



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2026 – 03:13 pm BST

PDB ID : 31XQ / pdb_000031xq
Title : Crystal structure of RAD52 N-terminal domain in complex with fragment Z448237394
Authors : Bocquet, N.; Gschell, M.; Powell, A.J.; Barker, I.A.
Deposited on : 2026-06-28
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

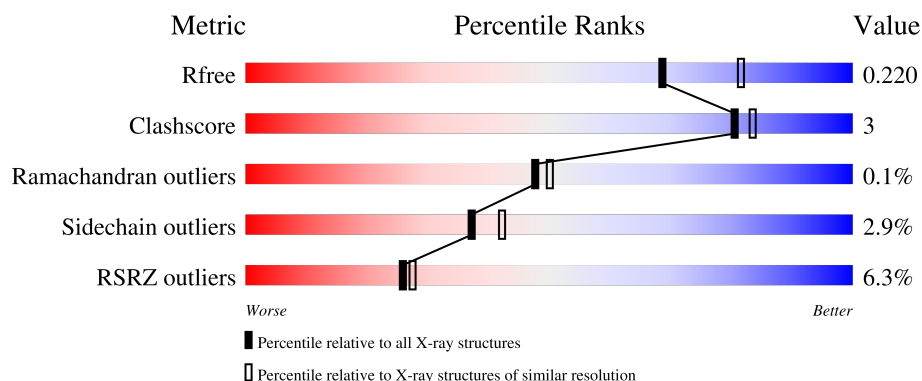
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	215	6% 81% 6% 13%
1	B	215	7% 81% 6% 13%
1	C	215	6% 83% •• 12%
1	D	215	4% 81% 6% 13%
1	E	215	3% 80% 7% 12%

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Mol	Chain	Length	Quality of chain
1	F	215	 3% 80% 5% • 13%
1	G	215	 5% 82% 5% 13%
1	H	215	 8% 80% 7% • 12%
1	I	215	 8% 79% 6% • 13%
1	J	215	 13% 77% 10% 13%
1	K	215	 12% 75% 10% • 13%
1	L	215	 4% 80% 5% • 13%
1	M	215	 4% 83% 5% 12%
1	N	215	 4% 78% 8% 13%
1	O	215	 5% 81% • 13%
1	P	215	 5% 81% 6% 13%
1	Q	215	 5% 79% 8% 13%
1	R	215	 2% 79% 8% 13%
1	S	215	 5% 83% • 13%
1	T	215	 6% 76% 11% 13%
1	U	215	 4% 81% • 13%
1	V	215	 3% 80% 6% • 13%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 35424 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 DNA repair protein RAD52 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1460	912	264	276	8			
1	B	188	Total	C	N	O	S	0	1	0
			1485	928	268	281	8			
1	C	189	Total	C	N	O	S	0	0	0
			1481	924	268	280	9			
1	D	188	Total	C	N	O	S	0	0	0
			1473	918	267	279	9			
1	E	189	Total	C	N	O	S	0	0	0
			1481	924	268	280	9			
1	F	187	Total	C	N	O	S	0	0	0
			1468	916	266	278	8			
1	G	188	Total	C	N	O	S	0	0	0
			1470	916	267	279	8			
1	H	189	Total	C	N	O	S	0	0	0
			1481	924	268	280	9			
1	I	187	Total	C	N	O	S	0	0	0
			1462	912	265	277	8			
1	J	188	Total	C	N	O	S	0	1	0
			1481	923	269	281	8			
1	K	187	Total	C	N	O	S	0	2	0
			1482	923	269	281	9			
1	L	187	Total	C	N	O	S	0	1	0
			1476	920	268	280	8			
1	M	189	Total	C	N	O	S	0	0	0
			1481	924	268	280	9			
1	N	187	Total	C	N	O	S	0	1	0
			1473	919	267	279	8			
1	O	187	Total	C	N	O	S	0	1	0
			1480	925	267	280	8			
1	P	187	Total	C	N	O	S	0	1	0
			1476	920	268	280	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	187	Total	C	N	O	S	0	2	0
			1488	929	269	282	8			
1	R	188	Total	C	N	O	S	0	1	0
			1481	923	269	281	8			
1	S	188	Total	C	N	O	S	0	0	0
			1473	919	267	279	8			
1	T	187	Total	C	N	O	S	0	2	0
			1488	929	269	282	8			
1	U	187	Total	C	N	O	S	0	0	0
			1468	916	266	278	8			
1	V	187	Total	C	N	O	S	0	0	0
			1468	916	266	278	8			

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P43351
A	-1	SER	-	expression tag	UNP P43351
A	0	HIS	-	expression tag	UNP P43351
A	102	ALA	LYS	engineered mutation	UNP P43351
A	133	ALA	LYS	engineered mutation	UNP P43351
B	-2	GLY	-	expression tag	UNP P43351
B	-1	SER	-	expression tag	UNP P43351
B	0	HIS	-	expression tag	UNP P43351
B	102	ALA	LYS	engineered mutation	UNP P43351
B	133	ALA	LYS	engineered mutation	UNP P43351
C	-2	GLY	-	expression tag	UNP P43351
C	-1	SER	-	expression tag	UNP P43351
C	0	HIS	-	expression tag	UNP P43351
C	102	ALA	LYS	engineered mutation	UNP P43351
C	133	ALA	LYS	engineered mutation	UNP P43351
D	-2	GLY	-	expression tag	UNP P43351
D	-1	SER	-	expression tag	UNP P43351
D	0	HIS	-	expression tag	UNP P43351
D	102	ALA	LYS	engineered mutation	UNP P43351
D	133	ALA	LYS	engineered mutation	UNP P43351
E	-2	GLY	-	expression tag	UNP P43351
E	-1	SER	-	expression tag	UNP P43351
E	0	HIS	-	expression tag	UNP P43351
E	102	ALA	LYS	engineered mutation	UNP P43351
E	133	ALA	LYS	engineered mutation	UNP P43351
F	-2	GLY	-	expression tag	UNP P43351
F	-1	SER	-	expression tag	UNP P43351

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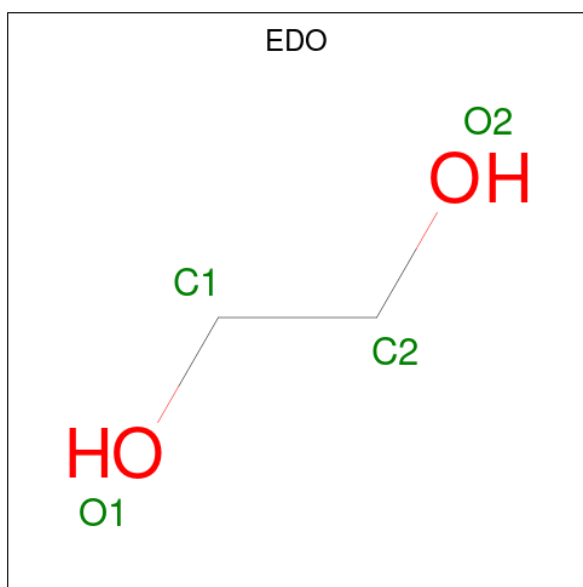
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	expression tag	UNP P43351
F	102	ALA	LYS	engineered mutation	UNP P43351
F	133	ALA	LYS	engineered mutation	UNP P43351
G	-2	GLY	-	expression tag	UNP P43351
G	-1	SER	-	expression tag	UNP P43351
G	0	HIS	-	expression tag	UNP P43351
G	102	ALA	LYS	engineered mutation	UNP P43351
G	133	ALA	LYS	engineered mutation	UNP P43351
H	-2	GLY	-	expression tag	UNP P43351
H	-1	SER	-	expression tag	UNP P43351
H	0	HIS	-	expression tag	UNP P43351
H	102	ALA	LYS	engineered mutation	UNP P43351
H	133	ALA	LYS	engineered mutation	UNP P43351
I	-2	GLY	-	expression tag	UNP P43351
I	-1	SER	-	expression tag	UNP P43351
I	0	HIS	-	expression tag	UNP P43351
I	102	ALA	LYS	engineered mutation	UNP P43351
I	133	ALA	LYS	engineered mutation	UNP P43351
J	-2	GLY	-	expression tag	UNP P43351
J	-1	SER	-	expression tag	UNP P43351
J	0	HIS	-	expression tag	UNP P43351
J	102	ALA	LYS	engineered mutation	UNP P43351
J	133	ALA	LYS	engineered mutation	UNP P43351
K	-2	GLY	-	expression tag	UNP P43351
K	-1	SER	-	expression tag	UNP P43351
K	0	HIS	-	expression tag	UNP P43351
K	102	ALA	LYS	engineered mutation	UNP P43351
K	133	ALA	LYS	engineered mutation	UNP P43351
L	-2	GLY	-	expression tag	UNP P43351
L	-1	SER	-	expression tag	UNP P43351
L	0	HIS	-	expression tag	UNP P43351
L	102	ALA	LYS	engineered mutation	UNP P43351
L	133	ALA	LYS	engineered mutation	UNP P43351
M	-2	GLY	-	expression tag	UNP P43351
M	-1	SER	-	expression tag	UNP P43351
M	0	HIS	-	expression tag	UNP P43351
M	102	ALA	LYS	engineered mutation	UNP P43351
M	133	ALA	LYS	engineered mutation	UNP P43351
N	-2	GLY	-	expression tag	UNP P43351
N	-1	SER	-	expression tag	UNP P43351
N	0	HIS	-	expression tag	UNP P43351
N	102	ALA	LYS	engineered mutation	UNP P43351

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Chain	Residue	Modelled	Actual	Comment	Reference
N	133	ALA	LYS	engineered mutation	UNP P43351
O	-2	GLY	-	expression tag	UNP P43351
O	-1	SER	-	expression tag	UNP P43351
O	0	HIS	-	expression tag	UNP P43351
O	102	ALA	LYS	engineered mutation	UNP P43351
O	133	ALA	LYS	engineered mutation	UNP P43351
P	-2	GLY	-	expression tag	UNP P43351
P	-1	SER	-	expression tag	UNP P43351
P	0	HIS	-	expression tag	UNP P43351
P	102	ALA	LYS	engineered mutation	UNP P43351
P	133	ALA	LYS	engineered mutation	UNP P43351
Q	-2	GLY	-	expression tag	UNP P43351
Q	-1	SER	-	expression tag	UNP P43351
Q	0	HIS	-	expression tag	UNP P43351
Q	102	ALA	LYS	engineered mutation	UNP P43351
Q	133	ALA	LYS	engineered mutation	UNP P43351
R	-2	GLY	-	expression tag	UNP P43351
R	-1	SER	-	expression tag	UNP P43351
R	0	HIS	-	expression tag	UNP P43351
R	102	ALA	LYS	engineered mutation	UNP P43351
R	133	ALA	LYS	engineered mutation	UNP P43351
S	-2	GLY	-	expression tag	UNP P43351
S	-1	SER	-	expression tag	UNP P43351
S	0	HIS	-	expression tag	UNP P43351
S	102	ALA	LYS	engineered mutation	UNP P43351
S	133	ALA	LYS	engineered mutation	UNP P43351
T	-2	GLY	-	expression tag	UNP P43351
T	-1	SER	-	expression tag	UNP P43351
T	0	HIS	-	expression tag	UNP P43351
T	102	ALA	LYS	engineered mutation	UNP P43351
T	133	ALA	LYS	engineered mutation	UNP P43351
U	-2	GLY	-	expression tag	UNP P43351
U	-1	SER	-	expression tag	UNP P43351
U	0	HIS	-	expression tag	UNP P43351
U	102	ALA	LYS	engineered mutation	UNP P43351
U	133	ALA	LYS	engineered mutation	UNP P43351
V	-2	GLY	-	expression tag	UNP P43351
V	-1	SER	-	expression tag	UNP P43351
V	0	HIS	-	expression tag	UNP P43351
V	102	ALA	LYS	engineered mutation	UNP P43351
V	133	ALA	LYS	engineered mutation	UNP P43351

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



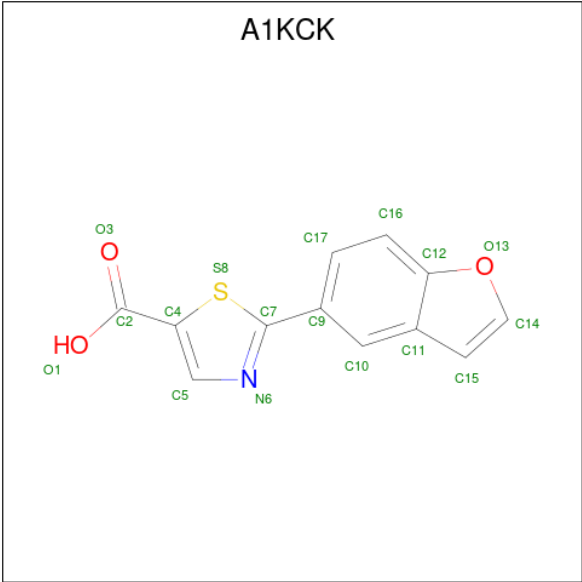
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	I	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	K	1	Total C O 4 2 2	0	0
2	L	1	Total C O 4 2 2	0	0
2	M	1	Total C O 4 2 2	0	0
2	N	1	Total C O 4 2 2	0	0
2	O	1	Total C O 4 2 2	0	0
2	P	1	Total C O 4 2 2	0	0
2	Q	1	Total C O 4 2 2	0	0
2	R	1	Total C O 4 2 2	0	0
2	S	1	Total C O 4 2 2	0	0
2	T	1	Total C O 4 2 2	0	0
2	U	1	Total C O 4 2 2	0	0
2	V	1	Total C O 4 2 2	0	0
2	V	1	Total C O 4 2 2	0	0
2	V	1	Total C O 4 2 2	0	0

- Molecule 3 is 2-(1-benzofuran-5-yl)-1,3-thiazole-5-carboxylic acid (CCD ID: A1KCK) (formula: C₁₂H₇NO₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			17	12	1	3	1		
3	A	1	Total	C	N	O	S	0	0
			17	12	1	3	1		
3	A	1	Total	C	N	O	S	0	0
			17	12	1	3	1		
3	B	1	Total	C	N	O	S	0	0
			17	12	1	3	1		
3	C	1	Total	C	N	O	S	0	0
			17	12	1	3	1		
3	C	1	Total	C	N	O	S	0	0
			17	12	1	3	1		
3	D	1	Total	C	N	O	S	0	0
			17	12	1	3	1		
3	D	1	Total	C	N	O	S	0	0
			17	12	1	3	1		
3	E	1	Total	C	N	O	S	0	0
			17	12	1	3	1		
3	E	1	Total	C	N	O	S	0	0
			17	12	1	3	1		
3	F	1	Total	C	N	O	S	0	0
			17	12	1	3	1		
3	F	1	Total	C	N	O	S	0	0
			17	12	1	3	1		
3	G	1	Total	C	N	O	S	0	0
			17	12	1	3	1		
3	G	1	Total	C	N	O	S	0	0
			17	12	1	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	H	1	Total 17	C 12	N 1	O 3	S 1	0	0
3	H	1	Total 17	C 12	N 1	O 3	S 1	0	0
3	I	1	Total 17	C 12	N 1	O 3	S 1	0	0
3	I	1	Total 17	C 12	N 1	O 3	S 1	0	0
3	J	1	Total 17	C 12	N 1	O 3	S 1	0	0
3	K	1	Total 17	C 12	N 1	O 3	S 1	0	0
3	K	1	Total 17	C 12	N 1	O 3	S 1	0	0
3	K	1	Total 17	C 12	N 1	O 3	S 1	0	0
3	L	1	Total 17	C 12	N 1	O 3	S 1	0	0
3	L	1	Total 17	C 12	N 1	O 3	S 1	0	0
3	L	1	Total 17	C 12	N 1	O 3	S 1	0	0
3	M	1	Total 17	C 12	N 1	O 3	S 1	0	0
3	M	1	Total 17	C 12	N 1	O 3	S 1	0	0
3	N	1	Total 17	C 12	N 1	O 3	S 1	0	0
3	N	1	Total 17	C 12	N 1	O 3	S 1	0	0
3	O	1	Total 17	C 12	N 1	O 3	S 1	0	0
3	O	1	Total 17	C 12	N 1	O 3	S 1	0	0
3	P	1	Total 17	C 12	N 1	O 3	S 1	0	0
3	P	1	Total 17	C 12	N 1	O 3	S 1	0	0
3	Q	1	Total 17	C 12	N 1	O 3	S 1	0	0
3	Q	1	Total 17	C 12	N 1	O 3	S 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	R	1	Total	C	N	O	S	0	0
			17	12	1	3	1		
3	R	1	Total	C	N	O	S	0	0
			17	12	1	3	1		
3	S	1	Total	C	N	O	S	0	0
			17	12	1	3	1		
3	S	1	Total	C	N	O	S	0	0
			17	12	1	3	1		
3	T	1	Total	C	N	O	S	0	0
			17	12	1	3	1		
3	T	1	Total	C	N	O	S	0	0
			17	12	1	3	1		
3	U	1	Total	C	N	O	S	0	0
			17	12	1	3	1		
3	V	1	Total	C	N	O	S	0	0
			17	12	1	3	1		
3	V	1	Total	C	N	O	S	0	0
			17	12	1	3	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	I	1	Total	Mg	0	0
			1	1		
4	M	1	Total	Mg	0	0
			1	1		
4	O	2	Total	Mg	0	0
			2	2		
4	T	1	Total	Mg	0	0
			1	1		
4	V	2	Total	Mg	0	0
			2	2		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	3	Total	Cl	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total 2	Cl 2	0	0
5	D	1	Total 1	Cl 1	0	0
5	E	1	Total 1	Cl 1	0	0
5	F	2	Total 2	Cl 2	0	0
5	G	2	Total 2	Cl 2	0	0
5	L	1	Total 1	Cl 1	0	0
5	N	1	Total 1	Cl 1	0	0
5	O	1	Total 1	Cl 1	0	0
5	P	2	Total 2	Cl 2	0	0
5	Q	2	Total 2	Cl 2	0	0
5	R	2	Total 2	Cl 2	0	0
5	S	2	Total 2	Cl 2	0	0
5	T	1	Total 1	Cl 1	0	0
5	U	3	Total 3	Cl 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	94	Total 94	O 94	0	0
6	B	108	Total 108	O 108	0	0
6	C	123	Total 123	O 123	0	0
6	D	100	Total 100	O 100	0	0
6	E	101	Total 101	O 101	0	0

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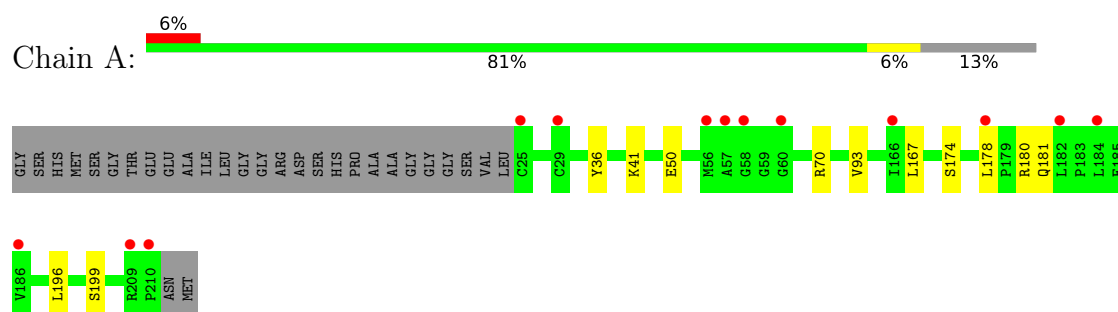
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	95	Total 95	O 95	0	0
6	G	65	Total 65	O 65	0	0
6	H	68	Total 68	O 68	0	0
6	I	51	Total 51	O 51	0	0
6	J	66	Total 66	O 66	0	0
6	K	63	Total 63	O 63	0	0
6	L	105	Total 105	O 105	0	0
6	M	108	Total 108	O 108	0	0
6	N	90	Total 90	O 90	0	0
6	O	89	Total 89	O 89	0	0
6	P	107	Total 107	O 107	0	0
6	Q	109	Total 109	O 109	0	0
6	R	119	Total 119	O 119	0	0
6	S	82	Total 82	O 82	0	0
6	T	88	Total 88	O 88	0	0
6	U	103	Total 103	O 103	0	0
6	V	111	Total 111	O 111	0	0

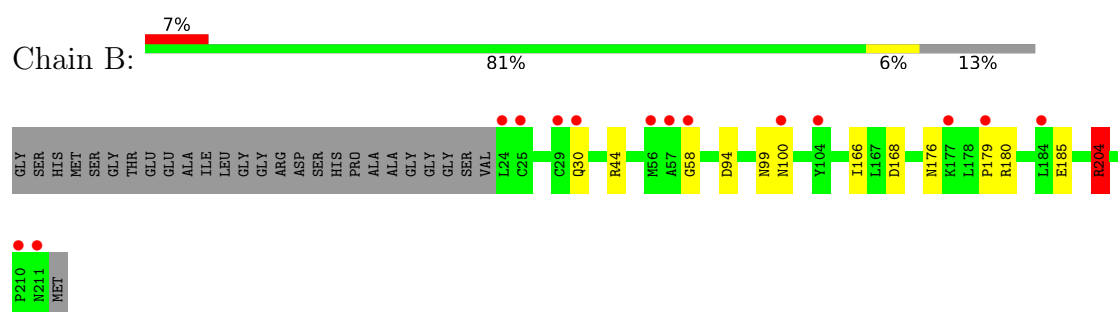
3 Residue-property plots [i](#)

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.

