



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 05:22 AM BST

PDB ID : 5FR9  
Title : Structure of transaminase ATA-117 arRmut11 from *Arthrobacter* sp. KNK168 inhibited with 1-(4-Bromophenyl)-2-fluoroethylamine  
Authors : Cuetos, A.; Kroutil, W.; Lavandera, I.; Grogan, G.  
Deposited on : 2015-12-16  
Resolution : 2.81 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.

---

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	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

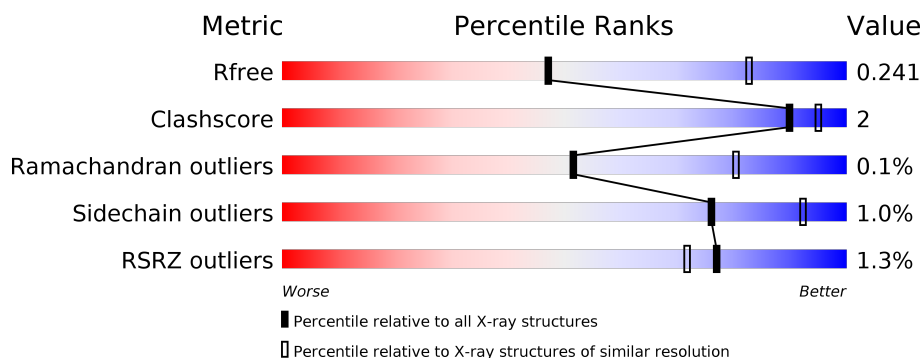
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.81 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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	333	91% 5% .
1	B	333	91% . . .
1	C	333	93% . . .
1	D	333	92% . . .
1	E	333	2% 92% . .
1	F	333	92% . . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	333	<div><div></div><div>94%</div><div></div><div></div></div>
1	H	333	<div><div>%</div><div></div><div>92%</div><div></div></div>
1	I	333	<div><div>3%</div><div></div><div>95%</div><div></div></div>
1	J	333	<div><div>2%</div><div></div><div>92%</div><div></div></div>
1	K	333	<div><div>3%</div><div></div><div>91%</div><div></div></div>
1	L	333	<div><div>3%</div><div></div><div>91%</div><div>5%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29531 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 (R)-AMINE TRANSAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2445	1559	413	467	6			
1	B	320	Total	C	N	O	S	0	0	0
			2473	1577	417	473	6			
1	C	321	Total	C	N	O	S	0	0	0
			2429	1553	408	462	6			
1	D	322	Total	C	N	O	S	0	0	0
			2496	1591	423	476	6			
1	E	321	Total	C	N	O	S	0	0	0
			2374	1519	403	446	6			
1	F	322	Total	C	N	O	S	0	0	0
			2461	1575	413	467	6			
1	G	321	Total	C	N	O	S	0	0	0
			2465	1574	415	470	6			
1	H	321	Total	C	N	O	S	0	0	0
			2469	1578	415	470	6			
1	I	320	Total	C	N	O	S	0	0	0
			2289	1465	392	427	5			
1	J	319	Total	C	N	O	S	0	0	0
			2406	1538	407	455	6			
1	K	319	Total	C	N	O	S	0	0	0
			2347	1492	407	442	6			
1	L	318	Total	C	N	O	S	0	0	0
			2280	1452	389	433	6			

There are 372 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	331	ALA	-	expression tag	UNP F7J696
A	332	LEU	-	expression tag	UNP F7J696
A	333	GLU	-	expression tag	UNP F7J696
A	8	PRO	SER	engineered mutation	UNP F7J696
A	60	PHE	TYR	engineered mutation	UNP F7J696

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	TYR	LEU	engineered mutation	UNP F7J696
A	62	THR	HIS	engineered mutation	UNP F7J696
A	65	ALA	VAL	engineered mutation	UNP F7J696
A	69	THR	VAL	engineered mutation	UNP F7J696
A	81	GLY	ASP	engineered mutation	UNP F7J696
A	94	ILE	MET	engineered mutation	UNP F7J696
A	96	LEU	ILE	engineered mutation	UNP F7J696
A	122	MET	PHE	engineered mutation	UNP F7J696
A	124	THR	SER	engineered mutation	UNP F7J696
A	126	THR	SER	engineered mutation	UNP F7J696
A	136	PHE	GLY	engineered mutation	UNP F7J696
A	150	SER	TYR	engineered mutation	UNP F7J696
A	152	CYS	VAL	engineered mutation	UNP F7J696
A	169	LEU	ALA	engineered mutation	UNP F7J696
A	199	ILE	VAL	engineered mutation	UNP F7J696
A	209	LEU	ALA	engineered mutation	UNP F7J696
A	215	CYS	GLY	engineered mutation	UNP F7J696
A	217	ASN	GLY	engineered mutation	UNP F7J696
A	223	PRO	SER	engineered mutation	UNP F7J696
A	269	PRO	LEU	engineered mutation	UNP F7J696
A	273	TYR	LEU	engineered mutation	UNP F7J696
A	282	SER	THR	engineered mutation	UNP F7J696
A	284	GLY	ALA	engineered mutation	UNP F7J696
A	297	SER	PRO	engineered mutation	UNP F7J696
A	306	VAL	ILE	engineered mutation	UNP F7J696
A	321	PRO	SER	engineered mutation	UNP F7J696
B	331	ALA	-	expression tag	UNP F7J696
B	332	LEU	-	expression tag	UNP F7J696
B	333	GLU	-	expression tag	UNP F7J696
B	8	PRO	SER	engineered mutation	UNP F7J696
B	60	PHE	TYR	engineered mutation	UNP F7J696
B	61	TYR	LEU	engineered mutation	UNP F7J696
B	62	THR	HIS	engineered mutation	UNP F7J696
B	65	ALA	VAL	engineered mutation	UNP F7J696
B	69	THR	VAL	engineered mutation	UNP F7J696
B	81	GLY	ASP	engineered mutation	UNP F7J696
B	94	ILE	MET	engineered mutation	UNP F7J696
B	96	LEU	ILE	engineered mutation	UNP F7J696
B	122	MET	PHE	engineered mutation	UNP F7J696
B	124	THR	SER	engineered mutation	UNP F7J696
B	126	THR	SER	engineered mutation	UNP F7J696
B	136	PHE	GLY	engineered mutation	UNP F7J696

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	150	SER	TYR	engineered mutation	UNP F7J696
B	152	CYS	VAL	engineered mutation	UNP F7J696
B	169	LEU	ALA	engineered mutation	UNP F7J696
B	199	ILE	VAL	engineered mutation	UNP F7J696
B	209	LEU	ALA	engineered mutation	UNP F7J696
B	215	CYS	GLY	engineered mutation	UNP F7J696
B	217	ASN	GLY	engineered mutation	UNP F7J696
B	223	PRO	SER	engineered mutation	UNP F7J696
B	269	PRO	LEU	engineered mutation	UNP F7J696
B	273	TYR	LEU	engineered mutation	UNP F7J696
B	282	SER	THR	engineered mutation	UNP F7J696
B	284	GLY	ALA	engineered mutation	UNP F7J696
B	297	SER	PRO	engineered mutation	UNP F7J696
B	306	VAL	ILE	engineered mutation	UNP F7J696
B	321	PRO	SER	engineered mutation	UNP F7J696
C	331	ALA	-	expression tag	UNP F7J696
C	332	LEU	-	expression tag	UNP F7J696
C	333	GLU	-	expression tag	UNP F7J696
C	8	PRO	SER	engineered mutation	UNP F7J696
C	60	PHE	TYR	engineered mutation	UNP F7J696
C	61	TYR	LEU	engineered mutation	UNP F7J696
C	62	THR	HIS	engineered mutation	UNP F7J696
C	65	ALA	VAL	engineered mutation	UNP F7J696
C	69	THR	VAL	engineered mutation	UNP F7J696
C	81	GLY	ASP	engineered mutation	UNP F7J696
C	94	ILE	MET	engineered mutation	UNP F7J696
C	96	LEU	ILE	engineered mutation	UNP F7J696
C	122	MET	PHE	engineered mutation	UNP F7J696
C	124	THR	SER	engineered mutation	UNP F7J696
C	126	THR	SER	engineered mutation	UNP F7J696
C	136	PHE	GLY	engineered mutation	UNP F7J696
C	150	SER	TYR	engineered mutation	UNP F7J696
C	152	CYS	VAL	engineered mutation	UNP F7J696
C	169	LEU	ALA	engineered mutation	UNP F7J696
C	199	ILE	VAL	engineered mutation	UNP F7J696
C	209	LEU	ALA	engineered mutation	UNP F7J696
C	215	CYS	GLY	engineered mutation	UNP F7J696
C	217	ASN	GLY	engineered mutation	UNP F7J696
C	223	PRO	SER	engineered mutation	UNP F7J696
C	269	PRO	LEU	engineered mutation	UNP F7J696
C	273	TYR	LEU	engineered mutation	UNP F7J696
C	282	SER	THR	engineered mutation	UNP F7J696

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	284	GLY	ALA	engineered mutation	UNP F7J696
C	297	SER	PRO	engineered mutation	UNP F7J696
C	306	VAL	ILE	engineered mutation	UNP F7J696
C	321	PRO	SER	engineered mutation	UNP F7J696
D	331	ALA	-	expression tag	UNP F7J696
D	332	LEU	-	expression tag	UNP F7J696
D	333	GLU	-	expression tag	UNP F7J696
D	8	PRO	SER	engineered mutation	UNP F7J696
D	60	PHE	TYR	engineered mutation	UNP F7J696
D	61	TYR	LEU	engineered mutation	UNP F7J696
D	62	THR	HIS	engineered mutation	UNP F7J696
D	65	ALA	VAL	engineered mutation	UNP F7J696
D	69	THR	VAL	engineered mutation	UNP F7J696
D	81	GLY	ASP	engineered mutation	UNP F7J696
D	94	ILE	MET	engineered mutation	UNP F7J696
D	96	LEU	ILE	engineered mutation	UNP F7J696
D	122	MET	PHE	engineered mutation	UNP F7J696
D	124	THR	SER	engineered mutation	UNP F7J696
D	126	THR	SER	engineered mutation	UNP F7J696
D	136	PHE	GLY	engineered mutation	UNP F7J696
D	150	SER	TYR	engineered mutation	UNP F7J696
D	152	CYS	VAL	engineered mutation	UNP F7J696
D	169	LEU	ALA	engineered mutation	UNP F7J696
D	199	ILE	VAL	engineered mutation	UNP F7J696
D	209	LEU	ALA	engineered mutation	UNP F7J696
D	215	CYS	GLY	engineered mutation	UNP F7J696
D	217	ASN	GLY	engineered mutation	UNP F7J696
D	223	PRO	SER	engineered mutation	UNP F7J696
D	269	PRO	LEU	engineered mutation	UNP F7J696
D	273	TYR	LEU	engineered mutation	UNP F7J696
D	282	SER	THR	engineered mutation	UNP F7J696
D	284	GLY	ALA	engineered mutation	UNP F7J696
D	297	SER	PRO	engineered mutation	UNP F7J696
D	306	VAL	ILE	engineered mutation	UNP F7J696
D	321	PRO	SER	engineered mutation	UNP F7J696
E	331	ALA	-	expression tag	UNP F7J696
E	332	LEU	-	expression tag	UNP F7J696
E	333	GLU	-	expression tag	UNP F7J696
E	8	PRO	SER	engineered mutation	UNP F7J696
E	60	PHE	TYR	engineered mutation	UNP F7J696
E	61	TYR	LEU	engineered mutation	UNP F7J696
E	62	THR	HIS	engineered mutation	UNP F7J696

