
N	114	THR	MET	engineered mutation	UNP P58154
O	104	HIS	ARG	engineered mutation	UNP P58154
O	112	GLN	LEU	engineered mutation	UNP P58154
O	114	THR	MET	engineered mutation	UNP P58154
Q	104	HIS	ARG	engineered mutation	UNP P58154
Q	112	GLN	LEU	engineered mutation	UNP P58154
Q	114	THR	MET	engineered mutation	UNP P58154
R	104	HIS	ARG	engineered mutation	UNP P58154
R	112	GLN	LEU	engineered mutation	UNP P58154
R	114	THR	MET	engineered mutation	UNP P58154
T	104	HIS	ARG	engineered mutation	UNP P58154
T	112	GLN	LEU	engineered mutation	UNP P58154
T	114	THR	MET	engineered mutation	UNP P58154
U	104	HIS	ARG	engineered mutation	UNP P58154
U	112	GLN	LEU	engineered mutation	UNP P58154
U	114	THR	MET	engineered mutation	UNP P58154
V	104	HIS	ARG	engineered mutation	UNP P58154
V	112	GLN	LEU	engineered mutation	UNP P58154
V	114	THR	MET	engineered mutation	UNP P58154
W	104	HIS	ARG	engineered mutation	UNP P58154
W	112	GLN	LEU	engineered mutation	UNP P58154
W	114	THR	MET	engineered mutation	UNP P58154
X	104	HIS	ARG	engineered mutation	UNP P58154
X	112	GLN	LEU	engineered mutation	UNP P58154
X	114	THR	MET	engineered mutation	UNP P58154
Y	104	HIS	ARG	engineered mutation	UNP P58154
Y	112	GLN	LEU	engineered mutation	UNP P58154
Y	114	THR	MET	engineered mutation	UNP P58154
Z	104	HIS	ARG	engineered mutation	UNP P58154
Z	112	GLN	LEU	engineered mutation	UNP P58154
Z	114	THR	MET	engineered mutation	UNP P58154
a	104	HIS	ARG	engineered mutation	UNP P58154
a	112	GLN	LEU	engineered mutation	UNP P58154
a	114	THR	MET	engineered mutation	UNP P58154
b	104	HIS	ARG	engineered mutation	UNP P58154
b	112	GLN	LEU	engineered mutation	UNP P58154
b	114	THR	MET	engineered mutation	UNP P58154

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Chain	Residue	Modelled	Actual	Comment	Reference
c	104	HIS	ARG	engineered mutation	UNP P58154
c	112	GLN	LEU	engineered mutation	UNP P58154
c	114	THR	MET	engineered mutation	UNP P58154
d	104	HIS	ARG	engineered mutation	UNP P58154
d	112	GLN	LEU	engineered mutation	UNP P58154
d	114	THR	MET	engineered mutation	UNP P58154
e	104	HIS	ARG	engineered mutation	UNP P58154
e	112	GLN	LEU	engineered mutation	UNP P58154
e	114	THR	MET	engineered mutation	UNP P58154
f	104	HIS	ARG	engineered mutation	UNP P58154
f	112	GLN	LEU	engineered mutation	UNP P58154
f	114	THR	MET	engineered mutation	UNP P58154
g	104	HIS	ARG	engineered mutation	UNP P58154
g	112	GLN	LEU	engineered mutation	UNP P58154
g	114	THR	MET	engineered mutation	UNP P58154
h	104	HIS	ARG	engineered mutation	UNP P58154
h	112	GLN	LEU	engineered mutation	UNP P58154
h	114	THR	MET	engineered mutation	UNP P58154
i	104	HIS	ARG	engineered mutation	UNP P58154
i	112	GLN	LEU	engineered mutation	UNP P58154
i	114	THR	MET	engineered mutation	UNP P58154
j	104	HIS	ARG	engineered mutation	UNP P58154
j	112	GLN	LEU	engineered mutation	UNP P58154
j	114	THR	MET	engineered mutation	UNP P58154
k	104	HIS	ARG	engineered mutation	UNP P58154
k	112	GLN	LEU	engineered mutation	UNP P58154
k	114	THR	MET	engineered mutation	UNP P58154
l	104	HIS	ARG	engineered mutation	UNP P58154
l	112	GLN	LEU	engineered mutation	UNP P58154
l	114	THR	MET	engineered mutation	UNP P58154
m	104	HIS	ARG	engineered mutation	UNP P58154
m	112	GLN	LEU	engineered mutation	UNP P58154
m	114	THR	MET	engineered mutation	UNP P58154
n	104	HIS	ARG	engineered mutation	UNP P58154
n	112	GLN	LEU	engineered mutation	UNP P58154
n	114	THR	MET	engineered mutation	UNP P58154

- Molecule 2 is a protein called ACETYLCHOLINE BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	201	Total	C	N	O	S	0	0	0
			1608	1007	278	319	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	104	HIS	ARG	engineered mutation	UNP P58154
P	112	GLN	LEU	engineered mutation	UNP P58154
P	114	THR	MET	engineered mutation	UNP P58154
P	?	-	ASP	deletion	UNP P58154

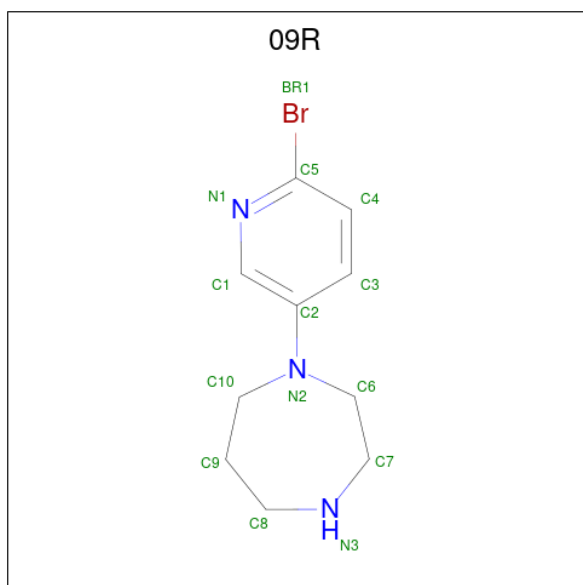
- Molecule 3 is a protein called ACETYLCHOLINE BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	201	Total	C	N	O	S	0	0	0
			1603	1004	276	319	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	104	HIS	ARG	engineered mutation	UNP P58154
S	112	GLN	LEU	engineered mutation	UNP P58154
S	114	THR	MET	engineered mutation	UNP P58154
S	131	GLN	GLU	conflict	UNP P58154

- Molecule 4 is 1-(6-bromopyridin-3-yl)-1,4-diazepane (CCD ID: 09R) (formula: C₁₀H₁₄BrN₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Br	C	N	0	0
			14	1	10	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	Br	C	N	0	0
			14	1	10	3		
4	C	1	Total	Br	C	N	0	0
			14	1	10	3		
4	D	1	Total	Br	C	N	0	0
			14	1	10	3		
4	E	1	Total	Br	C	N	0	0
			14	1	10	3		
4	F	1	Total	Br	C	N	0	0
			14	1	10	3		
4	G	1	Total	Br	C	N	0	0
			14	1	10	3		
4	H	1	Total	Br	C	N	0	0
			14	1	10	3		
4	I	1	Total	Br	C	N	0	0
			14	1	10	3		
4	J	1	Total	Br	C	N	0	0
			14	1	10	3		
4	K	1	Total	Br	C	N	0	0
			14	1	10	3		
4	L	1	Total	Br	C	N	0	0
			14	1	10	3		
4	M	1	Total	Br	C	N	0	0
			14	1	10	3		
4	N	1	Total	Br	C	N	0	0
			14	1	10	3		
4	O	1	Total	Br	C	N	0	0
			14	1	10	3		
4	P	1	Total	Br	C	N	0	0
			14	1	10	3		
4	Q	1	Total	Br	C	N	0	0
			14	1	10	3		
4	R	1	Total	Br	C	N	0	0
			14	1	10	3		
4	S	1	Total	Br	C	N	0	0
			14	1	10	3		
4	T	1	Total	Br	C	N	0	0
			14	1	10	3		
4	U	1	Total	Br	C	N	0	0
			14	1	10	3		
4	V	1	Total	Br	C	N	0	0
			14	1	10	3		

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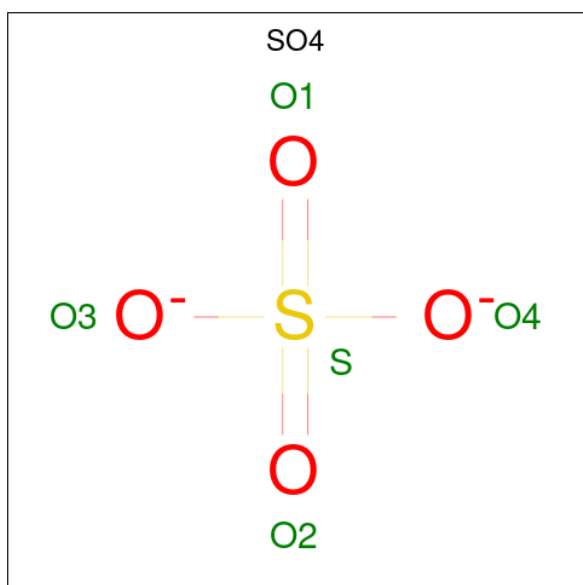
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	W	1	Total	Br	C	N	0	0
			14	1	10	3		
4	X	1	Total	Br	C	N	0	0
			14	1	10	3		
4	Y	1	Total	Br	C	N	0	0
			14	1	10	3		
4	Z	1	Total	Br	C	N	0	0
			14	1	10	3		
4	a	1	Total	Br	C	N	0	0
			14	1	10	3		
4	b	1	Total	Br	C	N	0	0
			14	1	10	3		
4	c	1	Total	Br	C	N	0	0
			14	1	10	3		
4	d	1	Total	Br	C	N	0	0
			14	1	10	3		
4	f	1	Total	Br	C	N	0	0
			14	1	10	3		
4	f	1	Total	Br	C	N	0	0
			14	1	10	3		
4	g	1	Total	Br	C	N	0	0
			14	1	10	3		
4	h	1	Total	Br	C	N	0	0
			14	1	10	3		
4	i	1	Total	Br	C	N	0	0
			14	1	10	3		
4	j	1	Total	Br	C	N	0	0
			14	1	10	3		
4	k	1	Total	Br	C	N	0	0
			14	1	10	3		
4	l	1	Total	Br	C	N	0	0
			14	1	10	3		
4	m	1	Total	Br	C	N	0	0
			14	1	10	3		
4	n	1	Total	Br	C	N	0	0
			14	1	10	3		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	O	1	Total	C	N	O	0	0
			14	8	1	5		
5	d	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	V	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	41	Total O 41 41	0	0
7	B	31	Total O 31 31	0	0
7	C	25	Total O 25 25	0	0
7	D	26	Total O 26 26	0	0
7	E	25	Total O 25 25	0	0
7	F	29	Total O 29 29	0	0
7	G	29	Total O 29 29	0	0
7	H	22	Total O 22 22	0	0
7	I	28	Total O 28 28	0	0
7	J	37	Total O 37 37	0	0
7	K	29	Total O 29 29	0	0
7	L	23	Total O 23 23	0	0
7	M	19	Total O 19 19	0	0
7	N	21	Total O 21 21	0	0
7	O	30	Total O 30 30	0	0
7	P	40	Total O 40 40	0	0
7	Q	37	Total O 37 37	0	0
7	R	27	Total O 27 27	0	0
7	S	28	Total O 28 28	0	0
7	T	31	Total O 31 31	0	0
7	U	30	Total O 30 30	0	0

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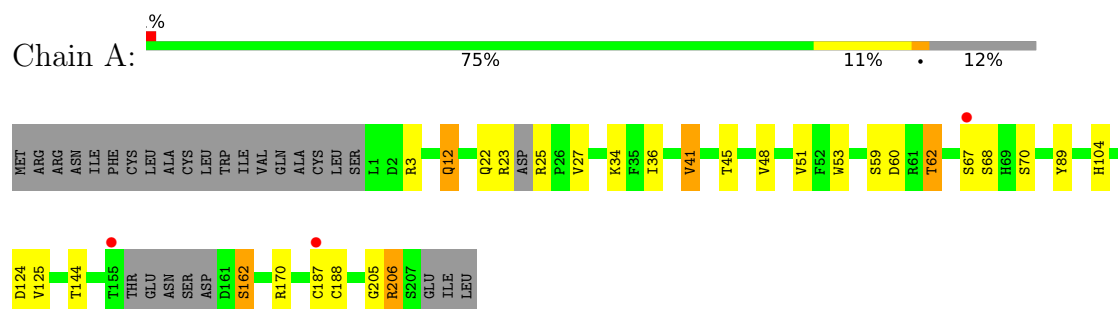
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	V	44	Total 44	O 44	0	0
7	W	28	Total 28	O 28	0	0
7	X	28	Total 28	O 28	0	0
7	Y	16	Total 16	O 16	0	0
7	Z	23	Total 23	O 23	0	0
7	a	16	Total 16	O 16	0	0
7	b	9	Total 9	O 9	0	0
7	c	3	Total 3	O 3	0	0
7	d	19	Total 19	O 19	0	0
7	e	3	Total 3	O 3	0	0
7	f	2	Total 2	O 2	0	0
7	g	1	Total 1	O 1	0	0
7	h	7	Total 7	O 7	0	0
7	i	5	Total 5	O 5	0	0
7	j	2	Total 2	O 2	0	0
7	k	7	Total 7	O 7	0	0
7	l	6	Total 6	O 6	0	0
7	m	2	Total 2	O 2	0	0
7	n	7	Total 7	O 7	0	0

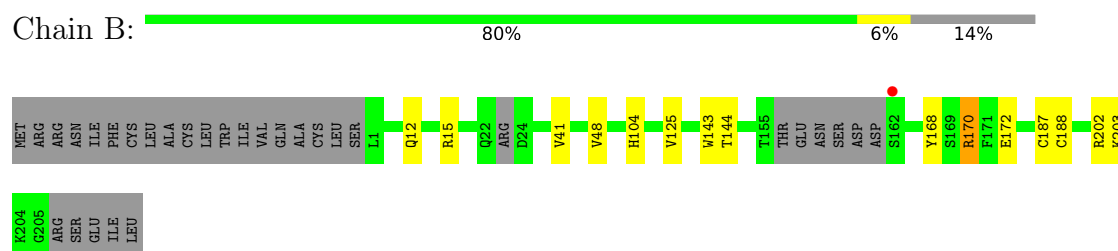
3 Residue-property plots [i](#)

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.

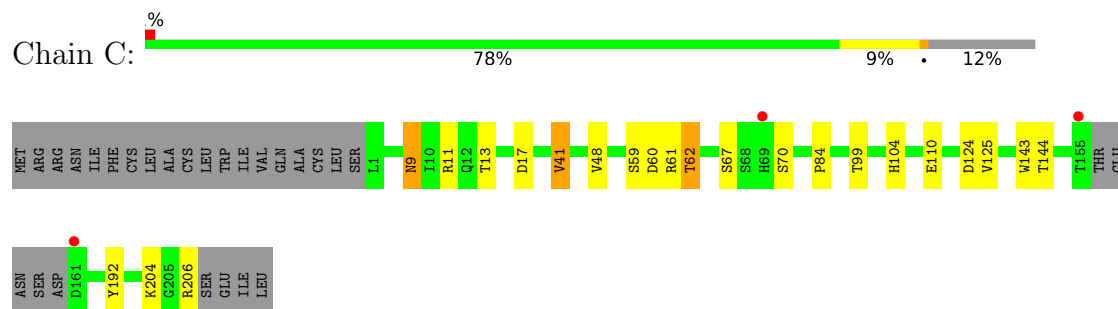
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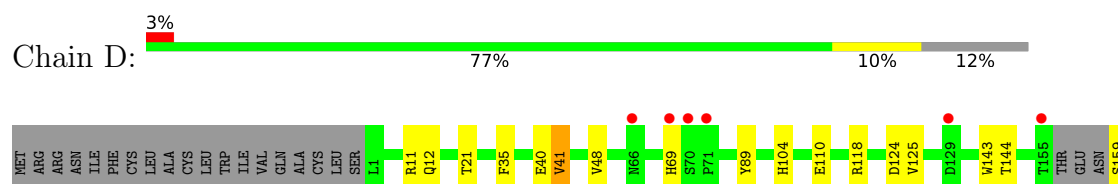
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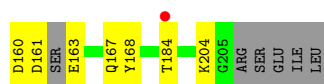


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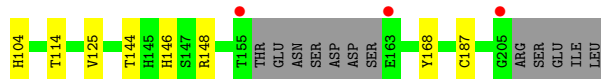
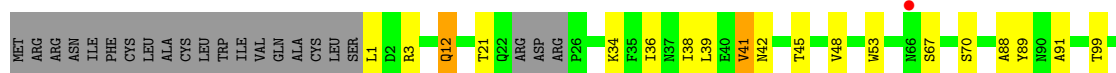


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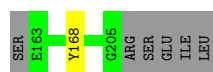
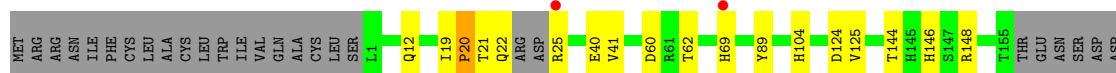
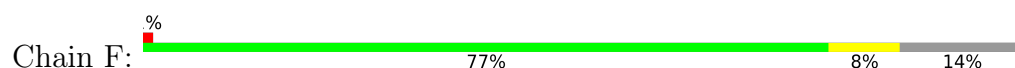




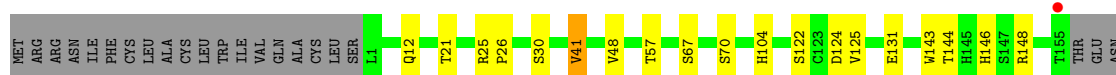
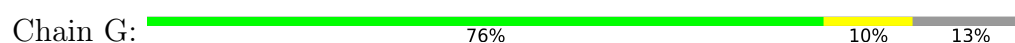
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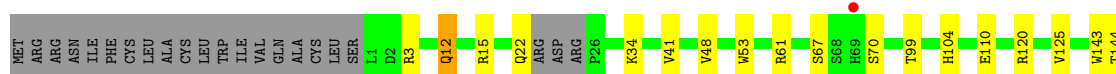
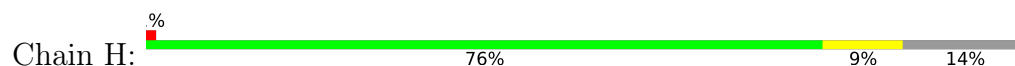
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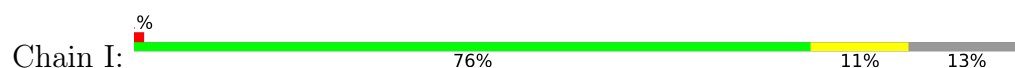
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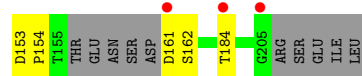


● Molecule 1: ACETYLCHOLINE BINDING PROTEIN

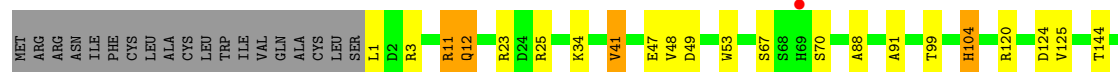
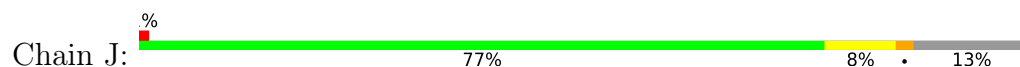


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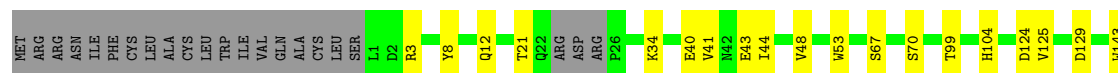
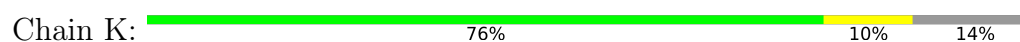




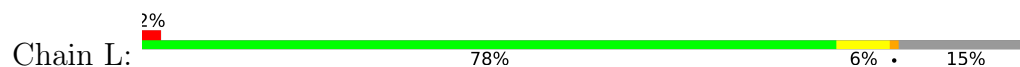
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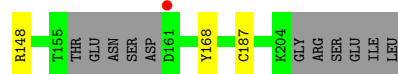
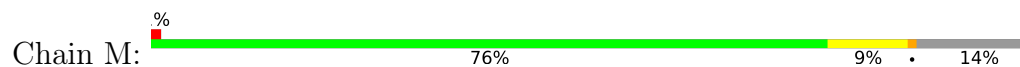
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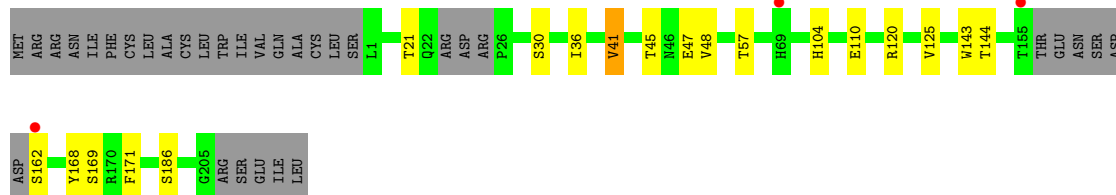
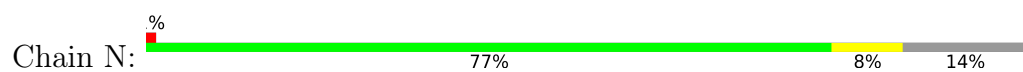
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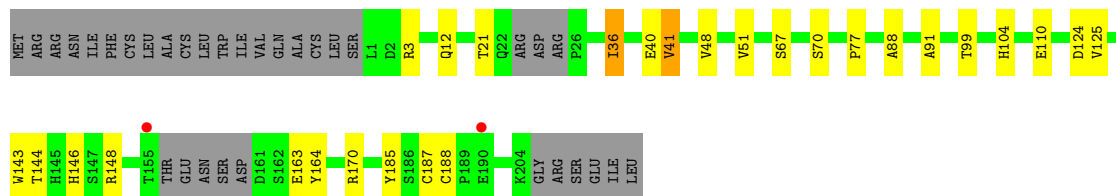
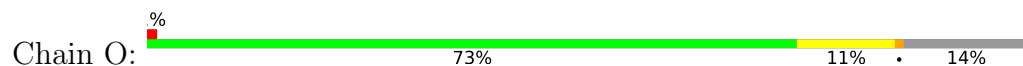
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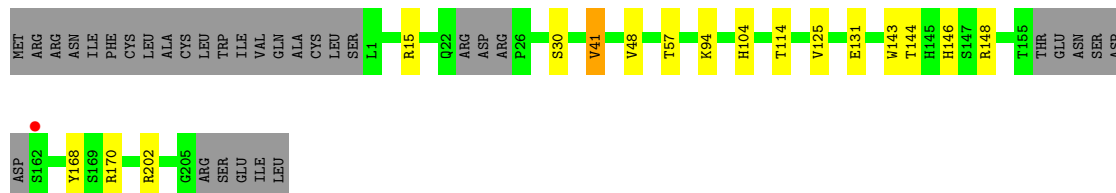
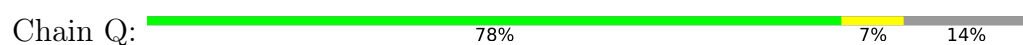
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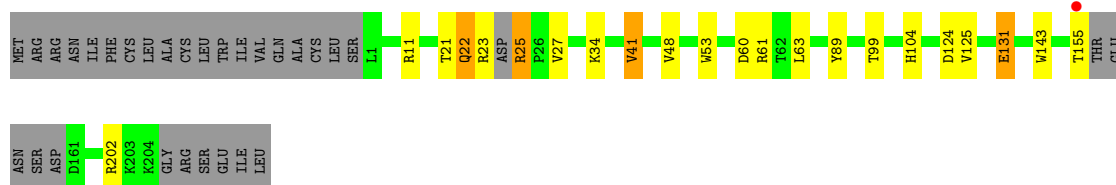
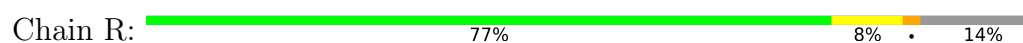
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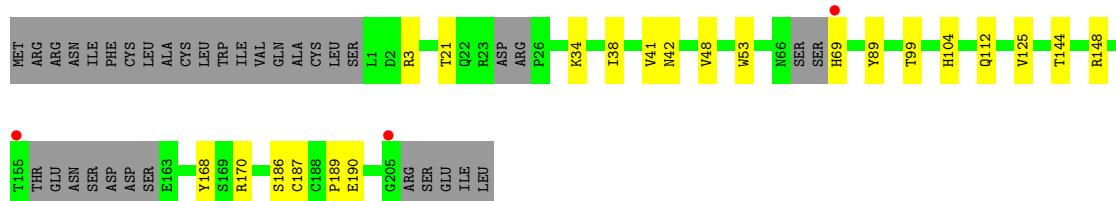
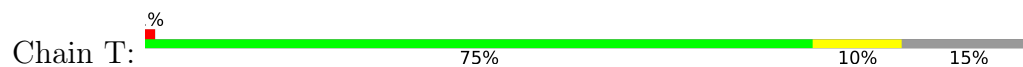
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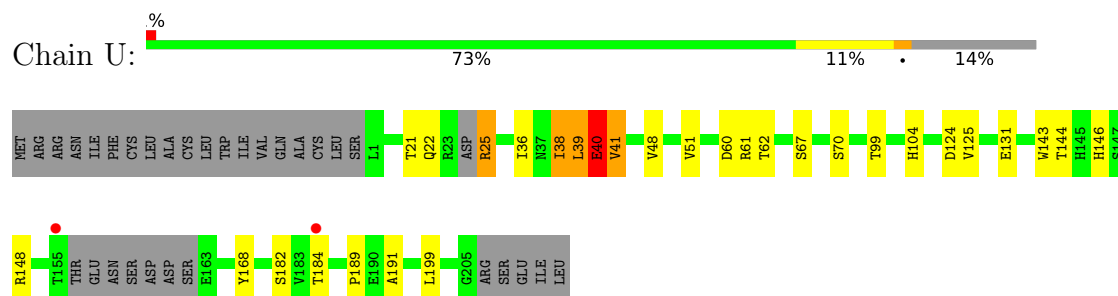
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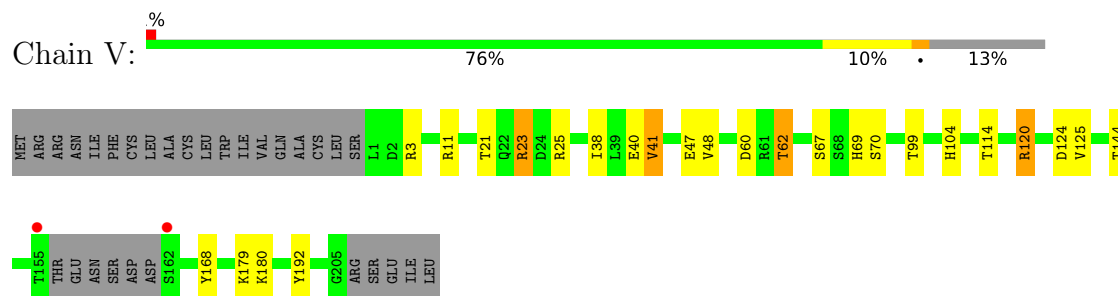
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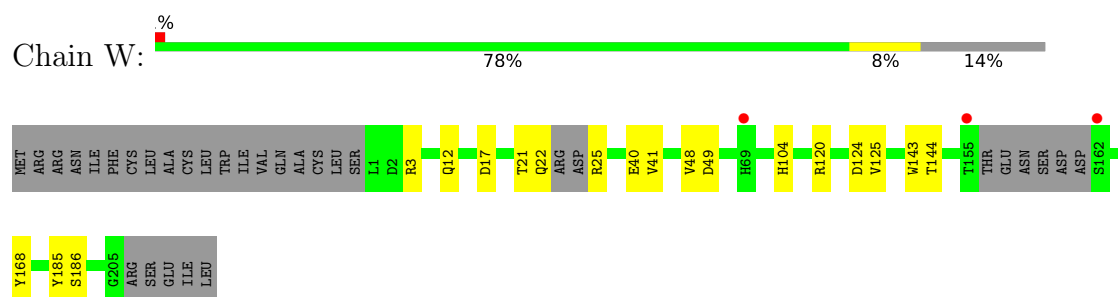
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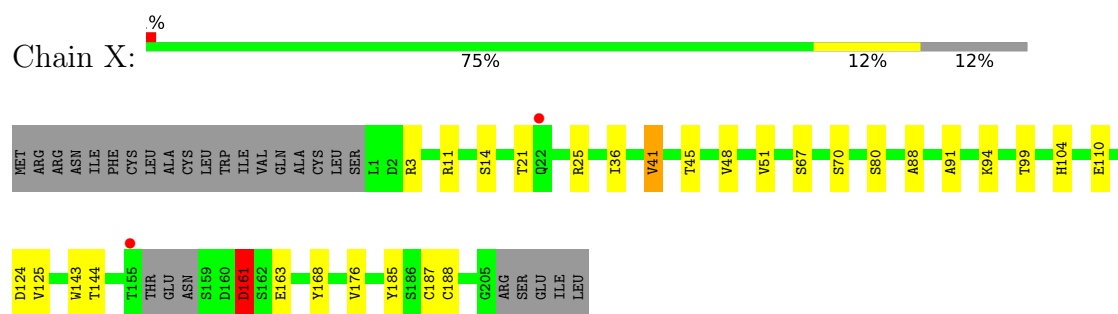
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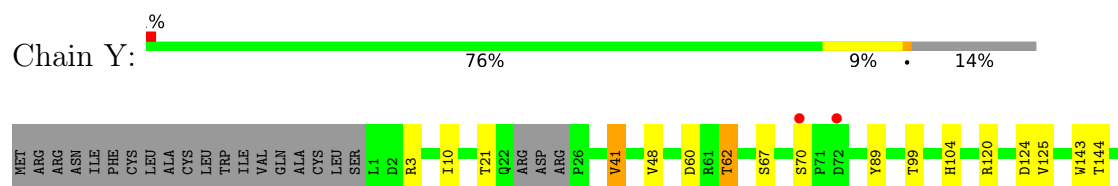
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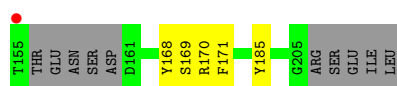


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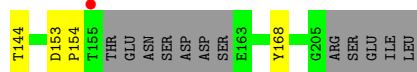
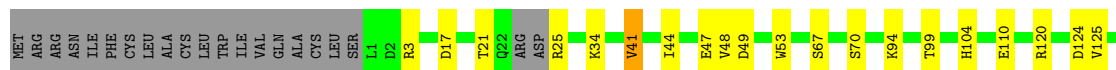
- Molecule 1: ACETYLCHOLINE BINDING PROTEIN





• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain Z: 75% 10% 14%



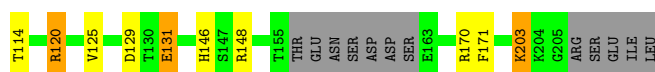
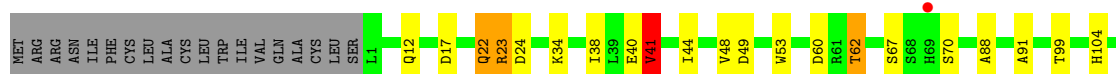
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain a: 78% 8% 14%



• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain b: 73% 10% 14%



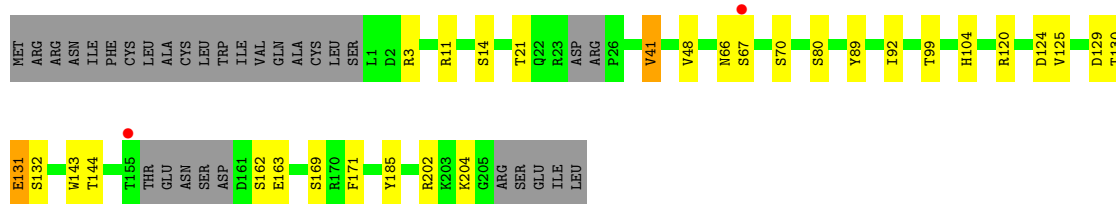
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain c: 76% 10% 13%

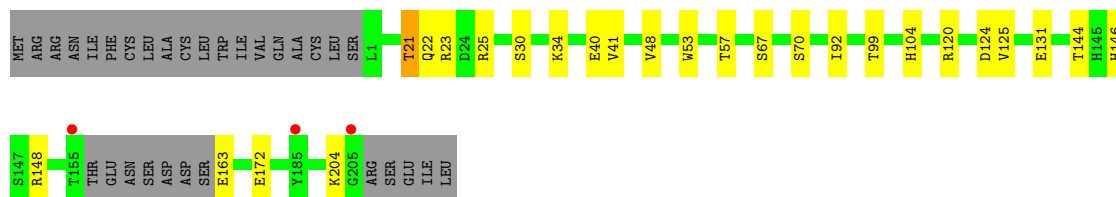


• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

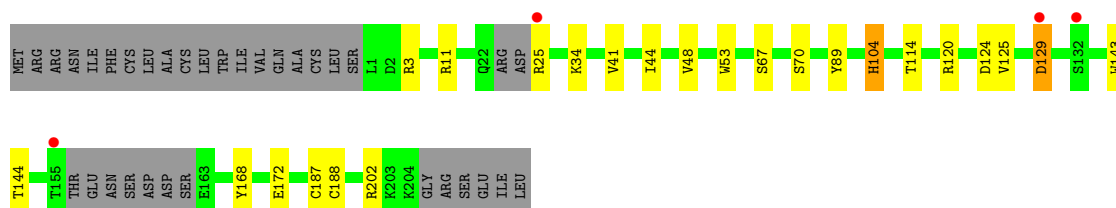
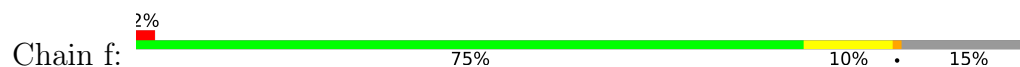
Chain d: 73% 12% 14%



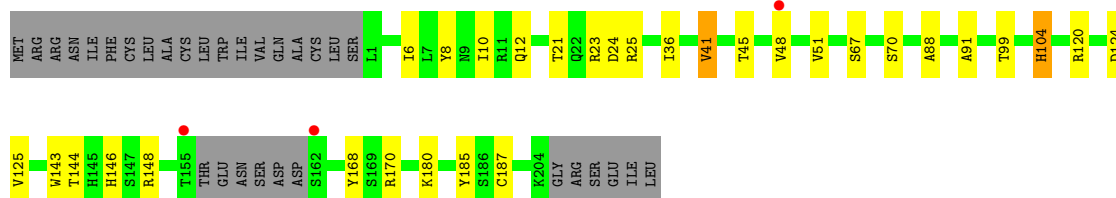
● Molecule 1: ACETYLCHOLINE BINDING PROTEIN



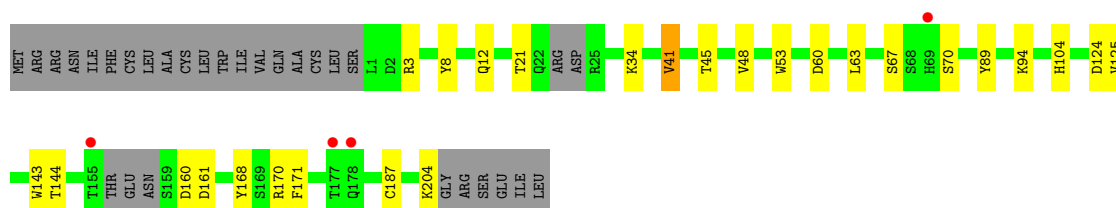
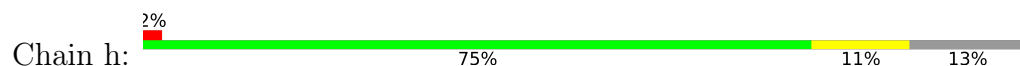
● Molecule 1: ACETYLCHOLINE BINDING PROTEIN



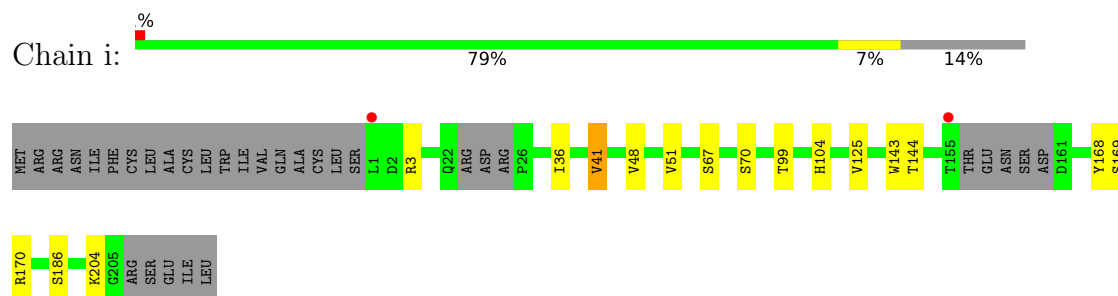
● Molecule 1: ACETYLCHOLINE BINDING PROTEIN



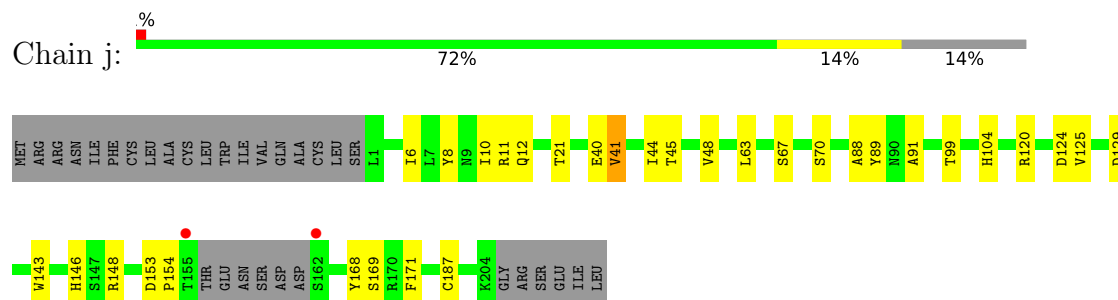
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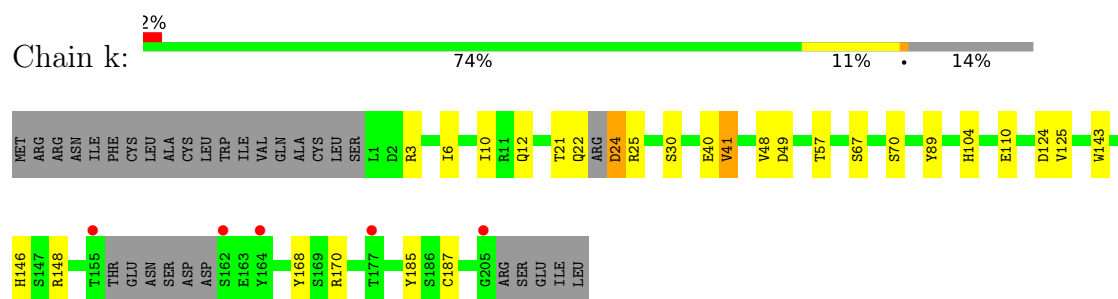
● Molecule 1: ACETYLCHOLINE BINDING PROTEIN