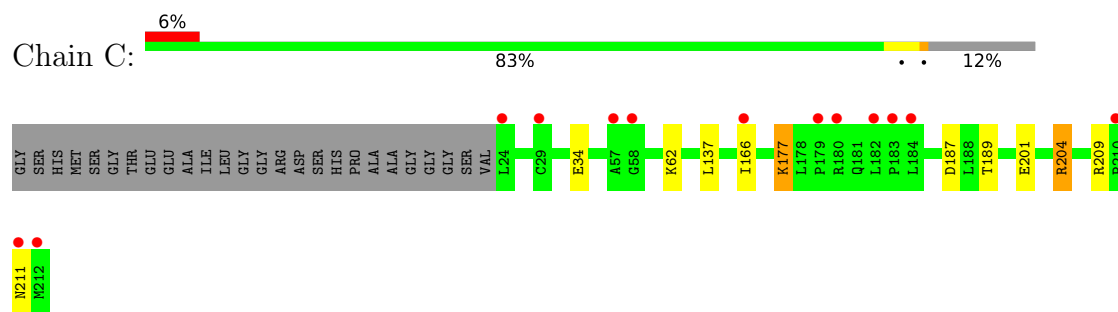
- Molecule 1: DNA repair protein RAD52 homolog



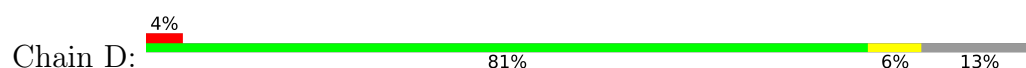
- Molecule 1: DNA repair protein RAD52 homolog

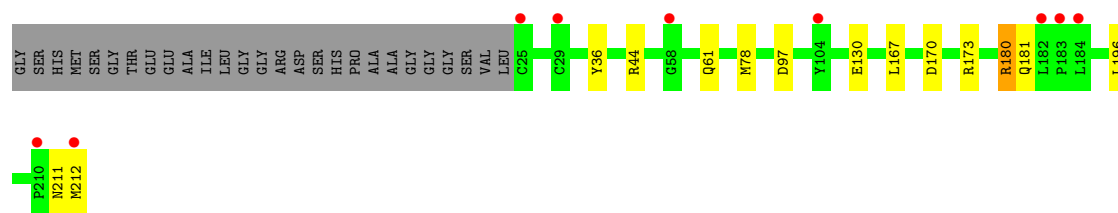


- Molecule 1: DNA repair protein RAD52 homolog

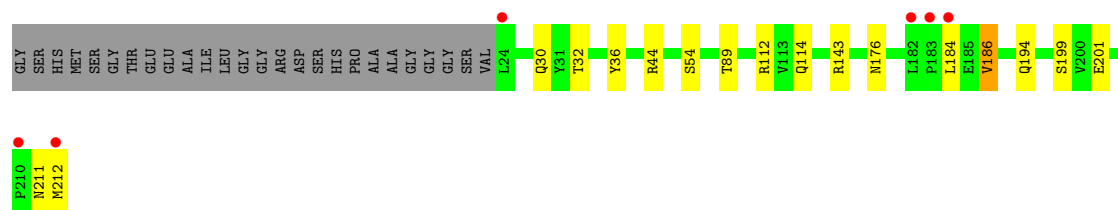
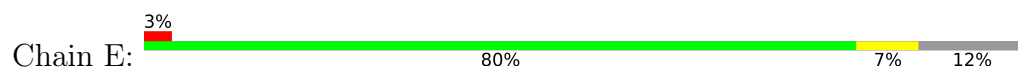


- Molecule 1: DNA repair protein RAD52 homolog

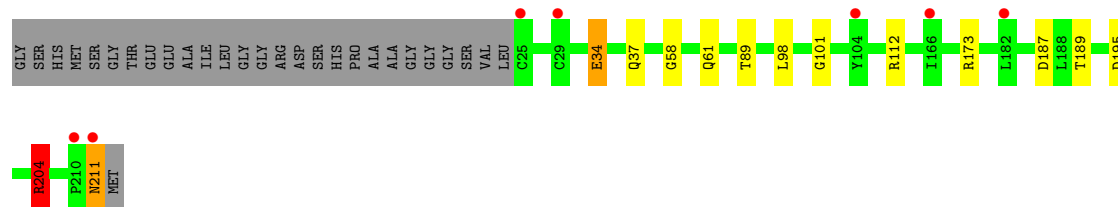
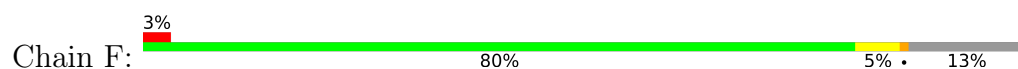




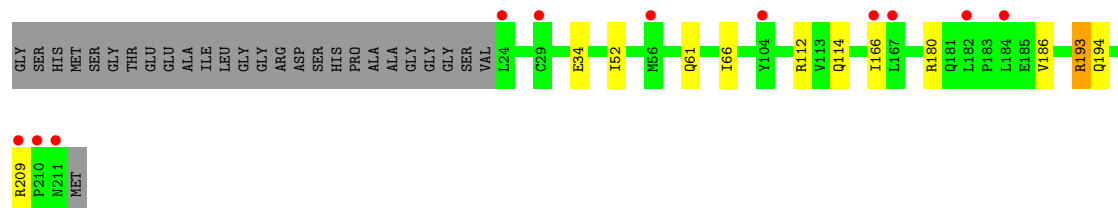
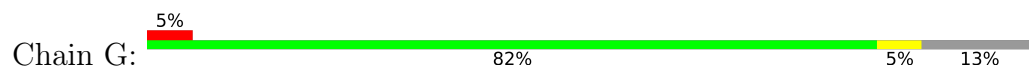
- Molecule 1: DNA repair protein RAD52 homolog



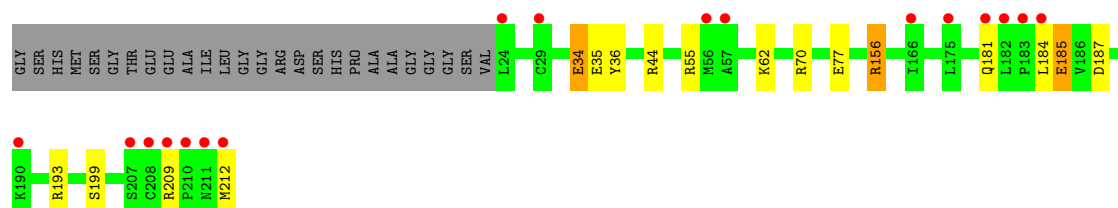
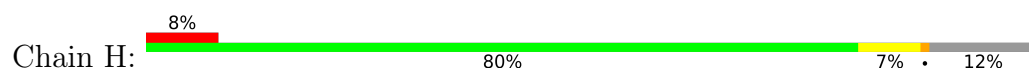
- Molecule 1: DNA repair protein RAD52 homolog



- Molecule 1: DNA repair protein RAD52 homolog

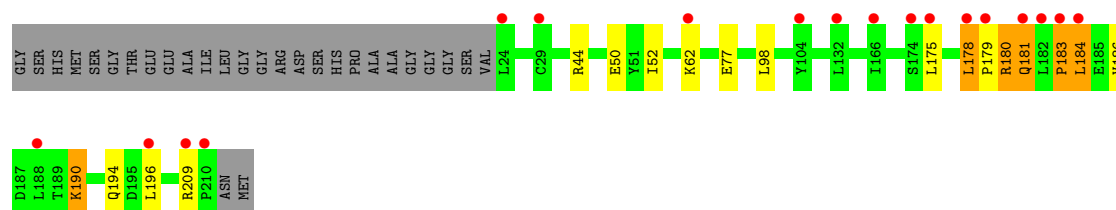


- Molecule 1: DNA repair protein RAD52 homolog



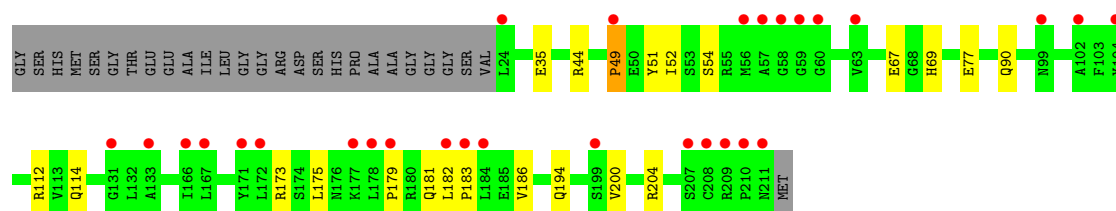
- Molecule 1: DNA repair protein RAD52 homolog

Chain I: 



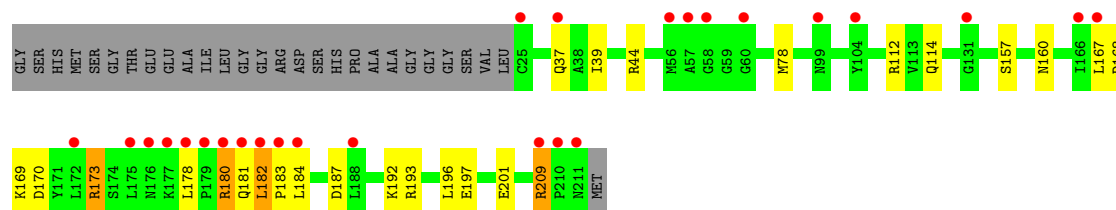
- Molecule 1: DNA repair protein RAD52 homolog

Chain J: 



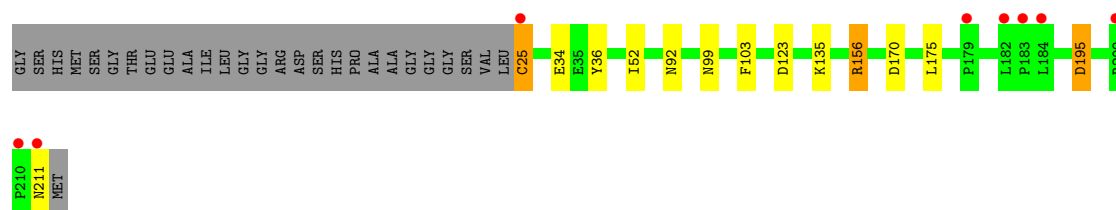
- Molecule 1: DNA repair protein RAD52 homolog

Chain K: 



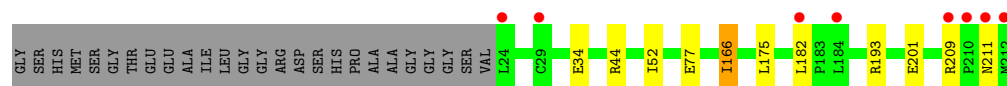
- Molecule 1: DNA repair protein RAD52 homolog

Chain L: 

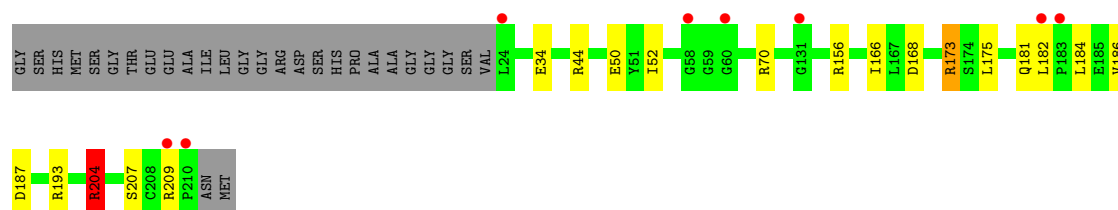
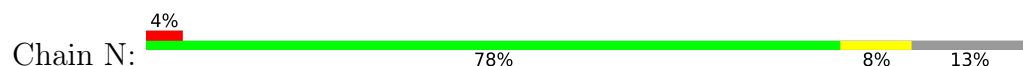


- Molecule 1: DNA repair protein RAD52 homolog

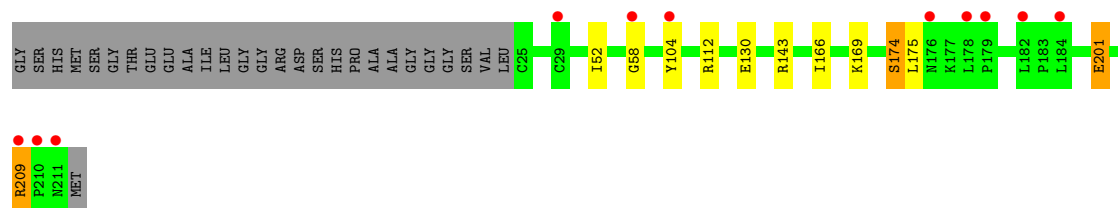
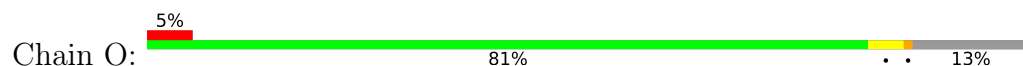
Chain M: 



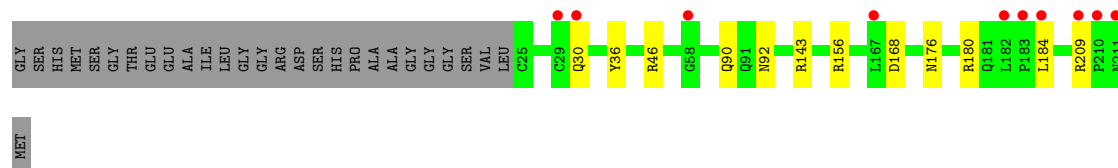
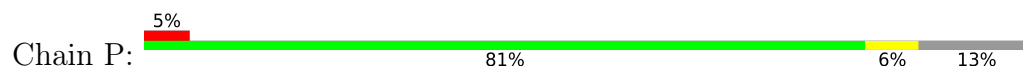
- Molecule 1: DNA repair protein RAD52 homolog



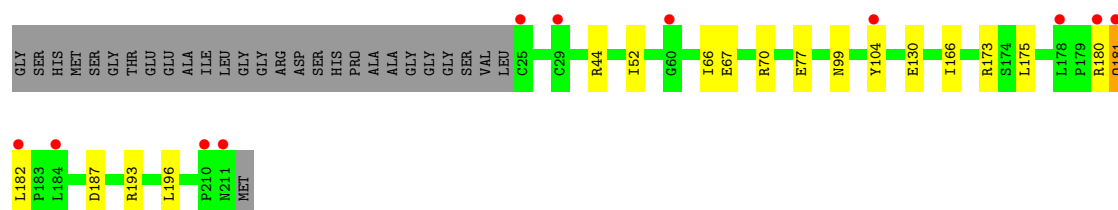
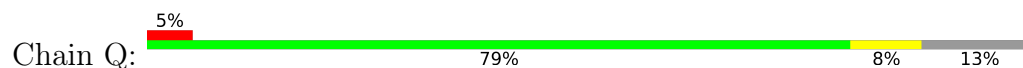
- Molecule 1: DNA repair protein RAD52 homolog



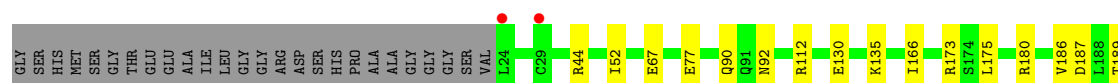
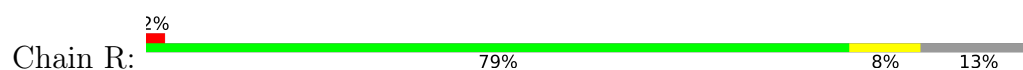
- Molecule 1: DNA repair protein RAD52 homolog



- Molecule 1: DNA repair protein RAD52 homolog

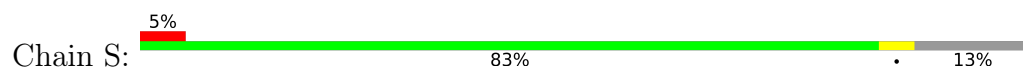


- Molecule 1: DNA repair protein RAD52 homolog

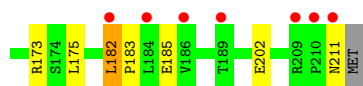
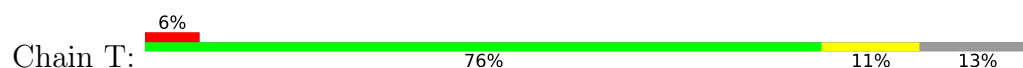




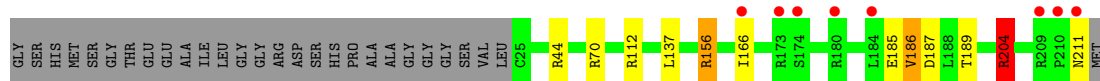
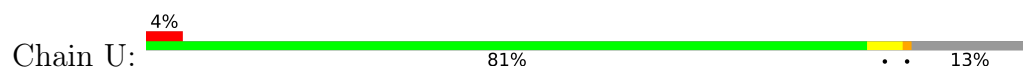
- Molecule 1: DNA repair protein RAD52 homolog



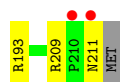
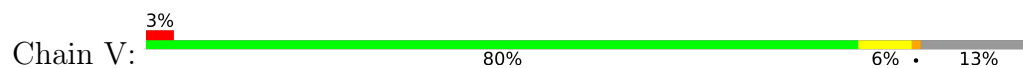
- Molecule 1: DNA repair protein RAD52 homolog



- Molecule 1: DNA repair protein RAD52 homolog



- Molecule 1: DNA repair protein RAD52 homolog



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	144.87Å 147.20Å 251.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	127.02 – 2.10 127.02 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (127.02-2.10) 100.0 (127.02-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.172 , 0.212 0.183 , 0.220	Depositor DCC
R_{free} test set	20882 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 70.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	35424	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL, EDO, A1KCK, MG

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	0.65	0/1485	1.05	0/1999
1	B	0.67	0/1511	1.11	5/2035 (0.2%)
1	C	0.68	0/1506	1.11	5/2027 (0.2%)
1	D	0.68	0/1498	1.09	5/2016 (0.2%)
1	E	0.69	0/1506	1.11	4/2027 (0.2%)
1	F	0.68	0/1493	1.09	4/2010 (0.2%)
1	G	0.66	0/1495	1.11	2/2013 (0.1%)
1	H	0.61	0/1506	1.11	5/2027 (0.2%)
1	I	0.64	0/1487	1.08	1/2002 (0.0%)
1	J	0.74	3/1506 (0.2%)	1.07	2/2028 (0.1%)
1	K	0.72	2/1507 (0.1%)	1.10	3/2029 (0.1%)
1	L	0.67	0/1501	1.09	3/2021 (0.1%)
1	M	0.71	0/1506	1.10	3/2027 (0.1%)
1	N	0.67	0/1498	1.08	6/2017 (0.3%)
1	O	0.66	0/1506	1.09	2/2028 (0.1%)
1	P	0.70	0/1501	1.09	1/2021 (0.0%)
1	Q	0.66	0/1514	1.11	3/2039 (0.1%)
1	R	0.67	0/1506	1.03	1/2028 (0.0%)
1	S	0.65	0/1498	1.03	0/2017
1	T	0.68	0/1514	1.06	2/2039 (0.1%)
1	U	0.65	0/1493	1.17	5/2010 (0.2%)
1	V	0.67	0/1493	1.08	8/2010 (0.4%)
All	All	0.67	5/33030 (0.0%)	1.09	70/44470 (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

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	3
1	I	0	1
1	K	0	1
1	L	0	1
1	N	0	6
1	O	0	1
1	P	0	2
1	Q	0	2
1	R	0	1
1	S	0	1
1	U	0	3
1	V	0	3
All	All	0	30

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	186	VAL	C-O	12.26	1.37	1.24
1	J	49	PRO	C-O	8.76	1.35	1.24
1	K	37	GLN	C-O	7.30	1.32	1.24
1	J	49	PRO	CA-C	6.52	1.63	1.52
1	K	160	ASN	C-O	5.63	1.30	1.24

