



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 8, 2026 – 04:39 PM EDT

PDB ID : 10HM / pdb_000010hm
Title : Trypanosoma brucei CLK1 kinase domain in complex with a covalent Amido-benzimidazole (AB4) inhibitor
Authors : Mamo, M.
Deposited on : 2026-01-20
Resolution : 2.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

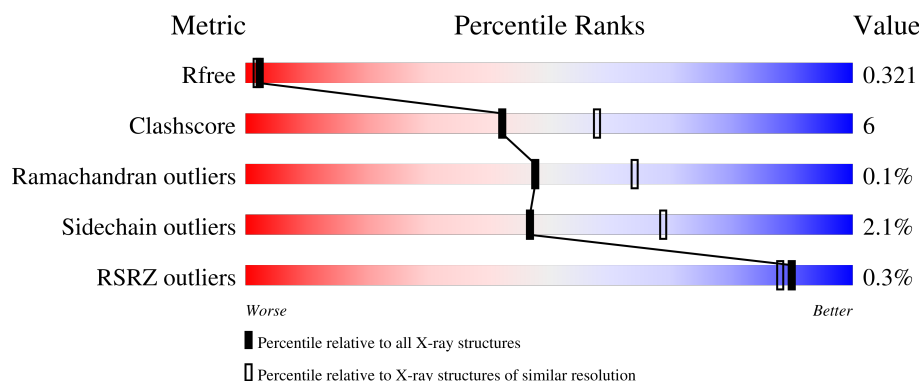
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	370	<div> <div>80%</div> <div>10%</div> <div>8%</div> </div>
1	B	370	<div> <div>79%</div> <div>11%</div> <div>8%</div> </div>
1	C	370	<div> <div>76%</div> <div>13%</div> <div>8%</div> </div>
1	D	370	<div> <div>76%</div> <div>13%</div> <div>8%</div> </div>
1	E	370	<div> <div>77%</div> <div>14%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	370	 77% 13% • 8%
1	G	370	 81% 10% • 8%
1	H	370	 78% 13% • 8%
1	I	370	 77% 12% • 8%
1	J	370	 79% 12% • 8%
1	K	370	 75% 13% • 9%
1	L	370	 78% 12% • 8%
1	M	370	 81% 10% • 8%
1	N	370	 76% 14% • 8%
1	O	370	 73% 16% • 9%
1	P	370	 73% 16% • 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 45259 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 Protein kinase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2672	1696	472	478	26			
1	B	339	Total	C	N	O	S	0	0	0
			2674	1697	475	476	26			
1	C	339	Total	C	N	O	S	0	0	0
			2673	1697	478	472	26			
1	D	339	Total	C	N	O	S	0	0	0
			2673	1697	478	472	26			
1	E	339	Total	C	N	O	S	0	0	0
			2674	1697	475	476	26			
1	F	339	Total	C	N	O	S	0	1	0
			2681	1700	477	478	26			
1	G	339	Total	C	N	O	S	0	0	0
			2674	1697	475	476	26			
1	H	339	Total	C	N	O	S	0	0	0
			2674	1697	475	476	26			
1	I	339	Total	C	N	O	S	0	0	0
			2674	1697	480	471	26			
1	J	339	Total	C	N	O	S	0	0	0
			2652	1686	471	470	25			
1	K	335	Total	C	N	O	S	0	0	0
			2637	1678	468	465	26			
1	L	339	Total	C	N	O	S	0	1	0
			2683	1702	481	474	26			
1	M	339	Total	C	N	O	S	0	0	0
			2673	1697	475	475	26			
1	N	339	Total	C	N	O	S	0	0	0
			2668	1693	475	474	26			
1	O	335	Total	C	N	O	S	0	1	0
			2618	1660	469	463	26			
1	P	339	Total	C	N	O	S	0	1	0
			2681	1702	483	470	26			

There are 336 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	MET	-	expression tag	UNP Q382U0
A	97	HIS	-	expression tag	UNP Q382U0
A	98	HIS	-	expression tag	UNP Q382U0
A	99	HIS	-	expression tag	UNP Q382U0
A	100	HIS	-	expression tag	UNP Q382U0
A	101	HIS	-	expression tag	UNP Q382U0
A	102	HIS	-	expression tag	UNP Q382U0
A	103	SER	-	expression tag	UNP Q382U0
A	104	SER	-	expression tag	UNP Q382U0
A	105	GLY	-	expression tag	UNP Q382U0
A	106	LEU	-	expression tag	UNP Q382U0
A	107	GLU	-	expression tag	UNP Q382U0
A	108	VAL	-	expression tag	UNP Q382U0
A	109	LEU	-	expression tag	UNP Q382U0
A	110	PHE	-	expression tag	UNP Q382U0
A	111	GLN	-	expression tag	UNP Q382U0
A	112	GLY	-	expression tag	UNP Q382U0
A	113	PRO	-	expression tag	UNP Q382U0
A	114	SER	-	expression tag	UNP Q382U0
A	115	MET	-	expression tag	UNP Q382U0
A	116	HIS	-	expression tag	UNP Q382U0
B	96	MET	-	expression tag	UNP Q382U0
B	97	HIS	-	expression tag	UNP Q382U0
B	98	HIS	-	expression tag	UNP Q382U0
B	99	HIS	-	expression tag	UNP Q382U0
B	100	HIS	-	expression tag	UNP Q382U0
B	101	HIS	-	expression tag	UNP Q382U0
B	102	HIS	-	expression tag	UNP Q382U0
B	103	SER	-	expression tag	UNP Q382U0
B	104	SER	-	expression tag	UNP Q382U0
B	105	GLY	-	expression tag	UNP Q382U0
B	106	LEU	-	expression tag	UNP Q382U0
B	107	GLU	-	expression tag	UNP Q382U0
B	108	VAL	-	expression tag	UNP Q382U0
B	109	LEU	-	expression tag	UNP Q382U0
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B	111	GLN	-	expression tag	UNP Q382U0
B	112	GLY	-	expression tag	UNP Q382U0
B	113	PRO	-	expression tag	UNP Q382U0
B	114	SER	-	expression tag	UNP Q382U0
B	115	MET	-	expression tag	UNP Q382U0
B	116	HIS	-	expression tag	UNP Q382U0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	96	MET	-	expression tag	UNP Q382U0
C	97	HIS	-	expression tag	UNP Q382U0
C	98	HIS	-	expression tag	UNP Q382U0
C	99	HIS	-	expression tag	UNP Q382U0
C	100	HIS	-	expression tag	UNP Q382U0
C	101	HIS	-	expression tag	UNP Q382U0
C	102	HIS	-	expression tag	UNP Q382U0
C	103	SER	-	expression tag	UNP Q382U0
C	104	SER	-	expression tag	UNP Q382U0
C	105	GLY	-	expression tag	UNP Q382U0
C	106	LEU	-	expression tag	UNP Q382U0
C	107	GLU	-	expression tag	UNP Q382U0
C	108	VAL	-	expression tag	UNP Q382U0
C	109	LEU	-	expression tag	UNP Q382U0
C	110	PHE	-	expression tag	UNP Q382U0
C	111	GLN	-	expression tag	UNP Q382U0
C	112	GLY	-	expression tag	UNP Q382U0
C	113	PRO	-	expression tag	UNP Q382U0
C	114	SER	-	expression tag	UNP Q382U0
C	115	MET	-	expression tag	UNP Q382U0
C	116	HIS	-	expression tag	UNP Q382U0
D	96	MET	-	expression tag	UNP Q382U0
D	97	HIS	-	expression tag	UNP Q382U0
D	98	HIS	-	expression tag	UNP Q382U0
D	99	HIS	-	expression tag	UNP Q382U0
D	100	HIS	-	expression tag	UNP Q382U0
D	101	HIS	-	expression tag	UNP Q382U0
D	102	HIS	-	expression tag	UNP Q382U0
D	103	SER	-	expression tag	UNP Q382U0
D	104	SER	-	expression tag	UNP Q382U0
D	105	GLY	-	expression tag	UNP Q382U0
D	106	LEU	-	expression tag	UNP Q382U0
D	107	GLU	-	expression tag	UNP Q382U0
D	108	VAL	-	expression tag	UNP Q382U0
D	109	LEU	-	expression tag	UNP Q382U0
D	110	PHE	-	expression tag	UNP Q382U0
D	111	GLN	-	expression tag	UNP Q382U0
D	112	GLY	-	expression tag	UNP Q382U0
D	113	PRO	-	expression tag	UNP Q382U0
D	114	SER	-	expression tag	UNP Q382U0
D	115	MET	-	expression tag	UNP Q382U0
D	116	HIS	-	expression tag	UNP Q382U0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	96	MET	-	expression tag	UNP Q382U0
E	97	HIS	-	expression tag	UNP Q382U0
E	98	HIS	-	expression tag	UNP Q382U0
E	99	HIS	-	expression tag	UNP Q382U0
E	100	HIS	-	expression tag	UNP Q382U0
E	101	HIS	-	expression tag	UNP Q382U0
E	102	HIS	-	expression tag	UNP Q382U0
E	103	SER	-	expression tag	UNP Q382U0
E	104	SER	-	expression tag	UNP Q382U0
E	105	GLY	-	expression tag	UNP Q382U0
E	106	LEU	-	expression tag	UNP Q382U0
E	107	GLU	-	expression tag	UNP Q382U0
E	108	VAL	-	expression tag	UNP Q382U0
E	109	LEU	-	expression tag	UNP Q382U0
E	110	PHE	-	expression tag	UNP Q382U0
E	111	GLN	-	expression tag	UNP Q382U0
E	112	GLY	-	expression tag	UNP Q382U0
E	113	PRO	-	expression tag	UNP Q382U0
E	114	SER	-	expression tag	UNP Q382U0
E	115	MET	-	expression tag	UNP Q382U0
E	116	HIS	-	expression tag	UNP Q382U0
F	96	MET	-	expression tag	UNP Q382U0
F	97	HIS	-	expression tag	UNP Q382U0
F	98	HIS	-	expression tag	UNP Q382U0
F	99	HIS	-	expression tag	UNP Q382U0
F	100	HIS	-	expression tag	UNP Q382U0
F	101	HIS	-	expression tag	UNP Q382U0
F	102	HIS	-	expression tag	UNP Q382U0
F	103	SER	-	expression tag	UNP Q382U0
F	104	SER	-	expression tag	UNP Q382U0
F	105	GLY	-	expression tag	UNP Q382U0
F	106	LEU	-	expression tag	UNP Q382U0
F	107	GLU	-	expression tag	UNP Q382U0
F	108	VAL	-	expression tag	UNP Q382U0
F	109	LEU	-	expression tag	UNP Q382U0
F	110	PHE	-	expression tag	UNP Q382U0
F	111	GLN	-	expression tag	UNP Q382U0
F	112	GLY	-	expression tag	UNP Q382U0
F	113	PRO	-	expression tag	UNP Q382U0
F	114	SER	-	expression tag	UNP Q382U0
F	115	MET	-	expression tag	UNP Q382U0
F	116	HIS	-	expression tag	UNP Q382U0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	96	MET	-	expression tag	UNP Q382U0
G	97	HIS	-	expression tag	UNP Q382U0
G	98	HIS	-	expression tag	UNP Q382U0
G	99	HIS	-	expression tag	UNP Q382U0
G	100	HIS	-	expression tag	UNP Q382U0
G	101	HIS	-	expression tag	UNP Q382U0
G	102	HIS	-	expression tag	UNP Q382U0
G	103	SER	-	expression tag	UNP Q382U0
G	104	SER	-	expression tag	UNP Q382U0
G	105	GLY	-	expression tag	UNP Q382U0
G	106	LEU	-	expression tag	UNP Q382U0
G	107	GLU	-	expression tag	UNP Q382U0
G	108	VAL	-	expression tag	UNP Q382U0
G	109	LEU	-	expression tag	UNP Q382U0
G	110	PHE	-	expression tag	UNP Q382U0
G	111	GLN	-	expression tag	UNP Q382U0
G	112	GLY	-	expression tag	UNP Q382U0
G	113	PRO	-	expression tag	UNP Q382U0
G	114	SER	-	expression tag	UNP Q382U0
G	115	MET	-	expression tag	UNP Q382U0
G	116	HIS	-	expression tag	UNP Q382U0
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H	97	HIS	-	expression tag	UNP Q382U0
H	98	HIS	-	expression tag	UNP Q382U0
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H	102	HIS	-	expression tag	UNP Q382U0
H	103	SER	-	expression tag	UNP Q382U0
H	104	SER	-	expression tag	UNP Q382U0
H	105	GLY	-	expression tag	UNP Q382U0
H	106	LEU	-	expression tag	UNP Q382U0
H	107	GLU	-	expression tag	UNP Q382U0
H	108	VAL	-	expression tag	UNP Q382U0
H	109	LEU	-	expression tag	UNP Q382U0
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H	111	GLN	-	expression tag	UNP Q382U0
H	112	GLY	-	expression tag	UNP Q382U0
H	113	PRO	-	expression tag	UNP Q382U0
H	114	SER	-	expression tag	UNP Q382U0
H	115	MET	-	expression tag	UNP Q382U0
H	116	HIS	-	expression tag	UNP Q382U0

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Chain	Residue	Modelled	Actual	Comment	Reference
I	96	MET	-	expression tag	UNP Q382U0
I	97	HIS	-	expression tag	UNP Q382U0
I	98	HIS	-	expression tag	UNP Q382U0
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I	100	HIS	-	expression tag	UNP Q382U0
I	101	HIS	-	expression tag	UNP Q382U0
I	102	HIS	-	expression tag	UNP Q382U0
I	103	SER	-	expression tag	UNP Q382U0
I	104	SER	-	expression tag	UNP Q382U0
I	105	GLY	-	expression tag	UNP Q382U0
I	106	LEU	-	expression tag	UNP Q382U0
I	107	GLU	-	expression tag	UNP Q382U0
I	108	VAL	-	expression tag	UNP Q382U0
I	109	LEU	-	expression tag	UNP Q382U0
I	110	PHE	-	expression tag	UNP Q382U0
I	111	GLN	-	expression tag	UNP Q382U0
I	112	GLY	-	expression tag	UNP Q382U0
I	113	PRO	-	expression tag	UNP Q382U0
I	114	SER	-	expression tag	UNP Q382U0
I	115	MET	-	expression tag	UNP Q382U0
I	116	HIS	-	expression tag	UNP Q382U0
J	96	MET	-	expression tag	UNP Q382U0
J	97	HIS	-	expression tag	UNP Q382U0
J	98	HIS	-	expression tag	UNP Q382U0
J	99	HIS	-	expression tag	UNP Q382U0
J	100	HIS	-	expression tag	UNP Q382U0
J	101	HIS	-	expression tag	UNP Q382U0
J	102	HIS	-	expression tag	UNP Q382U0
J	103	SER	-	expression tag	UNP Q382U0
J	104	SER	-	expression tag	UNP Q382U0
J	105	GLY	-	expression tag	UNP Q382U0
J	106	LEU	-	expression tag	UNP Q382U0
J	107	GLU	-	expression tag	UNP Q382U0
J	108	VAL	-	expression tag	UNP Q382U0
J	109	LEU	-	expression tag	UNP Q382U0
J	110	PHE	-	expression tag	UNP Q382U0
J	111	GLN	-	expression tag	UNP Q382U0
J	112	GLY	-	expression tag	UNP Q382U0
J	113	PRO	-	expression tag	UNP Q382U0
J	114	SER	-	expression tag	UNP Q382U0
J	115	MET	-	expression tag	UNP Q382U0
J	116	HIS	-	expression tag	UNP Q382U0

