



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2020 – 11:58 AM BST

PDB ID : 4J9A  
Title : Engineered Digoxigenin binder DIG10.3  
Authors : Stoddard, B.L.; Doyle, L.A.  
Deposited on : 2013-02-15  
Resolution : 3.20 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

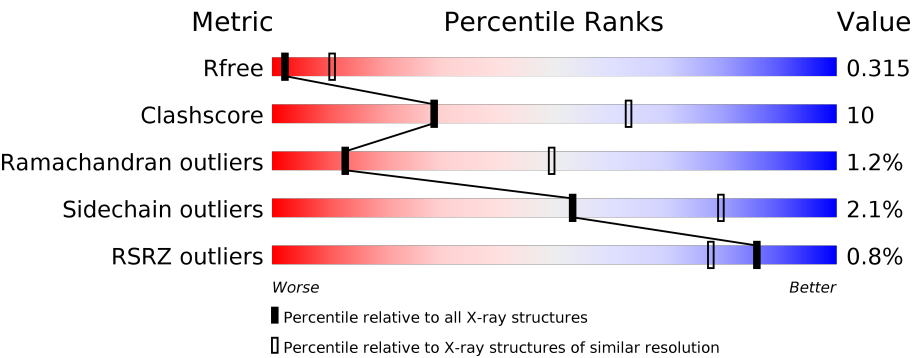
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	137	<div><div></div><div><div></div><div>64%</div><div>24%</div><div>•</div><div>11%</div></div></div>
1	B	137	<div><div>%</div><div><div></div><div>80%</div><div>7%</div><div>•</div><div>12%</div></div></div>
1	C	137	<div><div>%</div><div><div></div><div>79%</div><div>9%</div><div>•</div><div>11%</div></div></div>
1	D	137	<div><div></div><div><div></div><div>78%</div><div>12%</div><div>9%</div></div></div>
1	E	137	<div><div></div><div><div></div><div>70%</div><div>10%</div><div>•</div><div>19%</div></div></div>
1	F	137	<div><div>%</div><div><div></div><div>79%</div><div>10%</div><div>•</div><div>10%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	137	<div><div><div>%</div><div><div></div><div>69%</div><div>7%</div><div>••</div><div>23%</div></div></div></div>
1	H	137	<div><div><div>2%</div><div><div></div><div>74%</div><div>7%</div><div>•</div><div>18%</div></div></div></div>
1	I	137	<div><div><div></div><div><div></div><div>75%</div><div>5%</div><div>•</div><div>19%</div></div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7297 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 Engineered Digoxigenin binder protein DIG10.3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	122	Total	C	N	O	S	0	0	0
			906	595	146	163	2			
1	B	121	Total	C	N	O	S	0	0	0
			826	543	137	144	2			
1	C	122	Total	C	N	O	S	0	0	0
			812	526	139	146	1			
1	D	124	Total	C	N	O	S	0	0	0
			820	531	141	146	2			
1	E	111	Total	C	N	O	S	0	0	0
			731	477	126	127	1			
1	F	123	Total	C	N	O	S	0	0	0
			800	514	141	144	1			
1	G	105	Total	C	N	O		0	0	0
			657	421	117	119				
1	H	113	Total	C	N	O	S	0	0	0
			746	488	126	131	1			
1	I	111	Total	C	N	O		0	0	0
			747	483	128	136				

There are 234 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	VAL	LEU	ENGINEERED MUTATION	UNP Q9HYR3
A	10	ALA	SER	ENGINEERED MUTATION	UNP Q9HYR3
A	23	SER	CYS	ENGINEERED MUTATION	UNP Q9HYR3
A	34	TYR	PHE	ENGINEERED MUTATION	UNP Q9HYR3
A	37	PRO	ALA	ENGINEERED MUTATION	UNP Q9HYR3
A	41	TYR	TRP	ENGINEERED MUTATION	UNP Q9HYR3
A	61	TYR	HIS	ENGINEERED MUTATION	UNP Q9HYR3
A	62	MET	LEU	ENGINEERED MUTATION	UNP Q9HYR3
A	64	ILE	VAL	ENGINEERED MUTATION	UNP Q9HYR3
A	90	LEU	ALA	ENGINEERED MUTATION	UNP Q9HYR3
A	92	ALA	VAL	ENGINEERED MUTATION	UNP Q9HYR3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	99	TYR	GLN	ENGINEERED MUTATION	UNP Q9HYR3
A	103	ALA	SER	ENGINEERED MUTATION	UNP Q9HYR3
A	105	TRP	LEU	ENGINEERED MUTATION	UNP Q9HYR3
A	117	LEU	ASP	ENGINEERED MUTATION	UNP Q9HYR3
A	119	PHE	TRP	ENGINEERED MUTATION	UNP Q9HYR3
A	124	VAL	HIS	ENGINEERED MUTATION	UNP Q9HYR3
A	127	PRO	ALA	ENGINEERED MUTATION	UNP Q9HYR3
A	130	LEU	GLY	ENGINEERED MUTATION	UNP Q9HYR3
A	131	GLU	VAL	ENGINEERED MUTATION	UNP Q9HYR3
A	132	HIS	-	EXPRESSION TAG	UNP Q9HYR3
A	133	HIS	-	EXPRESSION TAG	UNP Q9HYR3
A	134	HIS	-	EXPRESSION TAG	UNP Q9HYR3
A	135	HIS	-	EXPRESSION TAG	UNP Q9HYR3
A	136	HIS	-	EXPRESSION TAG	UNP Q9HYR3
A	137	HIS	-	EXPRESSION TAG	UNP Q9HYR3
B	7	VAL	LEU	ENGINEERED MUTATION	UNP Q9HYR3
B	10	ALA	SER	ENGINEERED MUTATION	UNP Q9HYR3
B	23	SER	CYS	ENGINEERED MUTATION	UNP Q9HYR3
B	34	TYR	PHE	ENGINEERED MUTATION	UNP Q9HYR3
B	37	PRO	ALA	ENGINEERED MUTATION	UNP Q9HYR3
B	41	TYR	TRP	ENGINEERED MUTATION	UNP Q9HYR3
B	61	TYR	HIS	ENGINEERED MUTATION	UNP Q9HYR3
B	62	MET	LEU	ENGINEERED MUTATION	UNP Q9HYR3
B	64	ILE	VAL	ENGINEERED MUTATION	UNP Q9HYR3
B	90	LEU	ALA	ENGINEERED MUTATION	UNP Q9HYR3
B	92	ALA	VAL	ENGINEERED MUTATION	UNP Q9HYR3
B	99	TYR	GLN	ENGINEERED MUTATION	UNP Q9HYR3
B	103	ALA	SER	ENGINEERED MUTATION	UNP Q9HYR3
B	105	TRP	LEU	ENGINEERED MUTATION	UNP Q9HYR3
B	117	LEU	ASP	ENGINEERED MUTATION	UNP Q9HYR3
B	119	PHE	TRP	ENGINEERED MUTATION	UNP Q9HYR3
B	124	VAL	HIS	ENGINEERED MUTATION	UNP Q9HYR3
B	127	PRO	ALA	ENGINEERED MUTATION	UNP Q9HYR3
B	130	LEU	GLY	ENGINEERED MUTATION	UNP Q9HYR3
B	131	GLU	VAL	ENGINEERED MUTATION	UNP Q9HYR3
B	132	HIS	-	EXPRESSION TAG	UNP Q9HYR3
B	133	HIS	-	EXPRESSION TAG	UNP Q9HYR3
B	134	HIS	-	EXPRESSION TAG	UNP Q9HYR3
B	135	HIS	-	EXPRESSION TAG	UNP Q9HYR3
B	136	HIS	-	EXPRESSION TAG	UNP Q9HYR3
B	137	HIS	-	EXPRESSION TAG	UNP Q9HYR3
C	7	VAL	LEU	ENGINEERED MUTATION	UNP Q9HYR3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	10	ALA	SER	ENGINEERED MUTATION	UNP Q9HYR3
C	23	SER	CYS	ENGINEERED MUTATION	UNP Q9HYR3
C	34	TYR	PHE	ENGINEERED MUTATION	UNP Q9HYR3
C	37	PRO	ALA	ENGINEERED MUTATION	UNP Q9HYR3
C	41	TYR	TRP	ENGINEERED MUTATION	UNP Q9HYR3
C	61	TYR	HIS	ENGINEERED MUTATION	UNP Q9HYR3
C	62	MET	LEU	ENGINEERED MUTATION	UNP Q9HYR3
C	64	ILE	VAL	ENGINEERED MUTATION	UNP Q9HYR3
C	90	LEU	ALA	ENGINEERED MUTATION	UNP Q9HYR3
C	92	ALA	VAL	ENGINEERED MUTATION	UNP Q9HYR3
C	99	TYR	GLN	ENGINEERED MUTATION	UNP Q9HYR3
C	103	ALA	SER	ENGINEERED MUTATION	UNP Q9HYR3
C	105	TRP	LEU	ENGINEERED MUTATION	UNP Q9HYR3
C	117	LEU	ASP	ENGINEERED MUTATION	UNP Q9HYR3
C	119	PHE	TRP	ENGINEERED MUTATION	UNP Q9HYR3
C	124	VAL	HIS	ENGINEERED MUTATION	UNP Q9HYR3
C	127	PRO	ALA	ENGINEERED MUTATION	UNP Q9HYR3
C	130	LEU	GLY	ENGINEERED MUTATION	UNP Q9HYR3
C	131	GLU	VAL	ENGINEERED MUTATION	UNP Q9HYR3
C	132	HIS	-	EXPRESSION TAG	UNP Q9HYR3
C	133	HIS	-	EXPRESSION TAG	UNP Q9HYR3
C	134	HIS	-	EXPRESSION TAG	UNP Q9HYR3
C	135	HIS	-	EXPRESSION TAG	UNP Q9HYR3
C	136	HIS	-	EXPRESSION TAG	UNP Q9HYR3
C	137	HIS	-	EXPRESSION TAG	UNP Q9HYR3
D	7	VAL	LEU	ENGINEERED MUTATION	UNP Q9HYR3
D	10	ALA	SER	ENGINEERED MUTATION	UNP Q9HYR3
D	23	SER	CYS	ENGINEERED MUTATION	UNP Q9HYR3
D	34	TYR	PHE	ENGINEERED MUTATION	UNP Q9HYR3
D	37	PRO	ALA	ENGINEERED MUTATION	UNP Q9HYR3
D	41	TYR	TRP	ENGINEERED MUTATION	UNP Q9HYR3
D	61	TYR	HIS	ENGINEERED MUTATION	UNP Q9HYR3
D	62	MET	LEU	ENGINEERED MUTATION	UNP Q9HYR3
D	64	ILE	VAL	ENGINEERED MUTATION	UNP Q9HYR3
D	90	LEU	ALA	ENGINEERED MUTATION	UNP Q9HYR3
D	92	ALA	VAL	ENGINEERED MUTATION	UNP Q9HYR3
D	99	TYR	GLN	ENGINEERED MUTATION	UNP Q9HYR3
D	103	ALA	SER	ENGINEERED MUTATION	UNP Q9HYR3
D	105	TRP	LEU	ENGINEERED MUTATION	UNP Q9HYR3
D	117	LEU	ASP	ENGINEERED MUTATION	UNP Q9HYR3
D	119	PHE	TRP	ENGINEERED MUTATION	UNP Q9HYR3
D	124	VAL	HIS	ENGINEERED MUTATION	UNP Q9HYR3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	127	PRO	ALA	ENGINEERED MUTATION	UNP Q9HYR3
D	130	LEU	GLY	ENGINEERED MUTATION	UNP Q9HYR3
D	131	GLU	VAL	ENGINEERED MUTATION	UNP Q9HYR3
D	132	HIS	-	EXPRESSION TAG	UNP Q9HYR3
D	133	HIS	-	EXPRESSION TAG	UNP Q9HYR3
D	134	HIS	-	EXPRESSION TAG	UNP Q9HYR3
D	135	HIS	-	EXPRESSION TAG	UNP Q9HYR3
D	136	HIS	-	EXPRESSION TAG	UNP Q9HYR3
D	137	HIS	-	EXPRESSION TAG	UNP Q9HYR3
E	7	VAL	LEU	ENGINEERED MUTATION	UNP Q9HYR3
E	10	ALA	SER	ENGINEERED MUTATION	UNP Q9HYR3
E	23	SER	CYS	ENGINEERED MUTATION	UNP Q9HYR3
E	34	TYR	PHE	ENGINEERED MUTATION	UNP Q9HYR3
E	37	PRO	ALA	ENGINEERED MUTATION	UNP Q9HYR3
E	41	TYR	TRP	ENGINEERED MUTATION	UNP Q9HYR3
E	61	TYR	HIS	ENGINEERED MUTATION	UNP Q9HYR3
E	62	MET	LEU	ENGINEERED MUTATION	UNP Q9HYR3
E	64	ILE	VAL	ENGINEERED MUTATION	UNP Q9HYR3
E	90	LEU	ALA	ENGINEERED MUTATION	UNP Q9HYR3
E	92	ALA	VAL	ENGINEERED MUTATION	UNP Q9HYR3
E	99	TYR	GLN	ENGINEERED MUTATION	UNP Q9HYR3
E	103	ALA	SER	ENGINEERED MUTATION	UNP Q9HYR3
E	105	TRP	LEU	ENGINEERED MUTATION	UNP Q9HYR3
E	117	LEU	ASP	ENGINEERED MUTATION	UNP Q9HYR3
E	119	PHE	TRP	ENGINEERED MUTATION	UNP Q9HYR3
E	124	VAL	HIS	ENGINEERED MUTATION	UNP Q9HYR3
E	127	PRO	ALA	ENGINEERED MUTATION	UNP Q9HYR3
E	130	LEU	GLY	ENGINEERED MUTATION	UNP Q9HYR3
E	131	GLU	VAL	ENGINEERED MUTATION	UNP Q9HYR3
E	132	HIS	-	EXPRESSION TAG	UNP Q9HYR3
E	133	HIS	-	EXPRESSION TAG	UNP Q9HYR3
E	134	HIS	-	EXPRESSION TAG	UNP Q9HYR3
E	135	HIS	-	EXPRESSION TAG	UNP Q9HYR3
E	136	HIS	-	EXPRESSION TAG	UNP Q9HYR3
E	137	HIS	-	EXPRESSION TAG	UNP Q9HYR3
F	7	VAL	LEU	ENGINEERED MUTATION	UNP Q9HYR3
F	10	ALA	SER	ENGINEERED MUTATION	UNP Q9HYR3
F	23	SER	CYS	ENGINEERED MUTATION	UNP Q9HYR3
F	34	TYR	PHE	ENGINEERED MUTATION	UNP Q9HYR3
F	37	PRO	ALA	ENGINEERED MUTATION	UNP Q9HYR3
F	41	TYR	TRP	ENGINEERED MUTATION	UNP Q9HYR3
F	61	TYR	HIS	ENGINEERED MUTATION	UNP Q9HYR3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	62	MET	LEU	ENGINEERED MUTATION	UNP Q9HYR3
F	64	ILE	VAL	ENGINEERED MUTATION	UNP Q9HYR3
F	90	LEU	ALA	ENGINEERED MUTATION	UNP Q9HYR3
F	92	ALA	VAL	ENGINEERED MUTATION	UNP Q9HYR3
F	99	TYR	GLN	ENGINEERED MUTATION	UNP Q9HYR3
F	103	ALA	SER	ENGINEERED MUTATION	UNP Q9HYR3
F	105	TRP	LEU	ENGINEERED MUTATION	UNP Q9HYR3
F	117	LEU	ASP	ENGINEERED MUTATION	UNP Q9HYR3
F	119	PHE	TRP	ENGINEERED MUTATION	UNP Q9HYR3
F	124	VAL	HIS	ENGINEERED MUTATION	UNP Q9HYR3
F	127	PRO	ALA	ENGINEERED MUTATION	UNP Q9HYR3
F	130	LEU	GLY	ENGINEERED MUTATION	UNP Q9HYR3
F	131	GLU	VAL	ENGINEERED MUTATION	UNP Q9HYR3
F	132	HIS	-	EXPRESSION TAG	UNP Q9HYR3
F	133	HIS	-	EXPRESSION TAG	UNP Q9HYR3
F	134	HIS	-	EXPRESSION TAG	UNP Q9HYR3
F	135	HIS	-	EXPRESSION TAG	UNP Q9HYR3
F	136	HIS	-	EXPRESSION TAG	UNP Q9HYR3
F	137	HIS	-	EXPRESSION TAG	UNP Q9HYR3
G	7	VAL	LEU	ENGINEERED MUTATION	UNP Q9HYR3
G	10	ALA	SER	ENGINEERED MUTATION	UNP Q9HYR3
G	23	SER	CYS	ENGINEERED MUTATION	UNP Q9HYR3
G	34	TYR	PHE	ENGINEERED MUTATION	UNP Q9HYR3
G	37	PRO	ALA	ENGINEERED MUTATION	UNP Q9HYR3
G	41	TYR	TRP	ENGINEERED MUTATION	UNP Q9HYR3
G	61	TYR	HIS	ENGINEERED MUTATION	UNP Q9HYR3
G	62	MET	LEU	ENGINEERED MUTATION	UNP Q9HYR3
G	64	ILE	VAL	ENGINEERED MUTATION	UNP Q9HYR3
G	90	LEU	ALA	ENGINEERED MUTATION	UNP Q9HYR3
G	92	ALA	VAL	ENGINEERED MUTATION	UNP Q9HYR3
G	99	TYR	GLN	ENGINEERED MUTATION	UNP Q9HYR3
G	103	ALA	SER	ENGINEERED MUTATION	UNP Q9HYR3
G	105	TRP	LEU	ENGINEERED MUTATION	UNP Q9HYR3
G	117	LEU	ASP	ENGINEERED MUTATION	UNP Q9HYR3
G	119	PHE	TRP	ENGINEERED MUTATION	UNP Q9HYR3
G	124	VAL	HIS	ENGINEERED MUTATION	UNP Q9HYR3
G	127	PRO	ALA	ENGINEERED MUTATION	UNP Q9HYR3
G	130	LEU	GLY	ENGINEERED MUTATION	UNP Q9HYR3
G	131	GLU	VAL	ENGINEERED MUTATION	UNP Q9HYR3
G	132	HIS	-	EXPRESSION TAG	UNP Q9HYR3
G	133	HIS	-	EXPRESSION TAG	UNP Q9HYR3
G	134	HIS	-	EXPRESSION TAG	UNP Q9HYR3