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	204	ARG	CD-NE-CZ	13.06	142.68	124.40
1	U	204	ARG	CD-NE-CZ	11.87	141.02	124.40
1	C	204	ARG	CD-NE-CZ	10.27	138.78	124.40
1	B	204	ARG	NE-CZ-NH2	-9.89	110.30	119.20
1	C	204	ARG	NE-CZ-NH2	-9.85	110.34	119.20
1	U	204	ARG	NE-CZ-NH2	-7.94	112.06	119.20
1	M	44	ARG	CG-CD-NE	-7.81	94.81	112.00
1	M	44	ARG	CB-CA-C	-7.71	94.20	110.31
1	D	44	ARG	CB-CA-C	-7.61	94.42	110.31
1	I	184	LEU	N-CA-CB	-7.45	100.39	111.71
1	O	209	ARG	CB-CA-C	7.23	119.07	108.87
1	D	180	ARG	CB-CA-C	7.04	118.46	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	44	ARG	CG-CD-NE	-6.88	96.88	112.00
1	C	204	ARG	NE-CZ-NH1	6.73	128.23	121.50
1	V	34	GLU	CB-CG-CD	6.63	123.88	112.60
1	F	204	ARG	CD-NE-CZ	6.63	133.69	124.40
1	B	168	ASP	CA-CB-CG	6.46	119.06	112.60
1	B	204	ARG	NE-CZ-NH1	6.22	127.72	121.50
1	L	195	ASP	CA-CB-CG	6.16	118.76	112.60
1	Q	44	ARG	CB-CA-C	-6.13	97.17	109.99
1	E	44	ARG	CB-CA-C	-6.09	97.58	110.31
1	D	130	GLU	CB-CG-CD	5.94	122.70	112.60
1	D	97	ASP	CA-CB-CG	5.92	118.52	112.60
1	F	34	GLU	N-CA-CB	-5.91	101.42	110.16
1	J	49	PRO	O-C-N	5.88	129.28	122.17
1	U	186	VAL	N-CA-CB	5.86	118.02	110.99
1	V	44	ARG	CB-CA-C	-5.84	98.10	110.31
1	H	187	ASP	CA-CB-CG	5.76	118.36	112.60
1	F	204	ARG	NE-CZ-NH2	-5.71	114.06	119.20
1	N	168	ASP	CA-CB-CG	5.70	118.30	112.60
1	N	187	ASP	CA-CB-CG	5.69	118.29	112.60
1	H	156	ARG	CG-CD-NE	-5.68	99.49	112.00
1	R	130	GLU	CB-CG-CD	5.65	122.21	112.60
1	V	55	ARG	NE-CZ-NH2	5.63	124.27	119.20
1	T	44	ARG	CB-CA-C	-5.61	98.58	110.31
1	V	55	ARG	CD-NE-CZ	5.61	132.25	124.40
1	K	201	GLU	CB-CG-CD	5.59	122.11	112.60
1	K	168	ASP	CA-CB-CG	5.58	118.18	112.60
1	N	44	ARG	CB-CA-C	-5.51	98.80	110.31
1	K	187	ASP	CA-CB-CG	5.44	118.04	112.60
1	G	193	ARG	N-CA-CB	-5.43	103.78	111.00
1	V	176	ASN	CA-CB-CG	-5.41	107.19	112.60
1	N	44	ARG	CG-CD-NE	-5.40	100.12	112.00
1	V	44	ARG	CG-CD-NE	-5.40	100.12	112.00
1	E	201	GLU	CB-CG-CD	5.34	121.68	112.60
1	L	25	CYS	CB-CA-C	5.34	120.25	110.10
1	V	209	ARG	CB-CA-C	5.33	117.65	109.60
1	H	44	ARG	CB-CA-C	-5.33	98.85	109.99
1	C	201	GLU	CB-CG-CD	5.32	121.65	112.60
1	G	180	ARG	CB-CA-C	5.30	118.51	109.72
1	P	168	ASP	CB-CA-C	5.29	119.53	110.81
1	Q	44	ARG	CG-CD-NE	-5.25	100.46	112.00
1	E	186	VAL	N-CA-CB	5.17	117.19	110.99
1	M	201	GLU	CB-CG-CD	5.16	121.38	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	130	GLU	CB-CG-CD	5.16	121.37	112.60
1	H	35	GLU	CB-CG-CD	5.15	121.35	112.60
1	E	89	THR	CA-CB-OG1	-5.14	101.89	109.60
1	F	195	ASP	CA-CB-CG	5.14	117.74	112.60
1	L	170	ASP	CA-CB-CG	5.13	117.73	112.60
1	C	34	GLU	CB-CG-CD	5.11	121.28	112.60
1	U	44	ARG	CG-CD-NE	-5.08	100.83	112.00
1	Q	187	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	44	ARG	CB-CA-C	-5.06	99.73	110.31
1	N	34	GLU	CB-CG-CD	5.05	121.18	112.60
1	U	112	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	J	35	GLU	CB-CG-CD	5.03	121.15	112.60
1	H	185	GLU	CB-CA-C	5.03	118.33	110.19
1	N	204	ARG	CD-NE-CZ	5.02	131.43	124.40
1	T	202	GLU	CB-CG-CD	5.02	121.13	112.60
1	O	201	GLU	CB-CG-CD	5.01	121.12	112.60

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	70	ARG	Sidechain
1	B	204	ARG	Sidechain
1	E	143	ARG	Sidechain
1	F	204	ARG	Sidechain
1	G	193	ARG	Sidechain
1	H	156	ARG	Sidechain
1	H	55	ARG	Sidechain
1	H	70	ARG	Sidechain
1	I	180	ARG	Sidechain
1	K	180	ARG	Sidechain
1	L	156	ARG	Sidechain
1	N	156	ARG	Sidechain
1	N	173	ARG	Sidechain
1	N	193	ARG	Sidechain
1	N	204	ARG	Sidechain
1	N	209	ARG	Sidechain
1	N	70	ARG	Sidechain
1	O	143	ARG	Sidechain
1	P	143	ARG	Sidechain
1	P	46	ARG	Sidechain
1	Q	193	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	Q	70	ARG	Sidechain
1	R	173	ARG	Sidechain
1	S	70	ARG	Sidechain
1	U	156	ARG	Sidechain
1	U	204	ARG	Sidechain
1	U	70	ARG	Sidechain
1	V	173	ARG	Sidechain
1	V	46	ARG	Sidechain
1	V	55	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	1460	0	1437	7	0
1	B	1485	0	1453	8	0
1	C	1481	0	1454	8	0
1	D	1473	0	1443	11	0
1	E	1481	0	1454	13	0
1	F	1468	0	1443	14	0
1	G	1470	0	1436	9	0
1	H	1481	0	1454	8	0
1	I	1462	0	1430	10	0
1	J	1481	0	1450	17	0
1	K	1482	0	1452	18	0
1	L	1476	0	1448	13	0
1	M	1481	0	1454	7	0
1	N	1473	0	1444	8	0
1	O	1480	0	1451	6	0
1	P	1476	0	1448	7	0
1	Q	1488	0	1456	9	0
1	R	1481	0	1450	15	0
1	S	1473	0	1445	3	0
1	T	1488	0	1456	11	0
1	U	1468	0	1443	7	0
1	V	1468	0	1443	7	0
2	A	12	0	18	1	0
2	B	8	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	4	0	6	0	0
2	D	4	0	6	0	0
2	E	12	0	18	1	0
2	F	8	0	12	0	0
2	G	4	0	6	0	0
2	H	4	0	6	0	0
2	I	4	0	6	1	0
2	J	4	0	6	0	0
2	K	4	0	6	0	0
2	L	4	0	6	0	0
2	M	4	0	6	0	0
2	N	4	0	6	0	0
2	O	4	0	6	0	0
2	P	4	0	6	0	0
2	Q	4	0	6	0	0
2	R	4	0	6	1	0
2	S	4	0	6	0	0
2	T	4	0	6	0	0
2	U	4	0	6	0	0
2	V	12	0	18	1	0
3	A	51	0	0	1	0
3	B	17	0	0	0	0
3	C	34	0	0	0	0
3	D	34	0	0	0	0
3	E	34	0	0	0	0
3	F	34	0	0	0	0
3	G	34	0	0	0	0
3	H	34	0	0	0	0
3	I	34	0	0	0	0
3	J	17	0	0	1	0
3	K	51	0	0	0	0
3	L	51	0	0	0	0
3	M	34	0	0	0	0
3	N	34	0	0	3	0
3	O	34	0	0	0	0
3	P	34	0	0	1	0
3	Q	34	0	0	0	0
3	R	34	0	0	0	0
3	S	34	0	0	0	0
3	T	34	0	0	0	0
3	U	17	0	0	0	0
3	V	34	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	I	1	0	0	0	0
4	M	1	0	0	0	0
4	O	2	0	0	0	0
4	T	1	0	0	0	0
4	V	2	0	0	0	0
5	B	3	0	0	0	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	2	0	0	1	0
5	G	2	0	0	1	0
5	L	1	0	0	0	0
5	N	1	0	0	0	0
5	O	1	0	0	1	0
5	P	2	0	0	0	0
5	Q	2	0	0	0	0
5	R	2	0	0	1	0
5	S	2	0	0	0	0
5	T	1	0	0	1	0
5	U	3	0	0	0	0
6	A	94	0	0	2	0
6	B	108	0	0	0	0
6	C	123	0	0	3	0
6	D	100	0	0	2	0
6	E	101	0	0	3	0
6	F	95	0	0	2	0
6	G	65	0	0	1	0
6	H	68	0	0	0	0
6	I	51	0	0	0	0
6	J	66	0	0	1	0
6	K	63	0	0	2	0
6	L	105	0	0	3	0
6	M	108	0	0	0	0
6	N	90	0	0	3	0
6	O	89	0	0	2	0
6	P	107	0	0	3	0
6	Q	109	0	0	2	0
6	R	119	0	0	4	0
6	S	82	0	0	0	0
6	T	88	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	U	103	0	0	1	0
6	V	111	0	0	4	0
All	All	35424	0	32024	173	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 3.

All (173) 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:R:90:GLN:HE21	1:R:92[B]:ASN:HD21	1.12	0.96
1:E:211:ASN:HD21	1:G:34:GLU:H	1.27	0.83
1:G:112:ARG:HH22	1:G:114:GLN:HE21	1.25	0.83
1:J:112:ARG:HH12	1:J:114:GLN:HE21	1.24	0.83
1:R:67:GLU:HG2	6:R:495:HOH:O	1.82	0.78
3:N:303:A1KCK:C14	6:N:480:HOH:O	2.31	0.78
1:A:50:GLU:OE2	1:K:193:ARG:NH1	2.18	0.77
1:B:204:ARG:HD2	1:D:36:TYR:OH	1.84	0.77
1:F:37:GLN:NE2	6:F:2001:HOH:O	2.17	0.77
1:K:170:ASP:OD1	1:K:173:ARG:NH2	2.20	0.73
1:D:211:ASN:HD21	1:F:34:GLU:H	1.36	0.73
1:L:99:ASN:HB2	6:L:495:HOH:O	1.88	0.72
1:R:187:ASP:OD1	1:R:189:THR:HG23	1.89	0.72
1:Q:66:ILE:CD1	1:Q:166:ILE:HD11	2.19	0.72
1:R:90:GLN:NE2	1:R:92[B]:ASN:HD21	1.88	0.71
1:E:112:ARG:HH22	1:E:114:GLN:HE21	1.35	0.71
1:R:90:GLN:HE21	1:R:92[B]:ASN:ND2	1.88	0.71
1:O:201:GLU:OE1	6:O:401:HOH:O	2.09	0.71
1:I:181:GLN:HG2	1:I:183:PRO:HD3	1.73	0.70
1:M:52:ILE:HD12	1:M:166:ILE:HD11	1.73	0.70
1:A:36:TYR:OH	1:J:204:ARG:HD2	1.92	0.69
1:H:77:GLU:OE2	1:I:44:ARG:HD3	1.93	0.68
1:T:52:ILE:HG13	1:T:175:LEU:HD11	1.74	0.68
1:F:173:ARG:HD3	6:F:2084:HOH:O	1.93	0.67
1:K:78:MET:HE3	1:K:78:MET:HA	1.76	0.67
1:L:36:TYR:OH	1:U:204:ARG:HD2	1.96	0.66
3:J:301:A1KCK:O3	6:J:401:HOH:O	2.13	0.66
1:O:112:ARG:NE	5:O:306:CL:CL	2.67	0.65
1:J:200:VAL:HG21	1:K:78:MET:HE1	1.78	0.65
1:C:204:ARG:HD2	1:E:36:TYR:OH	1.98	0.63
1:T:90:GLN:NE2	1:T:92[B]:ASN:HD21	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:34:GLU:OE2	1:U:211:ASN:HB2	2.00	0.61
1:K:39:ILE:HG12	1:K:78:MET:HE2	1.83	0.61
1:C:177:LYS:HE2	6:C:510:HOH:O	2.01	0.60
1:L:52:ILE:HG13	1:L:175:LEU:HD21	1.81	0.60
1:F:204:ARG:HD2	1:H:36:TYR:OH	2.00	0.60
1:R:201:GLU:OE1	6:R:401:HOH:O	2.16	0.60
1:Q:67:GLU:HG2	6:Q:494:HOH:O	2.02	0.59
1:T:170:ASP:OD1	1:T:173:ARG:NH2	2.33	0.59
1:N:186:VAL:O	1:O:174:SER:OG	2.17	0.59
1:V:99:ASN:HB2	6:V:502:HOH:O	2.02	0.59
1:J:77:GLU:OE1	1:K:44:ARG:HD3	2.03	0.59
1:A:41:LYS:NZ	6:A:402:HOH:O	2.36	0.58
1:B:204:ARG:CD	1:D:36:TYR:OH	2.51	0.58
1:I:178:LEU:HD23	1:I:179:PRO:HD2	1.84	0.58
1:R:135:LYS:NZ	6:R:404:HOH:O	2.37	0.58
1:C:209:ARG:NH1	1:E:30:GLN:O	2.37	0.58
1:I:52:ILE:HG13	1:I:175:LEU:HD21	1.86	0.57
1:C:166:ILE:HG22	6:C:489:HOH:O	2.03	0.57
1:J:182:LEU:HB2	1:J:183:PRO:HD2	1.88	0.56
1:M:34:GLU:OE2	1:V:211:ASN:HB2	2.05	0.56
1:P:90:GLN:NE2	1:P:92[B]:ASN:HD21	2.04	0.56
1:R:77:GLU:OE1	1:S:44:ARG:HD3	2.04	0.56
3:N:303:A1KCK:C5	6:N:434:HOH:O	2.54	0.56
1:B:204:ARG:CD	1:D:36:TYR:CZ	2.89	0.56
1:E:112:ARG:HE	2:E:303:EDO:C1	2.19	0.55
1:A:93:VAL:HG23	2:A:302:EDO:H11	1.89	0.55
1:Q:67:GLU:OE2	6:Q:401:HOH:O	2.18	0.55
1:L:36:TYR:CZ	1:U:204:ARG:HD2	2.42	0.55
1:K:173:ARG:CG	1:K:173:ARG:HH11	2.19	0.54
1:J:77:GLU:OE2	1:K:44:ARG:NH1	2.40	0.54
1:Q:180:ARG:HH22	1:Q:181:GLN:HE21	1.55	0.53
1:E:211:ASN:HD21	1:G:34:GLU:N	2.03	0.52
1:K:181:GLN:HG2	1:K:182:LEU:N	2.25	0.52
1:B:204:ARG:HD2	1:D:36:TYR:CZ	2.44	0.52
1:K:112:ARG:HH22	1:K:114:GLN:HE21	1.57	0.52
1:K:173:ARG:HH11	1:K:173:ARG:CB	2.23	0.52
1:R:52:ILE:HD12	1:R:166:ILE:HD11	1.91	0.52
1:V:193:ARG:NH1	6:V:402:HOH:O	2.32	0.52
1:J:67:GLU:OE2	1:K:169:LYS:NZ	2.41	0.52
1:L:92[A]:ASN:CG	6:L:401:HOH:O	2.53	0.52
1:F:112:ARG:NE	5:F:306:CL:CL	2.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:46:ARG:NE	6:V:403:HOH:O	2.35	0.51
1:F:187:ASP:OD1	1:F:189:THR:HG23	2.11	0.51
1:V:130:GLU:OE2	6:V:401:HOH:O	2.19	0.51
1:B:204:ARG:HD3	1:D:36:TYR:CZ	2.45	0.51
1:J:77:GLU:CD	1:K:44:ARG:HH11	2.18	0.51
1:M:193:ARG:NH1	1:N:50:GLU:OE2	2.43	0.51
1:O:52:ILE:HG13	1:O:175:LEU:HD21	1.93	0.51
3:N:303:A1KCK:C15	6:N:480:HOH:O	2.56	0.51
1:P:156:ARG:CZ	6:P:403:HOH:O	2.59	0.50
1:D:170:ASP:OD1	1:D:173:ARG:NH2	2.45	0.49
1:D:167:LEU:HB2	6:D:470:HOH:O	2.12	0.49
1:L:92[A]:ASN:ND2	6:L:401:HOH:O	2.45	0.49
1:Q:77:GLU:OE2	1:R:44:ARG:HD3	2.12	0.49
1:R:112:ARG:NE	5:R:305:CL:CL	2.77	0.49
1:B:94:ASP:O	2:B:301:EDO:H22	2.13	0.49
1:Q:66:ILE:HD11	1:Q:166:ILE:HD11	1.92	0.49
1:G:112:ARG:NE	5:G:305:CL:CL	2.81	0.49
1:F:204:ARG:CD	1:H:36:TYR:CZ	2.97	0.48
6:E:412:HOH:O	1:F:89:THR:HG21	2.13	0.48
1:J:69:HIS:CD2	6:K:449:HOH:O	2.67	0.48
1:A:36:TYR:OH	1:J:204:ARG:CD	2.61	0.48
1:M:52:ILE:HD12	1:M:166:ILE:CD1	2.42	0.48
1:E:211:ASN:ND2	1:G:34:GLU:HB2	2.28	0.47
1:I:183:PRO:O	1:I:184:LEU:C	2.57	0.47
1:U:187:ASP:OD1	1:U:189:THR:HG23	2.13	0.47
1:F:204:ARG:HD3	1:H:36:TYR:CZ	2.49	0.47
1:D:211:ASN:HD21	1:F:34:GLU:N	2.09	0.47
1:E:211:ASN:CG	1:G:34:GLU:HB2	2.40	0.47
1:E:194:GLN:HG3	6:E:495:HOH:O	2.15	0.47
1:P:156:ARG:NH2	6:P:403:HOH:O	2.49	0.46
1:G:66:ILE:HG22	6:G:430:HOH:O	2.15	0.46
1:K:167:LEU:HD23	6:K:427:HOH:O	2.14	0.46
1:T:182:LEU:HD13	1:T:183:PRO:HD2	1.97	0.46
1:E:211:ASN:ND2	1:G:34:GLU:H	2.05	0.46
1:E:199:SER:HB2	6:E:451:HOH:O	2.16	0.46
1:S:210:PRO:O	1:S:211:ASN:C	2.58	0.46
1:L:103:PHE:CE2	1:L:135:LYS:HB2	2.51	0.46
1:N:204:ARG:HD2	1:P:36:TYR:OH	2.16	0.46
1:L:195:ASP:HB3	1:M:77:GLU:HG3	1.98	0.45
1:T:104[B]:TYR:CD1	1:T:130:GLU:HG2	2.51	0.45
1:C:187:ASP:OD1	1:C:189:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:50:GLU:H	1:S:50:GLU:CD	2.25	0.45
1:C:204:ARG:NH2	1:D:78:MET:O	2.46	0.45
1:K:173:ARG:HH11	1:K:173:ARG:HG3	1.81	0.45
1:M:211:ASN:OD1	1:N:207:SER:HA	2.17	0.44
1:J:112:ARG:HH12	1:J:114:GLN:NE2	2.04	0.44
1:R:52:ILE:HG13	1:R:175:LEU:HD21	1.98	0.44
1:R:90:GLN:HA	2:R:301:EDO:C1	2.47	0.44
1:A:36:TYR:CZ	1:J:204:ARG:CD	3.01	0.44
1:I:209:ARG:O	1:I:209:ARG:HG3	2.18	0.44
1:C:211:ASN:HD22	1:E:32:THR:HG21	1.83	0.44
1:I:190:LYS:HE3	1:I:190:LYS:HB3	1.76	0.44
1:A:174:SER:O	1:A:178:LEU:HD13	2.18	0.43
1:R:52:ILE:HD12	1:R:166:ILE:CD1	2.48	0.43
1:T:99:ASN:HB2	1:T:104[A]:TYR:CE2	2.53	0.43
1:Q:104[B]:TYR:CE2	1:Q:130:GLU:HB3	2.53	0.43
1:I:175:LEU:HD12	1:I:175:LEU:HA	1.90	0.43
1:D:211:ASN:O	1:D:212:MET:C	2.61	0.43
1:J:49:PRO:C	1:J:51:TYR:N	2.74	0.43
1:Q:52:ILE:HG13	1:Q:175:LEU:HD21	1.99	0.43
1:H:193:ARG:NH1	1:I:50:GLU:OE2	2.51	0.43
1:F:204:ARG:HD2	1:H:36:TYR:CZ	2.53	0.43
1:F:204:ARG:CD	1:H:36:TYR:OH	2.65	0.43
1:N:204:ARG:CD	1:P:36:TYR:OH	2.66	0.43
1:K:192:LYS:NZ	1:K:197:GLU:OE2	2.43	0.43
1:K:173:ARG:CB	1:K:173:ARG:NH1	2.82	0.43
1:V:52:ILE:HD12	1:V:166:ILE:CD1	2.49	0.43
1:L:103:PHE:CZ	1:L:135:LYS:HB2	2.54	0.43
1:N:204:ARG:HD3	1:P:36:TYR:CZ	2.53	0.42
1:T:57:ALA:O	1:T:58:GLY:C	2.63	0.42
1:J:49:PRO:C	1:J:51:TYR:H	2.28	0.42
1:M:52:ILE:HG13	1:M:175:LEU:HD21	2.02	0.42
3:P:303:A1KCK:C14	6:P:402:HOH:O	2.67	0.42
1:F:98:LEU:HD11	1:F:101:GLY:HA2	2.02	0.42
1:P:90:GLN:HE21	1:P:92[B]:ASN:HD21	1.68	0.42
1:C:137:LEU:HD23	6:C:402:HOH:O	2.19	0.42
1:T:99:ASN:HB2	1:T:104[A]:TYR:HE2	1.84	0.42
1:L:34:GLU:CD	1:U:211:ASN:HB2	2.45	0.41
1:V:53:SER:OG	2:V:303:EDO:H11	2.20	0.41
1:K:209:ARG:H	1:K:209:ARG:HD2	1.84	0.41
1:N:52:ILE:HG13	1:N:175:LEU:HD21	2.02	0.41
1:L:36:TYR:CZ	1:U:204:ARG:CD	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:52:ILE:HG13	1:J:175:LEU:HD21	2.02	0.41
1:T:112:ARG:NE	5:T:305:CL:CL	2.76	0.41
1:B:99:ASN:OD1	1:Q:99:ASN:OD1	2.39	0.41
1:I:77:GLU:OE2	1:J:44:ARG:HD3	2.20	0.41
1:F:211:ASN:HD22	1:F:211:ASN:HA	1.72	0.41
1:O:169:LYS:HG2	6:O:434:HOH:O	2.21	0.41
1:T:134:SER:HB3	1:T:137:LEU:HB2	2.03	0.41
1:B:179:PRO:O	1:B:180:ARG:C	2.63	0.41
3:A:304:A1KCK:C5	6:A:417:HOH:O	2.69	0.40
6:D:442:HOH:O	1:E:30:GLN:HG3	2.19	0.40
1:T:102:ALA:HB1	1:T:131:GLY:HA2	2.03	0.40
1:O:104[A]:TYR:CD1	1:O:130:GLU:HG2	2.57	0.40
1:U:137:LEU:HD23	6:U:405:HOH:O	2.21	0.40
1:H:34:GLU:CD	1:H:34:GLU:H	2.28	0.40
2:I:302:EDO:H11	1:J:90:GLN:OE1	2.21	0.40
1:N:166:ILE:HD12	1:N:166:ILE:HA	1.93	0.40
1:R:92[B]:ASN:ND2	6:R:411:HOH:O	2.55	0.40
1:L:123:ASP:OD2	1:L:156:ARG:NH2	2.54	0.40
1:G:52:ILE:HD12	1:G:166:ILE:CD1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	184/215 (86%)	184 (100%)	0	0	100	100
1	B	187/215 (87%)	182 (97%)	4 (2%)	1 (0%)	24	22
1	C	187/215 (87%)	183 (98%)	4 (2%)	0	100	100
1	D	186/215 (86%)	183 (98%)	3 (2%)	0	100	100
1	E	187/215 (87%)	186 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	185/215 (86%)	183 (99%)	1 (0%)	1 (0%)	24	22
1	G	186/215 (86%)	185 (100%)	1 (0%)	0	100	100
1	H	187/215 (87%)	184 (98%)	3 (2%)	0	100	100
1	I	185/215 (86%)	181 (98%)	3 (2%)	1 (0%)	24	22
1	J	187/215 (87%)	182 (97%)	4 (2%)	1 (0%)	24	22
1	K	187/215 (87%)	182 (97%)	4 (2%)	1 (0%)	24	22
1	L	186/215 (86%)	183 (98%)	3 (2%)	0	100	100
1	M	187/215 (87%)	183 (98%)	4 (2%)	0	100	100
1	N	186/215 (86%)	183 (98%)	3 (2%)	0	100	100
1	O	186/215 (86%)	183 (98%)	2 (1%)	1 (0%)	24	22
1	P	186/215 (86%)	184 (99%)	2 (1%)	0	100	100
1	Q	187/215 (87%)	185 (99%)	2 (1%)	0	100	100
1	R	187/215 (87%)	186 (100%)	1 (0%)	0	100	100
1	S	186/215 (86%)	183 (98%)	3 (2%)	0	100	100
1	T	187/215 (87%)	181 (97%)	6 (3%)	0	100	100
1	U	185/215 (86%)	184 (100%)	1 (0%)	0	100	100
1	V	185/215 (86%)	184 (100%)	1 (0%)	0	100	100
All	All	4096/4730 (87%)	4034 (98%)	56 (1%)	6 (0%)	48	50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	58	GLY
1	F	58	GLY
1	O	58	GLY
1	K	183	PRO
1	I	183	PRO
1	J	179	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	153/172 (89%)	148 (97%)	5 (3%)	33	37
1	B	155/172 (90%)	150 (97%)	5 (3%)	34	38
1	C	155/172 (90%)	153 (99%)	2 (1%)	61	69
1	D	154/172 (90%)	150 (97%)	4 (3%)	40	46
1	E	155/172 (90%)	150 (97%)	5 (3%)	34	38
1	F	154/172 (90%)	152 (99%)	2 (1%)	61	69
1	G	153/172 (89%)	149 (97%)	4 (3%)	40	46
1	H	155/172 (90%)	147 (95%)	8 (5%)	21	20
1	I	152/172 (88%)	143 (94%)	9 (6%)	18	16
1	J	155/172 (90%)	151 (97%)	4 (3%)	40	46
1	K	156/172 (91%)	148 (95%)	8 (5%)	21	21
1	L	155/172 (90%)	153 (99%)	2 (1%)	61	69
1	M	155/172 (90%)	152 (98%)	3 (2%)	50	58
1	N	154/172 (90%)	150 (97%)	4 (3%)	40	46
1	O	155/172 (90%)	152 (98%)	3 (2%)	50	58
1	P	155/172 (90%)	150 (97%)	5 (3%)	34	38
1	Q	156/172 (91%)	152 (97%)	4 (3%)	40	46
1	R	155/172 (90%)	152 (98%)	3 (2%)	50	58
1	S	154/172 (90%)	148 (96%)	6 (4%)	28	31
1	T	156/172 (91%)	151 (97%)	5 (3%)	34	38
1	U	154/172 (90%)	150 (97%)	4 (3%)	40	46
1	V	154/172 (90%)	151 (98%)	3 (2%)	50	58
All	All	3400/3784 (90%)	3302 (97%)	98 (3%)	37	42

