



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 03:38 AM UTC

PDB ID : 7JGM / pdb_00007jgm
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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

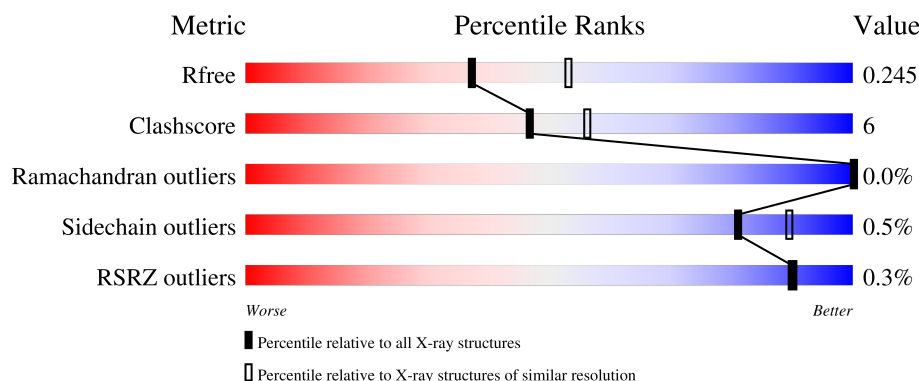
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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.



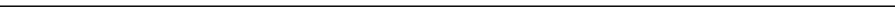
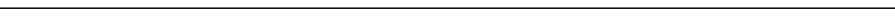
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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 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	182	 81% 15% .
1	B	182	 87% 9% .
1	C	182	 81% 14% .
1	D	182	 90% 6% .
1	E	182	 82% 13% .

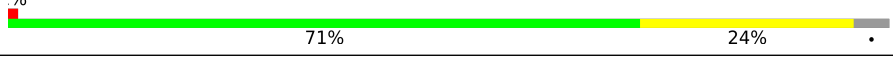
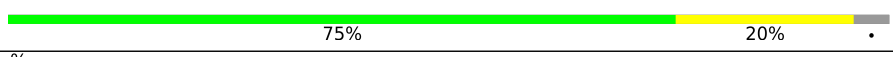
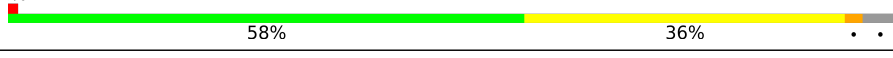
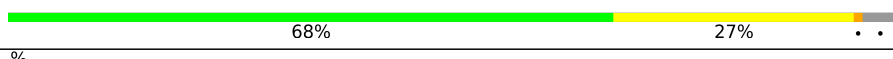
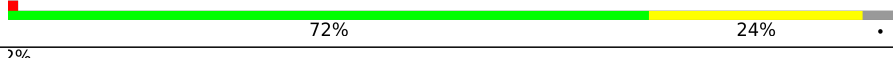
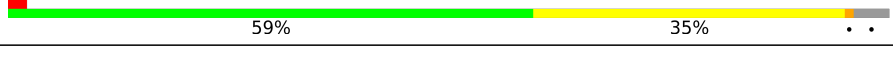
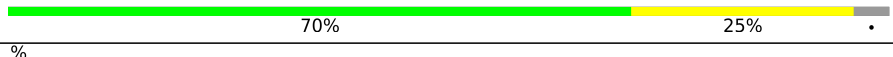
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Mol	Chain	Length	Quality of chain
1	F	182	 87% 8% . .
1	G	182	 89% 7% .
1	H	182	 88% 8% .
1	I	182	 86% 10% .
1	J	182	 85% 10% .
1	K	182	 88% 8% .
1	L	182	 82% 13% .
1	M	182	 79% 16% .
1	N	182	 86% 10% .
1	O	182	 82% 13% . .
1	P	182	 89% 7% .
1	Q	182	 81% 15% .
1	R	182	 88% 7% .
1	S	182	 85% 10% .
1	T	182	 88% 7% .
1	U	182	 87% 9% .
1	V	182	 82% 13% .
1	W	182	 89% 7% .
1	X	182	 81% 15% .
1	a	182	 % 76% 20% .
1	b	182	 % 76% 20% .
1	c	182	 % 69% 27% .
1	d	182	 % 75% 20% .
1	e	182	 % 66% 29% .
1	f	182	 69% 26% . .

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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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	V9D	R	202[D]	-	-	X	-

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 (CCD ID: NI) (formula: Ni).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	N	1	Total 1	Ni 1	0	0
2	O	2	Total 2	Ni 2	0	0
2	P	2	Total 2	Ni 2	0	0
2	Q	1	Total 1	Ni 1	0	0
2	R	1	Total 1	Ni 1	0	0
2	S	2	Total 2	Ni 2	0	0
2	T	1	Total 1	Ni 1	0	0
2	U	1	Total 1	Ni 1	0	0
2	V	1	Total 1	Ni 1	0	0
2	W	1	Total 1	Ni 1	0	0
2	X	2	Total 2	Ni 2	0	0
2	a	2	Total 4	Ni 4	0	2
2	b	1	Total 2	Ni 2	0	1
2	c	1	Total 2	Ni 2	0	1
2	d	3	Total 6	Ni 6	0	3
2	e	2	Total 4	Ni 4	0	2
2	f	2	Total 4	Ni 4	0	2
2	g	2	Total 4	Ni 4	0	2
2	h	1	Total 2	Ni 2	0	1
2	i	1	Total 2	Ni 2	0	1
2	j	2	Total 4	Ni 4	0	2

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	k	1	Total 2	Ni 2	0	1
2	l	1	Total 2	Ni 2	0	1
2	m	2	Total 4	Ni 4	0	2
2	n	1	Total 2	Ni 2	0	1
2	o	1	Total 2	Ni 2	0	1
2	p	2	Total 4	Ni 4	0	2
2	q	1	Total 2	Ni 2	0	1
2	r	1	Total 2	Ni 2	0	1
2	s	1	Total 2	Ni 2	0	1
2	t	2	Total 4	Ni 4	0	2
2	u	1	Total 2	Ni 2	0	1
2	v	3	Total 6	Ni 6	0	3
2	w	2	Total 4	Ni 4	0	2
2	x	2	Total 4	Ni 4	0	2

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

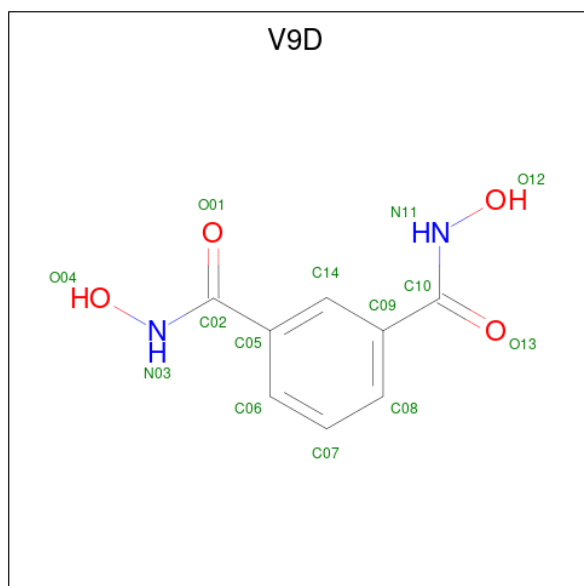
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Na 1	0	0
3	D	1	Total 1	Na 1	0	0
3	G	1	Total 1	Na 1	0	0
3	J	1	Total 1	Na 1	0	0
3	M	1	Total 1	Na 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total 1	Na 1	0	0
3	S	1	Total 1	Na 1	0	0
3	V	1	Total 1	Na 1	0	0
3	a	1	Total 2	Na 2	0	1
3	d	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	m	1	Total 2	Na 2	0	1
3	p	1	Total 2	Na 2	0	1
3	t	1	Total 2	Na 2	0	1
3	v	1	Total 2	Na 2	0	1

- Molecule 4 is N 1 ,N 3 -dihydroxybenzene-1,3-dicarboxamide (CCD ID: V9D) (formula: $C_8H_8N_2O_4$) (labeled as "Ligand of Interest" by depositor).



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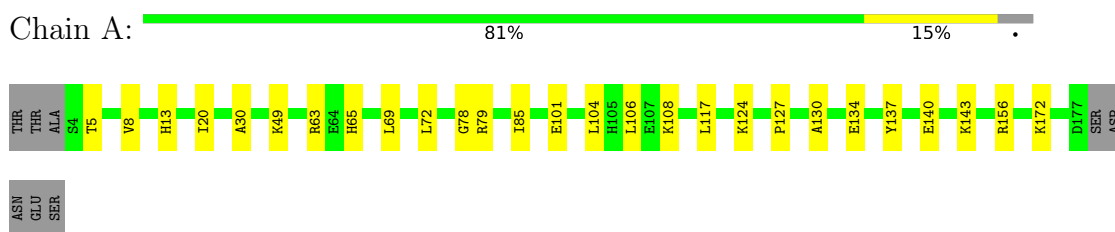
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	m	1	Total 1	O 1	0	0
5	n	2	Total 2	O 2	0	0
5	o	1	Total 1	O 1	0	0
5	p	1	Total 1	O 1	0	0
5	q	3	Total 3	O 3	0	0
5	r	2	Total 2	O 2	0	0
5	t	1	Total 1	O 1	0	0
5	u	1	Total 1	O 1	0	0

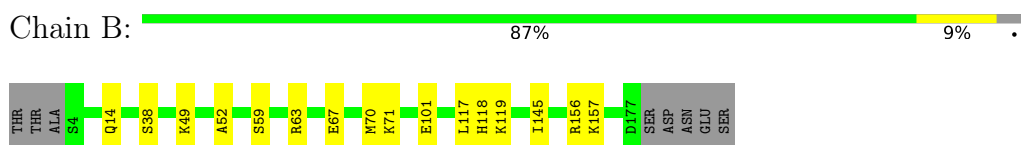
3 Residue-property plots

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.

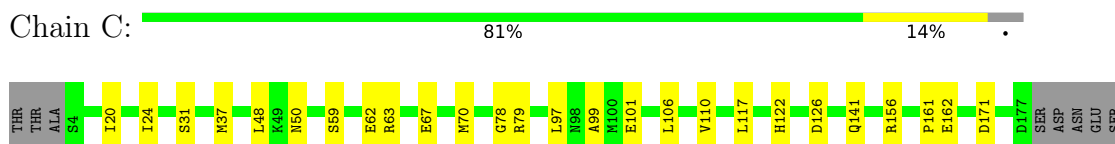
- Molecule 1: Ferritin heavy chain



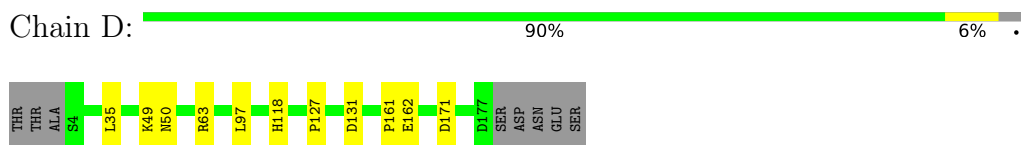
- Molecule 1: Ferritin heavy chain



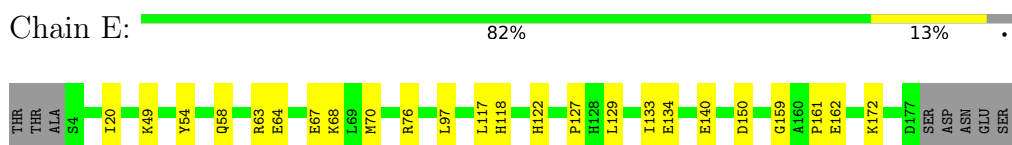
- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain

Chain F:  87% 8% . .



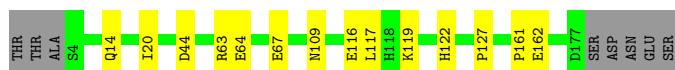
• Molecule 1: Ferritin heavy chain

Chain G:  89% 7% .



• Molecule 1: Ferritin heavy chain

Chain H:  88% 8% .



• Molecule 1: Ferritin heavy chain

Chain I:  86% 10% .



• Molecule 1: Ferritin heavy chain

Chain J:  85% 10% .



• Molecule 1: Ferritin heavy chain

Chain K:  88% 8% .



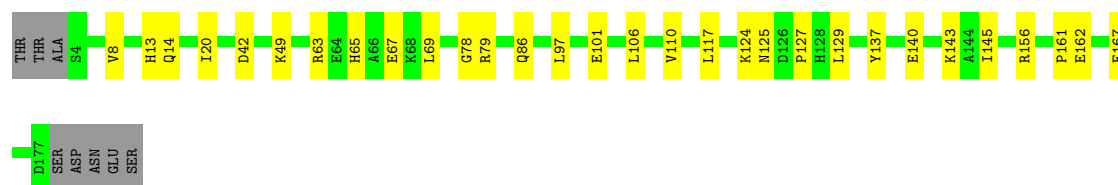
• Molecule 1: Ferritin heavy chain

Chain L:  82% 13% .



• Molecule 1: Ferritin heavy chain

Chain M:  79% 16% .



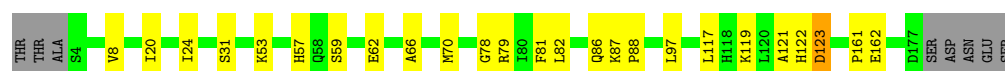
- Molecule 1: Ferritin heavy chain

Chain N:  86% 10% .



- Molecule 1: Ferritin heavy chain

Chain O:  82% 13% . .



- Molecule 1: Ferritin heavy chain

Chain P:  89% 7% .



- Molecule 1: Ferritin heavy chain

Chain Q:  81% 15% .



- Molecule 1: Ferritin heavy chain

Chain R:  88% 7% .



- Molecule 1: Ferritin heavy chain

Chain S:  85% 10% .



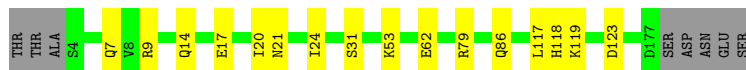
- Molecule 1: Ferritin heavy chain

Chain T:  88% 7% .



- Molecule 1: Ferritin heavy chain

Chain U:  87% 9% .



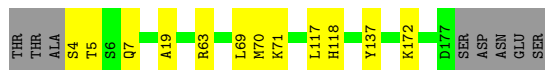
- Molecule 1: Ferritin heavy chain

Chain V:  82% 13% .



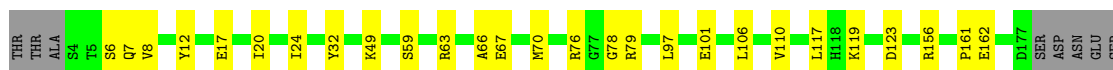
- Molecule 1: Ferritin heavy chain

Chain W:  89% 7% .



- Molecule 1: Ferritin heavy chain

Chain X:  81% 15% .



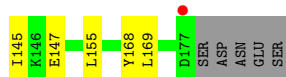
- Molecule 1: Ferritin heavy chain

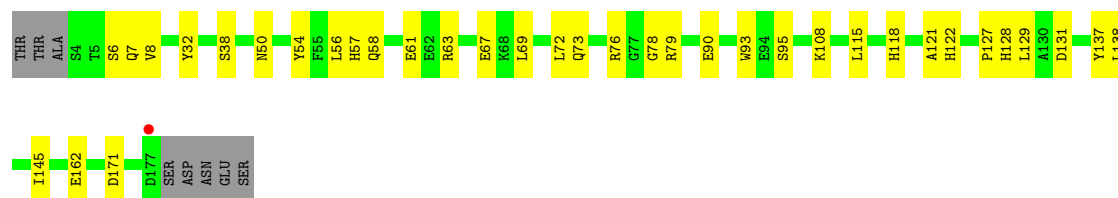
Chain a:  76% 20% .



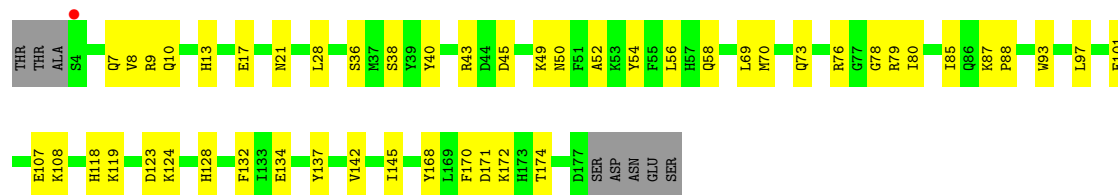
- Molecule 1: Ferritin heavy chain

Chain b:  76% 20% .

