



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 7, 2020 – 12:38 PM EDT

PDB ID : 7JGM
Title : Crystal Structure of the Ni-bound Human Heavy-chain variant 122H-delta C-star with meta-benzenedihydroxamate
Authors : Bailey, J.B.; Tezcan, F.A.
Deposited on : 2020-07-19
Resolution : 2.31 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

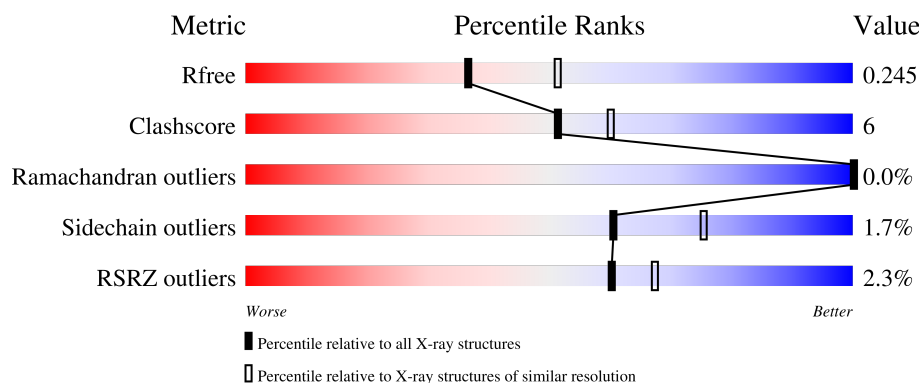
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 Å.

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






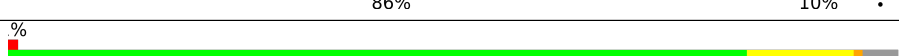

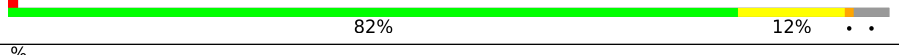

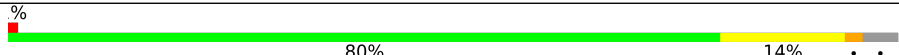
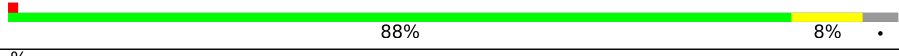
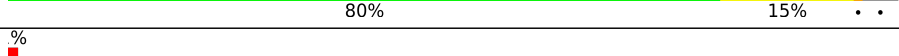
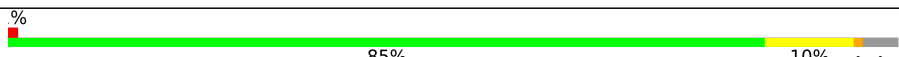


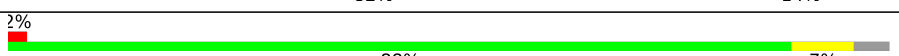

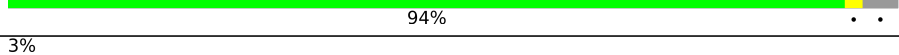
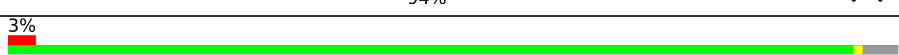
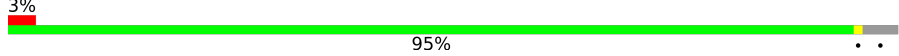
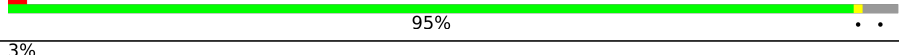
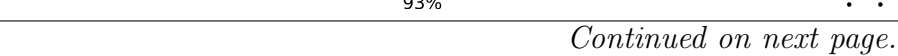


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	182	<div> <div>%</div> <div>79% 17% .</div> </div>
1	B	182	<div> <div>2%</div> <div>86% 8% . .</div> </div>
1	C	182	<div> <div>%</div> <div>82% 13% .</div> </div>
1	D	182	<div> <div>%</div> <div>88% 7% . .</div> </div>
1	E	182	<div> <div>%</div> <div>81% 14% .</div> </div>

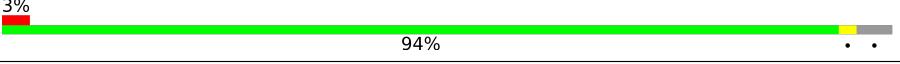
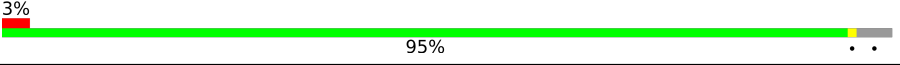
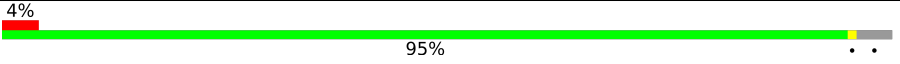
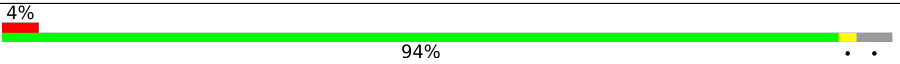
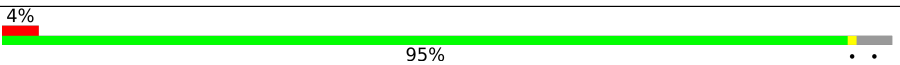
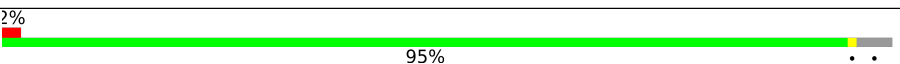
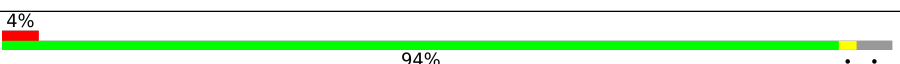
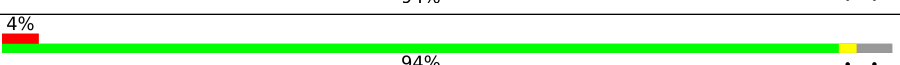
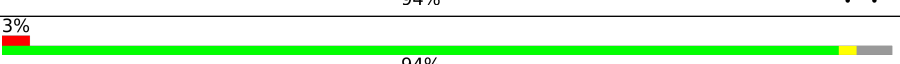
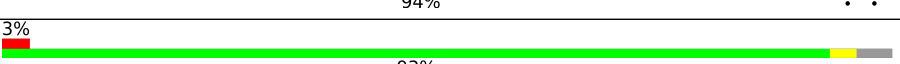
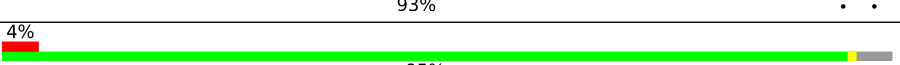
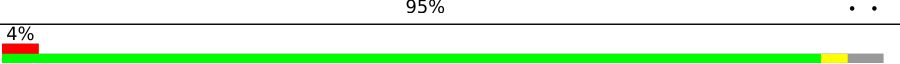
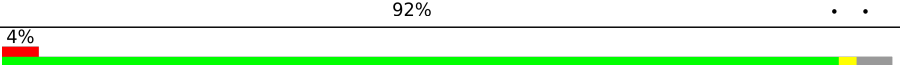
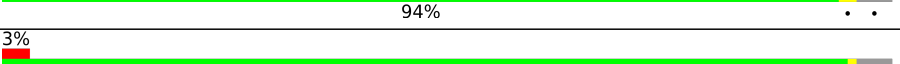
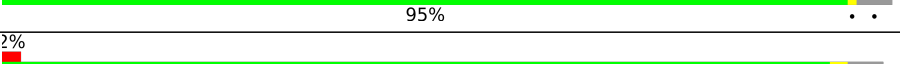
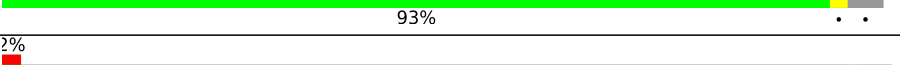
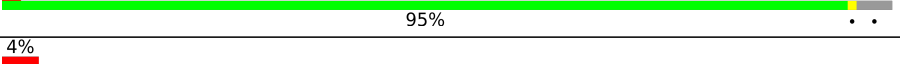
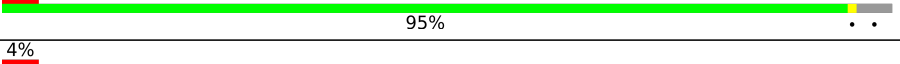
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Mol	Chain	Length	Quality of chain
1	F	182	
1	G	182	
1	H	182	
1	I	182	
1	J	182	
1	K	182	
1	L	182	
1	M	182	
1	N	182	
1	O	182	
1	P	182	
1	Q	182	
1	R	182	
1	S	182	
1	T	182	
1	U	182	
1	V	182	
1	W	182	
1	X	182	
1	a	182	
1	b	182	
1	c	182	
1	d	182	
1	e	182	
1	f	182	

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Mol	Chain	Length	Quality of chain
1	g	182	
1	h	182	
1	i	182	
1	j	182	
1	k	182	
1	l	182	
1	m	182	
1	n	182	
1	o	182	
1	p	182	
1	q	182	
1	r	182	
1	s	182	
1	t	182	
1	u	182	
1	v	182	
1	w	182	
1	x	182	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 105984 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 Ferritin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	0	0
			1431	896	252	279	4			
1	B	174	Total	C	N	O	S	0	0	0
			1431	896	252	279	4			
1	C	174	Total	C	N	O	S	0	0	0
			1431	896	252	279	4			
1	D	174	Total	C	N	O	S	0	1	0
			1436	899	252	281	4			
1	E	174	Total	C	N	O	S	0	0	0
			1431	896	252	279	4			
1	F	174	Total	C	N	O	S	0	1	0
			1437	900	253	280	4			
1	G	174	Total	C	N	O	S	0	1	0
			1436	899	252	281	4			
1	H	174	Total	C	N	O	S	0	0	0
			1431	896	252	279	4			
1	I	174	Total	C	N	O	S	0	0	0
			1431	896	252	279	4			
1	J	174	Total	C	N	O	S	0	0	0
			1431	896	252	279	4			
1	K	174	Total	C	N	O	S	0	0	0
			1431	896	252	279	4			
1	L	174	Total	C	N	O	S	0	0	0
			1431	896	252	279	4			
1	M	174	Total	C	N	O	S	0	0	0
			1431	896	252	279	4			
1	N	174	Total	C	N	O	S	0	0	0
			1431	896	252	279	4			
1	O	174	Total	C	N	O	S	0	0	0
			1431	896	252	279	4			
1	P	174	Total	C	N	O	S	0	0	0
			1431	896	252	279	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	174	Total	C	N	O	S	0	0	0
			1431	896	252	279	4			
1	R	174	Total	C	N	O	S	0	0	0
			1431	896	252	279	4			
1	S	174	Total	C	N	O	S	0	1	0
			1436	899	252	281	4			
1	T	174	Total	C	N	O	S	0	0	0
			1431	896	252	279	4			
1	U	174	Total	C	N	O	S	0	1	0
			1437	900	253	280	4			
1	V	174	Total	C	N	O	S	0	0	0
			1431	896	252	279	4			
1	W	174	Total	C	N	O	S	0	0	0
			1431	896	252	279	4			
1	X	174	Total	C	N	O	S	0	0	0
			1431	896	252	279	4			
1	a	174	Total	C	N	O	S	0	174	0
			2862	1792	504	558	8			
1	b	174	Total	C	N	O	S	0	174	0
			2862	1792	504	558	8			
1	c	174	Total	C	N	O	S	0	174	0
			2862	1792	504	558	8			
1	d	174	Total	C	N	O	S	0	174	0
			2862	1792	504	558	8			
1	e	174	Total	C	N	O	S	0	174	0
			2862	1792	504	558	8			
1	f	174	Total	C	N	O	S	0	174	0
			2862	1792	504	558	8			
1	g	174	Total	C	N	O	S	0	174	0
			2862	1792	504	558	8			
1	h	174	Total	C	N	O	S	0	174	0
			2862	1792	504	558	8			
1	i	174	Total	C	N	O	S	0	174	0
			2862	1792	504	558	8			
1	j	174	Total	C	N	O	S	0	174	0
			2862	1792	504	558	8			
1	k	174	Total	C	N	O	S	0	174	0
			2862	1792	504	558	8			
1	l	174	Total	C	N	O	S	0	174	0
			2862	1792	504	558	8			
1	m	174	Total	C	N	O	S	0	174	0
			2862	1792	504	558	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	n	174	Total	C	N	O	S	0	174	0
			2862	1792	504	558	8			
1	o	174	Total	C	N	O	S	0	174	0
			2862	1792	504	558	8			
1	p	174	Total	C	N	O	S	0	174	0
			2862	1792	504	558	8			
1	q	174	Total	C	N	O	S	0	174	0
			2862	1792	504	558	8			
1	r	174	Total	C	N	O	S	0	174	0
			2862	1792	504	558	8			
1	s	174	Total	C	N	O	S	0	174	0
			2862	1792	504	558	8			
1	t	174	Total	C	N	O	S	0	174	0
			2862	1792	504	558	8			
1	u	174	Total	C	N	O	S	0	174	0
			2862	1792	504	558	8			
1	v	174	Total	C	N	O	S	0	174	0
			2862	1792	504	558	8			
1	w	174	Total	C	N	O	S	0	174	0
			2862	1792	504	558	8			
1	x	174	Total	C	N	O	S	0	174	0
			2862	1792	504	558	8			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	GLN	LYS	engineered mutation	UNP P02794
A	90	GLU	CYS	engineered mutation	UNP P02794
A	102	ALA	CYS	engineered mutation	UNP P02794
A	122	HIS	THR	engineered mutation	UNP P02794
A	130	ALA	CYS	engineered mutation	UNP P02794
B	86	GLN	LYS	engineered mutation	UNP P02794
B	90	GLU	CYS	engineered mutation	UNP P02794
B	102	ALA	CYS	engineered mutation	UNP P02794
B	122	HIS	THR	engineered mutation	UNP P02794
B	130	ALA	CYS	engineered mutation	UNP P02794
C	86	GLN	LYS	engineered mutation	UNP P02794
C	90	GLU	CYS	engineered mutation	UNP P02794
C	102	ALA	CYS	engineered mutation	UNP P02794
C	122	HIS	THR	engineered mutation	UNP P02794
C	130	ALA	CYS	engineered mutation	UNP P02794
D	86	GLN	LYS	engineered mutation	UNP P02794
D	90	GLU	CYS	engineered mutation	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
D	102	ALA	CYS	engineered mutation	UNP P02794
D	122	HIS	THR	engineered mutation	UNP P02794
D	130	ALA	CYS	engineered mutation	UNP P02794
E	86	GLN	LYS	engineered mutation	UNP P02794
E	90	GLU	CYS	engineered mutation	UNP P02794
E	102	ALA	CYS	engineered mutation	UNP P02794
E	122	HIS	THR	engineered mutation	UNP P02794
E	130	ALA	CYS	engineered mutation	UNP P02794
F	86	GLN	LYS	engineered mutation	UNP P02794
F	90	GLU	CYS	engineered mutation	UNP P02794
F	102	ALA	CYS	engineered mutation	UNP P02794
F	122	HIS	THR	engineered mutation	UNP P02794
F	130	ALA	CYS	engineered mutation	UNP P02794
G	86	GLN	LYS	engineered mutation	UNP P02794
G	90	GLU	CYS	engineered mutation	UNP P02794
G	102	ALA	CYS	engineered mutation	UNP P02794
G	122	HIS	THR	engineered mutation	UNP P02794
G	130	ALA	CYS	engineered mutation	UNP P02794
H	86	GLN	LYS	engineered mutation	UNP P02794
H	90	GLU	CYS	engineered mutation	UNP P02794
H	102	ALA	CYS	engineered mutation	UNP P02794
H	122	HIS	THR	engineered mutation	UNP P02794
H	130	ALA	CYS	engineered mutation	UNP P02794
I	86	GLN	LYS	engineered mutation	UNP P02794
I	90	GLU	CYS	engineered mutation	UNP P02794
I	102	ALA	CYS	engineered mutation	UNP P02794
I	122	HIS	THR	engineered mutation	UNP P02794
I	130	ALA	CYS	engineered mutation	UNP P02794
J	86	GLN	LYS	engineered mutation	UNP P02794
J	90	GLU	CYS	engineered mutation	UNP P02794
J	102	ALA	CYS	engineered mutation	UNP P02794
J	122	HIS	THR	engineered mutation	UNP P02794
J	130	ALA	CYS	engineered mutation	UNP P02794
K	86	GLN	LYS	engineered mutation	UNP P02794
K	90	GLU	CYS	engineered mutation	UNP P02794
K	102	ALA	CYS	engineered mutation	UNP P02794
K	122	HIS	THR	engineered mutation	UNP P02794
K	130	ALA	CYS	engineered mutation	UNP P02794
L	86	GLN	LYS	engineered mutation	UNP P02794
L	90	GLU	CYS	engineered mutation	UNP P02794
L	102	ALA	CYS	engineered mutation	UNP P02794
L	122	HIS	THR	engineered mutation	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
L	130	ALA	CYS	engineered mutation	UNP P02794
M	86	GLN	LYS	engineered mutation	UNP P02794
M	90	GLU	CYS	engineered mutation	UNP P02794
M	102	ALA	CYS	engineered mutation	UNP P02794
M	122	HIS	THR	engineered mutation	UNP P02794
M	130	ALA	CYS	engineered mutation	UNP P02794
N	86	GLN	LYS	engineered mutation	UNP P02794
N	90	GLU	CYS	engineered mutation	UNP P02794
N	102	ALA	CYS	engineered mutation	UNP P02794
N	122	HIS	THR	engineered mutation	UNP P02794
N	130	ALA	CYS	engineered mutation	UNP P02794
O	86	GLN	LYS	engineered mutation	UNP P02794
O	90	GLU	CYS	engineered mutation	UNP P02794
O	102	ALA	CYS	engineered mutation	UNP P02794
O	122	HIS	THR	engineered mutation	UNP P02794
O	130	ALA	CYS	engineered mutation	UNP P02794
P	86	GLN	LYS	engineered mutation	UNP P02794
P	90	GLU	CYS	engineered mutation	UNP P02794
P	102	ALA	CYS	engineered mutation	UNP P02794
P	122	HIS	THR	engineered mutation	UNP P02794
P	130	ALA	CYS	engineered mutation	UNP P02794
Q	86	GLN	LYS	engineered mutation	UNP P02794
Q	90	GLU	CYS	engineered mutation	UNP P02794
Q	102	ALA	CYS	engineered mutation	UNP P02794
Q	122	HIS	THR	engineered mutation	UNP P02794
Q	130	ALA	CYS	engineered mutation	UNP P02794
R	86	GLN	LYS	engineered mutation	UNP P02794
R	90	GLU	CYS	engineered mutation	UNP P02794
R	102	ALA	CYS	engineered mutation	UNP P02794
R	122	HIS	THR	engineered mutation	UNP P02794
R	130	ALA	CYS	engineered mutation	UNP P02794
S	86	GLN	LYS	engineered mutation	UNP P02794
S	90	GLU	CYS	engineered mutation	UNP P02794
S	102	ALA	CYS	engineered mutation	UNP P02794
S	122	HIS	THR	engineered mutation	UNP P02794
S	130	ALA	CYS	engineered mutation	UNP P02794
T	86	GLN	LYS	engineered mutation	UNP P02794
T	90	GLU	CYS	engineered mutation	UNP P02794
T	102	ALA	CYS	engineered mutation	UNP P02794
T	122	HIS	THR	engineered mutation	UNP P02794
T	130	ALA	CYS	engineered mutation	UNP P02794
U	86	GLN	LYS	engineered mutation	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
U	90	GLU	CYS	engineered mutation	UNP P02794
U	102	ALA	CYS	engineered mutation	UNP P02794
U	122	HIS	THR	engineered mutation	UNP P02794
U	130	ALA	CYS	engineered mutation	UNP P02794
V	86	GLN	LYS	engineered mutation	UNP P02794
V	90	GLU	CYS	engineered mutation	UNP P02794
V	102	ALA	CYS	engineered mutation	UNP P02794
V	122	HIS	THR	engineered mutation	UNP P02794
V	130	ALA	CYS	engineered mutation	UNP P02794
W	86	GLN	LYS	engineered mutation	UNP P02794
W	90	GLU	CYS	engineered mutation	UNP P02794
W	102	ALA	CYS	engineered mutation	UNP P02794
W	122	HIS	THR	engineered mutation	UNP P02794
W	130	ALA	CYS	engineered mutation	UNP P02794
X	86	GLN	LYS	engineered mutation	UNP P02794
X	90	GLU	CYS	engineered mutation	UNP P02794
X	102	ALA	CYS	engineered mutation	UNP P02794
X	122	HIS	THR	engineered mutation	UNP P02794
X	130	ALA	CYS	engineered mutation	UNP P02794
a	86	GLN	LYS	engineered mutation	UNP P02794
a	90	GLU	CYS	engineered mutation	UNP P02794
a	102	ALA	CYS	engineered mutation	UNP P02794
a	122	HIS	THR	engineered mutation	UNP P02794
a	130	ALA	CYS	engineered mutation	UNP P02794
b	86	GLN	LYS	engineered mutation	UNP P02794
b	90	GLU	CYS	engineered mutation	UNP P02794
b	102	ALA	CYS	engineered mutation	UNP P02794
b	122	HIS	THR	engineered mutation	UNP P02794
b	130	ALA	CYS	engineered mutation	UNP P02794
c	86	GLN	LYS	engineered mutation	UNP P02794
c	90	GLU	CYS	engineered mutation	UNP P02794
c	102	ALA	CYS	engineered mutation	UNP P02794
c	122	HIS	THR	engineered mutation	UNP P02794
c	130	ALA	CYS	engineered mutation	UNP P02794
d	86	GLN	LYS	engineered mutation	UNP P02794
d	90	GLU	CYS	engineered mutation	UNP P02794
d	102	ALA	CYS	engineered mutation	UNP P02794
d	122	HIS	THR	engineered mutation	UNP P02794
d	130	ALA	CYS	engineered mutation	UNP P02794
e	86	GLN	LYS	engineered mutation	UNP P02794
e	90	GLU	CYS	engineered mutation	UNP P02794
e	102	ALA	CYS	engineered mutation	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
e	122	HIS	THR	engineered mutation	UNP P02794
e	130	ALA	CYS	engineered mutation	UNP P02794
f	86	GLN	LYS	engineered mutation	UNP P02794
f	90	GLU	CYS	engineered mutation	UNP P02794
f	102	ALA	CYS	engineered mutation	UNP P02794
f	122	HIS	THR	engineered mutation	UNP P02794
f	130	ALA	CYS	engineered mutation	UNP P02794
g	86	GLN	LYS	engineered mutation	UNP P02794
g	90	GLU	CYS	engineered mutation	UNP P02794
g	102	ALA	CYS	engineered mutation	UNP P02794
g	122	HIS	THR	engineered mutation	UNP P02794
g	130	ALA	CYS	engineered mutation	UNP P02794
h	86	GLN	LYS	engineered mutation	UNP P02794
h	90	GLU	CYS	engineered mutation	UNP P02794
h	102	ALA	CYS	engineered mutation	UNP P02794
h	122	HIS	THR	engineered mutation	UNP P02794
h	130	ALA	CYS	engineered mutation	UNP P02794
i	86	GLN	LYS	engineered mutation	UNP P02794
i	90	GLU	CYS	engineered mutation	UNP P02794
i	102	ALA	CYS	engineered mutation	UNP P02794
i	122	HIS	THR	engineered mutation	UNP P02794
i	130	ALA	CYS	engineered mutation	UNP P02794
j	86	GLN	LYS	engineered mutation	UNP P02794
j	90	GLU	CYS	engineered mutation	UNP P02794
j	102	ALA	CYS	engineered mutation	UNP P02794
j	122	HIS	THR	engineered mutation	UNP P02794
j	130	ALA	CYS	engineered mutation	UNP P02794
k	86	GLN	LYS	engineered mutation	UNP P02794
k	90	GLU	CYS	engineered mutation	UNP P02794
k	102	ALA	CYS	engineered mutation	UNP P02794
k	122	HIS	THR	engineered mutation	UNP P02794
k	130	ALA	CYS	engineered mutation	UNP P02794
l	86	GLN	LYS	engineered mutation	UNP P02794
l	90	GLU	CYS	engineered mutation	UNP P02794
l	102	ALA	CYS	engineered mutation	UNP P02794
l	122	HIS	THR	engineered mutation	UNP P02794
l	130	ALA	CYS	engineered mutation	UNP P02794
m	86	GLN	LYS	engineered mutation	UNP P02794
m	90	GLU	CYS	engineered mutation	UNP P02794
m	102	ALA	CYS	engineered mutation	UNP P02794
m	122	HIS	THR	engineered mutation	UNP P02794
m	130	ALA	CYS	engineered mutation	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
n	86	GLN	LYS	engineered mutation	UNP P02794
n	90	GLU	CYS	engineered mutation	UNP P02794
n	102	ALA	CYS	engineered mutation	UNP P02794
n	122	HIS	THR	engineered mutation	UNP P02794
n	130	ALA	CYS	engineered mutation	UNP P02794
o	86	GLN	LYS	engineered mutation	UNP P02794
o	90	GLU	CYS	engineered mutation	UNP P02794
o	102	ALA	CYS	engineered mutation	UNP P02794
o	122	HIS	THR	engineered mutation	UNP P02794
o	130	ALA	CYS	engineered mutation	UNP P02794
p	86	GLN	LYS	engineered mutation	UNP P02794
p	90	GLU	CYS	engineered mutation	UNP P02794
p	102	ALA	CYS	engineered mutation	UNP P02794
p	122	HIS	THR	engineered mutation	UNP P02794
p	130	ALA	CYS	engineered mutation	UNP P02794
q	86	GLN	LYS	engineered mutation	UNP P02794
q	90	GLU	CYS	engineered mutation	UNP P02794
q	102	ALA	CYS	engineered mutation	UNP P02794
q	122	HIS	THR	engineered mutation	UNP P02794
q	130	ALA	CYS	engineered mutation	UNP P02794
r	86	GLN	LYS	engineered mutation	UNP P02794
r	90	GLU	CYS	engineered mutation	UNP P02794
r	102	ALA	CYS	engineered mutation	UNP P02794
r	122	HIS	THR	engineered mutation	UNP P02794
r	130	ALA	CYS	engineered mutation	UNP P02794
s	86	GLN	LYS	engineered mutation	UNP P02794
s	90	GLU	CYS	engineered mutation	UNP P02794
s	102	ALA	CYS	engineered mutation	UNP P02794
s	122	HIS	THR	engineered mutation	UNP P02794
s	130	ALA	CYS	engineered mutation	UNP P02794
t	86	GLN	LYS	engineered mutation	UNP P02794
t	90	GLU	CYS	engineered mutation	UNP P02794
t	102	ALA	CYS	engineered mutation	UNP P02794
t	122	HIS	THR	engineered mutation	UNP P02794
t	130	ALA	CYS	engineered mutation	UNP P02794
u	86	GLN	LYS	engineered mutation	UNP P02794
u	90	GLU	CYS	engineered mutation	UNP P02794
u	102	ALA	CYS	engineered mutation	UNP P02794
u	122	HIS	THR	engineered mutation	UNP P02794
u	130	ALA	CYS	engineered mutation	UNP P02794
v	86	GLN	LYS	engineered mutation	UNP P02794
v	90	GLU	CYS	engineered mutation	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
v	102	ALA	CYS	engineered mutation	UNP P02794
v	122	HIS	THR	engineered mutation	UNP P02794
v	130	ALA	CYS	engineered mutation	UNP P02794
w	86	GLN	LYS	engineered mutation	UNP P02794
w	90	GLU	CYS	engineered mutation	UNP P02794
w	102	ALA	CYS	engineered mutation	UNP P02794
w	122	HIS	THR	engineered mutation	UNP P02794
w	130	ALA	CYS	engineered mutation	UNP P02794
x	86	GLN	LYS	engineered mutation	UNP P02794
x	90	GLU	CYS	engineered mutation	UNP P02794
x	102	ALA	CYS	engineered mutation	UNP P02794
x	122	HIS	THR	engineered mutation	UNP P02794
x	130	ALA	CYS	engineered mutation	UNP P02794