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	LEU
1	A	180	ARG
1	A	181	GLN
1	A	196	LEU
1	A	199	SER
1	B	30	GLN

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Mol	Chain	Res	Type
1	B	100	ASN
1	B	166	ILE
1	B	176	ASN
1	B	185	GLU
1	C	62	LYS
1	C	177	LYS
1	D	61	GLN
1	D	180	ARG
1	D	181	GLN
1	D	196	LEU
1	E	54	SER
1	E	176	ASN
1	E	184	LEU
1	E	186	VAL
1	E	212	MET
1	F	61	GLN
1	F	211	ASN
1	G	61	GLN
1	G	186	VAL
1	G	194	GLN
1	G	209	ARG
1	H	34	GLU
1	H	62	LYS
1	H	181	GLN
1	H	184	LEU
1	H	185	GLU
1	H	199	SER
1	H	209	ARG
1	H	212	MET
1	I	62	LYS
1	I	98	LEU
1	I	178	LEU
1	I	180	ARG
1	I	181	GLN
1	I	186	VAL
1	I	190	LYS
1	I	194	GLN
1	I	196	LEU
1	J	54	SER
1	J	173	ARG
1	J	181	GLN
1	J	194	GLN

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Mol	Chain	Res	Type
1	K	157	SER
1	K	173	ARG
1	K	178	LEU
1	K	180	ARG
1	K	182	LEU
1	K	184	LEU
1	K	196	LEU
1	K	209	ARG
1	L	25	CYS
1	L	211	ASN
1	M	166	ILE
1	M	182	LEU
1	M	209	ARG
1	N	173	ARG
1	N	181	GLN
1	N	182	LEU
1	N	184	LEU
1	O	166	ILE
1	O	174	SER
1	O	209	ARG
1	P	30	GLN
1	P	176	ASN
1	P	180	ARG
1	P	184	LEU
1	P	209	ARG
1	Q	173	ARG
1	Q	181	GLN
1	Q	182	LEU
1	Q	196	LEU
1	R	180	ARG
1	R	186	VAL
1	R	194	GLN
1	S	37	GLN
1	S	50	GLU
1	S	172	LEU
1	S	182	LEU
1	S	194	GLN
1	S	196	LEU
1	T	100	ASN
1	T	166	ILE
1	T	182	LEU
1	T	185	GLU

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Mol	Chain	Res	Type
1	T	211	ASN
1	U	156	ARG
1	U	166	ILE
1	U	185	GLU
1	U	186	VAL
1	V	37	GLN
1	V	55	ARG
1	V	184	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	45	GLN
1	B	28	GLN
1	B	30	GLN
1	B	69	HIS
1	C	181	GLN
1	C	211	ASN
1	D	211	ASN
1	E	69	HIS
1	E	92	ASN
1	E	114	GLN
1	E	206	ASN
1	E	211	ASN
1	F	37	GLN
1	F	45	GLN
1	F	61	GLN
1	F	211	ASN
1	G	45	GLN
1	G	69	HIS
1	G	114	GLN
1	H	30	GLN
1	H	92	ASN
1	H	181	GLN
1	I	45	GLN
1	J	114	GLN
1	J	181	GLN
1	J	194	GLN
1	J	211	ASN
1	K	114	GLN
1	K	206	ASN

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Mol	Chain	Res	Type
1	L	28	GLN
1	L	45	GLN
1	L	206	ASN
1	M	30	GLN
1	M	69	HIS
1	M	176	ASN
1	N	45	GLN
1	N	92	ASN
1	O	69	HIS
1	P	30	GLN
1	P	90	GLN
1	Q	61	GLN
1	Q	69	HIS
1	Q	90	GLN
1	Q	100	ASN
1	Q	181	GLN
1	Q	211	ASN
1	R	61	GLN
1	R	90	GLN
1	S	37	GLN
1	S	45	GLN
1	S	211	ASN
1	T	28	GLN
1	T	37	GLN
1	T	45	GLN
1	T	90	GLN
1	U	28	GLN
1	U	69	HIS
1	V	30	GLN
1	V	206	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 109 ligands modelled in this entry, 35 are monoatomic - leaving 74 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A1KCK	O	302	-	19,19,19	3.14	4 (21%)	26,27,27	1.61	3 (11%)
2	EDO	O	301	-	3,3,3	0.05	0	2,2,2	0.47	0
3	A1KCK	V	305	-	19,19,19	3.34	4 (21%)	26,27,27	1.63	4 (15%)
3	A1KCK	A	304	-	19,19,19	3.08	4 (21%)	26,27,27	1.62	4 (15%)
3	A1KCK	C	301	-	19,19,19	3.10	3 (15%)	26,27,27	1.65	3 (11%)
3	A1KCK	J	301	-	19,19,19	2.99	3 (15%)	26,27,27	1.66	3 (11%)
2	EDO	D	302	-	3,3,3	0.12	0	2,2,2	0.22	0
2	EDO	E	304	-	3,3,3	0.08	0	2,2,2	0.24	0
3	A1KCK	K	304	-	19,19,19	3.24	4 (21%)	26,27,27	1.63	3 (11%)
3	A1KCK	A	306	-	19,19,19	2.97	3 (15%)	26,27,27	1.80	3 (11%)
3	A1KCK	C	303	-	19,19,19	3.38	4 (21%)	26,27,27	1.67	4 (15%)
3	A1KCK	I	301	-	19,19,19	3.12	4 (21%)	26,27,27	1.76	3 (11%)
3	A1KCK	N	303	-	19,19,19	3.06	4 (21%)	26,27,27	1.67	3 (11%)
2	EDO	H	302	-	3,3,3	0.15	0	2,2,2	0.28	0
2	EDO	U	301	-	3,3,3	0.09	0	2,2,2	0.59	0
3	A1KCK	H	303	-	19,19,19	3.33	4 (21%)	26,27,27	1.60	3 (11%)
3	A1KCK	D	301	-	19,19,19	3.12	4 (21%)	26,27,27	1.74	3 (11%)
2	EDO	I	302	-	3,3,3	0.11	0	2,2,2	0.27	0
2	EDO	T	301	-	3,3,3	0.15	0	2,2,2	0.33	0
2	EDO	A	301	-	3,3,3	0.30	0	2,2,2	0.46	0
3	A1KCK	K	302	-	19,19,19	3.03	3 (15%)	26,27,27	1.78	3 (11%)
3	A1KCK	N	301	-	19,19,19	3.10	4 (21%)	26,27,27	1.57	3 (11%)
2	EDO	P	301	-	3,3,3	0.15	0	2,2,2	0.46	0
3	A1KCK	S	303	-	19,19,19	3.33	4 (21%)	26,27,27	1.63	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	F	302	-	3,3,3	0.12	0	2,2,2	0.51	0
3	A1KCK	K	301	-	19,19,19	3.11	4 (21%)	26,27,27	1.66	3 (11%)
3	A1KCK	V	304	-	19,19,19	3.18	4 (21%)	26,27,27	1.81	5 (19%)
3	A1KCK	B	303	-	19,19,19	3.23	5 (26%)	26,27,27	1.61	4 (15%)
2	EDO	M	301	-	3,3,3	0.09	0	2,2,2	0.10	0
3	A1KCK	R	303	-	19,19,19	3.35	4 (21%)	26,27,27	1.57	4 (15%)
2	EDO	A	302	-	3,3,3	0.71	0	2,2,2	1.27	0
3	A1KCK	Q	302	-	19,19,19	3.26	4 (21%)	26,27,27	2.03	7 (26%)
3	A1KCK	R	302	-	19,19,19	3.07	3 (15%)	26,27,27	1.59	4 (15%)
3	A1KCK	T	302	-	19,19,19	3.08	4 (21%)	26,27,27	1.55	4 (15%)
3	A1KCK	L	302	-	19,19,19	3.29	4 (21%)	26,27,27	1.64	4 (15%)
2	EDO	S	301	-	3,3,3	0.09	0	2,2,2	0.28	0
3	A1KCK	P	303	-	19,19,19	3.06	4 (21%)	26,27,27	1.66	3 (11%)
3	A1KCK	P	302	-	19,19,19	3.15	4 (21%)	26,27,27	1.57	3 (11%)
3	A1KCK	Q	303	-	19,19,19	3.24	5 (26%)	26,27,27	1.58	4 (15%)
2	EDO	E	301	-	3,3,3	0.08	0	2,2,2	0.45	0
2	EDO	B	302	-	3,3,3	0.01	0	2,2,2	0.28	0
2	EDO	V	301	-	3,3,3	0.19	0	2,2,2	0.77	0
3	A1KCK	I	303	-	19,19,19	3.10	4 (21%)	26,27,27	1.57	4 (15%)
3	A1KCK	M	302	-	19,19,19	2.97	3 (15%)	26,27,27	1.57	3 (11%)
2	EDO	B	301	-	3,3,3	0.13	0	2,2,2	0.64	0
3	A1KCK	G	301	-	19,19,19	3.10	4 (21%)	26,27,27	1.59	3 (11%)
3	A1KCK	D	303	-	19,19,19	3.23	5 (26%)	26,27,27	1.57	3 (11%)
3	A1KCK	L	303	-	19,19,19	3.06	3 (15%)	26,27,27	1.84	5 (19%)
2	EDO	V	302	-	3,3,3	0.06	0	2,2,2	0.04	0
2	EDO	G	302	-	3,3,3	0.07	0	2,2,2	0.60	0
3	A1KCK	H	301	-	19,19,19	3.14	4 (21%)	26,27,27	1.64	3 (11%)
2	EDO	A	303	-	3,3,3	0.20	0	2,2,2	0.78	0
3	A1KCK	F	304	-	19,19,19	3.31	4 (21%)	26,27,27	1.60	4 (15%)
2	EDO	E	303	-	3,3,3	0.06	0	2,2,2	0.53	0
2	EDO	Q	301	-	3,3,3	0.12	0	2,2,2	0.37	0
2	EDO	F	303	-	3,3,3	0.07	0	2,2,2	0.39	0
3	A1KCK	T	303	-	19,19,19	3.39	4 (21%)	26,27,27	1.80	5 (19%)
2	EDO	C	302	-	3,3,3	0.07	0	2,2,2	0.26	0
2	EDO	L	301	-	3,3,3	0.06	0	2,2,2	0.06	0
3	A1KCK	M	303	-	19,19,19	3.20	4 (21%)	26,27,27	1.60	4 (15%)
2	EDO	N	302	-	3,3,3	0.08	0	2,2,2	0.64	0
2	EDO	V	303	-	3,3,3	0.11	0	2,2,2	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	K	303	-	3,3,3	0.10	0	2,2,2	0.07	0
3	A1KCK	A	305	-	19,19,19	3.10	3 (15%)	26,27,27	1.60	3 (11%)
2	EDO	R	301	-	3,3,3	0.10	0	2,2,2	0.32	0
3	A1KCK	E	305	-	19,19,19	3.20	4 (21%)	26,27,27	1.60	4 (15%)
3	A1KCK	U	302	-	19,19,19	3.16	4 (21%)	26,27,27	1.91	6 (23%)
3	A1KCK	F	301	-	19,19,19	3.02	4 (21%)	26,27,27	1.64	3 (11%)
3	A1KCK	O	303	-	19,19,19	3.23	4 (21%)	26,27,27	1.60	4 (15%)
3	A1KCK	L	304	-	19,19,19	3.17	5 (26%)	26,27,27	1.59	4 (15%)
3	A1KCK	S	302	-	19,19,19	3.10	4 (21%)	26,27,27	1.57	3 (11%)
3	A1KCK	G	303	-	19,19,19	3.10	4 (21%)	26,27,27	1.63	4 (15%)
2	EDO	J	302	-	3,3,3	0.13	0	2,2,2	0.30	0
3	A1KCK	E	302	-	19,19,19	3.18	5 (26%)	26,27,27	1.59	4 (15%)

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
3	A1KCK	O	302	-	-	0/8/8/8	0/3/3/3
2	EDO	O	301	-	-	1/1/1/1	-
3	A1KCK	V	305	-	-	4/8/8/8	0/3/3/3
3	A1KCK	A	304	-	-	0/8/8/8	0/3/3/3
3	A1KCK	C	301	-	-	0/8/8/8	0/3/3/3
3	A1KCK	J	301	-	-	4/8/8/8	0/3/3/3
2	EDO	D	302	-	-	1/1/1/1	-
2	EDO	E	304	-	-	1/1/1/1	-
3	A1KCK	K	304	-	-	3/8/8/8	0/3/3/3
3	A1KCK	A	306	-	-	2/8/8/8	0/3/3/3
3	A1KCK	C	303	-	-	4/8/8/8	0/3/3/3
3	A1KCK	I	301	-	-	0/8/8/8	0/3/3/3
3	A1KCK	N	303	-	-	4/8/8/8	0/3/3/3
2	EDO	H	302	-	-	1/1/1/1	-
2	EDO	U	301	-	-	0/1/1/1	-
3	A1KCK	H	303	-	-	0/8/8/8	0/3/3/3
3	A1KCK	D	301	-	-	0/8/8/8	0/3/3/3
2	EDO	I	302	-	-	0/1/1/1	-
2	EDO	T	301	-	-	1/1/1/1	-
2	EDO	A	301	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1KCK	K	302	-	-	0/8/8/8	0/3/3/3
3	A1KCK	N	301	-	-	3/8/8/8	0/3/3/3
2	EDO	P	301	-	-	1/1/1/1	-
3	A1KCK	S	303	-	-	1/8/8/8	0/3/3/3
2	EDO	F	302	-	-	0/1/1/1	-
3	A1KCK	K	301	-	-	4/8/8/8	0/3/3/3
3	A1KCK	V	304	-	-	0/8/8/8	0/3/3/3
3	A1KCK	B	303	-	-	0/8/8/8	0/3/3/3
2	EDO	M	301	-	-	1/1/1/1	-
3	A1KCK	R	303	-	-	0/8/8/8	0/3/3/3
2	EDO	A	302	-	-	1/1/1/1	-
3	A1KCK	Q	302	-	-	0/8/8/8	0/3/3/3
3	A1KCK	R	302	-	-	0/8/8/8	0/3/3/3
3	A1KCK	T	302	-	-	0/8/8/8	0/3/3/3
3	A1KCK	L	302	-	-	2/8/8/8	0/3/3/3
2	EDO	S	301	-	-	1/1/1/1	-
3	A1KCK	P	303	-	-	4/8/8/8	0/3/3/3
3	A1KCK	P	302	-	-	0/8/8/8	0/3/3/3
3	A1KCK	Q	303	-	-	0/8/8/8	0/3/3/3
2	EDO	E	301	-	-	0/1/1/1	-
2	EDO	B	302	-	-	1/1/1/1	-
2	EDO	V	301	-	-	0/1/1/1	-
3	A1KCK	I	303	-	-	0/8/8/8	0/3/3/3
3	A1KCK	M	302	-	-	0/8/8/8	0/3/3/3
2	EDO	B	301	-	-	0/1/1/1	-
3	A1KCK	G	301	-	-	0/8/8/8	0/3/3/3
3	A1KCK	D	303	-	-	0/8/8/8	0/3/3/3
3	A1KCK	L	303	-	-	0/8/8/8	0/3/3/3
2	EDO	V	302	-	-	0/1/1/1	-
2	EDO	G	302	-	-	0/1/1/1	-
3	A1KCK	H	301	-	-	0/8/8/8	0/3/3/3
2	EDO	A	303	-	-	0/1/1/1	-
3	A1KCK	F	304	-	-	0/8/8/8	0/3/3/3
2	EDO	E	303	-	-	0/1/1/1	-
2	EDO	Q	301	-	-	1/1/1/1	-
2	EDO	F	303	-	-	1/1/1/1	-
3	A1KCK	T	303	-	-	0/8/8/8	0/3/3/3
2	EDO	C	302	-	-	1/1/1/1	-
2	EDO	L	301	-	-	0/1/1/1	-
3	A1KCK	M	303	-	-	0/8/8/8	0/3/3/3
2	EDO	N	302	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	V	303	-	-	1/1/1/1	-
2	EDO	K	303	-	-	1/1/1/1	-
3	A1KCK	A	305	-	-	0/8/8/8	0/3/3/3
2	EDO	R	301	-	-	1/1/1/1	-
3	A1KCK	E	305	-	-	0/8/8/8	0/3/3/3
3	A1KCK	U	302	-	-	0/8/8/8	0/3/3/3
3	A1KCK	F	301	-	-	0/8/8/8	0/3/3/3
3	A1KCK	O	303	-	-	0/8/8/8	0/3/3/3
3	A1KCK	L	304	-	-	0/8/8/8	0/3/3/3
3	A1KCK	S	302	-	-	0/8/8/8	0/3/3/3
3	A1KCK	G	303	-	-	0/8/8/8	0/3/3/3
2	EDO	J	302	-	-	1/1/1/1	-
3	A1KCK	E	302	-	-	0/8/8/8	0/3/3/3