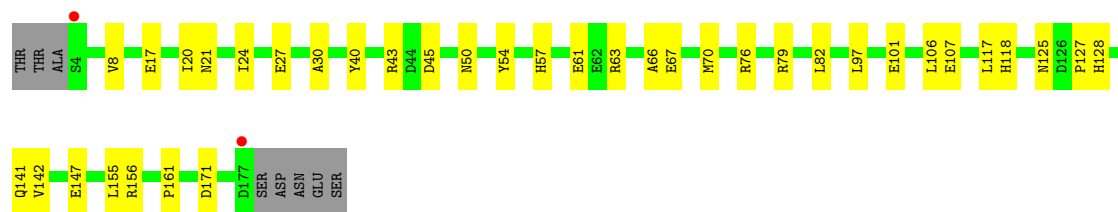
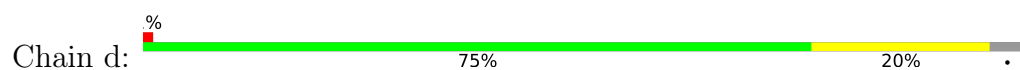




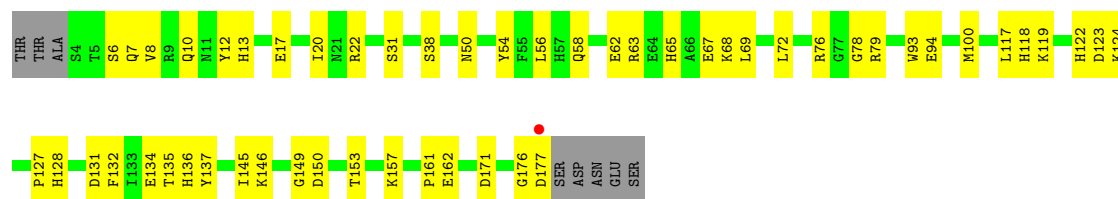
• Molecule 1: Ferritin heavy chain



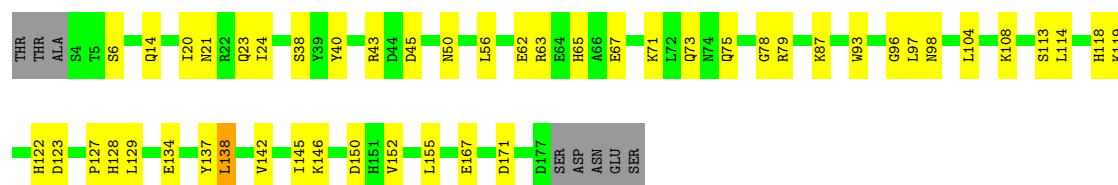
• Molecule 1: Ferritin heavy chain



• Molecule 1: Ferritin heavy chain



• Molecule 1: Ferritin heavy chain



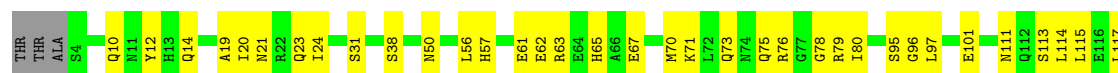
• Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



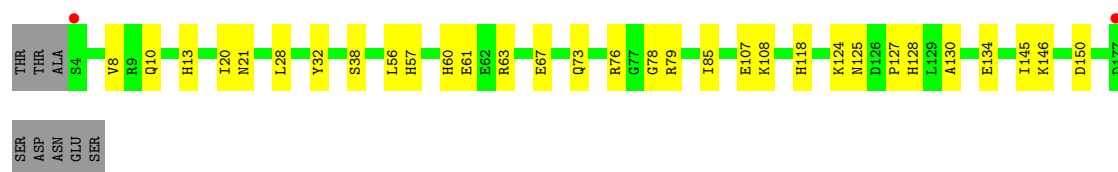
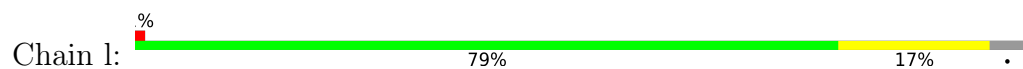
- Molecule 1: Ferritin heavy chain



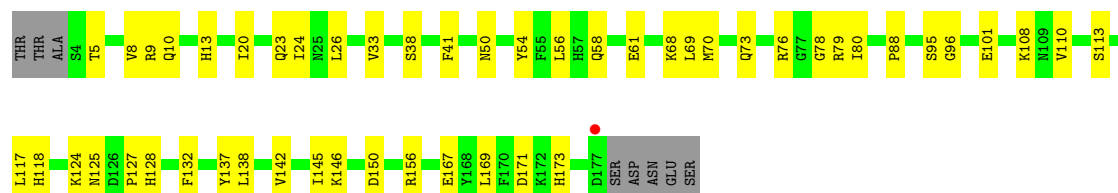
- Molecule 1: Ferritin heavy chain



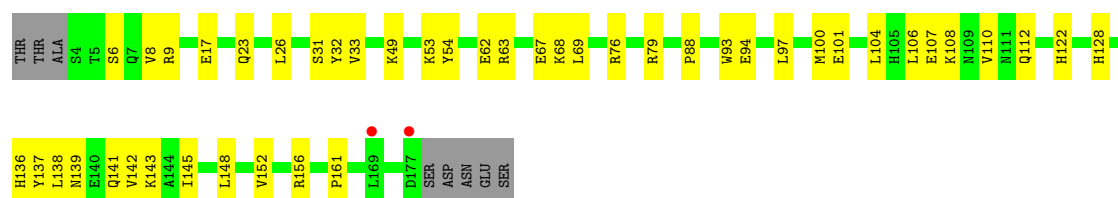
- Molecule 1: Ferritin heavy chain



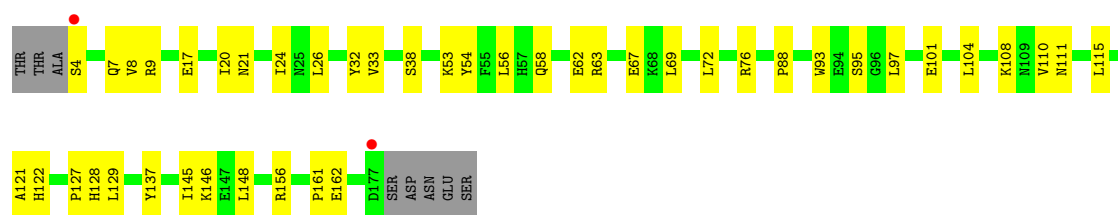
- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain

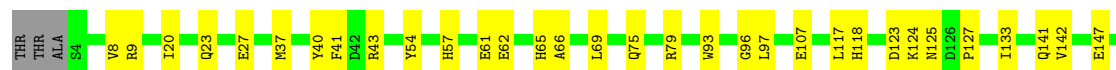
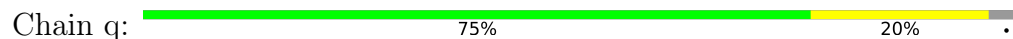


- Molecule 1: Ferritin heavy chain

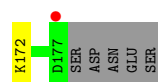




- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



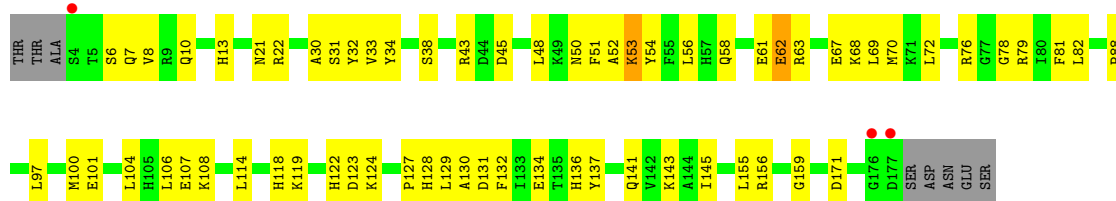
- Molecule 1: Ferritin heavy chain



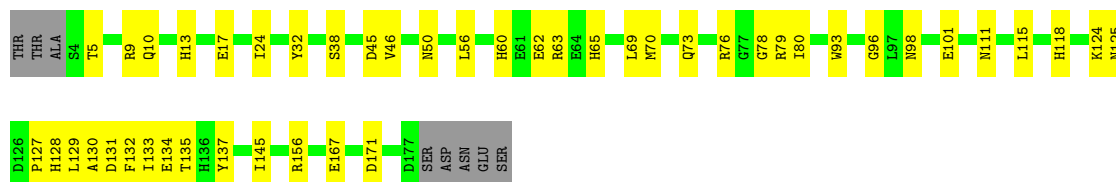
- Molecule 1: Ferritin heavy chain



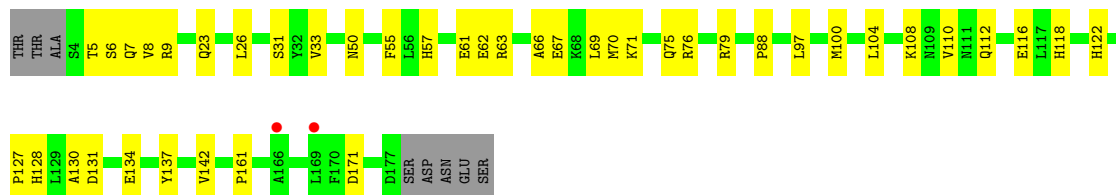
- Molecule 1: Ferritin heavy chain



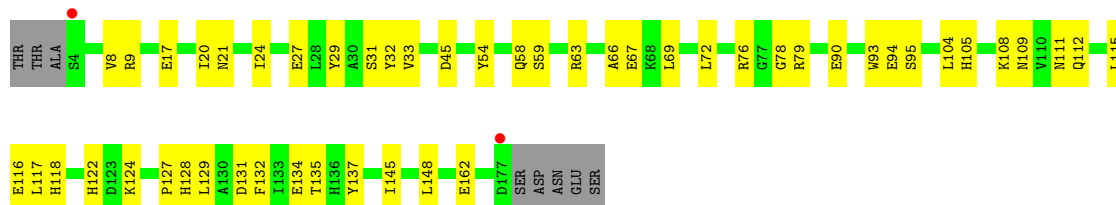
- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



- 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 38.46 – 2.31	Depositor EDS
% Data completeness (in resolution range)	98.2 (38.46-2.31) 90.8 (38.46-2.31)	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)	0.34 , 43.4	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	0.95	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

5.1 Standard geometry

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

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	0.51	0/1461	0.67	0/1969
1	B	0.50	0/1461	0.66	0/1969
1	C	0.50	0/1461	0.65	0/1969
1	D	0.50	0/1469	0.68	0/1980
1	E	0.51	0/1461	0.67	0/1969
1	F	0.53	0/1470	0.68	0/1981
1	G	0.51	0/1469	0.66	0/1980
1	H	0.51	0/1461	0.68	0/1969
1	I	0.54	0/1461	0.68	0/1969
1	J	0.49	0/1461	0.66	0/1969
1	K	0.49	0/1461	0.67	0/1969
1	L	0.49	0/1461	0.64	0/1969
1	M	0.50	0/1461	0.65	0/1969
1	N	0.50	0/1461	0.66	0/1969
1	O	0.49	0/1461	0.68	0/1969
1	P	0.51	0/1461	0.66	0/1969
1	Q	0.54	0/1461	0.68	0/1969
1	R	0.53	0/1461	0.67	0/1969
1	S	0.51	0/1469	0.70	0/1980
1	T	0.53	0/1461	0.69	0/1969
1	U	0.53	0/1470	0.67	0/1981
1	V	0.50	0/1461	0.65	0/1969
1	W	0.51	0/1461	0.65	0/1969
1	X	0.48	0/1461	0.65	0/1969
1	a	0.22	0/2922	0.32	0/3938
1	b	0.22	0/2922	0.34	0/3938
1	c	0.22	0/2922	0.35	0/3938
1	d	0.23	0/2922	0.33	0/3938
1	e	0.21	0/2922	0.32	0/3938
1	f	0.20	0/2922	0.31	0/3938
1	g	0.22	0/2922	0.33	0/3938
1	h	0.22	0/2922	0.33	0/3938

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	i	0.21	0/2922	0.33	0/3938
1	j	0.22	0/2922	0.33	0/3938
1	k	0.22	0/2922	0.33	0/3938
1	l	0.21	0/2922	0.33	0/3938
1	m	0.22	0/2922	0.34	0/3938
1	n	0.22	0/2922	0.33	0/3938
1	o	0.21	0/2922	0.33	0/3938
1	p	0.20	0/2922	0.32	0/3938
1	q	0.23	0/2922	0.34	0/3938
1	r	0.20	0/2922	0.32	0/3938
1	s	0.21	0/2922	0.34	0/3938
1	t	0.22	0/2922	0.33	0/3938
1	u	0.22	0/2922	0.32	0/3938
1	v	0.22	0/2922	0.35	0/3938
1	w	0.21	0/2922	0.34	0/3938
1	x	0.22	0/2922	0.34	0/3938
All	All	0.34	0/105234	0.47	0/141825

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.

There are no bond angle outliers.

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1431	0	1362	19	0
1	B	1431	0	1362	14	0
1	C	1431	0	1362	21	0
1	D	1436	0	1366	11	0
1	E	1431	0	1362	18	0
1	F	1437	0	1370	15	0
1	G	1436	0	1366	10	0
1	H	1431	0	1362	12	0
1	I	1431	0	1362	16	0
1	J	1431	0	1362	16	0
1	K	1431	0	1362	9	0
1	L	1431	0	1362	20	0
1	M	1431	0	1362	25	0
1	N	1431	0	1362	18	0
1	O	1431	0	1362	24	0
1	P	1431	0	1362	9	0
1	Q	1431	0	1362	20	0
1	R	1431	0	1362	15	0
1	S	1436	0	1366	12	0
1	T	1431	0	1362	10	0
1	U	1437	0	1370	14	0
1	V	1431	0	1362	20	0
1	W	1431	0	1362	10	0
1	X	1431	0	1362	23	0
1	a	2862	0	2704	27	0
1	b	2862	0	2705	33	0
1	c	2862	0	2701	38	0
1	d	2862	0	2705	28	0
1	e	2862	0	2704	45	0
1	f	2862	0	2704	33	0
1	g	2862	0	2707	41	0
1	h	2862	0	2700	44	0
1	i	2862	0	2704	39	0
1	j	2862	0	2705	32	0
1	k	2862	0	2706	43	0
1	l	2862	0	2698	21	0
1	m	2862	0	2703	42	0
1	n	2862	0	2707	32	0
1	o	2862	0	2703	40	0
1	p	2862	0	2705	49	0
1	q	2862	0	2707	29	0
1	r	2862	0	2706	57	0
1	s	2862	0	2703	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	t	2862	0	2707	34	0
1	u	2862	0	2704	57	0
1	v	2862	0	2704	31	0
1	w	2862	0	2705	31	0
1	x	2862	0	2709	40	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3	0
4	I	28	0	0	4	0
4	R	28	0	0	10	0
4	W	28	0	0	3	0
4	a	28	0	0	3	0
4	j	28	0	0	6	0
4	n	28	0	0	4	0
4	t	28	0	0	4	0
5	A	79	0	0	2	0
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	3	0
5	G	119	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	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	97622	1146	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 1146 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)
4:R:202[D]:V9D:O12	1:r:122[D]:HIS:CE1	1.86	1.27
4:a:204[C]:V9D:O12	1:b:122[C]:HIS:HE1	1.23	1.21
4:R:202[D]:V9D:O12	1:r:122[D]:HIS:HE1	1.24	1.13
1:j:72[C]:LEU:HD11	1:j:132[C]:PHE:CE2	1.86	1.10
4:j:204[C]:V9D:O12	1:k:122[C]:HIS:HE1	1.33	1.09

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
1	N	172/182 (94%)	169 (98%)	3 (2%)	0	100	100
1	O	172/182 (94%)	166 (96%)	5 (3%)	1 (1%)	21	25
1	P	172/182 (94%)	167 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	21	25
1	s	344/182 (189%)	326 (95%)	18 (5%)	0	100	100
1	t	344/182 (189%)	328 (95%)	16 (5%)	0	100	100
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	x	344/182 (189%)	336 (98%)	6 (2%)	2 (1%)	21	25
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%)	152 (99%)	1 (1%)	76	86
1	B	153/160 (96%)	153 (100%)	0	100	100
1	C	153/160 (96%)	153 (100%)	0	100	100
1	D	154/160 (96%)	154 (100%)	0	100	100
1	E	153/160 (96%)	153 (100%)	0	100	100
1	F	154/160 (96%)	152 (99%)	2 (1%)	61	76
1	G	154/160 (96%)	154 (100%)	0	100	100
1	H	153/160 (96%)	153 (100%)	0	100	100
1	I	153/160 (96%)	153 (100%)	0	100	100
1	J	153/160 (96%)	153 (100%)	0	100	100
1	K	153/160 (96%)	153 (100%)	0	100	100
1	L	153/160 (96%)	153 (100%)	0	100	100
1	M	153/160 (96%)	153 (100%)	0	100	100
1	N	153/160 (96%)	153 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	153/160 (96%)	153 (100%)	0	100	100
1	P	153/160 (96%)	153 (100%)	0	100	100
1	Q	153/160 (96%)	153 (100%)	0	100	100
1	R	153/160 (96%)	153 (100%)	0	100	100
1	S	154/160 (96%)	154 (100%)	0	100	100
1	T	153/160 (96%)	153 (100%)	0	100	100
1	U	154/160 (96%)	152 (99%)	2 (1%)	61	76
1	V	153/160 (96%)	153 (100%)	0	100	100
1	W	153/160 (96%)	153 (100%)	0	100	100
1	X	153/160 (96%)	153 (100%)	0	100	100
1	a	306/160 (191%)	306 (100%)	0	100	100
1	b	306/160 (191%)	304 (99%)	2 (1%)	76	86
1	c	306/160 (191%)	306 (100%)	0	100	100
1	d	306/160 (191%)	306 (100%)	0	100	100
1	e	306/160 (191%)	306 (100%)	0	100	100
1	f	306/160 (191%)	298 (97%)	8 (3%)	40	57
1	g	306/160 (191%)	302 (99%)	4 (1%)	61	76
1	h	306/160 (191%)	306 (100%)	0	100	100
1	i	306/160 (191%)	304 (99%)	2 (1%)	76	86
1	j	306/160 (191%)	306 (100%)	0	100	100
1	k	306/160 (191%)	304 (99%)	2 (1%)	76	86
1	l	306/160 (191%)	304 (99%)	2 (1%)	76	86
1	m	306/160 (191%)	304 (99%)	2 (1%)	76	86
1	n	306/160 (191%)	302 (99%)	4 (1%)	61	76
1	o	306/160 (191%)	300 (98%)	6 (2%)	48	66
1	p	306/160 (191%)	294 (96%)	12 (4%)	28	42
1	q	306/160 (191%)	306 (100%)	0	100	100
1	r	306/160 (191%)	298 (97%)	8 (3%)	40	57
1	s	306/160 (191%)	302 (99%)	4 (1%)	61	76
1	t	306/160 (191%)	306 (100%)	0	100	100
1	u	306/160 (191%)	298 (97%)	8 (3%)	40	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	v	306/160 (191%)	304 (99%)	2 (1%)	76	86
1	w	306/160 (191%)	306 (100%)	0	100	100
1	x	306/160 (191%)	304 (99%)	2 (1%)	76	86
All	All	11021/7680 (144%)	10948 (99%)	73 (1%)	81	86

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	s	5[C]	THR
1	x	32[C]	TYR
1	s	89[C]	ASP
1	u	61[C]	GLU
1	l	32[D]	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	141	GLN
1	X	112	GLN
1	P	111	ASN
1	X	14	GLN
1	T	154	ASN