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	2	Total Ni 2 2	0	0
2	g	2	Total Ni 4 4	0	2
2	q	1	Total Ni 2 2	0	1
2	K	1	Total Ni 1 1	0	0
2	h	1	Total Ni 2 2	0	1
2	B	3	Total Ni 3 3	0	0
2	c	1	Total Ni 2 2	0	1
2	W	1	Total Ni 1 1	0	0
2	t	2	Total Ni 4 4	0	2
2	N	1	Total Ni 1 1	0	0
2	X	2	Total Ni 2 2	0	0
2	o	1	Total Ni 2 2	0	1
2	S	2	Total Ni 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	f	2	Total Ni 4 4	0	2
2	p	2	Total Ni 4 4	0	2
2	J	1	Total Ni 1 1	0	0
2	k	1	Total Ni 2 2	0	1
2	E	1	Total Ni 1 1	0	0
2	b	1	Total Ni 2 2	0	1
2	V	1	Total Ni 1 1	0	0
2	w	2	Total Ni 4 4	0	2
2	A	2	Total Ni 2 2	0	0
2	n	1	Total Ni 2 2	0	1
2	x	2	Total Ni 4 4	0	2
2	R	1	Total Ni 1 1	0	0
2	s	1	Total Ni 2 2	0	1
2	M	2	Total Ni 2 2	0	0
2	j	2	Total Ni 4 4	0	2
2	D	2	Total Ni 2 2	0	0
2	e	2	Total Ni 4 4	0	2
2	I	1	Total Ni 1 1	0	0
2	v	3	Total Ni 6 6	0	3
2	a	2	Total Ni 4 4	0	2
2	U	1	Total Ni 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	r	1	Total 2	Ni 2	0	1
2	L	2	Total 2	Ni 2	0	0
2	m	2	Total 4	Ni 4	0	2
2	G	2	Total 2	Ni 2	0	0
2	Q	1	Total 1	Ni 1	0	0
2	d	3	Total 6	Ni 6	0	3
2	H	2	Total 2	Ni 2	0	0
2	i	1	Total 2	Ni 2	0	1
2	C	2	Total 2	Ni 2	0	0
2	T	1	Total 1	Ni 1	0	0
2	u	1	Total 2	Ni 2	0	1
2	O	2	Total 2	Ni 2	0	0
2	l	1	Total 2	Ni 2	0	1
2	F	2	Total 2	Ni 2	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

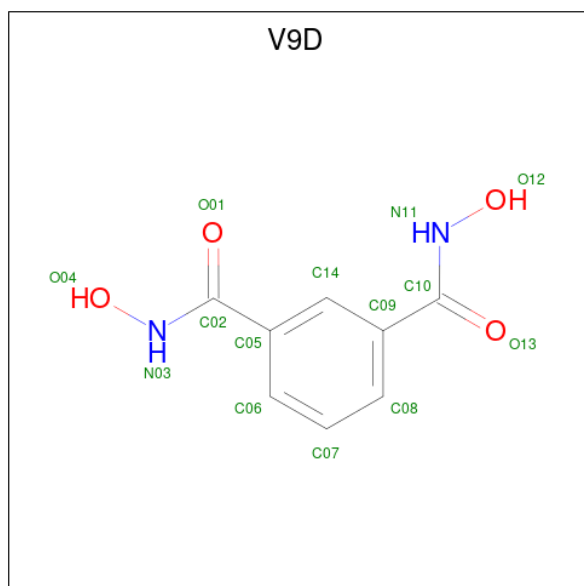
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total 1	Na 1	0	0
3	G	1	Total 1	Na 1	0	0
3	J	1	Total 1	Na 1	0	0
3	p	1	Total 2	Na 2	0	1
3	D	1	Total 1	Na 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	a	1	Total 2	Na 2	0	1
3	g	1	Total 2	Na 2	0	1
3	j	1	Total 2	Na 2	0	1
3	V	1	Total 1	Na 1	0	0
3	A	1	Total 1	Na 1	0	0
3	t	1	Total 2	Na 2	0	1
3	v	1	Total 2	Na 2	0	1
3	d	1	Total 2	Na 2	0	1
3	m	1	Total 2	Na 2	0	1
3	S	1	Total 1	Na 1	0	0
3	M	1	Total 1	Na 1	0	0

- Molecule 4 is N 1 ,N 3 -dihydroxybenzene-1,3-dicarboxamide (three-letter code: V9D) (formula: C₈H₈N₂O₄) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	F	1	Total	C	N	O	0	1
			28	16	4	8		
4	I	1	Total	C	N	O	0	1
			28	16	4	8		
4	R	1	Total	C	N	O	0	1
			28	16	4	8		
4	W	1	Total	C	N	O	0	1
			28	16	4	8		
4	a	1	Total	C	N	O	0	1
			28	16	4	8		
4	j	1	Total	C	N	O	0	1
			28	16	4	8		
4	n	1	Total	C	N	O	0	1
			28	16	4	8		
4	t	1	Total	C	N	O	0	1
			28	16	4	8		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	79	Total	O	0	0
			79	79		
5	B	108	Total	O	0	0
			108	108		
5	C	97	Total	O	0	0
			97	97		
5	D	112	Total	O	0	0
			112	112		
5	E	116	Total	O	0	0
			116	116		
5	F	117	Total	O	0	0
			117	117		
5	G	119	Total	O	0	0
			119	119		
5	H	110	Total	O	0	0
			110	110		
5	I	125	Total	O	0	0
			125	125		
5	J	81	Total	O	0	0
			81	81		
5	K	106	Total	O	0	0
			106	106		
5	L	84	Total	O	0	0
			84	84		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	90	Total 90	O 90	0	0
5	N	94	Total 94	O 94	0	0
5	O	90	Total 90	O 90	0	0
5	P	123	Total 123	O 123	0	0
5	Q	115	Total 115	O 115	0	0
5	R	112	Total 112	O 112	0	0
5	S	120	Total 120	O 120	0	0
5	T	124	Total 124	O 124	0	0
5	U	128	Total 128	O 128	0	0
5	V	92	Total 92	O 92	0	0
5	W	98	Total 98	O 98	0	0
5	X	95	Total 95	O 95	0	0
5	a	1	Total 1	O 1	0	0
5	c	3	Total 3	O 3	0	0
5	d	1	Total 1	O 1	0	0
5	e	2	Total 2	O 2	0	0
5	f	1	Total 1	O 1	0	0
5	g	2	Total 2	O 2	0	0
5	i	3	Total 3	O 3	0	0
5	j	2	Total 2	O 2	0	0
5	l	1	Total 1	O 1	0	0

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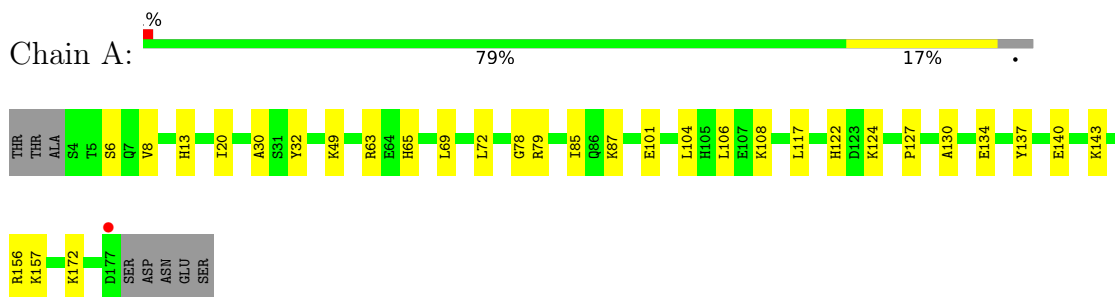
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	m	1	Total 1	O 1	0	0
5	n	2	Total 2	O 2	0	0
5	o	1	Total 1	O 1	0	0
5	p	1	Total 1	O 1	0	0
5	q	3	Total 3	O 3	0	0
5	r	2	Total 2	O 2	0	0
5	t	1	Total 1	O 1	0	0
5	u	1	Total 1	O 1	0	0

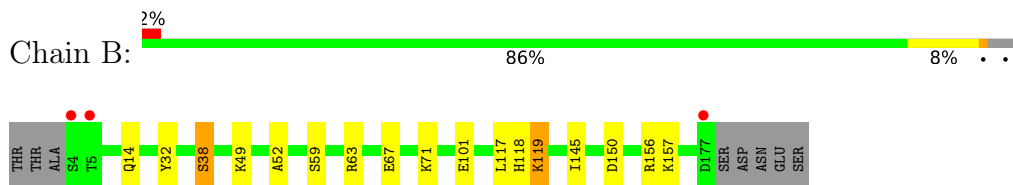
3 Residue-property plots [i](#)

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.

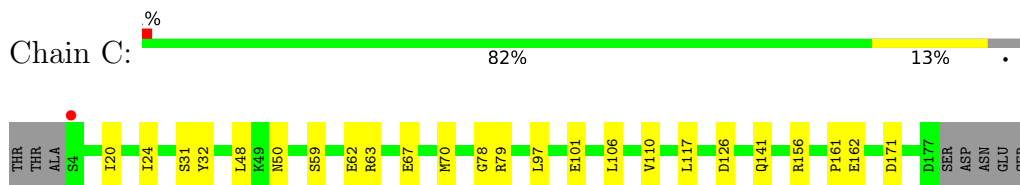
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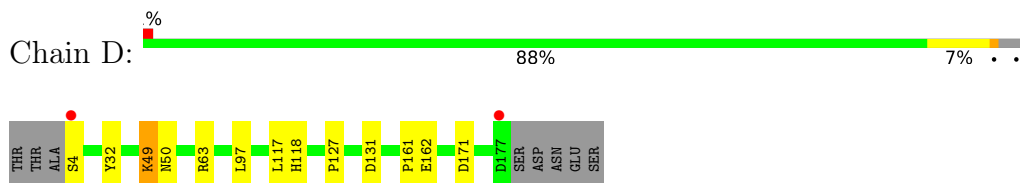
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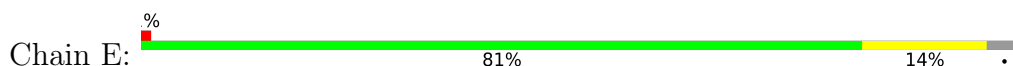
- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain

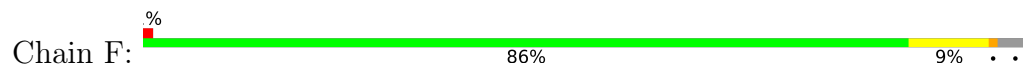


- Molecule 1: Ferritin heavy chain

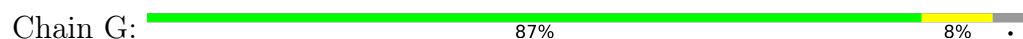




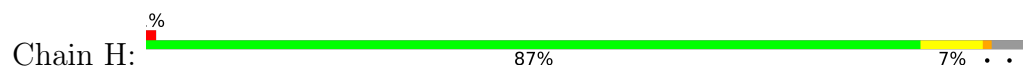
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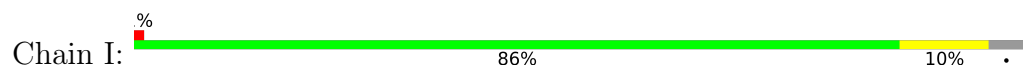
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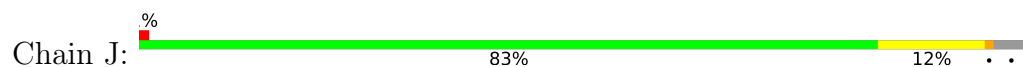
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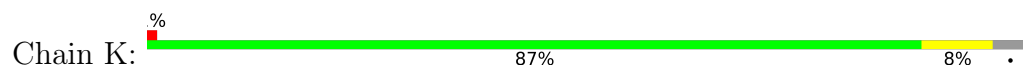
- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain

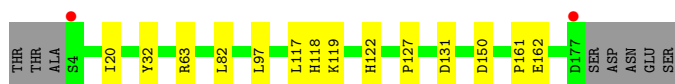


- Molecule 1: Ferritin heavy chain

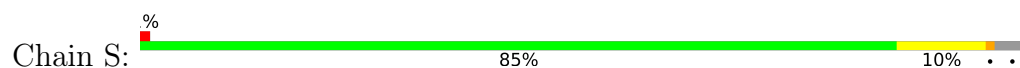


- Molecule 1: Ferritin heavy chain

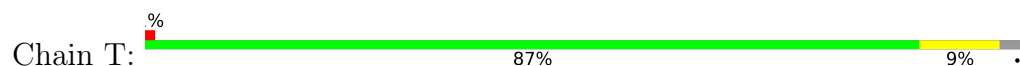




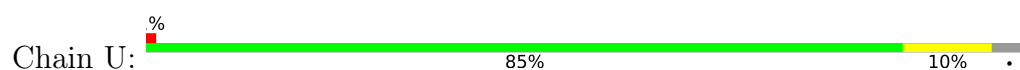
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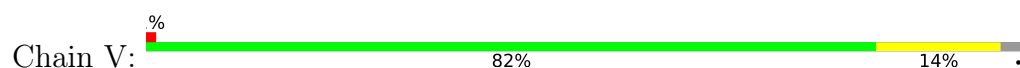
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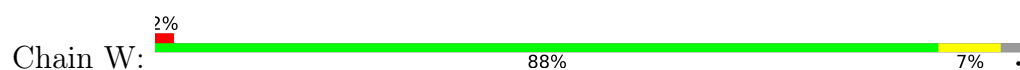
- Molecule 1: Ferritin heavy chain



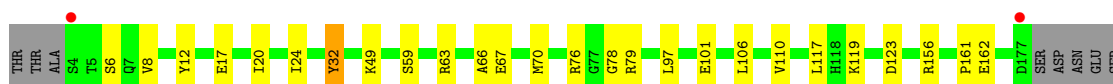
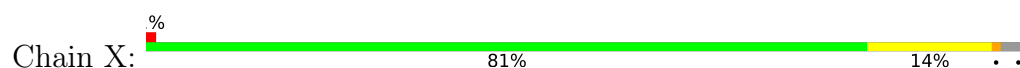
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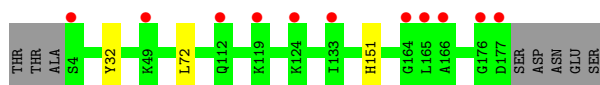
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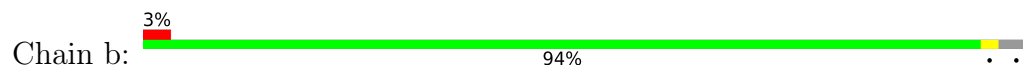
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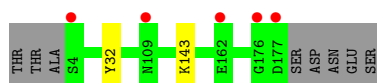
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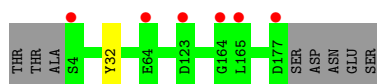
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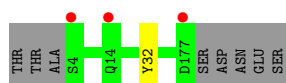
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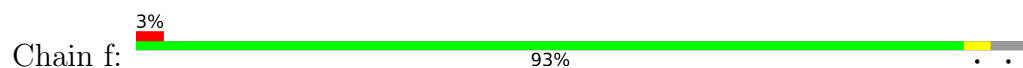
- Molecule 1: Ferritin heavy chain



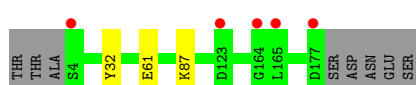
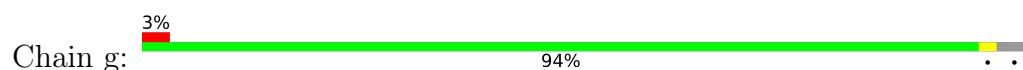
- Molecule 1: Ferritin heavy chain



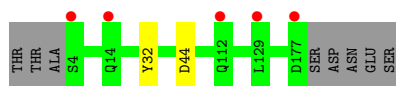
- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