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Chain	Residue	Modelled	Actual	Comment	Reference
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K	97	HIS	-	expression tag	UNP Q382U0
K	98	HIS	-	expression tag	UNP Q382U0
K	99	HIS	-	expression tag	UNP Q382U0
K	100	HIS	-	expression tag	UNP Q382U0
K	101	HIS	-	expression tag	UNP Q382U0
K	102	HIS	-	expression tag	UNP Q382U0
K	103	SER	-	expression tag	UNP Q382U0
K	104	SER	-	expression tag	UNP Q382U0
K	105	GLY	-	expression tag	UNP Q382U0
K	106	LEU	-	expression tag	UNP Q382U0
K	107	GLU	-	expression tag	UNP Q382U0
K	108	VAL	-	expression tag	UNP Q382U0
K	109	LEU	-	expression tag	UNP Q382U0
K	110	PHE	-	expression tag	UNP Q382U0
K	111	GLN	-	expression tag	UNP Q382U0
K	112	GLY	-	expression tag	UNP Q382U0
K	113	PRO	-	expression tag	UNP Q382U0
K	114	SER	-	expression tag	UNP Q382U0
K	115	MET	-	expression tag	UNP Q382U0
K	116	HIS	-	expression tag	UNP Q382U0
L	96	MET	-	expression tag	UNP Q382U0
L	97	HIS	-	expression tag	UNP Q382U0
L	98	HIS	-	expression tag	UNP Q382U0
L	99	HIS	-	expression tag	UNP Q382U0
L	100	HIS	-	expression tag	UNP Q382U0
L	101	HIS	-	expression tag	UNP Q382U0
L	102	HIS	-	expression tag	UNP Q382U0
L	103	SER	-	expression tag	UNP Q382U0
L	104	SER	-	expression tag	UNP Q382U0
L	105	GLY	-	expression tag	UNP Q382U0
L	106	LEU	-	expression tag	UNP Q382U0
L	107	GLU	-	expression tag	UNP Q382U0
L	108	VAL	-	expression tag	UNP Q382U0
L	109	LEU	-	expression tag	UNP Q382U0
L	110	PHE	-	expression tag	UNP Q382U0
L	111	GLN	-	expression tag	UNP Q382U0
L	112	GLY	-	expression tag	UNP Q382U0
L	113	PRO	-	expression tag	UNP Q382U0
L	114	SER	-	expression tag	UNP Q382U0
L	115	MET	-	expression tag	UNP Q382U0
L	116	HIS	-	expression tag	UNP Q382U0

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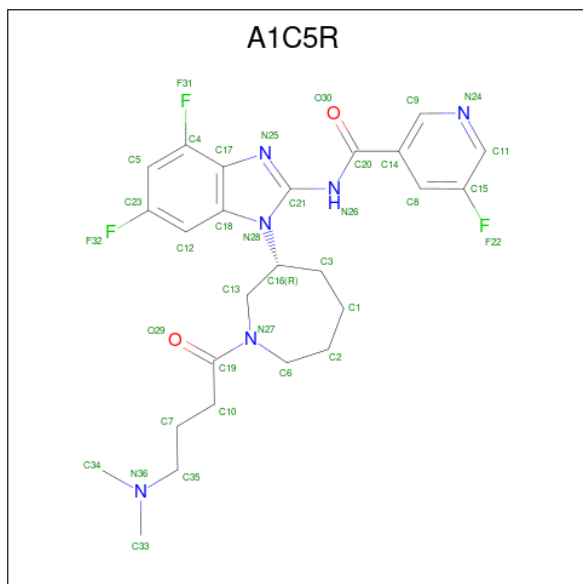
Chain	Residue	Modelled	Actual	Comment	Reference
M	96	MET	-	expression tag	UNP Q382U0
M	97	HIS	-	expression tag	UNP Q382U0
M	98	HIS	-	expression tag	UNP Q382U0
M	99	HIS	-	expression tag	UNP Q382U0
M	100	HIS	-	expression tag	UNP Q382U0
M	101	HIS	-	expression tag	UNP Q382U0
M	102	HIS	-	expression tag	UNP Q382U0
M	103	SER	-	expression tag	UNP Q382U0
M	104	SER	-	expression tag	UNP Q382U0
M	105	GLY	-	expression tag	UNP Q382U0
M	106	LEU	-	expression tag	UNP Q382U0
M	107	GLU	-	expression tag	UNP Q382U0
M	108	VAL	-	expression tag	UNP Q382U0
M	109	LEU	-	expression tag	UNP Q382U0
M	110	PHE	-	expression tag	UNP Q382U0
M	111	GLN	-	expression tag	UNP Q382U0
M	112	GLY	-	expression tag	UNP Q382U0
M	113	PRO	-	expression tag	UNP Q382U0
M	114	SER	-	expression tag	UNP Q382U0
M	115	MET	-	expression tag	UNP Q382U0
M	116	HIS	-	expression tag	UNP Q382U0
N	96	MET	-	expression tag	UNP Q382U0
N	97	HIS	-	expression tag	UNP Q382U0
N	98	HIS	-	expression tag	UNP Q382U0
N	99	HIS	-	expression tag	UNP Q382U0
N	100	HIS	-	expression tag	UNP Q382U0
N	101	HIS	-	expression tag	UNP Q382U0
N	102	HIS	-	expression tag	UNP Q382U0
N	103	SER	-	expression tag	UNP Q382U0
N	104	SER	-	expression tag	UNP Q382U0
N	105	GLY	-	expression tag	UNP Q382U0
N	106	LEU	-	expression tag	UNP Q382U0
N	107	GLU	-	expression tag	UNP Q382U0
N	108	VAL	-	expression tag	UNP Q382U0
N	109	LEU	-	expression tag	UNP Q382U0
N	110	PHE	-	expression tag	UNP Q382U0
N	111	GLN	-	expression tag	UNP Q382U0
N	112	GLY	-	expression tag	UNP Q382U0
N	113	PRO	-	expression tag	UNP Q382U0
N	114	SER	-	expression tag	UNP Q382U0
N	115	MET	-	expression tag	UNP Q382U0
N	116	HIS	-	expression tag	UNP Q382U0

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Chain	Residue	Modelled	Actual	Comment	Reference
O	96	MET	-	expression tag	UNP Q382U0
O	97	HIS	-	expression tag	UNP Q382U0
O	98	HIS	-	expression tag	UNP Q382U0
O	99	HIS	-	expression tag	UNP Q382U0
O	100	HIS	-	expression tag	UNP Q382U0
O	101	HIS	-	expression tag	UNP Q382U0
O	102	HIS	-	expression tag	UNP Q382U0
O	103	SER	-	expression tag	UNP Q382U0
O	104	SER	-	expression tag	UNP Q382U0
O	105	GLY	-	expression tag	UNP Q382U0
O	106	LEU	-	expression tag	UNP Q382U0
O	107	GLU	-	expression tag	UNP Q382U0
O	108	VAL	-	expression tag	UNP Q382U0
O	109	LEU	-	expression tag	UNP Q382U0
O	110	PHE	-	expression tag	UNP Q382U0
O	111	GLN	-	expression tag	UNP Q382U0
O	112	GLY	-	expression tag	UNP Q382U0
O	113	PRO	-	expression tag	UNP Q382U0
O	114	SER	-	expression tag	UNP Q382U0
O	115	MET	-	expression tag	UNP Q382U0
O	116	HIS	-	expression tag	UNP Q382U0
P	96	MET	-	expression tag	UNP Q382U0
P	97	HIS	-	expression tag	UNP Q382U0
P	98	HIS	-	expression tag	UNP Q382U0
P	99	HIS	-	expression tag	UNP Q382U0
P	100	HIS	-	expression tag	UNP Q382U0
P	101	HIS	-	expression tag	UNP Q382U0
P	102	HIS	-	expression tag	UNP Q382U0
P	103	SER	-	expression tag	UNP Q382U0
P	104	SER	-	expression tag	UNP Q382U0
P	105	GLY	-	expression tag	UNP Q382U0
P	106	LEU	-	expression tag	UNP Q382U0
P	107	GLU	-	expression tag	UNP Q382U0
P	108	VAL	-	expression tag	UNP Q382U0
P	109	LEU	-	expression tag	UNP Q382U0
P	110	PHE	-	expression tag	UNP Q382U0
P	111	GLN	-	expression tag	UNP Q382U0
P	112	GLY	-	expression tag	UNP Q382U0
P	113	PRO	-	expression tag	UNP Q382U0
P	114	SER	-	expression tag	UNP Q382U0
P	115	MET	-	expression tag	UNP Q382U0
P	116	HIS	-	expression tag	UNP Q382U0

- Molecule 2 is %N-(1-((3R)-1-[4-(dimethylamino)butanoyl]azepan-3-yl)-4,6-difluoro-1H-1,3-benzimidazol-2-yl)-5-fluoropyridine-3-carboxamide (CCD ID: A1C5R) (formula: C₂₅H₂₉F₃N₆O₂) (labeled as "Ligand of Interest" by depositor).



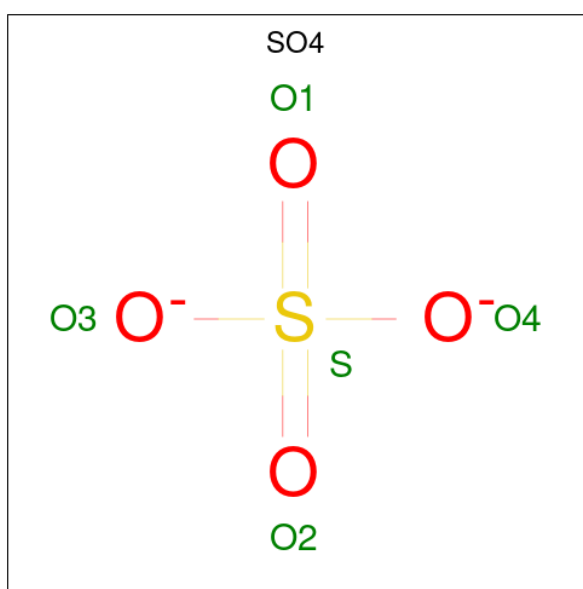
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			36	25	3	6	2		
2	B	1	Total	C	F	N	O	0	0
			36	25	3	6	2		
2	C	1	Total	C	F	N	O	0	0
			36	25	3	6	2		
2	D	1	Total	C	F	N	O	0	0
			36	25	3	6	2		
2	E	1	Total	C	F	N	O	0	0
			36	25	3	6	2		
2	F	1	Total	C	F	N	O	0	0
			36	25	3	6	2		
2	G	1	Total	C	F	N	O	0	0
			36	25	3	6	2		
2	H	1	Total	C	F	N	O	0	0
			36	25	3	6	2		
2	I	1	Total	C	F	N	O	0	0
			36	25	3	6	2		
2	J	1	Total	C	F	N	O	0	0
			36	25	3	6	2		
2	K	1	Total	C	F	N	O	0	0
			36	25	3	6	2		
2	L	1	Total	C	F	N	O	0	0
			36	25	3	6	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	M	1	Total	C	F	N	O	0	0
			36	25	3	6	2		
2	N	1	Total	C	F	N	O	0	0
			36	25	3	6	2		
2	O	1	Total	C	F	N	O	0	0
			36	25	3	6	2		
2	P	1	Total	C	F	N	O	0	0
			36	25	3	6	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



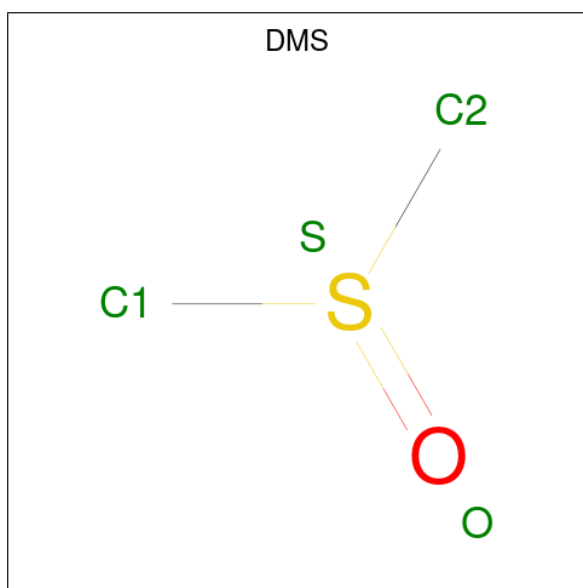
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	M	1	Total	O	S	0	0
			5	4	1		
3	M	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		
3	P	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	83	Total	O	0	0
			83	83		
5	B	120	Total	O	0	0
			120	120		
5	C	131	Total	O	0	0
			131	131		
5	D	89	Total	O	0	0
			89	89		
5	E	109	Total	O	0	0
			109	109		
5	F	126	Total	O	0	0
			126	126		
5	G	110	Total	O	0	0
			110	110		
5	H	129	Total	O	0	0
			129	129		
5	I	121	Total	O	0	0
			121	121		
5	J	127	Total	O	0	0
			127	127		

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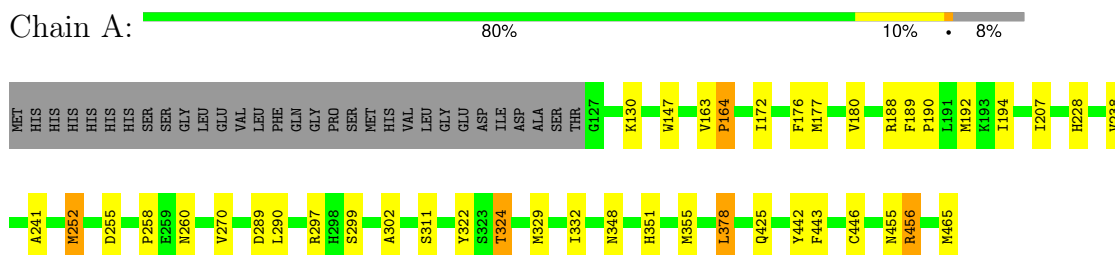
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	K	143	Total 143	O 143	0	0
5	L	93	Total 93	O 93	0	0
5	M	123	Total 123	O 123	0	0
5	N	114	Total 114	O 114	0	0
5	O	121	Total 121	O 121	0	0
5	P	119	Total 119	O 119	0	0