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

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	I	202[D]	2	14,14,14	3.76	3 (21%)	18,18,18	1.27	2 (11%)
4	V9D	n	202[C]	2	14,14,14	3.89	2 (14%)	18,18,18	1.72	2 (11%)
4	V9D	j	204[D]	2	14,14,14	3.82	2 (14%)	18,18,18	1.74	3 (16%)
4	V9D	I	202[C]	2	14,14,14	3.66	2 (14%)	18,18,18	1.83	7 (38%)
4	V9D	R	202[D]	2	14,14,14	3.40	2 (14%)	18,18,18	2.04	6 (33%)
4	V9D	j	204[C]	2	14,14,14	3.67	2 (14%)	18,18,18	2.34	6 (33%)
4	V9D	R	202[C]	2	14,14,14	3.85	2 (14%)	18,18,18	1.45	3 (16%)
4	V9D	F	203[D]	2	14,14,14	3.73	2 (14%)	18,18,18	1.35	3 (16%)
4	V9D	W	202[D]	2	14,14,14	3.75	2 (14%)	18,18,18	1.72	4 (22%)
4	V9D	t	204[D]	2	14,14,14	3.62	2 (14%)	18,18,18	1.68	5 (27%)
4	V9D	F	203[C]	2	14,14,14	3.67	2 (14%)	18,18,18	1.54	3 (16%)
4	V9D	W	202[C]	2	14,14,14	3.80	2 (14%)	18,18,18	1.84	5 (27%)
4	V9D	t	204[C]	2	14,14,14	3.82	2 (14%)	18,18,18	1.76	4 (22%)
4	V9D	n	202[D]	2	14,14,14	3.76	2 (14%)	18,18,18	1.90	4 (22%)
4	V9D	a	204[C]	2	14,14,14	3.75	2 (14%)	18,18,18	1.53	3 (16%)
4	V9D	a	204[D]	2	14,14,14	3.85	2 (14%)	18,18,18	1.77	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	I	202[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	j	204[D]	2	-	3/12/12/12	0/1/1/1
4	V9D	I	202[C]	2	-	4/12/12/12	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	V9D	R	202[D]	2	-	0/12/12/12	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	F	203[D]	2	-	3/12/12/12	0/1/1/1
4	V9D	W	202[D]	2	-	5/12/12/12	0/1/1/1
4	V9D	t	204[D]	2	-	4/12/12/12	0/1/1/1
4	V9D	F	203[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	t	204[C]	2	-	7/12/12/12	0/1/1/1
4	V9D	n	202[D]	2	-	4/12/12/12	0/1/1/1
4	V9D	a	204[C]	2	-	4/12/12/12	0/1/1/1
4	V9D	a	204[D]	2	-	4/12/12/12	0/1/1/1

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	a	204[D]	V9D	C10-N11	10.66	1.46	1.32
4	j	204[D]	V9D	C10-N11	10.64	1.46	1.32
4	n	202[C]	V9D	C10-N11	10.61	1.46	1.32
4	a	204[C]	V9D	C02-N03	10.46	1.46	1.32
4	W	202[D]	V9D	C02-N03	10.43	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	6.47	126.25	116.26
4	R	202[D]	V9D	O12-N11-C10	-5.18	106.77	119.73
4	W	202[C]	V9D	C05-C02-N03	5.07	124.09	116.26
4	a	204[D]	V9D	C05-C02-N03	4.99	123.97	116.26
4	n	202[C]	V9D	C05-C02-N03	4.81	123.69	116.26

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

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

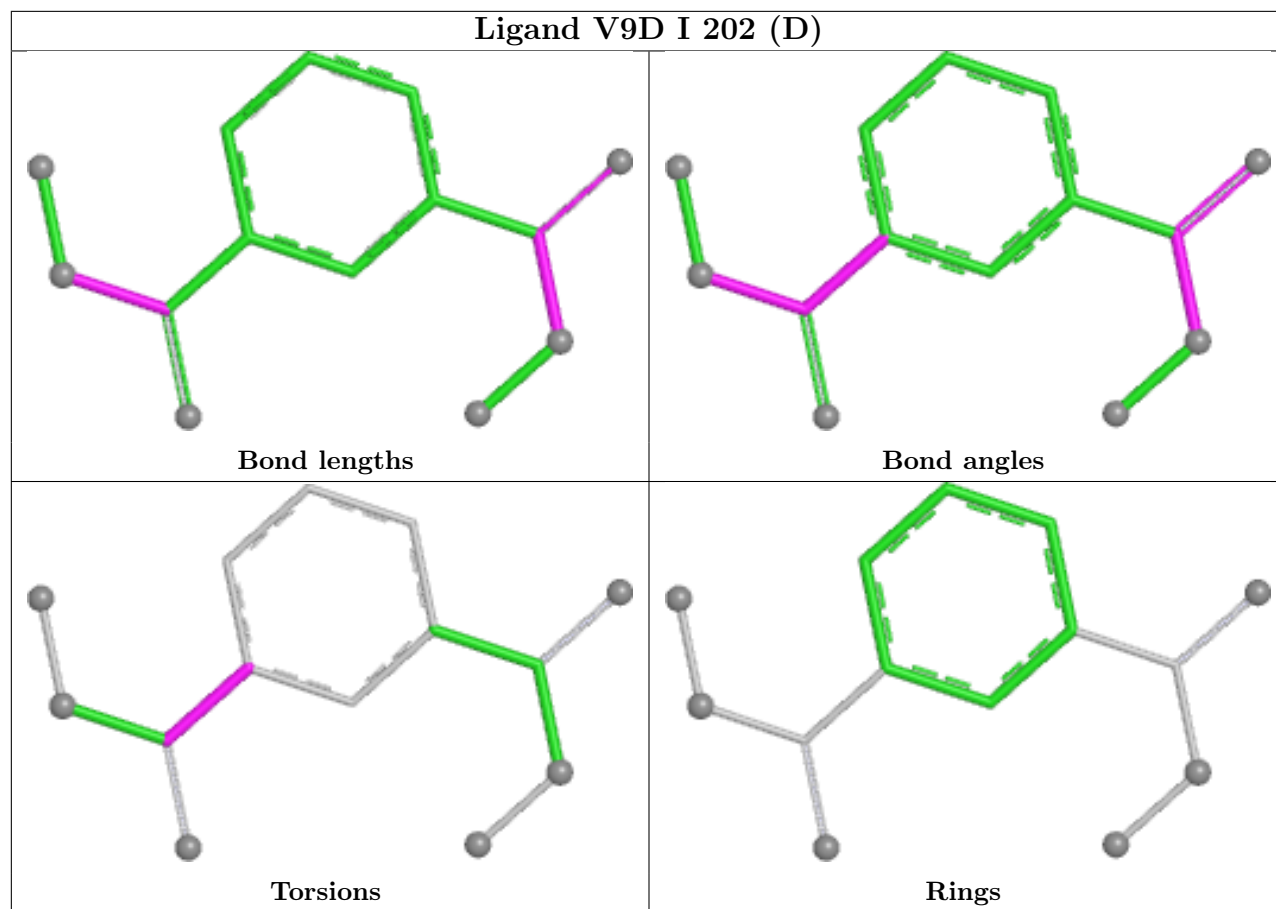
There are no ring outliers.

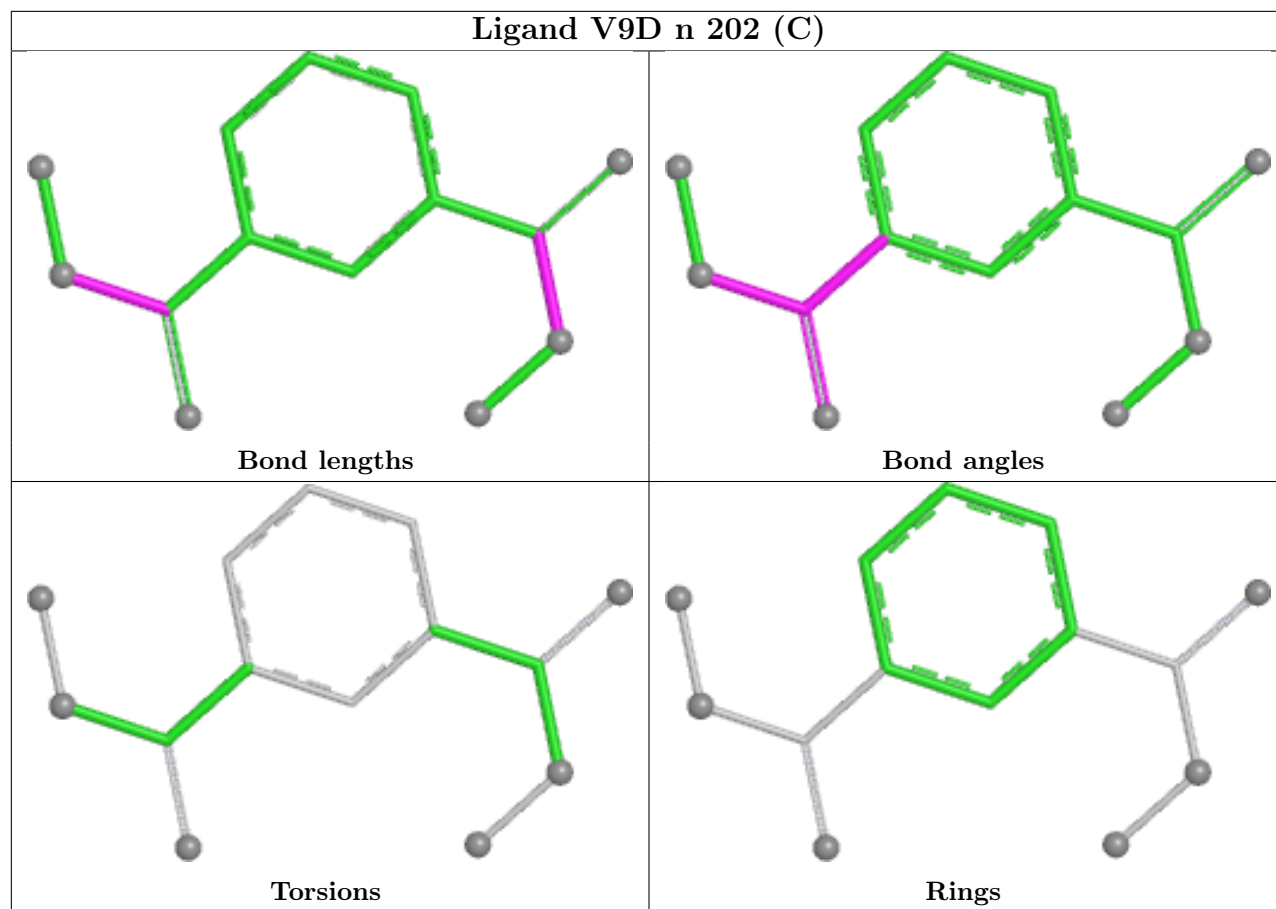
16 monomers are involved in 37 short contacts:

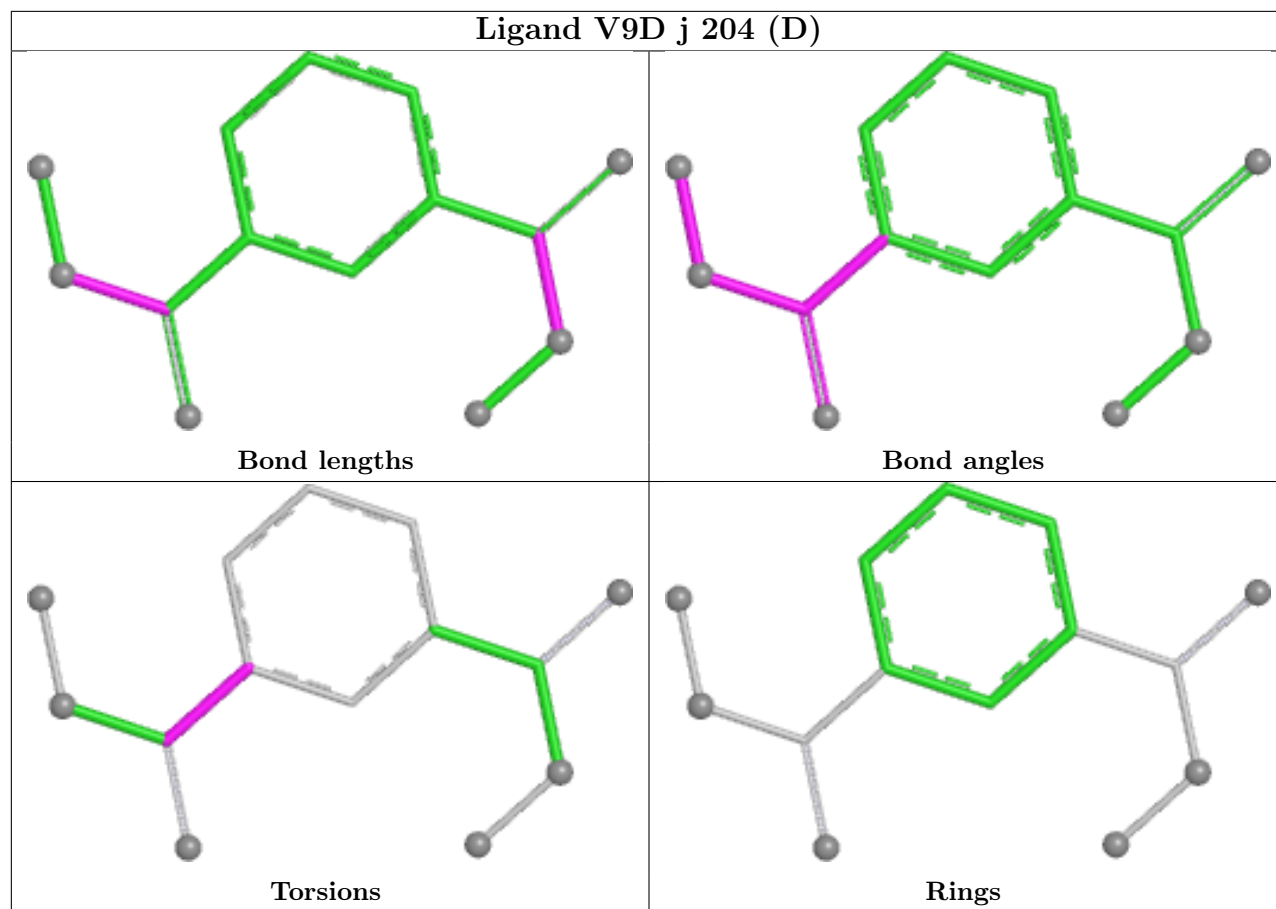
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	202[D]	V9D	1	0
4	n	202[C]	V9D	2	0
4	j	204[D]	V9D	3	0
4	I	202[C]	V9D	3	0
4	R	202[D]	V9D	8	0
4	j	204[C]	V9D	3	0
4	R	202[C]	V9D	2	0
4	F	203[D]	V9D	2	0
4	W	202[D]	V9D	2	0
4	t	204[D]	V9D	2	0
4	F	203[C]	V9D	1	0
4	W	202[C]	V9D	1	0
4	t	204[C]	V9D	2	0
4	n	202[D]	V9D	2	0
4	a	204[C]	V9D	2	0
4	a	204[D]	V9D	1	0

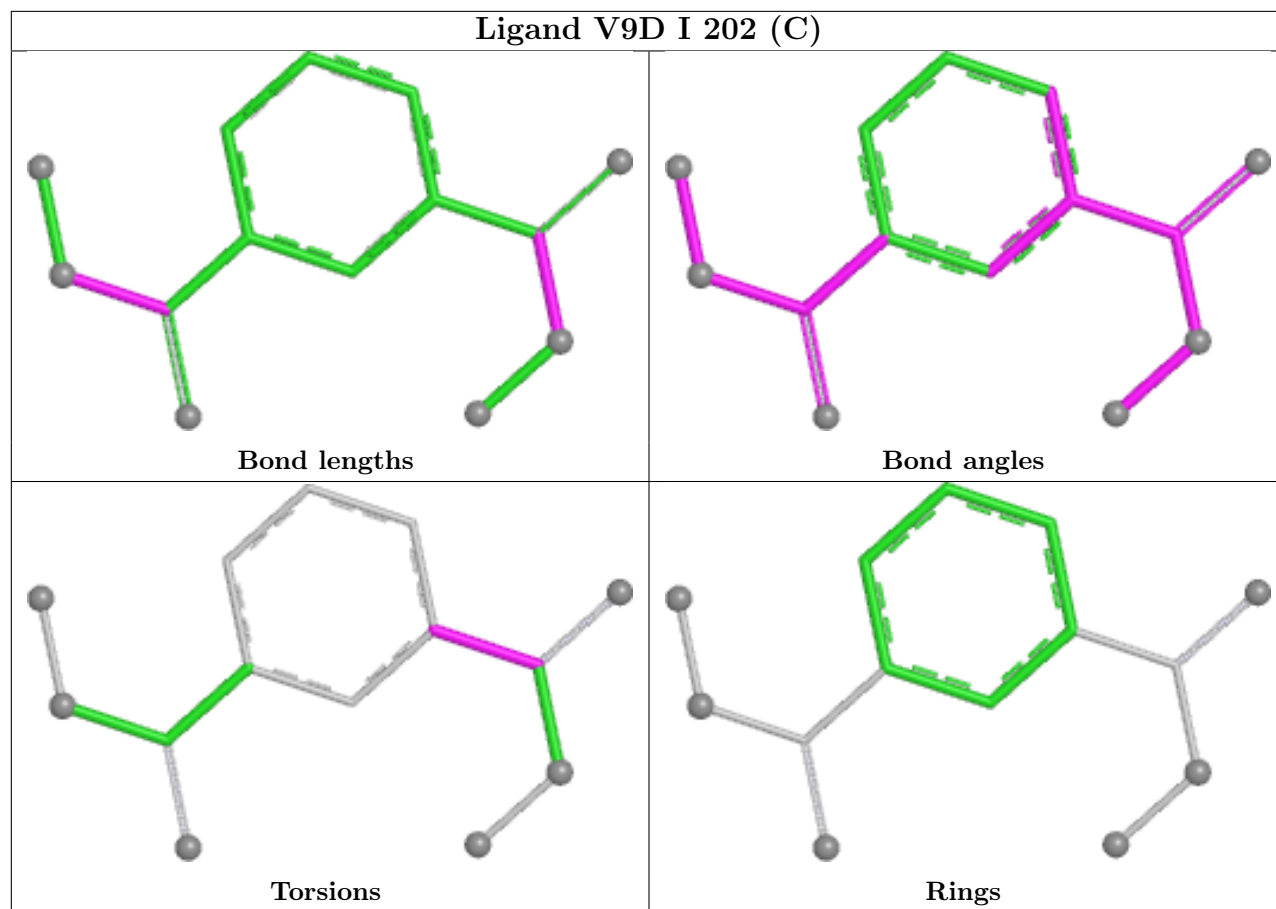
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand V9D I 202 (D)