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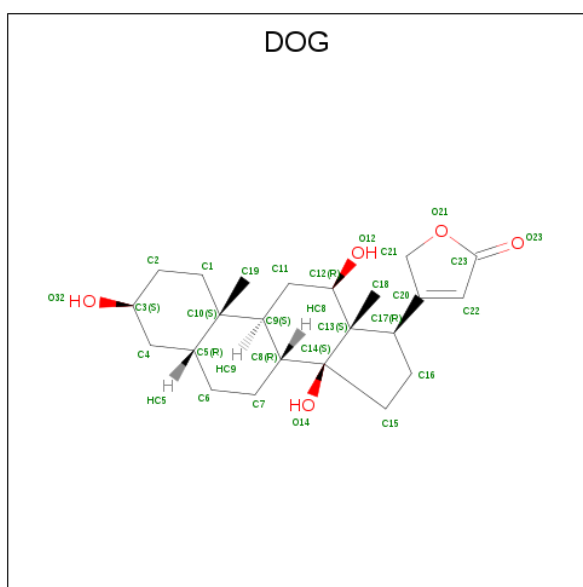
Chain	Residue	Modelled	Actual	Comment	Reference
G	135	HIS	-	EXPRESSION TAG	UNP Q9HYR3
G	136	HIS	-	EXPRESSION TAG	UNP Q9HYR3
G	137	HIS	-	EXPRESSION TAG	UNP Q9HYR3
H	7	VAL	LEU	ENGINEERED MUTATION	UNP Q9HYR3
H	10	ALA	SER	ENGINEERED MUTATION	UNP Q9HYR3
H	23	SER	CYS	ENGINEERED MUTATION	UNP Q9HYR3
H	34	TYR	PHE	ENGINEERED MUTATION	UNP Q9HYR3
H	37	PRO	ALA	ENGINEERED MUTATION	UNP Q9HYR3
H	41	TYR	TRP	ENGINEERED MUTATION	UNP Q9HYR3
H	61	TYR	HIS	ENGINEERED MUTATION	UNP Q9HYR3
H	62	MET	LEU	ENGINEERED MUTATION	UNP Q9HYR3
H	64	ILE	VAL	ENGINEERED MUTATION	UNP Q9HYR3
H	90	LEU	ALA	ENGINEERED MUTATION	UNP Q9HYR3
H	92	ALA	VAL	ENGINEERED MUTATION	UNP Q9HYR3
H	99	TYR	GLN	ENGINEERED MUTATION	UNP Q9HYR3
H	103	ALA	SER	ENGINEERED MUTATION	UNP Q9HYR3
H	105	TRP	LEU	ENGINEERED MUTATION	UNP Q9HYR3
H	117	LEU	ASP	ENGINEERED MUTATION	UNP Q9HYR3
H	119	PHE	TRP	ENGINEERED MUTATION	UNP Q9HYR3
H	124	VAL	HIS	ENGINEERED MUTATION	UNP Q9HYR3
H	127	PRO	ALA	ENGINEERED MUTATION	UNP Q9HYR3
H	130	LEU	GLY	ENGINEERED MUTATION	UNP Q9HYR3
H	131	GLU	VAL	ENGINEERED MUTATION	UNP Q9HYR3
H	132	HIS	-	EXPRESSION TAG	UNP Q9HYR3
H	133	HIS	-	EXPRESSION TAG	UNP Q9HYR3
H	134	HIS	-	EXPRESSION TAG	UNP Q9HYR3
H	135	HIS	-	EXPRESSION TAG	UNP Q9HYR3
H	136	HIS	-	EXPRESSION TAG	UNP Q9HYR3
H	137	HIS	-	EXPRESSION TAG	UNP Q9HYR3
I	7	VAL	LEU	ENGINEERED MUTATION	UNP Q9HYR3
I	10	ALA	SER	ENGINEERED MUTATION	UNP Q9HYR3
I	23	SER	CYS	ENGINEERED MUTATION	UNP Q9HYR3
I	34	TYR	PHE	ENGINEERED MUTATION	UNP Q9HYR3
I	37	PRO	ALA	ENGINEERED MUTATION	UNP Q9HYR3
I	41	TYR	TRP	ENGINEERED MUTATION	UNP Q9HYR3
I	61	TYR	HIS	ENGINEERED MUTATION	UNP Q9HYR3
I	62	MET	LEU	ENGINEERED MUTATION	UNP Q9HYR3
I	64	ILE	VAL	ENGINEERED MUTATION	UNP Q9HYR3
I	90	LEU	ALA	ENGINEERED MUTATION	UNP Q9HYR3
I	92	ALA	VAL	ENGINEERED MUTATION	UNP Q9HYR3
I	99	TYR	GLN	ENGINEERED MUTATION	UNP Q9HYR3
I	103	ALA	SER	ENGINEERED MUTATION	UNP Q9HYR3

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Chain	Residue	Modelled	Actual	Comment	Reference
I	105	TRP	LEU	ENGINEERED MUTATION	UNP Q9HYR3
I	117	LEU	ASP	ENGINEERED MUTATION	UNP Q9HYR3
I	119	PHE	TRP	ENGINEERED MUTATION	UNP Q9HYR3
I	124	VAL	HIS	ENGINEERED MUTATION	UNP Q9HYR3
I	127	PRO	ALA	ENGINEERED MUTATION	UNP Q9HYR3
I	130	LEU	GLY	ENGINEERED MUTATION	UNP Q9HYR3
I	131	GLU	VAL	ENGINEERED MUTATION	UNP Q9HYR3
I	132	HIS	-	EXPRESSION TAG	UNP Q9HYR3
I	133	HIS	-	EXPRESSION TAG	UNP Q9HYR3
I	134	HIS	-	EXPRESSION TAG	UNP Q9HYR3
I	135	HIS	-	EXPRESSION TAG	UNP Q9HYR3
I	136	HIS	-	EXPRESSION TAG	UNP Q9HYR3
I	137	HIS	-	EXPRESSION TAG	UNP Q9HYR3

- Molecule 2 is DIGOXIGENIN (three-letter code: DOG) (formula:  $C_{23}H_{34}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			28	23	5		
2	B	1	Total	C	O	0	0
			28	23	5		
2	C	1	Total	C	O	0	0
			28	23	5		
2	D	1	Total	C	O	0	0
			28	23	5		
2	E	1	Total	C	O	0	0
			28	23	5		