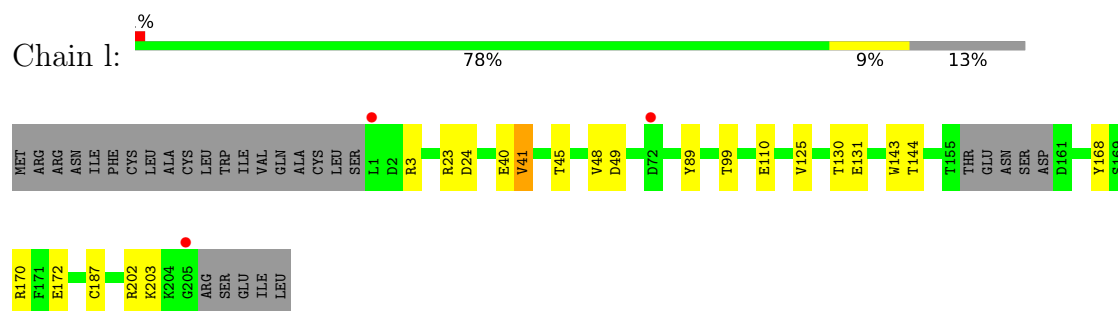
● Molecule 1: ACETYLCHOLINE BINDING PROTEIN



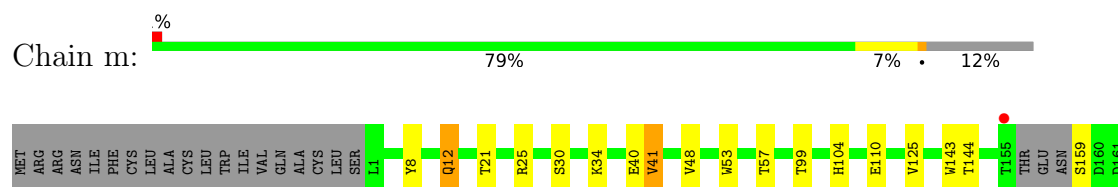
● Molecule 1: ACETYLCHOLINE BINDING PROTEIN



● Molecule 1: ACETYLCHOLINE BINDING PROTEIN

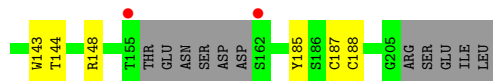
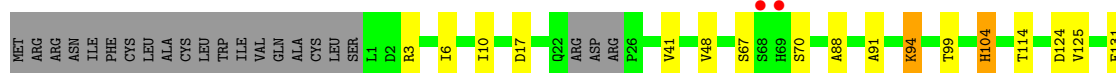
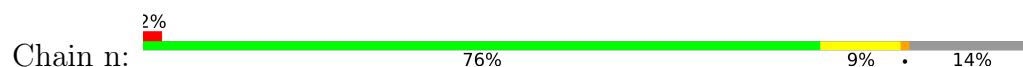


● Molecule 1: ACETYLCHOLINE BINDING PROTEIN

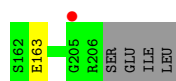
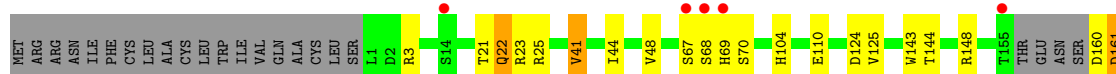
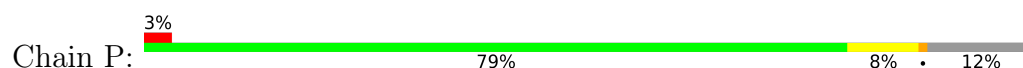




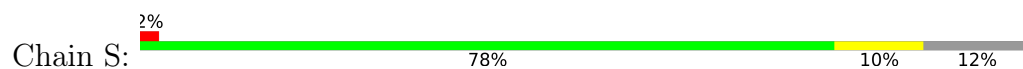
● Molecule 1: ACETYLCHOLINE BINDING PROTEIN



● Molecule 2: ACETYLCHOLINE BINDING PROTEIN



● Molecule 3: ACETYLCHOLINE BINDING PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.49Å 145.42Å 234.91Å 90.00° 101.29° 90.00°	Depositor
Resolution (Å)	30.07 – 2.70 30.07 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.07-2.70) 99.4 (30.07-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.72Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.198 , 0.244 0.207 , 0.246	Depositor DCC
R_{free} test set	4883 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	64774	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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: 09R, NAG, SO4

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	0.84	1/1661 (0.1%)	0.92	2/2264 (0.1%)
1	B	0.67	0/1613	0.82	1/2201 (0.0%)
1	C	0.73	0/1644	0.89	3/2243 (0.1%)
1	D	0.74	0/1640	0.85	0/2237
1	E	0.76	3/1599 (0.2%)	0.85	4/2182 (0.2%)
1	F	0.78	1/1610 (0.1%)	0.87	0/2196
1	G	0.67	0/1633	0.81	0/2229
1	H	0.67	0/1602	0.85	1/2186 (0.0%)
1	I	0.75	0/1642	0.86	0/2241
1	J	0.68	0/1644	0.85	1/2243 (0.0%)
1	K	0.61	0/1613	0.80	0/2200
1	L	0.61	0/1603	0.87	3/2187 (0.1%)
1	M	0.56	0/1628	0.77	2/2221 (0.1%)
1	N	0.65	0/1602	0.83	1/2187 (0.0%)
1	O	0.71	0/1598	0.80	2/2181 (0.1%)
1	Q	0.61	0/1616	0.83	0/2204
1	R	0.73	1/1620 (0.1%)	0.86	2/2210 (0.1%)
1	T	0.76	2/1586 (0.1%)	0.81	0/2162
1	U	0.82	4/1610 (0.2%)	0.86	2/2196 (0.1%)
1	V	0.80	3/1625 (0.2%)	0.91	0/2218
1	W	0.68	0/1605	0.86	1/2190 (0.0%)
1	X	0.66	0/1647	0.83	1/2248 (0.0%)
1	Y	0.64	1/1602 (0.1%)	0.83	0/2186
1	Z	0.62	0/1599	0.81	0/2182
1	a	0.66	0/1613	0.81	0/2201
1	b	0.73	2/1630 (0.1%)	0.81	2/2225 (0.1%)
1	c	0.64	0/1645	0.82	2/2245 (0.1%)
1	d	0.64	0/1613	0.83	0/2200
1	e	0.62	0/1619	0.81	0/2210
1	f	0.56	0/1595	0.80	0/2177
1	g	0.60	0/1621	0.79	0/2213
1	h	0.55	0/1634	0.79	0/2229

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	i	0.62	0/1602	0.81	0/2186
1	j	0.55	0/1621	0.79	0/2213
1	k	0.54	0/1613	0.79	1/2201 (0.0%)
1	l	0.56	0/1633	0.82	2/2229 (0.1%)
1	m	0.54	0/1640	0.82	3/2237 (0.1%)
1	n	0.54	0/1594	0.79	0/2175
2	P	0.78	0/1644	0.88	1/2243 (0.0%)
3	S	0.69	0/1638	0.81	0/2234
All	All	0.67	18/64797 (0.0%)	0.83	37/88412 (0.0%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	38	ILE	C-O	-6.55	1.17	1.24
1	U	38	ILE	C-O	-6.46	1.17	1.24
1	R	27	VAL	C-O	-6.29	1.17	1.24
1	U	40	GLU	CA-C	-6.29	1.45	1.52
1	b	38	ILE	C-O	-6.16	1.17	1.24
1	V	38	ILE	C-O	-5.97	1.17	1.24
1	b	41	VAL	CA-C	-5.85	1.45	1.52
1	E	42	ASN	C-O	-5.67	1.17	1.24
1	T	38	ILE	C-O	-5.48	1.18	1.24
1	A	27	VAL	C-O	-5.48	1.18	1.24
1	F	20	PRO	N-CA	-5.42	1.43	1.47
1	U	40	GLU	C-O	-5.42	1.17	1.23
1	V	41	VAL	C-O	-5.35	1.18	1.24
1	T	42	ASN	C-O	-5.33	1.18	1.24
1	E	41	VAL	C-O	-5.26	1.18	1.24
1	Y	10	ILE	C-O	-5.22	1.18	1.24
1	U	41	VAL	N-CA	-5.16	1.40	1.46
1	V	40	GLU	CA-C	-5.05	1.46	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	25	ARG	CA-C-N	-11.87	107.55	119.78
1	L	25	ARG	C-N-CA	-11.87	107.55	119.78
1	X	161	ASP	N-CA-C	7.31	119.33	111.36
1	W	12	GLN	N-CA-C	6.80	118.78	111.36
1	L	12	GLN	N-CA-C	6.66	118.62	111.36
1	H	12	GLN	N-CA-C	6.48	118.43	111.36
1	E	39	LEU	N-CA-C	6.36	121.39	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	9	ASN	N-CA-C	6.30	118.15	111.28
1	k	12	GLN	N-CA-C	6.11	118.02	111.36
1	U	41	VAL	N-CA-C	-6.04	99.77	108.53
1	m	25	ARG	CA-C-N	5.96	125.96	119.89
1	m	25	ARG	C-N-CA	5.96	125.96	119.89
1	J	12	GLN	N-CA-C	5.95	118.72	111.82
1	l	130	THR	CA-C-N	5.93	128.50	120.44
1	l	130	THR	C-N-CA	5.93	128.50	120.44
1	b	41	VAL	N-CA-C	-5.81	99.39	108.86
1	c	36	ILE	N-CA-C	-5.78	107.22	111.90
1	R	25	ARG	CA-C-N	-5.77	113.99	119.76
1	R	25	ARG	C-N-CA	-5.77	113.99	119.76
1	M	94	LYS	CA-C-N	-5.59	113.80	119.83
1	M	94	LYS	C-N-CA	-5.59	113.80	119.83
1	m	12	GLN	N-CA-C	5.57	117.43	111.36
1	C	204	LYS	N-CA-C	-5.55	102.67	110.50
1	A	27	VAL	CB-CA-C	-5.45	103.21	111.33
1	C	84	PRO	CA-C-O	-5.41	115.17	121.34
1	E	36	ILE	N-CA-C	-5.41	107.52	111.90
1	A	12	GLN	N-CA-C	5.39	117.23	111.36
1	N	36	ILE	N-CA-C	-5.33	107.58	111.90
1	B	170	ARG	N-CA-C	-5.33	106.61	113.01
1	O	36	ILE	N-CA-C	-5.27	107.69	112.12
1	E	12	GLN	N-CA-C	5.24	117.07	111.36
1	b	12	GLN	N-CA-C	5.18	117.01	111.36
1	c	160	ASP	N-CA-C	5.14	117.09	109.69
1	E	41	VAL	N-CA-C	-5.12	101.11	108.48
1	U	39	LEU	N-CA-C	5.11	119.99	113.55
2	P	161	ASP	N-CA-C	5.09	116.64	111.14
1	O	12	GLN	N-CA-C	5.05	117.67	111.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1619	0	1565	30	0
1	B	1578	0	1523	15	0
1	C	1608	0	1554	19	0
1	D	1605	0	1544	26	2
1	E	1560	0	1509	23	0
1	F	1572	0	1527	19	0
1	G	1597	0	1541	17	0
1	H	1567	0	1511	28	0
1	I	1603	0	1547	18	1
1	J	1605	0	1554	18	0
1	K	1575	0	1524	24	0
1	L	1565	0	1521	16	0
1	M	1590	0	1537	17	0
1	N	1564	0	1511	14	0
1	O	1563	0	1507	21	0
1	Q	1574	0	1527	19	0
1	R	1585	0	1533	22	0
1	T	1552	0	1504	24	0
1	U	1575	0	1527	28	0
1	V	1589	0	1537	27	1
1	W	1570	0	1519	15	0
1	X	1611	0	1550	23	0
1	Y	1567	0	1511	16	0
1	Z	1564	0	1514	20	0
1	a	1575	0	1523	21	0
1	b	1590	0	1539	21	0
1	c	1604	0	1545	21	0
1	d	1578	0	1522	29	1
1	e	1583	0	1532	16	0
1	f	1560	0	1511	28	0
1	g	1585	0	1534	26	0
1	h	1596	0	1542	24	0
1	i	1567	0	1511	16	0
1	j	1585	0	1536	32	0
1	k	1578	0	1523	20	1
1	l	1597	0	1541	14	0
1	m	1605	0	1544	15	0
1	n	1559	0	1507	18	0
2	P	1608	0	1554	21	0
3	S	1603	0	1547	18	0
4	A	14	0	14	1	0
4	B	14	0	14	3	0
4	C	14	0	14	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	14	0	14	4	0
4	E	14	0	14	2	0
4	F	14	0	14	2	0
4	G	14	0	14	3	0
4	H	14	0	14	2	0
4	I	14	0	14	0	0
4	J	14	0	14	2	0
4	K	14	0	14	0	0
4	L	14	0	14	2	0
4	M	14	0	14	2	0
4	N	14	0	14	1	0
4	O	14	0	14	2	0
4	P	14	0	14	5	0
4	Q	14	0	14	0	0
4	R	14	0	14	2	0
4	S	14	0	14	3	0
4	T	14	0	14	2	0
4	U	14	0	14	2	0
4	V	14	0	14	1	0
4	W	14	0	14	2	0
4	X	14	0	14	3	0
4	Y	14	0	14	2	0
4	Z	14	0	14	1	0
4	a	14	0	14	4	0
4	b	14	0	14	1	0
4	c	14	0	14	2	0
4	d	14	0	14	3	0
4	f	28	0	28	8	0
4	g	14	0	14	5	0
4	h	14	0	14	3	0
4	i	14	0	14	3	0
4	j	14	0	14	5	0
4	k	14	0	14	3	0
4	l	14	0	14	2	0
4	m	14	0	14	6	0
4	n	14	0	14	2	0
5	A	14	0	13	0	0
5	O	14	0	13	0	0
5	d	14	0	13	0	0
6	V	5	0	0	0	0
7	A	41	0	0	2	0
7	B	31	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	25	0	0	0	0
7	D	26	0	0	1	0
7	E	25	0	0	0	0
7	F	29	0	0	1	0
7	G	29	0	0	0	0
7	H	22	0	0	0	0
7	I	28	0	0	0	0
7	J	37	0	0	0	0
7	K	29	0	0	0	0
7	L	23	0	0	1	0
7	M	19	0	0	0	0
7	N	21	0	0	0	0
7	O	30	0	0	1	0
7	P	40	0	0	1	0
7	Q	37	0	0	1	0
7	R	27	0	0	2	0
7	S	28	0	0	0	0
7	T	31	0	0	1	0
7	U	30	0	0	0	0
7	V	44	0	0	0	0
7	W	28	0	0	0	0
7	X	28	0	0	0	0
7	Y	16	0	0	1	0
7	Z	23	0	0	0	0
7	a	16	0	0	0	0
7	b	9	0	0	1	0
7	c	3	0	0	0	0
7	d	19	0	0	0	0
7	e	3	0	0	0	0
7	f	2	0	0	0	0
7	g	1	0	0	0	0
7	h	7	0	0	0	0
7	i	5	0	0	0	0
7	j	2	0	0	0	0
7	k	7	0	0	0	0
7	l	6	0	0	0	0
7	m	2	0	0	0	0
7	n	7	0	0	0	0
All	All	64774	0	61807	636	3

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 5.