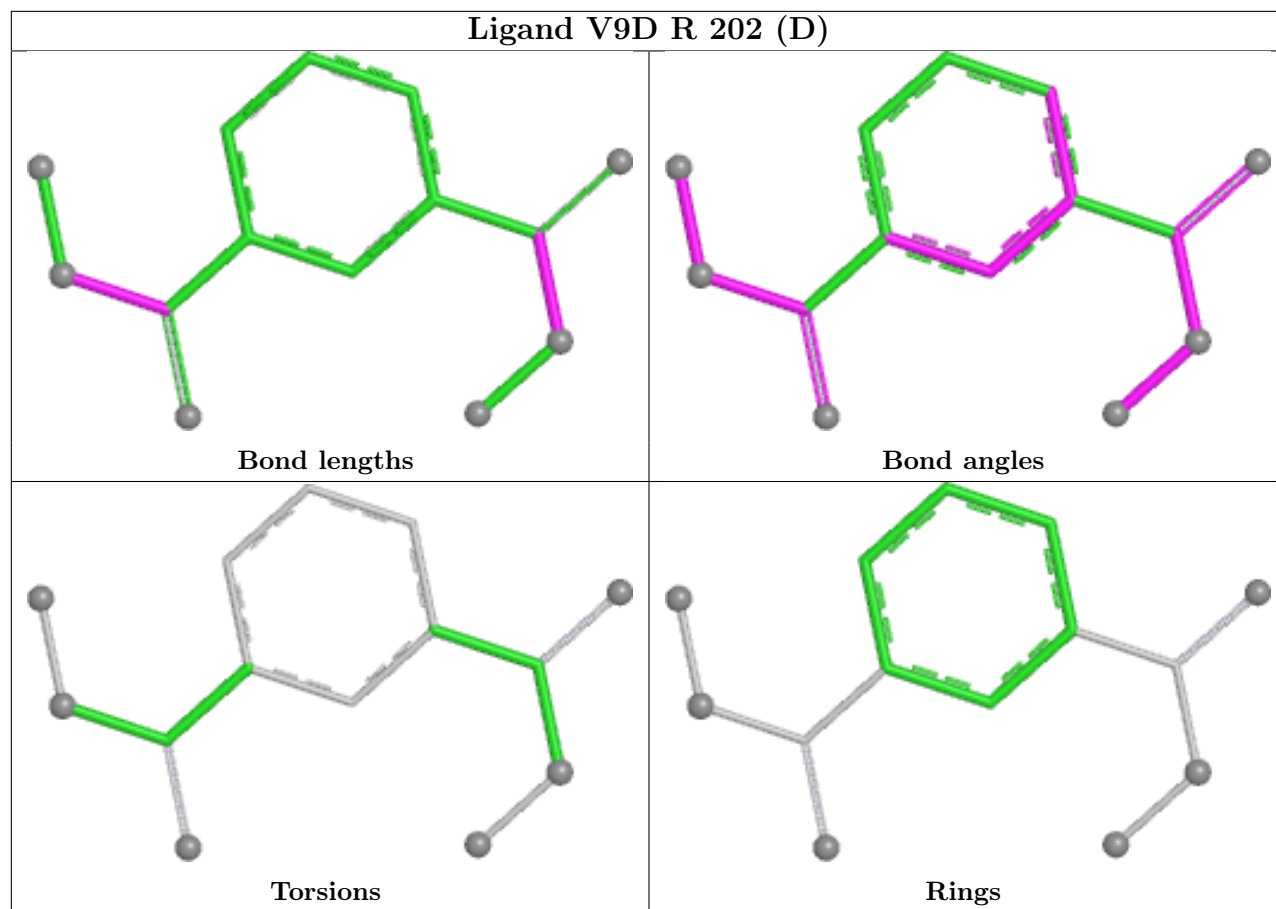


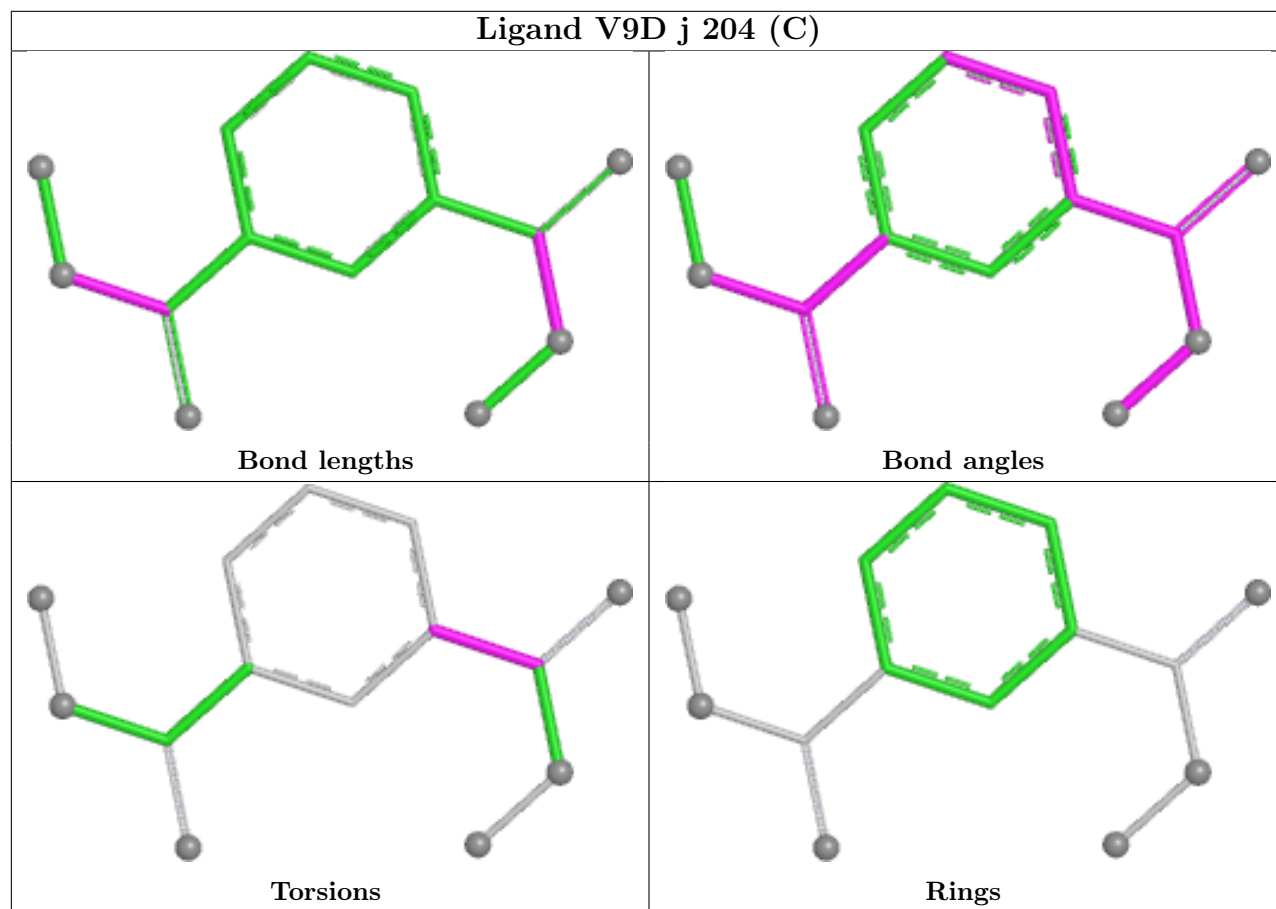


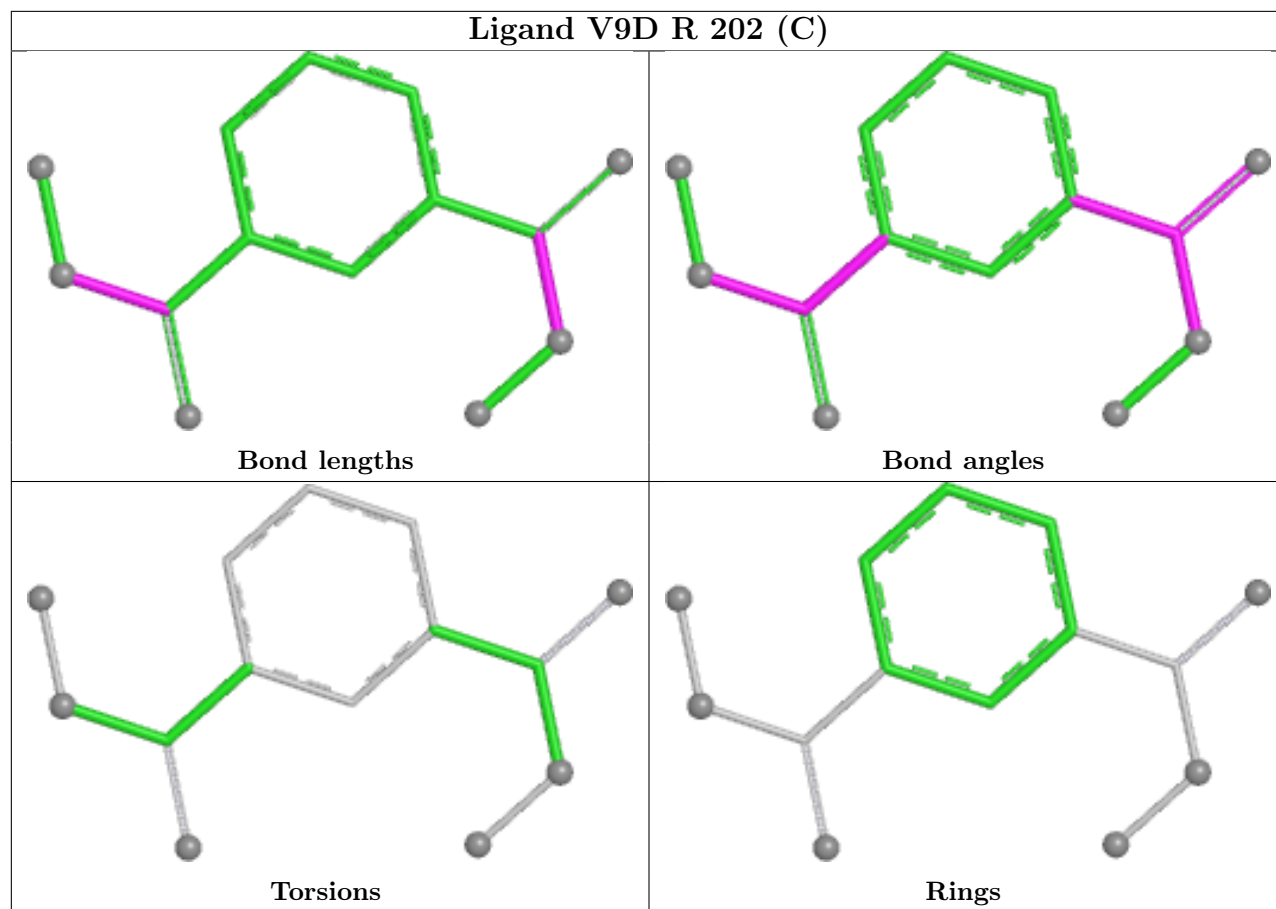




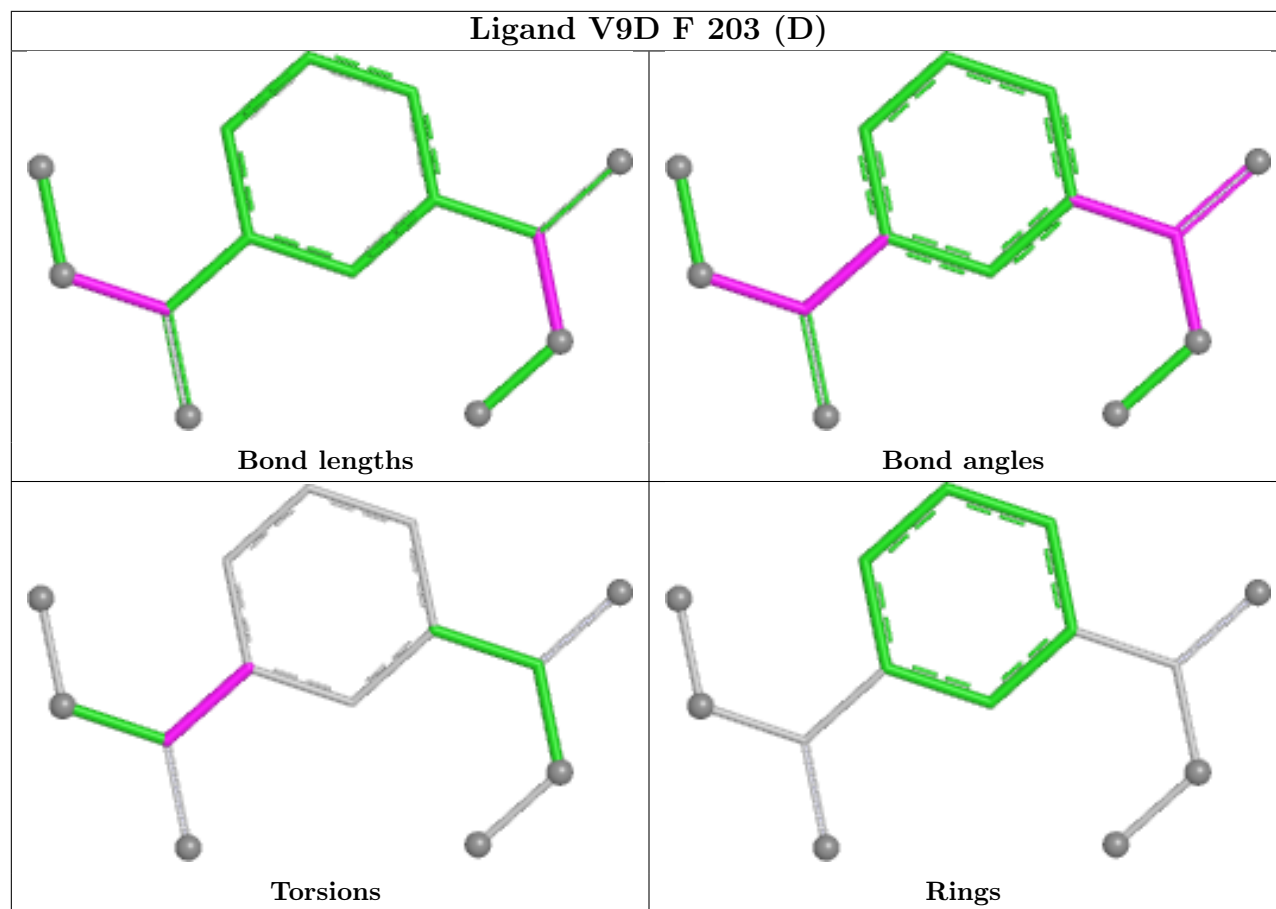
Ligand V9D R 202 (D)

