



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:00 PM UTC

PDB ID : 8AVP / pdb_00008avp
Title : Structure of short biotin complexed agroavidin with the Hoef tail.
Authors : Livnah, O.; Bana, J.; Warar, J.
Deposited on : 2022-08-26
Resolution : 2.87 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:

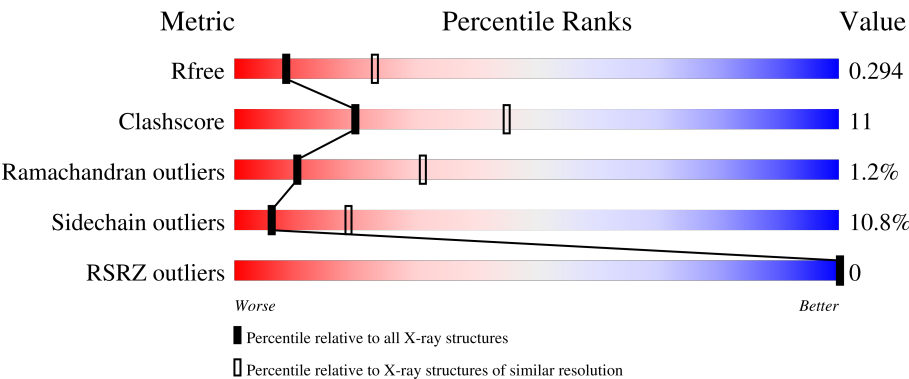
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	131	68%23%• 8%
1	B	131	68%19%5% 8%
1	C	131	63%27%• 8%
1	D	131	64%25%• 8%
1	E	131	66%26%• 8%

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Mol	Chain	Length	Quality of chain
1	F	131	 73%18%• 8%
1	G	131	 65%26%• 8%
1	H	131	 63%27%• 8%
1	I	131	 60%27%5% 8%
1	J	131	 67%24%• 8%
1	K	131	 75%16%• 8%
1	L	131	 73%18%• 8%
1	M	131	 73%18%• 8%
1	N	131	 67%24%• 8%
1	O	131	 63%26%• 8%
1	P	131	 68%22%• 8%
1	Q	131	 50%31%11% 8%
1	R	131	 52%33%8% 8%
1	S	131	 61%24%7% 8%
1	T	131	 70%21%• 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18172 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 agroavCH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	S	0	0	0
			892	560	154	175	3			
1	B	121	Total	C	N	O	S	0	0	0
			892	560	154	175	3			
1	C	121	Total	C	N	O	S	0	0	0
			892	560	154	175	3			
1	D	121	Total	C	N	O	S	0	1	0
			904	569	155	177	3			
1	E	121	Total	C	N	O	S	0	0	0
			892	560	154	175	3			
1	F	121	Total	C	N	O	S	0	0	0
			892	560	154	175	3			
1	G	121	Total	C	N	O	S	0	0	0
			892	560	154	175	3			
1	H	121	Total	C	N	O	S	0	0	0
			892	560	154	175	3			
1	I	121	Total	C	N	O	S	0	0	0
			892	560	154	175	3			
1	J	121	Total	C	N	O	S	0	0	0
			892	560	154	175	3			
1	K	121	Total	C	N	O	S	0	0	0
			892	560	154	175	3			
1	L	121	Total	C	N	O	S	0	0	0
			892	560	154	175	3			
1	M	121	Total	C	N	O	S	0	0	0
			892	560	154	175	3			
1	N	121	Total	C	N	O	S	0	0	0
			892	560	154	175	3			
1	O	121	Total	C	N	O	S	0	0	0
			892	560	154	175	3			
1	P	121	Total	C	N	O	S	0	0	0
			892	560	154	175	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	S	121	Total	C	N	O	S	0	0	0
			892	560	154	175	3			
1	T	121	Total	C	N	O	S	0	0	0
			892	560	154	175	3			
1	Q	121	Total	C	N	O	S	0	0	0
			892	560	154	175	3			
1	R	121	Total	C	N	O	S	0	0	0
			892	560	154	175	3			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A0N1ABZ3
A	36	TYR	PHE	conflict	UNP A0A0N1ABZ3
A	122	ALA	-	expression tag	UNP A0A0N1ABZ3
A	123	THR	-	expression tag	UNP A0A0N1ABZ3
A	124	VAL	-	expression tag	UNP A0A0N1ABZ3
A	125	SER	-	expression tag	UNP A0A0N1ABZ3
A	126	GLU	-	expression tag	UNP A0A0N1ABZ3
A	127	SER	-	expression tag	UNP A0A0N1ABZ3
A	128	LEU	-	expression tag	UNP A0A0N1ABZ3
A	129	LEU	-	expression tag	UNP A0A0N1ABZ3
A	130	THR	-	expression tag	UNP A0A0N1ABZ3
A	131	GLU	-	expression tag	UNP A0A0N1ABZ3
B	1	MET	-	initiating methionine	UNP A0A0N1ABZ3
B	36	TYR	PHE	conflict	UNP A0A0N1ABZ3
B	122	ALA	-	expression tag	UNP A0A0N1ABZ3
B	123	THR	-	expression tag	UNP A0A0N1ABZ3
B	124	VAL	-	expression tag	UNP A0A0N1ABZ3
B	125	SER	-	expression tag	UNP A0A0N1ABZ3
B	126	GLU	-	expression tag	UNP A0A0N1ABZ3
B	127	SER	-	expression tag	UNP A0A0N1ABZ3
B	128	LEU	-	expression tag	UNP A0A0N1ABZ3
B	129	LEU	-	expression tag	UNP A0A0N1ABZ3
B	130	THR	-	expression tag	UNP A0A0N1ABZ3
B	131	GLU	-	expression tag	UNP A0A0N1ABZ3
C	1	MET	-	initiating methionine	UNP A0A0N1ABZ3
C	36	TYR	PHE	conflict	UNP A0A0N1ABZ3
C	122	ALA	-	expression tag	UNP A0A0N1ABZ3
C	123	THR	-	expression tag	UNP A0A0N1ABZ3
C	124	VAL	-	expression tag	UNP A0A0N1ABZ3
C	125	SER	-	expression tag	UNP A0A0N1ABZ3
C	126	GLU	-	expression tag	UNP A0A0N1ABZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	127	SER	-	expression tag	UNP A0A0N1ABZ3
C	128	LEU	-	expression tag	UNP A0A0N1ABZ3
C	129	LEU	-	expression tag	UNP A0A0N1ABZ3
C	130	THR	-	expression tag	UNP A0A0N1ABZ3
C	131	GLU	-	expression tag	UNP A0A0N1ABZ3
D	1	MET	-	initiating methionine	UNP A0A0N1ABZ3
D	36	TYR	PHE	conflict	UNP A0A0N1ABZ3
D	122	ALA	-	expression tag	UNP A0A0N1ABZ3
D	123	THR	-	expression tag	UNP A0A0N1ABZ3
D	124	VAL	-	expression tag	UNP A0A0N1ABZ3
D	125	SER	-	expression tag	UNP A0A0N1ABZ3
D	126	GLU	-	expression tag	UNP A0A0N1ABZ3
D	127	SER	-	expression tag	UNP A0A0N1ABZ3
D	128	LEU	-	expression tag	UNP A0A0N1ABZ3
D	129	LEU	-	expression tag	UNP A0A0N1ABZ3
D	130	THR	-	expression tag	UNP A0A0N1ABZ3
D	131	GLU	-	expression tag	UNP A0A0N1ABZ3
E	1	MET	-	initiating methionine	UNP A0A0N1ABZ3
E	36	TYR	PHE	conflict	UNP A0A0N1ABZ3
E	122	ALA	-	expression tag	UNP A0A0N1ABZ3
E	123	THR	-	expression tag	UNP A0A0N1ABZ3
E	124	VAL	-	expression tag	UNP A0A0N1ABZ3
E	125	SER	-	expression tag	UNP A0A0N1ABZ3
E	126	GLU	-	expression tag	UNP A0A0N1ABZ3
E	127	SER	-	expression tag	UNP A0A0N1ABZ3
E	128	LEU	-	expression tag	UNP A0A0N1ABZ3
E	129	LEU	-	expression tag	UNP A0A0N1ABZ3
E	130	THR	-	expression tag	UNP A0A0N1ABZ3
E	131	GLU	-	expression tag	UNP A0A0N1ABZ3
F	1	MET	-	initiating methionine	UNP A0A0N1ABZ3
F	36	TYR	PHE	conflict	UNP A0A0N1ABZ3
F	122	ALA	-	expression tag	UNP A0A0N1ABZ3
F	123	THR	-	expression tag	UNP A0A0N1ABZ3
F	124	VAL	-	expression tag	UNP A0A0N1ABZ3
F	125	SER	-	expression tag	UNP A0A0N1ABZ3
F	126	GLU	-	expression tag	UNP A0A0N1ABZ3
F	127	SER	-	expression tag	UNP A0A0N1ABZ3
F	128	LEU	-	expression tag	UNP A0A0N1ABZ3
F	129	LEU	-	expression tag	UNP A0A0N1ABZ3
F	130	THR	-	expression tag	UNP A0A0N1ABZ3
F	131	GLU	-	expression tag	UNP A0A0N1ABZ3
G	1	MET	-	initiating methionine	UNP A0A0N1ABZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	36	TYR	PHE	conflict	UNP A0A0N1ABZ3
G	122	ALA	-	expression tag	UNP A0A0N1ABZ3
G	123	THR	-	expression tag	UNP A0A0N1ABZ3
G	124	VAL	-	expression tag	UNP A0A0N1ABZ3
G	125	SER	-	expression tag	UNP A0A0N1ABZ3
G	126	GLU	-	expression tag	UNP A0A0N1ABZ3
G	127	SER	-	expression tag	UNP A0A0N1ABZ3
G	128	LEU	-	expression tag	UNP A0A0N1ABZ3
G	129	LEU	-	expression tag	UNP A0A0N1ABZ3
G	130	THR	-	expression tag	UNP A0A0N1ABZ3
G	131	GLU	-	expression tag	UNP A0A0N1ABZ3
H	1	MET	-	initiating methionine	UNP A0A0N1ABZ3
H	36	TYR	PHE	conflict	UNP A0A0N1ABZ3
H	122	ALA	-	expression tag	UNP A0A0N1ABZ3
H	123	THR	-	expression tag	UNP A0A0N1ABZ3
H	124	VAL	-	expression tag	UNP A0A0N1ABZ3
H	125	SER	-	expression tag	UNP A0A0N1ABZ3
H	126	GLU	-	expression tag	UNP A0A0N1ABZ3
H	127	SER	-	expression tag	UNP A0A0N1ABZ3
H	128	LEU	-	expression tag	UNP A0A0N1ABZ3
H	129	LEU	-	expression tag	UNP A0A0N1ABZ3
H	130	THR	-	expression tag	UNP A0A0N1ABZ3
H	131	GLU	-	expression tag	UNP A0A0N1ABZ3
I	1	MET	-	initiating methionine	UNP A0A0N1ABZ3
I	36	TYR	PHE	conflict	UNP A0A0N1ABZ3
I	122	ALA	-	expression tag	UNP A0A0N1ABZ3
I	123	THR	-	expression tag	UNP A0A0N1ABZ3
I	124	VAL	-	expression tag	UNP A0A0N1ABZ3
I	125	SER	-	expression tag	UNP A0A0N1ABZ3
I	126	GLU	-	expression tag	UNP A0A0N1ABZ3
I	127	SER	-	expression tag	UNP A0A0N1ABZ3
I	128	LEU	-	expression tag	UNP A0A0N1ABZ3
I	129	LEU	-	expression tag	UNP A0A0N1ABZ3
I	130	THR	-	expression tag	UNP A0A0N1ABZ3
I	131	GLU	-	expression tag	UNP A0A0N1ABZ3
J	1	MET	-	initiating methionine	UNP A0A0N1ABZ3
J	36	TYR	PHE	conflict	UNP A0A0N1ABZ3
J	122	ALA	-	expression tag	UNP A0A0N1ABZ3
J	123	THR	-	expression tag	UNP A0A0N1ABZ3
J	124	VAL	-	expression tag	UNP A0A0N1ABZ3
J	125	SER	-	expression tag	UNP A0A0N1ABZ3
J	126	GLU	-	expression tag	UNP A0A0N1ABZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
J	127	SER	-	expression tag	UNP A0A0N1ABZ3
J	128	LEU	-	expression tag	UNP A0A0N1ABZ3
J	129	LEU	-	expression tag	UNP A0A0N1ABZ3
J	130	THR	-	expression tag	UNP A0A0N1ABZ3
J	131	GLU	-	expression tag	UNP A0A0N1ABZ3
K	1	MET	-	initiating methionine	UNP A0A0N1ABZ3
K	36	TYR	PHE	conflict	UNP A0A0N1ABZ3
K	122	ALA	-	expression tag	UNP A0A0N1ABZ3
K	123	THR	-	expression tag	UNP A0A0N1ABZ3
K	124	VAL	-	expression tag	UNP A0A0N1ABZ3
K	125	SER	-	expression tag	UNP A0A0N1ABZ3
K	126	GLU	-	expression tag	UNP A0A0N1ABZ3
K	127	SER	-	expression tag	UNP A0A0N1ABZ3
K	128	LEU	-	expression tag	UNP A0A0N1ABZ3
K	129	LEU	-	expression tag	UNP A0A0N1ABZ3
K	130	THR	-	expression tag	UNP A0A0N1ABZ3
K	131	GLU	-	expression tag	UNP A0A0N1ABZ3
L	1	MET	-	initiating methionine	UNP A0A0N1ABZ3
L	36	TYR	PHE	conflict	UNP A0A0N1ABZ3
L	122	ALA	-	expression tag	UNP A0A0N1ABZ3
L	123	THR	-	expression tag	UNP A0A0N1ABZ3
L	124	VAL	-	expression tag	UNP A0A0N1ABZ3
L	125	SER	-	expression tag	UNP A0A0N1ABZ3
L	126	GLU	-	expression tag	UNP A0A0N1ABZ3
L	127	SER	-	expression tag	UNP A0A0N1ABZ3
L	128	LEU	-	expression tag	UNP A0A0N1ABZ3
L	129	LEU	-	expression tag	UNP A0A0N1ABZ3
L	130	THR	-	expression tag	UNP A0A0N1ABZ3
L	131	GLU	-	expression tag	UNP A0A0N1ABZ3
M	1	MET	-	initiating methionine	UNP A0A0N1ABZ3
M	36	TYR	PHE	conflict	UNP A0A0N1ABZ3
M	122	ALA	-	expression tag	UNP A0A0N1ABZ3
M	123	THR	-	expression tag	UNP A0A0N1ABZ3
M	124	VAL	-	expression tag	UNP A0A0N1ABZ3
M	125	SER	-	expression tag	UNP A0A0N1ABZ3
M	126	GLU	-	expression tag	UNP A0A0N1ABZ3
M	127	SER	-	expression tag	UNP A0A0N1ABZ3
M	128	LEU	-	expression tag	UNP A0A0N1ABZ3
M	129	LEU	-	expression tag	UNP A0A0N1ABZ3
M	130	THR	-	expression tag	UNP A0A0N1ABZ3
M	131	GLU	-	expression tag	UNP A0A0N1ABZ3
N	1	MET	-	initiating methionine	UNP A0A0N1ABZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
N	36	TYR	PHE	conflict	UNP A0A0N1ABZ3
N	122	ALA	-	expression tag	UNP A0A0N1ABZ3
N	123	THR	-	expression tag	UNP A0A0N1ABZ3
N	124	VAL	-	expression tag	UNP A0A0N1ABZ3
N	125	SER	-	expression tag	UNP A0A0N1ABZ3
N	126	GLU	-	expression tag	UNP A0A0N1ABZ3
N	127	SER	-	expression tag	UNP A0A0N1ABZ3
N	128	LEU	-	expression tag	UNP A0A0N1ABZ3
N	129	LEU	-	expression tag	UNP A0A0N1ABZ3
N	130	THR	-	expression tag	UNP A0A0N1ABZ3
N	131	GLU	-	expression tag	UNP A0A0N1ABZ3
O	1	MET	-	initiating methionine	UNP A0A0N1ABZ3
O	36	TYR	PHE	conflict	UNP A0A0N1ABZ3
O	122	ALA	-	expression tag	UNP A0A0N1ABZ3
O	123	THR	-	expression tag	UNP A0A0N1ABZ3
O	124	VAL	-	expression tag	UNP A0A0N1ABZ3
O	125	SER	-	expression tag	UNP A0A0N1ABZ3
O	126	GLU	-	expression tag	UNP A0A0N1ABZ3
O	127	SER	-	expression tag	UNP A0A0N1ABZ3
O	128	LEU	-	expression tag	UNP A0A0N1ABZ3
O	129	LEU	-	expression tag	UNP A0A0N1ABZ3
O	130	THR	-	expression tag	UNP A0A0N1ABZ3
O	131	GLU	-	expression tag	UNP A0A0N1ABZ3
P	1	MET	-	initiating methionine	UNP A0A0N1ABZ3
P	36	TYR	PHE	conflict	UNP A0A0N1ABZ3
P	122	ALA	-	expression tag	UNP A0A0N1ABZ3
P	123	THR	-	expression tag	UNP A0A0N1ABZ3
P	124	VAL	-	expression tag	UNP A0A0N1ABZ3
P	125	SER	-	expression tag	UNP A0A0N1ABZ3
P	126	GLU	-	expression tag	UNP A0A0N1ABZ3
P	127	SER	-	expression tag	UNP A0A0N1ABZ3
P	128	LEU	-	expression tag	UNP A0A0N1ABZ3
P	129	LEU	-	expression tag	UNP A0A0N1ABZ3
P	130	THR	-	expression tag	UNP A0A0N1ABZ3
P	131	GLU	-	expression tag	UNP A0A0N1ABZ3
S	1	MET	-	initiating methionine	UNP A0A0N1ABZ3
S	36	TYR	PHE	conflict	UNP A0A0N1ABZ3
S	122	ALA	-	expression tag	UNP A0A0N1ABZ3
S	123	THR	-	expression tag	UNP A0A0N1ABZ3
S	124	VAL	-	expression tag	UNP A0A0N1ABZ3
S	125	SER	-	expression tag	UNP A0A0N1ABZ3
S	126	GLU	-	expression tag	UNP A0A0N1ABZ3

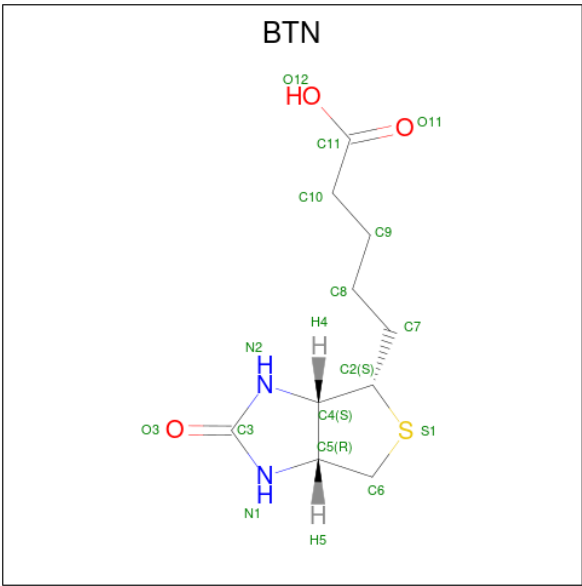
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Chain	Residue	Modelled	Actual	Comment	Reference
S	127	SER	-	expression tag	UNP A0A0N1ABZ3
S	128	LEU	-	expression tag	UNP A0A0N1ABZ3
S	129	LEU	-	expression tag	UNP A0A0N1ABZ3
S	130	THR	-	expression tag	UNP A0A0N1ABZ3
S	131	GLU	-	expression tag	UNP A0A0N1ABZ3
T	1	MET	-	initiating methionine	UNP A0A0N1ABZ3
T	36	TYR	PHE	conflict	UNP A0A0N1ABZ3
T	122	ALA	-	expression tag	UNP A0A0N1ABZ3
T	123	THR	-	expression tag	UNP A0A0N1ABZ3
T	124	VAL	-	expression tag	UNP A0A0N1ABZ3
T	125	SER	-	expression tag	UNP A0A0N1ABZ3
T	126	GLU	-	expression tag	UNP A0A0N1ABZ3
T	127	SER	-	expression tag	UNP A0A0N1ABZ3
T	128	LEU	-	expression tag	UNP A0A0N1ABZ3
T	129	LEU	-	expression tag	UNP A0A0N1ABZ3
T	130	THR	-	expression tag	UNP A0A0N1ABZ3
T	131	GLU	-	expression tag	UNP A0A0N1ABZ3
Q	1	MET	-	initiating methionine	UNP A0A0N1ABZ3
Q	36	TYR	PHE	conflict	UNP A0A0N1ABZ3
Q	122	ALA	-	expression tag	UNP A0A0N1ABZ3
Q	123	THR	-	expression tag	UNP A0A0N1ABZ3
Q	124	VAL	-	expression tag	UNP A0A0N1ABZ3
Q	125	SER	-	expression tag	UNP A0A0N1ABZ3
Q	126	GLU	-	expression tag	UNP A0A0N1ABZ3
Q	127	SER	-	expression tag	UNP A0A0N1ABZ3
Q	128	LEU	-	expression tag	UNP A0A0N1ABZ3
Q	129	LEU	-	expression tag	UNP A0A0N1ABZ3
Q	130	THR	-	expression tag	UNP A0A0N1ABZ3
Q	131	GLU	-	expression tag	UNP A0A0N1ABZ3
R	1	MET	-	initiating methionine	UNP A0A0N1ABZ3
R	36	TYR	PHE	conflict	UNP A0A0N1ABZ3
R	122	ALA	-	expression tag	UNP A0A0N1ABZ3
R	123	THR	-	expression tag	UNP A0A0N1ABZ3
R	124	VAL	-	expression tag	UNP A0A0N1ABZ3
R	125	SER	-	expression tag	UNP A0A0N1ABZ3
R	126	GLU	-	expression tag	UNP A0A0N1ABZ3
R	127	SER	-	expression tag	UNP A0A0N1ABZ3
R	128	LEU	-	expression tag	UNP A0A0N1ABZ3
R	129	LEU	-	expression tag	UNP A0A0N1ABZ3
R	130	THR	-	expression tag	UNP A0A0N1ABZ3
R	131	GLU	-	expression tag	UNP A0A0N1ABZ3

- Molecule 2 is BIOTIN (CCD ID: BTN) (formula: $C_{10}H_{16}N_2O_3S$) (labeled as "Ligand of

Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	B	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	C	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	D	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	E	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	F	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	G	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	H	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	I	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	J	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	K	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	L	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	M	1	Total	C	N	O	S	0	0
			16	10	2	3	1		