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	65	ALA	VAL	engineered mutation	UNP F7J696
E	69	THR	VAL	engineered mutation	UNP F7J696
E	81	GLY	ASP	engineered mutation	UNP F7J696
E	94	ILE	MET	engineered mutation	UNP F7J696
E	96	LEU	ILE	engineered mutation	UNP F7J696
E	122	MET	PHE	engineered mutation	UNP F7J696
E	124	THR	SER	engineered mutation	UNP F7J696
E	126	THR	SER	engineered mutation	UNP F7J696
E	136	PHE	GLY	engineered mutation	UNP F7J696
E	150	SER	TYR	engineered mutation	UNP F7J696
E	152	CYS	VAL	engineered mutation	UNP F7J696
E	169	LEU	ALA	engineered mutation	UNP F7J696
E	199	ILE	VAL	engineered mutation	UNP F7J696
E	209	LEU	ALA	engineered mutation	UNP F7J696
E	215	CYS	GLY	engineered mutation	UNP F7J696
E	217	ASN	GLY	engineered mutation	UNP F7J696
E	223	PRO	SER	engineered mutation	UNP F7J696
E	269	PRO	LEU	engineered mutation	UNP F7J696
E	273	TYR	LEU	engineered mutation	UNP F7J696
E	282	SER	THR	engineered mutation	UNP F7J696
E	284	GLY	ALA	engineered mutation	UNP F7J696
E	297	SER	PRO	engineered mutation	UNP F7J696
E	306	VAL	ILE	engineered mutation	UNP F7J696
E	321	PRO	SER	engineered mutation	UNP F7J696
F	331	ALA	-	expression tag	UNP F7J696
F	332	LEU	-	expression tag	UNP F7J696
F	333	GLU	-	expression tag	UNP F7J696
F	8	PRO	SER	engineered mutation	UNP F7J696
F	60	PHE	TYR	engineered mutation	UNP F7J696
F	61	TYR	LEU	engineered mutation	UNP F7J696
F	62	THR	HIS	engineered mutation	UNP F7J696
F	65	ALA	VAL	engineered mutation	UNP F7J696
F	69	THR	VAL	engineered mutation	UNP F7J696
F	81	GLY	ASP	engineered mutation	UNP F7J696
F	94	ILE	MET	engineered mutation	UNP F7J696
F	96	LEU	ILE	engineered mutation	UNP F7J696
F	122	MET	PHE	engineered mutation	UNP F7J696
F	124	THR	SER	engineered mutation	UNP F7J696
F	126	THR	SER	engineered mutation	UNP F7J696
F	136	PHE	GLY	engineered mutation	UNP F7J696
F	150	SER	TYR	engineered mutation	UNP F7J696
F	152	CYS	VAL	engineered mutation	UNP F7J696

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	169	LEU	ALA	engineered mutation	UNP F7J696
F	199	ILE	VAL	engineered mutation	UNP F7J696
F	209	LEU	ALA	engineered mutation	UNP F7J696
F	215	CYS	GLY	engineered mutation	UNP F7J696
F	217	ASN	GLY	engineered mutation	UNP F7J696
F	223	PRO	SER	engineered mutation	UNP F7J696
F	269	PRO	LEU	engineered mutation	UNP F7J696
F	273	TYR	LEU	engineered mutation	UNP F7J696
F	282	SER	THR	engineered mutation	UNP F7J696
F	284	GLY	ALA	engineered mutation	UNP F7J696
F	297	SER	PRO	engineered mutation	UNP F7J696
F	306	VAL	ILE	engineered mutation	UNP F7J696
F	321	PRO	SER	engineered mutation	UNP F7J696
G	331	ALA	-	expression tag	UNP F7J696
G	332	LEU	-	expression tag	UNP F7J696
G	333	GLU	-	expression tag	UNP F7J696
G	8	PRO	SER	engineered mutation	UNP F7J696
G	60	PHE	TYR	engineered mutation	UNP F7J696
G	61	TYR	LEU	engineered mutation	UNP F7J696
G	62	THR	HIS	engineered mutation	UNP F7J696
G	65	ALA	VAL	engineered mutation	UNP F7J696
G	69	THR	VAL	engineered mutation	UNP F7J696
G	81	GLY	ASP	engineered mutation	UNP F7J696
G	94	ILE	MET	engineered mutation	UNP F7J696
G	96	LEU	ILE	engineered mutation	UNP F7J696
G	122	MET	PHE	engineered mutation	UNP F7J696
G	124	THR	SER	engineered mutation	UNP F7J696
G	126	THR	SER	engineered mutation	UNP F7J696
G	136	PHE	GLY	engineered mutation	UNP F7J696
G	150	SER	TYR	engineered mutation	UNP F7J696
G	152	CYS	VAL	engineered mutation	UNP F7J696
G	169	LEU	ALA	engineered mutation	UNP F7J696
G	199	ILE	VAL	engineered mutation	UNP F7J696
G	209	LEU	ALA	engineered mutation	UNP F7J696
G	215	CYS	GLY	engineered mutation	UNP F7J696
G	217	ASN	GLY	engineered mutation	UNP F7J696
G	223	PRO	SER	engineered mutation	UNP F7J696
G	269	PRO	LEU	engineered mutation	UNP F7J696
G	273	TYR	LEU	engineered mutation	UNP F7J696
G	282	SER	THR	engineered mutation	UNP F7J696
G	284	GLY	ALA	engineered mutation	UNP F7J696
G	297	SER	PRO	engineered mutation	UNP F7J696

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
G	306	VAL	ILE	engineered mutation	UNP F7J696
G	321	PRO	SER	engineered mutation	UNP F7J696
H	331	ALA	-	expression tag	UNP F7J696
H	332	LEU	-	expression tag	UNP F7J696
H	333	GLU	-	expression tag	UNP F7J696
H	8	PRO	SER	engineered mutation	UNP F7J696
H	60	PHE	TYR	engineered mutation	UNP F7J696
H	61	TYR	LEU	engineered mutation	UNP F7J696
H	62	THR	HIS	engineered mutation	UNP F7J696
H	65	ALA	VAL	engineered mutation	UNP F7J696
H	69	THR	VAL	engineered mutation	UNP F7J696
H	81	GLY	ASP	engineered mutation	UNP F7J696
H	94	ILE	MET	engineered mutation	UNP F7J696
H	96	LEU	ILE	engineered mutation	UNP F7J696
H	122	MET	PHE	engineered mutation	UNP F7J696
H	124	THR	SER	engineered mutation	UNP F7J696
H	126	THR	SER	engineered mutation	UNP F7J696
H	136	PHE	GLY	engineered mutation	UNP F7J696
H	150	SER	TYR	engineered mutation	UNP F7J696
H	152	CYS	VAL	engineered mutation	UNP F7J696
H	169	LEU	ALA	engineered mutation	UNP F7J696
H	199	ILE	VAL	engineered mutation	UNP F7J696
H	209	LEU	ALA	engineered mutation	UNP F7J696
H	215	CYS	GLY	engineered mutation	UNP F7J696
H	217	ASN	GLY	engineered mutation	UNP F7J696
H	223	PRO	SER	engineered mutation	UNP F7J696
H	269	PRO	LEU	engineered mutation	UNP F7J696
H	273	TYR	LEU	engineered mutation	UNP F7J696
H	282	SER	THR	engineered mutation	UNP F7J696
H	284	GLY	ALA	engineered mutation	UNP F7J696
H	297	SER	PRO	engineered mutation	UNP F7J696
H	306	VAL	ILE	engineered mutation	UNP F7J696
H	321	PRO	SER	engineered mutation	UNP F7J696
I	331	ALA	-	expression tag	UNP F7J696
I	332	LEU	-	expression tag	UNP F7J696
I	333	GLU	-	expression tag	UNP F7J696
I	8	PRO	SER	engineered mutation	UNP F7J696
I	60	PHE	TYR	engineered mutation	UNP F7J696
I	61	TYR	LEU	engineered mutation	UNP F7J696
I	62	THR	HIS	engineered mutation	UNP F7J696
I	65	ALA	VAL	engineered mutation	UNP F7J696
I	69	THR	VAL	engineered mutation	UNP F7J696

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
I	81	GLY	ASP	engineered mutation	UNP F7J696
I	94	ILE	MET	engineered mutation	UNP F7J696
I	96	LEU	ILE	engineered mutation	UNP F7J696
I	122	MET	PHE	engineered mutation	UNP F7J696
I	124	THR	SER	engineered mutation	UNP F7J696
I	126	THR	SER	engineered mutation	UNP F7J696
I	136	PHE	GLY	engineered mutation	UNP F7J696
I	150	SER	TYR	engineered mutation	UNP F7J696
I	152	CYS	VAL	engineered mutation	UNP F7J696
I	169	LEU	ALA	engineered mutation	UNP F7J696
I	199	ILE	VAL	engineered mutation	UNP F7J696
I	209	LEU	ALA	engineered mutation	UNP F7J696
I	215	CYS	GLY	engineered mutation	UNP F7J696
I	217	ASN	GLY	engineered mutation	UNP F7J696
I	223	PRO	SER	engineered mutation	UNP F7J696
I	269	PRO	LEU	engineered mutation	UNP F7J696
I	273	TYR	LEU	engineered mutation	UNP F7J696
I	282	SER	THR	engineered mutation	UNP F7J696
I	284	GLY	ALA	engineered mutation	UNP F7J696
I	297	SER	PRO	engineered mutation	UNP F7J696
I	306	VAL	ILE	engineered mutation	UNP F7J696
I	321	PRO	SER	engineered mutation	UNP F7J696
J	331	ALA	-	expression tag	UNP F7J696
J	332	LEU	-	expression tag	UNP F7J696
J	333	GLU	-	expression tag	UNP F7J696
J	8	PRO	SER	engineered mutation	UNP F7J696
J	60	PHE	TYR	engineered mutation	UNP F7J696
J	61	TYR	LEU	engineered mutation	UNP F7J696
J	62	THR	HIS	engineered mutation	UNP F7J696
J	65	ALA	VAL	engineered mutation	UNP F7J696
J	69	THR	VAL	engineered mutation	UNP F7J696
J	81	GLY	ASP	engineered mutation	UNP F7J696
J	94	ILE	MET	engineered mutation	UNP F7J696
J	96	LEU	ILE	engineered mutation	UNP F7J696
J	122	MET	PHE	engineered mutation	UNP F7J696
J	124	THR	SER	engineered mutation	UNP F7J696
J	126	THR	SER	engineered mutation	UNP F7J696
J	136	PHE	GLY	engineered mutation	UNP F7J696
J	150	SER	TYR	engineered mutation	UNP F7J696
J	152	CYS	VAL	engineered mutation	UNP F7J696
J	169	LEU	ALA	engineered mutation	UNP F7J696
J	199	ILE	VAL	engineered mutation	UNP F7J696

*Continued on next page...*

*Continued from previous page...*

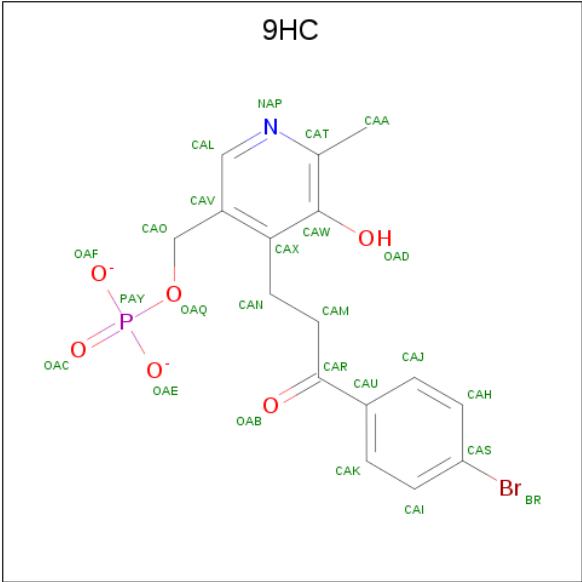
Chain	Residue	Modelled	Actual	Comment	Reference
J	209	LEU	ALA	engineered mutation	UNP F7J696
J	215	CYS	GLY	engineered mutation	UNP F7J696
J	217	ASN	GLY	engineered mutation	UNP F7J696
J	223	PRO	SER	engineered mutation	UNP F7J696
J	269	PRO	LEU	engineered mutation	UNP F7J696
J	273	TYR	LEU	engineered mutation	UNP F7J696
J	282	SER	THR	engineered mutation	UNP F7J696
J	284	GLY	ALA	engineered mutation	UNP F7J696
J	297	SER	PRO	engineered mutation	UNP F7J696
J	306	VAL	ILE	engineered mutation	UNP F7J696
J	321	PRO	SER	engineered mutation	UNP F7J696
K	331	ALA	-	expression tag	UNP F7J696
K	332	LEU	-	expression tag	UNP F7J696
K	333	GLU	-	expression tag	UNP F7J696
K	8	PRO	SER	engineered mutation	UNP F7J696
K	60	PHE	TYR	engineered mutation	UNP F7J696
K	61	TYR	LEU	engineered mutation	UNP F7J696
K	62	THR	HIS	engineered mutation	UNP F7J696
K	65	ALA	VAL	engineered mutation	UNP F7J696
K	69	THR	VAL	engineered mutation	UNP F7J696
K	81	GLY	ASP	engineered mutation	UNP F7J696
K	94	ILE	MET	engineered mutation	UNP F7J696
K	96	LEU	ILE	engineered mutation	UNP F7J696
K	122	MET	PHE	engineered mutation	UNP F7J696
K	124	THR	SER	engineered mutation	UNP F7J696
K	126	THR	SER	engineered mutation	UNP F7J696
K	136	PHE	GLY	engineered mutation	UNP F7J696
K	150	SER	TYR	engineered mutation	UNP F7J696
K	152	CYS	VAL	engineered mutation	UNP F7J696
K	169	LEU	ALA	engineered mutation	UNP F7J696
K	199	ILE	VAL	engineered mutation	UNP F7J696
K	209	LEU	ALA	engineered mutation	UNP F7J696
K	215	CYS	GLY	engineered mutation	UNP F7J696
K	217	ASN	GLY	engineered mutation	UNP F7J696
K	223	PRO	SER	engineered mutation	UNP F7J696
K	269	PRO	LEU	engineered mutation	UNP F7J696
K	273	TYR	LEU	engineered mutation	UNP F7J696
K	282	SER	THR	engineered mutation	UNP F7J696
K	284	GLY	ALA	engineered mutation	UNP F7J696
K	297	SER	PRO	engineered mutation	UNP F7J696
K	306	VAL	ILE	engineered mutation	UNP F7J696
K	321	PRO	SER	engineered mutation	UNP F7J696

