Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 02:20 AM EDT

PDB ID	:	7JGN
Title	:	Crystal Structure of the Zn-bound Human Heavy-chain variant 122H-delta C-star with meta-benzenedihyrdoxamate collected at 100K
Authors	:	Bailey, J.B.; Tezcan, F.A.
Deposited on	:	2020-07-19
Resolution	:	2.07 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

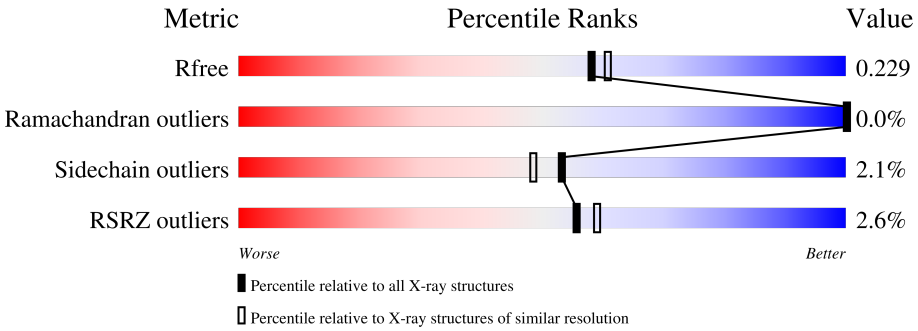
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.07 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	2684 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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 <=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	93%
1	B	182	93%
1	C	182	95%
1	D	182	94%
1	E	182	94%
1	F	182	% 95%

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Mol	Chain	Length	Quality of chain
1	G	182	95%
1	H	182	95%
1	I	182	94%
1	J	182	95%
1	K	182	95%
1	L	182	95%
1	M	182	94%
1	N	182	95%
1	O	182	95%
1	P	182	95%
1	Q	182	94%
1	R	182	94%
1	S	182	95%
1	T	182	94%
1	U	182	95%
1	V	182	94%
1	W	182	94%
1	X	182	93%
1	a	182	9% 93%
1	b	182	94%
1	c	182	4% 93%
1	d	182	7% 93%
1	e	182	4% 93%
1	f	182	7% 93%
1	g	182	5% 93%

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Mol	Chain	Length	Quality of chain
1	h	182	4% 92%
1	i	182	7% 94%
1	j	182	7% 93%
1	k	182	% 95%
1	l	182	7% 93%
1	m	182	5% 92%
1	n	182	5% 93%
1	o	182	2% 93%
1	p	182	6% 92%
1	q	182	3% 95%
1	r	182	3% 93%
1	s	182	5% 93%
1	t	182	5% 95%
1	u	182	2% 94%
1	v	182	4% 94%
1	w	182	10% 92%
1	x	182	% 93%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 108449 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	1	0
			1437	901	253	279	4			
1	C	174	Total	C	N	O	S	0	1	0
			1437	901	253	279	4			
1	D	174	Total	C	N	O	S	0	0	0
			1431	896	252	279	4			
1	E	174	Total	C	N	O	S	0	3	0
			1448	908	255	281	4			
1	F	174	Total	C	N	O	S	0	1	0
			1437	900	252	281	4			
1	G	174	Total	C	N	O	S	0	1	0
			1437	901	253	279	4			
1	H	174	Total	C	N	O	S	0	1	0
			1437	900	253	280	4			
1	I	174	Total	C	N	O	S	0	1	0
			1436	899	253	280	4			
1	J	174	Total	C	N	O	S	0	1	0
			1436	899	253	280	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	1	0
			1439	901	255	279	4			
1	O	174	Total	C	N	O	S	0	1	0
			1437	901	253	279	4			
1	P	174	Total	C	N	O	S	0	1	0
			1437	901	253	279	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	174	Total	C	N	O	S	0	2	0
			1443	905	254	280	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
			1437	901	253	279	4			
1	T	174	Total	C	N	O	S	0	1	0
			1436	899	253	280	4			
1	U	174	Total	C	N	O	S	0	2	0
			1444	904	256	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	3	0
			1453	911	259	279	4			
1	X	174	Total	C	N	O	S	0	1	0
			1437	901	253	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 ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Zn 4 4	0	0
2	B	3	Total Zn 3 3	0	0
2	C	3	Total Zn 3 3	0	0
2	D	3	Total Zn 3 3	0	0
2	E	2	Total Zn 2 2	0	0
2	F	3	Total Zn 3 3	0	0
2	G	3	Total Zn 3 3	0	0
2	H	3	Total Zn 3 3	0	0
2	I	2	Total Zn 2 2	0	0
2	J	3	Total Zn 3 3	0	0
2	K	2	Total Zn 2 2	0	0
2	L	2	Total Zn 2 2	0	0
2	M	2	Total Zn 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	N	2	Total Zn 2 2	0	0
2	O	4	Total Zn 4 4	0	0
2	P	3	Total Zn 3 3	0	0
2	Q	2	Total Zn 2 2	0	0
2	R	2	Total Zn 2 2	0	0
2	S	3	Total Zn 3 3	0	0
2	T	2	Total Zn 2 2	0	0
2	U	2	Total Zn 2 2	0	0
2	V	2	Total Zn 2 2	0	0
2	W	2	Total Zn 2 2	0	0
2	X	3	Total Zn 3 3	0	0
2	a	3	Total Zn 6 6	0	3
2	b	2	Total Zn 4 4	0	2
2	c	2	Total Zn 4 4	0	2
2	d	4	Total Zn 8 8	0	4
2	e	3	Total Zn 6 6	0	3
2	f	3	Total Zn 6 6	0	3
2	g	3	Total Zn 6 6	0	3
2	h	2	Total Zn 4 4	0	2
2	i	2	Total Zn 4 4	0	2
2	j	3	Total Zn 6 6	0	3

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	k	2	Total Zn 4 4	0	2
2	l	2	Total Zn 4 4	0	2
2	m	3	Total Zn 6 6	0	3
2	n	2	Total Zn 4 4	0	2
2	o	2	Total Zn 4 4	0	2
2	p	2	Total Zn 4 4	0	2
2	q	3	Total Zn 6 6	0	3
2	r	2	Total Zn 4 4	0	2
2	s	2	Total Zn 4 4	0	2
2	t	3	Total Zn 6 6	0	3
2	u	2	Total Zn 4 4	0	2
2	v	4	Total Zn 8 8	0	4
2	w	3	Total Zn 6 6	0	3
2	x	3	Total Zn 6 6	0	3

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

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

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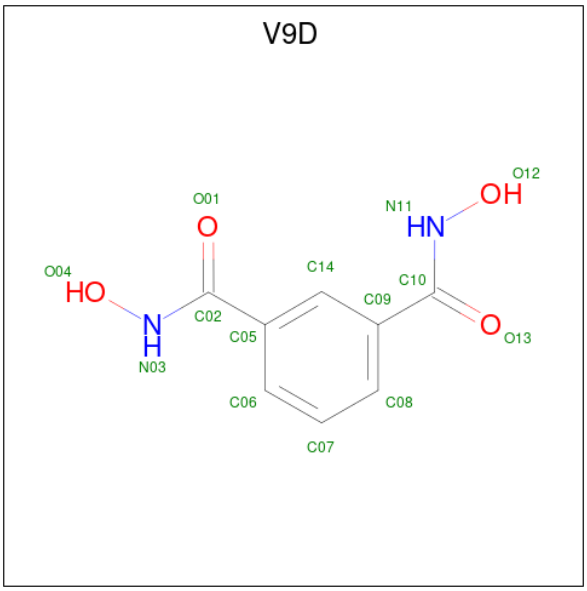
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	1	Total Na 1 1	0	0
3	S	1	Total Na 1 1	0	0
3	V	1	Total Na 1 1	0	0
3	a	1	Total Na 2 2	0	1
3	d	1	Total Na 2 2	0	1
3	g	1	Total Na 2 2	0	1
3	j	1	Total Na 2 2	0	1
3	m	1	Total Na 2 2	0	1
3	p	1	Total Na 2 2	0	1
3	s	1	Total Na 2 2	0	1
3	v	1	Total Na 2 2	0	1

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 28 16 4 8	0	1
4	E	1	Total C N O 28 16 4 8	0	1
4	H	1	Total C N O 28 16 4 8	0	1
4	K	1	Total C N O 28 16 4 8	0	1
4	O	1	Total C N O 28 16 4 8	0	1
4	Q	1	Total C N O 28 16 4 8	0	1
4	T	1	Total C N O 28 16 4 8	0	1
4	X	1	Total C N O 28 16 4 8	0	1

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	190	Total O 190 190	0	0
5	B	190	Total O 190 190	0	0
5	C	172	Total O 172 172	0	0
5	D	199	Total O 199 199	0	0
5	E	226	Total O 226 226	0	0
5	F	208	Total O 208 208	0	0
5	G	211	Total O 211 211	0	0
5	H	209	Total O 209 209	0	0
5	I	201	Total O 201 201	0	0
5	J	185	Total O 185 185	0	0
5	K	184	Total O 184 184	0	0
5	L	176	Total O 176 176	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	M	198	Total O 198 198	0	0
5	N	203	Total O 203 203	0	0
5	O	175	Total O 175 175	0	0
5	P	209	Total O 209 209	0	0
5	Q	221	Total O 221 221	0	0
5	R	200	Total O 200 200	0	0
5	S	211	Total O 211 211	0	0
5	T	223	Total O 223 223	0	0
5	U	218	Total O 218 218	0	0
5	V	190	Total O 190 190	0	0
5	W	183	Total O 183 183	0	0
5	X	184	Total O 184 184	0	0
5	a	3	Total O 3 3	0	0
5	b	2	Total O 2 2	0	0
5	c	3	Total O 3 3	0	0
5	d	3	Total O 3 3	0	0
5	e	1	Total O 1 1	0	0
5	f	5	Total O 5 5	0	0
5	g	4	Total O 4 4	0	0
5	h	2	Total O 2 2	0	0
5	i	3	Total O 3 3	0	0

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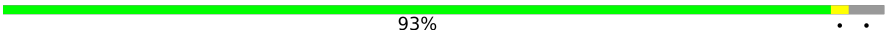
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	j	3	Total O 3 3	0	0
5	k	2	Total O 2 2	0	0
5	l	3	Total O 3 3	0	0
5	m	6	Total O 6 6	0	0
5	n	2	Total O 2 2	0	0
5	o	2	Total O 2 2	0	0
5	p	3	Total O 3 3	0	0
5	q	4	Total O 4 4	0	0
5	r	4	Total O 4 4	0	0
5	s	5	Total O 5 5	0	0
5	t	4	Total O 4 4	0	0
5	u	3	Total O 3 3	0	0
5	v	5	Total O 5 5	0	0
5	w	1	Total O 1 1	0	0
5	x	3	Total O 3 3	0	0

3 Residue-property plots (i)

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

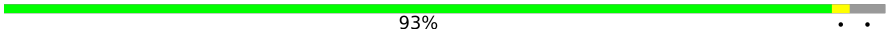
• Molecule 1: Ferritin heavy chain

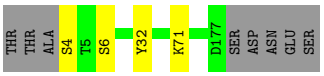
Chain A:



• Molecule 1: Ferritin heavy chain

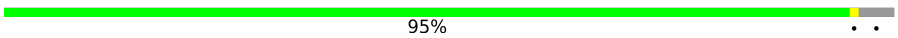
Chain B:

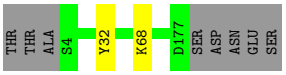




• Molecule 1: Ferritin heavy chain

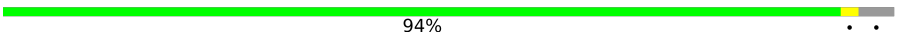
Chain C:

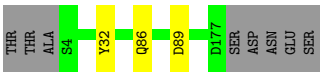




• Molecule 1: Ferritin heavy chain

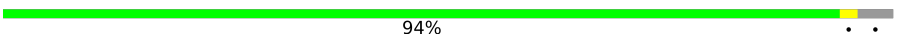
Chain D:

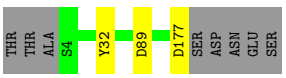




• Molecule 1: Ferritin heavy chain

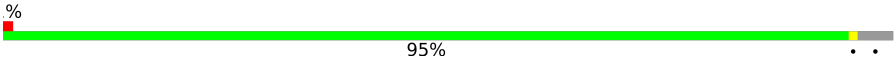
Chain E:

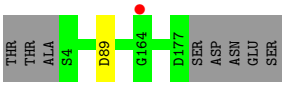




• Molecule 1: Ferritin heavy chain

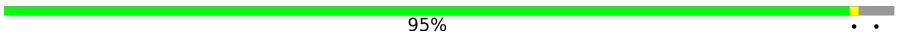
Chain F:

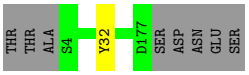




• Molecule 1: Ferritin heavy chain

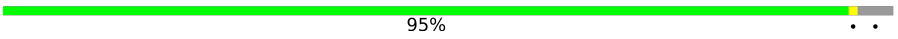
Chain G:

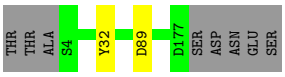




• Molecule 1: Ferritin heavy chain

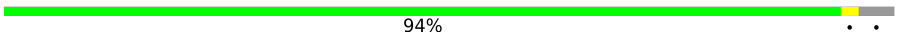
Chain H:

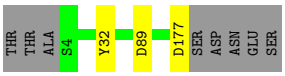




• Molecule 1: Ferritin heavy chain

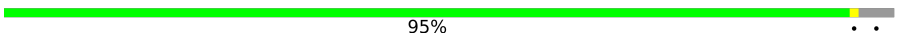
Chain I:

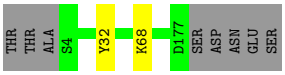




• Molecule 1: Ferritin heavy chain

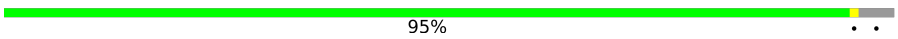
Chain J:





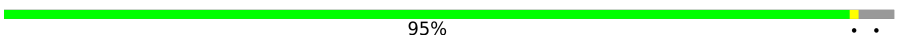
• Molecule 1: Ferritin heavy chain

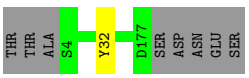
Chain K:



• Molecule 1: Ferritin heavy chain

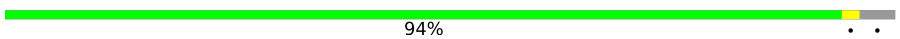
Chain L:

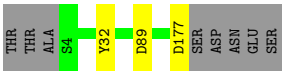




• Molecule 1: Ferritin heavy chain

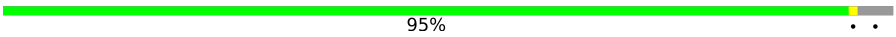
Chain M:

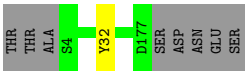




• Molecule 1: Ferritin heavy chain

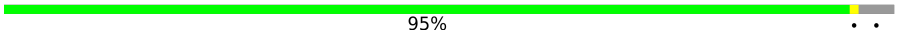
Chain N:





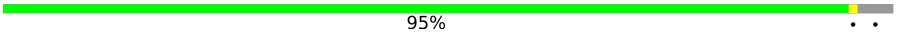
• Molecule 1: Ferritin heavy chain

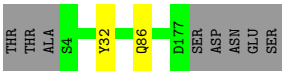
Chain O:



• Molecule 1: Ferritin heavy chain

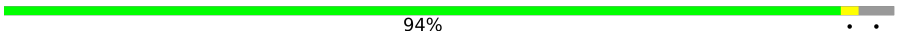
Chain P:





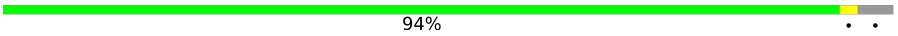
• Molecule 1: Ferritin heavy chain

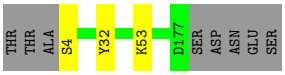
Chain Q:



• Molecule 1: Ferritin heavy chain

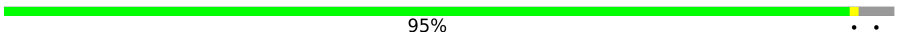
Chain R:

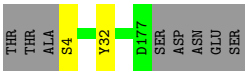




• Molecule 1: Ferritin heavy chain

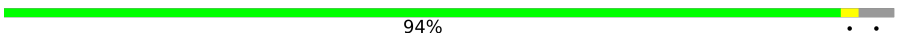
Chain S:





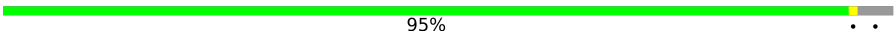
• Molecule 1: Ferritin heavy chain

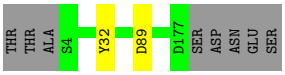
Chain T:



• Molecule 1: Ferritin heavy chain

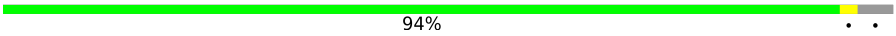
Chain U:





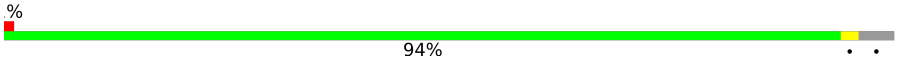
• Molecule 1: Ferritin heavy chain

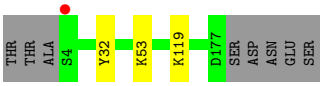
Chain V:



• Molecule 1: Ferritin heavy chain

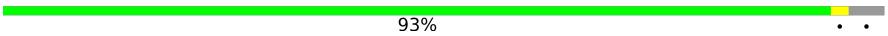
Chain W:





• Molecule 1: Ferritin heavy chain

Chain X:

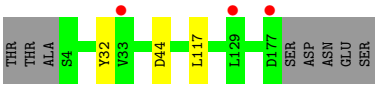


• Molecule 1: Ferritin heavy chain

Chain a:

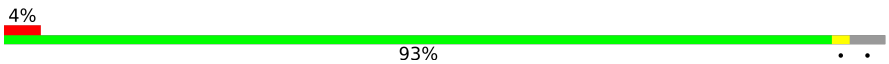
• Molecule 1: Ferritin heavy chain

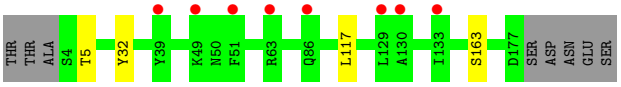
Chain b:



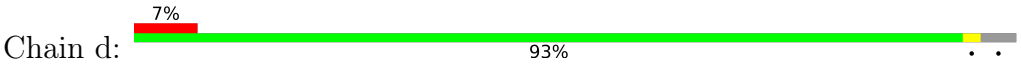
• Molecule 1: Ferritin heavy chain

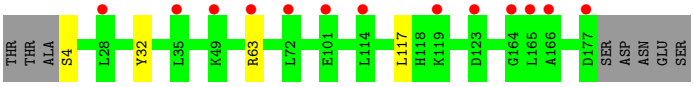
Chain c:



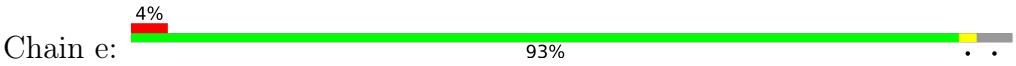


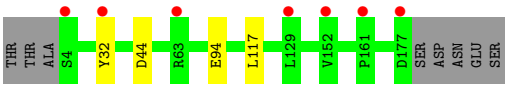
• Molecule 1: Ferritin heavy chain



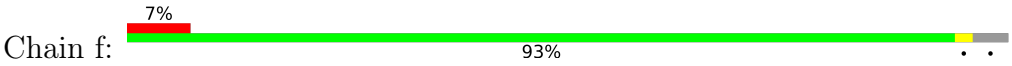


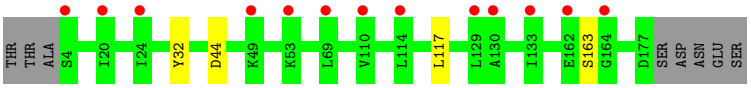
• Molecule 1: Ferritin heavy chain



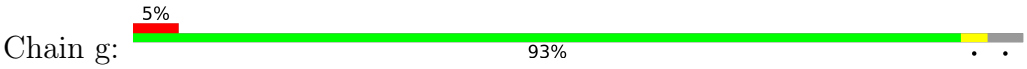


• Molecule 1: Ferritin heavy chain

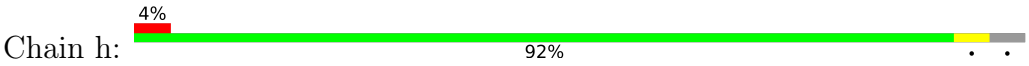


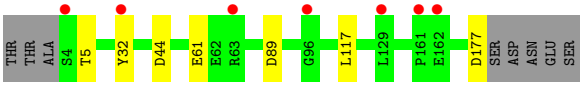


• Molecule 1: Ferritin heavy chain

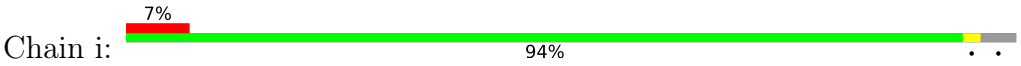


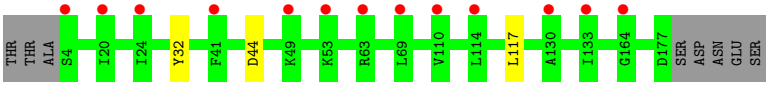
• Molecule 1: Ferritin heavy chain





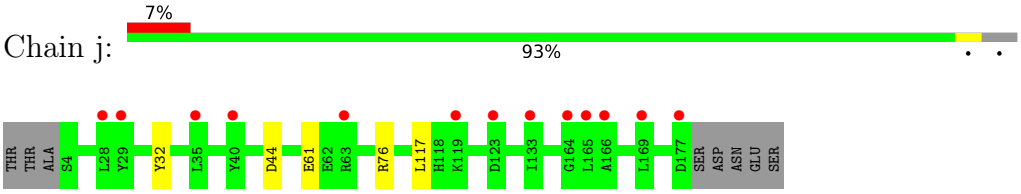
• Molecule 1: Ferritin heavy chain





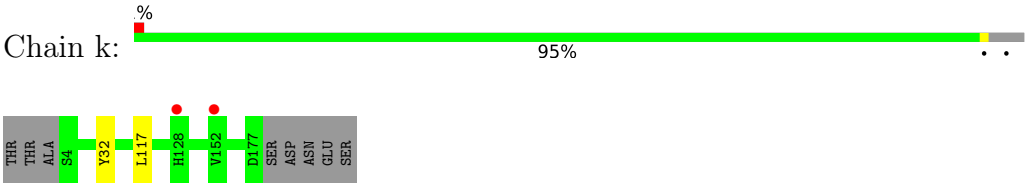
• Molecule 1: Ferritin heavy chain

Chain j:



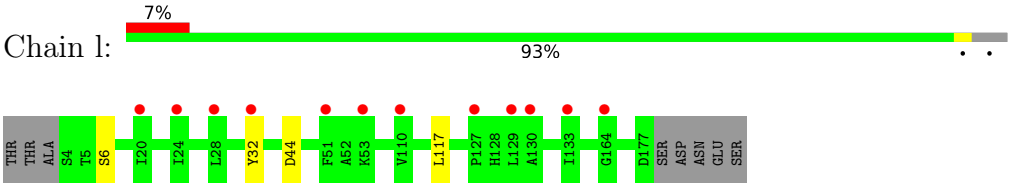
• Molecule 1: Ferritin heavy chain

Chain k:



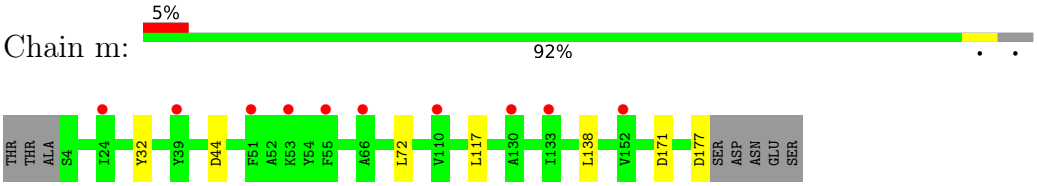
• Molecule 1: Ferritin heavy chain

Chain l:



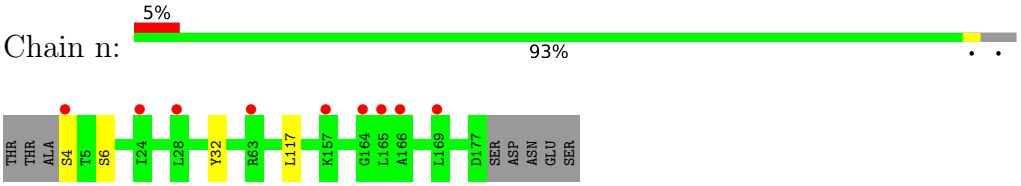
• Molecule 1: Ferritin heavy chain

Chain m:



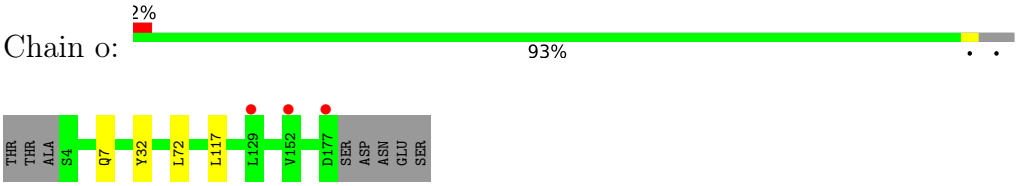
• Molecule 1: Ferritin heavy chain

Chain n:



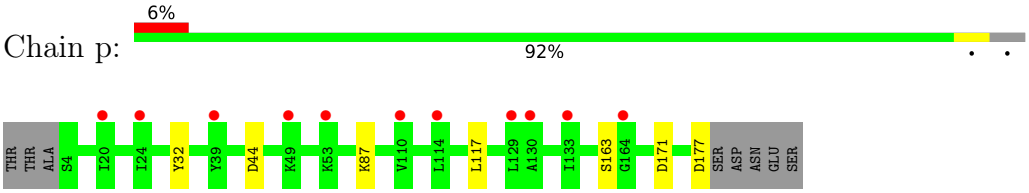
• Molecule 1: Ferritin heavy chain

Chain o:



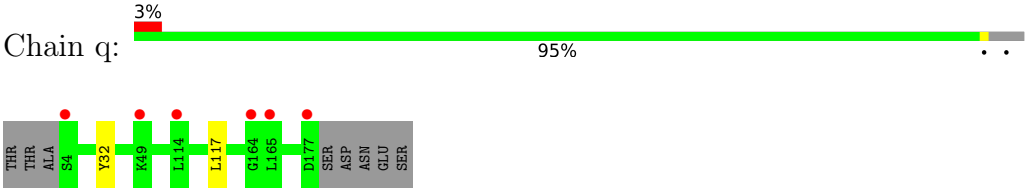
• Molecule 1: Ferritin heavy chain

Chain p:



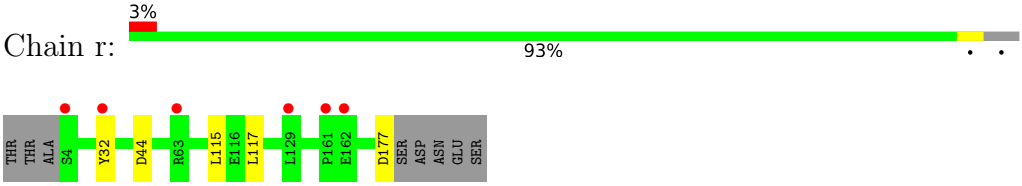
• Molecule 1: Ferritin heavy chain

Chain q:



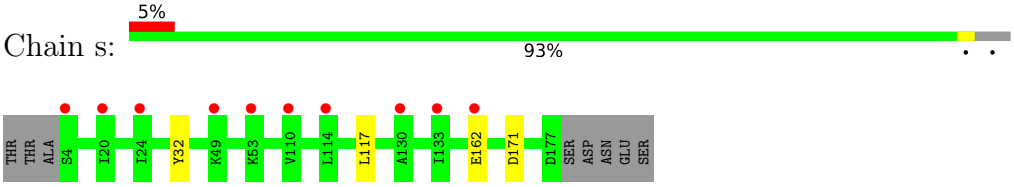
• Molecule 1: Ferritin heavy chain

Chain r:



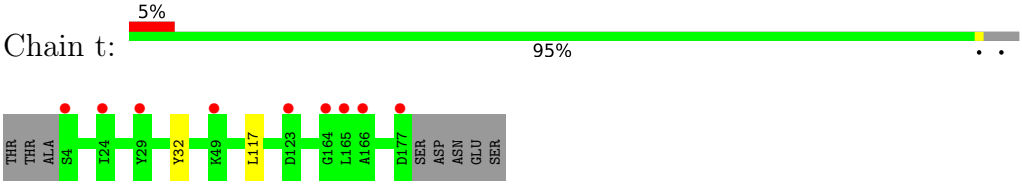
• Molecule 1: Ferritin heavy chain

Chain s:



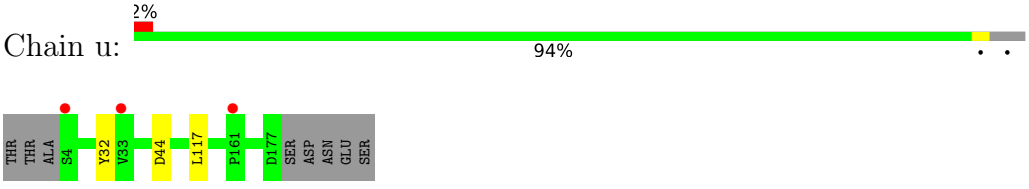
• Molecule 1: Ferritin heavy chain

Chain t:



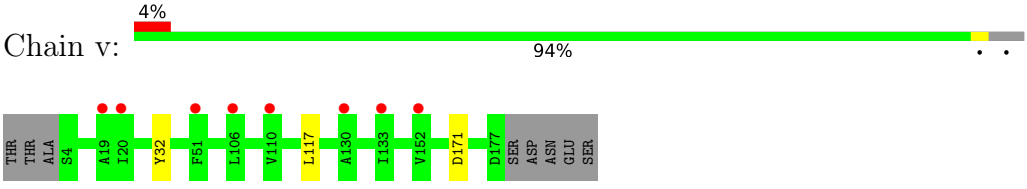
• Molecule 1: Ferritin heavy chain

Chain u:



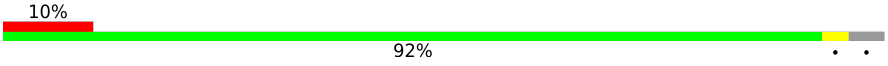
• Molecule 1: Ferritin heavy chain

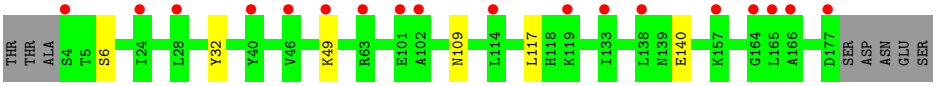
Chain v:



• Molecule 1: Ferritin heavy chain

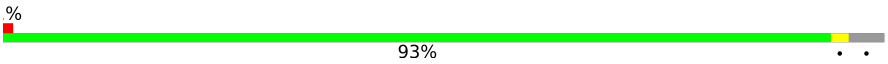
Chain w:





• Molecule 1: Ferritin heavy chain

Chain x:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	215.75Å 215.46Å 156.46Å 90.00° 89.95° 90.00°	Depositor
Resolution (Å)	37.80 – 2.07 39.32 – 2.07	Depositor EDS
% Data completeness (in resolution range)	97.5 (37.80-2.07) 90.4 (39.32-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 2.06Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.184 , 0.229 0.184 , 0.229	Depositor DCC
R_{free} test set	84387 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	26.2	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 41.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.477 for k,h,-l 0.477 for -k,-h,-l 0.478 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	108449	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NA, ZN, 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	0.50	0/1461	0.63	0/1969
1	B	0.49	0/1470	0.61	0/1980
1	C	0.48	0/1470	0.59	0/1980
1	D	0.53	0/1461	0.62	0/1969
1	E	0.53	0/1487	0.62	0/2003
1	F	0.51	0/1470	0.62	0/1981
1	G	0.53	0/1470	0.66	0/1980
1	H	0.54	0/1470	0.63	0/1981
1	I	0.54	0/1469	0.62	0/1980
1	J	0.52	0/1469	0.61	0/1980
1	K	0.52	0/1461	0.59	0/1969
1	L	0.49	0/1461	0.58	0/1969
1	M	0.48	0/1461	0.59	0/1969
1	N	0.50	0/1472	0.60	0/1983
1	O	0.48	0/1470	0.61	0/1980
1	P	0.53	0/1470	0.62	0/1980
1	Q	0.57	0/1479	0.62	0/1992
1	R	0.54	0/1461	0.62	0/1969
1	S	0.53	0/1470	0.65	0/1980
1	T	0.55	0/1469	0.63	0/1980
1	U	0.52	0/1480	0.63	0/1994
1	V	0.50	0/1461	0.60	0/1969
1	W	0.52	0/1492	0.60	0/2008
1	X	0.51	0/1470	0.60	0/1980
1	a	0.41	0/2922	0.54	2/3938 (0.1%)
1	b	0.39	0/2922	0.50	0/3938
1	c	0.40	0/2922	0.51	0/3938
1	d	0.42	0/2922	0.53	0/3938
1	e	0.40	0/2922	0.54	0/3938
1	f	0.40	0/2922	0.50	0/3938
1	g	0.43	0/2922	0.53	0/3938
1	h	0.39	0/2922	0.53	0/3938

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	i	0.40	0/2922	0.50	0/3938
1	j	0.40	0/2922	0.54	2/3938 (0.1%)
1	k	0.39	0/2922	0.49	0/3938
1	l	0.41	0/2922	0.54	0/3938
1	m	0.38	0/2922	0.53	0/3938
1	n	0.40	0/2922	0.52	0/3938
1	o	0.40	0/2922	0.54	0/3938
1	p	0.39	0/2922	0.52	0/3938
1	q	0.39	0/2922	0.49	0/3938
1	r	0.42	0/2922	0.53	0/3938
1	s	0.40	0/2922	0.53	0/3938
1	t	0.39	0/2922	0.52	0/3938
1	u	0.42	0/2922	0.52	0/3938
1	v	0.39	0/2922	0.52	0/3938
1	w	0.40	0/2922	0.52	0/3938
1	x	0.42	0/2922	0.53	0/3938
All	All	0.44	0/105402	0.55	4/142037 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	76[C]	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	a	76[D]	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	j	76[C]	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	j	76[D]	ARG	NE-CZ-NH2	-5.68	117.46	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	172/182 (94%)	168 (98%)	4 (2%)	0	100	100
1	B	173/182 (95%)	168 (97%)	5 (3%)	0	100	100
1	C	173/182 (95%)	170 (98%)	3 (2%)	0	100	100
1	D	172/182 (94%)	168 (98%)	4 (2%)	0	100	100
1	E	175/182 (96%)	173 (99%)	2 (1%)	0	100	100
1	F	173/182 (95%)	169 (98%)	4 (2%)	0	100	100
1	G	173/182 (95%)	169 (98%)	4 (2%)	0	100	100
1	H	173/182 (95%)	170 (98%)	3 (2%)	0	100	100
1	I	173/182 (95%)	170 (98%)	3 (2%)	0	100	100
1	J	173/182 (95%)	170 (98%)	3 (2%)	0	100	100
1	K	172/182 (94%)	165 (96%)	7 (4%)	0	100	100
1	L	172/182 (94%)	168 (98%)	4 (2%)	0	100	100
1	M	172/182 (94%)	169 (98%)	3 (2%)	0	100	100
1	N	173/182 (95%)	170 (98%)	3 (2%)	0	100	100
1	O	173/182 (95%)	168 (97%)	5 (3%)	0	100	100
1	P	173/182 (95%)	169 (98%)	4 (2%)	0	100	100
1	Q	174/182 (96%)	172 (99%)	2 (1%)	0	100	100
1	R	172/182 (94%)	169 (98%)	3 (2%)	0	100	100
1	S	173/182 (95%)	169 (98%)	4 (2%)	0	100	100
1	T	173/182 (95%)	170 (98%)	3 (2%)	0	100	100
1	U	174/182 (96%)	170 (98%)	4 (2%)	0	100	100
1	V	172/182 (94%)	169 (98%)	3 (2%)	0	100	100
1	W	175/182 (96%)	171 (98%)	4 (2%)	0	100	100
1	X	173/182 (95%)	169 (98%)	4 (2%)	0	100	100
1	a	344/182 (189%)	336 (98%)	8 (2%)	0	100	100
1	b	344/182 (189%)	338 (98%)	6 (2%)	0	100	100
1	c	344/182 (189%)	336 (98%)	8 (2%)	0	100	100
1	d	344/182 (189%)	334 (97%)	10 (3%)	0	100	100
1	e	344/182 (189%)	340 (99%)	2 (1%)	2 (1%)	25	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	f	344/182 (189%)	336 (98%)	6 (2%)	2 (1%)	25 15
1	g	344/182 (189%)	334 (97%)	10 (3%)	0	100 100
1	h	344/182 (189%)	340 (99%)	4 (1%)	0	100 100
1	i	344/182 (189%)	338 (98%)	6 (2%)	0	100 100
1	j	344/182 (189%)	336 (98%)	8 (2%)	0	100 100
1	k	344/182 (189%)	338 (98%)	6 (2%)	0	100 100
1	l	344/182 (189%)	338 (98%)	6 (2%)	0	100 100
1	m	344/182 (189%)	336 (98%)	8 (2%)	0	100 100
1	n	344/182 (189%)	338 (98%)	6 (2%)	0	100 100
1	o	344/182 (189%)	338 (98%)	6 (2%)	0	100 100
1	p	344/182 (189%)	334 (97%)	10 (3%)	0	100 100
1	q	344/182 (189%)	334 (97%)	10 (3%)	0	100 100
1	r	344/182 (189%)	340 (99%)	4 (1%)	0	100 100
1	s	344/182 (189%)	332 (96%)	10 (3%)	2 (1%)	25 15
1	t	344/182 (189%)	332 (96%)	12 (4%)	0	100 100
1	u	344/182 (189%)	342 (99%)	2 (1%)	0	100 100
1	v	344/182 (189%)	332 (96%)	12 (4%)	0	100 100
1	w	344/182 (189%)	338 (98%)	6 (2%)	0	100 100
1	x	344/182 (189%)	340 (99%)	4 (1%)	0	100 100
All	All	12407/8736 (142%)	12143 (98%)	258 (2%)	6 (0%)	100 100

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	f	163[C]	SER
1	f	163[D]	SER
1	s	162[C]	GLU
1	s	162[D]	GLU
1	e	94[C]	GLU
1	e	94[D]	GLU

5.3.2 Protein sidechains (i)

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%)	149 (97%)	4 (3%)	46	40
1	B	154/160 (96%)	150 (97%)	4 (3%)	46	40
1	C	154/160 (96%)	152 (99%)	2 (1%)	69	67
1	D	153/160 (96%)	150 (98%)	3 (2%)	55	51
1	E	156/160 (98%)	153 (98%)	3 (2%)	57	53
1	F	154/160 (96%)	153 (99%)	1 (1%)	86	86
1	G	154/160 (96%)	153 (99%)	1 (1%)	86	86
1	H	154/160 (96%)	152 (99%)	2 (1%)	69	67
1	I	154/160 (96%)	151 (98%)	3 (2%)	57	53
1	J	154/160 (96%)	152 (99%)	2 (1%)	69	67
1	K	153/160 (96%)	151 (99%)	2 (1%)	69	67
1	L	153/160 (96%)	152 (99%)	1 (1%)	84	84
1	M	153/160 (96%)	150 (98%)	3 (2%)	55	51
1	N	154/160 (96%)	153 (99%)	1 (1%)	86	86
1	O	154/160 (96%)	152 (99%)	2 (1%)	69	67
1	P	154/160 (96%)	152 (99%)	2 (1%)	69	67
1	Q	155/160 (97%)	152 (98%)	3 (2%)	57	53
1	R	153/160 (96%)	150 (98%)	3 (2%)	55	51
1	S	154/160 (96%)	152 (99%)	2 (1%)	69	67
1	T	154/160 (96%)	151 (98%)	3 (2%)	57	53
1	U	155/160 (97%)	153 (99%)	2 (1%)	69	67
1	V	153/160 (96%)	150 (98%)	3 (2%)	55	51
1	W	156/160 (98%)	153 (98%)	3 (2%)	57	53
1	X	154/160 (96%)	150 (97%)	4 (3%)	46	40
1	a	306/160 (191%)	298 (97%)	8 (3%)	46	40
1	b	306/160 (191%)	300 (98%)	6 (2%)	55	51
1	c	306/160 (191%)	298 (97%)	8 (3%)	46	40
1	d	306/160 (191%)	298 (97%)	8 (3%)	46	40
1	e	306/160 (191%)	300 (98%)	6 (2%)	55	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	f	306/160 (191%)	300 (98%)	6 (2%)	55	51
1	g	306/160 (191%)	296 (97%)	10 (3%)	38	31
1	h	306/160 (191%)	292 (95%)	14 (5%)	27	19
1	i	306/160 (191%)	300 (98%)	6 (2%)	55	51
1	j	306/160 (191%)	298 (97%)	8 (3%)	46	40
1	k	306/160 (191%)	302 (99%)	4 (1%)	69	67
1	l	306/160 (191%)	298 (97%)	8 (3%)	46	40
1	m	306/160 (191%)	292 (95%)	14 (5%)	27	19
1	n	306/160 (191%)	298 (97%)	8 (3%)	46	40
1	o	306/160 (191%)	298 (97%)	8 (3%)	46	40
1	p	306/160 (191%)	292 (95%)	14 (5%)	27	19
1	q	306/160 (191%)	302 (99%)	4 (1%)	69	67
1	r	306/160 (191%)	296 (97%)	10 (3%)	38	31
1	s	306/160 (191%)	300 (98%)	6 (2%)	55	51
1	t	306/160 (191%)	302 (99%)	4 (1%)	69	67
1	u	306/160 (191%)	300 (98%)	6 (2%)	55	51
1	v	306/160 (191%)	300 (98%)	6 (2%)	55	51
1	w	306/160 (191%)	294 (96%)	12 (4%)	32	25
1	x	306/160 (191%)	298 (97%)	8 (3%)	46	40
All	All	11039/7680 (144%)	10788 (98%)	251 (2%)	53	45

All (251) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	TYR
1	A	49	LYS
1	A	119	LYS
1	A	157	LYS
1	B	4	SER
1	B	6	SER
1	B	32	TYR
1	B	71	LYS
1	C	32	TYR
1	C	68	LYS
1	D	32	TYR

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Mol	Chain	Res	Type
1	D	86	GLN
1	D	89	ASP
1	E	32	TYR
1	E	89	ASP
1	E	177	ASP
1	F	89	ASP
1	G	32	TYR
1	H	32	TYR
1	H	89	ASP
1	I	32	TYR
1	I	89	ASP
1	I	177	ASP
1	J	32	TYR
1	J	68	LYS
1	K	32	TYR
1	K	177	ASP
1	L	32	TYR
1	M	32	TYR
1	M	89	ASP
1	M	177	ASP
1	N	32	TYR
1	O	32	TYR
1	O	177	ASP
1	P	32	TYR
1	P	86	GLN
1	Q	32	TYR
1	Q	68	LYS
1	Q	89	ASP
1	R	4	SER
1	R	32	TYR
1	R	53	LYS
1	S	4	SER
1	S	32	TYR
1	T	32	TYR
1	T	89	ASP
1	T	117	LEU
1	U	32	TYR
1	U	89	ASP
1	V	32	TYR
1	V	63	ARG
1	V	117	LEU
1	W	32	TYR

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Mol	Chain	Res	Type
1	W	53	LYS
1	W	119	LYS
1	X	4	SER
1	X	32	TYR
1	X	119	LYS
1	X	177	ASP
1	a	32[C]	TYR
1	a	32[D]	TYR
1	a	61[C]	GLU
1	a	61[D]	GLU
1	a	117[C]	LEU
1	a	117[D]	LEU
1	a	123[C]	ASP
1	a	123[D]	ASP
1	b	32[C]	TYR
1	b	32[D]	TYR
1	b	44[C]	ASP
1	b	44[D]	ASP
1	b	117[C]	LEU
1	b	117[D]	LEU
1	c	5[C]	THR
1	c	5[D]	THR
1	c	32[C]	TYR
1	c	32[D]	TYR
1	c	117[C]	LEU
1	c	117[D]	LEU
1	c	163[C]	SER
1	c	163[D]	SER
1	d	4[C]	SER
1	d	4[D]	SER
1	d	32[C]	TYR
1	d	32[D]	TYR
1	d	63[C]	ARG
1	d	63[D]	ARG
1	d	117[C]	LEU
1	d	117[D]	LEU
1	e	32[C]	TYR
1	e	32[D]	TYR
1	e	44[C]	ASP
1	e	44[D]	ASP
1	e	117[C]	LEU
1	e	117[D]	LEU

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Mol	Chain	Res	Type
1	f	32[C]	TYR
1	f	32[D]	TYR
1	f	44[C]	ASP
1	f	44[D]	ASP
1	f	117[C]	LEU
1	f	117[D]	LEU
1	g	32[C]	TYR
1	g	32[D]	TYR
1	g	61[C]	GLU
1	g	61[D]	GLU
1	g	63[C]	ARG
1	g	63[D]	ARG
1	g	91[C]	ASP
1	g	91[D]	ASP
1	g	117[C]	LEU
1	g	117[D]	LEU
1	h	5[C]	THR
1	h	5[D]	THR
1	h	32[C]	TYR
1	h	32[D]	TYR
1	h	44[C]	ASP
1	h	44[D]	ASP
1	h	61[C]	GLU
1	h	61[D]	GLU
1	h	89[C]	ASP
1	h	89[D]	ASP
1	h	117[C]	LEU
1	h	117[D]	LEU
1	h	177[C]	ASP
1	h	177[D]	ASP
1	i	32[C]	TYR
1	i	32[D]	TYR
1	i	44[C]	ASP
1	i	44[D]	ASP
1	i	117[C]	LEU
1	i	117[D]	LEU
1	j	32[C]	TYR
1	j	32[D]	TYR
1	j	44[C]	ASP
1	j	44[D]	ASP
1	j	61[C]	GLU
1	j	61[D]	GLU