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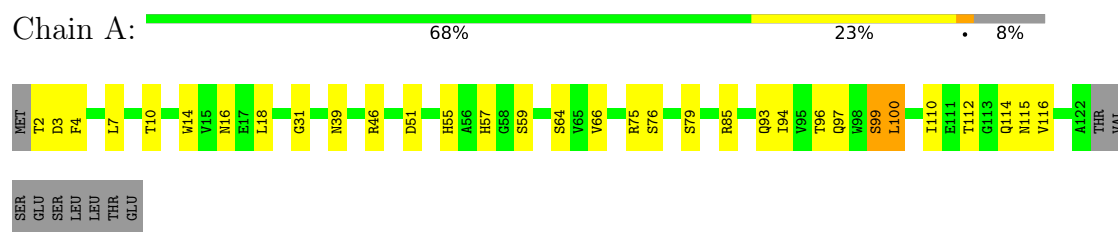
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	N	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	O	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	P	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	S	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	T	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	Q	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	R	1	Total	C	N	O	S	0	0
			16	10	2	3	1		

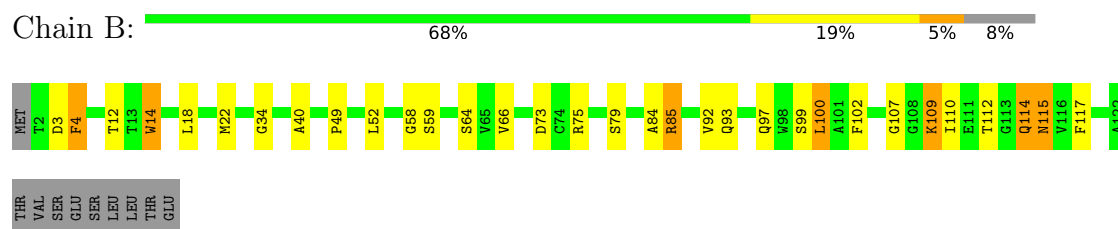
3 Residue-property plots

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

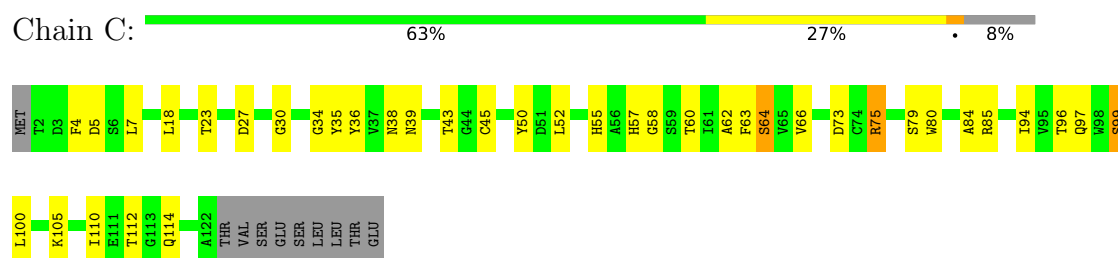
• Molecule 1: agroavCH



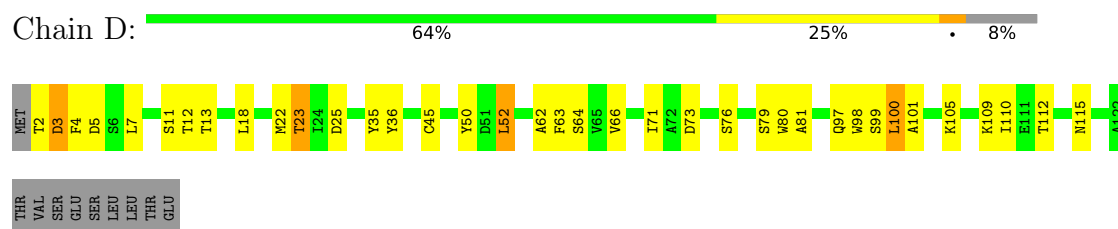
• Molecule 1: agroavCH



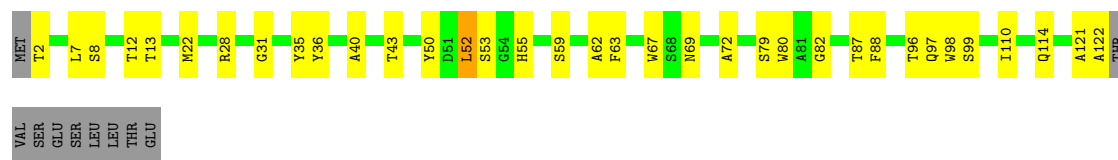
• Molecule 1: agroavCH



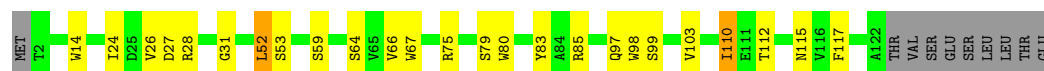
• Molecule 1: agroavCH



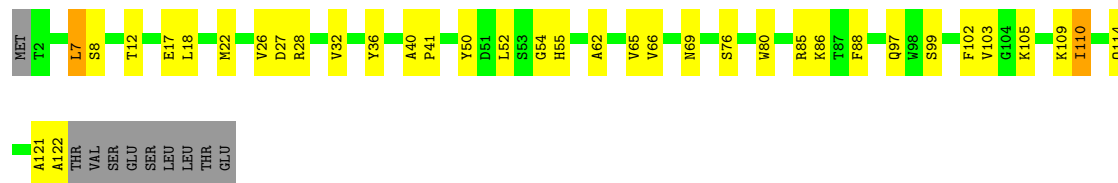
● Molecule 1: agroavCH

Chain E:  66% 26% 8%

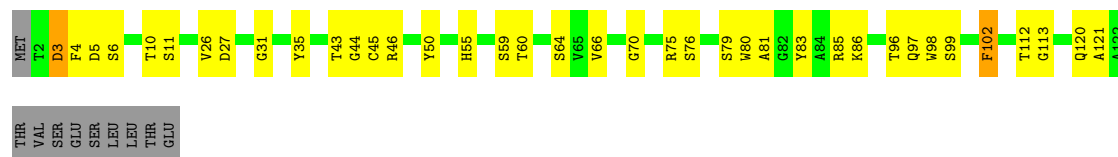
● Molecule 1: agroavCH

Chain F:  73% 18% 8%

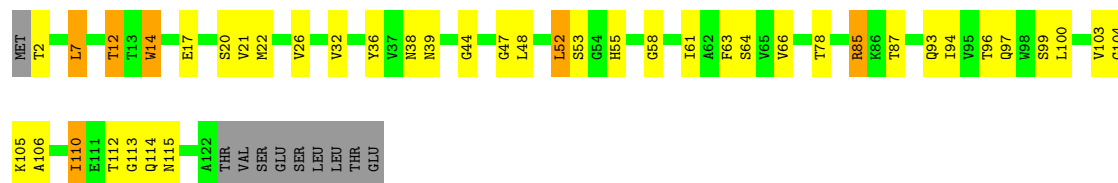
● Molecule 1: agroavCH

Chain G:  65% 26% 8%

● Molecule 1: agroavCH

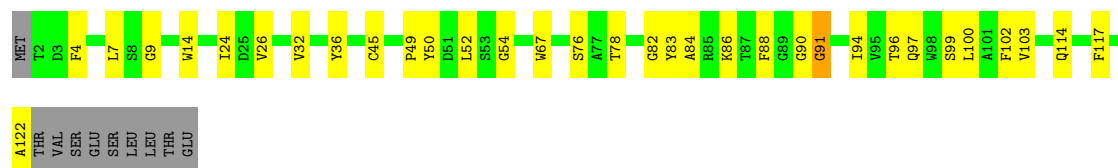
Chain H:  63% 27% 8%

● Molecule 1: agroavCH

Chain I:  60% 27% 5% 8%

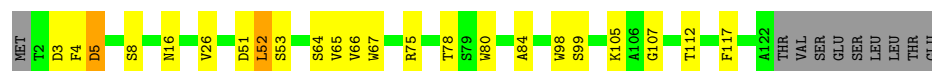
● Molecule 1: agroavCH

Chain J:  67% 24% 8%



- Molecule 1: agroavCH

Chain K: 75% 16% 8%



- Molecule 1: agroavCH

Chain L: 73% 18% 8%



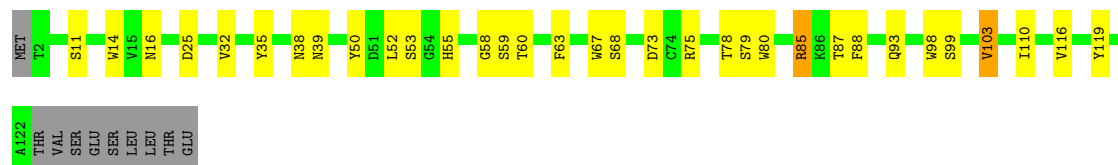
- Molecule 1: agroavCH

Chain M: 73% 18% 8%



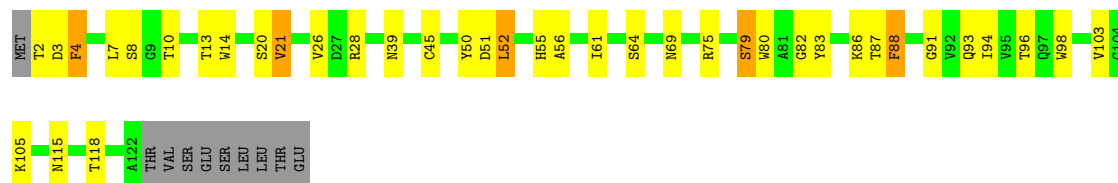
- Molecule 1: agroavCH

Chain N: 67% 24% 8%



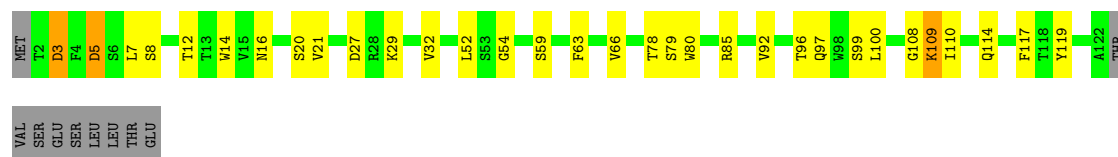
- Molecule 1: agroavCH

Chain O: 63% 26% 8%

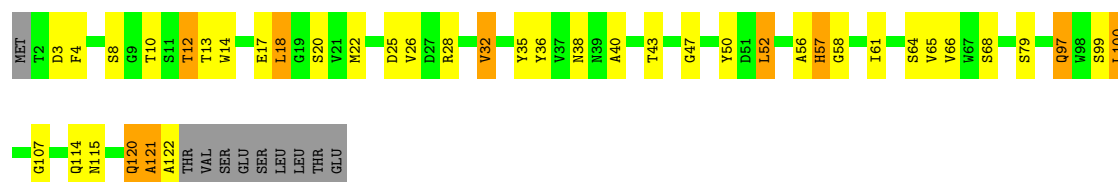


- Molecule 1: agroavCH

Chain P: 68% 22% 8%



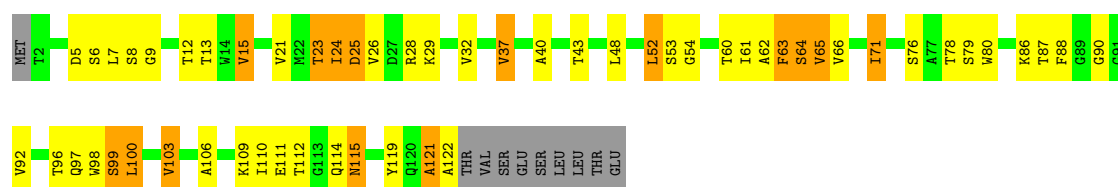
- Molecule 1: agroavCH



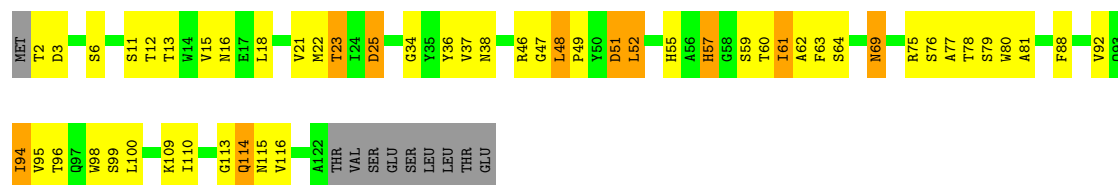
- Molecule 1: agroavCH



- Molecule 1: agroavCH



- Molecule 1: agroavCH



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	143.11Å 81.58Å 170.05Å 90.00° 114.87° 90.00°	Depositor
Resolution (Å)	50.00 – 2.87 50.00 – 2.87	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-2.87) 95.3 (50.00-2.87)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.231 , 0.297 0.234 , 0.294	Depositor DCC
R_{free} test set	4024 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	59.3	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.079 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18172	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.5317e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.09	1/913 (0.1%)	1.41	1/1242 (0.1%)
1	B	1.13	1/913 (0.1%)	1.47	8/1242 (0.6%)
1	C	1.12	0/913	1.40	2/1242 (0.2%)
1	D	1.07	0/926	1.43	2/1260 (0.2%)
1	E	1.09	0/913	1.42	0/1242
1	F	1.12	1/913 (0.1%)	1.46	0/1242
1	G	1.11	0/913	1.40	1/1242 (0.1%)
1	H	1.13	0/913	1.46	2/1242 (0.2%)
1	I	1.11	0/913	1.41	0/1242
1	J	1.06	0/913	1.39	1/1242 (0.1%)
1	K	1.08	0/913	1.43	2/1242 (0.2%)
1	L	1.05	0/913	1.39	1/1242 (0.1%)
1	M	1.11	0/913	1.33	0/1242
1	N	1.10	0/913	1.36	0/1242
1	O	1.08	0/913	1.41	0/1242
1	P	1.09	0/913	1.47	2/1242 (0.2%)
1	Q	1.08	0/913	1.48	0/1242
1	R	1.13	0/913	1.42	0/1242
1	S	1.11	0/913	1.46	2/1242 (0.2%)
1	T	1.09	0/913	1.40	2/1242 (0.2%)
All	All	1.10	3/18273 (0.0%)	1.42	26/24858 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	49	PRO	C-O	-5.39	1.17	1.23
1	A	57	HIS	C-O	5.06	1.29	1.23
1	F	53	SER	C-O	5.00	1.30	1.23

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	TRP	CA-C-O	-6.34	114.03	121.44
1	T	70	GLY	CA-C-N	5.98	128.10	120.56
1	T	70	GLY	C-N-CA	5.98	128.10	120.56
1	B	3	ASP	CA-C-N	5.93	132.87	121.54
1	B	3	ASP	C-N-CA	5.93	132.87	121.54
1	P	96	THR	CA-CB-OG1	-5.85	100.82	109.60
1	L	45	CYS	N-CA-C	-5.82	105.48	112.58
1	C	35	TYR	CB-CA-C	5.80	120.15	109.71
1	B	114	GLN	CB-CA-C	5.75	119.14	109.48
1	P	3	ASP	CA-CB-CG	5.66	118.26	112.60
1	B	73	ASP	CA-CB-CG	5.62	118.22	112.60
1	D	71	ILE	N-CA-C	-5.56	107.40	112.96
1	S	107	GLY	CA-C-N	5.42	126.07	120.60
1	S	107	GLY	C-N-CA	5.42	126.07	120.60
1	C	27	ASP	CA-CB-CG	5.32	117.92	112.60
1	H	70	GLY	CA-C-N	5.31	127.36	120.56
1	H	70	GLY	C-N-CA	5.31	127.36	120.56
1	B	107	GLY	CA-C-N	5.23	126.62	120.71
1	B	107	GLY	C-N-CA	5.23	126.62	120.71
1	K	107	GLY	CA-C-N	5.21	124.92	119.92
1	K	107	GLY	C-N-CA	5.21	124.92	119.92
1	G	110	ILE	CA-C-O	-5.15	114.34	120.78
1	D	115	ASN	CA-C-O	-5.11	115.33	121.11
1	J	86	LYS	CB-CA-C	5.09	118.22	109.51
1	A	51	ASP	CB-CA-C	-5.06	101.56	109.70
1	B	34	GLY	CA-C-O	-5.05	116.50	121.05