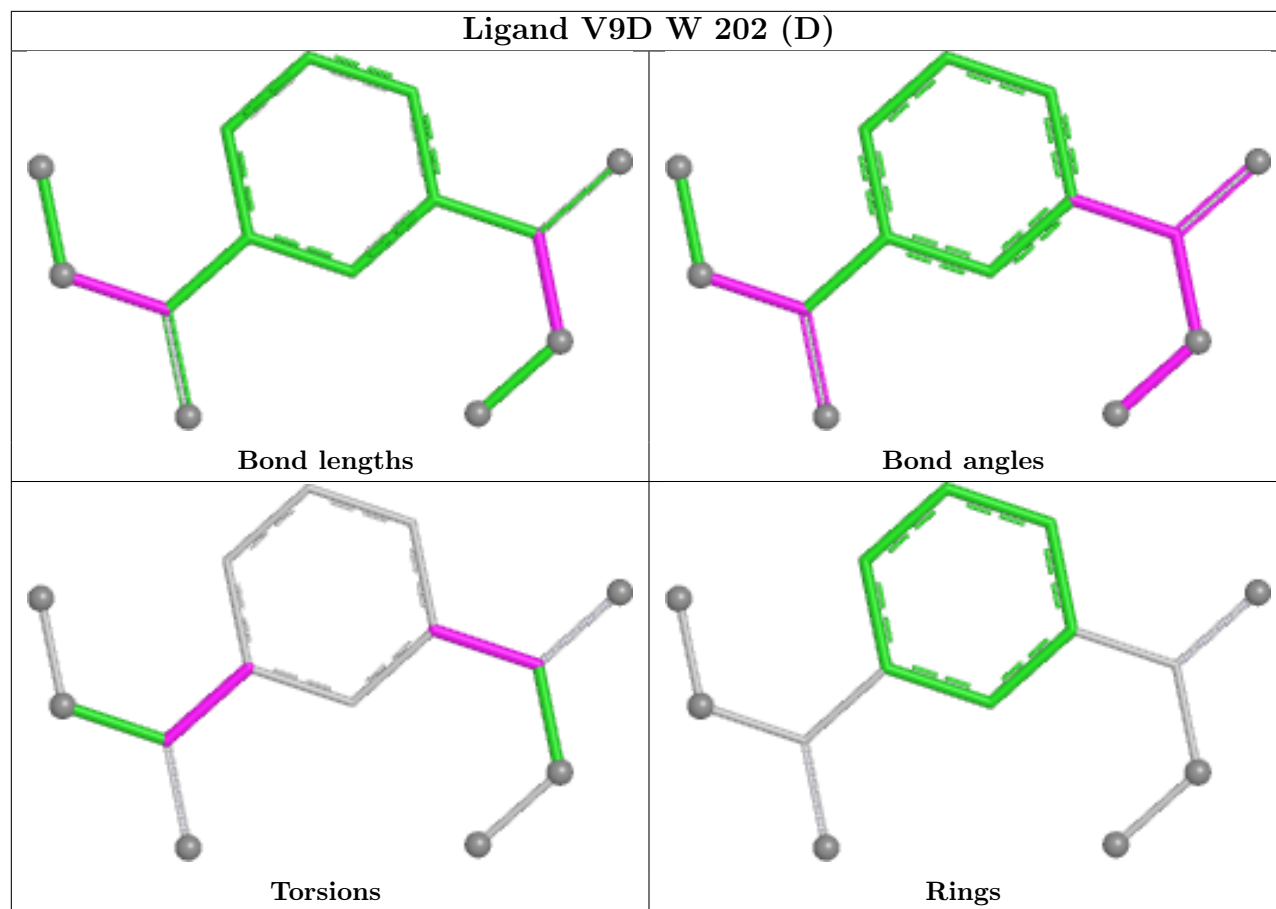


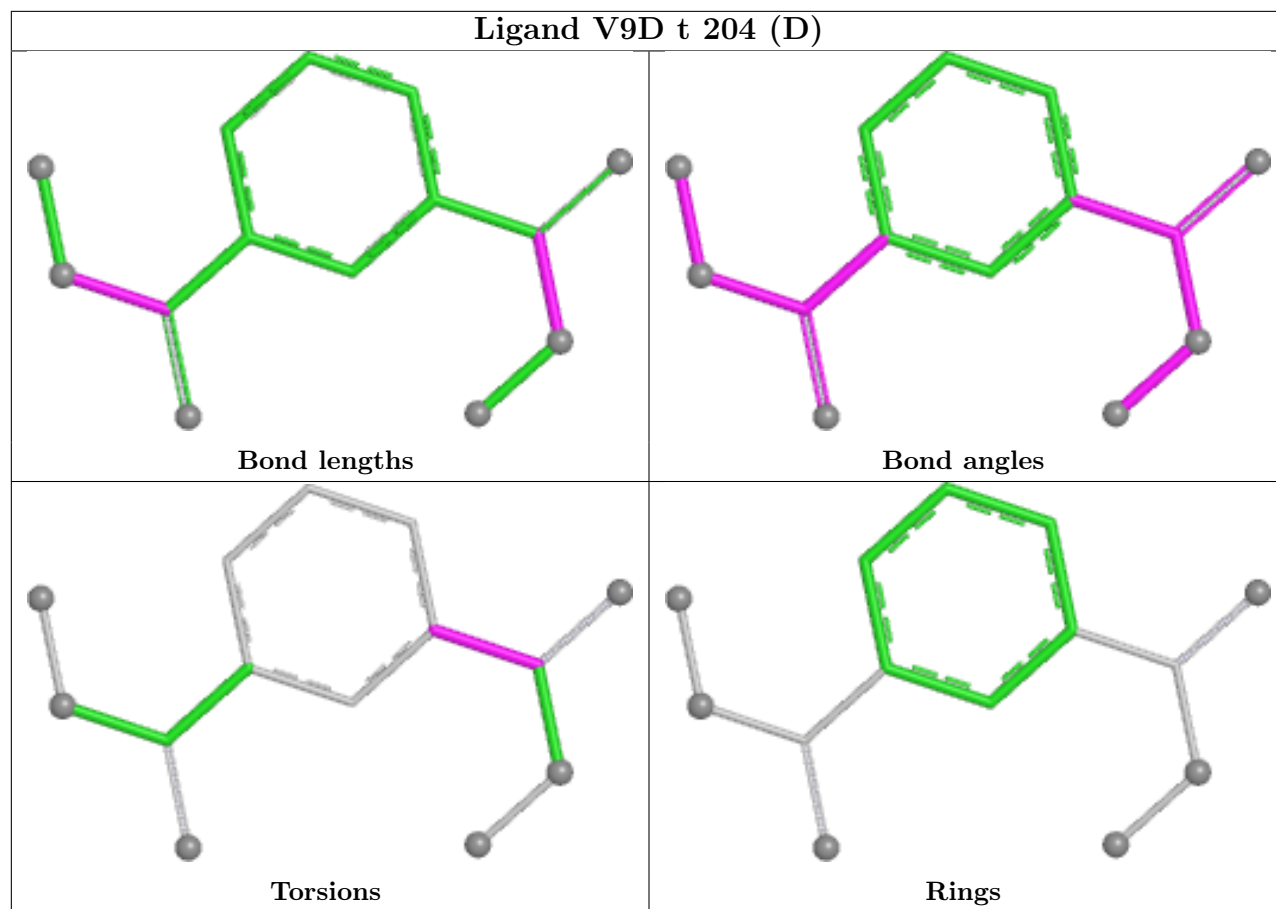


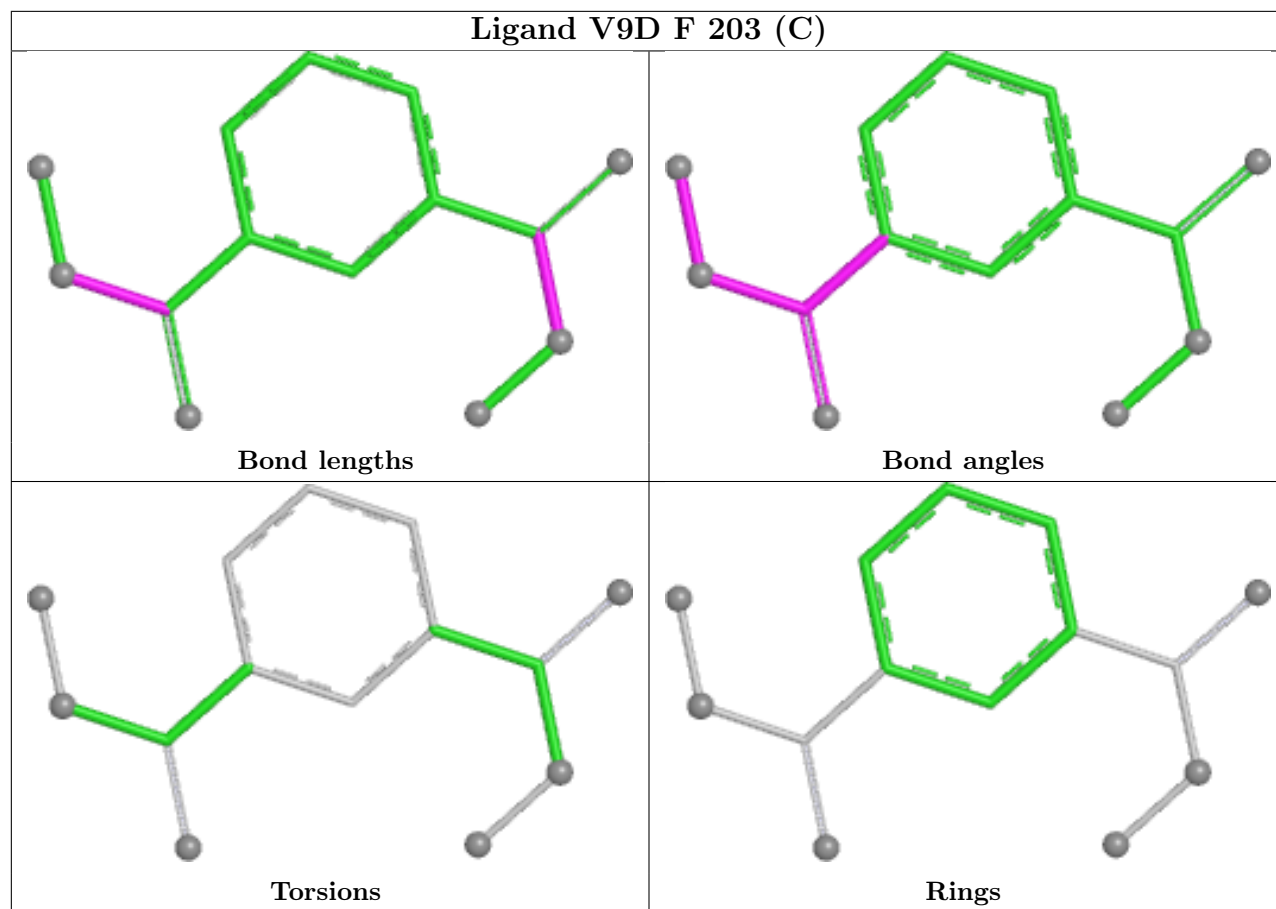


Ligand V9D F 203 (D)

