



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:13 PM UTC

PDB ID : 7JGN / pdb_00007jgn
Title : Crystal Structure of the Zn-bound Human Heavy-chain variant 122H-delta C-star with meta-benzenedihydroxamate 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

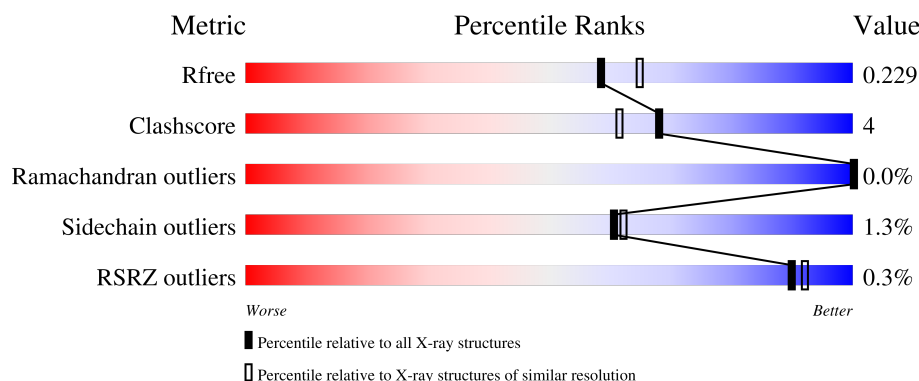
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

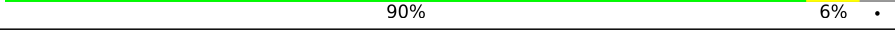
The reported resolution of this entry is 2.07 Å.

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.



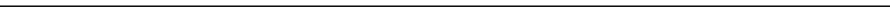
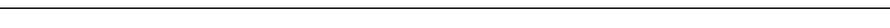
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	182	
1	B	182	
1	C	182	
1	D	182	
1	E	182	

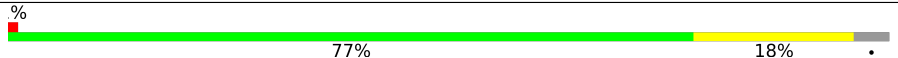
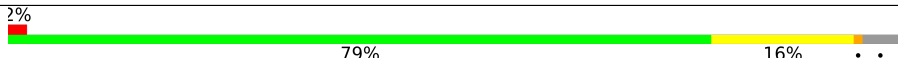
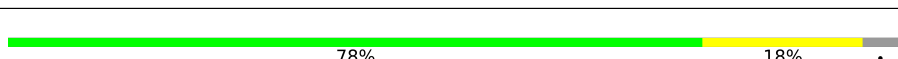
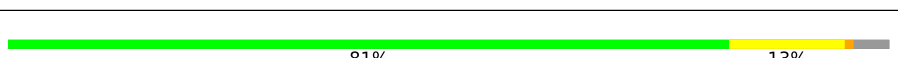
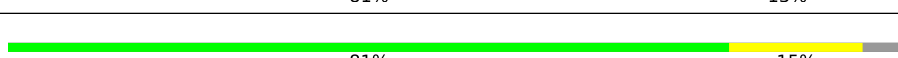
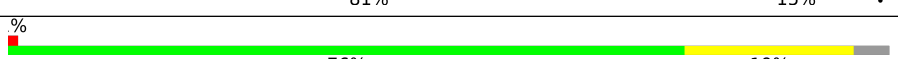
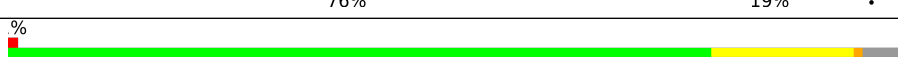
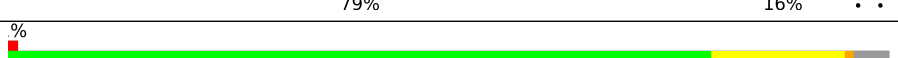
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Mol	Chain	Length	Quality of chain
1	F	182	 87% 8% .
1	G	182	 90% 6% .
1	H	182	 89% 7% .
1	I	182	 88% 8% .
1	J	182	 87% 8% .
1	K	182	 90% 5% .
1	L	182	 87% 9% .
1	M	182	 89% 7% .
1	N	182	 88% 7% .
1	O	182	 87% 8% . .
1	P	182	 91% 5% .
1	Q	182	 89% 7% .
1	R	182	 90% 5% .
1	S	182	 90% 6% .
1	T	182	 89% 7% .
1	U	182	 89% 7% .
1	V	182	 90% 6% .
1	W	182	 85% 10% .
1	X	182	 86% 9% .
1	a	182	 % 79% 15% . .
1	b	182	 78% 18% .
1	c	182	 84% 12% .
1	d	182	 % 82% 13% . .
1	e	182	 % 80% 15% . .
1	f	182	 74% 21% . .

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

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 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 (CCD ID: 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 2	Zn 2	0	0
2	O	4	Total 4	Zn 4	0	0
2	P	3	Total 3	Zn 3	0	0
2	Q	2	Total 2	Zn 2	0	0
2	R	2	Total 2	Zn 2	0	0
2	S	3	Total 3	Zn 3	0	0
2	T	2	Total 2	Zn 2	0	0
2	U	2	Total 2	Zn 2	0	0
2	V	2	Total 2	Zn 2	0	0
2	W	2	Total 2	Zn 2	0	0
2	X	3	Total 3	Zn 3	0	0
2	a	3	Total 6	Zn 6	0	3
2	b	2	Total 4	Zn 4	0	2
2	c	2	Total 4	Zn 4	0	2
2	d	4	Total 8	Zn 8	0	4
2	e	3	Total 6	Zn 6	0	3
2	f	3	Total 6	Zn 6	0	3
2	g	3	Total 6	Zn 6	0	3
2	h	2	Total 4	Zn 4	0	2
2	i	2	Total 4	Zn 4	0	2
2	j	3	Total 6	Zn 6	0	3

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

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

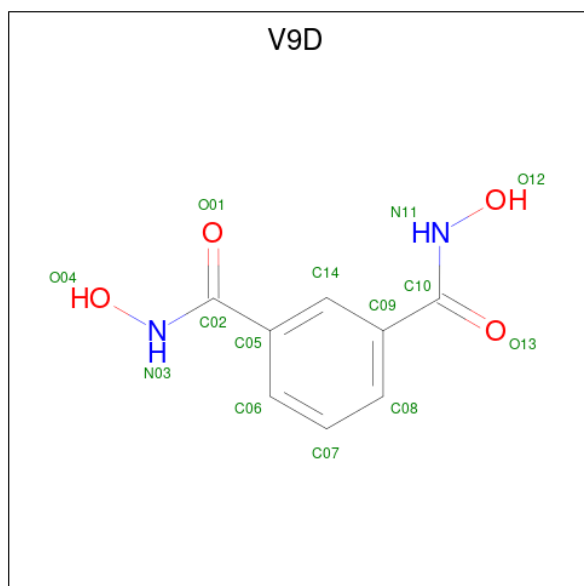
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Na 1	0	0
3	D	1	Total 1	Na 1	0	0
3	G	1	Total 1	Na 1	0	0
3	J	1	Total 1	Na 1	0	0
3	M	1	Total 1	Na 1	0	0

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

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



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

- Molecule 5 is water.

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

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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 3	O 3	0	0
5	k	2	Total 2	O 2	0	0
5	l	3	Total 3	O 3	0	0
5	m	6	Total 6	O 6	0	0
5	n	2	Total 2	O 2	0	0
5	o	2	Total 2	O 2	0	0
5	p	3	Total 3	O 3	0	0
5	q	4	Total 4	O 4	0	0
5	r	4	Total 4	O 4	0	0
5	s	5	Total 5	O 5	0	0
5	t	4	Total 4	O 4	0	0
5	u	3	Total 3	O 3	0	0
5	v	5	Total 5	O 5	0	0
5	w	1	Total 1	O 1	0	0
5	x	3	Total 3	O 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:  89% 7% .



- Molecule 1: Ferritin heavy chain

Chain B:  89% 7% .



- Molecule 1: Ferritin heavy chain

Chain C:  89% 7% .



- Molecule 1: Ferritin heavy chain

Chain D:  90% 6% .



- Molecule 1: Ferritin heavy chain

Chain E:  87% 8% .



- Molecule 1: Ferritin heavy chain

Chain F:  87% 8% .



- Molecule 1: Ferritin heavy chain

Chain G: 90% 6% .



- Molecule 1: Ferritin heavy chain

Chain H: 89% 7% .



- Molecule 1: Ferritin heavy chain

Chain I: 88% 8% .



- Molecule 1: Ferritin heavy chain

Chain J: 87% 8% .



- Molecule 1: Ferritin heavy chain

Chain K: 90% 5% .



- Molecule 1: Ferritin heavy chain

Chain L: 87% 9% .



- Molecule 1: Ferritin heavy chain

Chain M: 89% 7% .



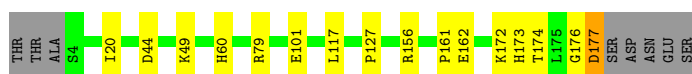
- Molecule 1: Ferritin heavy chain

Chain N: 88% 7% .



- Molecule 1: Ferritin heavy chain

Chain O: 87% 8% . .



- Molecule 1: Ferritin heavy chain

Chain P: 91% 5% .



- Molecule 1: Ferritin heavy chain

Chain Q: 89% 7% .



- Molecule 1: Ferritin heavy chain

Chain R: 90% 5% .



- Molecule 1: Ferritin heavy chain

Chain S: 90% 6% .



- Molecule 1: Ferritin heavy chain

Chain T: 89% 7% .



- Molecule 1: Ferritin heavy chain

Chain U: 89% 7% .



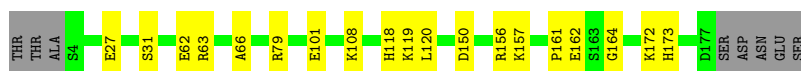
- Molecule 1: Ferritin heavy chain

Chain V: 90% 6% .



- Molecule 1: Ferritin heavy chain

Chain W: 85% 10% .



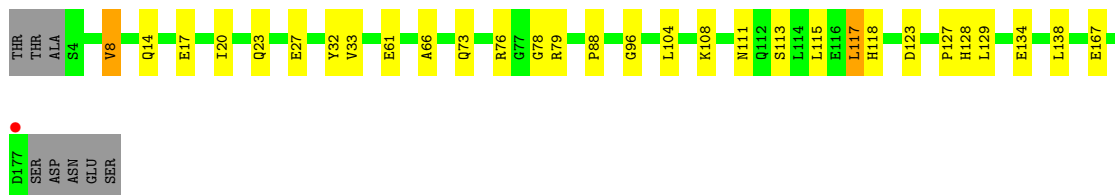
- Molecule 1: Ferritin heavy chain

Chain X: 86% 9% .



- Molecule 1: Ferritin heavy chain

Chain a: 79% 15% . .



- Molecule 1: Ferritin heavy chain

Chain b: 78% 18% .



SER
THR
ASP
ASN
GLU
SER

- Molecule 1: Ferritin heavy chain

Chain c:  84% 12%

THR THR ALA S4 T5 S6 Q7 V8 R43 D44 D45 L72 R79 M11 L115 E116 L117 M125 D126 P127 H128 L129 A130 D131 F132 I133 E134 L155 E162 E167 D177 SER ASP ASN GLU SER

- Molecule 1: Ferritin heavy chain

Chain d:  82% 13%

THR THR ALA S4 Q10 I20 Q23 Y32 V33 Y34 L35 E61 E62 E63 E67 R76 R79 P88 K108 N111 Q112 S113 L114 L115 E116 L117 H118 H128 L129 I133 I145 D177 SER ASP ASN GLU SER

- Molecule 1: Ferritin heavy chain

Chain e:  80% 15%

THR THR ALA S4 S6 Q7 V8 Y32 F41 Y46 A47 L48 Y54 Q58 L72 R76 G77 G78 R79 E94 S95 G96 L97 K108 N111 L117 H128 L129 I133 E134 L138 I145 P161 E162 Y168 K172 D177 SER ASP ASN

GLU
SER

- Molecule 1: Ferritin heavy chain

Chain f:  74% 21%

THR THR ALA S4 Q7 V8 Q14 I20 Q23 E27 V33 S38 F41 D42 R43 D44 D45 N50 L56 H57 Q58 E61 E62 A66 E67 K68 L69 M70 K71 L72 Q75 R76 R79 I80 P88 G96 S113 L114 L117 H118 K119

H122 D123 P127 H128 Y137 V152 S163 D171 D177 SER ASP ASN GLU SER

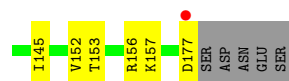
- Molecule 1: Ferritin heavy chain

Chain g:  77% 18%

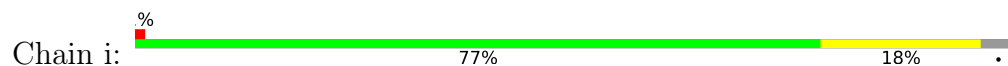
THR THR ALA S4 V8 E9 Q10 Q14 N21 E22 Q23 I24 L28 L35 F41 H57 E61 E62 R63 E67 K68 R76 R79 D91 G96 L97 E101 K108 N111 Q112 S113 L114 L115 E116 L117 H118 A121 K124 P127 H128 L129

F132 I133 E134 D177 SER ASP ASN GLU SER

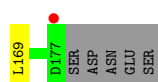
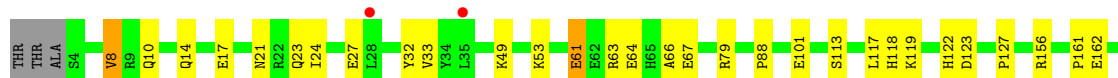
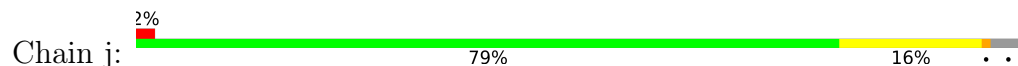
- Molecule 1: Ferritin heavy chain



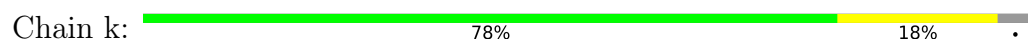
- Molecule 1: Ferritin heavy chain



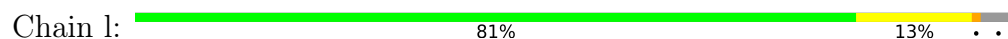
- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain

Chain m:  81% 15% .



• Molecule 1: Ferritin heavy chain

Chain n:  76% 19% .



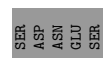
• Molecule 1: Ferritin heavy chain

Chain o:  79% 16% . .



• Molecule 1: Ferritin heavy chain

Chain p:  79% 15% . .



• Molecule 1: Ferritin heavy chain

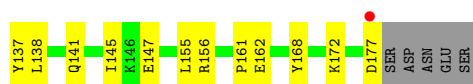
Chain q:  81% 14% . .



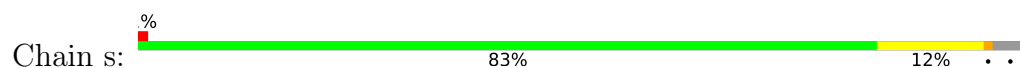
• Molecule 1: Ferritin heavy chain

Chain r:  70% 25% . .

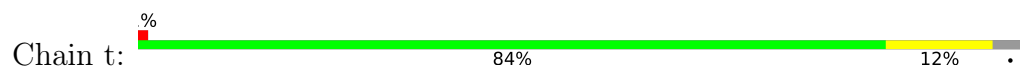




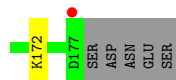
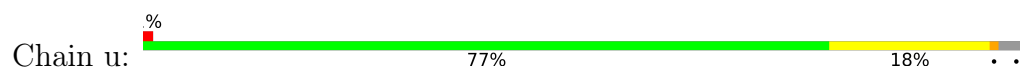
- Molecule 1: Ferritin heavy chain



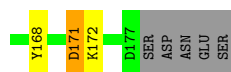
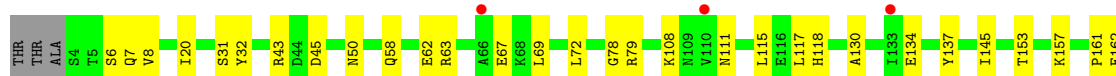
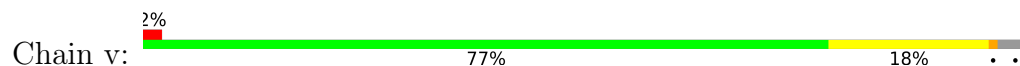
- Molecule 1: Ferritin heavy chain



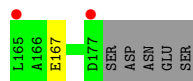
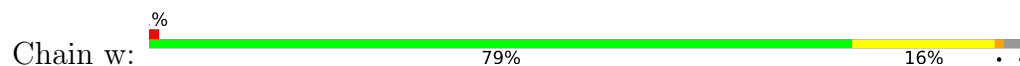
- Molecule 1: Ferritin heavy chain



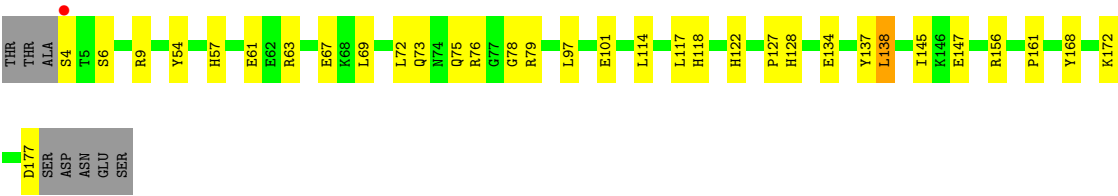
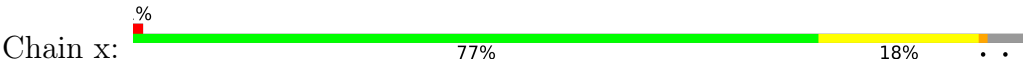
- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



● Molecule 1: Ferritin heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	215.75Å 215.46Å 156.46Å 90.00° 89.95° 90.00°	Depositor
Resolution (Å)	37.80 – 2.07 37.80 – 2.07	Depositor EDS
% Data completeness (in resolution range)	97.5 (37.80-2.07) 90.4 (37.80-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.33 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.45	0/1461	0.59	0/1969
1	B	0.45	0/1470	0.60	0/1980
1	C	0.44	0/1470	0.57	0/1980
1	D	0.47	0/1461	0.62	0/1969
1	E	0.48	0/1487	0.61	0/2003
1	F	0.48	0/1470	0.63	0/1981
1	G	0.49	0/1470	0.63	0/1980
1	H	0.49	0/1470	0.61	0/1981
1	I	0.48	0/1469	0.63	0/1980
1	J	0.46	0/1469	0.60	0/1980
1	K	0.47	0/1461	0.60	0/1969
1	L	0.45	0/1461	0.57	0/1969
1	M	0.43	0/1461	0.57	0/1969
1	N	0.45	0/1472	0.59	0/1983
1	O	0.44	0/1470	0.59	0/1980
1	P	0.48	0/1470	0.62	0/1980
1	Q	0.51	0/1479	0.61	0/1992
1	R	0.49	0/1461	0.61	0/1969
1	S	0.48	0/1470	0.63	0/1980
1	T	0.49	0/1469	0.62	0/1980
1	U	0.47	0/1480	0.62	0/1994
1	V	0.44	0/1461	0.58	0/1969
1	W	0.48	0/1492	0.60	0/2008
1	X	0.46	0/1470	0.58	0/1980
1	a	0.20	0/2922	0.31	0/3938
1	b	0.20	0/2922	0.32	0/3938
1	c	0.20	0/2922	0.32	0/3938
1	d	0.20	0/2922	0.32	0/3938
1	e	0.20	0/2922	0.33	0/3938
1	f	0.19	0/2922	0.30	0/3938
1	g	0.21	0/2922	0.31	0/3938
1	h	0.20	0/2922	0.33	0/3938

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	i	0.20	0/2922	0.31	0/3938
1	j	0.20	0/2922	0.32	0/3938
1	k	0.20	0/2922	0.31	0/3938
1	l	0.20	0/2922	0.34	0/3938
1	m	0.20	0/2922	0.34	0/3938
1	n	0.20	0/2922	0.33	0/3938
1	o	0.21	0/2922	0.31	0/3938
1	p	0.19	0/2922	0.31	0/3938
1	q	0.20	0/2922	0.31	0/3938
1	r	0.20	0/2922	0.32	0/3938
1	s	0.19	0/2922	0.31	0/3938
1	t	0.21	0/2922	0.31	0/3938
1	u	0.20	0/2922	0.32	0/3938
1	v	0.20	0/2922	0.34	0/3938
1	w	0.21	0/2922	0.33	0/3938
1	x	0.20	0/2922	0.32	0/3938
All	All	0.32	0/105402	0.44	0/142037