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	10	THR	Peptide

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	892	0	843	22	0
1	B	892	0	843	20	0
1	C	892	0	843	28	0
1	D	904	0	851	23	0
1	E	892	0	843	24	0
1	F	892	0	843	15	0
1	G	892	0	843	29	0
1	H	892	0	843	21	0
1	I	892	0	843	32	0
1	J	892	0	843	21	0
1	K	892	0	843	12	0
1	L	892	0	843	16	0
1	M	892	0	843	23	0
1	N	892	0	843	19	0
1	O	892	0	843	23	0
1	P	892	0	843	17	0
1	Q	892	0	843	45	0
1	R	892	0	843	34	0
1	S	892	0	843	25	0
1	T	892	0	843	24	0
2	A	16	0	15	0	0
2	B	16	0	15	0	0
2	C	16	0	15	1	0
2	D	16	0	15	0	0
2	E	16	0	15	1	0
2	F	16	0	15	2	0
2	G	16	0	15	0	0
2	H	16	0	15	1	0
2	I	16	0	15	0	0
2	J	16	0	15	2	0
2	K	16	0	15	1	0
2	L	16	0	15	0	0
2	M	16	0	15	1	0
2	N	16	0	15	1	0
2	O	16	0	15	0	0
2	P	16	0	15	0	0
2	Q	16	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	16	0	15	1	0
2	S	16	0	15	1	0
2	T	16	0	15	1	0
All	All	18172	0	17168	403	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (403) 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:S:97:GLN:HE22	1:S:114:GLN:HE21	1.09	0.92
1:Q:60:THR:HG21	1:R:76:SER:HA	1.49	0.91
1:C:97:GLN:HE22	1:C:114:GLN:HE21	1.26	0.83
1:N:85:ARG:NH1	1:N:93:GLN:OE1	2.11	0.83
1:S:97:GLN:NE2	1:S:114:GLN:HE21	1.77	0.81
1:E:97:GLN:HE22	1:E:114:GLN:HE21	1.29	0.81
1:T:40:ALA:O	1:T:43:THR:OG1	2.03	0.76
1:A:97:GLN:HE22	1:A:114:GLN:HE21	1.31	0.76
1:L:97:GLN:HE22	1:L:114:GLN:HE21	1.34	0.76
1:M:15:VAL:HG13	1:T:118:THR:HG21	1.68	0.76
1:S:97:GLN:HE22	1:S:114:GLN:NE2	1.84	0.75
1:Q:52:LEU:HB2	1:Q:65:VAL:HG22	1.70	0.74
1:I:26:VAL:HG22	1:I:32:VAL:HG12	1.69	0.73
1:I:20:SER:OG	1:I:39:ASN:N	2.21	0.72
1:E:52:LEU:HD12	1:E:53:SER:N	2.05	0.72
1:O:118:THR:HG21	1:Q:15:VAL:HG13	1.73	0.71
1:B:97:GLN:HE22	1:B:114:GLN:HG3	1.54	0.71
1:Q:5:ASP:O	1:Q:8:SER:OG	2.06	0.70
1:C:36:TYR:OH	2:C:201:BTN:O3	2.09	0.70
1:Q:78:THR:HG22	1:Q:80:TRP:CZ3	2.27	0.68
1:G:32:VAL:CG2	1:G:54:GLY:C	2.67	0.67
1:E:110:ILE:HG21	1:F:97:GLN:HB2	1.75	0.67
1:R:114:GLN:O	1:R:115:ASN:ND2	2.28	0.67
1:E:52:LEU:HD12	1:E:52:LEU:C	2.19	0.67
1:G:97:GLN:NE2	1:G:114:GLN:HE21	1.92	0.67
1:A:7:LEU:O	1:A:10:THR:OG1	2.12	0.66
1:L:36:TYR:HB2	1:L:52:LEU:HD23	1.78	0.66
1:B:4:PHE:HB2	1:B:58:GLY:O	1.96	0.65
1:Q:103:VAL:HG21	1:R:59:SER:HB3	1.77	0.65
1:E:59:SER:HB2	1:F:103:VAL:HG21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:22:MET:HB3	1:T:36:TYR:CD1	2.33	0.64
1:I:97:GLN:HE22	1:I:114:GLN:HE21	1.46	0.63
1:Q:40:ALA:O	1:Q:43:THR:OG1	2.16	0.63
1:R:16:ASN:ND2	2:R:201:BTN:O3	2.31	0.63
1:Q:80:TRP:O	1:R:79:SER:OG	2.16	0.63
1:G:32:VAL:HG23	1:G:54:GLY:C	2.24	0.62
1:B:22:MET:HE2	1:B:117:PHE:CD2	2.35	0.62
1:E:59:SER:CB	1:F:103:VAL:HG21	2.29	0.62
1:G:17:GLU:HG2	1:G:18:LEU:HD12	1.81	0.62
1:N:80:TRP:CD1	1:N:98:TRP:HB3	2.35	0.62
1:C:60:THR:HG21	1:D:76:SER:HA	1.83	0.61
1:Q:62:ALA:HB1	1:R:79:SER:HB3	1.81	0.61
1:R:52:LEU:HD12	1:R:52:LEU:C	2.24	0.61
1:C:73:ASP:OD1	1:C:75:ARG:HD2	2.00	0.61
1:H:3:ASP:OD2	1:H:5:ASP:HB2	2.01	0.61
1:Q:60:THR:HG21	1:R:76:SER:CA	2.27	0.61
1:R:23:THR:O	1:R:34:GLY:HA3	2.01	0.60
1:M:114:GLN:N	1:M:114:GLN:CD	2.60	0.59
1:J:9:GLY:N	1:J:26:VAL:O	2.26	0.59
1:M:52:LEU:HB2	1:M:65:VAL:HG22	1.83	0.59
1:R:52:LEU:HD13	1:R:63:PHE:HB2	1.85	0.59
1:D:52:LEU:C	1:D:52:LEU:HD12	2.28	0.59
1:I:47:GLY:O	1:I:48:LEU:HG	2.03	0.59
1:O:88:PHE:CD1	1:Q:37:VAL:HG21	2.38	0.59
1:Q:13:THR:OG1	1:Q:23:THR:HG23	2.03	0.59
1:Q:103:VAL:HG21	1:R:59:SER:CB	2.33	0.59
1:Q:109:LYS:O	1:Q:110:ILE:HG13	2.03	0.58
1:C:79:SER:HB2	1:D:79:SER:HB2	1.85	0.58
1:C:97:GLN:HB2	1:D:110:ILE:HG21	1.85	0.58
1:R:94:ILE:HG22	1:R:96:THR:HG22	1.85	0.58
1:I:7:LEU:HD22	1:I:26:VAL:CG2	2.33	0.58
1:I:52:LEU:HD12	1:I:53:SER:N	2.19	0.58
1:I:114:GLN:O	1:I:115:ASN:ND2	2.37	0.58
1:D:52:LEU:HD13	1:D:63:PHE:HB2	1.86	0.56
1:G:97:GLN:HE22	1:G:114:GLN:HE21	1.53	0.56
1:I:7:LEU:HD21	1:I:12:THR:CG2	2.35	0.56
1:E:97:GLN:HB2	1:F:110:ILE:HG21	1.87	0.56
1:I:97:GLN:NE2	1:I:114:GLN:HE21	2.03	0.56
1:O:103:VAL:HG23	1:O:103:VAL:O	2.06	0.56
1:K:78:THR:HA	1:K:99:SER:O	2.06	0.56
1:E:31:GLY:HA2	1:E:55:HIS:CD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LEU:C	1:B:52:LEU:HD12	2.31	0.55
1:K:5:ASP:N	1:K:5:ASP:OD1	2.39	0.55
1:C:4:PHE:O	1:C:7:LEU:HB2	2.07	0.55
1:C:38:ASN:ND2	1:C:43:THR:OG1	2.38	0.54
1:I:26:VAL:HG22	1:I:32:VAL:CG1	2.37	0.54
1:S:35:TYR:HA	1:S:50:TYR:O	2.08	0.54
1:O:20:SER:OG	1:O:39:ASN:N	2.40	0.54
1:A:39:ASN:ND2	1:A:46:ARG:HH11	2.05	0.54
1:F:67:TRP:CE2	2:F:201:BTN:H91	2.43	0.54
1:P:27:ASP:OD1	1:P:29:LYS:N	2.40	0.54
1:P:16:ASN:ND2	1:P:20:SER:HB2	2.22	0.54
1:B:85:ARG:NH1	1:B:93:GLN:OE1	2.26	0.54
1:R:15:VAL:HG23	1:R:21:VAL:HG22	1.88	0.54
1:F:80:TRP:CD1	1:F:98:TRP:HB3	2.43	0.54
1:G:76:SER:HA	1:H:60:THR:HG21	1.90	0.54
1:E:79:SER:HB2	1:F:79:SER:HB2	1.90	0.53
1:G:32:VAL:CG2	1:G:55:HIS:N	2.71	0.53
1:N:68:SER:OG	1:N:73:ASP:OD2	2.16	0.53
1:R:2:THR:HG22	1:R:6:SER:HB3	1.90	0.53
1:O:52:LEU:C	1:O:52:LEU:HD12	2.33	0.53
1:Q:60:THR:HB	1:R:77:ALA:HB3	1.90	0.53
1:C:5:ASP:OD1	1:C:58:GLY:N	2.36	0.53
1:P:78:THR:OG1	1:P:100:LEU:HD13	2.08	0.53
1:S:52:LEU:C	1:S:52:LEU:HD12	2.33	0.53
1:C:30:GLY:O	1:C:55:HIS:CD2	2.61	0.53
1:G:103:VAL:HG23	1:G:103:VAL:O	2.08	0.53
1:H:43:THR:HB	2:H:201:BTN:H102	1.89	0.53
1:J:94:ILE:HG22	1:J:96:THR:HG23	1.89	0.53
1:L:78:THR:HA	1:L:99:SER:O	2.09	0.53
1:A:97:GLN:HG2	1:B:112:THR:CG2	2.39	0.53
1:M:118:THR:HG21	1:T:15:VAL:HG13	1.91	0.53
1:Q:76:SER:HA	1:R:60:THR:HG21	1.91	0.53
1:Q:66:VAL:HG11	1:R:57:HIS:HB3	1.89	0.53
1:I:7:LEU:HD22	1:I:26:VAL:HB	1.90	0.53
1:Q:32:VAL:HB	1:Q:54:GLY:O	2.09	0.53
1:C:97:GLN:HE22	1:C:114:GLN:NE2	2.00	0.52
1:N:63:PHE:CE1	1:N:80:TRP:CE3	2.97	0.52
1:C:39:ASN:CG	1:C:39:ASN:O	2.52	0.52
1:G:32:VAL:HG22	1:G:55:HIS:N	2.24	0.52
1:B:102:PHE:CZ	1:B:109:LYS:HB2	2.44	0.52
1:J:83:TYR:HD2	1:J:84:ALA:O	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:4:PHE:CE1	1:O:56:ALA:HB1	2.44	0.52
1:C:4:PHE:CE2	1:C:84:ALA:HB2	2.44	0.52
1:I:110:ILE:HG21	1:J:97:GLN:HB2	1.91	0.52
1:C:45:CYS:HB3	1:C:50:TYR:CZ	2.45	0.52
1:I:97:GLN:HE22	1:I:114:GLN:NE2	2.07	0.52
1:S:12:THR:HA	1:S:122:ALA:CB	2.39	0.52
1:A:97:GLN:HB2	1:B:110:ILE:HG21	1.92	0.52
1:C:52:LEU:HD12	1:C:52:LEU:C	2.35	0.52
1:K:98:TRP:O	1:K:112:THR:HA	2.10	0.52
1:A:39:ASN:CG	1:A:39:ASN:O	2.53	0.51
1:S:12:THR:HA	1:S:122:ALA:HB1	1.92	0.51
1:S:114:GLN:O	1:S:115:ASN:ND2	2.41	0.51
1:F:14:TRP:HB3	1:F:117:PHE:HB3	1.93	0.51
1:G:97:GLN:HG2	1:H:112:THR:CG2	2.40	0.51
1:A:97:GLN:NE2	1:A:114:GLN:HE21	2.04	0.51
1:B:97:GLN:NE2	1:B:114:GLN:HG3	2.24	0.51
1:O:14:TRP:CZ3	1:O:94:ILE:HG13	2.45	0.51
1:M:52:LEU:HD12	1:M:52:LEU:C	2.36	0.51
1:N:87:THR:HG21	1:N:93:GLN:HG3	1.92	0.51
1:M:63:PHE:CE1	1:M:80:TRP:CE3	2.99	0.51
1:M:15:VAL:HG13	1:T:118:THR:CG2	2.38	0.51
1:J:36:TYR:OH	2:J:201:BTN:O3	2.25	0.51
1:Q:48:LEU:HD13	1:Q:71:ILE:CG2	2.41	0.50
1:A:79:SER:HB2	1:B:79:SER:HB2	1.92	0.50
1:T:35:TYR:HA	1:T:50:TYR:O	2.11	0.50
1:O:4:PHE:CZ	1:O:61:ILE:HB	2.47	0.50
1:T:119:TYR:CZ	1:T:121:ALA:HA	2.45	0.50
1:G:97:GLN:CD	1:G:114:GLN:HE21	2.19	0.50
1:I:85:ARG:NH2	1:I:93:GLN:OE1	2.43	0.50
1:S:40:ALA:O	1:S:43:THR:OG1	2.24	0.50
1:T:78:THR:HG21	1:T:80:TRP:CZ2	2.46	0.50
1:Q:32:VAL:HB	1:Q:54:GLY:C	2.37	0.50
1:H:59:SER:O	1:H:83:TYR:HA	2.12	0.50
1:Q:52:LEU:C	1:Q:52:LEU:HD12	2.36	0.50
1:E:87:THR:O	1:E:88:PHE:C	2.55	0.50
1:G:32:VAL:HG22	1:G:54:GLY:C	2.37	0.50
1:O:80:TRP:CD1	1:O:98:TRP:HB3	2.47	0.50
1:P:109:LYS:HD3	1:P:110:ILE:H	1.76	0.50
1:A:2:THR:HG22	1:A:2:THR:O	2.12	0.50
1:G:76:SER:HB3	1:G:102:PHE:HB3	1.93	0.50
1:P:5:ASP:N	1:P:5:ASP:OD1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:27:ASP:OD1	1:P:29:LYS:HB2	2.12	0.50
1:B:100:LEU:O	1:B:110:ILE:HA	2.11	0.50
1:N:78:THR:HG21	1:N:80:TRP:CZ2	2.47	0.49
1:G:50:TYR:CE1	1:G:69:ASN:ND2	2.80	0.49
1:S:64:SER:HB3	1:T:62:ALA:HB3	1.94	0.49
1:F:26:VAL:HA	1:F:31:GLY:O	2.11	0.49
1:Q:98:TRP:O	1:Q:98:TRP:CE3	2.66	0.49
1:R:25:ASP:N	1:R:25:ASP:OD1	2.45	0.49
1:I:22:MET:HB3	1:I:36:TYR:CD2	2.46	0.49
1:L:3:ASP:HB2	1:L:58:GLY:C	2.38	0.49
1:A:14:TRP:CZ3	1:A:94:ILE:HG13	2.47	0.49
1:O:82:GLY:HA3	1:O:96:THR:HG22	1.94	0.49
1:Q:12:THR:HA	1:Q:122:ALA:HB2	1.94	0.49
1:F:67:TRP:CD2	2:F:201:BTN:H91	2.48	0.49
1:T:87:THR:O	1:T:88:PHE:C	2.55	0.49
1:M:20:SER:OG	1:M:38:ASN:HA	2.13	0.49
1:O:87:THR:OG1	1:O:91:GLY:O	2.30	0.49
1:P:97:GLN:HE22	1:P:114:GLN:HG3	1.77	0.49
1:S:4:PHE:CE2	1:S:61:ILE:HB	2.48	0.49
1:D:80:TRP:CD1	1:D:98:TRP:HB3	2.48	0.49
1:L:52:LEU:C	1:L:52:LEU:HD12	2.37	0.49
1:A:97:GLN:HG2	1:B:112:THR:HG22	1.94	0.48
1:H:35:TYR:HA	1:H:50:TYR:O	2.13	0.48
1:H:98:TRP:CE2	1:H:113:GLY:HA3	2.48	0.48
1:J:94:ILE:HG22	1:J:96:THR:CG2	2.43	0.48
1:J:97:GLN:HE22	1:J:114:GLN:HE21	1.61	0.48
1:S:3:ASP:HA	1:S:58:GLY:O	2.13	0.48
1:A:112:THR:HG22	1:B:97:GLN:HG2	1.95	0.48
1:O:79:SER:HG	1:P:79:SER:CB	2.27	0.48
1:M:97:GLN:HB2	1:N:110:ILE:HG21	1.96	0.48
1:S:79:SER:HB3	1:T:62:ALA:HB1	1.96	0.48
1:E:28:ARG:CZ	1:J:122:ALA:HB3	2.43	0.48
1:N:35:TYR:HA	1:N:50:TYR:O	2.14	0.48
1:I:94:ILE:HG22	1:I:96:THR:CG2	2.44	0.48
1:E:80:TRP:CD1	1:E:98:TRP:HB3	2.49	0.48
1:G:12:THR:HA	1:G:122:ALA:HB1	1.95	0.48
1:E:88:PHE:C	1:E:88:PHE:CD1	2.91	0.48
1:G:80:TRP:C	1:H:79:SER:HG	2.21	0.48
1:G:97:GLN:HE22	1:G:114:GLN:NE2	2.11	0.48
1:O:87:THR:O	1:O:88:PHE:C	2.56	0.48
1:O:93:GLN:HG2	1:O:118:THR:OG1	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:16:ASN:HD21	1:P:20:SER:HB2	1.79	0.47
1:D:22:MET:HB3	1:D:36:TYR:CD2	2.49	0.47
1:E:50:TYR:OH	1:E:72:ALA:HB3	2.14	0.47
1:G:18:LEU:HD23	1:G:40:ALA:CB	2.44	0.47
1:J:78:THR:HG1	1:J:100:LEU:HD13	1.79	0.47
1:Q:63:PHE:O	1:Q:63:PHE:CD2	2.67	0.47
1:D:100:LEU:C	1:D:100:LEU:HD12	2.40	0.47
1:E:7:LEU:HD22	1:E:12:THR:HG21	1.95	0.47
1:J:67:TRP:CD1	2:J:201:BTN:H101	2.49	0.47
1:Q:100:LEU:C	1:Q:100:LEU:HD12	2.39	0.47
1:G:7:LEU:HD21	1:G:12:THR:HG21	1.95	0.47
1:I:52:LEU:HD13	1:I:63:PHE:HB2	1.97	0.47
1:A:112:THR:CG2	1:B:97:GLN:HG2	2.44	0.47
1:N:14:TRP:CZ3	1:N:119:TYR:HB2	2.50	0.47
1:N:32:VAL:O	1:N:53:SER:HA	2.15	0.47
1:O:45:CYS:HB3	1:O:50:TYR:CZ	2.50	0.47
1:S:12:THR:HB	1:S:14:TRP:HE1	1.79	0.47
1:A:76:SER:HB2	1:A:100:LEU:HD11	1.97	0.47
1:J:49:PRO:O	1:J:50:TYR:CD1	2.68	0.47
1:J:82:GLY:HA3	1:J:96:THR:HG22	1.96	0.47
1:M:37:VAL:HG11	1:T:88:PHE:CD2	2.50	0.47
1:A:110:ILE:HG21	1:B:97:GLN:HB2	1.97	0.46
1:E:69:ASN:OD1	1:E:69:ASN:C	2.56	0.46
1:E:82:GLY:HA3	1:E:96:THR:HG22	1.98	0.46
1:H:80:TRP:CD1	1:H:98:TRP:HB3	2.50	0.46
1:M:52:LEU:CB	1:M:65:VAL:HG22	2.46	0.46
1:Q:64:SER:O	1:Q:65:VAL:HG23	2.15	0.46
1:R:80:TRP:HE3	1:R:80:TRP:H	1.63	0.46
1:C:112:THR:CG2	1:D:97:GLN:HG2	2.44	0.46
1:J:45:CYS:HB3	1:J:50:TYR:CZ	2.51	0.46
1:L:14:TRP:CZ3	1:L:94:ILE:HG13	2.51	0.46
1:Q:64:SER:OG	1:Q:65:VAL:N	2.48	0.46
1:I:17:GLU:N	1:I:17:GLU:OE1	2.47	0.46
1:I:103:VAL:HG23	1:I:103:VAL:O	2.16	0.46
1:Q:114:GLN:O	1:Q:115:ASN:ND2	2.48	0.46
1:G:88:PHE:O	1:P:21:VAL:HG21	2.16	0.46
1:M:20:SER:OG	1:M:39:ASN:N	2.49	0.46
1:C:62:ALA:HA	1:C:80:TRP:O	2.14	0.46
1:Q:86:LYS:CE	1:Q:90:GLY:HA2	2.46	0.46
1:A:31:GLY:HA2	1:A:55:HIS:CD2	2.51	0.46
1:K:52:LEU:HD12	1:K:52:LEU:C	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:118:THR:HG21	1:T:15:VAL:CG1	2.46	0.46
1:R:22:MET:HB3	1:R:36:TYR:CD1	2.51	0.46
1:R:49:PRO:O	1:R:69:ASN:ND2	2.48	0.46
1:I:100:LEU:O	1:I:110:ILE:HA	2.16	0.46
1:Q:92:VAL:HG12	1:Q:119:TYR:HB2	1.98	0.46
1:G:110:ILE:HG21	1:H:97:GLN:HB2	1.97	0.45
1:A:4:PHE:O	1:A:7:LEU:HB2	2.16	0.45
1:R:95:VAL:HA	1:R:116:VAL:HG22	1.98	0.45
1:B:115:ASN:HD22	1:B:115:ASN:HA	1.54	0.45
1:R:98:TRP:CZ2	1:R:113:GLY:HA3	2.52	0.45
1:C:97:GLN:HG2	1:D:112:THR:CG2	2.46	0.45
1:M:59:SER:HB2	1:N:103:VAL:HG11	1.99	0.45
1:P:97:GLN:NE2	1:P:114:GLN:HG3	2.32	0.45
1:C:63:PHE:CE1	1:C:80:TRP:CE3	3.05	0.45
1:F:52:LEU:HD12	1:F:52:LEU:C	2.42	0.45
1:J:32:VAL:HB	1:J:54:GLY:O	2.17	0.45
1:O:118:THR:HG21	1:Q:15:VAL:CG1	2.43	0.45
1:L:7:LEU:HD22	1:L:12:THR:HG21	1.99	0.45
1:S:120:GLN:O	1:S:121:ALA:C	2.59	0.45
1:A:85:ARG:NH1	1:A:93:GLN:OE1	2.37	0.45
1:O:7:LEU:HD13	1:O:26:VAL:HG21	1.99	0.45
1:G:50:TYR:CZ	1:G:69:ASN:ND2	2.85	0.45
1:T:36:TYR:HH	1:T:117:PHE:HE1	1.62	0.45
1:C:57:HIS:NE2	1:D:73:ASP:OD2	2.49	0.45
1:J:114:GLN:N	1:J:114:GLN:CD	2.75	0.45
1:K:16:ASN:HB3	1:K:117:PHE:CD2	2.52	0.45
1:M:81:ALA:HB2	1:N:79:SER:OG	2.16	0.45
1:R:78:THR:CG2	1:R:80:TRP:CH2	3.00	0.45
1:D:35[A]:TYR:CD1	1:D:35[A]:TYR:C	2.96	0.44
1:E:22:MET:HB3	1:E:36:TYR:CD2	2.52	0.44
1:C:94:ILE:HG22	1:C:96:THR:HG23	1.99	0.44
1:G:27:ASP:OD1	1:G:27:ASP:C	2.59	0.44
1:C:110:ILE:HG21	1:D:97:GLN:HB2	1.98	0.44
1:R:48:LEU:HD22	1:R:48:LEU:HA	1.87	0.44
1:G:32:VAL:HG22	1:G:55:HIS:CA	2.48	0.44
1:I:104:GLY:O	1:I:106:ALA:N	2.39	0.44
1:T:78:THR:HG22	1:T:79:SER:N	2.32	0.44
1:Q:48:LEU:N	1:Q:48:LEU:HD23	2.32	0.44
1:S:17:GLU:HG2	1:S:18:LEU:HD13	1.99	0.44
1:I:104:GLY:C	1:I:106:ALA:H	2.23	0.44
1:C:99:SER:HB2	1:D:81:ALA:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:14:TRP:HB3	1:J:117:PHE:HB3	1.99	0.44
1:L:45:CYS:HB3	1:L:50:TYR:CZ	2.53	0.44
1:R:38:ASN:O	1:R:47:GLY:N	2.43	0.44
1:D:45:CYS:HB3	1:D:50:TYR:CE2	2.52	0.44
1:S:56:ALA:O	1:S:57:HIS:HB2	2.18	0.44
1:Q:6:SER:C	1:Q:8:SER:H	2.26	0.44
1:O:83:TYR:CE2	1:P:108:GLY:O	2.70	0.43
1:I:78:THR:HA	1:I:99:SER:O	2.17	0.43
1:K:8:SER:HA	1:K:26:VAL:O	2.18	0.43
1:M:57:HIS:O	1:M:58:GLY:C	2.61	0.43
1:G:62:ALA:HB1	1:H:79:SER:HB3	2.00	0.43
1:S:100:LEU:C	1:S:100:LEU:HD12	2.43	0.43
1:R:64:SER:HA	1:R:79:SER:HA	2.00	0.43
1:I:38:ASN:ND2	1:I:44:GLY:O	2.51	0.43
1:L:3:ASP:HB2	1:L:58:GLY:O	2.18	0.43
1:Q:25:ASP:OD1	1:Q:25:ASP:N	2.51	0.43
1:H:26:VAL:HA	1:H:31:GLY:O	2.18	0.43
1:P:12:THR:HG23	1:P:119:TYR:CE1	2.53	0.43
1:T:22:MET:O	1:T:22:MET:HG3	2.17	0.43
1:H:98:TRP:CZ2	1:H:113:GLY:HA3	2.53	0.43
1:I:113:GLY:C	1:I:114:GLN:NE2	2.76	0.43
1:K:66:VAL:HG23	1:L:55:HIS:HB3	1.99	0.43
1:P:32:VAL:N	1:P:54:GLY:O	2.46	0.43
1:D:13:THR:OG1	1:D:23:THR:OG1	2.31	0.43
1:J:90:GLY:C	1:J:91:GLY:O	2.62	0.43
1:H:76:SER:HB3	1:H:102:PHE:HB3	2.01	0.43
1:J:88:PHE:CD1	1:J:88:PHE:C	2.97	0.43
1:O:21:VAL:HG21	1:Q:88:PHE:HB3	1.99	0.43
1:H:44:GLY:O	1:H:45:CYS:C	2.61	0.42
1:S:20:SER:OG	1:S:38:ASN:HA	2.18	0.42
1:S:22:MET:HB3	1:S:36:TYR:CD2	2.54	0.42
1:G:26:VAL:HG22	1:G:32:VAL:HG12	2.00	0.42
1:S:66:VAL:HG11	1:T:57:HIS:HB2	2.01	0.42
1:C:110:ILE:HG21	1:D:97:GLN:CB	2.49	0.42
1:K:65:VAL:HG23	1:K:80:TRP:HZ3	1.85	0.42
1:O:115:ASN:HD22	1:O:115:ASN:HA	1.66	0.42
1:K:4:PHE:CZ	1:K:84:ALA:HB2	2.54	0.42
1:M:97:GLN:CB	1:N:110:ILE:HG21	2.49	0.42
1:A:2:THR:O	1:A:59:SER:OG	2.26	0.42
1:M:121:ALA:HB3	1:T:121:ALA:HB2	2.01	0.42
1:B:4:PHE:CE2	1:B:84:ALA:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:SER:HB3	1:D:62:ALA:HB1	2.02	0.42
1:H:46:ARG:HE	1:H:46:ARG:HB3	1.55	0.42
1:T:38:ASN:O	1:T:46:ARG:HA	2.19	0.42
1:E:52:LEU:HD13	1:E:63:PHE:HB2	2.01	0.42
1:E:121:ALA:O	1:E:122:ALA:HB3	2.20	0.42
1:K:67:TRP:CE2	2:K:201:BTN:H91	2.54	0.42
1:M:97:GLN:HE22	1:M:114:GLN:HE21	1.67	0.42
1:O:2:THR:HB	1:O:86:LYS:HG2	2.01	0.42
1:S:38:ASN:ND2	2:S:201:BTN:H72	2.35	0.42
1:Q:24:ILE:CG2	1:Q:52:LEU:HD21	2.49	0.42
1:E:62:ALA:HA	1:E:80:TRP:O	2.19	0.42
1:F:27:ASP:C	1:F:27:ASP:OD1	2.62	0.42
1:I:2:THR:HG23	1:I:2:THR:O	2.18	0.42
1:P:63:PHE:CE1	1:P:80:TRP:CE3	3.08	0.42
1:Q:92:VAL:CG1	1:Q:119:TYR:HB2	2.50	0.42
1:H:27:ASP:OD1	1:H:27:ASP:C	2.62	0.42
1:L:14:TRP:HB3	1:L:117:PHE:HB3	2.01	0.42
1:N:16:ASN:HA	1:N:116:VAL:O	2.20	0.42
1:N:38:ASN:OD1	1:N:39:ASN:N	2.53	0.42
1:T:52:LEU:HD12	1:T:52:LEU:C	2.45	0.42
1:Q:79:SER:OG	1:R:79:SER:HB2	2.20	0.42
1:R:37:VAL:HG13	1:R:47:GLY:HA2	2.01	0.42
1:B:18:LEU:HB3	1:B:40:ALA:HA	2.02	0.42
1:J:76:SER:HB3	1:J:102:PHE:HB3	2.02	0.42
1:L:78:THR:OG1	1:L:100:LEU:HD13	2.20	0.42
1:N:67:TRP:CZ2	2:N:201:BTN:H71	2.55	0.42
1:S:26:VAL:HG22	1:S:32:VAL:HG12	2.02	0.42
1:R:51:ASP:OD2	1:R:51:ASP:N	2.41	0.42
1:F:59:SER:O	1:F:83:TYR:HA	2.20	0.41
1:H:45:CYS:HB3	1:H:50:TYR:CZ	2.55	0.41
1:J:78:THR:OG1	1:J:100:LEU:HD13	2.20	0.41
1:M:78:THR:HA	1:M:99:SER:O	2.20	0.41
1:R:80:TRP:CE3	1:R:80:TRP:N	2.88	0.41
1:G:40:ALA:HA	1:G:41:PRO:HD2	1.87	0.41
1:I:12:THR:OG1	1:I:14:TRP:NE1	2.53	0.41
1:S:26:VAL:HG22	1:S:32:VAL:CG1	2.50	0.41
1:L:44:GLY:O	1:L:45:CYS:HB2	2.20	0.41
1:O:88:PHE:CD1	1:O:88:PHE:C	2.98	0.41
1:T:3:ASP:HB2	1:T:58:GLY:C	2.45	0.41
1:E:40:ALA:HB3	1:E:43:THR:OG1	2.21	0.41
1:E:67:TRP:CE2	2:E:201:BTN:H91	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:7:LEU:HD21	1:I:12:THR:HG23	2.02	0.41
1:Q:87:THR:HG23	1:Q:92:VAL:N	2.36	0.41
1:R:61:ILE:HD13	1:R:62:ALA:N	2.35	0.41
1:C:23:THR:O	1:C:34:GLY:HA3	2.20	0.41
1:N:39:ASN:O	1:N:39:ASN:CG	2.64	0.41
1:S:8:SER:OG	1:S:28:ARG:HA	2.21	0.41
1:T:78:THR:HG21	1:T:80:TRP:CH2	2.55	0.41
1:D:4:PHE:O	1:D:7:LEU:N	2.53	0.41
1:D:100:LEU:HD12	1:D:101:ALA:N	2.35	0.41
1:I:7:LEU:HD22	1:I:26:VAL:CB	2.50	0.41
1:I:32:VAL:HG22	1:I:55:HIS:N	2.35	0.41
1:M:67:TRP:CZ2	2:M:201:BTN:C8	3.04	0.41
1:T:79:SER:O	1:T:98:TRP:HA	2.20	0.41
1:E:97:GLN:HG2	1:F:112:THR:CG2	2.51	0.41
1:Q:119:TYR:CZ	1:Q:121:ALA:HA	2.55	0.41
1:A:16:ASN:HA	1:A:116:VAL:O	2.20	0.41
1:C:62:ALA:HB1	1:D:79:SER:HB3	2.03	0.41
1:D:3:ASP:OD2	1:D:5:ASP:HB2	2.21	0.41
1:G:22:MET:HB3	1:G:36:TYR:CD2	2.56	0.41
1:I:26:VAL:CG2	1:I:32:VAL:HG12	2.45	0.41
1:L:115:ASN:HD22	1:L:115:ASN:HA	1.66	0.41
1:M:76:SER:HA	1:N:60:THR:HG21	2.03	0.41
1:T:67:TRP:CE2	2:T:201:BTN:H91	2.56	0.41
1:Q:24:ILE:HG23	1:Q:52:LEU:HD21	2.02	0.41
1:G:66:VAL:CG2	1:H:55:HIS:HB3	2.51	0.41
1:P:14:TRP:HB3	1:P:117:PHE:HB3	2.03	0.41
1:P:27:ASP:OD1	1:P:27:ASP:C	2.64	0.41
1:Q:99:SER:HB2	1:R:81:ALA:HB3	2.02	0.41
1:C:97:GLN:HG2	1:D:112:THR:HG22	2.02	0.40
1:Q:78:THR:CG2	1:Q:80:TRP:CZ3	3.00	0.40
1:R:88:PHE:CD2	1:R:88:PHE:C	2.99	0.40
1:A:99:SER:HB3	1:B:97:GLN:HB3	2.04	0.40
1:H:81:ALA:O	1:H:96:THR:HA	2.20	0.40
1:J:4:PHE:HD1	1:J:7:LEU:HD12	1.87	0.40
1:Q:8:SER:HB3	1:Q:28:ARG:HA	2.01	0.40
1:A:94:ILE:HG22	1:A:96:THR:CG2	2.51	0.40
1:B:14:TRP:CD1	1:B:14:TRP:N	2.90	0.40
1:F:24:ILE:O	1:F:24:ILE:HG13	2.22	0.40
1:K:65:VAL:HG23	1:K:80:TRP:CZ3	2.56	0.40
1:O:88:PHE:O	1:Q:21:VAL:HG21	2.20	0.40
1:K:99:SER:HB2	1:L:81:ALA:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:4:PHE:C	1:H:6:SER:N	2.78	0.40
1:I:97:GLN:OE1	1:I:112:THR:HB	2.21	0.40
1:L:97:GLN:HE22	1:L:114:GLN:HG3	1.87	0.40
1:M:66:VAL:CG2	1:N:55:HIS:HB3	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	119/131 (91%)	114 (96%)	5 (4%)	0	100	100
1	B	119/131 (91%)	110 (92%)	8 (7%)	1 (1%)	16	41
1	C	119/131 (91%)	113 (95%)	6 (5%)	0	100	100
1	D	120/131 (92%)	111 (92%)	9 (8%)	0	100	100
1	E	119/131 (91%)	109 (92%)	10 (8%)	0	100	100
1	F	119/131 (91%)	115 (97%)	4 (3%)	0	100	100
1	G	119/131 (91%)	110 (92%)	8 (7%)	1 (1%)	16	41
1	H	119/131 (91%)	110 (92%)	7 (6%)	2 (2%)	7	23
1	I	119/131 (91%)	98 (82%)	20 (17%)	1 (1%)	16	41
1	J	119/131 (91%)	106 (89%)	12 (10%)	1 (1%)	16	41
1	K	119/131 (91%)	107 (90%)	11 (9%)	1 (1%)	16	41
1	L	119/131 (91%)	112 (94%)	6 (5%)	1 (1%)	16	41
1	M	119/131 (91%)	106 (89%)	11 (9%)	2 (2%)	7	23
1	N	119/131 (91%)	111 (93%)	6 (5%)	2 (2%)	7	23
1	O	119/131 (91%)	107 (90%)	10 (8%)	2 (2%)	7	23
1	P	119/131 (91%)	109 (92%)	10 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	119/131 (91%)	94 (79%)	19 (16%)	6 (5%)	1	5
1	R	119/131 (91%)	98 (82%)	18 (15%)	3 (2%)	4	15
1	S	119/131 (91%)	105 (88%)	10 (8%)	4 (3%)	3	11
1	T	119/131 (91%)	109 (92%)	9 (8%)	1 (1%)	16	41
All	All	2381/2620 (91%)	2154 (90%)	199 (8%)	28 (1%)	10	31