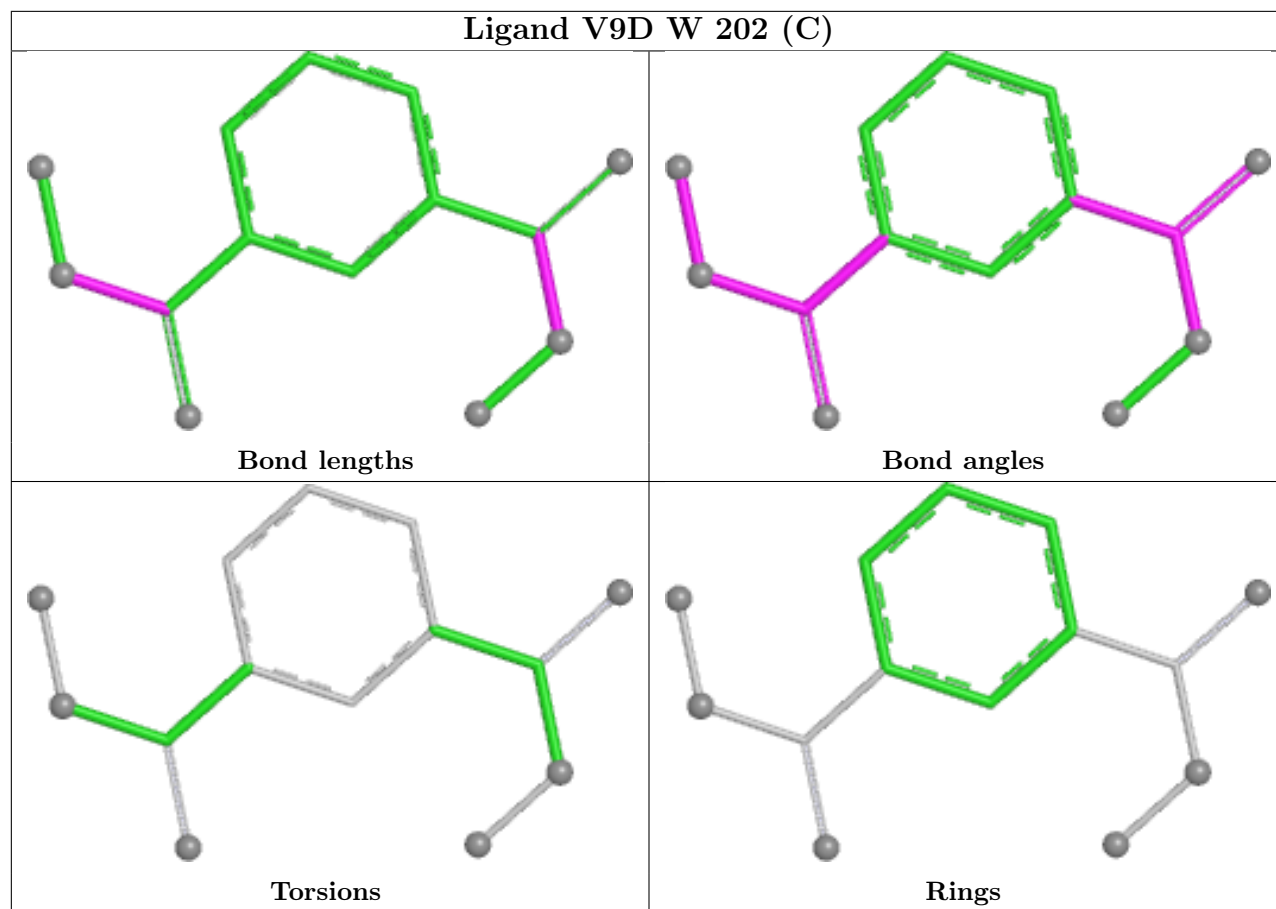


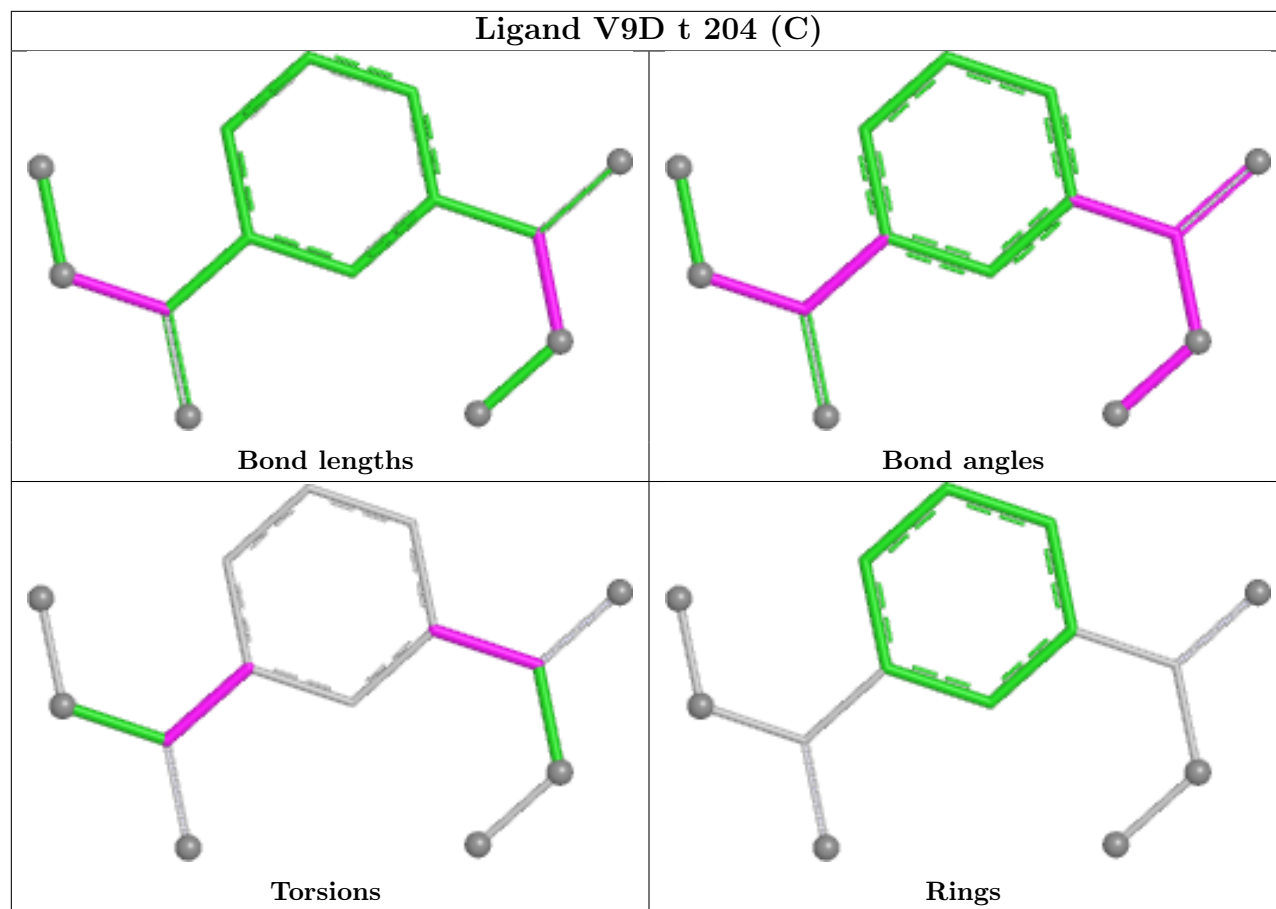


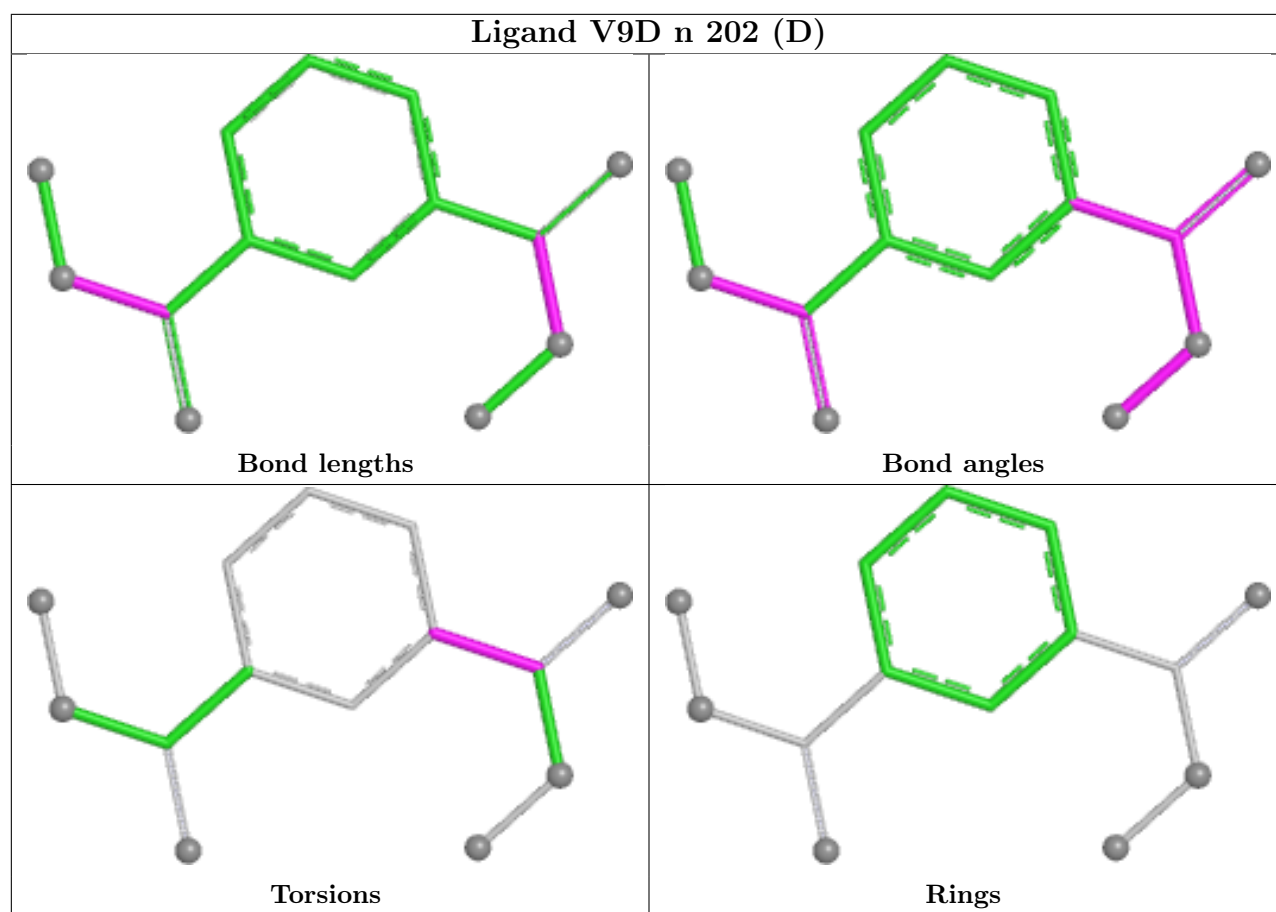


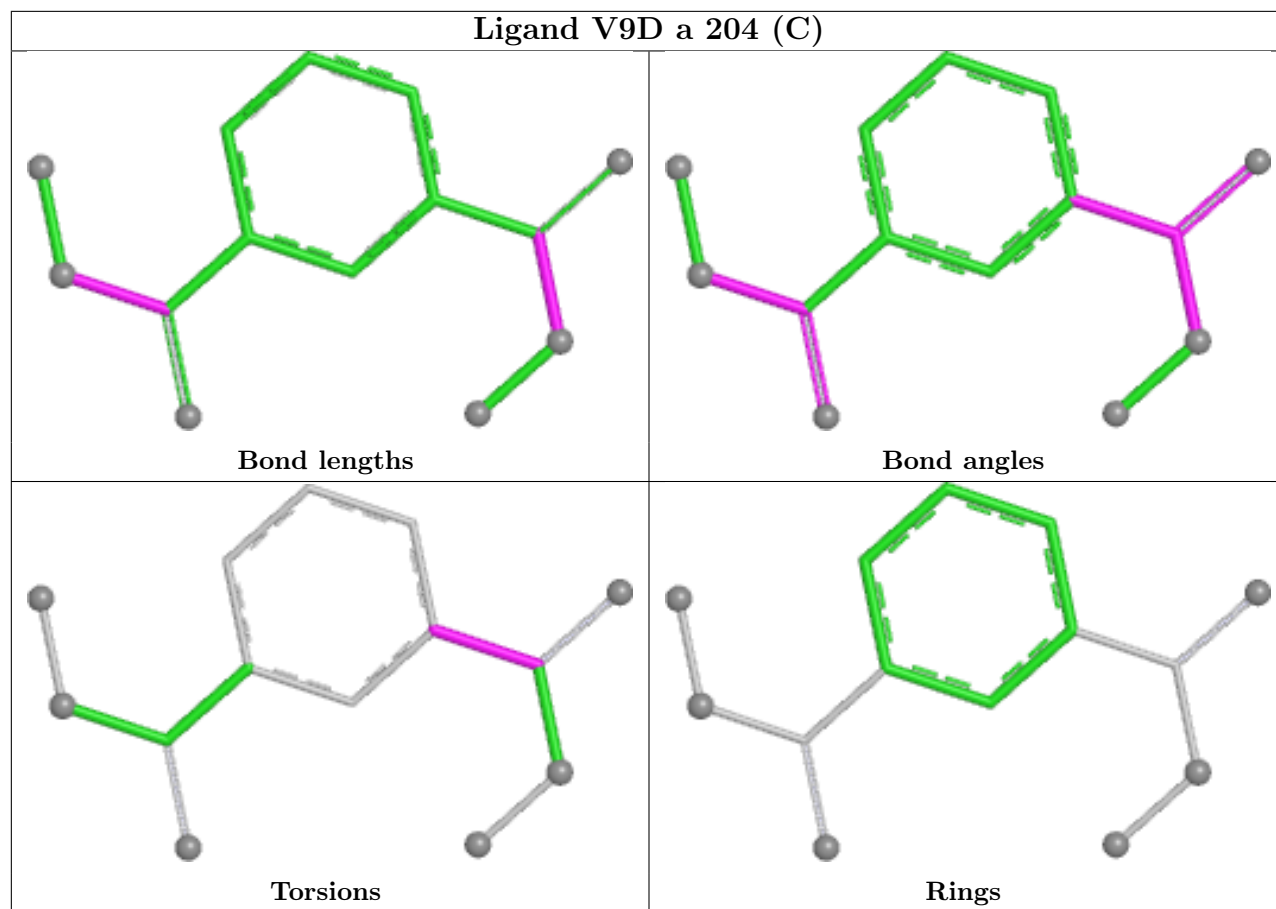


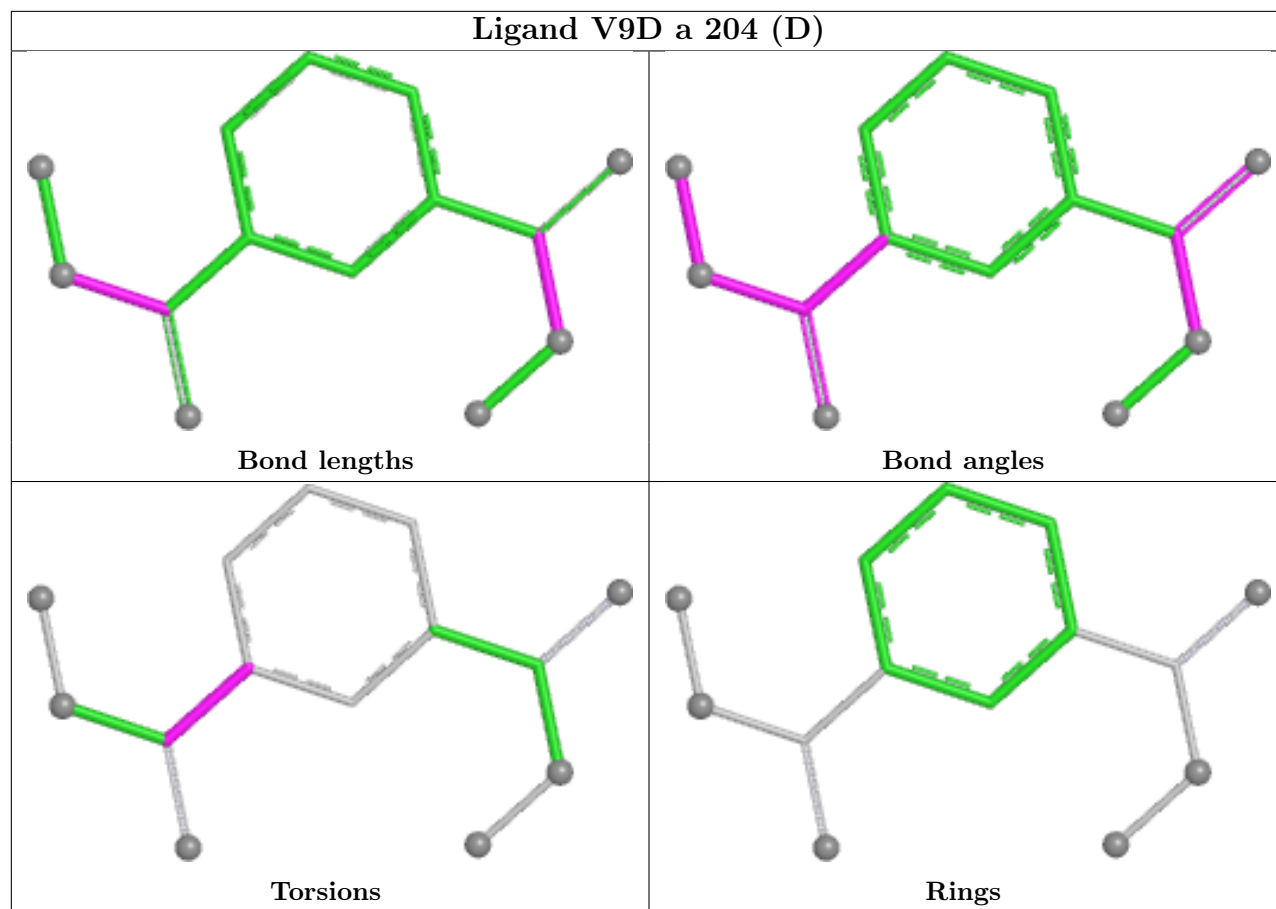
Ligand V9D W 202 (C)











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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	174/182 (95%)	-1.24	0 100 100	33, 42, 60, 89	0
1	B	174/182 (95%)	-1.28	0 100 100	30, 39, 56, 93	0
1	C	174/182 (95%)	-1.25	0 100 100	29, 42, 57, 90	0
1	D	174/182 (95%)	-1.30	0 100 100	30, 37, 53, 87	1 (0%)
1	E	174/182 (95%)	-1.35	0 100 100	29, 36, 54, 88	0
1	F	174/182 (95%)	-1.38	0 100 100	28, 36, 52, 92	1 (0%)
1	G	174/182 (95%)	-1.36	0 100 100	28, 37, 53, 82	1 (0%)
1	H	174/182 (95%)	-1.34	0 100 100	27, 35, 54, 90	0
1	I	174/182 (95%)	-1.33	0 100 100	28, 36, 52, 95	0
1	J	174/182 (95%)	-1.25	0 100 100	34, 42, 61, 86	0
1	K	174/182 (95%)	-1.34	0 100 100	30, 39, 57, 95	0
1	L	174/182 (95%)	-1.25	0 100 100	30, 41, 56, 93	0
1	M	174/182 (95%)	-1.22	0 100 100	32, 42, 60, 88	0
1	N	174/182 (95%)	-1.29	0 100 100	30, 39, 55, 96	0
1	O	174/182 (95%)	-1.33	0 100 100	31, 42, 56, 94	0
1	P	174/182 (95%)	-1.31	0 100 100	28, 37, 55, 89	0
1	Q	174/182 (95%)	-1.39	0 100 100	28, 36, 54, 88	0
1	R	174/182 (95%)	-1.31	0 100 100	28, 36, 51, 97	0
1	S	174/182 (95%)	-1.28	0 100 100	28, 36, 51, 87	1 (0%)
1	T	174/182 (95%)	-1.35	0 100 100	29, 36, 55, 91	0
1	U	174/182 (95%)	-1.34	0 100 100	28, 36, 53, 92	1 (0%)
1	V	174/182 (95%)	-1.28	0 100 100	33, 43, 61, 88	0
1	W	174/182 (95%)	-1.27	0 100 100	30, 39, 56, 91	0
1	X	174/182 (95%)	-1.25	0 100 100	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%)	-0.91	1 (0%) 85 86	15, 17, 22, 30	174 (100%)
1	b	174/182 (95%)	-0.85	1 (0%) 85 86	15, 17, 22, 31	174 (100%)
1	c	174/182 (95%)	-0.85	1 (0%) 85 86	16, 18, 23, 33	174 (100%)
1	d	174/182 (95%)	-0.86	2 (1%) 78 79	15, 17, 22, 33	174 (100%)
1	e	174/182 (95%)	-0.85	1 (0%) 85 86	15, 18, 23, 33	174 (100%)
1	f	174/182 (95%)	-0.91	0 100 100	16, 18, 23, 31	174 (100%)
1	g	174/182 (95%)	-0.91	2 (1%) 78 79	15, 17, 21, 31	174 (100%)
1	h	174/182 (95%)	-0.87	1 (0%) 85 86	15, 18, 22, 31	174 (100%)
1	i	174/182 (95%)	-0.88	0 100 100	15, 18, 23, 32	174 (100%)
1	j	174/182 (95%)	-0.88	0 100 100	15, 17, 22, 30	174 (100%)
1	k	174/182 (95%)	-0.85	1 (0%) 85 86	15, 17, 22, 31	174 (100%)
1	l	174/182 (95%)	-0.88	2 (1%) 78 79	16, 18, 23, 34	174 (100%)
1	m	174/182 (95%)	-0.80	1 (0%) 85 86	16, 18, 23, 31	174 (100%)
1	n	174/182 (95%)	-0.74	2 (1%) 78 79	15, 17, 22, 30	174 (100%)
1	o	174/182 (95%)	-0.74	2 (1%) 78 79	15, 18, 22, 33	174 (100%)
1	p	174/182 (95%)	-0.84	0 100 100	16, 18, 24, 35	174 (100%)
1	q	174/182 (95%)	-0.76	0 100 100	15, 17, 22, 31	174 (100%)
1	r	174/182 (95%)	-0.69	2 (1%) 78 79	15, 18, 23, 32	174 (100%)
1	s	174/182 (95%)	-0.79	0 100 100	16, 18, 23, 31	174 (100%)
1	t	174/182 (95%)	-0.75	2 (1%) 78 79	15, 17, 22, 31	174 (100%)
1	u	174/182 (95%)	-0.74	3 (1%) 69 71	15, 18, 22, 34	174 (100%)
1	v	174/182 (95%)	-0.75	0 100 100	16, 18, 23, 31	174 (100%)
1	w	174/182 (95%)	-0.76	2 (1%) 78 79	15, 17, 22, 30	174 (100%)
1	x	174/182 (95%)	-0.77	2 (1%) 78 79	15, 17, 22, 33	174 (100%)
All	All	8352/8736 (95%)	-1.06	28 (0%) 90 90	15, 29, 52, 97	4181 (50%)

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	l	4[C]	SER	3.3
1	x	4[C]	SER	3.3
1	c	4[C]	SER	3.3
1	u	177[C]	ASP	3.2
1	e	177[C]	ASP	3.2

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
3	NA	d	204[C]	1/1	0.97	0.03	39,39,39,39	1
3	NA	d	204[D]	1/1	0.97	0.03	39,39,39,39	1
3	NA	S	203	1/1	0.98	0.09	56,56,56,56	0
4	V9D	F	203[C]	14/14	0.98	0.07	41,53,59,60	14
4	V9D	F	203[D]	14/14	0.98	0.07	41,47,50,54	14
2	NI	v	203[D]	1/1	0.99	0.03	78,78,78,78	1
2	NI	x	201[C]	1/1	0.99	0.02	44,44,44,44	1
2	NI	x	201[D]	1/1	0.99	0.02	41,41,41,41	1
3	NA	D	203	1/1	0.99	0.07	54,54,54,54	0
3	NA	G	203	1/1	0.99	0.08	49,49,49,49	0
3	NA	P	203	1/1	0.99	0.08	54,54,54,54	0
2	NI	f	202[C]	1/1	0.99	0.03	11,11,11,11	1
3	NA	V	202	1/1	0.99	0.05	51,51,51,51	0
3	NA	a	203[C]	1/1	0.99	0.06	36,36,36,36	1
3	NA	a	203[D]	1/1	0.99	0.06	36,36,36,36	1
2	NI	f	202[D]	1/1	0.99	0.03	30,30,30,30	1
2	NI	h	201[C]	1/1	0.99	0.02	44,44,44,44	1
3	NA	g	203[C]	1/1	0.99	0.03	39,39,39,39	1
3	NA	g	203[D]	1/1	0.99	0.03	39,39,39,39	1
3	NA	j	203[C]	1/1	0.99	0.04	37,37,37,37	1
3	NA	j	203[D]	1/1	0.99	0.04	38,38,38,38	1
3	NA	t	203[C]	1/1	0.99	0.03	41,41,41,41	1
3	NA	t	203[D]	1/1	0.99	0.03	37,37,37,37	1
2	NI	h	201[D]	1/1	0.99	0.02	51,51,51,51	1
2	NI	v	203[C]	1/1	0.99	0.03	15,15,15,15	1
4	V9D	I	202[C]	14/14	0.99	0.06	44,53,59,60	14
4	V9D	I	202[D]	14/14	0.99	0.06	41,45,52,52	14