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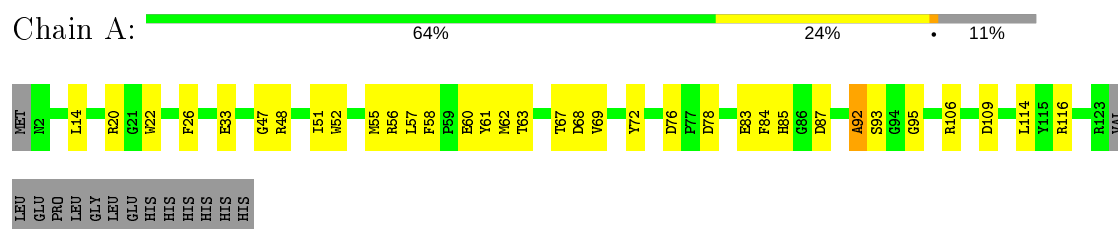
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	C	O	0	0
			28	23	5		
2	G	1	Total	C	O	0	0
			28	23	5		
2	H	1	Total	C	O	0	0
			28	23	5		
2	I	1	Total	C	O	0	0
			28	23	5		

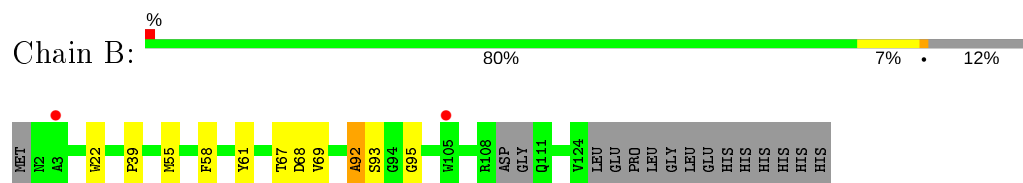
### 3 Residue-property plots [i](#)

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.

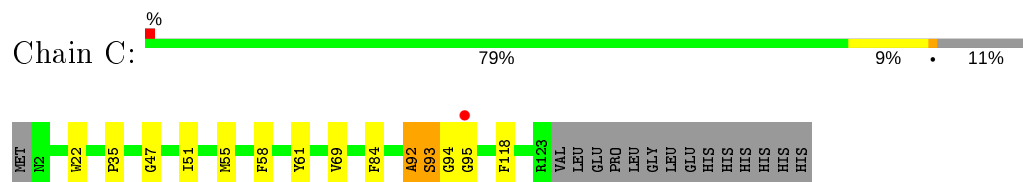
- Molecule 1: Engineered Digoxigenin binder protein DIG10.3



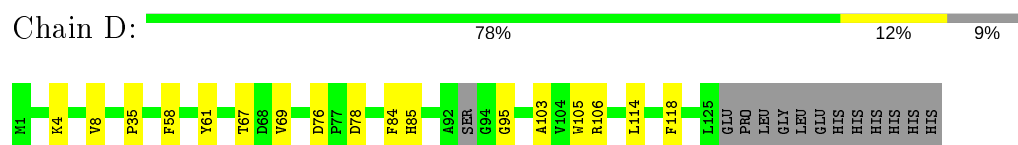
- Molecule 1: Engineered Digoxigenin binder protein DIG10.3



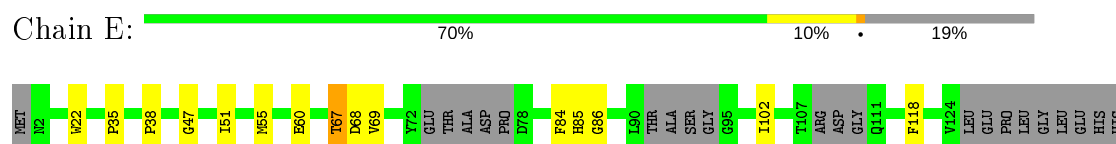
- Molecule 1: Engineered Digoxigenin binder protein DIG10.3



- Molecule 1: Engineered Digoxigenin binder protein DIG10.3



- Molecule 1: Engineered Digoxigenin binder protein DIG10.3



H1	T43	T67	D68	V69	D76	P77	D78	F84	H85	G86	D87	GLY	VAL	LEU	LEU	THR	ALA	SER	GLY	GLY	LYS	LEU	ALA	TYR	D100	R123	VAL	LEU	GLU	PRO	LEU	LEU	GLY	GLU	GLU	HIS	HIS	HIS	HIS	HIS
----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.79 Å 90.99 Å 110.08 Å 90.00° 92.68° 90.00°	Depositor
Resolution (Å)	45.54 – 3.20 45.50 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.5 (45.54-3.20) 97.5 (45.50-3.20)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.84 (at 3.19 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.262 , 0.317 0.263 , 0.315	Depositor DCC
$R_{free}$ test set	1082 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.5	Xtriage
Anisotropy	0.609	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 127.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	7297	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: DOG

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	0.57	0/939	0.73	0/1290
1	B	0.59	0/857	0.68	0/1181
1	C	0.49	0/844	0.64	0/1167
1	D	0.53	0/847	0.69	0/1167
1	E	0.55	0/756	0.66	0/1041
1	F	0.51	0/826	0.67	0/1141
1	G	0.52	0/677	0.73	2/935 (0.2%)
1	H	0.53	0/772	0.66	0/1067
1	I	0.54	0/773	0.68	0/1071
All	All	0.54	0/7291	0.68	2/10060 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	G	101	TYR	CB-CG-CD1	7.64	125.58	121.00
1	G	101	TYR	CB-CG-CD2	-6.31	117.21	121.00

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	906	0	762	29	0
1	B	826	0	613	12	0
1	C	812	0	572	10	0
1	D	820	0	605	12	0
1	E	731	0	507	22	0
1	F	800	0	566	11	0
1	G	657	0	439	9	0
1	H	746	0	535	14	0
1	I	747	0	547	7	0
2	A	28	0	34	1	0
2	B	28	0	34	0	0
2	C	28	0	34	0	0
2	D	28	0	34	1	0
2	E	28	0	34	3	0
2	F	28	0	34	2	0
2	G	28	0	34	3	0
2	H	28	0	34	4	0
2	I	28	0	34	0	0
All	All	7297	0	5452	123	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 10.

All (123) 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:E:35:PRO:HG2	1:E:118:PHE:CE1	1.71	1.25
1:A:60:GLU:OE1	1:B:92:ALA:HB2	1.58	1.02
1:E:35:PRO:HG2	1:E:118:PHE:HE1	1.26	0.99
1:E:35:PRO:CG	1:E:118:PHE:HE1	1.80	0.94
1:A:26:PHE:O	1:A:48:ARG:NH1	2.01	0.94
1:E:35:PRO:CG	1:E:118:PHE:CE1	2.51	0.93
1:F:26:PHE:O	1:F:48:ARG:NH1	2.03	0.91
1:H:67:THR:OG1	1:H:85:HIS:HB3	1.70	0.90
1:A:60:GLU:CD	1:B:92:ALA:HB2	1.92	0.89
1:H:108:ARG:O	1:H:110:GLY:N	2.08	0.85
1:H:67:THR:HG22	1:H:68:ASP:H	1.43	0.83
1:E:35:PRO:HG2	1:E:118:PHE:CD1	2.21	0.76
1:H:67:THR:HG22	1:H:68:ASP:N	2.02	0.73
1:E:35:PRO:CB	1:E:118:PHE:HE1	2.02	0.73
1:E:67:THR:CG2	1:E:85:HIS:HB3	2.20	0.72
1:I:67:THR:CG2	1:I:85:HIS:HB3	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:TRP:CZ2	1:A:56:ARG:HG2	2.29	0.67
1:A:52:TRP:CE2	1:A:56:ARG:HG2	2.31	0.66
1:E:35:PRO:CB	1:E:118:PHE:CE1	2.80	0.65
1:A:60:GLU:OE1	1:B:92:ALA:CB	2.41	0.64
1:G:18:ASP:O	1:G:20:ARG:N	2.29	0.64
1:A:106:ARG:HB2	1:A:114:LEU:HB3	1.80	0.64
1:D:4:LYS:O	1:D:8:VAL:HG23	1.99	0.63
1:A:57:LEU:HD21	1:B:61:TYR:CG	2.34	0.62
1:A:20:ARG:HG3	1:A:52:TRP:CH2	2.36	0.60
1:A:57:LEU:HD21	1:B:61:TYR:CD1	2.37	0.59
1:G:70:GLN:O	1:G:71:PHE:CB	2.51	0.59
1:D:106:ARG:HB2	1:D:114:LEU:HB3	1.83	0.58
1:A:76:ASP:OD1	1:A:78:ASP:N	2.34	0.58
1:H:108:ARG:O	1:H:109:ASP:C	2.43	0.57
1:E:102:ILE:HG23	1:E:118:PHE:HD2	1.69	0.57
1:C:93:SER:OG	1:C:94:GLY:N	2.35	0.56
1:G:101:TYR:OH	2:G:201:DOG:O12	2.21	0.56
1:B:67:THR:HA	1:B:68:ASP:CB	2.35	0.55
1:H:67:THR:HG1	1:H:85:HIS:HB3	1.70	0.55
1:D:35:PRO:HG2	1:D:118:PHE:CE1	2.41	0.55
1:A:22:TRP:CZ3	1:A:55:MET:HG3	2.41	0.55
1:F:35:PRO:HG2	1:F:118:PHE:CE1	2.42	0.55
1:D:76:ASP:OD1	1:D:78:ASP:N	2.37	0.54
1:G:122:LEU:O	1:G:123:ARG:CB	2.53	0.54
1:F:22:TRP:CZ3	1:F:55:MET:HG3	2.42	0.54
1:H:84:PHE:CE1	1:H:101:TYR:CD1	2.96	0.54
1:F:76:ASP:OD1	1:F:78:ASP:N	2.35	0.53
1:E:38:PRO:HG3	2:E:201:DOG:H191	1.90	0.53
1:G:72:TYR:OH	1:G:83:GLU:OE2	2.25	0.53
1:E:22:TRP:CZ3	1:E:55:MET:HG3	2.43	0.53
1:C:22:TRP:CZ3	1:C:55:MET:HG3	2.43	0.53
1:E:67:THR:OG1	1:E:68:ASP:N	2.42	0.53
1:B:92:ALA:N	1:B:93:SER:HA	2.23	0.52
1:I:76:ASP:OD1	1:I:78:ASP:N	2.36	0.52
1:A:61:TYR:HB3	1:B:61:TYR:HB3	1.89	0.52
1:D:58:PHE:HA	1:D:61:TYR:CE2	2.44	0.52
1:A:72:TYR:OH	1:A:83:GLU:OE2	2.27	0.52
1:B:22:TRP:CZ3	1:B:55:MET:HG3	2.45	0.52
1:C:61:TYR:HB3	1:D:61:TYR:HB3	1.89	0.52
1:F:67:THR:CG2	1:F:85:HIS:HB3	2.40	0.52
1:D:67:THR:CG2	1:D:85:HIS:HB3	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:PHE:HA	1:B:61:TYR:CE2	2.45	0.51
1:A:92:ALA:N	1:A:93:SER:HA	2.26	0.51
1:G:101:TYR:HE2	2:G:201:DOG:C22	2.24	0.51
1:I:67:THR:OG1	1:I:68:ASP:N	2.41	0.51
1:C:92:ALA:N	1:C:93:SER:HA	2.26	0.51
2:D:201:DOG:H183	2:D:201:DOG:H211	1.92	0.51
1:C:47:GLY:O	1:C:51:ILE:HG13	2.11	0.50
1:F:92:ALA:N	1:F:93:SER:HA	2.25	0.50
1:A:67:THR:CG2	1:A:85:HIS:HB3	2.42	0.50
1:C:35:PRO:HG2	1:C:118:PHE:CE1	2.47	0.49
1:A:58:PHE:HA	1:A:61:TYR:CE2	2.47	0.49
1:A:47:GLY:O	1:A:51:ILE:HG13	2.12	0.49
1:E:47:GLY:O	1:E:51:ILE:HG13	2.13	0.49
1:E:55:MET:CE	2:E:201:DOG:O14	2.61	0.49
1:E:67:THR:HG21	1:E:85:HIS:HB3	1.94	0.48
1:G:101:TYR:CD1	1:G:101:TYR:N	2.82	0.48
1:F:67:THR:HG21	1:F:85:HIS:HB3	1.96	0.47
1:C:58:PHE:HA	1:C:61:TYR:CE1	2.50	0.47
1:H:101:TYR:CD2	1:H:117:LEU:HD11	2.50	0.47
1:E:55:MET:HE1	2:E:201:DOG:O14	2.15	0.47
1:A:85:HIS:NE2	1:A:87:ASP:OD1	2.48	0.46
1:A:14:LEU:HG	1:A:22:TRP:CD1	2.51	0.46
1:A:33:GLU:OE1	1:A:116:ARG:HD2	2.16	0.46
1:H:99:TYR:CZ	2:H:201:DOG:H111	2.50	0.46
1:I:67:THR:HG23	1:I:85:HIS:H	1.82	0.45
1:F:69:VAL:HA	1:F:84:PHE:HB3	1.99	0.45
1:I:67:THR:HG21	1:I:85:HIS:HB3	1.95	0.45
1:D:67:THR:HG21	1:D:85:HIS:HB3	1.98	0.45
1:E:67:THR:HG23	1:E:85:HIS:H	1.81	0.45
1:F:92:ALA:HB3	1:F:93:SER:O	2.17	0.45
1:A:67:THR:HG21	1:A:85:HIS:HB3	1.98	0.44
1:F:35:PRO:CB	1:F:118:PHE:CE1	3.00	0.44
2:F:201:DOG:H211	2:F:201:DOG:O14	2.17	0.44
1:E:85:HIS:CD2	1:E:86:GLY:N	2.86	0.44
1:H:67:THR:OG1	1:H:85:HIS:CB	2.55	0.44
1:D:58:PHE:HA	1:D:61:TYR:CZ	2.53	0.44
1:B:92:ALA:HB3	1:B:93:SER:O	2.18	0.44
1:G:84:PHE:CZ	1:G:101:TYR:CD2	3.06	0.44
1:A:58:PHE:HA	1:A:61:TYR:CZ	2.53	0.43
1:E:60:GLU:HA	1:F:92:ALA:HA	1.98	0.43
1:A:55:MET:HE1	2:A:201:DOG:H161	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ALA:HB3	1:A:93:SER:O	2.19	0.43
1:B:58:PHE:HA	1:B:61:TYR:CZ	2.54	0.43
1:E:102:ILE:HG23	1:E:118:PHE:CD2	2.52	0.43
1:D:69:VAL:HA	1:D:84:PHE:HB3	2.01	0.43
2:F:201:DOG:H111	2:F:201:DOG:HC11	1.78	0.43
1:G:84:PHE:CZ	1:G:101:TYR:HD2	2.36	0.43
2:H:201:DOG:O14	2:H:201:DOG:H211	2.19	0.43
1:C:69:VAL:HA	1:C:84:PHE:HB3	2.01	0.42
1:C:92:ALA:HB3	1:C:93:SER:O	2.19	0.42
2:G:201:DOG:H211	2:G:201:DOG:H183	2.02	0.42
1:C:35:PRO:CB	1:C:118:PHE:CE1	3.03	0.42
1:E:69:VAL:HA	1:E:84:PHE:HB3	2.02	0.42
1:A:69:VAL:HA	1:A:84:PHE:HB3	2.01	0.41
1:E:35:PRO:HB2	1:E:118:PHE:CE1	2.54	0.41
1:A:76:ASP:OD1	1:A:78:ASP:HB2	2.20	0.41
1:H:99:TYR:OH	2:H:201:DOG:C2	2.69	0.41
1:D:103:ALA:HB3	1:D:105:TRP:CH2	2.56	0.41
1:H:99:TYR:OH	2:H:201:DOG:HC22	2.21	0.41
1:A:62:MET:CG	1:A:63:THR:N	2.84	0.41
1:D:35:PRO:CB	1:D:118:PHE:CE1	3.04	0.41
1:I:69:VAL:HA	1:I:84:PHE:HB3	2.03	0.40
1:A:55:MET:O	1:A:56:ARG:C	2.58	0.40
1:I:76:ASP:OD1	1:I:78:ASP:HB2	2.22	0.40
1:H:85:HIS:CD2	1:H:86:GLY:N	2.90	0.40
1:H:67:THR:CG2	1:H:68:ASP:H	2.24	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	120/137 (88%)	113 (94%)	5 (4%)	2 (2%)	9	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	117/137 (85%)	108 (92%)	6 (5%)	3 (3%)	5	31
1	C	120/137 (88%)	113 (94%)	5 (4%)	2 (2%)	9	42
1	D	120/137 (88%)	115 (96%)	4 (3%)	1 (1%)	19	58
1	E	103/137 (75%)	100 (97%)	3 (3%)	0	100	100
1	F	119/137 (87%)	114 (96%)	4 (3%)	1 (1%)	19	58
1	G	99/137 (72%)	89 (90%)	8 (8%)	2 (2%)	7	38
1	H	107/137 (78%)	99 (92%)	7 (6%)	1 (1%)	17	56
1	I	107/137 (78%)	103 (96%)	4 (4%)	0	100	100
All	All	1012/1233 (82%)	954 (94%)	46 (4%)	12 (1%)	13	49