All (636) 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:U:41:VAL:HG13	1:U:125:VAL:HG11	1.44	0.99
1:j:6:ILE:O	1:j:10:ILE:HG13	1.66	0.94
1:V:60:ASP:OD1	1:V:62:THR:HB	1.70	0.92
1:E:41:VAL:HG13	1:E:125:VAL:HG11	1.53	0.91
1:Y:60:ASP:OD1	1:Y:62:THR:HB	1.69	0.91
1:K:44:ILE:HD12	1:d:129:ASP:HB3	1.54	0.90
1:V:11:ARG:HG2	1:V:11:ARG:HH11	1.38	0.88
1:I:60:ASP:OD1	1:I:62:THR:HB	1.76	0.86
1:T:69:HIS:CD2	1:V:69:HIS:CD2	2.64	0.85
1:K:43:GLU:OE2	1:d:131:GLU:HB2	1.79	0.83
1:b:41:VAL:HG13	1:b:125:VAL:HG11	1.61	0.82
1:U:41:VAL:HG13	1:U:125:VAL:CG1	2.11	0.81
1:d:131:GLU:HG3	1:d:202:ARG:NH1	1.95	0.80
1:A:23:ARG:HH22	1:F:69:HIS:CB	1.95	0.80
1:D:12:GLN:HE21	1:H:12:GLN:HE21	1.30	0.78
1:T:41:VAL:HG13	1:T:125:VAL:HG11	1.65	0.77
1:W:186:SER:OG	1:X:163:GLU:OE2	2.01	0.77
1:K:129:ASP:OD2	1:d:132:SER:HB3	1.86	0.76
1:C:60:ASP:OD1	1:C:62:THR:HB	1.83	0.76
1:A:162:SER:OG	7:A:401:HOH:O	2.01	0.76
1:h:45:THR:HA	1:i:170:ARG:HD3	1.66	0.75
1:H:61:ARG:HH11	1:H:61:ARG:HG3	1.52	0.75
1:j:11:ARG:NH1	1:n:17:ASP:OD2	2.20	0.75
2:P:68:SER:HA	1:a:25:ARG:HG2	1.69	0.74
1:H:22:GLN:HE22	1:H:61:ARG:HH12	1.36	0.73
1:D:161:ASP:HA	1:D:163:GLU:N	2.05	0.72
1:c:106:VAL:HG11	1:g:25:ARG:HH21	1.55	0.72
1:A:60:ASP:OD1	1:A:62:THR:HB	1.89	0.72
1:c:41:VAL:HG13	1:c:125:VAL:HG11	1.71	0.71
1:C:59:SER:OG	1:C:61:ARG:NH2	2.24	0.71
1:T:69:HIS:CD2	1:V:69:HIS:HD2	2.09	0.70
1:K:43:GLU:CD	1:d:131:GLU:HB2	2.17	0.69
1:b:49:ASP:OD2	1:b:120:ARG:NH1	2.25	0.69
1:R:23:ARG:HG2	1:R:23:ARG:HH11	1.57	0.69
1:A:206:ARG:NH1	1:b:131:GLU:OE2	2.24	0.69
1:i:169:SER:O	1:i:204:LYS:NZ	2.25	0.69
1:A:23:ARG:HH22	1:F:69:HIS:HB2	1.58	0.69
1:U:41:VAL:CG1	1:U:125:VAL:HG11	2.23	0.68
1:V:41:VAL:HG13	1:V:125:VAL:HG11	1.75	0.68
1:T:89:TYR:OH	4:T:301:09R:N3	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:12:GLN:HA	1:j:12:GLN:NE2	2.09	0.68
2:P:22:GLN:C	2:P:23:ARG:HG3	2.19	0.67
1:D:144:THR:O	1:E:104[A]:HIS:HE1	1.78	0.67
1:h:89:TYR:OH	4:h:301:09R:N3	2.28	0.67
1:a:25:ARG:HB3	1:a:26:PRO:HD2	1.78	0.66
1:f:129:ASP:O	1:j:44:ILE:HG12	1.96	0.66
1:k:146:HIS:CE1	1:k:148:ARG:HB2	2.30	0.66
1:D:21:THR:HG21	1:E:3:ARG:NH1	2.11	0.66
1:E:41:VAL:HG13	1:E:125:VAL:CG1	2.23	0.65
1:c:159:SER:HA	1:g:180:LYS:H	1.60	0.65
3:S:21:THR:HG21	1:T:3:ARG:NH1	2.12	0.65
1:b:41:VAL:HG22	1:b:48:VAL:HG12	1.79	0.65
2:P:160:ASP:CG	2:P:161:ASP:H	2.04	0.64
1:V:124:ASP:HB2	1:W:168:TYR:CE1	2.32	0.64
1:k:6:ILE:O	1:k:10:ILE:HG13	1.97	0.64
1:B:172:GLU:OE2	1:B:202:ARG:NE	2.22	0.64
1:F:168:TYR:CE1	1:J:124:ASP:HB2	2.33	0.64
1:M:47:GLU:OE1	1:M:120[B]:ARG:NH2	2.31	0.63
1:U:60:ASP:OD1	1:U:62:THR:HB	1.99	0.63
1:D:160:ASP:O	1:D:161:ASP:OD1	2.17	0.63
1:N:47:GLU:OE1	1:N:120:ARG:NH2	2.31	0.63
1:d:169:SER:O	1:d:204:LYS:NZ	2.26	0.62
1:K:104:HIS:HE1	1:O:144:THR:O	1.83	0.62
1:F:104:HIS:HE1	1:J:144:THR:O	1.83	0.62
1:V:11:ARG:HH11	1:V:11:ARG:CG	2.13	0.62
1:b:60:ASP:OD1	1:b:62:THR:HG23	2.00	0.62
1:j:12:GLN:HA	1:j:12:GLN:HE21	1.64	0.62
1:g:185:TYR:CD1	4:g:301:09R:H10	2.35	0.61
1:U:38:ILE:HD11	1:U:199:LEU:HD21	1.81	0.61
1:f:129:ASP:OD1	1:j:44:ILE:CD1	2.49	0.61
1:B:144:THR:O	1:C:104:HIS:HE1	1.83	0.61
1:A:22:GLN:HG3	1:A:22:GLN:O	2.01	0.60
1:D:12:GLN:NE2	1:H:12:GLN:HE21	1.98	0.60
2:P:163:GLU:OE2	1:T:186:SER:OG	2.19	0.60
1:R:89:TYR:OH	4:R:301:09R:N3	2.35	0.60
1:C:206:ARG:HE	1:U:131:GLU:CD	2.10	0.60
1:V:144:THR:O	1:W:104:HIS:HE1	1.84	0.60
1:K:44:ILE:CD1	1:d:129:ASP:HB3	2.30	0.60
1:T:148:ARG:NH1	7:T:401:HOH:O	2.35	0.59
1:b:41:VAL:HG13	1:b:125:VAL:CG1	2.32	0.59
1:H:61:ARG:HH11	1:H:61:ARG:CG	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:144:THR:O	1:h:104:HIS:HE1	1.85	0.59
1:D:12:GLN:HE21	1:H:12:GLN:NE2	2.00	0.59
1:B:12:GLN:HB3	1:J:12:GLN:HB3	1.84	0.59
1:D:41:VAL:HG13	1:D:125:VAL:HG11	1.84	0.59
1:D:12:GLN:HB3	1:H:12:GLN:HB3	1.84	0.59
1:K:41:VAL:HG13	1:K:125:VAL:HG11	1.84	0.59
1:Z:47:GLU:OE1	1:Z:120:ARG:NH2	2.36	0.59
1:I:41:VAL:HG13	1:I:125:VAL:HG11	1.84	0.59
3:S:41:VAL:HG13	3:S:125:VAL:HG11	1.85	0.59
1:e:41:VAL:HG13	1:e:125:VAL:HG11	1.85	0.58
1:R:41:VAL:HG13	1:R:125:VAL:HG11	1.85	0.58
1:h:124:ASP:HB2	1:i:168:TYR:CE1	2.38	0.58
1:B:143:TRP:CZ2	1:C:99:THR:HG21	2.39	0.58
1:e:146:HIS:CE1	1:e:148:ARG:HB2	2.38	0.58
2:P:69:HIS:NE2	1:a:24:ASP:OD2	2.36	0.58
1:H:41:VAL:HG13	1:H:125:VAL:HG11	1.86	0.58
1:Y:41:VAL:HG13	1:Y:125:VAL:HG11	1.85	0.58
1:n:41:VAL:HG13	1:n:125:VAL:HG11	1.86	0.58
1:U:21:THR:HG21	1:V:3:ARG:NH1	2.19	0.58
1:U:22:GLN:OE1	1:U:61:ARG:NH1	2.36	0.58
1:d:41:VAL:HG13	1:d:125:VAL:HG11	1.85	0.58
1:Y:89:TYR:OH	4:Y:301:09R:N3	2.37	0.58
1:U:144:THR:O	1:V:104:HIS:HE1	1.87	0.57
1:g:45:THR:HA	1:h:170:ARG:HD3	1.85	0.57
3:S:144:THR:O	1:T:104:HIS:HE1	1.87	0.57
1:a:41:VAL:HG13	1:a:125:VAL:HG11	1.85	0.57
1:f:104:HIS:NE2	4:f:301:09R:H3	2.19	0.57
1:k:41:VAL:HG13	1:k:125:VAL:HG11	1.87	0.57
1:F:41:VAL:HG13	1:F:125:VAL:HG11	1.86	0.57
1:T:69:HIS:HD2	1:V:69:HIS:CD2	2.19	0.57
1:O:146:HIS:CE1	1:O:148:ARG:HB2	2.39	0.57
1:f:129:ASP:CG	1:j:44:ILE:HG13	2.29	0.57
1:W:40:GLU:HB2	1:W:120:ARG:HH12	1.68	0.57
1:C:41:VAL:HG13	1:C:125:VAL:HG11	1.87	0.57
1:U:146:HIS:CE1	1:U:148:ARG:HB2	2.40	0.57
1:L:143:TRP:CZ2	1:M:99:THR:HG21	2.40	0.57
1:O:41:VAL:HG13	1:O:125:VAL:HG11	1.87	0.57
1:m:144:THR:O	1:n:104:HIS:HE1	1.88	0.57
4:U:301:09R:H3	1:V:104:HIS:CD2	2.40	0.56
1:L:41:VAL:HG22	1:L:48:VAL:HG12	1.86	0.56
1:Z:21:THR:HG21	1:a:3:ARG:NH1	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:VAL:HG13	1:B:125:VAL:HG11	1.86	0.56
1:C:124:ASP:HB2	1:D:168:TYR:CE1	2.40	0.56
1:k:187:CYS:SG	4:k:301:09R:H2	2.45	0.56
1:X:41:VAL:HG13	1:X:125:VAL:HG11	1.88	0.56
1:R:124:ASP:HB2	3:S:168:TYR:CE1	2.41	0.56
1:W:41:VAL:HG13	1:W:125:VAL:HG11	1.87	0.56
1:A:41:VAL:HG13	1:A:125:VAL:HG11	1.88	0.56
1:C:41:VAL:HG22	1:C:48:VAL:HG12	1.88	0.56
1:Q:143:TRP:CZ2	1:R:99:THR:HG21	2.41	0.56
1:Z:41:VAL:HG13	1:Z:125:VAL:HG11	1.86	0.56
1:i:41:VAL:HG13	1:i:125:VAL:HG11	1.86	0.56
1:D:12:GLN:NE2	1:H:12:GLN:NE2	2.54	0.56
1:c:160:ASP:OD1	1:c:161:ASP:N	2.30	0.56
1:G:185:TYR:CD1	4:G:301:09R:H10	2.41	0.55
1:a:45:THR:HA	1:b:170:ARG:HD3	1.88	0.55
1:h:41:VAL:HG13	1:h:125:VAL:HG11	1.89	0.55
1:m:41:VAL:HG13	1:m:125:VAL:HG11	1.89	0.55
1:M:41:VAL:HG22	1:M:48:VAL:HG12	1.88	0.55
1:N:41:VAL:HG13	1:N:125:VAL:HG11	1.89	0.55
1:Z:104:HIS:HE1	1:d:144:THR:O	1.89	0.55
1:G:41:VAL:HG13	1:G:125:VAL:HG11	1.89	0.55
1:R:23:ARG:HG2	1:R:23:ARG:NH1	2.22	0.55
1:A:22:GLN:O	1:A:23:ARG:HB2	2.06	0.55
1:f:124:ASP:HB2	1:g:168:TYR:CE1	2.42	0.55
1:J:41:VAL:HG13	1:J:125:VAL:HG11	1.88	0.55
1:Q:144:THR:O	1:R:104:HIS:HE1	1.88	0.55
1:D:40:GLU:OE1	1:D:118:ARG:NH2	2.40	0.55
1:G:144:THR:O	1:H:104:HIS:HE1	1.90	0.55
1:f:41:VAL:HG13	1:f:125:VAL:HG11	1.89	0.55
1:Q:41:VAL:HG13	1:Q:125:VAL:HG11	1.89	0.55
2:P:41:VAL:HG13	2:P:125:VAL:HG11	1.89	0.55
1:f:202:ARG:HH22	1:j:129:ASP:HB3	1.72	0.55
1:f:202:ARG:NH1	1:j:129:ASP:OD2	2.40	0.54
1:B:187:CYS:SG	4:B:301:09R:H2	2.48	0.54
1:M:41:VAL:HG13	1:M:125:VAL:HG11	1.89	0.54
1:g:6:ILE:O	1:g:10:ILE:HG13	2.08	0.54
1:K:43:GLU:CD	1:d:131:GLU:H	2.15	0.54
1:c:41:VAL:CG1	1:c:125:VAL:HG11	2.36	0.54
1:T:41:VAL:HG22	1:T:48:VAL:HG12	1.89	0.54
1:V:11:ARG:HG2	1:V:11:ARG:NH1	2.14	0.54
1:X:187:CYS:SG	4:X:301:09R:H2	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:143:TRP:CZ2	1:b:99:THR:HG21	2.43	0.54
1:O:77:PRO:HD3	7:O:401:HOH:O	2.07	0.54
2:P:3:ARG:NH1	1:T:21:THR:HG21	2.23	0.54
1:L:89:TYR:OH	4:L:301:09R:N3	2.41	0.54
1:T:41:VAL:HG13	1:T:125:VAL:CG1	2.35	0.54
1:f:129:ASP:O	1:j:44:ILE:CG1	2.56	0.54
1:L:41:VAL:HG13	1:L:125:VAL:HG11	1.89	0.54
1:e:104:HIS:HE1	1:i:144:THR:O	1.91	0.54
1:e:144:THR:O	1:f:104:HIS:HE1	1.90	0.54
1:C:9:ASN:O	1:C:13:THR:OG1	2.20	0.54
1:j:41:VAL:HG13	1:j:125:VAL:HG11	1.90	0.53
1:l:41:VAL:HG13	1:l:125:VAL:HG11	1.88	0.53
1:F:21:THR:HG23	1:F:21:THR:O	2.06	0.53
1:V:47:GLU:HB2	1:V:120:ARG:HH21	1.73	0.53
1:j:99:THR:HG21	1:n:143:TRP:CZ2	2.43	0.53
1:n:6:ILE:O	1:n:10:ILE:HG13	2.08	0.53
1:A:104[A]:HIS:HD2	7:A:420:HOH:O	1.90	0.53
1:F:89:TYR:OH	4:F:301:09R:N3	2.42	0.53
1:K:168:TYR:CE1	1:O:124:ASP:HB2	2.43	0.53
1:R:25:ARG:HD3	1:R:25:ARG:N	2.23	0.53
1:L:17:ASP:OD2	1:M:11:ARG:NH2	2.41	0.53
1:U:22:GLN:O	1:U:25:ARG:HG2	2.09	0.53
1:k:40:GLU:HB2	1:k:49:ASP:HB2	1.90	0.53
2:P:104:HIS:CE1	1:T:144:THR:HB	2.44	0.53
1:U:41:VAL:CG1	1:U:125:VAL:CG1	2.83	0.53
1:f:172:GLU:OE2	1:f:202:ARG:NE	2.26	0.53
1:g:41:VAL:HG13	1:g:125:VAL:HG11	1.91	0.53
4:D:301:09R:H3	1:E:104[A]:HIS:CD2	2.44	0.53
1:m:41:VAL:HG22	1:m:48:VAL:HG12	1.91	0.53
1:X:41:VAL:HG22	1:X:48:VAL:HG12	1.91	0.52
1:h:41:VAL:HG22	1:h:48:VAL:HG12	1.91	0.52
1:k:24:ASP:OD1	1:k:24:ASP:N	2.39	0.52
1:D:144:THR:O	1:E:104[A]:HIS:CE1	2.57	0.52
2:P:104:HIS:HE1	1:T:144:THR:O	1.93	0.52
1:Z:168:TYR:CE1	1:d:124:ASP:HB2	2.44	0.52
1:B:143:TRP:CE2	1:C:99:THR:HG21	2.43	0.52
1:M:6:ILE:O	1:M:10:ILE:HG13	2.10	0.52
1:j:104:HIS:HE1	1:n:144:THR:O	1.92	0.52
1:l:187:CYS:SG	4:l:301:09R:H2	2.49	0.52
1:D:124:ASP:HB2	1:E:168:TYR:CE1	2.43	0.52
1:Q:41:VAL:HG22	1:Q:48:VAL:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:169:SER:C	1:j:171:PHE:H	2.17	0.52
1:N:41:VAL:HG22	1:N:48:VAL:HG12	1.92	0.52
4:P:301:09R:H3	1:Q:104[A]:HIS:CD2	2.44	0.52
1:k:124:ASP:HB2	1:l:168:TYR:CE1	2.44	0.52
1:I:21:THR:HG21	1:J:3:ARG:NH1	2.25	0.52
1:N:45:THR:HA	1:O:170:ARG:HD2	1.91	0.52
2:P:160:ASP:OD1	2:P:161:ASP:N	2.42	0.52
1:c:41:VAL:HG13	1:c:125:VAL:CG1	2.40	0.52
1:e:146:HIS:HE1	1:e:148:ARG:HB2	1.73	0.52
1:I:41:VAL:HG22	1:I:48:VAL:HG12	1.91	0.52
3:S:191:ALA:HB3	1:U:189:PRO:O	2.09	0.52
1:k:146:HIS:HE1	1:k:148:ARG:HB2	1.72	0.52
1:R:21:THR:OG1	1:R:25:ARG:O	2.27	0.52
1:Z:99:THR:HG21	1:d:143:TRP:CZ2	2.45	0.52
1:f:144:THR:O	1:g:104:HIS:HE1	1.93	0.52
1:k:41:VAL:HG22	1:k:48:VAL:HG12	1.92	0.51
1:D:41:VAL:HG22	1:D:48:VAL:HG12	1.92	0.51
1:Q:143:TRP:CE2	1:R:99:THR:HG21	2.44	0.51
3:S:124:ASP:HB2	1:T:168:TYR:CE1	2.45	0.51
1:O:41:VAL:HG22	1:O:48:VAL:HG12	1.91	0.51
3:S:41:VAL:HG22	3:S:48:VAL:HG12	1.91	0.51
1:V:179:LYS:HE3	1:V:180:LYS:O	2.11	0.51
1:a:143:TRP:CE2	1:b:99:THR:HG21	2.46	0.51
1:h:144:THR:O	1:i:104:HIS:HE1	1.94	0.51
1:X:124:ASP:HB2	1:Y:168:TYR:CE1	2.46	0.51
4:P:301:09R:H3	1:Q:104[B]:HIS:CE1	2.46	0.51
1:Z:41:VAL:HG22	1:Z:48:VAL:HG12	1.92	0.51
1:g:143:TRP:CE3	4:g:301:09R:H7	2.46	0.51
1:M:146:HIS:CE1	1:M:148:ARG:HB2	2.45	0.51
1:R:131:GLU:HG3	1:R:202:ARG:NH1	2.25	0.51
1:O:67:SER:HA	1:O:70:SER:HB2	1.93	0.51
1:V:11:ARG:CG	1:V:11:ARG:NH1	2.73	0.51
1:W:185:TYR:CD1	4:W:301:09R:H10	2.46	0.51
1:Z:144:THR:O	1:a:104:HIS:HE1	1.94	0.51
1:f:143:TRP:O	4:f:302:09R:H121	2.11	0.51
1:g:41:VAL:HG22	1:g:48:VAL:HG12	1.92	0.51
1:D:167:GLN:O	1:D:204:LYS:NZ	2.44	0.50
1:e:41:VAL:HG22	1:e:48:VAL:HG12	1.93	0.50
1:l:45:THR:HA	1:m:170:ARG:HD3	1.93	0.50
1:E:148:ARG:HD3	1:L:191:ALA:HB2	1.93	0.50
1:d:41:VAL:HG22	1:d:48:VAL:HG12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:8:TYR:O	1:m:12:GLN:HG2	2.12	0.50
3:S:93:SER:HB3	3:S:120:ARG:HD2	1.94	0.50
1:D:35:PHE:N	1:D:161:ASP:OD2	2.44	0.50
1:F:19:ILE:HG13	1:F:20:PRO:HD2	1.93	0.50
1:O:185:TYR:CD1	4:O:301:09R:H10	2.47	0.50
1:l:41:VAL:HG22	1:l:48:VAL:HG12	1.92	0.50
1:A:41:VAL:HG22	1:A:48:VAL:HG12	1.92	0.50
1:I:144:THR:O	1:J:104:HIS:HE1	1.94	0.50
1:Z:99:THR:HG21	1:d:143:TRP:CE2	2.46	0.50
1:m:143:TRP:CZ3	4:m:301:09R:H7	2.46	0.50
1:H:61:ARG:CG	1:H:61:ARG:NH1	2.73	0.50
1:h:143:TRP:O	4:h:301:09R:H121	2.11	0.50
1:A:3:ARG:NH1	1:E:21:THR:HG21	2.27	0.50
1:D:161:ASP:CA	1:D:163:GLU:N	2.73	0.50
1:X:45:THR:HA	1:Y:170:ARG:HD2	1.94	0.50
1:f:104:HIS:CD2	4:f:301:09R:H3	2.47	0.50
1:i:41:VAL:HG22	1:i:48:VAL:HG12	1.92	0.50
1:L:143:TRP:CE2	1:M:99:THR:HG21	2.47	0.50
4:a:301:09R:H3	1:b:104[A]:HIS:CD2	2.47	0.50
1:U:143:TRP:CE2	1:V:99:THR:HG21	2.47	0.49
1:g:187:CYS:SG	4:g:301:09R:H2	2.51	0.49
1:H:185:TYR:CD1	4:H:301:09R:H10	2.47	0.49
1:N:143:TRP:CE2	1:O:99:THR:HG21	2.47	0.49
2:P:23:ARG:HD2	2:P:25:ARG:HH21	1.77	0.49
1:m:21:THR:HG21	1:n:3:ARG:NH1	2.26	0.49
1:A:23:ARG:HH22	1:F:69:HIS:HB3	1.77	0.49
1:c:21:THR:HG21	1:d:3:ARG:NH1	2.26	0.49
1:h:21:THR:HG21	1:i:3:ARG:NH1	2.28	0.49
1:A:23:ARG:HH12	1:F:69:HIS:CD2	2.30	0.49
1:E:34:LYS:HB2	1:E:53:TRP:HB2	1.95	0.49
1:G:41:VAL:HG22	1:G:48:VAL:HG12	1.94	0.49
1:j:187:CYS:SG	4:j:301:09R:H2	2.52	0.49
1:A:170:ARG:HD3	1:E:45:THR:HA	1.93	0.49
1:E:12:GLN:HB3	1:G:12:GLN:HB3	1.93	0.49
1:c:93:SER:HB3	1:c:120[B]:ARG:HD2	1.94	0.49
1:K:41:VAL:HG22	1:K:48:VAL:HG12	1.94	0.49
1:j:21:THR:HG21	1:k:3:ARG:NH1	2.28	0.49
1:h:160:ASP:OD1	1:h:161:ASP:N	2.46	0.49
1:l:144:THR:O	1:m:104:HIS:HE1	1.95	0.49
1:K:44:ILE:CD1	1:d:129:ASP:C	2.86	0.49
1:V:21:THR:HG21	1:W:3:ARG:NH1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:170:ARG:NH1	1:l:203:LYS:HZ1	2.10	0.49
1:H:22:GLN:NE2	1:H:61:ARG:HH12	2.06	0.49
3:S:21:THR:OG1	3:S:25:ARG:O	2.30	0.49
3:S:184:THR:OG1	1:U:184:THR:OG1	2.25	0.49
1:V:41:VAL:HG13	1:V:125:VAL:CG1	2.41	0.48
1:Z:17:ASP:OD2	1:a:11:ARG:NH1	2.46	0.48
1:c:143:TRP:CE2	1:d:99:THR:HG21	2.48	0.48
1:f:143:TRP:CZ2	1:g:99:THR:HG21	2.48	0.48
1:j:41:VAL:HG22	1:j:48:VAL:HG12	1.94	0.48
1:A:205:GLY:HA3	1:b:129:ASP:CG	2.38	0.48
1:Q:94:LYS:HD3	7:Q:431:HOH:O	2.13	0.48
3:S:189:PRO:O	1:U:191:ALA:HB3	2.12	0.48
1:B:41:VAL:HG22	1:B:48:VAL:HG12	1.94	0.48
1:W:41:VAL:HG22	1:W:48:VAL:HG12	1.95	0.48
1:g:185:TYR:CG	4:g:301:09R:H10	2.47	0.48
1:A:144:THR:O	1:B:104:HIS:HE1	1.96	0.48
1:F:146:HIS:CE1	1:F:148:ARG:HB2	2.48	0.48
1:G:146:HIS:CE1	1:G:148:ARG:HB2	2.49	0.48
1:K:44:ILE:HG12	1:d:130:THR:HG22	1.95	0.48
1:M:12:GLN:NE2	1:M:12:GLN:HA	2.28	0.48
1:Z:144:THR:HB	1:a:104:HIS:CE1	2.48	0.48
4:G:301:09R:H3	1:H:104:HIS:CD2	2.47	0.48
1:M:25:ARG:HB2	1:M:26:PRO:HD2	1.95	0.48
1:N:186:SER:OG	1:O:163:GLU:OE2	2.31	0.48
2:P:41:VAL:HG22	2:P:48:VAL:HG12	1.95	0.48
4:S:301:09R:H3	1:T:104:HIS:CD2	2.49	0.48
1:k:89:TYR:OH	4:k:301:09R:N3	2.46	0.48
1:m:143:TRP:CE3	4:m:301:09R:H7	2.49	0.48
1:K:167:GLN:O	1:K:204:LYS:NZ	2.47	0.48
1:X:144:THR:O	1:Y:104:HIS:HE1	1.96	0.48
1:Y:185:TYR:CD1	4:Y:301:09R:H10	2.49	0.48
1:g:21:THR:HG21	1:h:3:ARG:NH1	2.28	0.48
1:K:99:THR:HG21	1:O:143:TRP:CE2	2.49	0.48
1:g:124:ASP:HB2	1:h:168:TYR:CE1	2.49	0.48
1:e:92:ILE:HD11	1:e:120:ARG:HG2	1.96	0.48
1:G:25:ARG:HG2	1:G:26:PRO:HD2	1.95	0.47
1:L:124:ASP:HB2	1:M:168:TYR:CE1	2.49	0.47
4:b:301:09R:H3	1:c:104:HIS:CD2	2.48	0.47
1:c:30:SER:HB2	1:c:57:THR:HB	1.96	0.47
1:c:144:THR:O	1:d:104:HIS:HE1	1.97	0.47
1:H:34:LYS:HB2	1:H:53:TRP:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:41:VAL:HG22	1:a:48:VAL:HG12	1.94	0.47
1:n:41:VAL:HG22	1:n:48:VAL:HG12	1.95	0.47
1:D:143:TRP:CE2	1:E:99:THR:HG21	2.50	0.47
1:D:161:ASP:C	1:D:163:GLU:N	2.72	0.47
1:T:190:GLU:HG3	1:a:182:SER:HB3	1.96	0.47
1:A:45:THR:HA	1:B:170:ARG:HD3	1.96	0.47
1:h:8:TYR:O	1:h:12:GLN:HG2	2.14	0.47
1:n:185:TYR:CD1	4:n:301:09R:H10	2.49	0.47
1:A:89:TYR:OH	4:A:301:09R:N3	2.47	0.47
1:E:41:VAL:HG22	1:E:48:VAL:HG12	1.97	0.47
1:N:21:THR:HG21	1:O:3:ARG:NH1	2.28	0.47
1:Z:94:LYS:HD2	1:a:96:GLU:HG3	1.96	0.47
1:D:89:TYR:OH	4:D:301:09R:N3	2.47	0.47
1:N:186:SER:H	1:O:164:TYR:HH	1.60	0.47
1:U:146:HIS:HE1	1:U:148:ARG:HB2	1.78	0.47
1:C:144:THR:HB	1:D:104:HIS:CE1	2.50	0.47
1:U:168:TYR:CE1	1:Y:124:ASP:HB2	2.50	0.47
1:G:67:SER:HA	1:G:70:SER:HB2	1.97	0.47
1:L:192:TYR:CD2	4:L:301:09R:H121	2.50	0.47
1:R:22:GLN:NE2	1:R:61:ARG:HG3	2.30	0.47
4:R:301:09R:BR1	3:S:112:GLN:O	2.88	0.47
1:W:49:ASP:HB2	1:W:120:ARG:NH1	2.30	0.47
1:f:44:ILE:HG22	1:g:170:ARG:HD3	1.97	0.47
1:G:131:GLU:HG3	1:G:202:ARG:NH1	2.30	0.46
1:Q:30:SER:HB2	1:Q:57:THR:HB	1.98	0.46
1:V:41:VAL:HG22	1:V:48:VAL:HG12	1.97	0.46
1:G:21:THR:HG21	1:H:3:ARG:NH1	2.30	0.46
1:X:21:THR:HG21	1:Y:3:ARG:NH1	2.31	0.46
1:Z:124:ASP:HB2	1:a:168:TYR:CE1	2.50	0.46
3:S:22:GLN:O	3:S:22:GLN:HG3	2.15	0.46
1:U:143:TRP:CZ2	1:V:99:THR:HG21	2.49	0.46
4:a:301:09R:C1	1:b:114:THR:HB	2.46	0.46
1:f:187:CYS:SG	4:f:302:09R:H2	2.55	0.46
1:k:21:THR:HG21	1:l:3:ARG:NH1	2.30	0.46
4:G:301:09R:H5	4:G:301:09R:H1	1.68	0.46
1:K:43:GLU:OE1	1:d:131:GLU:HB2	2.15	0.46
1:X:185:TYR:CD1	4:X:301:09R:H10	2.51	0.46
1:e:34:LYS:HB2	1:e:53:TRP:HB2	1.98	0.46
4:j:301:09R:H5	4:j:301:09R:H1	1.60	0.46
1:J:67:SER:HA	1:J:70:SER:HB2	1.98	0.46
1:Q:15:ARG:HH21	1:R:11:ARG:NH2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:143:TRP:CD2	4:g:301:09R:H7	2.51	0.46
1:H:15:ARG:NH2	1:I:11:ARG:NH2	2.64	0.46
1:K:99:THR:HG21	1:O:143:TRP:CZ2	2.50	0.46
1:f:129:ASP:OD1	1:j:44:ILE:HG13	2.15	0.46
1:j:12:GLN:HE21	1:j:12:GLN:CA	2.24	0.46
2:P:44:ILE:HG22	1:Q:170:ARG:HD3	1.98	0.46
2:P:160:ASP:CG	2:P:161:ASP:N	2.72	0.46
1:a:89:TYR:OH	4:a:301:09R:N3	2.49	0.46
1:j:10:ILE:HG23	1:j:63:LEU:HD22	1.96	0.46
1:O:36:ILE:HB	1:O:51:VAL:HG12	1.97	0.46
1:f:41:VAL:HG22	1:f:48:VAL:HG12	1.97	0.46
4:m:301:09R:H1	4:m:301:09R:H5	1.50	0.46
1:K:3:ARG:NH1	1:O:21:THR:HG21	2.31	0.46
2:P:148:ARG:NH1	7:P:404:HOH:O	2.46	0.46
1:Y:21:THR:HG22	7:Y:401:HOH:O	2.16	0.46
1:g:144:THR:HB	1:h:104:HIS:CE1	2.51	0.46
1:A:68:SER:HA	1:L:25:ARG:HG3	1.98	0.45
1:E:88:ALA:HB3	1:E:91:ALA:HB2	1.98	0.45
1:E:89:TYR:OH	4:E:301:09R:N3	2.39	0.45
4:U:301:09R:C1	1:V:114:THR:HB	2.46	0.45
1:b:104[A]:HIS:HD2	7:b:406:HOH:O	1.97	0.45
1:e:21:THR:HG21	1:f:3:ARG:NH1	2.31	0.45
1:F:104:HIS:CD2	4:J:301:09R:H3	2.51	0.45
3:S:184:THR:HG21	1:U:182:SER:OG	2.17	0.45
1:C:144:THR:O	1:D:104:HIS:HE1	1.99	0.45
1:K:21:THR:HG21	1:L:3:ARG:NH1	2.32	0.45
1:J:41:VAL:HG22	1:J:48:VAL:HG12	1.97	0.45
1:L:154:PRO:HD2	7:L:422:HOH:O	2.16	0.45
2:P:69:HIS:CE1	1:a:24:ASP:HB3	2.51	0.45
1:U:61:ARG:HG3	1:U:61:ARG:HH11	1.81	0.45
1:F:144:THR:O	1:G:104:HIS:HE1	1.98	0.45
1:H:61:ARG:HA	1:H:61:ARG:HD3	1.69	0.45
1:V:192:TYR:CD2	4:V:302:09R:H121	2.52	0.45
1:A:34:LYS:HB2	1:A:53:TRP:HB2	1.98	0.45
1:F:60:ASP:OD1	1:F:62:THR:OG1	2.30	0.45
1:G:30:SER:HB2	1:G:57:THR:HB	1.99	0.45
1:G:124:ASP:HB2	1:H:168:TYR:CE1	2.50	0.45
1:I:143:TRP:CZ2	1:J:99:THR:HG21	2.51	0.45
1:M:124:ASP:HB2	1:N:168:TYR:CE1	2.52	0.45
1:Z:3:ARG:NH1	1:d:21:THR:HG21	2.32	0.45
1:Z:104:HIS:CD2	4:d:301:09R:H3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:22:GLN:HG2	1:b:23:ARG:HG2	1.99	0.45
1:l:89:TYR:OH	4:l:301:09R:N3	2.50	0.45
1:Q:131:GLU:HG3	1:Q:202:ARG:NH1	2.31	0.45
1:d:92:ILE:HD11	1:d:120:ARG:HG2	1.99	0.45
1:j:8:TYR:O	1:j:12:GLN:HG2	2.17	0.45
1:E:146:HIS:CE1	1:E:148:ARG:HB2	2.52	0.45
1:E:187:CYS:SG	4:E:301:09R:H2	2.57	0.45
1:O:187:CYS:SG	4:O:301:09R:H2	2.57	0.45
1:Z:49:ASP:OD2	1:Z:120:ARG:HD3	2.16	0.45
1:g:67:SER:HA	1:g:70:SER:HB2	1.98	0.45
1:A:104[A]:HIS:HE1	1:E:144:THR:O	2.00	0.45
1:R:41:VAL:HG22	1:R:48:VAL:HG12	1.99	0.45
1:U:104:HIS:HE1	1:Y:144:THR:O	2.00	0.45
1:h:34:LYS:HB2	1:h:53:TRP:HB2	1.99	0.45
1:j:124:ASP:HB2	1:k:168:TYR:CE1	2.51	0.45
1:A:36:ILE:HB	1:A:51:VAL:HG12	1.99	0.45
2:P:124:ASP:HB2	1:Q:168:TYR:CE1	2.52	0.45
1:d:67:SER:HA	1:d:70:SER:HB2	1.99	0.45
1:h:143:TRP:CZ2	1:i:99:THR:HG21	2.52	0.44
1:V:67:SER:HA	1:V:70:SER:HB2	1.99	0.44
1:W:17:ASP:OD2	1:X:11:ARG:NH1	2.50	0.44
1:c:38:ILE:HD11	1:c:199:LEU:HD21	1.99	0.44
1:A:12:GLN:HB3	1:F:12:GLN:HB3	2.00	0.44
1:M:187:CYS:SG	4:M:301:09R:H2	2.57	0.44
1:Q:15:ARG:NH2	1:R:11:ARG:NH2	2.66	0.44
1:d:169:SER:C	1:d:171:PHE:H	2.25	0.44
1:C:143:TRP:CZ3	4:C:301:09R:H7	2.52	0.44
1:U:41:VAL:HG22	1:U:48:VAL:HG12	2.00	0.44
1:Y:41:VAL:HG22	1:Y:48:VAL:HG12	1.98	0.44
4:c:301:09R:H1	4:c:301:09R:H5	1.69	0.44
1:H:67:SER:HA	1:H:70:SER:HB2	2.00	0.44
1:I:124:ASP:HB2	1:J:168:TYR:CE1	2.53	0.44
1:O:88:ALA:HB3	1:O:91:ALA:HB2	1.99	0.44
1:l:40:GLU:HB3	1:l:49:ASP:HB2	1.99	0.44
1:G:143:TRP:CZ2	1:H:99:THR:HG21	2.53	0.44
1:I:34:LYS:HB2	1:I:53:TRP:HB2	1.98	0.44
1:J:88:ALA:HB3	1:J:91:ALA:HB2	2.00	0.44
1:N:30:SER:HB2	1:N:57:THR:HB	2.00	0.44
4:W:301:09R:H5	4:W:301:09R:H1	1.77	0.44
1:A:23:ARG:HD3	1:A:23:ARG:HA	1.72	0.44
1:C:67:SER:HA	1:C:70:SER:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:114:THR:HB	4:f:301:09R:C1	2.47	0.44
1:k:143:TRP:CE2	1:l:99:THR:HG21	2.52	0.44
1:j:45:THR:HA	1:k:170:ARG:HD3	1.99	0.44
1:j:99:THR:HG21	1:n:143:TRP:CE2	2.53	0.44
1:j:143:TRP:CE3	4:j:301:09R:H7	2.53	0.44
1:B:170:ARG:NH2	1:B:203:LYS:HE3	2.33	0.44
1:J:34:LYS:HB2	1:J:53:TRP:HB2	1.99	0.44
1:X:161:ASP:HB3	1:X:176:VAL:HG23	1.99	0.44
1:A:67:SER:HA	1:A:70:SER:HB2	2.00	0.43
1:X:36:ILE:HB	1:X:51:VAL:HG12	2.00	0.43
1:b:34:LYS:HB2	1:b:53:TRP:HB2	1.99	0.43
1:h:143:TRP:CE2	1:i:99:THR:HG21	2.53	0.43
1:E:67:SER:HA	1:E:70:SER:HB2	2.00	0.43
3:S:131:GLN:HG3	3:S:202:ARG:NH1	2.34	0.43
1:U:99:THR:HG21	1:Y:143:TRP:CE2	2.53	0.43
1:i:143:TRP:CE2	4:i:301:09R:H5	2.53	0.43
1:j:146:HIS:CE1	1:j:148:ARG:HB2	2.53	0.43
1:m:34:LYS:HB2	1:m:53:TRP:HB2	2.00	0.43
4:D:301:09R:H12	4:D:301:09R:H6	1.75	0.43
1:K:8:TYR:O	1:K:12:GLN:HG2	2.18	0.43
1:U:124:ASP:HB2	1:V:168:TYR:CE1	2.53	0.43
1:n:94:LYS:HB2	1:n:94:LYS:HE3	1.63	0.43
2:P:143:TRP:CE2	4:P:301:09R:H5	2.53	0.43
1:Q:15:ARG:NH2	1:R:11:ARG:HH22	2.16	0.43
1:b:171:PHE:CE2	1:b:203:LYS:HG3	2.54	0.43
3:S:44:ILE:HG22	1:T:170:ARG:HH11	1.83	0.43
1:T:34:LYS:HB2	1:T:53:TRP:HB2	2.01	0.43
1:V:23:ARG:HG3	1:V:25:ARG:NH1	2.34	0.43
1:W:144:THR:O	1:X:104:HIS:HE1	2.01	0.43
1:g:8:TYR:O	1:g:12:GLN:HG2	2.19	0.43
1:g:36:ILE:HB	1:g:51:VAL:HG12	2.01	0.43
4:m:301:09R:C1	1:n:114:THR:HB	2.49	0.43
1:H:41:VAL:HG22	1:H:48:VAL:HG12	2.01	0.43
1:H:144:THR:O	1:I:104:HIS:HE1	2.02	0.43
1:j:89:TYR:OH	4:j:301:09R:N3	2.52	0.43
1:A:206:ARG:H	1:A:206:ARG:HG3	1.55	0.43
1:B:144:THR:O	1:C:104:HIS:CE1	2.68	0.43
4:H:301:09R:H5	4:H:301:09R:H1	1.72	0.43
1:Z:67:SER:HA	1:Z:70:SER:HB2	2.01	0.43
1:e:30:SER:HB2	1:e:57:THR:HB	2.01	0.43
1:e:124:ASP:HB2	1:f:168:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:302:09R:H12	4:f:302:09R:H6	1.71	0.43
1:k:40:GLU:HB2	1:k:49:ASP:CB	2.48	0.43
1:A:22:GLN:HG3	1:A:25:ARG:HD3	2.01	0.43
4:F:301:09R:H3	1:G:104:HIS:CD2	2.54	0.43
1:H:143:TRP:CE2	1:I:99:THR:HG21	2.53	0.43
1:f:187:CYS:SG	1:f:188:CYS:N	2.92	0.43
1:F:124:ASP:HB2	1:G:168:TYR:CE1	2.54	0.42
1:X:94:LYS:HB2	1:X:94:LYS:HE3	1.82	0.42
1:N:144:THR:O	1:O:104:HIS:HE1	2.02	0.42
1:R:23:ARG:O	1:R:25:ARG:NE	2.52	0.42
1:K:67:SER:HA	1:K:70:SER:HB2	2.01	0.42
1:X:67:SER:HA	1:X:70:SER:HB2	2.01	0.42
1:b:67:SER:HA	1:b:70:SER:HB2	2.01	0.42
1:A:187:CYS:SG	1:A:188:CYS:N	2.91	0.42
4:D:301:09R:C1	1:E:114:THR:HB	2.49	0.42
1:M:144:THR:O	1:N:104:HIS:HE1	2.02	0.42
1:c:186:SER:OG	1:d:163:GLU:OE2	2.37	0.42
1:e:99:THR:HG21	1:i:143:TRP:CE2	2.55	0.42
1:g:144:THR:O	1:h:104:HIS:CE1	2.70	0.42
1:j:88:ALA:HB3	1:j:91:ALA:HB2	2.01	0.42
1:k:185:TYR:CE1	4:k:301:09R:H9	2.54	0.42
1:H:169:SER:C	1:H:171:PHE:H	2.26	0.42
1:T:189:PRO:HB3	1:a:180:LYS:O	2.19	0.42
1:d:185:TYR:CE1	4:d:301:09R:H9	2.55	0.42
1:C:192:TYR:CD2	4:C:301:09R:H121	2.54	0.42
1:D:204:LYS:HE2	7:D:420:HOH:O	2.19	0.42
4:S:301:09R:H1	4:S:301:09R:H5	1.80	0.42
1:Z:44:ILE:HG22	1:a:170:ARG:HD3	2.01	0.42
1:b:17:ASP:OD2	1:c:11:ARG:NH1	2.52	0.42
1:b:44:ILE:HG22	1:c:170:ARG:HD3	2.01	0.42
1:b:146:HIS:CE1	1:b:148:ARG:HB2	2.54	0.42
1:f:67:SER:HA	1:f:70:SER:HB2	2.02	0.42
1:m:143:TRP:CZ2	1:n:99:THR:HG21	2.55	0.42
1:A:12:GLN:HE21	1:F:12:GLN:NE2	2.18	0.42
1:D:143:TRP:CZ2	1:E:99:THR:HG21	2.54	0.42
1:F:25:ARG:NH1	7:F:401:HOH:O	2.51	0.42
1:K:34:LYS:HB2	1:K:53:TRP:HB2	2.00	0.42
1:R:60:ASP:HB3	1:R:63:LEU:HD12	2.01	0.42
1:c:67:SER:HA	1:c:70:SER:HB2	2.02	0.42
1:c:143:TRP:CZ2	1:d:99:THR:HG21	2.53	0.42
1:i:143:TRP:CZ3	4:i:301:09R:H7	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:TRP:CE2	4:C:301:09R:H5	2.54	0.42
1:G:169:SER:C	1:G:171:PHE:H	2.28	0.42
1:H:22:GLN:HE22	1:H:61:ARG:NH1	2.09	0.42
1:L:144:THR:O	1:M:104:HIS:HE1	2.02	0.42
1:h:67:SER:HA	1:h:70:SER:HB2	2.02	0.42
1:A:124:ASP:HB2	1:B:168:TYR:CE1	2.55	0.42
1:R:11:ARG:O	7:R:401:HOH:O	2.21	0.42
1:X:14:SER:OG	1:X:80:SER:O	2.29	0.42
1:h:60:ASP:HB3	1:h:63:LEU:HD12	2.02	0.42
4:i:301:09R:H5	4:i:301:09R:H1	1.70	0.42
4:P:301:09R:C1	1:Q:114:THR:HB	2.50	0.42
1:U:39:LEU:C	1:U:40:GLU:HG2	2.44	0.42
1:X:161:ASP:OD1	1:X:161:ASP:N	2.52	0.42
1:a:185:TYR:CE1	4:a:301:09R:H9	2.54	0.42
1:k:67:SER:HA	1:k:70:SER:HB2	2.02	0.42
1:n:187:CYS:SG	4:n:301:09R:H2	2.60	0.42
1:I:143:TRP:CE2	1:J:99:THR:HG21	2.55	0.41
4:Z:301:09R:H4	1:a:53:TRP:CZ3	2.54	0.41
1:f:114:THR:HB	4:f:301:09R:N1	2.34	0.41
1:i:36:ILE:HB	1:i:51:VAL:HG12	2.02	0.41
1:K:124:ASP:HB2	1:L:168:TYR:CE1	2.54	0.41
1:h:187:CYS:SG	4:h:301:09R:H2	2.60	0.41
1:e:23:ARG:HA	1:e:23:ARG:HD3	1.77	0.41
1:j:67:SER:HA	1:j:70:SER:HB2	2.02	0.41
1:n:67:SER:HA	1:n:70:SER:HB2	2.03	0.41
2:P:67:SER:HA	2:P:70:SER:HB2	2.03	0.41
1:T:187:CYS:SG	4:T:301:09R:H2	2.60	0.41
1:U:67:SER:HA	1:U:70:SER:HB2	2.03	0.41
1:b:88:ALA:HB3	1:b:91:ALA:HB2	2.03	0.41
1:c:143:TRP:CE3	4:c:301:09R:H7	2.56	0.41
1:c:159:SER:HB2	1:c:160:ASP:H	1.66	0.41
1:j:168:TYR:CE1	1:n:124:ASP:HB2	2.55	0.41
1:J:49:ASP:OD2	1:J:120[B]:ARG:HD3	2.21	0.41
2:P:104:HIS:CE1	1:T:144:THR:O	2.73	0.41
1:W:21:THR:HG21	1:X:3:ARG:NH1	2.35	0.41
1:n:88:ALA:HB3	1:n:91:ALA:HB2	2.02	0.41
1:N:169:SER:C	1:N:171:PHE:H	2.29	0.41
1:g:146:HIS:CE1	1:g:148:ARG:HB2	2.55	0.41
1:h:171:PHE:O	1:h:204:LYS:HE3	2.20	0.41
1:J:47:GLU:OE1	1:J:120[B]:ARG:NH2	2.52	0.41
1:e:172:GLU:OE1	1:e:204:LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:89:TYR:OH	4:f:302:09R:N3	2.37	0.41
1:k:30:SER:HB2	1:k:57:THR:HB	2.03	0.41
1:C:17:ASP:OD2	1:D:11:ARG:NH2	2.49	0.41
1:I:153:ASP:HA	1:I:154:PRO:HD3	1.97	0.41
1:J:23:ARG:HG3	1:J:25:ARG:NH2	2.36	0.41
1:M:89:TYR:OH	4:M:301:09R:N3	2.53	0.41
1:R:155:THR:HG21	7:R:420:HOH:O	2.21	0.41
1:W:143:TRP:CE2	1:X:99:THR:HG21	2.55	0.41
1:d:89:TYR:OH	4:d:301:09R:N3	2.53	0.41
1:e:163:GLU:OE2	1:i:186:SER:OG	2.38	0.41
1:l:172:GLU:OE2	1:l:202:ARG:NE	2.46	0.41
1:m:30:SER:HB2	1:m:57:THR:HB	2.03	0.41
1:B:15:ARG:NH2	1:C:11:ARG:HH22	2.19	0.41
1:F:19:ILE:C	1:F:21:THR:H	2.29	0.41
4:N:301:09R:H5	4:N:301:09R:H1	1.73	0.41
2:P:144:THR:O	1:Q:104[A]:HIS:HE1	2.04	0.41
3:S:143:TRP:CE2	1:T:99:THR:HG21	2.56	0.41
1:Y:67:SER:HA	1:Y:70:SER:HB2	2.03	0.41
1:Z:153:ASP:HA	1:Z:154:PRO:HD3	1.97	0.41
1:f:143:TRP:CE2	1:g:99:THR:HG21	2.55	0.41
1:g:88:ALA:HB3	1:g:91:ALA:HB2	2.02	0.41
1:j:12:GLN:NE2	1:j:12:GLN:CA	2.73	0.41
1:l:143:TRP:CE2	1:m:99:THR:HG21	2.56	0.41
1:K:144:THR:O	1:L:104:HIS:HE1	2.04	0.41
1:N:162:SER:O	1:N:162:SER:OG	2.33	0.41
1:d:14:SER:OG	1:d:80:SER:O	2.29	0.41
1:e:67:SER:HA	1:e:70:SER:HB2	2.03	0.41
1:f:34:LYS:HB2	1:f:53:TRP:HB2	2.02	0.41
1:h:94:LYS:HB2	1:h:94:LYS:HE3	1.79	0.41
1:m:143:TRP:CH2	4:m:301:09R:H7	2.55	0.41
1:X:188:CYS:SG	4:X:301:09R:H2	2.61	0.40
1:c:170:ARG:HH22	1:c:203:LYS:NZ	2.19	0.40
1:k:143:TRP:CZ2	1:l:99:THR:HG21	2.56	0.40
4:B:301:09R:H5	4:B:301:09R:H1	1.83	0.40
1:E:1:LEU:HB2	1:E:70:SER:OG	2.21	0.40
1:I:30:SER:HB2	1:I:57:THR:HB	2.04	0.40
1:J:1:LEU:HB2	1:J:70:SER:OG	2.21	0.40
4:P:301:09R:N1	1:Q:114:THR:HB	2.36	0.40
1:U:36:ILE:HB	1:U:51:VAL:HG12	2.04	0.40
1:Z:34:LYS:HB2	1:Z:53:TRP:HB2	2.02	0.40
4:j:301:09R:H2	4:j:301:09R:H11	2.00	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:67:SER:HA	1:I:70:SER:HB2	2.02	0.40
4:J:301:09R:H5	4:J:301:09R:H1	1.78	0.40
1:M:67:SER:HA	1:M:70:SER:HB2	2.03	0.40
4:S:301:09R:BR1	1:T:112:GLN:O	2.94	0.40
1:n:187:CYS:SG	1:n:188:CYS:N	2.95	0.40
1:B:188:CYS:SG	4:B:301:09R:H2	2.61	0.40
1:I:15:ARG:NH2	1:J:11:ARG:HH22	2.20	0.40
1:K:143:TRP:CE2	1:L:99:THR:HG21	2.57	0.40
1:O:187:CYS:SG	1:O:188:CYS:N	2.94	0.40
1:Q:146:HIS:CE1	1:Q:148:ARG:HB2	2.56	0.40
1:V:124:ASP:HB2	1:W:168:TYR:CZ	2.57	0.40
1:X:143:TRP:CE2	1:Y:99:THR:HG21	2.55	0.40
1:Y:169:SER:C	1:Y:171:PHE:H	2.29	0.40
1:i:67:SER:HA	1:i:70:SER:HB2	2.03	0.40
1:j:153:ASP:HA	1:j:154:PRO:HD3	1.97	0.40
1:m:143:TRP:CD2	4:m:301:09R:H7	2.56	0.40
1:H:15:ARG:HH21	1:I:11:ARG:NH2	2.18	0.40
1:H:15:ARG:HH21	1:I:11:ARG:HH21	1.68	0.40
1:R:34:LYS:HB2	1:R:53:TRP:HB2	2.03	0.40
1:R:143:TRP:CZ2	3:S:99:THR:HG21	2.56	0.40
1:W:124:ASP:HB2	1:X:168:TYR:CE1	2.57	0.40
1:X:88:ALA:HB3	1:X:91:ALA:HB2	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:HIS:NE2	1:k:22:GLN:NE2[2_454]	1.66	0.54
1:D:184:THR:OG1	1:I:184:THR:OG1[2_454]	1.81	0.39
1:V:25:ARG:NH2	1:d:66:ASN:OD1[1_455]	2.19	0.01

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	197/229 (86%)	194 (98%)	3 (2%)	0	100	100
1	B	192/229 (84%)	192 (100%)	0	0	100	100
1	C	197/229 (86%)	195 (99%)	2 (1%)	0	100	100
1	D	195/229 (85%)	195 (100%)	0	0	100	100
1	E	190/229 (83%)	190 (100%)	0	0	100	100
1	F	191/229 (83%)	190 (100%)	1 (0%)	0	100	100
1	G	196/229 (86%)	194 (99%)	2 (1%)	0	100	100
1	H	191/229 (83%)	188 (98%)	3 (2%)	0	100	100
1	I	197/229 (86%)	195 (99%)	2 (1%)	0	100	100
1	J	197/229 (86%)	194 (98%)	3 (2%)	0	100	100
1	K	192/229 (84%)	189 (98%)	3 (2%)	0	100	100
1	L	190/229 (83%)	189 (100%)	1 (0%)	0	100	100
1	M	193/229 (84%)	190 (98%)	3 (2%)	0	100	100
1	N	191/229 (83%)	189 (99%)	2 (1%)	0	100	100
1	O	190/229 (83%)	188 (99%)	2 (1%)	0	100	100
1	Q	192/229 (84%)	191 (100%)	1 (0%)	0	100	100
1	R	192/229 (84%)	191 (100%)	1 (0%)	0	100	100
1	T	186/229 (81%)	186 (100%)	0	0	100	100
1	U	191/229 (83%)	191 (100%)	0	0	100	100
1	V	195/229 (85%)	195 (100%)	0	0	100	100
1	W	191/229 (83%)	190 (100%)	1 (0%)	0	100	100
1	X	198/229 (86%)	197 (100%)	1 (0%)	0	100	100
1	Y	191/229 (83%)	189 (99%)	2 (1%)	0	100	100
1	Z	190/229 (83%)	188 (99%)	2 (1%)	0	100	100
1	a	192/229 (84%)	191 (100%)	1 (0%)	0	100	100
1	b	195/229 (85%)	194 (100%)	1 (0%)	0	100	100
1	c	196/229 (86%)	193 (98%)	3 (2%)	0	100	100
1	d	192/229 (84%)	190 (99%)	2 (1%)	0	100	100
1	e	194/229 (85%)	193 (100%)	1 (0%)	0	100	100
1	f	189/229 (82%)	187 (99%)	2 (1%)	0	100	100
1	g	194/229 (85%)	193 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	h	194/229 (85%)	190 (98%)	4 (2%)	0	100	100
1	i	191/229 (83%)	190 (100%)	1 (0%)	0	100	100
1	j	194/229 (85%)	192 (99%)	2 (1%)	0	100	100
1	k	192/229 (84%)	191 (100%)	1 (0%)	0	100	100
1	l	196/229 (86%)	195 (100%)	1 (0%)	0	100	100
1	m	195/229 (85%)	192 (98%)	3 (2%)	0	100	100
1	n	190/229 (83%)	188 (99%)	2 (1%)	0	100	100
2	P	197/228 (86%)	194 (98%)	3 (2%)	0	100	100
3	S	195/229 (85%)	194 (100%)	1 (0%)	0	100	100
All	All	7721/9159 (84%)	7657 (99%)	64 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	189/213 (89%)	184 (97%)	5 (3%)	40	70
1	B	184/213 (86%)	184 (100%)	0	100	100
1	C	187/213 (88%)	184 (98%)	3 (2%)	55	80
1	D	187/213 (88%)	184 (98%)	3 (2%)	55	80
1	E	182/213 (85%)	182 (100%)	0	100	100
1	F	183/213 (86%)	181 (99%)	2 (1%)	65	85
1	G	186/213 (87%)	183 (98%)	3 (2%)	55	80
1	H	183/213 (86%)	181 (99%)	2 (1%)	65	85
1	I	187/213 (88%)	182 (97%)	5 (3%)	39	69
1	J	187/213 (88%)	184 (98%)	3 (2%)	55	80
1	K	184/213 (86%)	183 (100%)	1 (0%)	81	92
1	L	183/213 (86%)	181 (99%)	2 (1%)	65	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	186/213 (87%)	184 (99%)	2 (1%)	65	85
1	N	183/213 (86%)	181 (99%)	2 (1%)	65	85
1	O	183/213 (86%)	180 (98%)	3 (2%)	55	80
1	Q	184/213 (86%)	183 (100%)	1 (0%)	81	92
1	R	185/213 (87%)	182 (98%)	3 (2%)	55	80
1	T	180/213 (84%)	180 (100%)	0	100	100
1	U	183/213 (86%)	181 (99%)	2 (1%)	65	85
1	V	185/213 (87%)	182 (98%)	3 (2%)	55	80
1	W	183/213 (86%)	181 (99%)	2 (1%)	65	85
1	X	188/213 (88%)	184 (98%)	4 (2%)	47	75
1	Y	183/213 (86%)	180 (98%)	3 (2%)	55	80
1	Z	182/213 (85%)	179 (98%)	3 (2%)	55	80
1	a	184/213 (86%)	183 (100%)	1 (0%)	81	92
1	b	185/213 (87%)	176 (95%)	9 (5%)	22	49
1	c	188/213 (88%)	183 (97%)	5 (3%)	39	69
1	d	184/213 (86%)	180 (98%)	4 (2%)	45	74
1	e	184/213 (86%)	179 (97%)	5 (3%)	39	69
1	f	182/213 (85%)	177 (97%)	5 (3%)	39	69
1	g	185/213 (87%)	180 (97%)	5 (3%)	39	69
1	h	187/213 (88%)	186 (100%)	1 (0%)	81	92
1	i	183/213 (86%)	182 (100%)	1 (0%)	81	92
1	j	185/213 (87%)	182 (98%)	3 (2%)	55	80
1	k	184/213 (86%)	179 (97%)	5 (3%)	39	69
1	l	186/213 (87%)	181 (97%)	5 (3%)	39	69
1	m	187/213 (88%)	183 (98%)	4 (2%)	47	75
1	n	182/213 (85%)	178 (98%)	4 (2%)	45	74
2	P	187/212 (88%)	183 (98%)	4 (2%)	47	75
3	S	187/213 (88%)	185 (99%)	2 (1%)	65	85
All	All	7387/8519 (87%)	7267 (98%)	120 (2%)	55	80

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	VAL
1	A	59	SER
1	A	62	THR
1	A	162	SER
1	A	206	ARG
1	C	41	VAL
1	C	62	THR
1	C	110	GLU
1	D	41	VAL
1	D	110	GLU
1	D	159	SER
1	F	22	GLN
1	F	40	GLU
1	G	41	VAL
1	G	122	SER
1	G	162	SER
1	H	110	GLU
1	H	120	ARG
1	I	24	ASP
1	I	40	GLU
1	I	62	THR
1	I	161	ASP
1	I	162	SER
1	J	11	ARG
1	J	41	VAL
1	J	104	HIS
1	K	40	GLU
1	L	41	VAL
1	L	104	HIS
1	M	41	VAL
1	M	94	LYS
1	N	41	VAL
1	N	110	GLU
1	O	40	GLU
1	O	41	VAL
1	O	110	GLU
2	P	21	THR
2	P	22	GLN
2	P	41	VAL
2	P	110	GLU
1	Q	41	VAL
1	R	22	GLN
1	R	41	VAL

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Mol	Chain	Res	Type
1	R	131	GLU
3	S	24	ASP
3	S	61	ARG
1	U	25	ARG
1	U	40	GLU
1	V	23	ARG
1	V	62	THR
1	V	120	ARG
1	W	22	GLN
1	W	25	ARG
1	X	25	ARG
1	X	41	VAL
1	X	110	GLU
1	X	161	ASP
1	Y	41	VAL
1	Y	62	THR
1	Y	120	ARG
1	Z	25	ARG
1	Z	41	VAL
1	Z	110	GLU
1	a	25	ARG
1	b	22	GLN
1	b	23	ARG
1	b	24	ASP
1	b	40	GLU
1	b	41	VAL
1	b	62	THR
1	b	120	ARG
1	b	131	GLU
1	b	203	LYS
1	c	24	ASP
1	c	110	GLU
1	c	120[A]	ARG
1	c	120[B]	ARG
1	c	159	SER
1	d	11	ARG
1	d	41	VAL
1	d	131	GLU
1	d	162	SER
1	e	21	THR
1	e	22	GLN
1	e	25	ARG

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Mol	Chain	Res	Type
1	e	40	GLU
1	e	131	GLU
1	f	11	ARG
1	f	25	ARG
1	f	104	HIS
1	f	120	ARG
1	f	129	ASP
1	g	23	ARG
1	g	24	ASP
1	g	41	VAL
1	g	104	HIS
1	g	120	ARG
1	h	41	VAL
1	i	41	VAL
1	j	40	GLU
1	j	41	VAL
1	j	120	ARG
1	k	24	ASP
1	k	25	ARG
1	k	41	VAL
1	k	104	HIS
1	k	110	GLU
1	l	23	ARG
1	l	24	ASP
1	l	41	VAL
1	l	110	GLU
1	l	131	GLU
1	m	40	GLU
1	m	41	VAL
1	m	110	GLU
1	m	159	SER
1	n	94	LYS
1	n	104	HIS
1	n	131	GLU
1	n	148	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (159) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	73	GLN
1	A	167	GLN