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
L	331	ALA	-	expression tag	UNP F7J696
L	332	LEU	-	expression tag	UNP F7J696
L	333	GLU	-	expression tag	UNP F7J696
L	8	PRO	SER	engineered mutation	UNP F7J696
L	60	PHE	TYR	engineered mutation	UNP F7J696
L	61	TYR	LEU	engineered mutation	UNP F7J696
L	62	THR	HIS	engineered mutation	UNP F7J696
L	65	ALA	VAL	engineered mutation	UNP F7J696
L	69	THR	VAL	engineered mutation	UNP F7J696
L	81	GLY	ASP	engineered mutation	UNP F7J696
L	94	ILE	MET	engineered mutation	UNP F7J696
L	96	LEU	ILE	engineered mutation	UNP F7J696
L	122	MET	PHE	engineered mutation	UNP F7J696
L	124	THR	SER	engineered mutation	UNP F7J696
L	126	THR	SER	engineered mutation	UNP F7J696
L	136	PHE	GLY	engineered mutation	UNP F7J696
L	150	SER	TYR	engineered mutation	UNP F7J696
L	152	CYS	VAL	engineered mutation	UNP F7J696
L	169	LEU	ALA	engineered mutation	UNP F7J696
L	199	ILE	VAL	engineered mutation	UNP F7J696
L	209	LEU	ALA	engineered mutation	UNP F7J696
L	215	CYS	GLY	engineered mutation	UNP F7J696
L	217	ASN	GLY	engineered mutation	UNP F7J696
L	223	PRO	SER	engineered mutation	UNP F7J696
L	269	PRO	LEU	engineered mutation	UNP F7J696
L	273	TYR	LEU	engineered mutation	UNP F7J696
L	282	SER	THR	engineered mutation	UNP F7J696
L	284	GLY	ALA	engineered mutation	UNP F7J696
L	297	SER	PRO	engineered mutation	UNP F7J696
L	306	VAL	ILE	engineered mutation	UNP F7J696
L	321	PRO	SER	engineered mutation	UNP F7J696

- Molecule 2 is [4-[3-(4-bromophenyl)-3-oxidanylidene-propyl]-6-methyl-5-oxidanyl-pyridin-3-yl]methyl phosphate (three-letter code: 9HC) (formula: C<sub>16</sub>H<sub>15</sub>BrNO<sub>6</sub>P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	P	0	0
			25	1	16	1	6	1		
2	B	1	Total	Br	C	N	O	P	0	0
			25	1	16	1	6	1		
2	C	1	Total	Br	C	N	O	P	0	0
			25	1	16	1	6	1		
2	D	1	Total	Br	C	N	O	P	0	0
			25	1	16	1	6	1		
2	E	1	Total	Br	C	N	O	P	0	0
			25	1	16	1	6	1		
2	F	1	Total	Br	C	N	O	P	0	0
			25	1	16	1	6	1		
2	G	1	Total	Br	C	N	O	P	0	0
			25	1	16	1	6	1		
2	H	1	Total	Br	C	N	O	P	0	0
			25	1	16	1	6	1		
2	I	1	Total	Br	C	N	O	P	0	0
			25	1	16	1	6	1		
2	J	1	Total	Br	C	N	O	P	0	0
			25	1	16	1	6	1		
2	K	1	Total	Br	C	N	O	P	0	0
			25	1	16	1	6	1		
2	L	1	Total	Br	C	N	O	P	0	0
			25	1	16	1	6	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total 35	O 35	0	0
3	B	41	Total 41	O 41	0	0
3	C	20	Total 20	O 20	0	0
3	D	60	Total 60	O 60	0	0
3	E	6	Total 6	O 6	0	0
3	F	22	Total 22	O 22	0	0
3	G	40	Total 40	O 40	0	0
3	H	28	Total 28	O 28	0	0
3	I	5	Total 5	O 5	0	0
3	J	28	Total 28	O 28	0	0
3	K	4	Total 4	O 4	0	0
3	L	8	Total 8	O 8	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: (R)-AMINE TRANSAMINASE

Chain A: 



- Molecule 1: (R)-AMINE TRANSAMINASE

Chain B: 



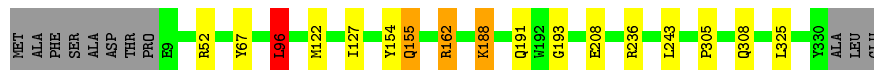
- Molecule 1: (R)-AMINE TRANSAMINASE

Chain C: 



- Molecule 1: (R)-AMINE TRANSAMINASE

Chain D: 



- Molecule 1: (R)-AMINE TRANSAMINASE

Chain E: 



- Molecule 1: (R)-AMINE TRANSAMINASE

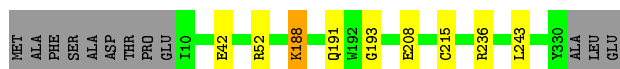


Chain F:  92% ..



• Molecule 1: (R)-AMINE TRANSAMINASE

Chain G:  94% ..



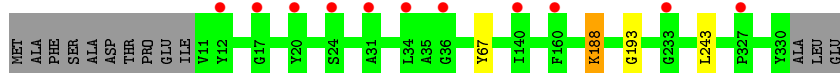
• Molecule 1: (R)-AMINE TRANSAMINASE

Chain H:  92% ..



• Molecule 1: (R)-AMINE TRANSAMINASE

Chain I:  95% ..




• Molecule 1: (R)-AMINE TRANSAMINASE

Chain J:  92% ..




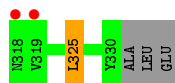
• Molecule 1: (R)-AMINE TRANSAMINASE

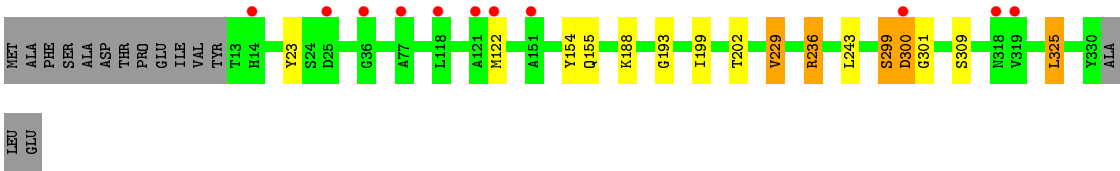
Chain K:  91% ..



• Molecule 1: (R)-AMINE TRANSAMINASE

Chain L:  91% .. 5%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.15Å 135.51Å 197.32Å 90.00° 100.40° 90.00°	Depositor
Resolution (Å)	194.08 – 2.81 48.52 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.3 (194.08-2.81) 99.3 (48.52-2.81)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.52 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.210 , 0.239 0.214 , 0.241	Depositor DCC
$R_{free}$ test set	5274 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.2	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	29531	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.21 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.0435e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: 9HC

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	0.62	0/2508	0.73	3/3435 (0.1%)
1	B	0.64	1/2537 (0.0%)	0.73	3/3473 (0.1%)
1	C	0.64	1/2493 (0.0%)	0.77	6/3419 (0.2%)
1	D	0.67	0/2560	0.83	9/3503 (0.3%)
1	E	0.67	4/2437 (0.2%)	0.75	6/3346 (0.2%)
1	F	0.64	0/2525	0.79	10/3460 (0.3%)
1	G	0.67	1/2529 (0.0%)	0.73	2/3464 (0.1%)
1	H	0.62	0/2533	0.76	6/3469 (0.2%)
1	I	0.61	0/2347	0.69	0/3231
1	J	0.67	1/2469 (0.0%)	0.80	3/3385 (0.1%)
1	K	0.64	0/2409	0.82	11/3308 (0.3%)
1	L	0.66	0/2338	0.78	5/3216 (0.2%)
All	All	0.64	8/29685 (0.0%)	0.77	64/40709 (0.2%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	85	GLU	CD-OE1	-9.46	1.15	1.25
1	E	85	GLU	CD-OE2	-7.59	1.17	1.25
1	E	85	GLU	CD-OE1	7.45	1.33	1.25
1	G	215	CYS	CB-SG	-7.16	1.70	1.82
1	C	323	SER	CA-CB	6.65	1.62	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	161	ASP	CB-CG-OD2	16.71	133.34	118.30
1	J	161	ASP	CB-CG-OD1	-13.11	106.50	118.30
1	D	162	ARG	NE-CZ-NH2	-10.72	114.94	120.30
1	D	162	ARG	NE-CZ-NH1	10.43	125.52	120.30
1	L	325	LEU	CB-CG-CD1	-10.25	93.57	111.00

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	2445	0	2348	13	0
1	B	2473	0	2383	15	0
1	C	2429	0	2301	13	1
1	D	2496	0	2413	14	0
1	E	2374	0	2191	6	0
1	F	2461	0	2364	10	0
1	G	2465	0	2368	6	0
1	H	2469	0	2379	8	0
1	I	2289	0	2091	3	0
1	J	2406	0	2284	7	0
1	K	2347	0	2163	15	1
1	L	2280	0	2053	11	0
2	A	25	0	0	1	0
2	B	25	0	0	0	0
2	C	25	0	0	1	0
2	D	25	0	0	1	0
2	E	25	0	0	0	0
2	F	25	0	0	0	0
2	G	25	0	0	0	0
2	H	25	0	0	0	0
2	I	25	0	0	0	0
2	J	25	0	0	0	0
2	K	25	0	0	0	0
2	L	25	0	0	0	0
3	A	35	0	0	0	0
3	B	41	0	0	0	0
3	C	20	0	0	0	0
3	D	60	0	0	0	0
3	E	6	0	0	0	0
3	F	22	0	0	0	0
3	G	40	0	0	0	0
3	H	28	0	0	0	0
3	I	5	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	28	0	0	0	0
3	K	4	0	0	0	0
3	L	8	0	0	0	0
All	All	29531	0	27338	103	1

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 2.