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1431	0	1362	12	0
1	B	1437	0	1375	15	0
1	C	1437	0	1375	17	0
1	D	1431	0	1362	11	0
1	E	1448	0	1389	15	0
1	F	1437	0	1368	20	0
1	G	1437	0	1375	10	0
1	H	1437	0	1370	11	0
1	I	1436	0	1368	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1436	0	1368	14	0
1	K	1431	0	1362	9	0
1	L	1431	0	1362	14	0
1	M	1431	0	1362	16	0
1	N	1439	0	1375	12	0
1	O	1437	0	1375	18	0
1	P	1437	0	1375	12	0
1	Q	1443	0	1383	19	0
1	R	1431	0	1362	9	0
1	S	1437	0	1375	12	0
1	T	1436	0	1368	11	0
1	U	1444	0	1381	10	0
1	V	1431	0	1362	14	0
1	W	1453	0	1401	20	0
1	X	1437	0	1375	17	0
1	a	2862	0	2716	22	0
1	b	2862	0	2712	24	0
1	c	2862	0	2705	13	0
1	d	2862	0	2718	14	0
1	e	2862	0	2713	20	0
1	f	2862	0	2704	25	0
1	g	2862	0	2717	26	0
1	h	2862	0	2711	28	0
1	i	2862	0	2703	21	0
1	j	2862	0	2715	22	0
1	k	2862	0	2714	25	0
1	l	2862	0	2707	14	0
1	m	2862	0	2703	13	0
1	n	2862	0	2717	21	0
1	o	2862	0	2712	18	0
1	p	2862	0	2703	21	0
1	q	2862	0	2719	21	0
1	r	2862	0	2712	32	0
1	s	2862	0	2701	14	0
1	t	2862	0	2716	15	0
1	u	2862	0	2713	25	0
1	v	2862	0	2708	19	0
1	w	2862	0	2714	17	0
1	x	2862	0	2713	24	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3	0	0	0	0
2	E	2	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
2	I	2	0	0	0	0
2	J	3	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	O	4	0	0	0	0
2	P	3	0	0	0	0
2	Q	2	0	0	0	0
2	R	2	0	0	0	0
2	S	3	0	0	0	0
2	T	2	0	0	0	0
2	U	2	0	0	0	0
2	V	2	0	0	0	0
2	W	2	0	0	0	0
2	X	3	0	0	0	0
2	a	6	0	0	0	0
2	b	4	0	0	0	0
2	c	4	0	0	0	0
2	d	8	0	0	0	0
2	e	6	0	0	0	0
2	f	6	0	0	0	0
2	g	6	0	0	0	0
2	h	4	0	0	0	0
2	i	4	0	0	0	0
2	j	6	0	0	0	0
2	k	4	0	0	0	0
2	l	4	0	0	0	0
2	m	6	0	0	0	0
2	n	4	0	0	0	0
2	o	4	0	0	0	0
2	p	4	0	0	0	0
2	q	6	0	0	0	0
2	r	4	0	0	0	0
2	s	4	0	0	0	0
2	t	6	0	0	0	0
2	u	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	v	8	0	0	0	0
2	w	6	0	0	0	0
2	x	6	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
3	G	1	0	0	0	0
3	J	1	0	0	0	0
3	M	1	0	0	0	0
3	P	1	0	0	0	0
3	S	1	0	0	0	0
3	V	1	0	0	0	0
3	a	2	0	0	0	0
3	d	2	0	0	0	0
3	g	2	0	0	0	0
3	j	2	0	0	0	0
3	m	2	0	0	0	0
3	p	2	0	0	0	0
3	s	2	0	0	0	0
3	v	2	0	0	0	0
4	B	28	0	0	1	0
4	E	28	0	0	2	0
4	H	28	0	0	3	0
4	K	28	0	0	2	0
4	O	28	0	0	2	0
4	Q	28	0	0	3	0
4	T	28	0	0	2	0
4	X	28	0	0	2	0
5	A	190	0	0	5	0
5	B	190	0	0	8	0
5	C	172	0	0	1	0
5	D	199	0	0	8	0
5	E	226	0	0	4	0
5	F	208	0	0	2	0
5	G	211	0	0	1	0
5	H	209	0	0	2	0
5	I	201	0	0	5	0
5	J	185	0	0	5	0
5	K	184	0	0	6	0
5	L	176	0	0	4	0
5	M	198	0	0	3	0
5	N	203	0	0	5	0
5	O	175	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	209	0	0	3	0
5	Q	221	0	0	3	0
5	R	200	0	0	5	0
5	S	211	0	0	1	0
5	T	223	0	0	5	0
5	U	218	0	0	0	0
5	V	190	0	0	5	0
5	W	183	0	0	7	0
5	X	184	0	0	6	0
5	a	3	0	0	1	0
5	b	2	0	0	0	0
5	c	3	0	0	0	0
5	d	3	0	0	0	0
5	e	1	0	0	0	0
5	f	5	0	0	2	0
5	g	4	0	0	1	0
5	h	2	0	0	0	0
5	i	3	0	0	0	0
5	j	3	0	0	1	0
5	k	2	0	0	0	0
5	l	3	0	0	0	0
5	m	6	0	0	0	0
5	n	2	0	0	1	0
5	o	2	0	0	0	0
5	p	3	0	0	1	0
5	q	4	0	0	1	0
5	r	4	0	0	0	0
5	s	5	0	0	0	0
5	t	4	0	0	1	0
5	u	3	0	0	1	0
5	v	5	0	0	0	0
5	w	1	0	0	0	0
5	x	3	0	0	0	0
All	All	108449	0	97996	721	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (721) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:32:TYR:OH	1:Q:82:LEU:HB3	1.40	1.19
1:C:63:ARG:HG2	1:M:63:ARG:NH2	1.59	1.16
1:g:108[D]:LYS:NZ	1:i:7[D]:GLN:O	1.86	1.08
1:p:7[C]:GLN:O	1:q:108[C]:LYS:NZ	1.89	1.05
1:C:63:ARG:CG	1:M:63:ARG:HH22	1.72	1.03
1:s:7[C]:GLN:O	1:t:108[C]:LYS:NZ	1.91	1.03
1:d:108[D]:LYS:NZ	1:f:7[D]:GLN:O	1.92	1.00
1:C:63:ARG:HG2	1:M:63:ARG:HH22	0.85	1.00
1:I:33:VAL:HG12	1:I:37:MET:HE2	1.49	0.94
1:F:32:TYR:CE2	1:F:87:LYS:HA	2.02	0.94
1:C:63:ARG:CG	1:M:63:ARG:NH2	2.29	0.91
1:P:122:HIS:HE1	4:Q:203[D]:V9D:O01	1.55	0.89
1:o:63[C]:ARG:NE	1:o:67[C]:GLU:OE2	2.05	0.88
1:C:155:LEU:HA	1:C:158:MET:HE2	1.56	0.88
1:v:7[C]:GLN:O	1:w:108[C]:LYS:NZ	2.07	0.87
1:b:101[C]:GLU:OE2	1:b:156[C]:ARG:NH2	2.08	0.86
1:C:158:MET:HE1	1:C:170:PHE:HB2	1.57	0.85
1:F:32:TYR:HE2	1:F:87:LYS:HA	1.39	0.84
4:Q:203[D]:V9D:O12	1:r:122[D]:HIS:HE1	1.61	0.83
1:s:101[C]:GLU:OE2	1:s:156[C]:ARG:NH2	2.12	0.82
4:T:203[D]:V9D:O12	1:u:122[D]:HIS:HE1	1.63	0.81
1:F:32:TYR:CE2	1:F:88:PRO:HD3	2.15	0.81
1:S:122:HIS:HE1	4:T:203[D]:V9D:O01	1.63	0.80
1:x:101[D]:GLU:OE2	1:x:156[D]:ARG:NH2	2.12	0.78
1:R:53:LYS:NZ	5:R:301:HOH:O	2.16	0.78
1:C:161:PRO:HD2	1:C:162:GLU:OE2	1.85	0.77
1:B:157:LYS:HE2	5:B:310:HOH:O	1.84	0.76
4:H:204[D]:V9D:O12	1:i:122[D]:HIS:HE1	1.65	0.76
1:R:157:LYS:HE3	5:R:333:HOH:O	1.84	0.76
1:N:19:ALA:HB1	1:N:117:LEU:HD13	1.67	0.76
1:F:32:TYR:OH	1:Q:82:LEU:CB	2.29	0.75
1:D:122:HIS:HE1	4:E:203[C]:V9D:O01	1.69	0.75
1:W:101:GLU:OE2	1:W:156[A]:ARG:NH2	2.19	0.75
1:S:168:TYR:OH	1:X:174:THR:HG23	1.87	0.75
1:q:63[D]:ARG:NE	1:q:67[D]:GLU:OE2	2.19	0.75
4:H:204[C]:V9D:O12	1:h:122[C]:HIS:HE1	1.69	0.75
1:V:122:HIS:HE1	4:X:204[D]:V9D:O01	1.70	0.75
1:N:156[A]:ARG:NH1	5:N:301:HOH:O	2.18	0.75
1:h:101[C]:GLU:OE2	1:h:156[C]:ARG:NH2	2.20	0.75
1:k:101[C]:GLU:OE2	1:k:156[C]:ARG:NH2	2.18	0.74
1:g:76[C]:ARG:HH11	1:g:128[C]:HIS:HD1	1.32	0.74
1:R:161:PRO:HD2	1:R:162:GLU:OE2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:173:HIS:HB3	1:P:172[B]:LYS:HD3	1.70	0.73
1:v:78[C]:GLY:O	1:v:79[C]:ARG:NH1	2.22	0.73
1:b:63[D]:ARG:NE	1:b:67[D]:GLU:OE2	2.23	0.72
1:p:14[D]:GLN:NE2	5:p:301:HOH:O	2.22	0.72
1:F:32:TYR:CE1	1:Q:82:LEU:HD13	2.25	0.71
1:S:53:LYS:NZ	5:S:301:HOH:O	2.20	0.70
1:D:112:GLN:OE1	5:D:301:HOH:O	2.09	0.70
1:C:157:LYS:HG2	1:D:164:GLY:HA3	1.74	0.69
1:r:101[D]:GLU:OE2	1:r:156[D]:ARG:NH2	2.23	0.69
1:w:101[C]:GLU:OE2	1:w:156[C]:ARG:NH2	2.21	0.69
1:j:21[C]:ASN:HA	1:j:24[C]:ILE:HD12	1.73	0.69
1:l:161[C]:PRO:HD2	1:l:162[C]:GLU:OE2	1.92	0.69
1:S:63:ARG:HG2	1:W:63[B]:ARG:HH21	1.58	0.68
1:B:157:LYS:CE	5:B:310:HOH:O	2.41	0.68
1:t:10[C]:GLN:OE1	1:u:111[C]:ASN:ND2	2.16	0.68
1:x:54[D]:TYR:OH	1:x:147[D]:GLU:OE2	2.06	0.68
1:O:101:GLU:OE2	1:O:156:ARG:NH2	2.24	0.67
1:j:10[D]:GLN:OE1	1:k:111[D]:ASN:ND2	2.23	0.67
1:j:63[D]:ARG:NE	1:j:67[D]:GLU:OE2	2.25	0.67
1:m:161[D]:PRO:HD2	1:m:162[D]:GLU:OE2	1.93	0.67
1:t:76[D]:ARG:HH11	1:t:128[D]:HIS:HD1	1.42	0.67
1:M:122:HIS:HE1	4:O:205[D]:V9D:O01	1.78	0.67
1:X:172[A]:LYS:NZ	5:X:301:HOH:O	2.10	0.67
1:n:63[D]:ARG:NE	1:n:67[D]:GLU:OE2	2.15	0.67
1:F:63:ARG:HG2	1:Q:63:ARG:NH1	2.10	0.66
1:v:63[D]:ARG:NE	1:v:67[D]:GLU:OE2	2.24	0.66
1:e:78[C]:GLY:O	1:e:79[C]:ARG:NH1	2.26	0.66
1:d:33[D]:VAL:HG22	1:d:88[D]:PRO:HB3	1.78	0.66
1:n:101[C]:GLU:OE2	1:n:156[C]:ARG:NH2	2.28	0.66
1:o:76[C]:ARG:NH1	1:o:128[C]:HIS:HD1	1.94	0.66
1:O:49:LYS:HD2	5:O:331:HOH:O	1.95	0.66
1:t:14[C]:GLN:NE2	5:t:301:HOH:O	2.29	0.66
1:A:122:HIS:HE1	4:B:204[C]:V9D:O01	1.79	0.65
1:Q:117:LEU:HD23	1:Q:117:LEU:O	1.96	0.65
1:V:14:GLN:OE1	5:V:301:HOH:O	2.13	0.65
1:I:34:TYR:HA	1:I:37:MET:HE3	1.79	0.65
1:g:21[C]:ASN:HA	1:g:24[C]:ILE:HD12	1.79	0.65
1:r:78[D]:GLY:O	1:r:79[D]:ARG:NH1	2.31	0.64
1:a:14[D]:GLN:NE2	5:a:301:HOH:O	2.29	0.64
1:x:118[D]:HIS:NE2	1:x:134[D]:GLU:OE1	2.30	0.64
1:l:78[D]:GLY:O	1:l:79[D]:ARG:NH1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:63[C]:ARG:NE	1:j:67[C]:GLU:OE2	2.20	0.64
1:J:19:ALA:HB1	1:J:117:LEU:HD13	1.79	0.63
1:C:63:ARG:CB	1:M:63:ARG:NH2	2.61	0.62
1:w:96[C]:GLY:N	1:w:167[C]:GLU:OE2	2.32	0.62
1:N:31:SER:HB2	1:N:62:GLU:HB2	1.80	0.62
1:H:63:ARG:HG2	1:U:63[A]:ARG:NH1	2.15	0.62
1:u:101[D]:GLU:OE2	1:u:156[D]:ARG:NH2	2.28	0.62
1:w:23[C]:GLN:OE1	1:w:113[C]:SER:OG	2.17	0.62
1:F:42:ASP:HA	1:F:49:LYS:NZ	2.14	0.62
1:r:119[D]:LYS:HE2	1:r:123[D]:ASP:OD2	2.00	0.62
1:x:57[D]:HIS:NE2	1:x:61[D]:GLU:OE2	2.32	0.62
1:v:161[D]:PRO:HD2	1:v:162[D]:GLU:OE2	2.00	0.62
1:A:164:GLY:N	5:A:303:HOH:O	2.32	0.62
1:X:14:GLN:CD	1:X:14:GLN:H	2.07	0.62
1:B:172[B]:LYS:HG3	1:E:173:HIS:HB3	1.80	0.61
1:j:101[D]:GLU:OE2	1:j:156[D]:ARG:NH2	2.25	0.61
1:e:108[D]:LYS:HG2	1:e:145[D]:ILE:HD13	1.81	0.61
1:j:14[D]:GLN:NE2	5:j:301:HOH:O	2.32	0.61
1:b:76[D]:ARG:NH1	1:b:128[D]:HIS:HD1	1.99	0.61
1:F:32:TYR:CD2	1:F:88:PRO:HD3	2.36	0.60
1:S:63:ARG:HG2	1:W:63[B]:ARG:NH2	2.16	0.60
4:K:203[C]:V9D:O13	1:j:122[C]:HIS:HE1	1.81	0.60
1:b:168[D]:TYR:O	1:b:172[D]:LYS:HG2	2.02	0.60
1:B:71:LYS:HD2	5:D:338:HOH:O	2.01	0.60
1:J:167:GLU:HB2	1:V:157:LYS:NZ	2.16	0.60
1:M:108:LYS:NZ	5:M:302:HOH:O	2.35	0.60
1:X:161:PRO:HD2	1:X:162:GLU:OE2	2.01	0.60
1:E:63:ARG:HG2	1:I:63:ARG:HH21	1.67	0.59
1:U:161:PRO:HD2	1:U:162:GLU:OE1	2.03	0.59
1:H:172:LYS:HE2	5:H:372:HOH:O	2.02	0.59
1:L:172:LYS:NZ	5:L:301:HOH:O	2.24	0.59
1:T:49:LYS:HD3	5:T:374:HOH:O	2.02	0.59
1:b:118[D]:HIS:NE2	1:b:134[D]:GLU:OE1	2.25	0.59
1:i:78[D]:GLY:O	1:i:79[D]:ARG:NH1	2.36	0.59
1:k:76[D]:ARG:NH1	1:k:128[D]:HIS:HD1	2.01	0.59
1:e:76[D]:ARG:NH1	1:e:128[D]:HIS:HD1	2.00	0.58
1:o:118[C]:HIS:NE2	1:o:134[C]:GLU:OE1	2.24	0.58
1:T:63:ARG:HD2	1:T:67:GLU:OE2	2.02	0.58
1:d:76[C]:ARG:HH11	1:d:128[C]:HIS:HD1	1.51	0.58
1:K:156:ARG:HD3	5:K:424:HOH:O	2.02	0.58
1:Q:20:ILE:HD13	1:Q:117:LEU:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:161[C]:PRO:HD2	1:j:162[C]:GLU:OE2	2.04	0.58
1:s:118[C]:HIS:NE2	1:s:134[C]:GLU:OE1	2.25	0.58
1:x:76[C]:ARG:NH1	1:x:128[C]:HIS:HD1	2.02	0.58
1:r:68[C]:LYS:HZ2	1:r:136[C]:HIS:CE1	2.22	0.57
1:F:42:ASP:HA	1:F:49:LYS:HZ3	1.68	0.57
1:A:87:LYS:HE3	5:A:388:HOH:O	2.04	0.57
1:A:156:ARG:NE	5:A:304:HOH:O	2.37	0.57
1:i:101[D]:GLU:OE2	1:i:156[D]:ARG:NH2	2.35	0.57
1:F:20:ILE:HD13	1:F:117:LEU:HD21	1.87	0.57
1:I:20:ILE:HD13	1:I:117:LEU:HD21	1.86	0.57
1:p:161[D]:PRO:HD2	1:p:162[D]:GLU:OE2	2.04	0.57
1:a:96[D]:GLY:N	1:a:167[D]:GLU:OE2	2.38	0.57
1:B:164:GLY:N	5:B:304:HOH:O	2.38	0.56
1:t:63[D]:ARG:NE	1:t:67[D]:GLU:OE2	2.35	0.56
1:T:49:LYS:NZ	5:T:303:HOH:O	2.34	0.56
1:s:50[C]:ASN:HB2	1:s:171[C]:ASP:OD2	2.05	0.56
1:J:127:PRO:HB3	1:K:118:HIS:CE1	2.41	0.56
1:g:134[C]:GLU:HG2	1:i:131[C]:ASP:HB2	1.87	0.56
1:q:23[C]:GLN:OE1	1:q:113[C]:SER:OG	2.24	0.56
1:q:76[D]:ARG:HH11	1:q:128[D]:HIS:HD1	1.54	0.56
1:B:157:LYS:HE3	5:L:373:HOH:O	2.04	0.56
1:Q:108:LYS:NZ	5:Q:303:HOH:O	2.39	0.56
1:h:68[D]:LYS:HZ2	1:h:136[D]:HIS:CE1	2.24	0.56
1:o:97[D]:LEU:HD23	1:o:161[D]:PRO:HD3	1.86	0.56
1:a:23[D]:GLN:OE1	1:a:113[D]:SER:OG	2.24	0.56
1:k:168[D]:TYR:O	1:k:172[D]:LYS:HG2	2.06	0.56
1:o:78[D]:GLY:O	1:o:79[D]:ARG:NH1	2.37	0.56
1:w:63[D]:ARG:NE	1:w:67[D]:GLU:OE2	2.25	0.56
1:k:57[C]:HIS:NE2	1:k:61[C]:GLU:OE2	2.38	0.56
1:B:156:ARG:HD3	5:B:433:HOH:O	2.05	0.55
1:G:172[B]:LYS:HG3	1:L:173:HIS:HB3	1.88	0.55
1:a:76[C]:ARG:HH11	1:a:128[C]:HIS:HD1	1.54	0.55
1:c:130[C]:ALA:O	1:c:134[C]:GLU:HG3	2.06	0.55
1:f:14[C]:GLN:NE2	5:f:301:HOH:O	2.35	0.55
1:f:33[D]:VAL:HG22	1:f:88[D]:PRO:HB3	1.87	0.55
1:I:63:ARG:NH1	5:I:301:HOH:O	2.12	0.55
1:C:156:ARG:NE	5:C:301:HOH:O	2.22	0.55
1:k:161[D]:PRO:HD2	1:k:162[D]:GLU:OE2	2.07	0.55
1:u:68[C]:LYS:HZ2	1:u:136[C]:HIS:CE1	2.24	0.55
1:M:20:ILE:HD13	1:M:117:LEU:HD21	1.89	0.55
1:b:105[C]:HIS:CD2	1:b:109[C]:ASN:HD21	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:168[C]:TYR:O	1:o:172[C]:LYS:HG2	2.06	0.55
5:B:345:HOH:O	1:E:157:LYS:HE2	2.06	0.54
1:X:101:GLU:OE2	1:X:156:ARG:NH2	2.36	0.54
1:h:108[D]:LYS:HG2	1:h:145[D]:ILE:HD13	1.89	0.54
1:K:164:GLY:N	5:K:305:HOH:O	2.41	0.54
1:i:38[D]:SER:OG	1:i:56[D]:LEU:HB2	2.08	0.54
1:V:61:GLU:HG2	5:V:442:HOH:O	2.07	0.54
1:h:78[C]:GLY:O	1:h:79[C]:ARG:NH1	2.41	0.54
1:o:76[C]:ARG:HH11	1:o:128[C]:HIS:HD1	1.56	0.54
1:x:63[C]:ARG:NE	1:x:67[C]:GLU:OE2	2.40	0.54
1:M:164:GLY:N	5:M:304:HOH:O	2.40	0.54
1:j:33[C]:VAL:HG22	1:j:88[C]:PRO:HB3	1.89	0.54
1:k:168[D]:TYR:CZ	1:k:172[D]:LYS:HE2	2.43	0.54
1:A:49:LYS:NZ	5:A:305:HOH:O	2.40	0.53
1:m:20[D]:ILE:HD12	1:m:69[D]:LEU:HD22	1.90	0.53
1:u:146[D]:LYS:NZ	1:u:150[D]:ASP:OD2	2.39	0.53
1:s:43[C]:ARG:NH2	1:s:45[C]:ASP:OD2	2.41	0.53
1:X:64:GLU:HG2	5:X:438:HOH:O	2.08	0.53
1:k:76[D]:ARG:HH11	1:k:128[D]:HIS:HD1	1.56	0.53
1:H:157:LYS:HB3	1:H:157:LYS:NZ	2.23	0.53
1:i:50[D]:ASN:HB2	1:i:171[D]:ASP:OD2	2.08	0.53
1:n:8[C]:VAL:HB	1:o:145[C]:ILE:HG22	1.90	0.53
1:r:68[C]:LYS:NZ	1:r:136[C]:HIS:CE1	2.76	0.53
1:g:76[C]:ARG:NH1	1:g:128[C]:HIS:HD1	2.03	0.53
1:w:127[C]:PRO:HG2	1:x:138[C]:LEU:HD11	1.91	0.53
1:d:118[C]:HIS:CE1	1:f:127[C]:PRO:HB3	2.43	0.53
1:E:14:GLN:HG3	5:E:322:HOH:O	2.08	0.53
1:F:161:PRO:HD2	1:F:162:GLU:OE1	2.09	0.53
1:M:161:PRO:HD2	1:M:162:GLU:OE2	2.09	0.53
1:h:129[C]:LEU:O	1:h:133[C]:ILE:HG12	2.08	0.53
5:R:316:HOH:O	1:r:123[D]:ASP:HB3	2.08	0.53
1:f:43[D]:ARG:NH2	1:f:45[D]:ASP:OD2	2.42	0.53
1:u:114[D]:LEU:HD13	1:u:137[D]:TYR:HB3	1.91	0.53
1:H:164:GLY:N	5:H:303:HOH:O	2.41	0.52
1:h:119[C]:LYS:HE2	1:h:123[C]:ASP:OD2	2.09	0.52
1:i:119[C]:LYS:HE2	1:i:123[C]:ASP:OD2	2.10	0.52
1:J:167:GLU:HB2	1:V:157:LYS:HZ1	1.74	0.52
1:f:119[C]:LYS:HE2	1:f:123[C]:ASP:OD2	2.09	0.52
1:o:101[D]:GLU:OE2	1:o:156[D]:ARG:NH2	2.42	0.52
1:k:118[C]:HIS:NE2	1:k:134[C]:GLU:OE1	2.32	0.52
1:x:168[C]:TYR:O	1:x:172[C]:LYS:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:164:GLY:N	5:T:306:HOH:O	2.41	0.52
1:g:14[D]:GLN:NE2	5:g:301:HOH:O	2.42	0.52
1:N:161:PRO:HD2	1:N:162:GLU:OE1	2.10	0.52
1:b:76[D]:ARG:HH11	1:b:128[D]:HIS:HD1	1.57	0.52
1:g:127[D]:PRO:HG2	1:h:138[D]:LEU:HD11	1.91	0.52
1:j:49[D]:LYS:O	1:j:53[D]:LYS:HG3	2.10	0.52
1:p:108[D]:LYS:HG2	1:p:145[D]:ILE:HD13	1.92	0.52
1:D:172:LYS:HE2	5:D:318:HOH:O	2.09	0.52
1:E:123:ASP:HB3	5:f:305:HOH:O	2.09	0.52
1:m:38[C]:SER:OG	1:m:56[C]:LEU:HB2	2.09	0.52
1:v:130[D]:ALA:O	1:v:134[D]:GLU:HG3	2.10	0.52
1:F:32:TYR:CZ	1:Q:82:LEU:HB3	2.37	0.52
1:b:168[D]:TYR:CZ	1:b:172[D]:LYS:HE2	2.45	0.52
1:p:43[C]:ARG:NH2	1:p:45[C]:ASP:OD2	2.41	0.52
1:D:19:ALA:HB1	1:D:117:LEU:HD13	1.91	0.51
1:F:32:TYR:HE1	1:Q:82:LEU:HD13	1.73	0.51
1:M:71:LYS:HE3	5:M:462:HOH:O	2.10	0.51
1:P:172[B]:LYS:HE2	5:P:341:HOH:O	2.09	0.51
1:V:87:LYS:HE2	5:V:422:HOH:O	2.09	0.51
1:k:78[C]:GLY:O	1:k:79[C]:ARG:NH1	2.42	0.51
1:K:72:LEU:HD22	1:K:132:PHE:CE1	2.45	0.51
1:O:156:ARG:NE	5:O:302:HOH:O	2.28	0.51
1:r:161[D]:PRO:HD2	1:r:162[D]:GLU:OE2	2.09	0.51
1:v:168[D]:TYR:CE1	1:v:172[D]:LYS:HE3	2.45	0.51
1:B:162:GLU:CD	1:B:162:GLU:H	2.19	0.51
1:X:162:GLU:CD	1:X:162:GLU:H	2.19	0.51
1:b:6[C]:SER:HB3	1:b:9[C]:ARG:HB2	1.92	0.51
1:f:27[C]:GLU:HB2	1:f:66[C]:ALA:HB2	1.93	0.51
5:B:358:HOH:O	1:E:157:LYS:HE3	2.11	0.51
1:N:19:ALA:CB	1:N:117:LEU:HD13	2.38	0.51
1:Q:127:PRO:HB3	1:R:118:HIS:CE1	2.45	0.51
1:X:72:LEU:C	1:X:72:LEU:HD13	2.35	0.51
1:s:127[D]:PRO:HB3	1:t:118[D]:HIS:CE1	2.45	0.51
1:g:111[D]:ASN:O	1:g:115[D]:LEU:HG	2.11	0.50
1:u:121[D]:ALA:HB2	1:u:129[D]:LEU:HD23	1.93	0.50
1:l:101[D]:GLU:OE2	1:l:156[D]:ARG:NH2	2.44	0.50
1:f:20[C]:ILE:HD13	1:f:117[C]:LEU:HD11	1.94	0.50
1:u:78[D]:GLY:O	1:u:79[D]:ARG:NH1	2.44	0.50
1:w:119[D]:LYS:HE2	1:w:123[D]:ASP:OD2	2.11	0.50
1:B:63:ARG:HG2	5:D:476:HOH:O	2.12	0.50
1:N:71:LYS:HE3	5:N:475:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:t:111[C]:ASN:O	1:t:115[C]:LEU:HG	2.11	0.50
1:X:164:GLY:N	5:X:305:HOH:O	2.44	0.50
1:f:23[C]:GLN:OE1	1:f:113[C]:SER:OG	2.24	0.50
1:n:61[D]:GLU:HG2	1:n:64[D]:GLU:OE2	2.12	0.50
1:r:69[D]:LEU:HG	1:r:137[D]:TYR:OH	2.12	0.50
1:C:101:GLU:OE2	1:C:156:ARG:NH2	2.38	0.50
1:W:63[A]:ARG:NH1	5:W:304:HOH:O	2.44	0.50
1:x:118[C]:HIS:NE2	1:x:134[C]:GLU:OE1	2.35	0.50
1:e:97[C]:LEU:HD23	1:e:161[C]:PRO:HD3	1.94	0.50
1:N:164:GLY:N	5:N:304:HOH:O	2.45	0.49
1:d:10[D]:GLN:OE1	1:e:111[D]:ASN:ND2	2.21	0.49
1:j:10[D]:GLN:CD	1:k:111[D]:ASN:HD22	2.16	0.49
1:r:168[C]:TYR:CZ	1:r:172[C]:LYS:HE3	2.47	0.49
1:i:111[C]:ASN:O	1:i:115[C]:LEU:HG	2.12	0.49
1:p:177[C]:ASP:OD1	1:p:177[C]:ASP:N	2.44	0.49
1:q:63[C]:ARG:O	1:q:67[C]:GLU:HG3	2.13	0.49
1:v:43[C]:ARG:NH2	1:v:45[C]:ASP:OD2	2.45	0.49
1:C:157:LYS:HD2	5:D:331:HOH:O	2.12	0.49
1:T:127:PRO:HB3	1:U:118:HIS:CE1	2.47	0.49
1:a:118[D]:HIS:CE1	1:c:127[D]:PRO:HB3	2.47	0.49
1:b:97[C]:LEU:HD23	1:b:161[C]:PRO:HD3	1.93	0.49
1:j:119[C]:LYS:HE2	1:j:123[C]:ASP:OD2	2.11	0.49
1:M:122:HIS:HE1	4:O:205[C]:V9D:O04	1.93	0.49
1:O:49:LYS:NZ	5:O:305:HOH:O	2.44	0.49
1:h:9[C]:ARG:O	1:i:108[C]:LYS:NZ	2.45	0.49
1:p:127[D]:PRO:HB3	1:q:118[D]:HIS:CE1	2.47	0.49
1:v:50[C]:ASN:HB2	1:v:171[C]:ASP:OD2	2.12	0.49
1:L:162:GLU:OE1	1:L:162:GLU:N	2.45	0.49
5:N:397:HOH:O	1:Q:157:LYS:HE3	2.12	0.49
1:d:129[D]:LEU:O	1:d:133[D]:ILE:HG12	2.11	0.49
1:v:118[D]:HIS:CE1	1:x:127[D]:PRO:HB3	2.46	0.49
1:O:49:LYS:HE3	5:W:386:HOH:O	2.12	0.49
1:O:20:ILE:HD13	1:O:117:LEU:HD11	1.95	0.49
1:k:118[D]:HIS:NE2	1:k:134[D]:GLU:OE1	2.26	0.49
1:n:111[C]:ASN:O	1:n:115[C]:LEU:HG	2.12	0.49
1:q:10[C]:GLN:OE1	1:r:111[C]:ASN:ND2	2.18	0.49
1:D:72:LEU:HD22	1:D:132:PHE:CE2	2.48	0.49
1:G:101:GLU:OE2	1:G:156:ARG:NH2	2.42	0.49
1:S:19:ALA:HB1	1:S:117:LEU:HD12	1.95	0.49
1:H:20:ILE:HD13	1:H:117:LEU:HD21	1.95	0.49
1:L:161:PRO:HD2	1:L:162:GLU:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:176:GLY:O	1:O:177:ASP:HB3	2.11	0.49
1:i:71[C]:LYS:O	1:i:75[C]:GLN:HG3	2.12	0.49
1:v:168[D]:TYR:CZ	1:v:172[D]:LYS:HE3	2.48	0.49
1:B:157:LYS:NZ	5:B:310:HOH:O	2.44	0.49
1:b:176[D]:GLY:O	1:b:177[D]:ASP:HB2	2.13	0.49
1:q:14[C]:GLN:NE2	5:q:301:HOH:O	2.44	0.49
1:q:97[C]:LEU:O	1:q:101[C]:GLU:HG3	2.12	0.49
1:r:129[D]:LEU:O	1:r:133[D]:ILE:HG12	2.13	0.49
1:c:162[D]:GLU:N	1:c:162[D]:GLU:OE1	2.46	0.48
1:K:172:LYS:HE2	5:K:328:HOH:O	2.13	0.48
1:V:164:GLY:N	5:V:307:HOH:O	2.45	0.48
1:h:54[D]:TYR:O	1:h:58[D]:GLN:HG2	2.14	0.48
1:k:97[C]:LEU:HD23	1:k:161[C]:PRO:HD3	1.95	0.48
1:E:172[B]:LYS:HG3	1:G:173:HIS:HB3	1.95	0.48
1:F:35:LEU:HG	1:Q:70:MET:HE1	1.95	0.48
1:H:127:PRO:HB3	1:I:118:HIS:CE1	2.48	0.48
1:N:4:SER:N	5:N:305:HOH:O	2.46	0.48
4:X:204[D]:V9D:O12	1:x:122[D]:HIS:HE1	1.96	0.48
1:h:79[C]:ARG:HD3	1:h:79[C]:ARG:HA	1.63	0.48
1:t:76[D]:ARG:HD3	1:t:128[D]:HIS:ND1	2.29	0.48
1:w:20[C]:ILE:HD13	1:w:117[C]:LEU:HD11	1.96	0.48
1:g:121[C]:ALA:HB2	1:g:129[C]:LEU:HD23	1.95	0.48
1:u:63[C]:ARG:NE	1:u:67[C]:GLU:OE2	2.47	0.48
1:u:168[C]:TYR:O	1:u:172[C]:LYS:HG2	2.13	0.48
1:x:78[D]:GLY:O	1:x:79[D]:ARG:NH1	2.45	0.48
1:E:20:ILE:HD13	1:E:117:LEU:HD21	1.96	0.48
1:I:112:GLN:OE1	5:I:302:HOH:O	2.20	0.48
1:O:161:PRO:HD2	1:O:162:GLU:CD	2.39	0.48
1:E:109[B]:ASN:ND2	5:E:303:HOH:O	2.46	0.48
1:F:65:HIS:CE1	5:F:303:HOH:O	2.67	0.48
1:I:161:PRO:HD2	1:I:162:GLU:OE1	2.14	0.48
1:V:140:GLU:OE1	1:V:143:LYS:NZ	2.47	0.48
1:X:65:HIS:HE1	5:X:411:HOH:O	1.97	0.48
1:d:111[D]:ASN:O	1:d:115[D]:LEU:HG	2.14	0.48
1:n:14[C]:GLN:NE2	5:n:301:HOH:O	2.46	0.48
1:b:78[C]:GLY:O	1:b:79[C]:ARG:NH1	2.47	0.48
1:x:97[D]:LEU:HD23	1:x:161[D]:PRO:HD3	1.96	0.48
1:S:60:HIS:CD2	1:W:63[B]:ARG:NH1	2.82	0.47
1:X:174:THR:HG21	5:X:436:HOH:O	2.13	0.47
1:a:8[D]:VAL:HB	1:b:145[D]:ILE:HG22	1.95	0.47
1:n:31[D]:SER:HB2	1:n:62[D]:GLU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:27[D]:GLU:HB2	1:f:66[D]:ALA:HB2	1.96	0.47
1:u:76[C]:ARG:NH1	1:u:128[C]:HIS:HD1	2.12	0.47
1:E:127:PRO:HB3	1:F:118:HIS:CE1	2.49	0.47
1:X:79:ARG:HD3	1:X:79:ARG:HA	1.72	0.47
1:d:63[C]:ARG:NE	1:d:67[C]:GLU:OE2	2.47	0.47
1:p:162[D]:GLU:CD	1:p:162[D]:GLU:H	2.22	0.47
1:K:161:PRO:HD2	1:K:162:GLU:OE2	2.14	0.47
1:U:20:ILE:HD13	1:U:117:LEU:HD21	1.96	0.47
1:a:17[C]:GLU:OE2	1:a:79[C]:ARG:N	2.47	0.47
1:m:161[D]:PRO:HD2	1:m:162[D]:GLU:CD	2.39	0.47
1:u:54[C]:TYR:O	1:u:58[C]:GLN:HG2	2.13	0.47
1:f:71[C]:LYS:O	1:f:75[C]:GLN:HG3	2.14	0.47
1:m:78[C]:GLY:O	1:m:79[C]:ARG:NH1	2.47	0.47
1:n:21[D]:ASN:HA	1:n:24[D]:ILE:HD12	1.97	0.47
1:o:114[C]:LEU:HD13	1:o:137[C]:TYR:HB3	1.96	0.47
1:u:79[C]:ARG:HA	1:u:79[C]:ARG:HD3	1.66	0.47
1:M:127:PRO:HB3	1:N:118:HIS:CE1	2.49	0.47
1:O:172[B]:LYS:HG3	1:W:173:HIS:HB3	1.97	0.47
1:g:10[D]:GLN:OE1	1:h:111[D]:ASN:ND2	2.28	0.47
1:h:68[D]:LYS:NZ	1:h:136[D]:HIS:CE1	2.82	0.47
1:h:69[C]:LEU:HG	1:h:137[C]:TYR:OH	2.15	0.47
1:u:108[C]:LYS:HG2	1:u:145[C]:ILE:HD13	1.97	0.47
1:e:6[C]:SER:OG	1:e:8[C]:VAL:HG22	2.14	0.47
1:J:48:LEU:HD21	1:V:157:LYS:HZ2	1.80	0.47
1:R:86:GLN:HG2	5:R:406:HOH:O	2.14	0.47
1:a:104[D]:LEU:O	1:a:108[D]:LYS:HG3	2.15	0.47
1:b:118[C]:HIS:NE2	1:b:134[C]:GLU:OE1	2.42	0.47
1:h:76[D]:ARG:NH1	1:h:128[D]:HIS:HD1	2.13	0.47
1:I:97:LEU:HD23	1:I:161:PRO:HD3	1.97	0.47
1:J:177:ASP:OD2	5:J:301:HOH:O	2.21	0.47
1:P:161:PRO:HD2	1:P:162:GLU:OE2	2.15	0.47
1:f:38[D]:SER:OG	1:f:56[D]:LEU:HB2	2.15	0.47
1:j:17[C]:GLU:OE2	1:j:79[C]:ARG:N	2.48	0.47
1:m:101[C]:GLU:OE2	1:m:156[C]:ARG:NH2	2.45	0.47
1:T:172:LYS:HE2	5:T:388:HOH:O	2.14	0.46
1:h:129[D]:LEU:O	1:h:133[D]:ILE:HG12	2.14	0.46
1:R:79:ARG:HD3	1:R:79:ARG:HA	1.73	0.46
1:l:129[D]:LEU:O	1:l:133[D]:ILE:HG12	2.15	0.46
1:s:38[C]:SER:OG	1:s:56[C]:LEU:HB2	2.14	0.46
1:a:73[C]:GLN:OE1	1:a:78[C]:GLY:HA3	2.15	0.46
1:f:114[D]:LEU:HD13	1:f:137[D]:TYR:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:57[D]:HIS:NE2	1:g:61[D]:GLU:OE2	2.49	0.46
1:w:111[C]:ASN:O	1:w:115[C]:LEU:HG	2.15	0.46
1:g:118[C]:HIS:CE1	1:i:127[C]:PRO:HB3	2.51	0.46
1:S:172[B]:LYS:HG3	1:X:173:HIS:HB3	1.97	0.46
1:h:12[D]:TYR:CE1	1:h:76[D]:ARG:HG3	2.51	0.46
1:t:9[C]:ARG:NH2	1:t:17[C]:GLU:OE1	2.43	0.46
1:x:114[C]:LEU:HD13	1:x:137[C]:TYR:HB3	1.97	0.46
1:i:23[C]:GLN:OE1	1:i:113[C]:SER:OG	2.29	0.46
1:r:168[C]:TYR:O	1:r:172[C]:LYS:HG2	2.15	0.46
1:u:117[D]:LEU:O	1:u:120[D]:LEU:HB3	2.16	0.46
1:O:172[A]:LYS:HG2	5:O:362:HOH:O	2.16	0.46
1:n:61[D]:GLU:HA	1:n:64[D]:GLU:HG3	1.97	0.46
1:E:108:LYS:NZ	5:E:304:HOH:O	2.49	0.46
1:T:14:GLN:HG2	5:T:432:HOH:O	2.15	0.46
1:n:73[D]:GLN:OE1	1:n:78[D]:GLY:HA3	2.16	0.46
1:F:79:ARG:HA	1:F:79:ARG:HD3	1.66	0.46
1:S:127:PRO:HB3	1:T:118:HIS:CE1	2.51	0.46
1:v:118[C]:HIS:CE1	1:x:127[C]:PRO:HB3	2.51	0.46
1:e:41[D]:PHE:HA	1:e:46[D]:VAL:HG11	1.97	0.45
1:g:68[C]:LYS:HG2	1:g:132[C]:PHE:HZ	1.81	0.45
1:q:121[D]:ALA:HB2	1:q:129[D]:LEU:HD23	1.98	0.45
1:w:21[D]:ASN:HA	1:w:24[D]:ILE:HD12	1.97	0.45
1:e:79[D]:ARG:HA	1:e:79[D]:ARG:HD3	1.69	0.45
1:g:129[D]:LEU:O	1:g:133[D]:ILE:HG12	2.17	0.45
1:n:139[C]:ASN:ND2	1:n:143[C]:LYS:HD2	2.31	0.45
1:x:6[D]:SER:HB3	1:x:9[D]:ARG:HB2	1.98	0.45
1:A:35:LEU:HG	1:L:70:MET:HE1	1.99	0.45
1:A:118:HIS:CE1	1:C:127:PRO:HB3	2.51	0.45
1:i:50[C]:ASN:OD1	1:i:53[C]:LYS:NZ	2.30	0.45
1:k:14[C]:GLN:HA	1:k:17[C]:GLU:HB3	1.98	0.45
1:q:127[D]:PRO:HB3	1:r:118[D]:HIS:CE1	2.51	0.45
1:r:76[C]:ARG:NH1	1:r:128[C]:HIS:HD1	2.14	0.45
1:O:161:PRO:HD2	1:O:162:GLU:OE2	2.17	0.45
1:a:20[D]:ILE:HD13	1:a:117[D]:LEU:HD11	1.98	0.45
1:d:20[C]:ILE:HD13	1:d:117[C]:LEU:HD11	1.97	0.45
1:e:76[D]:ARG:HH11	1:e:128[D]:HIS:HD1	1.63	0.45
1:C:14:GLN:H	1:C:14:GLN:CD	2.25	0.45
1:e:129[D]:LEU:O	1:e:133[D]:ILE:HG12	2.16	0.45
1:j:127[C]:PRO:HB3	1:k:118[C]:HIS:CE1	2.52	0.45
1:n:119[D]:LYS:HE2	1:n:123[D]:ASP:OD2	2.15	0.45
1:t:33[C]:VAL:HG22	1:t:88[C]:PRO:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:t:129[C]:LEU:O	1:t:133[C]:ILE:HG12	2.17	0.45
1:R:172:LYS:HE3	1:U:173:HIS:HB3	1.98	0.45
1:g:57[D]:HIS:CE1	1:g:61[D]:GLU:OE2	2.70	0.45
1:j:79[C]:ARG:HA	1:j:79[C]:ARG:HD3	1.81	0.45
1:v:111[C]:ASN:O	1:v:115[C]:LEU:HG	2.17	0.45
1:A:70:MET:HE1	1:L:35:LEU:HG	1.99	0.45
1:D:63:ARG:HG2	5:D:487:HOH:O	2.15	0.45
5:I:323:HOH:O	1:h:123[C]:ASP:HB3	2.15	0.45
1:L:156:ARG:NE	5:L:302:HOH:O	2.27	0.45
1:a:79[C]:ARG:HA	1:a:79[C]:ARG:HD3	1.74	0.45
1:c:129[D]:LEU:O	1:c:133[D]:ILE:HG12	2.17	0.45
1:c:155[C]:LEU:HD22	1:c:167[C]:GLU:HG2	1.98	0.45
1:e:79[C]:ARG:HA	1:e:79[C]:ARG:HD3	1.76	0.45
1:g:76[C]:ARG:HD3	1:g:128[C]:HIS:CE1	2.52	0.45
1:g:127[C]:PRO:HB3	1:h:118[C]:HIS:CE1	2.52	0.45
1:o:79[C]:ARG:HA	1:o:79[C]:ARG:HD3	1.61	0.45
1:r:76[C]:ARG:HH11	1:r:128[C]:HIS:HD1	1.63	0.45
1:u:12[C]:TYR:CE1	1:u:76[C]:ARG:HG3	2.52	0.45
1:I:86:GLN:HE21	1:I:86:GLN:HB2	1.55	0.45
1:O:60:HIS:HD2	5:O:450:HOH:O	1.99	0.45
1:W:157:LYS:HE2	5:W:330:HOH:O	2.16	0.45
1:W:164:GLY:N	5:W:305:HOH:O	2.49	0.45
1:j:61[C]:GLU:HA	1:j:64[C]:GLU:HG3	1.99	0.45
1:p:118[D]:HIS:CE1	1:r:127[D]:PRO:HB3	2.52	0.45
1:s:21[D]:ASN:HA	1:s:24[D]:ILE:HD12	1.99	0.45
1:D:160:ALA:O	5:D:302:HOH:O	2.21	0.45
1:a:111[D]:ASN:O	1:a:115[D]:LEU:HG	2.17	0.45
1:e:54[C]:TYR:O	1:e:58[C]:GLN:HG2	2.17	0.45
1:p:108[D]:LYS:HA	1:p:145[D]:ILE:HD11	1.98	0.45
1:W:172[A]:LYS:HG2	5:W:328:HOH:O	2.16	0.44
1:g:8[D]:VAL:HB	1:h:145[D]:ILE:HG22	1.98	0.44
1:m:54[C]:TYR:O	1:m:58[C]:GLN:HG2	2.16	0.44
1:n:127[D]:PRO:HB3	1:o:118[D]:HIS:CE1	2.52	0.44
1:D:173:HIS:HB3	1:Q:172[B]:LYS:HG3	1.99	0.44
1:I:79:ARG:HA	1:I:79:ARG:HD3	1.73	0.44
1:a:27[D]:GLU:HB2	1:a:66[D]:ALA:HB2	1.99	0.44
1:h:63[D]:ARG:NE	1:h:67[D]:GLU:OE2	2.34	0.44
1:n:13[C]:HIS:CE1	1:n:124[C]:LYS:HE3	2.52	0.44
1:S:53:LYS:HA	1:S:53:LYS:HD2	1.79	0.44
1:V:127:PRO:HB3	1:W:118:HIS:CE1	2.53	0.44
1:X:161:PRO:HD2	1:X:162:GLU:CD	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:43[D]:ARG:NH2	1:c:45[D]:ASP:OD2	2.45	0.44
1:m:119[D]:LYS:HE2	1:m:123[D]:ASP:OD2	2.17	0.44
1:p:118[C]:HIS:NE2	1:p:134[C]:GLU:OE1	2.39	0.44
1:w:27[C]:GLU:HB2	1:w:66[C]:ALA:HB2	1.98	0.44
1:A:127:PRO:HB3	1:B:118:HIS:CE1	2.51	0.44
1:G:127:PRO:HB3	1:H:118:HIS:CE1	2.53	0.44
1:L:79:ARG:HA	1:L:79:ARG:HD3	1.80	0.44
1:O:49:LYS:HD2	1:O:49:LYS:H	1.82	0.44
1:l:20[C]:ILE:HD13	1:l:117[C]:LEU:HD11	1.99	0.44
1:l:130[C]:ALA:O	1:l:134[C]:GLU:HG3	2.18	0.44
1:q:76[D]:ARG:HD3	1:q:128[D]:HIS:ND1	2.32	0.44
1:V:108:LYS:NZ	5:V:312:HOH:O	2.50	0.44
1:W:31:SER:HB2	1:W:62:GLU:HB2	1.99	0.44
1:g:97[D]:LEU:O	1:g:101[D]:GLU:HG3	2.18	0.44
1:G:123:ASP:OD1	1:g:124[D]:LYS:NZ	2.40	0.44
1:l:86[D]:GLN:HA	1:l:86[D]:GLN:OE1	2.18	0.44
1:o:176[C]:GLY:O	1:o:177[C]:ASP:HB2	2.17	0.44
1:e:41[C]:PHE:CZ	1:e:96[C]:GLY:HA2	2.52	0.44
1:e:168[D]:TYR:CZ	1:e:172[D]:LYS:HE3	2.53	0.44
1:m:20[D]:ILE:HD13	1:m:20[D]:ILE:HA	1.72	0.44
1:t:6[C]:SER:OG	1:t:8[C]:VAL:HG22	2.18	0.44
1:t:76[D]:ARG:HD3	1:t:128[D]:HIS:CE1	2.53	0.44
1:B:150:ASP:OD1	1:L:44:ASP:HA	2.18	0.44
1:O:174:THR:OG1	1:P:172[B]:LYS:HE3	2.18	0.44
1:u:79[D]:ARG:HD3	1:u:79[D]:ARG:HA	1.77	0.44
1:w:79[C]:ARG:HA	1:w:79[C]:ARG:HD3	1.84	0.44
1:W:119:LYS:HD2	1:W:120:LEU:N	2.32	0.44
1:W:161:PRO:HD2	1:W:162:GLU:OE1	2.18	0.44
1:c:6[C]:SER:OG	1:c:8[C]:VAL:HG22	2.18	0.44
1:d:23[D]:GLN:OE1	1:d:113[D]:SER:OG	2.31	0.44
1:e:161[C]:PRO:HD2	1:e:162[C]:GLU:OE2	2.17	0.44
1:i:43[D]:ARG:HB2	1:i:46[D]:VAL:HG23	2.00	0.44
1:s:145[C]:ILE:HG22	1:u:8[C]:VAL:HB	2.00	0.44
1:u:129[C]:LEU:O	1:u:133[C]:ILE:HG12	2.17	0.44
1:a:8[C]:VAL:HB	1:b:145[C]:ILE:HG22	2.00	0.43
1:u:54[D]:TYR:O	1:u:58[D]:GLN:HG2	2.18	0.43
1:x:79[D]:ARG:HA	1:x:79[D]:ARG:HD3	1.87	0.43
1:F:9:ARG:HD2	5:F:420:HOH:O	2.18	0.43
1:I:86:GLN:NE2	5:I:309:HOH:O	2.44	0.43
1:N:19:ALA:CB	1:N:117:LEU:CD1	2.96	0.43
1:f:76[D]:ARG:HD3	1:f:128[D]:HIS:CE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:31[C]:SER:HB2	1:l:62[C]:GLU:HB2	1.99	0.43
1:x:168[C]:TYR:CZ	1:x:172[C]:LYS:HE2	2.52	0.43
1:C:157:LYS:HB2	1:C:157:LYS:HE3	1.85	0.43
1:F:63:ARG:HG2	1:Q:63:ARG:HH12	1.83	0.43
1:V:79:ARG:HD3	1:V:79:ARG:HA	1.84	0.43
1:t:127[C]:PRO:HB3	1:u:118[C]:HIS:CE1	2.53	0.43
1:E:70:MET:HE1	1:I:35:LEU:HG	2.00	0.43
1:J:104:LEU:O	1:J:108:LYS:HG3	2.18	0.43
1:P:118:HIS:CE1	1:R:127:PRO:HB3	2.53	0.43
1:Q:164:GLY:N	5:Q:308:HOH:O	2.50	0.43
1:Q:172[B]:LYS:HE2	5:Q:448:HOH:O	2.17	0.43
1:n:172[D]:LYS:HD3	1:n:172[D]:LYS:HA	1.87	0.43
1:u:68[C]:LYS:NZ	1:u:136[C]:HIS:CE1	2.85	0.43
1:v:58[D]:GLN:O	1:v:62[D]:GLU:HG2	2.18	0.43
1:x:79[C]:ARG:HA	1:x:79[C]:ARG:HD3	1.68	0.43
1:J:108:LYS:NZ	5:J:313:HOH:O	2.52	0.43
1:P:122:HIS:HE1	4:Q:203[C]:V9D:O04	2.02	0.43
1:S:8:VAL:HB	1:T:145:ILE:HG22	2.00	0.43
1:S:118:HIS:CE1	1:U:127:PRO:HB3	2.54	0.43
1:b:60[D]:HIS:O	1:b:64[D]:GLU:HG3	2.18	0.43
1:b:161[C]:PRO:HD2	1:b:162[C]:GLU:OE1	2.19	0.43
1:p:145[C]:ILE:HG22	1:r:8[C]:VAL:HB	2.00	0.43
1:d:79[C]:ARG:HD3	1:d:79[C]:ARG:HA	1.87	0.43
1:h:54[C]:TYR:O	1:h:58[C]:GLN:HG2	2.18	0.43
1:h:79[D]:ARG:HA	1:h:79[D]:ARG:HD3	1.69	0.43
1:u:123[C]:ASP:OD2	5:u:301:HOH:O	2.21	0.43
1:C:63:ARG:CB	1:M:63:ARG:HH21	2.29	0.43
1:J:118:HIS:CE1	1:L:127:PRO:HB3	2.53	0.43
4:K:203[C]:V9D:C10	1:j:122[C]:HIS:HE1	2.32	0.43
1:c:111[D]:ASN:O	1:c:115[D]:LEU:HG	2.18	0.43
1:k:7[C]:GLN:O	1:l:108[C]:LYS:NZ	2.51	0.43
1:k:50[D]:ASN:HB2	1:k:171[D]:ASP:OD2	2.18	0.43
1:n:17[D]:GLU:OE2	1:n:79[D]:ARG:N	2.49	0.43
1:n:118[C]:HIS:NE2	1:n:134[C]:GLU:OE1	2.52	0.43
1:q:8[D]:VAL:HB	1:r:145[D]:ILE:HG22	2.01	0.43
1:q:20[D]:ILE:HD13	1:q:117[D]:LEU:HD11	2.00	0.43
1:B:79:ARG:HD3	1:B:79:ARG:HA	1.88	0.43
1:L:97:LEU:HD23	1:L:161:PRO:HD3	2.01	0.43
1:P:119:LYS:NZ	5:P:313:HOH:O	2.51	0.43
1:f:50[C]:ASN:HB2	1:f:171[C]:ASP:CG	2.43	0.43
1:p:27[D]:GLU:HB2	1:p:66[D]:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:6[D]:SER:OG	1:v:8[D]:VAL:HG22	2.19	0.43
1:E:172[A]:LYS:HE2	5:E:356:HOH:O	2.19	0.43
1:G:72:LEU:C	1:G:72:LEU:HD13	2.44	0.43
1:i:97[D]:LEU:HD23	1:i:161[D]:PRO:HD3	2.01	0.43
1:p:79[D]:ARG:HA	1:p:79[D]:ARG:HD3	1.79	0.43
4:E:203[D]:V9D:O12	1:f:122[D]:HIS:HE1	2.01	0.43
4:H:204[D]:V9D:N11	1:i:122[D]:HIS:HE1	2.17	0.43
1:L:63:ARG:NE	1:L:67:GLU:OE2	2.40	0.43
1:s:68[C]:LYS:HB2	1:s:68[C]:LYS:HE2	1.74	0.43
1:s:79[C]:ARG:HA	1:s:79[C]:ARG:HD3	1.86	0.43
1:u:162[D]:GLU:CD	1:u:162[D]:GLU:H	2.27	0.43
1:v:20[D]:ILE:HD13	1:v:20[D]:ILE:HA	1.82	0.43
1:H:82:LEU:HD12	1:U:36:SER:HB2	2.01	0.42
1:M:118:HIS:CE1	1:O:127:PRO:HB3	2.54	0.42
1:J:172:LYS:HE2	5:J:307:HOH:O	2.19	0.42
1:P:162:GLU:H	1:P:162:GLU:CD	2.27	0.42
1:W:156[A]:ARG:HH11	1:W:156[A]:ARG:HG2	1.84	0.42
1:a:134[C]:GLU:HA	1:a:138[C]:LEU:HD12	2.01	0.42
1:b:68[D]:LYS:HG2	1:b:132[D]:PHE:HZ	1.83	0.42
1:b:105[C]:HIS:CD2	1:b:109[C]:ASN:ND2	2.87	0.42
1:d:79[D]:ARG:HA	1:d:79[D]:ARG:HD3	1.81	0.42
1:j:118[C]:HIS:CE1	1:l:127[C]:PRO:HB3	2.54	0.42
1:m:130[D]:ALA:O	1:m:134[D]:GLU:HG3	2.19	0.42
1:r:70[D]:MET:HE3	1:r:82[D]:LEU:HD21	2.01	0.42
1:L:6:SER:HB3	1:L:9:ARG:HB2	2.01	0.42
1:a:20[C]:ILE:HD11	1:a:129[C]:LEU:HD11	2.00	0.42
1:h:58[C]:GLN:O	1:h:62[C]:GLU:HG2	2.19	0.42
1:l:69[C]:LEU:HG	1:l:137[C]:TYR:OH	2.18	0.42
1:w:73[D]:GLN:OE1	1:w:78[D]:GLY:HA3	2.19	0.42
1:x:69[C]:LEU:HG	1:x:137[C]:TYR:OH	2.19	0.42
1:C:79:ARG:HA	1:C:79:ARG:HD3	1.84	0.42
1:b:79[D]:ARG:HA	1:b:79[D]:ARG:HD3	1.65	0.42
1:r:63[C]:ARG:NE	1:r:67[C]:GLU:OE2	2.36	0.42
1:D:172:LYS:HG2	5:D:318:HOH:O	2.19	0.42
1:G:49:LYS:HE2	5:G:399:HOH:O	2.20	0.42
1:N:79:ARG:HD3	1:N:79:ARG:HA	1.90	0.42
1:a:118[C]:HIS:CE1	1:c:127[C]:PRO:HB3	2.54	0.42
1:c:125[D]:ASN:O	1:c:127[D]:PRO:HD3	2.20	0.42
1:p:23[D]:GLN:OE1	1:p:113[D]:SER:OG	2.36	0.42
1:x:73[D]:GLN:OE1	1:x:78[D]:GLY:HA3	2.18	0.42
1:X:172[A]:LYS:HG2	5:X:337:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:27[C]:GLU:HB2	1:i:66[C]:ALA:HB2	2.01	0.42
1:o:69[C]:LEU:HG	1:o:137[C]:TYR:OH	2.18	0.42
1:o:79[D]:ARG:HA	1:o:79[D]:ARG:HD3	1.77	0.42
1:p:38[C]:SER:OG	1:p:56[C]:LEU:HB2	2.20	0.42
1:r:76[D]:ARG:HH11	1:r:128[D]:HIS:ND1	2.18	0.42
1:v:31[D]:SER:HB2	1:v:62[D]:GLU:HB2	2.01	0.42
1:A:49:LYS:HE2	1:A:49:LYS:HB2	1.80	0.42
1:H:161:PRO:HD2	1:H:162:GLU:OE2	2.19	0.42
1:J:161:PRO:HG3	5:J:476:HOH:O	2.19	0.42
1:d:112[C]:GLN:O	1:d:116[C]:GLU:HG3	2.20	0.42
1:g:23[D]:GLN:OE1	1:g:113[D]:SER:OG	2.26	0.42
1:l:33[D]:VAL:HG22	1:l:88[D]:PRO:HB3	2.01	0.42
1:l:72[C]:LEU:HG	1:l:132[C]:PHE:CE2	2.54	0.42
1:n:127[C]:PRO:HG2	1:o:138[C]:LEU:HD11	2.02	0.42
1:G:8:VAL:HB	1:H:145:ILE:HG22	2.02	0.42
1:J:72:LEU:C	1:J:72:LEU:HD13	2.45	0.42
1:K:4:SER:N	5:K:309:HOH:O	2.51	0.42
1:K:172:LYS:HG2	5:K:328:HOH:O	2.20	0.42
1:b:69[D]:LEU:HG	1:b:137[D]:TYR:OH	2.19	0.42
1:b:114[D]:LEU:HD13	1:b:137[D]:TYR:HB3	2.01	0.42
1:g:79[C]:ARG:HA	1:g:79[C]:ARG:HD3	1.81	0.42
1:m:76[C]:ARG:HD3	1:m:128[C]:HIS:ND1	2.35	0.42
1:s:92[D]:ASP:OD1	1:s:92[D]:ASP:C	2.63	0.42
1:x:63[D]:ARG:O	1:x:67[D]:GLU:HG3	2.19	0.42
1:i:79[C]:ARG:HD3	1:i:79[C]:ARG:HA	1.82	0.42
1:j:27[D]:GLU:HB2	1:j:66[D]:ALA:HB2	2.01	0.42
1:k:153[D]:THR:O	1:k:157[D]:LYS:HG3	2.20	0.42
1:r:54[D]:TYR:OH	1:r:147[D]:GLU:OE2	2.33	0.42
1:w:17[D]:GLU:OE2	1:w:79[D]:ARG:N	2.48	0.42
1:w:79[D]:ARG:HA	1:w:79[D]:ARG:HD3	1.91	0.42
1:W:119:LYS:HD2	1:W:119:LYS:C	2.45	0.42
1:a:108[D]:LYS:NZ	1:c:7[D]:GLN:O	2.40	0.42
1:g:41[C]:PHE:CZ	1:g:96[C]:GLY:HA2	2.54	0.42
1:n:27[C]:GLU:HB2	1:n:66[C]:ALA:HB2	2.01	0.42
1:p:6[C]:SER:OG	1:p:8[C]:VAL:HG22	2.20	0.42
1:v:108[C]:LYS:HG2	1:v:145[C]:ILE:HD13	2.01	0.42
1:A:20:ILE:HD13	1:A:117:LEU:HD21	2.02	0.41
1:Q:117:LEU:HD23	1:Q:117:LEU:C	2.45	0.41
1:W:63[B]:ARG:HD2	5:W:411:HOH:O	2.19	0.41
1:i:68[D]:LYS:HE2	1:i:68[D]:LYS:HB2	1.78	0.41
1:l:6[C]:SER:OG	1:l:8[C]:VAL:HG22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:155[C]:LEU:HD23	1:m:155[C]:LEU:HA	1.87	0.41
1:h:63:ARG:HG2	1:u:63[A]:ARG:HH12	1.84	0.41
1:a:33[C]:VAL:HG22	1:a:88[C]:PRO:HB3	2.02	0.41
1:g:63[C]:ARG:NE	1:g:67[C]:GLU:OE2	2.53	0.41
1:k:114[D]:LEU:HD13	1:k:137[D]:TYR:HB3	2.02	0.41
1:q:7[C]:GLN:O	1:r:108[C]:LYS:NZ	2.41	0.41
1:r:41[C]:PHE:CZ	1:r:96[C]:GLY:HA2	2.55	0.41
1:A:71:LYS:NZ	5:A:311:HOH:O	2.51	0.41
1:E:79:ARG:HD3	1:E:79:ARG:HA	1.92	0.41
1:J:164:GLY:O	1:V:157:LYS:HE2	2.20	0.41
1:T:101:GLU:OE2	1:T:156:ARG:NH2	2.46	0.41
1:a:115[C]:LEU:HD23	1:a:115[C]:LEU:HA	1.92	0.41
1:d:145[C]:ILE:HG22	1:f:8[C]:VAL:HB	2.01	0.41
1:f:79[C]:ARG:HD3	1:f:79[C]:ARG:HA	1.90	0.41
1:h:68[D]:LYS:HZ2	1:h:136[D]:HIS:ND1	2.19	0.41
1:k:79[C]:ARG:HA	1:k:79[C]:ARG:HD3	1.82	0.41
1:k:79[D]:ARG:HA	1:k:79[D]:ARG:HD3	1.66	0.41
1:r:27[C]:GLU:HB2	1:r:66[C]:ALA:HB2	2.03	0.41
1:s:27[D]:GLU:HB2	1:s:66[D]:ALA:HB2	2.03	0.41
1:u:69[D]:LEU:HG	1:u:137[D]:TYR:OH	2.20	0.41
1:w:8[D]:VAL:HB	1:x:145[D]:ILE:HG22	2.01	0.41
5:J:302:HOH:O	1:V:157:LYS:HE3	2.20	0.41
1:W:79:ARG:HA	1:W:79:ARG:HD3	1.88	0.41
1:W:108:LYS:NZ	5:W:309:HOH:O	2.54	0.41
1:e:48[C]:LEU:HD23	1:e:48[C]:LEU:HA	1.94	0.41
1:f:41[C]:PHE:CZ	1:f:96[C]:GLY:HA2	2.55	0.41
1:h:66[D]:ALA:O	1:h:70[D]:MET:HG3	2.20	0.41
1:k:111[C]:ASN:O	1:k:115[C]:LEU:HG	2.19	0.41
1:n:79[C]:ARG:HA	1:n:79[C]:ARG:HD3	1.88	0.41
1:r:76[D]:ARG:HD3	1:r:128[D]:HIS:CE1	2.55	0.41
1:v:69[D]:LEU:HG	1:v:137[D]:TYR:OH	2.20	0.41
1:B:161:PRO:HD2	1:B:162:GLU:OE1	2.20	0.41
1:f:70[D]:MET:HE3	1:f:80[D]:ILE:HG21	2.03	0.41
1:g:28[C]:LEU:HD23	1:g:28[C]:LEU:HA	1.85	0.41
1:i:41[D]:PHE:CZ	1:i:96[D]:GLY:HA2	2.56	0.41
1:k:6[C]:SER:OG	1:k:8[C]:VAL:HG22	2.21	0.41
1:o:6[D]:SER:OG	1:o:8[D]:VAL:HG22	2.20	0.41
1:G:53:LYS:HE2	1:G:53:LYS:HA	2.01	0.41
1:J:129:LEU:O	1:J:133:ILE:HG12	2.21	0.41
1:L:164:GLY:N	5:L:310:HOH:O	2.53	0.41
1:X:20:ILE:HD13	1:X:117:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:76[C]:ARG:HD3	1:a:128[C]:HIS:ND1	2.35	0.41
1:e:129[C]:LEU:O	1:e:133[C]:ILE:HG12	2.20	0.41
1:e:134[D]:GLU:HA	1:e:138[D]:LEU:HG	2.01	0.41
1:s:79[D]:ARG:HA	1:s:79[D]:ARG:HD3	1.89	0.41
1:x:76[C]:ARG:HH11	1:x:128[C]:HIS:HD1	1.69	0.41
1:N:59:SER:OG	1:P:63:ARG:NH2	2.52	0.41
1:O:44:ASP:HA	1:W:150:ASP:OD1	2.21	0.41
1:T:72:LEU:C	1:T:72:LEU:HD13	2.46	0.41
1:e:168[D]:TYR:O	1:e:172[D]:LYS:HG2	2.20	0.41
1:f:41[D]:PHE:CZ	1:f:96[D]:GLY:HA2	2.56	0.41
1:h:37[C]:MET:HA	1:h:93[C]:TRP:CD1	2.55	0.41
1:h:153[C]:THR:O	1:h:157[C]:LYS:HG3	2.20	0.41
1:j:23[D]:GLN:OE1	1:j:113[D]:SER:OG	2.35	0.41
1:q:79[D]:ARG:HD3	1:q:79[D]:ARG:HA	1.81	0.41
1:r:93[C]:TRP:O	1:r:95[C]:SER:N	2.51	0.41
1:D:72:LEU:HD22	1:D:132:PHE:CD2	2.56	0.41
1:I:63:ARG:HD2	5:I:301:HOH:O	2.20	0.41
1:f:57[D]:HIS:O	1:f:61[D]:GLU:HG3	2.20	0.41
1:m:86[C]:GLN:OE1	1:m:86[C]:GLN:HA	2.20	0.41
1:o:54[C]:TYR:O	1:o:58[C]:GLN:HG2	2.21	0.41
1:K:67:GLU:OE1	5:K:301:HOH:O	2.22	0.41
1:M:159:GLY:O	1:M:162:GLU:HG2	2.21	0.41
1:O:79:ARG:HD3	1:O:79:ARG:HA	1.77	0.41
1:P:61:GLU:HG3	5:P:429:HOH:O	2.20	0.41
1:R:49:LYS:HE2	5:R:337:HOH:O	2.21	0.41
1:W:27:GLU:HB2	1:W:66:ALA:HB2	2.03	0.41
1:a:127[C]:PRO:HB3	1:b:118[C]:HIS:CE1	2.55	0.41
1:b:6[C]:SER:OG	1:b:8[C]:VAL:HG22	2.21	0.41
1:c:72[C]:LEU:HG	1:c:132[C]:PHE:CE2	2.56	0.41
1:f:68[D]:LYS:HE2	1:f:68[D]:LYS:HB2	1.92	0.41
1:j:8[C]:VAL:HB	1:k:145[C]:ILE:HG22	2.03	0.41
1:p:50[C]:ASN:HB2	1:p:171[C]:ASP:OD2	2.20	0.41
1:q:31[D]:SER:HB2	1:q:62[D]:GLU:HB2	2.03	0.41
1:q:33[C]:VAL:HG22	1:q:88[C]:PRO:HB3	2.03	0.41
1:q:68[C]:LYS:HE2	1:q:68[C]:LYS:HB2	1.91	0.41
1:q:129[C]:LEU:O	1:q:133[C]:ILE:HG12	2.21	0.41
1:r:79[D]:ARG:HD3	1:r:79[D]:ARG:HA	1.75	0.41
1:v:153[C]:THR:O	1:v:157[C]:LYS:HG3	2.21	0.41
1:B:4:SER:N	5:B:315:HOH:O	2.54	0.40
1:E:161:PRO:HD2	1:E:162:GLU:OE2	2.21	0.40
1:P:127:PRO:HB3	1:Q:118:HIS:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:6:SER:OG	1:U:8:VAL:HG22	2.21	0.40
1:U:79:ARG:HD3	1:U:79:ARG:HA	1.76	0.40
1:k:24[C]:ILE:HG12	1:k:70[C]:MET:HG3	2.03	0.40
1:p:79[C]:ARG:HD3	1:p:79[C]:ARG:HA	1.84	0.40
1:c:79[C]:ARG:HD3	1:c:79[C]:ARG:HA	1.88	0.40
1:f:58[C]:GLN:O	1:f:62[C]:GLU:HG2	2.20	0.40
1:q:76[D]:ARG:HD3	1:q:128[D]:HIS:CE1	2.56	0.40
1:r:134[C]:GLU:HA	1:r:138[C]:LEU:HG	2.04	0.40
1:g:76[C]:ARG:HD3	1:g:128[C]:HIS:ND1	2.37	0.40
1:n:20[C]:ILE:HD13	1:n:20[C]:ILE:HA	1.94	0.40
1:p:33[C]:VAL:HG22	1:p:88[C]:PRO:HB3	2.03	0.40
1:G:79:ARG:HD3	1:G:79:ARG:HA	1.88	0.40
1:I:33:VAL:HG12	1:I:37:MET:CE	2.36	0.40
1:Q:156:ARG:HH11	1:Q:156:ARG:HD2	1.75	0.40
1:e:76[C]:ARG:HD3	1:e:128[C]:HIS:CE1	2.56	0.40
1:w:33[D]:VAL:HG22	1:w:88[D]:PRO:HB3	2.02	0.40
1:X:24:ILE:HD13	1:X:70:MET:HG2	2.03	0.40
1:f:50[D]:ASN:HB2	1:f:171[D]:ASP:OD2	2.21	0.40
1:j:169[D]:LEU:HD23	1:j:169[D]:LEU:HA	1.89	0.40
1:p:50[D]:ASN:HB2	1:p:171[D]:ASP:CG	2.47	0.40
1:r:41[C]:PHE:HA	1:r:46[C]:VAL:HG11	2.02	0.40
1:r:155[C]:LEU:HD23	1:r:155[C]:LEU:HA	1.82	0.40
1:t:79[C]:ARG:HD3	1:t:79[C]:ARG:HA	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	172/182 (94%)	168 (98%)	4 (2%)	0	100	100
1	B	173/182 (95%)	168 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	21	13
1	f	344/182 (189%)	336 (98%)	6 (2%)	2 (1%)	21	13
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	21	13
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 ⓘ