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4	PHE
1	G	121	ALA
1	H	11	SER
1	H	121	ALA
1	L	121	ALA
1	O	105	LYS
1	Q	61	ILE
1	Q	65	VAL
1	R	57	HIS
1	R	92	VAL
1	J	91	GLY
1	N	88	PHE
1	S	65	VAL
1	S	121	ALA
1	Q	121	ALA
1	S	57	HIS
1	Q	63	PHE
1	K	51	ASP
1	N	58	GLY
1	I	58	GLY
1	M	58	GLY
1	S	47	GLY
1	O	88	PHE
1	Q	106	ALA
1	R	69	ASN
1	T	58	GLY
1	Q	9	GLY
1	M	104	GLY

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	91/101 (90%)	83 (91%)	8 (9%)	9	27
1	B	91/101 (90%)	80 (88%)	11 (12%)	5	14
1	C	91/101 (90%)	83 (91%)	8 (9%)	9	27
1	D	92/101 (91%)	78 (85%)	14 (15%)	3	8
1	E	91/101 (90%)	85 (93%)	6 (7%)	15	40
1	F	91/101 (90%)	82 (90%)	9 (10%)	7	22
1	G	91/101 (90%)	81 (89%)	10 (11%)	6	18
1	H	91/101 (90%)	82 (90%)	9 (10%)	7	22
1	I	91/101 (90%)	79 (87%)	12 (13%)	4	11
1	J	91/101 (90%)	87 (96%)	4 (4%)	25	56
1	K	91/101 (90%)	84 (92%)	7 (8%)	12	33
1	L	91/101 (90%)	86 (94%)	5 (6%)	19	48
1	M	91/101 (90%)	86 (94%)	5 (6%)	19	48
1	N	91/101 (90%)	83 (91%)	8 (9%)	9	27
1	O	91/101 (90%)	77 (85%)	14 (15%)	2	8
1	P	91/101 (90%)	80 (88%)	11 (12%)	5	14
1	Q	91/101 (90%)	71 (78%)	20 (22%)	1	2
1	R	91/101 (90%)	71 (78%)	20 (22%)	1	2
1	S	91/101 (90%)	79 (87%)	12 (13%)	4	11
1	T	91/101 (90%)	87 (96%)	4 (4%)	25	56
All	All	1821/2020 (90%)	1624 (89%)	197 (11%)	6	19

All (197) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	18	LEU
1	A	64	SER

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Mol	Chain	Res	Type
1	A	66	VAL
1	A	75	ARG
1	A	99	SER
1	A	100	LEU
1	A	115	ASN
1	B	12	THR
1	B	59	SER
1	B	64	SER
1	B	66	VAL
1	B	75	ARG
1	B	85	ARG
1	B	92	VAL
1	B	99	SER
1	B	100	LEU
1	B	109	LYS
1	B	115	ASN
1	C	18	LEU
1	C	64	SER
1	C	66	VAL
1	C	75	ARG
1	C	85	ARG
1	C	99	SER
1	C	100	LEU
1	C	105	LYS
1	D	2	THR
1	D	3	ASP
1	D	11	SER
1	D	12	THR
1	D	18	LEU
1	D	23	THR
1	D	25	ASP
1	D	52	LEU
1	D	64	SER
1	D	66	VAL
1	D	99	SER
1	D	100	LEU
1	D	105	LYS
1	D	109	LYS
1	E	2	THR
1	E	8	SER
1	E	13	THR
1	E	35	TYR

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Mol	Chain	Res	Type
1	E	52	LEU
1	E	99	SER
1	F	28	ARG
1	F	52	LEU
1	F	64	SER
1	F	66	VAL
1	F	75	ARG
1	F	85	ARG
1	F	99	SER
1	F	110	ILE
1	F	115	ASN
1	G	7	LEU
1	G	8	SER
1	G	28	ARG
1	G	52	LEU
1	G	65	VAL
1	G	85	ARG
1	G	86	LYS
1	G	99	SER
1	G	105	LYS
1	G	109	LYS
1	H	3	ASP
1	H	64	SER
1	H	66	VAL
1	H	75	ARG
1	H	85	ARG
1	H	86	LYS
1	H	99	SER
1	H	102	PHE
1	H	120	GLN
1	I	7	LEU
1	I	12	THR
1	I	14	TRP
1	I	21	VAL
1	I	52	LEU
1	I	61	ILE
1	I	64	SER
1	I	66	VAL
1	I	85	ARG
1	I	87	THR
1	I	105	LYS
1	I	110	ILE

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Mol	Chain	Res	Type
1	J	24	ILE
1	J	52	LEU
1	J	99	SER
1	J	103	VAL
1	K	3	ASP
1	K	5	ASP
1	K	52	LEU
1	K	53	SER
1	K	64	SER
1	K	75	ARG
1	K	105	LYS
1	L	52	LEU
1	L	64	SER
1	L	75	ARG
1	L	86	LYS
1	L	92	VAL
1	M	7	LEU
1	M	15	VAL
1	M	52	LEU
1	M	92	VAL
1	M	103	VAL
1	N	11	SER
1	N	25	ASP
1	N	52	LEU
1	N	59	SER
1	N	75	ARG
1	N	85	ARG
1	N	99	SER
1	N	103	VAL
1	O	3	ASP
1	O	4	PHE
1	O	8	SER
1	O	10	THR
1	O	13	THR
1	O	21	VAL
1	O	28	ARG
1	O	51	ASP
1	O	52	LEU
1	O	55	HIS
1	O	64	SER
1	O	69	ASN
1	O	75	ARG

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Mol	Chain	Res	Type
1	O	79	SER
1	P	3	ASP
1	P	5	ASP
1	P	7	LEU
1	P	8	SER
1	P	52	LEU
1	P	59	SER
1	P	66	VAL
1	P	85	ARG
1	P	92	VAL
1	P	99	SER
1	P	109	LYS
1	S	10	THR
1	S	12	THR
1	S	13	THR
1	S	18	LEU
1	S	25	ASP
1	S	32	VAL
1	S	52	LEU
1	S	68	SER
1	S	97	GLN
1	S	99	SER
1	S	100	LEU
1	S	120	GLN
1	T	52	LEU
1	T	66	VAL
1	T	75	ARG
1	T	99	SER
1	Q	7	LEU
1	Q	15	VAL
1	Q	23	THR
1	Q	24	ILE
1	Q	25	ASP
1	Q	26	VAL
1	Q	29	LYS
1	Q	37	VAL
1	Q	52	LEU
1	Q	53	SER
1	Q	64	SER
1	Q	71	ILE
1	Q	96	THR
1	Q	97	GLN

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Mol	Chain	Res	Type
1	Q	99	SER
1	Q	100	LEU
1	Q	103	VAL
1	Q	111	GLU
1	Q	112	THR
1	Q	115	ASN
1	R	3	ASP
1	R	11	SER
1	R	12	THR
1	R	13	THR
1	R	18	LEU
1	R	23	THR
1	R	25	ASP
1	R	46	ARG
1	R	48	LEU
1	R	51	ASP
1	R	52	LEU
1	R	55	HIS
1	R	61	ILE
1	R	75	ARG
1	R	94	ILE
1	R	99	SER
1	R	100	LEU
1	R	109	LYS
1	R	110	ILE
1	R	114	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	39	ASN
1	A	97	GLN
1	B	97	GLN
1	B	114	GLN
1	C	97	GLN
1	D	97	GLN
1	D	114	GLN
1	E	55	HIS
1	E	97	GLN
1	E	114	GLN
1	G	39	ASN

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Mol	Chain	Res	Type
1	G	97	GLN
1	G	114	GLN
1	H	97	GLN
1	I	97	GLN
1	I	114	GLN
1	J	97	GLN
1	J	120	GLN
1	K	39	ASN
1	K	93	GLN
1	L	39	ASN
1	L	97	GLN
1	M	97	GLN
1	N	97	GLN
1	O	39	ASN
1	O	55	HIS
1	O	57	HIS
1	O	69	ASN
1	O	97	GLN
1	P	97	GLN
1	S	39	ASN
1	S	97	GLN
1	T	55	HIS
1	T	97	GLN
1	T	120	GLN
1	Q	97	GLN
1	R	114	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

20 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$
2	BTN	T	201	-	17,17,17	0.68	0	23,23,23	1.13	1 (4%)
2	BTN	F	201	-	17,17,17	0.67	0	23,23,23	1.02	1 (4%)
2	BTN	J	201	-	17,17,17	0.64	0	23,23,23	1.61	3 (13%)
2	BTN	E	201	-	17,17,17	0.63	0	23,23,23	1.15	2 (8%)
2	BTN	G	201	-	17,17,17	0.82	0	23,23,23	1.12	2 (8%)
2	BTN	N	201	-	17,17,17	0.70	0	23,23,23	1.28	3 (13%)
2	BTN	I	201	-	17,17,17	0.65	0	23,23,23	1.33	3 (13%)
2	BTN	O	201	-	17,17,17	0.61	0	23,23,23	0.73	0
2	BTN	Q	201	-	17,17,17	0.65	0	23,23,23	1.36	2 (8%)
2	BTN	K	201	-	17,17,17	0.67	0	23,23,23	0.81	1 (4%)
2	BTN	D	201	-	17,17,17	0.64	0	23,23,23	1.01	2 (8%)
2	BTN	B	201	-	17,17,17	0.65	0	23,23,23	1.25	2 (8%)
2	BTN	H	201	-	17,17,17	0.73	1 (5%)	23,23,23	1.00	1 (4%)
2	BTN	R	201	-	17,17,17	0.76	0	23,23,23	1.16	1 (4%)
2	BTN	S	201	-	17,17,17	0.62	0	23,23,23	1.12	1 (4%)
2	BTN	C	201	-	17,17,17	0.66	0	23,23,23	1.01	2 (8%)
2	BTN	M	201	-	17,17,17	0.59	0	23,23,23	0.77	0
2	BTN	P	201	-	17,17,17	0.63	0	23,23,23	1.21	2 (8%)
2	BTN	L	201	-	17,17,17	0.70	0	23,23,23	0.81	1 (4%)
2	BTN	A	201	-	17,17,17	0.67	0	23,23,23	1.32	3 (13%)

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
2	BTN	T	201	-	-	0/7/28/28	0/2/2/2
2	BTN	F	201	-	-	1/7/28/28	0/2/2/2
2	BTN	J	201	-	-	0/7/28/28	0/2/2/2
2	BTN	E	201	-	-	0/7/28/28	0/2/2/2
2	BTN	G	201	-	-	5/7/28/28	0/2/2/2
2	BTN	N	201	-	-	5/7/28/28	0/2/2/2
2	BTN	I	201	-	-	4/7/28/28	0/2/2/2
2	BTN	O	201	-	-	6/7/28/28	0/2/2/2
2	BTN	Q	201	-	-	2/7/28/28	0/2/2/2
2	BTN	K	201	-	-	4/7/28/28	0/2/2/2
2	BTN	D	201	-	-	4/7/28/28	0/2/2/2
2	BTN	B	201	-	-	5/7/28/28	0/2/2/2
2	BTN	H	201	-	-	1/7/28/28	0/2/2/2
2	BTN	R	201	-	-	6/7/28/28	0/2/2/2
2	BTN	S	201	-	-	6/7/28/28	0/2/2/2
2	BTN	C	201	-	-	0/7/28/28	0/2/2/2
2	BTN	M	201	-	-	3/7/28/28	0/2/2/2
2	BTN	P	201	-	-	0/7/28/28	0/2/2/2
2	BTN	L	201	-	-	3/7/28/28	0/2/2/2
2	BTN	A	201	-	-	0/7/28/28	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	201	BTN	O12-C11	-2.15	1.23	1.30

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	201	BTN	C6-S1-C2	-4.50	80.64	89.98
2	Q	201	BTN	C2-C4-N2	4.10	117.69	113.34
2	J	201	BTN	C2-C4-C5	-3.76	104.29	108.89
2	T	201	BTN	C2-C4-N2	3.61	117.17	113.34
2	A	201	BTN	C2-C4-N2	3.49	117.04	113.34
2	I	201	BTN	C2-C4-C5	-3.43	104.70	108.89
2	P	201	BTN	C6-S1-C2	-3.42	82.88	89.98
2	E	201	BTN	C6-S1-C2	-3.24	83.25	89.98
2	R	201	BTN	C2-C4-N2	3.22	116.75	113.34
2	H	201	BTN	C6-S1-C2	-3.10	83.53	89.98
2	B	201	BTN	C7-C2-S1	-3.01	104.10	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	BTN	C6-S1-C2	-2.92	83.92	89.98
2	I	201	BTN	C6-S1-C2	-2.90	83.96	89.98
2	S	201	BTN	C4-C2-S1	-2.87	101.78	105.03
2	Q	201	BTN	C4-C2-S1	2.80	108.22	105.03
2	N	201	BTN	C2-C4-C5	-2.79	105.48	108.89
2	B	201	BTN	C8-C7-C2	2.54	119.88	114.04
2	P	201	BTN	C2-C4-C5	-2.42	105.93	108.89
2	C	201	BTN	C6-S1-C2	-2.42	84.96	89.98
2	K	201	BTN	C6-S1-C2	-2.37	85.06	89.98
2	G	201	BTN	C5-C4-N2	-2.34	100.04	102.68
2	A	201	BTN	C2-C4-C5	-2.33	106.04	108.89
2	N	201	BTN	C6-S1-C2	-2.33	85.15	89.98
2	D	201	BTN	C8-C7-C2	2.30	119.33	114.04
2	N	201	BTN	C4-C2-S1	-2.29	102.43	105.03
2	E	201	BTN	O11-C11-C10	-2.24	116.00	123.09
2	I	201	BTN	C6-C5-N1	2.22	116.04	113.18
2	C	201	BTN	C6-C5-N1	2.18	115.99	113.18
2	F	201	BTN	C6-S1-C2	-2.09	85.64	89.98
2	G	201	BTN	C5-C6-S1	2.08	108.93	106.06
2	L	201	BTN	C6-S1-C2	-2.07	85.69	89.98
2	J	201	BTN	C2-C4-N2	2.05	115.51	113.34
2	D	201	BTN	O11-C11-C10	-2.00	116.74	123.09

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	201	BTN	S1-C2-C7-C8
2	B	201	BTN	C4-C2-C7-C8
2	G	201	BTN	S1-C2-C7-C8
2	G	201	BTN	C4-C2-C7-C8
2	I	201	BTN	S1-C2-C7-C8
2	I	201	BTN	C4-C2-C7-C8
2	K	201	BTN	S1-C2-C7-C8
2	K	201	BTN	C4-C2-C7-C8
2	N	201	BTN	S1-C2-C7-C8
2	N	201	BTN	C4-C2-C7-C8
2	O	201	BTN	C2-C7-C8-C9
2	O	201	BTN	S1-C2-C7-C8
2	O	201	BTN	C4-C2-C7-C8
2	S	201	BTN	S1-C2-C7-C8
2	S	201	BTN	C4-C2-C7-C8