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Mol	Chain	Res	Type
1	j	117[C]	LEU
1	j	117[D]	LEU
1	k	32[C]	TYR
1	k	32[D]	TYR
1	k	117[C]	LEU
1	k	117[D]	LEU
1	l	6[C]	SER
1	l	6[D]	SER
1	l	32[C]	TYR
1	l	32[D]	TYR
1	l	44[C]	ASP
1	l	44[D]	ASP
1	l	117[C]	LEU
1	l	117[D]	LEU
1	m	32[C]	TYR
1	m	32[D]	TYR
1	m	44[C]	ASP
1	m	44[D]	ASP
1	m	72[C]	LEU
1	m	72[D]	LEU
1	m	117[C]	LEU
1	m	117[D]	LEU
1	m	138[C]	LEU
1	m	138[D]	LEU
1	m	171[C]	ASP
1	m	171[D]	ASP
1	m	177[C]	ASP
1	m	177[D]	ASP
1	n	4[C]	SER
1	n	4[D]	SER
1	n	6[C]	SER
1	n	6[D]	SER
1	n	32[C]	TYR
1	n	32[D]	TYR
1	n	117[C]	LEU
1	n	117[D]	LEU
1	o	7[C]	GLN
1	o	7[D]	GLN
1	o	32[C]	TYR
1	o	32[D]	TYR
1	o	72[C]	LEU
1	o	72[D]	LEU

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Mol	Chain	Res	Type
1	o	117[C]	LEU
1	o	117[D]	LEU
1	p	32[C]	TYR
1	p	32[D]	TYR
1	p	44[C]	ASP
1	p	44[D]	ASP
1	p	87[C]	LYS
1	p	87[D]	LYS
1	p	117[C]	LEU
1	p	117[D]	LEU
1	p	163[C]	SER
1	p	163[D]	SER
1	p	171[C]	ASP
1	p	171[D]	ASP
1	p	177[C]	ASP
1	p	177[D]	ASP
1	q	32[C]	TYR
1	q	32[D]	TYR
1	q	117[C]	LEU
1	q	117[D]	LEU
1	r	32[C]	TYR
1	r	32[D]	TYR
1	r	44[C]	ASP
1	r	44[D]	ASP
1	r	115[C]	LEU
1	r	115[D]	LEU
1	r	117[C]	LEU
1	r	117[D]	LEU
1	r	177[C]	ASP
1	r	177[D]	ASP
1	s	32[C]	TYR
1	s	32[D]	TYR
1	s	117[C]	LEU
1	s	117[D]	LEU
1	s	171[C]	ASP
1	s	171[D]	ASP
1	t	32[C]	TYR
1	t	32[D]	TYR
1	t	117[C]	LEU
1	t	117[D]	LEU
1	u	32[C]	TYR
1	u	32[D]	TYR

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Mol	Chain	Res	Type
1	u	44[C]	ASP
1	u	44[D]	ASP
1	u	117[C]	LEU
1	u	117[D]	LEU
1	v	32[C]	TYR
1	v	32[D]	TYR
1	v	117[C]	LEU
1	v	117[D]	LEU
1	v	171[C]	ASP
1	v	171[D]	ASP
1	w	6[C]	SER
1	w	6[D]	SER
1	w	32[C]	TYR
1	w	32[D]	TYR
1	w	49[C]	LYS
1	w	49[D]	LYS
1	w	109[C]	ASN
1	w	109[D]	ASN
1	w	117[C]	LEU
1	w	117[D]	LEU
1	w	140[C]	GLU
1	w	140[D]	GLU
1	x	4[C]	SER
1	x	4[D]	SER
1	x	32[C]	TYR
1	x	32[D]	TYR
1	x	117[C]	LEU
1	x	117[D]	LEU
1	x	177[C]	ASP
1	x	177[D]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	122	HIS
1	F	122	HIS
1	I	86	GLN
1	I	122	HIS
1	L	122	HIS
1	Q	57	HIS
1	Q	58	GLN
1	R	86	GLN

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Mol	Chain	Res	Type
1	W	14	GLN
1	W	86	GLN
1	X	122	HIS

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 226 ligands modelled in this entry, 210 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	E	203[C]	2	14,14,14	3.92	3 (21%)	18,18,18	1.09	3 (16%)
4	V9D	K	203[C]	2	14,14,14	3.98	3 (21%)	18,18,18	1.81	4 (22%)
4	V9D	T	203[C]	2	14,14,14	3.84	2 (14%)	18,18,18	1.34	3 (16%)
4	V9D	X	204[C]	2	14,14,14	3.72	3 (21%)	18,18,18	1.49	4 (22%)
4	V9D	O	205[D]	2	14,14,14	4.05	4 (28%)	18,18,18	1.48	4 (22%)
4	V9D	B	204[C]	2	14,14,14	3.96	3 (21%)	18,18,18	1.53	4 (22%)
4	V9D	E	203[D]	2	14,14,14	3.81	2 (14%)	18,18,18	1.39	4 (22%)
4	V9D	K	203[D]	2	14,14,14	3.74	3 (21%)	18,18,18	1.37	4 (22%)
4	V9D	T	203[D]	2	14,14,14	3.98	3 (21%)	18,18,18	1.23	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	V9D	X	204[D]	2	14,14,14	3.99	4 (28%)	18,18,18	1.71	4 (22%)
4	V9D	H	204[C]	2	14,14,14	3.93	3 (21%)	18,18,18	1.24	4 (22%)
4	V9D	Q	203[C]	2	14,14,14	3.80	3 (21%)	18,18,18	1.34	4 (22%)
4	V9D	B	204[D]	2	14,14,14	3.77	3 (21%)	18,18,18	1.41	4 (22%)
4	V9D	O	205[C]	2	14,14,14	3.73	3 (21%)	18,18,18	1.32	4 (22%)
4	V9D	Q	203[D]	2	14,14,14	3.91	2 (14%)	18,18,18	1.10	3 (16%)
4	V9D	H	204[D]	2	14,14,14	3.84	3 (21%)	18,18,18	1.45	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	E	203[C]	2	-	4/12/12/12	0/1/1/1
4	V9D	K	203[C]	2	-	4/12/12/12	0/1/1/1
4	V9D	T	203[C]	2	-	4/12/12/12	0/1/1/1
4	V9D	X	204[C]	2	-	4/12/12/12	0/1/1/1
4	V9D	O	205[D]	2	-	4/12/12/12	0/1/1/1
4	V9D	B	204[C]	2	-	4/12/12/12	0/1/1/1
4	V9D	E	203[D]	2	-	7/12/12/12	0/1/1/1
4	V9D	K	203[D]	2	-	4/12/12/12	0/1/1/1
4	V9D	T	203[D]	2	-	4/12/12/12	0/1/1/1
4	V9D	X	204[D]	2	-	4/12/12/12	0/1/1/1
4	V9D	H	204[C]	2	-	4/12/12/12	0/1/1/1
4	V9D	Q	203[C]	2	-	5/12/12/12	0/1/1/1
4	V9D	B	204[D]	2	-	4/12/12/12	0/1/1/1
4	V9D	O	205[C]	2	-	4/12/12/12	0/1/1/1
4	V9D	Q	203[D]	2	-	4/12/12/12	0/1/1/1
4	V9D	H	204[D]	2	-	8/12/12/12	0/1/1/1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	205[D]	V9D	C10-N11	10.64	1.46	1.32
4	K	203[C]	V9D	C10-N11	10.37	1.46	1.32
4	H	204[D]	V9D	C02-N03	10.34	1.46	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	203[D]	V9D	C02-N03	10.33	1.46	1.32
4	T	203[C]	V9D	C02-N03	10.33	1.46	1.32
4	T	203[D]	V9D	C10-N11	10.31	1.46	1.32
4	B	204[C]	V9D	C10-N11	10.30	1.46	1.32
4	O	205[C]	V9D	C02-N03	10.27	1.46	1.32
4	X	204[C]	V9D	C02-N03	10.27	1.46	1.32
4	X	204[D]	V9D	C10-N11	10.26	1.46	1.32
4	H	204[C]	V9D	C10-N11	10.26	1.46	1.32
4	B	204[D]	V9D	C02-N03	10.18	1.46	1.32
4	K	203[D]	V9D	C02-N03	10.12	1.45	1.32
4	Q	203[D]	V9D	C10-N11	10.11	1.45	1.32
4	Q	203[C]	V9D	C02-N03	10.10	1.45	1.32
4	T	203[D]	V9D	C02-N03	10.08	1.45	1.32
4	E	203[C]	V9D	C10-N11	10.07	1.45	1.32
4	X	204[D]	V9D	C02-N03	10.01	1.45	1.32
4	E	203[C]	V9D	C02-N03	9.99	1.45	1.32
4	O	205[D]	V9D	C02-N03	9.98	1.45	1.32
4	Q	203[D]	V9D	C02-N03	9.91	1.45	1.32
4	B	204[C]	V9D	C02-N03	9.88	1.45	1.32
4	K	203[C]	V9D	C02-N03	9.84	1.45	1.32
4	H	204[C]	V9D	C02-N03	9.82	1.45	1.32
4	H	204[D]	V9D	C10-N11	9.35	1.44	1.32
4	Q	203[C]	V9D	C10-N11	9.35	1.44	1.32
4	T	203[C]	V9D	C10-N11	9.31	1.44	1.32
4	E	203[D]	V9D	C10-N11	9.20	1.44	1.32
4	B	204[D]	V9D	C10-N11	9.08	1.44	1.32
4	K	203[D]	V9D	C10-N11	8.96	1.44	1.32
4	O	205[C]	V9D	C10-N11	8.74	1.44	1.32
4	X	204[C]	V9D	C10-N11	8.60	1.43	1.32
4	K	203[C]	V9D	C09-C10	2.36	1.55	1.50
4	X	204[D]	V9D	C09-C10	2.33	1.55	1.50
4	B	204[D]	V9D	C09-C10	2.30	1.55	1.50
4	O	205[D]	V9D	C09-C10	2.24	1.54	1.50
4	X	204[C]	V9D	C09-C10	2.22	1.54	1.50
4	O	205[C]	V9D	C09-C10	2.17	1.54	1.50
4	K	203[D]	V9D	C09-C10	2.16	1.54	1.50
4	O	205[D]	V9D	C05-C02	2.09	1.54	1.50
4	T	203[D]	V9D	C05-C02	2.09	1.54	1.50
4	B	204[C]	V9D	C05-C02	2.09	1.54	1.50
4	H	204[C]	V9D	C05-C02	2.07	1.54	1.50
4	Q	203[C]	V9D	C09-C10	2.04	1.54	1.50
4	X	204[D]	V9D	C05-C02	2.04	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	203[C]	V9D	C05-C02	2.01	1.54	1.50
4	H	204[D]	V9D	C09-C10	2.01	1.54	1.50

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	X	204[D]	V9D	C09-C10-N11	4.08	122.70	116.16
4	K	203[C]	V9D	C09-C10-N11	4.04	122.64	116.16
4	B	204[C]	V9D	C09-C10-N11	3.86	122.36	116.16
4	K	203[C]	V9D	C05-C02-N03	3.76	122.19	116.16
4	X	204[C]	V9D	O13-C10-N11	-3.64	116.15	122.94
4	H	204[D]	V9D	O13-C10-N11	-3.44	116.52	122.94
4	B	204[D]	V9D	O13-C10-N11	-3.42	116.55	122.94
4	E	203[D]	V9D	O13-C10-N11	-3.41	116.58	122.94
4	O	205[D]	V9D	C09-C10-N11	3.30	121.46	116.16
4	K	203[C]	V9D	O13-C10-N11	-3.30	116.78	122.94
4	X	204[D]	V9D	C05-C02-N03	3.24	121.36	116.16
4	K	203[D]	V9D	O13-C10-N11	-3.16	117.05	122.94
4	X	204[D]	V9D	O13-C10-N11	-3.13	117.10	122.94
4	T	203[C]	V9D	O13-C10-N11	-3.10	117.15	122.94
4	O	205[D]	V9D	O01-C02-N03	-3.08	117.20	122.94
4	X	204[C]	V9D	O13-C10-C09	3.06	126.40	120.94
4	Q	203[C]	V9D	O13-C10-N11	-3.05	117.25	122.94
4	O	205[C]	V9D	O13-C10-N11	-3.04	117.27	122.94
4	K	203[C]	V9D	O01-C02-N03	-3.02	117.31	122.94
4	B	204[D]	V9D	O13-C10-C09	2.98	126.26	120.94
4	O	205[D]	V9D	C05-C02-N03	2.96	120.91	116.16
4	B	204[C]	V9D	O01-C02-N03	-2.94	117.46	122.94
4	T	203[C]	V9D	O01-C02-N03	-2.91	117.51	122.94
4	X	204[D]	V9D	O01-C02-N03	-2.88	117.56	122.94
4	Q	203[D]	V9D	C09-C10-N11	2.88	120.78	116.16
4	H	204[C]	V9D	C09-C10-N11	2.88	120.77	116.16
4	Q	203[C]	V9D	O01-C02-N03	-2.83	117.67	122.94
4	H	204[D]	V9D	O01-C02-N03	-2.81	117.70	122.94
4	K	203[D]	V9D	O13-C10-C09	2.79	125.91	120.94
4	E	203[D]	V9D	O01-C02-N03	-2.76	117.78	122.94
4	K	203[D]	V9D	O01-C02-N03	-2.76	117.79	122.94
4	O	205[C]	V9D	O01-C02-N03	-2.72	117.87	122.94
4	O	205[C]	V9D	O13-C10-C09	2.70	125.75	120.94
4	H	204[C]	V9D	O01-C02-N03	-2.67	117.95	122.94
4	X	204[C]	V9D	O01-C02-N03	-2.66	117.98	122.94
4	T	203[D]	V9D	C05-C02-N03	2.62	120.36	116.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	T	203[D]	V9D	C09-C10-N11	2.61	120.34	116.16
4	T	203[D]	V9D	O01-C02-N03	-2.61	118.08	122.94
4	E	203[C]	V9D	C09-C10-N11	2.59	120.31	116.16
4	B	204[D]	V9D	O01-C02-N03	-2.58	118.12	122.94
4	B	204[C]	V9D	O13-C10-N11	-2.57	118.14	122.94
4	O	205[D]	V9D	O13-C10-N11	-2.56	118.16	122.94
4	B	204[D]	V9D	C05-C02-N03	2.39	119.99	116.16
4	B	204[C]	V9D	C05-C02-N03	2.39	119.99	116.16
4	O	205[C]	V9D	C05-C02-N03	2.33	119.89	116.16
4	X	204[C]	V9D	C05-C02-N03	2.31	119.86	116.16
4	K	203[D]	V9D	C05-C02-N03	2.31	119.86	116.16
4	Q	203[C]	V9D	C05-C02-N03	2.28	119.81	116.16
4	H	204[D]	V9D	C09-C10-N11	2.26	119.78	116.16
4	T	203[C]	V9D	C05-C02-N03	2.25	119.77	116.16
4	E	203[D]	V9D	C05-C02-N03	2.24	119.75	116.16
4	E	203[C]	V9D	O01-C02-N03	-2.22	118.79	122.94
4	H	204[C]	V9D	C05-C02-N03	2.22	119.72	116.16
4	H	204[C]	V9D	O13-C10-N11	-2.20	118.84	122.94
4	H	204[D]	V9D	C05-C02-N03	2.19	119.68	116.16
4	E	203[C]	V9D	O13-C10-N11	-2.13	118.97	122.94
4	Q	203[D]	V9D	O13-C10-N11	-2.08	119.07	122.94
4	E	203[D]	V9D	O13-C10-C09	2.04	124.57	120.94
4	Q	203[D]	V9D	O01-C02-N03	-2.04	119.14	122.94
4	Q	203[C]	V9D	O13-C10-C09	2.03	124.56	120.94

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	204[C]	V9D	N03-C02-C05-C06
4	B	204[C]	V9D	N03-C02-C05-C14
4	B	204[D]	V9D	C08-C09-C10-N11
4	B	204[D]	V9D	C14-C09-C10-N11
4	E	203[C]	V9D	N03-C02-C05-C06
4	E	203[C]	V9D	N03-C02-C05-C14
4	E	203[D]	V9D	N03-C02-C05-C06
4	E	203[D]	V9D	C08-C09-C10-N11
4	E	203[D]	V9D	C14-C09-C10-N11
4	H	204[C]	V9D	N03-C02-C05-C06
4	H	204[C]	V9D	N03-C02-C05-C14
4	H	204[D]	V9D	N03-C02-C05-C06
4	H	204[D]	V9D	C08-C09-C10-N11

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Mol	Chain	Res	Type	Atoms
4	H	204[D]	V9D	C14-C09-C10-N11
4	K	203[C]	V9D	N03-C02-C05-C06
4	K	203[C]	V9D	N03-C02-C05-C14
4	K	203[D]	V9D	C08-C09-C10-N11
4	K	203[D]	V9D	C14-C09-C10-N11
4	O	205[C]	V9D	C08-C09-C10-N11
4	O	205[C]	V9D	C14-C09-C10-N11
4	O	205[D]	V9D	N03-C02-C05-C06
4	O	205[D]	V9D	N03-C02-C05-C14
4	Q	203[C]	V9D	C08-C09-C10-N11
4	Q	203[C]	V9D	C14-C09-C10-N11
4	Q	203[D]	V9D	N03-C02-C05-C06
4	Q	203[D]	V9D	N03-C02-C05-C14
4	T	203[C]	V9D	C08-C09-C10-N11
4	T	203[C]	V9D	C14-C09-C10-N11
4	T	203[D]	V9D	N03-C02-C05-C06
4	T	203[D]	V9D	N03-C02-C05-C14
4	X	204[C]	V9D	C08-C09-C10-N11
4	X	204[C]	V9D	C14-C09-C10-N11
4	X	204[D]	V9D	N03-C02-C05-C06
4	X	204[D]	V9D	N03-C02-C05-C14
4	B	204[C]	V9D	O01-C02-C05-C06
4	B	204[C]	V9D	O01-C02-C05-C14
4	E	203[C]	V9D	O01-C02-C05-C06
4	E	203[C]	V9D	O01-C02-C05-C14
4	H	204[C]	V9D	O01-C02-C05-C06
4	H	204[C]	V9D	O01-C02-C05-C14
4	K	203[C]	V9D	O01-C02-C05-C06
4	K	203[C]	V9D	O01-C02-C05-C14
4	O	205[D]	V9D	O01-C02-C05-C06
4	O	205[D]	V9D	O01-C02-C05-C14
4	Q	203[C]	V9D	C08-C09-C10-O13
4	Q	203[C]	V9D	C14-C09-C10-O13
4	Q	203[D]	V9D	O01-C02-C05-C06
4	Q	203[D]	V9D	O01-C02-C05-C14
4	T	203[C]	V9D	C08-C09-C10-O13
4	T	203[C]	V9D	C14-C09-C10-O13
4	T	203[D]	V9D	O01-C02-C05-C14
4	X	204[D]	V9D	O01-C02-C05-C06
4	X	204[D]	V9D	O01-C02-C05-C14
4	T	203[D]	V9D	O01-C02-C05-C06
4	E	203[D]	V9D	C14-C09-C10-O13

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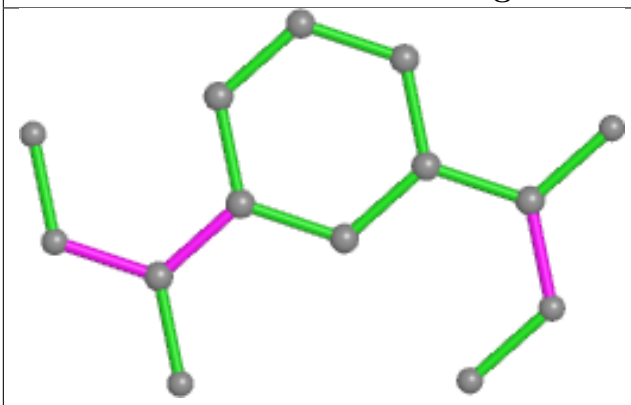
Mol	Chain	Res	Type	Atoms
4	E	203[D]	V9D	C08-C09-C10-O13
4	B	204[D]	V9D	C08-C09-C10-O13
4	O	205[C]	V9D	C08-C09-C10-O13
4	B	204[D]	V9D	C14-C09-C10-O13
4	O	205[C]	V9D	C14-C09-C10-O13
4	X	204[C]	V9D	C08-C09-C10-O13
4	K	203[D]	V9D	C08-C09-C10-O13
4	X	204[C]	V9D	C14-C09-C10-O13
4	H	204[D]	V9D	C14-C09-C10-O13
4	K	203[D]	V9D	C14-C09-C10-O13
4	H	204[D]	V9D	C08-C09-C10-O13
4	H	204[D]	V9D	N03-C02-C05-C14
4	H	204[D]	V9D	O01-C02-C05-C06
4	E	203[D]	V9D	N03-C02-C05-C14
4	E	203[D]	V9D	O01-C02-C05-C06
4	Q	203[C]	V9D	N03-C02-C05-C06
4	H	204[D]	V9D	O01-C02-C05-C14

There are no ring outliers.

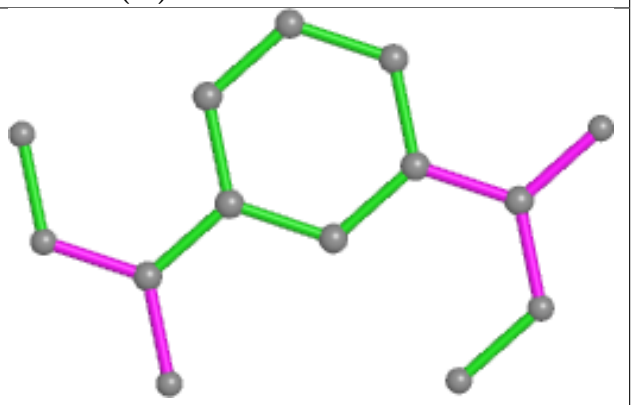
No monomer is involved in short contacts.