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%)	153 (100%)	0	100	100
1	B	154/160 (96%)	154 (100%)	0	100	100
1	C	154/160 (96%)	154 (100%)	0	100	100
1	D	153/160 (96%)	153 (100%)	0	100	100
1	E	156/160 (98%)	156 (100%)	0	100	100
1	F	154/160 (96%)	154 (100%)	0	100	100
1	G	154/160 (96%)	154 (100%)	0	100	100
1	H	154/160 (96%)	154 (100%)	0	100	100
1	I	154/160 (96%)	154 (100%)	0	100	100
1	J	154/160 (96%)	154 (100%)	0	100	100
1	K	153/160 (96%)	153 (100%)	0	100	100
1	L	153/160 (96%)	153 (100%)	0	100	100
1	M	153/160 (96%)	153 (100%)	0	100	100
1	N	154/160 (96%)	154 (100%)	0	100	100
1	O	154/160 (96%)	153 (99%)	1 (1%)	78	82
1	P	154/160 (96%)	154 (100%)	0	100	100
1	Q	155/160 (97%)	155 (100%)	0	100	100
1	R	153/160 (96%)	153 (100%)	0	100	100
1	S	154/160 (96%)	154 (100%)	0	100	100
1	T	154/160 (96%)	154 (100%)	0	100	100
1	U	155/160 (97%)	155 (100%)	0	100	100
1	V	153/160 (96%)	153 (100%)	0	100	100
1	W	156/160 (98%)	156 (100%)	0	100	100
1	X	154/160 (96%)	154 (100%)	0	100	100
1	a	306/160 (191%)	296 (97%)	10 (3%)	33	28
1	b	306/160 (191%)	302 (99%)	4 (1%)	61	62
1	c	306/160 (191%)	302 (99%)	4 (1%)	61	62
1	d	306/160 (191%)	298 (97%)	8 (3%)	40	37
1	e	306/160 (191%)	298 (97%)	8 (3%)	40	37
1	f	306/160 (191%)	300 (98%)	6 (2%)	48	47
1	g	306/160 (191%)	300 (98%)	6 (2%)	48	47
1	h	306/160 (191%)	290 (95%)	16 (5%)	21	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	i	306/160 (191%)	302 (99%)	4 (1%)	61	62
1	j	306/160 (191%)	298 (97%)	8 (3%)	40	37
1	k	306/160 (191%)	304 (99%)	2 (1%)	76	79
1	l	306/160 (191%)	300 (98%)	6 (2%)	48	47
1	m	306/160 (191%)	292 (95%)	14 (5%)	24	17
1	n	306/160 (191%)	298 (97%)	8 (3%)	40	37
1	o	306/160 (191%)	294 (96%)	12 (4%)	28	23
1	p	306/160 (191%)	292 (95%)	14 (5%)	24	17
1	q	306/160 (191%)	300 (98%)	6 (2%)	48	47
1	r	306/160 (191%)	294 (96%)	12 (4%)	28	23
1	s	306/160 (191%)	298 (97%)	8 (3%)	40	37
1	t	306/160 (191%)	304 (99%)	2 (1%)	76	79
1	u	306/160 (191%)	300 (98%)	6 (2%)	48	47
1	v	306/160 (191%)	298 (97%)	8 (3%)	40	37
1	w	306/160 (191%)	296 (97%)	10 (3%)	33	28
1	x	306/160 (191%)	294 (96%)	12 (4%)	28	23
All	All	11039/7680 (144%)	10844 (98%)	195 (2%)	61	51