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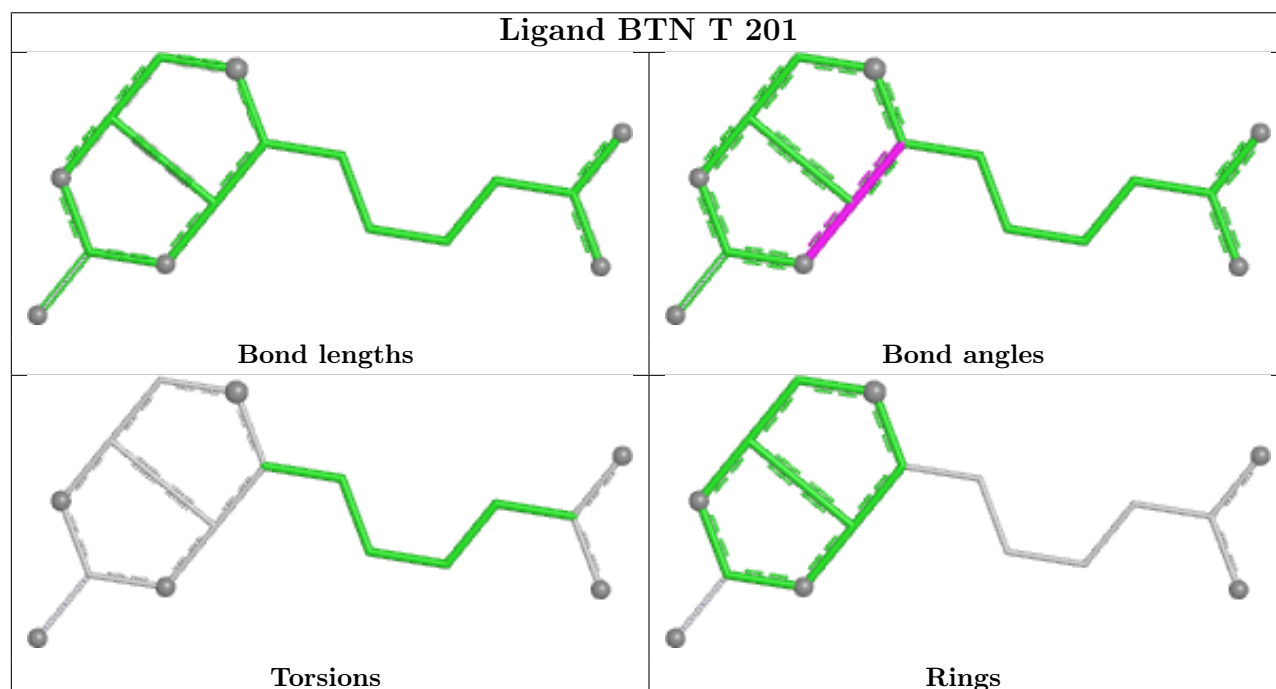
Mol	Chain	Res	Type	Atoms
2	R	201	BTN	C2-C7-C8-C9
2	R	201	BTN	S1-C2-C7-C8
2	R	201	BTN	C4-C2-C7-C8
2	G	201	BTN	C11-C10-C9-C8
2	G	201	BTN	C7-C8-C9-C10
2	I	201	BTN	C7-C8-C9-C10
2	M	201	BTN	C7-C8-C9-C10
2	H	201	BTN	C7-C8-C9-C10
2	K	201	BTN	C11-C10-C9-C8
2	D	201	BTN	C11-C10-C9-C8
2	B	201	BTN	C2-C7-C8-C9
2	K	201	BTN	C2-C7-C8-C9
2	N	201	BTN	C2-C7-C8-C9
2	S	201	BTN	C7-C8-C9-C10
2	O	201	BTN	C11-C10-C9-C8
2	I	201	BTN	C11-C10-C9-C8
2	F	201	BTN	C7-C8-C9-C10
2	S	201	BTN	C2-C7-C8-C9
2	Q	201	BTN	C2-C7-C8-C9
2	N	201	BTN	C7-C8-C9-C10
2	L	201	BTN	C11-C10-C9-C8
2	Q	201	BTN	C7-C8-C9-C10
2	O	201	BTN	C9-C10-C11-O12
2	O	201	BTN	C9-C10-C11-O11
2	M	201	BTN	C9-C10-C11-O11
2	D	201	BTN	C9-C10-C11-O11
2	R	201	BTN	C9-C10-C11-O11
2	R	201	BTN	C9-C10-C11-O12
2	D	201	BTN	C9-C10-C11-O12
2	D	201	BTN	S1-C2-C7-C8
2	M	201	BTN	C9-C10-C11-O12
2	S	201	BTN	C9-C10-C11-O12
2	B	201	BTN	C9-C10-C11-O11
2	B	201	BTN	C9-C10-C11-O12
2	S	201	BTN	C9-C10-C11-O11
2	R	201	BTN	C7-C8-C9-C10
2	L	201	BTN	C9-C10-C11-O11
2	G	201	BTN	C9-C10-C11-O12
2	L	201	BTN	C9-C10-C11-O12
2	N	201	BTN	C9-C10-C11-O12

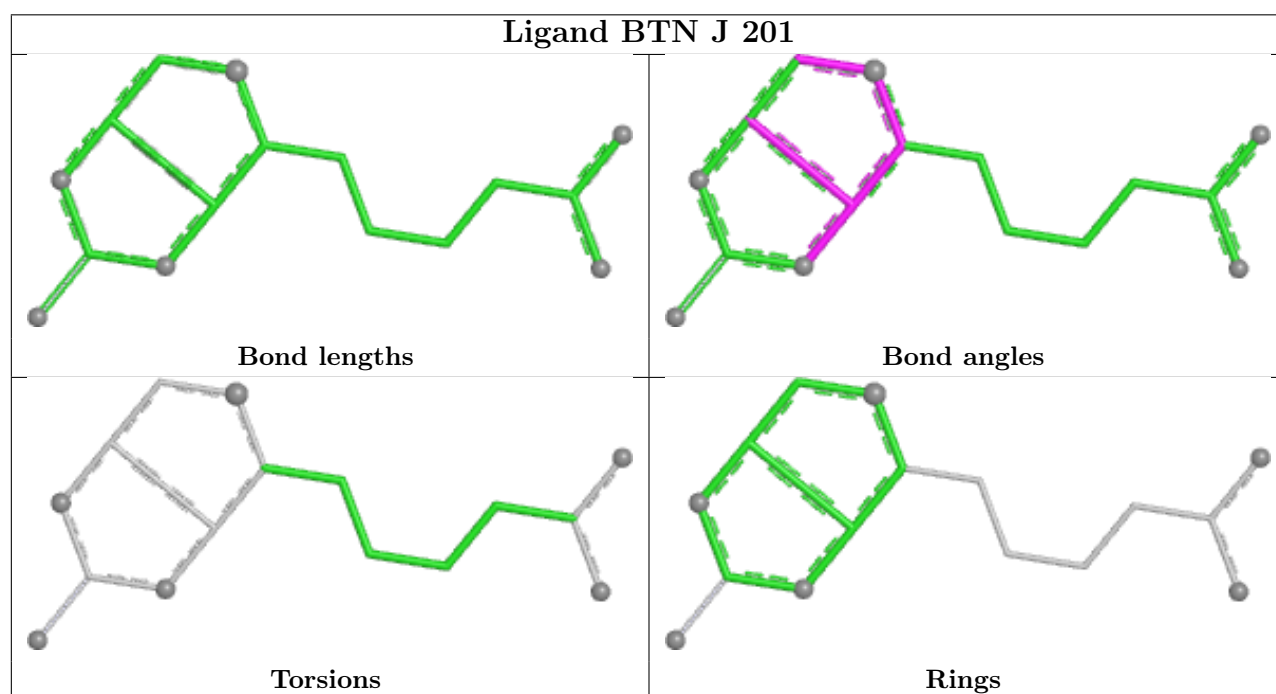
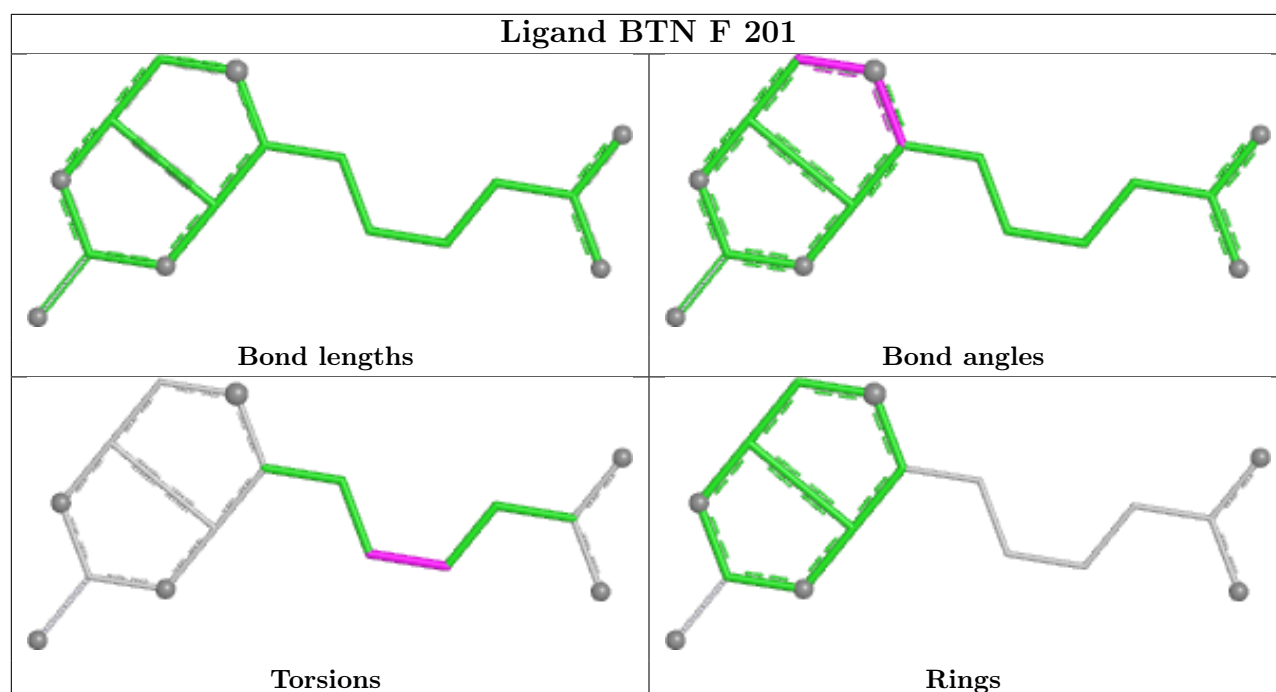
There are no ring outliers.

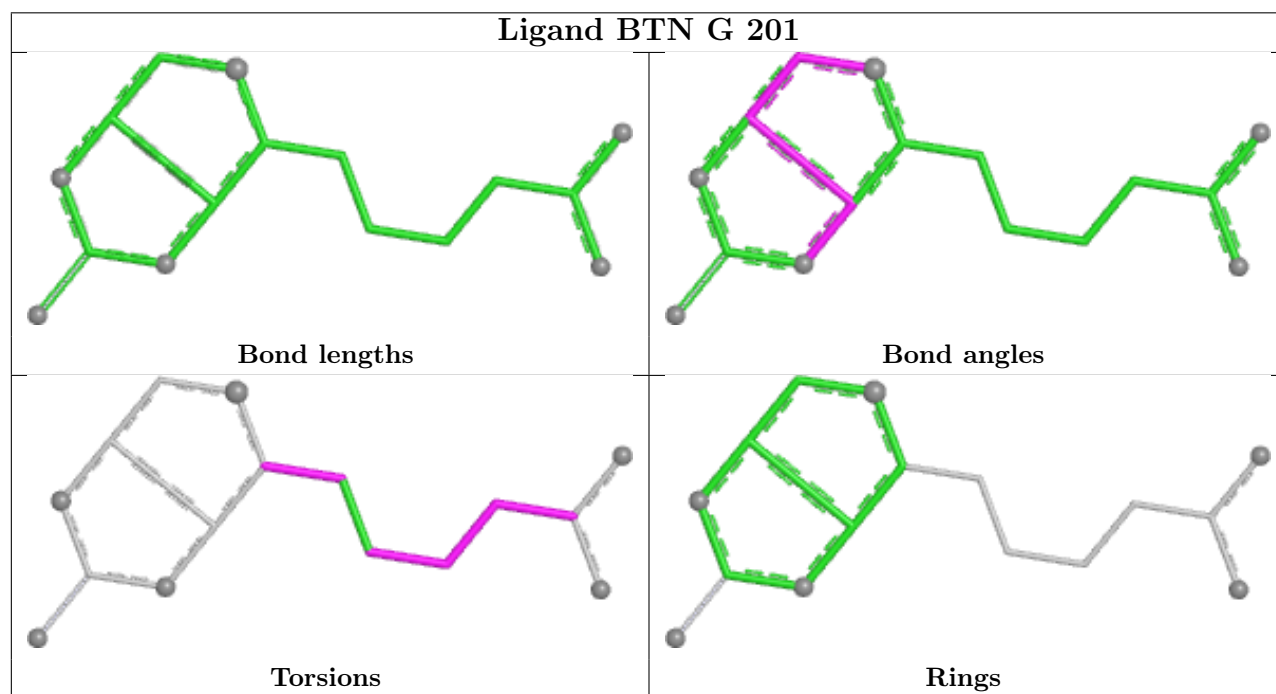
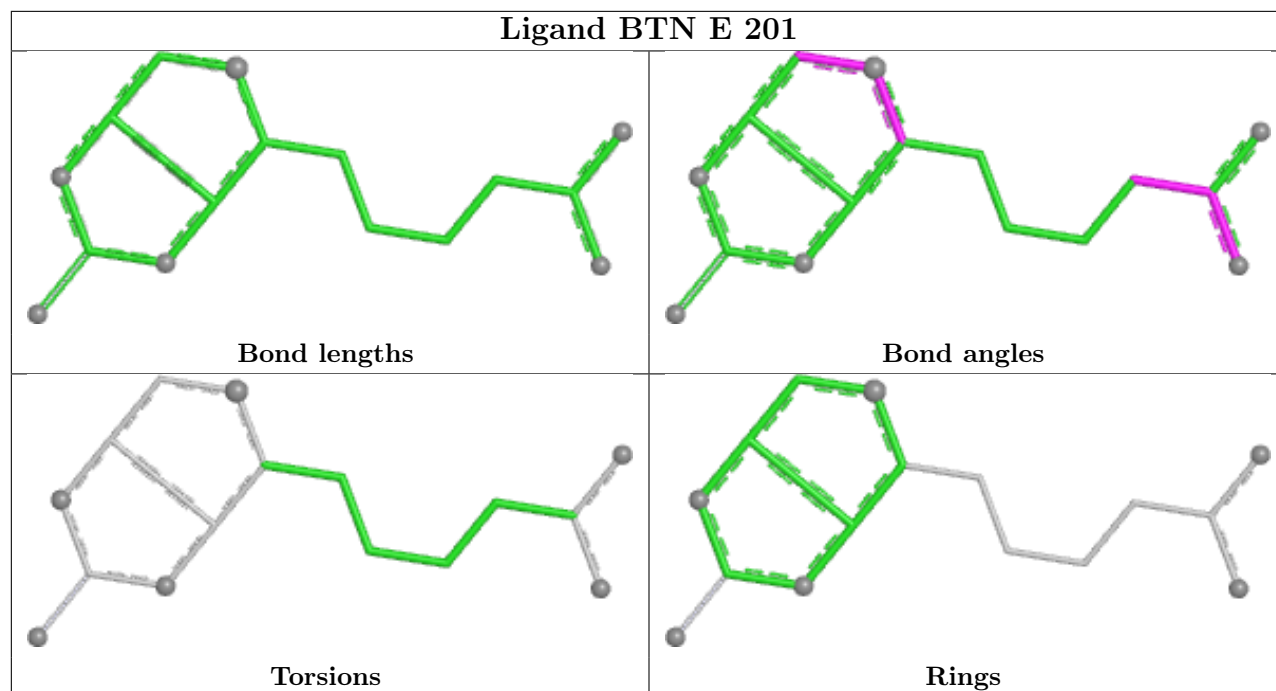
11 monomers are involved in 13 short contacts:

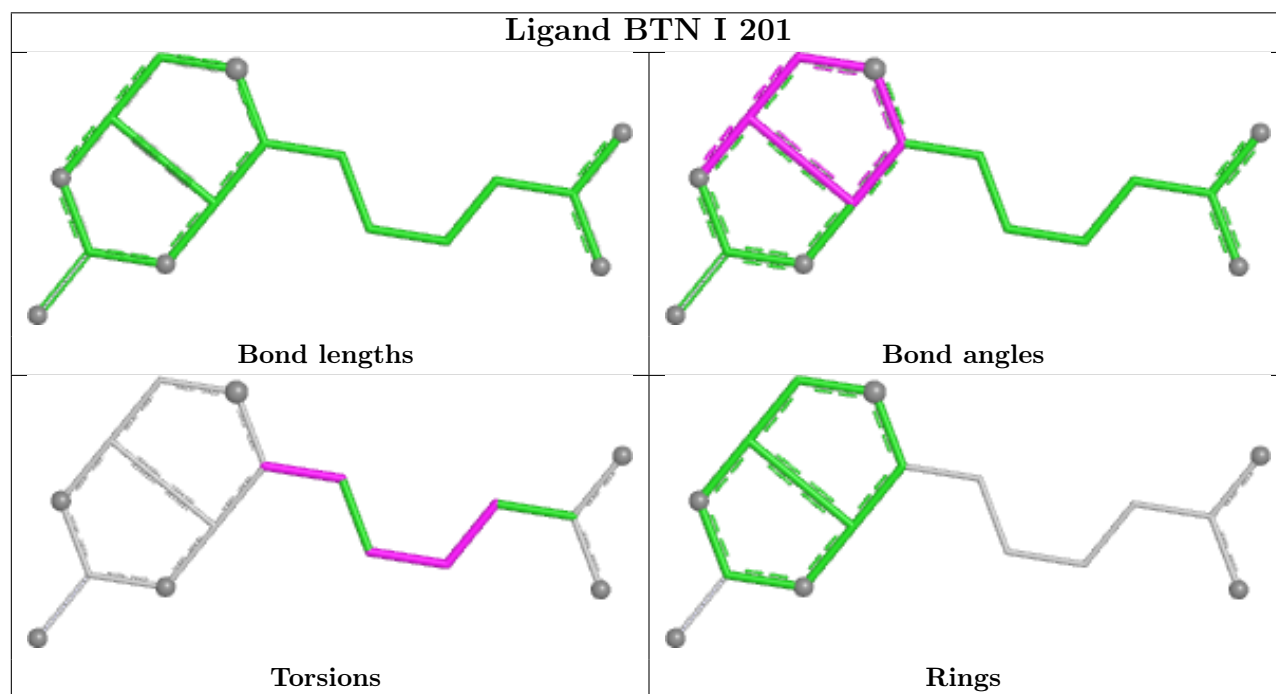
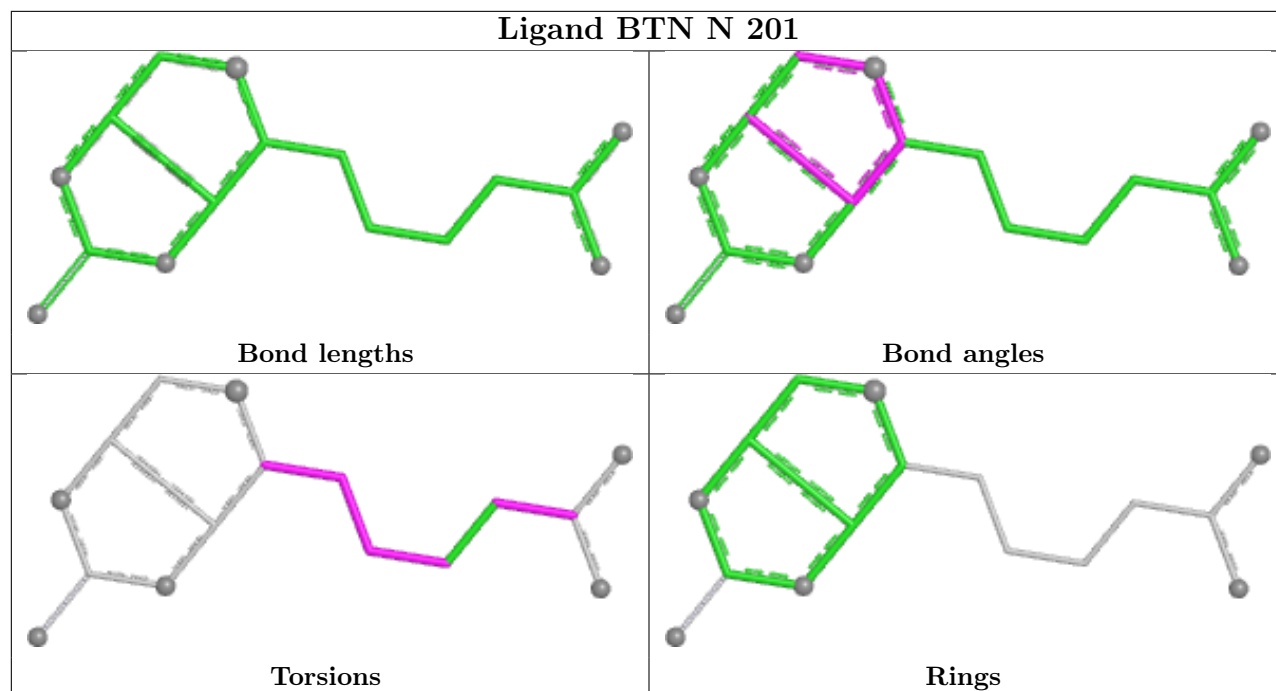
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	201	BTN	1	0
2	F	201	BTN	2	0
2	J	201	BTN	2	0
2	E	201	BTN	1	0
2	N	201	BTN	1	0
2	K	201	BTN	1	0
2	H	201	BTN	1	0
2	R	201	BTN	1	0
2	S	201	BTN	1	0
2	C	201	BTN	1	0
2	M	201	BTN	1	0