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	V9D	R	202[C]	14/14	0.99	0.07	44,48,54,55	14
4	V9D	R	202[D]	14/14	0.99	0.07	48,54,60,64	14
4	V9D	W	202[C]	14/14	0.99	0.05	41,46,51,54	14
4	V9D	W	202[D]	14/14	0.99	0.05	48,54,60,62	14
4	V9D	a	204[C]	14/14	0.99	0.07	49,53,62,63	14
4	V9D	a	204[D]	14/14	0.99	0.07	43,45,54,61	14
4	V9D	j	204[C]	14/14	0.99	0.06	51,54,59,62	14
4	V9D	j	204[D]	14/14	0.99	0.06	42,45,50,56	14
4	V9D	n	202[C]	14/14	0.99	0.04	41,47,52,60	14
4	V9D	n	202[D]	14/14	0.99	0.04	48,55,60,64	14
4	V9D	t	204[C]	14/14	0.99	0.08	40,46,49,50	14
4	V9D	t	204[D]	14/14	0.99	0.08	46,55,59,60	14
2	NI	a	201[D]	1/1	1.00	0.01	47,47,47,47	1
2	NI	a	202[C]	1/1	1.00	0.02	45,45,45,45	1
2	NI	a	202[D]	1/1	1.00	0.02	47,47,47,47	1
2	NI	b	201[C]	1/1	1.00	0.01	41,41,41,41	1
2	NI	b	201[D]	1/1	1.00	0.01	44,44,44,44	1
2	NI	c	201[C]	1/1	1.00	0.01	49,49,49,49	1
2	NI	c	201[D]	1/1	1.00	0.01	53,53,53,53	1
2	NI	d	201[C]	1/1	1.00	0.02	40,40,40,40	1
2	NI	d	201[D]	1/1	1.00	0.02	44,44,44,44	1
2	NI	d	202[C]	1/1	1.00	0.02	50,50,50,50	1
2	NI	d	202[D]	1/1	1.00	0.02	41,41,41,41	1
2	NI	d	203[C]	1/1	1.00	0.01	27,27,27,27	1
2	NI	d	203[D]	1/1	1.00	0.01	35,35,35,35	1
2	NI	e	201[C]	1/1	1.00	0.02	41,41,41,41	1
2	NI	e	201[D]	1/1	1.00	0.02	53,53,53,53	1
2	NI	e	202[C]	1/1	1.00	0.01	31,31,31,31	1
2	NI	e	202[D]	1/1	1.00	0.01	32,32,32,32	1
2	NI	f	201[C]	1/1	1.00	0.02	43,43,43,43	1
2	NI	f	201[D]	1/1	1.00	0.02	45,45,45,45	1
2	NI	A	201	1/1	1.00	0.01	52,52,52,52	0
2	NI	A	202	1/1	1.00	0.01	37,37,37,37	1
2	NI	g	201[C]	1/1	1.00	0.01	39,39,39,39	1
2	NI	g	201[D]	1/1	1.00	0.01	73,73,73,73	1
2	NI	g	202[C]	1/1	1.00	0.03	48,48,48,48	1
2	NI	g	202[D]	1/1	1.00	0.03	44,44,44,44	1
2	NI	B	201	1/1	1.00	0.01	53,53,53,53	0
2	NI	B	202	1/1	1.00	0.00	50,50,50,50	0
2	NI	i	201[C]	1/1	1.00	0.01	42,42,42,42	1
2	NI	i	201[D]	1/1	1.00	0.01	46,46,46,46	1
2	NI	j	201[C]	1/1	1.00	0.01	39,39,39,39	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NI	j	201[D]	1/1	1.00	0.01	77,77,77,77	1
2	NI	j	202[C]	1/1	1.00	0.02	47,47,47,47	1
2	NI	j	202[D]	1/1	1.00	0.02	46,46,46,46	1
2	NI	k	201[C]	1/1	1.00	0.01	44,44,44,44	1
2	NI	k	201[D]	1/1	1.00	0.01	45,45,45,45	1
2	NI	l	201[C]	1/1	1.00	0.02	48,48,48,48	1
2	NI	l	201[D]	1/1	1.00	0.02	48,48,48,48	1
2	NI	m	201[C]	1/1	1.00	0.01	51,51,51,51	1
2	NI	m	201[D]	1/1	1.00	0.01	49,49,49,49	1
2	NI	m	202[C]	1/1	1.00	0.01	43,43,43,43	1
2	NI	m	202[D]	1/1	1.00	0.01	48,48,48,48	1
2	NI	n	201[C]	1/1	1.00	0.02	44,44,44,44	1
2	NI	n	201[D]	1/1	1.00	0.02	43,43,43,43	1
2	NI	o	201[C]	1/1	1.00	0.01	46,46,46,46	1
2	NI	o	201[D]	1/1	1.00	0.01	42,42,42,42	1
2	NI	p	201[C]	1/1	1.00	0.01	48,48,48,48	1
2	NI	p	201[D]	1/1	1.00	0.01	44,44,44,44	1
2	NI	p	202[C]	1/1	1.00	0.02	44,44,44,44	1
2	NI	p	202[D]	1/1	1.00	0.02	53,53,53,53	1
2	NI	q	201[C]	1/1	1.00	0.02	46,46,46,46	1
2	NI	q	201[D]	1/1	1.00	0.02	44,44,44,44	1
2	NI	r	201[C]	1/1	1.00	0.02	49,49,49,49	1
2	NI	r	201[D]	1/1	1.00	0.02	44,44,44,44	1
2	NI	s	201[C]	1/1	1.00	0.01	45,45,45,45	1
2	NI	s	201[D]	1/1	1.00	0.01	44,44,44,44	1
2	NI	t	201[C]	1/1	1.00	0.02	45,45,45,45	1
2	NI	t	201[D]	1/1	1.00	0.02	41,41,41,41	1
2	NI	t	202[C]	1/1	1.00	0.01	46,46,46,46	1
2	NI	t	202[D]	1/1	1.00	0.01	52,52,52,52	1
2	NI	u	201[C]	1/1	1.00	0.03	50,50,50,50	1
2	NI	u	201[D]	1/1	1.00	0.03	44,44,44,44	1
2	NI	v	201[C]	1/1	1.00	0.02	48,48,48,48	1
2	NI	v	201[D]	1/1	1.00	0.02	50,50,50,50	1
2	NI	v	202[C]	1/1	1.00	0.01	47,47,47,47	1
2	NI	v	202[D]	1/1	1.00	0.01	47,47,47,47	1
2	NI	B	203	1/1	1.00	0.01	29,29,29,29	1
2	NI	C	201	1/1	1.00	0.01	50,50,50,50	0
2	NI	w	201[C]	1/1	1.00	0.02	45,45,45,45	1
2	NI	w	201[D]	1/1	1.00	0.02	41,41,41,41	1
2	NI	w	202[C]	1/1	1.00	0.17	56,56,56,56	1
2	NI	w	202[D]	1/1	1.00	0.17	30,30,30,30	1
2	NI	C	202	1/1	1.00	0.01	27,27,27,27	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NI	D	201	1/1	1.00	0.01	50,50,50,50	0
2	NI	x	202[C]	1/1	1.00	0.01	28,28,28,28	1
2	NI	x	202[D]	1/1	1.00	0.01	27,27,27,27	1
3	NA	A	203	1/1	1.00	0.04	42,42,42,42	0
2	NI	D	202	1/1	1.00	0.01	46,46,46,46	0
2	NI	E	201	1/1	1.00	0.01	48,48,48,48	0
3	NA	J	202	1/1	1.00	0.04	44,44,44,44	0
3	NA	M	203	1/1	1.00	0.04	49,49,49,49	0
2	NI	F	201	1/1	1.00	0.01	48,48,48,48	0
2	NI	F	202	1/1	1.00	0.03	32,32,32,32	1
2	NI	G	201	1/1	1.00	0.01	49,49,49,49	0
2	NI	G	202	1/1	1.00	0.01	45,45,45,45	0
2	NI	H	201	1/1	1.00	0.01	47,47,47,47	0
2	NI	H	202	1/1	1.00	0.02	32,32,32,32	1
2	NI	I	201	1/1	1.00	0.01	48,48,48,48	0
2	NI	J	201	1/1	1.00	0.01	52,52,52,52	0
2	NI	K	201	1/1	1.00	0.01	49,49,49,49	0
2	NI	L	201	1/1	1.00	0.01	53,53,53,53	0
2	NI	L	202	1/1	1.00	0.01	54,54,54,54	0
3	NA	m	203[C]	1/1	1.00	0.03	37,37,37,37	1
3	NA	m	203[D]	1/1	1.00	0.03	37,37,37,37	1
3	NA	p	203[C]	1/1	1.00	0.01	40,40,40,40	1
3	NA	p	203[D]	1/1	1.00	0.01	40,40,40,40	1
2	NI	M	201	1/1	1.00	0.01	51,51,51,51	0
2	NI	M	202	1/1	1.00	0.01	50,50,50,50	0
3	NA	v	204[C]	1/1	1.00	0.02	39,39,39,39	1
3	NA	v	204[D]	1/1	1.00	0.02	42,42,42,42	1
2	NI	N	201	1/1	1.00	0.01	52,52,52,52	0
2	NI	O	201	1/1	1.00	0.03	55,55,55,55	0
2	NI	O	202	1/1	1.00	0.02	34,34,34,34	1
2	NI	P	201	1/1	1.00	0.01	54,54,54,54	0
2	NI	P	202	1/1	1.00	0.01	47,47,47,47	0
2	NI	Q	201	1/1	1.00	0.01	51,51,51,51	0
2	NI	R	201	1/1	1.00	0.01	48,48,48,48	0
2	NI	S	201	1/1	1.00	0.01	50,50,50,50	0
2	NI	S	202	1/1	1.00	0.01	46,46,46,46	0
2	NI	T	201	1/1	1.00	0.01	50,50,50,50	0
2	NI	U	201	1/1	1.00	0.01	48,48,48,48	0
2	NI	V	201	1/1	1.00	0.01	55,55,55,55	0
2	NI	W	201	1/1	1.00	0.01	53,53,53,53	0
2	NI	X	201	1/1	1.00	0.01	54,54,54,54	0
2	NI	X	202	1/1	1.00	0.00	51,51,51,51	0

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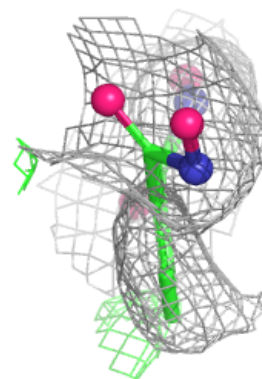
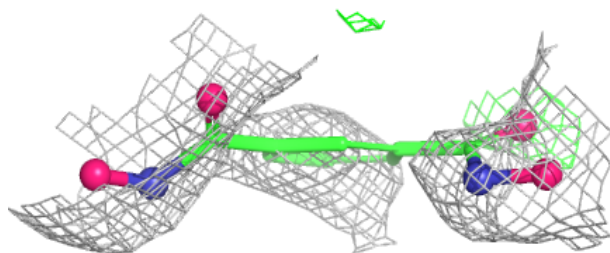
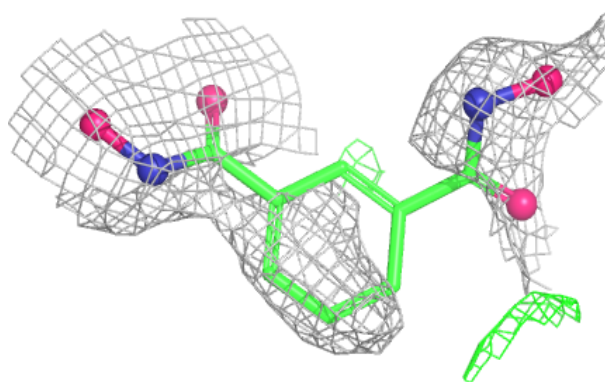
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NI	a	201[C]	1/1	1.00	0.01	40,40,40,40	1

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.

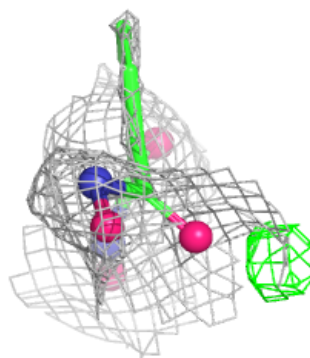
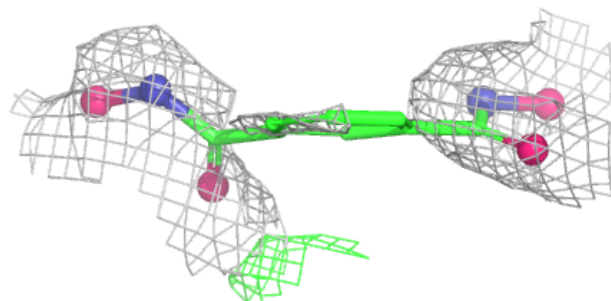
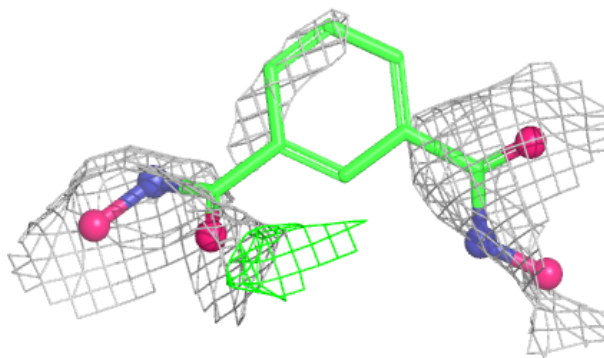
Electron density around V9D F 203 (C):

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

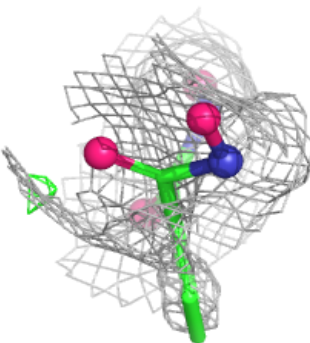
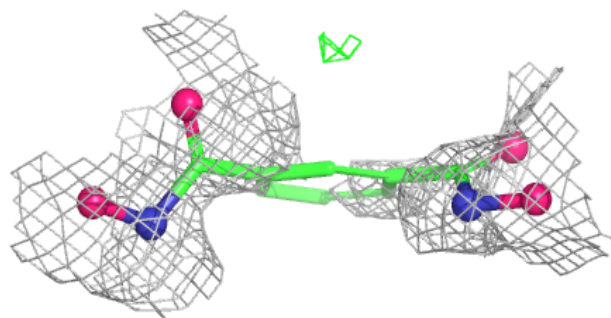
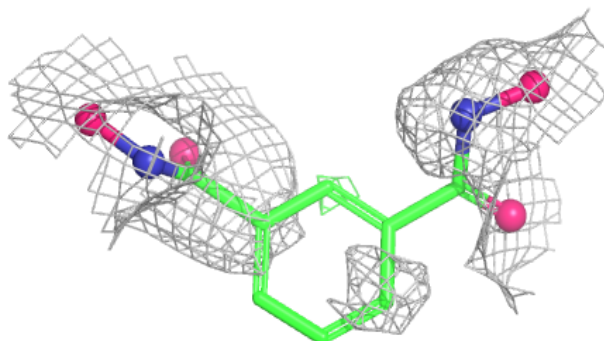


Electron density around V9D F 203 (D):

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

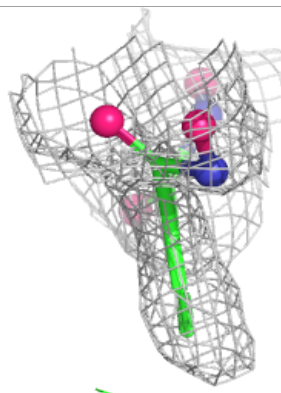
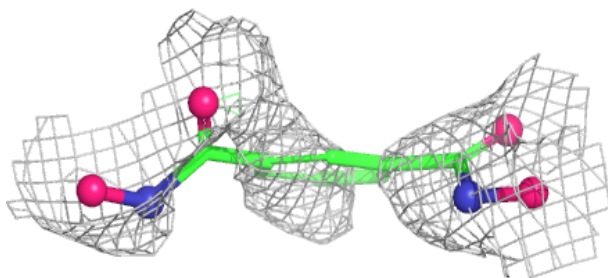
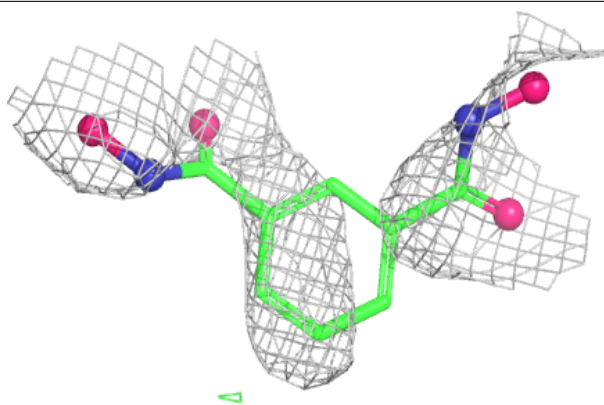
**Electron density around V9D I 202 (C):**

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

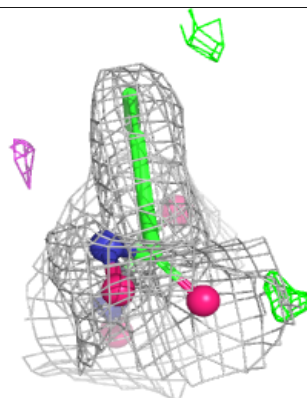
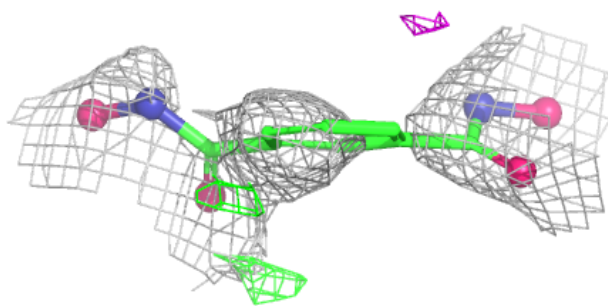
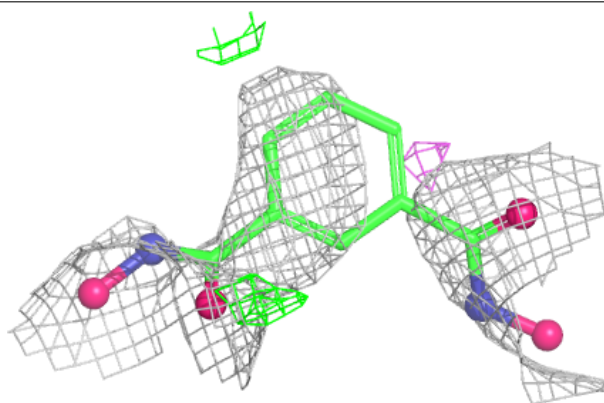


Electron density around V9D I 202 (D):

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

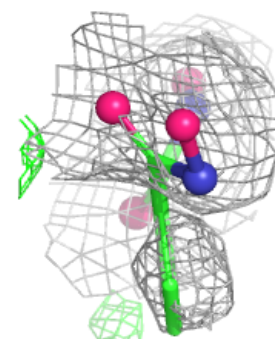
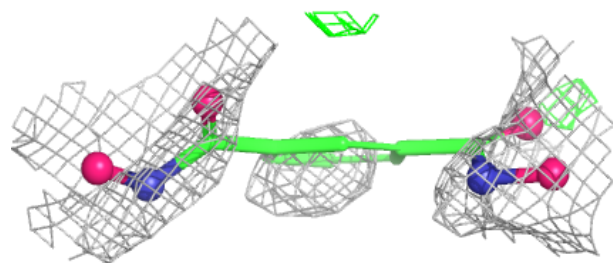
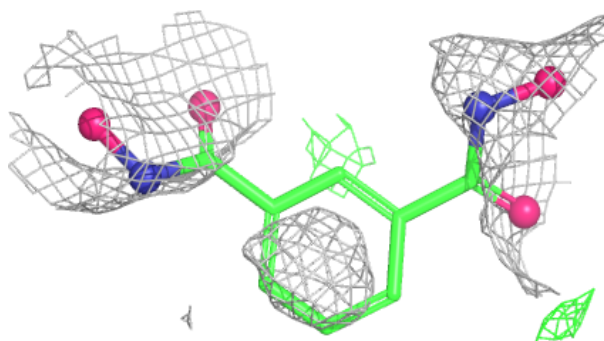
**Electron density around V9D R 202 (C):**

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and green (positive)

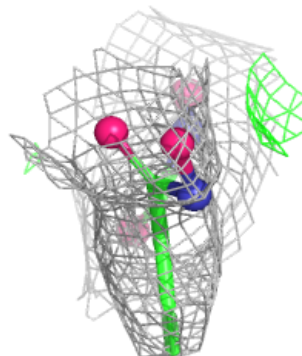
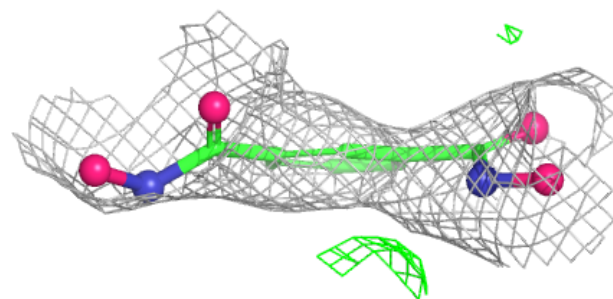
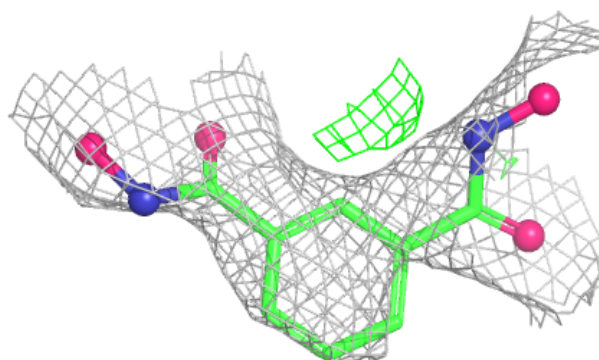