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Mol	Chain	Res	Type
1	B	104	HIS
1	B	112	GLN
1	C	69	HIS
1	C	104	HIS
1	C	112	GLN
1	D	12	GLN
1	D	69	HIS
1	D	104	HIS
1	D	112	GLN
1	D	145	HIS
1	E	112	GLN
1	F	9	ASN
1	F	12	GLN
1	F	69	HIS
1	F	104	HIS
1	G	12	GLN
1	G	69	HIS
1	G	104	HIS
1	G	112	GLN
1	H	12	GLN
1	H	22	GLN
1	H	55	GLN
1	H	69	HIS
1	H	104	HIS
1	H	112	GLN
1	H	167	GLN
1	H	200	ASN
1	I	69	HIS
1	I	104	HIS
1	I	112	GLN
1	I	119	GLN
1	J	55	GLN
1	J	104	HIS
1	J	112	GLN
1	K	12	GLN
1	K	69	HIS
1	K	104	HIS
1	K	112	GLN
1	K	200	ASN
1	L	12	GLN
1	L	69	HIS
1	L	104	HIS

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Mol	Chain	Res	Type
1	L	112	GLN
1	M	12	GLN
1	M	69	HIS
1	M	104	HIS
1	M	200	ASN
1	N	69	HIS
1	N	104	HIS
1	N	112	GLN
1	N	167	GLN
1	O	12	GLN
1	O	22	GLN
1	O	55	GLN
1	O	104	HIS
1	O	112	GLN
1	O	145	HIS
2	P	55	GLN
2	P	104	HIS
2	P	112	GLN
1	Q	69	HIS
1	Q	119	GLN
1	Q	167	GLN
1	R	22	GLN
1	R	55	GLN
1	R	69	HIS
1	R	104	HIS
1	R	112	GLN
1	R	167	GLN
3	S	69	HIS
3	S	112	GLN
3	S	145	HIS
3	S	200	ASN
1	T	12	GLN
1	T	69	HIS
1	T	73	GLN
1	T	104	HIS
1	T	112	GLN
1	U	69	HIS
1	U	104	HIS
1	U	112	GLN
1	V	12	GLN
1	V	55	GLN
1	V	69	HIS

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Mol	Chain	Res	Type
1	V	104	HIS
1	W	55	GLN
1	W	69	HIS
1	W	104	HIS
1	W	112	GLN
1	W	200	ASN
1	X	55	GLN
1	X	69	HIS
1	X	104	HIS
1	X	112	GLN
1	Y	55	GLN
1	Y	69	HIS
1	Y	104	HIS
1	Y	119	GLN
1	Y	167	GLN
1	Z	69	HIS
1	Z	200	ASN
1	a	12	GLN
1	a	69	HIS
1	a	104	HIS
1	a	112	GLN
1	b	55	GLN
1	b	69	HIS
1	b	167	GLN
1	c	69	HIS
1	c	112	GLN
1	c	167	GLN
1	d	12	GLN
1	d	55	GLN
1	d	104	HIS
1	d	112	GLN
1	e	12	GLN
1	e	69	HIS
1	e	104	HIS
1	e	167	GLN
1	f	12	GLN
1	f	69	HIS
1	f	104	HIS
1	f	112	GLN
1	f	167	GLN
1	g	12	GLN
1	g	55	GLN

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Mol	Chain	Res	Type
1	g	69	HIS
1	g	112	GLN
1	h	69	HIS
1	h	104	HIS
1	h	167	GLN
1	i	55	GLN
1	i	69	HIS
1	i	104	HIS
1	i	112	GLN
1	j	12	GLN
1	j	55	GLN
1	j	69	HIS
1	j	104	HIS
1	j	119	GLN
1	j	167	GLN
1	k	69	HIS
1	k	167	GLN
1	l	55	GLN
1	l	69	HIS
1	l	119	GLN
1	m	12	GLN
1	m	69	HIS
1	m	104	HIS
1	m	167	GLN
1	n	55	GLN
1	n	69	HIS
1	n	73	GLN
1	n	104	HIS
1	n	112	GLN
1	n	167	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

44 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$
4	09R	L	301	-	14,15,15	3.22	4 (28%)	14,19,19	2.97	7 (50%)
4	09R	F	301	-	14,15,15	3.45	3 (21%)	14,19,19	1.89	4 (28%)
4	09R	Y	301	-	14,15,15	3.27	4 (28%)	14,19,19	2.61	7 (50%)
4	09R	U	301	-	14,15,15	3.34	3 (21%)	14,19,19	1.94	5 (35%)
4	09R	X	301	-	14,15,15	3.33	3 (21%)	14,19,19	2.64	5 (35%)
4	09R	N	301	-	14,15,15	3.63	3 (21%)	14,19,19	2.13	5 (35%)
4	09R	D	301	-	14,15,15	3.08	3 (21%)	14,19,19	2.30	5 (35%)
4	09R	T	301	-	14,15,15	3.47	4 (28%)	14,19,19	1.71	3 (21%)
4	09R	M	301	-	14,15,15	3.38	4 (28%)	14,19,19	1.92	5 (35%)
4	09R	P	301	-	14,15,15	3.33	4 (28%)	14,19,19	2.05	6 (42%)
4	09R	S	301	-	14,15,15	3.37	4 (28%)	14,19,19	1.98	3 (21%)
4	09R	c	301	-	14,15,15	3.39	4 (28%)	14,19,19	1.94	5 (35%)
4	09R	R	301	-	14,15,15	3.38	3 (21%)	14,19,19	1.40	2 (14%)
4	09R	O	301	-	14,15,15	3.19	4 (28%)	14,19,19	1.77	6 (42%)
4	09R	A	301	-	14,15,15	3.10	4 (28%)	14,19,19	2.32	6 (42%)
4	09R	I	301	-	14,15,15	3.85	3 (21%)	14,19,19	2.81	7 (50%)
4	09R	k	301	-	14,15,15	3.37	3 (21%)	14,19,19	2.49	7 (50%)
4	09R	g	301	-	14,15,15	3.35	3 (21%)	14,19,19	2.02	5 (35%)
4	09R	Q	301	-	14,15,15	3.50	4 (28%)	14,19,19	1.18	2 (14%)
4	09R	l	301	-	14,15,15	3.36	3 (21%)	14,19,19	2.40	5 (35%)
4	09R	i	301	-	14,15,15	3.56	3 (21%)	14,19,19	2.00	5 (35%)
5	NAG	A	302	1	14,14,15	0.70	0	17,19,21	3.49	11 (64%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	09R	a	301	-	14,15,15	3.25	3 (21%)	14,19,19	2.73	7 (50%)
5	NAG	O	302	1	14,14,15	1.59	2 (14%)	17,19,21	3.63	10 (58%)
4	09R	j	301	-	14,15,15	3.47	3 (21%)	14,19,19	2.35	6 (42%)
4	09R	n	301	-	14,15,15	3.50	4 (28%)	14,19,19	2.32	5 (35%)
4	09R	B	301	-	14,15,15	3.35	3 (21%)	14,19,19	1.94	5 (35%)
4	09R	W	301	-	14,15,15	3.31	4 (28%)	14,19,19	2.58	7 (50%)
4	09R	E	301	-	14,15,15	3.42	3 (21%)	14,19,19	2.23	5 (35%)
4	09R	f	302	-	14,15,15	3.51	4 (28%)	14,19,19	2.21	5 (35%)
4	09R	K	301	-	14,15,15	3.42	4 (28%)	14,19,19	1.89	4 (28%)
4	09R	b	301	-	14,15,15	3.24	4 (28%)	14,19,19	2.71	7 (50%)
4	09R	V	302	-	14,15,15	3.54	5 (35%)	14,19,19	1.94	3 (21%)
4	09R	d	301	-	14,15,15	3.61	3 (21%)	14,19,19	2.45	6 (42%)
4	09R	m	301	-	14,15,15	3.76	3 (21%)	14,19,19	2.53	7 (50%)
4	09R	f	301	-	14,15,15	3.15	4 (28%)	14,19,19	3.43	9 (64%)
4	09R	H	301	-	14,15,15	3.22	3 (21%)	14,19,19	2.62	8 (57%)
5	NAG	d	302	1	14,14,15	0.71	0	17,19,21	3.49	11 (64%)
6	SO4	V	301	-	4,4,4	0.23	0	6,6,6	0.25	0
4	09R	C	301	-	14,15,15	3.39	5 (35%)	14,19,19	1.49	3 (21%)
4	09R	Z	301	-	14,15,15	3.33	3 (21%)	14,19,19	1.78	3 (21%)
4	09R	h	301	-	14,15,15	3.30	3 (21%)	14,19,19	2.40	7 (50%)
4	09R	J	301	-	14,15,15	3.42	3 (21%)	14,19,19	2.03	5 (35%)
4	09R	G	301	-	14,15,15	2.91	3 (21%)	14,19,19	2.66	6 (42%)

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
4	09R	L	301	-	-	0/4/13/13	0/2/2/2
4	09R	F	301	-	-	0/4/13/13	0/2/2/2
4	09R	Y	301	-	-	0/4/13/13	0/2/2/2
4	09R	U	301	-	-	0/4/13/13	0/2/2/2
4	09R	X	301	-	-	0/4/13/13	0/2/2/2
4	09R	N	301	-	-	0/4/13/13	0/2/2/2
4	09R	D	301	-	-	0/4/13/13	0/2/2/2
4	09R	T	301	-	-	0/4/13/13	0/2/2/2
4	09R	M	301	-	-	0/4/13/13	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	09R	P	301	-	-	0/4/13/13	0/2/2/2
4	09R	S	301	-	-	0/4/13/13	0/2/2/2
4	09R	c	301	-	-	0/4/13/13	0/2/2/2
4	09R	R	301	-	-	0/4/13/13	0/2/2/2
4	09R	O	301	-	-	0/4/13/13	0/2/2/2
4	09R	A	301	-	-	0/4/13/13	0/2/2/2
4	09R	I	301	-	-	0/4/13/13	0/2/2/2
4	09R	k	301	-	-	2/4/13/13	0/2/2/2
4	09R	g	301	-	-	0/4/13/13	0/2/2/2
4	09R	Q	301	-	-	0/4/13/13	0/2/2/2
4	09R	l	301	-	-	0/4/13/13	0/2/2/2
4	09R	i	301	-	-	0/4/13/13	0/2/2/2
5	NAG	A	302	1	-	4/6/23/26	0/1/1/1
4	09R	a	301	-	-	1/4/13/13	0/2/2/2
5	NAG	O	302	1	-	2/6/23/26	0/1/1/1
4	09R	j	301	-	-	0/4/13/13	0/2/2/2
4	09R	n	301	-	-	4/4/13/13	0/2/2/2
4	09R	B	301	-	-	0/4/13/13	0/2/2/2
4	09R	W	301	-	-	0/4/13/13	0/2/2/2
4	09R	E	301	-	-	0/4/13/13	0/2/2/2
4	09R	f	302	-	-	0/4/13/13	0/2/2/2
4	09R	K	301	-	-	0/4/13/13	0/2/2/2
4	09R	b	301	-	-	0/4/13/13	0/2/2/2
4	09R	V	302	-	-	0/4/13/13	0/2/2/2
4	09R	d	301	-	-	0/4/13/13	0/2/2/2
4	09R	m	301	-	-	0/4/13/13	0/2/2/2
4	09R	f	301	-	-	0/4/13/13	0/2/2/2
4	09R	H	301	-	-	0/4/13/13	0/2/2/2
5	NAG	d	302	1	-	4/6/23/26	0/1/1/1
4	09R	C	301	-	-	0/4/13/13	0/2/2/2
4	09R	Z	301	-	-	0/4/13/13	0/2/2/2
4	09R	h	301	-	-	0/4/13/13	0/2/2/2
4	09R	J	301	-	-	0/4/13/13	0/2/2/2
4	09R	G	301	-	-	0/4/13/13	0/2/2/2

All (142) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	301	09R	BR1-C5	-13.50	1.71	1.90
4	m	301	09R	BR1-C5	-12.93	1.71	1.90
4	N	301	09R	BR1-C5	-12.32	1.72	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	301	09R	BR1-C5	-12.19	1.72	1.90
4	i	301	09R	BR1-C5	-12.13	1.73	1.90
4	V	302	09R	BR1-C5	-12.00	1.73	1.90
4	f	302	09R	BR1-C5	-11.97	1.73	1.90
4	j	301	09R	BR1-C5	-11.97	1.73	1.90
4	n	301	09R	BR1-C5	-11.80	1.73	1.90
4	F	301	09R	BR1-C5	-11.77	1.73	1.90
4	Q	301	09R	BR1-C5	-11.75	1.73	1.90
4	J	301	09R	BR1-C5	-11.74	1.73	1.90
4	T	301	09R	BR1-C5	-11.63	1.73	1.90
4	g	301	09R	BR1-C5	-11.55	1.73	1.90
4	R	301	09R	BR1-C5	-11.46	1.74	1.90
4	S	301	09R	BR1-C5	-11.43	1.74	1.90
4	E	301	09R	BR1-C5	-11.40	1.74	1.90
4	P	301	09R	BR1-C5	-11.40	1.74	1.90
4	k	301	09R	BR1-C5	-11.39	1.74	1.90
4	K	301	09R	BR1-C5	-11.37	1.74	1.90
4	B	301	09R	BR1-C5	-11.33	1.74	1.90
4	Z	301	09R	BR1-C5	-11.30	1.74	1.90
4	M	301	09R	BR1-C5	-11.30	1.74	1.90
4	X	301	09R	BR1-C5	-11.28	1.74	1.90
4	l	301	09R	BR1-C5	-11.23	1.74	1.90
4	c	301	09R	BR1-C5	-11.17	1.74	1.90
4	h	301	09R	BR1-C5	-11.16	1.74	1.90
4	C	301	09R	BR1-C5	-11.07	1.74	1.90
4	U	301	09R	BR1-C5	-11.02	1.74	1.90
4	a	301	09R	BR1-C5	-10.83	1.74	1.90
4	O	301	09R	BR1-C5	-10.63	1.75	1.90
4	H	301	09R	BR1-C5	-10.61	1.75	1.90
4	L	301	09R	BR1-C5	-10.49	1.75	1.90
4	b	301	09R	BR1-C5	-10.42	1.75	1.90
4	f	301	09R	BR1-C5	-10.37	1.75	1.90
4	A	301	09R	BR1-C5	-10.36	1.75	1.90
4	W	301	09R	BR1-C5	-10.34	1.75	1.90
4	Y	301	09R	BR1-C5	-10.24	1.75	1.90
4	D	301	09R	BR1-C5	-10.24	1.75	1.90
4	G	301	09R	BR1-C5	-9.67	1.76	1.90
5	O	302	NAG	C1-C2	3.80	1.57	1.52
4	Y	301	09R	C4-C5	3.52	1.43	1.38
4	W	301	09R	C4-C5	3.37	1.43	1.38
4	f	301	09R	C4-C5	3.37	1.43	1.38
4	W	301	09R	C3-C2	3.34	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	301	09R	C4-C5	3.23	1.43	1.38
5	O	302	NAG	C2-N2	3.21	1.51	1.46
4	Y	301	09R	C3-C2	3.20	1.45	1.39
4	K	301	09R	C4-C5	3.20	1.43	1.38
4	H	301	09R	C4-C5	3.19	1.43	1.38
4	d	301	09R	C4-C5	3.17	1.43	1.38
4	O	301	09R	C4-C5	3.16	1.43	1.38
4	N	301	09R	C3-C2	3.16	1.45	1.39
4	m	301	09R	C4-C5	3.11	1.43	1.38
4	E	301	09R	C4-C5	3.09	1.43	1.38
4	N	301	09R	C4-C5	3.08	1.43	1.38
4	a	301	09R	C4-C5	3.05	1.43	1.38
4	C	301	09R	C3-C2	3.03	1.45	1.39
4	l	301	09R	C4-C5	3.01	1.43	1.38
4	U	301	09R	C4-C5	2.99	1.43	1.38
4	m	301	09R	C3-C2	2.96	1.44	1.39
4	k	301	09R	C4-C5	2.96	1.43	1.38
4	T	301	09R	C3-C2	2.95	1.44	1.39
4	n	301	09R	C3-C2	2.95	1.44	1.39
4	d	301	09R	C3-C2	2.94	1.44	1.39
4	L	301	09R	C3-C2	2.93	1.44	1.39
4	G	301	09R	C4-C5	2.93	1.42	1.38
4	l	301	09R	C3-C2	2.92	1.44	1.39
4	i	301	09R	C4-C5	2.91	1.42	1.38
4	i	301	09R	C3-C2	2.90	1.44	1.39
4	E	301	09R	C3-C2	2.89	1.44	1.39
4	c	301	09R	C4-C5	2.88	1.42	1.38
4	b	301	09R	C3-C2	2.88	1.44	1.39
4	Q	301	09R	C3-C2	2.84	1.44	1.39
4	b	301	09R	C4-C5	2.84	1.42	1.38
4	Q	301	09R	C4-C5	2.82	1.42	1.38
4	H	301	09R	C3-C2	2.81	1.44	1.39
4	I	301	09R	C4-C5	2.80	1.42	1.38
4	K	301	09R	C3-C2	2.79	1.44	1.39
4	B	301	09R	C4-C5	2.79	1.42	1.38
4	f	302	09R	C3-C2	2.77	1.44	1.39
4	h	301	09R	C4-C5	2.77	1.42	1.38
4	a	301	09R	C3-C2	2.76	1.44	1.39
4	c	301	09R	C3-C2	2.75	1.44	1.39
4	f	301	09R	C3-C2	2.74	1.44	1.39
4	R	301	09R	C3-C2	2.73	1.44	1.39
4	B	301	09R	C3-C2	2.71	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	n	301	09R	C4-C5	2.71	1.42	1.38
4	X	301	09R	C3-C2	2.70	1.44	1.39
4	A	301	09R	C4-C5	2.70	1.42	1.38
4	D	301	09R	C4-C5	2.70	1.42	1.38
4	T	301	09R	C4-C5	2.67	1.42	1.38
4	D	301	09R	C3-C2	2.63	1.44	1.39
4	M	301	09R	C4-C5	2.62	1.42	1.38
4	F	301	09R	C3-C2	2.62	1.44	1.39
4	Z	301	09R	C3-C2	2.61	1.44	1.39
4	Z	301	09R	C4-C5	2.60	1.42	1.38
4	g	301	09R	C4-C5	2.59	1.42	1.38
4	C	301	09R	C5-N1	2.58	1.38	1.32
4	F	301	09R	C4-C5	2.57	1.42	1.38
4	k	301	09R	C3-C2	2.56	1.44	1.39
4	g	301	09R	C3-C2	2.54	1.44	1.39
4	J	301	09R	C4-C5	2.53	1.42	1.38
4	G	301	09R	C3-C2	2.53	1.44	1.39
4	X	301	09R	C4-C5	2.53	1.42	1.38
4	U	301	09R	C3-C2	2.49	1.44	1.39
4	C	301	09R	C4-C5	2.46	1.42	1.38
4	J	301	09R	C3-C2	2.45	1.43	1.39
4	Q	301	09R	C1-C2	2.44	1.43	1.38
4	S	301	09R	C3-C2	2.39	1.43	1.39
4	f	302	09R	C4-C5	2.38	1.42	1.38
4	b	301	09R	C8-N3	2.38	1.52	1.47
4	M	301	09R	C3-C2	2.34	1.43	1.39
4	V	302	09R	C8-N3	2.33	1.52	1.47
4	V	302	09R	C3-C2	2.32	1.43	1.39
4	S	301	09R	C4-C5	2.31	1.42	1.38
4	h	301	09R	C3-C2	2.31	1.43	1.39
4	P	301	09R	C3-C2	2.30	1.43	1.39
4	j	301	09R	C3-C2	2.29	1.43	1.39
4	C	301	09R	C1-C2	2.22	1.42	1.38
4	I	301	09R	C3-C2	2.22	1.43	1.39
4	V	302	09R	C4-C5	2.22	1.41	1.38
4	L	301	09R	C4-C3	2.21	1.42	1.38
4	Y	301	09R	C1-C2	2.21	1.42	1.38
4	T	301	09R	C5-N1	2.20	1.37	1.32
4	j	301	09R	C4-C5	2.19	1.41	1.38
4	A	301	09R	C3-C2	2.17	1.43	1.39
4	P	301	09R	C1-C2	2.15	1.42	1.38
4	f	301	09R	C4-C3	2.14	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	301	09R	C1-C2	2.13	1.42	1.38
4	S	301	09R	C8-N3	2.13	1.51	1.47
4	P	301	09R	C4-C5	2.11	1.41	1.38
4	K	301	09R	C1-C2	2.11	1.42	1.38
4	W	301	09R	C1-C2	2.11	1.42	1.38
4	c	301	09R	C1-C2	2.10	1.42	1.38
4	R	301	09R	C5-N1	2.06	1.37	1.32
4	O	301	09R	C1-C2	2.05	1.42	1.38
4	V	302	09R	C10-N2	2.05	1.49	1.46
4	A	301	09R	C1-C2	2.04	1.42	1.38
4	n	301	09R	C1-C2	2.03	1.42	1.38
4	f	302	09R	C10-N2	2.02	1.49	1.46
4	O	301	09R	C3-C2	2.01	1.43	1.39

All (245) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	302	NAG	C1-O5-C5	7.99	122.89	112.19
5	d	302	NAG	C1-O5-C5	7.98	122.88	112.19
5	A	302	NAG	C2-N2-C7	7.74	133.27	122.90
5	d	302	NAG	C2-N2-C7	7.73	133.26	122.90
5	O	302	NAG	C1-O5-C5	6.92	121.46	112.19
5	O	302	NAG	C2-N2-C7	6.75	131.94	122.90
5	O	302	NAG	C4-C3-C2	6.74	120.90	111.02
4	f	301	09R	BR1-C5-C4	6.71	125.52	118.69
4	G	301	09R	C1-N1-C5	6.21	120.79	116.58
4	L	301	09R	BR1-C5-C4	6.05	124.85	118.69
4	I	301	09R	BR1-C5-C4	5.85	124.64	118.69
4	b	301	09R	C1-N1-C5	5.62	120.39	116.58
4	X	301	09R	C1-N1-C5	5.59	120.38	116.58
4	X	301	09R	BR1-C5-C4	5.59	124.38	118.69
4	f	301	09R	C3-C4-C5	5.45	121.05	117.41
4	b	301	09R	BR1-C5-C4	5.26	124.04	118.69
4	D	301	09R	C1-N1-C5	5.23	120.13	116.58
4	a	301	09R	BR1-C5-C4	5.15	123.93	118.69
4	d	301	09R	BR1-C5-C4	5.13	123.91	118.69
4	H	301	09R	BR1-C5-C4	5.06	123.84	118.69
4	A	301	09R	C3-C4-C5	4.97	120.73	117.41
4	Y	301	09R	BR1-C5-C4	4.91	123.69	118.69
4	L	301	09R	C1-N1-C5	4.89	119.90	116.58
4	l	301	09R	C1-N1-C5	4.83	119.86	116.58
4	k	301	09R	BR1-C5-C4	4.83	123.60	118.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	f	301	09R	C3-C2-N2	4.82	128.09	121.39
4	I	301	09R	C1-N1-C5	4.81	119.85	116.58
4	a	301	09R	C1-N1-C5	4.79	119.83	116.58
4	G	301	09R	BR1-C5-C4	4.79	123.56	118.69
4	W	301	09R	BR1-C5-C4	4.76	123.53	118.69
5	O	302	NAG	C1-C2-N2	4.66	117.77	110.43
4	V	302	09R	C9-C10-N2	4.66	121.75	113.63
4	l	301	09R	BR1-C5-C4	4.64	123.42	118.69
4	W	301	09R	C1-N1-C5	4.63	119.72	116.58
4	h	301	09R	BR1-C5-C4	4.60	123.37	118.69
4	j	301	09R	BR1-C5-C4	4.59	123.36	118.69
4	m	301	09R	BR1-C5-C4	4.59	123.36	118.69
4	H	301	09R	C1-N1-C5	4.57	119.68	116.58
4	Y	301	09R	C1-N1-C5	4.50	119.64	116.58
4	S	301	09R	C1-N1-C5	4.50	119.64	116.58
4	m	301	09R	C1-C2-N2	-4.45	115.05	121.80
4	a	301	09R	C9-C10-N2	4.38	121.27	113.63
4	f	302	09R	C1-N1-C5	4.37	119.54	116.58
4	B	301	09R	C1-N1-C5	4.30	119.50	116.58
4	D	301	09R	BR1-C5-C4	4.28	123.05	118.69
4	N	301	09R	C1-N1-C5	4.26	119.47	116.58
5	O	302	NAG	C3-C4-C5	4.24	117.92	110.23
4	f	301	09R	C1-C2-N2	-4.18	115.45	121.80
4	L	301	09R	C3-C2-N2	4.16	127.17	121.39
4	f	302	09R	BR1-C5-C4	4.15	122.91	118.69
4	E	301	09R	C1-N1-C5	4.14	119.39	116.58
4	f	301	09R	C1-N1-C5	4.05	119.33	116.58
4	i	301	09R	BR1-C5-C4	4.02	122.78	118.69
4	P	301	09R	C3-C4-C5	4.01	120.09	117.41
4	R	301	09R	C1-N1-C5	3.96	119.27	116.58
4	T	301	09R	C1-N1-C5	3.87	119.20	116.58
4	d	301	09R	C1-C2-N2	-3.86	115.95	121.80
4	n	301	09R	BR1-C5-C4	3.84	122.60	118.69
5	d	302	NAG	C1-C2-N2	3.80	116.42	110.43
4	J	301	09R	C9-C10-N2	3.80	120.25	113.63
5	A	302	NAG	C1-C2-N2	3.79	116.40	110.43
4	E	301	09R	BR1-C5-C4	3.78	122.53	118.69
4	m	301	09R	BR1-C5-N1	-3.77	111.92	116.32
4	g	301	09R	C9-C10-N2	3.76	120.20	113.63
4	S	301	09R	C9-C10-N2	3.74	120.15	113.63
4	W	301	09R	C9-C10-N2	3.73	120.13	113.63
4	j	301	09R	C1-N1-C5	3.71	119.10	116.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Y	301	09R	C3-C2-N2	3.71	126.54	121.39
4	l	301	09R	C9-C10-N2	3.69	120.07	113.63
4	Z	301	09R	BR1-C5-C4	3.68	122.43	118.69
4	n	301	09R	C9-C10-N2	3.67	120.03	113.63
4	U	301	09R	C1-N1-C5	3.66	119.06	116.58
4	F	301	09R	C1-N1-C5	3.64	119.05	116.58
4	A	301	09R	BR1-C5-C4	3.63	122.39	118.69
4	k	301	09R	C1-N1-C5	3.63	119.04	116.58
5	d	302	NAG	O5-C5-C6	3.62	114.71	107.66
5	A	302	NAG	O5-C5-C6	3.61	114.70	107.66
5	d	302	NAG	O7-C7-C8	-3.61	115.62	122.05
5	A	302	NAG	O7-C7-C8	-3.60	115.64	122.05
4	i	301	09R	C1-C2-N2	-3.59	116.35	121.80
4	n	301	09R	C1-N1-C5	3.59	119.02	116.58
4	d	301	09R	C3-C2-N2	3.56	126.34	121.39
4	E	301	09R	C1-C2-N2	-3.55	116.41	121.80
5	O	302	NAG	O7-C7-C8	-3.55	115.73	122.05
4	g	301	09R	C1-N1-C5	3.52	118.97	116.58
4	L	301	09R	C1-C2-N2	-3.52	116.46	121.80
4	W	301	09R	C3-C2-N2	3.52	126.28	121.39
4	M	301	09R	BR1-C5-C4	3.49	122.24	118.69
4	k	301	09R	C9-C10-N2	3.48	119.70	113.63
4	N	301	09R	C1-C2-N2	-3.48	116.52	121.80
4	P	301	09R	BR1-C5-C4	3.46	122.21	118.69
4	U	301	09R	C9-C10-N2	3.45	119.65	113.63
4	c	301	09R	BR1-C5-C4	3.43	122.18	118.69
4	h	301	09R	C1-N1-C5	3.43	118.91	116.58
4	Y	301	09R	C9-C10-N2	3.41	119.58	113.63
4	J	301	09R	BR1-C5-C4	3.41	122.16	118.69
4	F	301	09R	BR1-C5-C4	3.40	122.16	118.69
4	h	301	09R	C3-C4-C5	3.38	119.67	117.41
4	m	301	09R	C7-C6-N2	-3.36	107.15	113.11
5	O	302	NAG	O5-C1-C2	3.35	116.48	111.29
4	I	301	09R	C9-C10-N2	3.32	119.42	113.63
4	J	301	09R	C1-N1-C5	3.31	118.83	116.58
4	Z	301	09R	C1-N1-C5	3.27	118.80	116.58
4	N	301	09R	BR1-C5-C4	3.26	122.01	118.69
4	I	301	09R	C3-C4-C5	3.25	119.58	117.41
4	C	301	09R	C1-N1-C5	3.25	118.78	116.58
4	d	301	09R	BR1-C5-N1	-3.25	112.53	116.32
4	K	301	09R	BR1-C5-C4	3.25	121.99	118.69
4	c	301	09R	C1-N1-C5	3.24	118.78	116.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	301	09R	C3-C2-N2	3.22	125.86	121.39
4	G	301	09R	C3-C4-C5	3.20	119.55	117.41
4	G	301	09R	C4-C5-N1	-3.20	119.96	124.83
4	m	301	09R	C3-C2-N2	3.20	125.83	121.39
4	j	301	09R	C3-C2-N2	3.19	125.82	121.39
4	K	301	09R	C9-C10-N2	3.16	119.15	113.63
4	H	301	09R	C3-C2-N2	3.14	125.75	121.39
4	K	301	09R	C1-C2-N2	-3.13	117.04	121.80
4	b	301	09R	C3-C2-N2	3.13	125.74	121.39
4	g	301	09R	C7-C6-N2	-3.12	107.58	113.11
5	A	302	NAG	O6-C6-C5	3.10	121.90	111.33
4	f	301	09R	C4-C5-N1	-3.10	120.11	124.83
5	d	302	NAG	O6-C6-C5	3.09	121.87	111.33
4	E	301	09R	C3-C2-N2	3.06	125.64	121.39
4	h	301	09R	C9-C10-N2	3.06	118.96	113.63
4	f	302	09R	C9-C10-N2	3.03	118.92	113.63
4	Y	301	09R	C1-C2-N2	-3.02	117.22	121.80
4	a	301	09R	C1-C2-N2	-3.01	117.24	121.80
4	F	301	09R	C1-C2-N2	-2.99	117.26	121.80
4	b	301	09R	C1-C2-N2	-2.99	117.26	121.80
4	n	301	09R	C3-C2-N2	2.98	125.53	121.39
4	a	301	09R	C3-C2-N2	2.98	125.53	121.39
4	J	301	09R	C1-C2-N2	-2.95	117.33	121.80
4	n	301	09R	C7-C6-N2	-2.95	107.89	113.11
4	O	301	09R	C1-N1-C5	2.94	118.58	116.58
4	O	301	09R	BR1-C5-C4	2.94	121.68	118.69
4	L	301	09R	C9-C10-N2	2.91	118.71	113.63
4	B	301	09R	BR1-C5-C4	2.90	121.64	118.69
4	j	301	09R	C1-C2-N2	-2.89	117.41	121.80
4	H	301	09R	C3-C4-C5	2.89	119.34	117.41
4	S	301	09R	BR1-C5-C4	2.86	121.61	118.69
4	i	301	09R	C3-C2-N2	2.86	125.36	121.39
4	h	301	09R	C3-C2-N2	2.85	125.35	121.39
4	M	301	09R	C3-C4-C5	2.84	119.31	117.41
4	c	301	09R	C9-C10-N2	2.84	118.58	113.63
4	A	301	09R	C1-N1-C5	2.84	118.50	116.58
4	W	301	09R	C1-C2-N2	-2.83	117.50	121.80
4	g	301	09R	BR1-C5-C4	2.83	121.57	118.69
4	c	301	09R	C3-C2-N2	2.82	125.31	121.39
4	k	301	09R	C3-C4-C5	2.82	119.29	117.41
4	V	302	09R	C1-N1-C5	2.81	118.49	116.58
4	i	301	09R	BR1-C5-N1	-2.81	113.05	116.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	301	09R	BR1-C5-C4	2.80	121.54	118.69
4	k	301	09R	C3-C2-N2	2.79	125.27	121.39
4	d	301	09R	C1-N1-C5	2.79	118.47	116.58
4	i	301	09R	C1-N1-C5	2.78	118.46	116.58
4	b	301	09R	C9-C10-N2	2.78	118.47	113.63
4	I	301	09R	C4-C5-N1	-2.77	120.62	124.83
4	H	301	09R	C1-C2-N2	-2.75	117.62	121.80
5	d	302	NAG	C8-C7-N2	2.74	120.67	116.12
5	A	302	NAG	C8-C7-N2	2.74	120.66	116.12
4	B	301	09R	C9-C10-N2	2.73	118.40	113.63
4	Z	301	09R	C3-C4-C5	2.73	119.23	117.41
4	f	302	09R	C3-C2-N2	2.70	125.14	121.39
4	A	301	09R	C3-C2-N2	2.67	125.11	121.39
4	k	301	09R	C1-C2-N2	-2.66	117.76	121.80
4	M	301	09R	C9-C10-N2	2.66	118.26	113.63
4	L	301	09R	C3-C4-C5	2.65	119.18	117.41
4	K	301	09R	C3-C2-N2	2.64	125.06	121.39
4	F	301	09R	C3-C2-N2	2.63	125.05	121.39
4	H	301	09R	C9-C10-N2	2.63	118.21	113.63
4	P	301	09R	C3-C2-N2	2.62	125.03	121.39
4	L	301	09R	C4-C5-N1	-2.62	120.85	124.83
4	A	301	09R	C4-C5-N1	-2.62	120.85	124.83
4	I	301	09R	C3-C2-N2	2.62	125.02	121.39
4	b	301	09R	C4-C5-N1	-2.61	120.87	124.83
4	l	301	09R	C3-C2-N2	2.59	124.98	121.39
4	N	301	09R	BR1-C5-N1	-2.56	113.34	116.32
4	f	301	09R	C9-C10-N2	2.55	118.07	113.63
4	U	301	09R	C3-C4-C5	2.53	119.10	117.41
4	D	301	09R	C3-C2-N2	2.52	124.88	121.39
4	J	301	09R	C3-C2-N2	2.49	124.85	121.39
4	D	301	09R	C4-C5-N1	-2.49	121.04	124.83
5	O	302	NAG	C8-C7-N2	2.47	120.21	116.12
4	C	301	09R	C3-C2-N2	2.46	124.81	121.39
4	X	301	09R	C4-C5-N1	-2.46	121.09	124.83
4	H	301	09R	C4-C5-N1	-2.45	121.11	124.83
5	A	302	NAG	O3-C3-C2	-2.44	104.33	109.40
4	W	301	09R	C4-C5-N1	-2.43	121.13	124.83
5	d	302	NAG	O3-C3-C2	-2.43	104.35	109.40
4	a	301	09R	C4-C5-N1	-2.43	121.14	124.83
4	C	301	09R	C1-C2-N2	-2.42	118.12	121.80
4	b	301	09R	C3-C4-C5	2.41	119.02	117.41
5	A	302	NAG	C3-C4-C5	2.40	114.59	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	09R	C3-C2-N2	2.40	124.73	121.39
4	f	302	09R	C1-C2-N2	-2.39	118.18	121.80
4	A	301	09R	C1-C2-N2	-2.39	118.18	121.80
5	d	302	NAG	C3-C4-C5	2.38	114.56	110.23
4	O	301	09R	C3-C4-C5	2.36	118.98	117.41
4	Y	301	09R	C4-C5-N1	-2.35	121.25	124.83
4	Q	301	09R	C9-C10-N2	2.33	117.69	113.63
4	d	301	09R	C9-C10-N2	2.33	117.69	113.63
4	T	301	09R	C1-C2-N2	-2.32	118.28	121.80
4	j	301	09R	C9-C10-N2	2.31	117.66	113.63
4	h	301	09R	C4-C5-N1	-2.29	121.35	124.83
4	f	301	09R	C7-C6-N2	-2.28	109.07	113.11
5	d	302	NAG	O5-C1-C2	2.28	114.82	111.29
5	A	302	NAG	O5-C1-C2	2.27	114.80	111.29
5	d	302	NAG	O4-C4-C5	2.26	114.89	109.32
4	I	301	09R	C10-C9-C8	2.26	119.21	113.91
4	M	301	09R	C1-N1-C5	2.26	118.11	116.58
4	E	301	09R	C10-C9-C8	2.25	119.19	113.91
4	m	301	09R	C4-C3-C2	-2.25	117.45	120.30
5	A	302	NAG	O4-C4-C5	2.25	114.87	109.32
4	Y	301	09R	C3-C4-C5	2.25	118.91	117.41
5	O	302	NAG	O6-C6-C5	2.24	118.97	111.33
4	m	301	09R	C9-C10-N2	2.24	117.54	113.63
4	B	301	09R	C1-C2-N2	-2.24	118.40	121.80
4	N	301	09R	C3-C4-C5	-2.24	115.91	117.41
4	G	301	09R	C3-C2-N2	2.23	124.49	121.39
4	c	301	09R	C1-C2-N2	-2.22	118.43	121.80
4	M	301	09R	C3-C2-N2	2.21	124.46	121.39
4	j	301	09R	C3-C4-C5	2.21	118.89	117.41
4	f	301	09R	C4-C3-C2	-2.21	117.50	120.30
4	Q	301	09R	C7-C6-N2	-2.19	109.23	113.11
4	H	301	09R	C7-C6-N2	-2.19	109.23	113.11
4	V	302	09R	BR1-C5-C4	2.19	120.92	118.69
4	X	301	09R	C1-C2-N2	-2.18	118.49	121.80
4	R	301	09R	C9-C10-N2	2.17	117.42	113.63
4	P	301	09R	C9-C10-N2	2.17	117.41	113.63
4	P	301	09R	C4-C5-N1	-2.16	121.54	124.83
4	O	301	09R	C1-C2-N2	-2.15	118.53	121.80
4	O	301	09R	C9-C10-N2	2.15	117.37	113.63
4	W	301	09R	C3-C4-C5	2.14	118.84	117.41
4	P	301	09R	C1-N1-C5	2.12	118.02	116.58
4	h	301	09R	C1-C2-N2	-2.10	118.61	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	301	09R	C9-C10-N2	2.08	117.26	113.63
4	l	301	09R	C4-C5-N1	-2.08	121.67	124.83
4	k	301	09R	C4-C5-N1	-2.07	121.68	124.83
4	g	301	09R	C1-C2-N2	-2.07	118.66	121.80
4	G	301	09R	C1-C2-N2	-2.07	118.67	121.80
4	a	301	09R	C10-C9-C8	2.06	118.73	113.91
4	T	301	09R	C3-C2-N2	2.06	124.25	121.39
5	O	302	NAG	C6-C5-C4	-2.04	108.01	113.02
4	U	301	09R	C4-C5-N1	-2.03	121.75	124.83
4	O	301	09R	C4-C5-N1	-2.00	121.78	124.83

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	O	302	NAG	O5-C5-C6-O6
5	O	302	NAG	C4-C5-C6-O6
5	A	302	NAG	O5-C5-C6-O6
5	d	302	NAG	O5-C5-C6-O6
5	A	302	NAG	C8-C7-N2-C2
5	A	302	NAG	O7-C7-N2-C2
5	d	302	NAG	C8-C7-N2-C2
5	d	302	NAG	O7-C7-N2-C2
4	n	301	09R	C1-C2-N2-C10
5	A	302	NAG	C4-C5-C6-O6
5	d	302	NAG	C4-C5-C6-O6
4	k	301	09R	C1-C2-N2-C6
4	n	301	09R	C1-C2-N2-C6
4	n	301	09R	C3-C2-N2-C6
4	n	301	09R	C3-C2-N2-C10
4	a	301	09R	C3-C2-N2-C6
4	k	301	09R	C3-C2-N2-C6

There are no ring outliers.