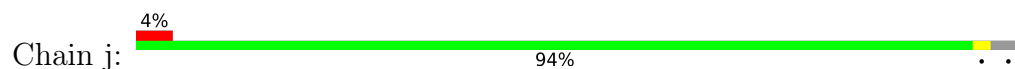
● Molecule 1: Ferritin heavy chain



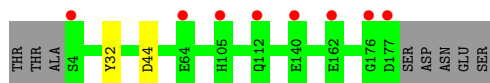
● Molecule 1: Ferritin heavy chain



● Molecule 1: Ferritin heavy chain



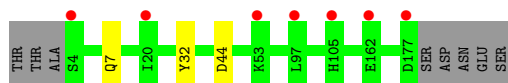
● Molecule 1: Ferritin heavy chain



● Molecule 1: Ferritin heavy chain

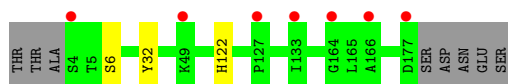


● Molecule 1: Ferritin heavy chain

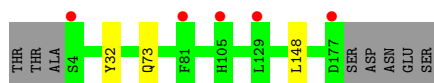


● Molecule 1: Ferritin heavy chain

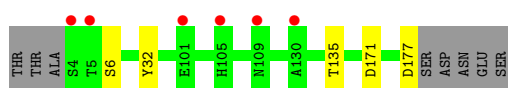
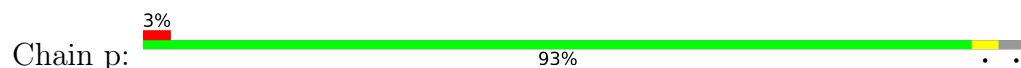




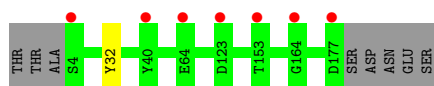
- Molecule 1: Ferritin heavy chain



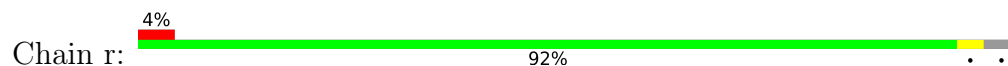
- Molecule 1: Ferritin heavy chain



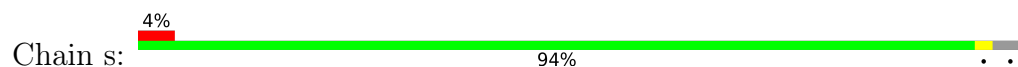
- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



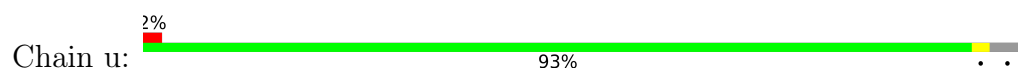
- Molecule 1: Ferritin heavy chain



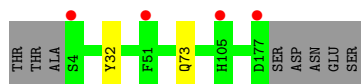
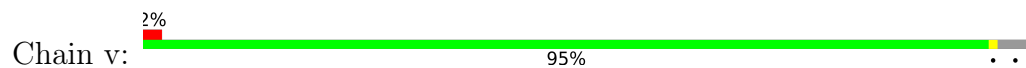
- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



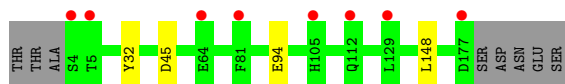
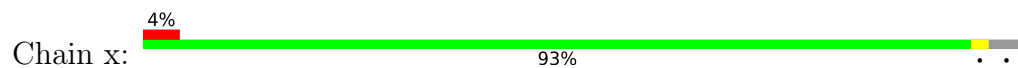
- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	213.55Å 213.75Å 155.93Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	38.46 – 2.31 39.09 – 2.31	Depositor EDS
% Data completeness (in resolution range)	98.2 (38.46-2.31) 90.8 (39.09-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.187 , 0.245 0.187 , 0.245	Depositor DCC
R_{free} test set	59846 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.469 for -k,-h,-l 0.469 for k,h,-l 0.467 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	105984	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.81% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NI, V9D, NA

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	0.56	0/1461	0.65	0/1969
1	B	0.56	0/1461	0.66	1/1969 (0.1%)
1	C	0.54	0/1461	0.63	0/1969
1	D	0.54	0/1469	0.64	0/1980
1	E	0.57	0/1461	0.66	0/1969
1	F	0.59	0/1470	0.65	0/1981
1	G	0.55	0/1469	0.64	0/1980
1	H	0.55	0/1461	0.66	0/1969
1	I	0.61	0/1461	0.66	0/1969
1	J	0.53	0/1461	0.64	0/1969
1	K	0.56	0/1461	0.66	1/1969 (0.1%)
1	L	0.56	0/1461	0.63	1/1969 (0.1%)
1	M	0.55	0/1461	0.64	0/1969
1	N	0.57	0/1461	0.65	1/1969 (0.1%)
1	O	0.53	0/1461	0.64	0/1969
1	P	0.54	0/1461	0.63	0/1969
1	Q	0.60	0/1461	0.69	0/1969
1	R	0.59	0/1461	0.64	0/1969
1	S	0.55	0/1469	0.68	0/1980
1	T	0.58	0/1461	0.66	0/1969
1	U	0.59	0/1470	0.63	0/1981
1	V	0.57	0/1461	0.64	0/1969
1	W	0.57	0/1461	0.66	1/1969 (0.1%)
1	X	0.53	0/1461	0.65	0/1969
1	a	0.42	0/2922	0.56	2/3938 (0.1%)
1	b	0.43	0/2922	0.56	2/3938 (0.1%)
1	c	0.45	0/2922	0.54	0/3938
1	d	0.41	0/2922	0.54	0/3938
1	e	0.42	0/2922	0.56	0/3938
1	f	0.41	0/2922	0.54	0/3938
1	g	0.43	0/2922	0.57	0/3938
1	h	0.42	0/2922	0.57	2/3938 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	i	0.42	0/2922	0.55	0/3938
1	j	0.42	0/2922	0.59	2/3938 (0.1%)
1	k	0.43	0/2922	0.55	0/3938
1	l	0.43	0/2922	0.56	2/3938 (0.1%)
1	m	0.44	0/2922	0.54	0/3938
1	n	0.42	0/2922	0.55	0/3938
1	o	0.42	0/2922	0.57	2/3938 (0.1%)
1	p	0.40	0/2922	0.52	0/3938
1	q	0.41	0/2922	0.55	0/3938
1	r	0.43	0/2922	0.57	0/3938
1	s	0.44	0/2922	0.54	0/3938
1	t	0.42	0/2922	0.57	0/3938
1	u	0.43	0/2922	0.56	2/3938 (0.1%)
1	v	0.42	0/2922	0.55	0/3938
1	w	0.43	0/2922	0.54	0/3938
1	x	0.41	0/2922	0.56	2/3938 (0.1%)
All	All	0.47	0/105234	0.59	21/141825 (0.0%)

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

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

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	u	171[C]	ASP	CB-CG-OD2	6.05	123.75	118.30
1	u	171[D]	ASP	CB-CG-OD2	6.05	123.75	118.30
1	N	150	ASP	CB-CG-OD1	5.59	123.34	118.30
1	W	150	ASP	CB-CG-OD1	5.58	123.32	118.30
1	b	150[C]	ASP	CB-CG-OD1	5.54	123.29	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	121	ALA	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	1431	0	1362	18	0
1	B	1431	0	1362	13	0
1	C	1431	0	1362	18	0
1	D	1436	0	1366	10	0
1	E	1431	0	1362	17	0
1	F	1437	0	1370	15	0
1	G	1436	0	1366	9	0
1	H	1431	0	1362	12	0
1	I	1431	0	1362	15	0
1	J	1431	0	1362	15	0
1	K	1431	0	1362	7	0
1	L	1431	0	1362	16	0
1	M	1431	0	1362	24	0
1	N	1431	0	1362	14	0
1	O	1431	0	1362	24	0
1	P	1431	0	1362	9	0
1	Q	1431	0	1362	19	0
1	R	1431	0	1362	14	0
1	S	1436	0	1366	11	0
1	T	1431	0	1362	8	0
1	U	1437	0	1370	13	0
1	V	1431	0	1362	18	0
1	W	1431	0	1362	9	0
1	X	1431	0	1362	21	0
1	a	2862	0	2704	0	0
1	b	2862	0	2705	0	0
1	c	2862	0	2700	0	0
1	d	2862	0	2705	0	0
1	e	2862	0	2704	0	0
1	f	2862	0	2704	0	0
1	g	2862	0	2707	0	0
1	h	2862	0	2700	0	0
1	i	2862	0	2704	0	0
1	j	2862	0	2705	0	0
1	k	2862	0	2706	0	0
1	l	2862	0	2698	0	0
1	m	2862	0	2703	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	n	2862	0	2707	0	0
1	o	2862	0	2703	0	0
1	p	2862	0	2705	0	0
1	q	2862	0	2707	0	0
1	r	2862	0	2706	0	0
1	s	2862	0	2703	0	0
1	t	2862	0	2707	0	0
1	u	2862	0	2704	0	0
1	v	2862	0	2704	0	0
1	w	2862	0	2705	0	0
1	x	2862	0	2709	0	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	1	0	0	0	0
2	O	2	0	0	0	0
2	P	2	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
2	S	2	0	0	0	0
2	T	1	0	0	0	0
2	U	1	0	0	0	0
2	V	1	0	0	0	0
2	W	1	0	0	0	0
2	X	2	0	0	0	0
2	a	4	0	0	0	0
2	b	2	0	0	0	0
2	c	2	0	0	0	0
2	d	6	0	0	0	0
2	e	4	0	0	0	0
2	f	4	0	0	0	0
2	g	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	h	2	0	0	0	0
2	i	2	0	0	0	0
2	j	4	0	0	0	0
2	k	2	0	0	0	0
2	l	2	0	0	0	0
2	m	4	0	0	0	0
2	n	2	0	0	0	0
2	o	2	0	0	0	0
2	p	4	0	0	0	0
2	q	2	0	0	0	0
2	r	2	0	0	0	0
2	s	2	0	0	0	0
2	t	4	0	0	0	0
2	u	2	0	0	0	0
2	v	6	0	0	0	0
2	w	4	0	0	0	0
2	x	4	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
3	G	1	0	0	0	0
3	J	1	0	0	0	0
3	M	1	0	0	0	0
3	P	1	0	0	0	0
3	S	1	0	0	0	0
3	V	1	0	0	0	0
3	a	2	0	0	0	0
3	d	2	0	0	0	0
3	g	2	0	0	0	0
3	j	2	0	0	0	0
3	m	2	0	0	0	0
3	p	2	0	0	0	0
3	t	2	0	0	0	0
3	v	2	0	0	0	0
4	F	28	0	0	1	0
4	I	28	0	0	3	0
4	R	28	0	0	5	0
4	W	28	0	0	0	0
4	a	28	0	0	0	0
4	j	28	0	0	0	0
4	n	28	0	0	0	0
4	t	28	0	0	0	0
5	A	79	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	108	0	0	3	0
5	C	97	0	0	2	0
5	D	112	0	0	0	0
5	E	116	0	0	5	0
5	F	117	0	0	2	0
5	G	119	0	0	1	0
5	H	110	0	0	2	0
5	I	125	0	0	1	0
5	J	81	0	0	1	0
5	K	106	0	0	0	0
5	L	84	0	0	3	0
5	M	90	0	0	3	0
5	N	94	0	0	3	0
5	O	90	0	0	3	0
5	P	123	0	0	0	0
5	Q	115	0	0	5	0
5	R	112	0	0	0	0
5	S	120	0	0	1	0
5	T	124	0	0	1	0
5	U	128	0	0	2	0
5	V	92	0	0	0	0
5	W	98	0	0	3	0
5	X	95	0	0	1	0
5	a	1	0	0	0	0
5	c	3	0	0	0	0
5	d	1	0	0	0	0
5	e	2	0	0	0	0
5	f	1	0	0	0	0
5	g	2	0	0	0	0
5	i	3	0	0	0	0
5	j	2	0	0	0	0
5	l	1	0	0	0	0
5	m	1	0	0	0	0
5	n	2	0	0	0	0
5	o	1	0	0	0	0
5	p	1	0	0	0	0
5	q	3	0	0	0	0
5	r	2	0	0	0	0
5	t	1	0	0	0	0
5	u	1	0	0	0	0
All	All	105984	0	97621	301	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 301 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:M:42:ASP:HA	1:M:49:LYS:HZ1	1.06	1.18
1:Q:49:LYS:NZ	5:Q:301:HOH:O	1.77	1.17
1:M:42:ASP:HA	1:M:49:LYS:NZ	1.75	1.02
1:R:161:PRO:HD2	1:R:162:GLU:OE2	1.70	0.92
1:X:119:LYS:NZ	1:X:123:ASP:OD1	2.05	0.87

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	172/182 (94%)	168 (98%)	4 (2%)	0	100	100
1	B	172/182 (94%)	168 (98%)	4 (2%)	0	100	100
1	C	172/182 (94%)	167 (97%)	5 (3%)	0	100	100
1	D	173/182 (95%)	168 (97%)	5 (3%)	0	100	100
1	E	172/182 (94%)	168 (98%)	4 (2%)	0	100	100
1	F	173/182 (95%)	166 (96%)	7 (4%)	0	100	100
1	G	173/182 (95%)	169 (98%)	4 (2%)	0	100	100
1	H	172/182 (94%)	166 (96%)	6 (4%)	0	100	100
1	I	172/182 (94%)	167 (97%)	5 (3%)	0	100	100
1	J	172/182 (94%)	169 (98%)	3 (2%)	0	100	100
1	K	172/182 (94%)	168 (98%)	4 (2%)	0	100	100
1	L	172/182 (94%)	166 (96%)	6 (4%)	0	100	100
1	M	172/182 (94%)	168 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	172/182 (94%)	169 (98%)	3 (2%)	0	100	100
1	O	172/182 (94%)	166 (96%)	5 (3%)	1 (1%)	25	30
1	P	172/182 (94%)	167 (97%)	5 (3%)	0	100	100
1	Q	172/182 (94%)	167 (97%)	5 (3%)	0	100	100
1	R	172/182 (94%)	167 (97%)	5 (3%)	0	100	100
1	S	173/182 (95%)	168 (97%)	5 (3%)	0	100	100
1	T	172/182 (94%)	167 (97%)	5 (3%)	0	100	100
1	U	173/182 (95%)	167 (96%)	6 (4%)	0	100	100
1	V	172/182 (94%)	167 (97%)	5 (3%)	0	100	100
1	W	172/182 (94%)	169 (98%)	3 (2%)	0	100	100
1	X	172/182 (94%)	168 (98%)	4 (2%)	0	100	100
1	a	344/182 (189%)	330 (96%)	14 (4%)	0	100	100
1	b	344/182 (189%)	334 (97%)	10 (3%)	0	100	100
1	c	344/182 (189%)	330 (96%)	14 (4%)	0	100	100
1	d	344/182 (189%)	334 (97%)	10 (3%)	0	100	100
1	e	344/182 (189%)	338 (98%)	6 (2%)	0	100	100
1	f	344/182 (189%)	334 (97%)	10 (3%)	0	100	100
1	g	344/182 (189%)	336 (98%)	8 (2%)	0	100	100
1	h	344/182 (189%)	328 (95%)	16 (5%)	0	100	100
1	i	344/182 (189%)	332 (96%)	12 (4%)	0	100	100
1	j	344/182 (189%)	330 (96%)	14 (4%)	0	100	100
1	k	344/182 (189%)	336 (98%)	8 (2%)	0	100	100
1	l	344/182 (189%)	330 (96%)	14 (4%)	0	100	100
1	m	344/182 (189%)	334 (97%)	10 (3%)	0	100	100
1	n	344/182 (189%)	328 (95%)	16 (5%)	0	100	100
1	o	344/182 (189%)	334 (97%)	10 (3%)	0	100	100
1	p	344/182 (189%)	330 (96%)	14 (4%)	0	100	100
1	q	344/182 (189%)	336 (98%)	8 (2%)	0	100	100
1	r	344/182 (189%)	332 (96%)	10 (3%)	2 (1%)	25	30
1	s	344/182 (189%)	326 (95%)	18 (5%)	0	100	100
1	t	344/182 (189%)	328 (95%)	16 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	u	344/182 (189%)	328 (95%)	16 (5%)	0	100	100
1	v	344/182 (189%)	330 (96%)	14 (4%)	0	100	100
1	w	344/182 (189%)	330 (96%)	14 (4%)	0	100	100
1	x	344/182 (189%)	336 (98%)	6 (2%)	2 (1%)	25	30
All	All	12389/8736 (142%)	11984 (97%)	400 (3%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	123	ASP
1	r	94[C]	GLU
1	r	94[D]	GLU
1	x	94[C]	GLU
1	x	94[D]	GLU

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	153/160 (96%)	148 (97%)	5 (3%)	38	52
1	B	153/160 (96%)	150 (98%)	3 (2%)	55	71
1	C	153/160 (96%)	152 (99%)	1 (1%)	84	92
1	D	154/160 (96%)	150 (97%)	4 (3%)	46	62
1	E	153/160 (96%)	150 (98%)	3 (2%)	55	71
1	F	154/160 (96%)	151 (98%)	3 (2%)	57	73
1	G	154/160 (96%)	150 (97%)	4 (3%)	46	62
1	H	153/160 (96%)	150 (98%)	3 (2%)	55	71
1	I	153/160 (96%)	152 (99%)	1 (1%)	84	92
1	J	153/160 (96%)	147 (96%)	6 (4%)	32	45
1	K	153/160 (96%)	151 (99%)	2 (1%)	69	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	153/160 (96%)	149 (97%)	4 (3%)	46	62
1	M	153/160 (96%)	151 (99%)	2 (1%)	69	81
1	N	153/160 (96%)	150 (98%)	3 (2%)	55	71
1	O	153/160 (96%)	148 (97%)	5 (3%)	38	52
1	P	153/160 (96%)	151 (99%)	2 (1%)	69	81
1	Q	153/160 (96%)	149 (97%)	4 (3%)	46	62
1	R	153/160 (96%)	152 (99%)	1 (1%)	84	92
1	S	154/160 (96%)	151 (98%)	3 (2%)	57	73
1	T	153/160 (96%)	149 (97%)	4 (3%)	46	62
1	U	154/160 (96%)	150 (97%)	4 (3%)	46	62
1	V	153/160 (96%)	150 (98%)	3 (2%)	55	71
1	W	153/160 (96%)	152 (99%)	1 (1%)	84	92
1	X	153/160 (96%)	152 (99%)	1 (1%)	84	92
1	a	306/160 (191%)	302 (99%)	4 (1%)	69	81
1	b	306/160 (191%)	302 (99%)	4 (1%)	69	81
1	c	306/160 (191%)	302 (99%)	4 (1%)	69	81
1	d	306/160 (191%)	304 (99%)	2 (1%)	84	92
1	e	306/160 (191%)	304 (99%)	2 (1%)	84	92
1	f	306/160 (191%)	296 (97%)	10 (3%)	38	52
1	g	306/160 (191%)	300 (98%)	6 (2%)	55	71
1	h	306/160 (191%)	304 (99%)	2 (1%)	84	92
1	i	306/160 (191%)	302 (99%)	4 (1%)	69	81
1	j	306/160 (191%)	302 (99%)	4 (1%)	69	81
1	k	306/160 (191%)	302 (99%)	4 (1%)	69	81
1	l	306/160 (191%)	304 (99%)	2 (1%)	84	92
1	m	306/160 (191%)	300 (98%)	6 (2%)	55	71
1	n	306/160 (191%)	300 (98%)	6 (2%)	55	71
1	o	306/160 (191%)	302 (99%)	4 (1%)	69	81
1	p	306/160 (191%)	296 (97%)	10 (3%)	38	52
1	q	306/160 (191%)	304 (99%)	2 (1%)	84	92
1	r	306/160 (191%)	296 (97%)	10 (3%)	38	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	s	306/160 (191%)	300 (98%)	6 (2%)	55	71
1	t	306/160 (191%)	304 (99%)	2 (1%)	84	92
1	u	306/160 (191%)	300 (98%)	6 (2%)	55	71
1	v	306/160 (191%)	302 (99%)	4 (1%)	69	81
1	w	306/160 (191%)	302 (99%)	4 (1%)	69	81
1	x	306/160 (191%)	302 (99%)	4 (1%)	69	81
All	All	11021/7680 (144%)	10837 (98%)	184 (2%)	60	75

5 of 184 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	c	143[D]	LYS
1	g	87[C]	LYS
1	u	62[C]	GLU
1	d	32[D]	TYR
1	f	32[D]	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	14	GLN
1	P	109	ASN
1	S	122	HIS
1	H	109	ASN
1	J	86	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 154 ligands modelled in this entry, 138 are monoatomic - leaving 16 for Mogul analysis.