Electron density around V9D R 202 (D):

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

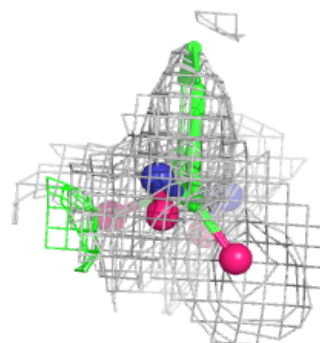
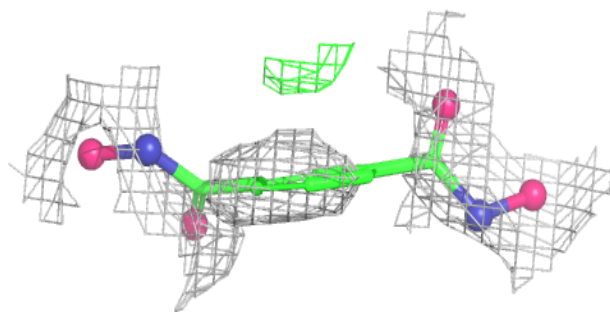
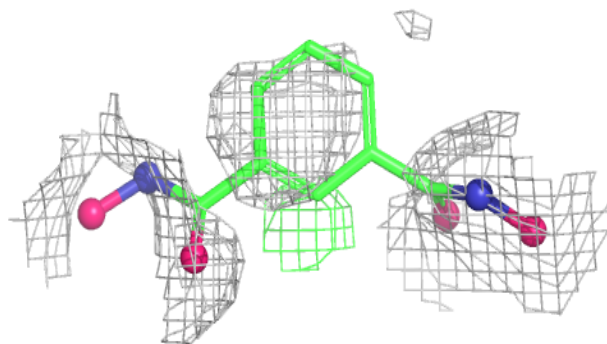
**Electron density around V9D W 202 (C):**

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

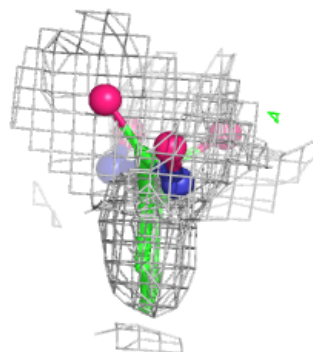
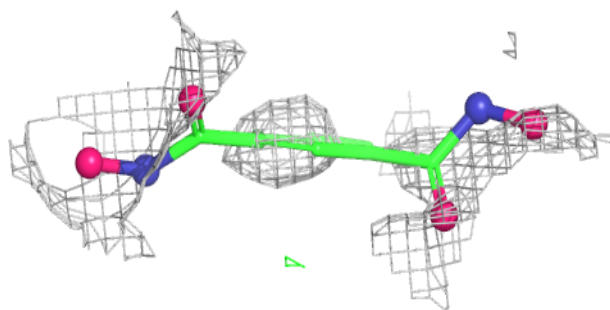
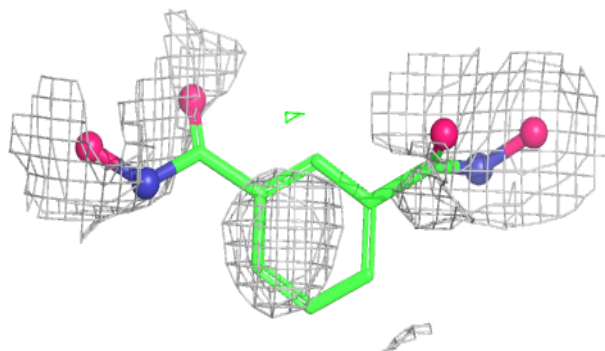


Electron density around V9D W 202 (D):

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

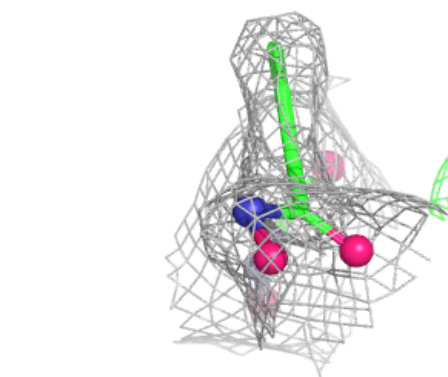
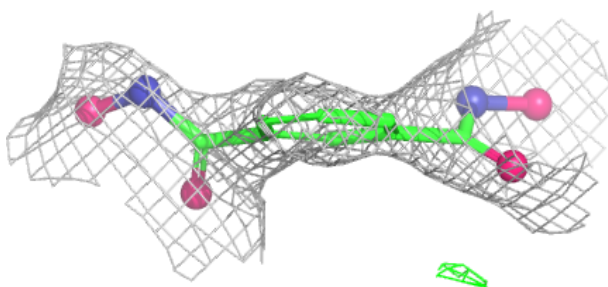
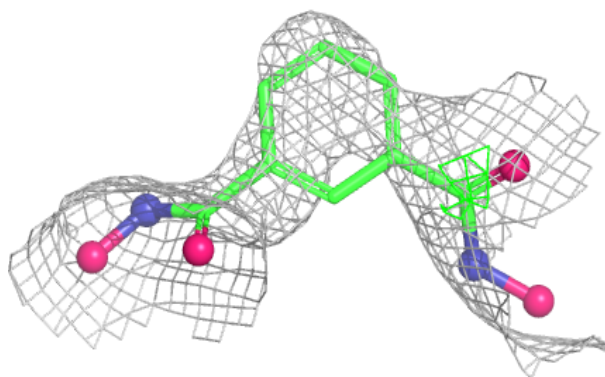
**Electron density around V9D a 204 (C):**

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

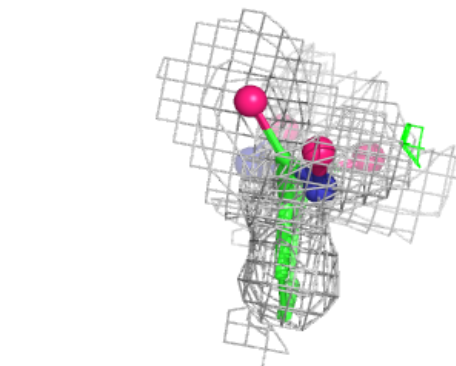
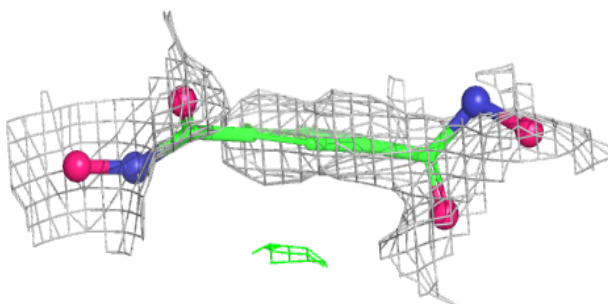
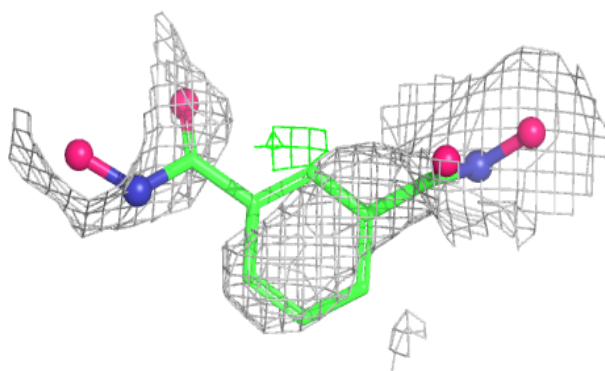


Electron density around V9D a 204 (D):

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

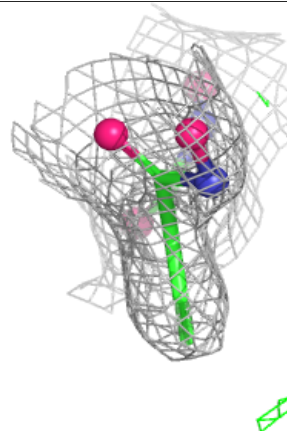
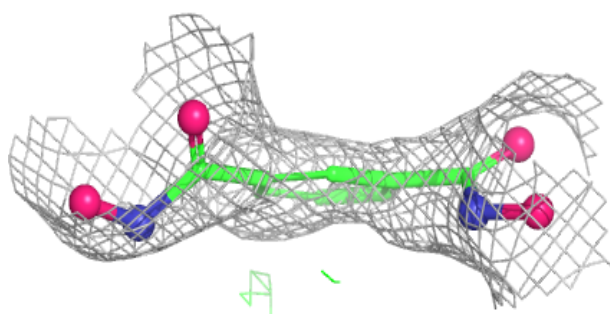
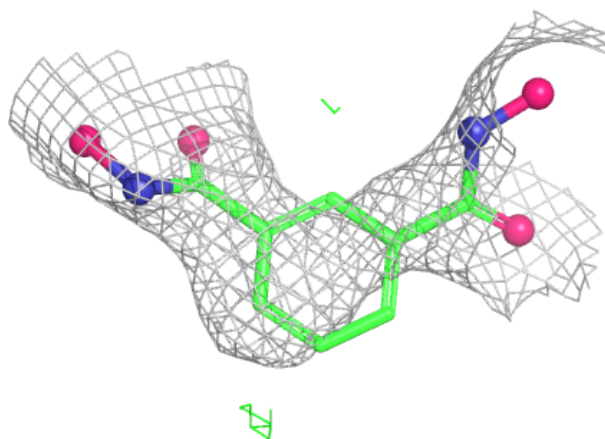
**Electron density around V9D j 204 (C):**

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

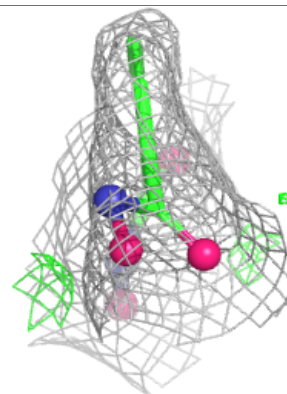
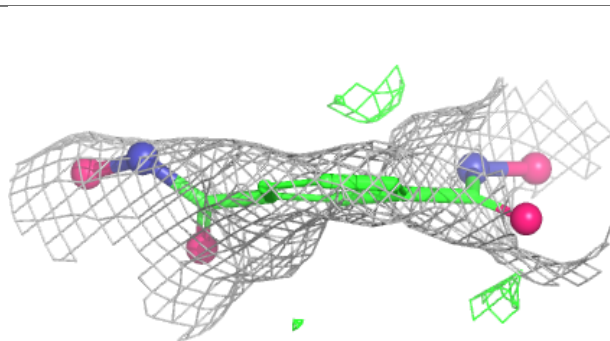
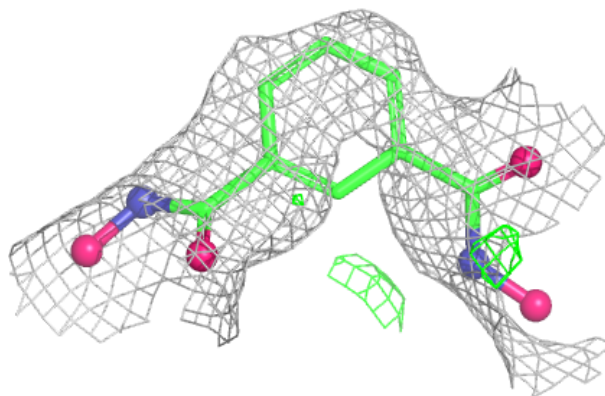


Electron density around V9D j 204 (D):

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

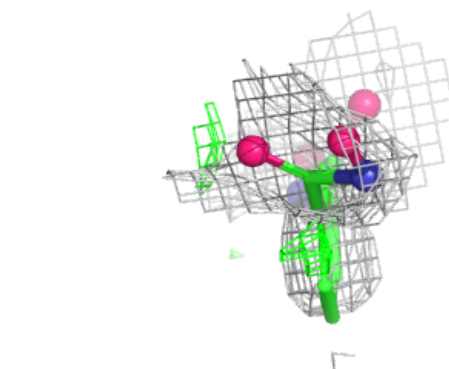
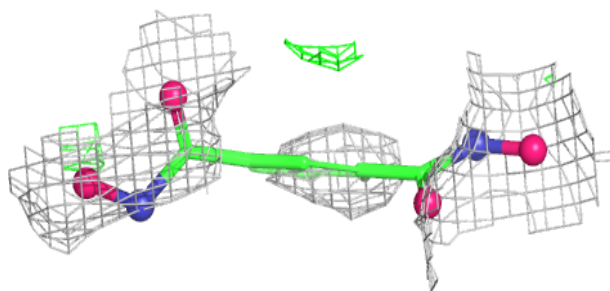
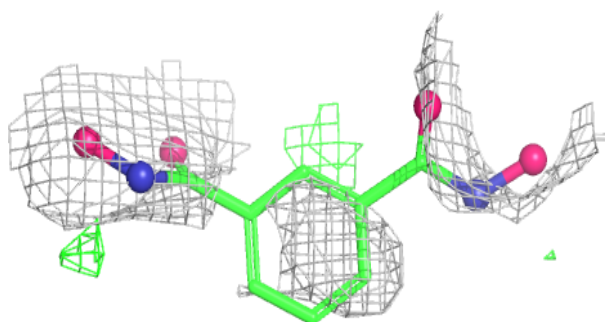
**Electron density around V9D n 202 (C):**

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

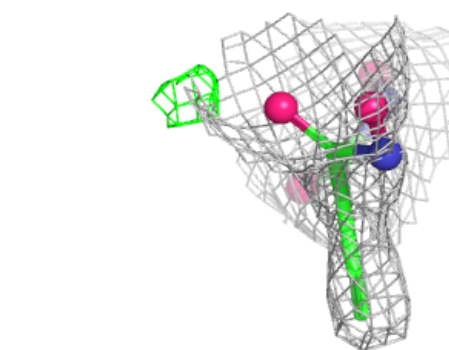
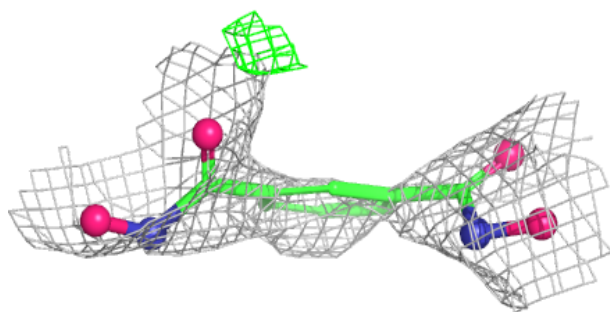
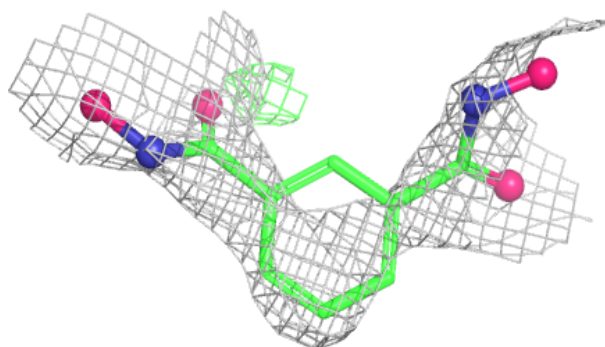


Electron density around V9D n 202 (D):

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

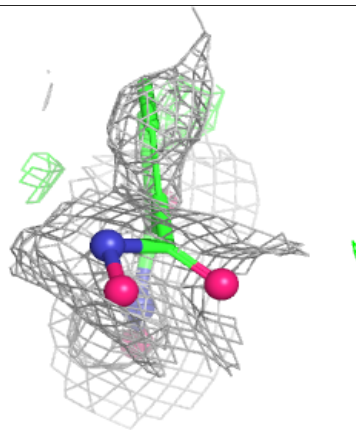
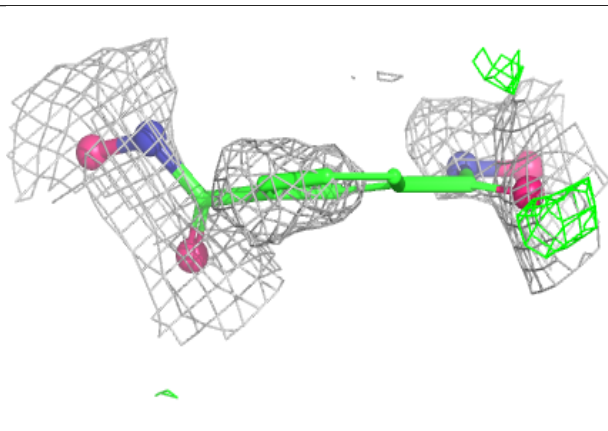
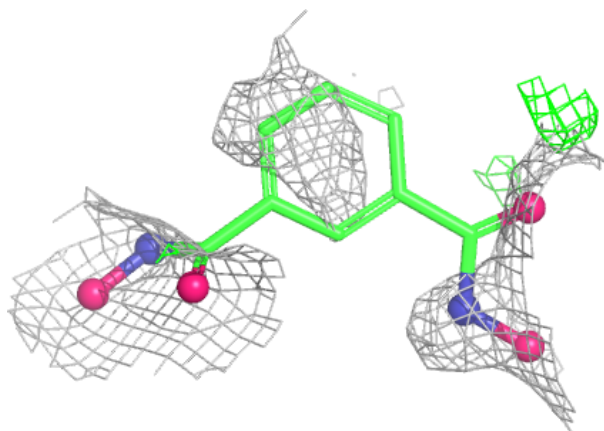
**Electron density around V9D t 204 (C):**

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



Electron density around V9D 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.