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

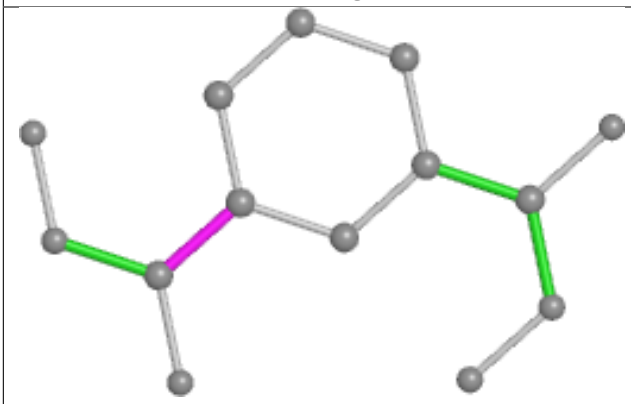
Ligand V9D E 203 (C)



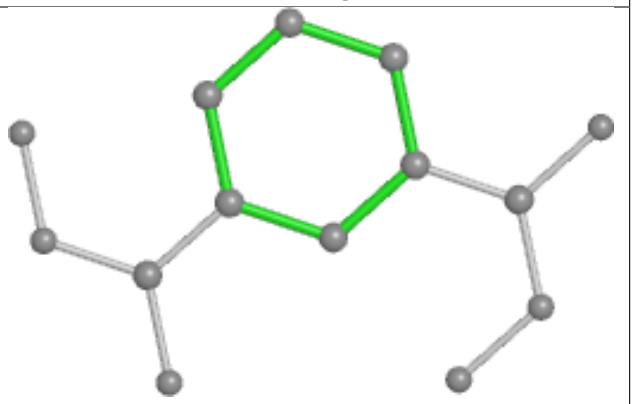
Bond lengths



Bond angles

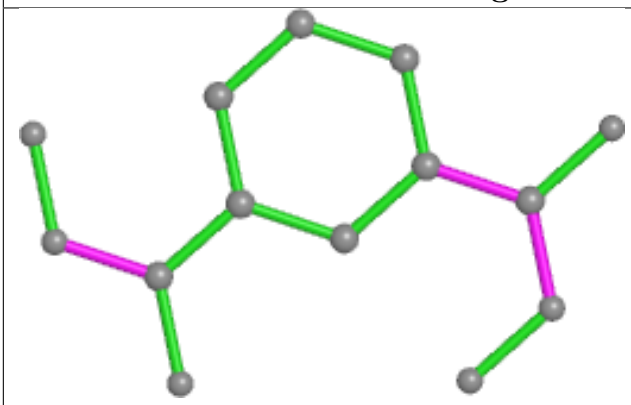


Torsions

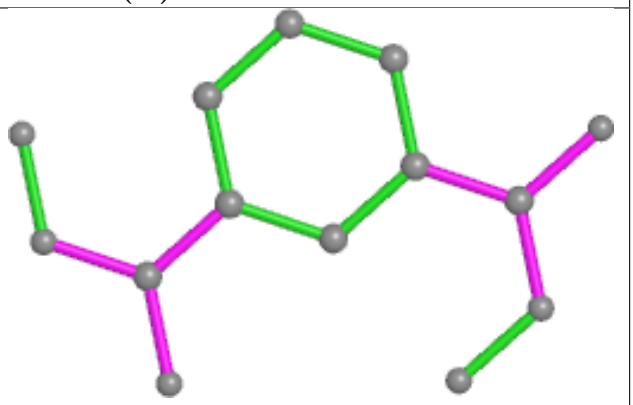


Rings

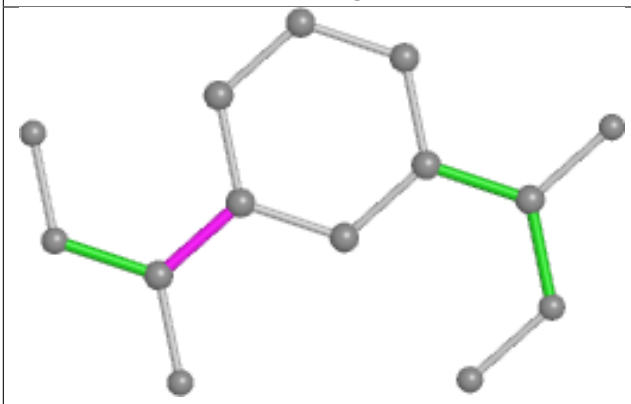
Ligand V9D K 203 (C)



Bond lengths



Bond angles



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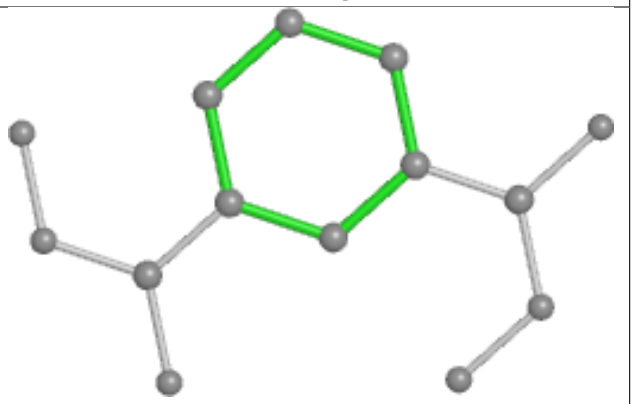
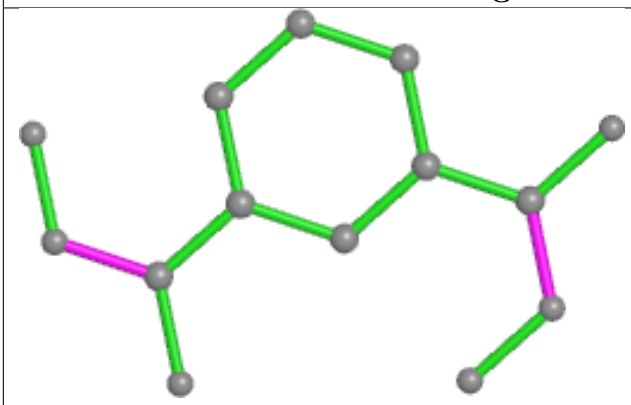
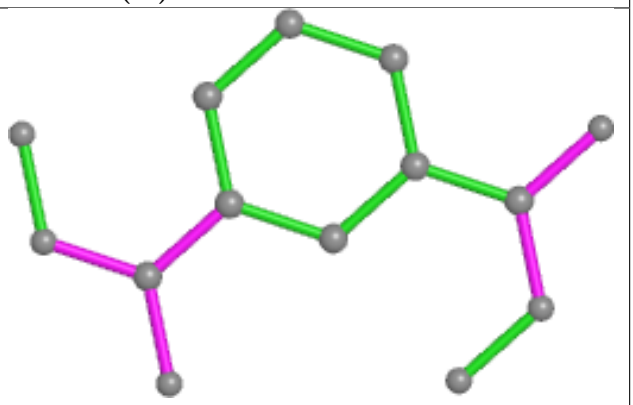


Rings

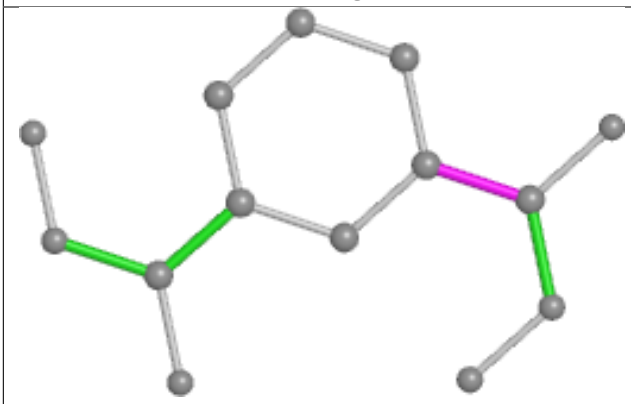
Ligand V9D T 203 (C)



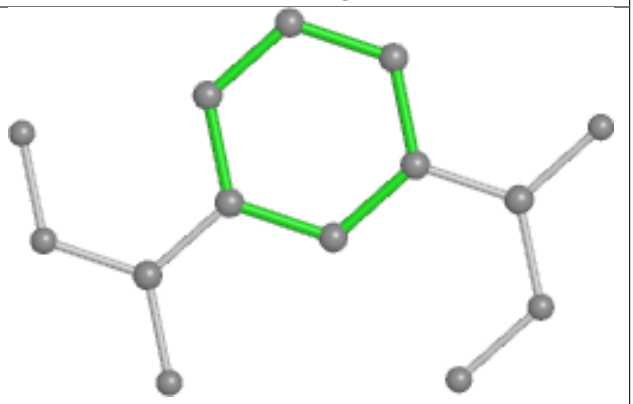
Bond lengths



Bond angles

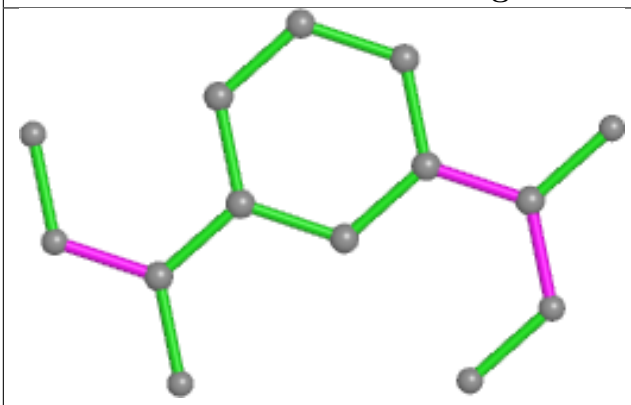


Torsions

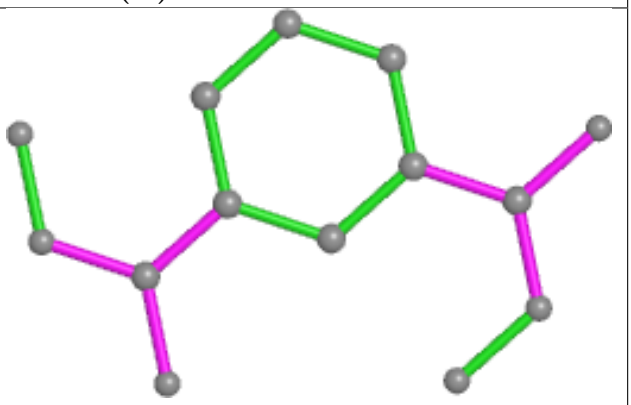


Rings

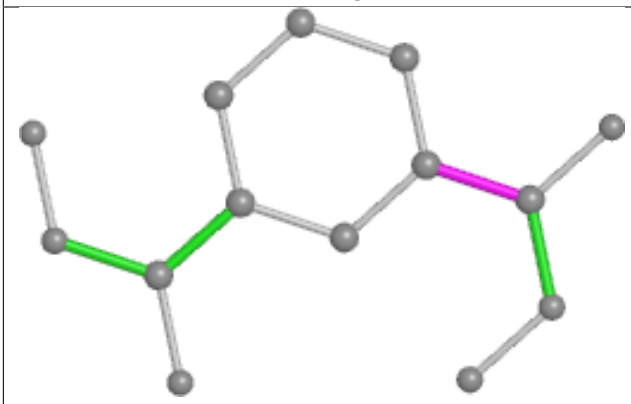
Ligand V9D X 204 (C)



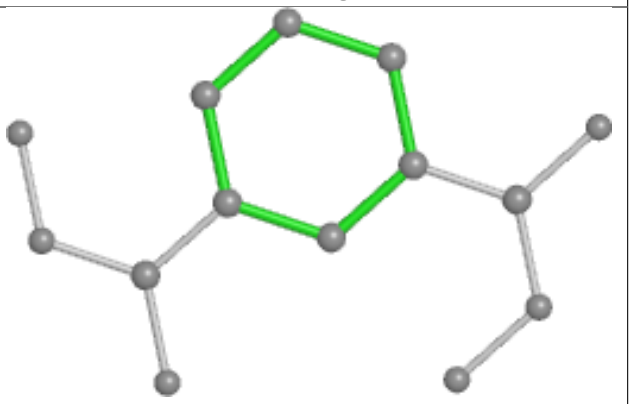
Bond lengths



Bond angles

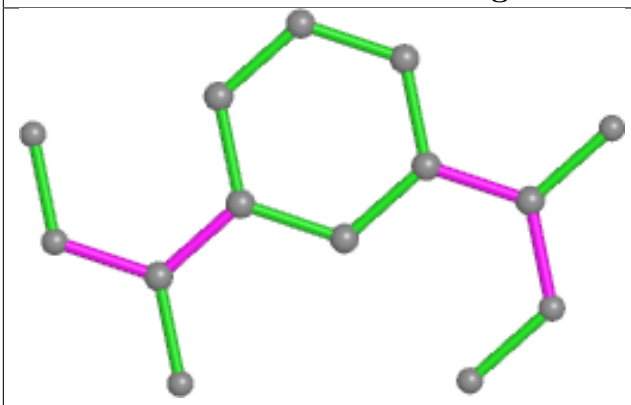


Torsions

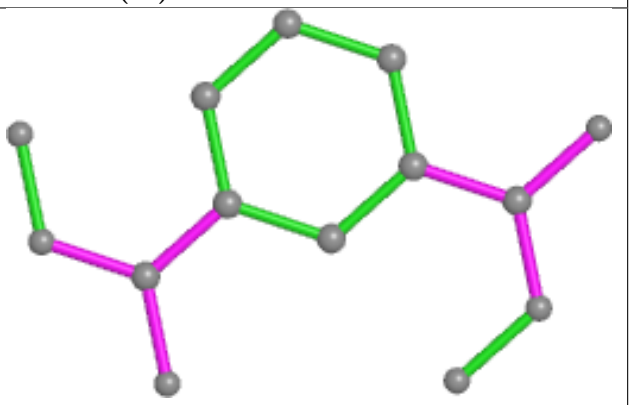


Rings

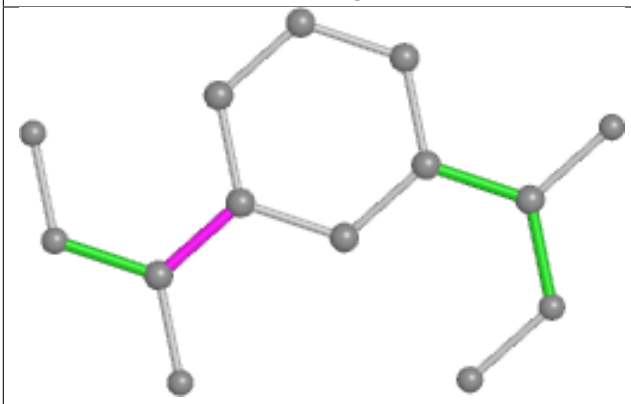
Ligand V9D O 205 (D)



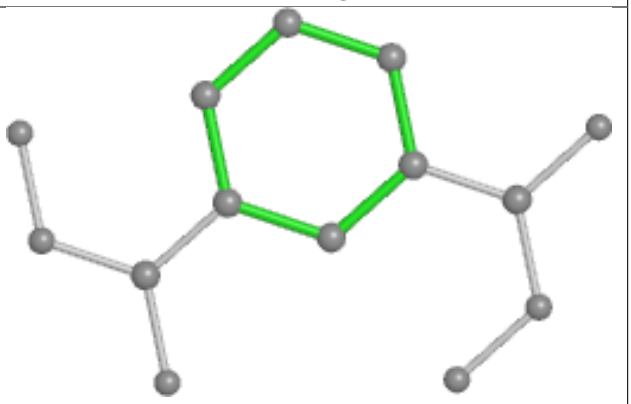
Bond lengths



Bond angles

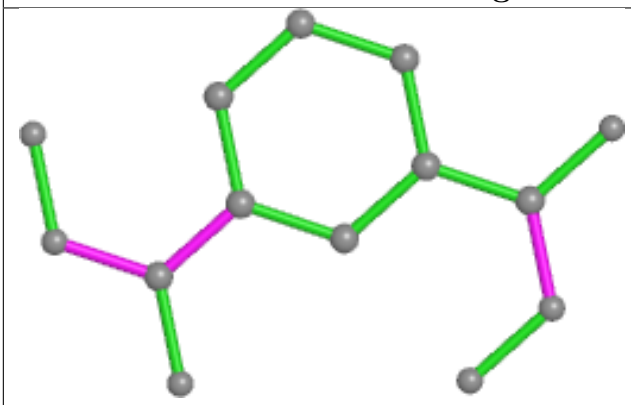


Torsions

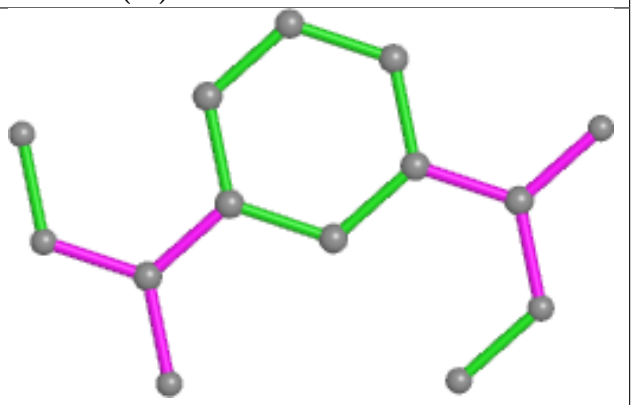


Rings

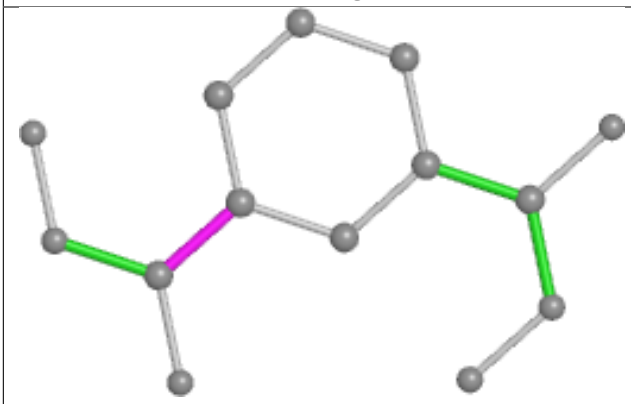
Ligand V9D B 204 (C)



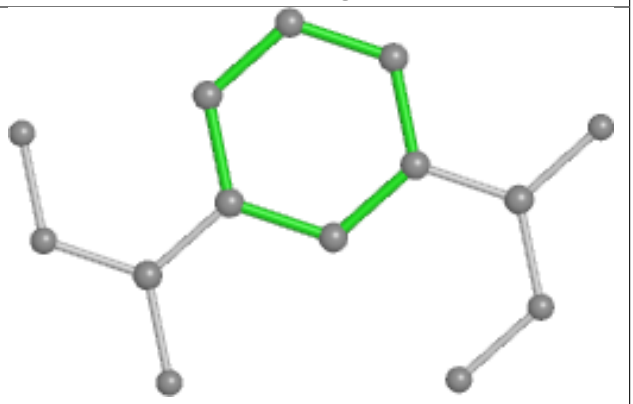
Bond lengths



Bond angles

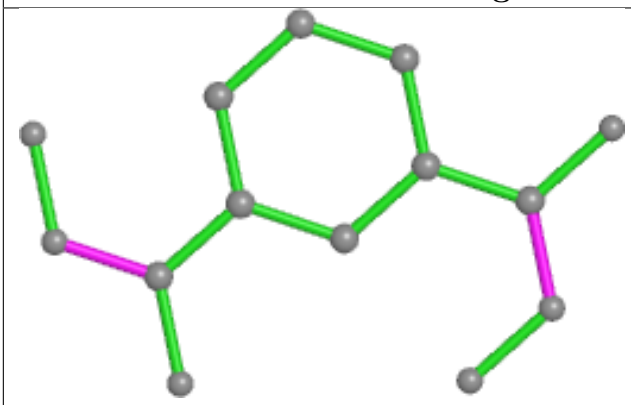


Torsions

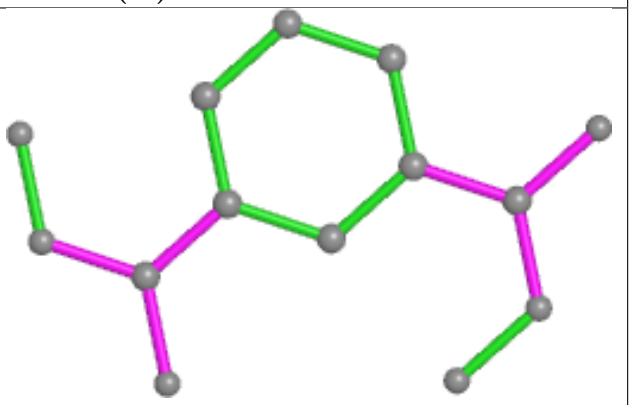


Rings

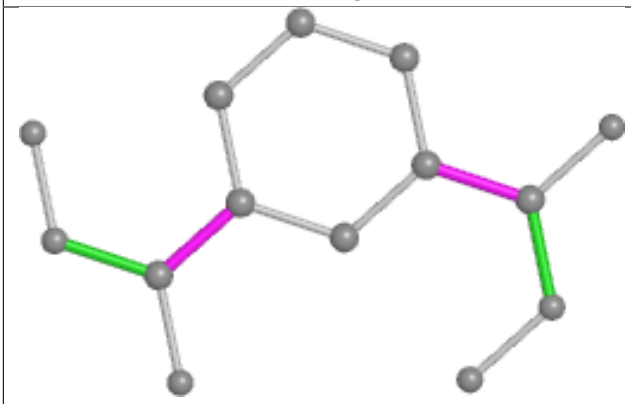
Ligand V9D E 203 (D)



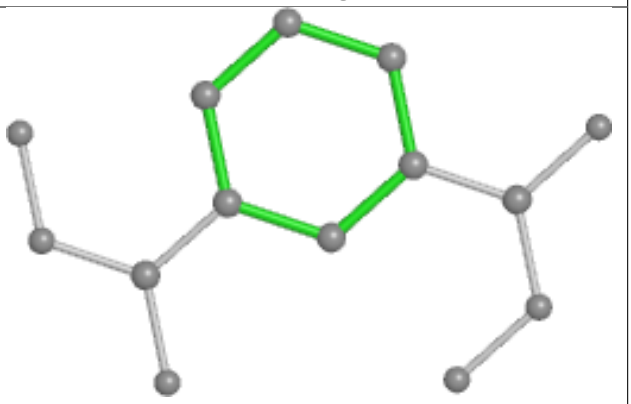
Bond lengths



Bond angles

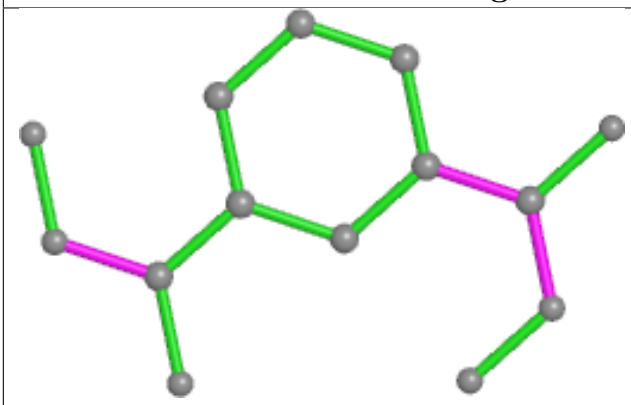


Torsions

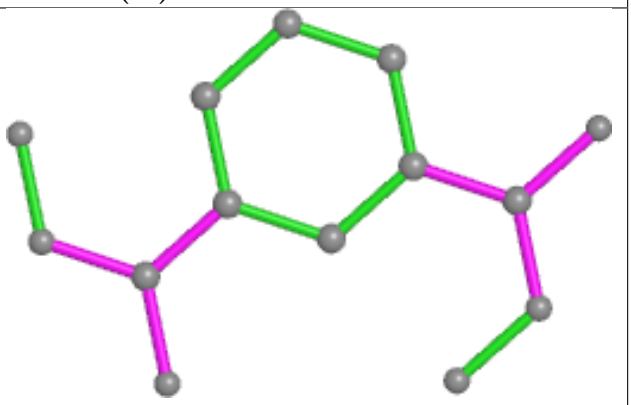


Rings

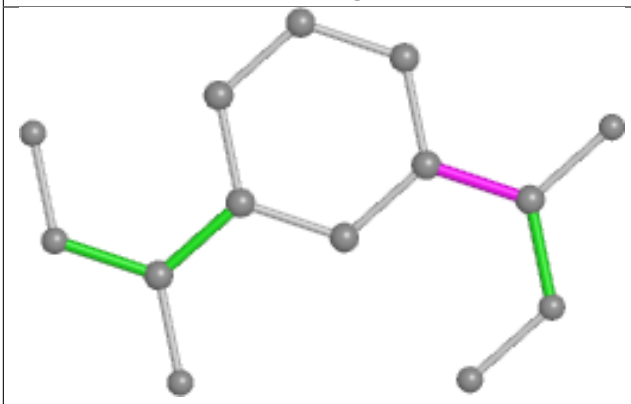
Ligand V9D K 203 (D)