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	V9D	a	204[C]	2	14,14,14	3.69	2 (14%)	18,18,18	1.51	3 (16%)
4	V9D	t	204[D]	2	14,14,14	3.56	2 (14%)	18,18,18	1.66	5 (27%)
4	V9D	F	203[D]	2	14,14,14	3.68	2 (14%)	18,18,18	1.38	3 (16%)
4	V9D	j	204[D]	2	14,14,14	3.77	3 (21%)	18,18,18	1.73	3 (16%)
4	V9D	I	202[D]	2	14,14,14	3.71	3 (21%)	18,18,18	1.26	2 (11%)
4	V9D	j	204[C]	2	14,14,14	3.62	3 (21%)	18,18,18	2.31	5 (27%)
4	V9D	R	202[C]	2	14,14,14	3.80	2 (14%)	18,18,18	1.44	3 (16%)
4	V9D	a	204[D]	2	14,14,14	3.80	2 (14%)	18,18,18	1.74	4 (22%)
4	V9D	n	202[C]	2	14,14,14	3.84	3 (21%)	18,18,18	1.70	2 (11%)
4	V9D	W	202[C]	2	14,14,14	3.75	2 (14%)	18,18,18	1.83	5 (27%)
4	V9D	W	202[D]	2	14,14,14	3.70	2 (14%)	18,18,18	1.70	5 (27%)
4	V9D	R	202[D]	2	14,14,14	3.35	2 (14%)	18,18,18	2.03	6 (33%)
4	V9D	I	202[C]	2	14,14,14	3.61	3 (21%)	18,18,18	1.80	6 (33%)
4	V9D	n	202[D]	2	14,14,14	3.71	2 (14%)	18,18,18	1.89	5 (27%)
4	V9D	F	203[C]	2	14,14,14	3.61	2 (14%)	18,18,18	1.53	3 (16%)
4	V9D	t	204[C]	2	14,14,14	3.77	2 (14%)	18,18,18	1.75	4 (22%)

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	V9D	a	204[C]	2	-	4/12/12/12	0/1/1/1
4	V9D	t	204[D]	2	-	4/12/12/12	0/1/1/1
4	V9D	F	203[D]	2	-	3/12/12/12	0/1/1/1
4	V9D	j	204[D]	2	-	4/12/12/12	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	V9D	I	202[D]	2	-	4/12/12/12	0/1/1/1
4	V9D	j	204[C]	2	-	4/12/12/12	0/1/1/1
4	V9D	R	202[C]	2	-	0/12/12/12	0/1/1/1
4	V9D	a	204[D]	2	-	4/12/12/12	0/1/1/1
4	V9D	n	202[C]	2	-	0/12/12/12	0/1/1/1
4	V9D	W	202[C]	2	-	0/12/12/12	0/1/1/1
4	V9D	W	202[D]	2	-	5/12/12/12	0/1/1/1
4	V9D	R	202[D]	2	-	0/12/12/12	0/1/1/1
4	V9D	I	202[C]	2	-	4/12/12/12	0/1/1/1
4	V9D	n	202[D]	2	-	4/12/12/12	0/1/1/1
4	V9D	F	203[C]	2	-	0/12/12/12	0/1/1/1
4	V9D	t	204[C]	2	-	7/12/12/12	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	a	204[D]	V9D	C10-N11	10.47	1.46	1.32
4	j	204[D]	V9D	C10-N11	10.45	1.46	1.32
4	n	202[C]	V9D	C10-N11	10.42	1.46	1.32
4	a	204[C]	V9D	C02-N03	10.27	1.46	1.32
4	W	202[D]	V9D	C02-N03	10.24	1.46	1.32

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	j	204[C]	V9D	C09-C10-N11	6.29	126.25	116.16
4	R	202[D]	V9D	O12-N11-C10	-5.21	106.77	119.64
4	W	202[C]	V9D	C05-C02-N03	4.95	124.09	116.16
4	a	204[D]	V9D	C05-C02-N03	4.87	123.97	116.16
4	n	202[D]	V9D	C09-C10-N11	4.70	123.70	116.16

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

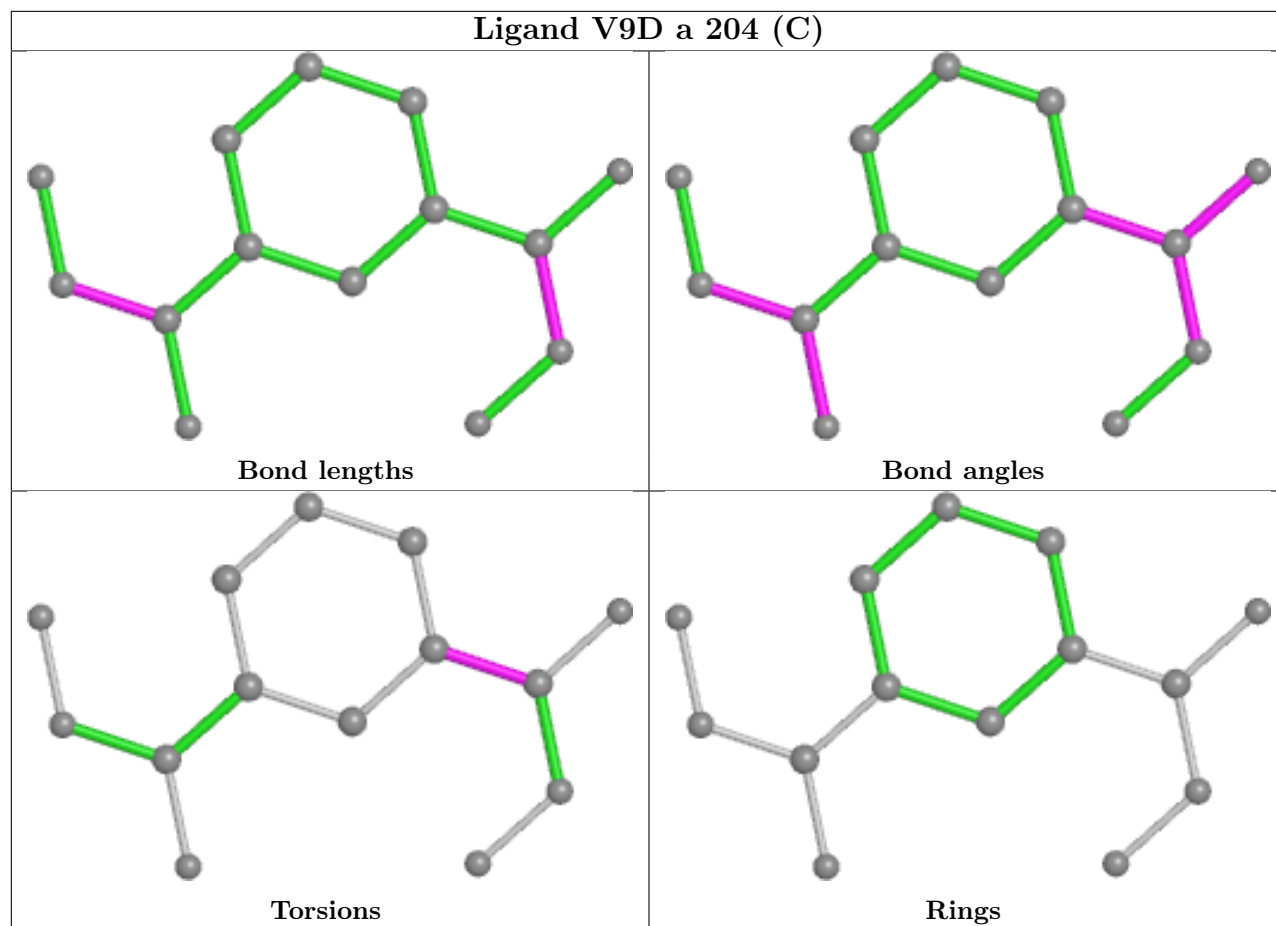
Mol	Chain	Res	Type	Atoms
4	W	202[D]	V9D	C08-C09-C10-N11
4	W	202[D]	V9D	C14-C09-C10-N11
4	a	204[D]	V9D	N03-C02-C05-C14
4	a	204[C]	V9D	C08-C09-C10-N11
4	a	204[C]	V9D	C14-C09-C10-N11

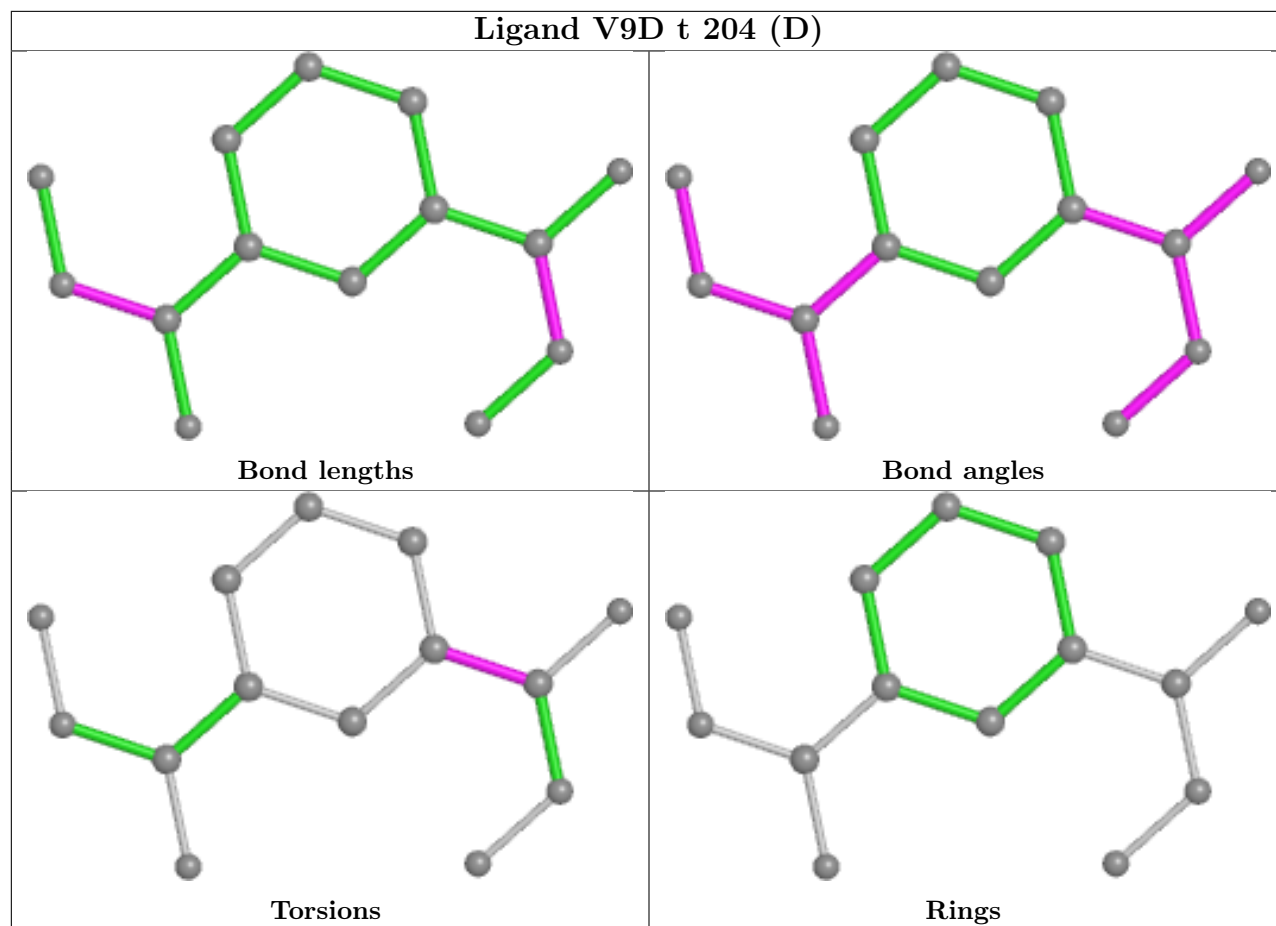
There are no ring outliers.

5 monomers are involved in 9 short contacts:

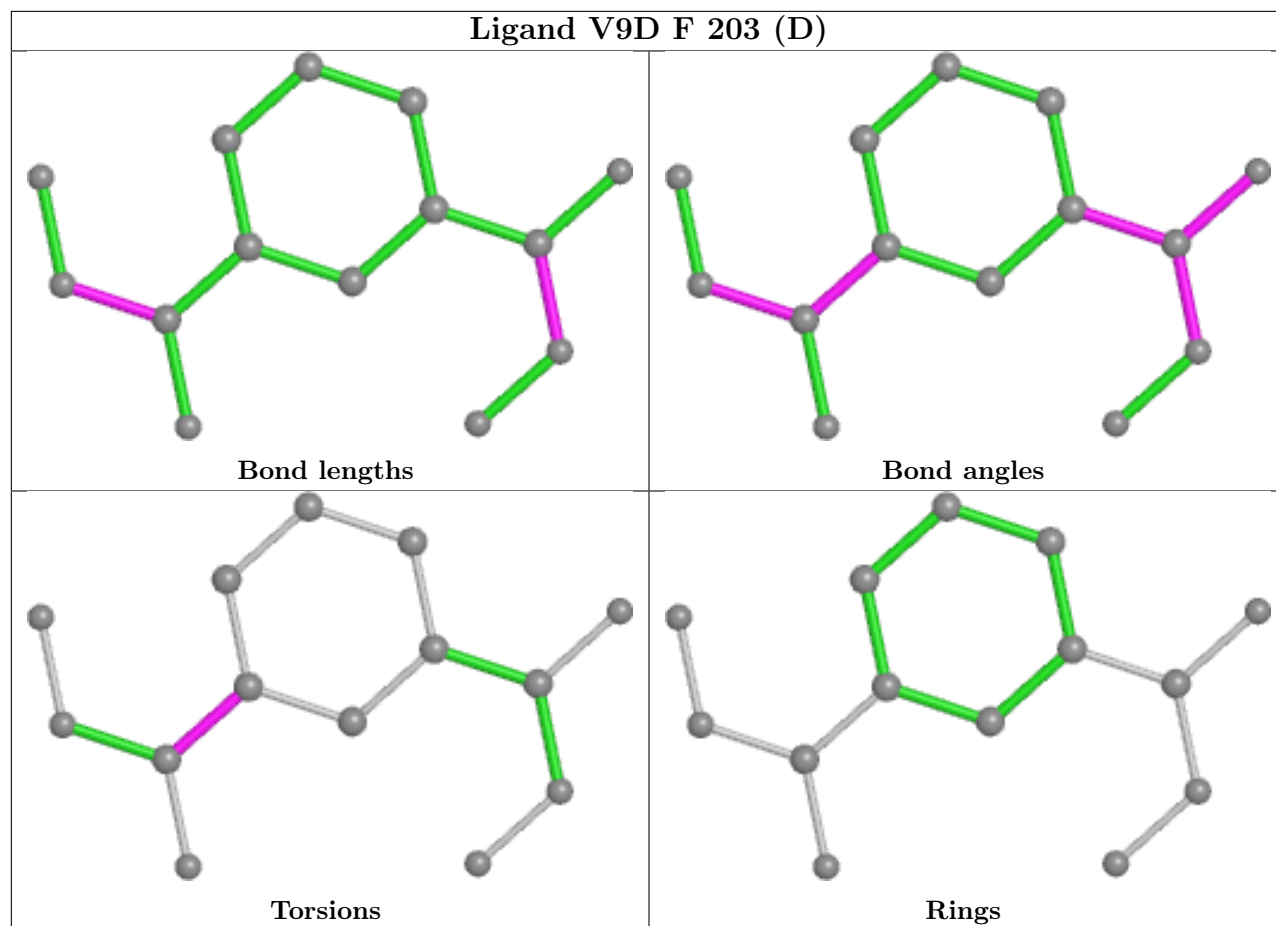
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	203[D]	V9D	1	0
4	I	202[D]	V9D	1	0
4	R	202[C]	V9D	1	0
4	R	202[D]	V9D	4	0
4	I	202[C]	V9D	2	0

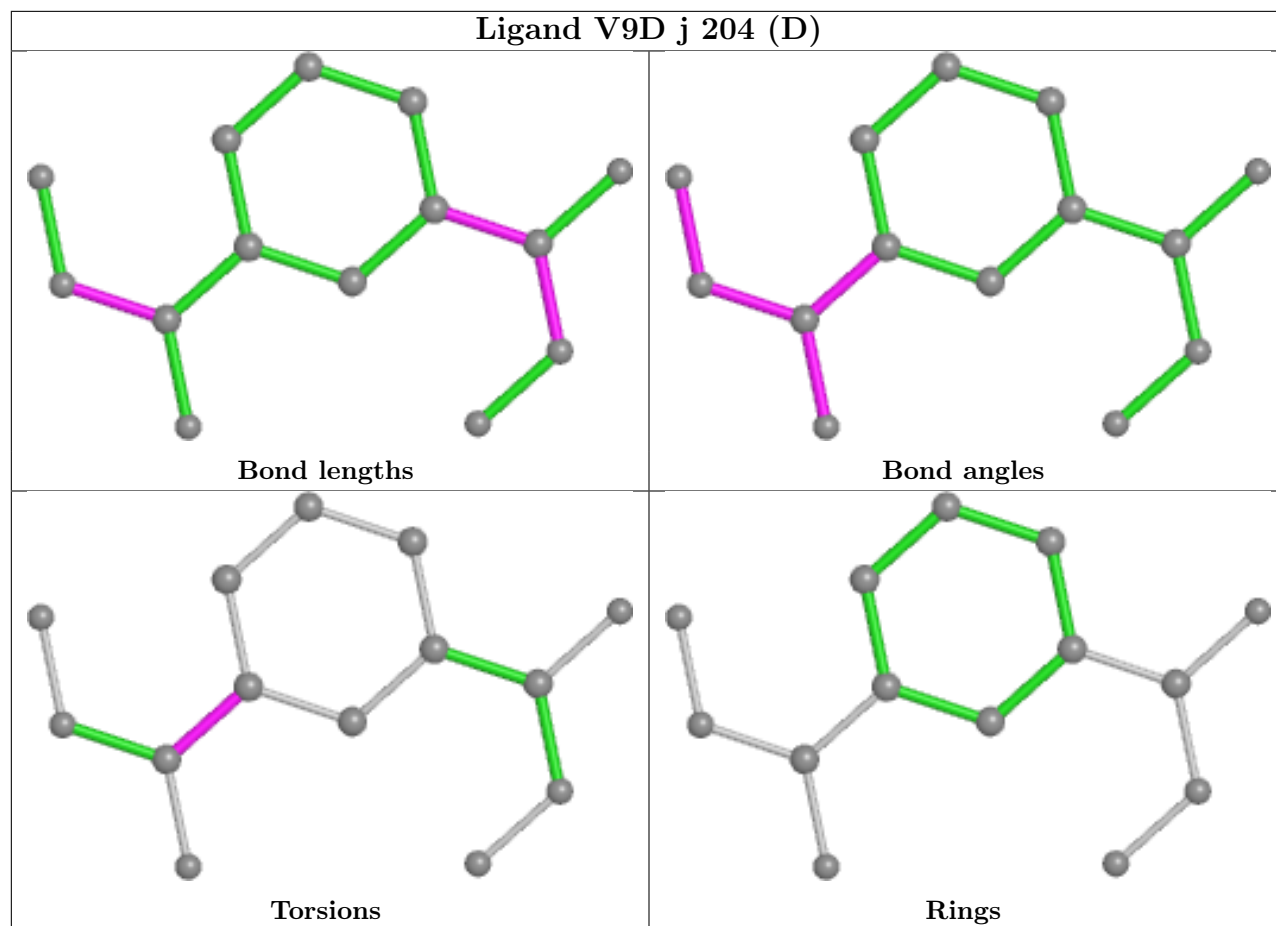
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