37 monomers are involved in 99 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	301	09R	2	0
4	F	301	09R	2	0
4	Y	301	09R	2	0
4	U	301	09R	2	0

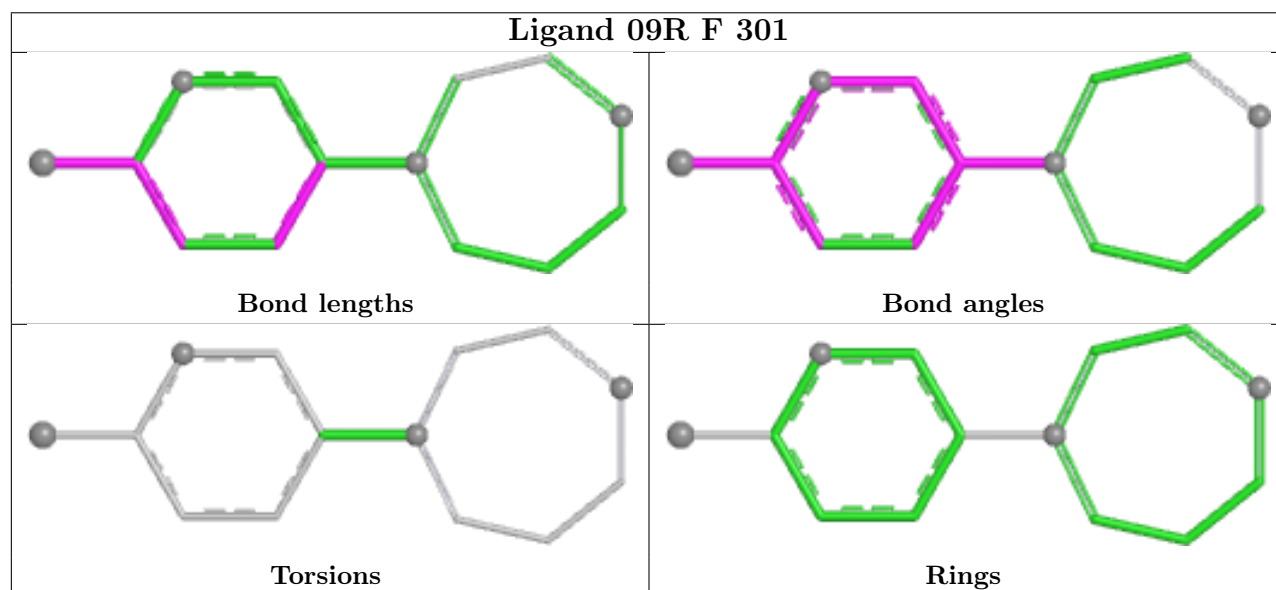
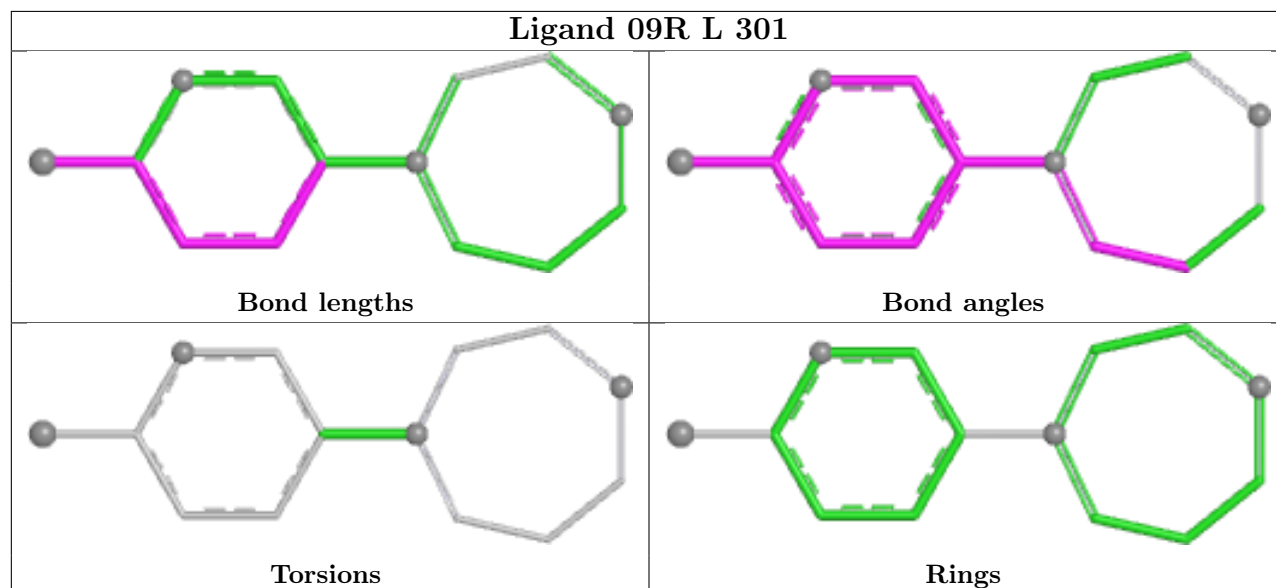
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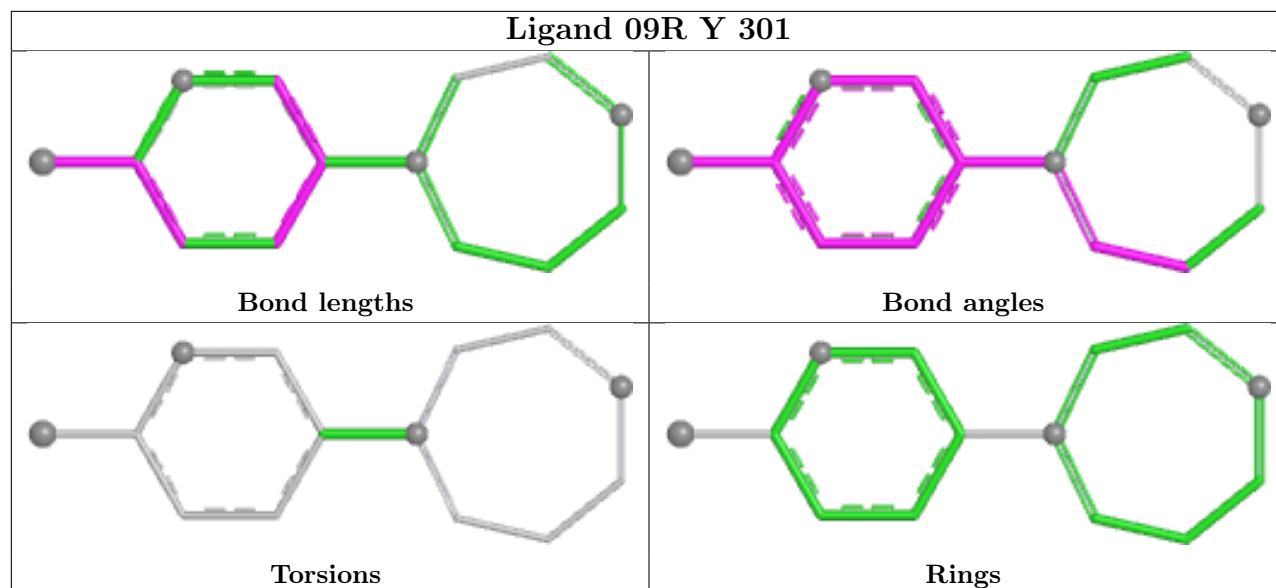
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	301	09R	3	0
4	N	301	09R	1	0
4	D	301	09R	4	0
4	T	301	09R	2	0
4	M	301	09R	2	0
4	P	301	09R	5	0
4	S	301	09R	3	0
4	c	301	09R	2	0
4	R	301	09R	2	0
4	O	301	09R	2	0
4	A	301	09R	1	0
4	k	301	09R	3	0
4	g	301	09R	5	0
4	l	301	09R	2	0
4	i	301	09R	3	0
4	a	301	09R	4	0
4	j	301	09R	5	0
4	n	301	09R	2	0
4	B	301	09R	3	0
4	W	301	09R	2	0
4	E	301	09R	2	0
4	f	302	09R	4	0
4	b	301	09R	1	0
4	V	302	09R	1	0
4	d	301	09R	3	0
4	m	301	09R	6	0
4	f	301	09R	4	0
4	H	301	09R	2	0
4	C	301	09R	3	0
4	Z	301	09R	1	0
4	h	301	09R	3	0
4	J	301	09R	2	0
4	G	301	09R	3	0

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

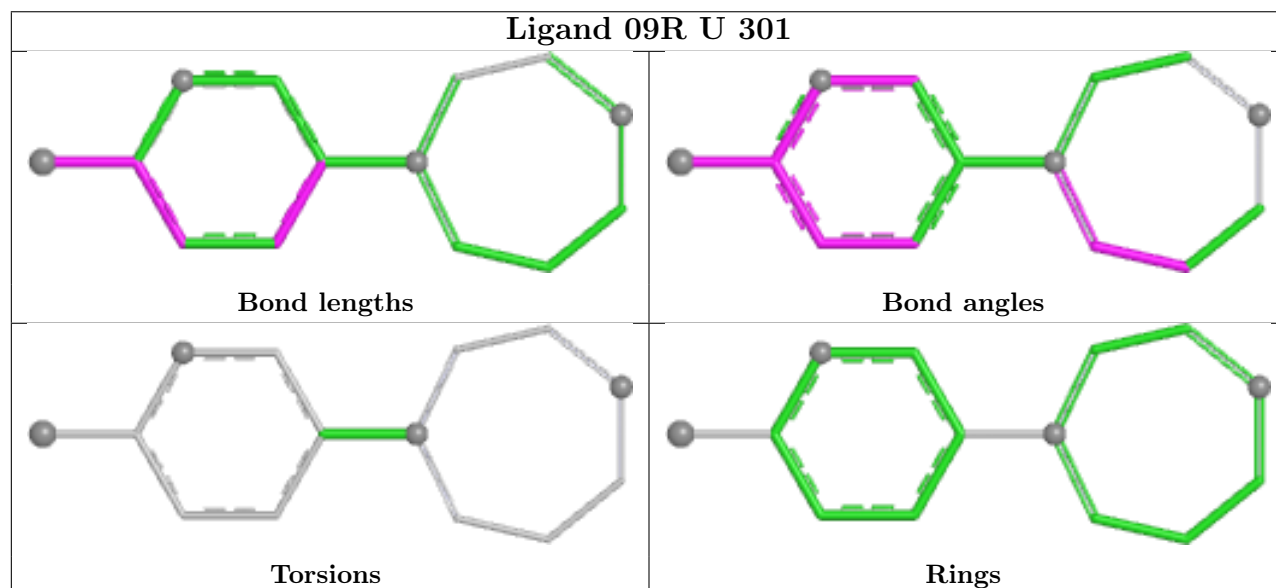
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



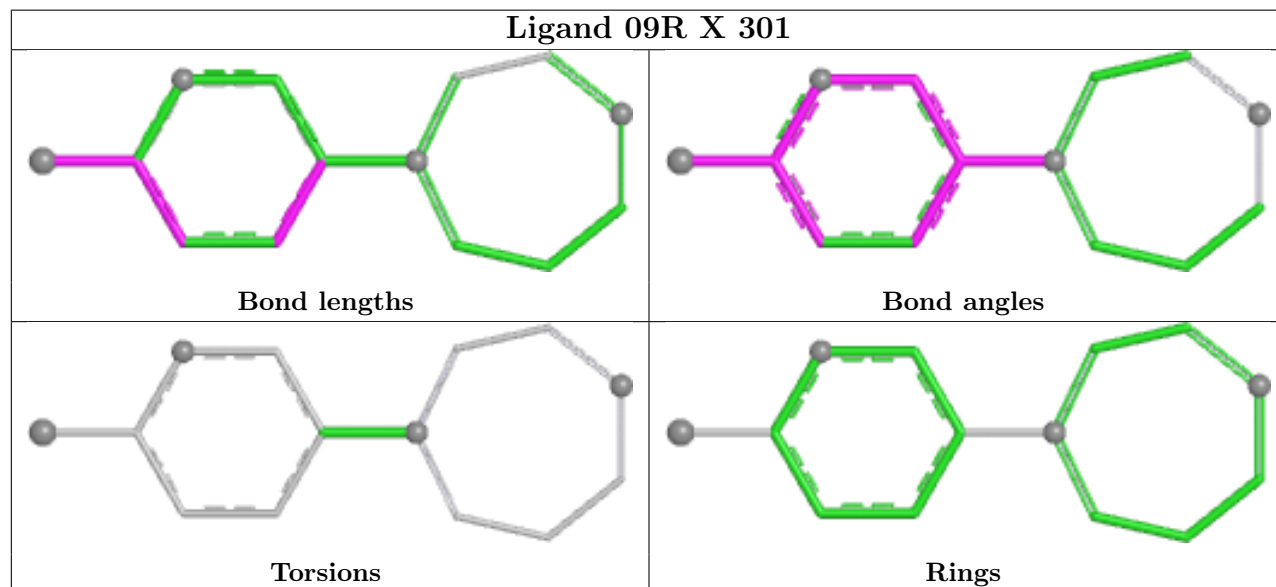
Ligand 09R Y 301



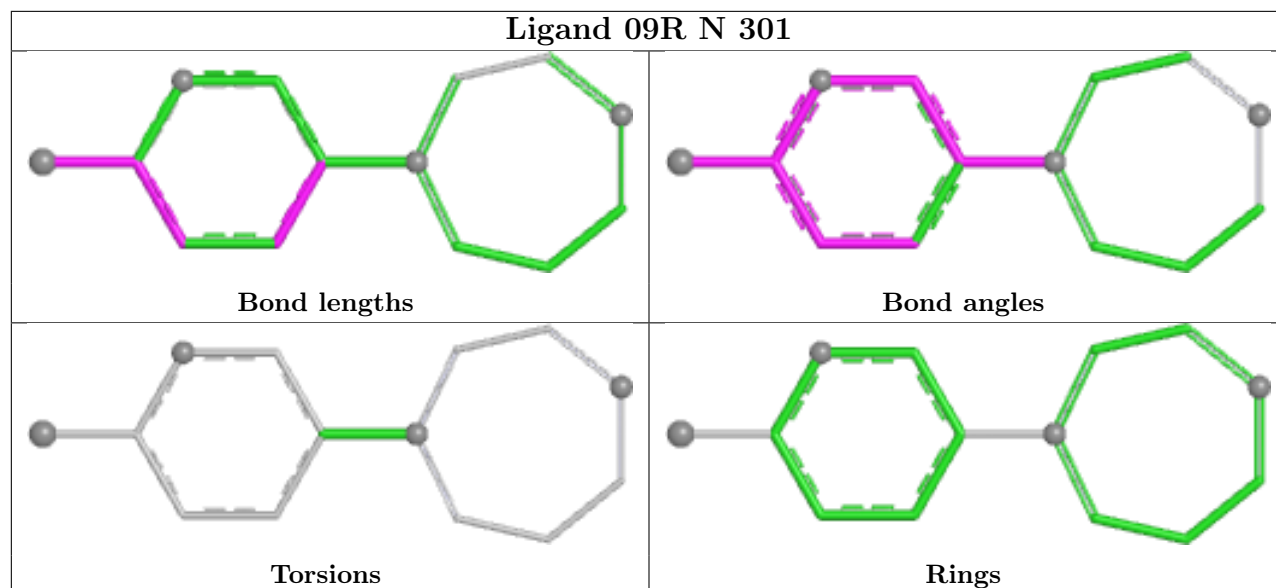
Ligand 09R U 301



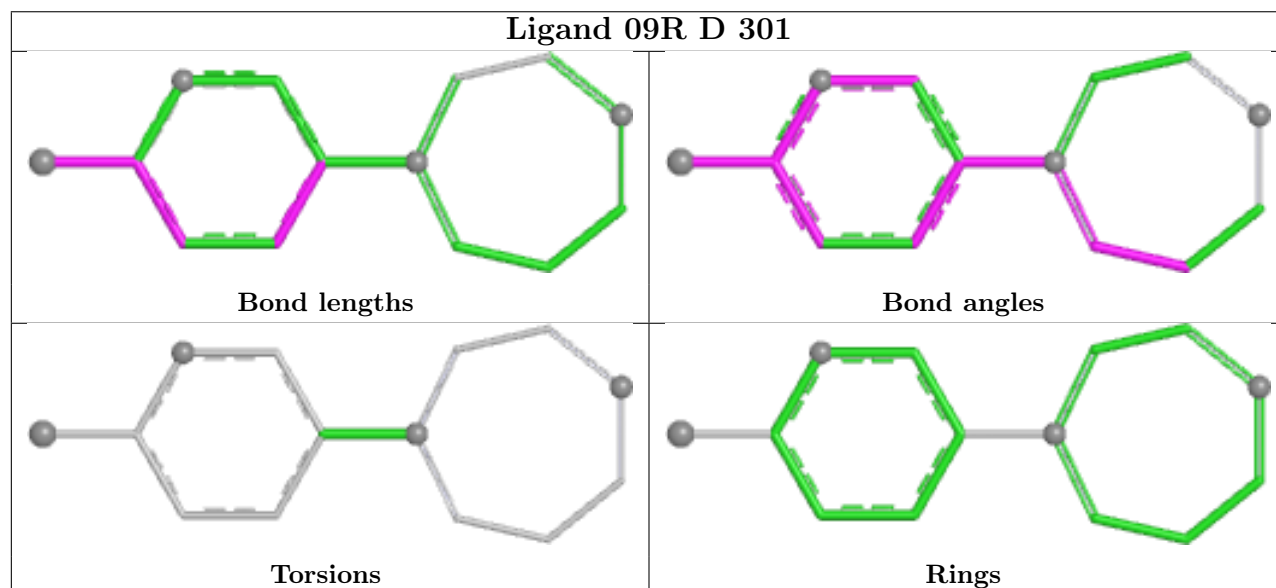
Ligand 09R X 301



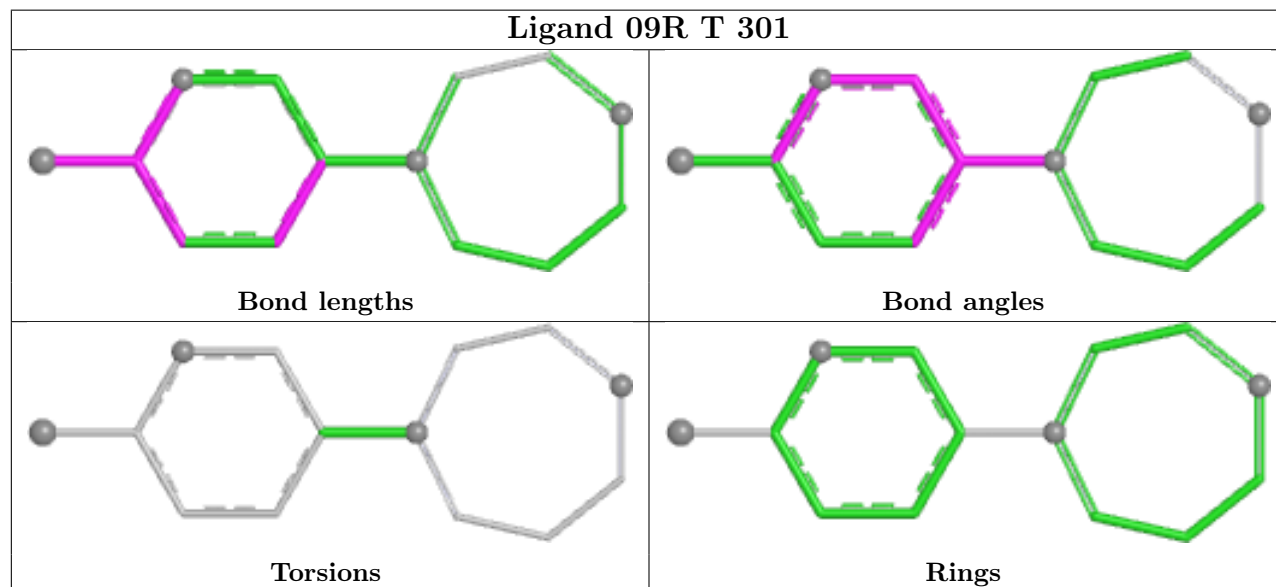
Ligand 09R N 301



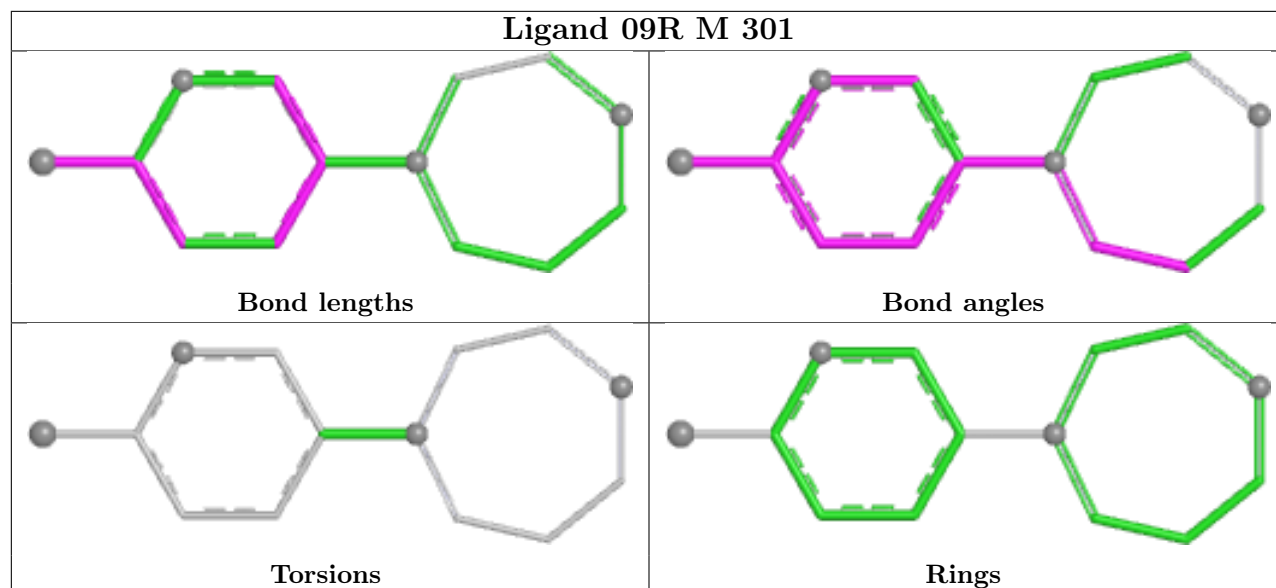
Ligand 09R D 301



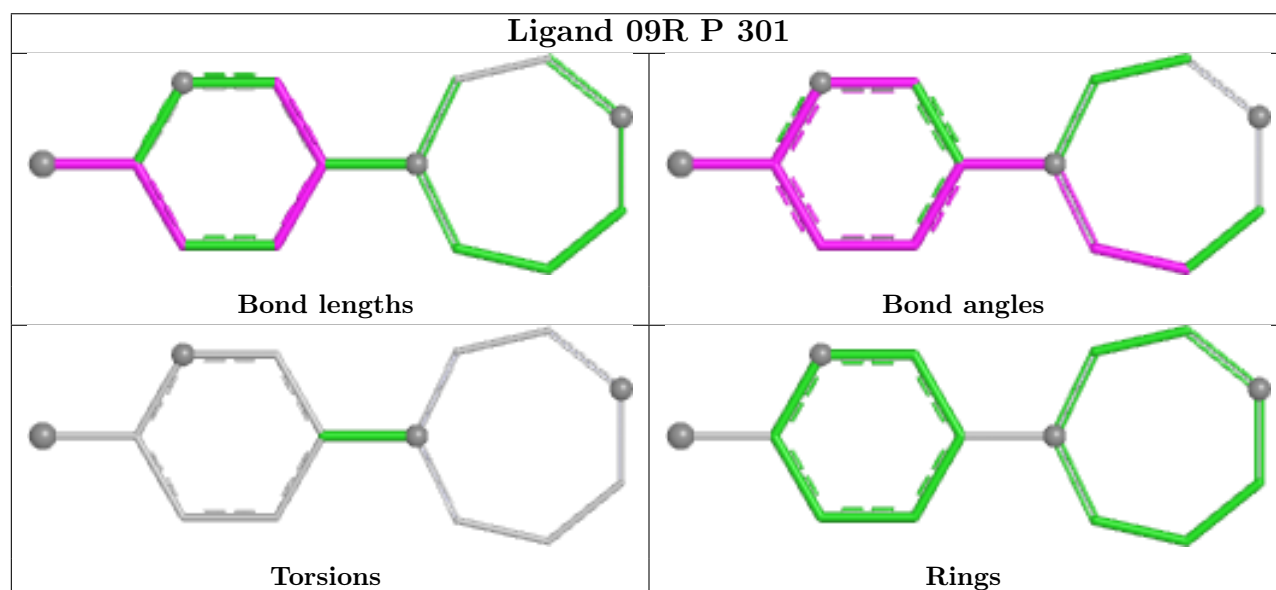
Ligand 09R T 301



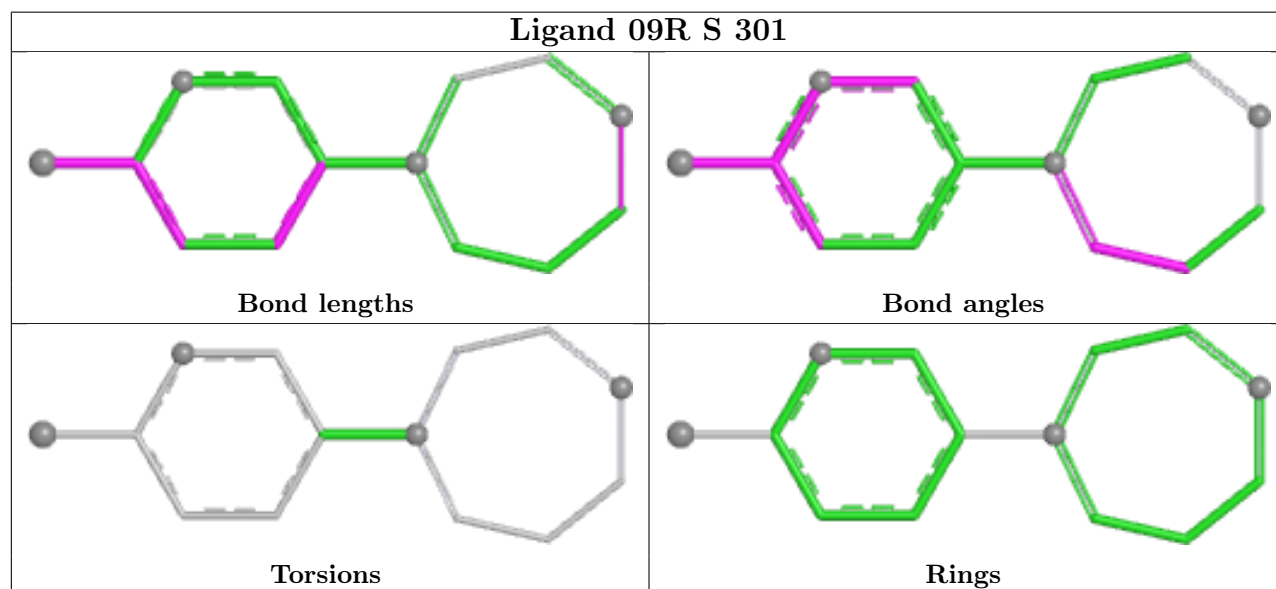
Ligand 09R M 301

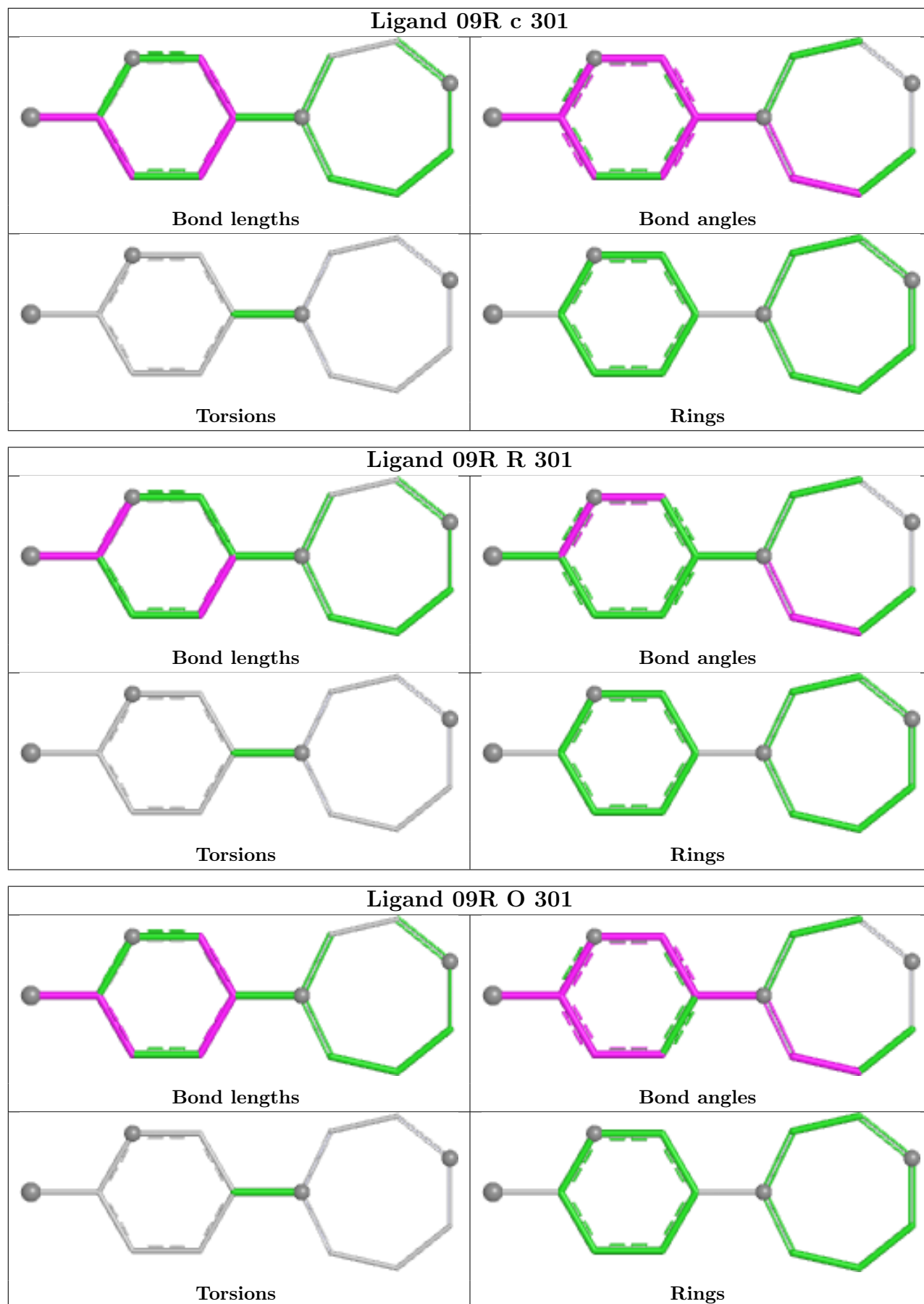


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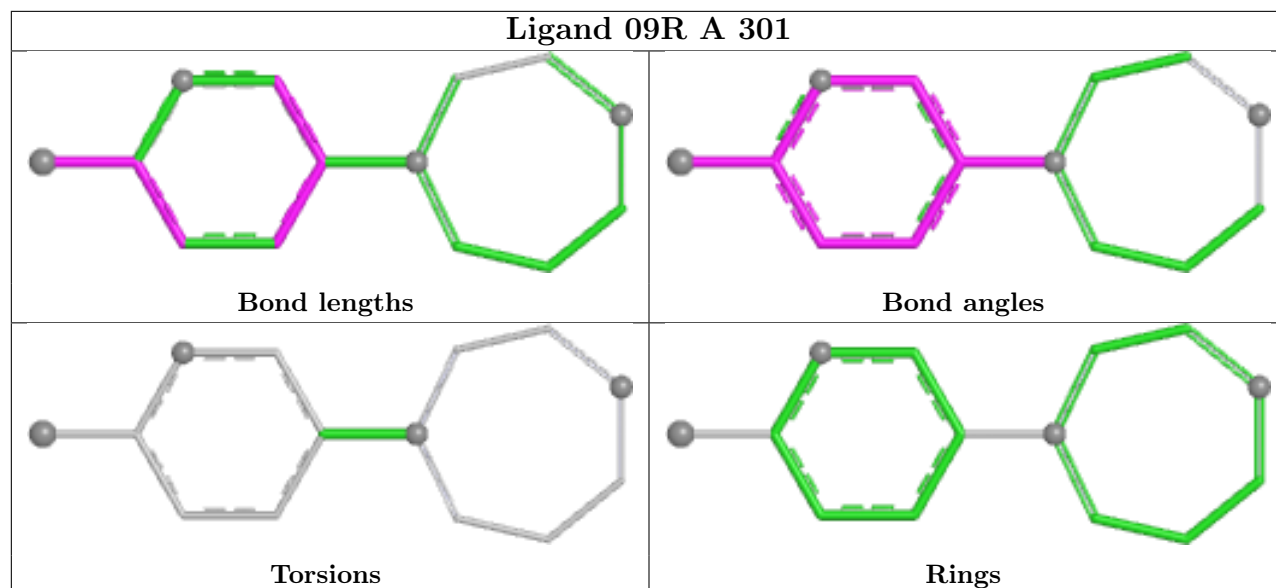


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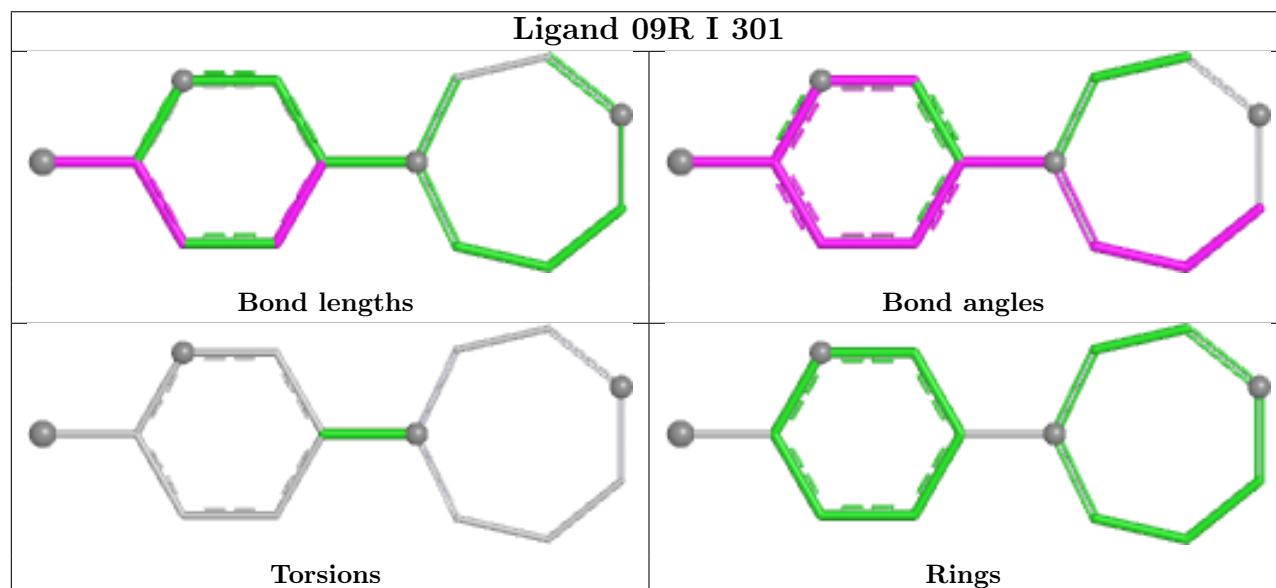