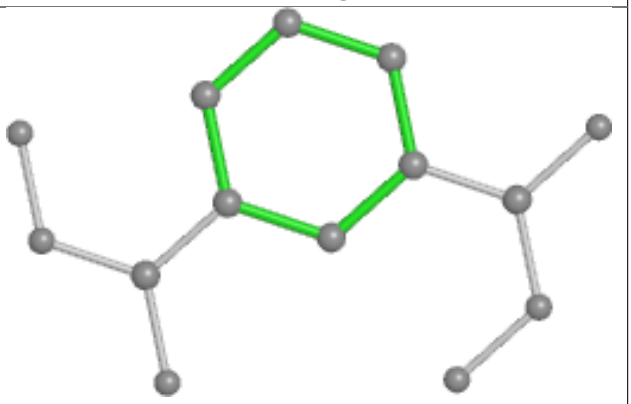
Bond lengths



Bond angles

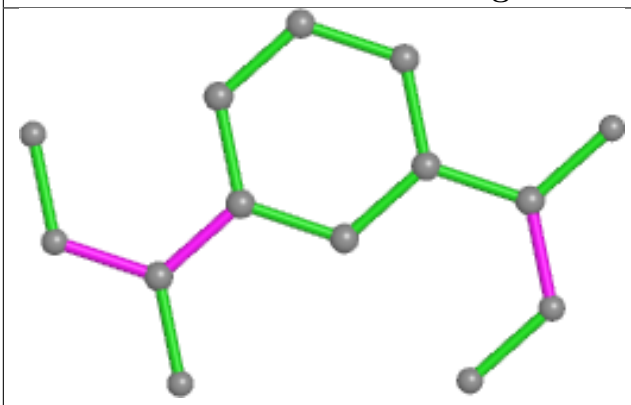


Torsions

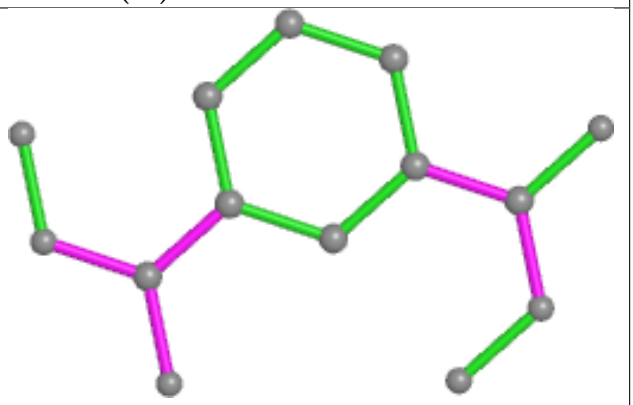


Rings

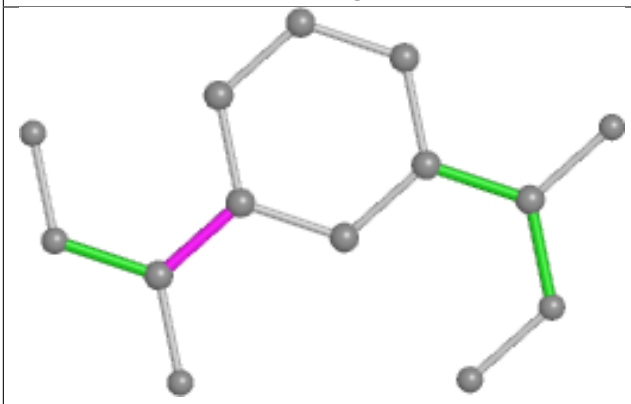
Ligand V9D T 203 (D)



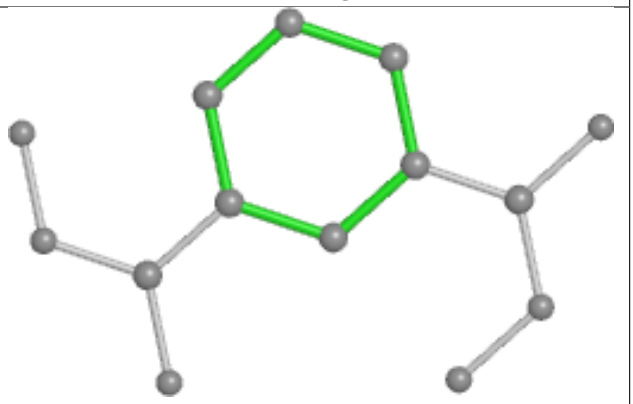
Bond lengths



Bond angles

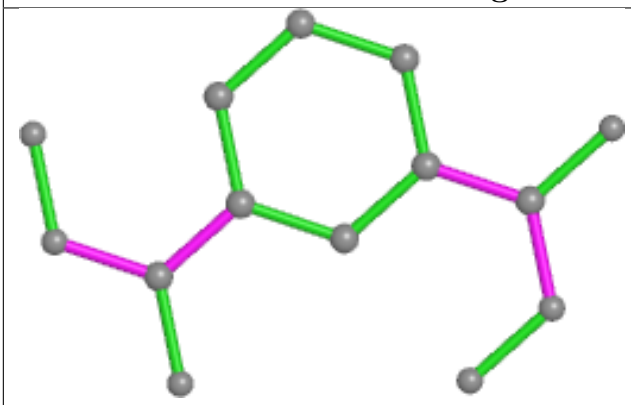


Torsions

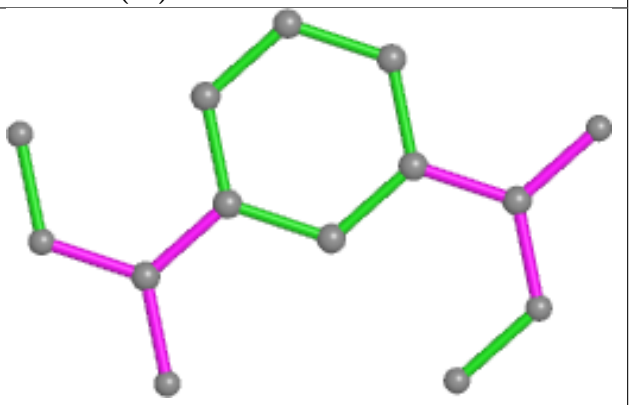


Rings

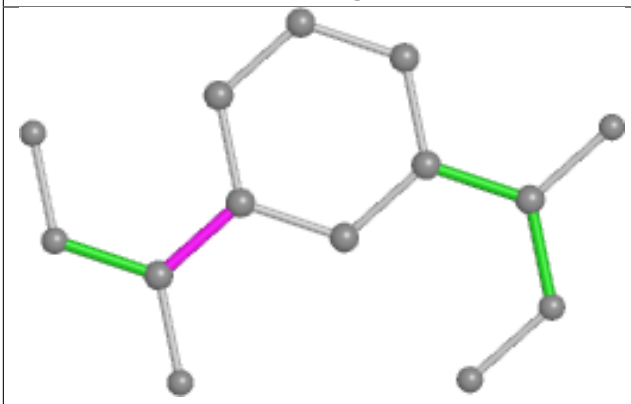
Ligand V9D X 204 (D)



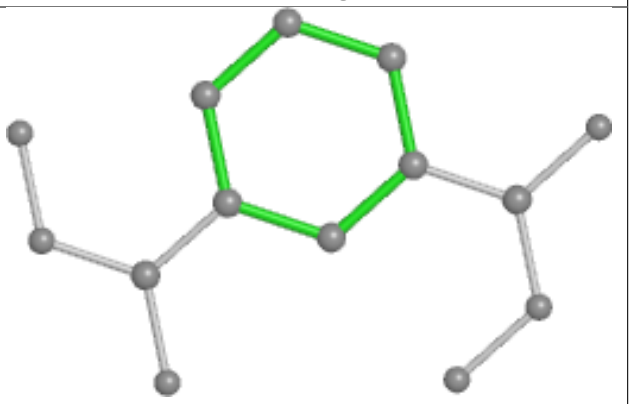
Bond lengths



Bond angles

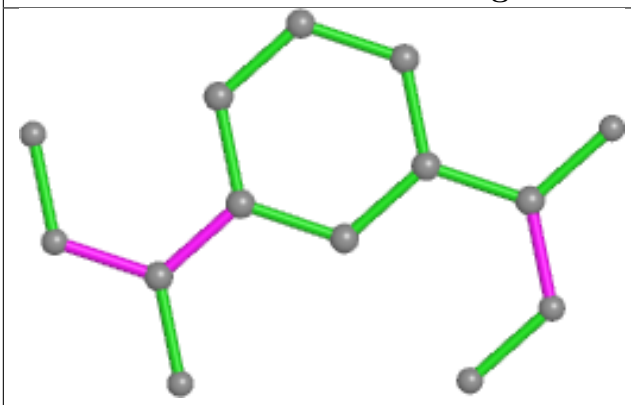


Torsions

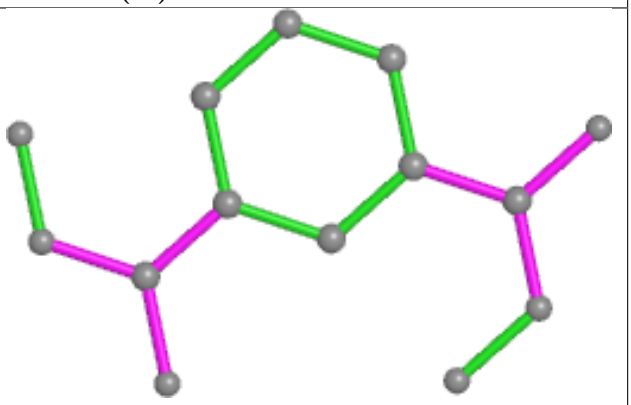


Rings

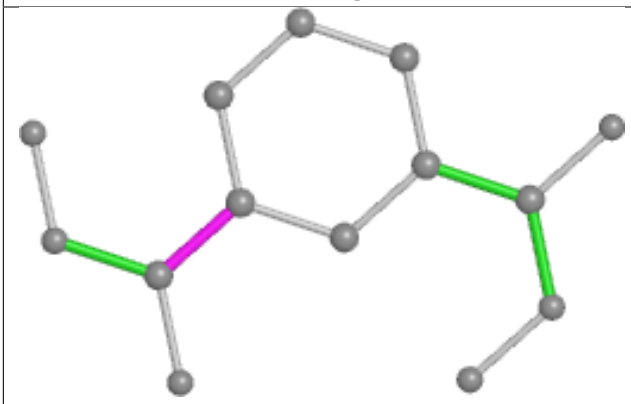
Ligand V9D H 204 (C)



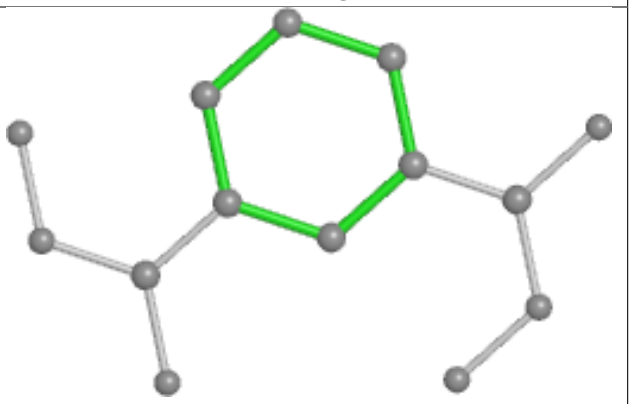
Bond lengths



Bond angles

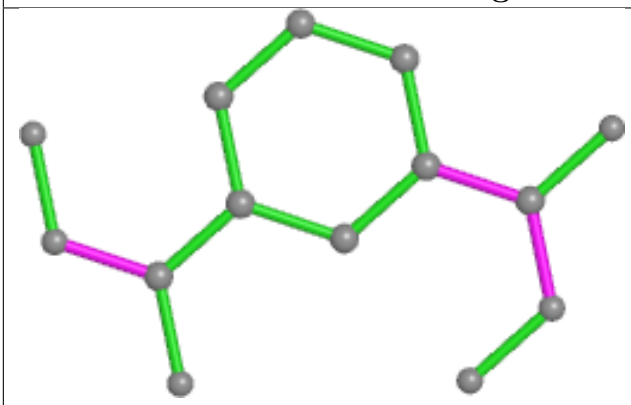


Torsions

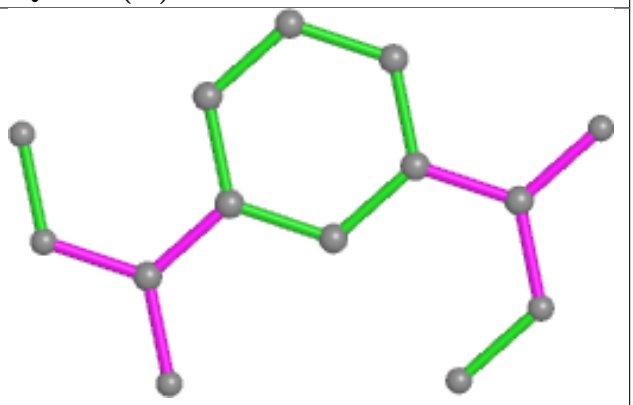


Rings

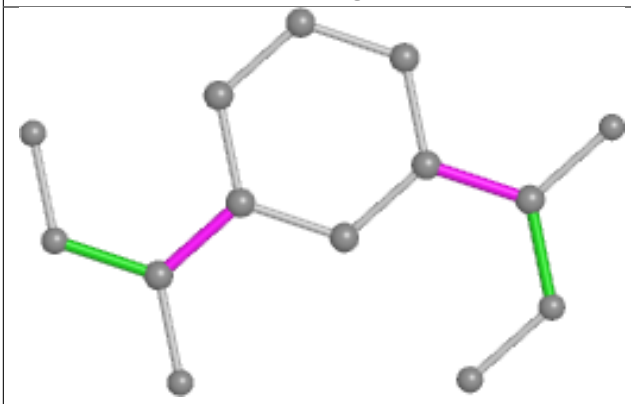
Ligand V9D Q 203 (C)



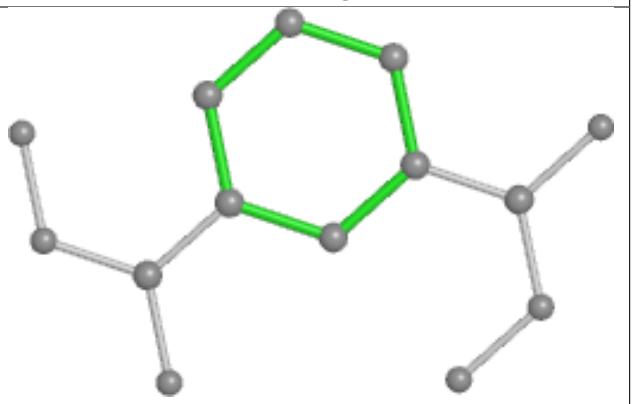
Bond lengths



Bond angles

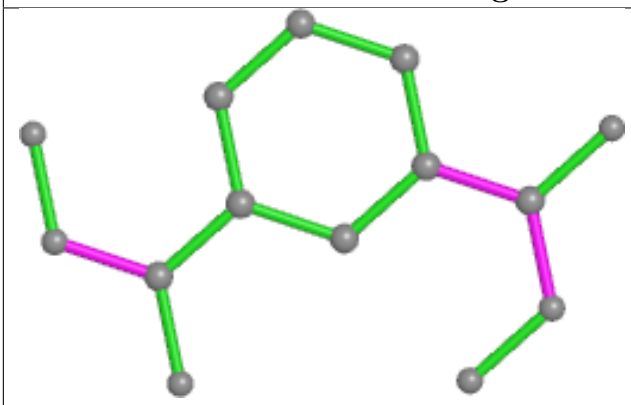


Torsions

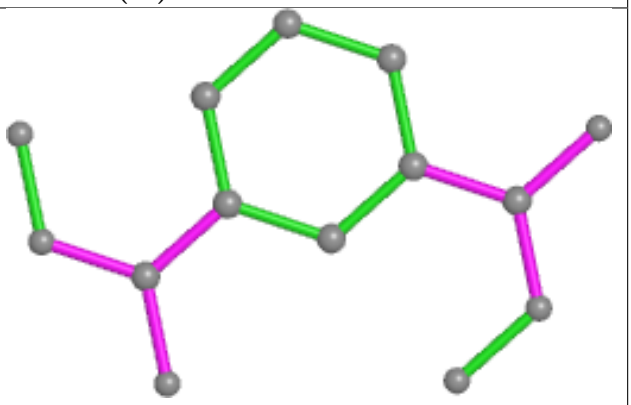


Rings

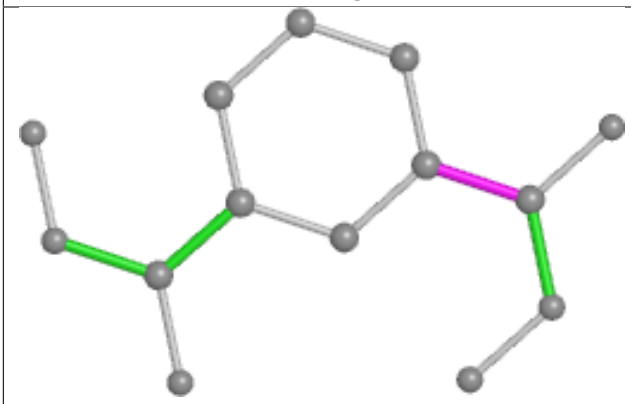
Ligand V9D B 204 (D)



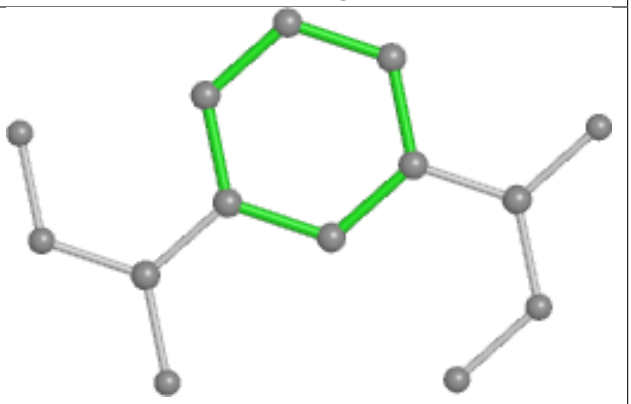
Bond lengths



Bond angles

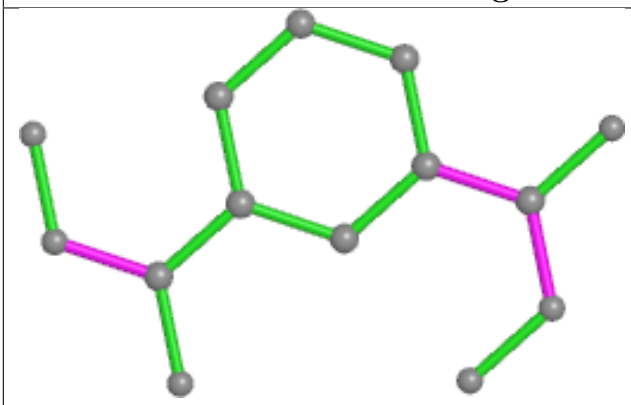


Torsions

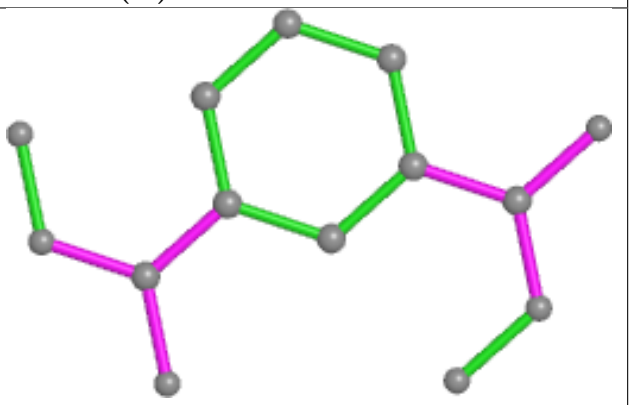


Rings

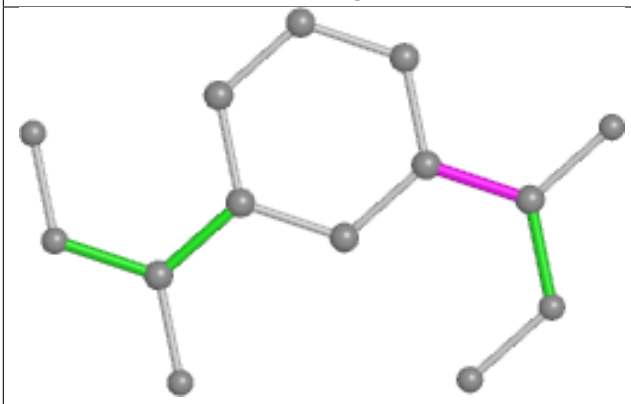
Ligand V9D O 205 (C)



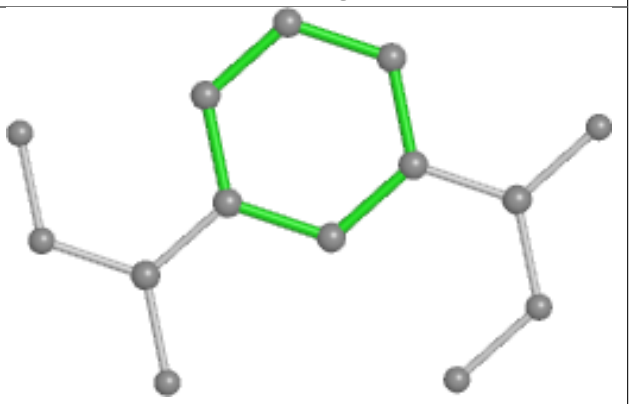
Bond lengths



Bond angles

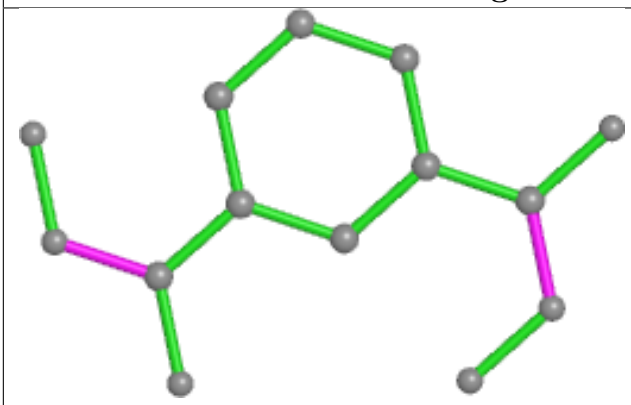


Torsions

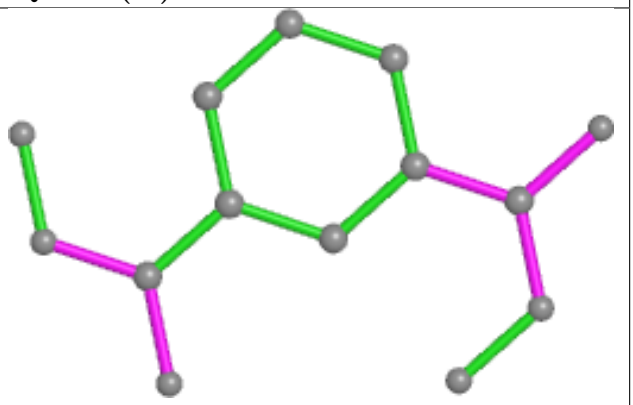


Rings

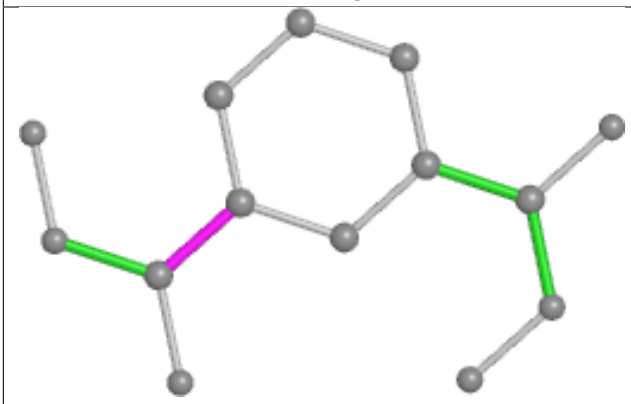
Ligand V9D Q 203 (D)