All (173) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	302	A1KCK	C15-C14	12.57	1.55	1.33
3	V	304	A1KCK	C15-C14	12.51	1.54	1.33
3	Q	303	A1KCK	C15-C14	12.46	1.54	1.33
3	T	303	A1KCK	C15-C14	12.41	1.54	1.33
3	R	303	A1KCK	C15-C14	12.39	1.54	1.33
3	B	303	A1KCK	C15-C14	12.31	1.54	1.33
3	K	304	A1KCK	C15-C14	12.24	1.54	1.33
3	L	304	A1KCK	C15-C14	12.23	1.54	1.33
3	S	303	A1KCK	C15-C14	12.20	1.54	1.33
3	M	303	A1KCK	C15-C14	12.18	1.54	1.33
3	V	305	A1KCK	C15-C14	12.12	1.54	1.33
3	G	303	A1KCK	C15-C14	12.07	1.54	1.33
3	F	304	A1KCK	C15-C14	12.06	1.54	1.33
3	D	303	A1KCK	C15-C14	12.06	1.54	1.33
3	C	303	A1KCK	C15-C14	12.05	1.54	1.33
3	I	301	A1KCK	C15-C14	11.99	1.54	1.33
3	L	302	A1KCK	C15-C14	11.97	1.54	1.33
3	E	302	A1KCK	C15-C14	11.97	1.54	1.33
3	P	302	A1KCK	C15-C14	11.95	1.53	1.33
3	U	302	A1KCK	C15-C14	11.94	1.53	1.33
3	N	303	A1KCK	C15-C14	11.94	1.53	1.33
3	R	302	A1KCK	C15-C14	11.94	1.53	1.33
3	A	305	A1KCK	C15-C14	11.93	1.53	1.33
3	O	303	A1KCK	C15-C14	11.93	1.53	1.33
3	D	301	A1KCK	C15-C14	11.93	1.53	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	A1KCK	C15-C14	11.89	1.53	1.33
3	L	303	A1KCK	C15-C14	11.89	1.53	1.33
3	O	302	A1KCK	C15-C14	11.88	1.53	1.33
3	H	301	A1KCK	C15-C14	11.87	1.53	1.33
3	H	303	A1KCK	C15-C14	11.81	1.53	1.33
3	T	302	A1KCK	C15-C14	11.78	1.53	1.33
3	E	305	A1KCK	C15-C14	11.75	1.53	1.33
3	K	301	A1KCK	C15-C14	11.70	1.53	1.33
3	G	301	A1KCK	C15-C14	11.70	1.53	1.33
3	S	302	A1KCK	C15-C14	11.65	1.53	1.33
3	I	303	A1KCK	C15-C14	11.58	1.53	1.33
3	K	302	A1KCK	C15-C14	11.57	1.53	1.33
3	J	301	A1KCK	C15-C14	11.57	1.53	1.33
3	A	306	A1KCK	C15-C14	11.55	1.53	1.33
3	F	301	A1KCK	C15-C14	11.50	1.53	1.33
3	P	303	A1KCK	C15-C14	11.46	1.53	1.33
3	N	301	A1KCK	C15-C14	11.43	1.53	1.33
3	M	302	A1KCK	C15-C14	11.32	1.52	1.33
3	A	304	A1KCK	C15-C14	10.95	1.52	1.33
3	C	303	A1KCK	O13-C14	5.97	1.48	1.38
3	A	304	A1KCK	O13-C14	5.71	1.47	1.38
3	S	302	A1KCK	O13-C14	5.47	1.47	1.38
3	V	305	A1KCK	O13-C14	5.47	1.47	1.38
3	S	303	A1KCK	O13-C14	5.40	1.47	1.38
3	L	302	A1KCK	O13-C14	5.39	1.47	1.38
3	H	303	A1KCK	C2-C4	5.38	1.60	1.47
3	E	305	A1KCK	O13-C14	5.35	1.47	1.38
3	P	303	A1KCK	O13-C14	5.28	1.47	1.38
3	M	302	A1KCK	O13-C14	5.23	1.46	1.38
3	B	303	A1KCK	O13-C14	5.21	1.46	1.38
3	O	303	A1KCK	O13-C14	5.20	1.46	1.38
3	A	305	A1KCK	O13-C14	5.17	1.46	1.38
3	E	302	A1KCK	O13-C14	5.16	1.46	1.38
3	R	303	A1KCK	O13-C14	5.16	1.46	1.38
3	N	301	A1KCK	O13-C14	5.14	1.46	1.38
3	H	303	A1KCK	O13-C14	5.13	1.46	1.38
3	K	301	A1KCK	O13-C14	5.09	1.46	1.38
3	D	303	A1KCK	O13-C14	5.09	1.46	1.38
3	F	304	A1KCK	O13-C14	5.08	1.46	1.38
3	C	301	A1KCK	O13-C14	5.07	1.46	1.38
3	P	302	A1KCK	O13-C14	5.07	1.46	1.38
3	T	302	A1KCK	O13-C14	5.02	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	303	A1KCK	O13-C14	5.01	1.46	1.38
3	U	302	A1KCK	O13-C14	5.01	1.46	1.38
3	G	301	A1KCK	O13-C14	5.01	1.46	1.38
3	O	302	A1KCK	O13-C14	5.01	1.46	1.38
3	M	303	A1KCK	O13-C14	5.00	1.46	1.38
3	I	303	A1KCK	O13-C14	4.99	1.46	1.38
3	K	304	A1KCK	O13-C14	4.96	1.46	1.38
3	F	301	A1KCK	O13-C14	4.94	1.46	1.38
3	D	301	A1KCK	O13-C14	4.91	1.46	1.38
3	F	304	A1KCK	C2-C4	4.89	1.59	1.47
3	R	302	A1KCK	O13-C14	4.88	1.46	1.38
3	J	301	A1KCK	O13-C14	4.78	1.46	1.38
3	L	304	A1KCK	O13-C14	4.78	1.46	1.38
3	H	301	A1KCK	O13-C14	4.77	1.46	1.38
3	A	306	A1KCK	O13-C14	4.72	1.46	1.38
3	Q	302	A1KCK	O13-C14	4.72	1.46	1.38
3	L	303	A1KCK	O13-C14	4.70	1.46	1.38
3	Q	303	A1KCK	O13-C14	4.70	1.46	1.38
3	G	303	A1KCK	O13-C14	4.69	1.46	1.38
3	I	301	A1KCK	O13-C14	4.69	1.46	1.38
3	K	302	A1KCK	O13-C14	4.65	1.46	1.38
3	N	303	A1KCK	O13-C14	4.64	1.46	1.38
3	C	303	A1KCK	C2-C4	4.60	1.58	1.47
3	T	303	A1KCK	C2-C4	4.56	1.58	1.47
3	V	304	A1KCK	O13-C14	4.50	1.45	1.38
3	L	302	A1KCK	C2-C4	4.40	1.58	1.47
3	V	305	A1KCK	C2-C4	4.40	1.58	1.47
3	S	303	A1KCK	C2-C4	4.34	1.57	1.47
3	R	303	A1KCK	C2-C4	4.13	1.57	1.47
3	E	305	A1KCK	C2-C4	4.00	1.57	1.47
3	O	303	A1KCK	C2-C4	3.98	1.57	1.47
3	A	304	A1KCK	C2-C4	3.67	1.56	1.47
3	I	303	A1KCK	C2-C4	3.48	1.55	1.47
3	H	301	A1KCK	C2-C4	3.47	1.55	1.47
3	K	304	A1KCK	C2-C4	3.41	1.55	1.47
3	N	301	A1KCK	C2-C4	3.04	1.54	1.47
3	K	301	A1KCK	C2-C4	3.03	1.54	1.47
3	D	303	A1KCK	C2-C4	3.01	1.54	1.47
3	O	302	A1KCK	C2-C4	3.00	1.54	1.47
3	G	301	A1KCK	C2-C4	2.93	1.54	1.47
3	Q	303	A1KCK	O1-C2	-2.91	1.22	1.30
3	M	303	A1KCK	C2-C4	2.84	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	302	A1KCK	C2-C4	2.76	1.54	1.47
3	D	303	A1KCK	O1-C2	-2.75	1.22	1.30
3	P	303	A1KCK	C2-C4	2.73	1.54	1.47
3	B	303	A1KCK	C2-C4	2.72	1.54	1.47
3	C	303	A1KCK	C11-C15	2.60	1.51	1.43
3	P	302	A1KCK	C2-C4	2.50	1.53	1.47
3	V	305	A1KCK	C11-C15	2.49	1.51	1.43
3	S	303	A1KCK	C11-C15	2.47	1.51	1.43
3	C	301	A1KCK	C11-C15	2.46	1.51	1.43
3	T	303	A1KCK	C11-C15	2.46	1.51	1.43
3	A	304	A1KCK	C11-C15	2.45	1.51	1.43
3	M	302	A1KCK	C11-C15	2.44	1.51	1.43
3	S	302	A1KCK	O1-C2	-2.44	1.23	1.30
3	K	301	A1KCK	C11-C15	2.44	1.51	1.43
3	L	304	A1KCK	C2-C4	2.44	1.53	1.47
3	P	302	A1KCK	C11-C15	2.43	1.51	1.43
3	F	304	A1KCK	C11-C15	2.43	1.51	1.43
3	L	302	A1KCK	C11-C15	2.43	1.51	1.43
3	E	302	A1KCK	C11-C15	2.43	1.51	1.43
3	G	301	A1KCK	C11-C15	2.42	1.51	1.43
3	I	303	A1KCK	C11-C15	2.42	1.51	1.43
3	H	303	A1KCK	C11-C15	2.42	1.51	1.43
3	O	303	A1KCK	C11-C15	2.42	1.51	1.43
3	O	302	A1KCK	C11-C15	2.40	1.51	1.43
3	N	301	A1KCK	C11-C15	2.40	1.51	1.43
3	A	305	A1KCK	C11-C15	2.39	1.51	1.43
3	D	301	A1KCK	C11-C15	2.38	1.51	1.43
3	K	304	A1KCK	C11-C15	2.37	1.51	1.43
3	P	303	A1KCK	C11-C15	2.37	1.51	1.43
3	E	305	A1KCK	C11-C15	2.37	1.51	1.43
3	R	303	A1KCK	C11-C15	2.37	1.51	1.43
3	F	301	A1KCK	C11-C15	2.36	1.51	1.43
3	S	302	A1KCK	C11-C15	2.36	1.51	1.43
3	I	301	A1KCK	C11-C15	2.36	1.51	1.43
3	T	302	A1KCK	C11-C15	2.35	1.51	1.43
3	H	301	A1KCK	C11-C15	2.34	1.51	1.43
3	M	303	A1KCK	C11-C15	2.33	1.50	1.43
3	D	303	A1KCK	C11-C15	2.33	1.50	1.43
3	L	304	A1KCK	C11-C15	2.32	1.50	1.43
3	G	303	A1KCK	C11-C15	2.31	1.50	1.43
3	N	303	A1KCK	O1-C2	-2.31	1.23	1.30
3	U	302	A1KCK	C11-C15	2.29	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	303	A1KCK	O1-C2	-2.29	1.23	1.30
3	R	302	A1KCK	C11-C15	2.28	1.50	1.43
3	J	301	A1KCK	C11-C15	2.28	1.50	1.43
3	A	306	A1KCK	C11-C15	2.28	1.50	1.43
3	D	301	A1KCK	C2-C4	2.26	1.53	1.47
3	F	301	A1KCK	C2-C4	2.26	1.53	1.47
3	K	302	A1KCK	C11-C15	2.25	1.50	1.43
3	Q	303	A1KCK	C2-C4	2.25	1.53	1.47
3	V	304	A1KCK	C11-C15	2.23	1.50	1.43
3	Q	302	A1KCK	C11-C15	2.21	1.50	1.43
3	L	303	A1KCK	C11-C15	2.21	1.50	1.43
3	V	304	A1KCK	C7-S8	2.19	1.78	1.74
3	B	303	A1KCK	C11-C15	2.13	1.50	1.43
3	E	302	A1KCK	O3-C2	2.11	1.28	1.22
3	N	303	A1KCK	C11-C15	2.11	1.50	1.43
3	Q	302	A1KCK	C7-S8	2.10	1.78	1.74
3	I	301	A1KCK	C2-C4	2.09	1.52	1.47
3	L	304	A1KCK	O1-C2	-2.05	1.24	1.30
3	U	302	A1KCK	O1-C2	-2.05	1.24	1.30
3	Q	303	A1KCK	C11-C15	2.05	1.50	1.43
3	T	302	A1KCK	C2-C4	2.01	1.52	1.47
3	G	303	A1KCK	C2-C4	2.01	1.52	1.47

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	306	A1KCK	O13-C14-C15	-5.94	107.24	112.46
3	C	303	A1KCK	O13-C14-C15	-5.89	107.29	112.46
3	I	301	A1KCK	O13-C14-C15	-5.73	107.43	112.46
3	H	301	A1KCK	O13-C14-C15	-5.66	107.49	112.46
3	S	303	A1KCK	O13-C14-C15	-5.66	107.49	112.46
3	P	303	A1KCK	O13-C14-C15	-5.63	107.51	112.46
3	K	302	A1KCK	O13-C14-C15	-5.59	107.54	112.46
3	K	301	A1KCK	O13-C14-C15	-5.56	107.58	112.46
3	F	301	A1KCK	O13-C14-C15	-5.54	107.59	112.46
3	J	301	A1KCK	O13-C14-C15	-5.54	107.59	112.46
3	Q	302	A1KCK	O13-C14-C15	-5.45	107.67	112.46
3	L	302	A1KCK	O13-C14-C15	-5.43	107.69	112.46
3	F	304	A1KCK	O13-C14-C15	-5.41	107.70	112.46
3	A	304	A1KCK	O13-C14-C15	-5.41	107.70	112.46
3	V	305	A1KCK	O13-C14-C15	-5.36	107.75	112.46
3	L	303	A1KCK	O13-C14-C15	-5.34	107.77	112.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	303	A1KCK	O13-C14-C15	-5.34	107.77	112.46
3	R	303	A1KCK	O13-C14-C15	-5.33	107.77	112.46
3	B	303	A1KCK	O13-C14-C15	-5.31	107.79	112.46
3	D	301	A1KCK	O13-C14-C15	-5.31	107.79	112.46
3	U	302	A1KCK	O13-C14-C15	-5.29	107.81	112.46
3	T	303	A1KCK	O13-C14-C15	-5.26	107.84	112.46
3	V	304	A1KCK	O13-C14-C15	-5.26	107.84	112.46
3	K	304	A1KCK	O13-C14-C15	-5.25	107.84	112.46
3	N	301	A1KCK	O13-C14-C15	-5.24	107.86	112.46
3	G	303	A1KCK	O13-C14-C15	-5.23	107.86	112.46
3	E	302	A1KCK	O13-C14-C15	-5.20	107.89	112.46
3	P	302	A1KCK	O13-C14-C15	-5.16	107.92	112.46
3	A	305	A1KCK	O13-C14-C15	-5.15	107.93	112.46
3	D	303	A1KCK	O13-C14-C15	-5.15	107.93	112.46
3	O	302	A1KCK	O13-C14-C15	-5.14	107.94	112.46
3	G	301	A1KCK	O13-C14-C15	-5.14	107.94	112.46
3	C	301	A1KCK	O13-C14-C15	-5.11	107.97	112.46
3	E	305	A1KCK	O13-C14-C15	-5.10	107.98	112.46
3	N	303	A1KCK	O13-C14-C15	-5.09	107.98	112.46
3	O	303	A1KCK	O13-C14-C15	-5.08	107.99	112.46
3	S	302	A1KCK	O13-C14-C15	-5.05	108.02	112.46
3	L	304	A1KCK	O13-C14-C15	-5.03	108.04	112.46
3	Q	303	A1KCK	O13-C14-C15	-5.03	108.04	112.46
3	I	303	A1KCK	O13-C14-C15	-5.01	108.06	112.46
3	A	306	A1KCK	C11-C15-C14	-4.99	100.99	106.47
3	M	302	A1KCK	O13-C14-C15	-4.98	108.08	112.46
3	M	303	A1KCK	O13-C14-C15	-4.98	108.08	112.46
3	R	302	A1KCK	O13-C14-C15	-4.98	108.08	112.46
3	T	302	A1KCK	O13-C14-C15	-4.88	108.17	112.46
3	K	302	A1KCK	C11-C15-C14	-4.82	101.19	106.47
3	I	301	A1KCK	C11-C15-C14	-4.60	101.43	106.47
3	J	301	A1KCK	C11-C15-C14	-4.58	101.44	106.47
3	N	303	A1KCK	C11-C15-C14	-4.54	101.49	106.47
3	F	301	A1KCK	C11-C15-C14	-4.53	101.50	106.47
3	D	301	A1KCK	C11-C15-C14	-4.51	101.52	106.47
3	U	302	A1KCK	C11-C15-C14	-4.48	101.56	106.47
3	L	303	A1KCK	C11-C15-C14	-4.45	101.58	106.47
3	Q	302	A1KCK	C11-C15-C14	-4.45	101.59	106.47
3	P	303	A1KCK	C11-C15-C14	-4.44	101.60	106.47
3	H	301	A1KCK	C11-C15-C14	-4.42	101.62	106.47
3	C	301	A1KCK	C11-C15-C14	-4.38	101.66	106.47
3	K	301	A1KCK	C11-C15-C14	-4.37	101.68	106.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	305	A1KCK	C11-C15-C14	-4.36	101.69	106.47
3	S	302	A1KCK	C11-C15-C14	-4.35	101.70	106.47
3	G	301	A1KCK	C11-C15-C14	-4.30	101.76	106.47
3	V	304	A1KCK	C11-C15-C14	-4.25	101.80	106.47
3	K	304	A1KCK	C11-C15-C14	-4.25	101.81	106.47
3	N	301	A1KCK	C11-C15-C14	-4.20	101.86	106.47
3	R	302	A1KCK	C11-C15-C14	-4.20	101.86	106.47
3	O	302	A1KCK	C11-C15-C14	-4.17	101.89	106.47
3	L	304	A1KCK	C11-C15-C14	-4.15	101.92	106.47
3	P	302	A1KCK	C11-C15-C14	-4.13	101.94	106.47
3	O	303	A1KCK	C11-C15-C14	-4.12	101.95	106.47
3	H	303	A1KCK	C11-C15-C14	-4.11	101.97	106.47
3	L	302	A1KCK	C11-C15-C14	-4.10	101.97	106.47
3	Q	303	A1KCK	C11-C15-C14	-4.09	101.98	106.47
3	M	302	A1KCK	C11-C15-C14	-4.09	101.98	106.47
3	M	303	A1KCK	C11-C15-C14	-4.09	101.99	106.47
3	E	305	A1KCK	C11-C15-C14	-4.06	102.01	106.47
3	T	302	A1KCK	C11-C15-C14	-4.06	102.01	106.47
3	T	303	A1KCK	C11-C15-C14	-4.04	102.03	106.47
3	V	305	A1KCK	C11-C15-C14	-4.01	102.07	106.47
3	R	303	A1KCK	C11-C15-C14	-4.01	102.08	106.47
3	E	302	A1KCK	C11-C15-C14	-3.98	102.10	106.47
3	F	304	A1KCK	C11-C15-C14	-3.98	102.11	106.47
3	S	303	A1KCK	C11-C15-C14	-3.96	102.12	106.47
3	D	303	A1KCK	C11-C15-C14	-3.95	102.14	106.47
3	G	303	A1KCK	C11-C15-C14	-3.95	102.14	106.47
3	I	303	A1KCK	C11-C15-C14	-3.93	102.16	106.47
3	B	303	A1KCK	C11-C15-C14	-3.93	102.16	106.47
3	C	303	A1KCK	C11-C15-C14	-3.82	102.27	106.47
3	A	304	A1KCK	C11-C15-C14	-3.65	102.46	106.47
3	Q	302	A1KCK	C17-C9-C7	-3.37	115.61	120.73
3	C	303	A1KCK	C12-C11-C15	2.96	109.46	105.54
3	Q	302	A1KCK	C10-C9-C7	2.88	125.28	120.15
3	V	305	A1KCK	C12-C11-C15	2.86	109.34	105.54
3	E	305	A1KCK	C12-C11-C15	2.83	109.30	105.54
3	E	302	A1KCK	C12-C11-C15	2.79	109.24	105.54
3	T	302	A1KCK	C12-C11-C15	2.78	109.23	105.54
3	B	303	A1KCK	C12-C11-C15	2.78	109.23	105.54
3	L	302	A1KCK	C12-C11-C15	2.78	109.23	105.54
3	S	303	A1KCK	C12-C11-C15	2.78	109.23	105.54
3	U	302	A1KCK	C2-C4-S8	2.77	126.32	120.06
3	R	302	A1KCK	C12-C11-C15	2.77	109.21	105.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	304	A1KCK	C12-C11-C15	2.74	109.18	105.54
3	F	304	A1KCK	C12-C11-C15	2.74	109.17	105.54
3	T	303	A1KCK	C12-C11-C15	2.73	109.16	105.54
3	I	303	A1KCK	C12-C11-C15	2.72	109.16	105.54
3	M	303	A1KCK	C12-C11-C15	2.71	109.14	105.54
3	N	303	A1KCK	C12-C11-C15	2.71	109.14	105.54
3	S	302	A1KCK	C12-C11-C15	2.71	109.13	105.54
3	A	305	A1KCK	C12-C11-C15	2.70	109.12	105.54
3	P	302	A1KCK	C12-C11-C15	2.70	109.12	105.54
3	G	301	A1KCK	C12-C11-C15	2.69	109.11	105.54
3	R	303	A1KCK	C12-C11-C15	2.68	109.10	105.54
3	O	302	A1KCK	C12-C11-C15	2.67	109.08	105.54
3	H	303	A1KCK	C12-C11-C15	2.65	109.06	105.54
3	Q	303	A1KCK	C12-C11-C15	2.64	109.04	105.54
3	P	303	A1KCK	C12-C11-C15	2.63	109.03	105.54
3	L	304	A1KCK	C12-C11-C15	2.63	109.03	105.54
3	C	301	A1KCK	C12-C11-C15	2.62	109.02	105.54
3	K	301	A1KCK	C12-C11-C15	2.61	109.00	105.54
3	G	303	A1KCK	C12-C11-C15	2.60	108.99	105.54
3	N	301	A1KCK	C12-C11-C15	2.59	108.98	105.54
3	U	302	A1KCK	C12-C11-C15	2.59	108.98	105.54
3	M	302	A1KCK	C12-C11-C15	2.59	108.98	105.54
3	V	304	A1KCK	C17-C9-C7	-2.57	116.83	120.73
3	L	303	A1KCK	C17-C9-C7	-2.57	116.83	120.73
3	F	301	A1KCK	C12-C11-C15	2.56	108.94	105.54
3	D	303	A1KCK	C12-C11-C15	2.55	108.93	105.54
3	H	301	A1KCK	C12-C11-C15	2.54	108.92	105.54
3	K	304	A1KCK	C12-C11-C15	2.54	108.91	105.54
3	C	303	A1KCK	C12-O13-C14	2.51	107.81	105.19
3	D	301	A1KCK	C12-C11-C15	2.49	108.85	105.54
3	U	302	A1KCK	C5-C4-C2	-2.48	124.36	129.75
3	J	301	A1KCK	C12-C11-C15	2.47	108.82	105.54
3	A	304	A1KCK	C12-O13-C14	2.46	107.75	105.19
3	T	303	A1KCK	C2-C4-S8	2.44	125.58	120.06
3	V	305	A1KCK	C12-O13-C14	2.42	107.71	105.19
3	T	303	A1KCK	C12-O13-C14	2.41	107.69	105.19
3	O	303	A1KCK	C12-C11-C15	2.40	108.73	105.54
3	V	304	A1KCK	C12-C11-C15	2.38	108.70	105.54
3	I	303	A1KCK	C12-O13-C14	2.38	107.66	105.19
3	L	304	A1KCK	C12-O13-C14	2.36	107.65	105.19
3	I	301	A1KCK	C12-C11-C15	2.36	108.67	105.54
3	K	302	A1KCK	C12-C11-C15	2.36	108.67	105.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	302	A1KCK	C12-C11-C15	2.35	108.66	105.54
3	E	302	A1KCK	C12-O13-C14	2.34	107.63	105.19
3	G	303	A1KCK	C12-O13-C14	2.32	107.60	105.19
3	F	304	A1KCK	C12-O13-C14	2.31	107.59	105.19
3	L	303	A1KCK	C12-C11-C15	2.29	108.57	105.54
3	B	303	A1KCK	C12-O13-C14	2.28	107.57	105.19
3	T	302	A1KCK	C12-O13-C14	2.28	107.56	105.19
3	S	303	A1KCK	C12-O13-C14	2.27	107.55	105.19
3	R	302	A1KCK	C12-O13-C14	2.27	107.55	105.19
3	L	302	A1KCK	C12-O13-C14	2.25	107.53	105.19
3	A	306	A1KCK	C12-C11-C15	2.24	108.52	105.54
3	Q	302	A1KCK	C2-C4-S8	2.23	125.11	120.06
3	V	304	A1KCK	C10-C9-C7	2.22	124.10	120.15
3	L	303	A1KCK	C10-C9-C7	2.20	124.08	120.15
3	E	305	A1KCK	C12-O13-C14	2.15	107.43	105.19
3	O	303	A1KCK	C12-O13-C14	2.12	107.39	105.19
3	Q	303	A1KCK	C12-O13-C14	2.11	107.39	105.19
3	Q	302	A1KCK	O3-C2-C4	-2.10	115.76	121.16
3	M	303	A1KCK	C12-O13-C14	2.06	107.33	105.19
3	U	302	A1KCK	O3-C2-C4	-2.06	115.86	121.16
3	R	303	A1KCK	C12-O13-C14	2.05	107.33	105.19