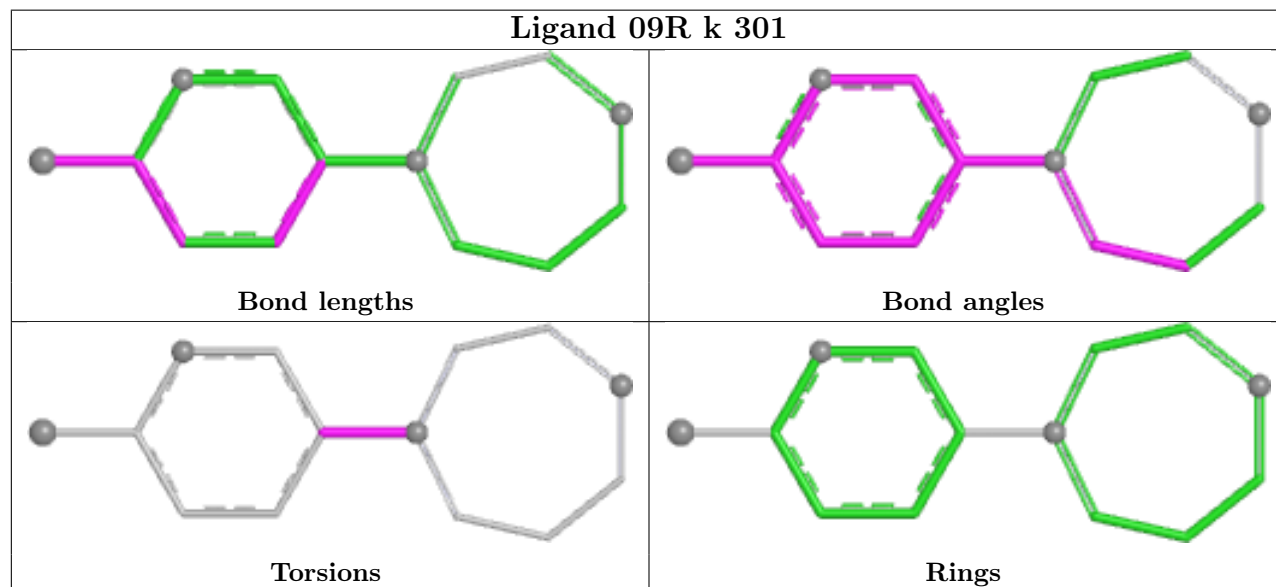
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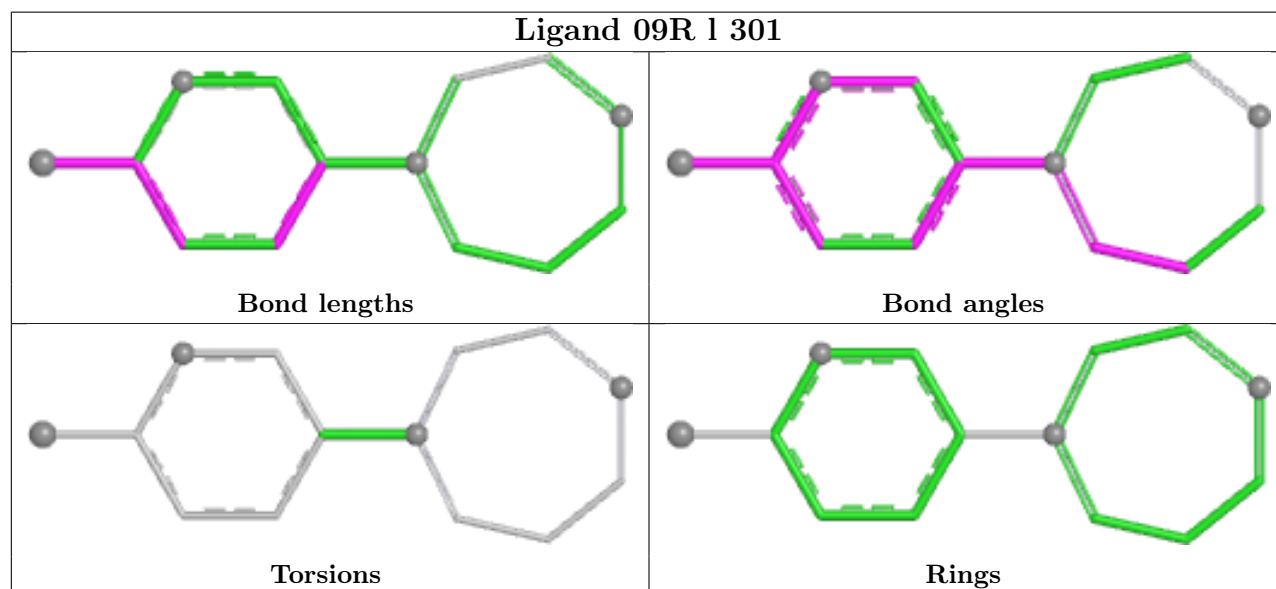
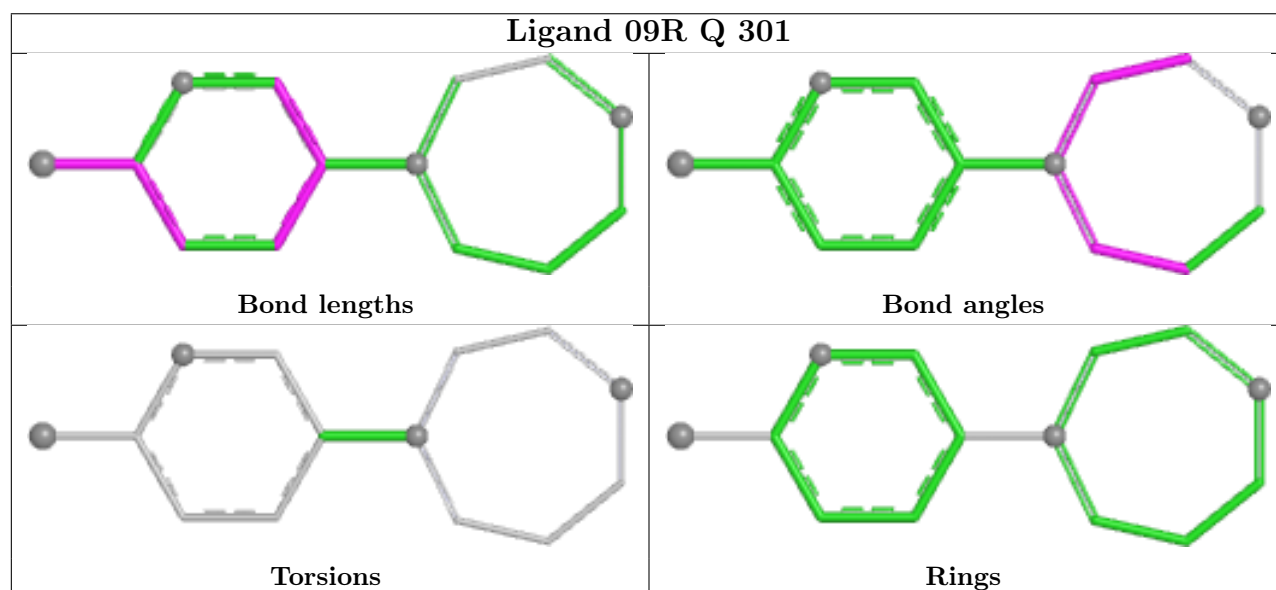
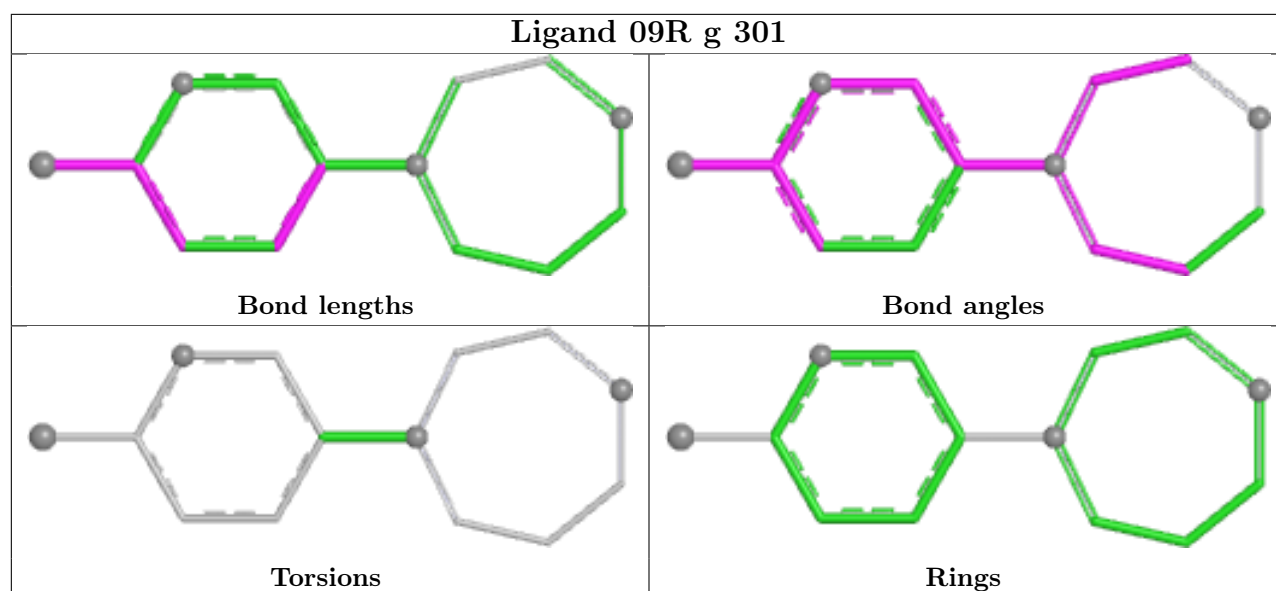


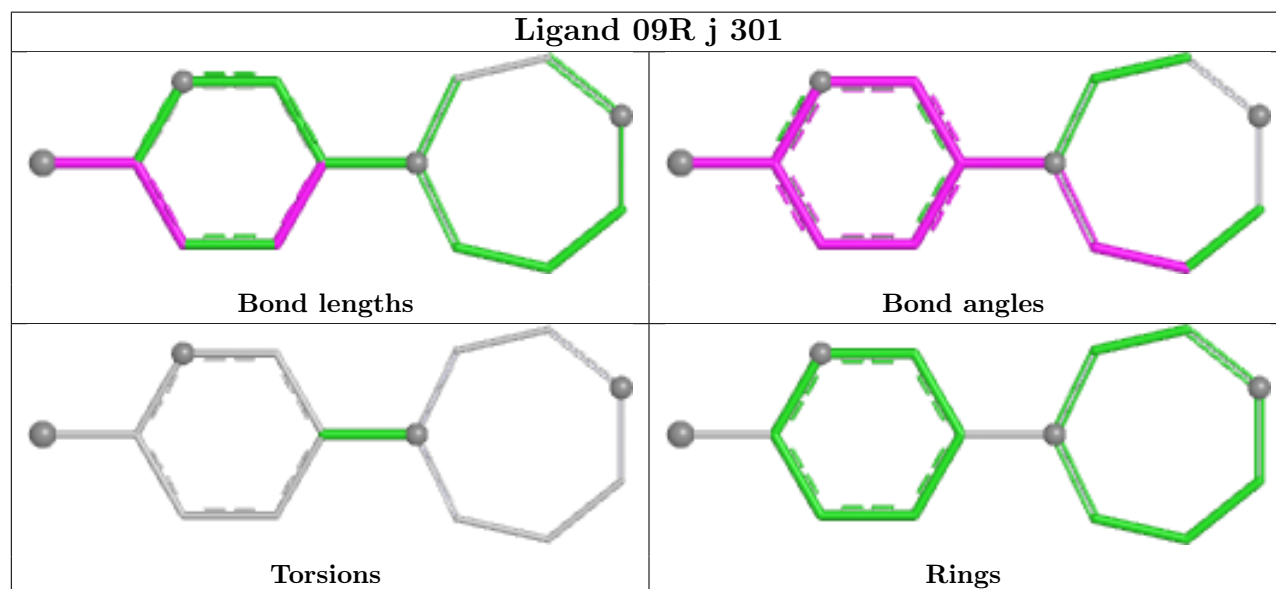
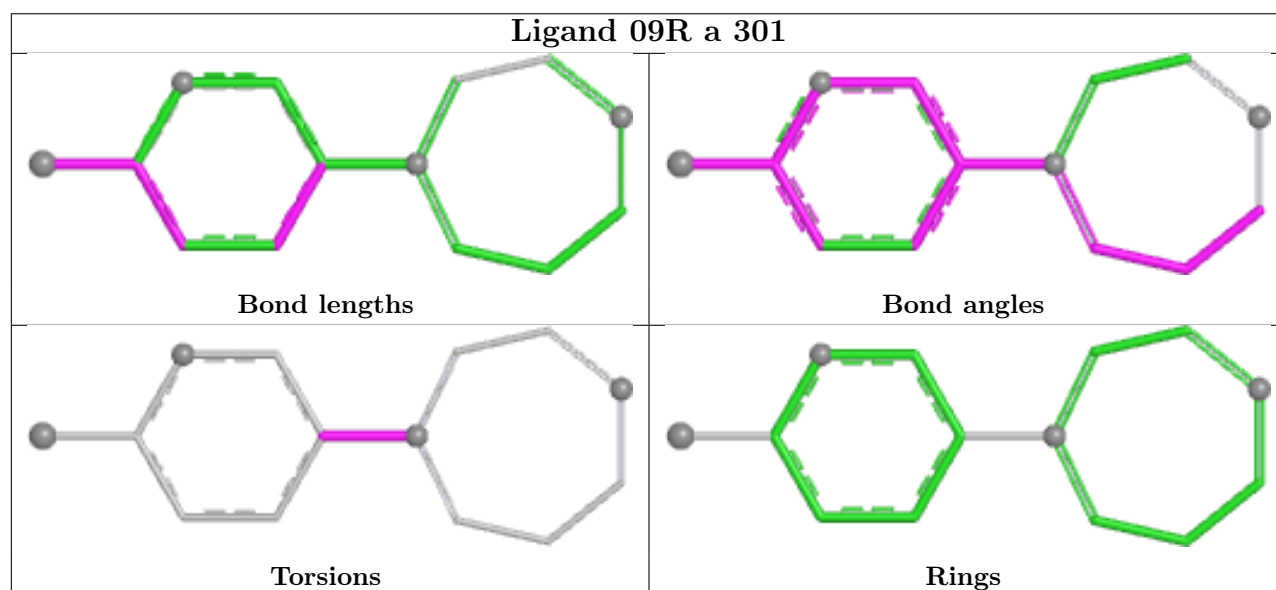
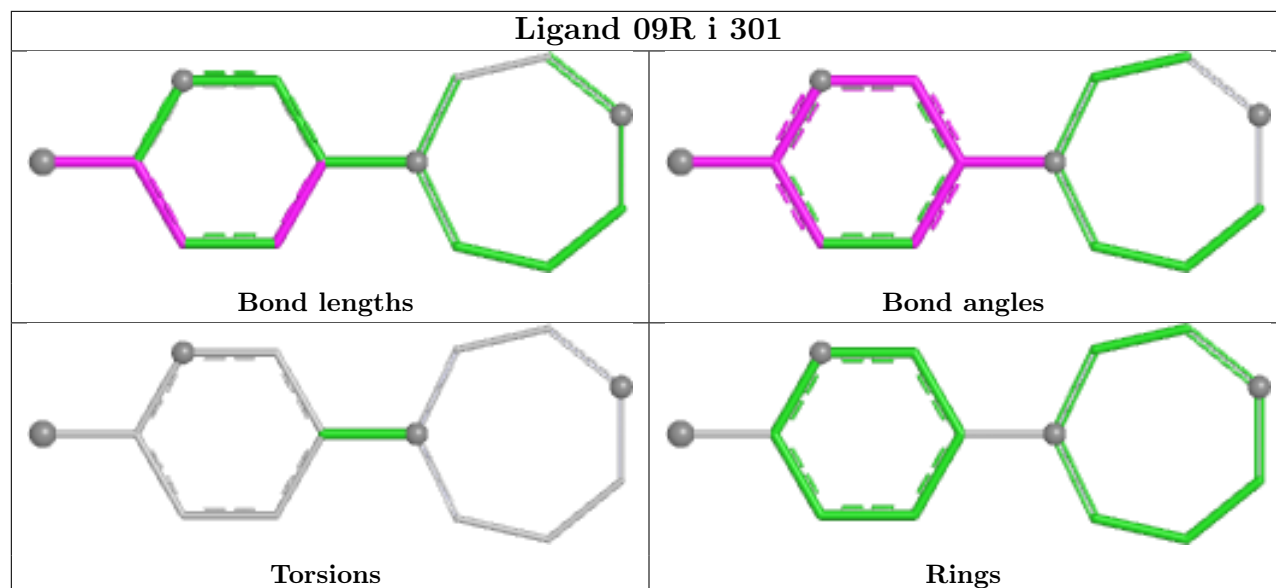
Ligand 09R I 301

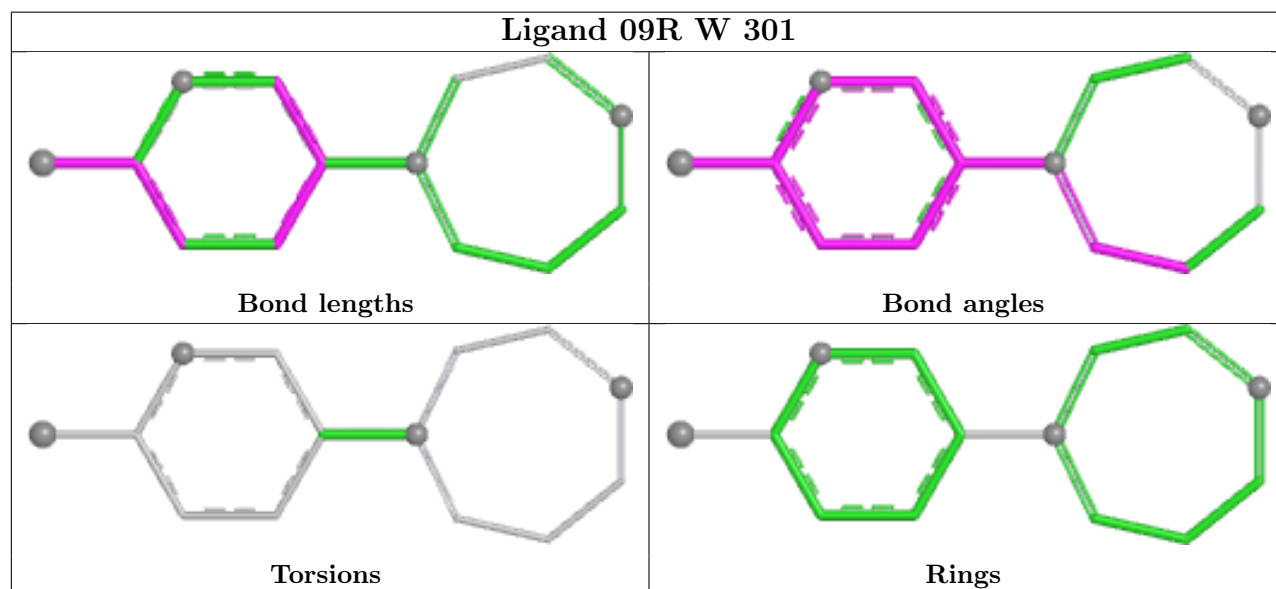
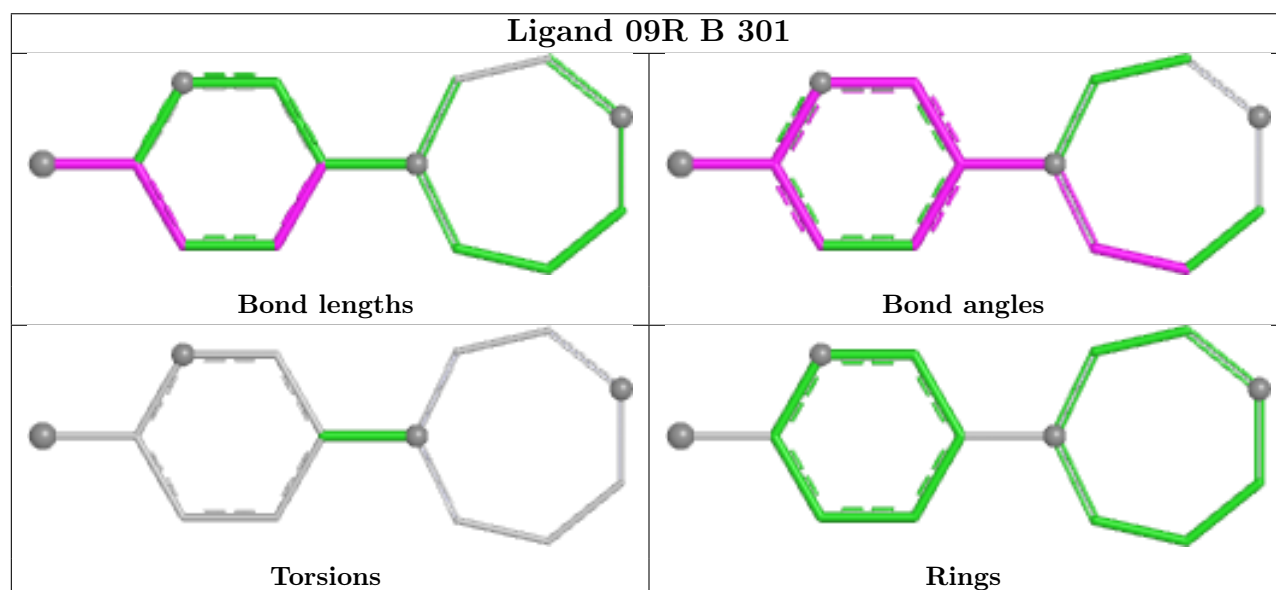
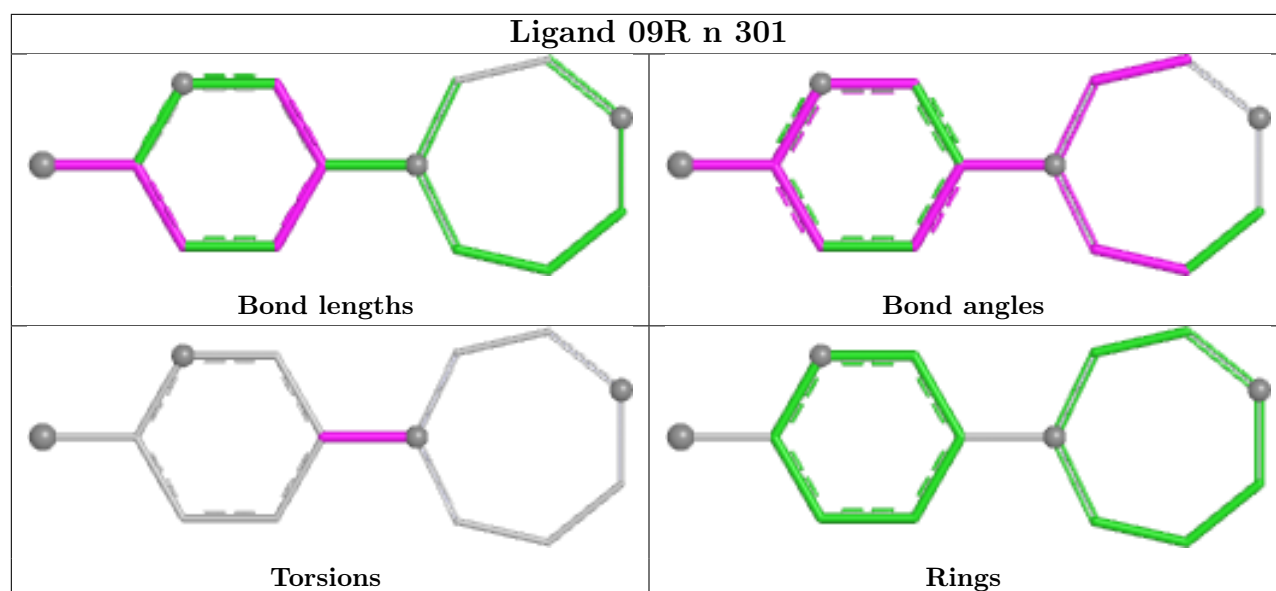


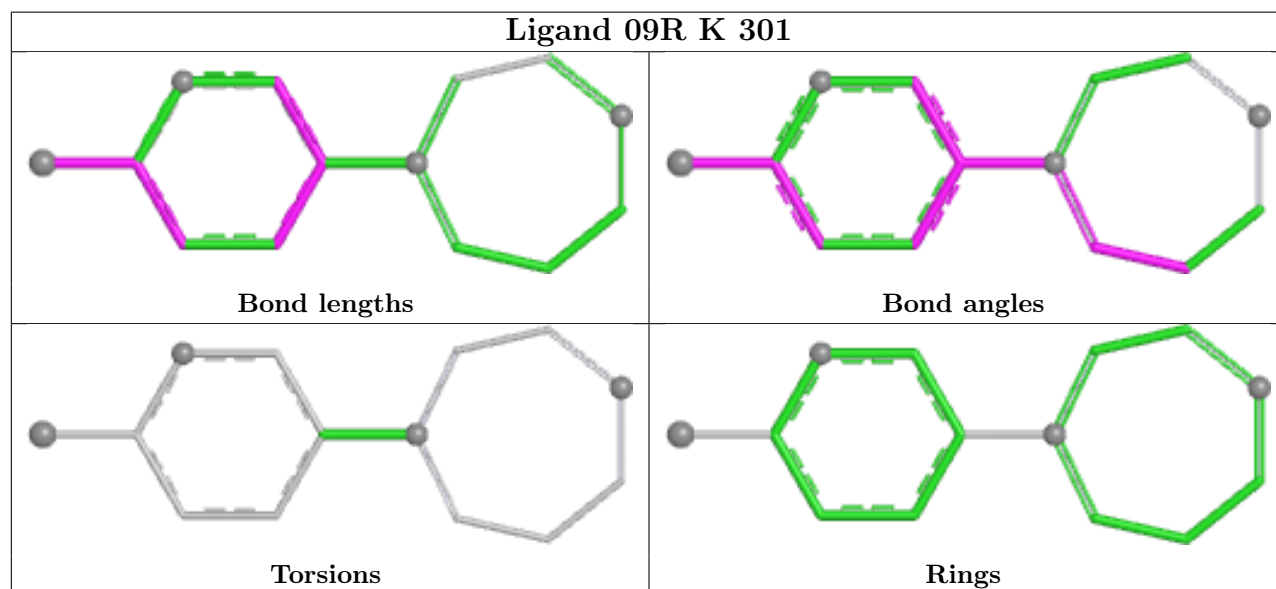
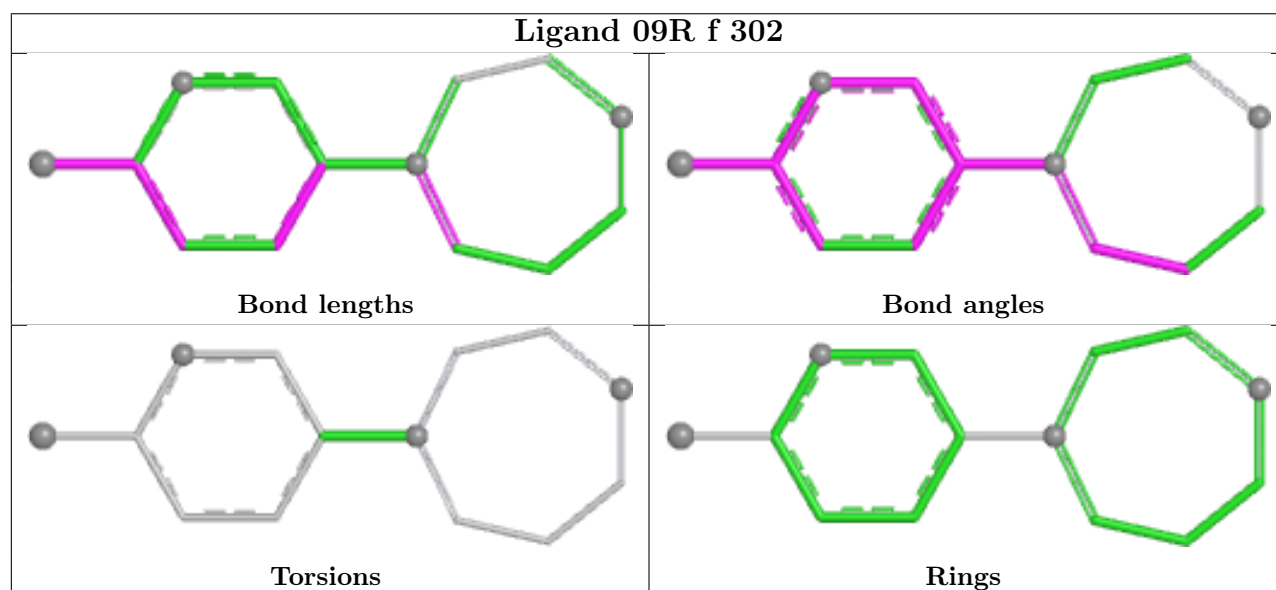
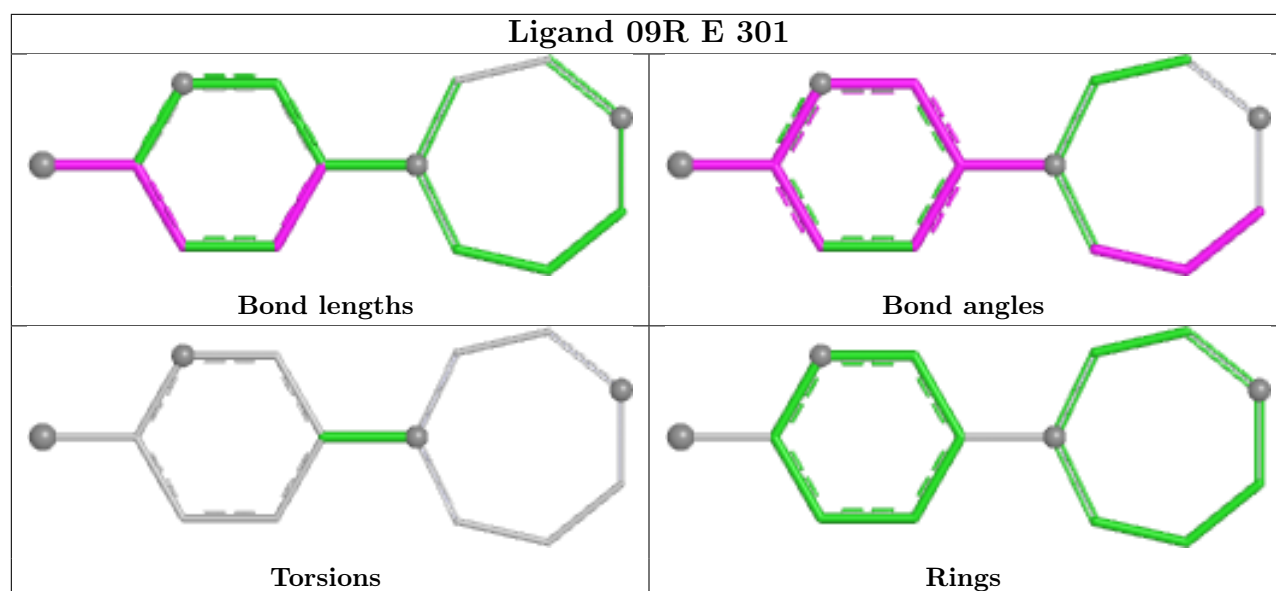
Ligand 09R k 301