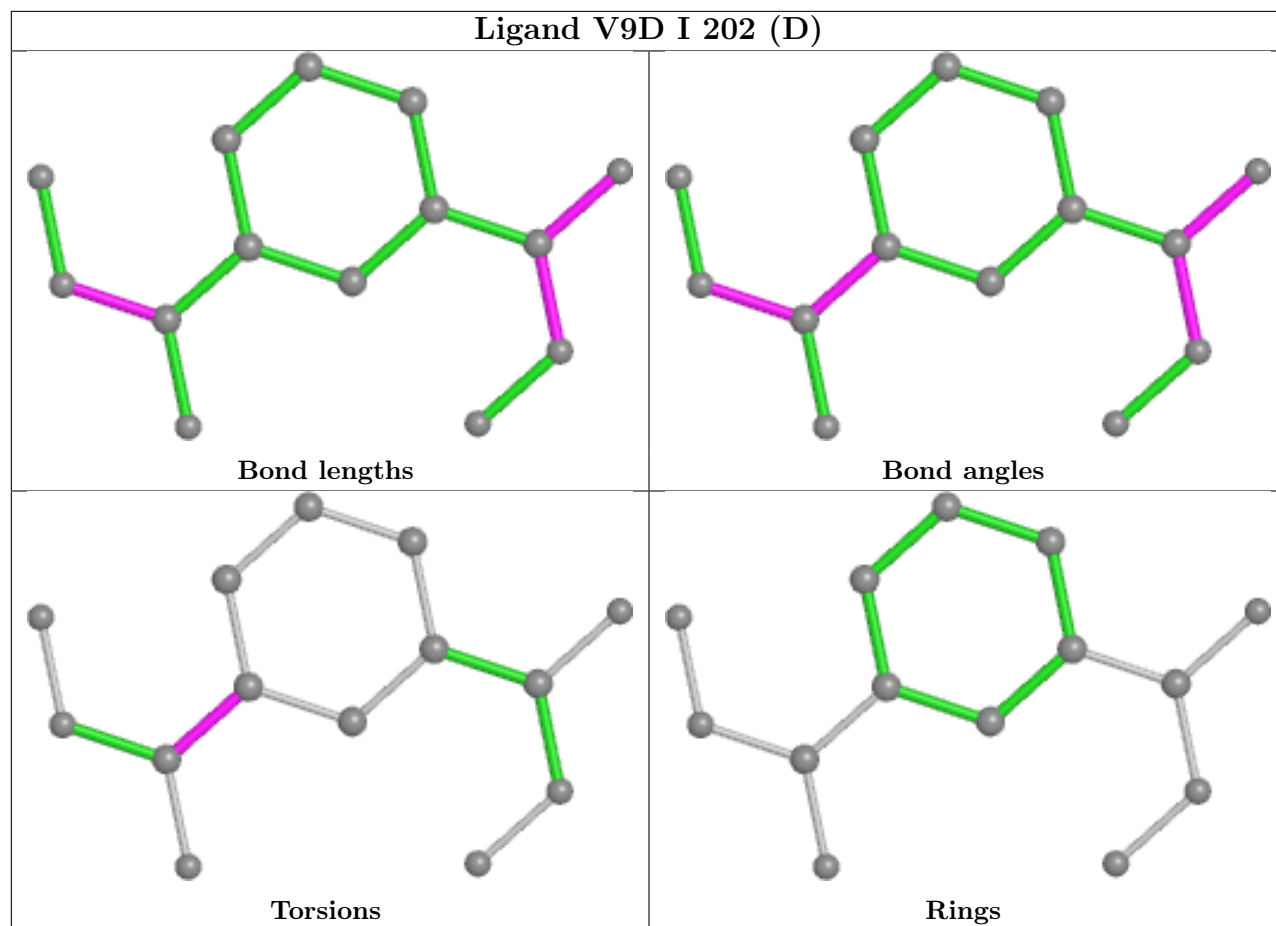


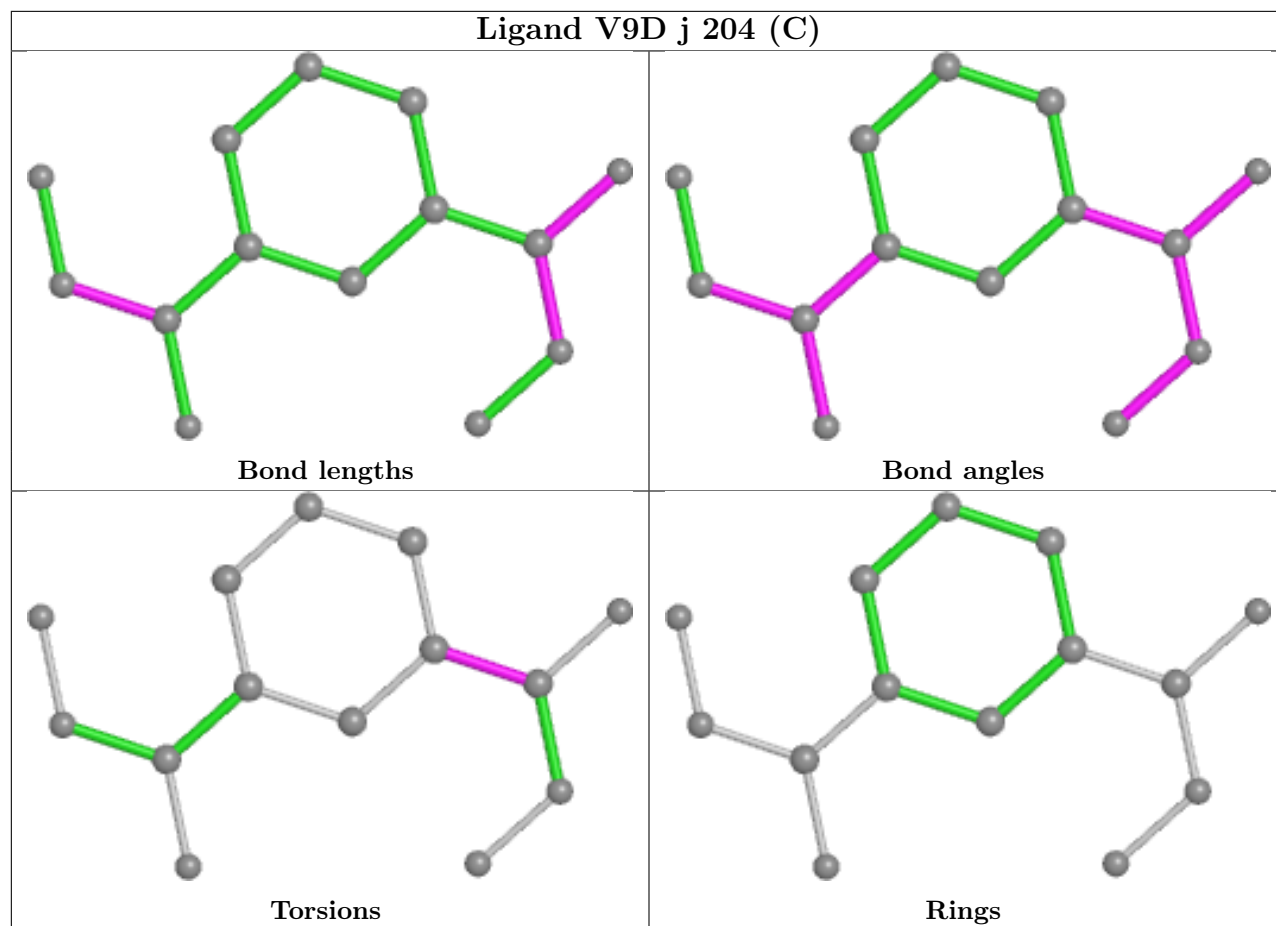


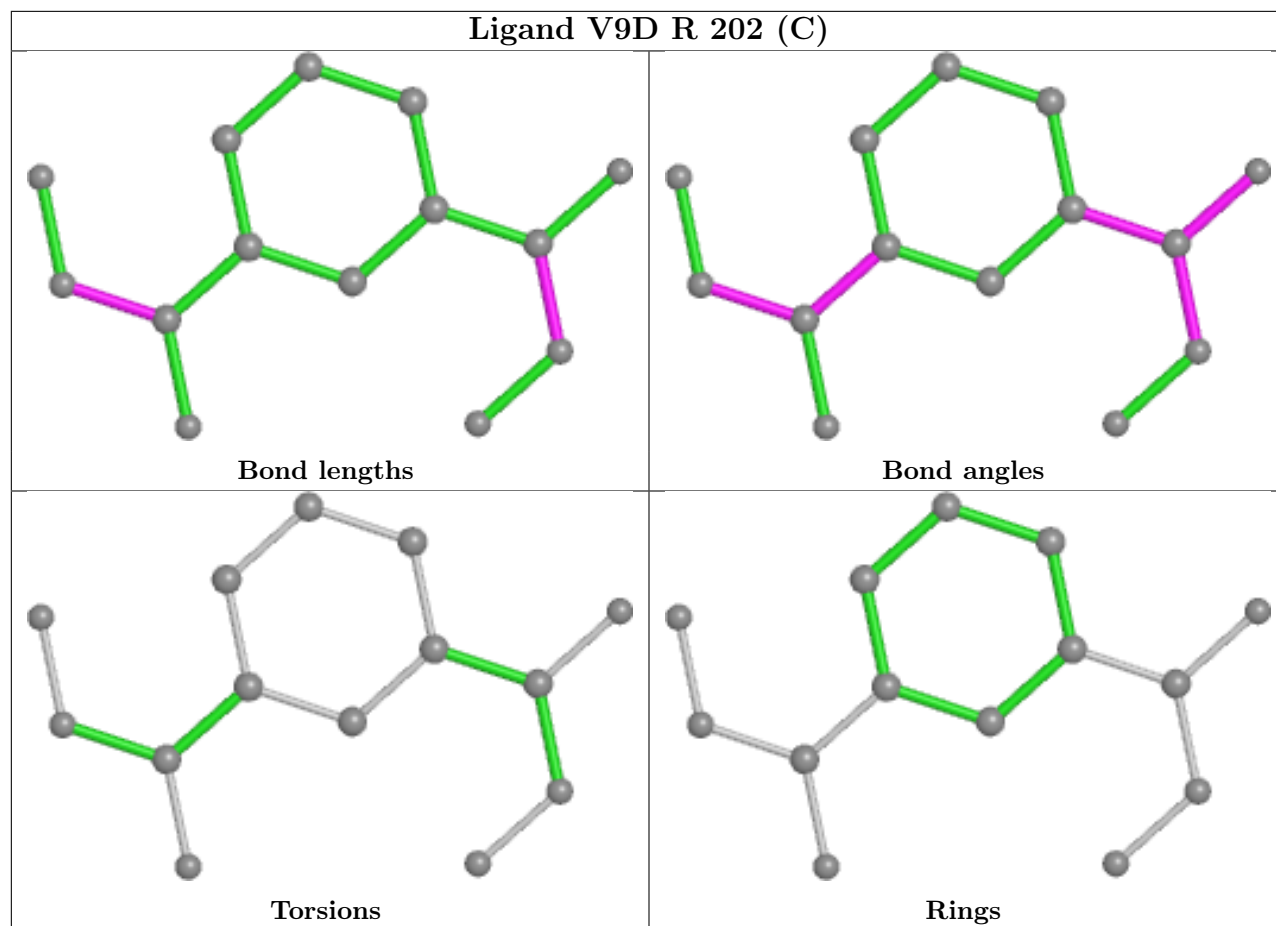
Ligand V9D F 203 (D)