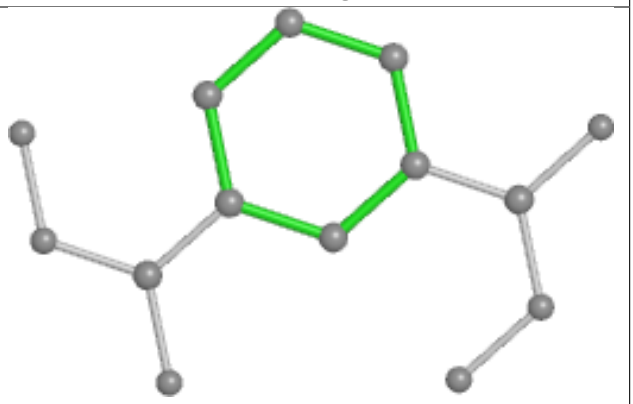
Bond lengths



Bond angles

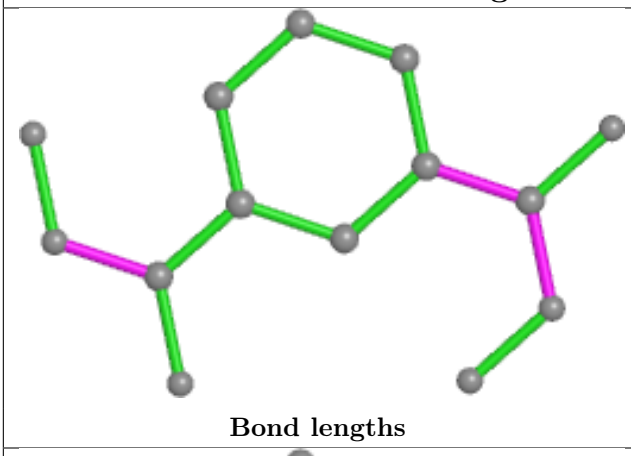


Torsions

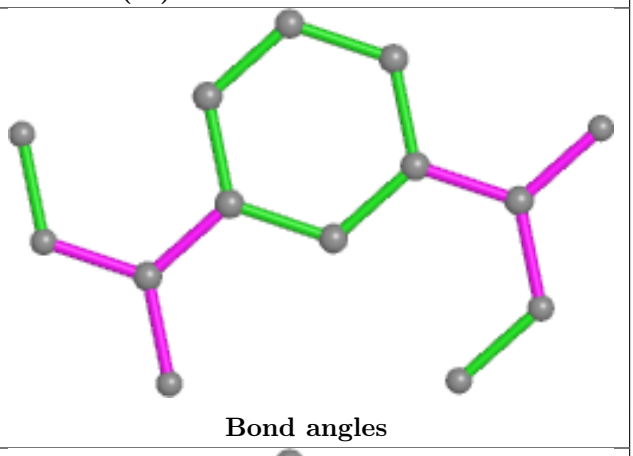


Rings

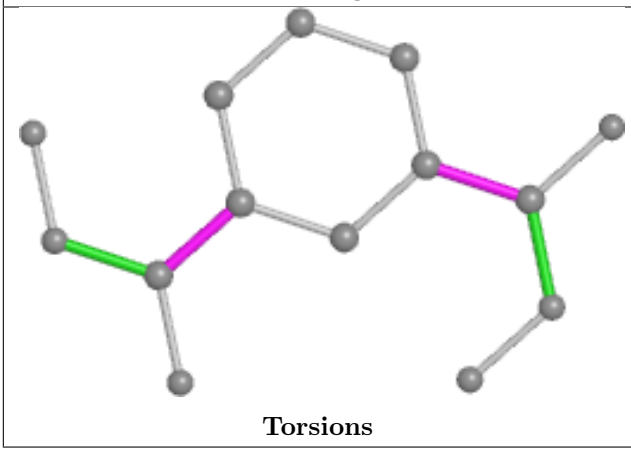
Ligand V9D H 204 (D)



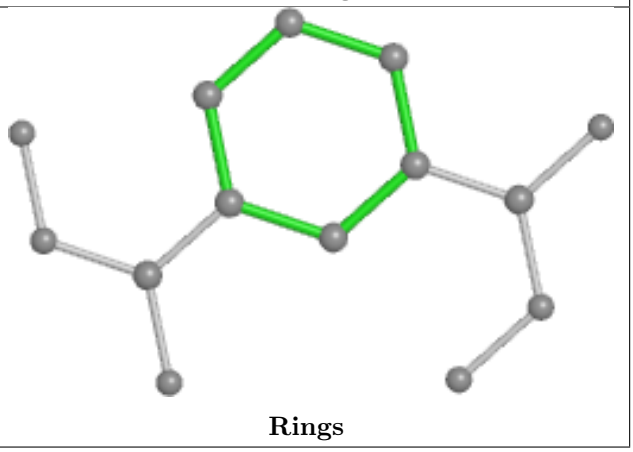
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	-0.65	0	100	100	25, 30, 48, 85	0
1	B	174/182 (95%)	-0.59	0	100	100	24, 29, 46, 84	0
1	C	174/182 (95%)	-0.58	0	100	100	22, 31, 48, 80	0
1	D	174/182 (95%)	-0.58	0	100	100	22, 27, 44, 78	0
1	E	174/182 (95%)	-0.60	0	100	100	22, 27, 44, 73	0
1	F	174/182 (95%)	-0.63	1 (0%)	89	90	22, 27, 43, 73	0
1	G	174/182 (95%)	-0.65	0	100	100	22, 28, 44, 75	0
1	H	174/182 (95%)	-0.63	0	100	100	22, 27, 45, 79	0
1	I	174/182 (95%)	-0.54	0	100	100	22, 27, 43, 75	0
1	J	174/182 (95%)	-0.56	0	100	100	25, 30, 48, 79	0
1	K	174/182 (95%)	-0.68	0	100	100	23, 29, 48, 85	0
1	L	174/182 (95%)	-0.62	0	100	100	24, 30, 47, 80	0
1	M	174/182 (95%)	-0.63	0	100	100	25, 30, 47, 80	0
1	N	174/182 (95%)	-0.66	0	100	100	23, 29, 48, 82	0
1	O	174/182 (95%)	-0.63	0	100	100	25, 30, 47, 83	0
1	P	174/182 (95%)	-0.64	0	100	100	23, 27, 45, 73	0
1	Q	174/182 (95%)	-0.62	0	100	100	21, 26, 44, 73	0
1	R	174/182 (95%)	-0.57	0	100	100	21, 26, 42, 72	0
1	S	174/182 (95%)	-0.61	0	100	100	22, 27, 43, 80	0
1	T	174/182 (95%)	-0.58	0	100	100	22, 27, 45, 75	0
1	U	174/182 (95%)	-0.60	0	100	100	21, 26, 44, 71	0
1	V	174/182 (95%)	-0.68	0	100	100	25, 30, 48, 78	0
1	W	174/182 (95%)	-0.59	1 (0%)	89	90	23, 29, 47, 82	0
1	X	174/182 (95%)	-0.59	0	100	100	24, 30, 47, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	a	174/182 (95%)	0.53	17 (9%) 7 7	23, 27, 36, 58	0
1	b	174/182 (95%)	0.40	3 (1%) 70 71	22, 27, 35, 57	0
1	c	174/182 (95%)	0.54	8 (4%) 32 33	24, 27, 37, 52	0
1	d	174/182 (95%)	0.51	13 (7%) 14 14	22, 26, 36, 56	0
1	e	174/182 (95%)	0.43	7 (4%) 38 40	23, 27, 35, 60	0
1	f	174/182 (95%)	0.57	13 (7%) 14 14	23, 27, 37, 56	0
1	g	174/182 (95%)	0.50	9 (5%) 27 27	23, 26, 35, 53	0
1	h	174/182 (95%)	0.46	7 (4%) 38 40	23, 27, 36, 56	0
1	i	174/182 (95%)	0.55	13 (7%) 14 14	23, 27, 38, 55	0
1	j	174/182 (95%)	0.54	13 (7%) 14 14	23, 27, 36, 59	0
1	k	174/182 (95%)	0.37	2 (1%) 80 81	23, 26, 34, 57	0
1	l	174/182 (95%)	0.55	12 (6%) 16 17	23, 27, 36, 52	0
1	m	174/182 (95%)	0.51	10 (5%) 23 24	23, 27, 37, 54	0
1	n	174/182 (95%)	0.48	9 (5%) 27 27	22, 27, 36, 57	0
1	o	174/182 (95%)	0.38	3 (1%) 70 71	23, 27, 36, 55	0
1	p	174/182 (95%)	0.53	11 (6%) 20 20	22, 28, 38, 58	0
1	q	174/182 (95%)	0.45	6 (3%) 45 47	22, 26, 35, 55	0
1	r	174/182 (95%)	0.37	6 (3%) 45 47	23, 27, 36, 57	0
1	s	174/182 (95%)	0.55	10 (5%) 23 24	23, 27, 37, 54	0
1	t	174/182 (95%)	0.49	9 (5%) 27 27	22, 26, 35, 56	0
1	u	174/182 (95%)	0.42	3 (1%) 70 71	24, 27, 35, 57	0
1	v	174/182 (95%)	0.55	8 (4%) 32 33	23, 27, 37, 52	0
1	w	174/182 (95%)	0.59	18 (10%) 6 6	23, 27, 36, 58	0
1	x	174/182 (95%)	0.41	2 (1%) 80 81	23, 27, 35, 55	0
All	All	8352/8736 (95%)	-0.06	214 (2%) 56 59	21, 28, 43, 85	0

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	n	165[C]	LEU	6.8
1	a	165[C]	LEU	6.0
1	j	165[C]	LEU	6.0
1	h	161[C]	PRO	5.6
1	q	177[C]	ASP	5.5

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Mol	Chain	Res	Type	RSRZ
1	h	4[C]	SER	5.5
1	w	165[C]	LEU	4.9
1	f	133[C]	ILE	4.8
1	u	4[C]	SER	4.7
1	a	164[C]	GLY	4.5
1	i	24[C]	ILE	4.5
1	p	164[C]	GLY	4.2
1	t	164[C]	GLY	4.2
1	u	161[C]	PRO	4.1
1	j	164[C]	GLY	4.1
1	r	161[C]	PRO	4.0
1	l	53[C]	LYS	4.0
1	n	164[C]	GLY	4.0
1	j	28[C]	LEU	4.0
1	d	165[C]	LEU	3.8
1	s	24[C]	ILE	3.8
1	j	177[C]	ASP	3.8
1	s	133[C]	ILE	3.8
1	t	165[C]	LEU	3.8
1	t	49[C]	LYS	3.7
1	c	133[C]	ILE	3.7
1	m	133[C]	ILE	3.7
1	v	133[C]	ILE	3.6
1	j	166[C]	ALA	3.6
1	g	49[C]	LYS	3.6
1	w	28[C]	LEU	3.6
1	w	133[C]	ILE	3.6
1	c	51[C]	PHE	3.5
1	l	164[C]	GLY	3.5
1	d	177[C]	ASP	3.5
1	n	28[C]	LEU	3.4
1	m	51[C]	PHE	3.4
1	l	133[C]	ILE	3.4
1	f	164[C]	GLY	3.4
1	p	130[C]	ALA	3.4
1	g	165[C]	LEU	3.3
1	i	110[C]	VAL	3.3
1	i	4[C]	SER	3.3
1	p	114[C]	LEU	3.3
1	w	164[C]	GLY	3.3
1	w	138[C]	LEU	3.2
1	f	4[C]	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	w	24[C]	ILE	3.2
1	p	110[C]	VAL	3.2
1	e	161[C]	PRO	3.2
1	h	129[C]	LEU	3.2
1	v	51[C]	PHE	3.2
1	s	130[C]	ALA	3.2
1	t	177[C]	ASP	3.1
1	f	24[C]	ILE	3.1
1	q	165[C]	LEU	3.1
1	l	51[C]	PHE	3.1
1	i	133[C]	ILE	3.1
1	a	40[C]	TYR	3.0
1	s	110[C]	VAL	3.0
1	q	49[C]	LYS	3.0
1	p	20[C]	ILE	3.0
1	w	119[C]	LYS	3.0
1	p	133[C]	ILE	2.9
1	w	40[C]	TYR	2.9
1	w	166[C]	ALA	2.9
1	a	119[C]	LYS	2.9
1	n	157[C]	LYS	2.9
1	e	177[C]	ASP	2.9
1	a	32[C]	TYR	2.9
1	j	133[C]	ILE	2.9
1	j	29[C]	TYR	2.8
1	m	53[C]	LYS	2.8
1	p	129[C]	LEU	2.8
1	w	4[C]	SER	2.8
1	e	129[C]	LEU	2.8
1	f	110[C]	VAL	2.8
1	n	166[C]	ALA	2.8
1	m	130[C]	ALA	2.8
1	i	49[C]	LYS	2.8
1	a	169[C]	LEU	2.8
1	m	39[C]	TYR	2.7
1	f	20[C]	ILE	2.7
1	w	49[C]	LYS	2.7
1	c	130[C]	ALA	2.7
1	r	4[C]	SER	2.7
1	s	4[C]	SER	2.7
1	o	129[C]	LEU	2.7
1	t	4[C]	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	s	20[C]	ILE	2.7
1	t	166[C]	ALA	2.6
1	l	130[C]	ALA	2.6
1	m	24[C]	ILE	2.6
1	a	63[C]	ARG	2.6
1	r	32[C]	TYR	2.6
1	d	123[C]	ASP	2.6
1	l	24[C]	ILE	2.6
1	v	110[C]	VAL	2.6
1	i	114[C]	LEU	2.6
1	n	63[C]	ARG	2.5
1	e	4[C]	SER	2.5
1	q	164[C]	GLY	2.5
1	p	24[C]	ILE	2.5
1	f	114[C]	LEU	2.5
1	a	28[C]	LEU	2.5
1	r	162[C]	GLU	2.5
1	q	4[C]	SER	2.5
1	e	63[C]	ARG	2.5
1	q	114[C]	LEU	2.5
1	a	123[C]	ASP	2.5
1	j	119[C]	LYS	2.5
1	d	35[C]	LEU	2.4
1	l	129[C]	LEU	2.4
1	l	127[C]	PRO	2.4
1	r	63[C]	ARG	2.4
1	j	63[C]	ARG	2.4
1	g	4[C]	SER	2.4
1	d	72[C]	LEU	2.4
1	c	39[C]	TYR	2.4
1	t	24[C]	ILE	2.4
1	h	63[C]	ARG	2.4
1	m	110[C]	VAL	2.4
1	d	49[C]	LYS	2.4
1	d	119[C]	LYS	2.4
1	i	69[C]	LEU	2.4
1	j	169[C]	LEU	2.4
1	j	40[C]	TYR	2.4
1	p	39[C]	TYR	2.4
1	v	20[C]	ILE	2.3
1	p	53[C]	LYS	2.3
1	i	20[C]	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	i	63[C]	ARG	2.3
1	a	138[C]	LEU	2.3
1	r	129[C]	LEU	2.3
1	g	177[C]	ASP	2.3
1	w	63[C]	ARG	2.3
1	c	129[C]	LEU	2.3
1	f	162[C]	GLU	2.3
1	F	164	GLY	2.3
1	v	130[C]	ALA	2.3
1	a	49[C]	LYS	2.2
1	j	35[C]	LEU	2.2
1	v	19[C]	ALA	2.2
1	o	152[C]	VAL	2.2
1	a	163[C]	SER	2.2
1	g	35[C]	LEU	2.2
1	n	169[C]	LEU	2.2
1	l	110[C]	VAL	2.2
1	W	4	SER	2.2
1	h	96[C]	GLY	2.2
1	m	66[C]	ALA	2.2
1	d	164[C]	GLY	2.2
1	i	41[C]	PHE	2.2
1	v	152[C]	VAL	2.2
1	a	102[C]	ALA	2.2
1	g	28[C]	LEU	2.2
1	k	152[C]	VAL	2.2
1	w	46[C]	VAL	2.2
1	f	130[C]	ALA	2.2
1	w	157[C]	LYS	2.2
1	m	152[C]	VAL	2.2
1	a	166[C]	ALA	2.2
1	w	102[C]	ALA	2.2
1	s	162[C]	GLU	2.1
1	e	32[C]	TYR	2.1
1	f	49[C]	LYS	2.1
1	x	129[C]	LEU	2.1
1	s	49[C]	LYS	2.1
1	t	123[C]	ASP	2.1
1	n	4[C]	SER	2.1
1	f	53[C]	LYS	2.1
1	h	162[C]	GLU	2.1
1	i	164[C]	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	i	130[C]	ALA	2.1
1	l	32[C]	TYR	2.1
1	x	177[C]	ASP	2.1
1	d	28[C]	LEU	2.1
1	d	114[C]	LEU	2.1
1	f	129[C]	LEU	2.1
1	l	28[C]	LEU	2.1
1	s	114[C]	LEU	2.1
1	w	114[C]	LEU	2.1
1	c	49[C]	LYS	2.1
1	c	63[C]	ARG	2.1
1	g	123[C]	ASP	2.1
1	t	29[C]	TYR	2.1
1	c	86[C]	GLN	2.1
1	w	101[C]	GLU	2.1
1	g	164[C]	GLY	2.1
1	b	129[C]	LEU	2.1
1	f	69[C]	LEU	2.1
1	v	106[C]	LEU	2.1
1	b	177[C]	ASP	2.1
1	o	177[C]	ASP	2.1
1	d	166[C]	ALA	2.1
1	l	20[C]	ILE	2.0
1	n	24[C]	ILE	2.0
1	b	33[C]	VAL	2.0
1	p	49[C]	LYS	2.0
1	m	55[C]	PHE	2.0
1	a	162[C]	GLU	2.0
1	h	32[C]	TYR	2.0
1	a	177[C]	ASP	2.0
1	w	177[C]	ASP	2.0
1	k	128[C]	HIS	2.0
1	u	33[C]	VAL	2.0
1	d	63[C]	ARG	2.0
1	a	86[C]	GLN	2.0
1	g	29[C]	TYR	2.0
1	i	53[C]	LYS	2.0
1	s	53[C]	LYS	2.0
1	d	101[C]	GLU	2.0
1	e	152[C]	VAL	2.0
1	j	123[C]	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no 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, 95^{th} 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	ZN	l	202[C]	1/1	0.82	0.13	46,46,46,46	1
2	ZN	l	202[D]	1/1	0.82	0.13	45,45,45,45	1
2	ZN	q	203[C]	1/1	0.83	0.11	45,45,45,45	1
2	ZN	q	203[D]	1/1	0.83	0.11	42,42,42,42	1
2	ZN	d	204[C]	1/1	0.84	0.16	41,41,41,41	1
2	ZN	d	204[D]	1/1	0.84	0.16	43,43,43,43	1
2	ZN	c	202[C]	1/1	0.85	0.11	41,41,41,41	1
2	ZN	c	202[D]	1/1	0.85	0.11	47,47,47,47	1
2	ZN	g	203[C]	1/1	0.85	0.10	45,45,45,45	1
2	ZN	g	203[D]	1/1	0.85	0.10	43,43,43,43	1
2	ZN	w	203[C]	1/1	0.85	0.12	47,47,47,47	1
2	ZN	w	203[D]	1/1	0.85	0.12	47,47,47,47	1
2	ZN	p	202[C]	1/1	0.86	0.15	47,47,47,47	1
2	ZN	p	202[D]	1/1	0.86	0.15	42,42,42,42	1
2	ZN	j	203[C]	1/1	0.86	0.11	47,47,47,47	1
2	ZN	j	203[D]	1/1	0.86	0.11	46,46,46,46	1
2	ZN	i	202[C]	1/1	0.86	0.11	46,46,46,46	1
2	ZN	i	202[D]	1/1	0.86	0.11	46,46,46,46	1
4	V9D	T	203[C]	14/14	0.86	0.20	38,43,51,51	14
4	V9D	T	203[D]	14/14	0.86	0.20	43,45,52,54	14
4	V9D	H	204[C]	14/14	0.88	0.16	41,45,50,56	14
4	V9D	H	204[D]	14/14	0.88	0.16	38,41,53,55	14
2	ZN	v	204[C]	1/1	0.88	0.19	48,48,48,48	1
2	ZN	v	204[D]	1/1	0.88	0.19	44,44,44,44	1
2	ZN	n	202[C]	1/1	0.90	0.09	47,47,47,47	1
2	ZN	n	202[D]	1/1	0.90	0.09	43,43,43,43	1
3	NA	G	204	1/1	0.90	0.36	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NA	M	203	1/1	0.90	0.27	39,39,39,39	0
2	ZN	a	203[D]	1/1	0.91	0.11	49,49,49,49	1
2	ZN	s	202[C]	1/1	0.91	0.06	47,47,47,47	1
2	ZN	s	202[D]	1/1	0.91	0.06	39,39,39,39	1
3	NA	D	204	1/1	0.91	0.36	42,42,42,42	0
2	ZN	a	203[C]	1/1	0.91	0.11	45,45,45,45	1
2	ZN	x	203[C]	1/1	0.92	0.09	47,47,47,47	1
2	ZN	x	203[D]	1/1	0.92	0.09	43,43,43,43	1
2	ZN	N	202	1/1	0.92	0.05	53,53,53,53	1
2	ZN	t	203[C]	1/1	0.92	0.12	43,43,43,43	1
3	NA	J	204	1/1	0.92	0.29	42,42,42,42	0
2	ZN	t	203[D]	1/1	0.92	0.12	42,42,42,42	1
4	V9D	B	204[C]	14/14	0.92	0.16	40,45,51,55	14
4	V9D	B	204[D]	14/14	0.92	0.16	37,42,54,54	14
2	ZN	m	203[C]	1/1	0.92	0.12	47,47,47,47	1
2	ZN	m	203[D]	1/1	0.92	0.12	45,45,45,45	1
2	ZN	W	202	1/1	0.92	0.05	55,55,55,55	1
2	ZN	K	202	1/1	0.92	0.07	55,55,55,55	1
4	V9D	E	203[C]	14/14	0.93	0.18	38,42,50,53	14
4	V9D	K	203[C]	14/14	0.93	0.15	40,43,57,58	14
4	V9D	K	203[D]	14/14	0.93	0.15	33,42,57,58	14
4	V9D	E	203[D]	14/14	0.93	0.18	40,44,50,52	14
3	NA	S	204	1/1	0.93	0.37	42,42,42,42	0
2	ZN	f	203[C]	1/1	0.94	0.10	40,40,40,40	1
2	ZN	f	203[D]	1/1	0.94	0.10	45,45,45,45	1
2	ZN	k	202[C]	1/1	0.94	0.09	40,40,40,40	1
4	V9D	O	205[C]	14/14	0.94	0.12	34,41,54,55	14
4	V9D	O	205[D]	14/14	0.94	0.12	38,45,53,56	14
4	V9D	Q	203[C]	14/14	0.94	0.14	38,44,51,55	14
4	V9D	Q	203[D]	14/14	0.94	0.14	37,44,51,56	14
2	ZN	k	202[D]	1/1	0.94	0.09	47,47,47,47	1
3	NA	A	205	1/1	0.94	0.25	42,42,42,42	0
2	ZN	e	203[C]	1/1	0.95	0.06	47,47,47,47	1
2	ZN	e	203[D]	1/1	0.95	0.06	49,49,49,49	1
2	ZN	O	204	1/1	0.95	0.04	55,55,55,55	1
2	ZN	o	202[C]	1/1	0.95	0.08	46,46,46,46	1
2	ZN	o	202[D]	1/1	0.95	0.08	39,39,39,39	1
3	NA	g	204[C]	1/1	0.95	0.18	33,33,33,33	1
3	NA	g	204[D]	1/1	0.95	0.18	33,33,33,33	1
2	ZN	G	203	1/1	0.96	0.05	53,53,53,53	1
2	ZN	r	201[C]	1/1	0.96	0.08	36,36,36,36	1
2	ZN	r	201[D]	1/1	0.96	0.08	37,37,37,37	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	r	202[C]	1/1	0.96	0.08	51,51,51,51	1
2	ZN	r	202[D]	1/1	0.96	0.08	45,45,45,45	1
2	ZN	m	201[C]	1/1	0.96	0.07	37,37,37,37	1
2	ZN	m	201[D]	1/1	0.96	0.07	31,31,31,31	1
2	ZN	E	202	1/1	0.96	0.04	53,53,53,53	1
2	ZN	P	203	1/1	0.96	0.05	54,54,54,54	1
3	NA	V	203	1/1	0.96	0.25	39,39,39,39	0
2	ZN	q	201[C]	1/1	0.96	0.08	34,34,34,34	1
2	ZN	q	201[D]	1/1	0.96	0.08	34,34,34,34	1
2	ZN	T	202	1/1	0.96	0.06	54,54,54,54	1
4	V9D	X	204[C]	14/14	0.96	0.12	36,43,54,57	14
4	V9D	X	204[D]	14/14	0.96	0.12	37,45,56,57	14
3	NA	s	203[D]	1/1	0.97	0.19	35,35,35,35	1
2	ZN	H	202	1/1	0.97	0.13	101,101,101,101	1
2	ZN	d	203[C]	1/1	0.97	0.27	48,48,48,48	1
2	ZN	d	203[D]	1/1	0.97	0.27	48,48,48,48	1
2	ZN	l	201[C]	1/1	0.97	0.06	32,32,32,32	1
2	ZN	l	201[D]	1/1	0.97	0.06	39,39,39,39	1
2	ZN	X	203	1/1	0.97	0.03	57,57,57,57	1
2	ZN	h	202[C]	1/1	0.97	0.07	46,46,46,46	1
2	ZN	h	202[D]	1/1	0.97	0.07	49,49,49,49	1
2	ZN	Q	202	1/1	0.97	0.06	48,48,48,48	1
3	NA	d	205[C]	1/1	0.97	0.20	34,34,34,34	1
3	NA	d	205[D]	1/1	0.97	0.20	34,34,34,34	1
2	ZN	C	203	1/1	0.97	0.06	54,54,54,54	1
2	ZN	U	202	1/1	0.97	0.04	48,48,48,48	1
3	NA	p	203[C]	1/1	0.97	0.18	34,34,34,34	1
3	NA	p	203[D]	1/1	0.97	0.18	35,35,35,35	1
3	NA	s	203[C]	1/1	0.97	0.19	34,34,34,34	1
2	ZN	u	201[D]	1/1	0.98	0.06	33,33,33,33	1
2	ZN	u	202[C]	1/1	0.98	0.04	49,49,49,49	1
2	ZN	u	202[D]	1/1	0.98	0.04	46,46,46,46	1
2	ZN	v	202[C]	1/1	0.98	0.10	34,34,34,34	1
2	ZN	v	202[D]	1/1	0.98	0.10	32,32,32,32	1
2	ZN	A	204	1/1	0.98	0.05	55,55,55,55	1
2	ZN	D	203	1/1	0.98	0.05	53,53,53,53	1
2	ZN	w	201[C]	1/1	0.98	0.10	36,36,36,36	1
2	ZN	w	201[D]	1/1	0.98	0.10	35,35,35,35	1
2	ZN	w	202[C]	1/1	0.98	0.26	45,45,45,45	1
2	ZN	w	202[D]	1/1	0.98	0.26	44,44,44,44	1
2	ZN	H	203	1/1	0.98	0.05	51,51,51,51	1
2	ZN	R	202	1/1	0.98	0.05	52,52,52,52	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	x	202[C]	1/1	0.98	0.28	46,46,46,46	1
2	ZN	x	202[D]	1/1	0.98	0.28	48,48,48,48	1
2	ZN	S	203	1/1	0.98	0.05	54,54,54,54	1
2	ZN	I	202	1/1	0.98	0.04	47,47,47,47	1
2	ZN	e	201[C]	1/1	0.98	0.07	34,34,34,34	1
2	ZN	e	201[D]	1/1	0.98	0.07	38,38,38,38	1
2	ZN	n	201[C]	1/1	0.98	0.09	37,37,37,37	1
2	ZN	n	201[D]	1/1	0.98	0.09	35,35,35,35	1
2	ZN	e	202[C]	1/1	0.98	0.35	46,46,46,46	1
2	ZN	e	202[D]	1/1	0.98	0.35	47,47,47,47	1
2	ZN	o	201[C]	1/1	0.98	0.05	33,33,33,33	1
3	NA	a	204[C]	1/1	0.98	0.24	36,36,36,36	1
3	NA	a	204[D]	1/1	0.98	0.24	27,27,27,27	1
2	ZN	o	201[D]	1/1	0.98	0.05	35,35,35,35	1
2	ZN	J	201	1/1	0.98	0.08	37,37,37,37	0
2	ZN	V	202	1/1	0.98	0.05	54,54,54,54	1
2	ZN	p	201[C]	1/1	0.98	0.09	36,36,36,36	1
3	NA	j	204[C]	1/1	0.98	0.16	33,33,33,33	1
3	NA	j	204[D]	1/1	0.98	0.16	29,29,29,29	1
3	NA	m	204[C]	1/1	0.98	0.19	32,32,32,32	1
3	NA	m	204[D]	1/1	0.98	0.19	35,35,35,35	1
2	ZN	p	201[D]	1/1	0.98	0.09	32,32,32,32	1
2	ZN	J	203	1/1	0.98	0.03	61,61,61,61	1
2	ZN	B	203	1/1	0.98	0.04	51,51,51,51	1
2	ZN	g	202[C]	1/1	0.98	0.08	31,31,31,31	1
3	NA	v	205[C]	1/1	0.98	0.20	31,31,31,31	1
3	NA	v	205[D]	1/1	0.98	0.20	31,31,31,31	1
2	ZN	g	202[D]	1/1	0.98	0.08	32,32,32,32	1
2	ZN	q	202[C]	1/1	0.98	0.08	30,30,30,30	1
2	ZN	q	202[D]	1/1	0.98	0.08	32,32,32,32	1
2	ZN	a	201[C]	1/1	0.98	0.07	36,36,36,36	1
2	ZN	a	201[D]	1/1	0.98	0.07	35,35,35,35	1
2	ZN	F	202	1/1	0.98	0.08	77,77,77,77	1
2	ZN	O	203	1/1	0.98	0.11	94,94,94,94	1
2	ZN	b	201[C]	1/1	0.98	0.07	35,35,35,35	1
2	ZN	b	201[D]	1/1	0.98	0.07	34,34,34,34	1
2	ZN	s	201[C]	1/1	0.98	0.10	37,37,37,37	1
2	ZN	s	201[D]	1/1	0.98	0.10	31,31,31,31	1
2	ZN	b	202[C]	1/1	0.98	0.06	41,41,41,41	1
2	ZN	b	202[D]	1/1	0.98	0.06	48,48,48,48	1
2	ZN	c	201[C]	1/1	0.98	0.06	31,31,31,31	1
2	ZN	c	201[D]	1/1	0.98	0.06	38,38,38,38	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	u	201[C]	1/1	0.98	0.06	36,36,36,36	1
2	ZN	a	202[D]	1/1	0.99	0.09	33,33,33,33	1
2	ZN	B	202	1/1	0.99	0.08	76,76,76,76	1
2	ZN	f	201[C]	1/1	0.99	0.10	33,33,33,33	1
2	ZN	f	201[D]	1/1	0.99	0.10	37,37,37,37	1
2	ZN	x	201[C]	1/1	0.99	0.06	33,33,33,33	1
2	ZN	x	201[D]	1/1	0.99	0.06	35,35,35,35	1
2	ZN	f	202[C]	1/1	0.99	0.21	45,45,45,45	1
2	ZN	f	202[D]	1/1	0.99	0.21	49,49,49,49	1
2	ZN	P	201	1/1	0.99	0.10	35,35,35,35	0
2	ZN	A	203	1/1	0.99	0.06	69,69,69,69	1
2	ZN	g	201[C]	1/1	0.99	0.07	31,31,31,31	1
2	ZN	g	201[D]	1/1	0.99	0.07	35,35,35,35	1
2	ZN	Q	201	1/1	0.99	0.09	36,36,36,36	0
2	ZN	C	202	1/1	0.99	0.10	79,79,79,79	1
2	ZN	J	202	1/1	0.99	0.09	40,40,40,40	0
3	NA	P	204	1/1	0.99	0.26	41,41,41,41	0
2	ZN	S	201	1/1	0.99	0.09	36,36,36,36	0
2	ZN	h	201[C]	1/1	0.99	0.07	35,35,35,35	1
2	ZN	h	201[D]	1/1	0.99	0.07	35,35,35,35	1
2	ZN	F	203	1/1	0.99	0.03	49,49,49,49	1
2	ZN	G	202	1/1	0.99	0.10	37,37,37,37	0
2	ZN	i	201[C]	1/1	0.99	0.07	33,33,33,33	1
2	ZN	i	201[D]	1/1	0.99	0.07	36,36,36,36	1
2	ZN	L	201	1/1	0.99	0.08	40,40,40,40	0
2	ZN	d	201[C]	1/1	0.99	0.07	32,32,32,32	1
2	ZN	j	201[C]	1/1	0.99	0.07	34,34,34,34	1
2	ZN	j	201[D]	1/1	0.99	0.07	38,38,38,38	1
2	ZN	d	201[D]	1/1	0.99	0.07	35,35,35,35	1
2	ZN	d	202[C]	1/1	0.99	0.09	33,33,33,33	1
2	ZN	k	201[C]	1/1	0.99	0.06	35,35,35,35	1
2	ZN	t	201[C]	1/1	0.99	0.07	35,35,35,35	1
2	ZN	t	201[D]	1/1	0.99	0.07	32,32,32,32	1
2	ZN	t	202[C]	1/1	0.99	0.08	31,31,31,31	1
2	ZN	t	202[D]	1/1	0.99	0.08	32,32,32,32	1
2	ZN	k	201[D]	1/1	0.99	0.06	35,35,35,35	1
2	ZN	d	202[D]	1/1	0.99	0.09	34,34,34,34	1
2	ZN	V	201	1/1	0.99	0.07	39,39,39,39	0
2	ZN	L	202	1/1	0.99	0.04	54,54,54,54	1
2	ZN	M	201	1/1	0.99	0.09	40,40,40,40	0
2	ZN	X	202	1/1	0.99	0.09	38,38,38,38	0
2	ZN	v	201[C]	1/1	0.99	0.06	39,39,39,39	1