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	303	A1KCK	O1-C2-C4-C5
3	C	303	A1KCK	O3-C2-C4-C5
3	C	303	A1KCK	O1-C2-C4-S8
3	C	303	A1KCK	O3-C2-C4-S8
3	N	301	A1KCK	O3-C2-C4-C5
3	N	303	A1KCK	O1-C2-C4-C5
3	N	303	A1KCK	O3-C2-C4-C5
3	N	303	A1KCK	O1-C2-C4-S8
3	N	303	A1KCK	O3-C2-C4-S8
3	P	303	A1KCK	O1-C2-C4-C5
3	P	303	A1KCK	O3-C2-C4-C5
3	P	303	A1KCK	O1-C2-C4-S8
3	P	303	A1KCK	O3-C2-C4-S8
3	V	305	A1KCK	O1-C2-C4-S8
3	N	301	A1KCK	O1-C2-C4-C5
2	A	302	EDO	O1-C1-C2-O2

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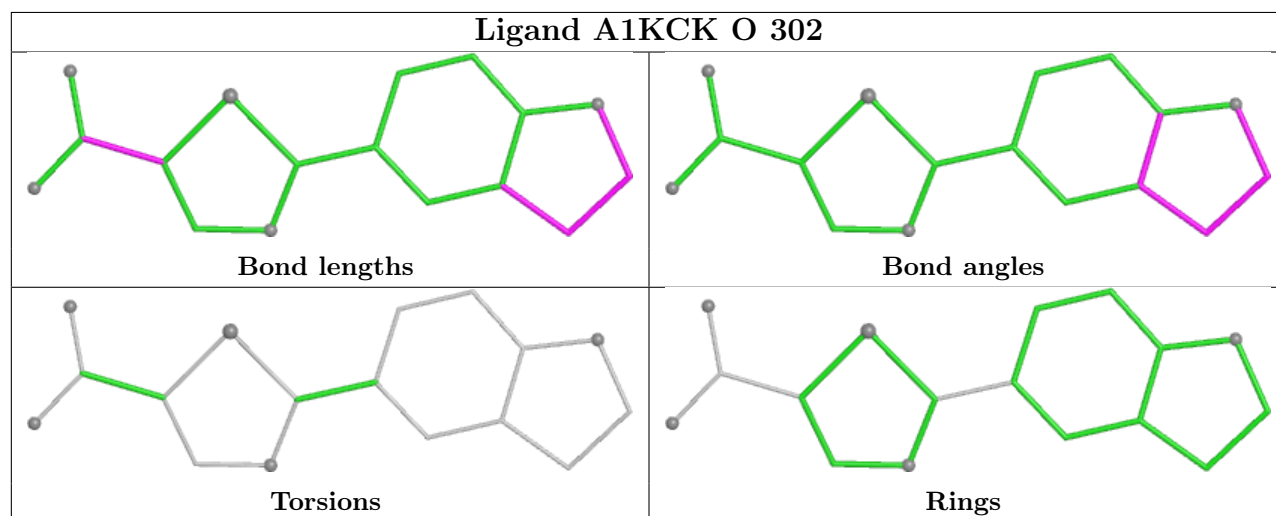
Mol	Chain	Res	Type	Atoms
2	B	302	EDO	O1-C1-C2-O2
2	E	304	EDO	O1-C1-C2-O2
2	H	302	EDO	O1-C1-C2-O2
2	K	303	EDO	O1-C1-C2-O2
2	O	301	EDO	O1-C1-C2-O2
2	P	301	EDO	O1-C1-C2-O2
2	Q	301	EDO	O1-C1-C2-O2
2	S	301	EDO	O1-C1-C2-O2
2	T	301	EDO	O1-C1-C2-O2
2	C	302	EDO	O1-C1-C2-O2
2	R	301	EDO	O1-C1-C2-O2
3	N	301	A1KCK	O3-C2-C4-S8
3	V	305	A1KCK	O3-C2-C4-S8
3	A	306	A1KCK	O3-C2-C4-C5
3	J	301	A1KCK	O1-C2-C4-C5
3	J	301	A1KCK	O3-C2-C4-C5
3	V	305	A1KCK	O1-C2-C4-C5
2	D	302	EDO	O1-C1-C2-O2
2	F	303	EDO	O1-C1-C2-O2
3	J	301	A1KCK	O3-C2-C4-S8
3	K	301	A1KCK	O1-C2-C4-S8
3	K	301	A1KCK	O3-C2-C4-S8
3	K	304	A1KCK	O1-C2-C4-S8
3	K	301	A1KCK	O1-C2-C4-C5
3	K	301	A1KCK	O3-C2-C4-C5
3	V	305	A1KCK	O3-C2-C4-C5
2	J	302	EDO	O1-C1-C2-O2
2	A	301	EDO	O1-C1-C2-O2
2	V	303	EDO	O1-C1-C2-O2
3	L	302	A1KCK	S8-C7-C9-C17
3	S	303	A1KCK	O1-C2-C4-S8
3	A	306	A1KCK	O1-C2-C4-C5
3	K	304	A1KCK	O1-C2-C4-C5
2	M	301	EDO	O1-C1-C2-O2
3	L	302	A1KCK	N6-C7-C9-C17
3	J	301	A1KCK	O1-C2-C4-S8
3	K	304	A1KCK	O3-C2-C4-S8

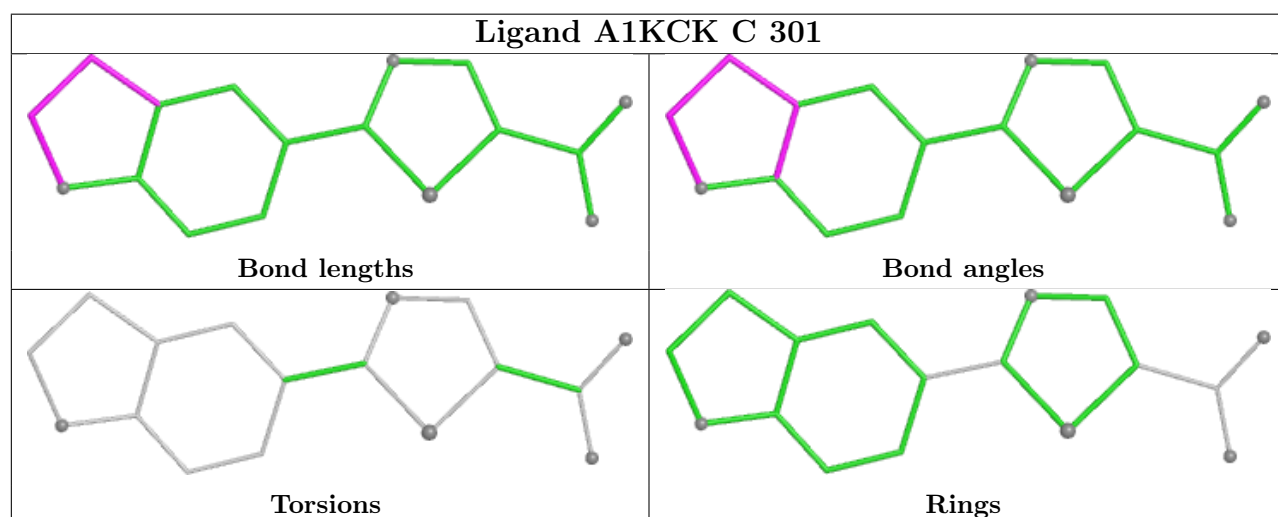
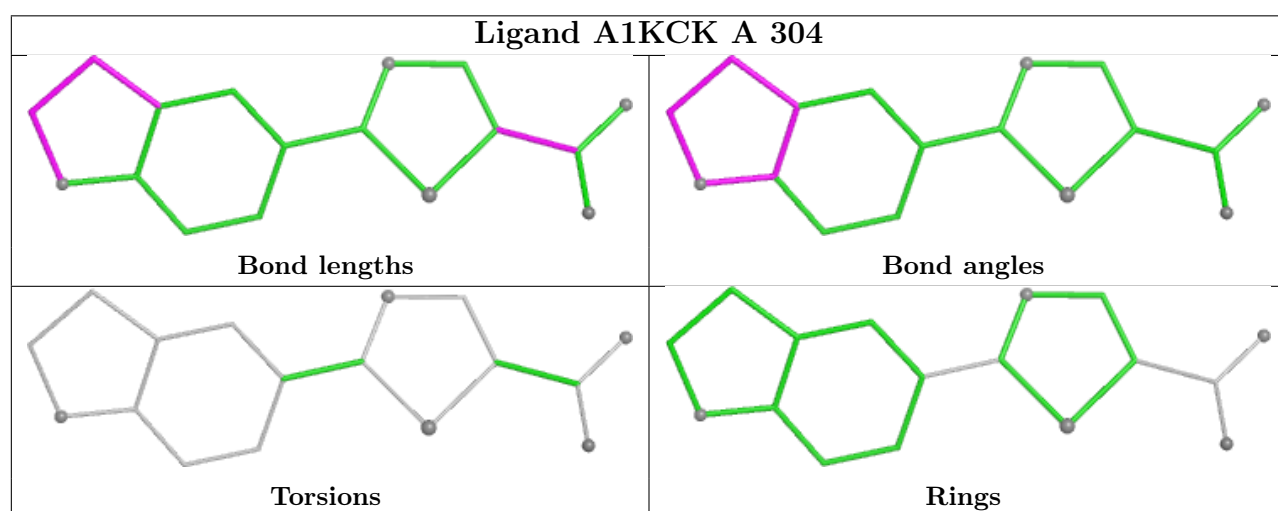
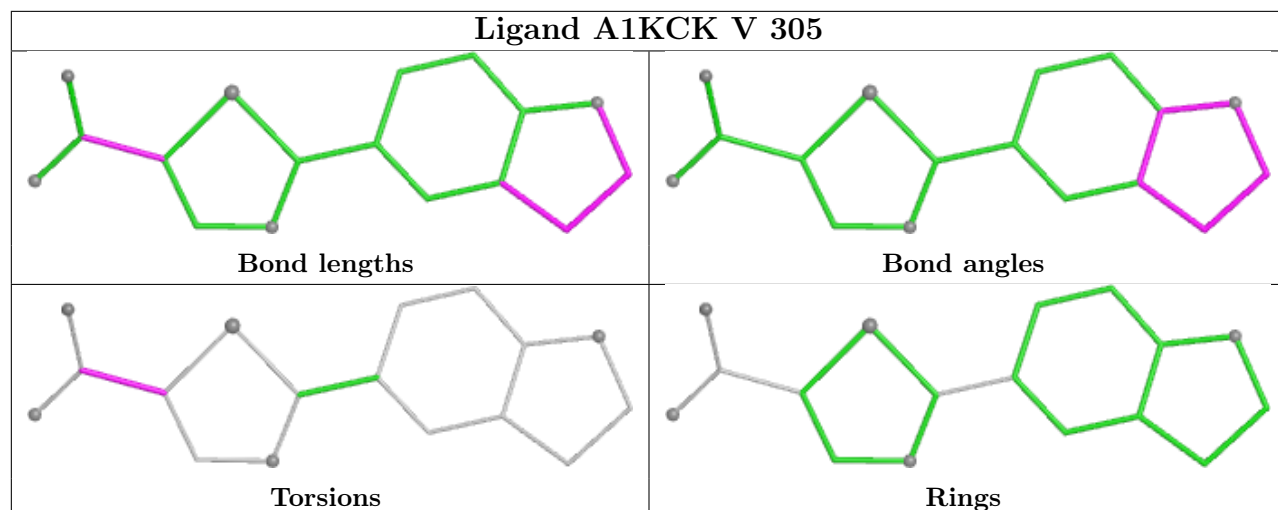
There are no ring outliers.

10 monomers are involved in 12 short contacts:

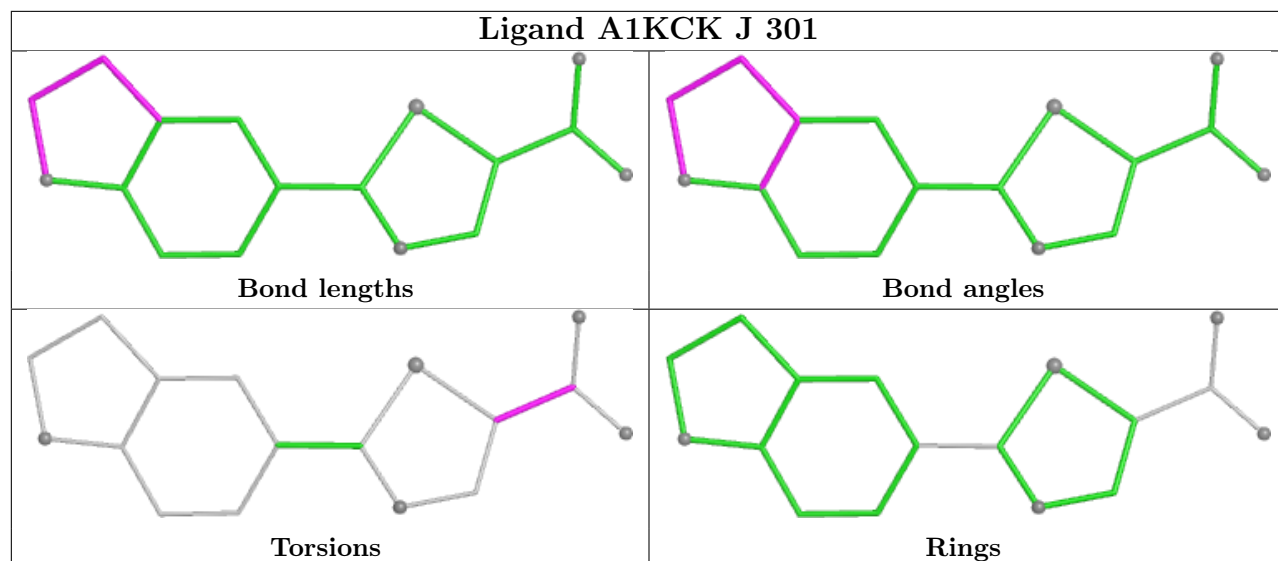
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	304	A1KCK	1	0
3	J	301	A1KCK	1	0
3	N	303	A1KCK	3	0
2	I	302	EDO	1	0
2	A	302	EDO	1	0
3	P	303	A1KCK	1	0
2	B	301	EDO	1	0
2	E	303	EDO	1	0
2	V	303	EDO	1	0
2	R	301	EDO	1	0

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.