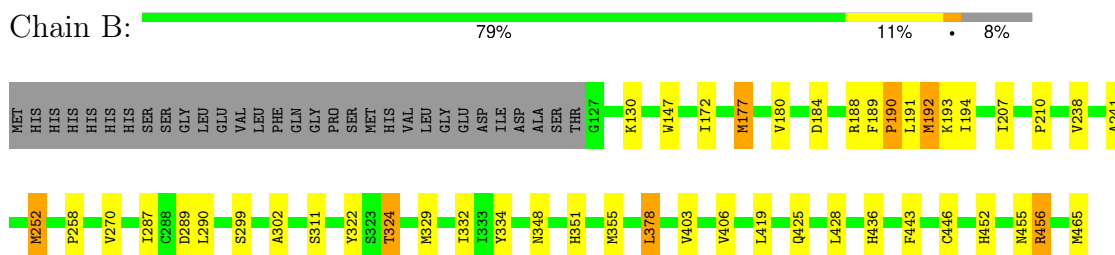
3 Residue-property plots

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

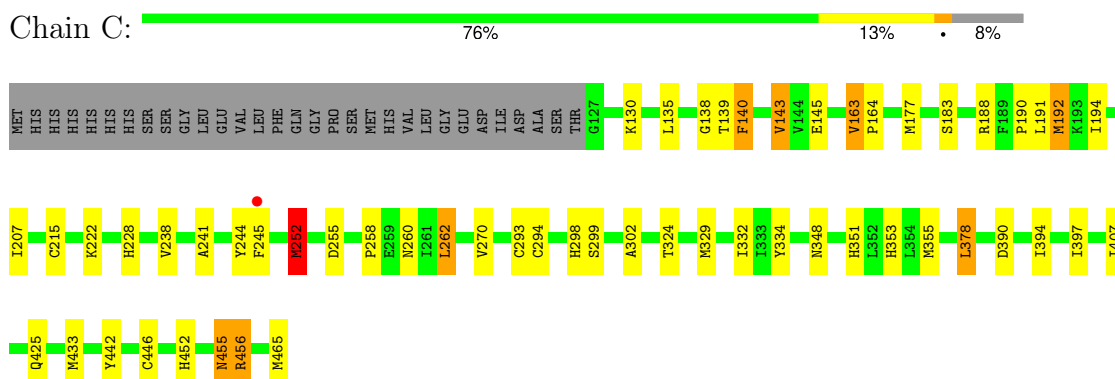
- Molecule 1: Protein kinase, putative



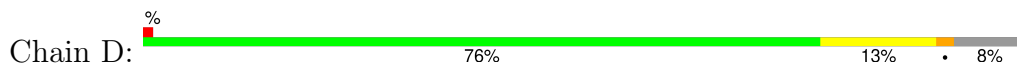
- Molecule 1: Protein kinase, putative

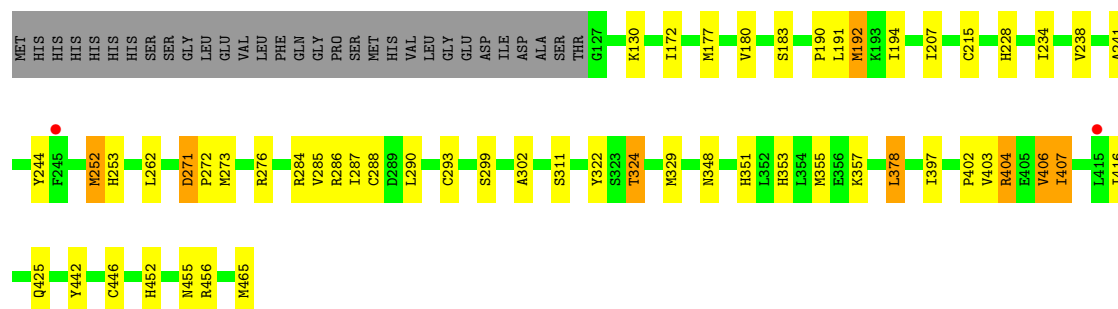


- Molecule 1: Protein kinase, putative



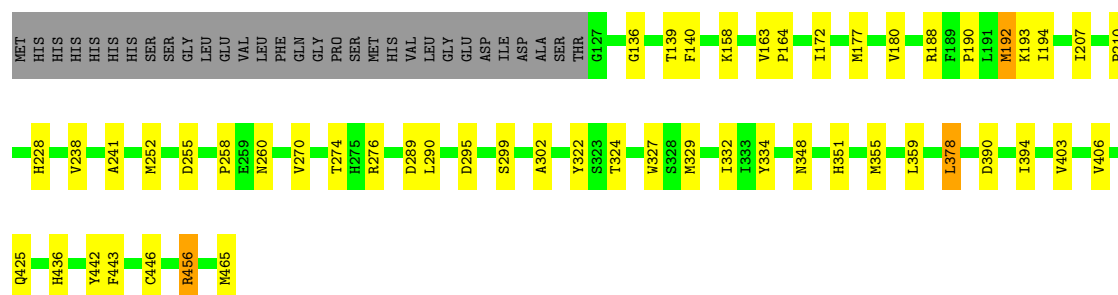
- Molecule 1: Protein kinase, putative





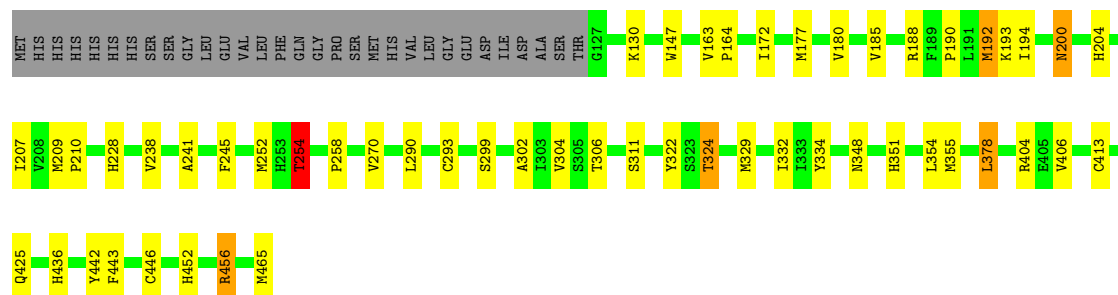
- Molecule 1: Protein kinase, putative

Chain E: 77% 14% 8%



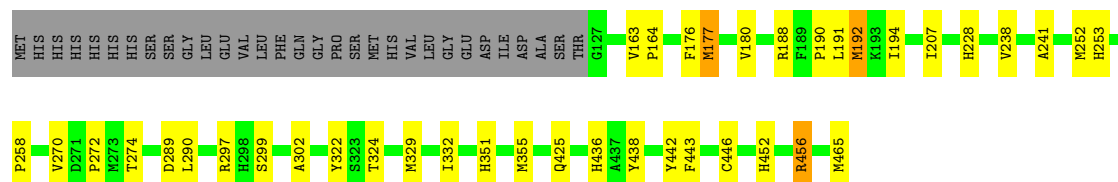
- Molecule 1: Protein kinase, putative

Chain F: 77% 13% 8%



- Molecule 1: Protein kinase, putative


Chain G: 81% 10% 8%

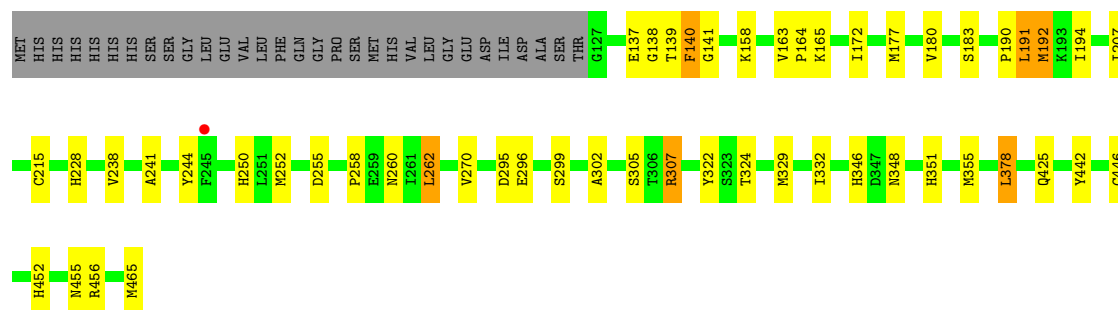


- Molecule 1: Protein kinase, putative


Chain H: 78% 13% 8%

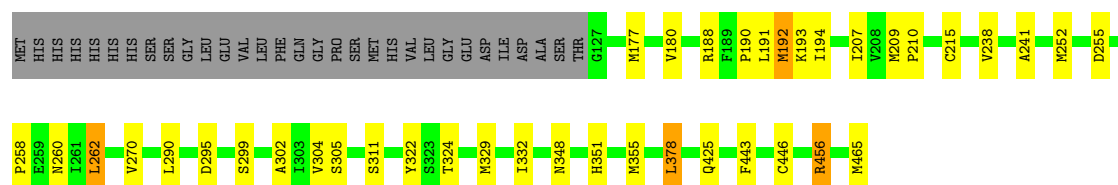
- Molecule 1: Protein kinase, putative

Chain L:  78% 12% 8%




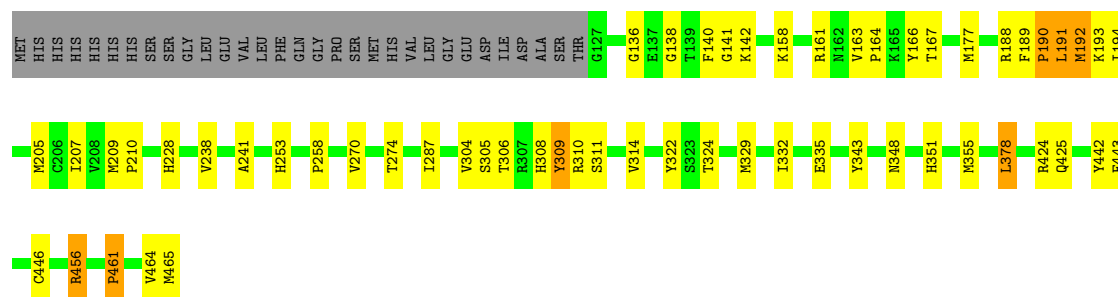
- Molecule 1: Protein kinase, putative

Chain M:  81% 10% 8%




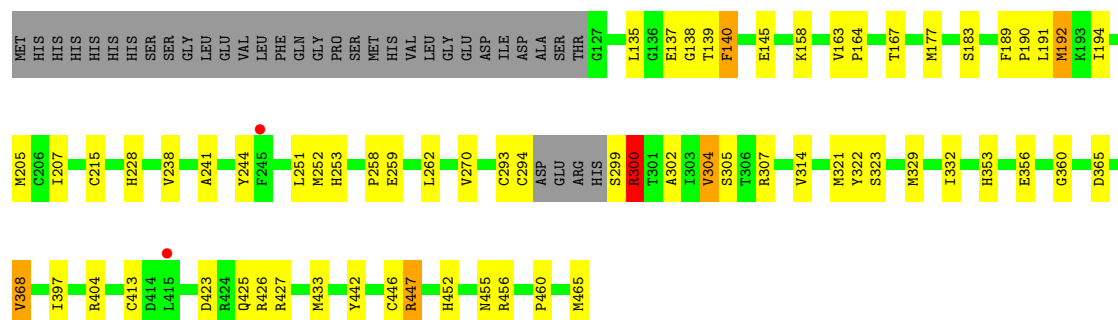
- Molecule 1: Protein kinase, putative

Chain N:  76% 14% 8%

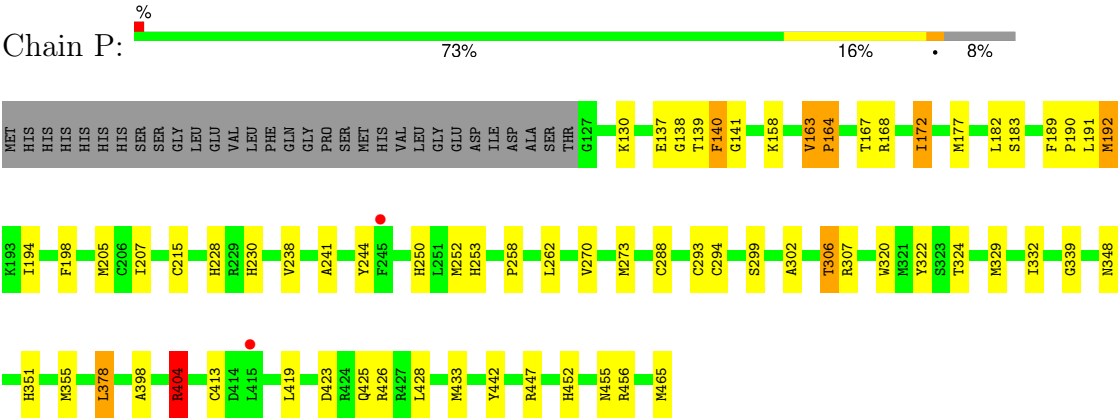


- Molecule 1: Protein kinase, putative

Chain O:  73% 16% 9%



● Molecule 1: Protein kinase, putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	147.68Å 147.68Å 265.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	127.89 – 2.40 127.89 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (127.89-2.40) 98.9 (127.89-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.40Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.296 , 0.335 0.285 , 0.321	Depositor DCC
R_{free} test set	12444 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.418 for -h,-k,l 0.427 for h,-h-k,-l 0.420 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	45259	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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 52.14 % 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 5.0721e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, A1C5R, DMS

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	0.72	0/2744	1.11	2/3733 (0.1%)
1	B	0.73	1/2746 (0.0%)	1.09	2/3735 (0.1%)
1	C	0.84	4/2745 (0.1%)	1.23	10/3733 (0.3%)
1	D	1.20	3/2745 (0.1%)	1.36	13/3733 (0.3%)
1	E	0.72	0/2746	1.11	1/3735 (0.0%)
1	F	0.73	0/2753	1.10	1/3744 (0.0%)
1	G	0.80	3/2746 (0.1%)	1.15	7/3735 (0.2%)
1	H	0.81	1/2746 (0.0%)	1.16	8/3735 (0.2%)
1	I	0.85	2/2746 (0.1%)	1.17	8/3734 (0.2%)
1	J	0.85	2/2724 (0.1%)	1.18	6/3709 (0.2%)
1	K	1.12	1/2707 (0.0%)	1.22	9/3681 (0.2%)
1	L	0.90	2/2755 (0.1%)	1.27	9/3746 (0.2%)
1	M	0.80	2/2745 (0.1%)	1.16	8/3734 (0.2%)
1	N	0.77	0/2740	1.22	11/3727 (0.3%)
1	O	0.90	3/2687 (0.1%)	1.30	13/3656 (0.4%)
1	P	0.95	2/2753 (0.1%)	1.29	16/3744 (0.4%)
All	All	0.87	26/43828 (0.1%)	1.20	124/59614 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	5
1	E	0	1
1	F	0	2
1	G	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	3
1	L	0	3
1	M	0	1
1	N	0	2
1	O	0	3
1	P	0	6
All	All	0	33

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	406	VAL	C-N	-43.68	0.77	1.33
1	K	406	VAL	C-N	-42.94	0.92	1.33
1	P	191	LEU	C-N	-29.78	0.94	1.33
1	L	191	LEU	C-N	-25.66	0.99	1.33
1	O	191	LEU	C-N	-21.91	1.04	1.33

The worst 5 of 124 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	406	VAL	CA-C-N	21.04	149.04	122.95
1	D	406	VAL	C-N-CA	21.04	149.04	122.95
1	D	406	VAL	O-C-N	-17.75	103.55	121.83
1	N	322	TYR	CB-CA-C	-17.38	84.58	111.17
1	L	191	LEU	O-C-N	-15.59	105.48	122.94

There are no chirality outliers.

5 of 33 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	456	ARG	Sidechain
1	B	456	ARG	Sidechain
1	C	456	ARG	Sidechain
1	D	276	ARG	Sidechain
1	D	284	ARG	Sidechain

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	2672	0	2560	31	0
1	B	2674	0	2567	32	0
1	C	2673	0	2571	36	0
1	D	2673	0	2570	44	0
1	E	2674	0	2567	33	0
1	F	2681	0	2571	35	0
1	G	2674	0	2567	27	0
1	H	2674	0	2566	30	0
1	I	2674	0	2574	33	0
1	J	2652	0	2531	27	0
1	K	2637	0	2545	40	0
1	L	2683	0	2579	29	0
1	M	2673	0	2563	21	0
1	N	2668	0	2556	36	0
1	O	2618	0	2499	42	0
1	P	2681	0	2582	46	0
2	A	36	0	0	0	0
2	B	36	0	0	0	0
2	C	36	0	0	0	0
2	D	36	0	0	0	0
2	E	36	0	0	1	0
2	F	36	0	0	0	0
2	G	36	0	0	0	0
2	H	36	0	0	1	0
2	I	36	0	0	0	0
2	J	36	0	0	0	0
2	K	36	0	0	0	0
2	L	36	0	0	0	0
2	M	36	0	0	0	0
2	N	36	0	0	1	0
2	O	36	0	0	0	0
2	P	36	0	0	0	0
3	A	10	0	0	0	0
3	B	15	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
3	E	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	15	0	0	0	0
3	G	10	0	0	0	0
3	H	10	0	0	0	0
3	I	5	0	0	0	0
3	J	5	0	0	1	0
3	K	5	0	0	0	0
3	L	10	0	0	0	0
3	M	10	0	0	0	0
3	N	10	0	0	0	0
3	P	5	0	0	0	0
4	C	4	0	6	0	0
5	A	83	0	0	2	0
5	B	120	0	0	6	0
5	C	131	0	0	2	0
5	D	89	0	0	7	0
5	E	109	0	0	9	0
5	F	126	0	0	7	0
5	G	110	0	0	3	0
5	H	129	0	0	1	0
5	I	121	0	0	8	0
5	J	127	0	0	4	0
5	K	143	0	0	3	0
5	L	93	0	0	3	0
5	M	123	0	0	0	0
5	N	114	0	0	1	0
5	O	121	0	0	12	0
5	P	119	0	0	13	0
All	All	45259	0	40974	530	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 530 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:D:406:VAL:O	1:D:407:ILE:N	1.60	1.29
1:O:294:CYS:HB2	5:O:692:HOH:O	1.36	1.25
1:D:406:VAL:C	1:D:407:ILE:CA	2.16	1.18
1:P:293:CYS:HB3	5:P:695:HOH:O	1.43	1.17
1:I:416:ILE:HD13	5:I:711:HOH:O	1.43	1.14

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	337/370 (91%)	329 (98%)	8 (2%)	0	100	100
1	B	337/370 (91%)	330 (98%)	7 (2%)	0	100	100
1	C	337/370 (91%)	330 (98%)	7 (2%)	0	100	100
1	D	337/370 (91%)	329 (98%)	8 (2%)	0	100	100
1	E	337/370 (91%)	330 (98%)	7 (2%)	0	100	100
1	F	338/370 (91%)	329 (97%)	9 (3%)	0	100	100
1	G	337/370 (91%)	329 (98%)	8 (2%)	0	100	100
1	H	337/370 (91%)	330 (98%)	7 (2%)	0	100	100
1	I	337/370 (91%)	327 (97%)	10 (3%)	0	100	100
1	J	337/370 (91%)	327 (97%)	9 (3%)	1 (0%)	36	50
1	K	331/370 (90%)	322 (97%)	8 (2%)	1 (0%)	36	50
1	L	338/370 (91%)	330 (98%)	7 (2%)	1 (0%)	36	50
1	M	337/370 (91%)	329 (98%)	7 (2%)	1 (0%)	36	50
1	N	337/370 (91%)	330 (98%)	6 (2%)	1 (0%)	36	50
1	O	332/370 (90%)	324 (98%)	7 (2%)	1 (0%)	36	50
1	P	338/370 (91%)	328 (97%)	10 (3%)	0	100	100
All	All	5384/5920 (91%)	5253 (98%)	125 (2%)	6 (0%)	48	64

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	305	SER
1	N	305	SER
1	K	305	SER
1	L	305	SER

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Mol	Chain	Res	Type
1	M	305	SER