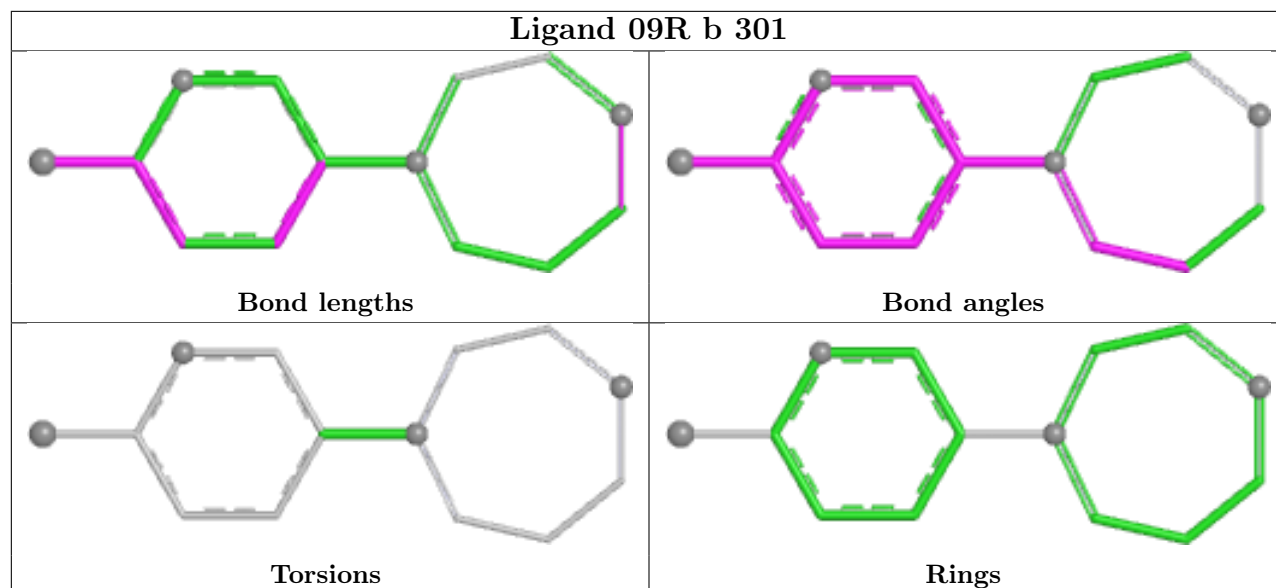




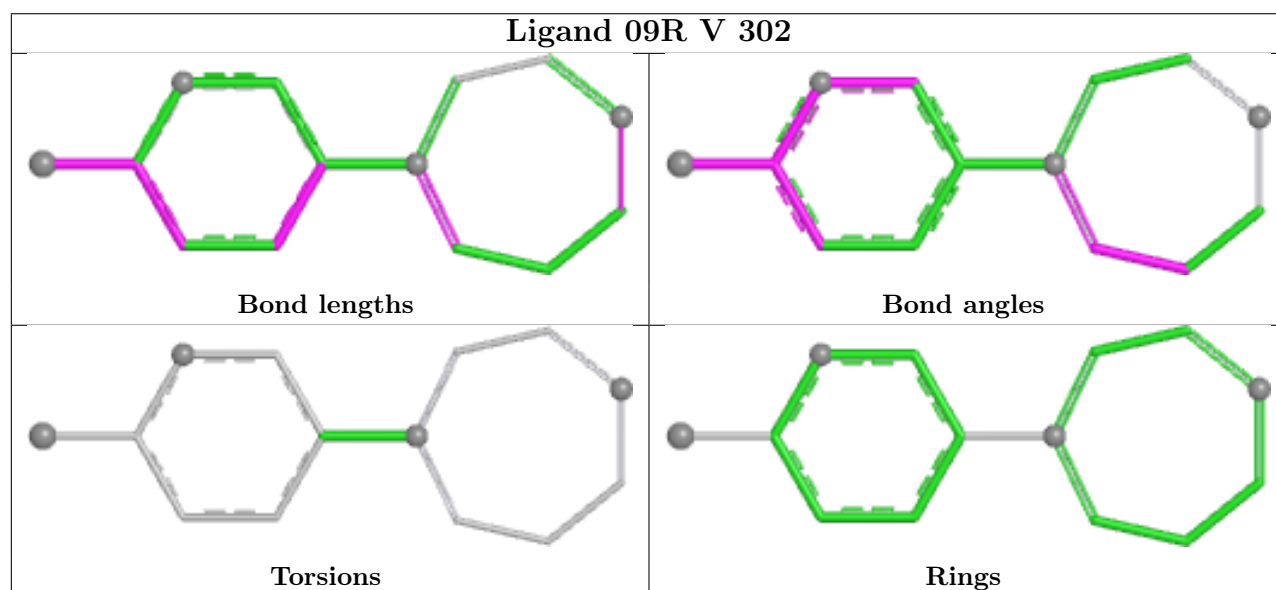




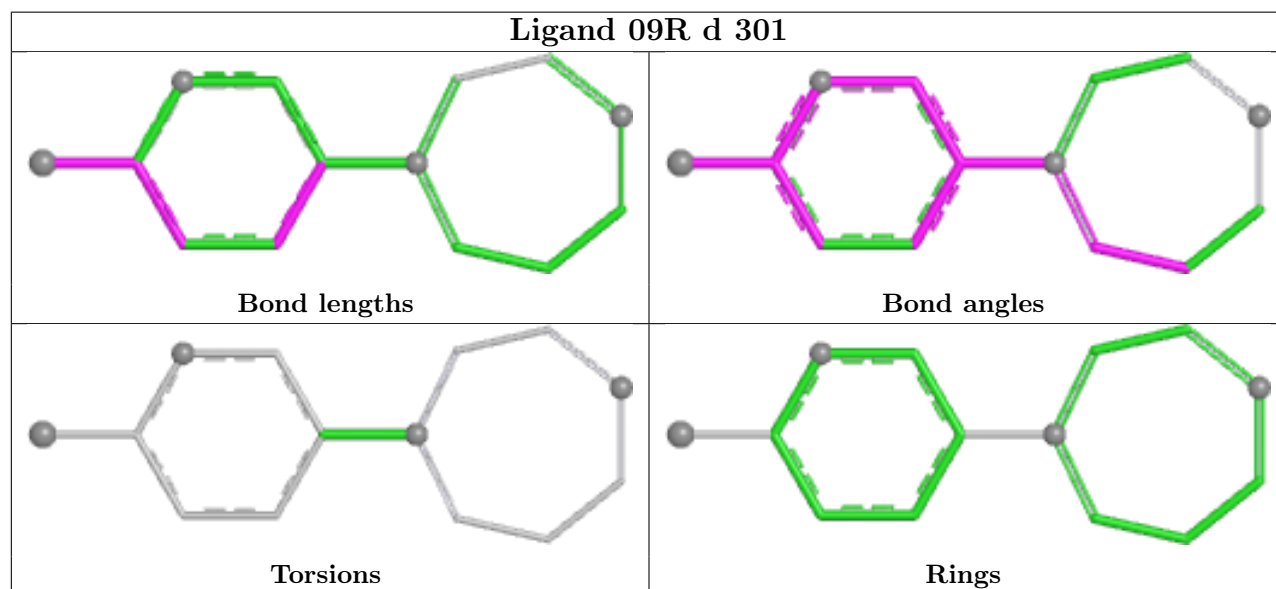
Ligand 09R b 301

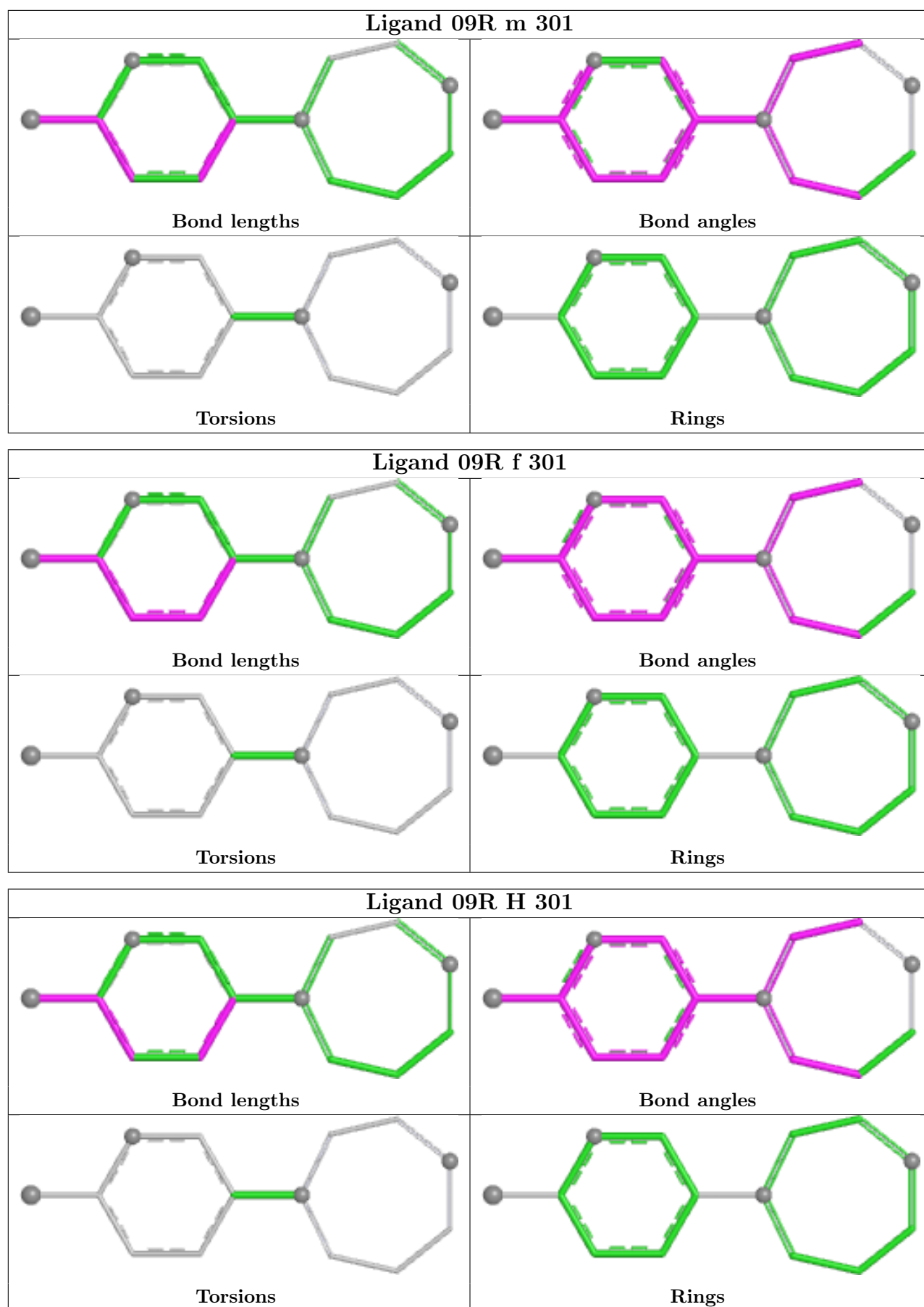


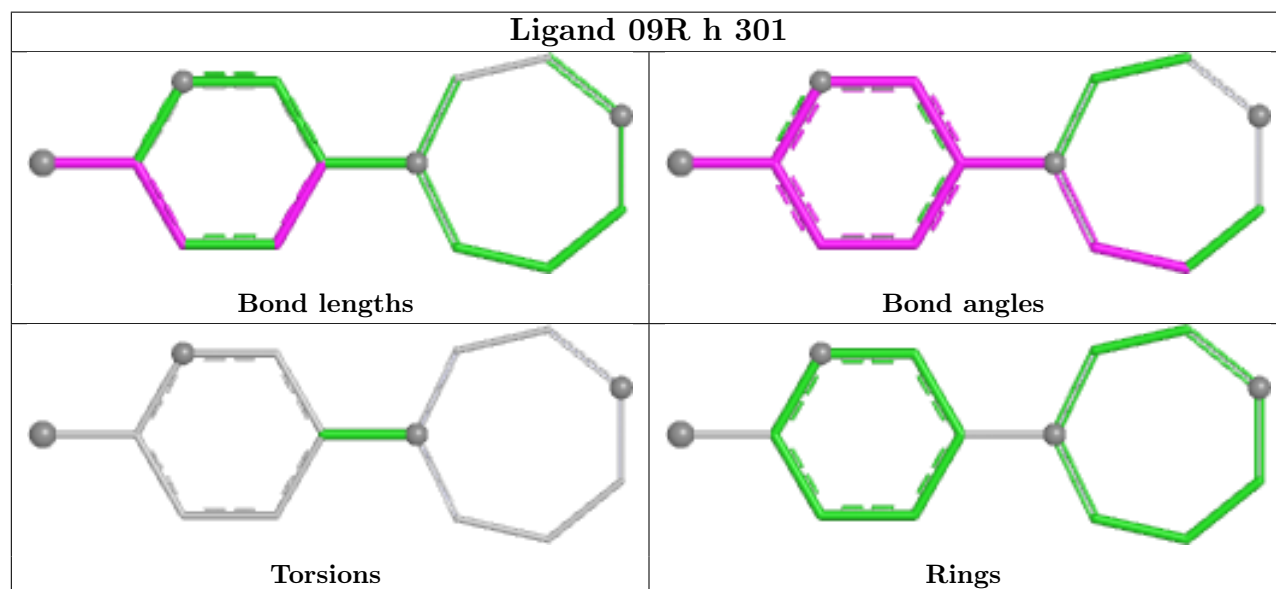
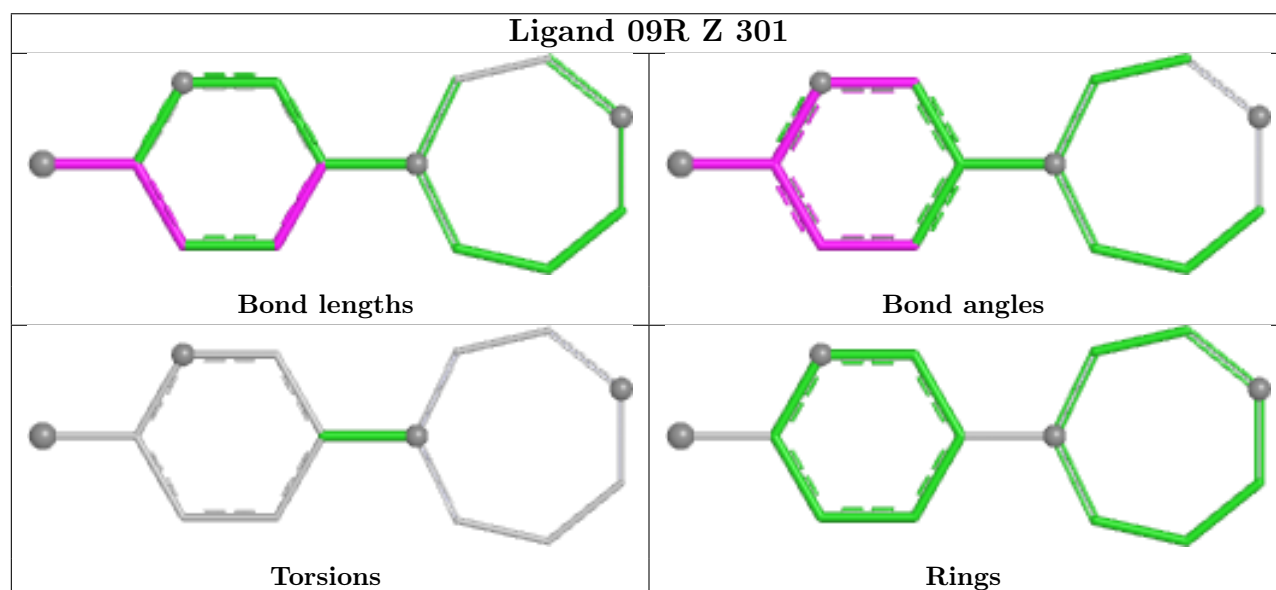
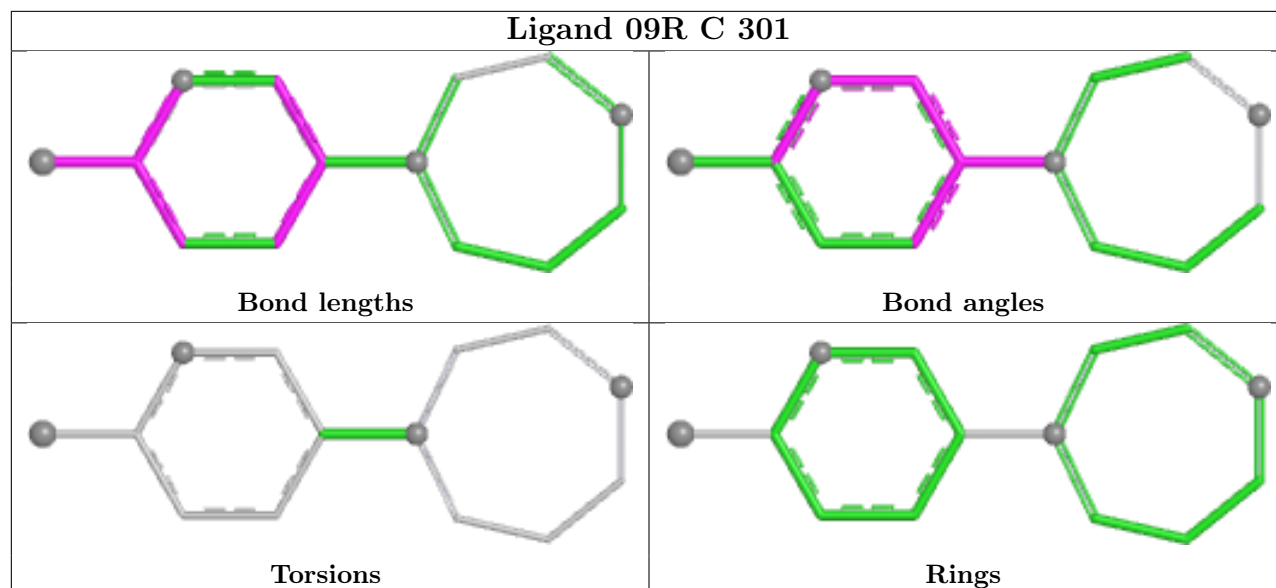
Ligand 09R V 302

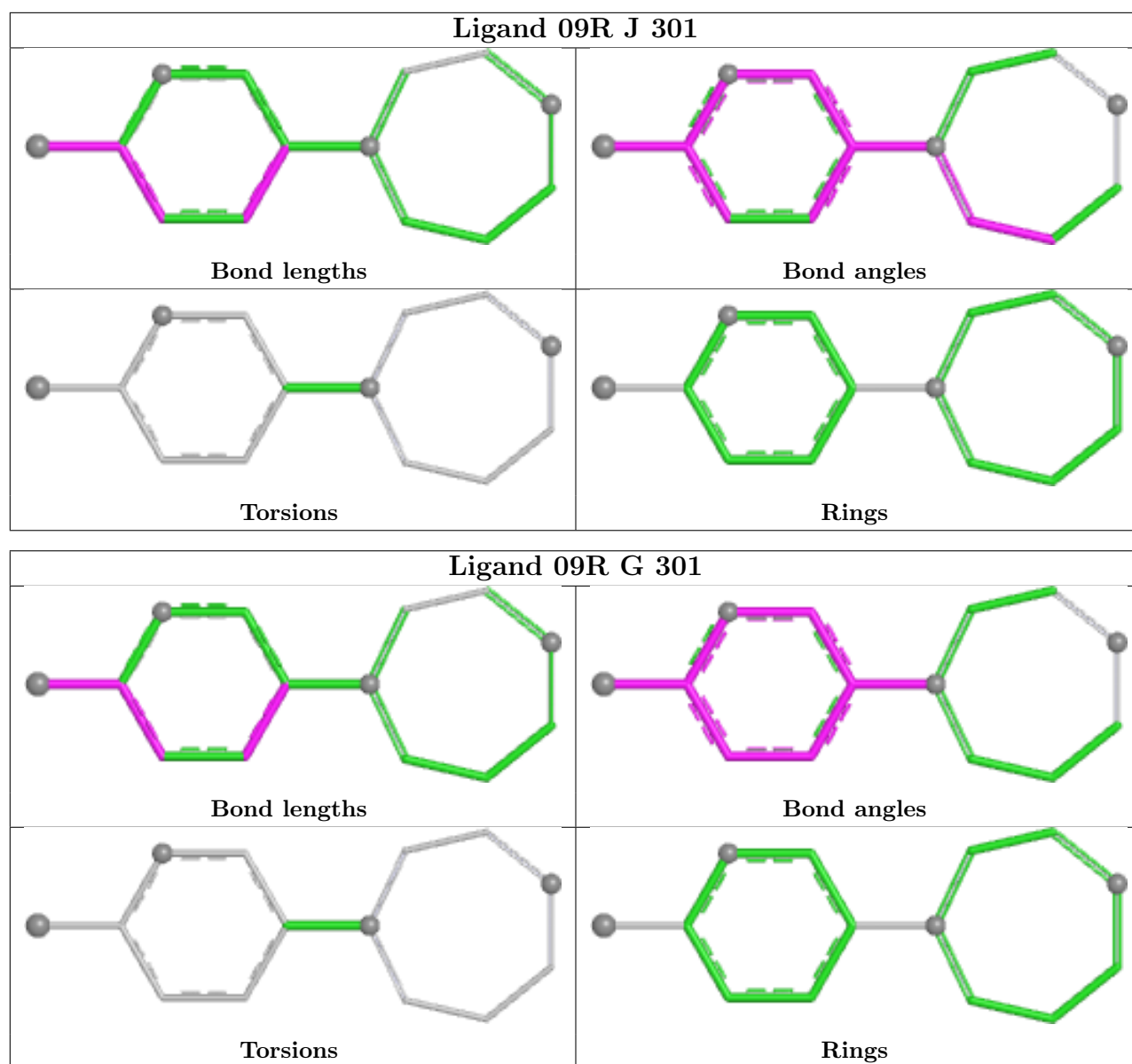


Ligand 09R d 301









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	201/229 (87%)	-0.43	3 (1%) 72 70	16, 33, 61, 95	3 (1%)
1	B	198/229 (86%)	-0.34	1 (0%) 87 86	13, 35, 68, 86	0
1	C	201/229 (87%)	-0.33	3 (1%) 72 70	18, 37, 68, 104	0
1	D	201/229 (87%)	-0.09	7 (3%) 47 43	22, 40, 74, 142	0
1	E	195/229 (85%)	-0.33	4 (2%) 63 61	17, 35, 74, 106	1 (0%)
1	F	196/229 (85%)	-0.27	2 (1%) 79 78	17, 38, 64, 78	2 (1%)
1	G	200/229 (87%)	-0.16	1 (0%) 87 86	21, 43, 76, 107	0
1	H	197/229 (86%)	-0.09	3 (1%) 72 70	24, 44, 77, 96	0
1	I	200/229 (87%)	-0.28	3 (1%) 72 70	15, 35, 75, 109	1 (0%)
1	J	200/229 (87%)	-0.40	2 (1%) 79 78	11, 32, 66, 103	1 (0%)
1	K	197/229 (86%)	-0.03	1 (0%) 87 86	19, 44, 82, 114	1 (0%)
1	L	195/229 (85%)	-0.20	4 (2%) 63 61	16, 41, 73, 99	1 (0%)
1	M	198/229 (86%)	-0.12	3 (1%) 72 70	22, 46, 80, 107	1 (0%)
1	N	196/229 (85%)	-0.24	3 (1%) 72 70	21, 40, 72, 105	2 (1%)
1	O	196/229 (85%)	-0.26	2 (1%) 79 78	22, 40, 70, 86	1 (0%)
1	Q	196/229 (85%)	-0.31	1 (0%) 87 86	17, 37, 68, 93	2 (1%)
1	R	198/229 (86%)	-0.20	1 (0%) 87 86	24, 41, 73, 96	0
1	T	194/229 (84%)	-0.29	3 (1%) 72 70	20, 37, 69, 94	0
1	U	197/229 (86%)	-0.35	2 (1%) 79 78	19, 35, 68, 97	0
1	V	199/229 (86%)	-0.42	2 (1%) 79 78	18, 32, 62, 93	0
1	W	197/229 (86%)	-0.27	3 (1%) 72 70	20, 37, 72, 101	0
1	X	202/229 (88%)	-0.22	2 (0%) 79 78	23, 43, 75, 107	1 (0%)
1	Y	197/229 (86%)	-0.05	3 (1%) 72 70	28, 44, 78, 93	0
1	Z	196/229 (85%)	-0.12	1 (0%) 87 86	26, 45, 80, 105	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	a	197/229 (86%)	-0.27	3 (1%) 72 70	21, 40, 71, 105	1 (0%)
1	b	198/229 (86%)	-0.31	1 (0%) 87 86	22, 38, 78, 104	1 (0%)
1	c	200/229 (87%)	-0.20	1 (0%) 87 86	19, 40, 86, 124	2 (1%)
1	d	198/229 (86%)	-0.14	2 (1%) 79 78	24, 44, 83, 101	0
1	e	198/229 (86%)	0.10	3 (1%) 72 70	27, 53, 87, 114	0
1	f	195/229 (85%)	0.19	4 (2%) 63 61	30, 58, 97, 123	0
1	g	198/229 (86%)	0.01	3 (1%) 72 70	27, 53, 81, 104	0
1	h	199/229 (86%)	0.08	4 (2%) 65 62	21, 52, 92, 113	1 (0%)
1	i	197/229 (86%)	-0.18	2 (1%) 79 78	21, 40, 69, 94	0
1	j	198/229 (86%)	0.18	2 (1%) 79 78	34, 57, 88, 93	0
1	k	198/229 (86%)	0.23	5 (2%) 58 55	32, 59, 97, 112	0
1	l	200/229 (87%)	-0.04	3 (1%) 72 70	27, 51, 80, 98	0
1	m	201/229 (87%)	0.19	2 (0%) 79 78	32, 60, 89, 109	0
1	n	196/229 (85%)	0.10	4 (2%) 65 62	34, 56, 87, 119	0
2	P	201/228 (88%)	-0.36	6 (2%) 52 49	14, 34, 65, 94	1 (0%)
3	S	201/229 (87%)	-0.07	4 (1%) 65 62	25, 44, 88, 147	1 (0%)
All	All	7922/9159 (86%)	-0.16	109 (1%) 73 72	11, 43, 80, 147	24 (0%)

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	f	155	THR	4.6
1	m	155	THR	4.5
1	n	155	THR	4.2
2	P	205	GLY	4.1
1	e	155	THR	4.1
1	Y	155	THR	4.0
1	d	155	THR	4.0
3	S	162	SER	3.9
1	H	155	THR	3.8
1	n	162	SER	3.7
1	K	155	THR	3.6
3	S	69	HIS	3.5
1	i	155	THR	3.4
1	c	155	THR	3.4
1	O	155	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	f	129	ASP	3.2
1	B	162	SER	3.2
2	P	68	SER	3.2
1	I	161	ASP	3.2
1	I	184	THR	3.1
1	a	162	SER	2.9
1	C	155	THR	2.9
1	k	177	THR	2.9
1	k	205	GLY	2.9
1	D	69	HIS	2.9
1	O	190	GLU	2.8
1	D	66	ASN	2.7
1	n	69	HIS	2.7
1	V	162	SER	2.7
1	a	155	THR	2.7
1	W	162	SER	2.7
1	k	162	SER	2.7
1	R	155	THR	2.7
1	T	155	THR	2.7
1	k	155	THR	2.7
1	A	67	SER	2.6
1	M	22	GLN	2.6
1	W	69	HIS	2.6
1	D	155	THR	2.6
1	A	155	THR	2.6
1	G	155	THR	2.5
1	N	162	SER	2.5
1	Y	70	SER	2.5
1	C	161	ASP	2.5
1	F	69	HIS	2.5
1	e	185	TYR	2.5
1	N	155	THR	2.5
1	X	155	THR	2.5
1	X	22	GLN	2.5
1	h	155	THR	2.5
1	I	205	GLY	2.5
1	D	70	SER	2.4
1	D	129	ASP	2.4
1	E	163	GLU	2.4
1	D	184	THR	2.4
1	i	1	LEU	2.4
1	A	187	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	m	167	GLN	2.4
1	L	162	SER	2.4
1	M	161	ASP	2.4
1	N	69	HIS	2.3
1	T	69	HIS	2.3
1	D	71	PRO	2.3
1	e	205	GLY	2.3
1	h	69	HIS	2.3
2	P	14	SER	2.3
1	E	205	GLY	2.3
1	J	205	GLY	2.3
1	h	178	GLN	2.3
1	E	155	THR	2.3
1	Y	72	ASP	2.3
1	f	132	SER	2.3
2	P	69	HIS	2.3
1	g	155	THR	2.3
1	f	25	ARG	2.3
1	h	177	THR	2.2
1	H	162	SER	2.2
1	n	68	SER	2.2
3	S	70	SER	2.2
1	C	69	HIS	2.2
1	H	69	HIS	2.2
1	b	69	HIS	2.2
1	j	155	THR	2.2
1	M	66	ASN	2.2
1	T	205	GLY	2.2
1	Q	162	SER	2.2
1	J	69	HIS	2.2
1	L	25	ARG	2.2
1	a	67	SER	2.2
1	L	69	HIS	2.2
2	P	155	THR	2.1
1	l	72	ASP	2.1
1	F	25	ARG	2.1
1	Z	155	THR	2.1
3	S	129	ASP	2.1
1	g	162	SER	2.1
1	E	66	ASN	2.1
1	j	162	SER	2.1
1	L	21	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	U	184	THR	2.1
1	V	155	THR	2.1
1	k	164	TYR	2.1
1	g	48	VAL	2.1
2	P	67	SER	2.0
1	U	155	THR	2.0
1	d	67	SER	2.0
1	W	155	THR	2.0
1	l	1	LEU	2.0
1	l	205	GLY	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, 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
5	NAG	A	302	14/15	0.70	0.13	44,50,53,54	0
5	NAG	d	302	14/15	0.71	0.14	44,50,53,54	0
5	NAG	O	302	14/15	0.80	0.12	25,49,66,72	0
6	SO4	V	301	5/5	0.82	0.10	88,93,96,97	0
4	09R	l	301	14/14	0.91	0.11	39,44,61,109	0
4	09R	m	301	14/14	0.92	0.10	38,54,75,90	0
4	09R	f	301	14/14	0.93	0.09	36,49,73,98	0
4	09R	i	301	14/14	0.93	0.10	17,37,57,88	0
4	09R	H	301	14/14	0.93	0.10	37,41,56,89	0
4	09R	Q	301	14/14	0.93	0.10	30,43,53,70	0
4	09R	j	301	14/14	0.94	0.08	37,51,60,102	0
4	09R	n	301	14/14	0.94	0.08	30,54,73,102	0
4	09R	f	302	14/14	0.94	0.11	43,64,81,87	0

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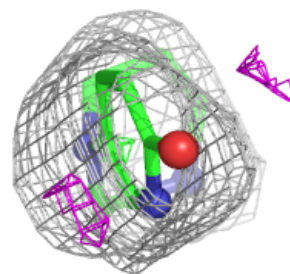
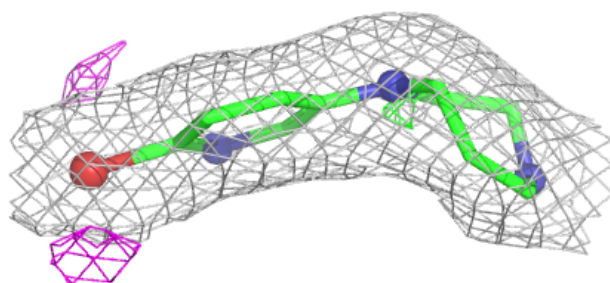
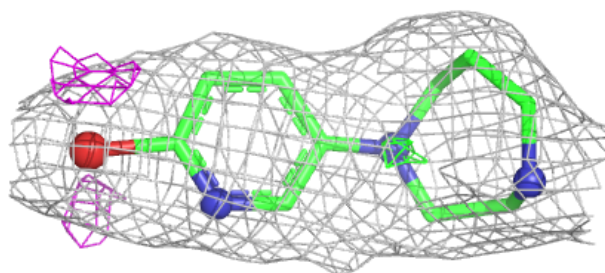
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	09R	d	301	14/14	0.95	0.09	32,45,63,91	0
4	09R	B	301	14/14	0.95	0.09	27,34,58,67	0
4	09R	L	301	14/14	0.95	0.10	34,40,63,79	0
4	09R	M	301	14/14	0.95	0.08	24,48,61,81	0
4	09R	N	301	14/14	0.95	0.08	23,29,43,75	0
4	09R	G	301	14/14	0.95	0.09	23,34,58,72	0
4	09R	K	301	14/14	0.96	0.08	29,45,59,67	0
4	09R	O	301	14/14	0.96	0.08	29,38,53,68	0
4	09R	F	301	14/14	0.96	0.07	20,27,46,75	0
4	09R	S	301	14/14	0.96	0.08	23,40,53,60	0
4	09R	U	301	14/14	0.96	0.08	18,36,59,68	0
4	09R	X	301	14/14	0.96	0.10	43,52,71,74	0
4	09R	Y	301	14/14	0.96	0.08	18,42,57,84	0
4	09R	Z	301	14/14	0.96	0.09	28,46,61,66	0
4	09R	a	301	14/14	0.96	0.09	23,35,61,74	0
4	09R	b	301	14/14	0.96	0.08	17,39,54,70	0
4	09R	I	301	14/14	0.96	0.09	19,34,49,99	0
4	09R	k	301	14/14	0.97	0.08	33,62,76,77	0
4	09R	c	301	14/14	0.97	0.07	34,43,58,62	0
4	09R	A	301	14/14	0.97	0.08	26,42,50,64	0
4	09R	C	301	14/14	0.97	0.08	28,36,52,54	0
4	09R	D	301	14/14	0.97	0.08	20,42,57,61	0
4	09R	g	301	14/14	0.97	0.06	29,39,58,79	0
4	09R	T	301	14/14	0.97	0.07	15,25,41,67	0
4	09R	E	301	14/14	0.97	0.06	15,23,54,76	0
4	09R	R	301	14/14	0.98	0.06	17,34,41,63	0
4	09R	W	301	14/14	0.98	0.07	23,40,53,71	0
4	09R	P	301	14/14	0.98	0.06	19,27,32,57	0
4	09R	J	301	14/14	0.98	0.05	16,30,41,68	0
4	09R	h	301	14/14	0.98	0.07	28,45,58,59	0
4	09R	V	302	14/14	0.99	0.05	8,27,50,66	0

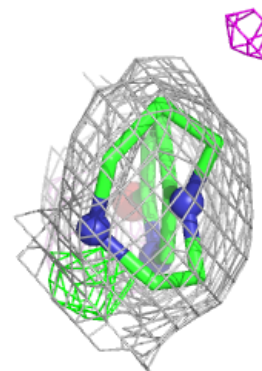
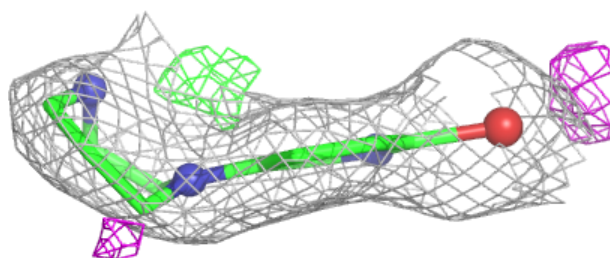
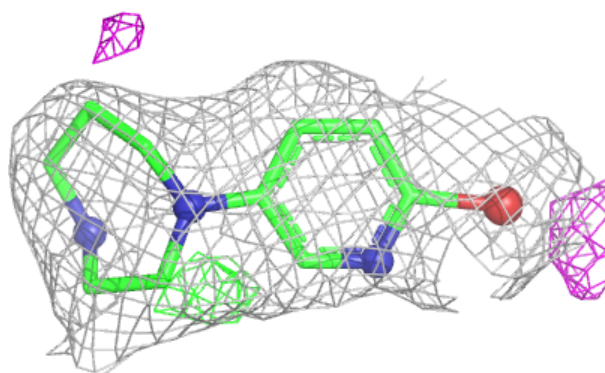
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 09R 1 301:

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

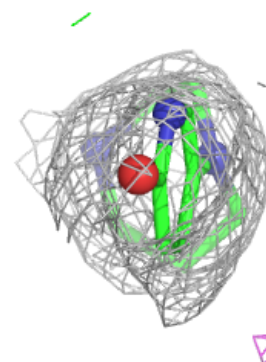
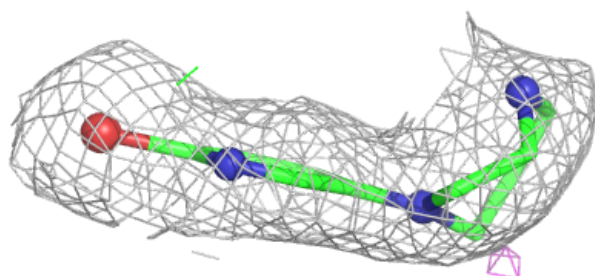
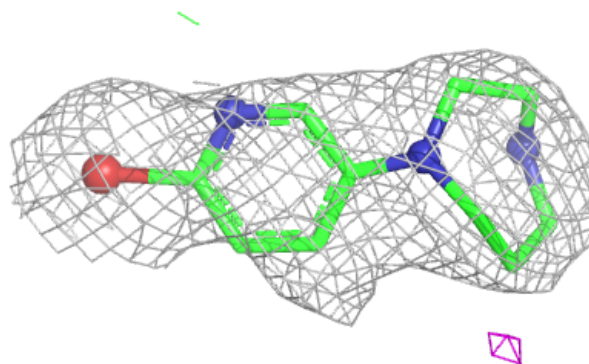
**Electron density around 09R m 301:**

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

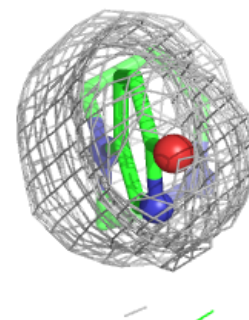
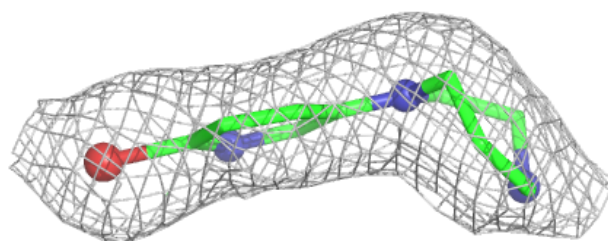
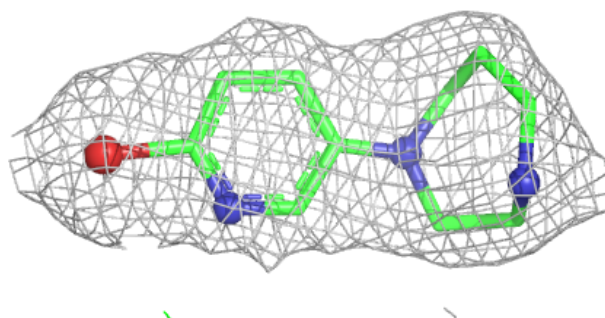


Electron density around 09R f 301:

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

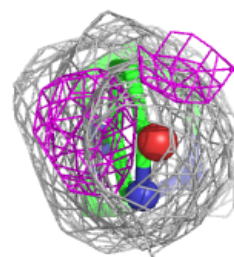
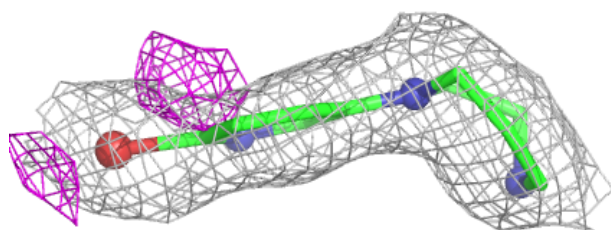
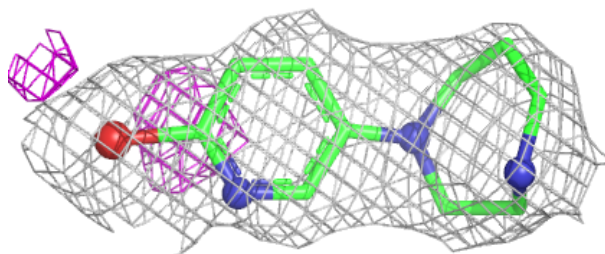
**Electron density around 09R i 301:**

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

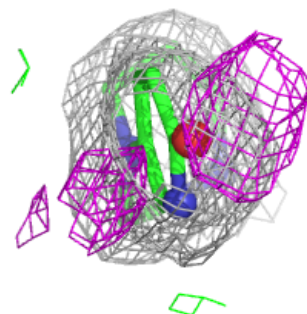
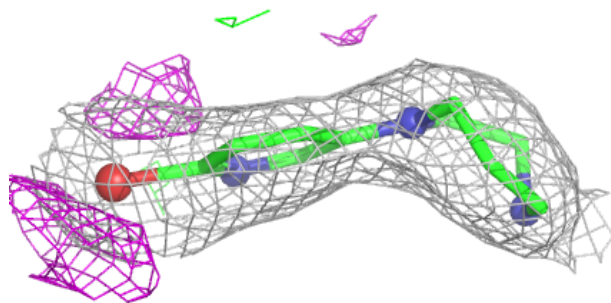
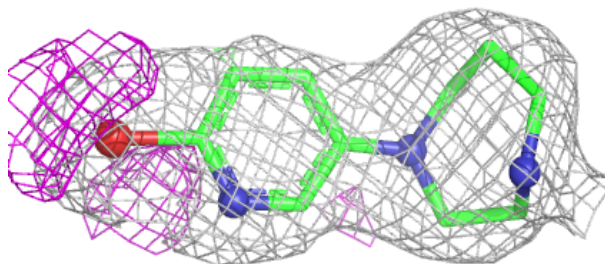


Electron density around 09R H 301:

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

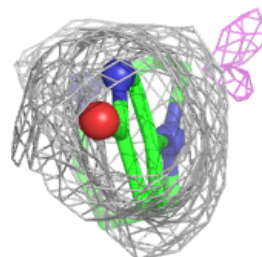
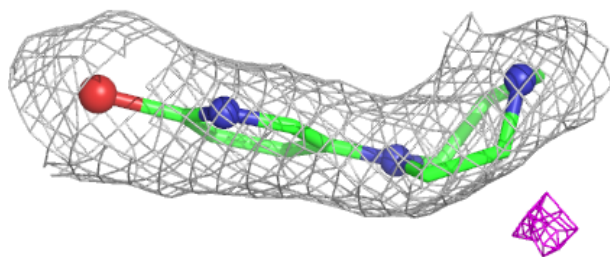
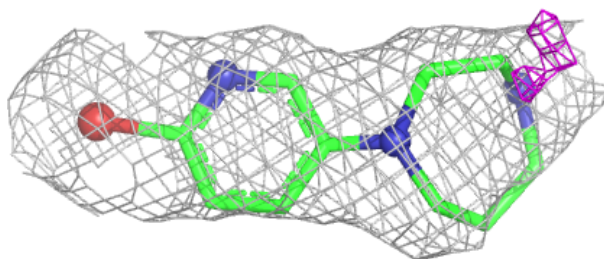
**Electron density around 09R Q 301:**

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

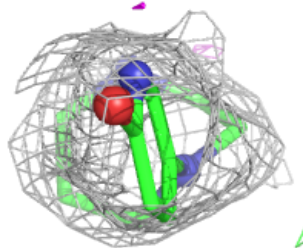
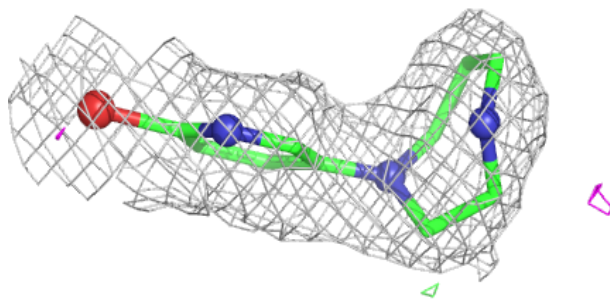
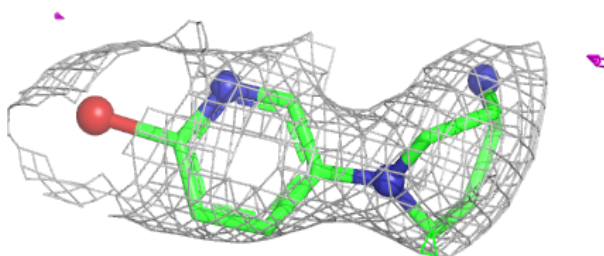


Electron density around 09R j 301:

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

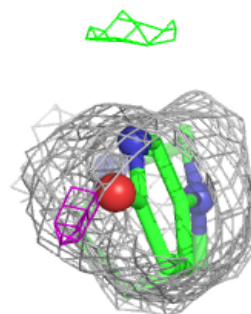
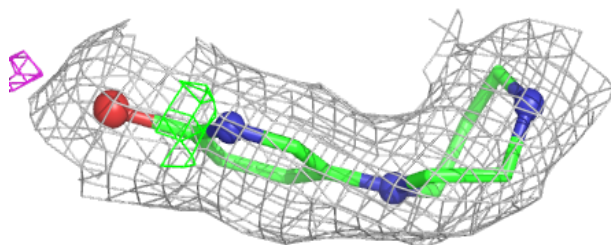
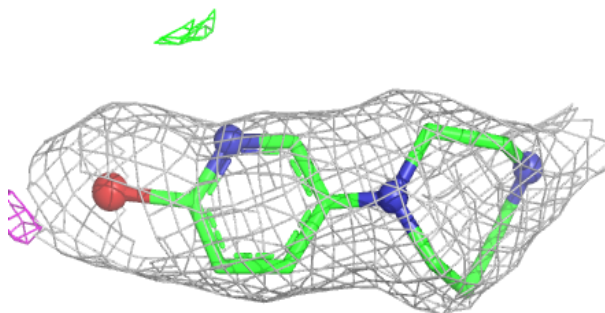
**Electron density around 09R n 301:**

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

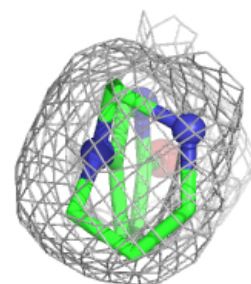
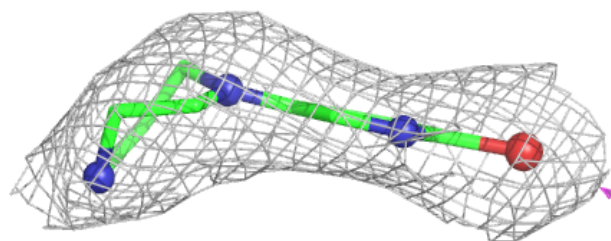
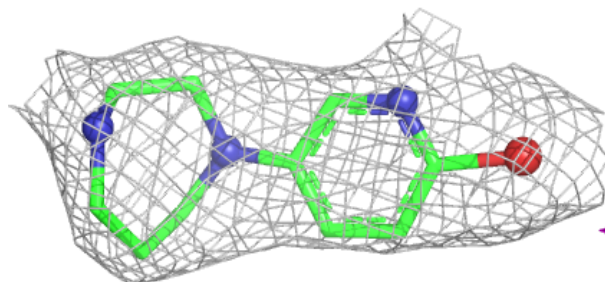


Electron density around 09R f 302:

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

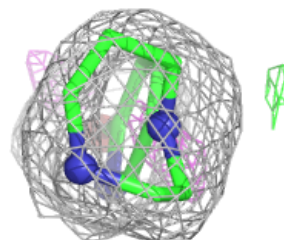
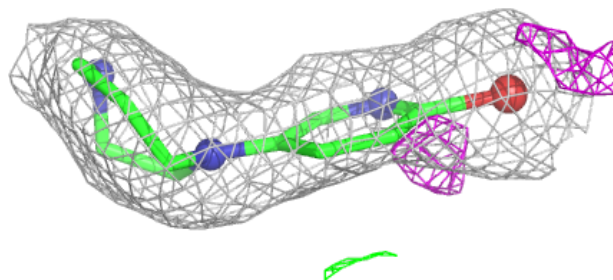
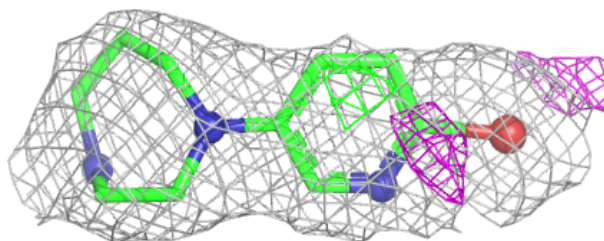
**Electron density around 09R d 301:**

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

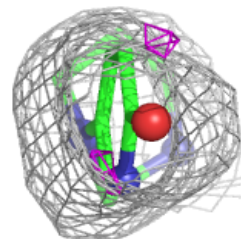
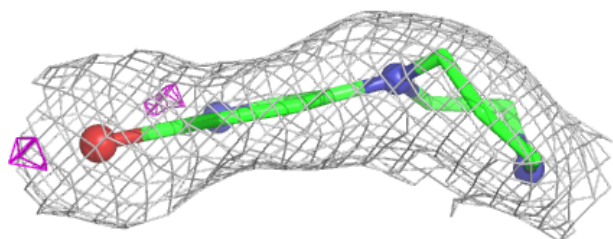
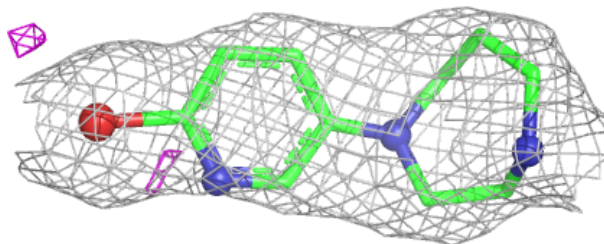