The worst 5 of 103 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:K:122:MET:HE2	1:K:155:GLN:H	1.05	1.17
1:F:122:MET:HE2	1:F:155:GLN:H	1.03	1.12
1:D:122:MET:HE2	1:D:155:GLN:H	0.93	1.09
1:L:122:MET:HE2	1:L:155:GLN:N	1.67	1.08
1:K:122:MET:HE2	1:K:155:GLN:N	1.70	1.06

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:SER:OG	1:K:19:ASP:OD1[1_455]	2.16	0.04

## 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	317/333 (95%)	307 (97%)	10 (3%)	0	100	100
1	B	318/333 (96%)	307 (96%)	10 (3%)	1 (0%)	41	70
1	C	319/333 (96%)	308 (97%)	11 (3%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	320/333 (96%)	310 (97%)	10 (3%)	0	100	100
1	E	319/333 (96%)	308 (97%)	10 (3%)	1 (0%)	41	70
1	F	320/333 (96%)	310 (97%)	10 (3%)	0	100	100
1	G	319/333 (96%)	308 (97%)	11 (3%)	0	100	100
1	H	319/333 (96%)	308 (97%)	11 (3%)	0	100	100
1	I	318/333 (96%)	307 (96%)	11 (4%)	0	100	100
1	J	317/333 (95%)	307 (97%)	10 (3%)	0	100	100
1	K	317/333 (95%)	307 (97%)	10 (3%)	0	100	100
1	L	316/333 (95%)	304 (96%)	11 (4%)	1 (0%)	41	70
All	All	3819/3996 (96%)	3691 (97%)	125 (3%)	3 (0%)	51	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	300	ASP
1	B	17	GLY
1	E	321	PRO

### 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	260/283 (92%)	257 (99%)	3 (1%)	71	91
1	B	265/283 (94%)	262 (99%)	3 (1%)	73	91
1	C	252/283 (89%)	249 (99%)	3 (1%)	71	91
1	D	268/283 (95%)	265 (99%)	3 (1%)	73	91
1	E	232/283 (82%)	231 (100%)	1 (0%)	91	97
1	F	260/283 (92%)	258 (99%)	2 (1%)	81	94
1	G	262/283 (93%)	261 (100%)	1 (0%)	91	97
1	H	263/283 (93%)	259 (98%)	4 (2%)	65	88

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	216/283 (76%)	215 (100%)	1 (0%)	88	96
1	J	249/283 (88%)	244 (98%)	5 (2%)	55	83
1	K	231/283 (82%)	229 (99%)	2 (1%)	78	93
1	L	215/283 (76%)	212 (99%)	3 (1%)	67	89
All	All	2973/3396 (88%)	2942 (99%)	31 (1%)	76	92

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	188	LYS
1	H	52	ARG
1	L	229	VAL
1	G	188	LYS
1	H	159	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	83	HIS
1	F	155	GLN
1	K	83	HIS
1	F	83	HIS
1	F	173	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.



## 5.6 Ligand geometry

12 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	9HC	B	1331	1	26,26,26	0.39	0	35,37,37	0.71	1 (2%)
2	9HC	C	1331	1	26,26,26	0.41	0	35,37,37	0.75	0
2	9HC	F	1331	1	26,26,26	0.44	0	35,37,37	0.83	1 (2%)
2	9HC	A	1331	1	26,26,26	0.38	0	35,37,37	0.68	0
2	9HC	D	1331	1	26,26,26	0.48	0	35,37,37	0.85	0
2	9HC	G	1331	1	26,26,26	0.43	0	35,37,37	0.93	2 (5%)
2	9HC	J	1331	1	26,26,26	0.43	0	35,37,37	0.81	1 (2%)
2	9HC	H	1331	1	26,26,26	0.47	0	35,37,37	0.74	0
2	9HC	K	1331	1	26,26,26	0.43	0	35,37,37	0.84	0
2	9HC	I	1331	1	26,26,26	0.42	0	35,37,37	0.79	0
2	9HC	L	1331	1	26,26,26	0.40	0	35,37,37	0.89	2 (5%)
2	9HC	E	1331	1	26,26,26	0.41	0	35,37,37	0.86	1 (2%)

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	9HC	B	1331	1	-	3/15/15/15	0/2/2/2
2	9HC	C	1331	1	-	0/15/15/15	0/2/2/2
2	9HC	F	1331	1	-	5/15/15/15	0/2/2/2
2	9HC	A	1331	1	-	4/15/15/15	0/2/2/2
2	9HC	D	1331	1	-	0/15/15/15	0/2/2/2
2	9HC	G	1331	1	-	3/15/15/15	0/2/2/2
2	9HC	J	1331	1	-	3/15/15/15	0/2/2/2
2	9HC	H	1331	1	-	0/15/15/15	0/2/2/2
2	9HC	K	1331	1	-	1/15/15/15	0/2/2/2
2	9HC	I	1331	1	-	4/15/15/15	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	9HC	L	1331	1	-	4/15/15/15	0/2/2/2
2	9HC	E	1331	1	-	0/15/15/15	0/2/2/2

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1331	9HC	CAM-CAN-CAX	-3.13	107.28	112.62
2	G	1331	9HC	OAQ-CAO-CAV	2.72	114.53	109.35
2	L	1331	9HC	CAM-CAN-CAX	-2.63	108.13	112.62
2	B	1331	9HC	CAM-CAN-CAX	-2.36	108.59	112.62
2	L	1331	9HC	OAQ-CAO-CAV	2.25	113.63	109.35

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1331	9HC	OAQ-CAO-CAV-CAX
2	F	1331	9HC	OAQ-CAO-CAV-CAL
2	F	1331	9HC	OAQ-CAO-CAV-CAX
2	F	1331	9HC	CAO-OAQ-PAY-OAC
2	F	1331	9HC	CAO-OAQ-PAY-OAE

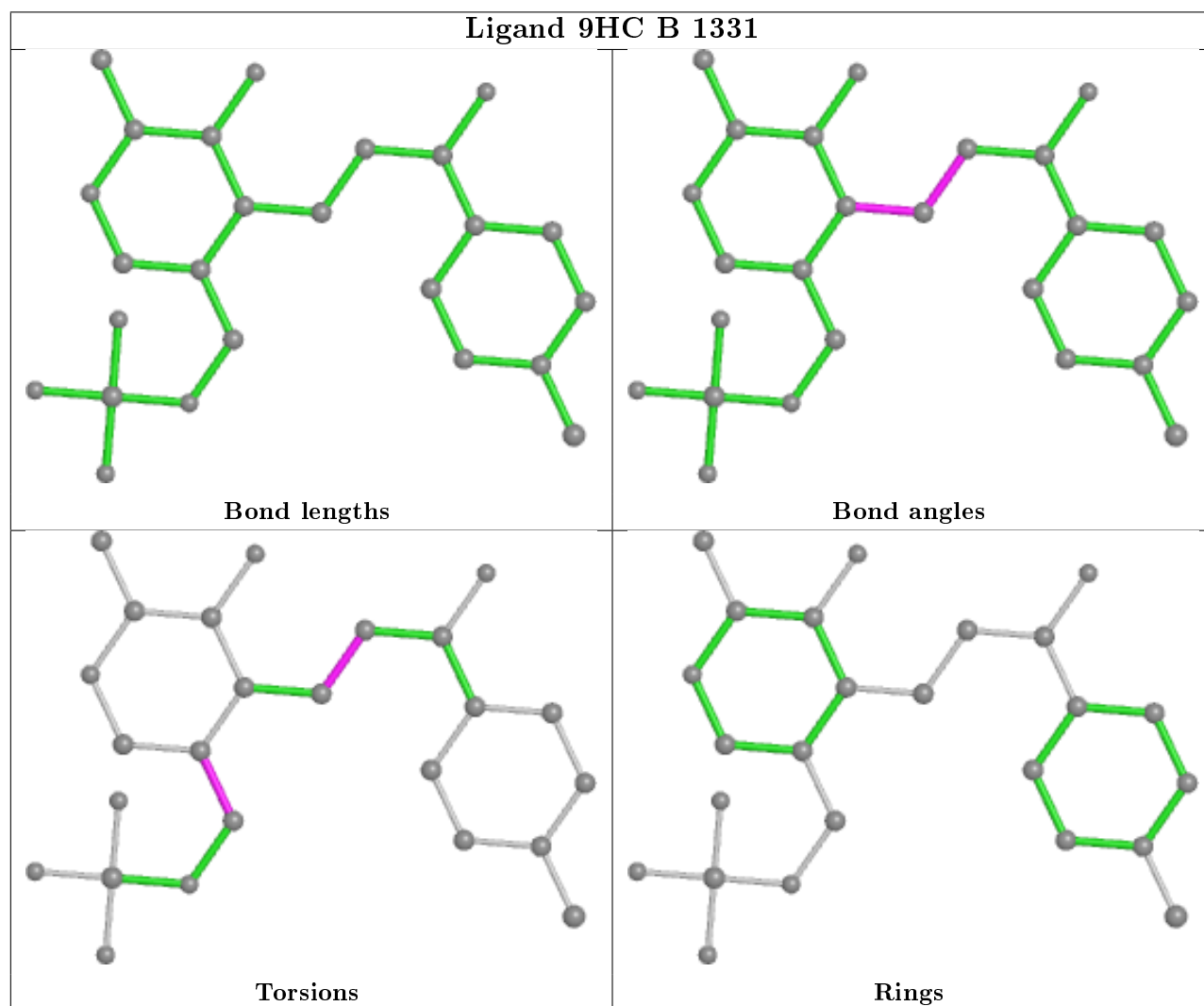
There are no ring outliers.

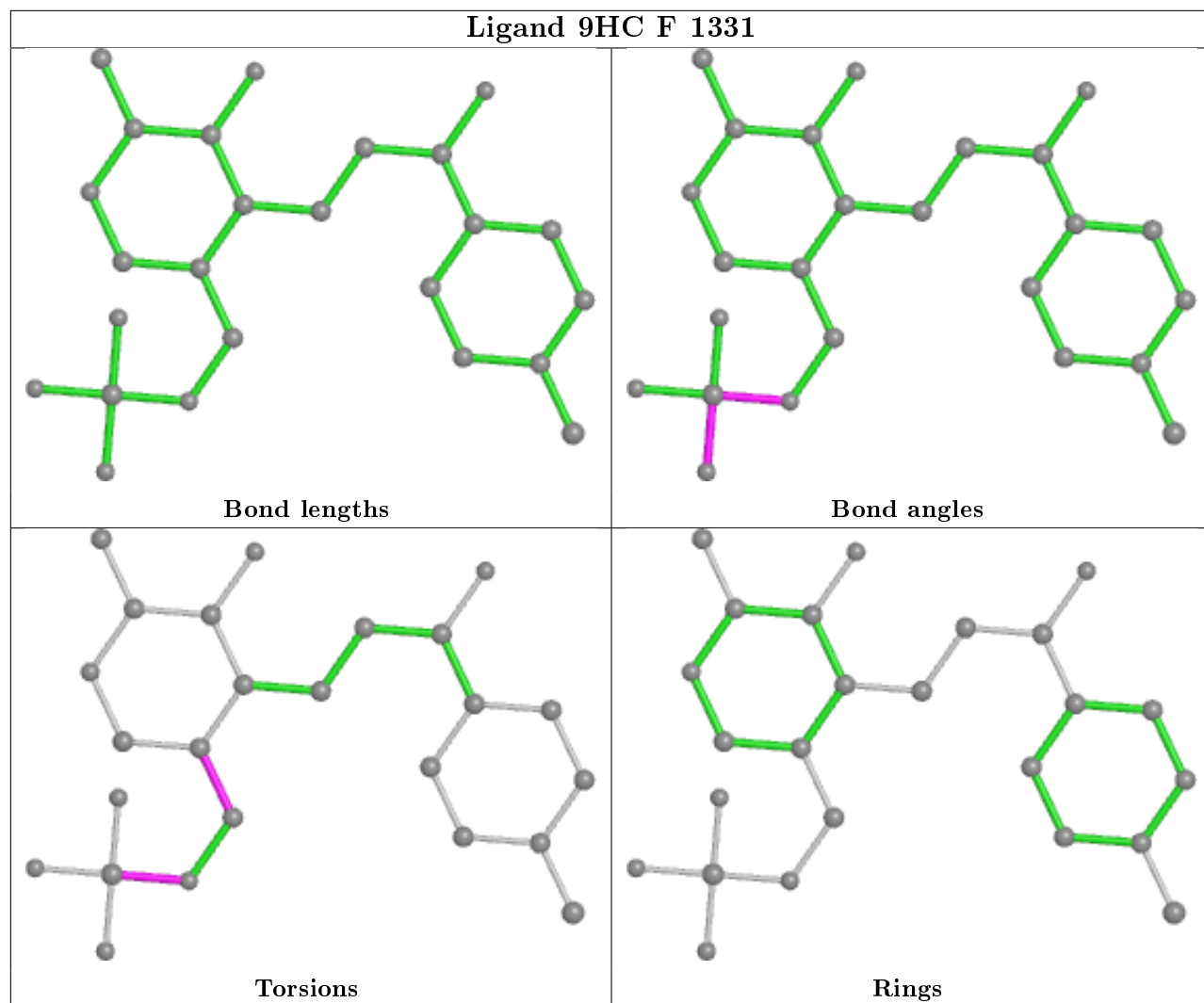
3 monomers are involved in 3 short contacts:

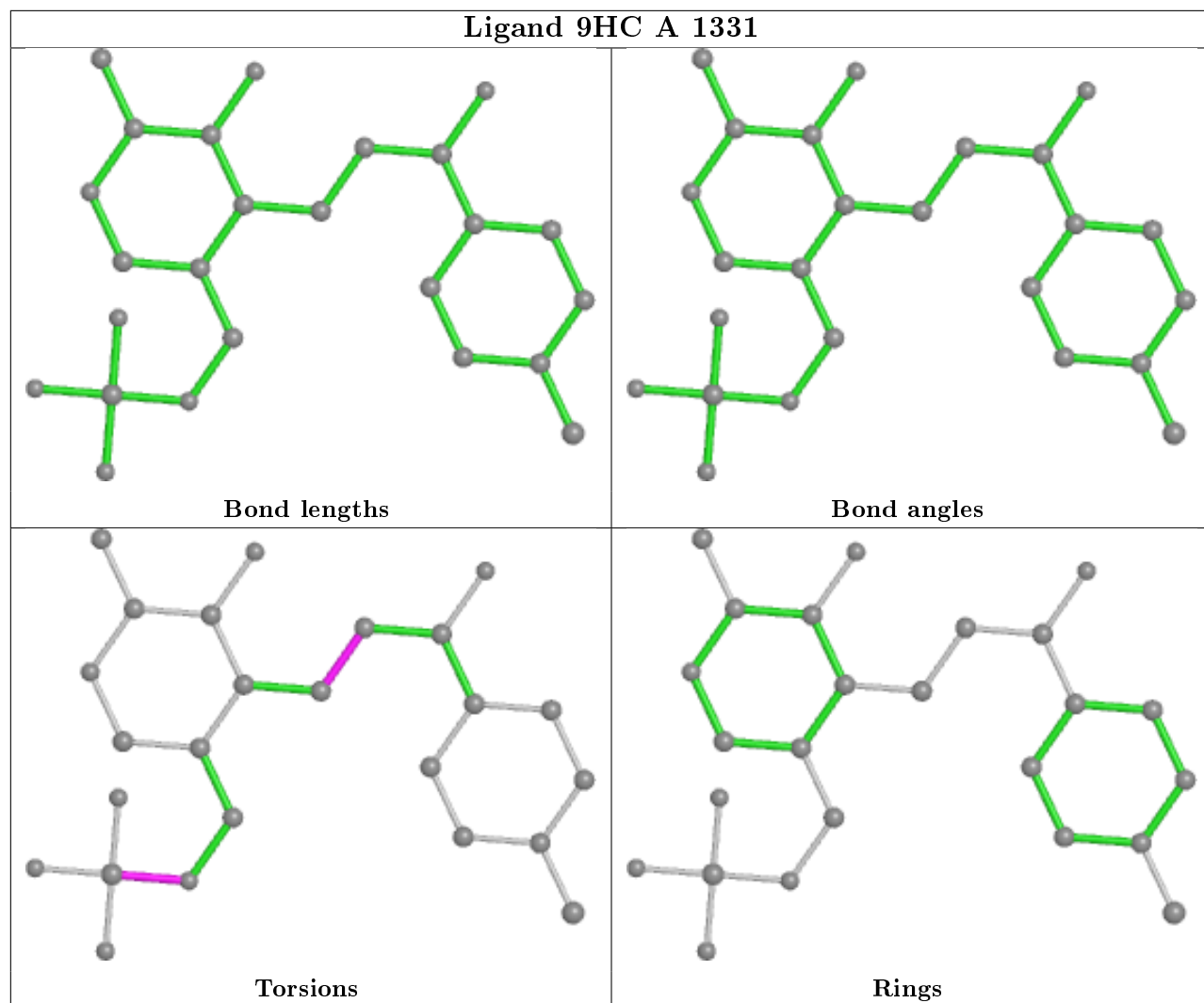
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1331	9HC	1	0
2	A	1331	9HC	1	0
2	D	1331	9HC	1	0

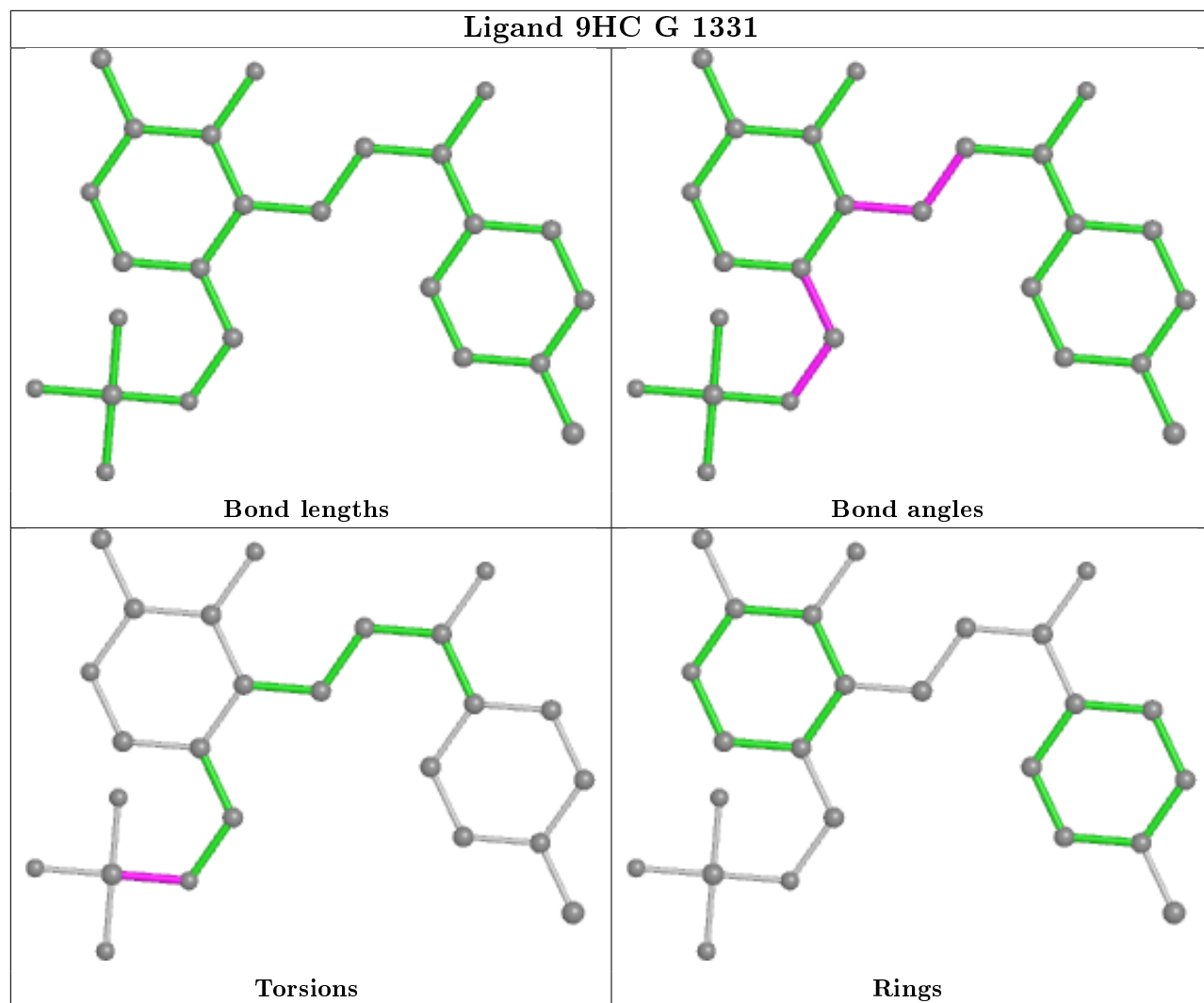
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

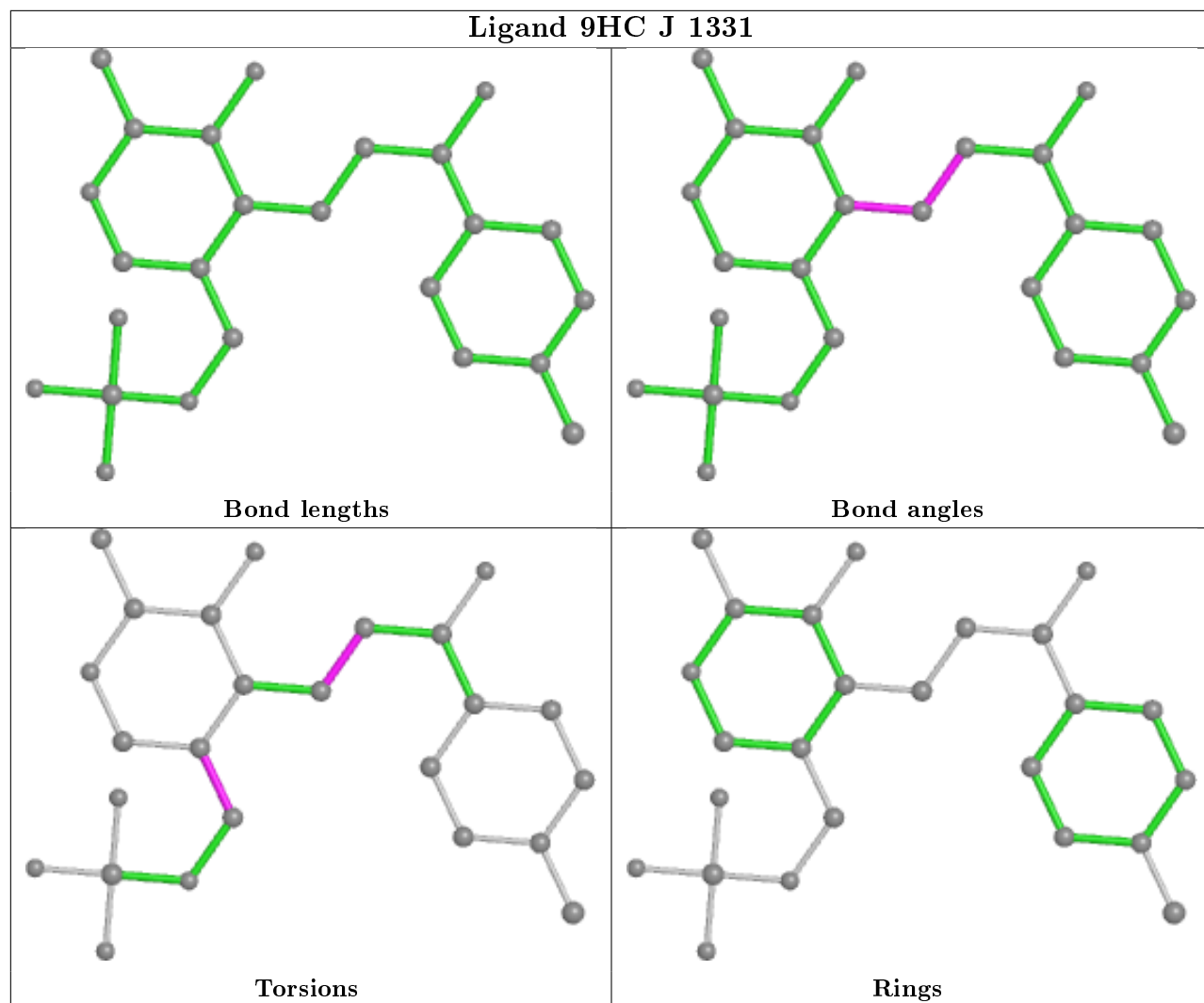
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