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	284/332 (86%)	279 (98%)	5 (2%)	51	73
1	B	284/332 (86%)	278 (98%)	6 (2%)	47	69
1	C	283/332 (85%)	277 (98%)	6 (2%)	47	69
1	D	283/332 (85%)	278 (98%)	5 (2%)	51	73
1	E	284/332 (86%)	278 (98%)	6 (2%)	47	69
1	F	285/332 (86%)	277 (97%)	8 (3%)	38	60
1	G	284/332 (86%)	282 (99%)	2 (1%)	76	88
1	H	284/332 (86%)	278 (98%)	6 (2%)	47	69
1	I	283/332 (85%)	274 (97%)	9 (3%)	34	56
1	J	278/332 (84%)	273 (98%)	5 (2%)	51	73
1	K	280/332 (84%)	273 (98%)	7 (2%)	42	64
1	L	284/332 (86%)	276 (97%)	8 (3%)	38	60
1	M	283/332 (85%)	280 (99%)	3 (1%)	65	82
1	N	282/332 (85%)	276 (98%)	6 (2%)	47	69
1	O	274/332 (82%)	268 (98%)	6 (2%)	45	67
1	P	283/332 (85%)	277 (98%)	6 (2%)	47	69
All	All	4518/5312 (85%)	4424 (98%)	94 (2%)	47	69

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	378	LEU
1	L	324	THR
1	K	270	VAL
1	L	137	GLU

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Mol	Chain	Res	Type
1	M	378	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	448	GLN
1	L	250	HIS
1	P	230	HIS
1	K	275	HIS
1	L	275	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

45 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	$\# Z > 2$
3	SO4	J	502	-	4,4,4	0.31	0	6,6,6	0.64	0
2	A1C5R	E	501	1	39,39,39	0.49	0	45,55,55	1.12	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	G	503	-	4,4,4	0.31	0	6,6,6	0.32	0
2	A1C5R	K	501	1	39,39,39	0.49	0	45,55,55	1.07	1 (2%)
2	A1C5R	P	501	1	39,39,39	0.51	0	45,55,55	1.10	1 (2%)
3	SO4	B	502	-	4,4,4	0.28	0	6,6,6	0.53	0
3	SO4	N	502	-	4,4,4	0.29	0	6,6,6	0.59	0
2	A1C5R	F	501	1	39,39,39	0.49	0	45,55,55	1.15	1 (2%)
3	SO4	C	504	-	4,4,4	0.27	0	6,6,6	0.37	0
2	A1C5R	C	501	1	39,39,39	0.49	0	45,55,55	1.11	1 (2%)
2	A1C5R	M	501	1	39,39,39	0.47	0	45,55,55	1.13	2 (4%)
3	SO4	H	502	-	4,4,4	0.29	0	6,6,6	0.70	0
3	SO4	L	502	-	4,4,4	0.28	0	6,6,6	0.66	0
2	A1C5R	I	501	1	39,39,39	0.50	0	45,55,55	1.06	1 (2%)
3	SO4	M	502	-	4,4,4	0.31	0	6,6,6	0.43	0
2	A1C5R	J	501	1	39,39,39	0.49	0	45,55,55	1.08	1 (2%)
3	SO4	H	503	-	4,4,4	0.31	0	6,6,6	0.27	0
2	A1C5R	A	501	1	39,39,39	0.49	0	45,55,55	1.14	2 (4%)
2	A1C5R	G	501	1	39,39,39	0.50	0	45,55,55	1.19	3 (6%)
3	SO4	F	502	-	4,4,4	0.30	0	6,6,6	0.68	0
3	SO4	N	503	-	4,4,4	0.31	0	6,6,6	0.39	0
2	A1C5R	D	501	1	39,39,39	0.50	0	45,55,55	1.09	1 (2%)
3	SO4	B	504	-	4,4,4	0.31	0	6,6,6	0.67	0
3	SO4	E	502	-	4,4,4	0.28	0	6,6,6	0.50	0
2	A1C5R	B	501	1	39,39,39	0.50	0	45,55,55	1.12	2 (4%)
3	SO4	A	502	-	4,4,4	0.34	0	6,6,6	0.74	0
3	SO4	A	503	-	4,4,4	0.28	0	6,6,6	0.68	0
3	SO4	F	504	-	4,4,4	0.30	0	6,6,6	0.51	0
3	SO4	P	502	-	4,4,4	0.30	0	6,6,6	0.58	0
3	SO4	K	502	-	4,4,4	0.31	0	6,6,6	0.53	0
3	SO4	F	503	-	4,4,4	0.30	0	6,6,6	0.71	0
2	A1C5R	L	501	1	39,39,39	0.48	0	45,55,55	1.09	1 (2%)
2	A1C5R	O	501	1	39,39,39	0.48	0	45,55,55	1.04	1 (2%)
3	SO4	G	502	-	4,4,4	0.27	0	6,6,6	1.05	1 (16%)
3	SO4	L	503	-	4,4,4	0.30	0	6,6,6	0.32	0
3	SO4	B	503	-	4,4,4	0.30	0	6,6,6	0.49	0
3	SO4	D	503	-	4,4,4	0.29	0	6,6,6	0.15	0
3	SO4	D	502	-	4,4,4	0.30	0	6,6,6	0.42	0
3	SO4	C	503	-	4,4,4	0.30	0	6,6,6	0.30	0
3	SO4	M	503	-	4,4,4	0.27	0	6,6,6	0.23	0
2	A1C5R	N	501	1	39,39,39	0.48	0	45,55,55	1.14	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMS	C	502	-	3,3,3	0.20	0	3,3,3	0.09	0
2	A1C5R	H	501	1	39,39,39	0.49	0	45,55,55	1.15	2 (4%)
3	SO4	E	503	-	4,4,4	0.31	0	6,6,6	0.65	0
3	SO4	I	502	-	4,4,4	0.29	0	6,6,6	0.38	0

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	A1C5R	O	501	1	-	3/20/33/33	0/4/4/4
2	A1C5R	H	501	1	-	3/20/33/33	0/4/4/4
2	A1C5R	I	501	1	-	3/20/33/33	0/4/4/4
2	A1C5R	D	501	1	-	3/20/33/33	0/4/4/4
2	A1C5R	E	501	1	-	3/20/33/33	0/4/4/4
2	A1C5R	J	501	1	-	3/20/33/33	0/4/4/4
2	A1C5R	K	501	1	-	3/20/33/33	0/4/4/4
2	A1C5R	B	501	1	-	2/20/33/33	0/4/4/4
2	A1C5R	P	501	1	-	3/20/33/33	0/4/4/4
2	A1C5R	N	501	1	-	1/20/33/33	0/4/4/4
2	A1C5R	F	501	1	-	3/20/33/33	0/4/4/4
2	A1C5R	A	501	1	-	3/20/33/33	0/4/4/4
2	A1C5R	G	501	1	-	3/20/33/33	0/4/4/4
2	A1C5R	C	501	1	-	3/20/33/33	0/4/4/4
2	A1C5R	M	501	1	-	3/20/33/33	0/4/4/4
2	A1C5R	L	501	1	-	3/20/33/33	0/4/4/4

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	501	A1C5R	C35-C7-C10	6.68	128.91	111.97
2	H	501	A1C5R	C35-C7-C10	6.44	128.30	111.97
2	F	501	A1C5R	C35-C7-C10	6.42	128.25	111.97
2	A	501	A1C5R	C35-C7-C10	6.42	128.25	111.97
2	B	501	A1C5R	C35-C7-C10	6.35	128.06	111.97

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	501	A1C5R	C7-C35-N36-C34
2	N	501	A1C5R	N36-C35-C7-C10
2	A	501	A1C5R	N36-C35-C7-C10
2	B	501	A1C5R	N36-C35-C7-C10
2	E	501	A1C5R	N36-C35-C7-C10

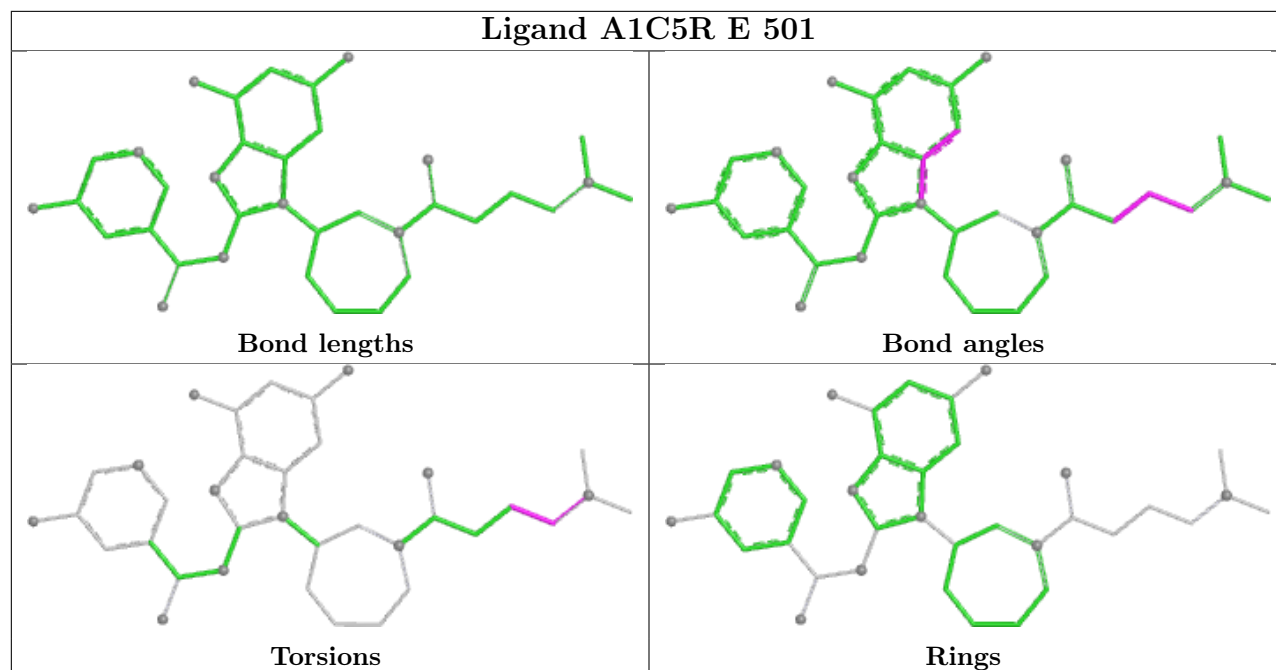
There are no ring outliers.

4 monomers are involved in 4 short contacts:

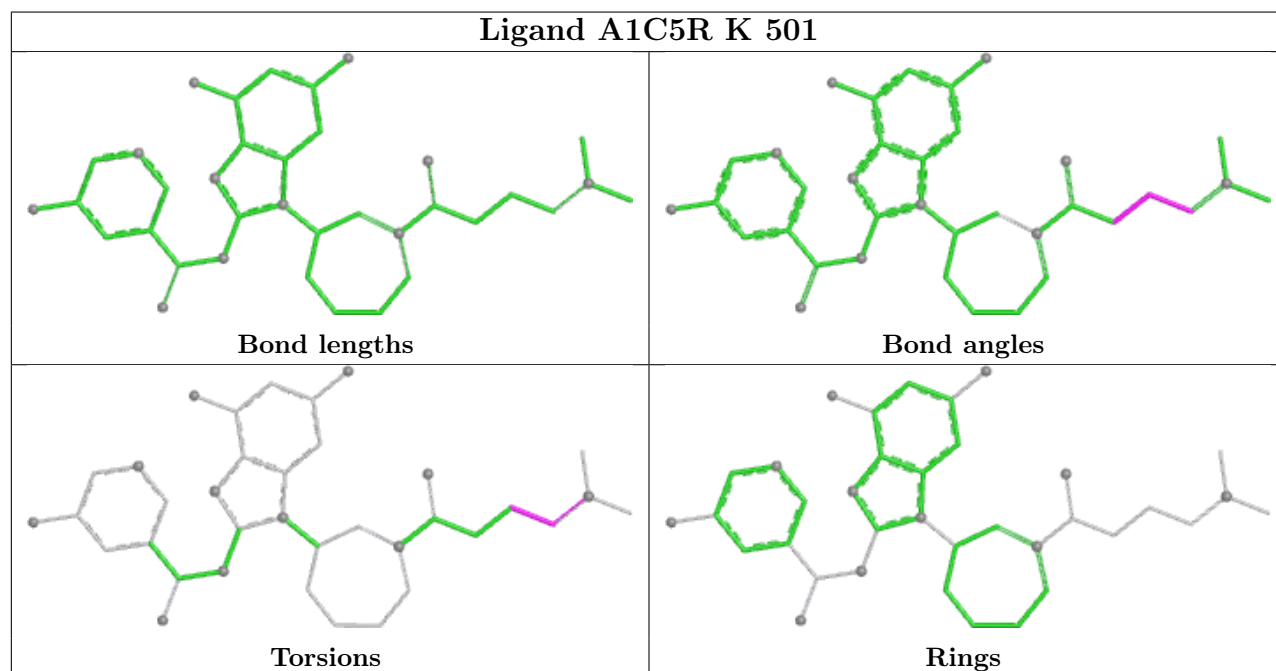
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	502	SO4	1	0
2	E	501	A1C5R	1	0
2	N	501	A1C5R	1	0
2	H	501	A1C5R	1	0

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.