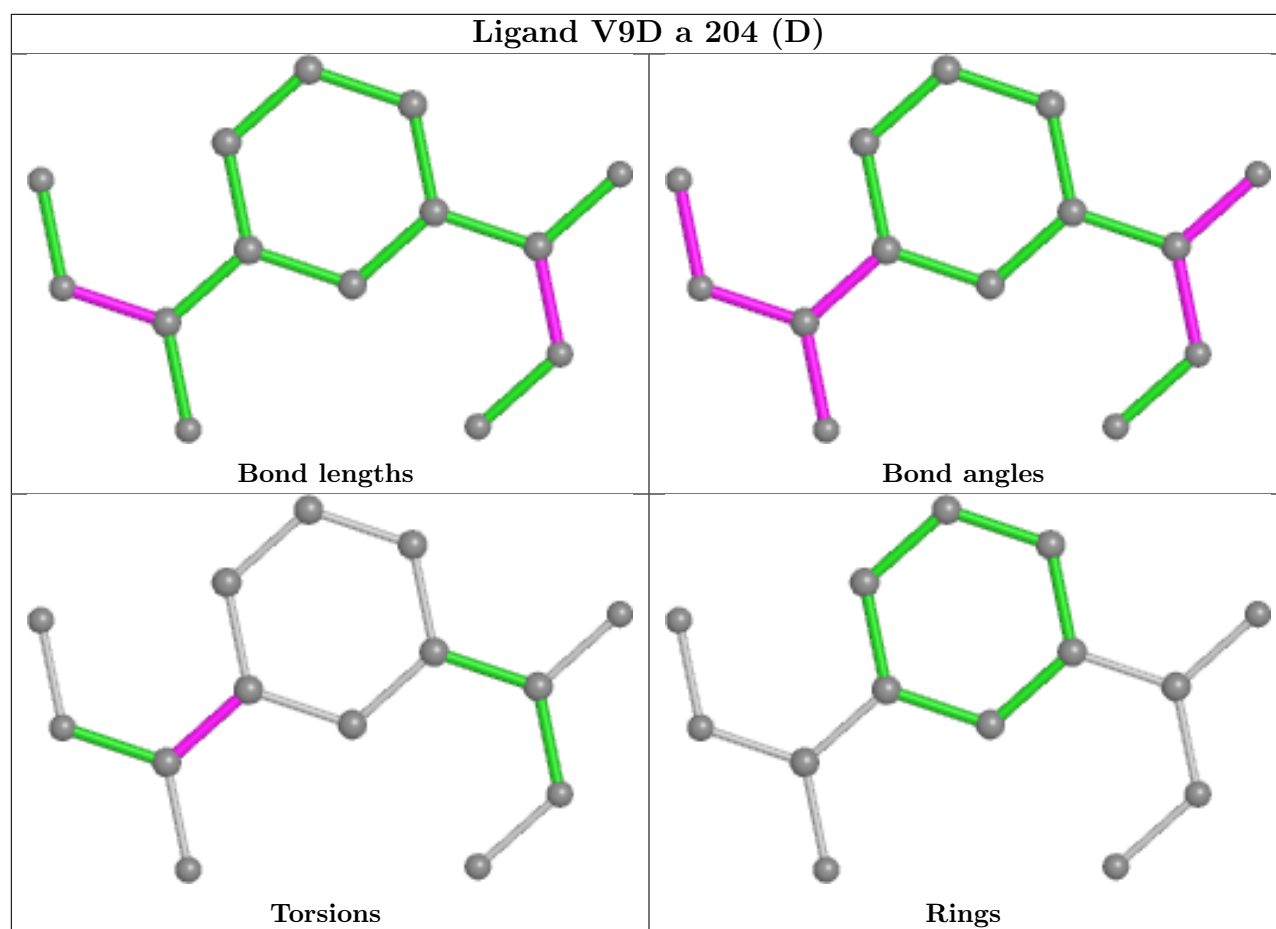


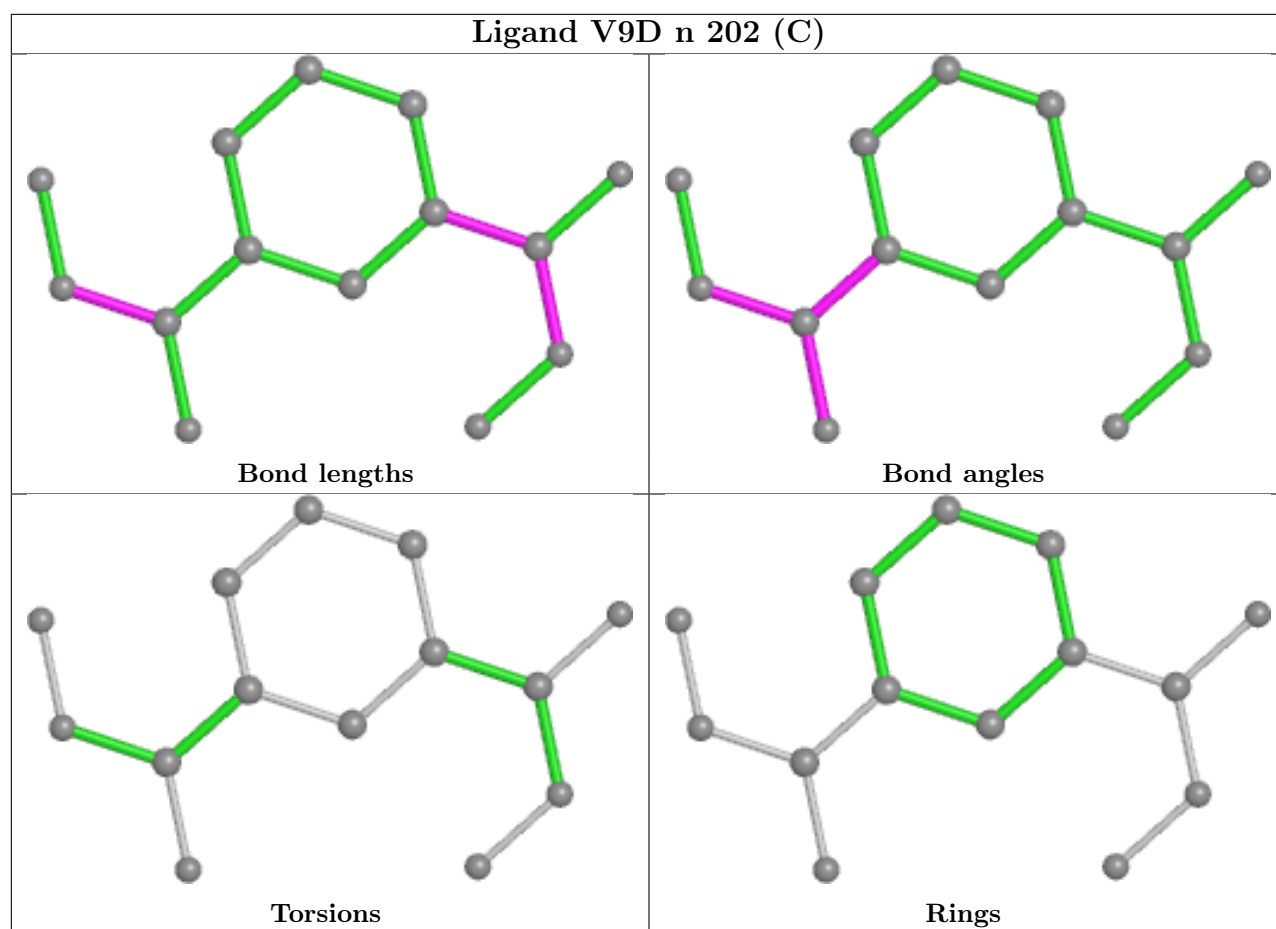


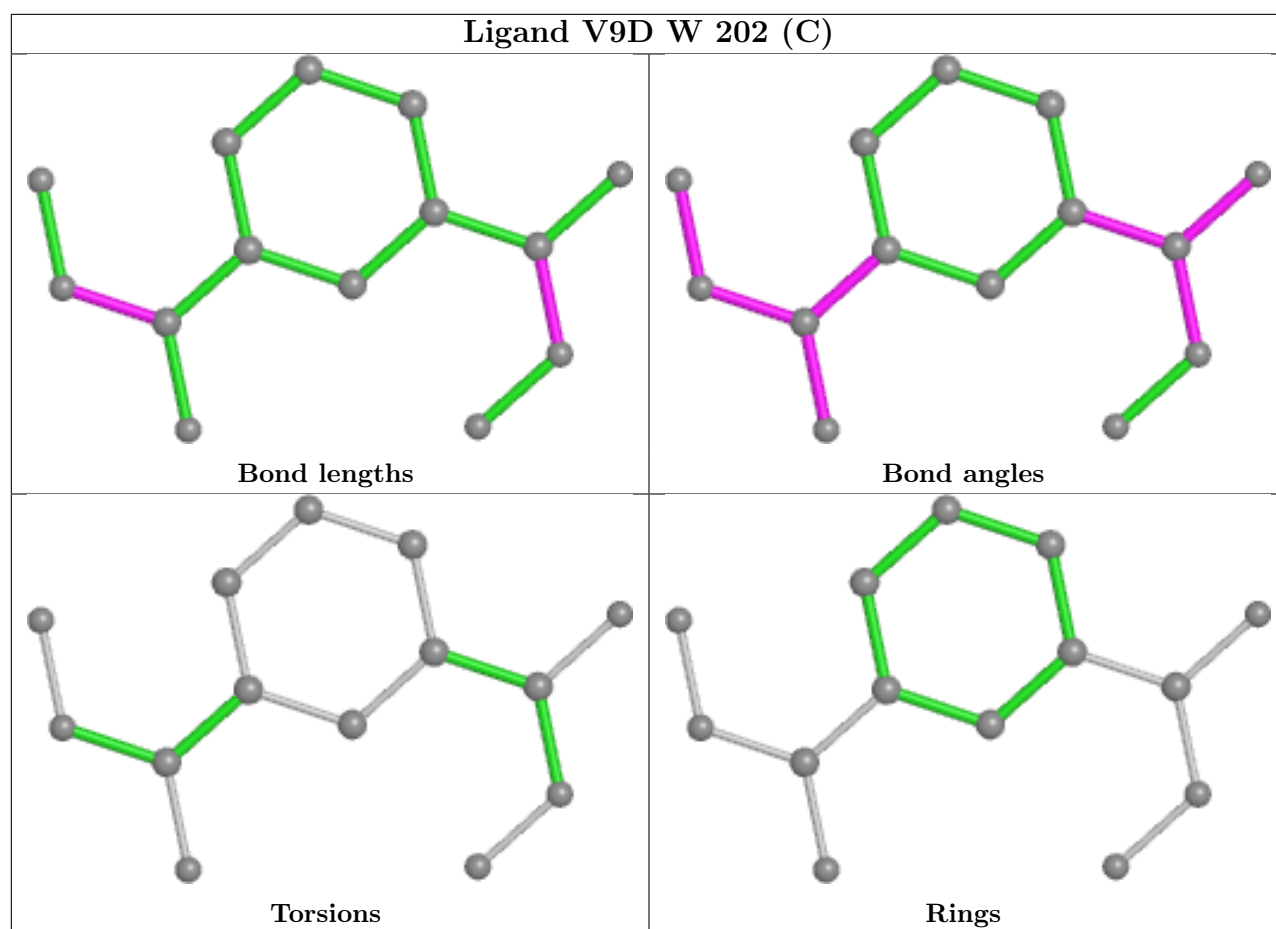


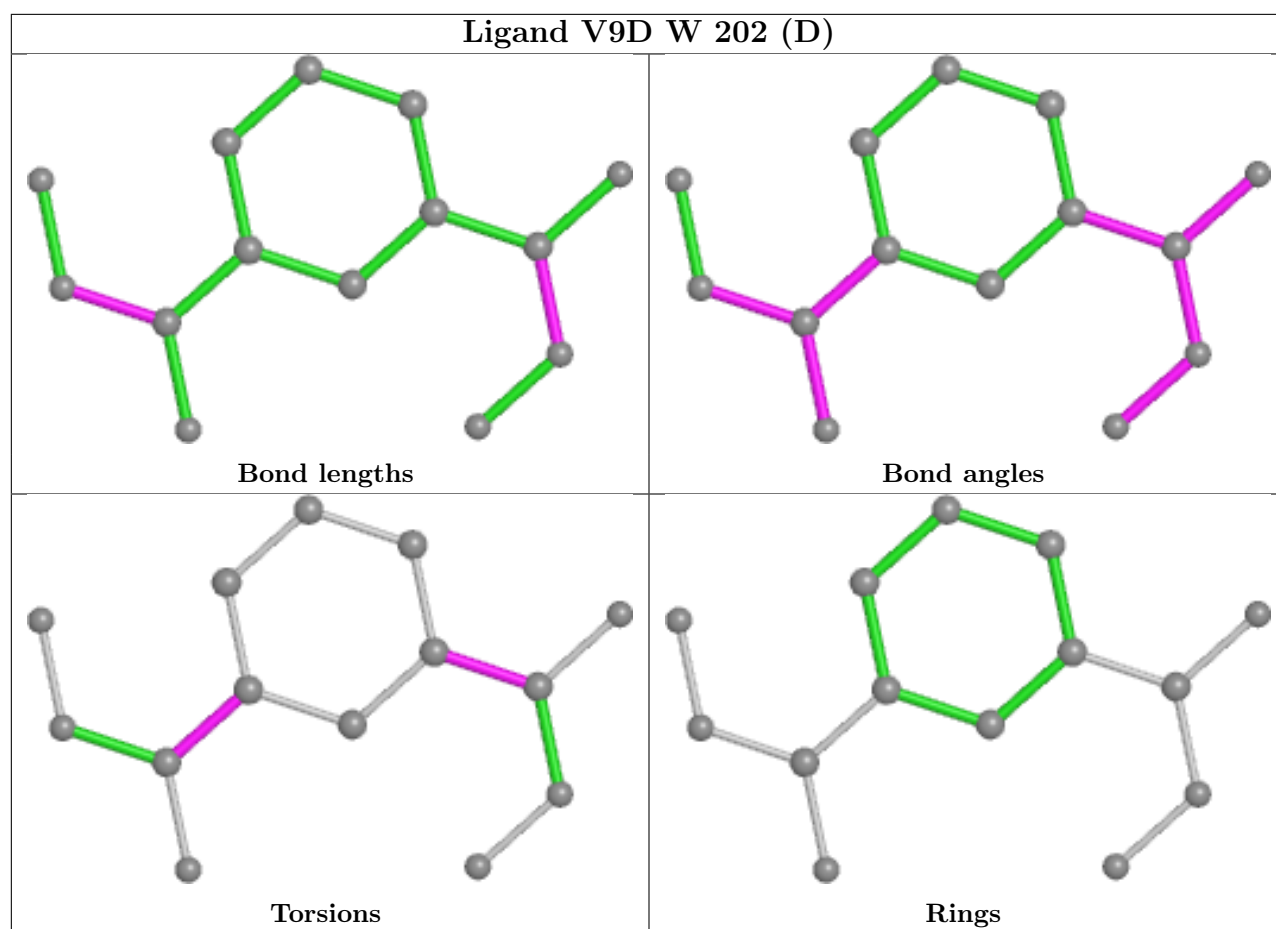


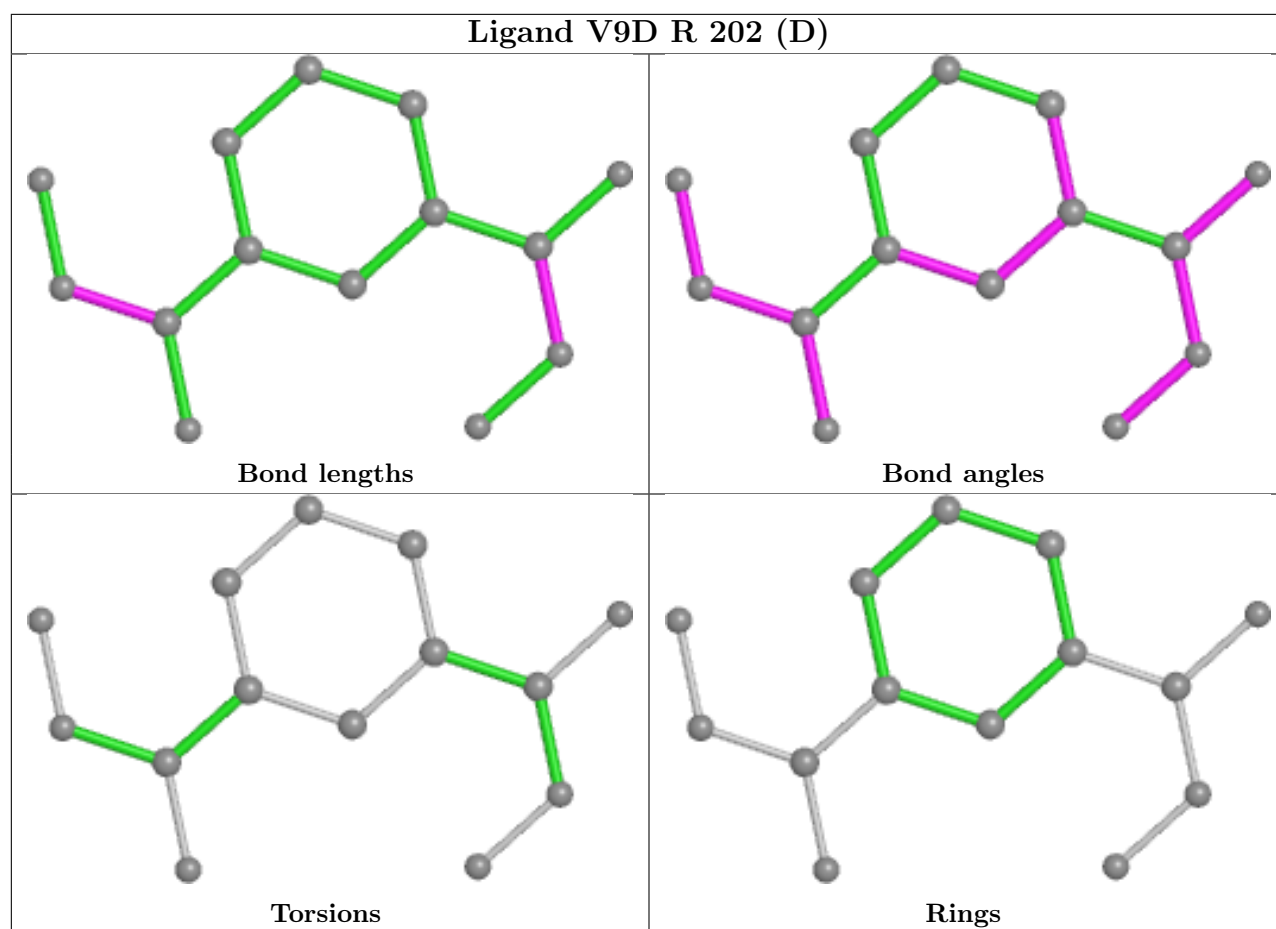


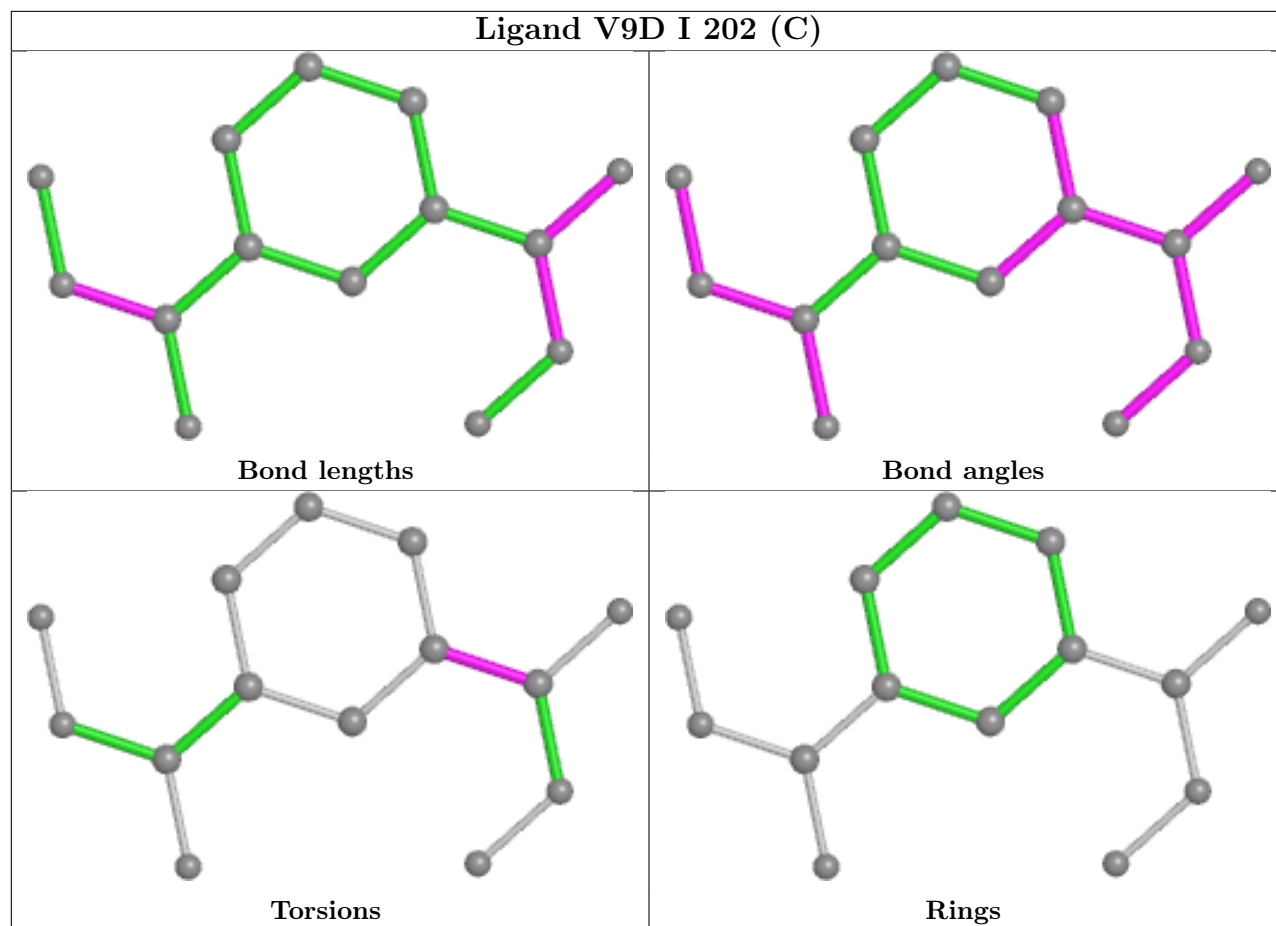


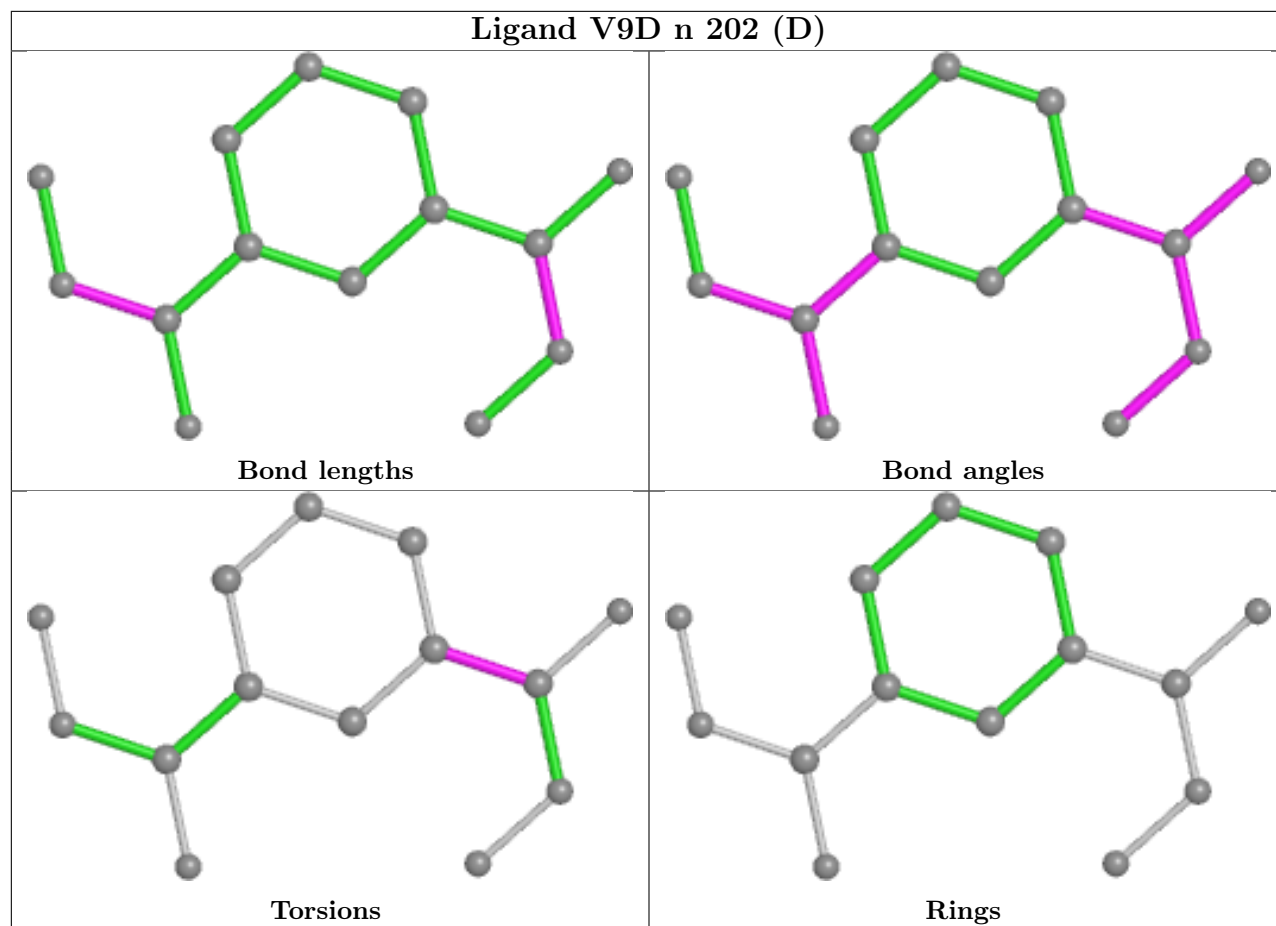




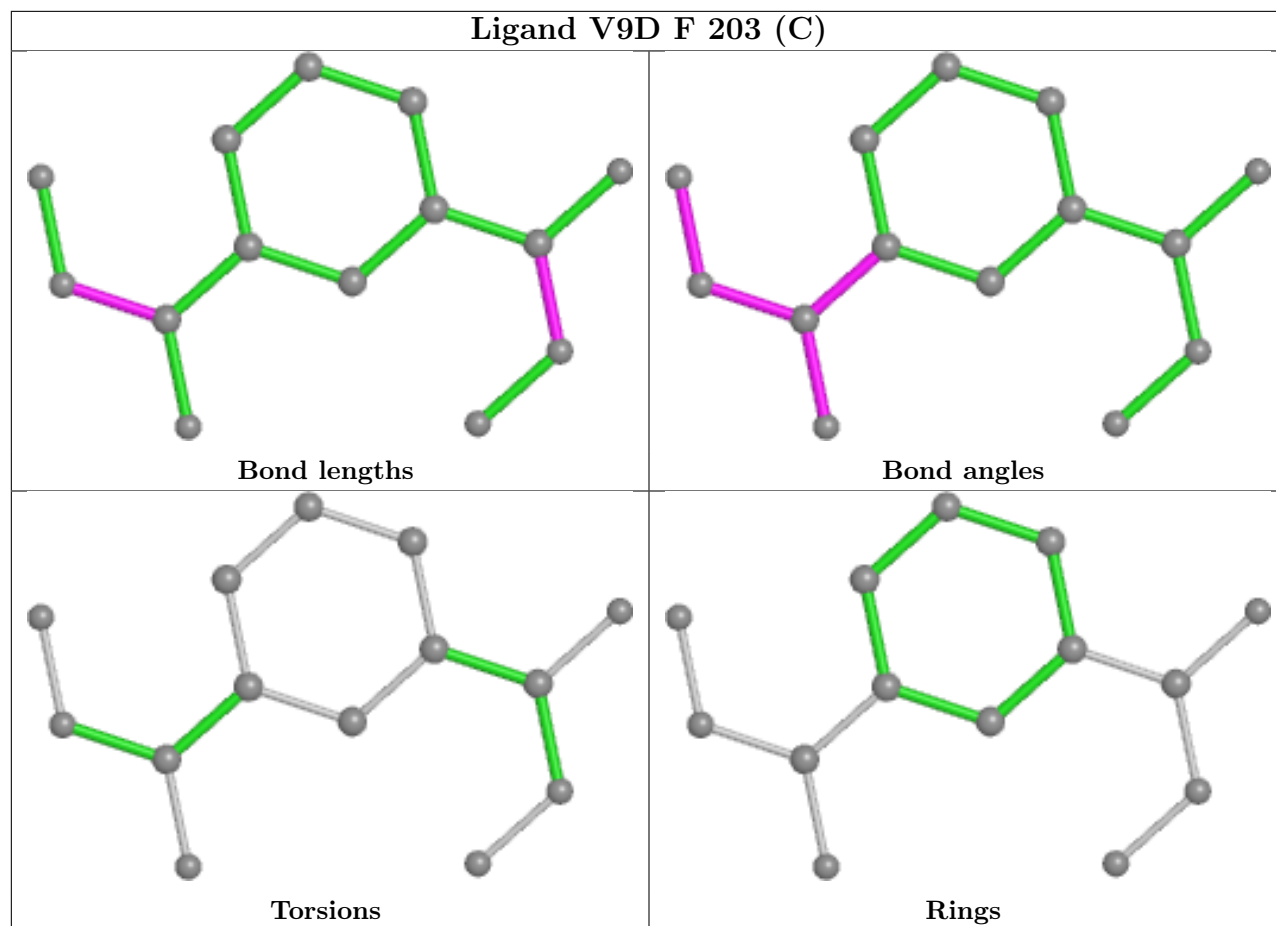


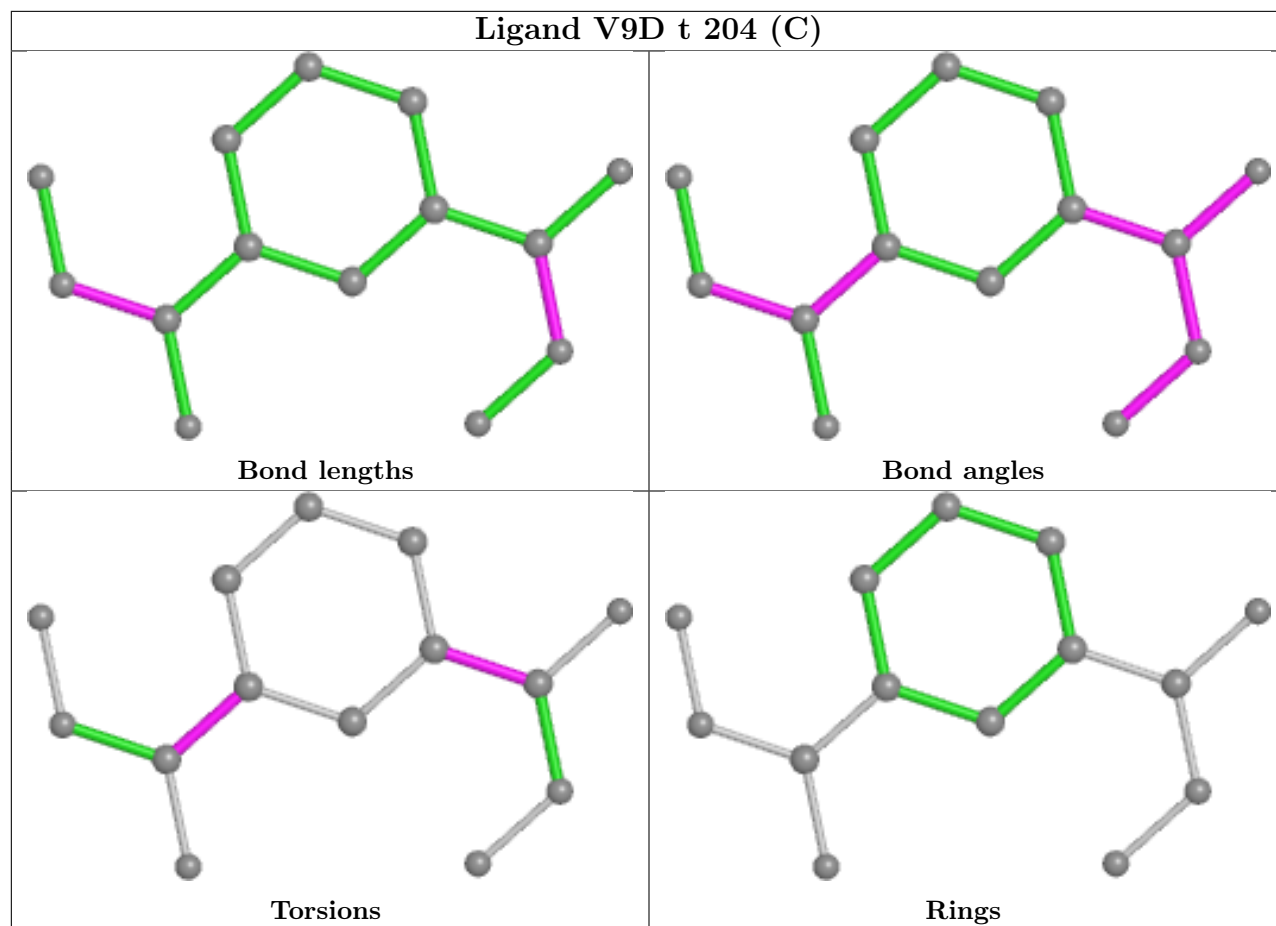






Ligand V9D F 203 (C)





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	174/182 (95%)	-0.62	1 (0%) 89 92	33, 42, 60, 89	0
1	B	174/182 (95%)	-0.66	3 (1%) 70 76	30, 39, 56, 93	0
1	C	174/182 (95%)	-0.62	1 (0%) 89 92	29, 42, 57, 90	0
1	D	174/182 (95%)	-0.70	2 (1%) 80 85	30, 37, 53, 87	0
1	E	174/182 (95%)	-0.70	2 (1%) 80 85	29, 36, 54, 88	0
1	F	174/182 (95%)	-0.81	2 (1%) 80 85	28, 36, 52, 92	0
1	G	174/182 (95%)	-0.83	0 100 100	28, 37, 53, 82	0
1	H	174/182 (95%)	-0.73	2 (1%) 80 85	27, 35, 54, 90	0
1	I	174/182 (95%)	-0.73	2 (1%) 80 85	28, 36, 52, 95	0
1	J	174/182 (95%)	-0.63	2 (1%) 80 85	34, 42, 61, 86	0
1	K	174/182 (95%)	-0.73	2 (1%) 80 85	30, 39, 57, 95	0
1	L	174/182 (95%)	-0.61	2 (1%) 80 85	30, 41, 56, 93	0
1	M	174/182 (95%)	-0.59	2 (1%) 80 85	32, 42, 60, 88	0
1	N	174/182 (95%)	-0.67	2 (1%) 80 85	30, 39, 55, 96	0
1	O	174/182 (95%)	-0.71	1 (0%) 89 92	31, 42, 56, 94	0
1	P	174/182 (95%)	-0.77	1 (0%) 89 92	28, 37, 55, 89	0
1	Q	174/182 (95%)	-0.79	2 (1%) 80 85	28, 36, 54, 88	0
1	R	174/182 (95%)	-0.74	2 (1%) 80 85	28, 36, 51, 97	0
1	S	174/182 (95%)	-0.66	2 (1%) 80 85	28, 37, 51, 87	0
1	T	174/182 (95%)	-0.67	2 (1%) 80 85	29, 36, 55, 91	0
1	U	174/182 (95%)	-0.69	2 (1%) 80 85	28, 36, 53, 93	0
1	V	174/182 (95%)	-0.72	2 (1%) 80 85	33, 43, 61, 88	0
1	W	174/182 (95%)	-0.62	3 (1%) 70 76	30, 39, 56, 91	0
1	X	174/182 (95%)	-0.65	2 (1%) 80 85	31, 42, 56, 90	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	a	174/182 (95%)	0.19	11 (6%) 20 26	30, 34, 44, 60	0
1	b	174/182 (95%)	0.20	6 (3%) 45 52	29, 35, 44, 63	0
1	c	174/182 (95%)	0.28	5 (2%) 51 59	31, 36, 45, 65	0
1	d	174/182 (95%)	0.15	6 (3%) 45 52	30, 34, 43, 65	0
1	e	174/182 (95%)	0.22	3 (1%) 70 76	31, 36, 46, 67	0
1	f	174/182 (95%)	0.27	6 (3%) 45 52	31, 36, 46, 62	0
1	g	174/182 (95%)	0.09	5 (2%) 51 59	30, 34, 42, 62	0
1	h	174/182 (95%)	0.17	5 (2%) 51 59	31, 35, 44, 62	0
1	i	174/182 (95%)	0.22	7 (4%) 38 45	30, 36, 45, 63	0
1	j	174/182 (95%)	0.21	8 (4%) 32 40	30, 34, 44, 59	0
1	k	174/182 (95%)	0.14	8 (4%) 32 40	30, 35, 44, 62	0
1	l	174/182 (95%)	0.21	4 (2%) 60 67	31, 36, 46, 68	0
1	m	174/182 (95%)	0.22	7 (4%) 38 45	32, 37, 46, 63	0
1	n	174/182 (95%)	0.14	7 (4%) 38 45	30, 34, 44, 60	0
1	o	174/182 (95%)	0.16	5 (2%) 51 59	29, 35, 44, 65	0
1	p	174/182 (95%)	0.18	6 (3%) 45 52	31, 37, 48, 71	0
1	q	174/182 (95%)	0.18	7 (4%) 38 45	30, 34, 44, 62	0
1	r	174/182 (95%)	0.23	8 (4%) 32 40	31, 36, 46, 64	0
1	s	174/182 (95%)	0.21	8 (4%) 32 40	32, 36, 46, 61	0
1	t	174/182 (95%)	0.16	6 (3%) 45 52	31, 34, 43, 61	0
1	u	174/182 (95%)	0.25	4 (2%) 60 67	31, 35, 44, 67	0
1	v	174/182 (95%)	0.24	4 (2%) 60 67	32, 37, 47, 62	0
1	w	174/182 (95%)	0.11	8 (4%) 32 40	30, 35, 43, 61	0
1	x	174/182 (95%)	0.18	8 (4%) 32 40	30, 35, 43, 66	0
All	All	8352/8736 (95%)	-0.25	196 (2%) 60 67	27, 36, 53, 97	0