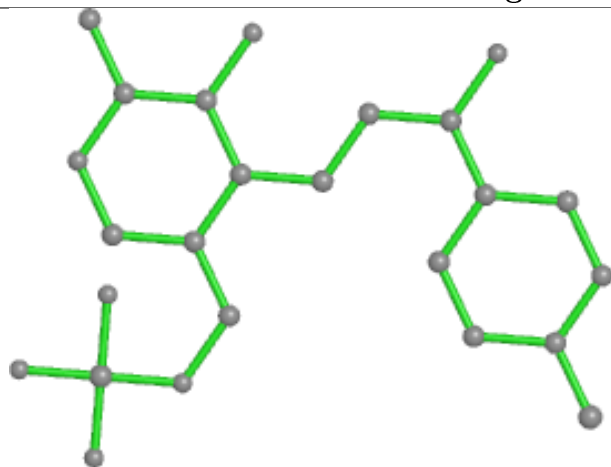




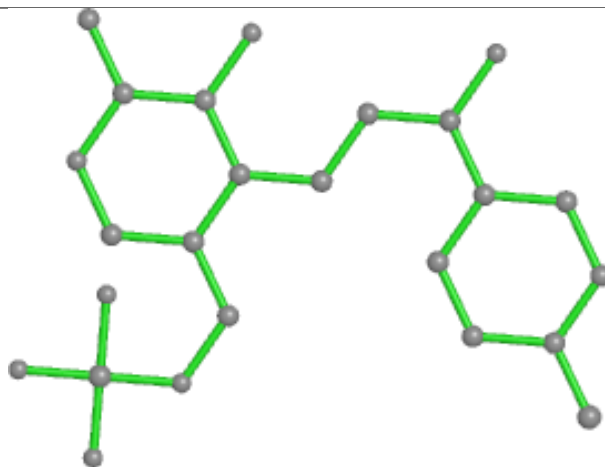




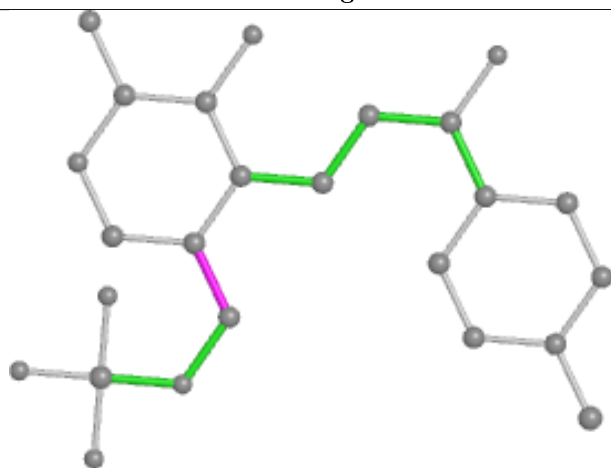
## Ligand 9HC K 1331



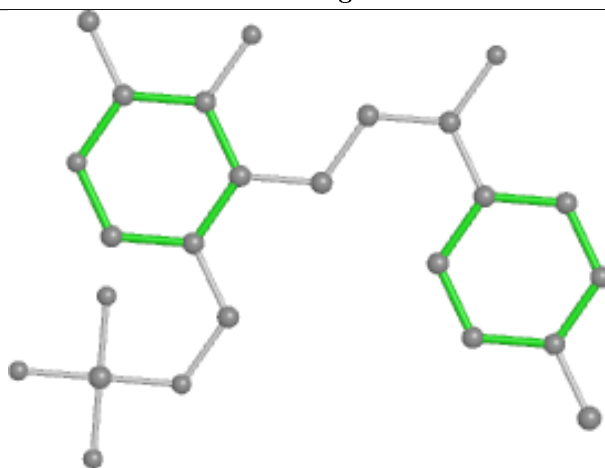
Bond lengths



Bond angles

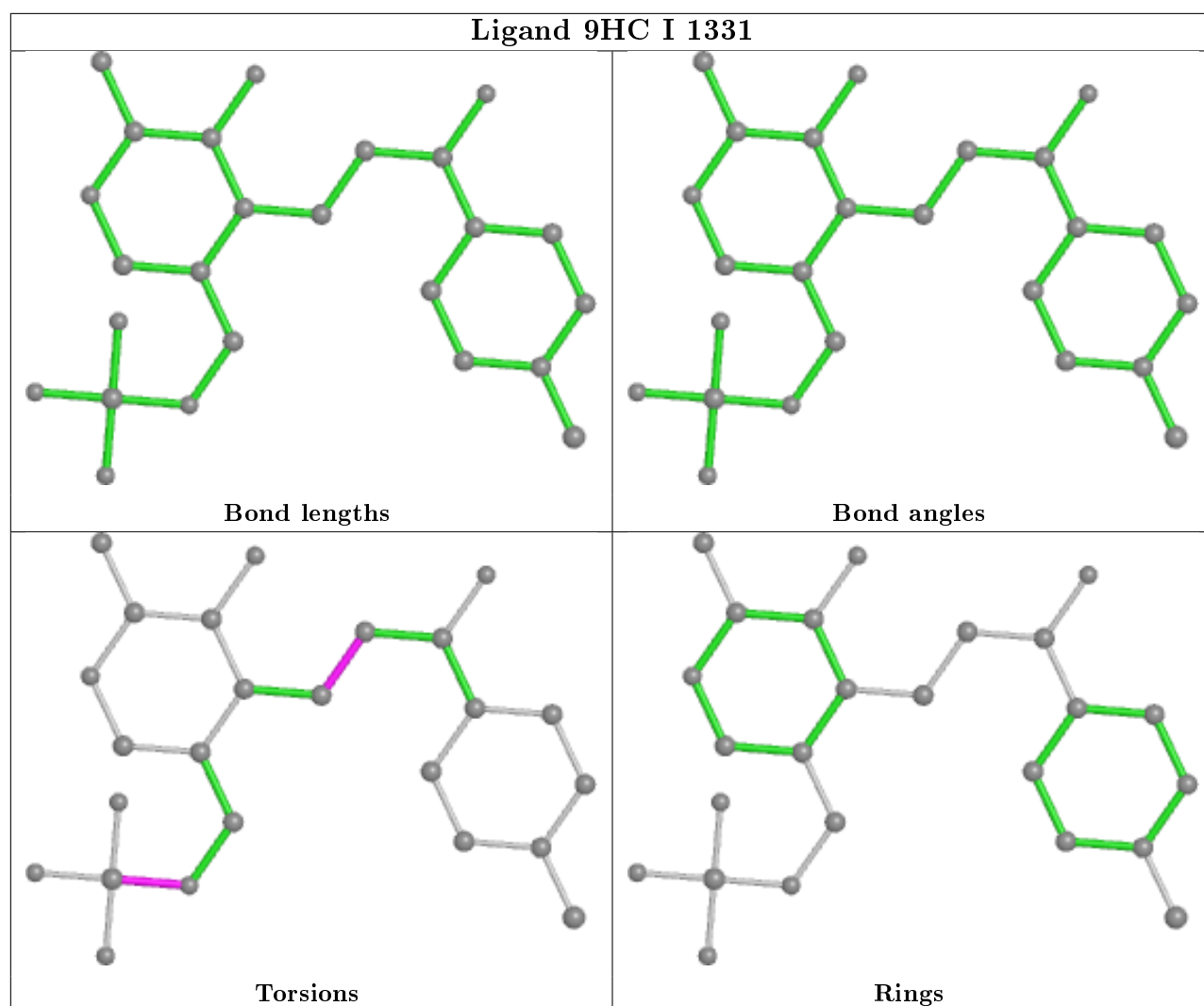


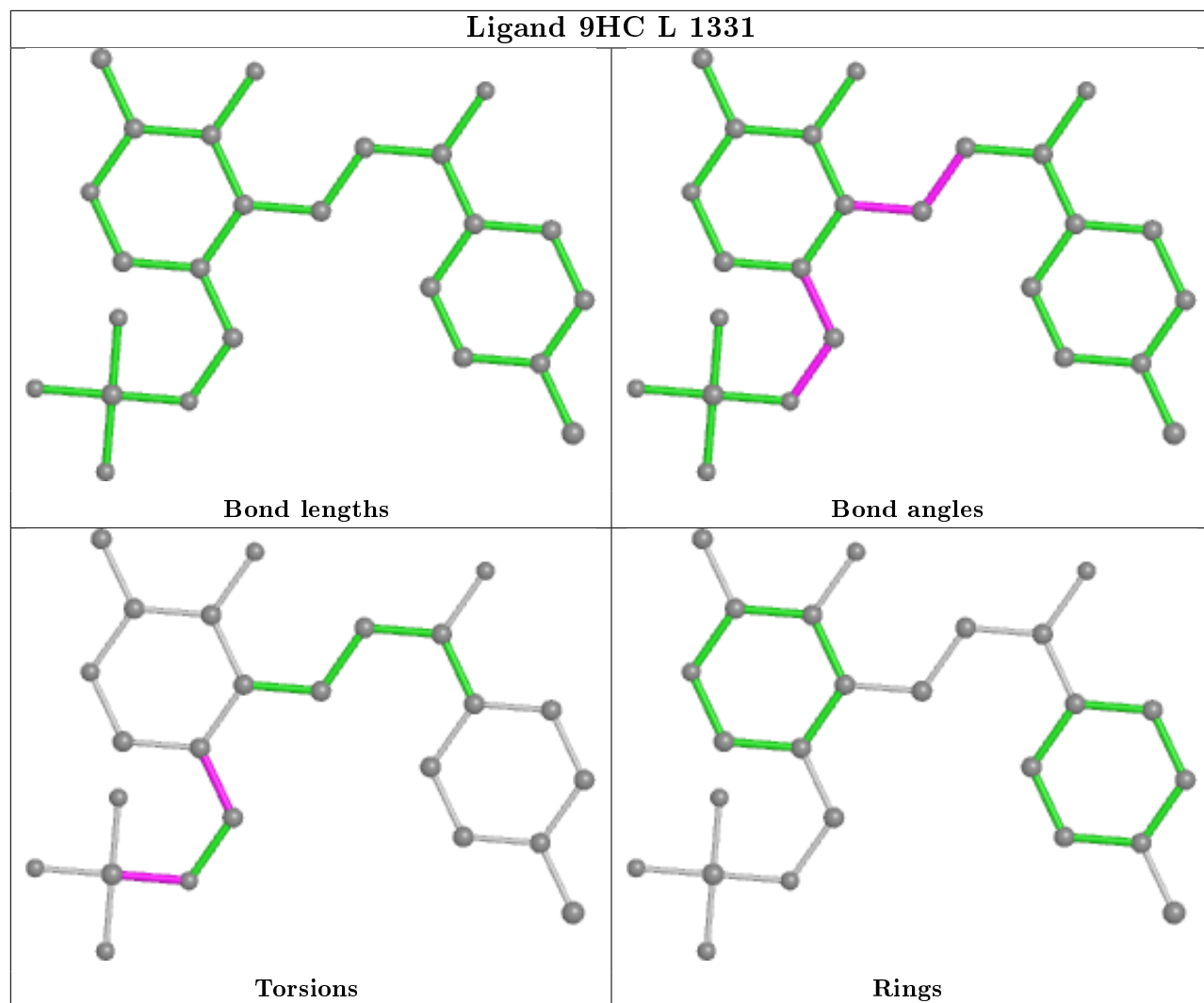
Torsions

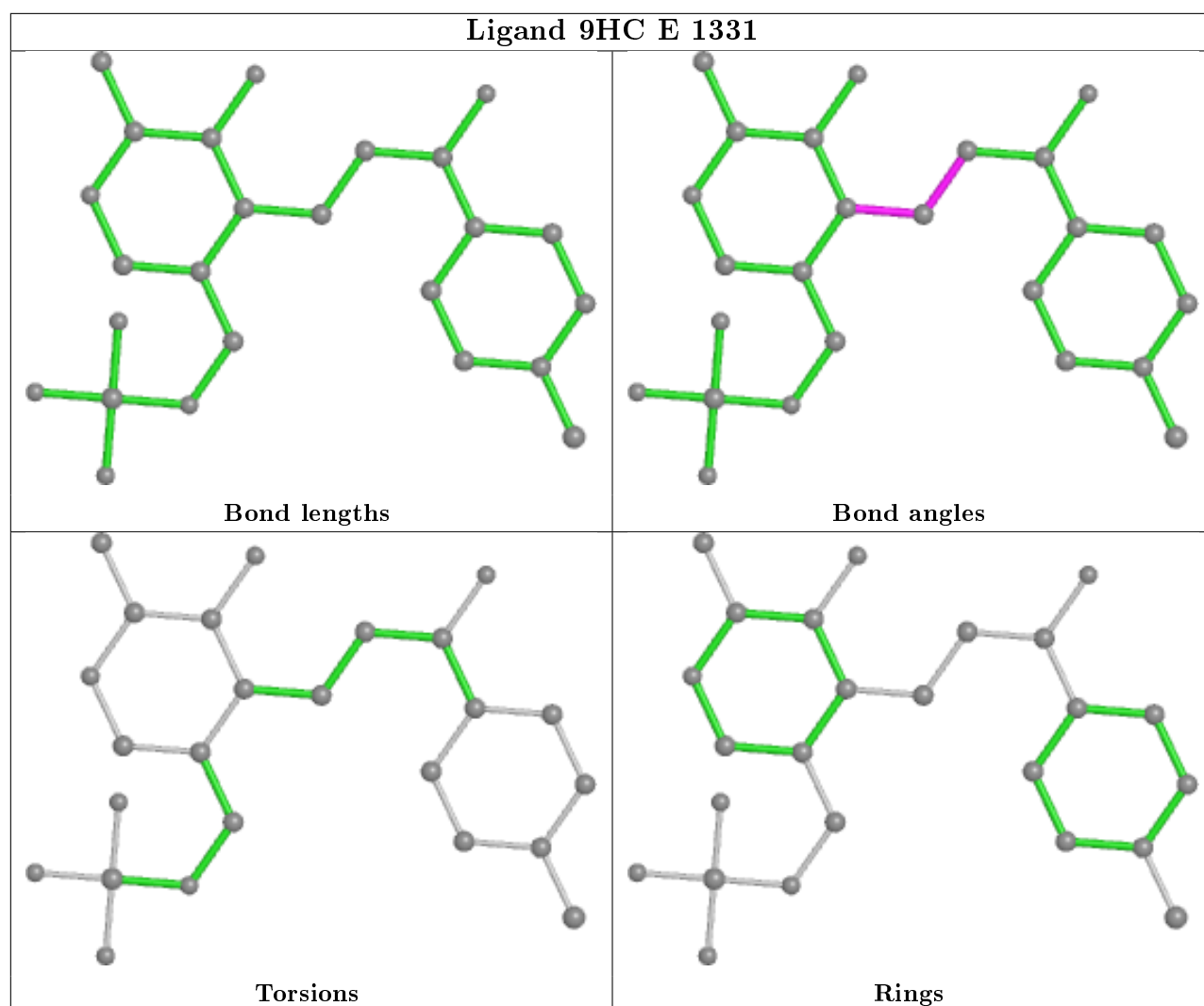


Rings









## 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	319/333 (95%)	-0.22	1 (0%) 94 93	42, 61, 88, 109	0
1	B	320/333 (96%)	-0.29	0 100 100	40, 59, 80, 96	0
1	C	321/333 (96%)	-0.29	1 (0%) 94 93	45, 66, 97, 125	0
1	D	322/333 (96%)	-0.44	0 100 100	39, 53, 76, 114	0
1	E	321/333 (96%)	0.01	7 (2%) 62 52	49, 81, 104, 116	0
1	F	322/333 (96%)	-0.27	1 (0%) 94 93	42, 62, 83, 110	0
1	G	321/333 (96%)	-0.40	0 100 100	39, 57, 83, 114	0
1	H	321/333 (96%)	-0.34	2 (0%) 89 86	40, 60, 85, 100	0
1	I	320/333 (96%)	0.11	11 (3%) 45 35	54, 81, 120, 140	0
1	J	319/333 (95%)	-0.24	6 (1%) 66 59	41, 63, 93, 115	0
1	K	319/333 (95%)	0.12	11 (3%) 45 35	51, 77, 99, 119	0
1	L	318/333 (95%)	0.15	11 (3%) 44 34	49, 81, 113, 136	0
All	All	3843/3996 (96%)	-0.18	51 (1%) 77 72	39, 66, 99, 140	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	35	ALA	5.2
1	L	121	ALA	4.8
1	I	12	TYR	4.4
1	E	328	VAL	3.7
1	I	24	SER	3.7

### 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

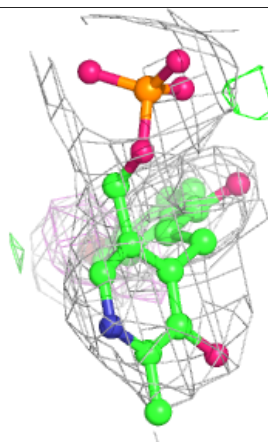