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	177	ASP
1	a	8[C]	VAL
1	a	8[D]	VAL
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	72[C]	LEU
1	b	72[D]	LEU
1	b	117[C]	LEU
1	b	117[D]	LEU

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Mol	Chain	Res	Type
1	c	5[C]	THR
1	c	5[D]	THR
1	c	117[C]	LEU
1	c	117[D]	LEU
1	d	4[C]	SER
1	d	4[D]	SER
1	d	32[C]	TYR
1	d	32[D]	TYR
1	d	61[C]	GLU
1	d	61[D]	GLU
1	d	117[C]	LEU
1	d	117[D]	LEU
1	e	32[C]	TYR
1	e	32[D]	TYR
1	e	72[C]	LEU
1	e	72[D]	LEU
1	e	117[C]	LEU
1	e	117[D]	LEU
1	e	138[C]	LEU
1	e	138[D]	LEU
1	f	72[C]	LEU
1	f	72[D]	LEU
1	f	117[C]	LEU
1	f	117[D]	LEU
1	f	152[C]	VAL
1	f	152[D]	VAL
1	g	61[C]	GLU
1	g	61[D]	GLU
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	61[C]	GLU
1	h	61[D]	GLU
1	h	72[C]	LEU
1	h	72[D]	LEU
1	h	89[C]	ASP
1	h	89[D]	ASP

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Mol	Chain	Res	Type
1	h	117[C]	LEU
1	h	117[D]	LEU
1	h	152[C]	VAL
1	h	152[D]	VAL
1	h	177[C]	ASP
1	h	177[D]	ASP
1	i	117[C]	LEU
1	i	117[D]	LEU
1	i	152[C]	VAL
1	i	152[D]	VAL
1	j	8[C]	VAL
1	j	8[D]	VAL
1	j	32[C]	TYR
1	j	32[D]	TYR
1	j	61[C]	GLU
1	j	61[D]	GLU
1	j	117[C]	LEU
1	j	117[D]	LEU
1	k	117[C]	LEU
1	k	117[D]	LEU
1	l	5[C]	THR
1	l	5[D]	THR
1	l	6[C]	SER
1	l	6[D]	SER
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

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Mol	Chain	Res	Type
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
1	o	75[C]	GLN
1	o	75[D]	GLN
1	o	117[C]	LEU
1	o	117[D]	LEU
1	o	138[C]	LEU
1	o	138[D]	LEU
1	p	32[C]	TYR
1	p	32[D]	TYR
1	p	87[C]	LYS
1	p	87[D]	LYS
1	p	117[C]	LEU
1	p	117[D]	LEU
1	p	141[C]	GLN
1	p	141[D]	GLN
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	8[C]	VAL
1	q	8[D]	VAL
1	q	117[C]	LEU
1	q	117[D]	LEU
1	q	177[C]	ASP
1	q	177[D]	ASP
1	r	8[C]	VAL
1	r	8[D]	VAL
1	r	32[C]	TYR
1	r	32[D]	TYR

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Mol	Chain	Res	Type
1	r	115[C]	LEU
1	r	115[D]	LEU
1	r	117[C]	LEU
1	r	117[D]	LEU
1	r	141[C]	GLN
1	r	141[D]	GLN
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	156[C]	ARG
1	s	156[D]	ARG
1	s	171[C]	ASP
1	s	171[D]	ASP
1	t	117[C]	LEU
1	t	117[D]	LEU
1	u	8[C]	VAL
1	u	8[D]	VAL
1	u	32[C]	TYR
1	u	32[D]	TYR
1	u	117[C]	LEU
1	u	117[D]	LEU
1	v	32[C]	TYR
1	v	32[D]	TYR
1	v	72[C]	LEU
1	v	72[D]	LEU
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	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

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Mol	Chain	Res	Type
1	x	4[C]	SER
1	x	4[D]	SER
1	x	72[C]	LEU
1	x	72[D]	LEU
1	x	75[C]	GLN
1	x	75[D]	GLN
1	x	117[C]	LEU
1	x	117[D]	LEU
1	x	138[C]	LEU
1	x	138[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 (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	109	ASN
1	A	111	ASN
1	A	125	ASN
1	B	7	GLN
1	B	105	HIS
1	B	109	ASN
1	B	111	ASN
1	C	111	ASN
1	C	122	HIS
1	C	125	ASN
1	D	7	GLN
1	E	25	ASN
1	F	50	ASN
1	F	57	HIS
1	F	109	ASN
1	F	122	HIS
1	G	111	ASN
1	H	14	GLN
1	H	105	HIS
1	I	86	GLN
1	I	122	HIS
1	J	111	ASN
1	K	105	HIS
1	K	111	ASN
1	K	136	HIS

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Mol	Chain	Res	Type
1	L	122	HIS
1	M	105	HIS
1	M	109	ASN
1	M	111	ASN
1	M	154	ASN
1	N	111	ASN
1	N	125	ASN
1	N	136	HIS
1	N	173	HIS
1	O	111	ASN
1	O	122	HIS
1	P	7	GLN
1	P	105	HIS
1	Q	25	ASN
1	Q	58	GLN
1	Q	109	ASN
1	R	86	GLN
1	R	111	ASN
1	S	98	ASN
1	S	111	ASN
1	T	10	GLN
1	T	111	ASN
1	U	111	ASN
1	U	112	GLN
1	V	111	ASN
1	W	14	GLN
1	W	86	GLN
1	W	111	ASN
1	X	7	GLN
1	X	111	ASN
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	O	205[C]	2	14,14,14	3.78	3 (21%)	18,18,18	1.31	4 (22%)
4	V9D	T	203[D]	2	14,14,14	4.03	2 (14%)	18,18,18	1.24	3 (16%)
4	V9D	Q	203[D]	2	14,14,14	3.96	2 (14%)	18,18,18	1.10	3 (16%)
4	V9D	K	203[D]	2	14,14,14	3.79	3 (21%)	18,18,18	1.36	4 (22%)
4	V9D	T	203[C]	2	14,14,14	3.89	2 (14%)	18,18,18	1.35	3 (16%)
4	V9D	X	204[D]	2	14,14,14	4.04	3 (21%)	18,18,18	1.74	4 (22%)
4	V9D	Q	203[C]	2	14,14,14	3.85	2 (14%)	18,18,18	1.34	3 (16%)
4	V9D	H	204[D]	2	14,14,14	3.89	2 (14%)	18,18,18	1.45	4 (22%)
4	V9D	H	204[C]	2	14,14,14	3.97	2 (14%)	18,18,18	1.26	4 (22%)
4	V9D	B	204[D]	2	14,14,14	3.82	3 (21%)	18,18,18	1.39	4 (22%)
4	V9D	K	203[C]	2	14,14,14	4.02	3 (21%)	18,18,18	1.84	4 (22%)
4	V9D	E	203[D]	2	14,14,14	3.86	2 (14%)	18,18,18	1.39	3 (16%)
4	V9D	X	204[C]	2	14,14,14	3.76	3 (21%)	18,18,18	1.47	4 (22%)
4	V9D	E	203[C]	2	14,14,14	3.97	2 (14%)	18,18,18	1.10	3 (16%)
4	V9D	O	205[D]	2	14,14,14	4.10	3 (21%)	18,18,18	1.49	4 (22%)
4	V9D	B	204[C]	2	14,14,14	4.01	2 (14%)	18,18,18	1.55	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	O	205[C]	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	Q	203[D]	2	-	4/12/12/12	0/1/1/1
4	V9D	K	203[D]	2	-	4/12/12/12	0/1/1/1
4	V9D	T	203[C]	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	Q	203[C]	2	-	5/12/12/12	0/1/1/1
4	V9D	H	204[D]	2	-	8/12/12/12	0/1/1/1
4	V9D	H	204[C]	2	-	4/12/12/12	0/1/1/1
4	V9D	B	204[D]	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	E	203[D]	2	-	7/12/12/12	0/1/1/1
4	V9D	X	204[C]	2	-	4/12/12/12	0/1/1/1
4	V9D	E	203[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

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	205[D]	V9D	C10-N11	10.83	1.46	1.32
4	K	203[C]	V9D	C10-N11	10.56	1.46	1.32
4	H	204[D]	V9D	C02-N03	10.53	1.46	1.32
4	E	203[D]	V9D	C02-N03	10.52	1.46	1.32
4	T	203[C]	V9D	C02-N03	10.51	1.46	1.32
4	T	203[D]	V9D	C10-N11	10.49	1.46	1.32
4	B	204[C]	V9D	C10-N11	10.48	1.46	1.32
4	O	205[C]	V9D	C02-N03	10.46	1.46	1.32
4	X	204[C]	V9D	C02-N03	10.46	1.46	1.32
4	X	204[D]	V9D	C10-N11	10.45	1.46	1.32
4	H	204[C]	V9D	C10-N11	10.44	1.46	1.32
4	B	204[D]	V9D	C02-N03	10.37	1.46	1.32
4	K	203[D]	V9D	C02-N03	10.30	1.45	1.32
4	Q	203[D]	V9D	C10-N11	10.30	1.45	1.32
4	Q	203[C]	V9D	C02-N03	10.29	1.45	1.32
4	T	203[D]	V9D	C02-N03	10.26	1.45	1.32
4	E	203[C]	V9D	C10-N11	10.25	1.45	1.32
4	X	204[D]	V9D	C02-N03	10.19	1.45	1.32
4	E	203[C]	V9D	C02-N03	10.18	1.45	1.32
4	O	205[D]	V9D	C02-N03	10.16	1.45	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	203[D]	V9D	C02-N03	10.09	1.45	1.32
4	B	204[C]	V9D	C02-N03	10.06	1.45	1.32
4	K	203[C]	V9D	C02-N03	10.02	1.45	1.32
4	H	204[C]	V9D	C02-N03	10.01	1.45	1.32
4	H	204[D]	V9D	C10-N11	9.53	1.44	1.32
4	Q	203[C]	V9D	C10-N11	9.53	1.44	1.32
4	T	203[C]	V9D	C10-N11	9.48	1.44	1.32
4	E	203[D]	V9D	C10-N11	9.38	1.44	1.32
4	B	204[D]	V9D	C10-N11	9.26	1.44	1.32
4	K	203[D]	V9D	C10-N11	9.13	1.44	1.32
4	O	205[C]	V9D	C10-N11	8.90	1.44	1.32
4	X	204[C]	V9D	C10-N11	8.77	1.43	1.32
4	K	203[C]	V9D	C09-C10	2.23	1.55	1.50
4	X	204[D]	V9D	C09-C10	2.20	1.55	1.50
4	B	204[D]	V9D	C09-C10	2.17	1.55	1.50
4	O	205[D]	V9D	C09-C10	2.12	1.54	1.50
4	X	204[C]	V9D	C09-C10	2.10	1.54	1.50
4	O	205[C]	V9D	C09-C10	2.06	1.54	1.50
4	K	203[D]	V9D	C09-C10	2.04	1.54	1.50

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	204[D]	V9D	C09-C10-N11	4.17	122.70	116.26
4	K	203[C]	V9D	C09-C10-N11	4.13	122.64	116.26
4	B	204[C]	V9D	C09-C10-N11	3.95	122.36	116.26
4	K	203[C]	V9D	C05-C02-N03	3.84	122.19	116.26
4	X	204[C]	V9D	O13-C10-N11	-3.67	116.15	122.90
4	H	204[D]	V9D	O13-C10-N11	-3.46	116.52	122.90
4	B	204[D]	V9D	O13-C10-N11	-3.45	116.55	122.90
4	E	203[D]	V9D	O13-C10-N11	-3.43	116.58	122.90
4	O	205[D]	V9D	C09-C10-N11	3.37	121.46	116.26
4	K	203[C]	V9D	O13-C10-N11	-3.32	116.78	122.90
4	X	204[D]	V9D	C05-C02-N03	3.30	121.36	116.26
4	K	203[D]	V9D	O13-C10-N11	-3.18	117.04	122.90
4	X	204[D]	V9D	O13-C10-N11	-3.15	117.10	122.90
4	T	203[C]	V9D	O13-C10-N11	-3.12	117.15	122.90
4	O	205[D]	V9D	O01-C02-N03	-3.10	117.20	122.90
4	Q	203[C]	V9D	O13-C10-N11	-3.07	117.25	122.90
4	O	205[C]	V9D	O13-C10-N11	-3.06	117.27	122.90
4	K	203[C]	V9D	O01-C02-N03	-3.03	117.31	122.90
4	O	205[D]	V9D	C05-C02-N03	3.01	120.91	116.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	204[C]	V9D	O01-C02-N03	-2.95	117.46	122.90
4	Q	203[D]	V9D	C09-C10-N11	2.93	120.78	116.26
4	T	203[C]	V9D	O01-C02-N03	-2.93	117.51	122.90
4	H	204[C]	V9D	C09-C10-N11	2.93	120.78	116.26
4	X	204[D]	V9D	O01-C02-N03	-2.90	117.56	122.90
4	Q	203[C]	V9D	O01-C02-N03	-2.84	117.67	122.90
4	H	204[D]	V9D	O01-C02-N03	-2.82	117.71	122.90
4	E	203[D]	V9D	O01-C02-N03	-2.78	117.79	122.90
4	X	204[C]	V9D	O13-C10-C09	2.77	126.40	120.90
4	K	203[D]	V9D	O01-C02-N03	-2.77	117.79	122.90
4	O	205[C]	V9D	O01-C02-N03	-2.73	117.87	122.90
4	B	204[D]	V9D	O13-C10-C09	2.71	126.26	120.90
4	H	204[C]	V9D	O01-C02-N03	-2.69	117.95	122.90
4	X	204[C]	V9D	O01-C02-N03	-2.68	117.97	122.90
4	T	203[D]	V9D	C05-C02-N03	2.65	120.36	116.26
4	T	203[D]	V9D	C09-C10-N11	2.64	120.34	116.26
4	E	203[C]	V9D	C09-C10-N11	2.63	120.32	116.26
4	T	203[D]	V9D	O01-C02-N03	-2.62	118.08	122.90
4	B	204[D]	V9D	O01-C02-N03	-2.59	118.12	122.90
4	B	204[C]	V9D	O13-C10-N11	-2.59	118.14	122.90
4	O	205[D]	V9D	O13-C10-N11	-2.57	118.17	122.90
4	K	203[D]	V9D	O13-C10-C09	2.53	125.91	120.90
4	O	205[C]	V9D	O13-C10-C09	2.45	125.75	120.90
4	B	204[D]	V9D	C05-C02-N03	2.42	119.99	116.26
4	B	204[C]	V9D	C05-C02-N03	2.42	119.99	116.26
4	O	205[C]	V9D	C05-C02-N03	2.35	119.89	116.26
4	X	204[C]	V9D	C05-C02-N03	2.34	119.87	116.26
4	K	203[D]	V9D	C05-C02-N03	2.33	119.86	116.26
4	Q	203[C]	V9D	C05-C02-N03	2.30	119.81	116.26
4	H	204[D]	V9D	C09-C10-N11	2.28	119.78	116.26
4	T	203[C]	V9D	C05-C02-N03	2.27	119.77	116.26
4	E	203[D]	V9D	C05-C02-N03	2.26	119.75	116.26
4	H	204[C]	V9D	C05-C02-N03	2.24	119.72	116.26
4	E	203[C]	V9D	O01-C02-N03	-2.23	118.79	122.90
4	H	204[D]	V9D	C05-C02-N03	2.21	119.68	116.26
4	H	204[C]	V9D	O13-C10-N11	-2.21	118.84	122.90
4	E	203[C]	V9D	O13-C10-N11	-2.13	118.97	122.90
4	Q	203[D]	V9D	O13-C10-N11	-2.08	119.07	122.90
4	Q	203[D]	V9D	O01-C02-N03	-2.04	119.14	122.90

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
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	H	204[C]	V9D	O01-C02-C05-C06
4	T	203[C]	V9D	C08-C09-C10-O13
4	B	204[C]	V9D	O01-C02-C05-C06
4	E	203[C]	V9D	O01-C02-C05-C06
4	Q	203[D]	V9D	O01-C02-C05-C06
4	Q	203[D]	V9D	O01-C02-C05-C14
4	B	204[C]	V9D	O01-C02-C05-C14
4	E	203[C]	V9D	O01-C02-C05-C14
4	H	204[C]	V9D	O01-C02-C05-C14

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

There are no ring outliers.