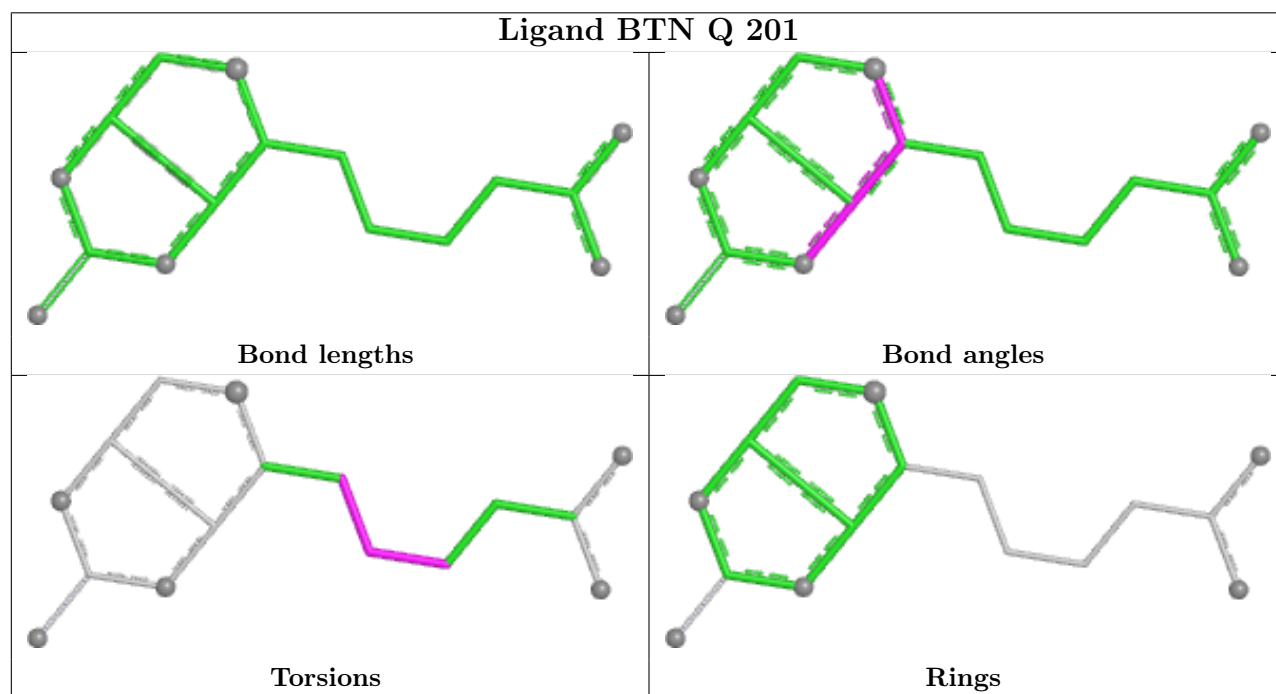
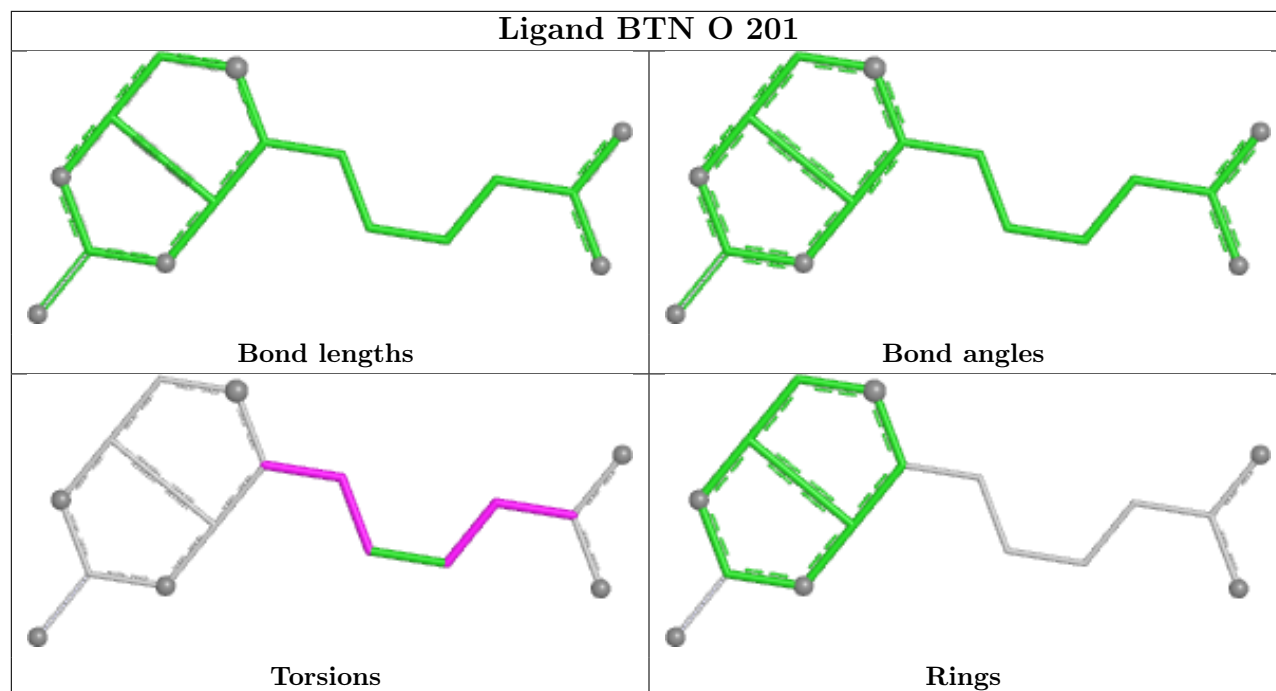
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

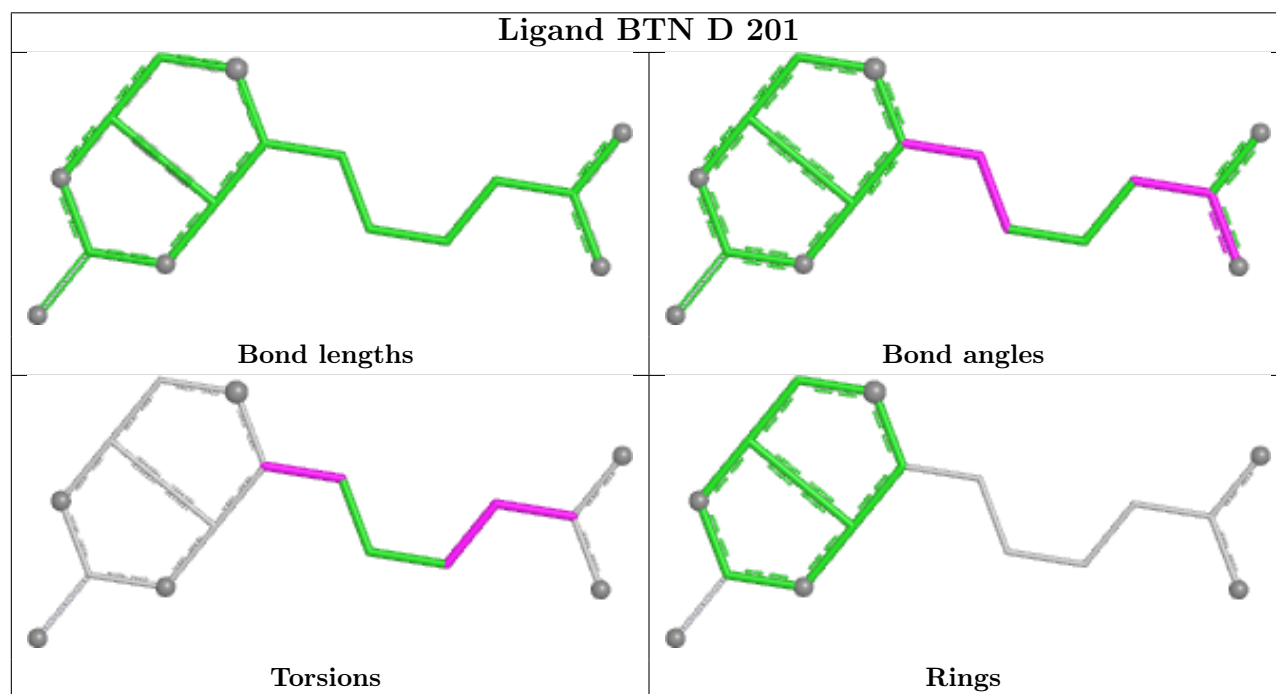
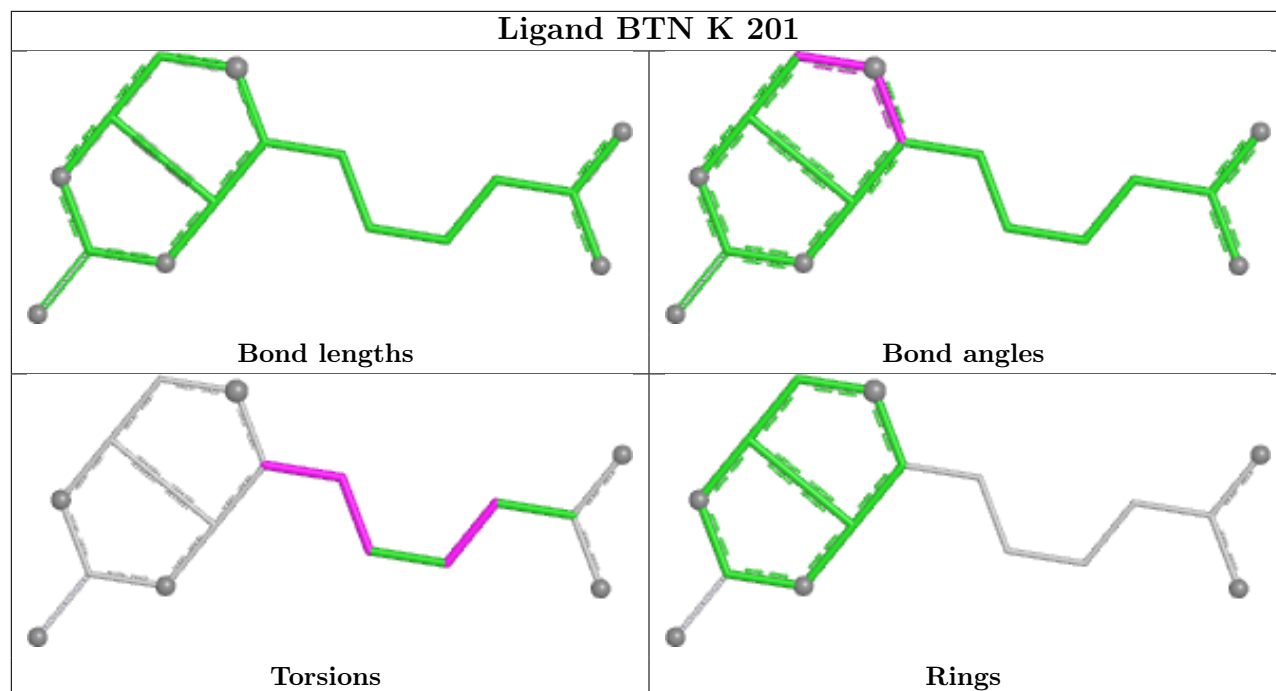


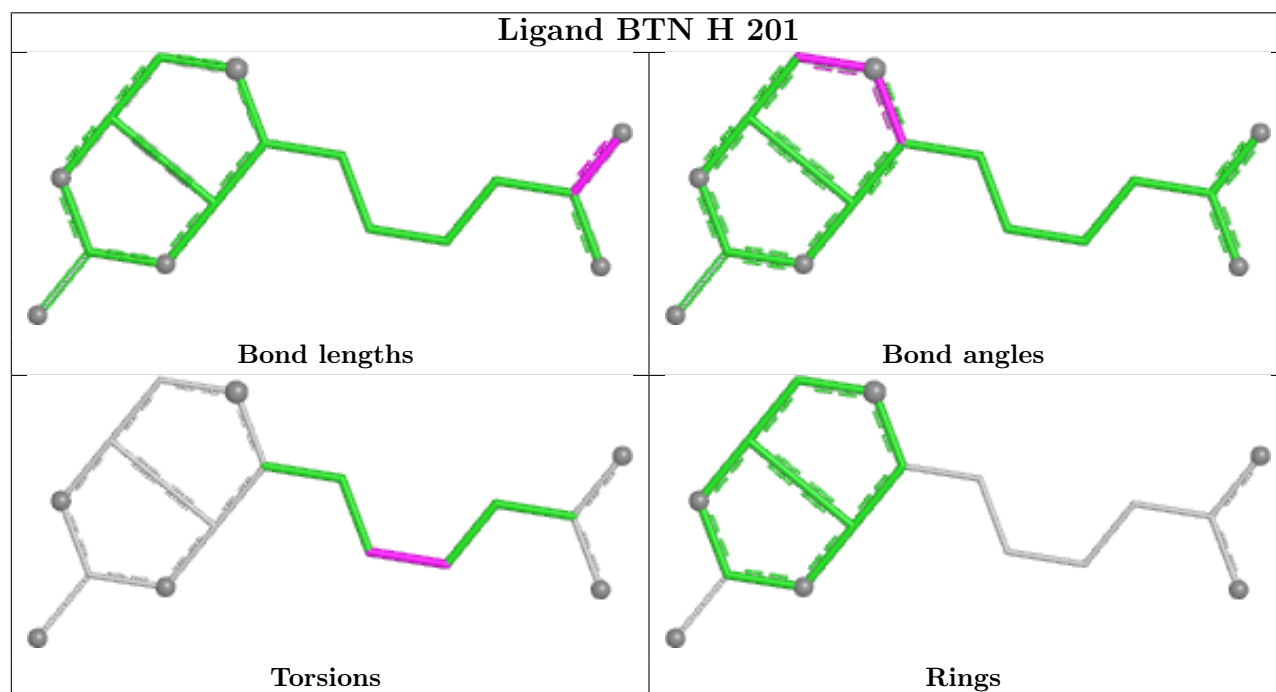
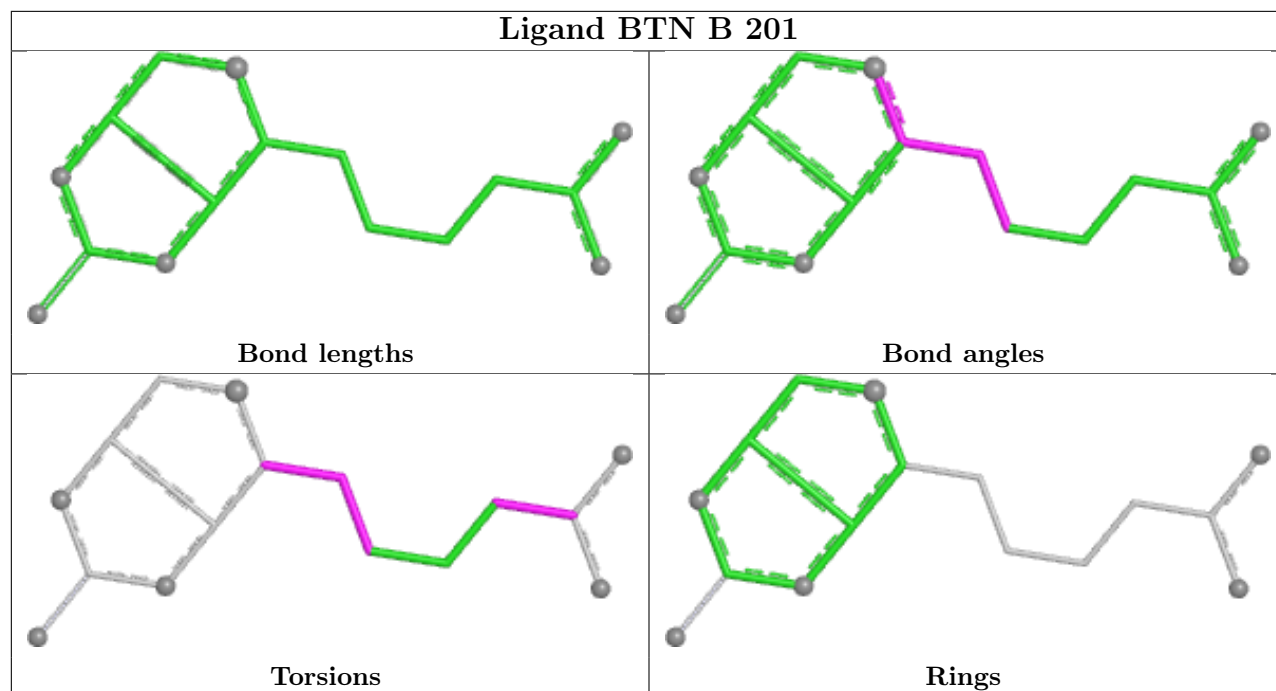


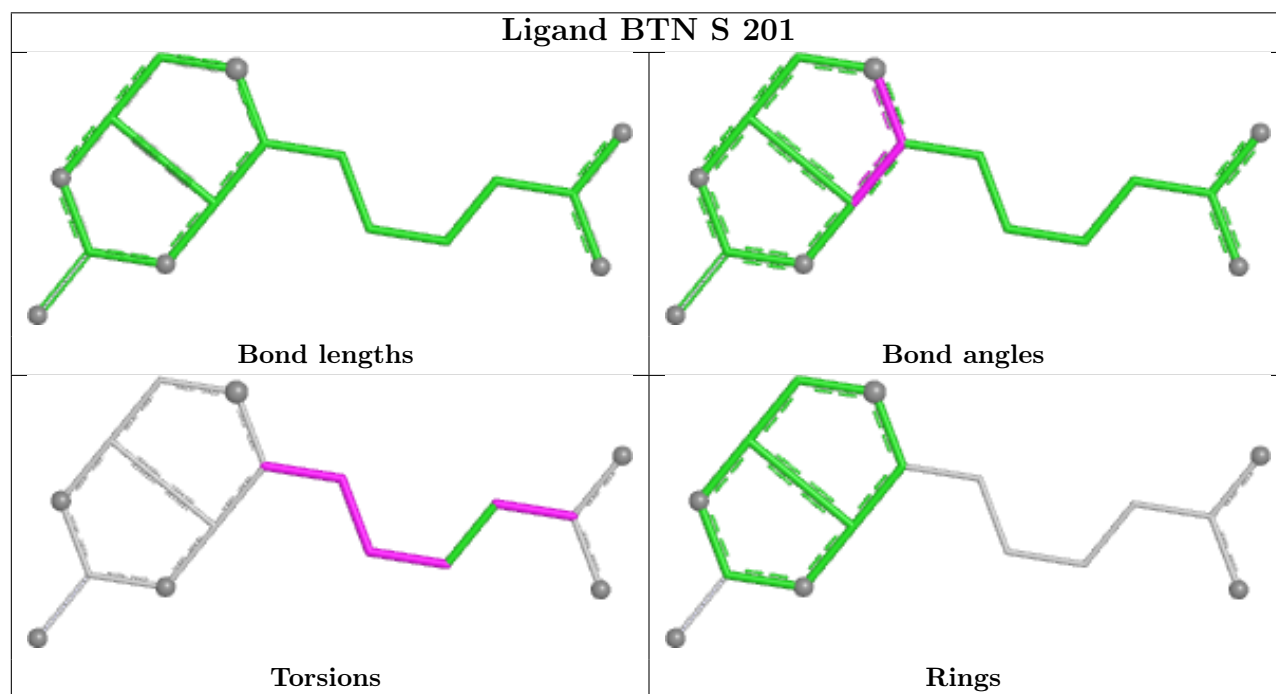
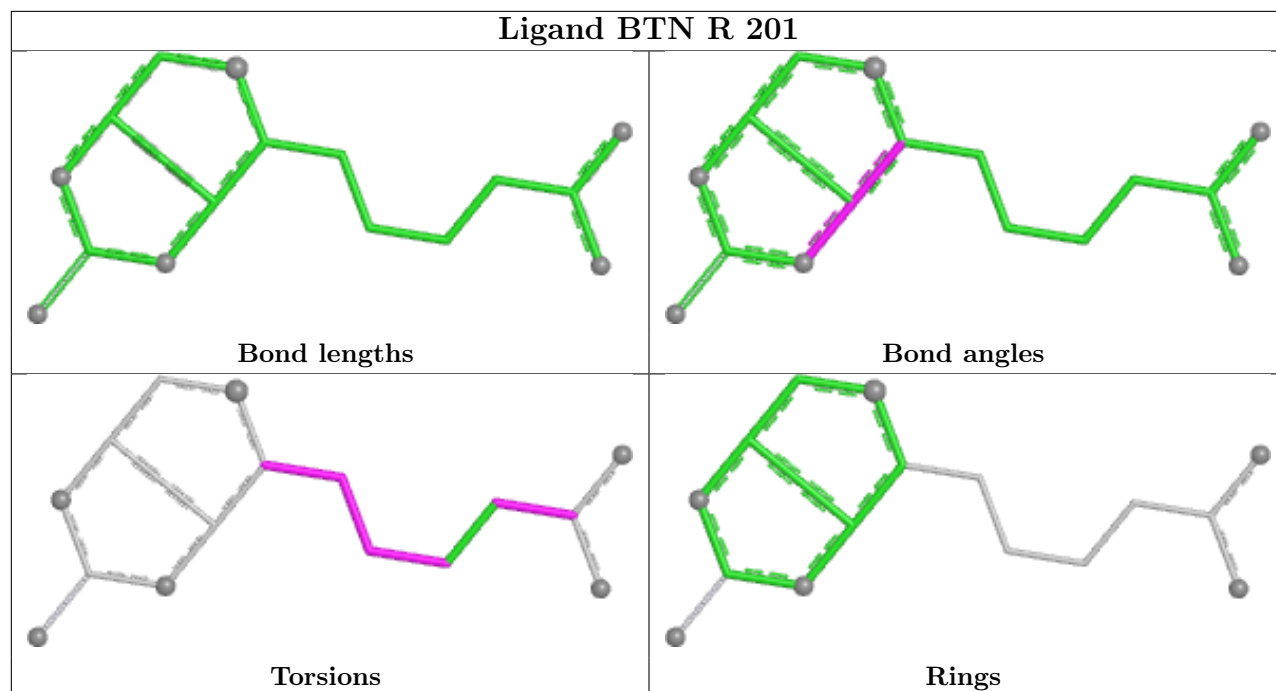