The worst 5 of 196 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	i	4[C]	SER	7.4
1	f	4[C]	SER	7.4
1	N	4	SER	7.1
1	r	4[C]	SER	7.0
1	d	177[C]	ASP	6.7

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	NI	l	201[C]	1/1	0.87	0.09	48,48,48,48	1
2	NI	l	201[D]	1/1	0.87	0.09	48,48,48,48	1
3	NA	j	203[C]	1/1	0.88	0.13	37,37,37,37	1
3	NA	j	203[D]	1/1	0.88	0.13	38,38,38,38	1
3	NA	V	202	1/1	0.90	0.24	51,51,51,51	0
2	NI	g	202[D]	1/1	0.91	0.05	44,44,44,44	1
2	NI	g	202[C]	1/1	0.91	0.05	48,48,48,48	1
2	NI	u	201[C]	1/1	0.92	0.09	50,50,50,50	1
2	NI	u	201[D]	1/1	0.92	0.09	44,44,44,44	1
3	NA	a	203[D]	1/1	0.92	0.17	36,36,36,36	1
3	NA	a	203[C]	1/1	0.92	0.17	36,36,36,36	1
3	NA	S	203	1/1	0.93	0.28	56,56,56,56	0
3	NA	D	203	1/1	0.93	0.26	54,54,54,54	0
2	NI	d	202[C]	1/1	0.93	0.04	50,50,50,50	1
2	NI	f	201[D]	1/1	0.93	0.09	45,45,45,45	1
2	NI	f	201[C]	1/1	0.93	0.09	43,43,43,43	1
2	NI	d	202[D]	1/1	0.93	0.04	41,41,41,41	1
2	NI	c	201[C]	1/1	0.94	0.07	49,49,49,49	1
4	V9D	R	202[D]	14/14	0.94	0.19	48,54,60,64	14
4	V9D	F	203[C]	14/14	0.94	0.20	41,53,59,60	14
4	V9D	F	203[D]	14/14	0.94	0.20	41,47,50,54	14
4	V9D	R	202[C]	14/14	0.94	0.19	44,48,54,55	14
2	NI	v	201[C]	1/1	0.94	0.08	48,48,48,48	1
2	NI	v	201[D]	1/1	0.94	0.08	50,50,50,50	1
4	V9D	a	204[D]	14/14	0.94	0.18	43,45,54,61	14
4	V9D	a	204[C]	14/14	0.94	0.18	49,53,62,63	14
2	NI	c	201[D]	1/1	0.94	0.07	53,53,53,53	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NI	h	201[D]	1/1	0.95	0.06	51,51,51,51	1
4	V9D	j	204[D]	14/14	0.95	0.16	42,45,50,56	14
4	V9D	t	204[C]	14/14	0.95	0.18	40,46,49,50	14
4	V9D	I	202[D]	14/14	0.95	0.16	41,45,52,52	14
4	V9D	t	204[D]	14/14	0.95	0.18	46,55,59,60	14
4	V9D	j	204[C]	14/14	0.95	0.16	51,54,59,62	14
4	V9D	I	202[C]	14/14	0.95	0.16	44,53,59,60	14
2	NI	h	201[C]	1/1	0.95	0.06	44,44,44,44	1
3	NA	p	203[D]	1/1	0.95	0.14	40,40,40,40	1
3	NA	p	203[C]	1/1	0.95	0.14	40,40,40,40	1
2	NI	e	201[C]	1/1	0.95	0.07	41,41,41,41	1
3	NA	P	203	1/1	0.95	0.30	54,54,54,54	0
2	NI	e	201[D]	1/1	0.95	0.07	53,53,53,53	1
2	NI	a	202[C]	1/1	0.96	0.07	45,45,45,45	1
3	NA	v	204[C]	1/1	0.96	0.16	39,39,39,39	1
2	NI	m	202[C]	1/1	0.96	0.06	43,43,43,43	1
2	NI	m	202[D]	1/1	0.96	0.06	48,48,48,48	1
2	NI	p	201[C]	1/1	0.96	0.04	48,48,48,48	1
3	NA	J	202	1/1	0.96	0.18	44,44,44,44	0
2	NI	p	201[D]	1/1	0.96	0.04	44,44,44,44	1
4	V9D	n	202[C]	14/14	0.96	0.16	41,47,52,60	14
2	NI	w	201[C]	1/1	0.96	0.04	45,45,45,45	1
2	NI	w	201[D]	1/1	0.96	0.04	41,41,41,41	1
3	NA	g	203[C]	1/1	0.96	0.17	39,39,39,39	1
4	V9D	W	202[D]	14/14	0.96	0.15	48,54,60,62	14
3	NA	g	203[D]	1/1	0.96	0.17	39,39,39,39	1
4	V9D	W	202[C]	14/14	0.96	0.15	41,46,51,54	14
3	NA	v	204[D]	1/1	0.96	0.16	42,42,42,42	1
4	V9D	n	202[D]	14/14	0.96	0.16	48,55,60,64	14
2	NI	a	202[D]	1/1	0.96	0.07	47,47,47,47	1
2	NI	m	201[C]	1/1	0.97	0.05	51,51,51,51	1
2	NI	r	201[C]	1/1	0.97	0.07	49,49,49,49	1
2	NI	b	201[D]	1/1	0.97	0.04	44,44,44,44	1
2	NI	b	201[C]	1/1	0.97	0.04	41,41,41,41	1
3	NA	M	203	1/1	0.97	0.21	49,49,49,49	0
2	NI	B	201	1/1	0.97	0.06	53,53,53,53	0
3	NA	m	203[C]	1/1	0.97	0.15	37,37,37,37	1
2	NI	p	202[D]	1/1	0.97	0.03	53,53,53,53	1
2	NI	v	202[C]	1/1	0.97	0.07	47,47,47,47	1
3	NA	m	203[D]	1/1	0.97	0.15	37,37,37,37	1
2	NI	v	202[D]	1/1	0.97	0.07	47,47,47,47	1
3	NA	d	204[C]	1/1	0.97	0.13	39,39,39,39	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NA	d	204[D]	1/1	0.97	0.13	39,39,39,39	1
2	NI	m	201[D]	1/1	0.97	0.05	49,49,49,49	1
2	NI	p	202[C]	1/1	0.97	0.03	44,44,44,44	1
2	NI	r	201[D]	1/1	0.97	0.07	44,44,44,44	1
2	NI	P	202	1/1	0.98	0.05	47,47,47,47	0
3	NA	t	203[D]	1/1	0.98	0.15	37,37,37,37	1
2	NI	i	201[D]	1/1	0.98	0.05	46,46,46,46	1
2	NI	j	202[C]	1/1	0.98	0.06	47,47,47,47	1
2	NI	j	202[D]	1/1	0.98	0.06	46,46,46,46	1
2	NI	w	202[D]	1/1	0.98	0.14	30,30,30,30	1
2	NI	w	202[C]	1/1	0.98	0.14	56,56,56,56	1
3	NA	t	203[C]	1/1	0.98	0.15	41,41,41,41	1
2	NI	g	201[C]	1/1	0.98	0.06	39,39,39,39	1
2	NI	M	202	1/1	0.98	0.05	50,50,50,50	0
2	NI	O	202	1/1	0.98	0.12	34,34,34,34	1
2	NI	j	201[D]	1/1	0.98	0.07	77,77,77,77	1
2	NI	s	201[D]	1/1	0.98	0.05	44,44,44,44	1
2	NI	g	201[D]	1/1	0.98	0.06	73,73,73,73	1
2	NI	k	201[C]	1/1	0.98	0.04	44,44,44,44	1
2	NI	n	201[C]	1/1	0.98	0.04	44,44,44,44	1
2	NI	o	201[C]	1/1	0.98	0.04	46,46,46,46	1
2	NI	d	203[D]	1/1	0.98	0.08	35,35,35,35	1
2	NI	o	201[D]	1/1	0.98	0.04	42,42,42,42	1
2	NI	n	201[D]	1/1	0.98	0.04	43,43,43,43	1
2	NI	d	203[C]	1/1	0.98	0.08	27,27,27,27	1
2	NI	a	201[C]	1/1	0.98	0.04	40,40,40,40	1
2	NI	v	203[D]	1/1	0.98	0.24	78,78,78,78	1
2	NI	k	201[D]	1/1	0.98	0.04	45,45,45,45	1
2	NI	a	201[D]	1/1	0.98	0.04	47,47,47,47	1
2	NI	D	202	1/1	0.98	0.05	46,46,46,46	0
2	NI	s	201[C]	1/1	0.98	0.05	45,45,45,45	1
2	NI	j	201[C]	1/1	0.98	0.07	39,39,39,39	1
2	NI	x	201[D]	1/1	0.98	0.04	41,41,41,41	1
2	NI	O	201	1/1	0.98	0.09	55,55,55,55	0
2	NI	e	202[C]	1/1	0.98	0.10	31,31,31,31	1
2	NI	S	202	1/1	0.98	0.05	46,46,46,46	0
2	NI	t	202[C]	1/1	0.98	0.04	46,46,46,46	1
2	NI	x	201[C]	1/1	0.98	0.04	44,44,44,44	1
2	NI	x	202[D]	1/1	0.98	0.07	27,27,27,27	1
3	NA	A	203	1/1	0.98	0.17	42,42,42,42	0
2	NI	x	202[C]	1/1	0.98	0.07	28,28,28,28	1
2	NI	i	201[C]	1/1	0.98	0.05	42,42,42,42	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NI	t	202[D]	1/1	0.98	0.04	52,52,52,52	1
3	NA	G	203	1/1	0.98	0.29	49,49,49,49	0
2	NI	e	202[D]	1/1	0.98	0.10	32,32,32,32	1
2	NI	v	203[C]	1/1	0.98	0.24	15,15,15,15	1
2	NI	d	201[D]	1/1	0.99	0.04	44,44,44,44	1
2	NI	G	202	1/1	0.99	0.04	45,45,45,45	0
2	NI	X	202	1/1	0.99	0.06	51,51,51,51	0
2	NI	H	202	1/1	0.99	0.10	32,32,32,32	1
2	NI	W	201	1/1	0.99	0.06	53,53,53,53	0
2	NI	F	202	1/1	0.99	0.12	32,32,32,32	1
2	NI	D	201	1/1	0.99	0.05	50,50,50,50	0
2	NI	d	201[C]	1/1	0.99	0.04	40,40,40,40	1
2	NI	C	201	1/1	0.99	0.03	50,50,50,50	0
2	NI	S	201	1/1	0.99	0.09	50,50,50,50	0
2	NI	L	202	1/1	0.99	0.04	54,54,54,54	0
2	NI	N	201	1/1	0.99	0.05	52,52,52,52	0
2	NI	H	201	1/1	0.99	0.06	47,47,47,47	0
2	NI	q	201[C]	1/1	0.99	0.05	46,46,46,46	1
2	NI	t	201[D]	1/1	0.99	0.04	41,41,41,41	1
2	NI	P	201	1/1	0.99	0.05	54,54,54,54	0
2	NI	t	201[C]	1/1	0.99	0.04	45,45,45,45	1
2	NI	J	201	1/1	0.99	0.07	52,52,52,52	0
2	NI	A	201	1/1	0.99	0.04	52,52,52,52	0
2	NI	F	201	1/1	0.99	0.03	48,48,48,48	0
2	NI	q	201[D]	1/1	0.99	0.05	44,44,44,44	1
2	NI	L	201	1/1	0.99	0.08	53,53,53,53	0
2	NI	I	201	1/1	0.99	0.06	48,48,48,48	0
2	NI	B	203	1/1	0.99	0.07	29,29,29,29	1
2	NI	f	202[D]	1/1	0.99	0.18	30,30,30,30	1
2	NI	T	201	1/1	0.99	0.06	50,50,50,50	0
2	NI	A	202	1/1	0.99	0.06	37,37,37,37	1
2	NI	f	202[C]	1/1	0.99	0.18	11,11,11,11	1
2	NI	B	202	1/1	0.99	0.05	50,50,50,50	0
2	NI	U	201	1/1	0.99	0.05	48,48,48,48	0
2	NI	V	201	1/1	0.99	0.07	55,55,55,55	0
2	NI	X	201	1/1	0.99	0.04	54,54,54,54	0
2	NI	K	201	1/1	1.00	0.04	49,49,49,49	0
2	NI	E	201	1/1	1.00	0.06	48,48,48,48	0
2	NI	C	202	1/1	1.00	0.07	27,27,27,27	1
2	NI	Q	201	1/1	1.00	0.07	51,51,51,51	0
2	NI	G	201	1/1	1.00	0.06	49,49,49,49	0
2	NI	M	201	1/1	1.00	0.05	51,51,51,51	0

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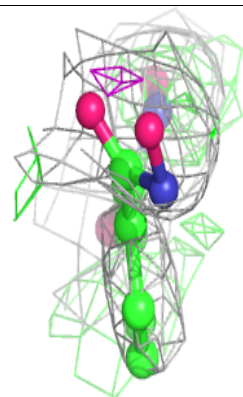
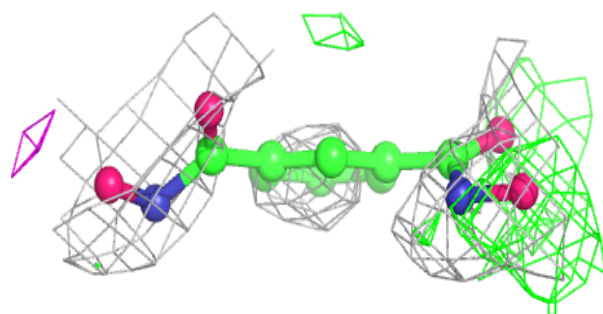
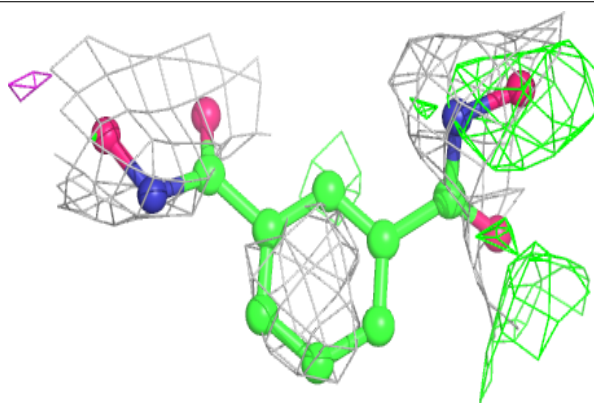
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NI	R	201	1/1	1.00	0.04	48,48,48,48	0

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.

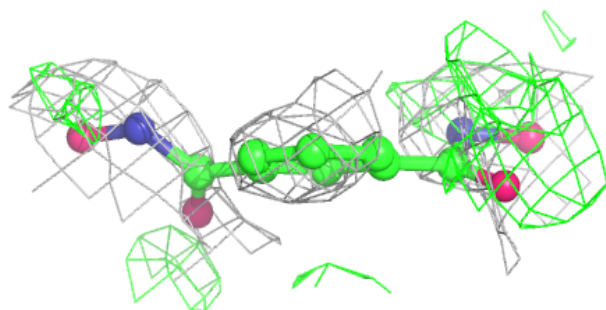
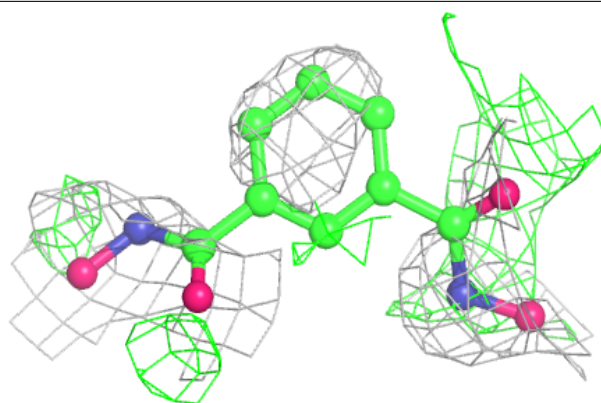
Electron density around V9D R 202 (D):

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

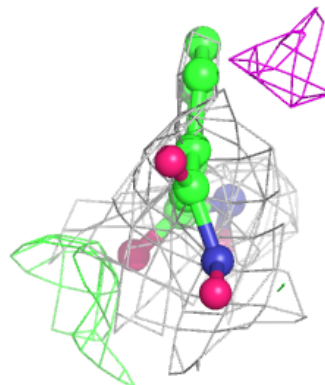
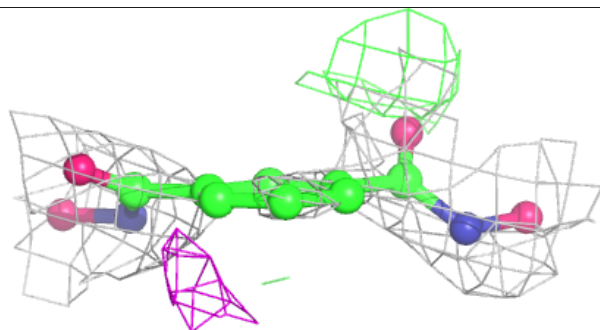
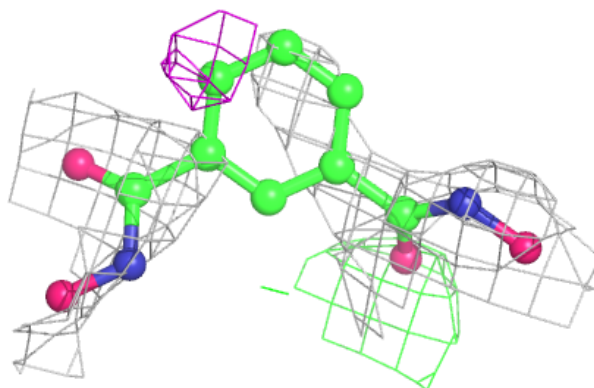


Electron density around V9D F 203 (C):

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

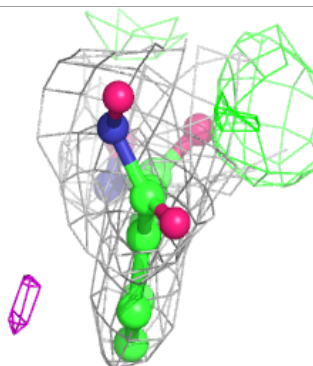
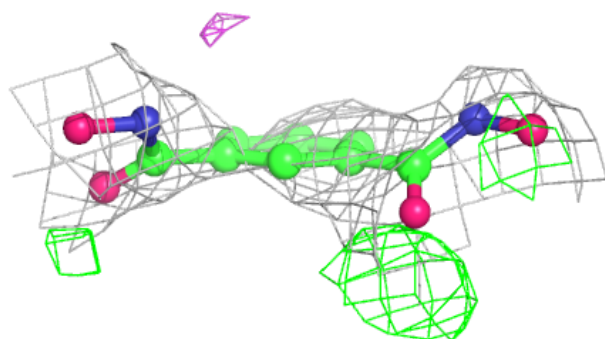
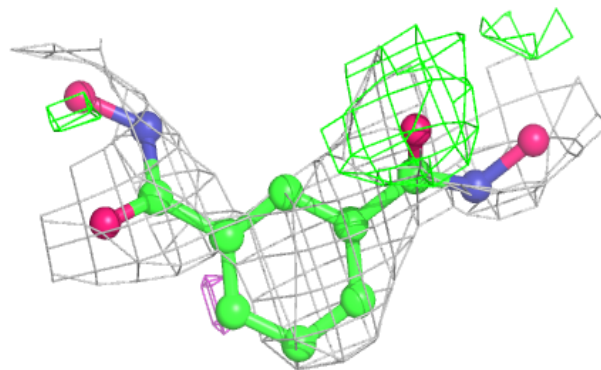
**Electron density around V9D F 203 (D):**

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

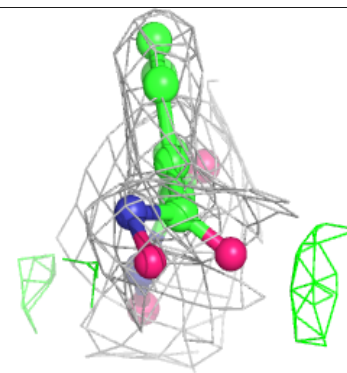
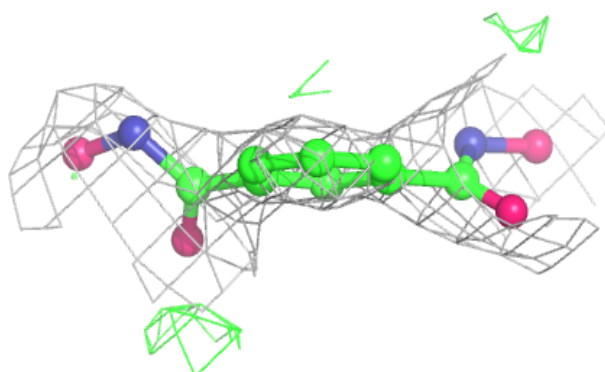
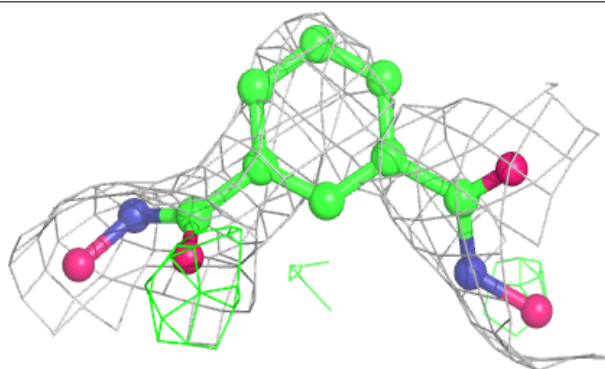