12 monomers are involved in 17 short contacts:

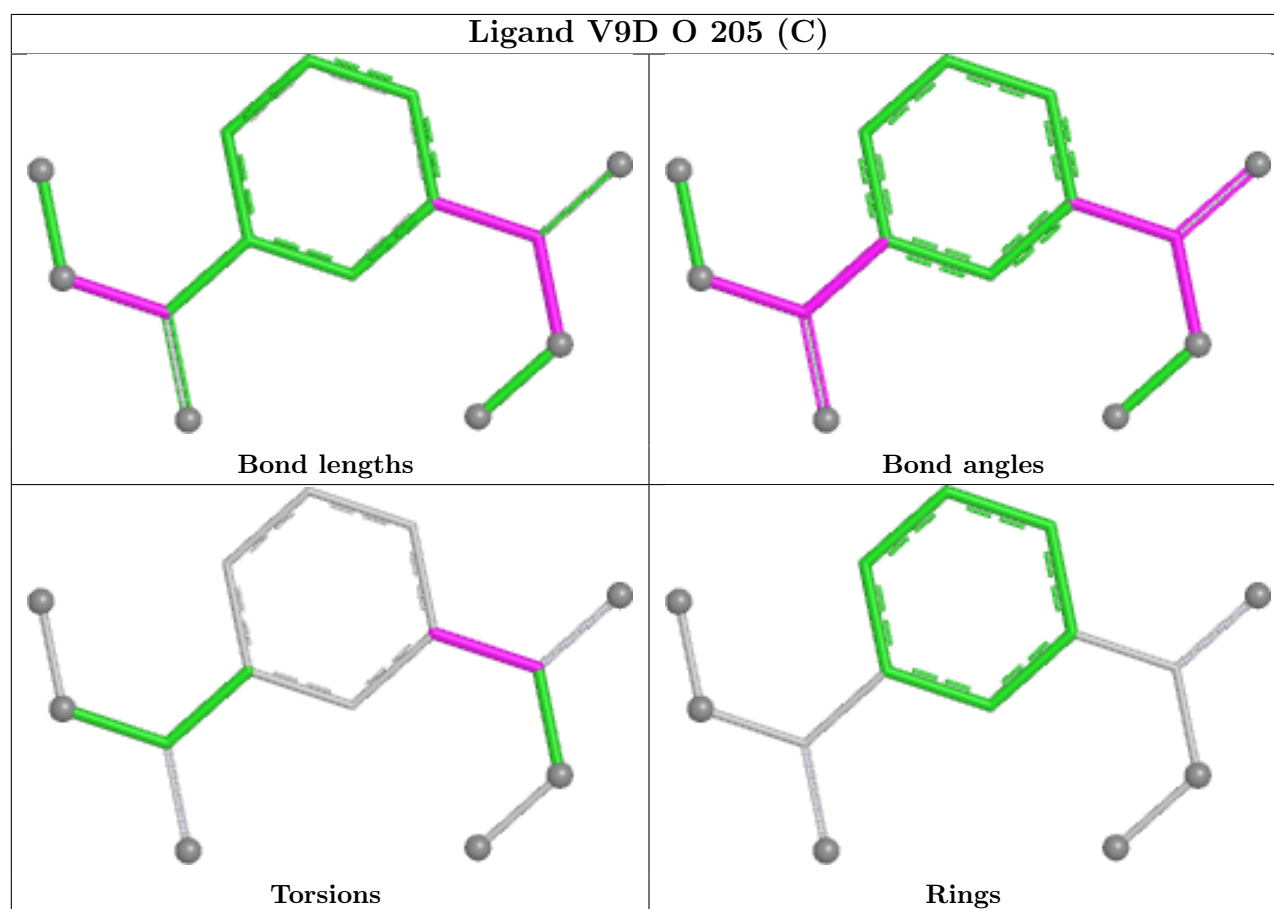
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	O	205[C]	V9D	1	0
4	T	203[D]	V9D	2	0
4	Q	203[D]	V9D	2	0
4	X	204[D]	V9D	2	0
4	Q	203[C]	V9D	1	0
4	H	204[D]	V9D	2	0
4	H	204[C]	V9D	1	0
4	K	203[C]	V9D	2	0

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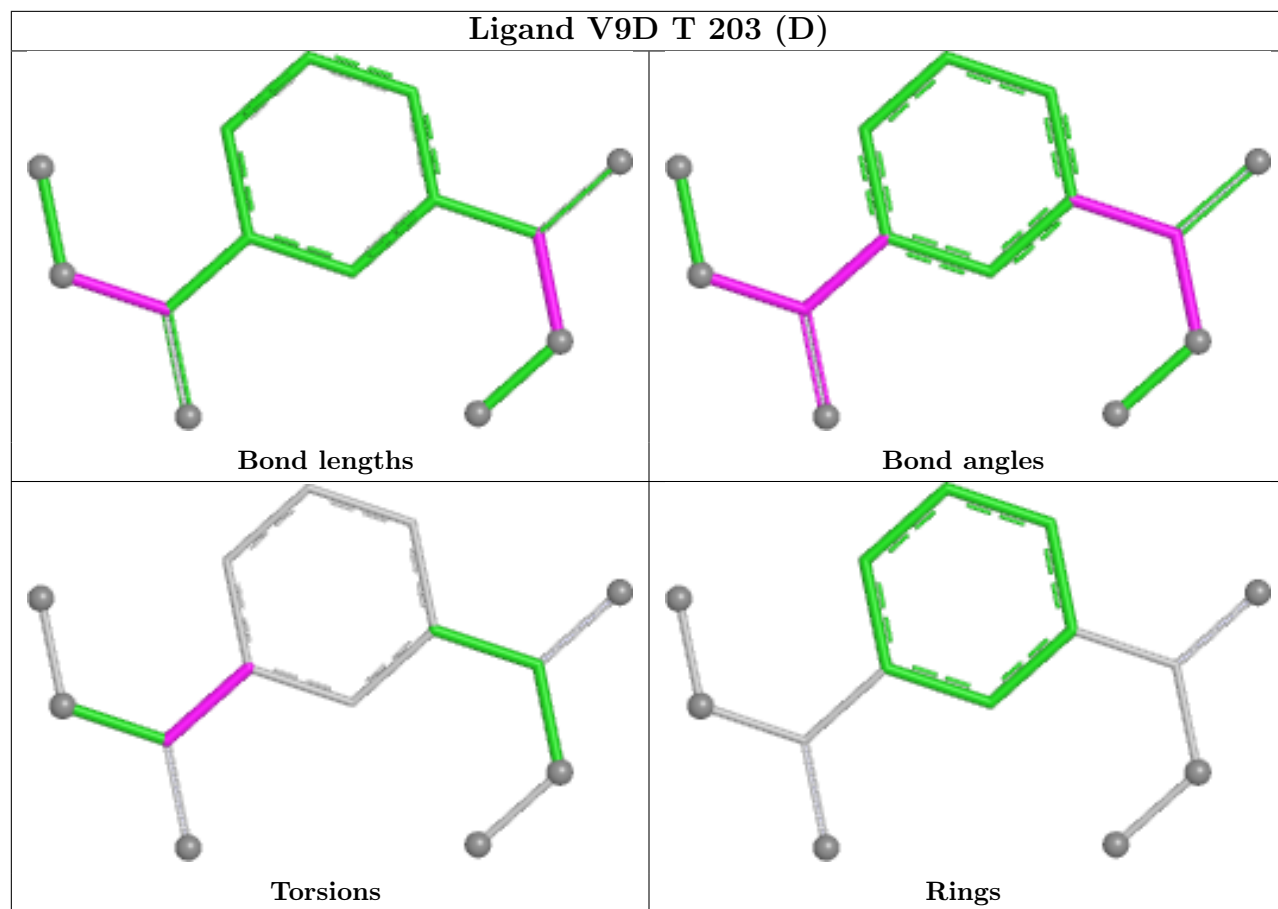
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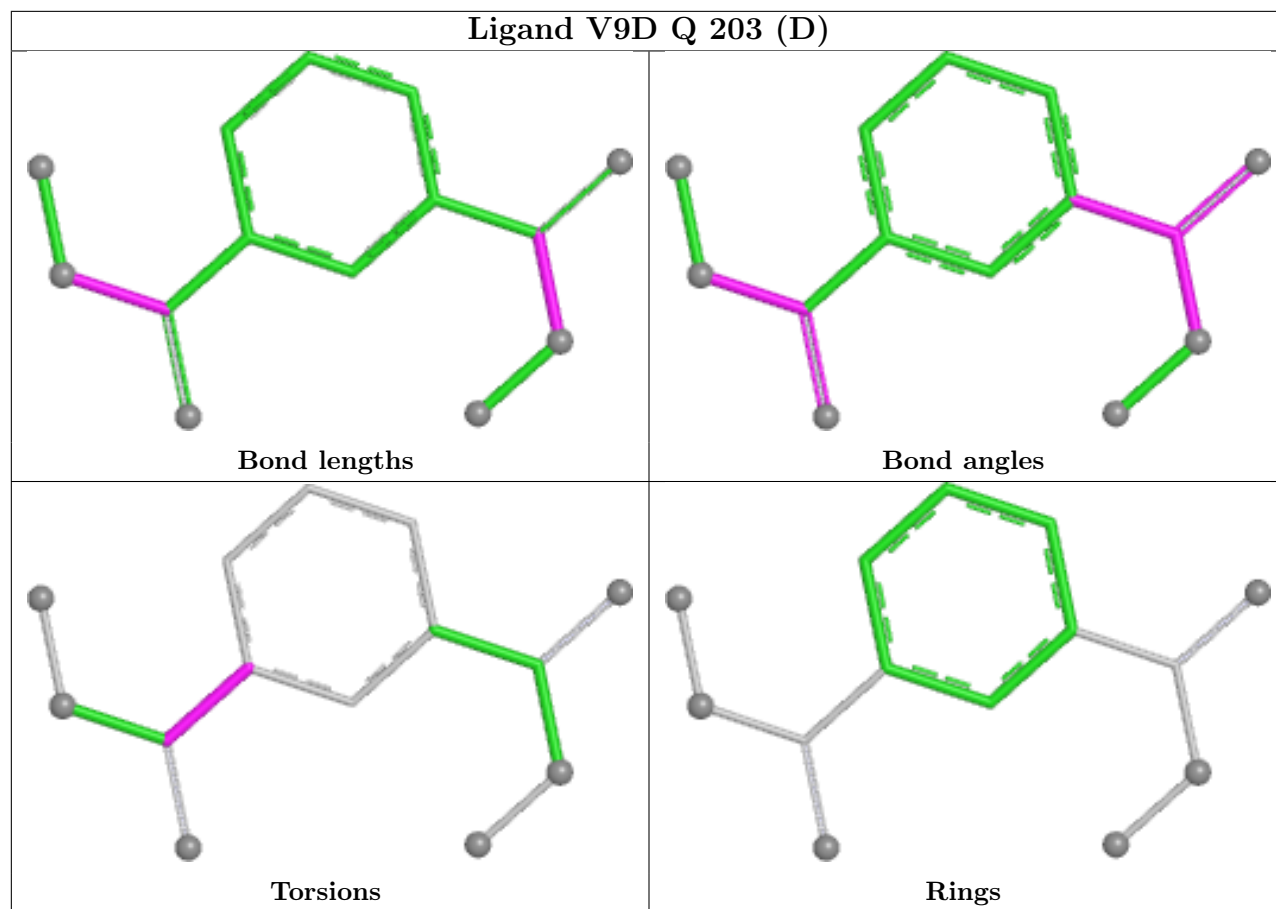
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	203[D]	V9D	1	0
4	E	203[C]	V9D	1	0
4	O	205[D]	V9D	1	0
4	B	204[C]	V9D	1	0

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

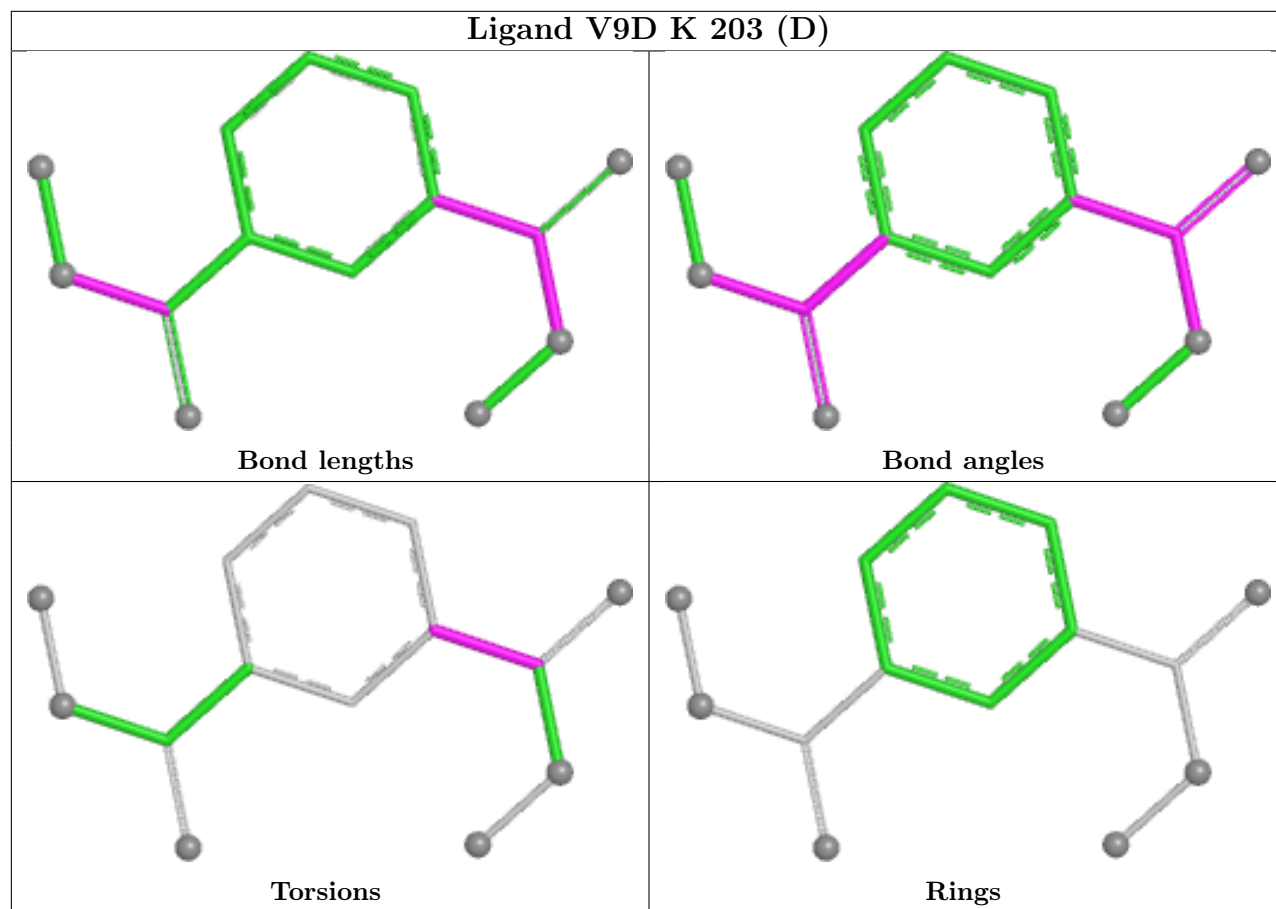


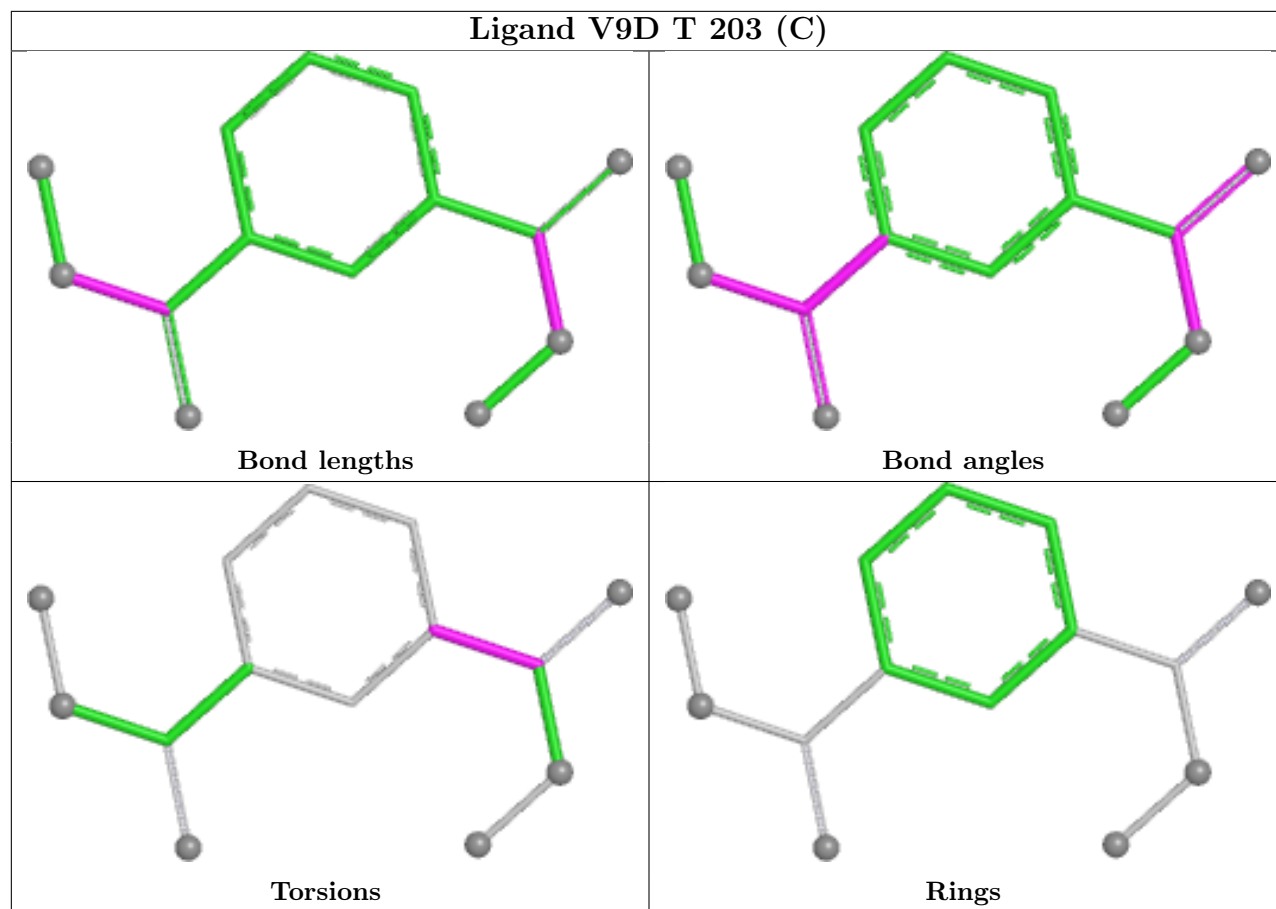
Ligand V9D T 203 (D)

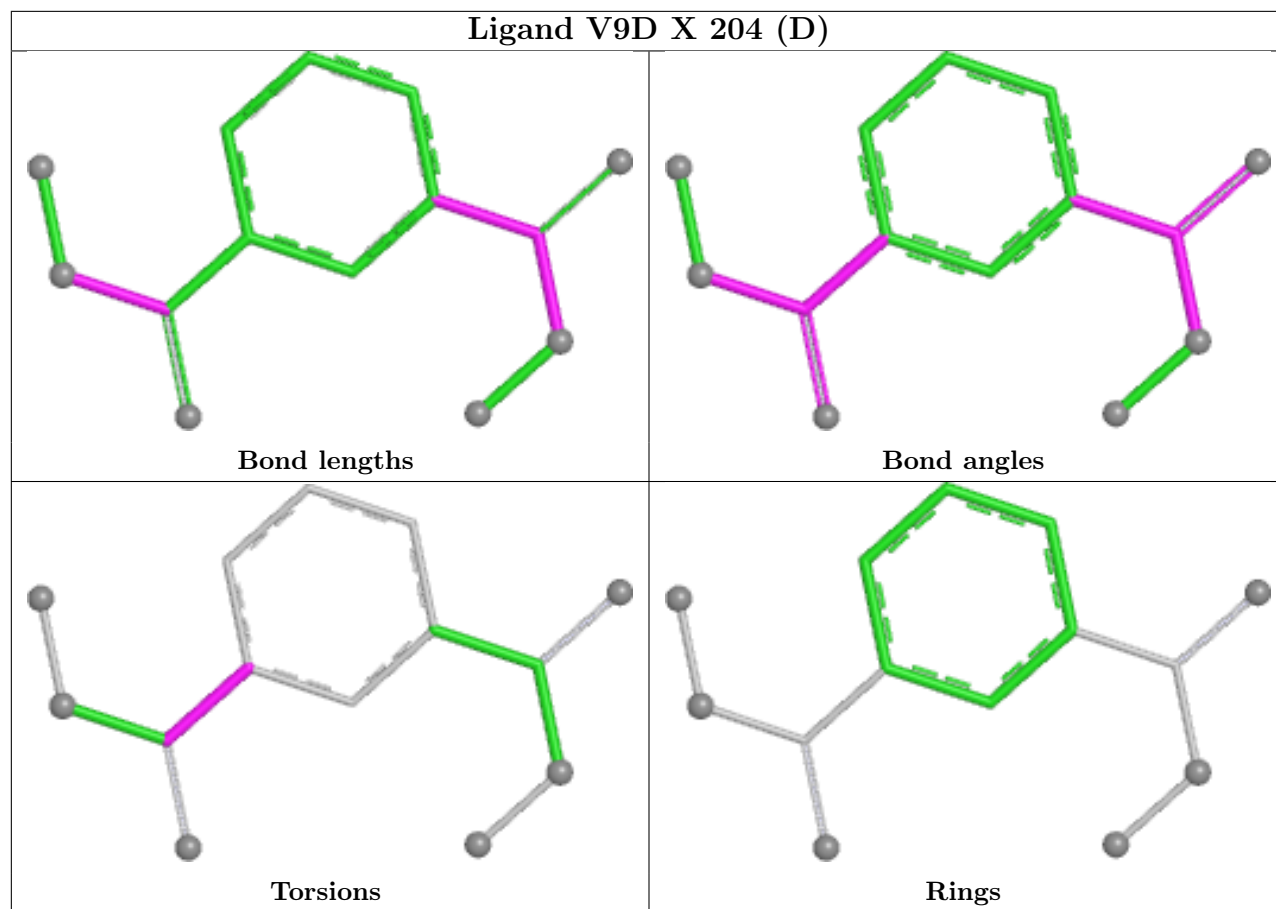


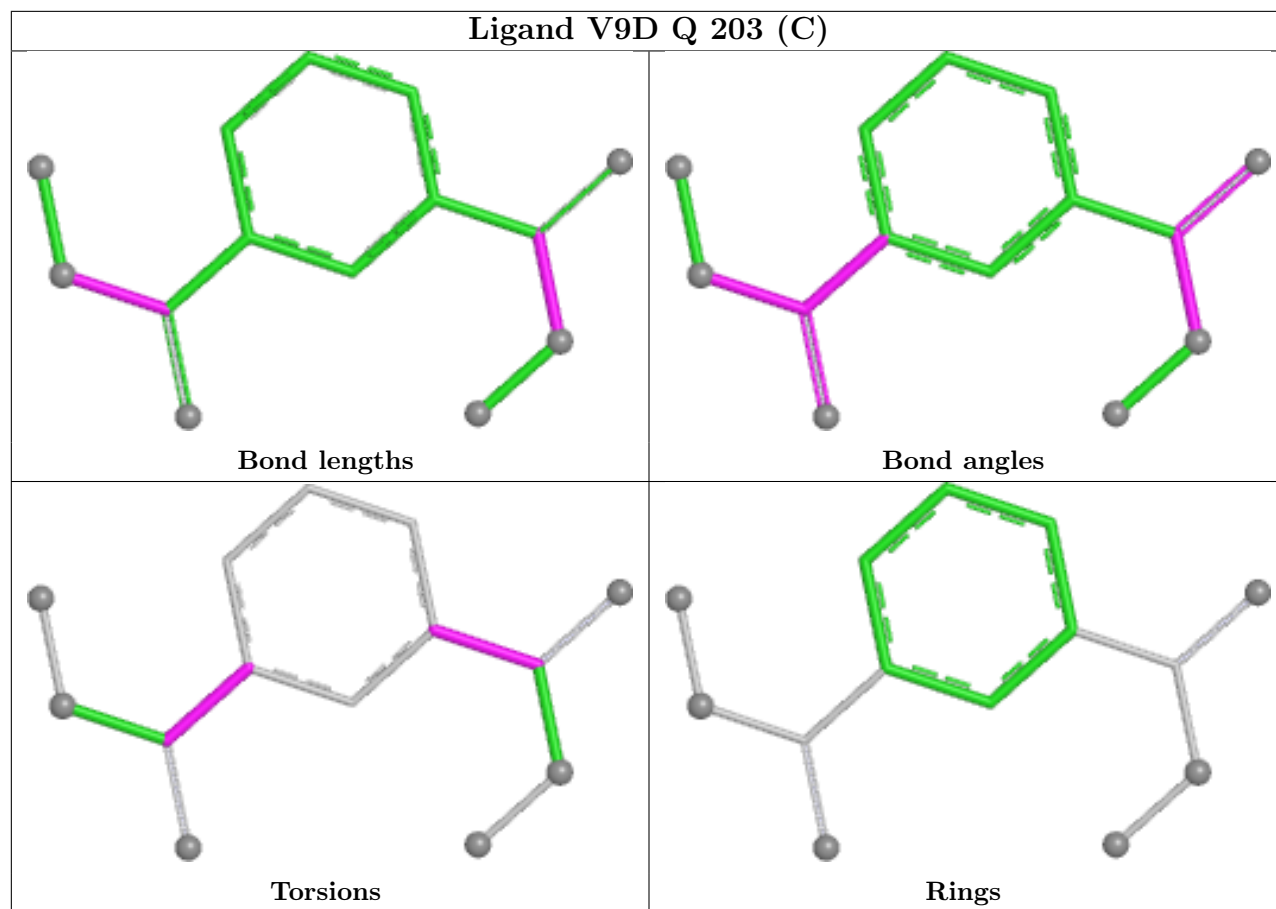


Ligand V9D K 203 (D)