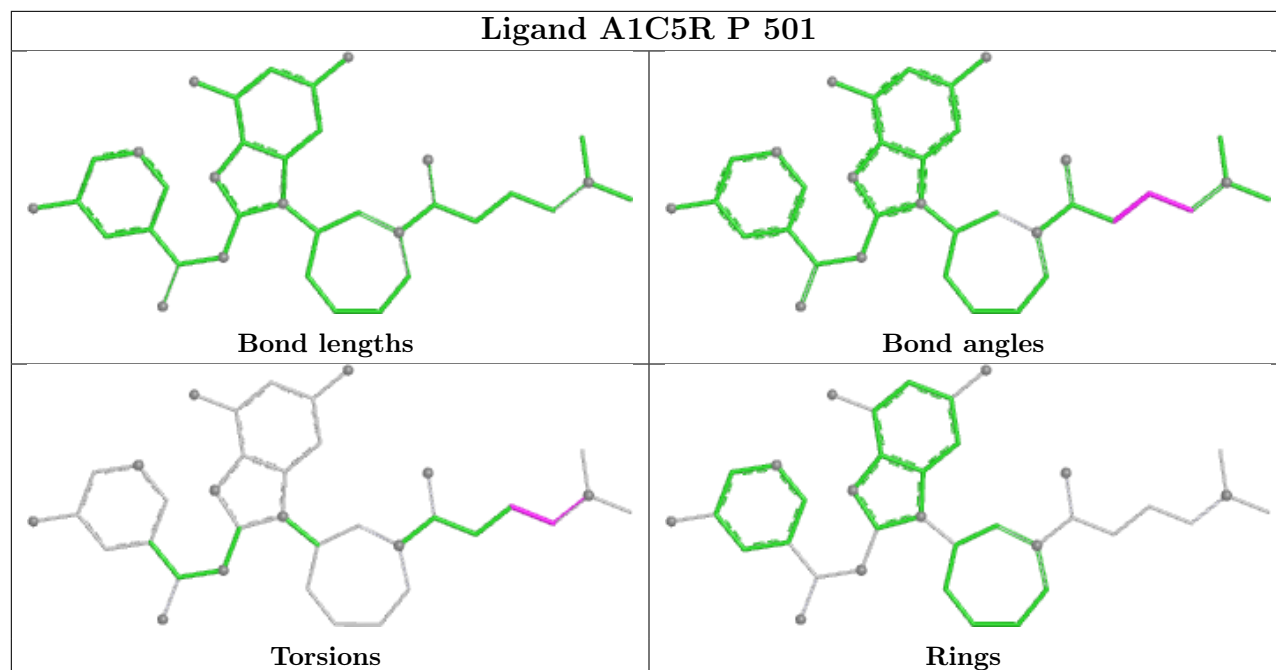
Ligand A1C5R E 501



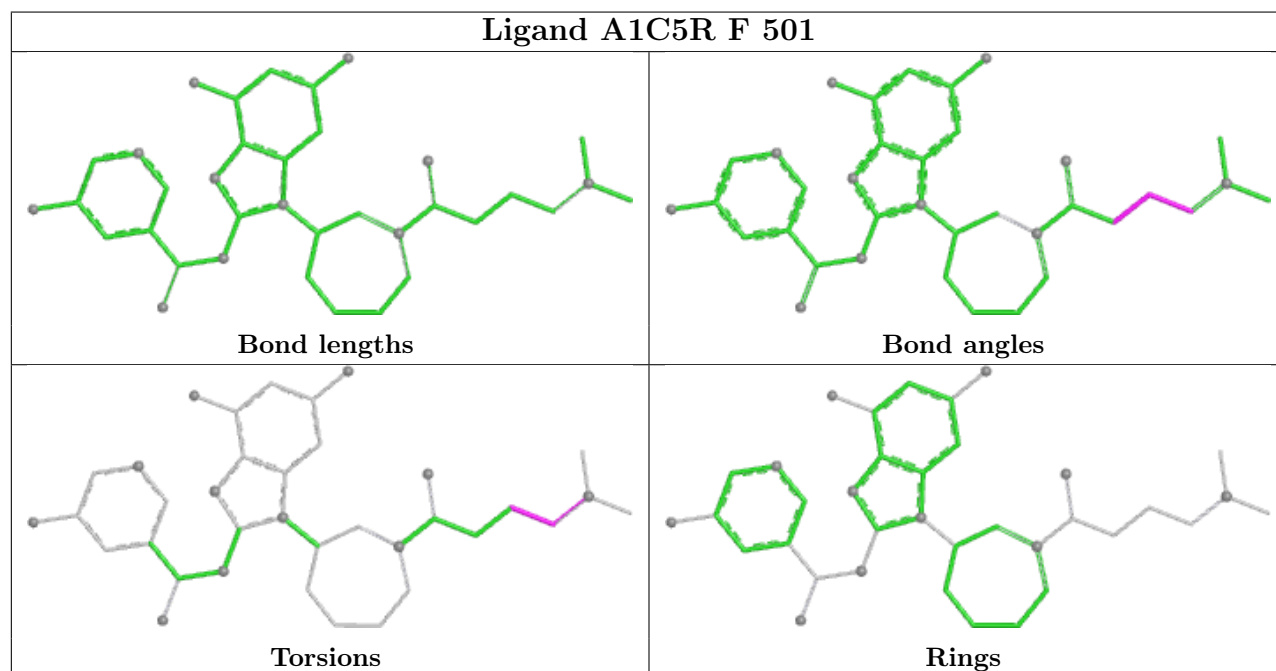
Ligand A1C5R K 501



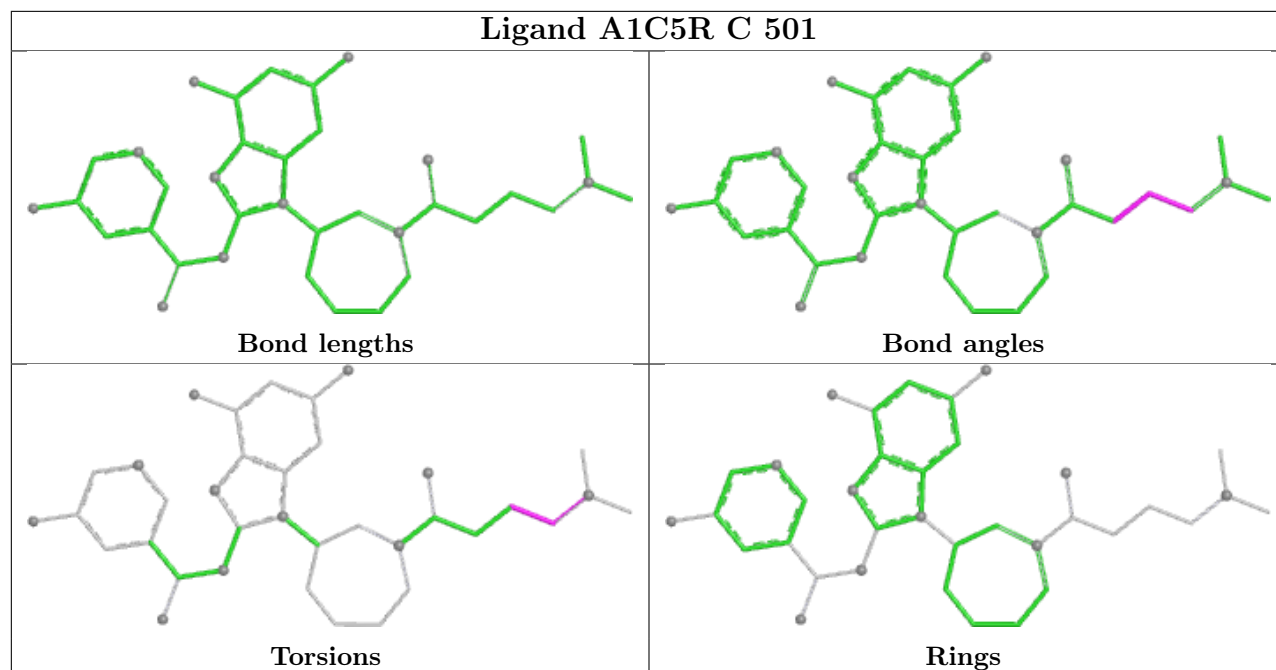
Ligand A1C5R P 501



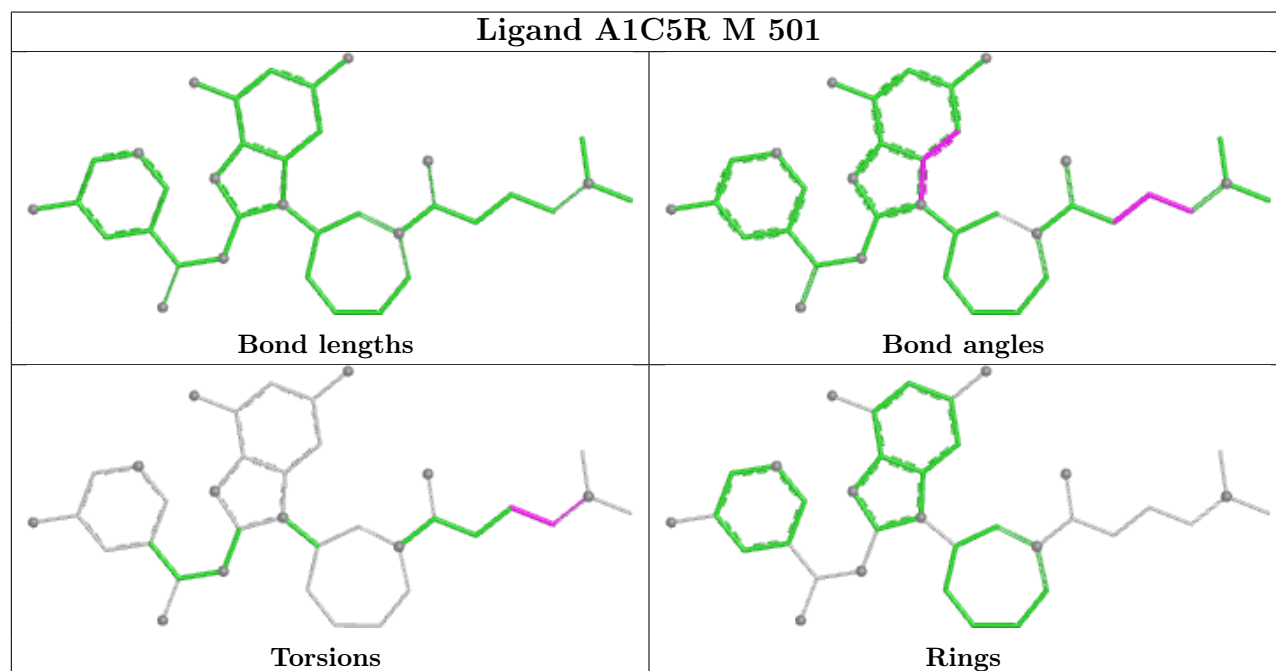
Ligand A1C5R F 501



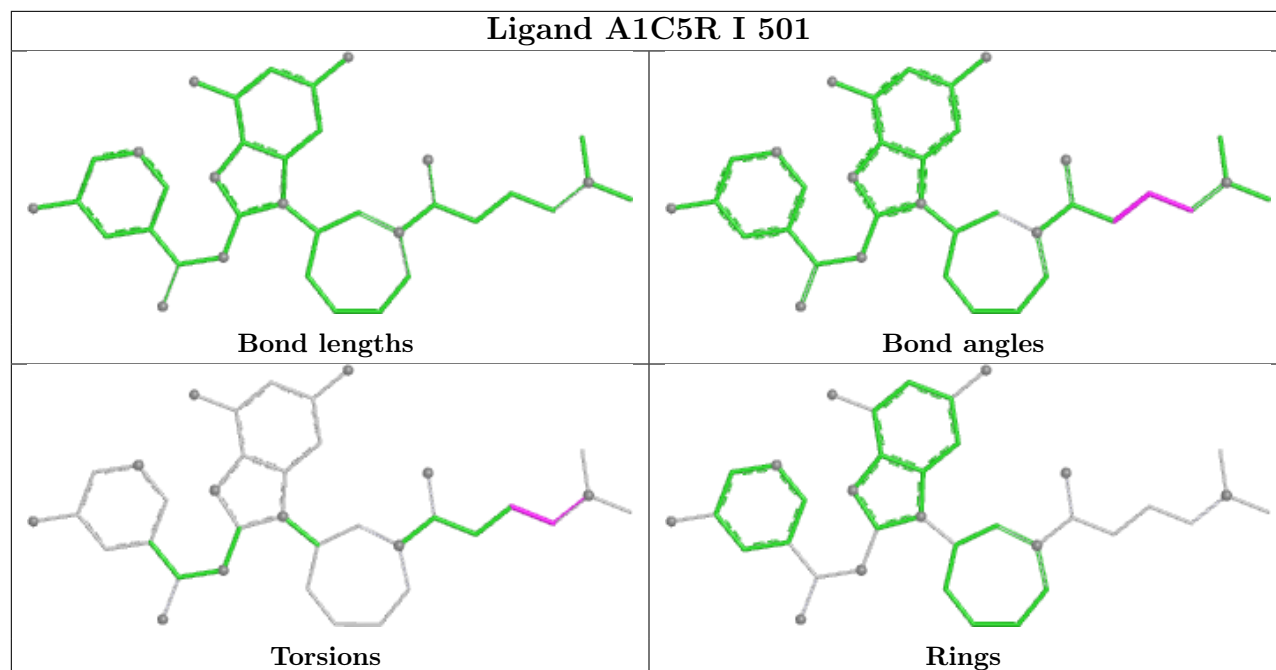
Ligand A1C5R C 501



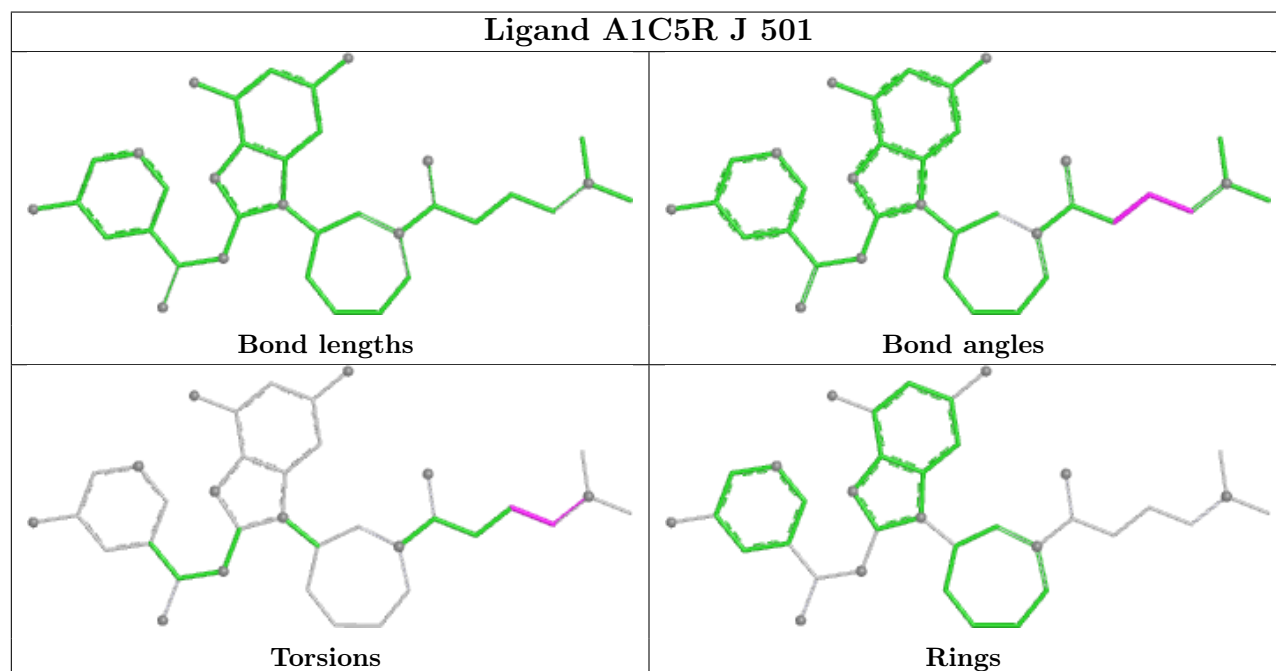
Ligand A1C5R M 501



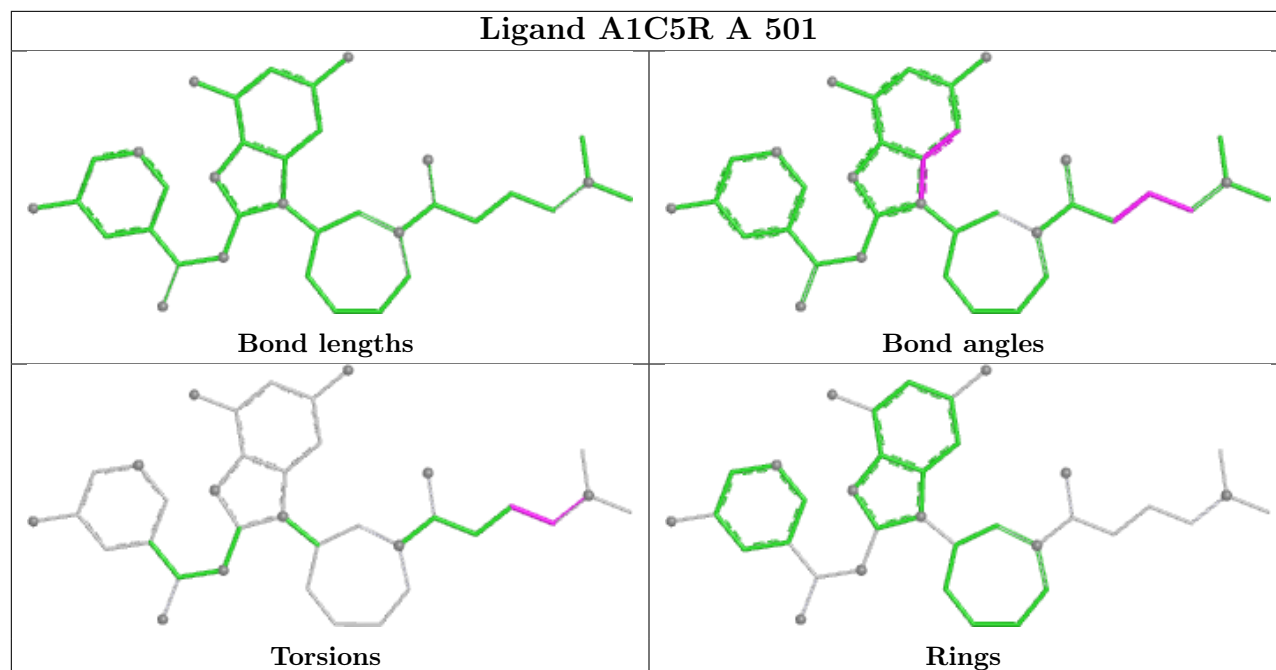
Ligand A1C5R I 501



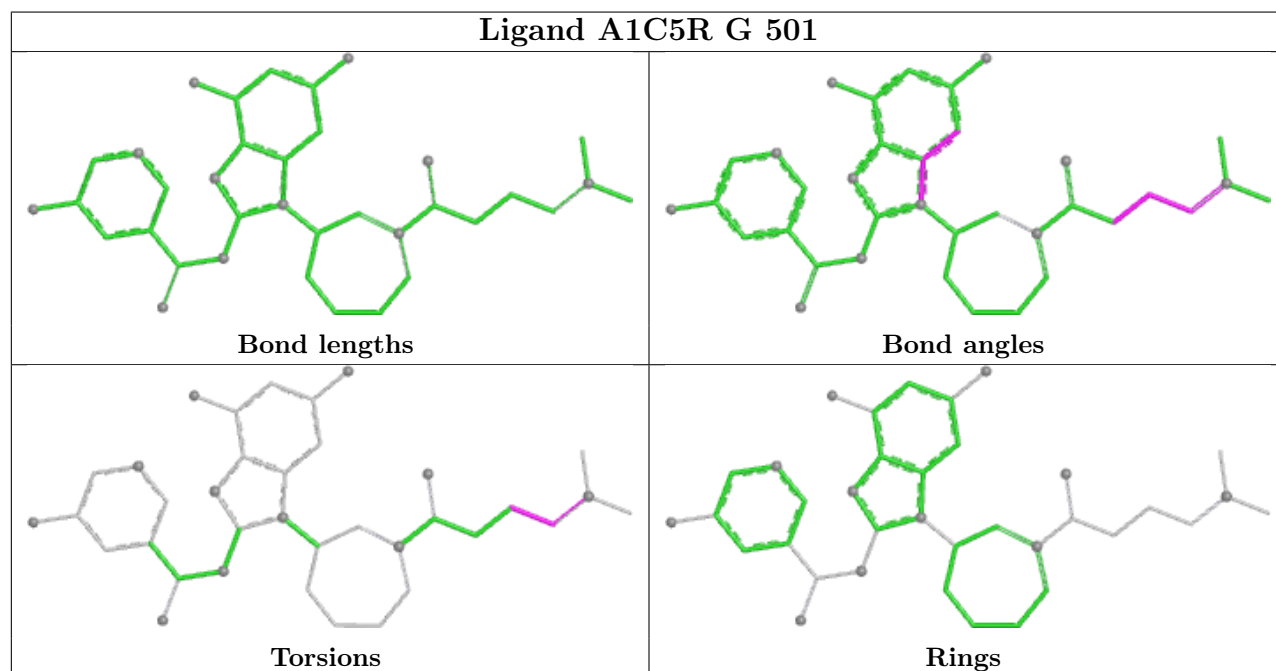
Ligand A1C5R J 501



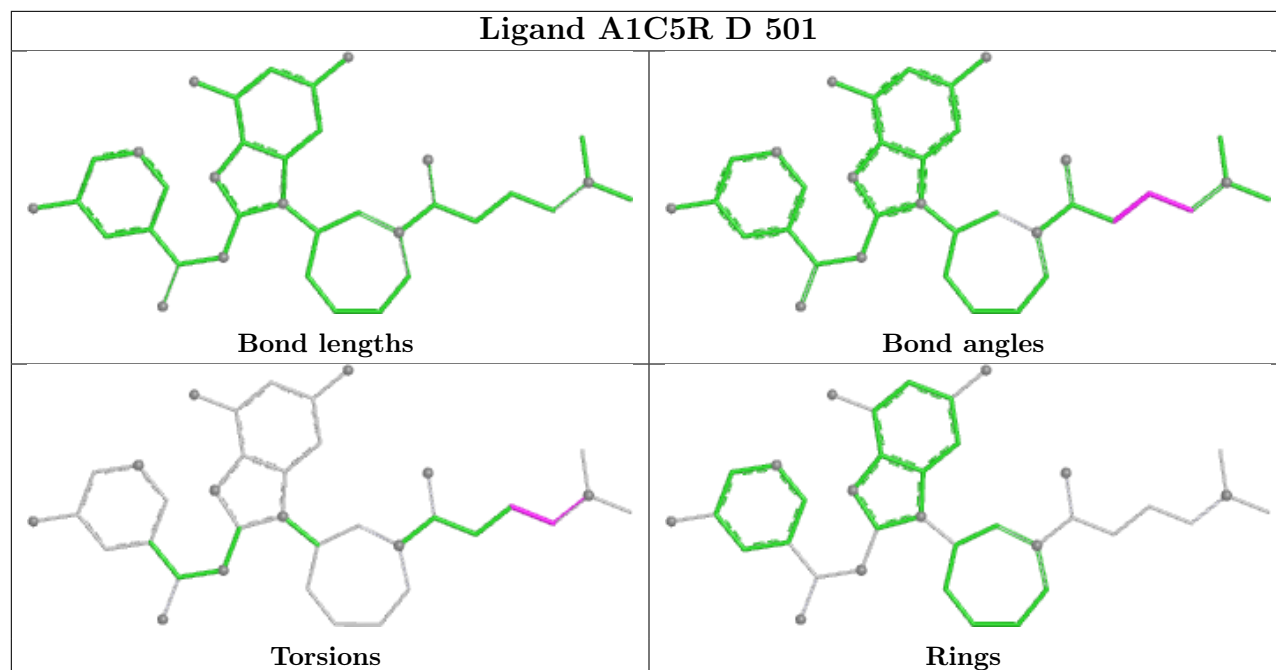
Ligand A1C5R A 501