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	19	ALA
1	H	109	ASP
1	A	95	GLY
1	B	95	GLY
1	C	95	GLY
1	D	95	GLY
1	G	71	PHE
1	A	92	ALA
1	B	92	ALA
1	C	92	ALA
1	F	92	ALA
1	B	69	VAL

### 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	74/116 (64%)	72 (97%)	2 (3%)	44	75
1	B	52/116 (45%)	51 (98%)	1 (2%)	57	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	48/116 (41%)	47 (98%)	1 (2%)	53	79
1	D	50/116 (43%)	50 (100%)	0	100	100
1	E	40/116 (34%)	39 (98%)	1 (2%)	47	77
1	F	46/116 (40%)	45 (98%)	1 (2%)	52	79
1	G	32/116 (28%)	31 (97%)	1 (3%)	40	72
1	H	43/116 (37%)	43 (100%)	0	100	100
1	I	48/116 (41%)	46 (96%)	2 (4%)	30	65
All	All	433/1044 (42%)	424 (98%)	9 (2%)	53	79

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ASP
1	A	109	ASP
1	B	39	PRO
1	C	93	SER
1	E	67	THR
1	F	122	LEU
1	G	101	TYR
1	I	43	THR
1	I	67	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	DOG	I	201	-	32,32,32	1.24	4 (12%)	48,53,53	1.33	6 (12%)
2	DOG	B	201	-	32,32,32	1.32	4 (12%)	48,53,53	1.26	5 (10%)
2	DOG	D	201	-	32,32,32	1.35	3 (9%)	48,53,53	1.30	6 (12%)
2	DOG	F	201	-	32,32,32	1.21	3 (9%)	48,53,53	1.64	10 (20%)
2	DOG	H	201	-	32,32,32	1.29	4 (12%)	48,53,53	1.61	11 (22%)
2	DOG	C	201	-	32,32,32	1.30	2 (6%)	48,53,53	1.23	6 (12%)
2	DOG	G	201	-	32,32,32	1.47	5 (15%)	48,53,53	1.61	9 (18%)
2	DOG	A	201	-	32,32,32	1.72	4 (12%)	48,53,53	1.30	6 (12%)
2	DOG	E	201	-	32,32,32	1.10	2 (6%)	48,53,53	1.57	10 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DOG	I	201	-	-	0/4/81/81	0/5/5/5
2	DOG	B	201	-	-	0/4/81/81	0/5/5/5
2	DOG	D	201	-	-	0/4/81/81	0/5/5/5
2	DOG	F	201	-	-	0/4/81/81	0/5/5/5
2	DOG	H	201	-	-	0/4/81/81	0/5/5/5
2	DOG	C	201	-	-	0/4/81/81	0/5/5/5
2	DOG	G	201	-	-	0/4/81/81	0/5/5/5
2	DOG	A	201	-	-	0/4/81/81	0/5/5/5
2	DOG	E	201	-	-	0/4/81/81	0/5/5/5

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	DOG	C14-C13	-6.35	1.49	1.56
2	G	201	DOG	C14-C13	-4.92	1.51	1.56
2	D	201	DOG	C14-C13	-4.27	1.51	1.56
2	H	201	DOG	C14-C13	-4.14	1.52	1.56
2	B	201	DOG	C13-C17	-4.02	1.51	1.57
2	E	201	DOG	C13-C17	-3.99	1.51	1.57
2	G	201	DOG	O21-C23	3.73	1.46	1.36
2	I	201	DOG	C13-C17	-3.42	1.52	1.57
2	F	201	DOG	O21-C23	3.39	1.45	1.36
2	C	201	DOG	C14-C13	-3.31	1.52	1.56
2	A	201	DOG	C15-C14	-3.24	1.49	1.54
2	C	201	DOG	O21-C23	3.18	1.44	1.36
2	B	201	DOG	C14-C13	-3.14	1.52	1.56
2	I	201	DOG	C14-C13	-3.14	1.52	1.56
2	B	201	DOG	C15-C14	-3.01	1.49	1.54
2	A	201	DOG	O21-C23	2.98	1.44	1.36
2	A	201	DOG	C13-C17	-2.95	1.53	1.57
2	E	201	DOG	O21-C23	2.95	1.43	1.36
2	H	201	DOG	O21-C23	2.84	1.43	1.36
2	H	201	DOG	C15-C14	-2.84	1.49	1.54
2	D	201	DOG	O21-C23	2.71	1.43	1.36
2	I	201	DOG	O21-C23	2.63	1.43	1.36
2	D	201	DOG	C10-C5	-2.58	1.51	1.55
2	G	201	DOG	C13-C17	-2.52	1.53	1.57
2	B	201	DOG	O21-C23	2.43	1.42	1.36
2	F	201	DOG	C13-C17	-2.43	1.53	1.57
2	G	201	DOG	C15-C14	-2.38	1.50	1.54
2	G	201	DOG	C10-C5	-2.32	1.51	1.55
2	H	201	DOG	C13-C17	-2.22	1.54	1.57
2	I	201	DOG	C15-C14	-2.21	1.50	1.54
2	F	201	DOG	O23-C23	2.16	1.25	1.21