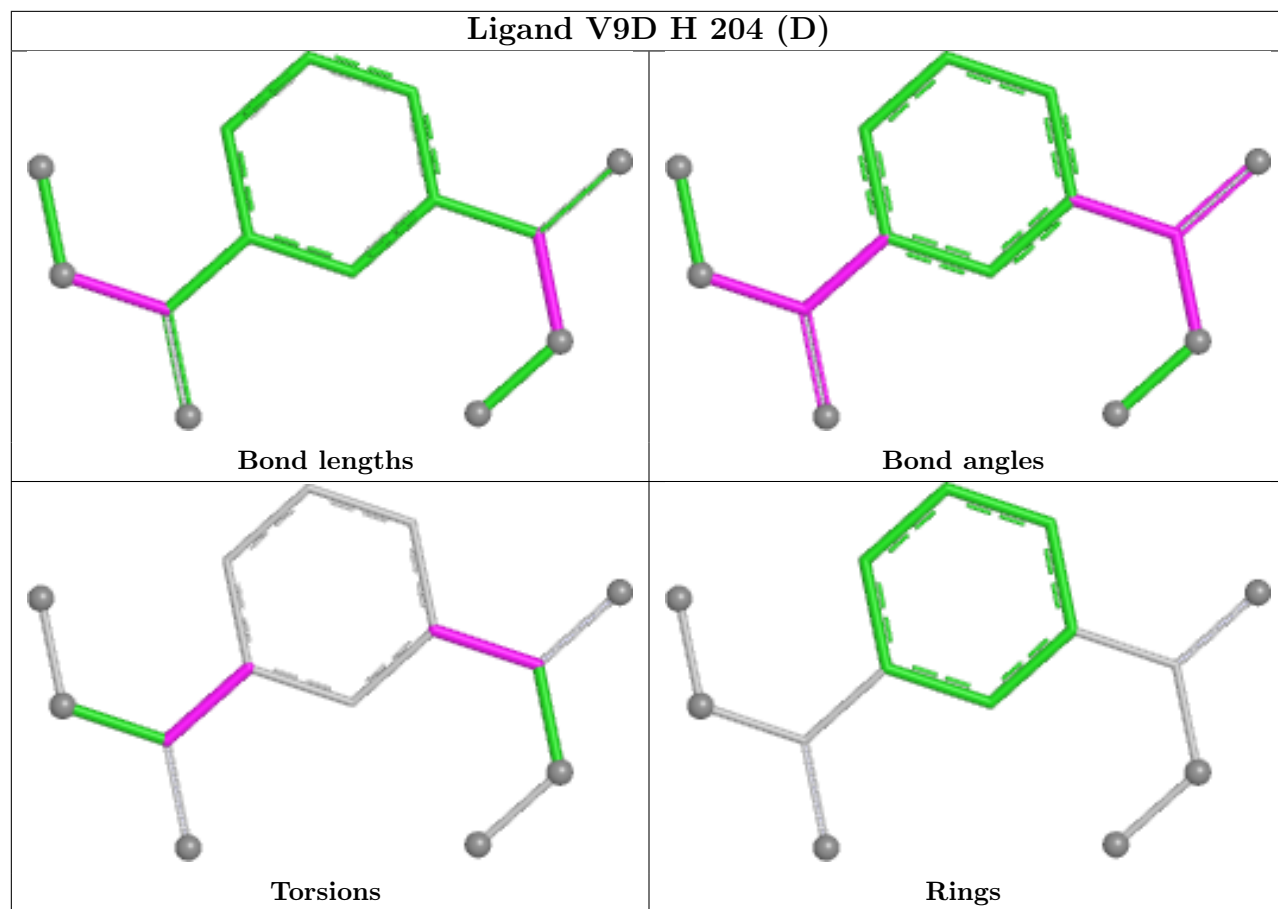


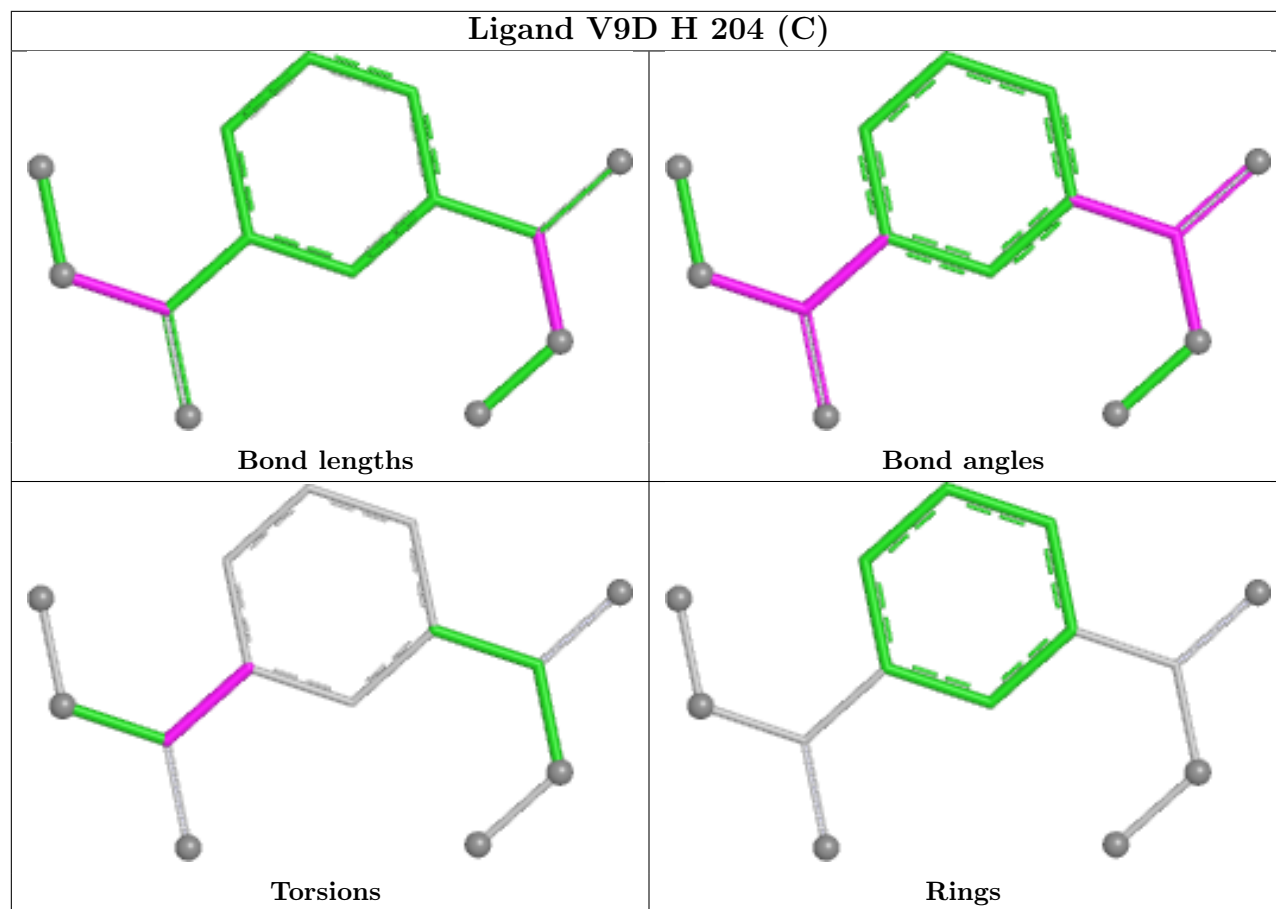


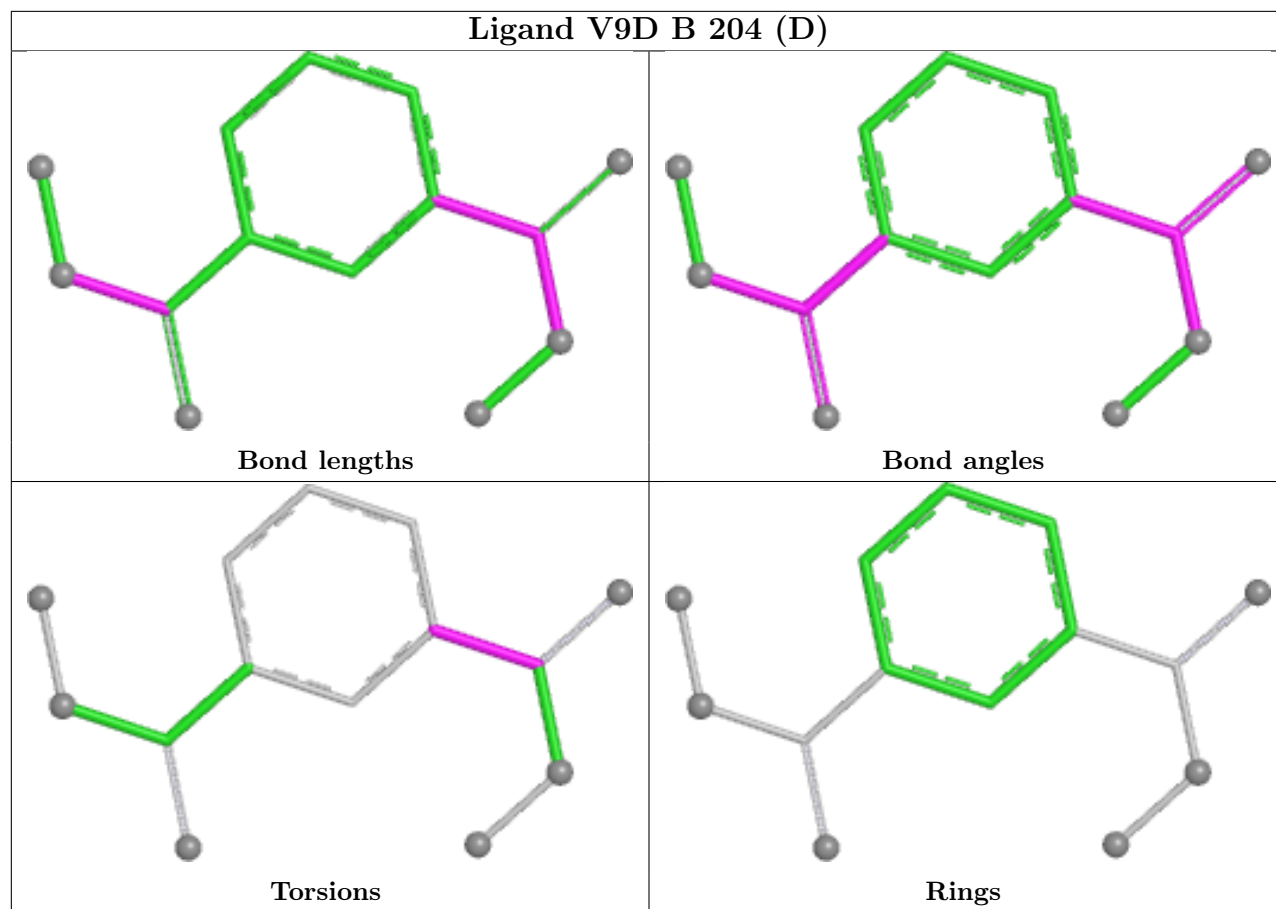


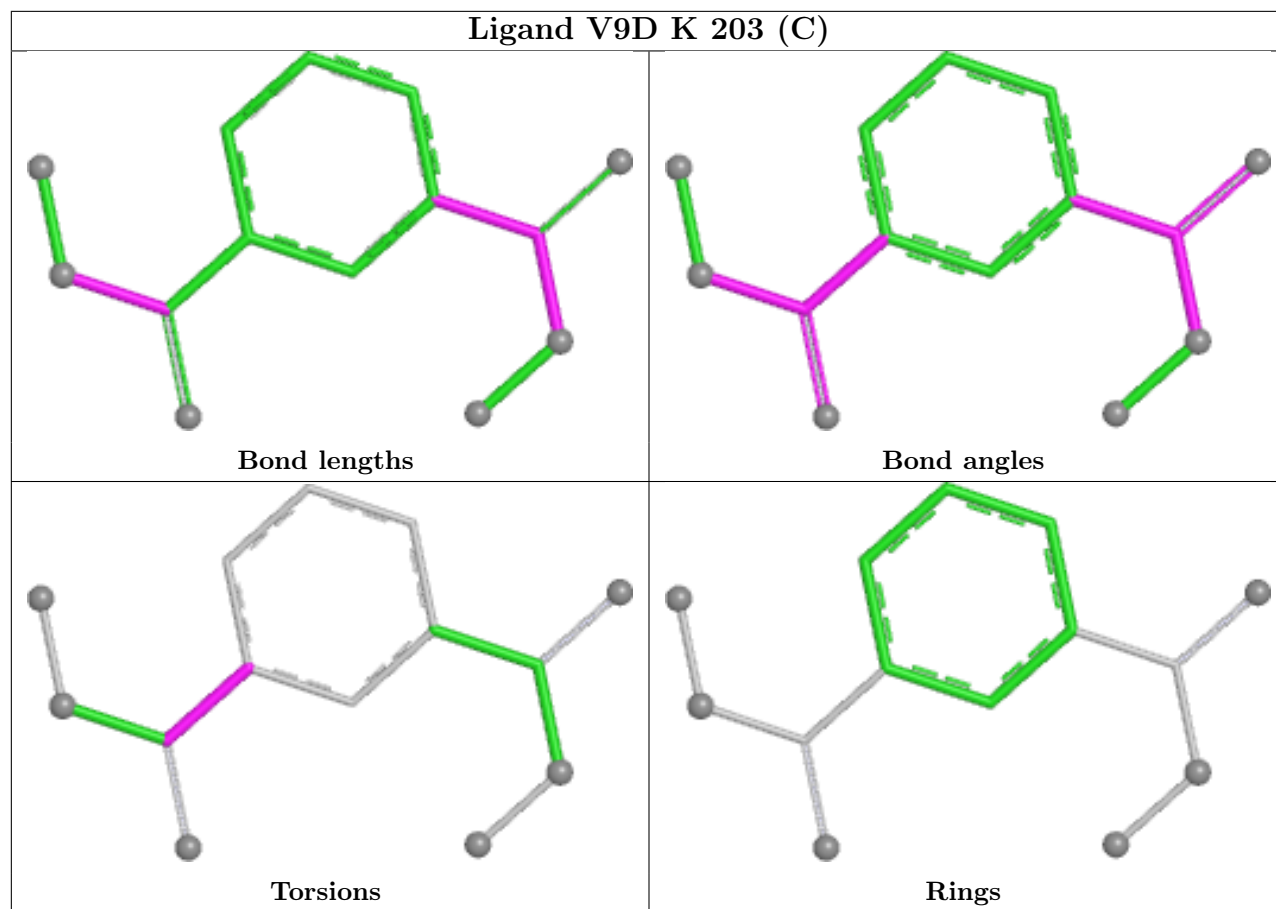


Ligand V9D H 204 (D)

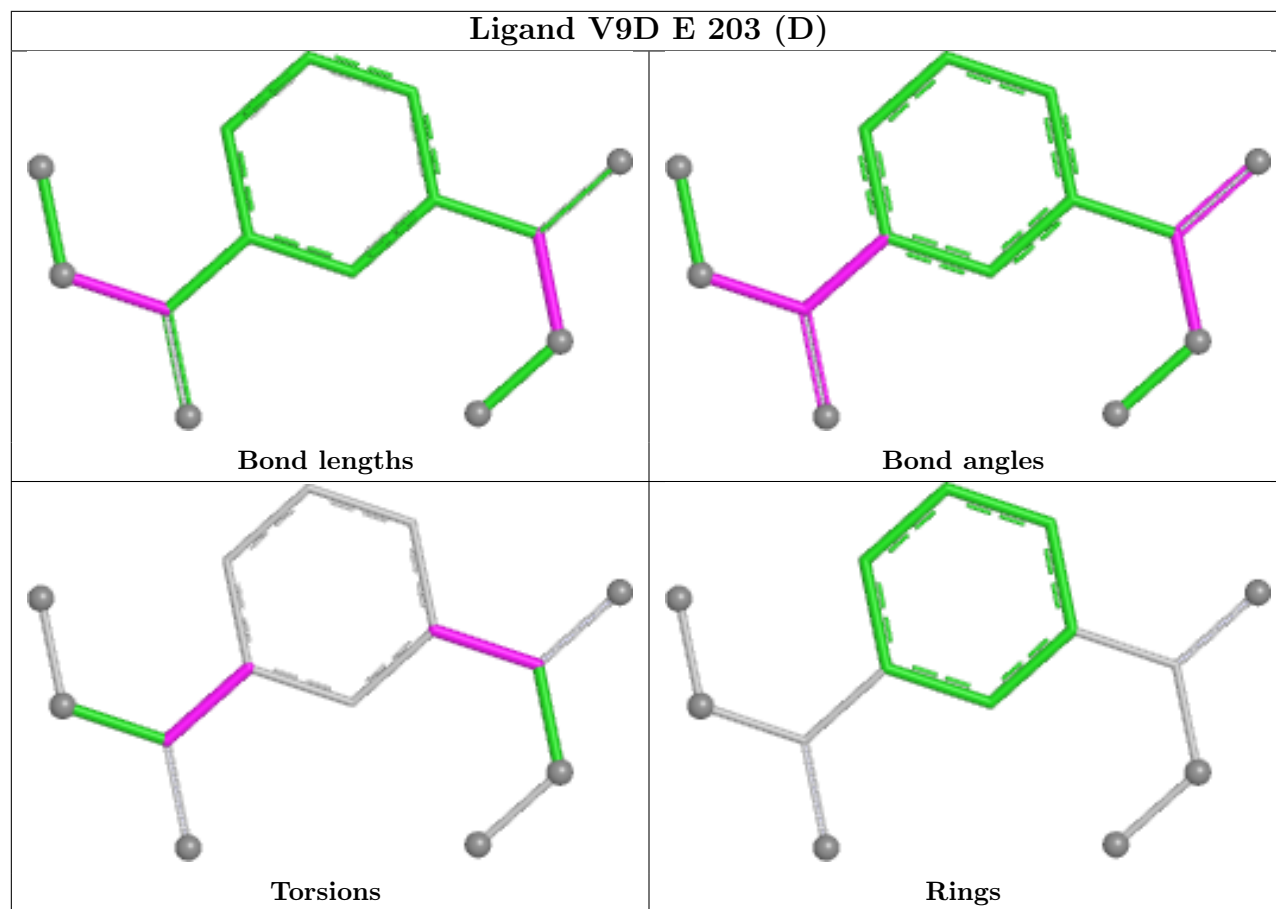


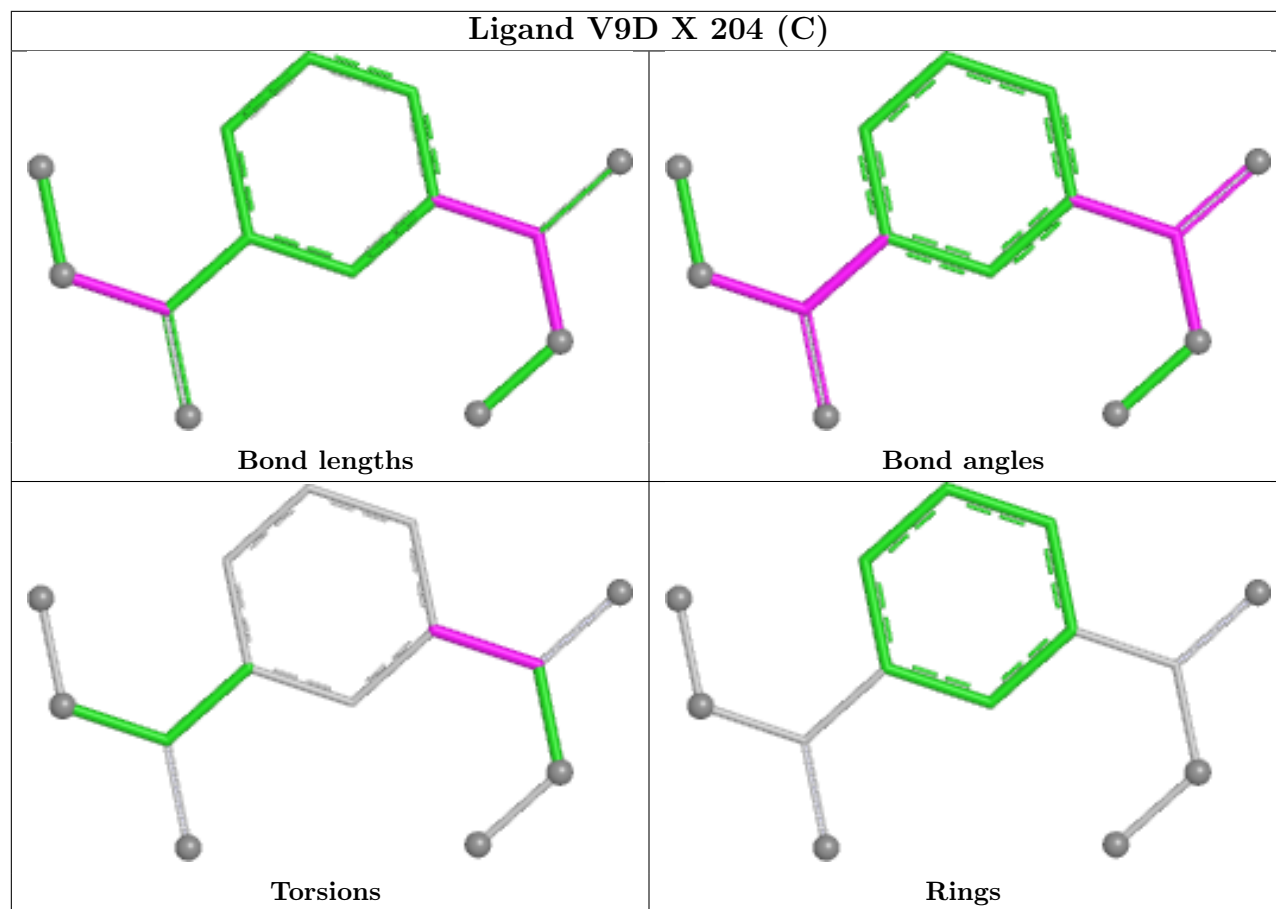


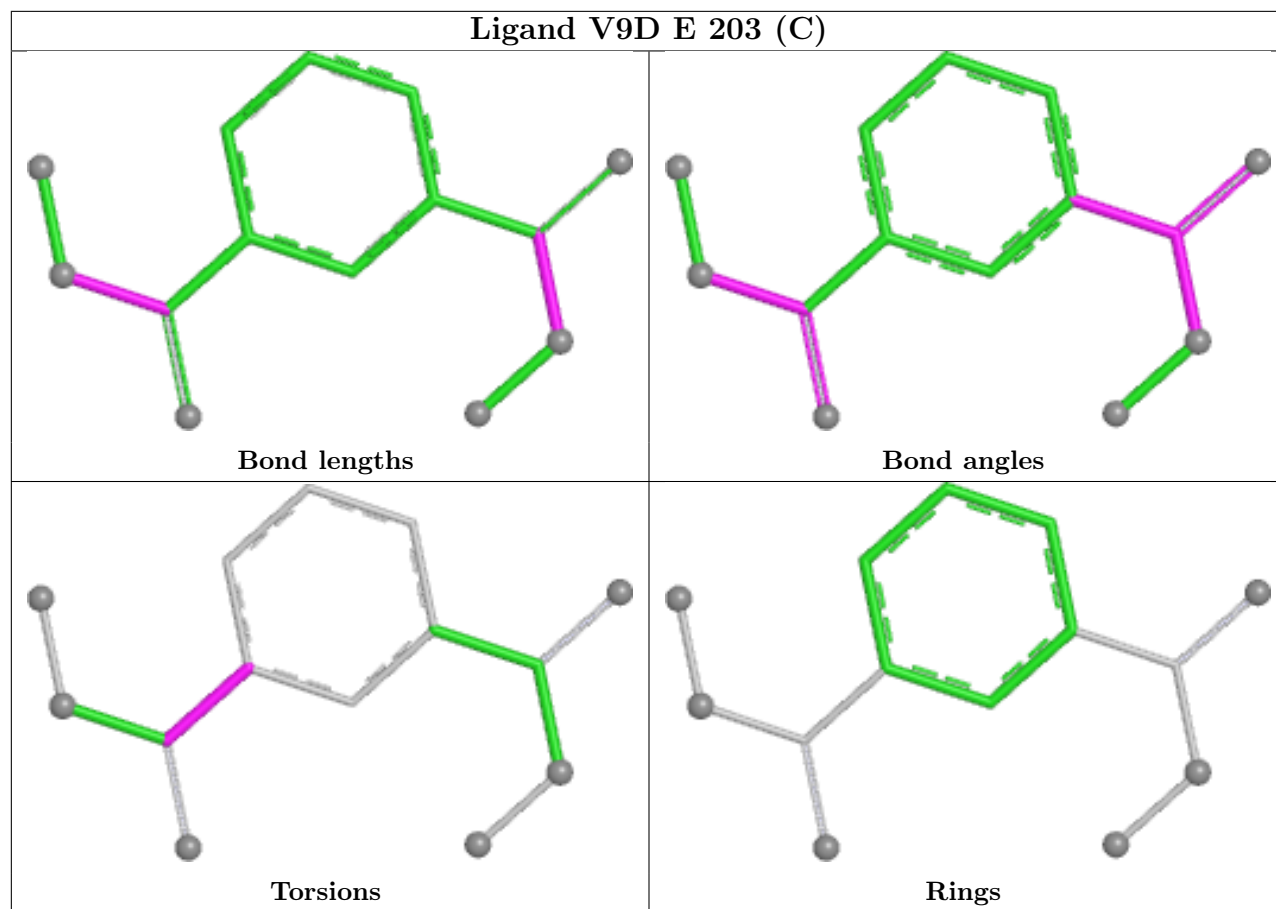




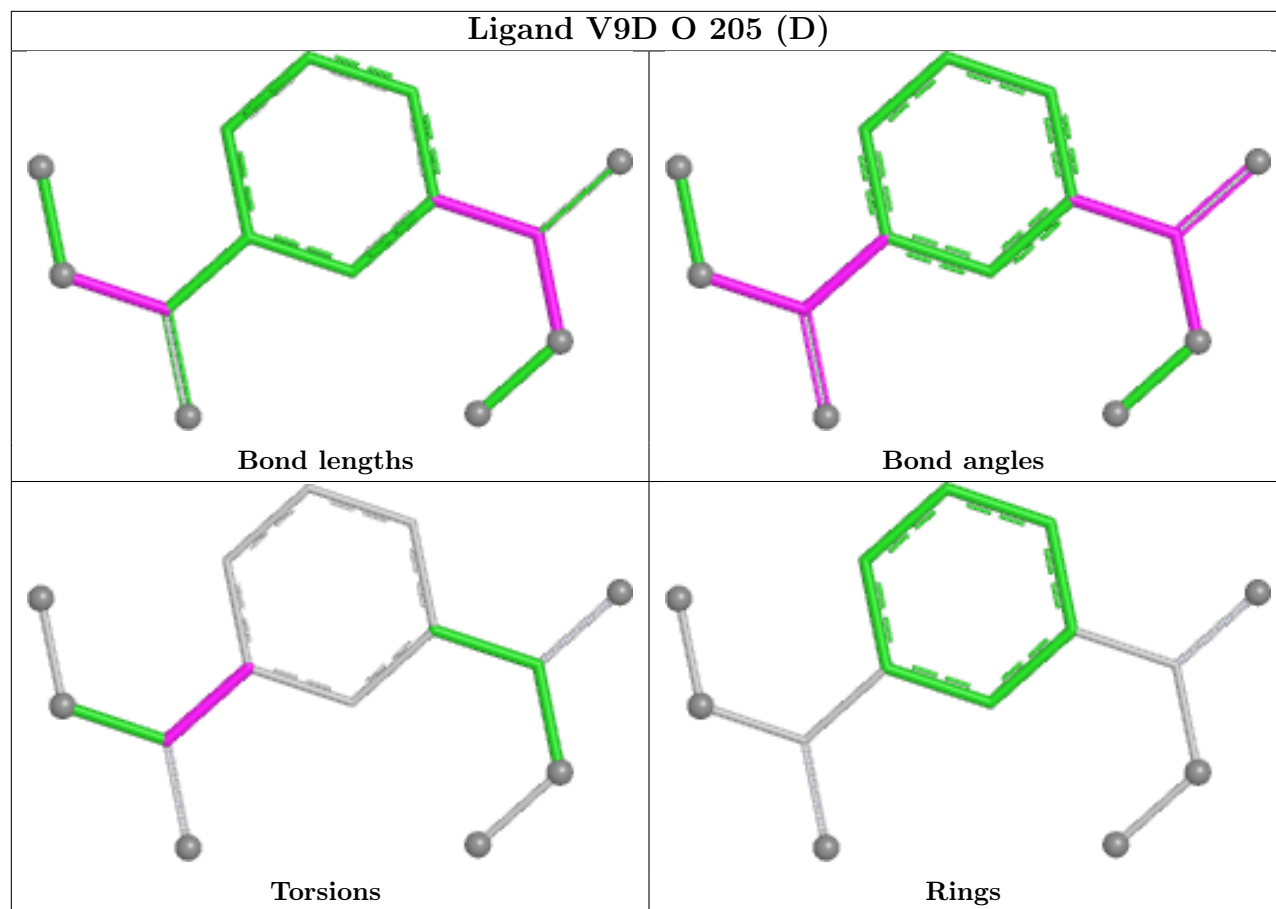
Ligand V9D E 203 (D)

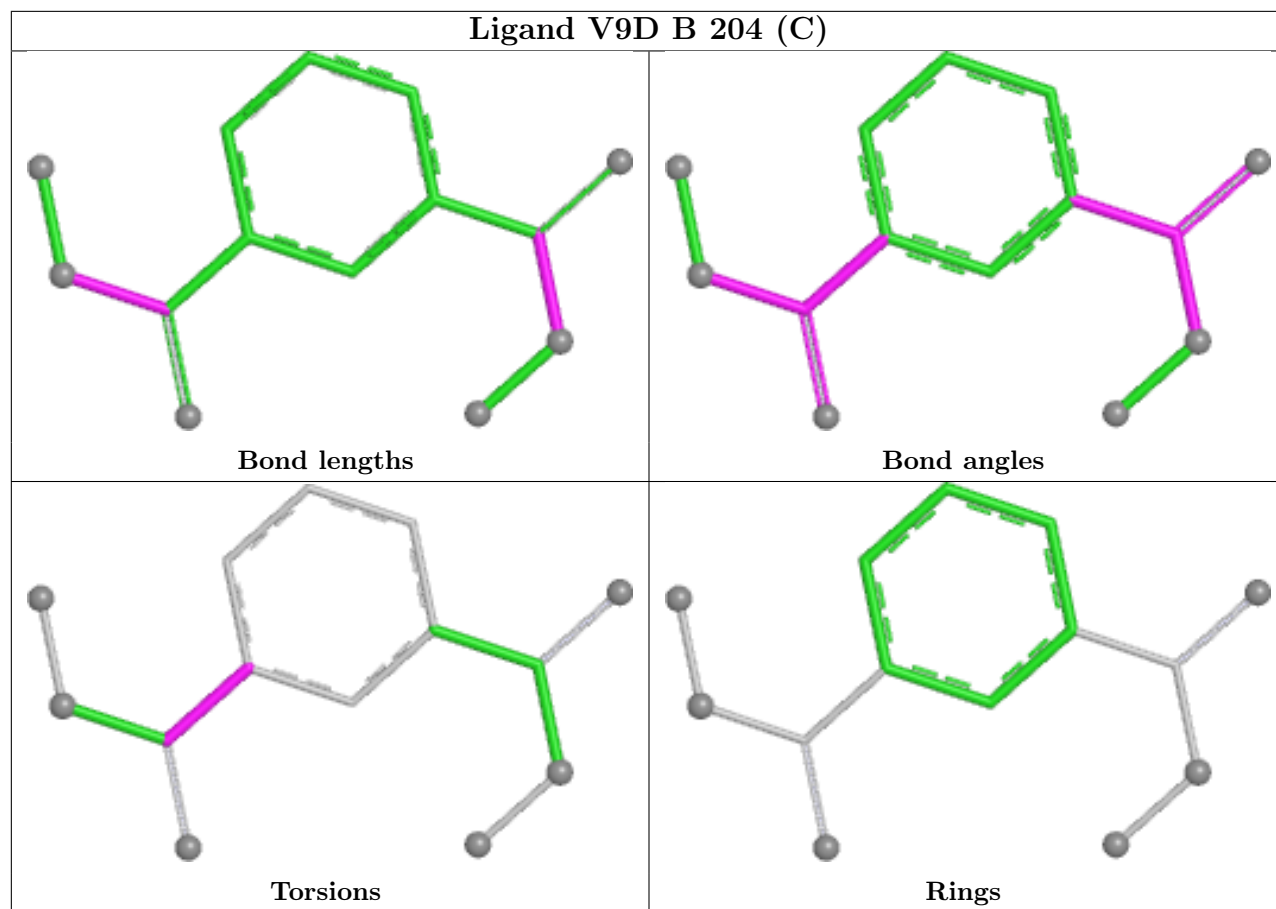






Ligand V9D O 205 (D)