Electron density around 09R B 301:

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

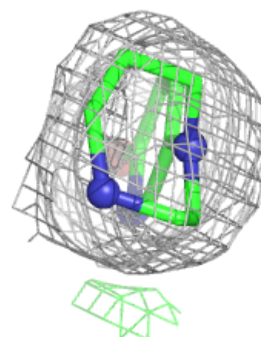
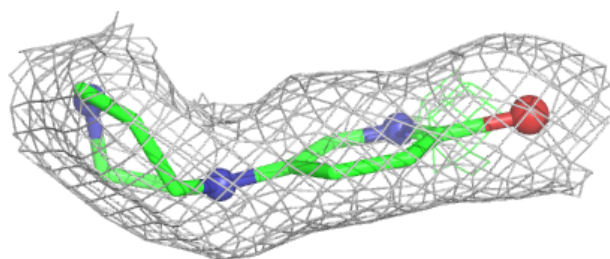
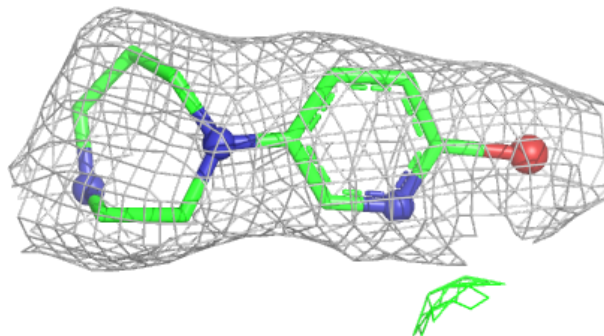
**Electron density around 09R L 301:**

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

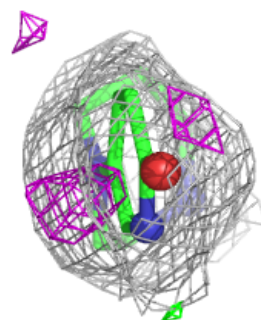
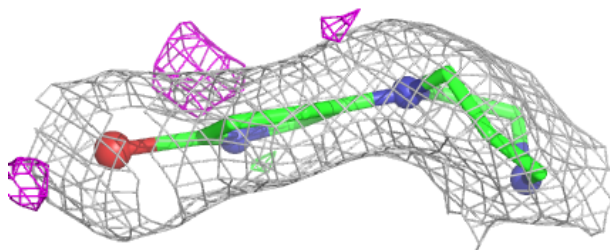
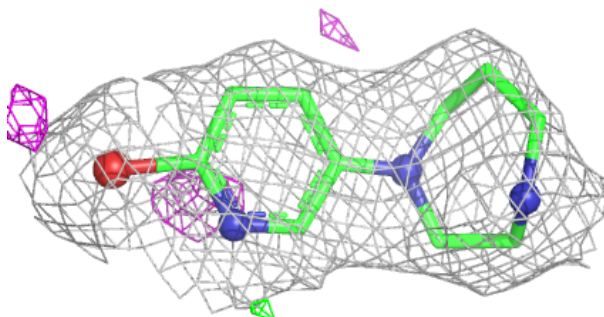


Electron density around 09R M 301:

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

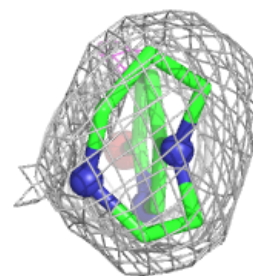
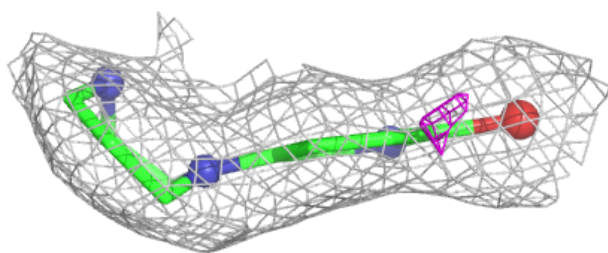
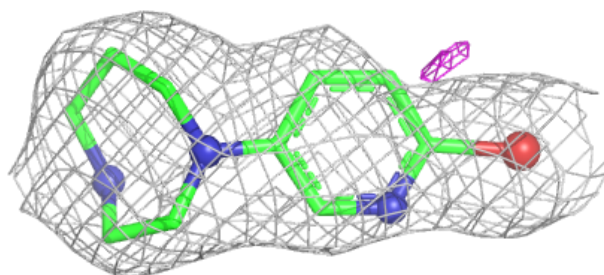
**Electron density around 09R N 301:**

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

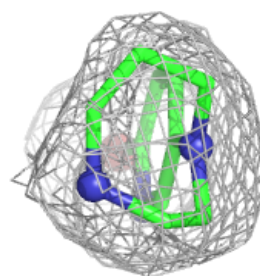
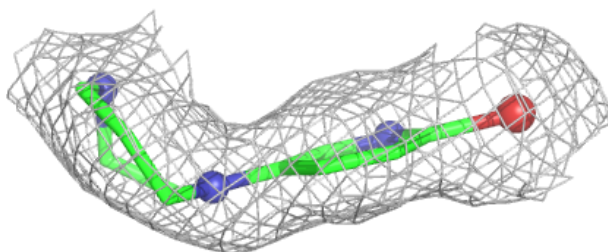
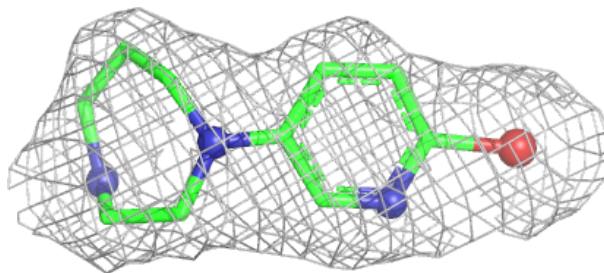


Electron density around 09R G 301:

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

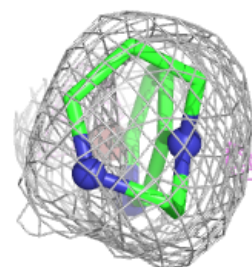
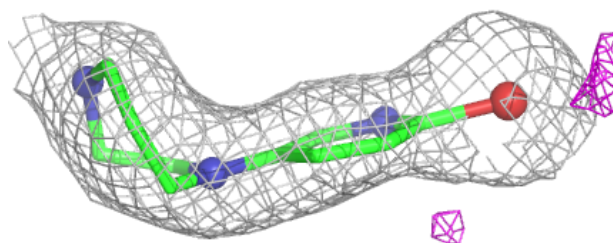
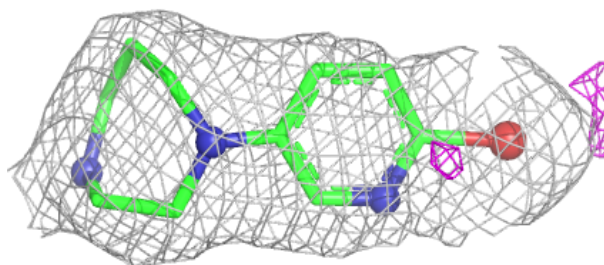
**Electron density around 09R K 301:**

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

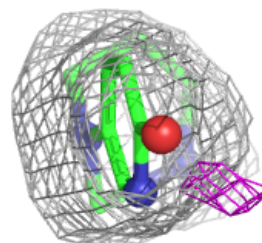
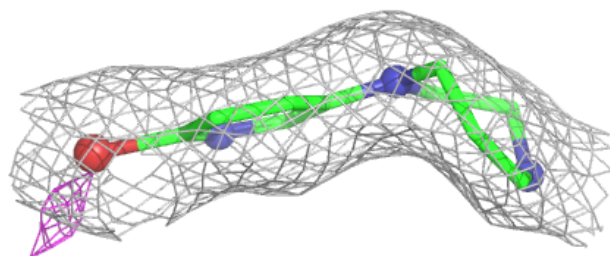
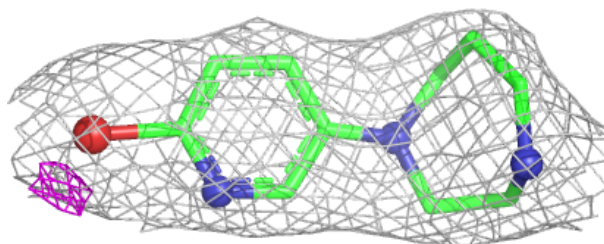


Electron density around 09R O 301:

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

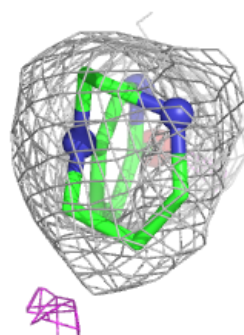
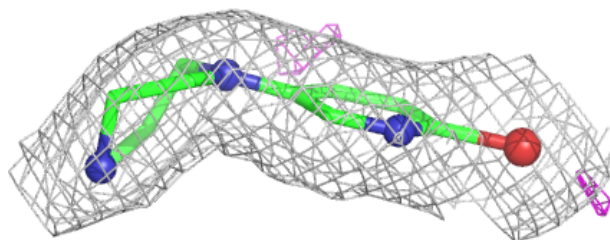
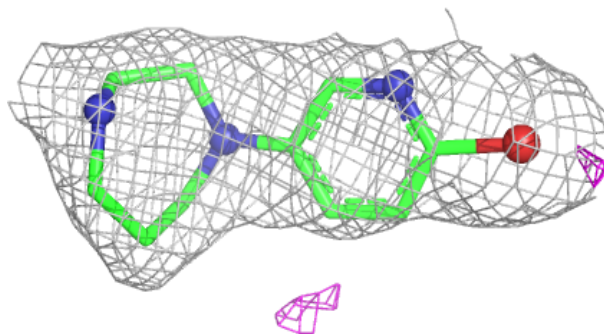
**Electron density around 09R F 301:**

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

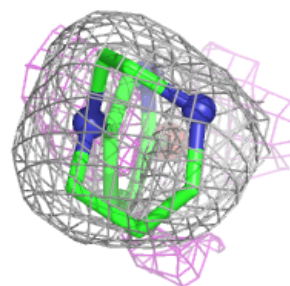
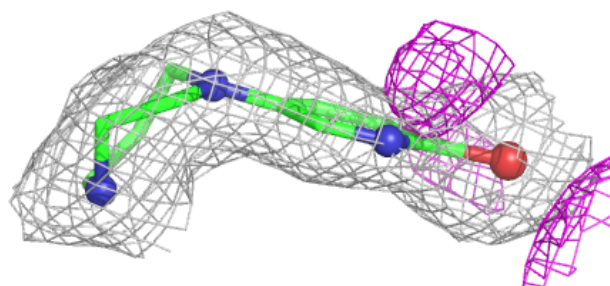
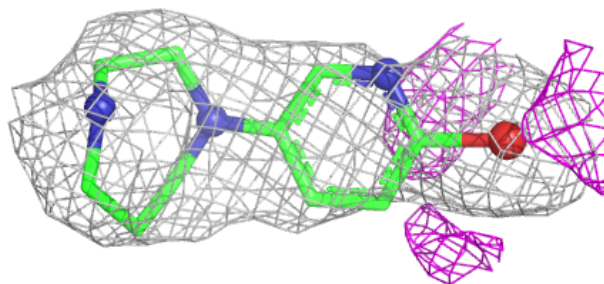


Electron density around 09R S 301:

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

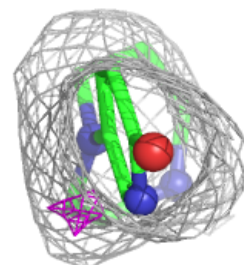
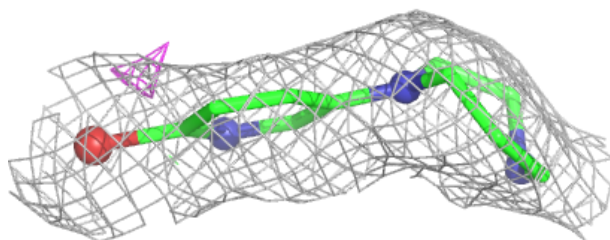
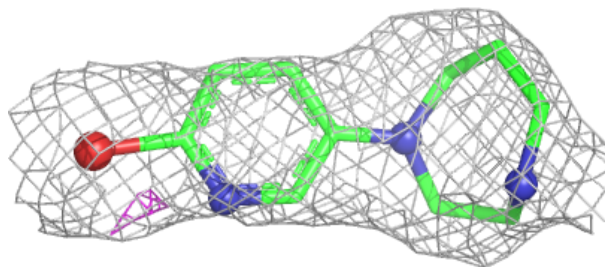
**Electron density around 09R U 301:**

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

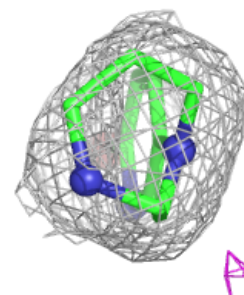
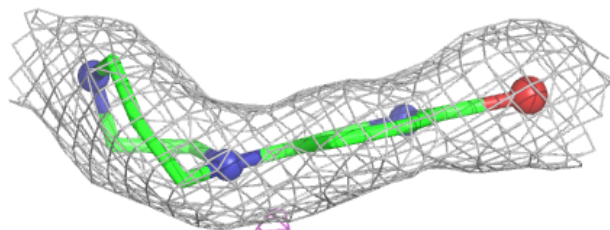
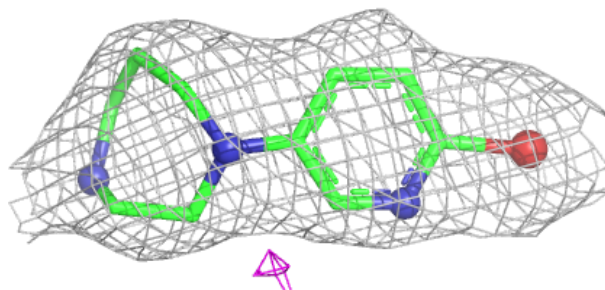


Electron density around 09R X 301:

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

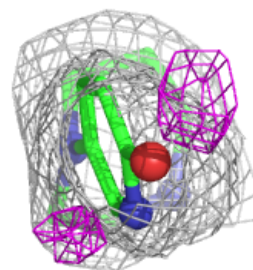
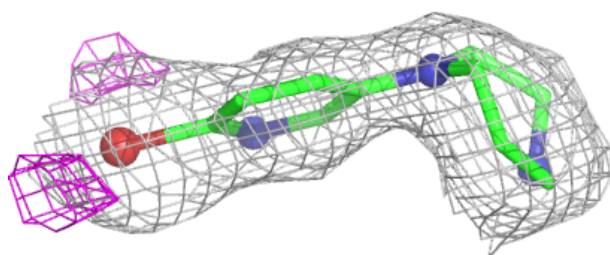
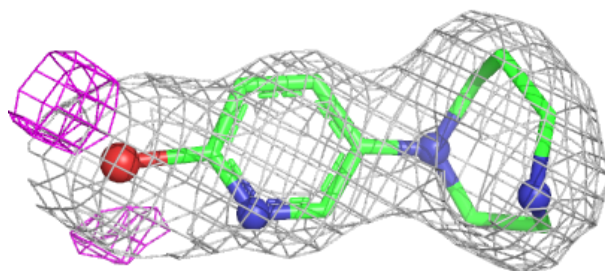
**Electron density around 09R Y 301:**

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

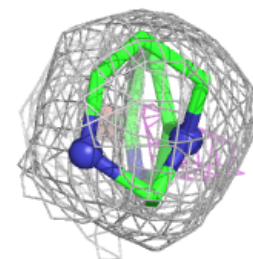
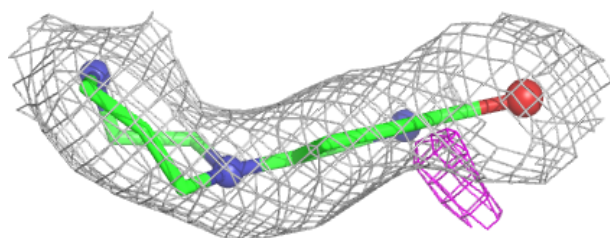
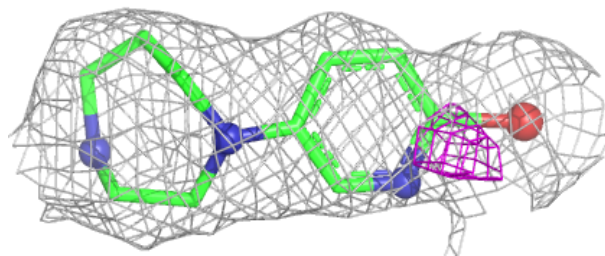


Electron density around 09R Z 301:

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

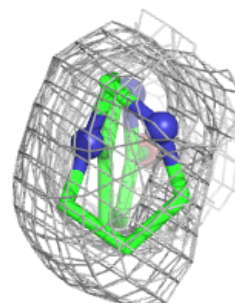
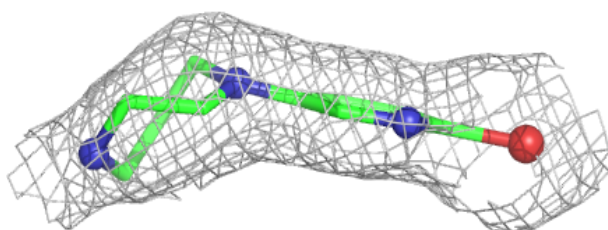
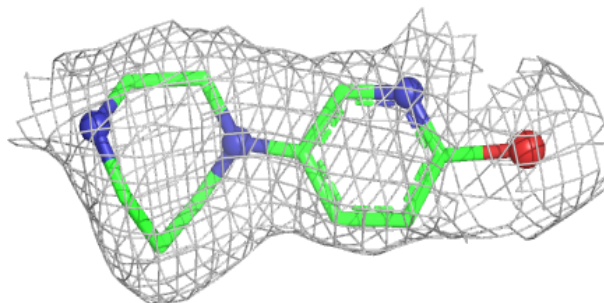
**Electron density around 09R a 301:**

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

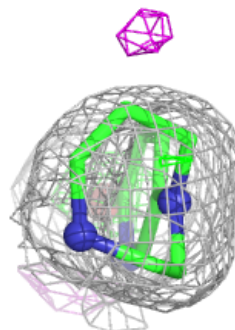
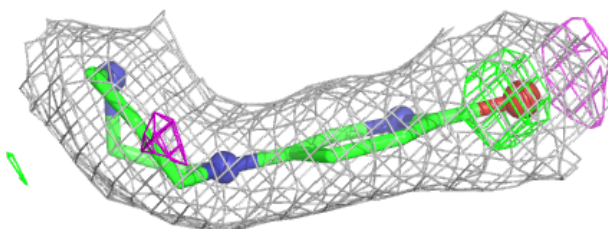
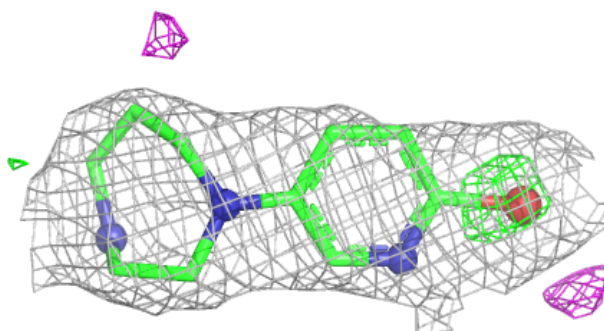


Electron density around 09R b 301:

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

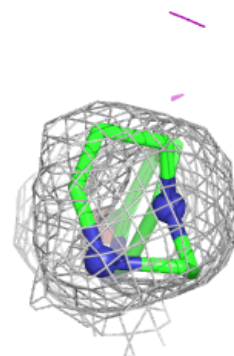
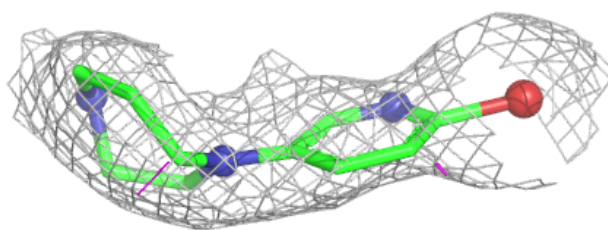
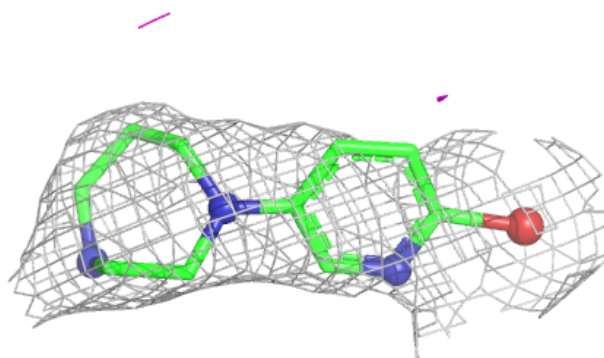
**Electron density around 09R I 301:**

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

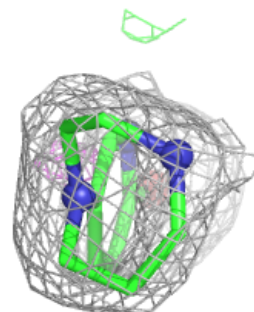
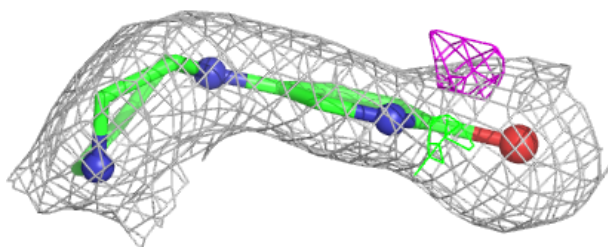
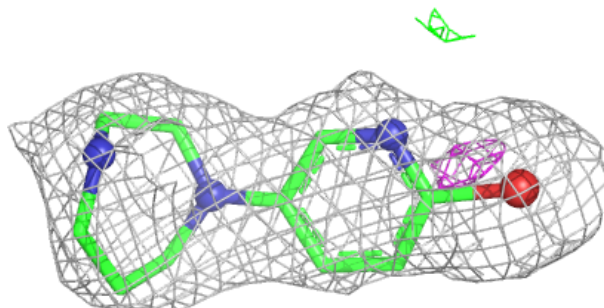


Electron density around 09R k 301:

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

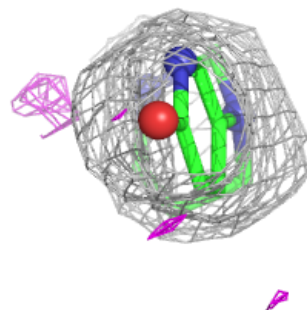
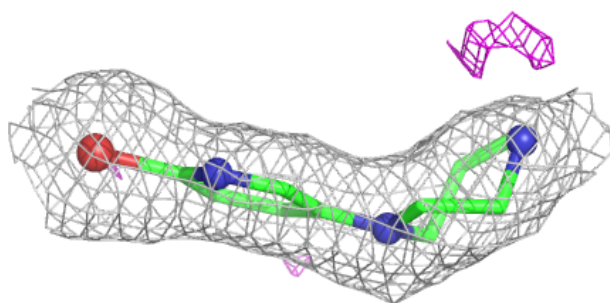
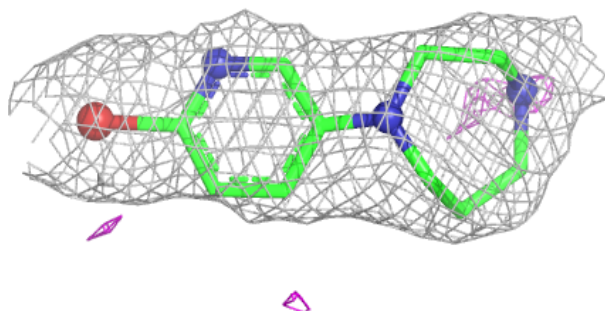
**Electron density around 09R c 301:**

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

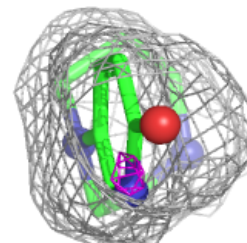
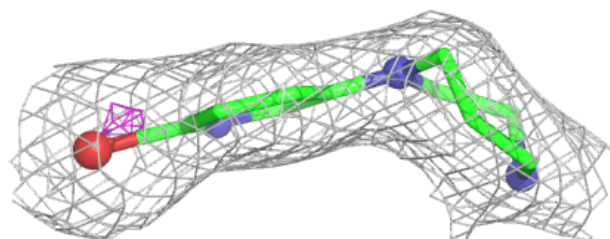
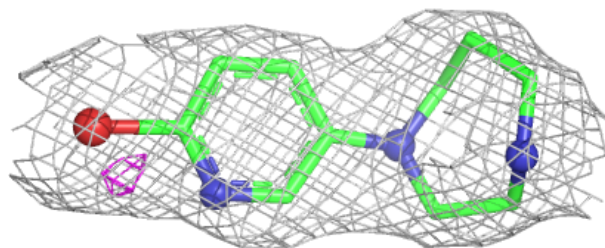


Electron density around 09R A 301:

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

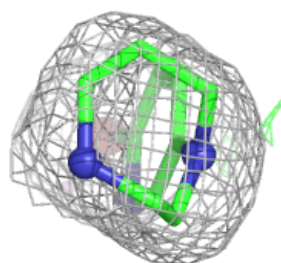
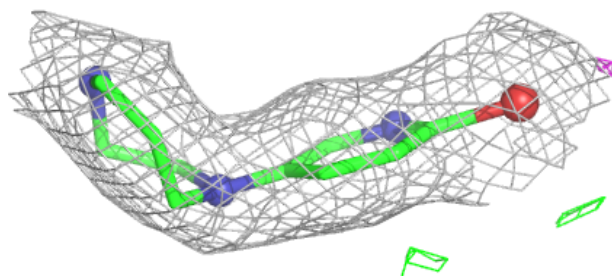
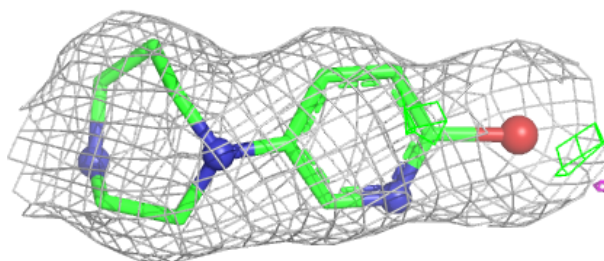
**Electron density around 09R C 301:**

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

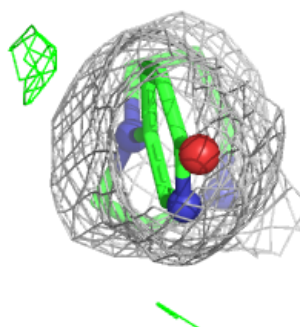
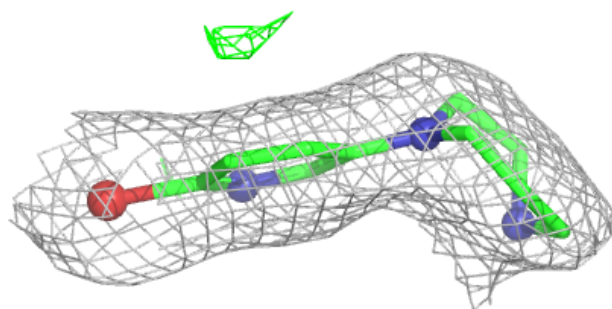
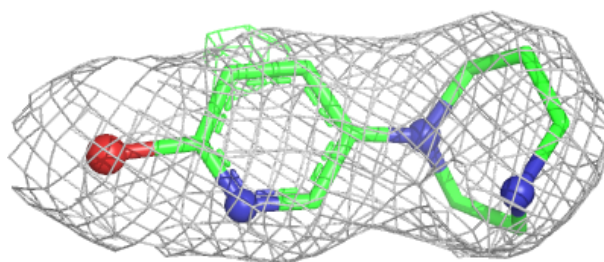


Electron density around 09R D 301:

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

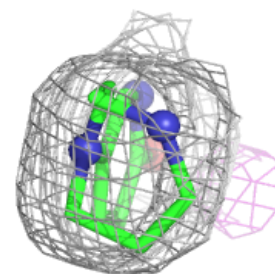
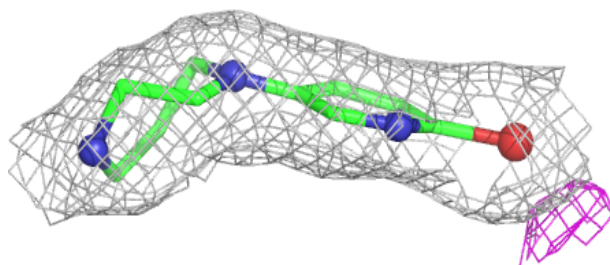
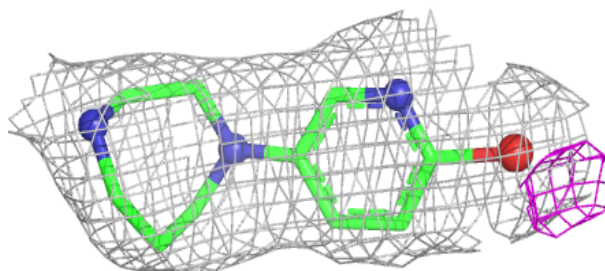
**Electron density around 09R g 301:**

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

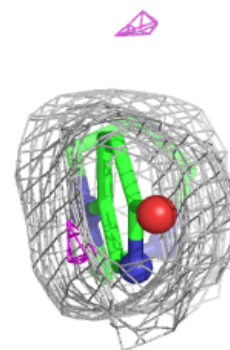
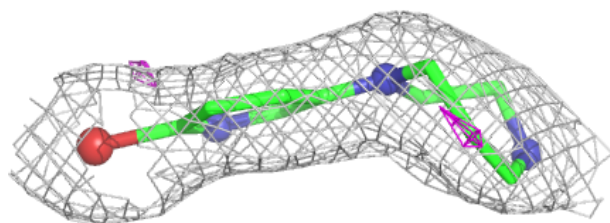
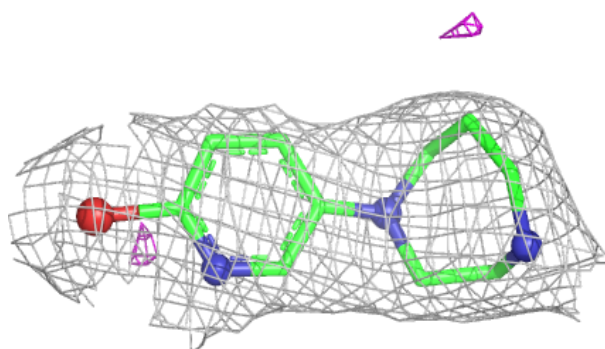


Electron density around 09R T 301:

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

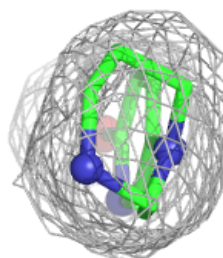
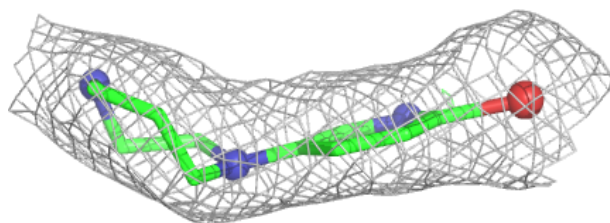
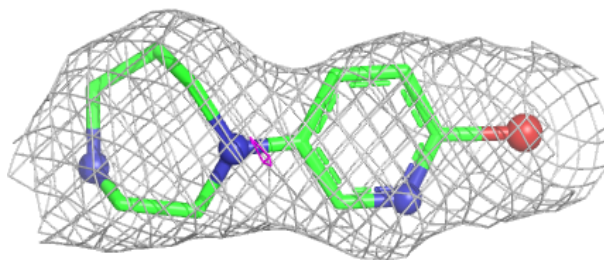
**Electron density around 09R E 301:**

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

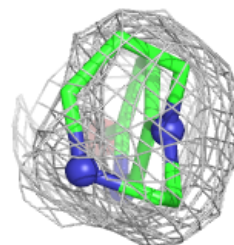
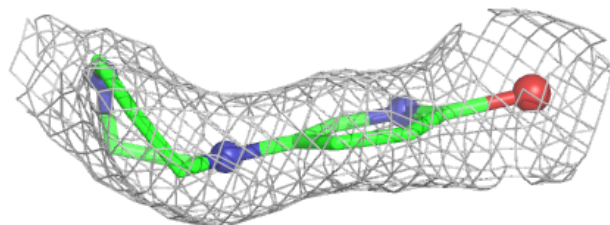
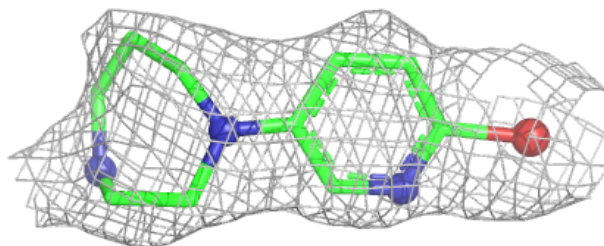


Electron density around 09R R 301:

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

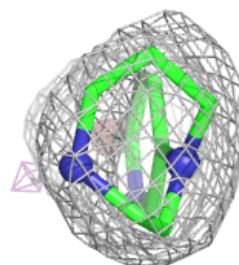
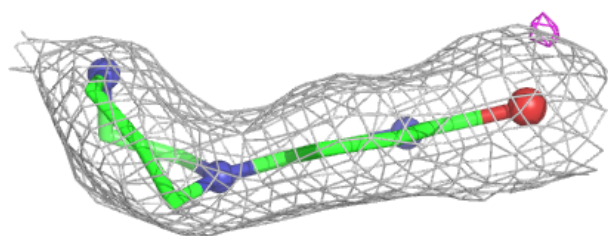
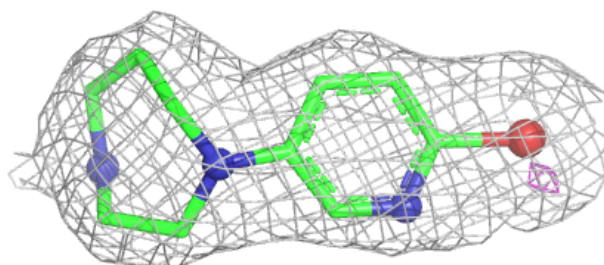
**Electron density around 09R W 301:**

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

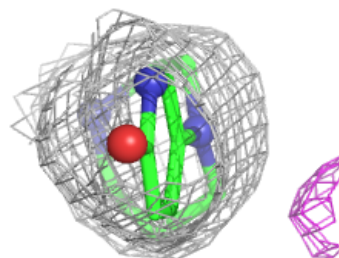
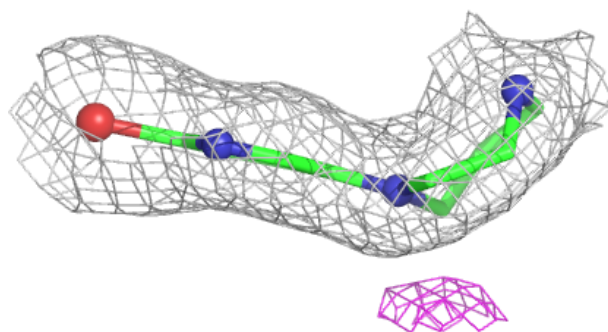
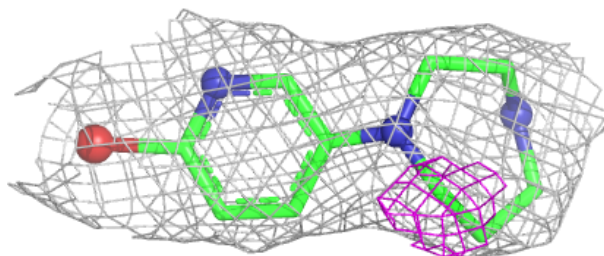


Electron density around 09R P 301:

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

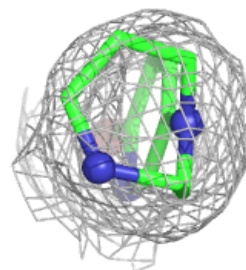
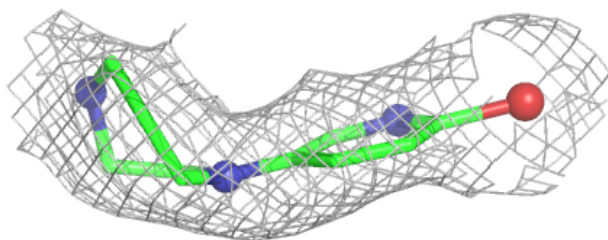
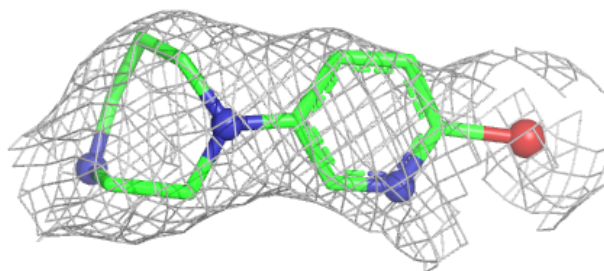
**Electron density around 09R J 301:**

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

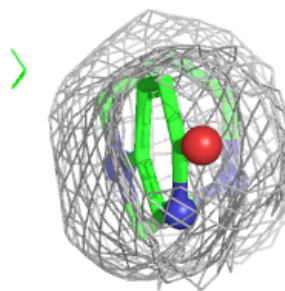
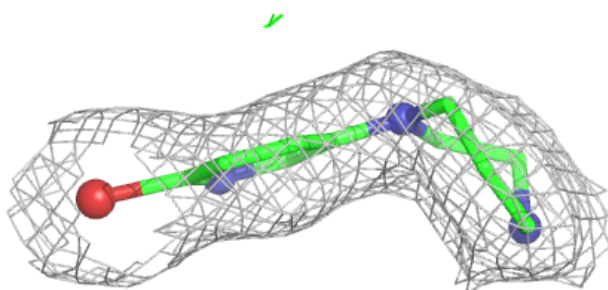
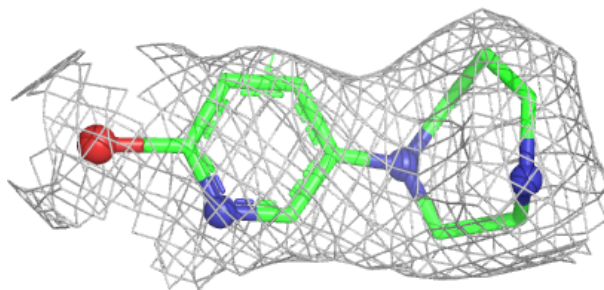


Electron density around 09R h 301:

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

**Electron density around 09R V 302:**

$2mF_o - DF_c$ (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.