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	201	DOG	O14-C14-C8	-4.05	101.80	108.42
2	D	201	DOG	O14-C14-C8	-4.04	101.82	108.42
2	E	201	DOG	C1-C2-C3	3.96	115.55	110.47
2	E	201	DOG	C9-C11-C12	-3.80	109.29	114.30
2	H	201	DOG	C7-C6-C5	3.74	119.34	111.84
2	B	201	DOG	C15-C16-C17	3.56	111.56	104.24
2	E	201	DOG	C13-C17-C20	-3.50	111.05	115.78
2	G	201	DOG	C7-C6-C5	3.50	118.86	111.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	201	DOG	C15-C14-C8	3.47	120.92	116.05
2	B	201	DOG	C19-C10-C1	-3.40	102.78	108.26
2	D	201	DOG	C19-C10-C9	3.29	115.72	111.18
2	F	201	DOG	C1-C10-C9	-3.22	106.30	111.35
2	F	201	DOG	C9-C11-C12	-3.21	110.06	114.30
2	F	201	DOG	C19-C10-C5	-3.17	104.98	110.36
2	B	201	DOG	C16-C15-C14	-3.16	99.82	105.19
2	I	201	DOG	C18-C13-C12	3.13	114.37	109.34
2	E	201	DOG	C15-C16-C17	3.09	110.59	104.24
2	A	201	DOG	C19-C10-C1	-3.08	103.29	108.26
2	G	201	DOG	C9-C11-C12	-3.08	110.23	114.30
2	A	201	DOG	C19-C10-C9	3.07	115.42	111.18
2	H	201	DOG	C11-C9-C10	-3.07	110.56	113.73
2	H	201	DOG	C7-C8-C14	3.07	114.42	111.39
2	G	201	DOG	C18-C13-C14	-3.07	107.66	112.40
2	F	201	DOG	C19-C10-C9	3.00	115.32	111.18
2	C	201	DOG	O12-C12-C11	-2.99	103.04	109.12
2	H	201	DOG	O12-C12-C11	-2.93	103.15	109.12
2	I	201	DOG	C9-C11-C12	-2.89	110.48	114.30
2	F	201	DOG	C1-C2-C3	-2.86	106.80	110.47
2	H	201	DOG	C7-C8-C9	-2.82	106.62	110.84
2	I	201	DOG	O12-C12-C13	-2.82	104.24	110.85
2	C	201	DOG	C13-C17-C20	2.79	119.56	115.78
2	F	201	DOG	O21-C23-C22	-2.79	105.02	108.67
2	F	201	DOG	C1-C10-C5	2.78	111.88	107.77
2	D	201	DOG	C16-C17-C20	-2.72	108.34	113.68
2	G	201	DOG	O14-C14-C15	-2.71	99.37	108.60
2	C	201	DOG	O14-C14-C8	-2.69	104.02	108.42
2	I	201	DOG	C17-C13-C12	-2.68	100.55	111.83
2	A	201	DOG	C4-C5-C6	-2.67	106.85	111.74
2	G	201	DOG	C17-C20-C22	-2.65	121.77	128.84
2	A	201	DOG	C13-C17-C20	2.65	119.37	115.78
2	G	201	DOG	C19-C10-C9	2.63	114.81	111.18
2	D	201	DOG	C11-C12-C13	2.53	116.33	112.54
2	H	201	DOG	C18-C13-C14	-2.50	108.54	112.40
2	C	201	DOG	C11-C12-C13	2.45	116.21	112.54
2	D	201	DOG	C10-C9-C8	-2.42	108.43	112.00
2	H	201	DOG	C18-C13-C12	2.40	113.19	109.34
2	I	201	DOG	C15-C16-C17	2.39	109.15	104.24
2	H	201	DOG	C15-C16-C17	2.38	109.13	104.24
2	H	201	DOG	O32-C3-C4	2.34	114.51	109.85
2	G	201	DOG	C19-C10-C5	-2.31	106.44	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	201	DOG	C18-C13-C14	-2.30	108.84	112.40
2	B	201	DOG	C9-C11-C12	-2.28	111.29	114.30
2	C	201	DOG	C15-C16-C17	2.27	108.91	104.24
2	H	201	DOG	C19-C10-C1	-2.25	104.64	108.26
2	E	201	DOG	C17-C13-C12	-2.24	102.40	111.83
2	I	201	DOG	C5-C4-C3	-2.23	109.49	112.76
2	H	201	DOG	C11-C9-C8	2.22	115.09	110.50
2	F	201	DOG	C11-C9-C10	-2.21	111.44	113.73
2	E	201	DOG	C19-C10-C1	-2.19	104.74	108.26
2	A	201	DOG	C16-C17-C20	-2.13	109.50	113.68
2	B	201	DOG	C7-C8-C9	2.12	114.02	110.84
2	D	201	DOG	C5-C4-C3	2.11	115.85	112.76
2	E	201	DOG	C9-C10-C5	2.10	111.53	108.58
2	E	201	DOG	O12-C12-C13	-2.08	105.96	110.85
2	C	201	DOG	C19-C10-C1	-2.08	104.91	108.26
2	G	201	DOG	C19-C10-C1	-2.08	104.91	108.26
2	E	201	DOG	C4-C3-C2	-2.03	108.12	110.55
2	E	201	DOG	C1-C10-C9	2.02	114.53	111.35
2	A	201	DOG	O14-C14-C15	-2.01	101.77	108.60

There are no chirality outliers.

There are no torsion outliers.

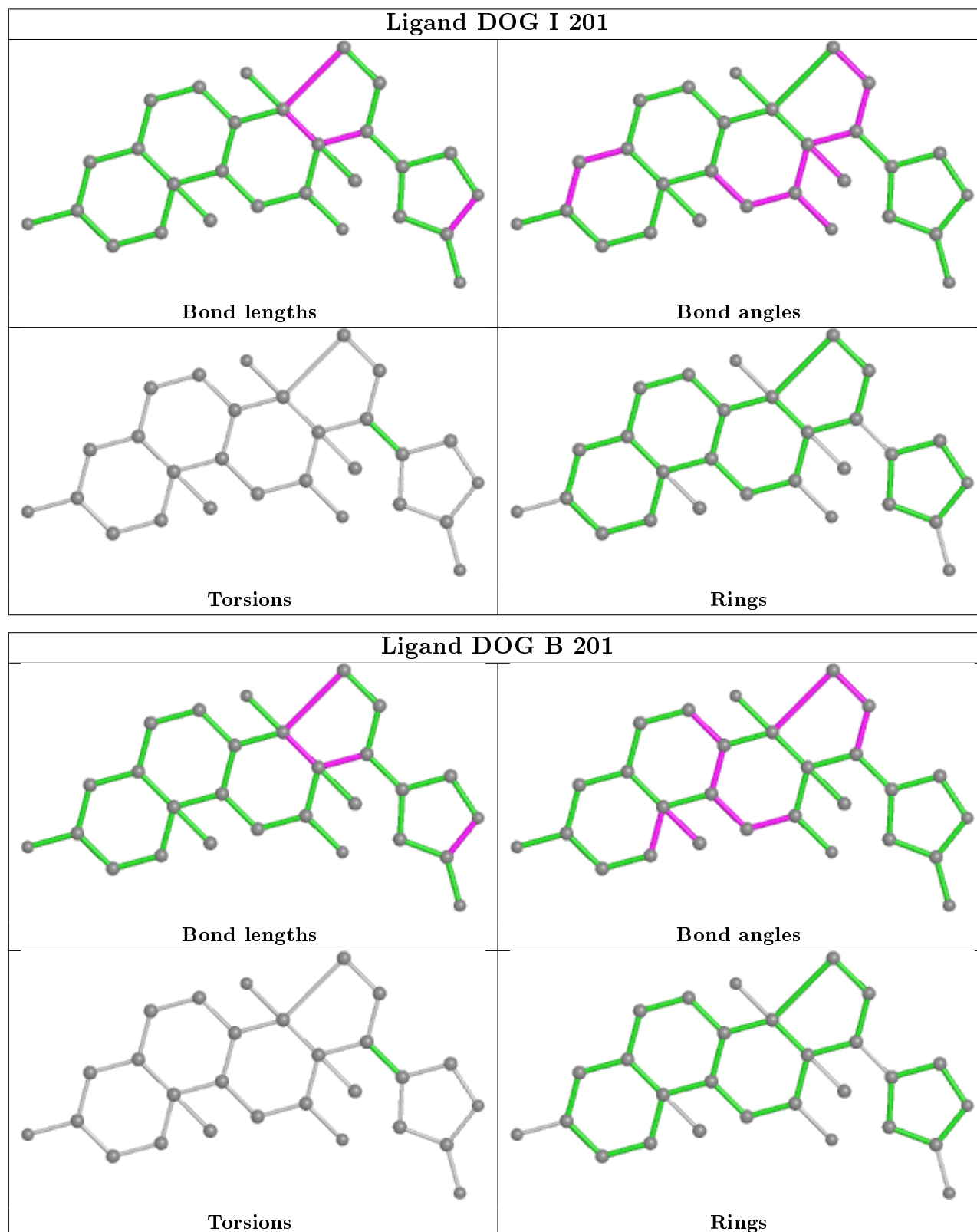
There are no ring outliers.

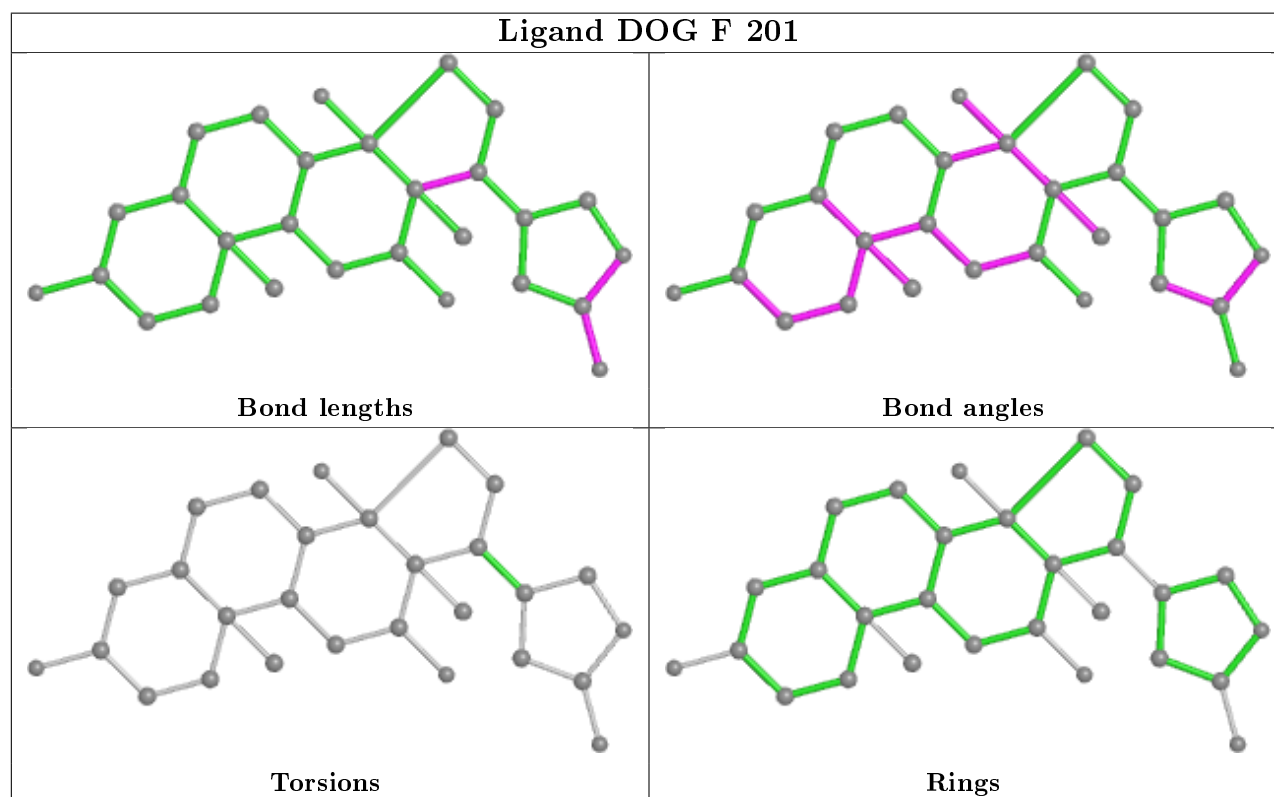
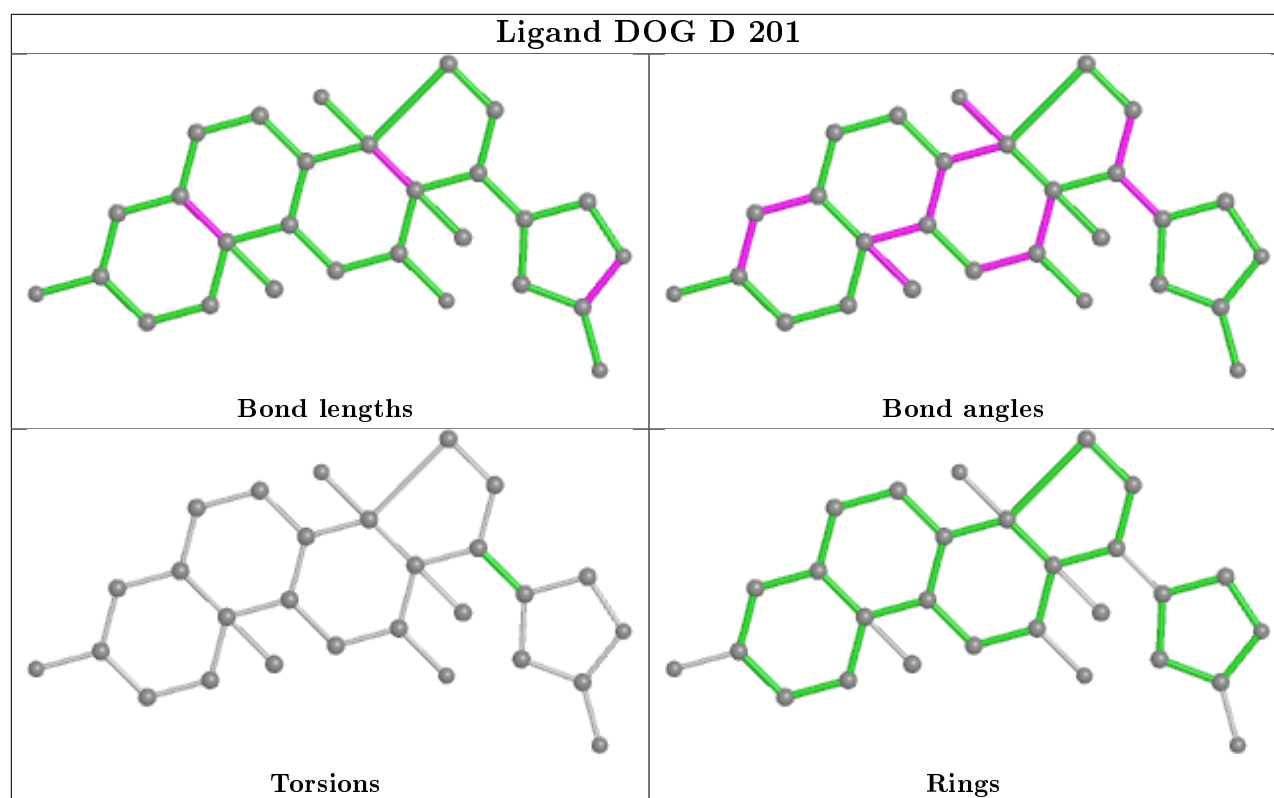
6 monomers are involved in 14 short contacts:

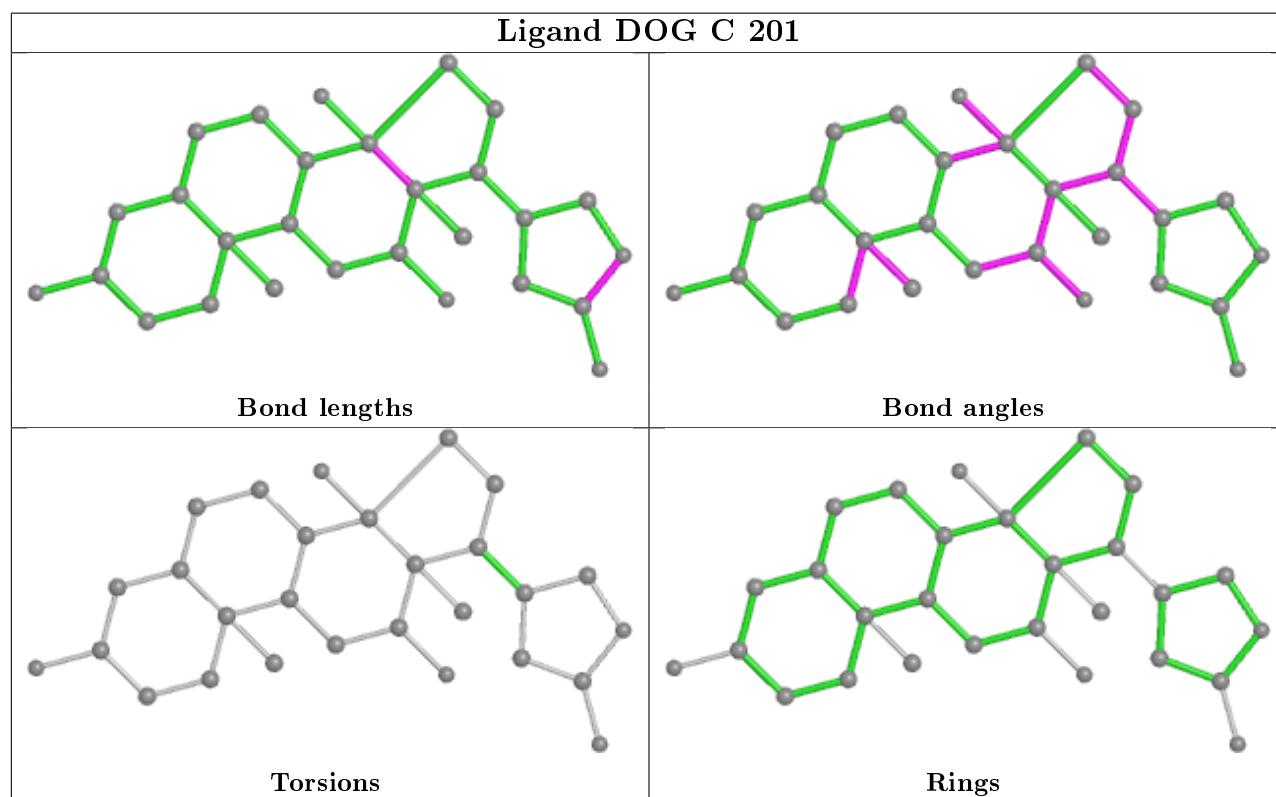
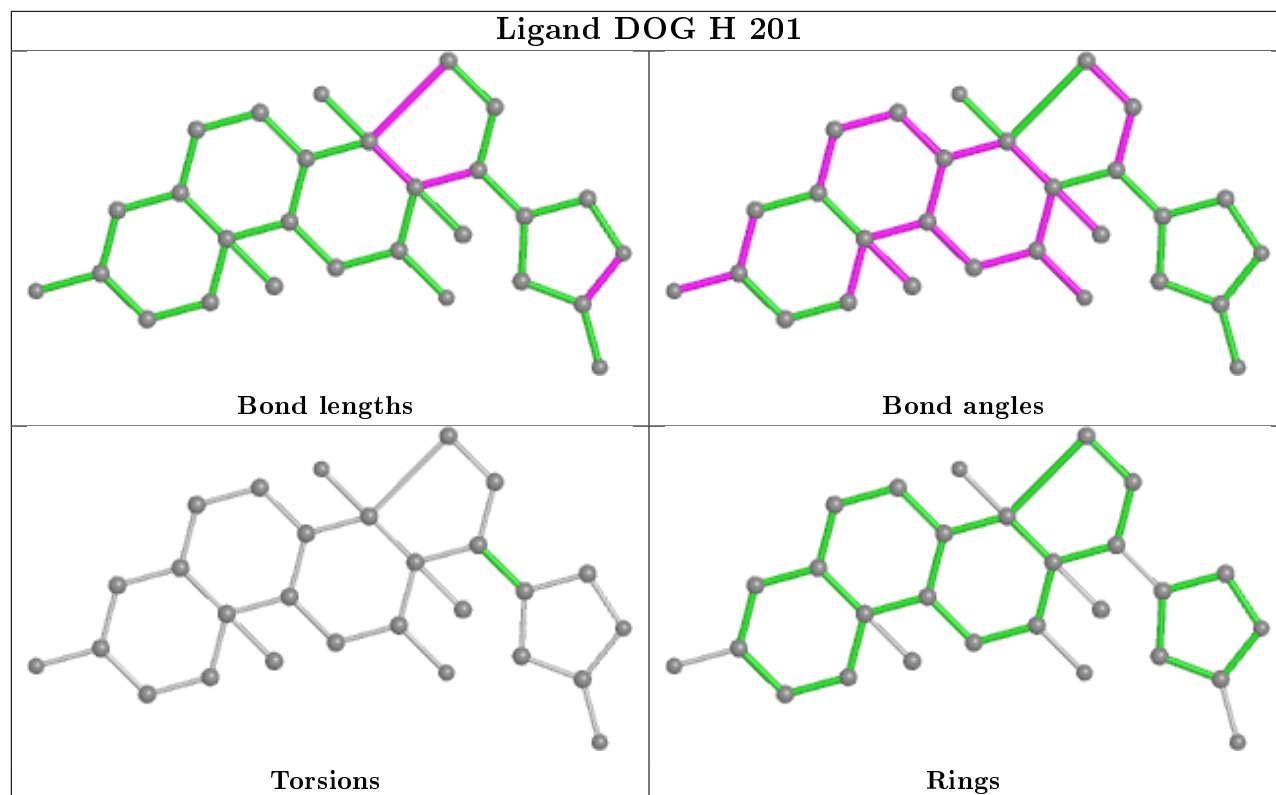
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	201	DOG	1	0
2	F	201	DOG	2	0
2	H	201	DOG	4	0
2	G	201	DOG	3	0
2	A	201	DOG	1	0
2	E	201	DOG	3	0

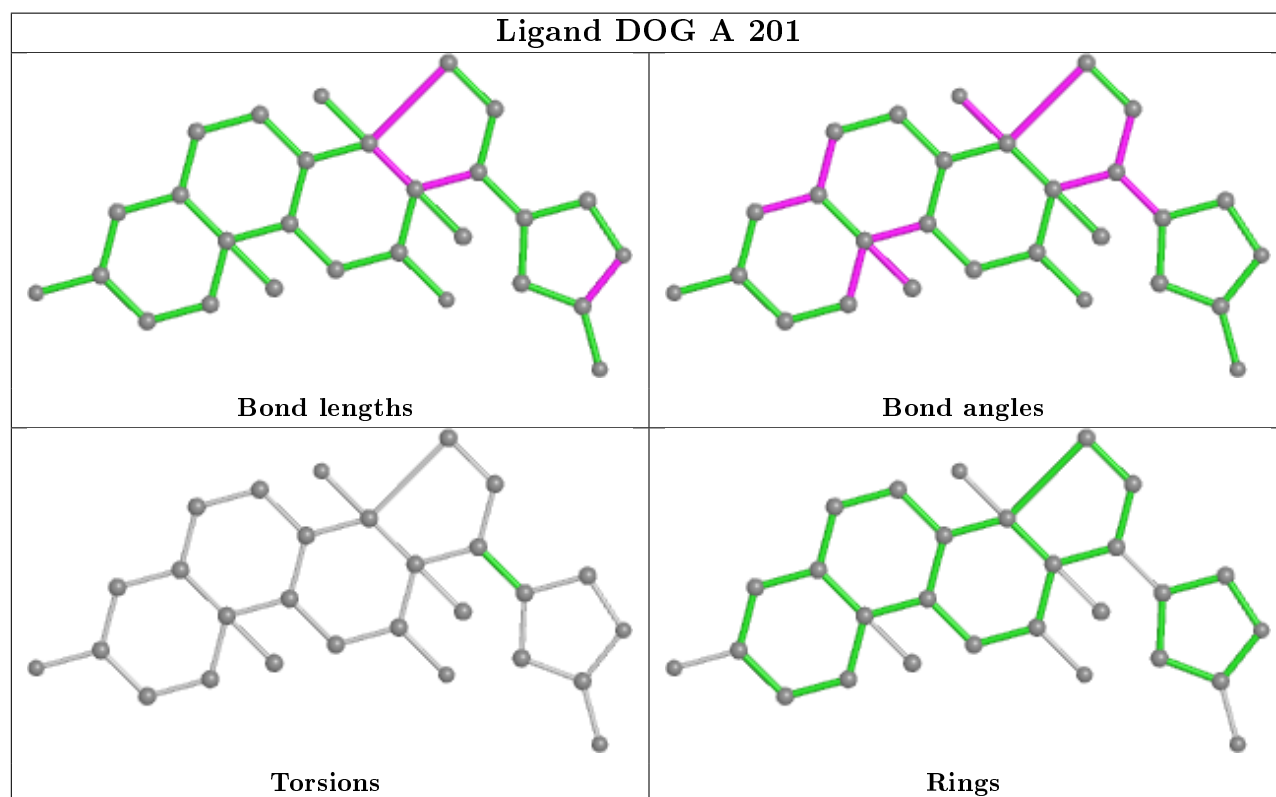
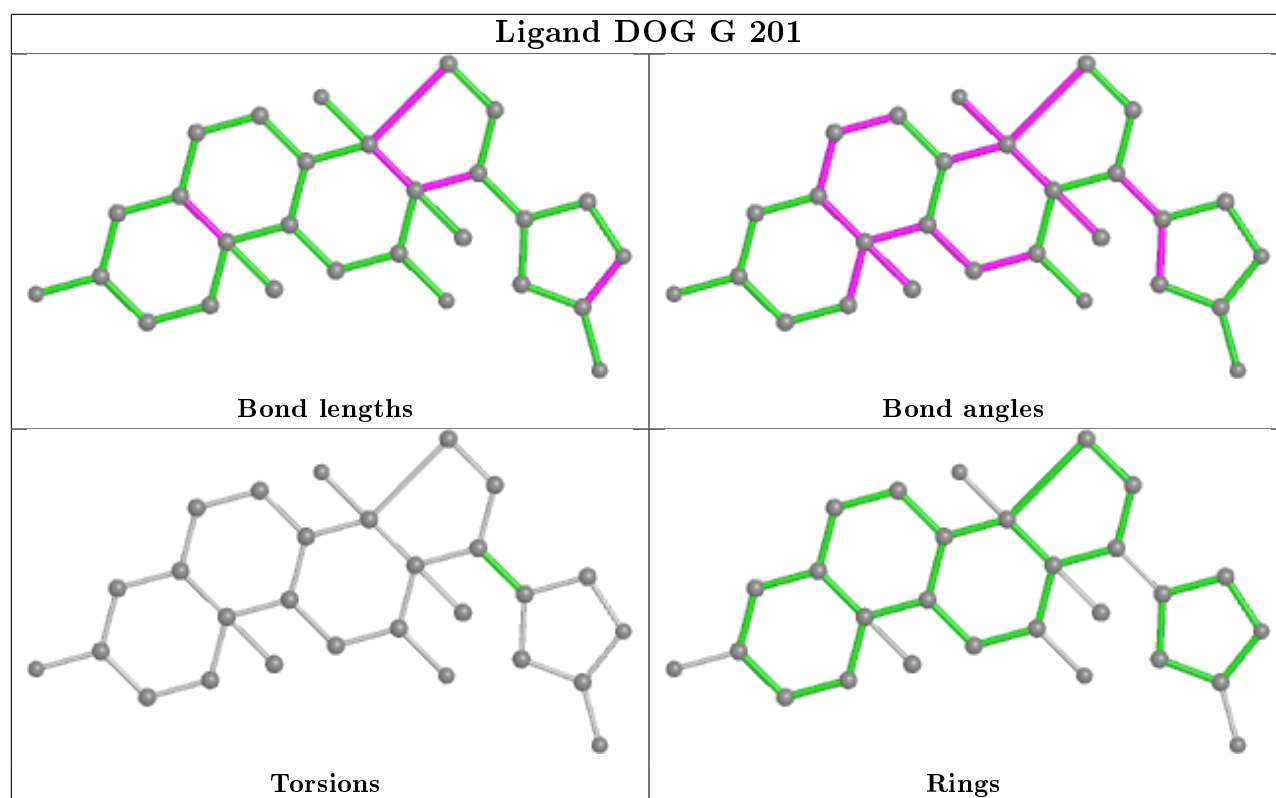
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