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	174/182 (95%)	-1.34	0 100 100	25, 30, 48, 85	0
1	B	174/182 (95%)	-1.36	0 100 100	16, 29, 46, 84	1 (0%)
1	C	174/182 (95%)	-1.34	0 100 100	15, 31, 48, 80	1 (0%)
1	D	174/182 (95%)	-1.37	0 100 100	22, 27, 44, 78	0
1	E	174/182 (95%)	-1.38	0 100 100	16, 27, 44, 73	3 (1%)
1	F	174/182 (95%)	-1.39	0 100 100	22, 27, 43, 73	1 (0%)
1	G	174/182 (95%)	-1.38	0 100 100	16, 28, 44, 75	1 (0%)
1	H	174/182 (95%)	-1.37	0 100 100	19, 27, 45, 79	1 (0%)
1	I	174/182 (95%)	-1.37	0 100 100	19, 26, 43, 75	1 (0%)
1	J	174/182 (95%)	-1.33	0 100 100	22, 30, 48, 79	1 (0%)
1	K	174/182 (95%)	-1.38	0 100 100	23, 29, 48, 85	0
1	L	174/182 (95%)	-1.34	0 100 100	24, 30, 47, 80	0
1	M	174/182 (95%)	-1.33	0 100 100	25, 30, 47, 80	0
1	N	174/182 (95%)	-1.36	0 100 100	20, 29, 48, 82	1 (0%)
1	O	174/182 (95%)	-1.35	0 100 100	16, 30, 47, 83	1 (0%)
1	P	174/182 (95%)	-1.37	0 100 100	16, 27, 45, 73	1 (0%)
1	Q	174/182 (95%)	-1.36	0 100 100	16, 26, 44, 73	2 (1%)
1	R	174/182 (95%)	-1.38	0 100 100	21, 26, 42, 72	0
1	S	174/182 (95%)	-1.37	0 100 100	16, 27, 43, 80	1 (0%)
1	T	174/182 (95%)	-1.36	0 100 100	19, 27, 45, 75	1 (0%)
1	U	174/182 (95%)	-1.39	0 100 100	18, 26, 44, 71	2 (1%)
1	V	174/182 (95%)	-1.37	0 100 100	25, 30, 48, 78	0
1	W	174/182 (95%)	-1.35	0 100 100	15, 29, 47, 82	3 (1%)
1	X	174/182 (95%)	-1.34	0 100 100	14, 30, 47, 80	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	a	174/182 (95%)	-0.69	1 (0%) 85 88	12, 13, 18, 29	174 (100%)
1	b	174/182 (95%)	-0.82	0 100 100	11, 13, 18, 29	174 (100%)
1	c	174/182 (95%)	-0.76	0 100 100	12, 14, 19, 26	174 (100%)
1	d	174/182 (95%)	-0.71	1 (0%) 85 88	11, 13, 18, 28	174 (100%)
1	e	174/182 (95%)	-0.69	1 (0%) 85 88	12, 13, 18, 30	174 (100%)
1	f	174/182 (95%)	-0.74	0 100 100	12, 14, 19, 28	174 (100%)
1	g	174/182 (95%)	-0.69	1 (0%) 85 88	11, 13, 17, 26	174 (100%)
1	h	174/182 (95%)	-0.66	2 (1%) 78 80	12, 13, 18, 28	174 (100%)
1	i	174/182 (95%)	-0.76	1 (0%) 85 88	12, 14, 19, 27	174 (100%)
1	j	174/182 (95%)	-0.71	3 (1%) 69 71	12, 13, 18, 29	174 (100%)
1	k	174/182 (95%)	-0.74	0 100 100	12, 13, 17, 28	174 (100%)
1	l	174/182 (95%)	-0.79	0 100 100	11, 14, 18, 26	174 (100%)
1	m	174/182 (95%)	-0.68	0 100 100	12, 14, 19, 27	174 (100%)
1	n	174/182 (95%)	-0.66	2 (1%) 78 80	11, 13, 18, 28	174 (100%)
1	o	174/182 (95%)	-0.68	1 (0%) 85 88	11, 13, 18, 28	174 (100%)
1	p	174/182 (95%)	-0.67	2 (1%) 78 80	11, 14, 19, 29	174 (100%)
1	q	174/182 (95%)	-0.74	2 (1%) 78 80	11, 13, 17, 28	174 (100%)
1	r	174/182 (95%)	-0.71	1 (0%) 85 88	12, 13, 18, 28	174 (100%)
1	s	174/182 (95%)	-0.68	1 (0%) 85 88	12, 13, 19, 27	174 (100%)
1	t	174/182 (95%)	-0.73	1 (0%) 85 88	11, 13, 18, 28	174 (100%)
1	u	174/182 (95%)	-0.73	1 (0%) 85 88	12, 13, 18, 29	174 (100%)
1	v	174/182 (95%)	-0.69	3 (1%) 69 71	12, 14, 18, 26	174 (100%)
1	w	174/182 (95%)	-0.59	2 (1%) 78 80	12, 13, 18, 29	174 (100%)
1	x	174/182 (95%)	-0.68	1 (0%) 85 88	11, 13, 17, 27	174 (100%)
All	All	8352/8736 (95%)	-1.04	27 (0%) 90 92	11, 23, 41, 85	4199 (50%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	n	165[C]	LEU	4.7
1	p	133[C]	ILE	3.5
1	s	133[C]	ILE	3.3
1	w	177[C]	ASP	3.2
1	q	177[C]	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	w	165[C]	LEU	3.1
1	h	129[C]	LEU	2.9
1	r	177[C]	ASP	2.9
1	a	177[C]	ASP	2.9
1	v	66[C]	ALA	2.9
1	u	177[C]	ASP	2.7
1	e	177[C]	ASP	2.7
1	g	35[C]	LEU	2.5
1	j	177[C]	ASP	2.5
1	n	177[C]	ASP	2.4
1	i	4[C]	SER	2.3
1	d	35[C]	LEU	2.3
1	v	133[C]	ILE	2.3
1	v	110[C]	VAL	2.3
1	p	110[C]	VAL	2.2
1	h	177[C]	ASP	2.2
1	t	177[C]	ASP	2.2
1	x	4[C]	SER	2.2
1	j	35[C]	LEU	2.1
1	j	28[C]	LEU	2.0
1	o	4[C]	SER	2.0
1	q	96[C]	GLY	2.0

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

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

6.3 Carbohydrates [\(i\)](#)

There are no oligosaccharides in this entry.

6.4 Ligands [\(i\)](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NA	a	204[C]	1/1	0.97	0.09	36,36,36,36	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	a	204[D]	1/1	0.97	0.09	27,27,27,27	1
4	V9D	B	204[C]	14/14	0.97	0.07	40,45,51,55	14
4	V9D	B	204[D]	14/14	0.97	0.07	37,42,54,54	14
4	V9D	H	204[C]	14/14	0.97	0.06	41,45,50,56	14
4	V9D	H	204[D]	14/14	0.97	0.06	38,41,53,55	14
2	ZN	l	202[D]	1/1	0.98	0.04	45,45,45,45	1
3	NA	d	205[C]	1/1	0.98	0.08	34,34,34,34	1
3	NA	d	205[D]	1/1	0.98	0.08	34,34,34,34	1
3	NA	j	204[C]	1/1	0.98	0.05	33,33,33,33	1
3	NA	j	204[D]	1/1	0.98	0.05	29,29,29,29	1
3	NA	D	204	1/1	0.98	0.14	42,42,42,42	0
3	NA	G	204	1/1	0.98	0.14	42,42,42,42	0
4	V9D	E	203[C]	14/14	0.98	0.06	38,42,50,53	14
4	V9D	E	203[D]	14/14	0.98	0.06	40,44,50,52	14
3	NA	S	204	1/1	0.98	0.13	42,42,42,42	0
2	ZN	l	202[C]	1/1	0.98	0.04	46,46,46,46	1
4	V9D	K	203[C]	14/14	0.98	0.06	40,43,57,58	14
4	V9D	K	203[D]	14/14	0.98	0.06	33,42,57,58	14
4	V9D	O	205[C]	14/14	0.98	0.05	34,41,54,55	14
4	V9D	O	205[D]	14/14	0.98	0.05	38,45,53,56	14
4	V9D	X	204[C]	14/14	0.98	0.06	36,43,54,57	14
4	V9D	X	204[D]	14/14	0.98	0.06	37,45,56,57	14
2	ZN	H	202	1/1	0.99	0.13	101,101,101,101	1
2	ZN	K	202	1/1	0.99	0.04	55,55,55,55	1
2	ZN	m	203[C]	1/1	0.99	0.04	47,47,47,47	1
2	ZN	m	203[D]	1/1	0.99	0.04	45,45,45,45	1
2	ZN	n	201[C]	1/1	0.99	0.02	37,37,37,37	1
2	ZN	n	201[D]	1/1	0.99	0.02	35,35,35,35	1
2	ZN	n	202[C]	1/1	0.99	0.04	47,47,47,47	1
2	ZN	n	202[D]	1/1	0.99	0.04	43,43,43,43	1
2	ZN	o	202[C]	1/1	0.99	0.04	46,46,46,46	1
2	ZN	o	202[D]	1/1	0.99	0.04	39,39,39,39	1
2	ZN	p	201[C]	1/1	0.99	0.02	36,36,36,36	1
2	ZN	p	201[D]	1/1	0.99	0.02	32,32,32,32	1
2	ZN	p	202[C]	1/1	0.99	0.08	47,47,47,47	1
2	ZN	p	202[D]	1/1	0.99	0.08	42,42,42,42	1
2	ZN	q	201[C]	1/1	0.99	0.02	34,34,34,34	1
2	ZN	q	201[D]	1/1	0.99	0.02	34,34,34,34	1
2	ZN	q	203[C]	1/1	0.99	0.07	45,45,45,45	1
2	ZN	q	203[D]	1/1	0.99	0.07	42,42,42,42	1
2	ZN	r	202[C]	1/1	0.99	0.03	51,51,51,51	1
2	ZN	r	202[D]	1/1	0.99	0.03	45,45,45,45	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	s	201[C]	1/1	0.99	0.02	37,37,37,37	1
2	ZN	s	201[D]	1/1	0.99	0.02	31,31,31,31	1
2	ZN	s	202[C]	1/1	0.99	0.04	47,47,47,47	1
2	ZN	s	202[D]	1/1	0.99	0.04	39,39,39,39	1
2	ZN	t	203[C]	1/1	0.99	0.07	43,43,43,43	1
2	ZN	t	203[D]	1/1	0.99	0.07	42,42,42,42	1
2	ZN	u	202[C]	1/1	0.99	0.03	49,49,49,49	1
2	ZN	u	202[D]	1/1	0.99	0.03	46,46,46,46	1
2	ZN	v	203[C]	1/1	0.99	0.11	44,44,44,44	1
2	ZN	v	203[D]	1/1	0.99	0.11	46,46,46,46	1
2	ZN	v	204[C]	1/1	0.99	0.07	48,48,48,48	1
2	ZN	v	204[D]	1/1	0.99	0.07	44,44,44,44	1
2	ZN	w	202[C]	1/1	0.99	0.19	45,45,45,45	1
2	ZN	w	202[D]	1/1	0.99	0.19	44,44,44,44	1
2	ZN	w	203[C]	1/1	0.99	0.05	47,47,47,47	1
2	ZN	w	203[D]	1/1	0.99	0.05	47,47,47,47	1
2	ZN	x	202[C]	1/1	0.99	0.15	46,46,46,46	1
2	ZN	x	202[D]	1/1	0.99	0.15	48,48,48,48	1
2	ZN	x	203[C]	1/1	0.99	0.07	47,47,47,47	1
2	ZN	x	203[D]	1/1	0.99	0.07	43,43,43,43	1
3	NA	A	205	1/1	0.99	0.08	42,42,42,42	0
2	ZN	O	203	1/1	0.99	0.14	94,94,94,94	1
2	ZN	a	203[C]	1/1	0.99	0.04	45,45,45,45	1
3	NA	J	204	1/1	0.99	0.07	42,42,42,42	0
3	NA	M	203	1/1	0.99	0.10	39,39,39,39	0
3	NA	P	204	1/1	0.99	0.11	41,41,41,41	0
2	ZN	a	203[D]	1/1	0.99	0.04	49,49,49,49	1
2	ZN	c	202[C]	1/1	0.99	0.04	41,41,41,41	1
2	ZN	c	202[D]	1/1	0.99	0.04	47,47,47,47	1
2	ZN	d	203[C]	1/1	0.99	0.15	48,48,48,48	1
2	ZN	d	203[D]	1/1	0.99	0.15	48,48,48,48	1
3	NA	g	204[C]	1/1	0.99	0.05	33,33,33,33	1
3	NA	g	204[D]	1/1	0.99	0.05	33,33,33,33	1
2	ZN	d	204[C]	1/1	0.99	0.06	41,41,41,41	1
2	ZN	d	204[D]	1/1	0.99	0.06	43,43,43,43	1
3	NA	m	204[C]	1/1	0.99	0.04	32,32,32,32	1
3	NA	m	204[D]	1/1	0.99	0.04	35,35,35,35	1
3	NA	v	205[C]	1/1	0.99	0.06	31,31,31,31	1
3	NA	v	205[D]	1/1	0.99	0.06	31,31,31,31	1
2	ZN	e	202[C]	1/1	0.99	0.23	46,46,46,46	1
2	ZN	e	202[D]	1/1	0.99	0.23	47,47,47,47	1
2	ZN	f	202[C]	1/1	0.99	0.13	45,45,45,45	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	f	202[D]	1/1	0.99	0.13	49,49,49,49	1
2	ZN	g	203[C]	1/1	0.99	0.03	45,45,45,45	1
2	ZN	g	203[D]	1/1	0.99	0.03	43,43,43,43	1
2	ZN	i	202[C]	1/1	0.99	0.07	46,46,46,46	1
2	ZN	i	202[D]	1/1	0.99	0.07	46,46,46,46	1
2	ZN	j	203[C]	1/1	0.99	0.02	47,47,47,47	1
2	ZN	j	203[D]	1/1	0.99	0.02	46,46,46,46	1
4	V9D	Q	203[C]	14/14	0.99	0.05	38,44,51,55	14
4	V9D	Q	203[D]	14/14	0.99	0.05	37,44,51,56	14
4	V9D	T	203[C]	14/14	0.99	0.06	38,43,51,51	14
4	V9D	T	203[D]	14/14	0.99	0.06	43,45,52,54	14
2	ZN	k	202[C]	1/1	0.99	0.02	40,40,40,40	1
2	ZN	k	202[D]	1/1	0.99	0.02	47,47,47,47	1
2	ZN	g	202[C]	1/1	1.00	0.01	31,31,31,31	1
2	ZN	g	202[D]	1/1	1.00	0.01	32,32,32,32	1
2	ZN	F	201	1/1	1.00	0.01	37,37,37,37	0
2	ZN	F	202	1/1	1.00	0.13	77,77,77,77	1
2	ZN	h	201[C]	1/1	1.00	0.01	35,35,35,35	1
2	ZN	h	201[D]	1/1	1.00	0.01	35,35,35,35	1
2	ZN	h	202[C]	1/1	1.00	0.03	46,46,46,46	1
2	ZN	h	202[D]	1/1	1.00	0.03	49,49,49,49	1
2	ZN	i	201[C]	1/1	1.00	0.02	33,33,33,33	1
2	ZN	i	201[D]	1/1	1.00	0.02	36,36,36,36	1
2	ZN	F	203	1/1	1.00	0.03	49,49,49,49	1
2	ZN	G	201	1/1	1.00	0.01	36,36,36,36	0
2	ZN	j	201[C]	1/1	1.00	0.01	34,34,34,34	1
2	ZN	j	201[D]	1/1	1.00	0.01	38,38,38,38	1
2	ZN	j	202[C]	1/1	1.00	0.01	30,30,30,30	1
2	ZN	j	202[D]	1/1	1.00	0.01	33,33,33,33	1
2	ZN	G	202	1/1	1.00	0.01	37,37,37,37	0
2	ZN	G	203	1/1	1.00	0.03	53,53,53,53	1
2	ZN	k	201[C]	1/1	1.00	0.01	35,35,35,35	1
2	ZN	k	201[D]	1/1	1.00	0.01	35,35,35,35	1
2	ZN	H	201	1/1	1.00	0.01	33,33,33,33	0
2	ZN	A	201	1/1	1.00	0.01	38,38,38,38	0
2	ZN	l	201[C]	1/1	1.00	0.02	32,32,32,32	1
2	ZN	l	201[D]	1/1	1.00	0.02	39,39,39,39	1
2	ZN	H	203	1/1	1.00	0.02	51,51,51,51	1
2	ZN	I	201	1/1	1.00	0.01	32,32,32,32	0
2	ZN	m	201[C]	1/1	1.00	0.03	37,37,37,37	1
2	ZN	m	201[D]	1/1	1.00	0.03	31,31,31,31	1
2	ZN	m	202[C]	1/1	1.00	0.01	34,34,34,34	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	m	202[D]	1/1	1.00	0.01	31,31,31,31	1
2	ZN	I	202	1/1	1.00	0.03	47,47,47,47	1
2	ZN	J	201	1/1	1.00	0.01	37,37,37,37	0
2	ZN	J	202	1/1	1.00	0.01	40,40,40,40	0
2	ZN	J	203	1/1	1.00	0.02	61,61,61,61	1
2	ZN	K	201	1/1	1.00	0.01	36,36,36,36	0
2	ZN	A	202	1/1	1.00	0.01	38,38,38,38	0
2	ZN	o	201[C]	1/1	1.00	0.02	33,33,33,33	1
2	ZN	o	201[D]	1/1	1.00	0.02	35,35,35,35	1
2	ZN	L	201	1/1	1.00	0.01	40,40,40,40	0
2	ZN	L	202	1/1	1.00	0.02	54,54,54,54	1
2	ZN	M	201	1/1	1.00	0.01	40,40,40,40	0
2	ZN	M	202	1/1	1.00	0.02	53,53,53,53	1
2	ZN	N	201	1/1	1.00	0.02	37,37,37,37	0
2	ZN	N	202	1/1	1.00	0.03	53,53,53,53	1
2	ZN	O	201	1/1	1.00	0.01	40,40,40,40	0
2	ZN	O	202	1/1	1.00	0.01	38,38,38,38	0
2	ZN	q	202[C]	1/1	1.00	0.01	30,30,30,30	1
2	ZN	q	202[D]	1/1	1.00	0.01	32,32,32,32	1
2	ZN	A	203	1/1	1.00	0.04	69,69,69,69	1
2	ZN	O	204	1/1	1.00	0.03	55,55,55,55	1
2	ZN	r	201[C]	1/1	1.00	0.01	36,36,36,36	1
2	ZN	r	201[D]	1/1	1.00	0.01	37,37,37,37	1
2	ZN	P	201	1/1	1.00	0.01	35,35,35,35	0
2	ZN	P	202	1/1	1.00	0.01	36,36,36,36	0
2	ZN	P	203	1/1	1.00	0.03	54,54,54,54	1
2	ZN	Q	201	1/1	1.00	0.01	36,36,36,36	0
2	ZN	Q	202	1/1	1.00	0.02	48,48,48,48	1
2	ZN	R	201	1/1	1.00	0.01	35,35,35,35	0
2	ZN	t	201[C]	1/1	1.00	0.02	35,35,35,35	1
2	ZN	t	201[D]	1/1	1.00	0.02	32,32,32,32	1
2	ZN	t	202[C]	1/1	1.00	0.01	31,31,31,31	1
2	ZN	t	202[D]	1/1	1.00	0.01	32,32,32,32	1
2	ZN	R	202	1/1	1.00	0.02	52,52,52,52	1
2	ZN	S	201	1/1	1.00	0.01	36,36,36,36	0
2	ZN	u	201[C]	1/1	1.00	0.02	36,36,36,36	1
2	ZN	u	201[D]	1/1	1.00	0.02	33,33,33,33	1
2	ZN	S	202	1/1	1.00	0.01	35,35,35,35	0
2	ZN	S	203	1/1	1.00	0.01	54,54,54,54	1
2	ZN	v	201[C]	1/1	1.00	0.02	39,39,39,39	1
2	ZN	v	201[D]	1/1	1.00	0.02	31,31,31,31	1
2	ZN	v	202[C]	1/1	1.00	0.01	34,34,34,34	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	v	202[D]	1/1	1.00	0.01	32,32,32,32	1
2	ZN	T	201	1/1	1.00	0.01	36,36,36,36	0
2	ZN	T	202	1/1	1.00	0.02	54,54,54,54	1
2	ZN	U	201	1/1	1.00	0.01	36,36,36,36	0
2	ZN	U	202	1/1	1.00	0.03	48,48,48,48	1
2	ZN	w	201[C]	1/1	1.00	0.02	36,36,36,36	1
2	ZN	w	201[D]	1/1	1.00	0.02	35,35,35,35	1
2	ZN	V	201	1/1	1.00	0.01	39,39,39,39	0
2	ZN	V	202	1/1	1.00	0.02	54,54,54,54	1
2	ZN	W	201	1/1	1.00	0.01	36,36,36,36	0
2	ZN	W	202	1/1	1.00	0.03	55,55,55,55	1
2	ZN	x	201[C]	1/1	1.00	0.03	33,33,33,33	1
2	ZN	x	201[D]	1/1	1.00	0.03	35,35,35,35	1
2	ZN	X	201	1/1	1.00	0.01	40,40,40,40	0
2	ZN	X	202	1/1	1.00	0.01	38,38,38,38	0
2	ZN	X	203	1/1	1.00	0.03	57,57,57,57	1
2	ZN	a	201[C]	1/1	1.00	0.01	36,36,36,36	1
2	ZN	a	201[D]	1/1	1.00	0.01	35,35,35,35	1
2	ZN	a	202[C]	1/1	1.00	0.01	29,29,29,29	1
2	ZN	a	202[D]	1/1	1.00	0.01	33,33,33,33	1
2	ZN	A	204	1/1	1.00	0.02	55,55,55,55	1
2	ZN	B	201	1/1	1.00	0.01	37,37,37,37	0
2	ZN	b	201[C]	1/1	1.00	0.01	35,35,35,35	1
2	ZN	b	201[D]	1/1	1.00	0.01	34,34,34,34	1
3	NA	V	203	1/1	1.00	0.06	39,39,39,39	0
2	ZN	b	202[C]	1/1	1.00	0.02	41,41,41,41	1
2	ZN	b	202[D]	1/1	1.00	0.02	48,48,48,48	1
2	ZN	c	201[C]	1/1	1.00	0.02	31,31,31,31	1
2	ZN	c	201[D]	1/1	1.00	0.02	38,38,38,38	1
2	ZN	B	202	1/1	1.00	0.15	76,76,76,76	1
2	ZN	B	203	1/1	1.00	0.02	51,51,51,51	1
2	ZN	d	201[C]	1/1	1.00	0.01	32,32,32,32	1
2	ZN	d	201[D]	1/1	1.00	0.01	35,35,35,35	1
2	ZN	d	202[C]	1/1	1.00	0.01	33,33,33,33	1
2	ZN	d	202[D]	1/1	1.00	0.01	34,34,34,34	1
3	NA	p	203[C]	1/1	1.00	0.03	34,34,34,34	1
3	NA	p	203[D]	1/1	1.00	0.03	35,35,35,35	1
3	NA	s	203[C]	1/1	1.00	0.04	34,34,34,34	1
3	NA	s	203[D]	1/1	1.00	0.04	35,35,35,35	1
2	ZN	C	201	1/1	1.00	0.01	40,40,40,40	0
2	ZN	C	202	1/1	1.00	0.12	79,79,79,79	1
2	ZN	C	203	1/1	1.00	0.02	54,54,54,54	1

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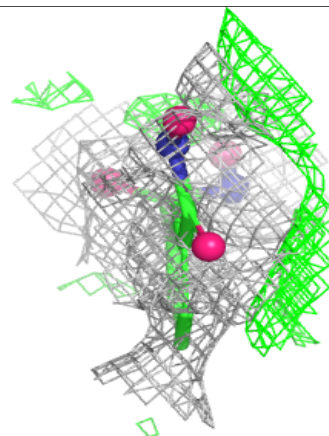
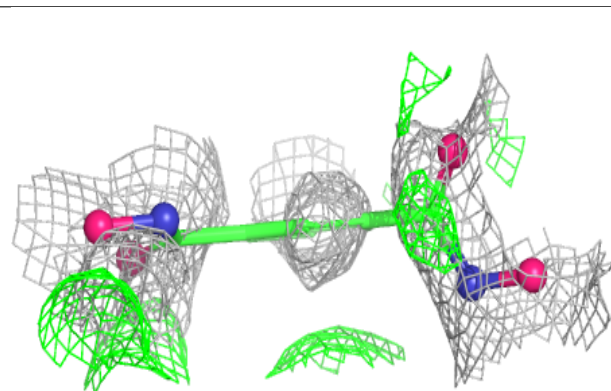
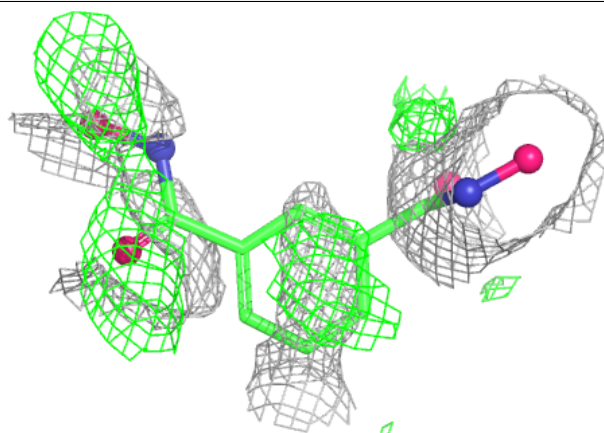
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	D	201	1/1	1.00	0.01	36,36,36,36	0
2	ZN	e	201[C]	1/1	1.00	0.01	34,34,34,34	1
2	ZN	e	201[D]	1/1	1.00	0.01	38,38,38,38	1
2	ZN	D	202	1/1	1.00	0.01	37,37,37,37	0
2	ZN	D	203	1/1	1.00	0.02	53,53,53,53	1
2	ZN	e	203[C]	1/1	1.00	0.02	47,47,47,47	1
2	ZN	e	203[D]	1/1	1.00	0.02	49,49,49,49	1
2	ZN	f	201[C]	1/1	1.00	0.01	33,33,33,33	1
2	ZN	f	201[D]	1/1	1.00	0.01	37,37,37,37	1
2	ZN	E	201	1/1	1.00	0.02	34,34,34,34	0
2	ZN	E	202	1/1	1.00	0.03	53,53,53,53	1
2	ZN	f	203[C]	1/1	1.00	0.06	40,40,40,40	1
2	ZN	f	203[D]	1/1	1.00	0.06	45,45,45,45	1
2	ZN	g	201[C]	1/1	1.00	0.01	31,31,31,31	1
2	ZN	g	201[D]	1/1	1.00	0.01	35,35,35,35	1

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

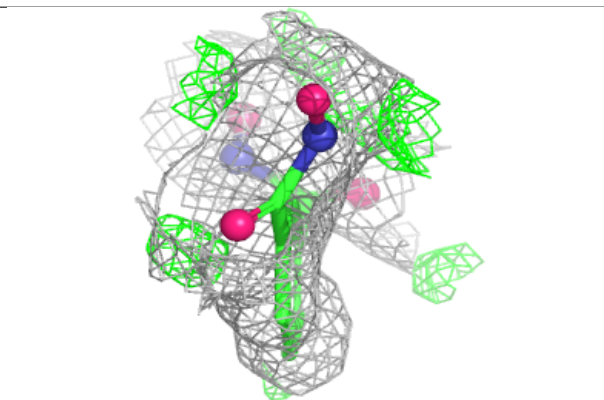
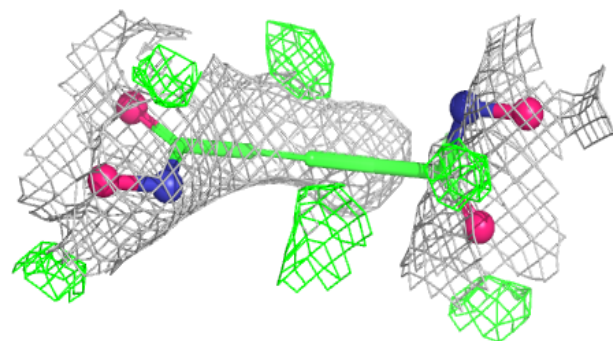
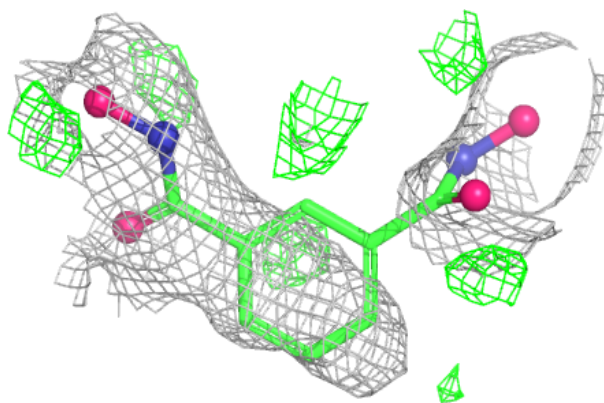
Electron density around V9D B 204 (C):