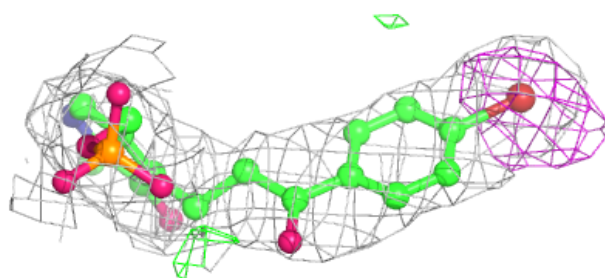
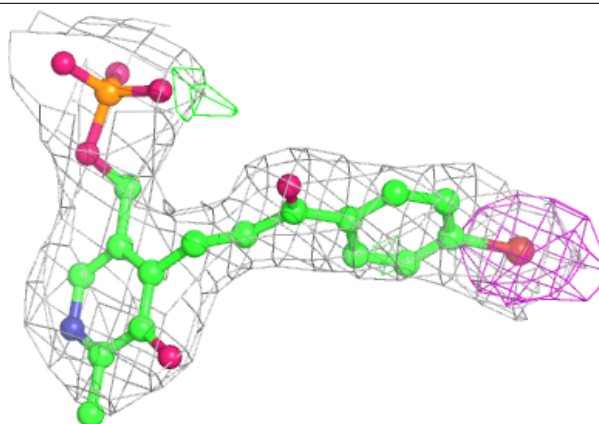
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	9HC	K	1331	25/25	0.91	0.14	62,75,84,101	0
2	9HC	E	1331	25/25	0.92	0.13	60,76,89,101	0
2	9HC	I	1331	25/25	0.93	0.16	53,66,77,93	0
2	9HC	L	1331	25/25	0.94	0.13	59,73,97,113	0
2	9HC	A	1331	25/25	0.94	0.16	43,61,70,86	0
2	9HC	C	1331	25/25	0.95	0.14	47,59,71,80	0
2	9HC	J	1331	25/25	0.95	0.17	42,51,76,88	0
2	9HC	F	1331	25/25	0.96	0.14	45,53,67,75	0
2	9HC	H	1331	25/25	0.96	0.14	44,53,68,77	0
2	9HC	B	1331	25/25	0.96	0.14	45,54,69,78	0
2	9HC	D	1331	25/25	0.97	0.14	36,43,58,61	0
2	9HC	G	1331	25/25	0.97	0.12	36,50,63,78	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.

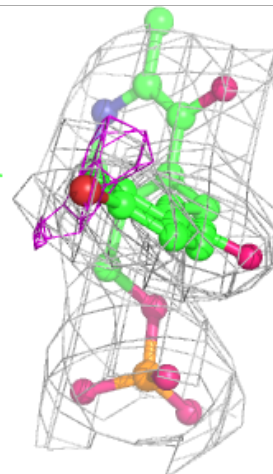
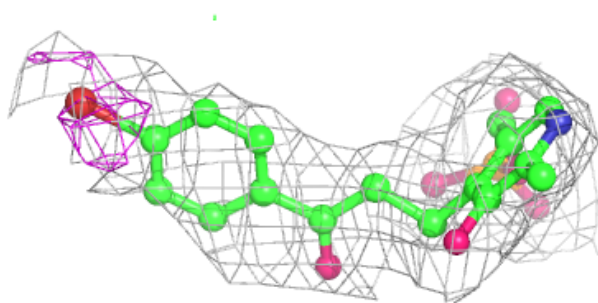
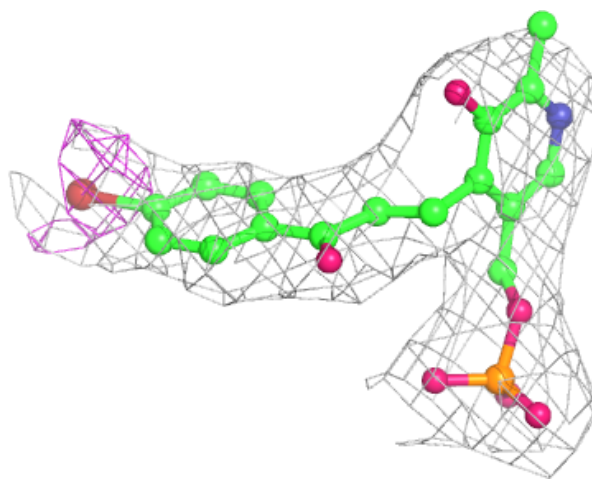
**Electron density around 9HC K 1331:**

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



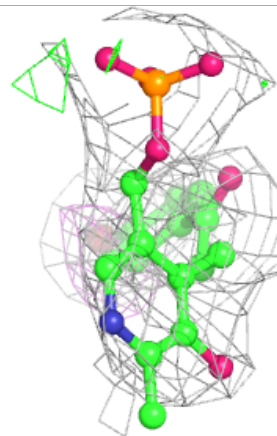
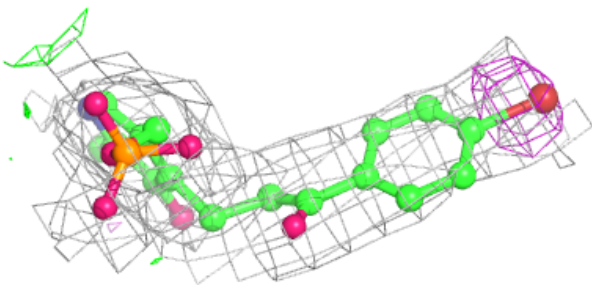
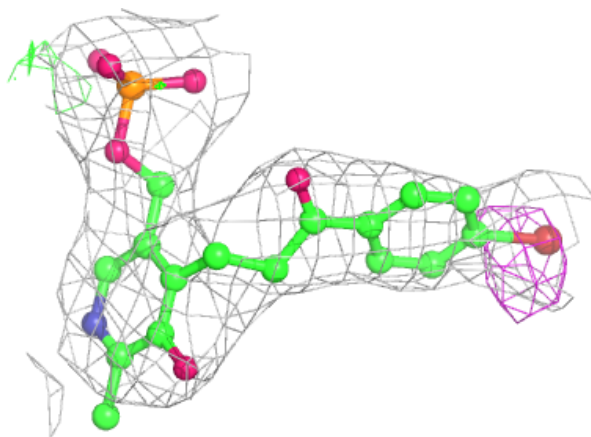
**Electron density around 9HC E 1331:**

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



**Electron density around 9HC I 1331:**

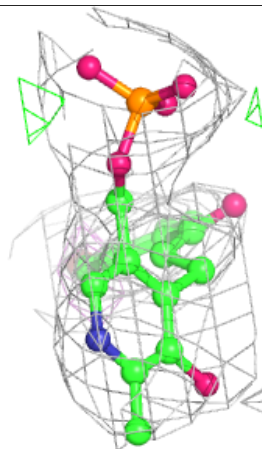
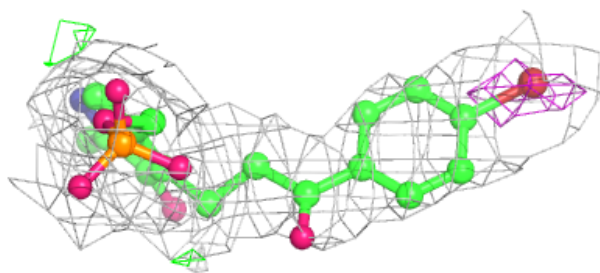
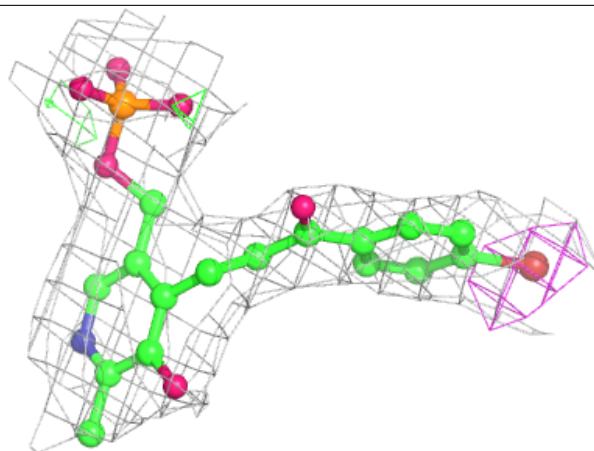
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