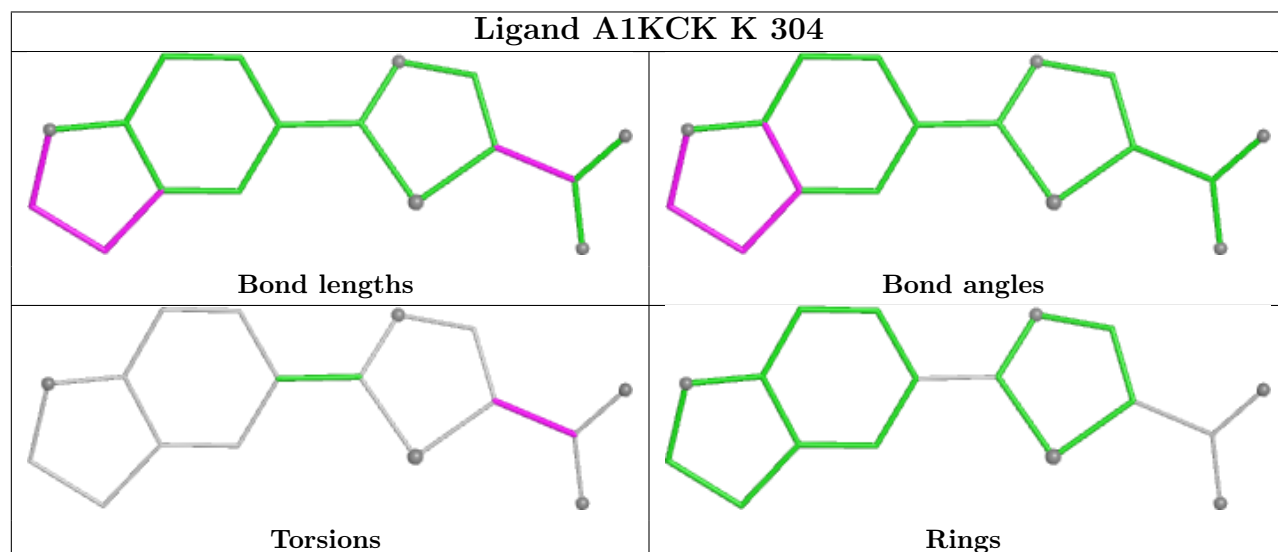




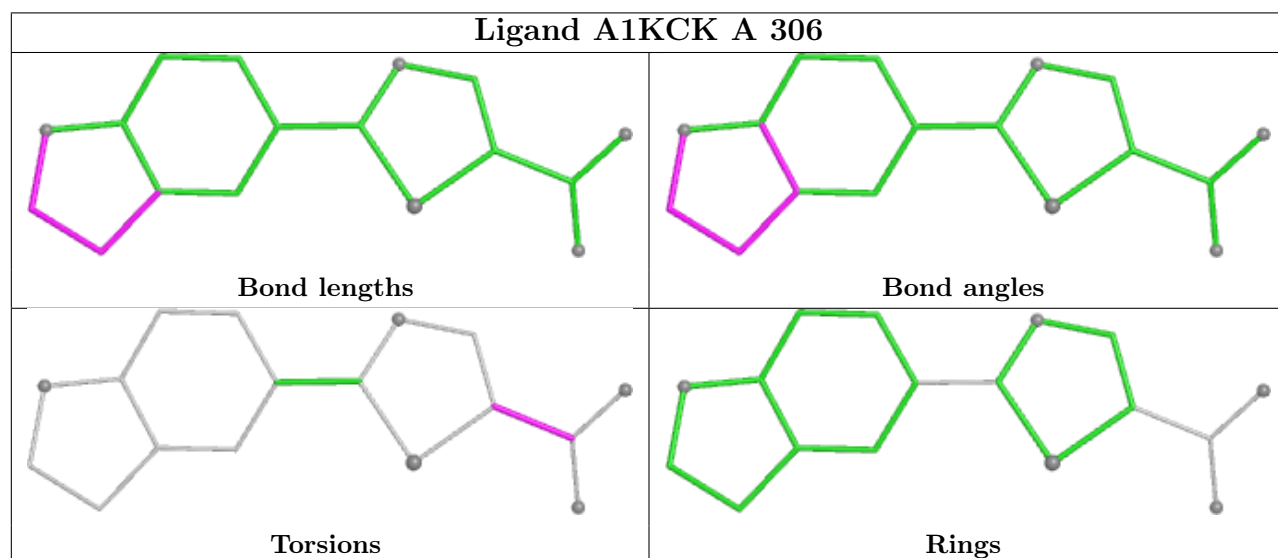
Ligand A1KCK J 301

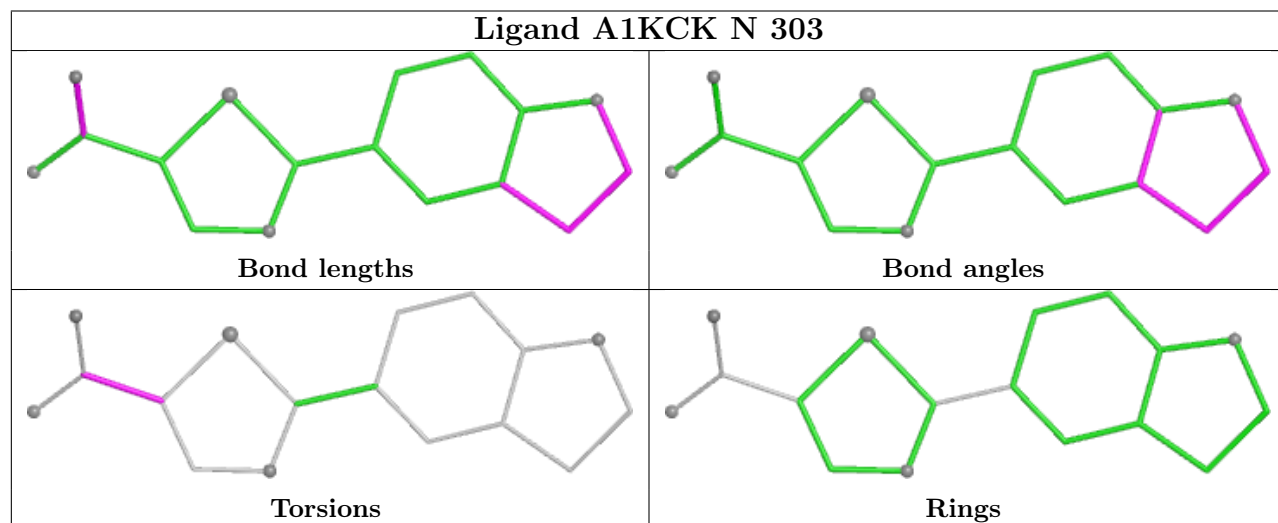
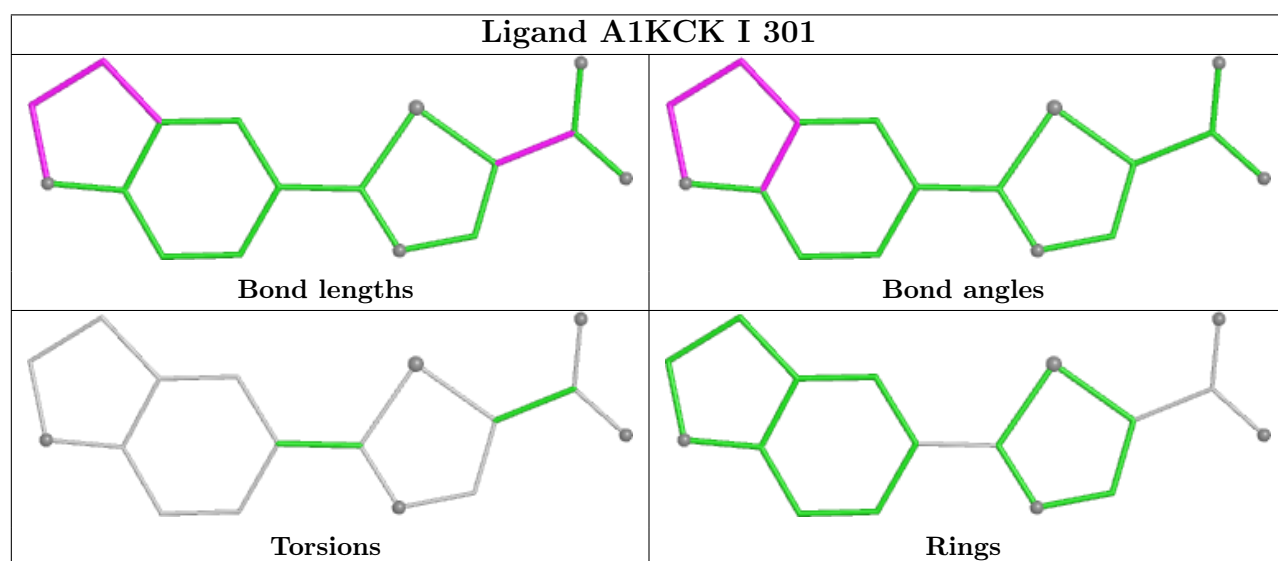
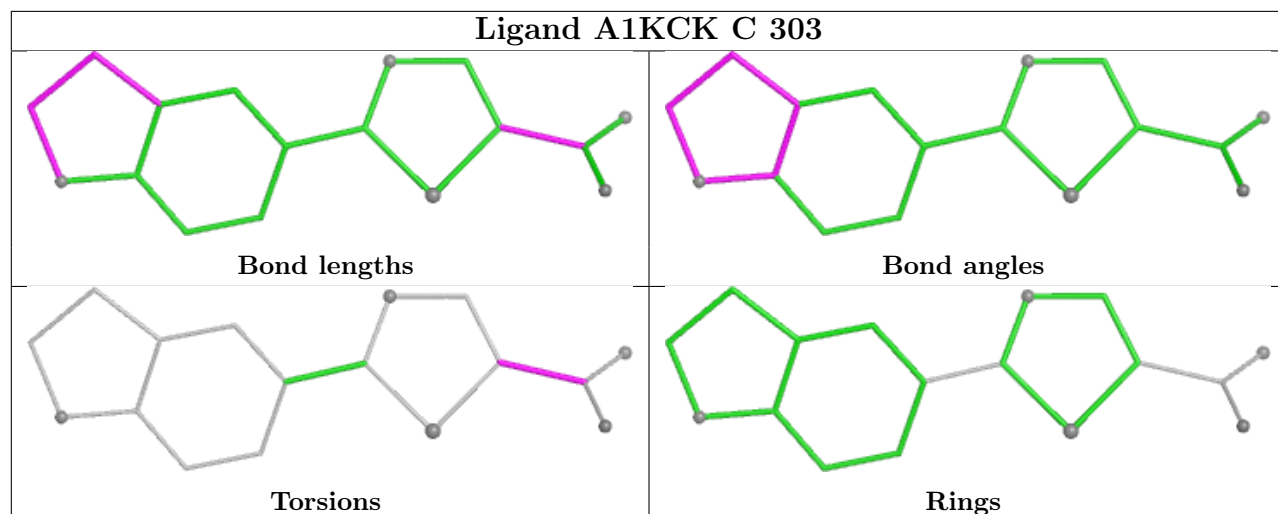


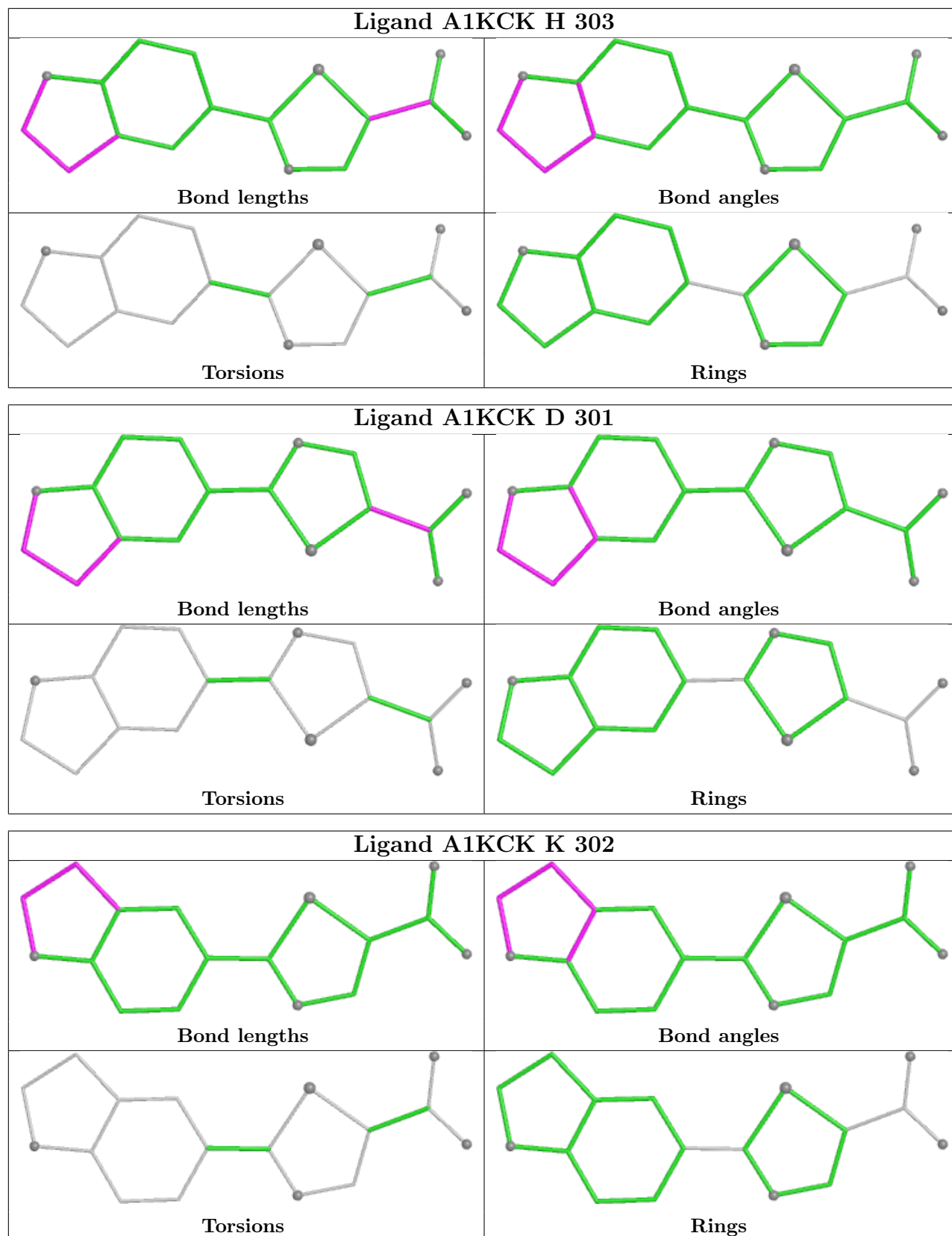
Ligand A1KCK K 304



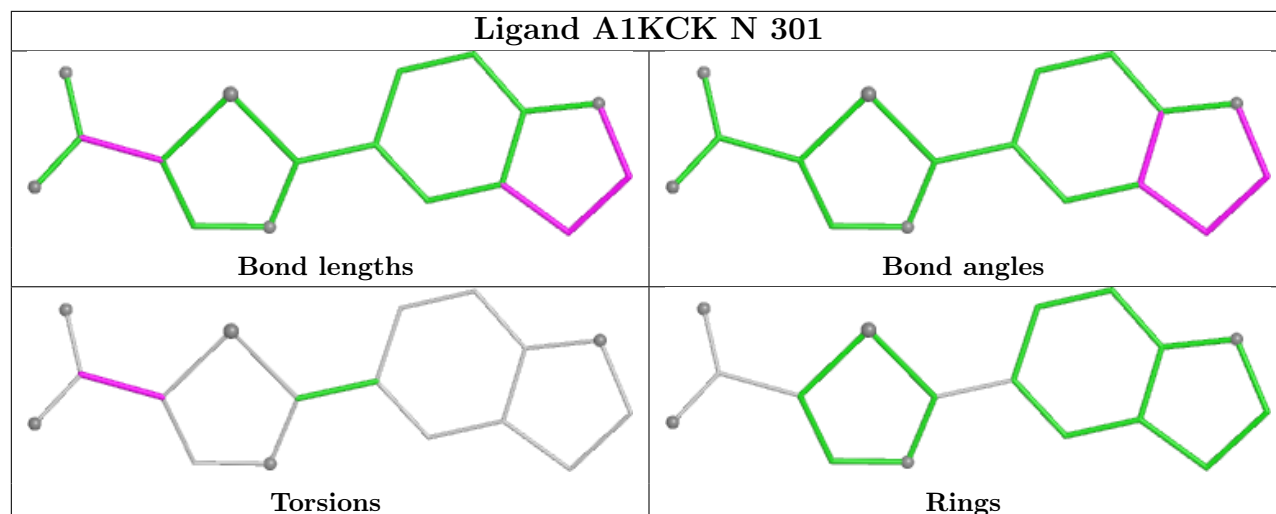
Ligand A1KCK A 306



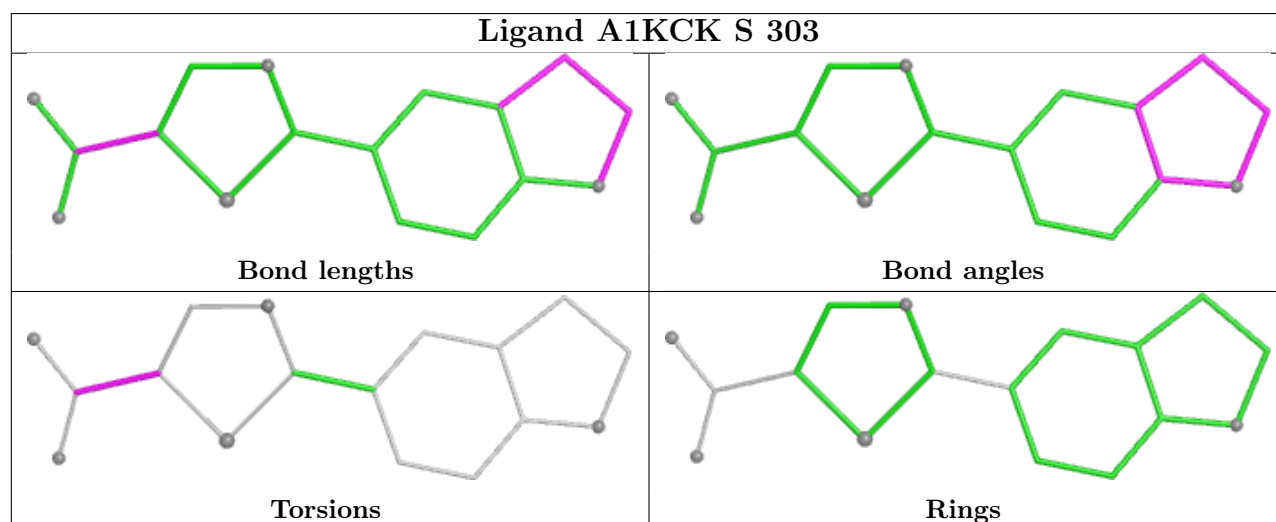




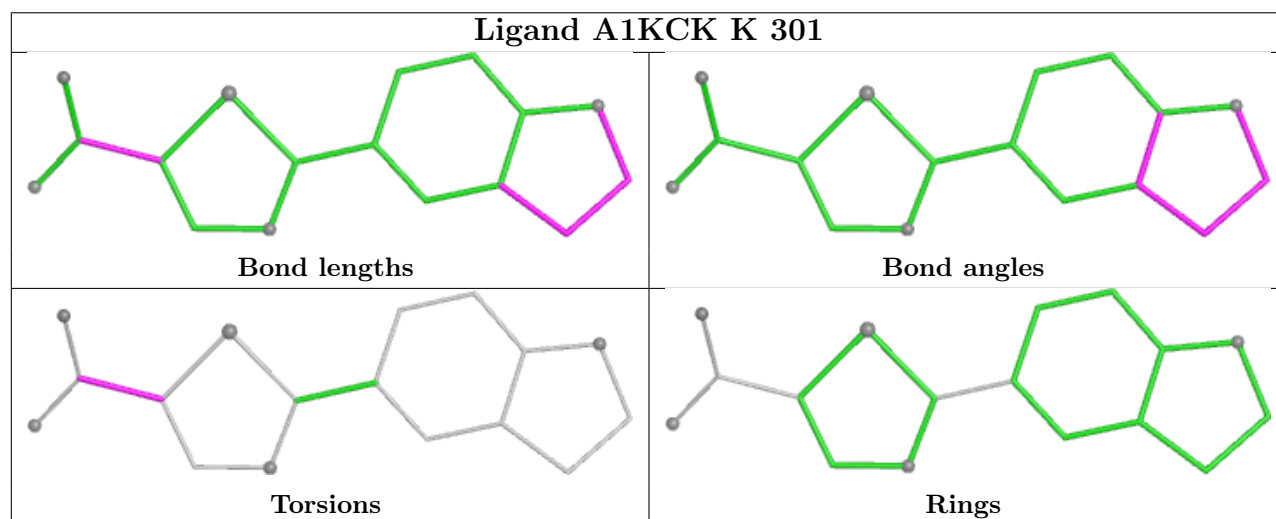
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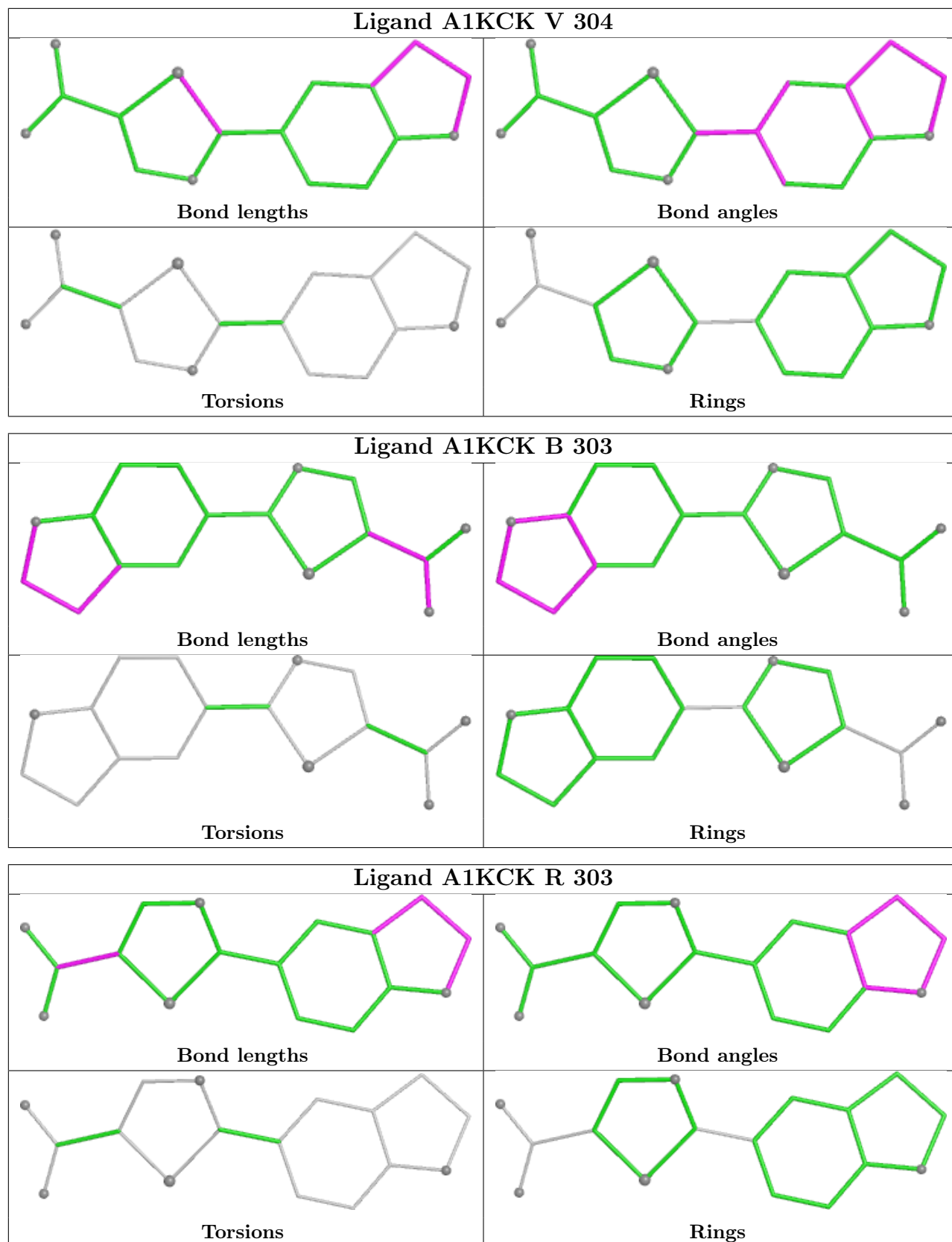