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

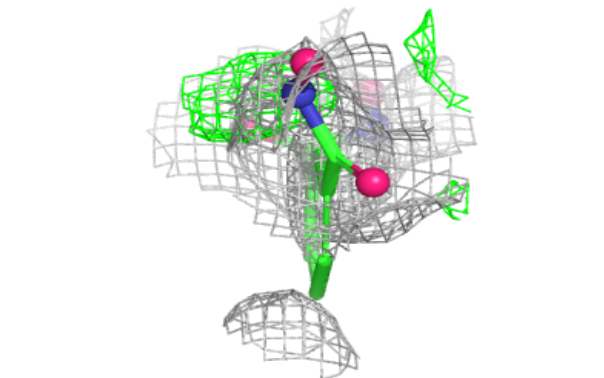
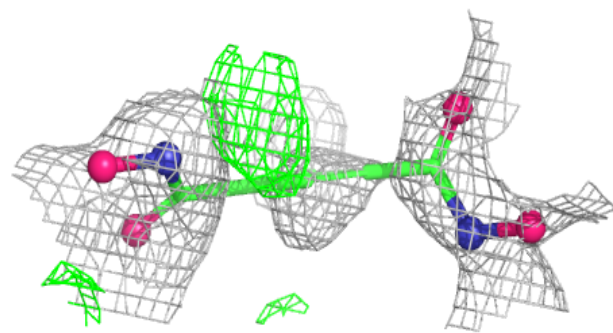
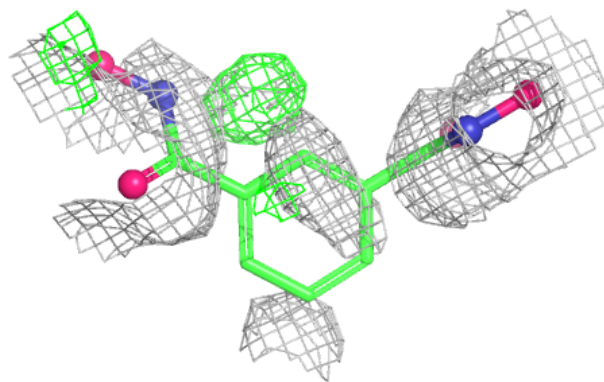


Electron density around V9D B 204 (D):

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

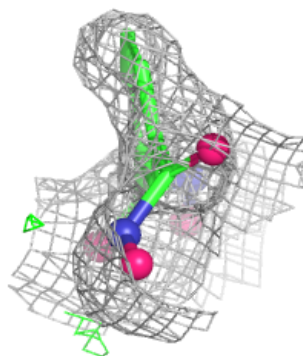
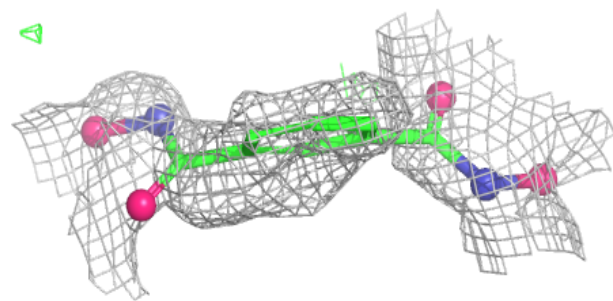
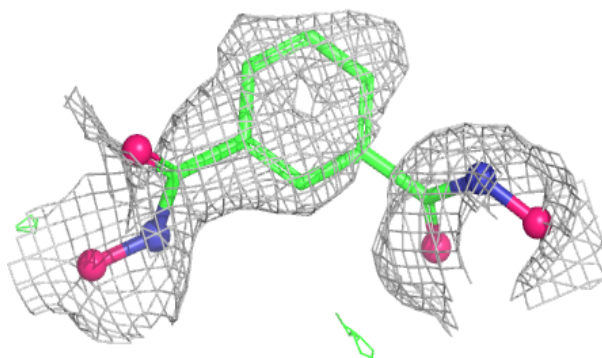
**Electron density around V9D H 204 (C):**

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

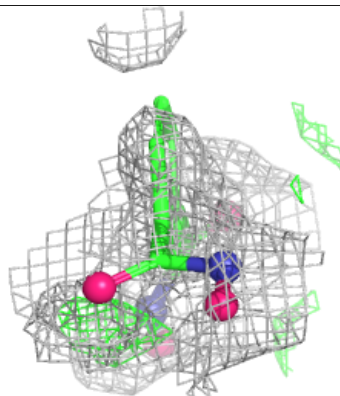
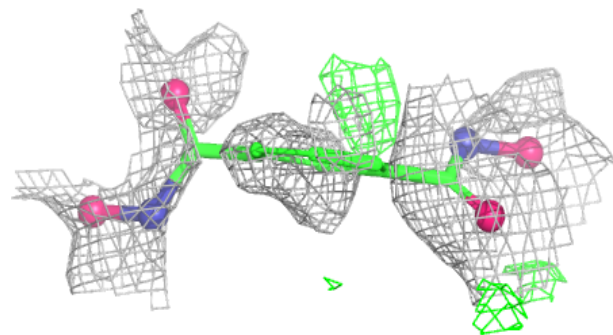
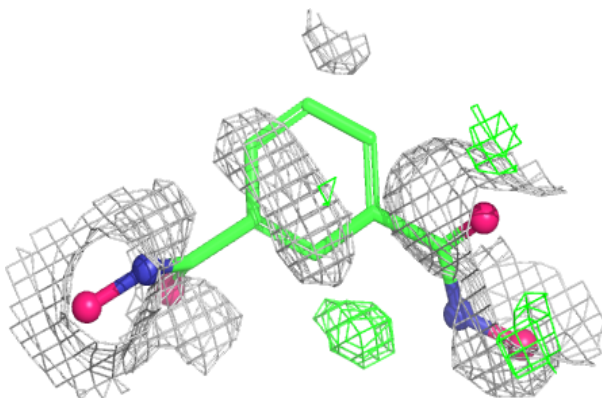


Electron density around V9D H 204 (D):

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

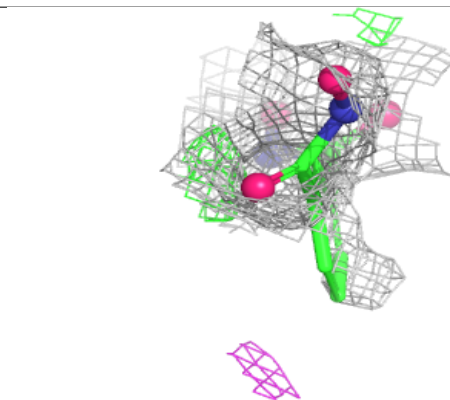
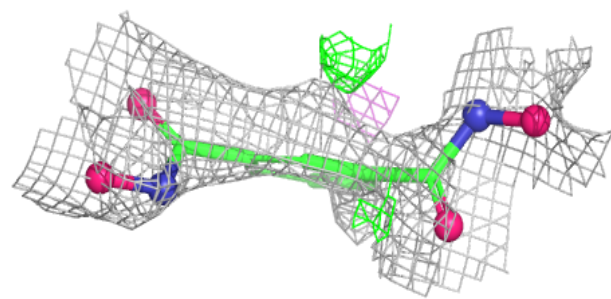
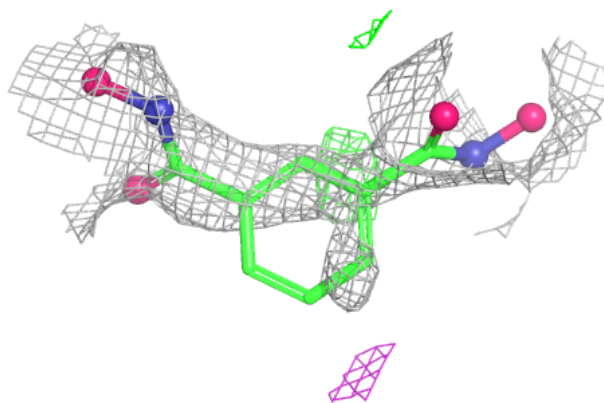
**Electron density around V9D E 203 (C):**

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

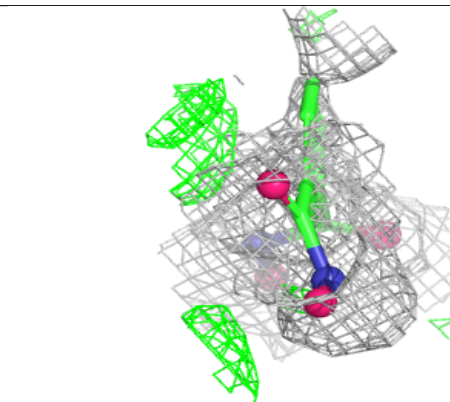
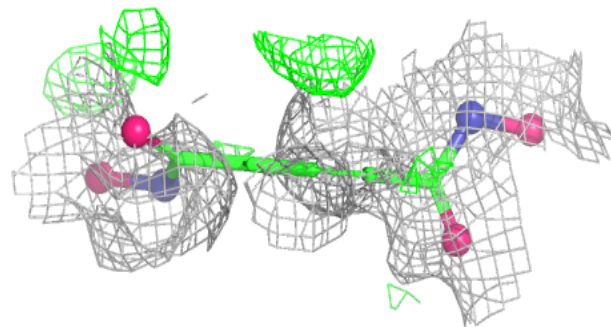
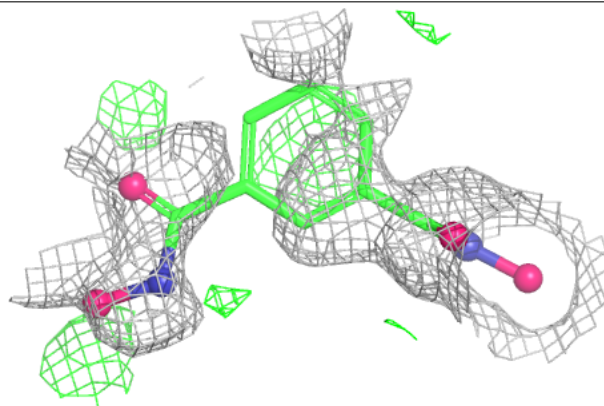


Electron density around V9D E 203 (D):

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

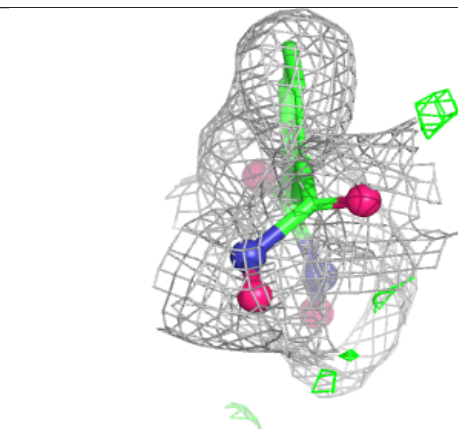
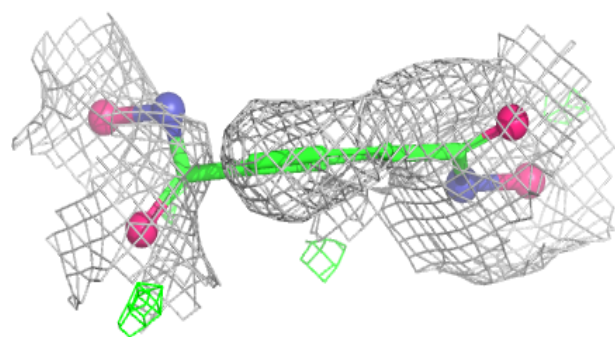
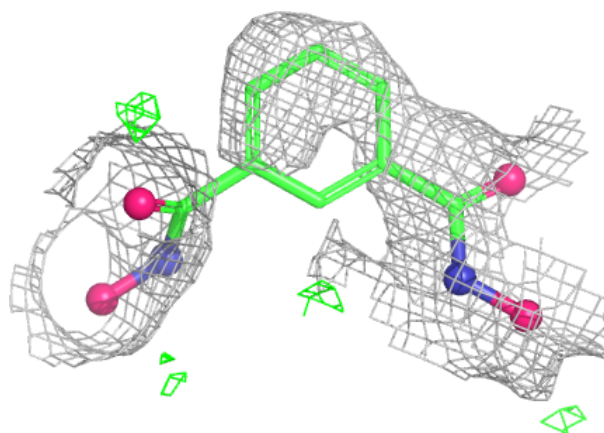
**Electron density around V9D K 203 (C):**

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

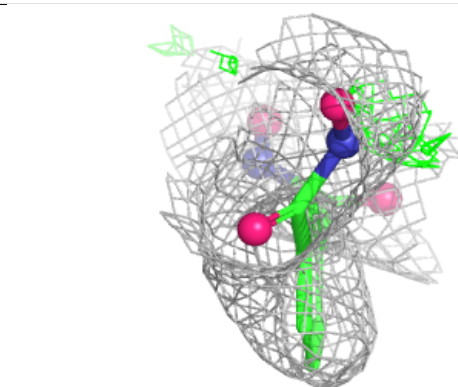
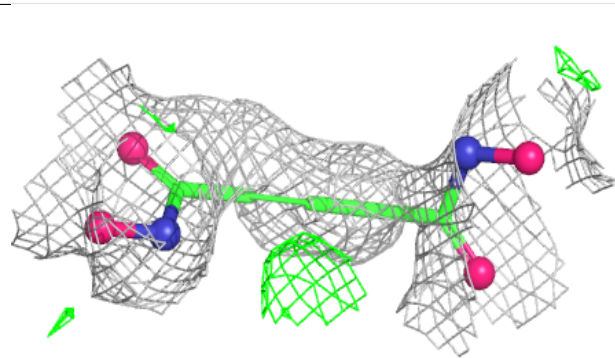
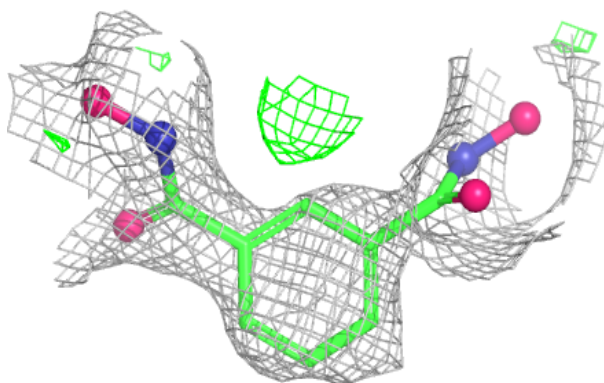


Electron density around V9D K 203 (D):

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

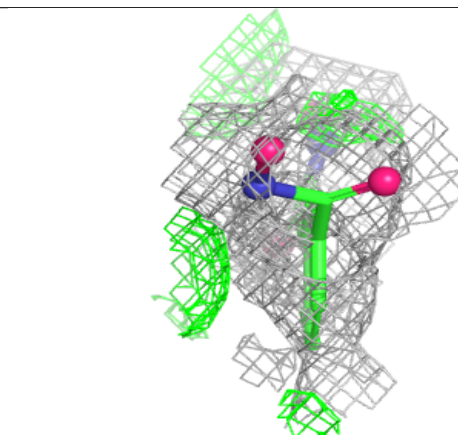
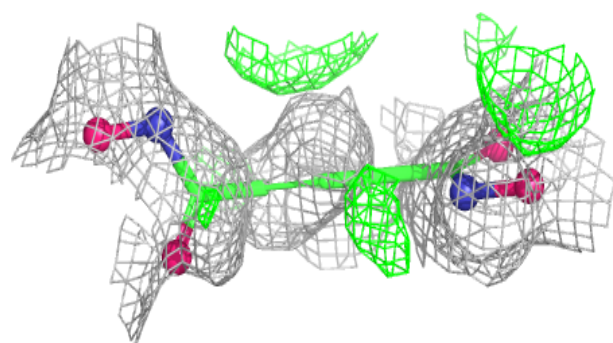
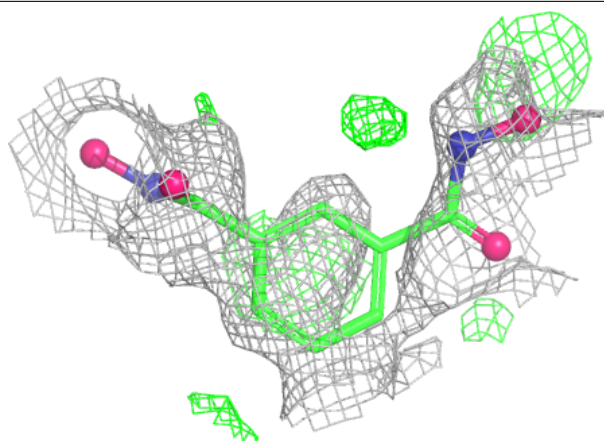
**Electron density around V9D O 205 (C):**

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

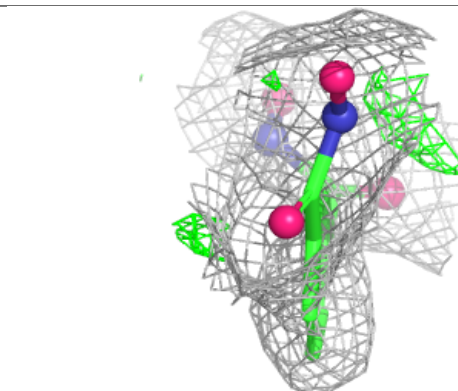
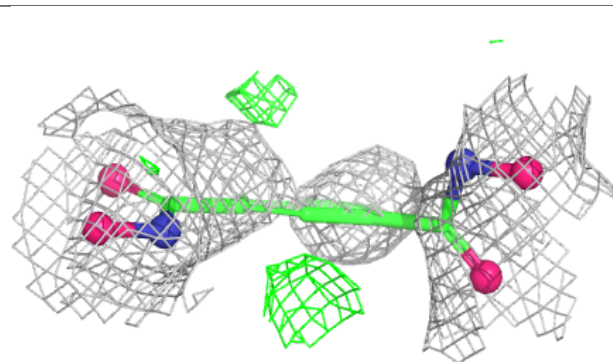
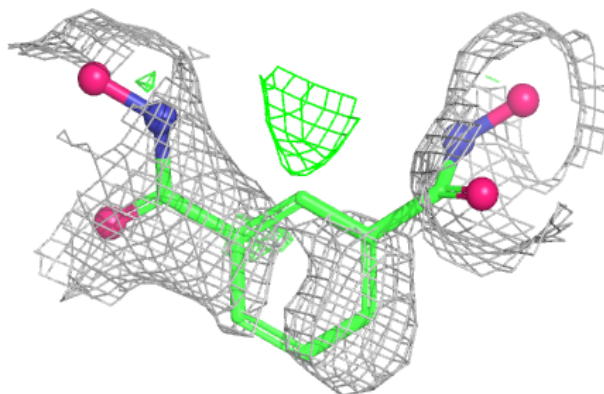


Electron density around V9D O 205 (D):

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

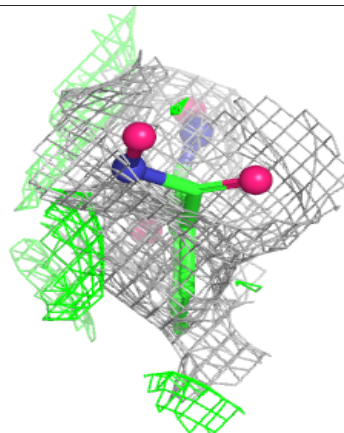
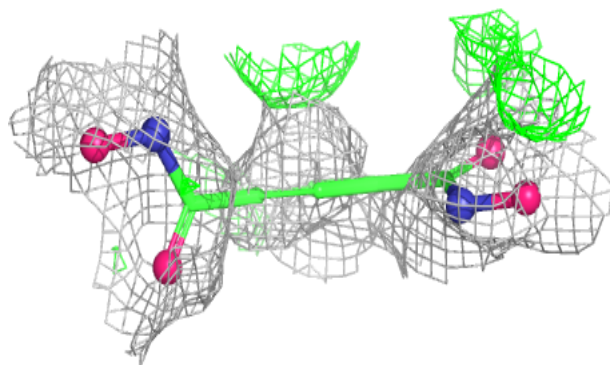
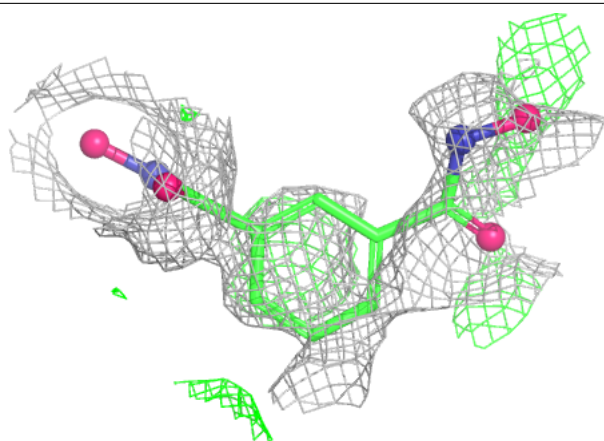
**Electron density around V9D X 204 (C):**

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



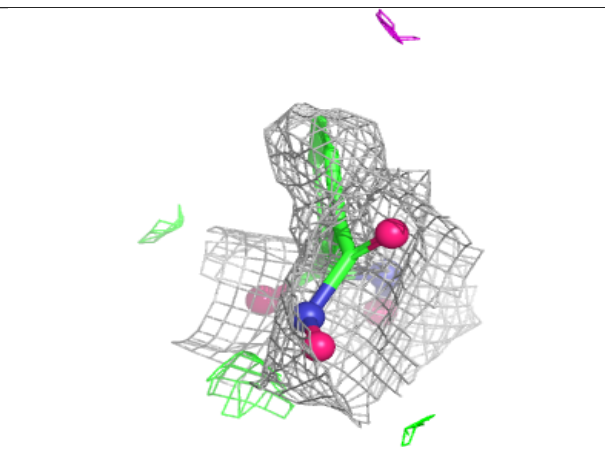
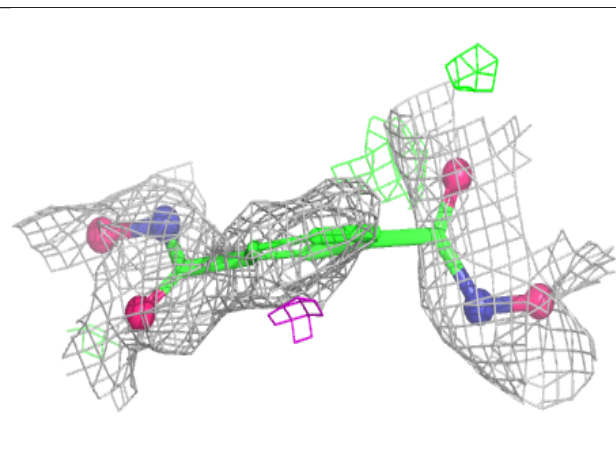
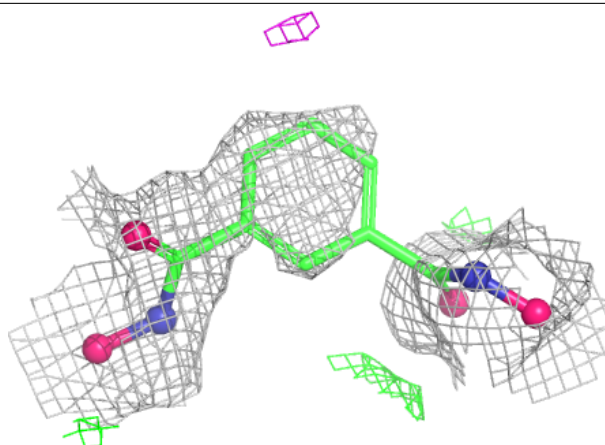
Electron density around V9D X 204 (D):

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

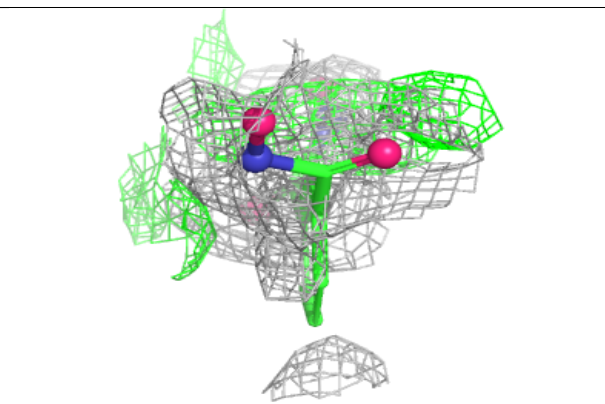
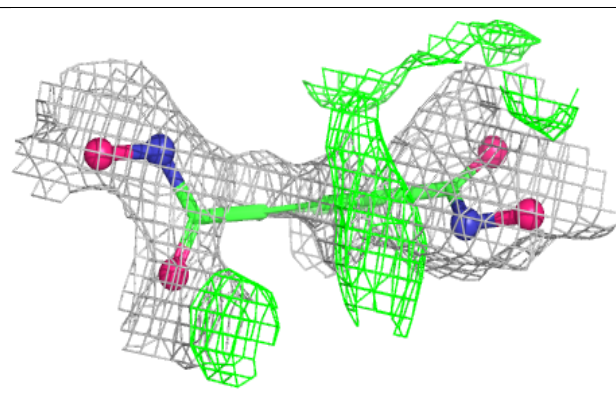
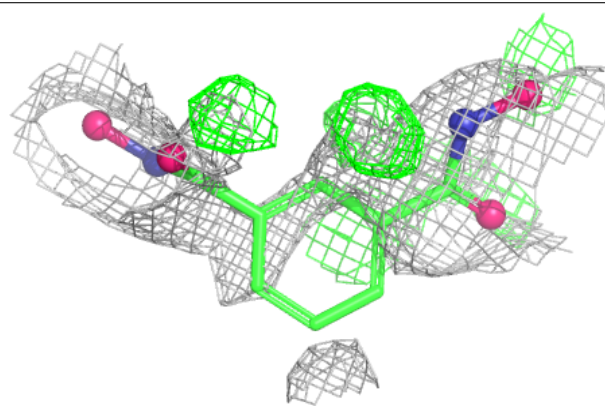


Electron density around V9D Q 203 (C):

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

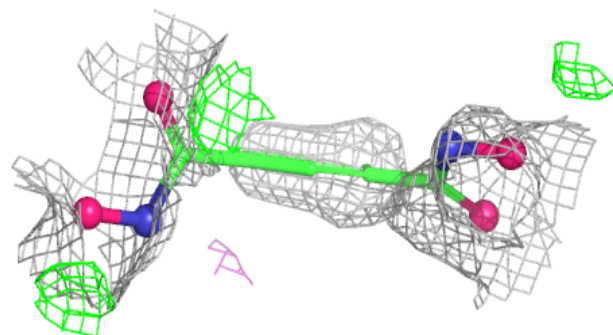
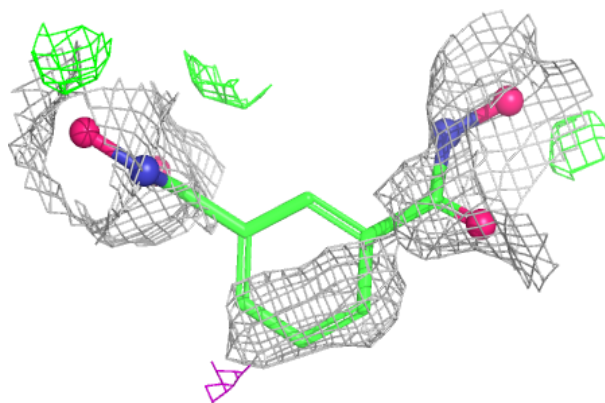
**Electron density around V9D Q 203 (D):**

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

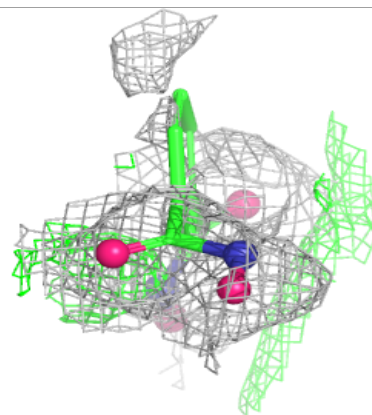
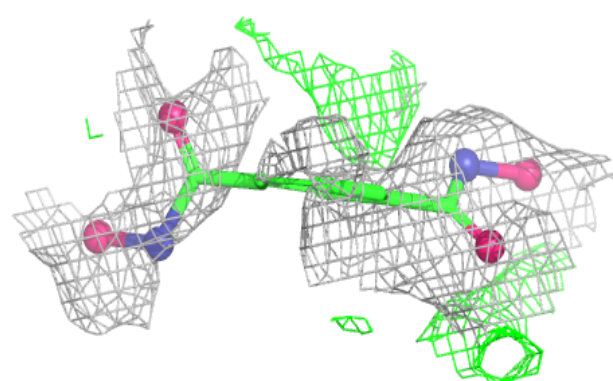
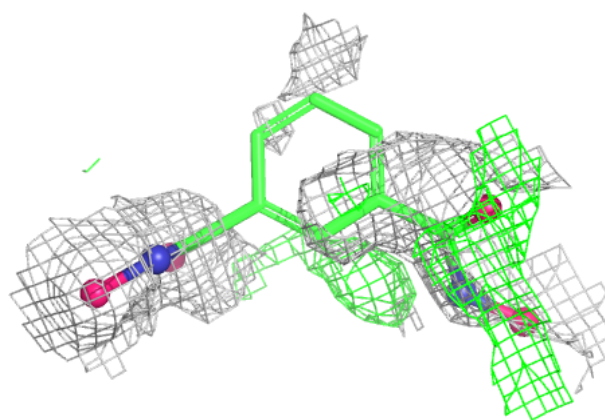


Electron density around V9D T 203 (C):

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.