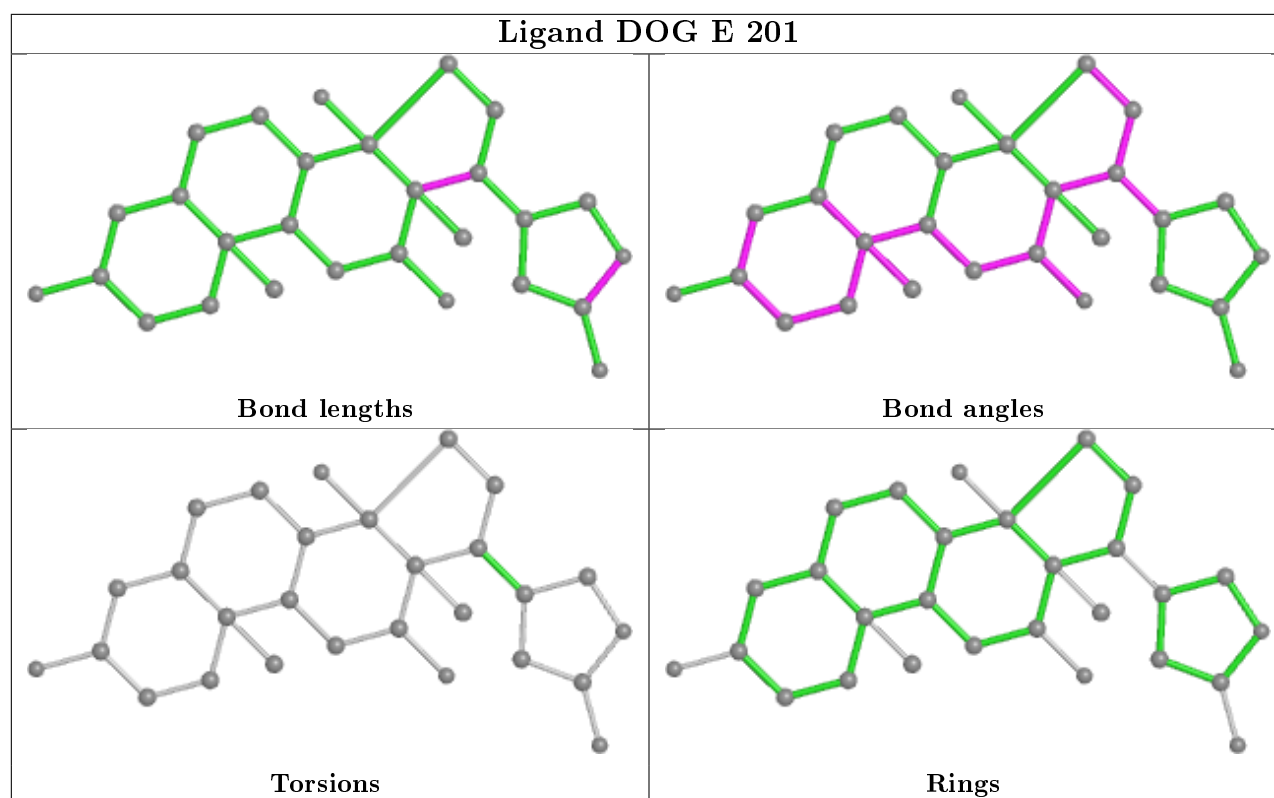
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	122/137 (89%)	-0.24	0 100 100	38, 57, 78, 94	0
1	B	121/137 (88%)	-0.15	2 (1%) 70 57	48, 68, 96, 123	0
1	C	122/137 (89%)	-0.22	1 (0%) 86 78	50, 73, 96, 129	0
1	D	124/137 (90%)	-0.25	0 100 100	46, 64, 87, 95	0
1	E	111/137 (81%)	-0.20	0 100 100	53, 79, 99, 107	0
1	F	123/137 (89%)	-0.26	1 (0%) 86 78	52, 76, 94, 110	0
1	G	105/137 (76%)	-0.17	1 (0%) 82 72	52, 84, 111, 124	0
1	H	113/137 (82%)	0.09	3 (2%) 54 39	54, 78, 109, 117	0
1	I	111/137 (81%)	-0.10	0 100 100	45, 71, 107, 146	0
All	All	1052/1233 (85%)	-0.17	8 (0%) 86 78	38, 73, 101, 146	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	30	GLY	3.2
1	H	39	PRO	2.7
1	B	105	TRP	2.7
1	F	66	PHE	2.3
1	G	80	ALA	2.3
1	C	95	GLY	2.2
1	H	114	LEU	2.1
1	B	3	ALA	2.0

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

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

### 6.3 Carbohydrates

There are no monosaccharides in this entry.

### 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

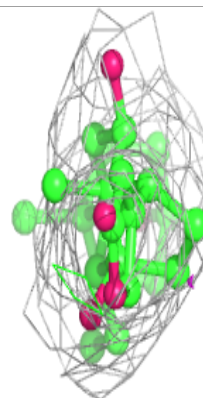
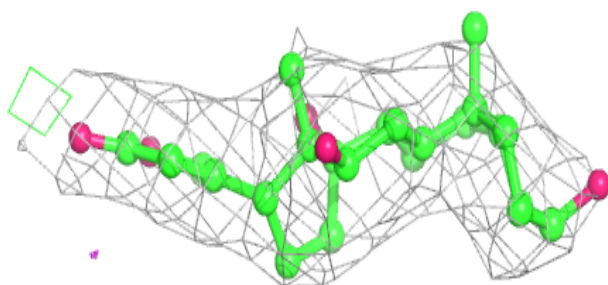
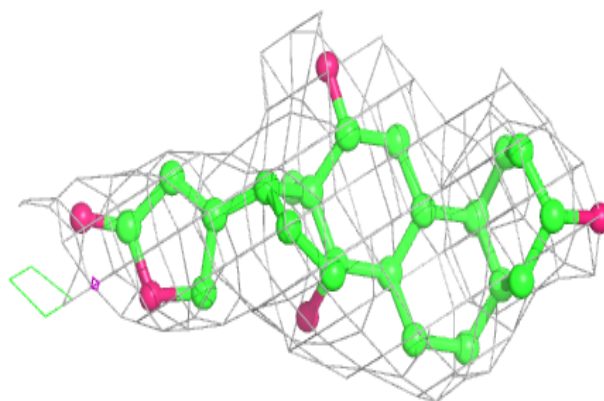
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	DOG	F	201	28/28	0.92	0.32	53,63,68,73	0
2	DOG	E	201	28/28	0.93	0.26	58,71,78,79	0
2	DOG	H	201	28/28	0.94	0.23	53,68,79,85	0
2	DOG	G	201	28/28	0.94	0.28	51,63,78,86	0
2	DOG	D	201	28/28	0.94	0.27	43,49,58,65	0
2	DOG	B	201	28/28	0.95	0.26	52,57,61,67	0
2	DOG	I	201	28/28	0.95	0.25	51,61,74,75	0
2	DOG	A	201	28/28	0.96	0.26	43,49,59,74	0
2	DOG	C	201	28/28	0.97	0.24	47,52,61,63	0

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

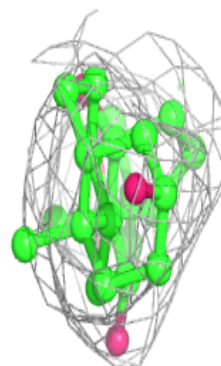
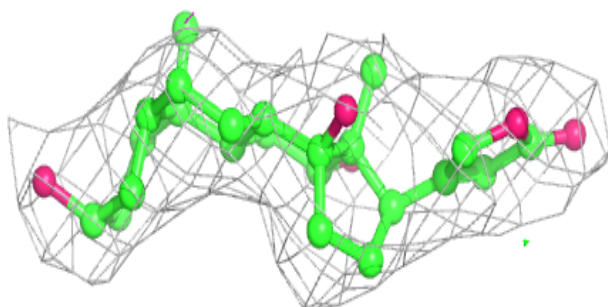
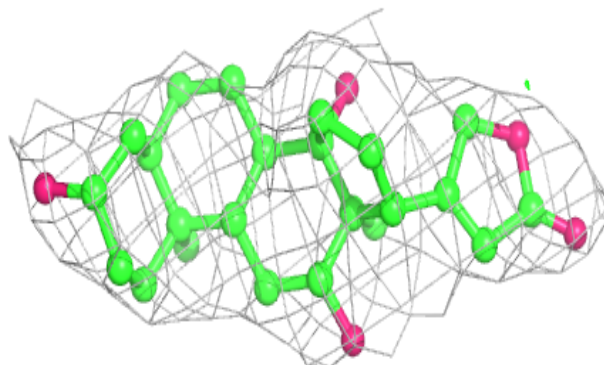


**Electron density around DOG F 201:**

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

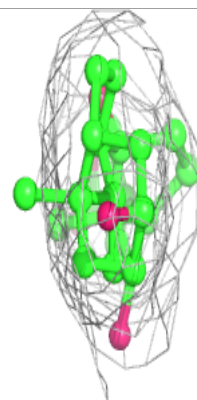
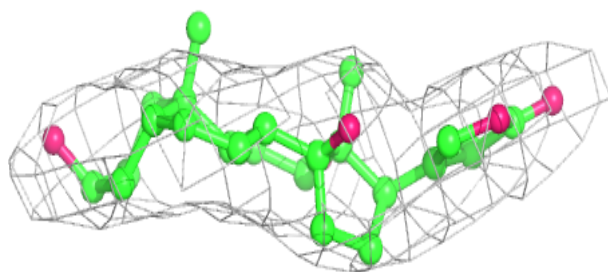
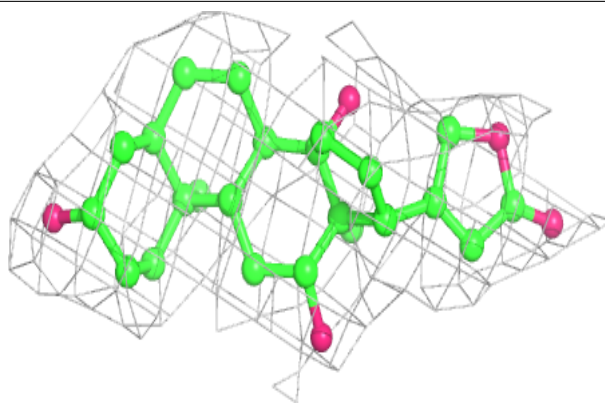
**Electron density around DOG E 201:**