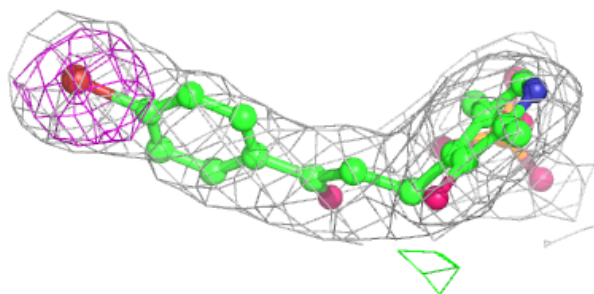
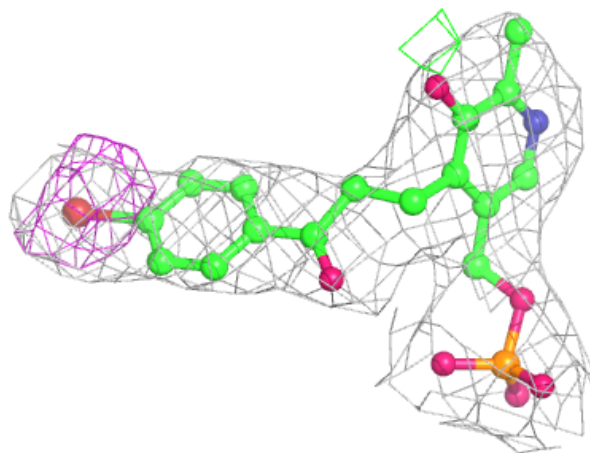
**Electron density around 9HC L 1331:**

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



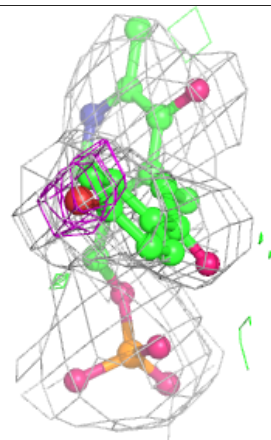
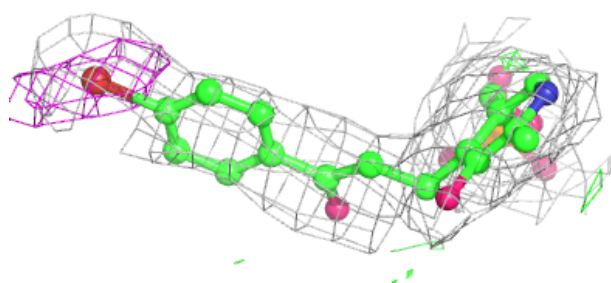
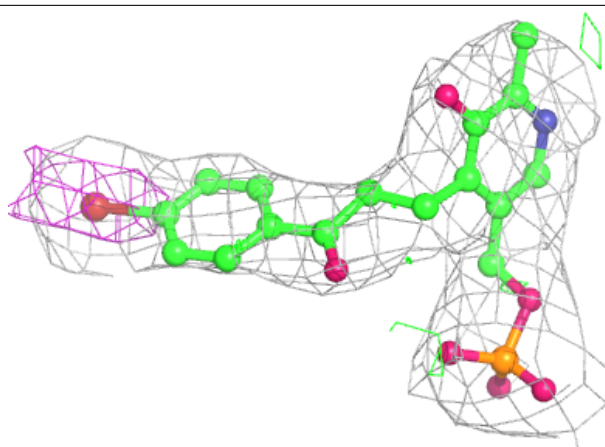
**Electron density around 9HC A 1331:**

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



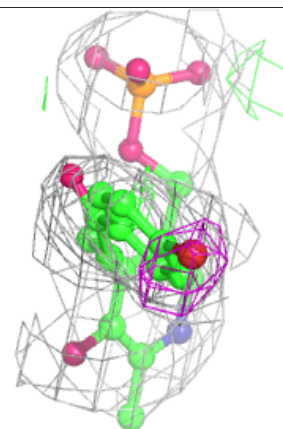
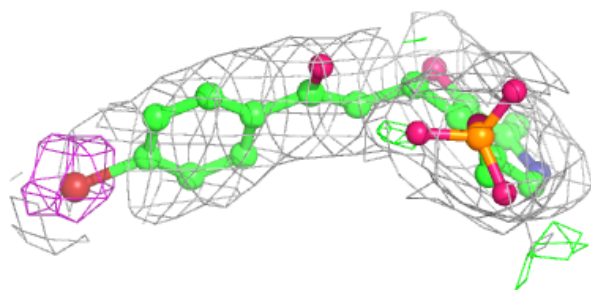
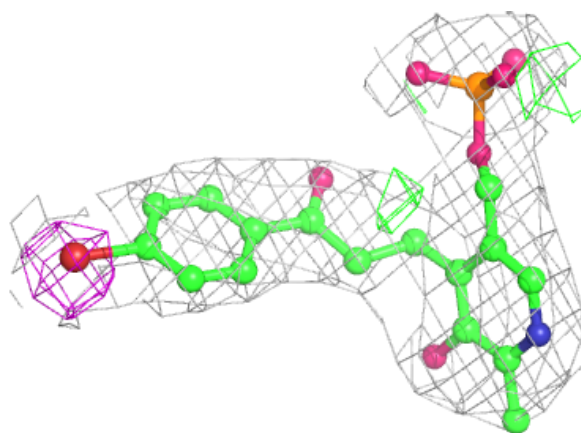
**Electron density around 9HC J 1331:**

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



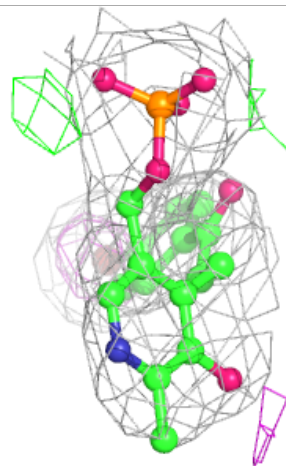
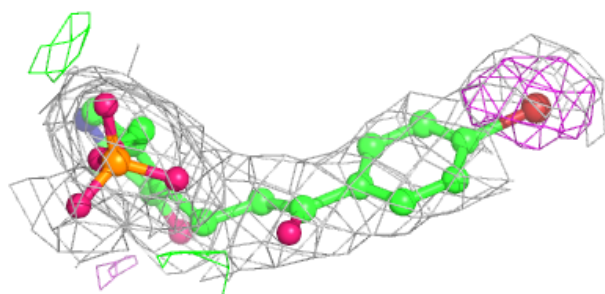
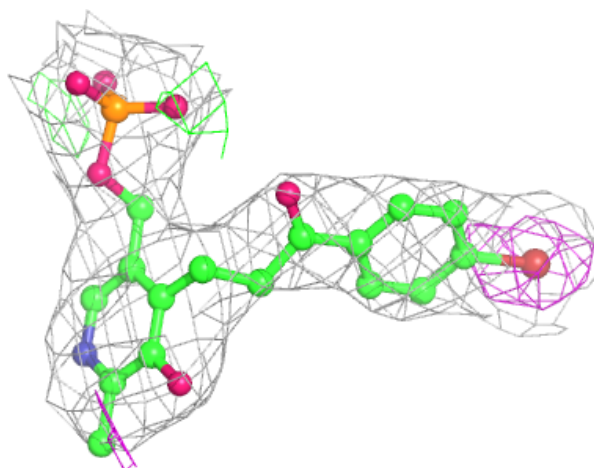
**Electron density around 9HC F 1331:**

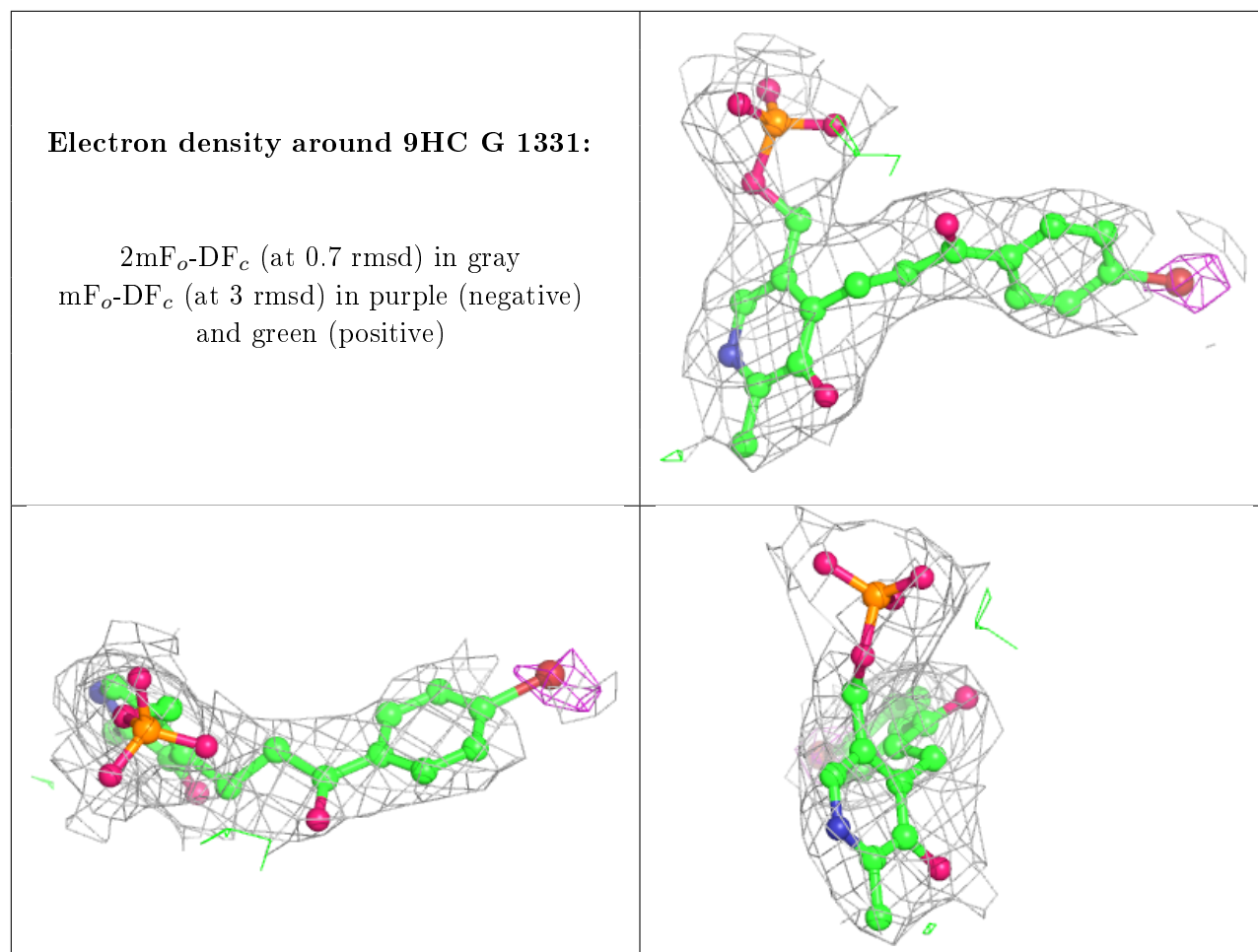
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 9HC B 1331:**

$2mF_o-DF_c$  (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.