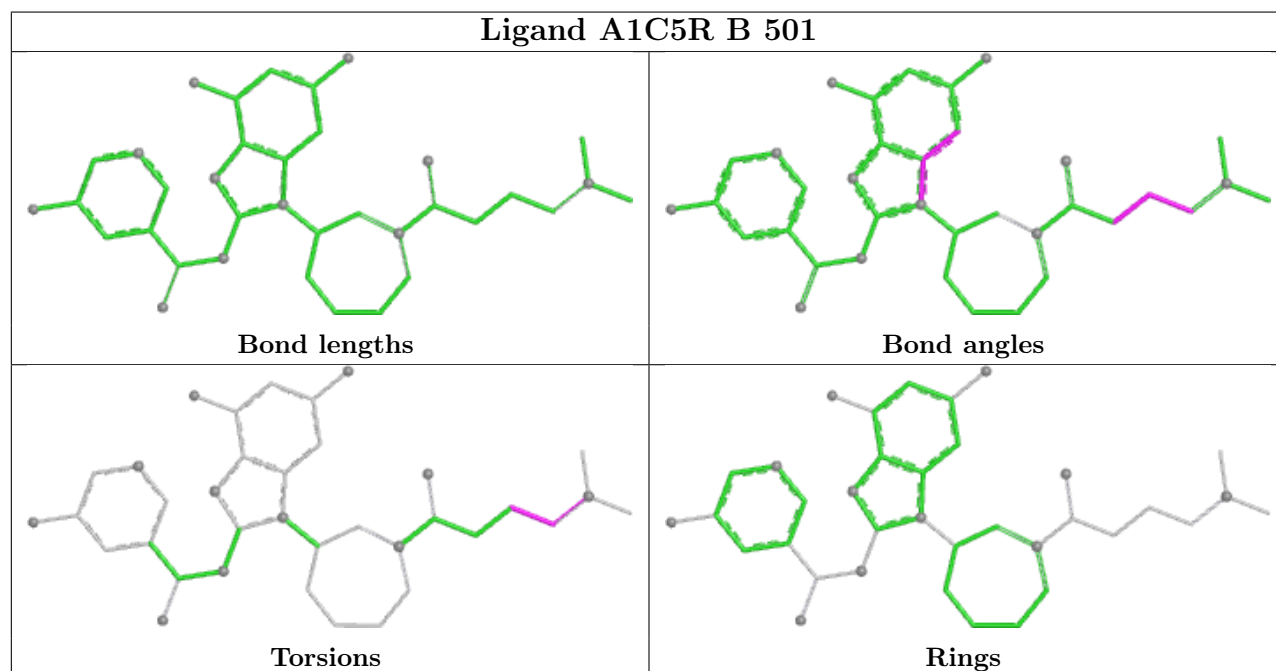
Ligand A1C5R G 501



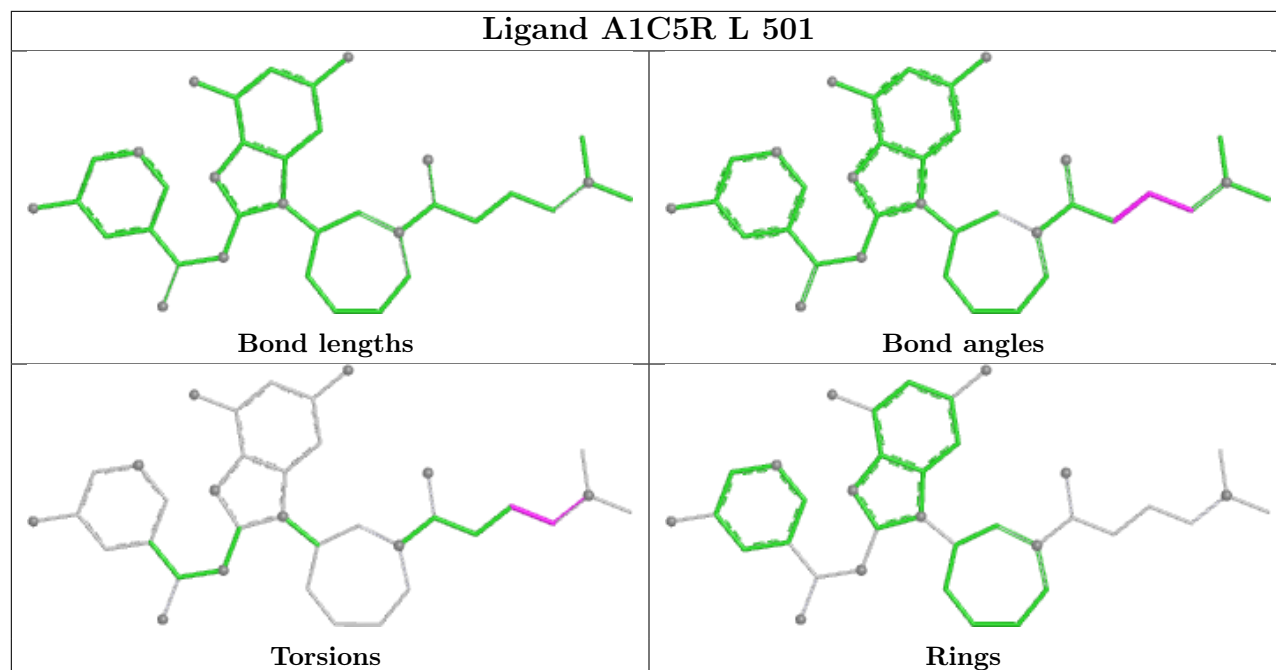
Ligand A1C5R D 501



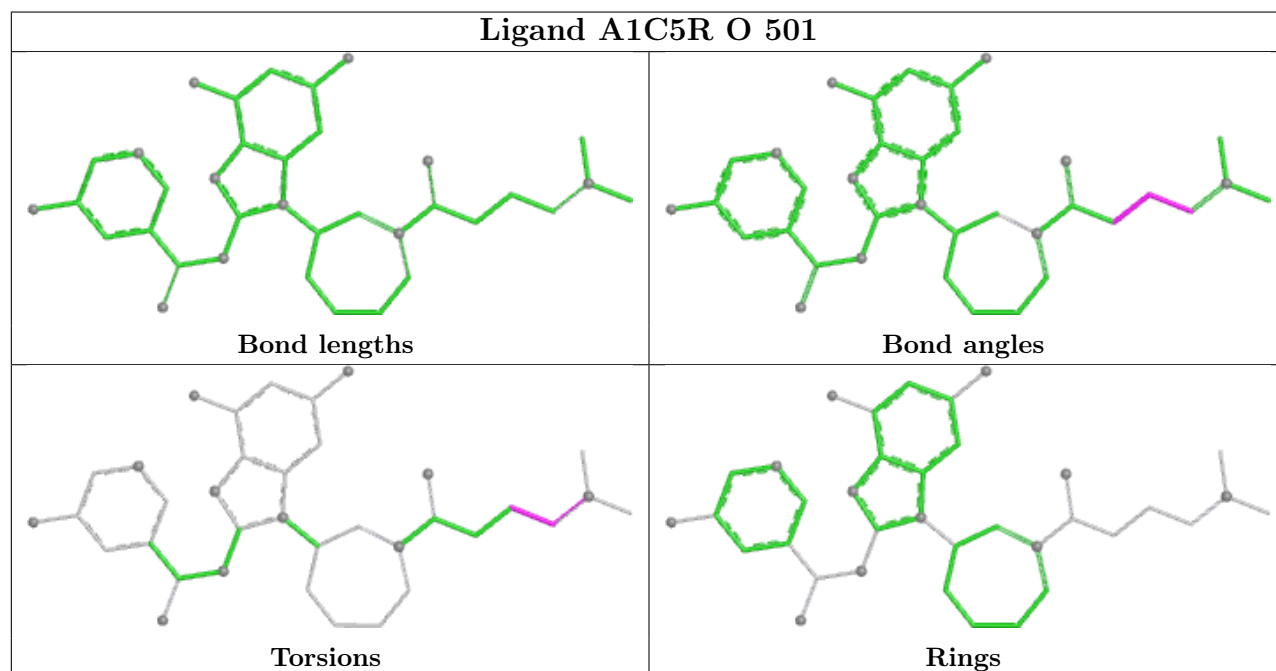
Ligand A1C5R B 501

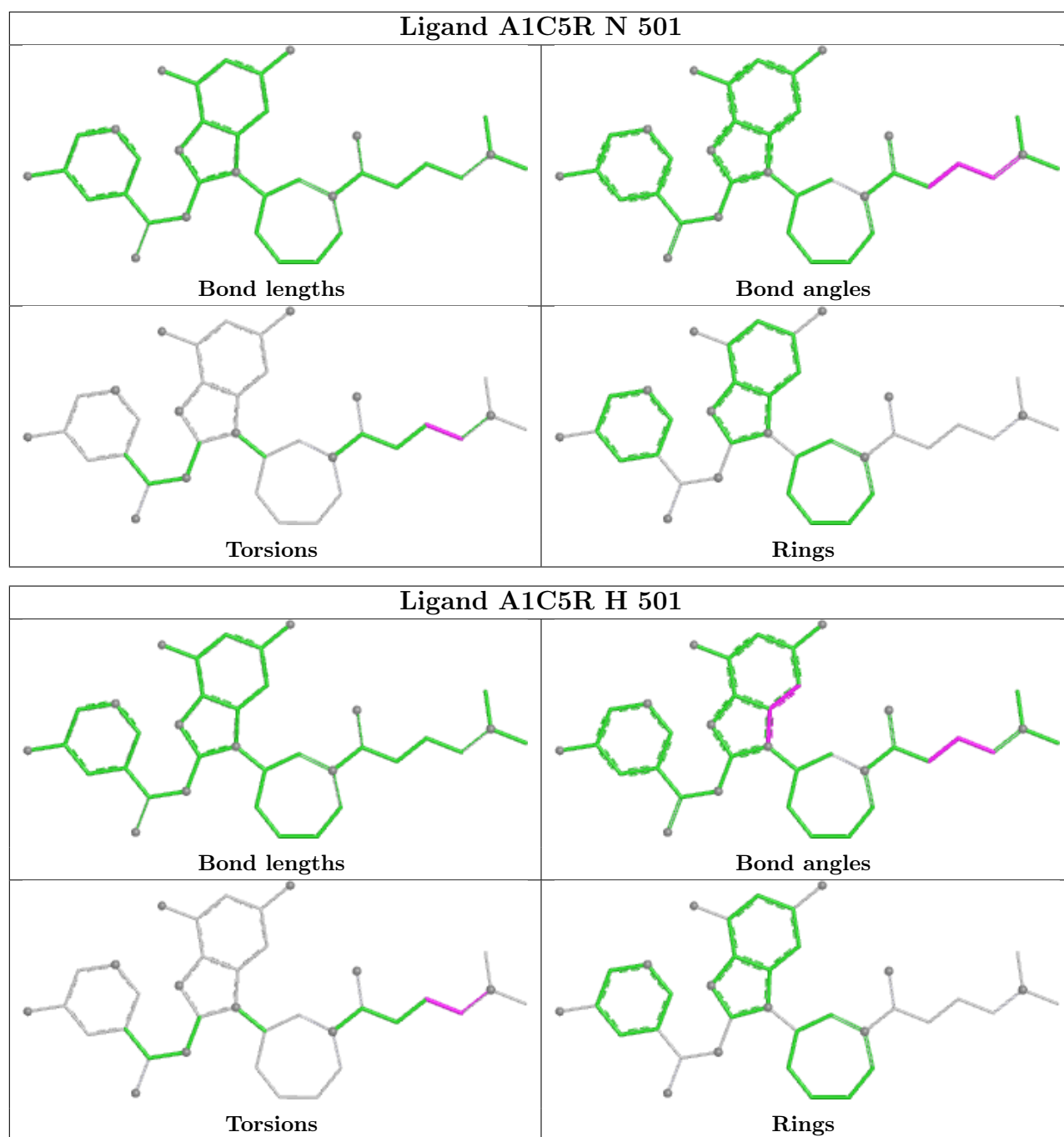


Ligand A1C5R L 501



Ligand A1C5R O 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	3
1	M	2
1	C	2
1	I	2
1	G	1
1	H	1
1	J	1
1	O	1
1	L	1
1	P	1
1	K	1

The worst 5 of 16 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	192:MET	C	193:LYS	N	1.19
1	M	192:MET	C	193:LYS	N	1.17
1	C	192:MET	C	193:LYS	N	1.15
1	M	191:LEU	C	192:MET	N	1.14
1	I	192:MET	C	193:LYS	N	1.13