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

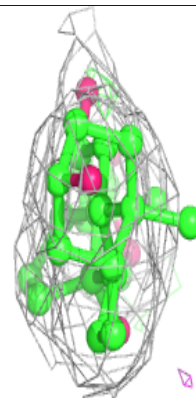
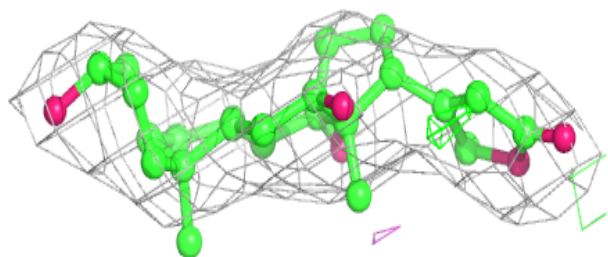
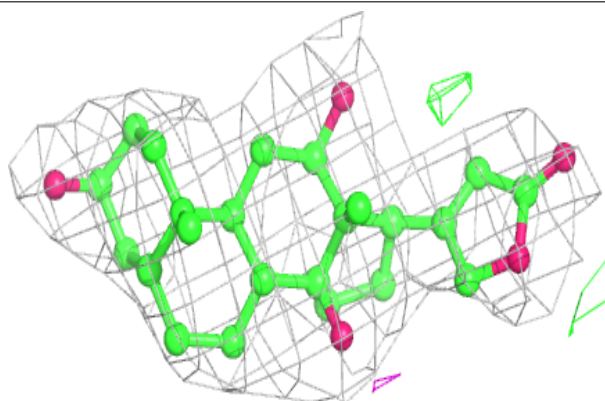


**Electron density around DOG H 201:**

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

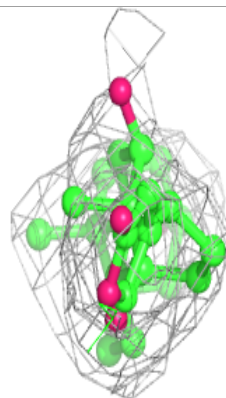
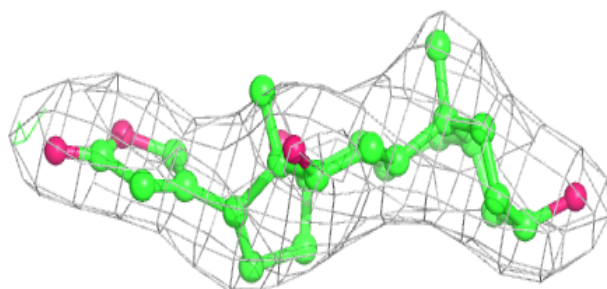
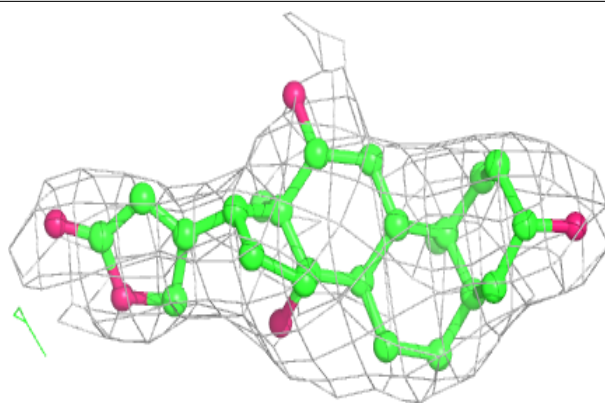
**Electron density around DOG G 201:**

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

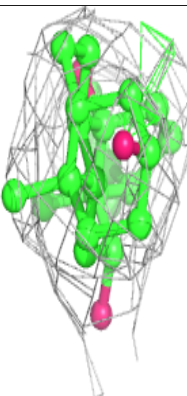
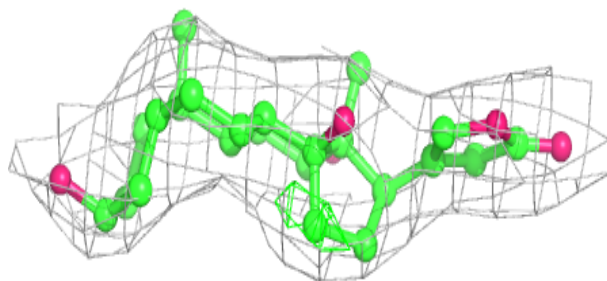
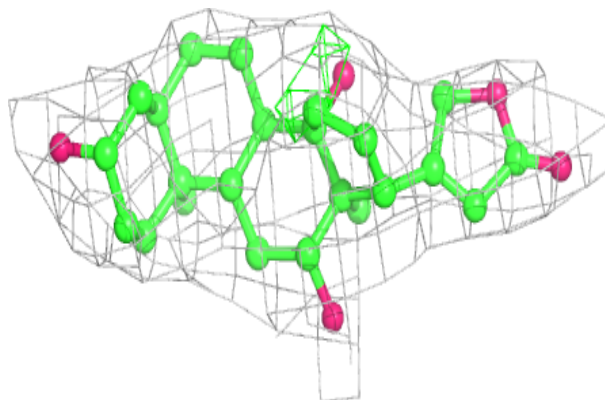


**Electron density around DOG D 201:**

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

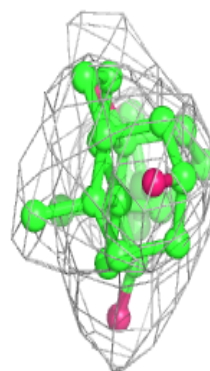
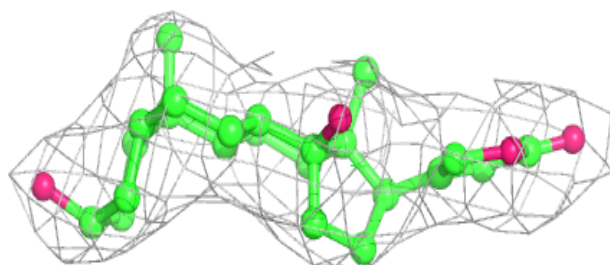
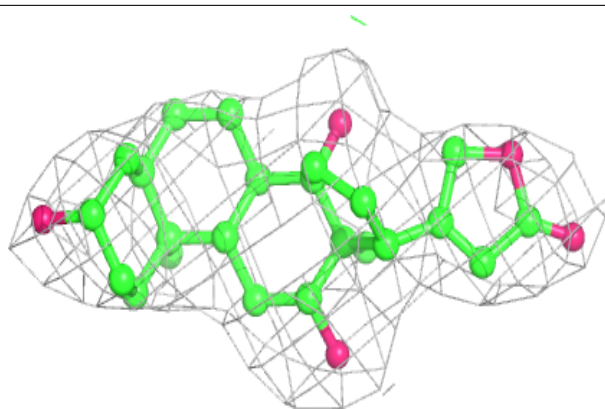
**Electron density around DOG B 201:**

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

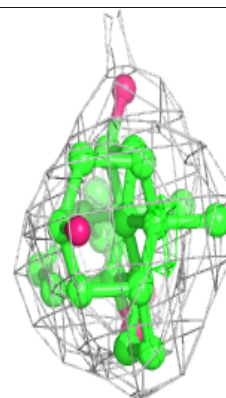
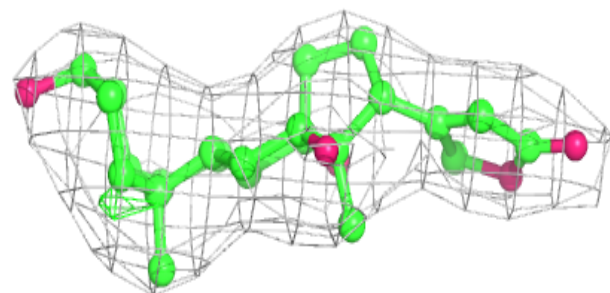
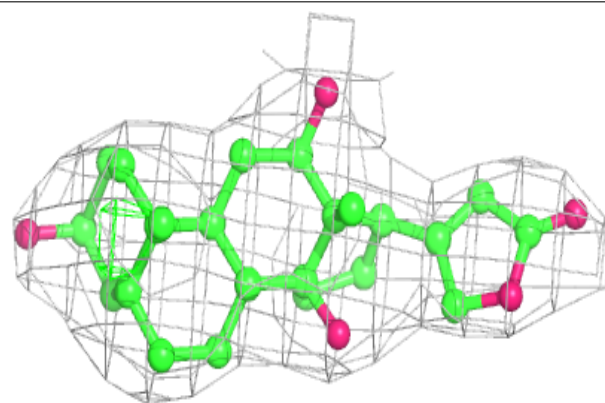


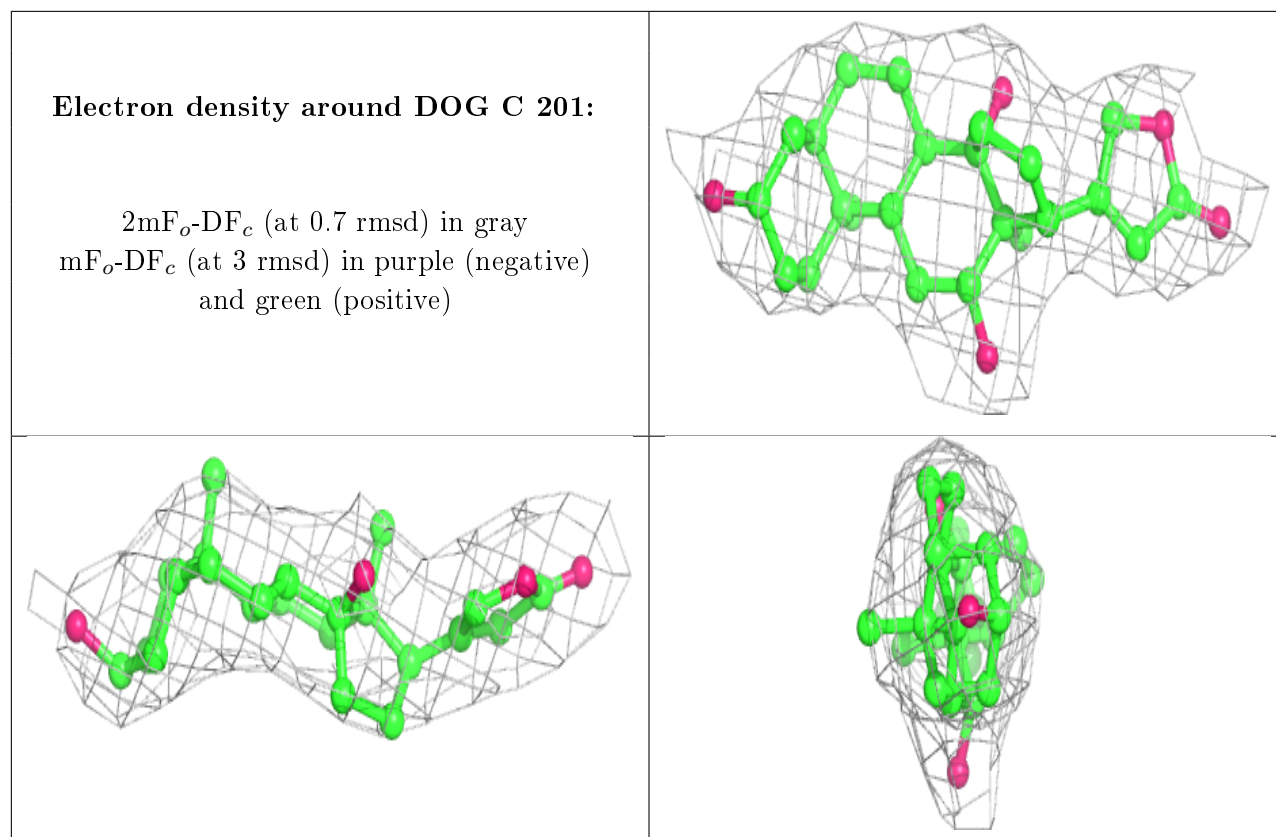
**Electron density around DOG I 201:**

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

**Electron density around DOG A 201:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.