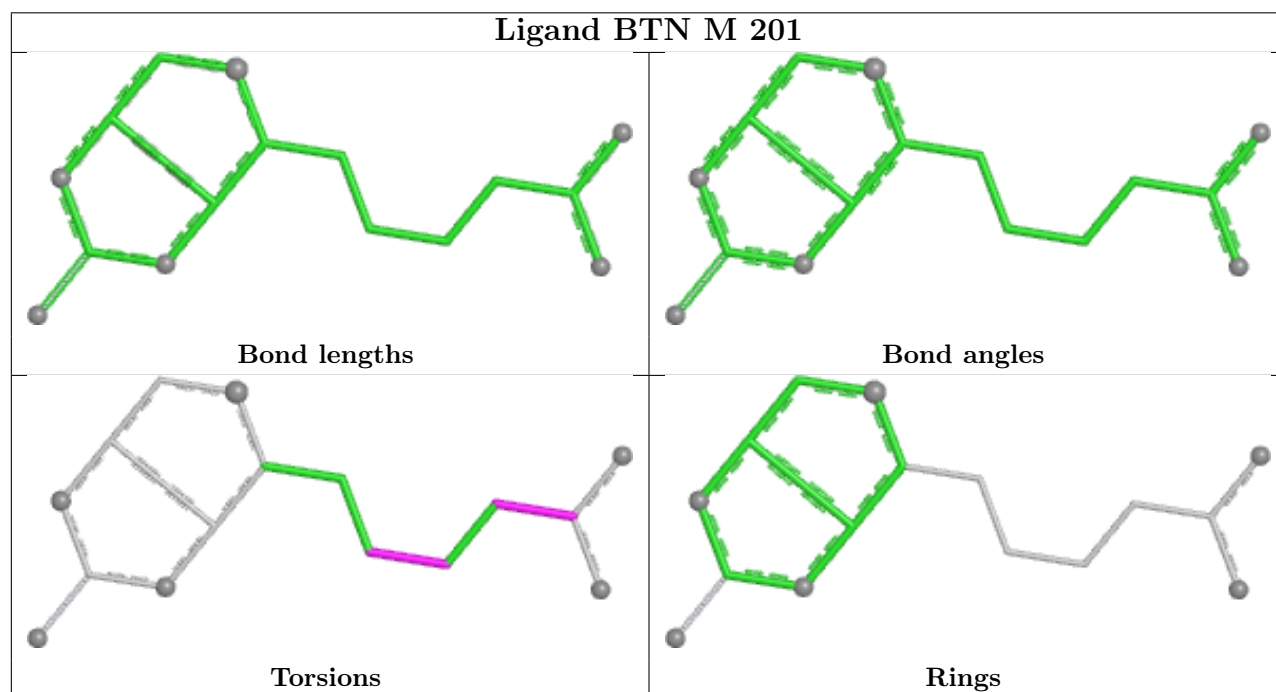
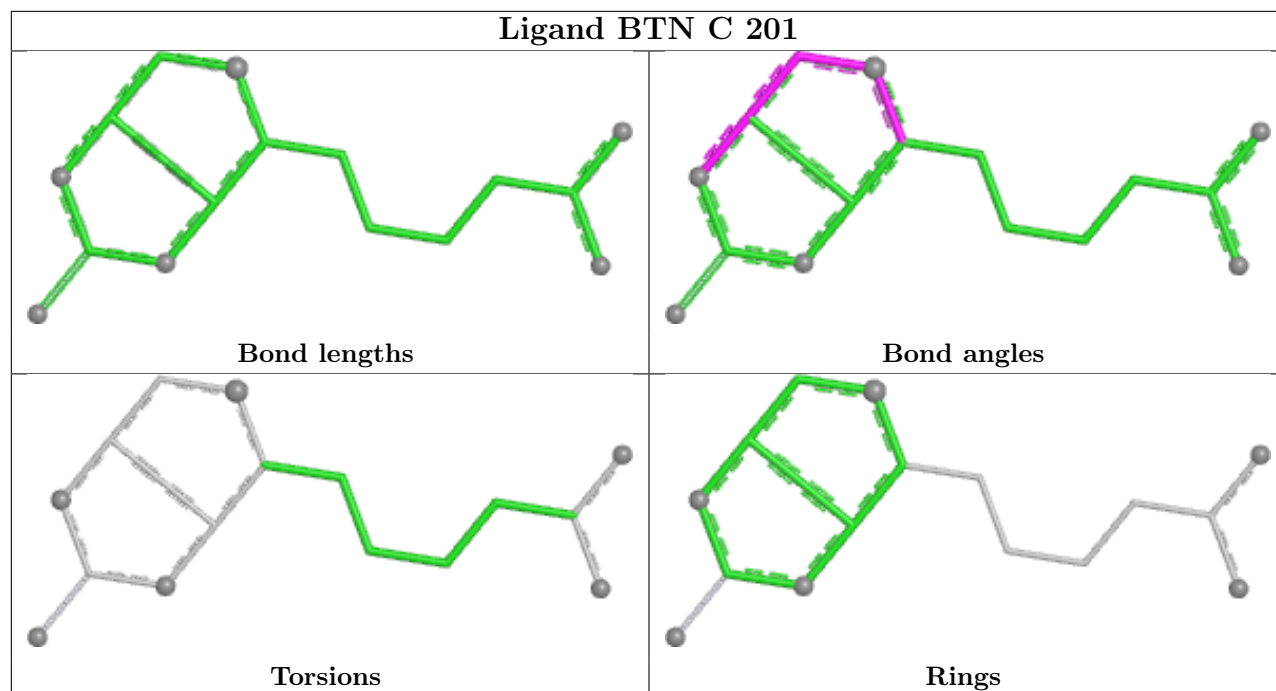


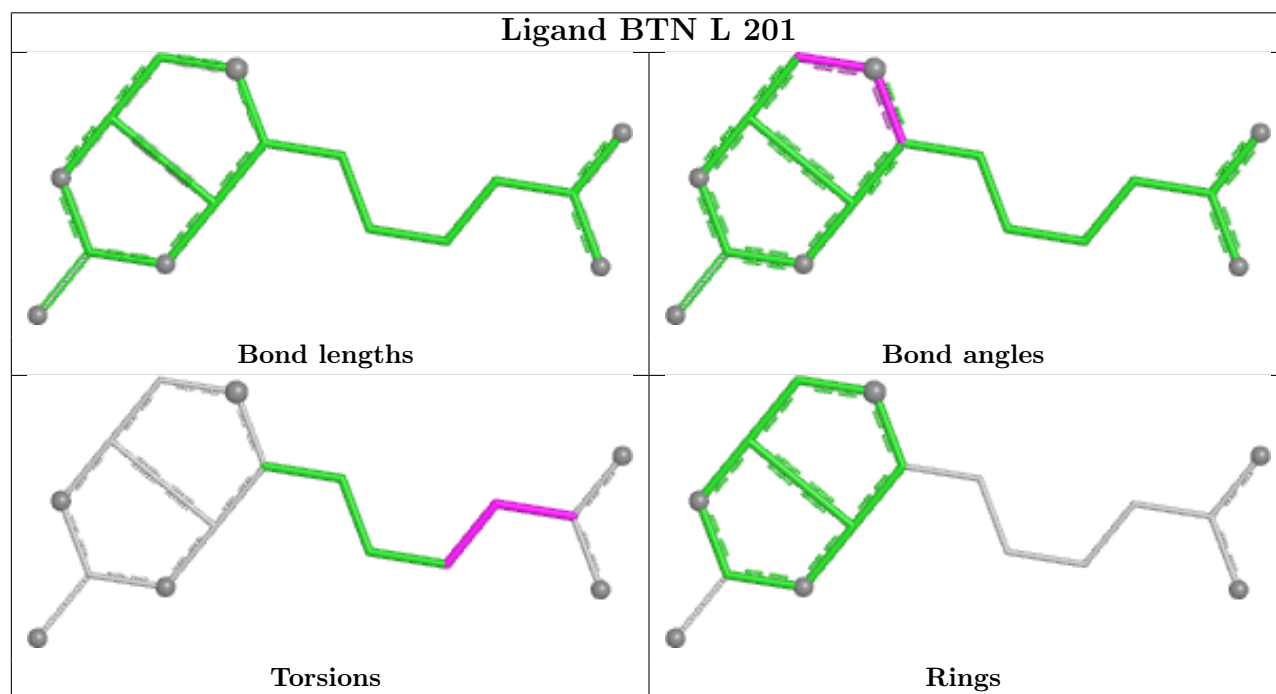
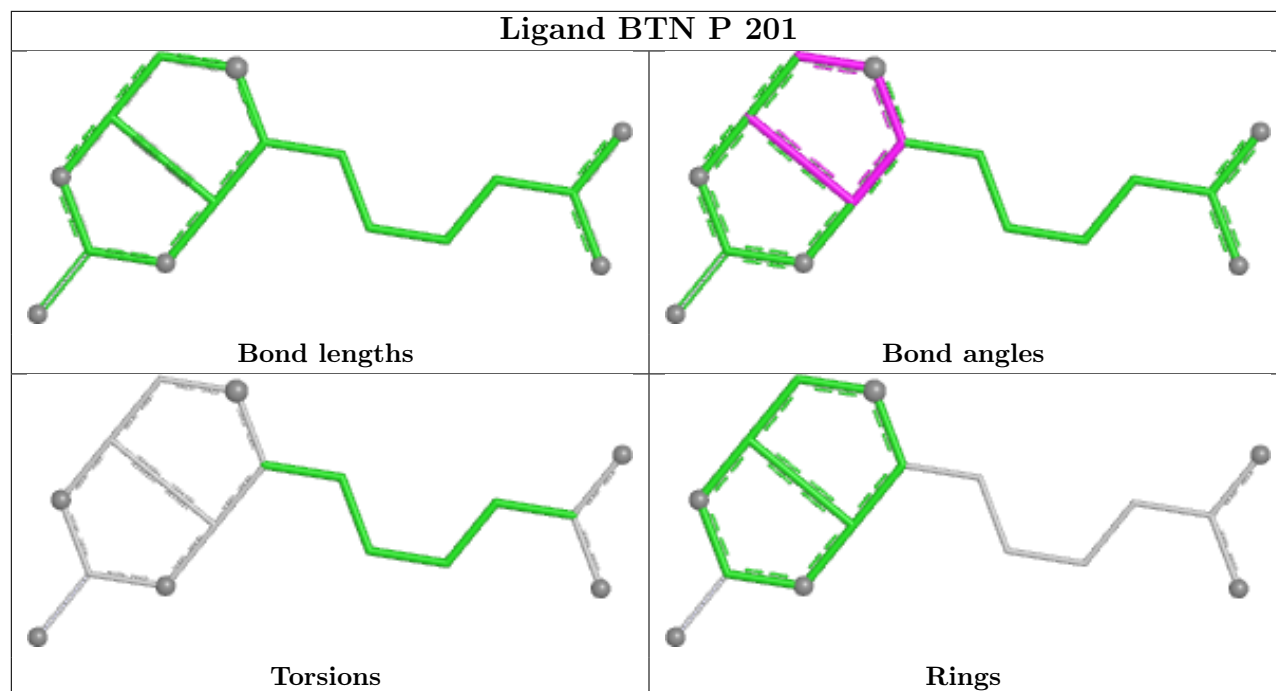


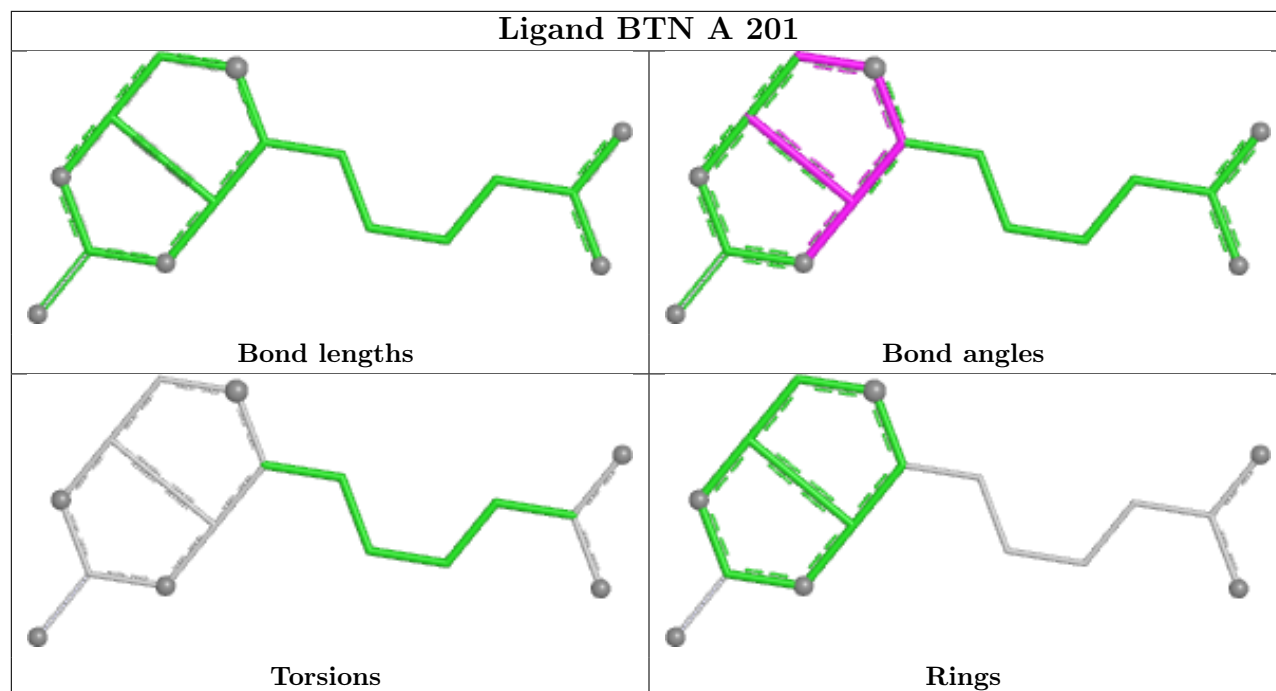












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	121/131 (92%)	-1.53	0 100 100	30, 45, 85, 116	0
1	B	121/131 (92%)	-1.48	0 100 100	29, 46, 90, 130	0
1	C	121/131 (92%)	-1.45	0 100 100	32, 47, 91, 118	0
1	D	121/131 (92%)	-1.50	0 100 100	20, 49, 81, 104	1 (0%)
1	E	121/131 (92%)	-1.42	0 100 100	38, 55, 98, 116	0
1	F	121/131 (92%)	-1.47	0 100 100	35, 51, 83, 122	0
1	G	121/131 (92%)	-1.37	0 100 100	37, 53, 97, 127	0
1	H	121/131 (92%)	-1.44	0 100 100	34, 51, 86, 110	0
1	I	121/131 (92%)	-1.03	0 100 100	57, 100, 134, 149	0
1	J	121/131 (92%)	-1.19	0 100 100	34, 82, 121, 144	0
1	K	121/131 (92%)	-1.22	0 100 100	51, 82, 111, 145	0
1	L	121/131 (92%)	-1.23	0 100 100	32, 69, 115, 134	0
1	M	121/131 (92%)	-1.03	0 100 100	56, 92, 135, 151	0
1	N	121/131 (92%)	-1.15	0 100 100	51, 86, 124, 141	0
1	O	121/131 (92%)	-1.12	0 100 100	62, 91, 133, 150	0
1	P	121/131 (92%)	-1.17	0 100 100	51, 85, 120, 139	0
1	Q	121/131 (92%)	-1.11	0 100 100	61, 89, 128, 134	0
1	R	121/131 (92%)	-0.96	0 100 100	73, 102, 132, 152	0
1	S	121/131 (92%)	-1.23	0 100 100	55, 80, 113, 146	0
1	T	121/131 (92%)	-1.09	0 100 100	64, 91, 127, 161	0
All	All	2420/2620 (92%)	-1.26	0 100 100	20, 76, 123, 161	1 (0%)

There are no RSRZ outliers to report.

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](#)

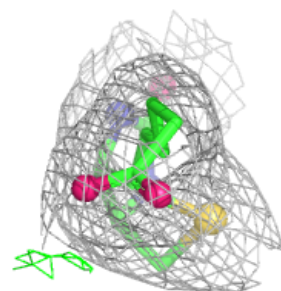
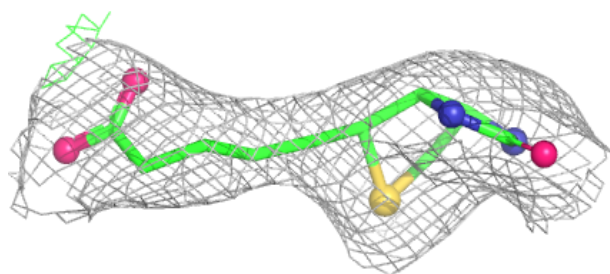
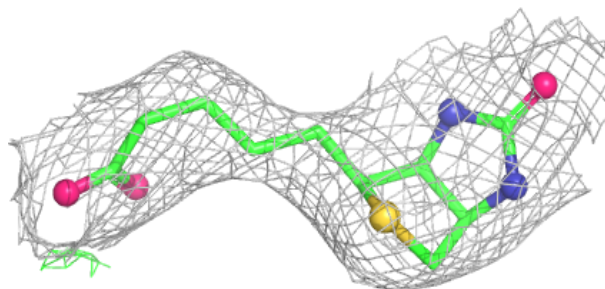
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BTN	A	201	16/16	0.99	0.03	36,39,45,46	0
2	BTN	F	201	16/16	0.99	0.03	30,39,49,56	0
2	BTN	H	201	16/16	0.99	0.04	39,52,61,64	0
2	BTN	I	201	16/16	0.99	0.04	66,79,84,87	0
2	BTN	J	201	16/16	0.99	0.03	60,70,82,83	0
2	BTN	K	201	16/16	0.99	0.04	69,76,87,92	0
2	BTN	L	201	16/16	0.99	0.04	52,62,73,76	0
2	BTN	N	201	16/16	0.99	0.04	64,71,82,96	0
2	BTN	O	201	16/16	0.99	0.04	71,77,86,89	0
2	BTN	S	201	16/16	0.99	0.03	59,65,69,73	0
2	BTN	T	201	16/16	0.99	0.04	65,71,77,77	0
2	BTN	Q	201	16/16	0.99	0.04	64,72,91,102	0
2	BTN	R	201	16/16	0.99	0.04	66,74,87,93	0
2	BTN	C	201	16/16	1.00	0.02	33,38,46,47	0
2	BTN	D	201	16/16	1.00	0.03	37,46,49,50	0
2	BTN	P	201	16/16	1.00	0.03	63,72,80,83	0
2	BTN	E	201	16/16	1.00	0.03	29,42,50,50	0
2	BTN	B	201	16/16	1.00	0.02	41,43,47,51	0
2	BTN	G	201	16/16	1.00	0.03	41,45,53,55	0
2	BTN	M	201	16/16	1.00	0.03	75,83,93,94	0

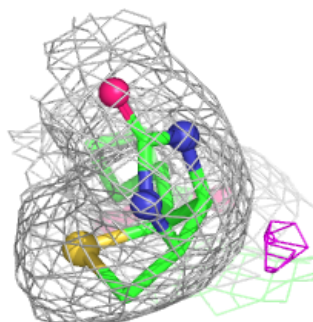
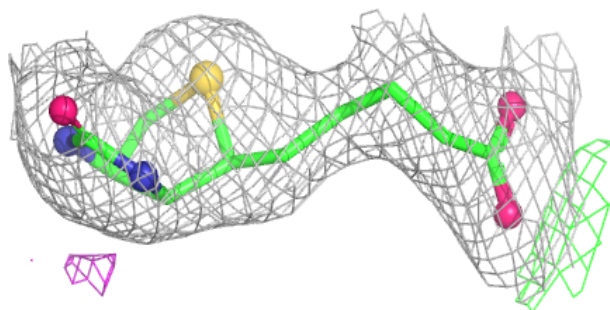
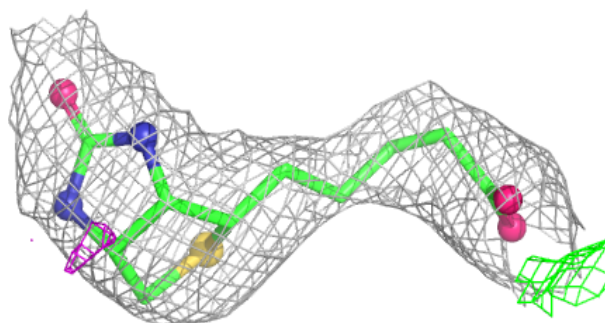
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BTN A 201:

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

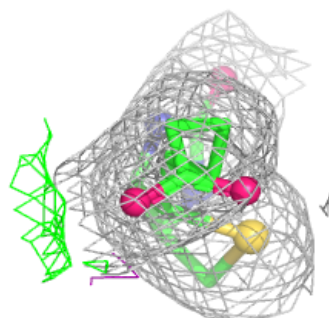
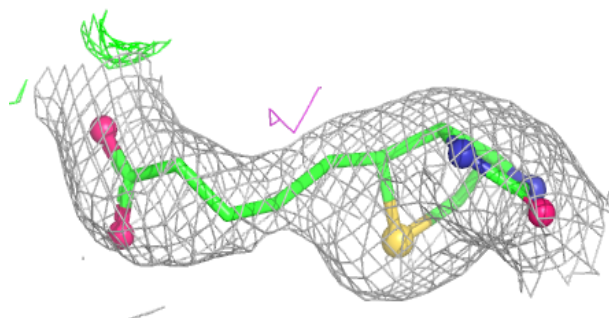
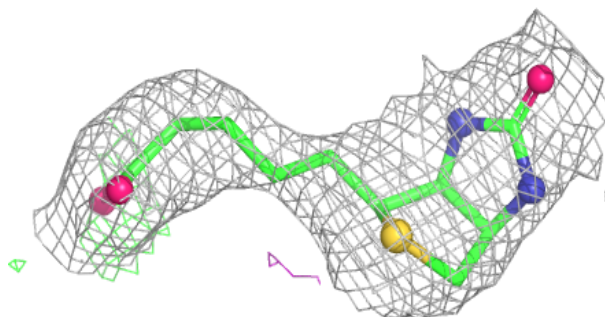
**Electron density around BTN F 201:**

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

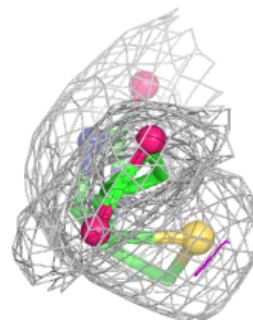
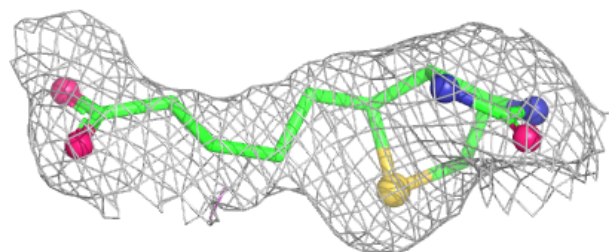
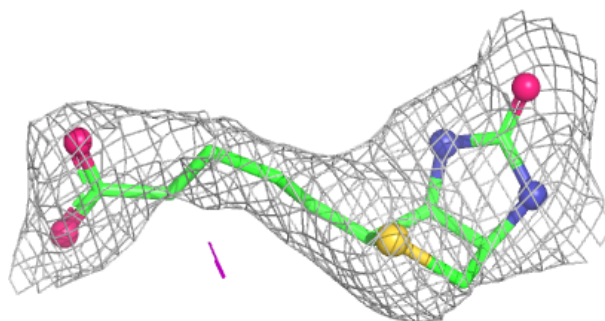