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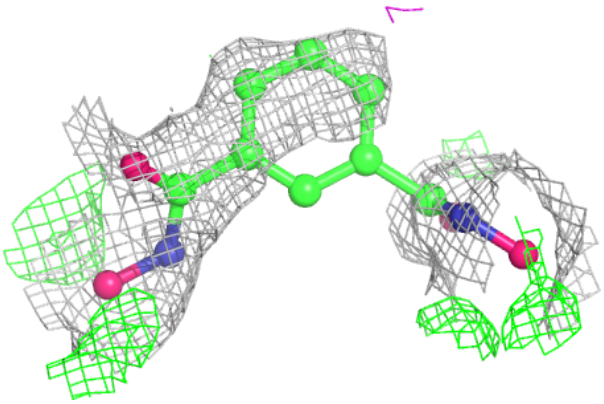
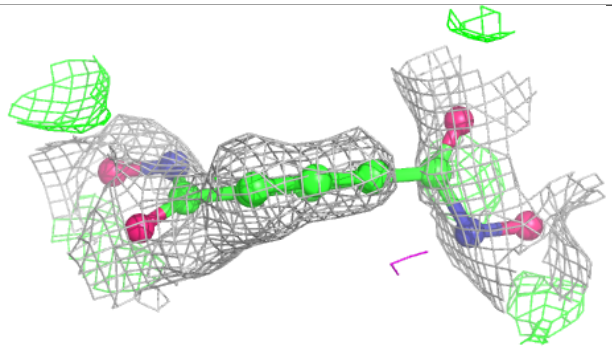
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	v	201[D]	1/1	0.99	0.06	31,31,31,31	1
2	ZN	A	202	1/1	0.99	0.08	38,38,38,38	0
2	ZN	O	202	1/1	0.99	0.07	38,38,38,38	0
2	ZN	v	203[C]	1/1	0.99	0.22	44,44,44,44	1
2	ZN	v	203[D]	1/1	0.99	0.22	46,46,46,46	1
2	ZN	D	202	1/1	0.99	0.09	37,37,37,37	0
2	ZN	m	202[C]	1/1	0.99	0.09	34,34,34,34	1
2	ZN	m	202[D]	1/1	0.99	0.09	31,31,31,31	1
2	ZN	a	202[C]	1/1	0.99	0.09	29,29,29,29	1
2	ZN	I	201	1/1	1.00	0.08	32,32,32,32	0
2	ZN	O	201	1/1	1.00	0.08	40,40,40,40	0
2	ZN	D	201	1/1	1.00	0.10	36,36,36,36	0
2	ZN	W	201	1/1	1.00	0.09	36,36,36,36	0
2	ZN	C	201	1/1	1.00	0.09	40,40,40,40	0
2	ZN	X	201	1/1	1.00	0.10	40,40,40,40	0
2	ZN	G	201	1/1	1.00	0.09	36,36,36,36	0
2	ZN	A	201	1/1	1.00	0.07	38,38,38,38	0
2	ZN	P	202	1/1	1.00	0.08	36,36,36,36	0
2	ZN	K	201	1/1	1.00	0.07	36,36,36,36	0
2	ZN	E	201	1/1	1.00	0.08	34,34,34,34	0
2	ZN	H	201	1/1	1.00	0.10	33,33,33,33	0
2	ZN	R	201	1/1	1.00	0.12	35,35,35,35	0
2	ZN	B	201	1/1	1.00	0.09	37,37,37,37	0
2	ZN	F	201	1/1	1.00	0.09	37,37,37,37	0
2	ZN	S	202	1/1	1.00	0.09	35,35,35,35	0
2	ZN	M	202	1/1	1.00	0.04	53,53,53,53	1
2	ZN	T	201	1/1	1.00	0.09	36,36,36,36	0
2	ZN	j	202[C]	1/1	1.00	0.08	30,30,30,30	1
2	ZN	j	202[D]	1/1	1.00	0.08	33,33,33,33	1
2	ZN	N	201	1/1	1.00	0.07	37,37,37,37	0
2	ZN	U	201	1/1	1.00	0.08	36,36,36,36	0

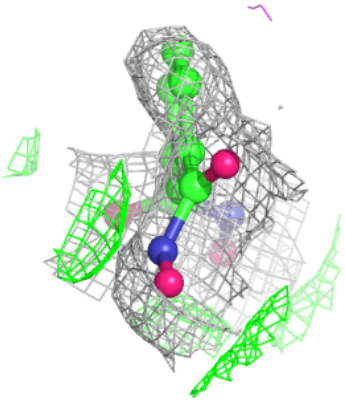
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around V9D T 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)

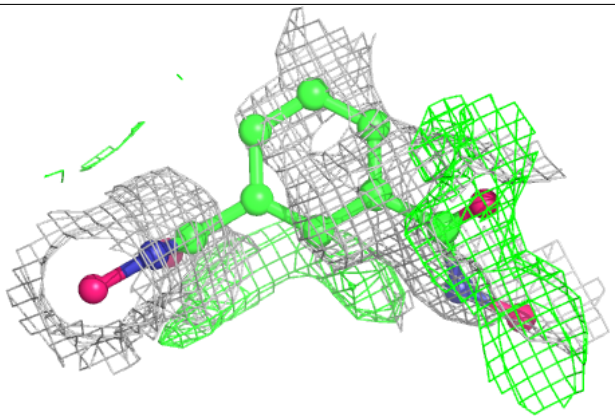


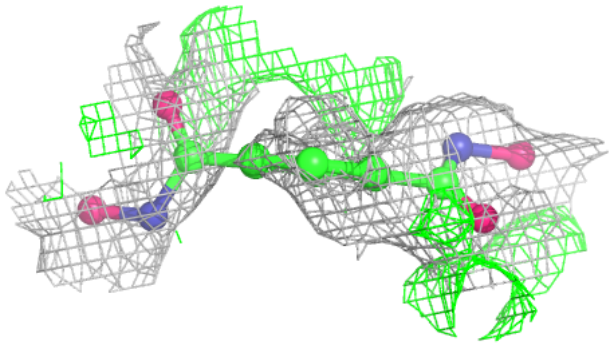


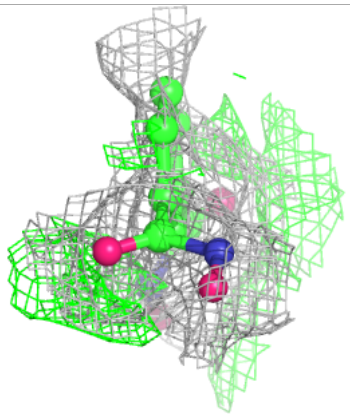


Electron density around V9D T 203 (D):

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

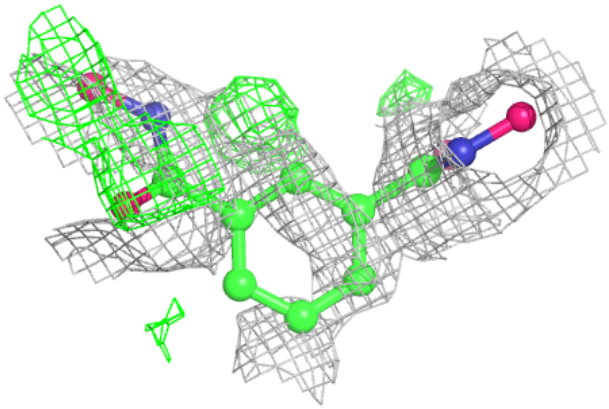


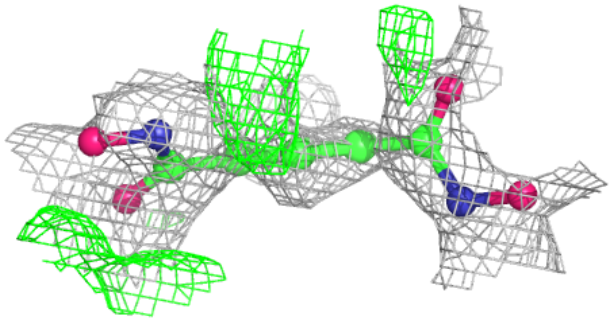


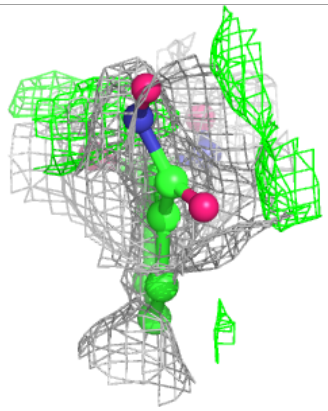


Electron density around V9D H 204 (C):

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

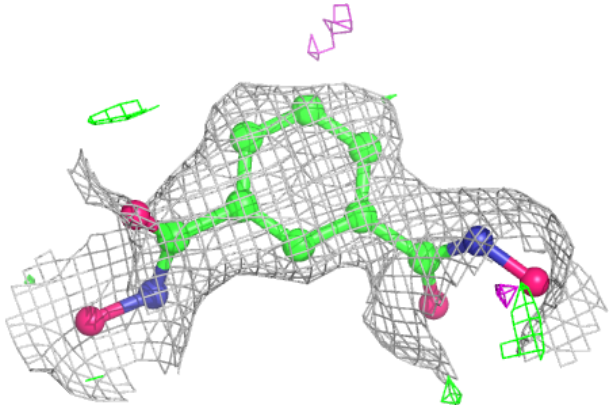


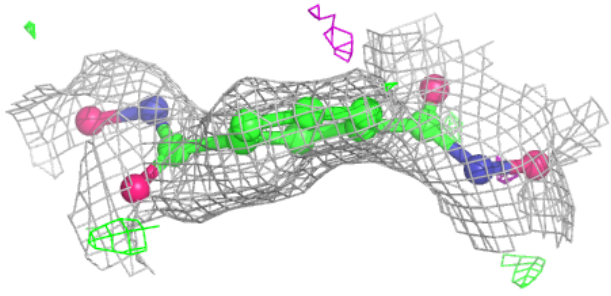


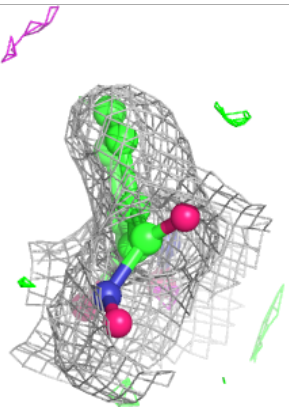


Electron density around V9D H 204 (D):

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

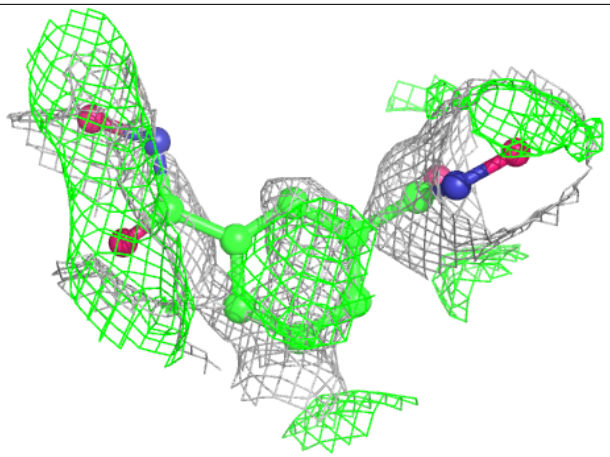


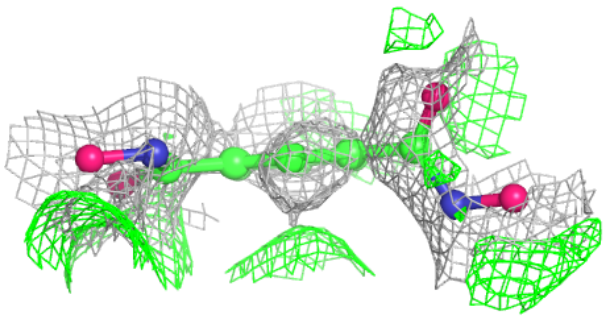


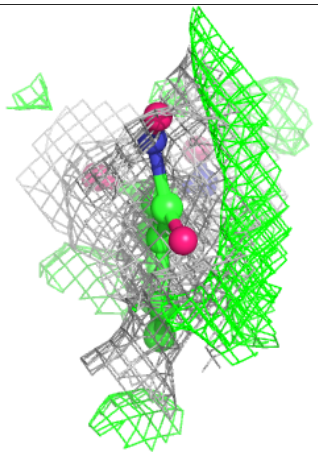


Electron density around V9D B 204 (C):