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	339/370 (91%)	-0.97	0 100 100	15, 29, 55, 67	0
1	B	339/370 (91%)	-0.96	0 100 100	14, 29, 56, 68	0
1	C	339/370 (91%)	-0.75	1 (0%) 90 88	17, 39, 75, 88	0
1	D	339/370 (91%)	-0.79	2 (0%) 85 83	14, 37, 71, 87	0
1	E	339/370 (91%)	-0.94	0 100 100	16, 29, 57, 68	0
1	F	339/370 (91%)	-0.94	0 100 100	15, 28, 57, 68	1 (0%)
1	G	339/370 (91%)	-0.99	0 100 100	15, 29, 57, 68	0
1	H	339/370 (91%)	-0.96	0 100 100	15, 30, 57, 67	0
1	I	339/370 (91%)	-0.73	3 (0%) 81 78	17, 40, 76, 90	0
1	J	339/370 (91%)	-0.82	2 (0%) 85 83	15, 35, 70, 88	0
1	K	335/370 (90%)	-0.73	2 (0%) 85 83	15, 39, 81, 93	0
1	L	339/370 (91%)	-0.77	1 (0%) 90 88	16, 36, 75, 86	1 (0%)
1	M	339/370 (91%)	-0.95	0 100 100	16, 30, 58, 72	0
1	N	339/370 (91%)	-0.97	0 100 100	13, 29, 57, 70	0
1	O	335/370 (90%)	-0.76	2 (0%) 85 83	17, 39, 77, 91	1 (0%)
1	P	339/370 (91%)	-0.78	2 (0%) 85 83	16, 36, 74, 88	1 (0%)
All	All	5416/5920 (91%)	-0.86	15 (0%) 90 88	13, 33, 67, 93	4 (0%)

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	245	PHE	3.5
1	J	245	PHE	3.3
1	D	245	PHE	3.2
1	K	245	PHE	3.2
1	C	245	PHE	3.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	A1C5R	F	501	36/36	0.97	0.05	18,21,26,26	0
3	SO4	C	503	5/5	0.97	0.07	93,93,93,93	0
3	SO4	L	503	5/5	0.97	0.09	109,109,109,109	0
2	A1C5R	D	501	36/36	0.98	0.05	22,24,28,28	0
2	A1C5R	E	501	36/36	0.98	0.05	13,17,26,26	0
2	A1C5R	A	501	36/36	0.98	0.05	17,20,26,26	0
2	A1C5R	G	501	36/36	0.98	0.05	16,18,24,24	0
2	A1C5R	H	501	36/36	0.98	0.05	16,19,28,28	0
2	A1C5R	I	501	36/36	0.98	0.05	20,23,27,27	0
2	A1C5R	J	501	36/36	0.98	0.04	19,20,25,25	0
2	A1C5R	K	501	36/36	0.98	0.06	23,25,26,26	0
2	A1C5R	L	501	36/36	0.98	0.06	20,22,26,26	0
2	A1C5R	M	501	36/36	0.98	0.06	19,20,25,25	0
2	A1C5R	N	501	36/36	0.98	0.05	16,21,26,26	0
2	A1C5R	O	501	36/36	0.98	0.05	20,21,25,26	0
2	A1C5R	P	501	36/36	0.98	0.05	21,22,26,26	0
3	SO4	A	502	5/5	0.98	0.06	57,57,57,57	0
3	SO4	A	503	5/5	0.98	0.05	49,49,50,50	0
3	SO4	B	503	5/5	0.98	0.05	75,76,76,76	0
2	A1C5R	B	501	36/36	0.98	0.05	16,20,27,28	0
3	SO4	D	502	5/5	0.98	0.05	84,84,85,85	0
3	SO4	D	503	5/5	0.98	0.06	122,122,122,122	0
3	SO4	G	503	5/5	0.98	0.05	65,65,65,65	0
2	A1C5R	C	501	36/36	0.98	0.06	25,26,27,28	0
3	SO4	M	503	5/5	0.98	0.06	65,65,65,65	0
3	SO4	N	503	5/5	0.98	0.06	76,76,76,76	0
3	SO4	E	503	5/5	0.99	0.04	57,57,57,57	0

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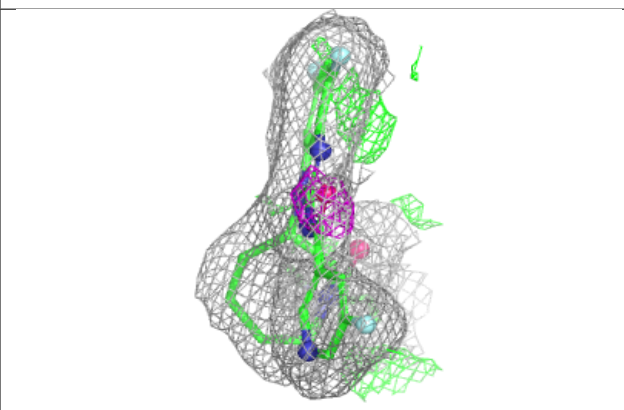
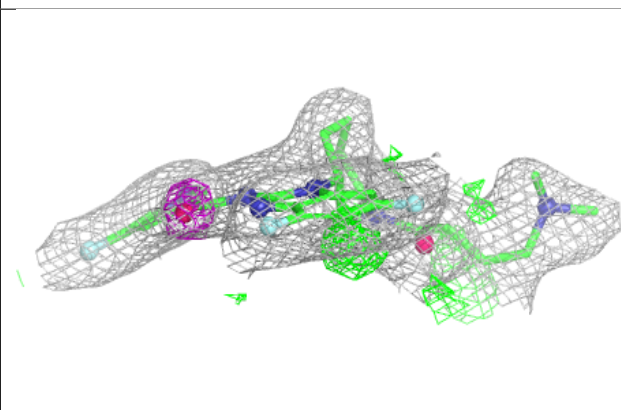
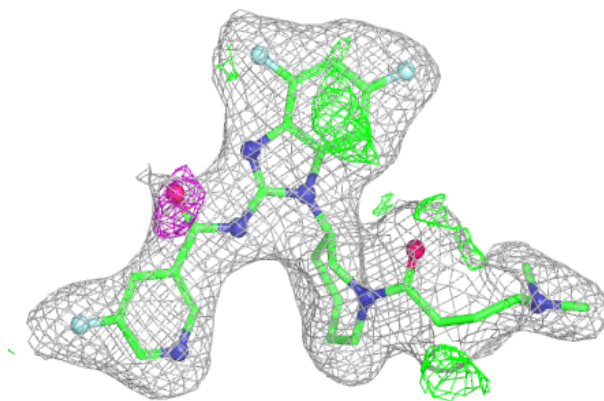
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	F	502	5/5	0.99	0.05	48,48,48,48	0
3	SO4	F	503	5/5	0.99	0.05	61,61,61,61	0
3	SO4	F	504	5/5	0.99	0.05	74,74,74,74	0
3	SO4	G	502	5/5	0.99	0.03	45,46,46,46	0
3	SO4	C	504	5/5	0.99	0.04	76,76,76,77	0
3	SO4	H	502	5/5	0.99	0.04	51,51,51,51	0
3	SO4	H	503	5/5	0.99	0.05	68,69,69,69	0
3	SO4	I	502	5/5	0.99	0.05	74,74,74,74	0
3	SO4	J	502	5/5	0.99	0.05	77,78,78,78	0
3	SO4	K	502	5/5	0.99	0.06	50,51,51,51	0
3	SO4	L	502	5/5	0.99	0.07	58,58,58,59	0
3	SO4	B	504	5/5	0.99	0.07	61,61,61,61	0
3	SO4	B	502	5/5	0.99	0.04	46,46,46,46	0
3	SO4	N	502	5/5	0.99	0.05	49,49,49,49	0
3	SO4	E	502	5/5	0.99	0.03	47,47,48,48	0
3	SO4	P	502	5/5	0.99	0.10	69,69,69,69	0
4	DMS	C	502	4/4	0.99	0.04	25,25,26,26	0
3	SO4	M	502	5/5	1.00	0.03	41,41,42,42	0

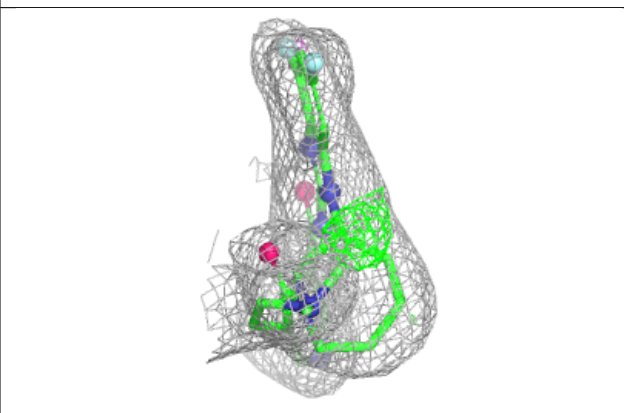
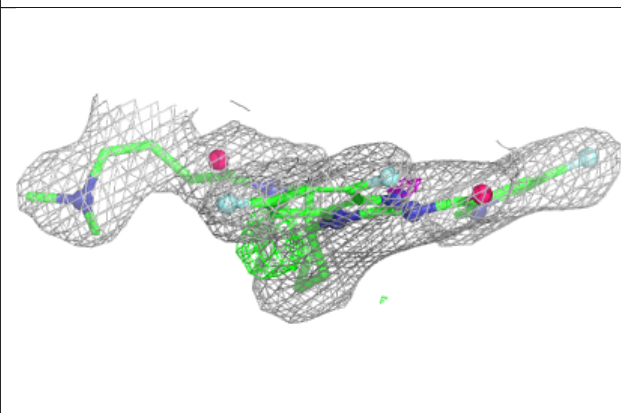
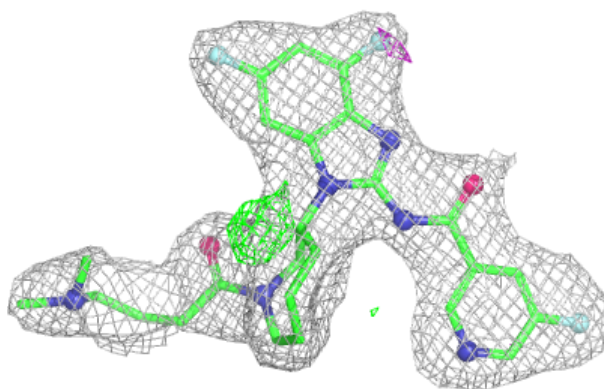
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1C5R F 501:

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

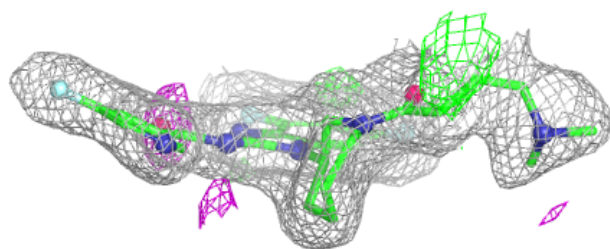
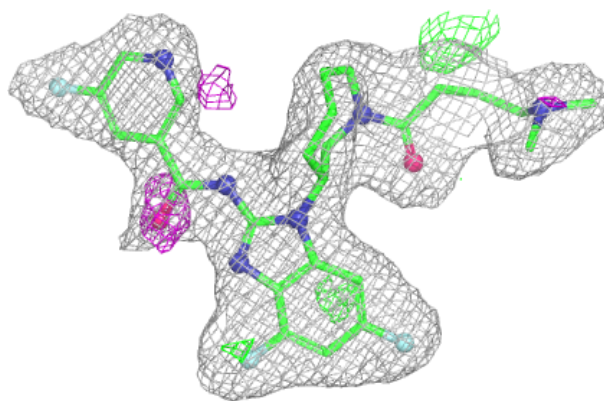
**Electron density around A1C5R D 501:**

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

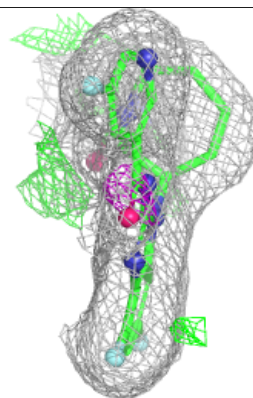
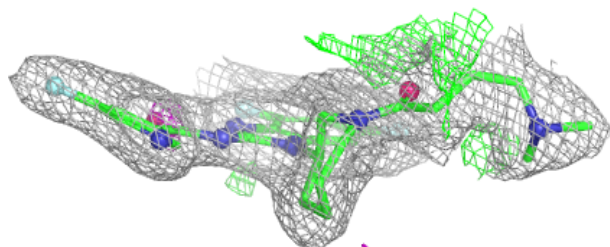
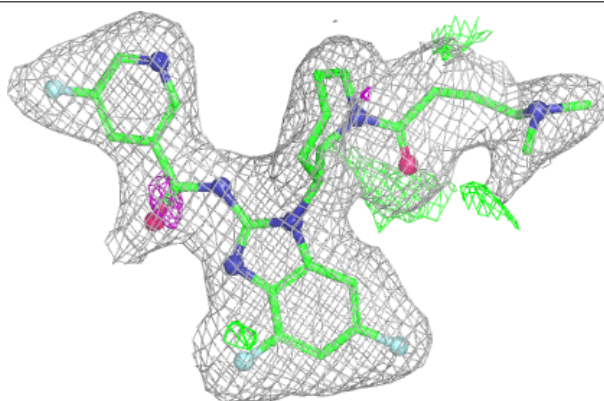


Electron density around A1C5R E 501:

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

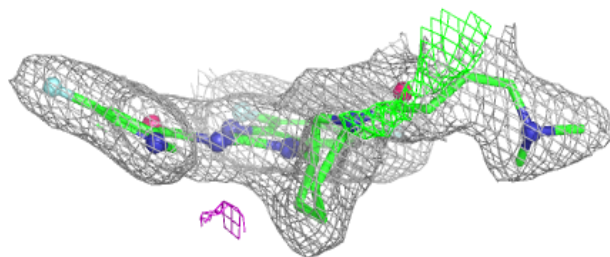
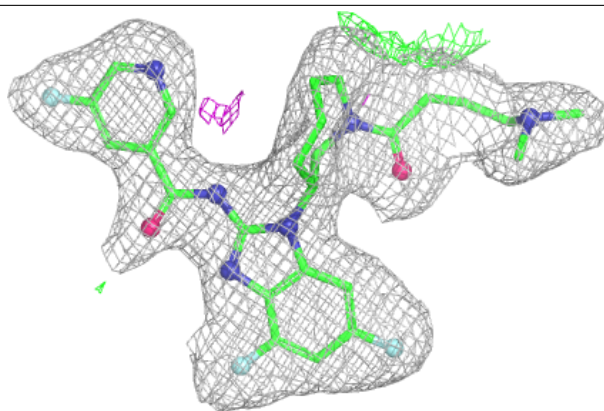
**Electron density around A1C5R A 501:**

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

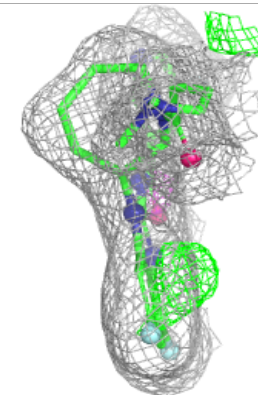
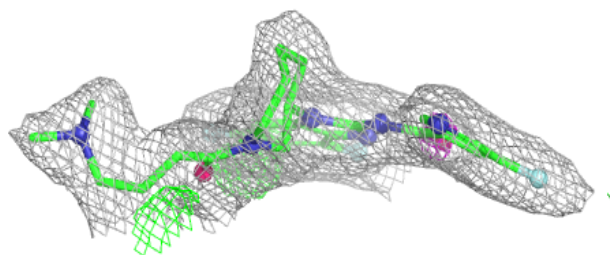
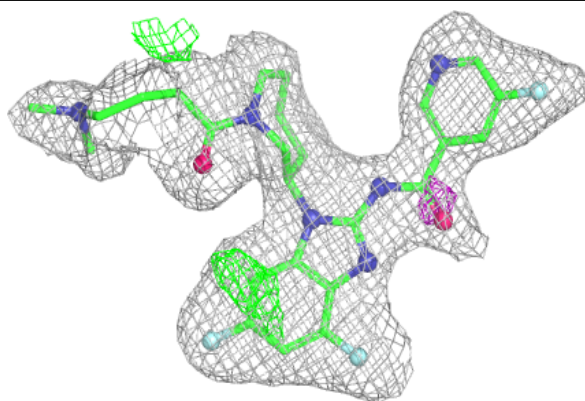


Electron density around A1C5R G 501:

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

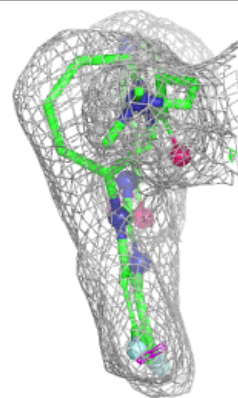
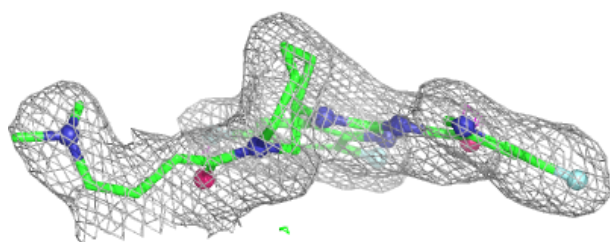
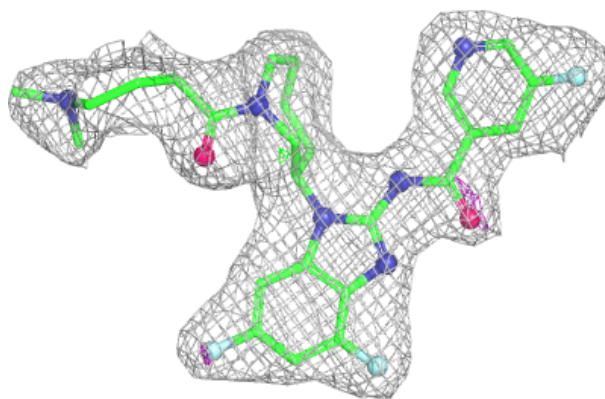
**Electron density around A1C5R H 501:**

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

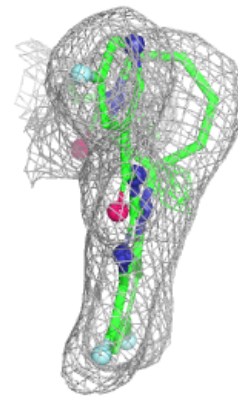
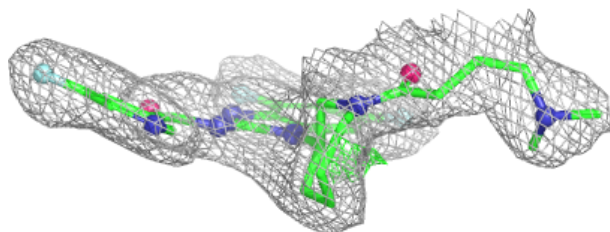
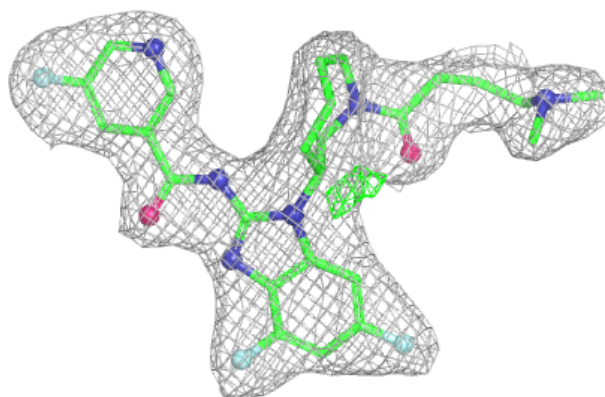


Electron density around A1C5R I 501:

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

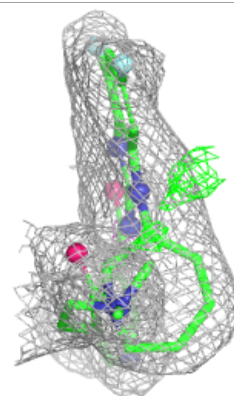
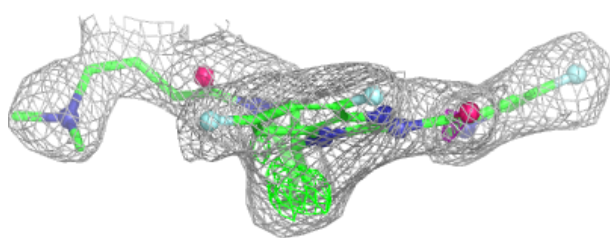
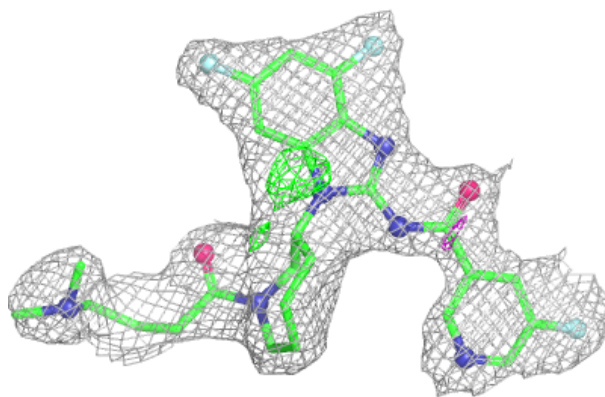
**Electron density around A1C5R J 501:**

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

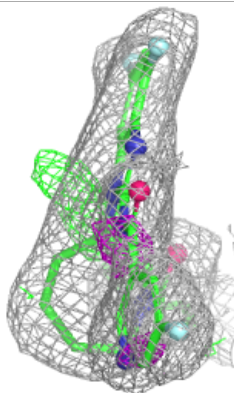
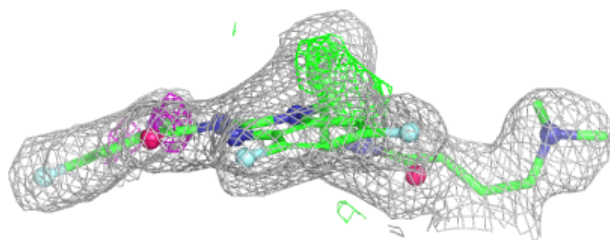
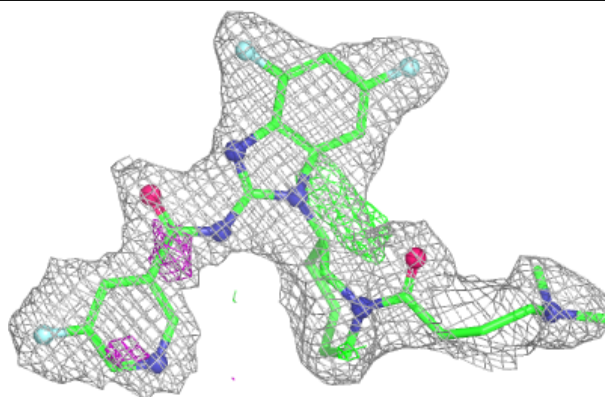


Electron density around A1C5R K 501:

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

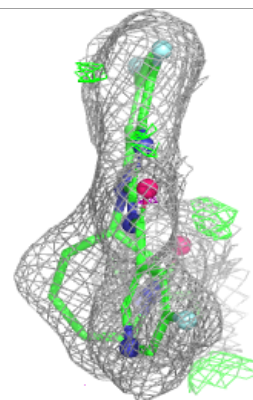
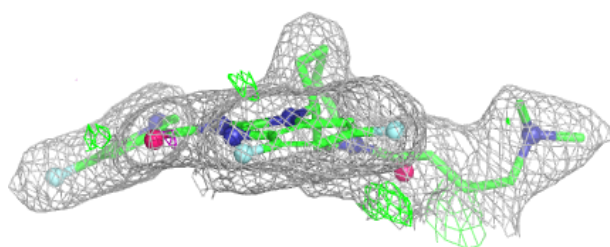
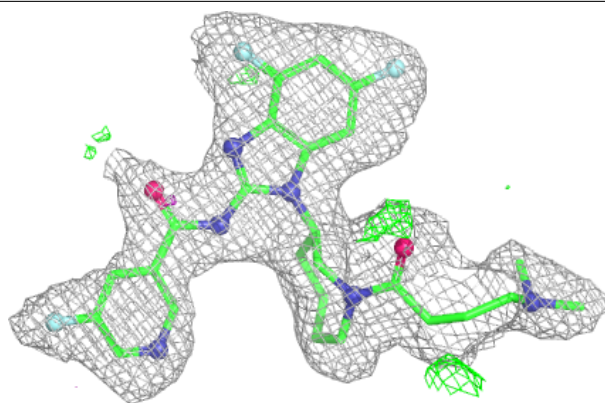
**Electron density around A1C5R L 501:**

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and green (positive)

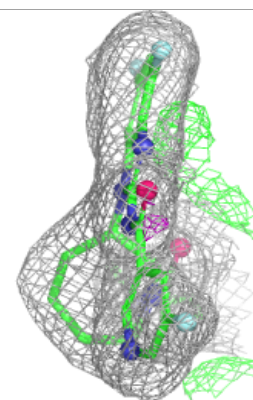
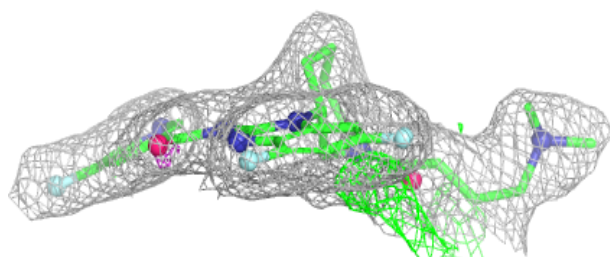
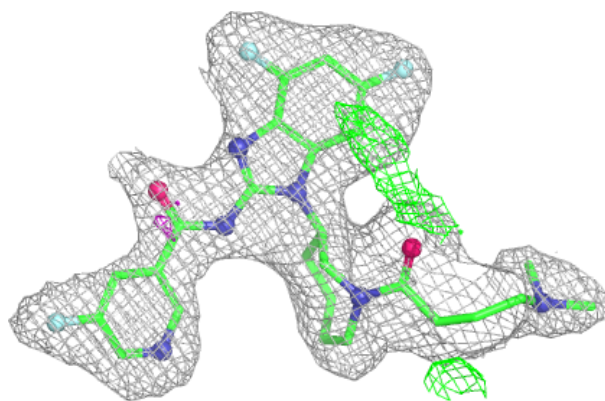


Electron density around A1C5R M 501:

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

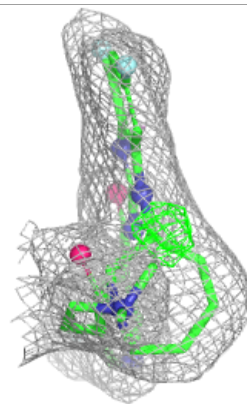
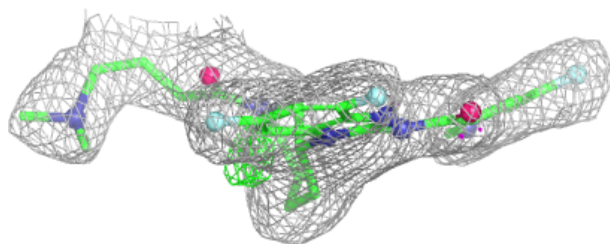
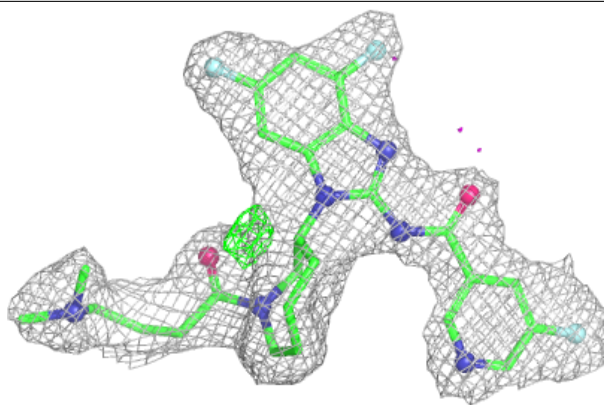
**Electron density around A1C5R N 501:**

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and green (positive)

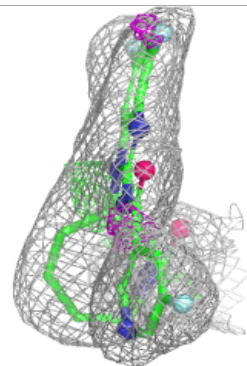
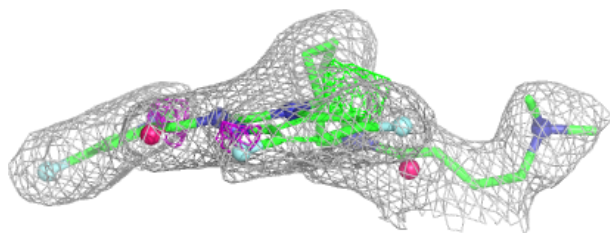
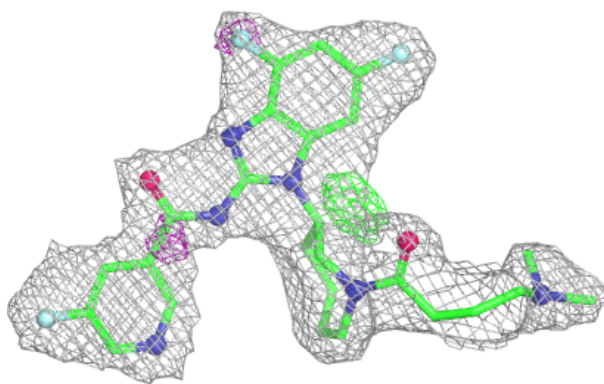


Electron density around A1C5R O 501:

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

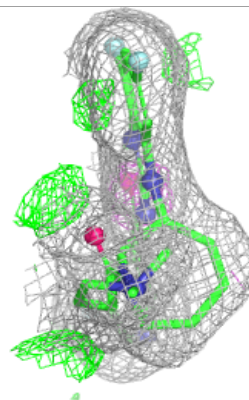
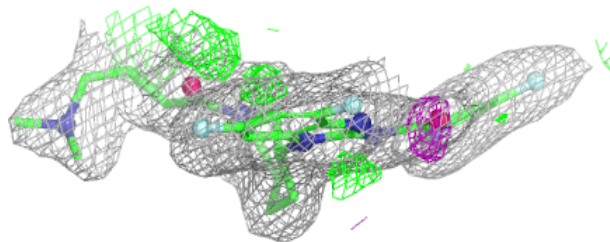
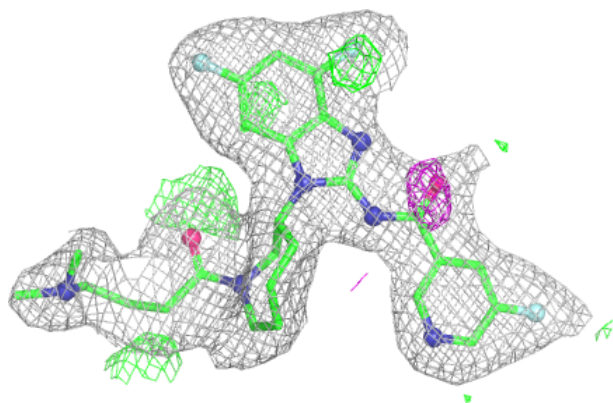
**Electron density around A1C5R P 501:**

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

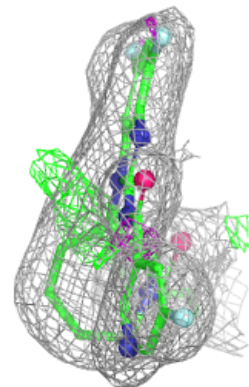
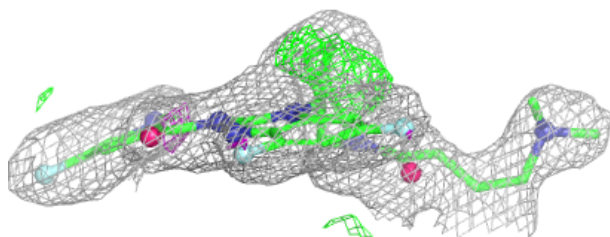
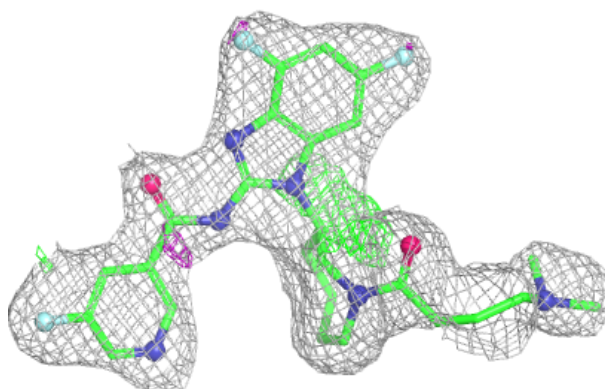


Electron density around A1C5R B 501:

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

**Electron density around A1C5R C 501:**

$2mF_o-DF_c$ (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.