Electron density around BTN H 201:

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

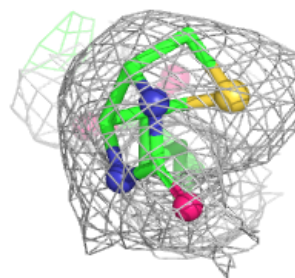
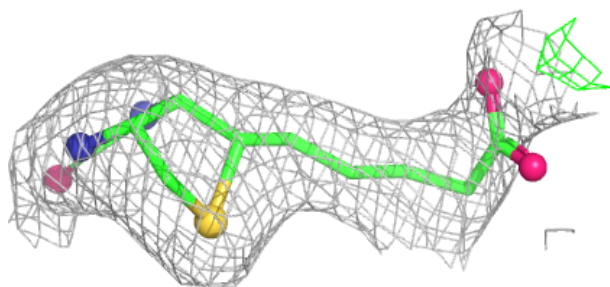
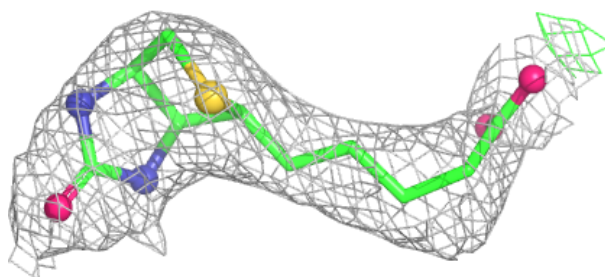
**Electron density around BTN I 201:**

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

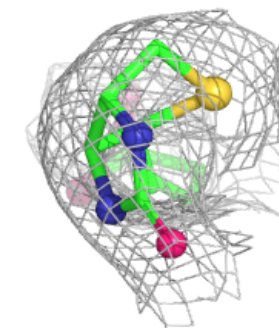
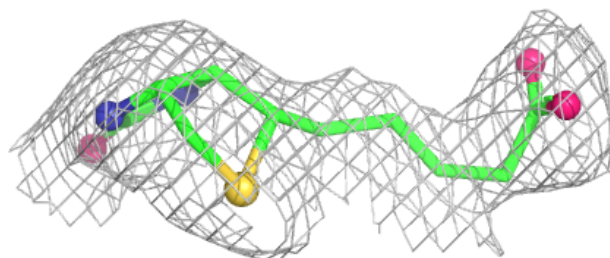
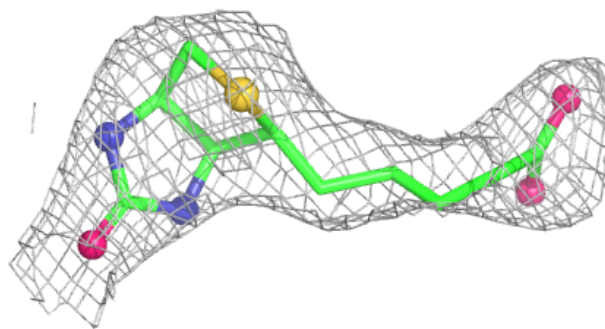


Electron density around BTN J 201:

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

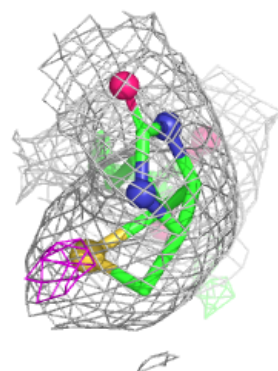
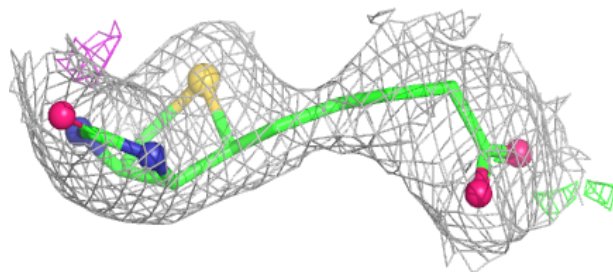
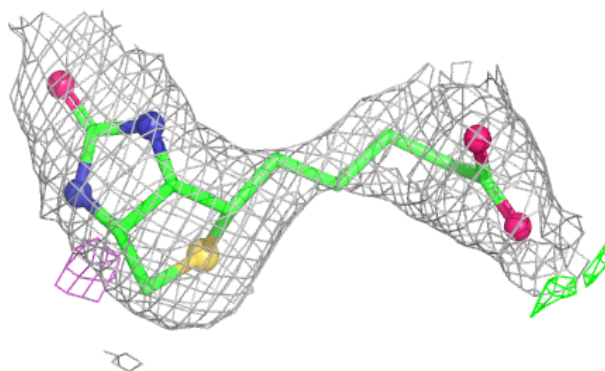
**Electron density around BTN K 201:**

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

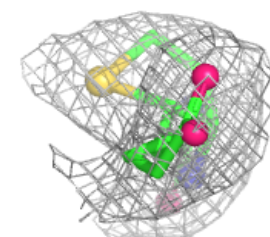
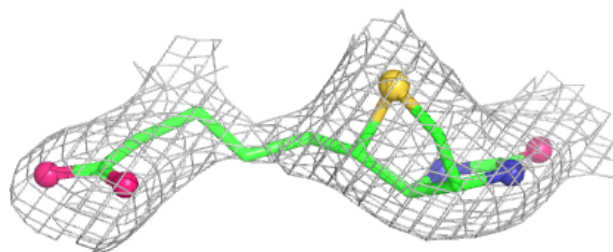
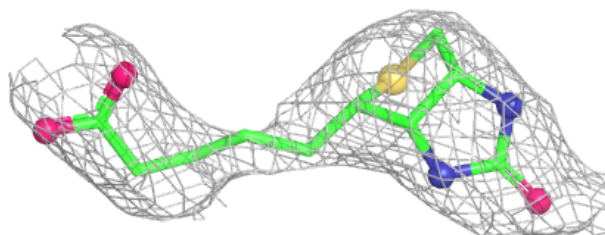


Electron density around BTN L 201:

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

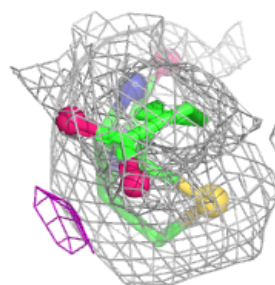
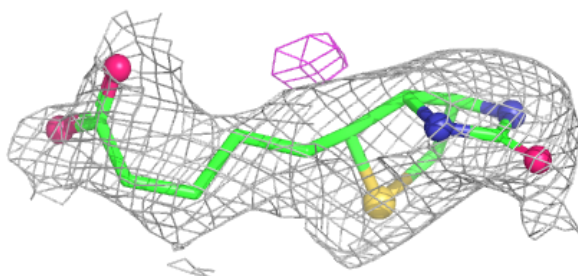
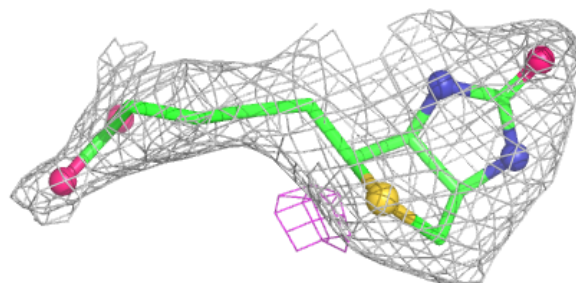
**Electron density around BTN N 201:**

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

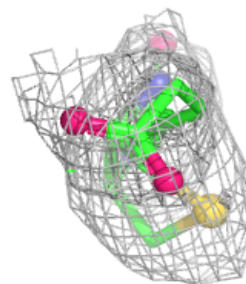
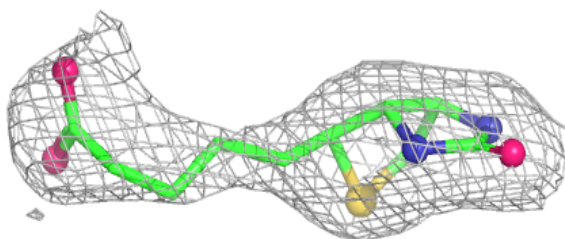
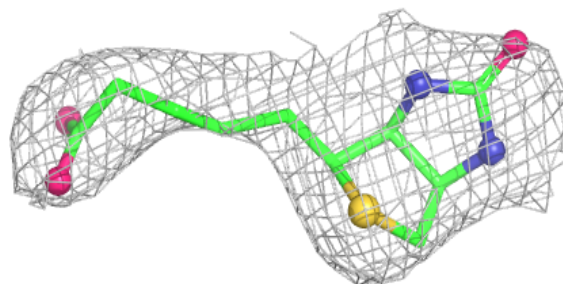


Electron density around BTN O 201:

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

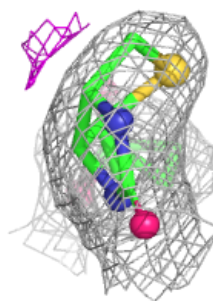
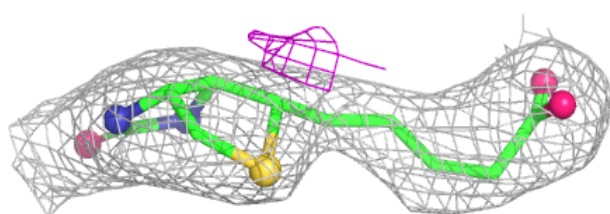
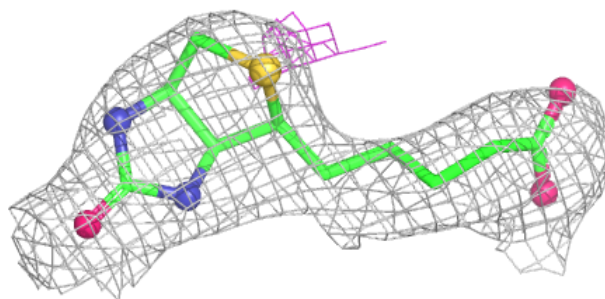
**Electron density around BTN S 201:**

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

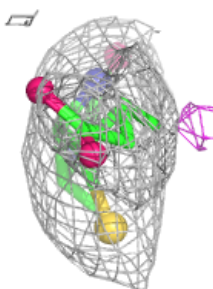
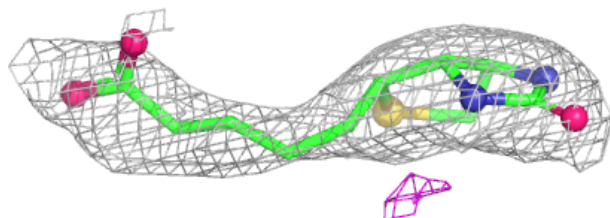


Electron density around BTN T 201:

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

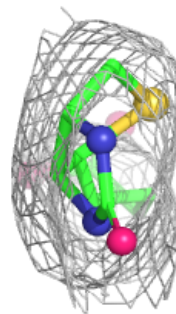
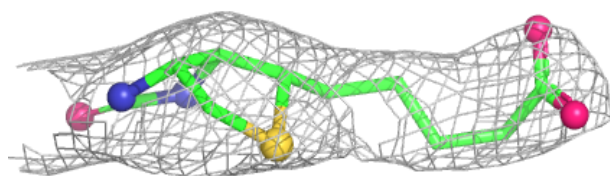
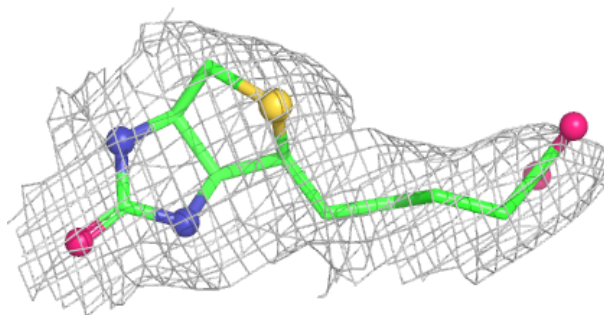
**Electron density around BTN Q 201:**

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

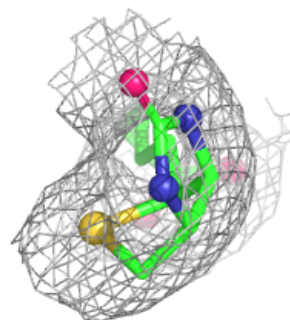
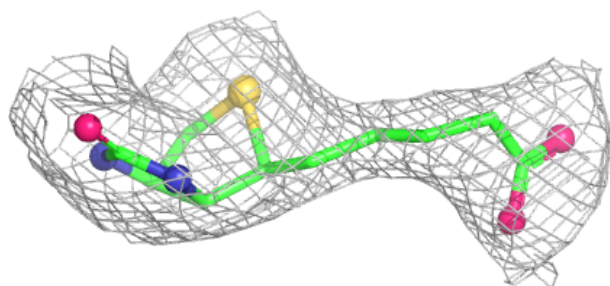
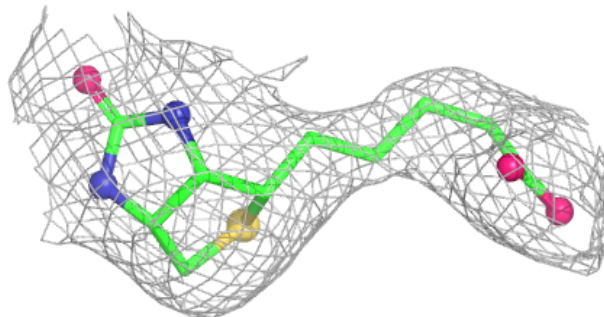


Electron density around BTN R 201:

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

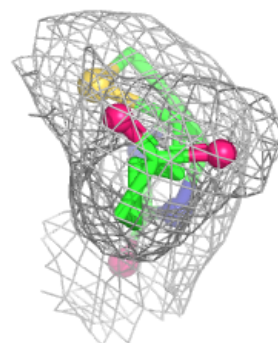
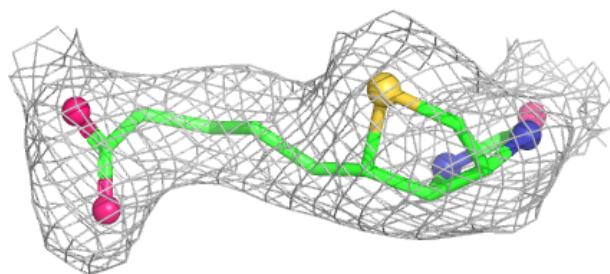
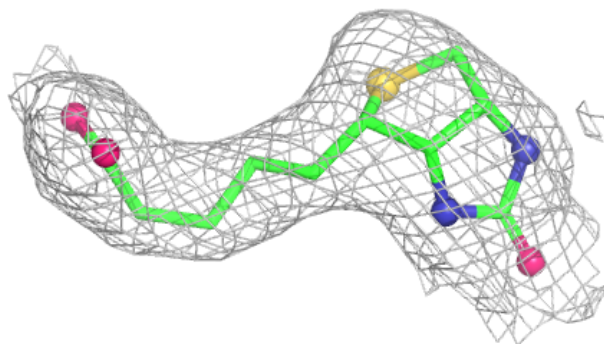
**Electron density around BTN C 201:**

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

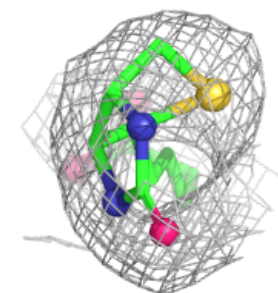
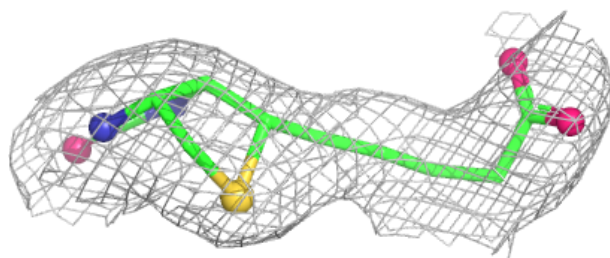
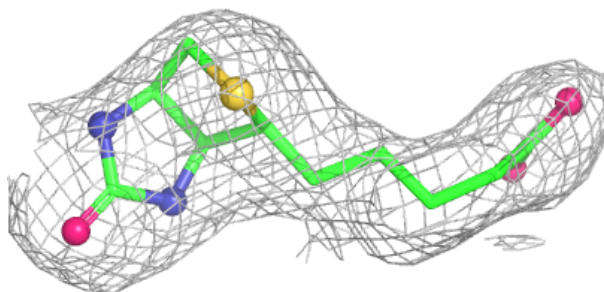


Electron density around BTN D 201:

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

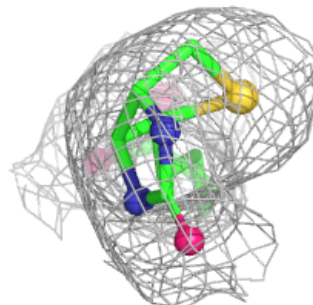
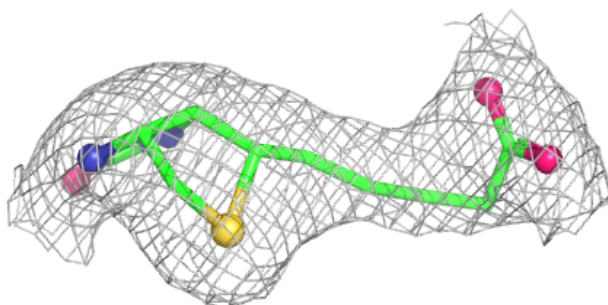
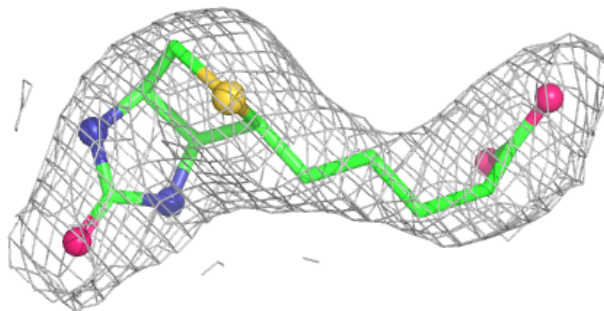
**Electron density around BTN P 201:**

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

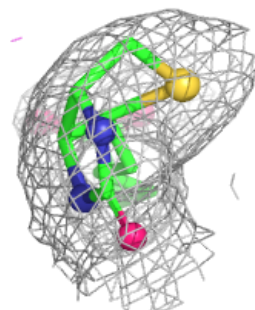
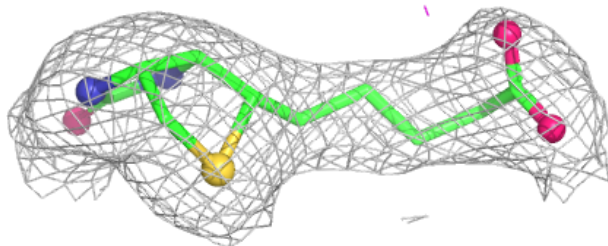
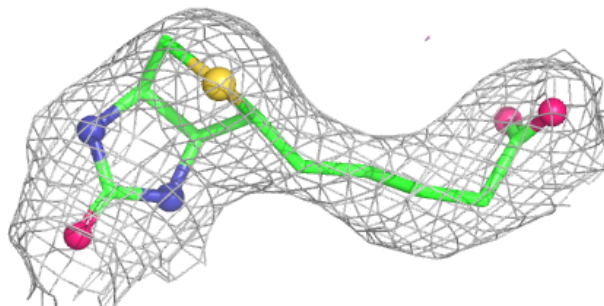


Electron density around BTN E 201:

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

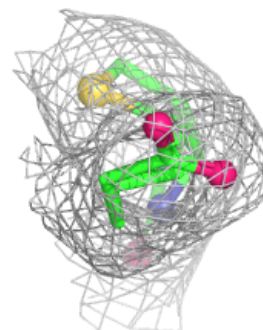
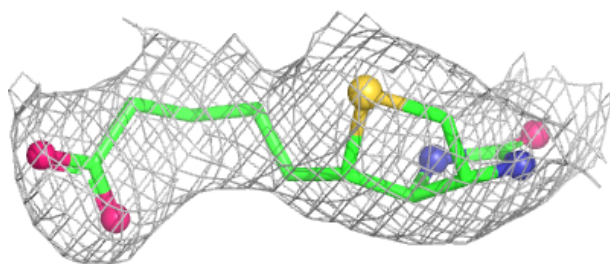
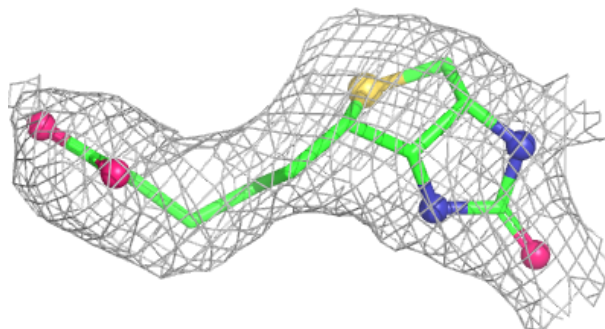
**Electron density around BTN B 201:**

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

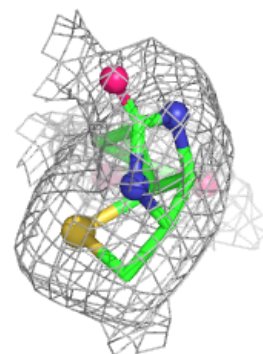
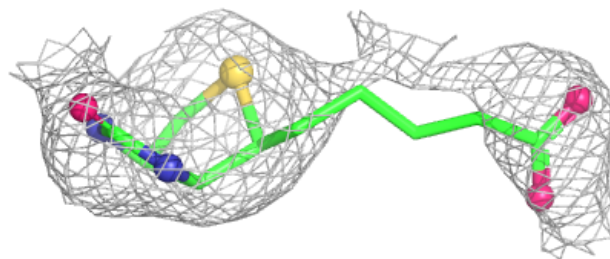
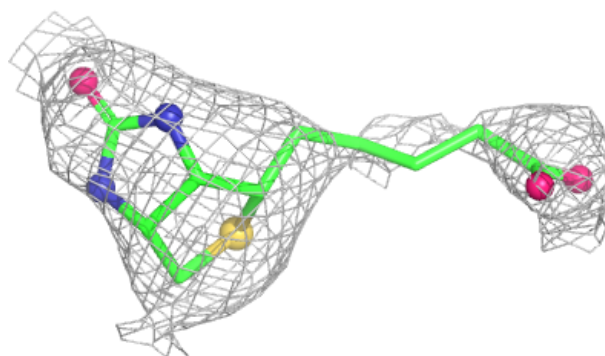


Electron density around BTN G 201:

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

**Electron density around BTN M 201:**

$2mF_o-DF_c$ (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.