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

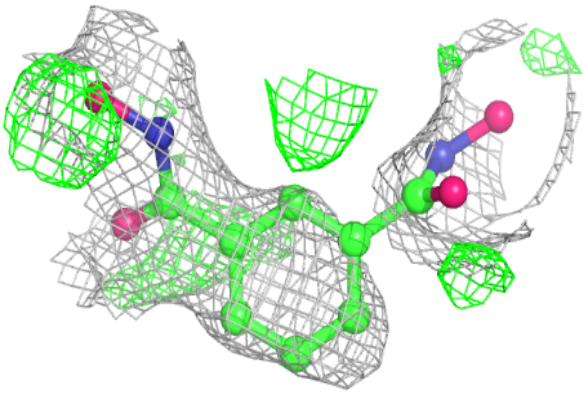


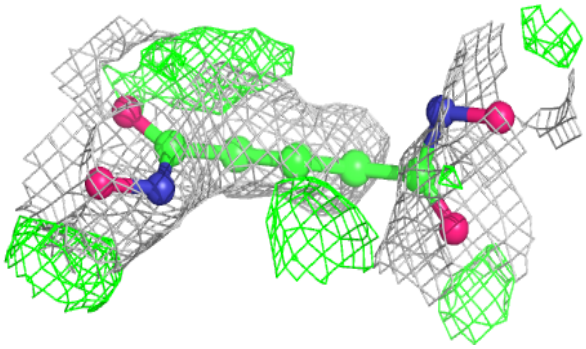


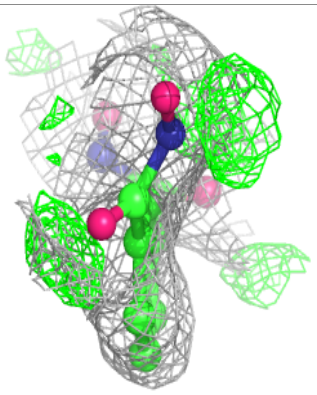


Electron density around V9D B 204 (D):

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

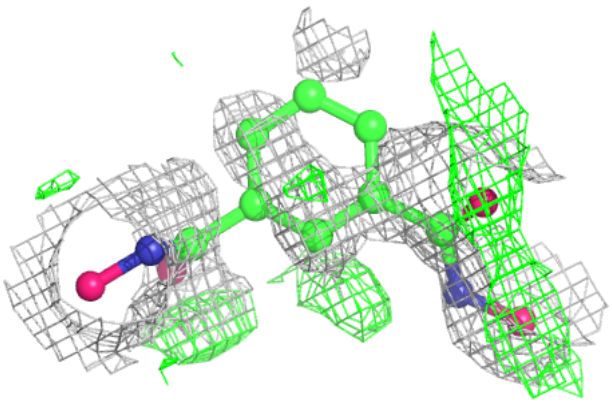


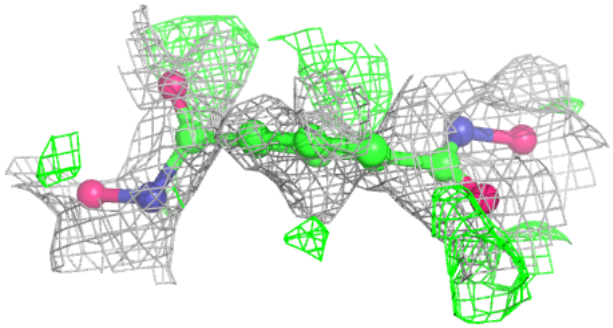


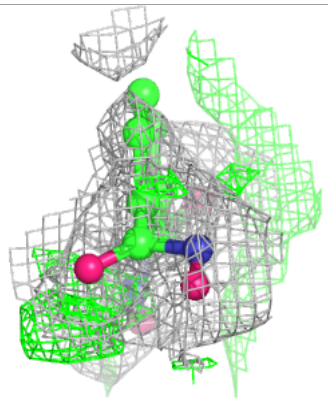


Electron density around V9D E 203 (C):

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

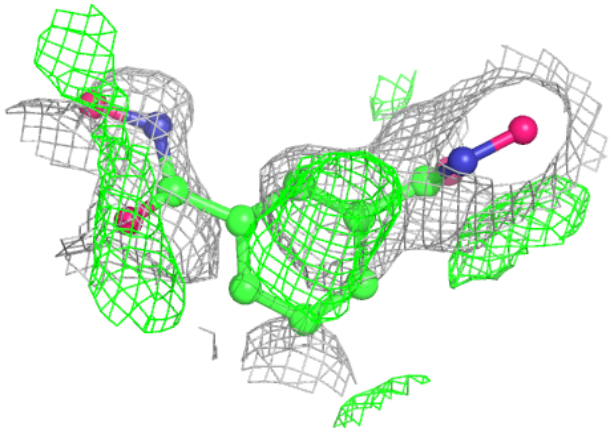


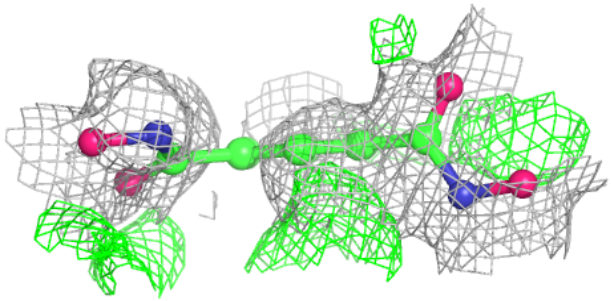


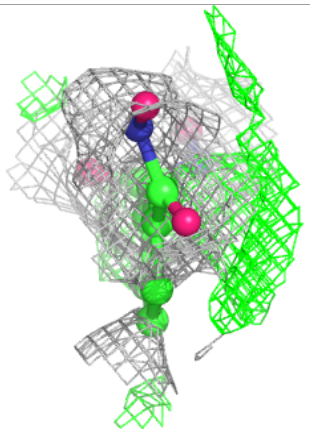


Electron density around V9D K 203 (C):

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

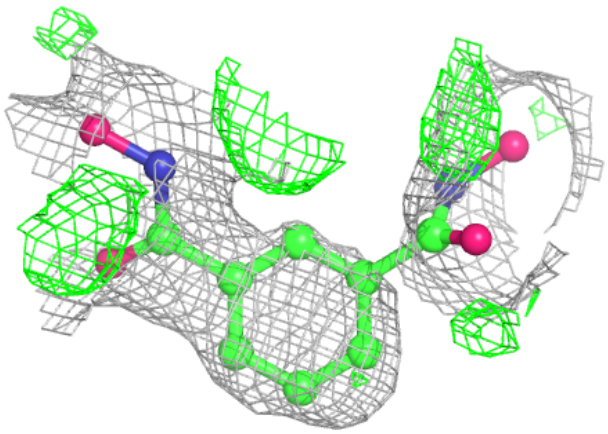


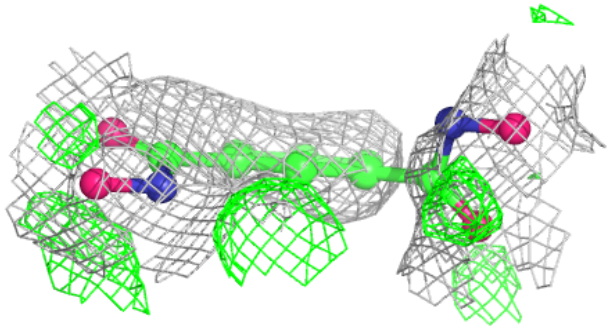


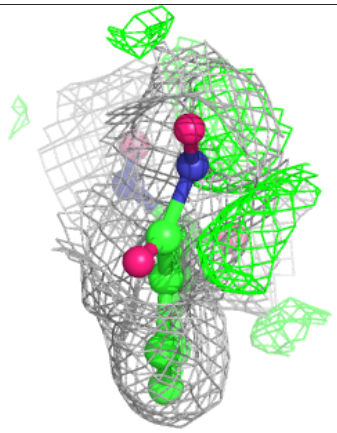


Electron density around V9D K 203 (D):

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

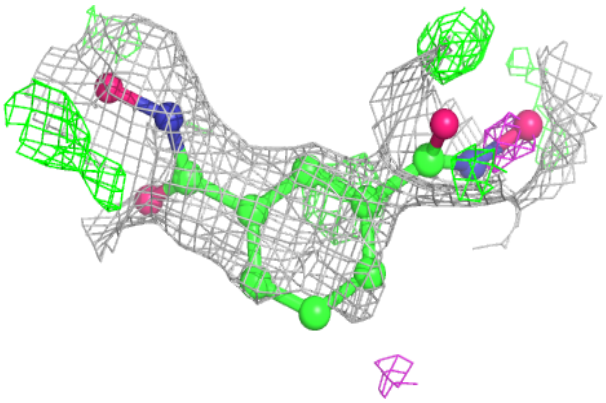


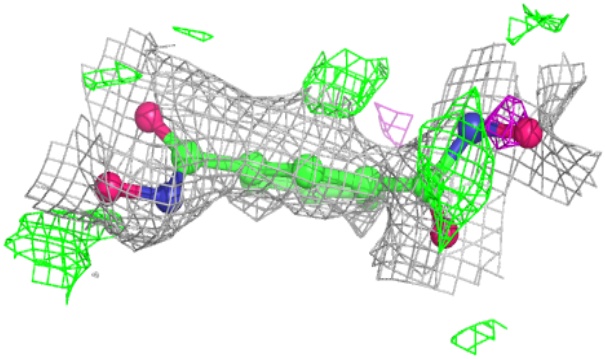


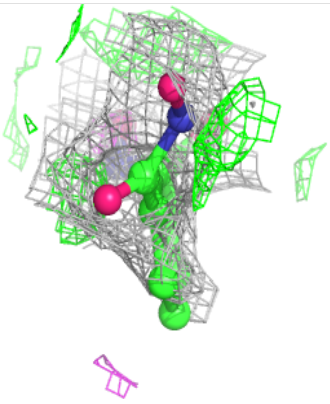


Electron density around V9D E 203 (D):

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

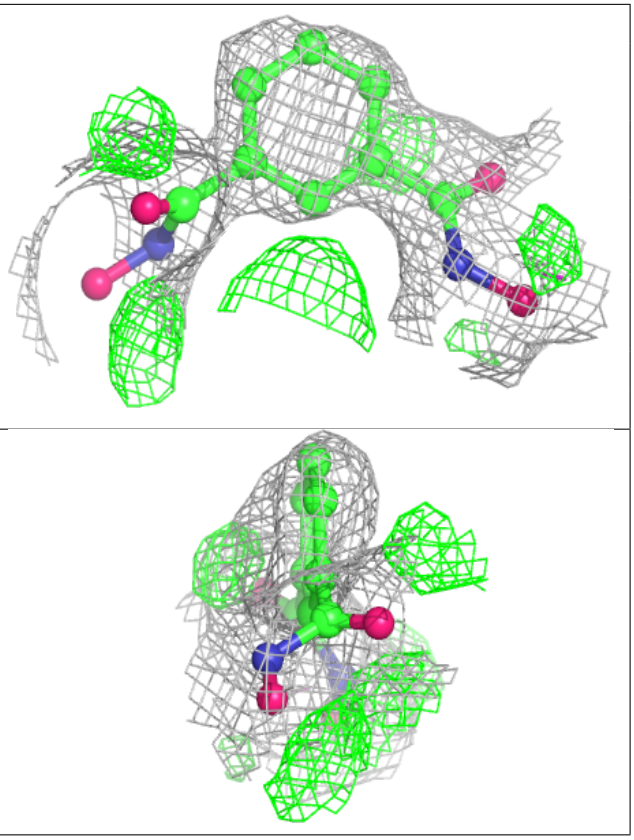


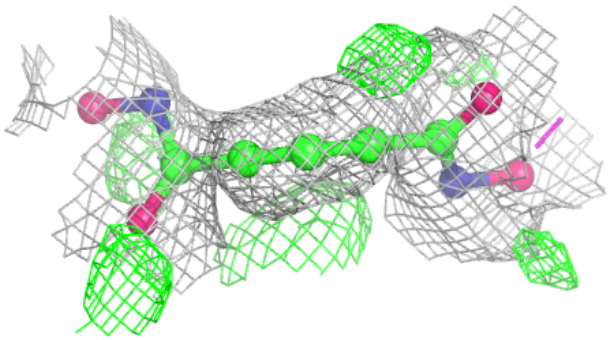




Electron density around V9D O 205 (C):

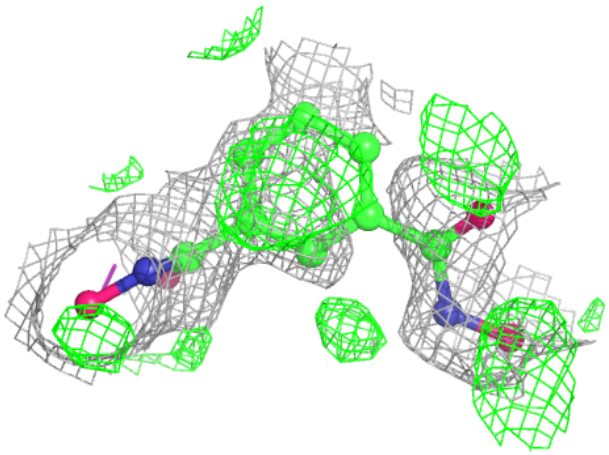
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

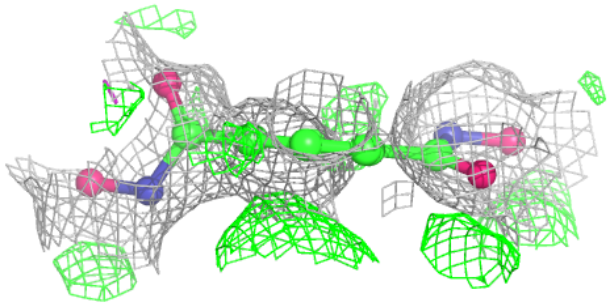


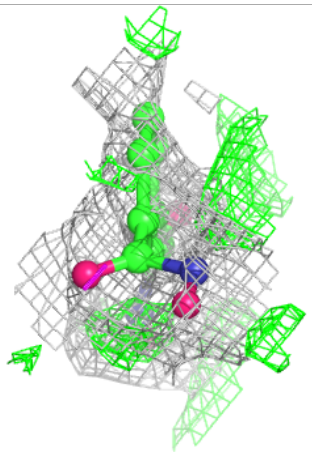


Electron density around V9D O 205 (D):

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

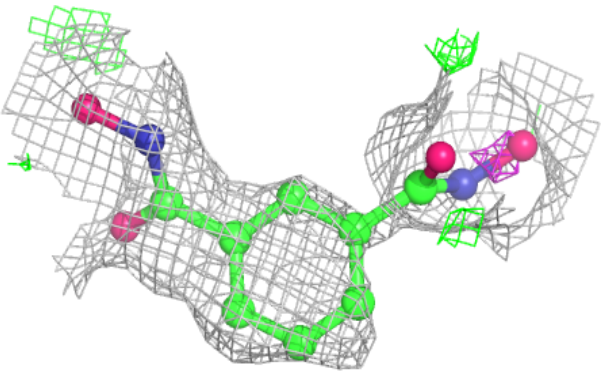


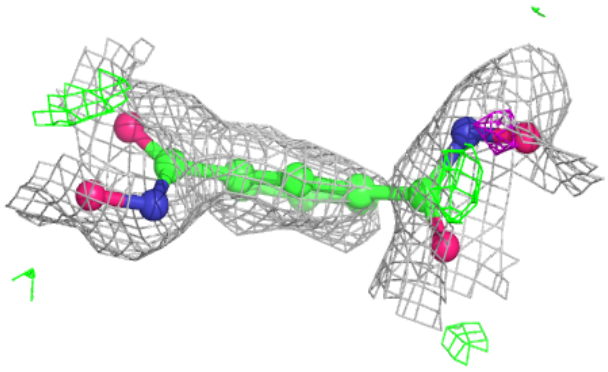


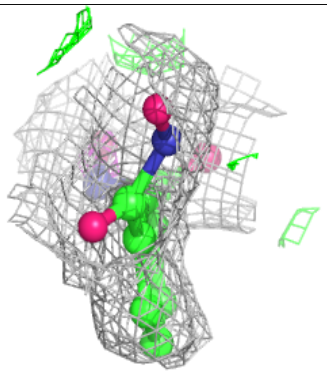


Electron density around V9D Q 203 (C):

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

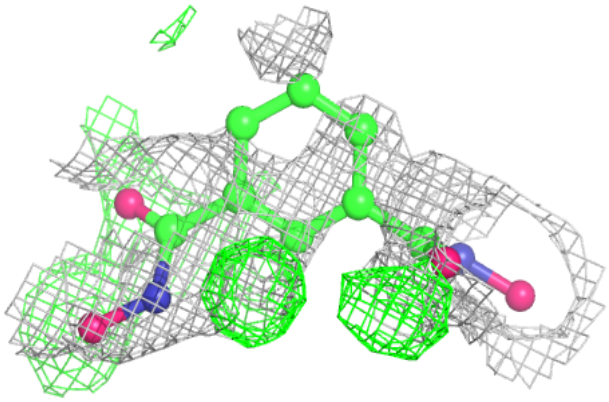


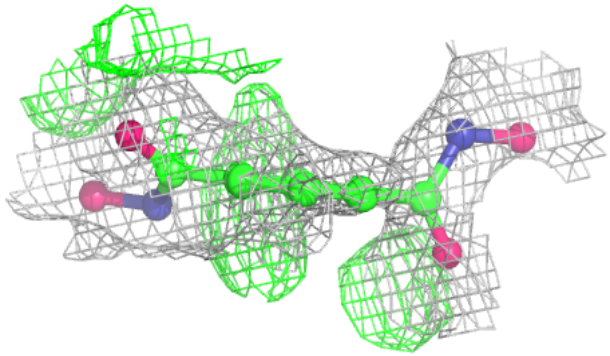


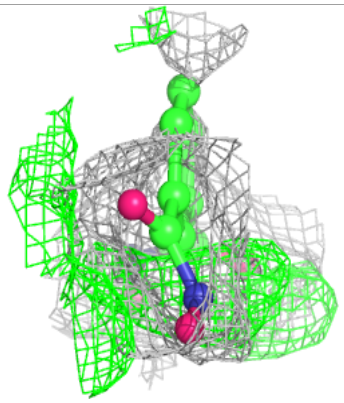


Electron density around V9D Q 203 (D):

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

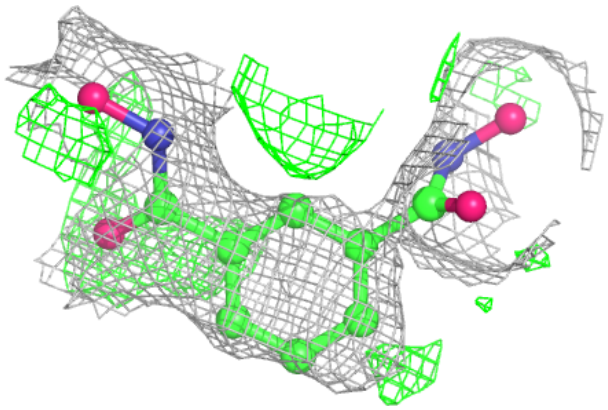


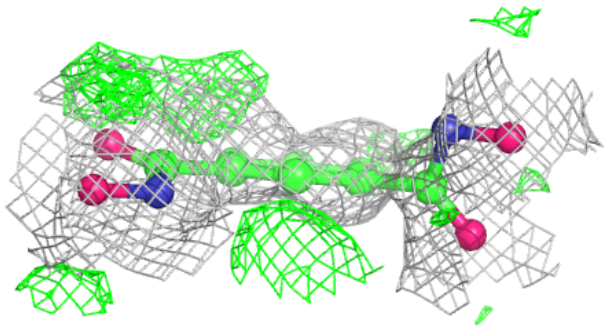




Electron density around V9D X 204 (C):

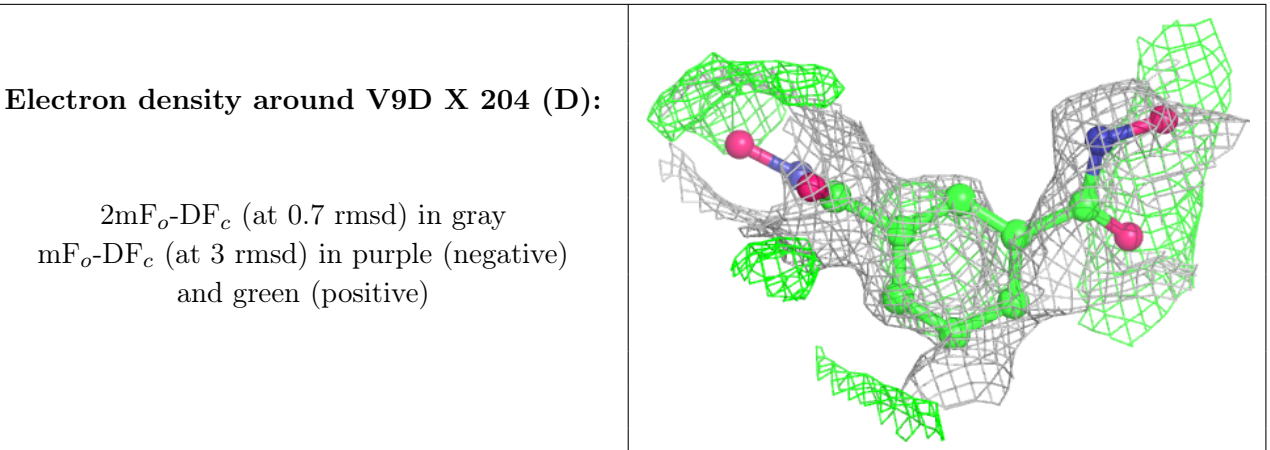
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

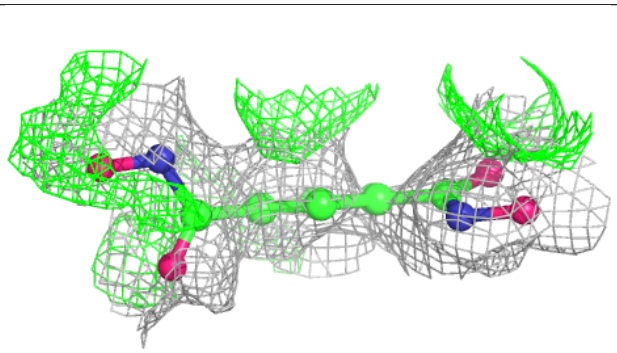


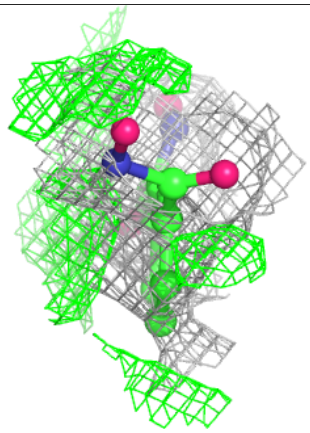


Electron density around V9D X 204 (D):

$2mF_o$-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

There are no such residues in this entry.