Electron density around V9D R 202 (C):

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

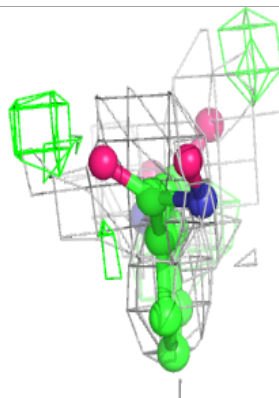
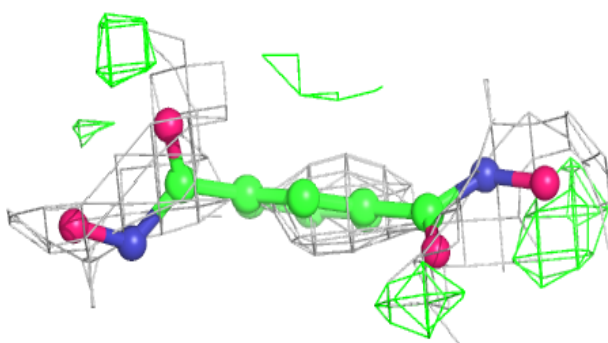
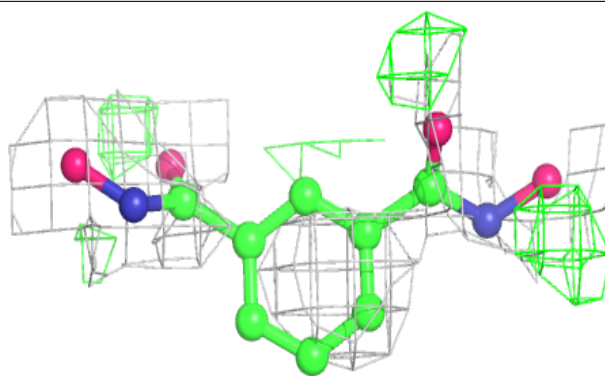
**Electron density around V9D a 204 (D):**

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

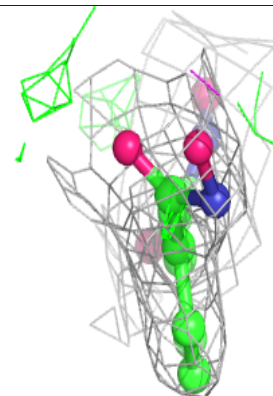
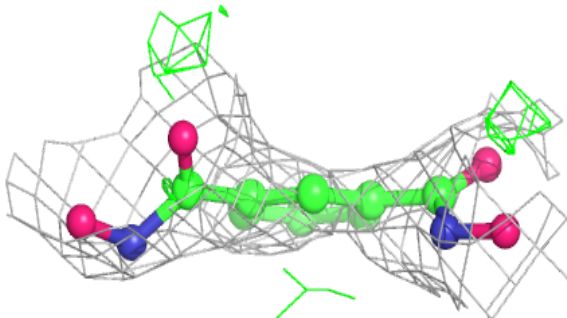
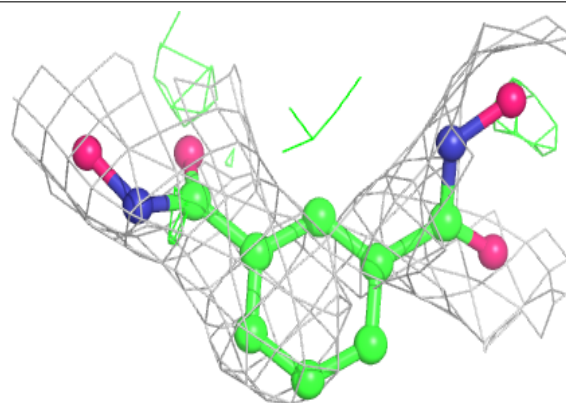


Electron density around V9D a 204 (C):

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

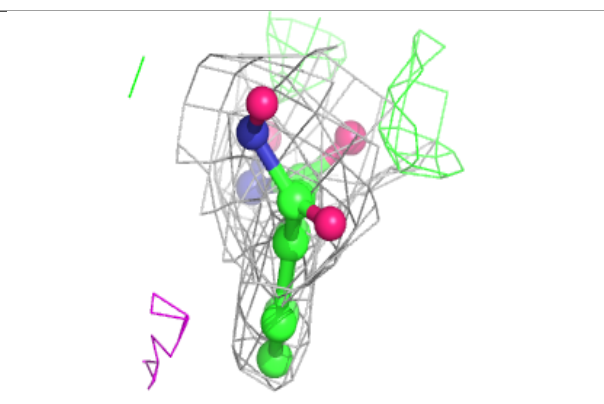
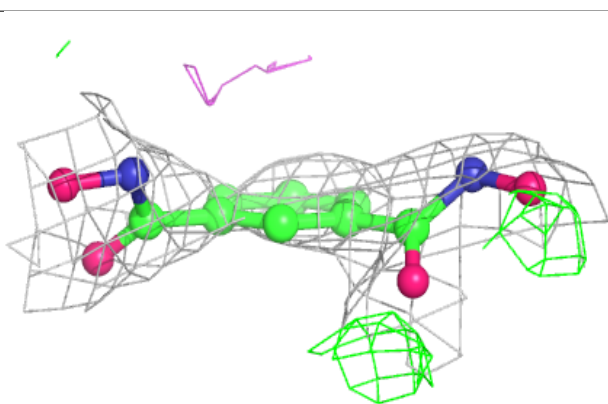
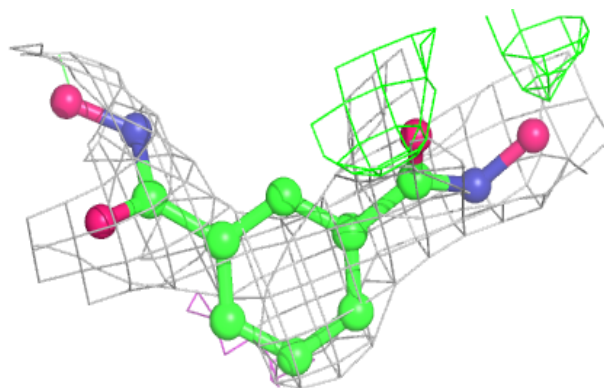
**Electron density around V9D j 204 (D):**

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

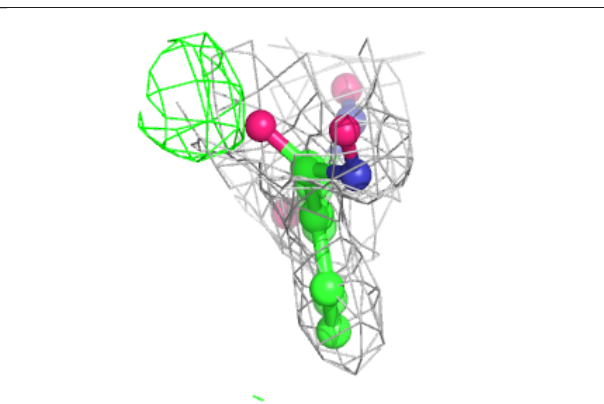
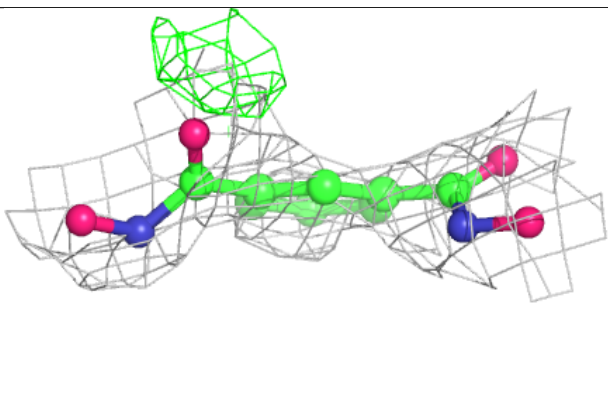
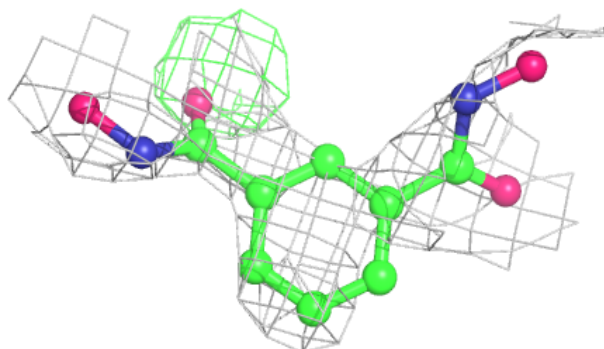


Electron density around V9D t 204 (C):

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

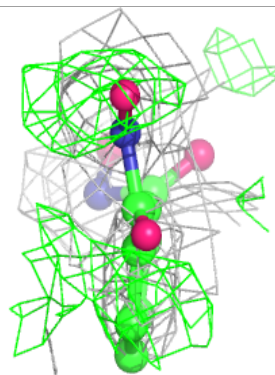
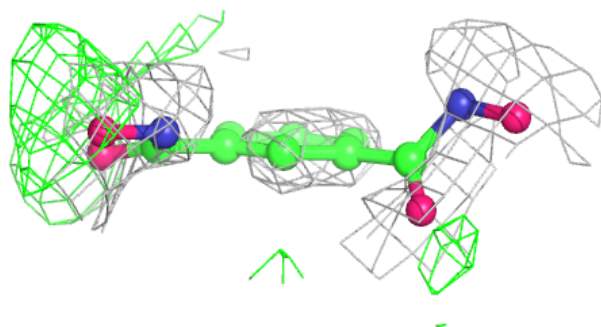
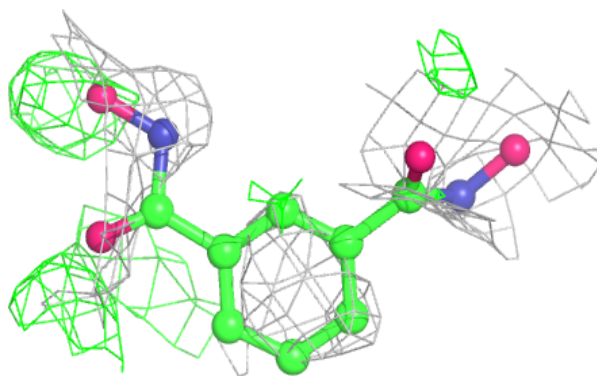
**Electron density around V9D I 202 (D):**

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

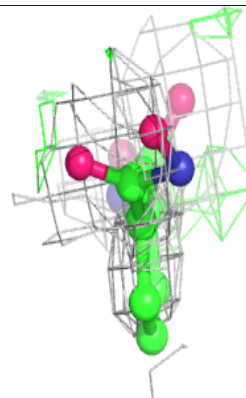
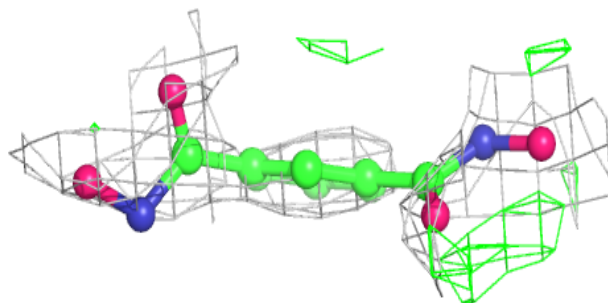
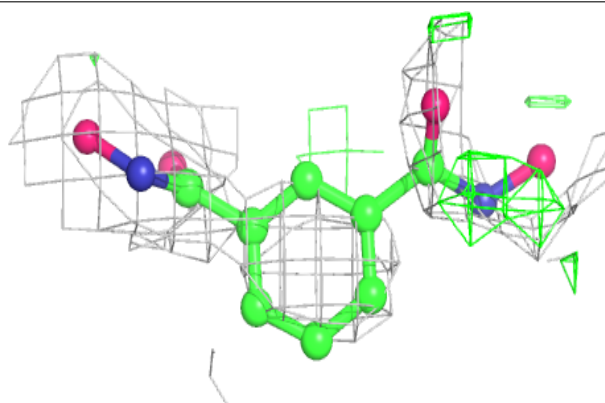


Electron density around V9D t 204 (D):

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

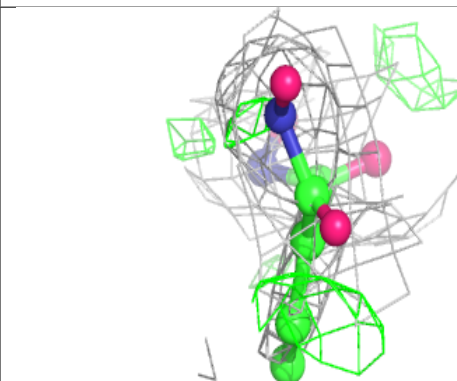
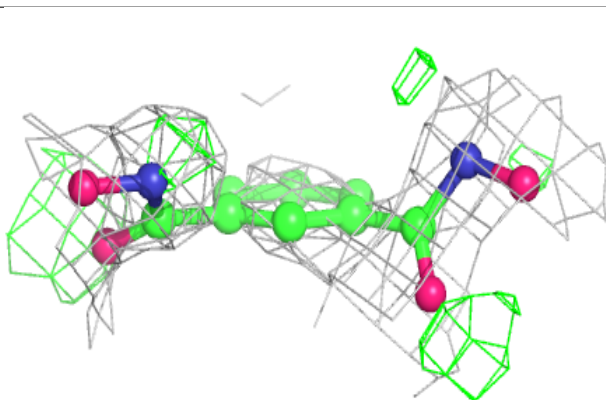
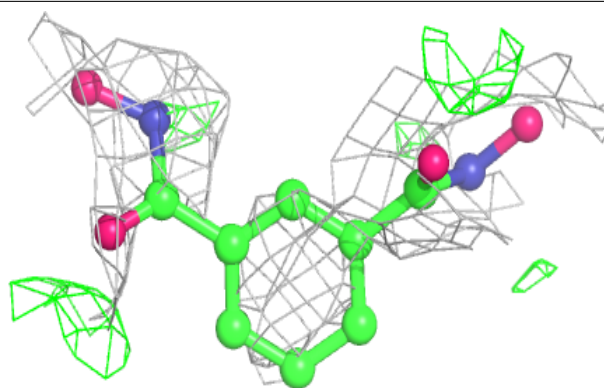
**Electron density around V9D j 204 (C):**

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

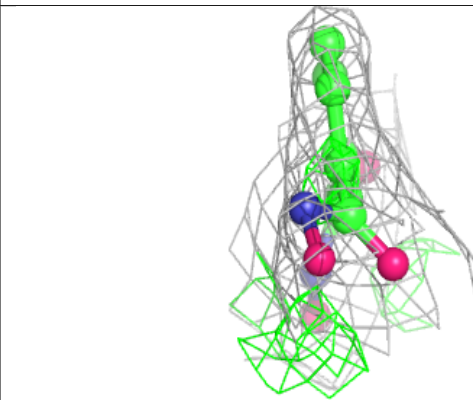
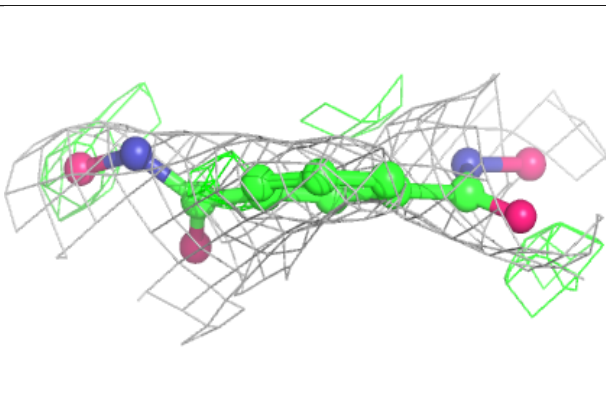
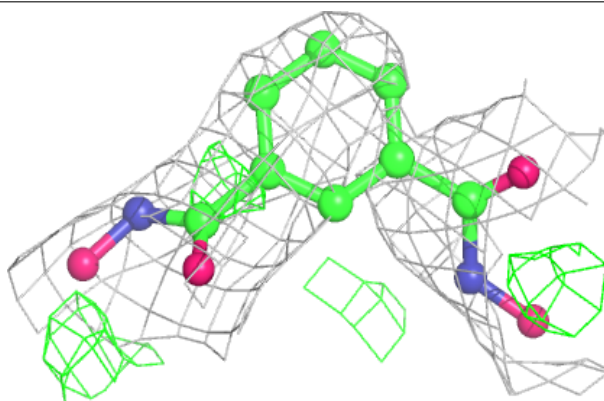


Electron density around V9D I 202 (C):

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

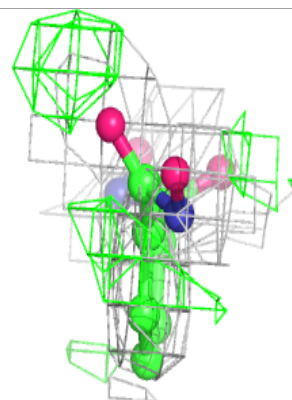
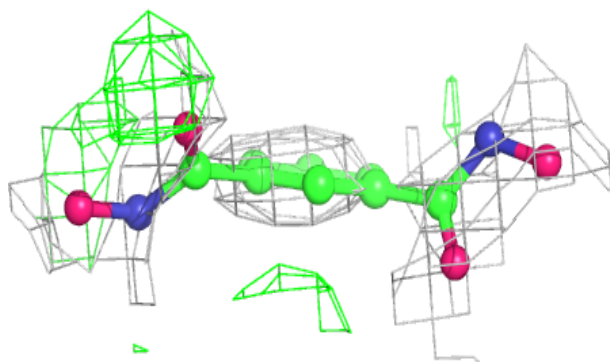
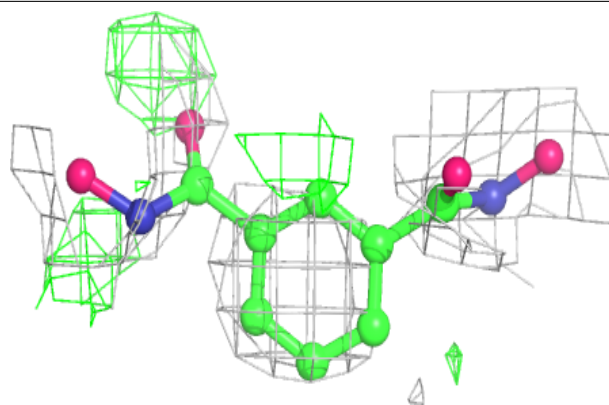
**Electron density around V9D n 202 (C):**

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

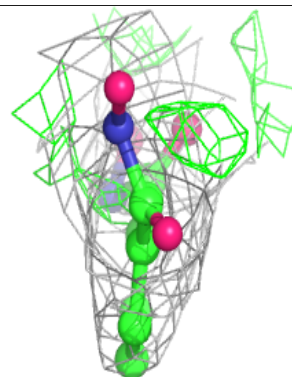
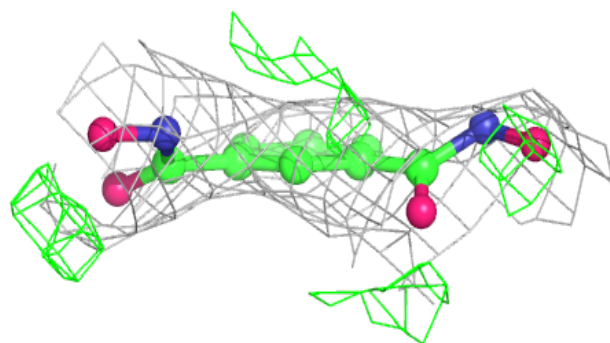
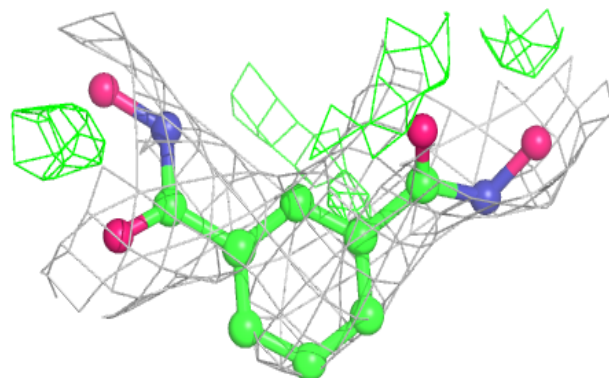


Electron density around V9D W 202 (D):

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

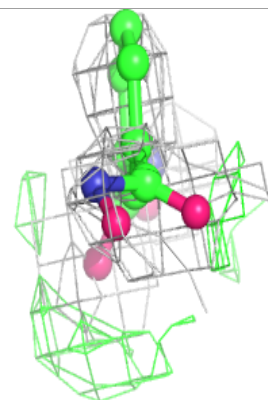
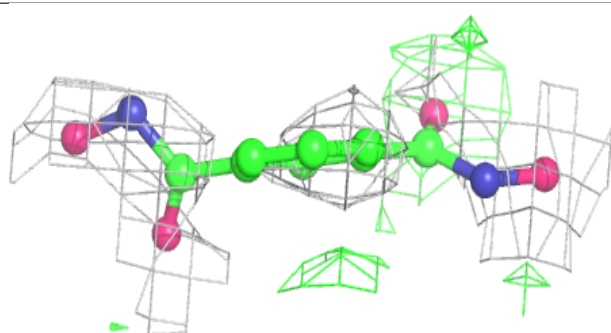
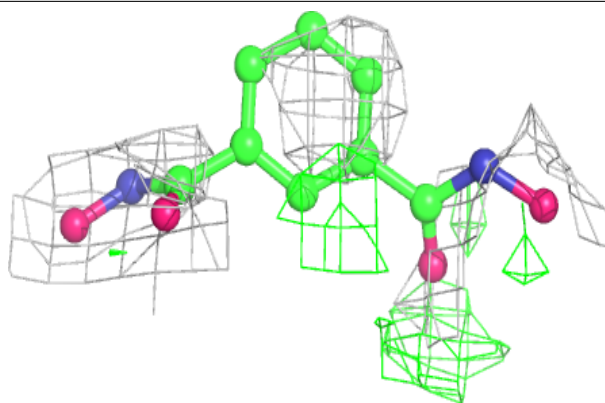
**Electron density around V9D W 202 (C):**

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



Electron density around V9D n 202 (D):

$2mF_o - DF_c$ (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.