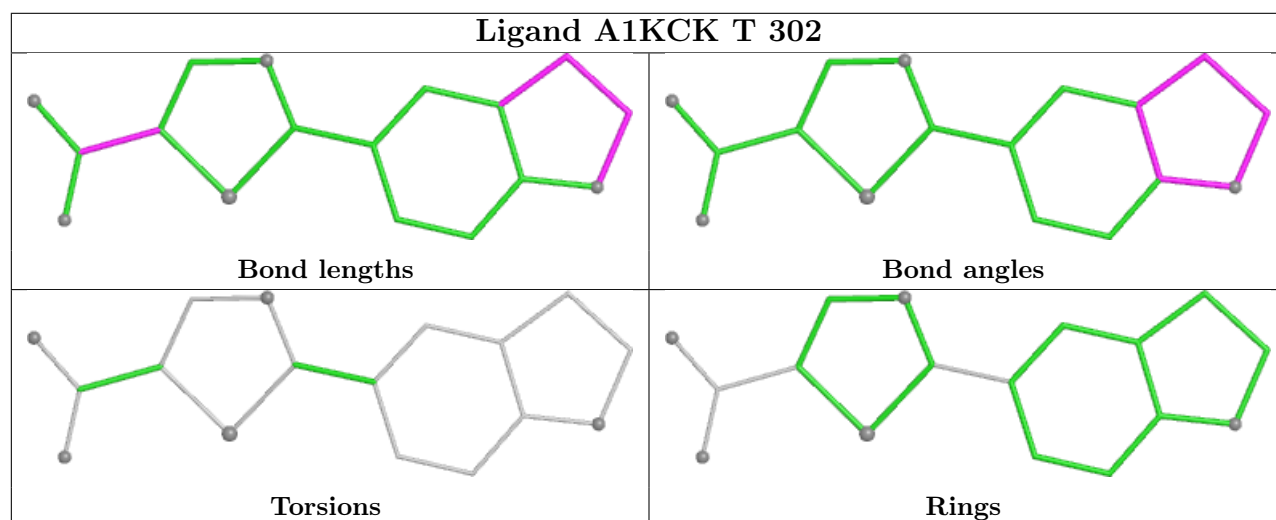
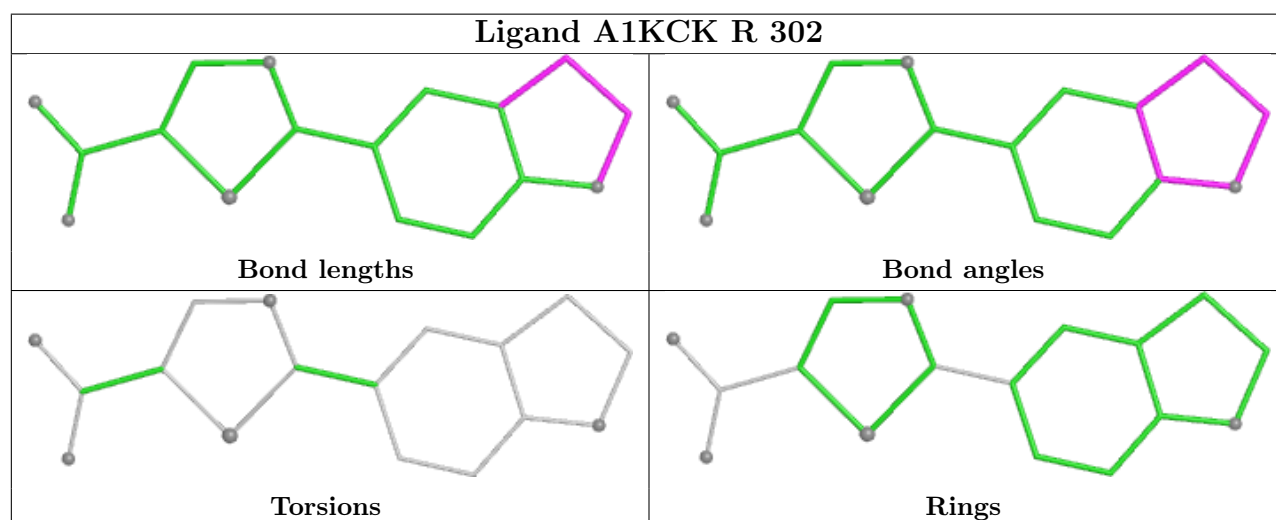
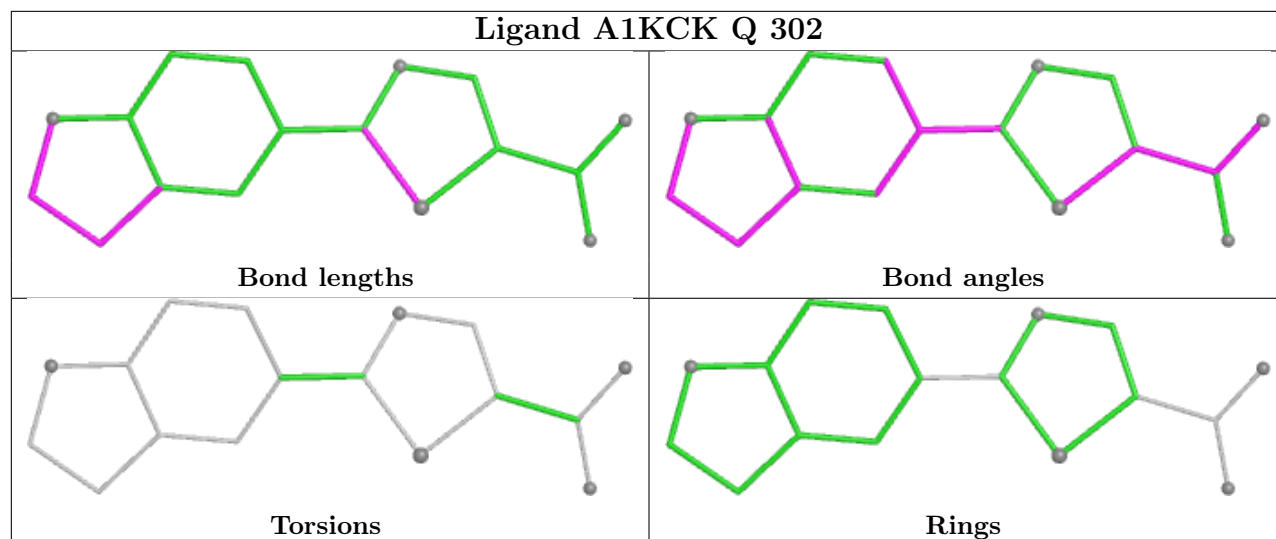
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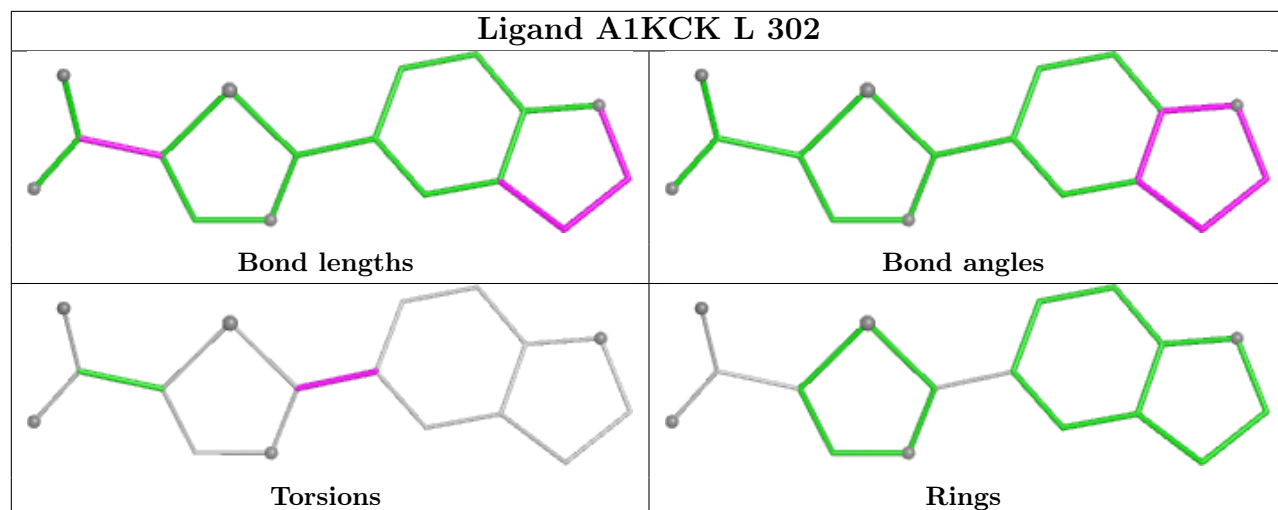
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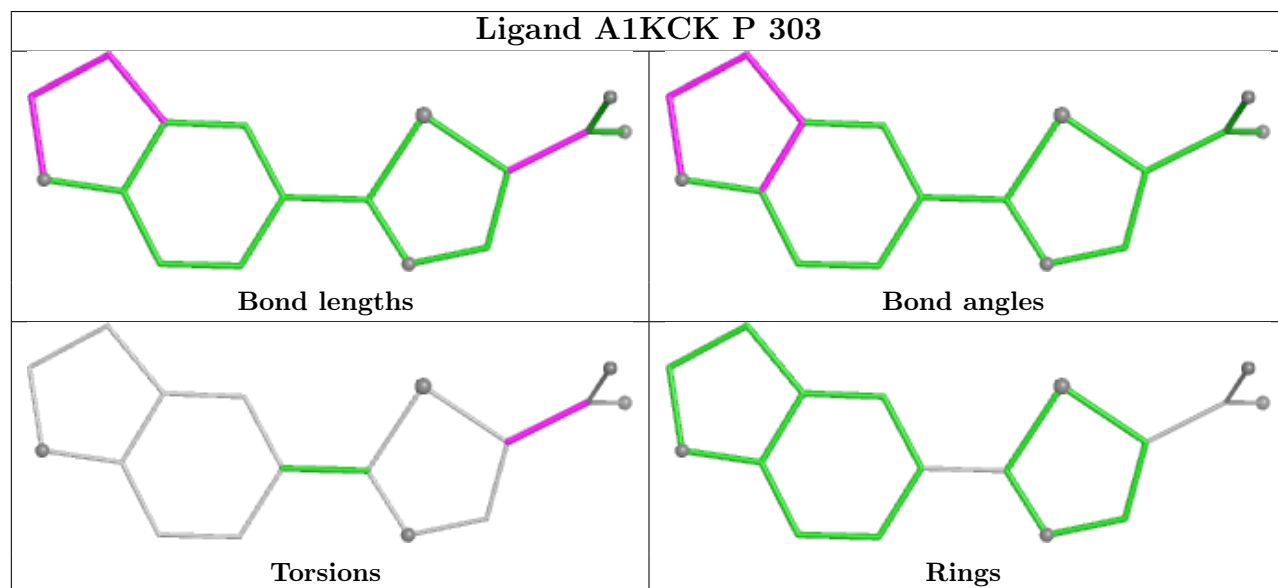




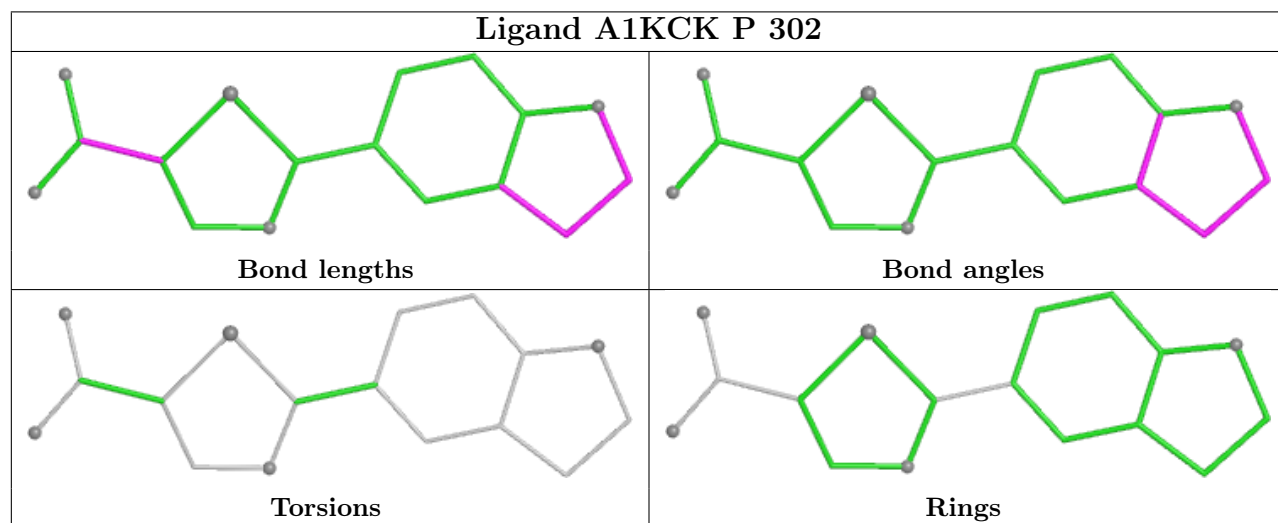
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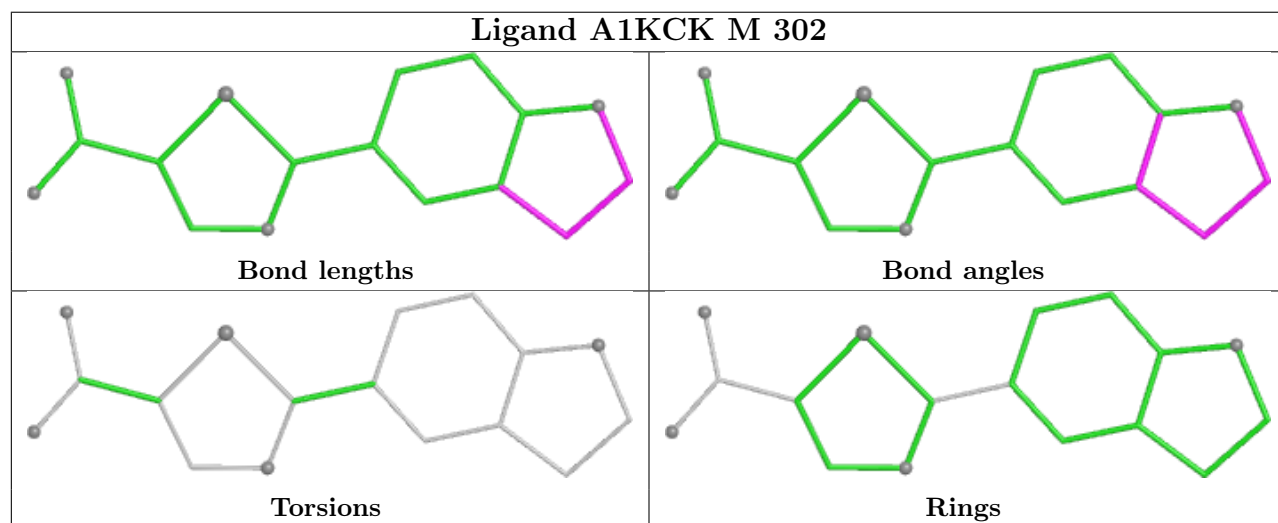
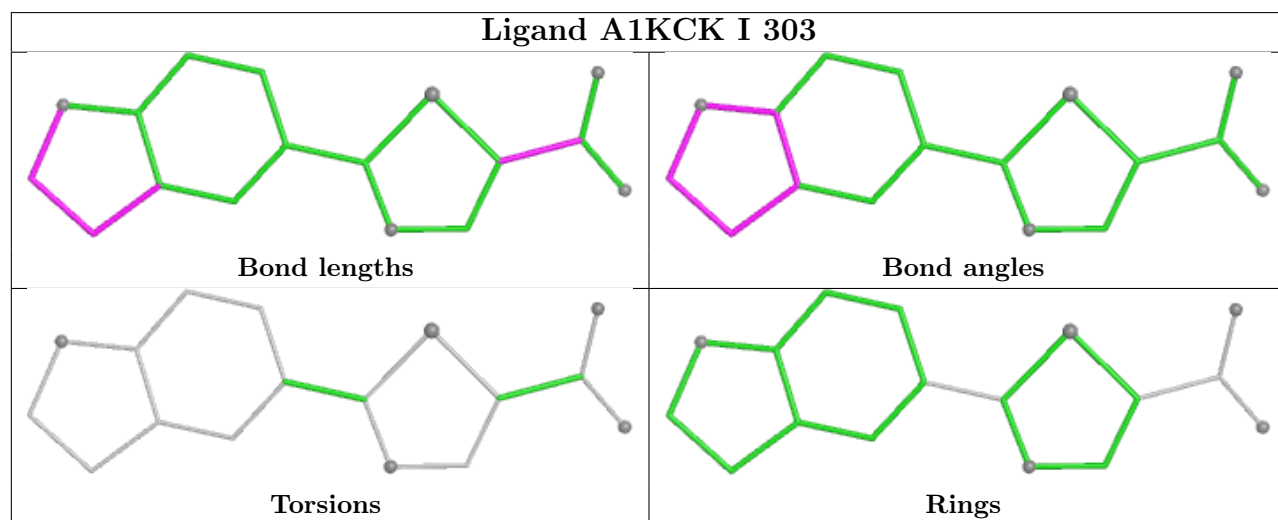
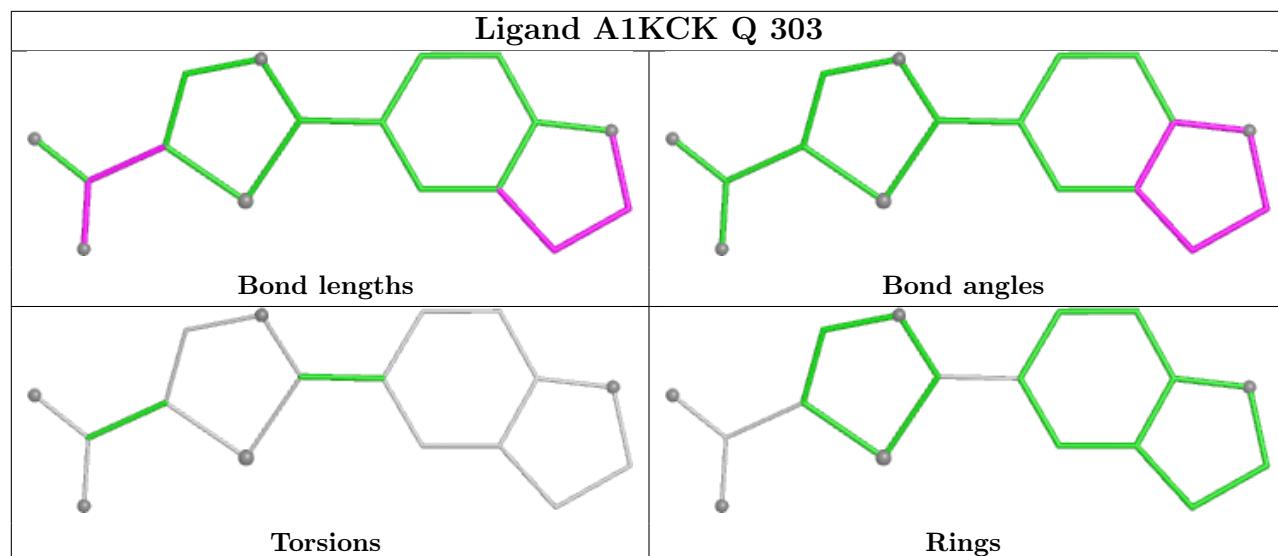


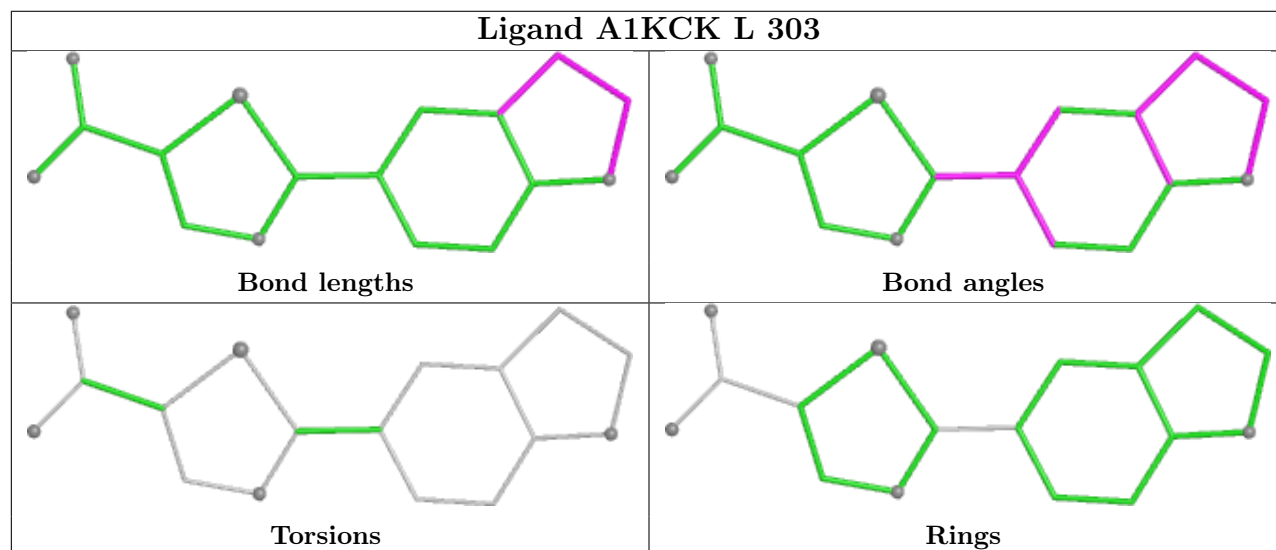
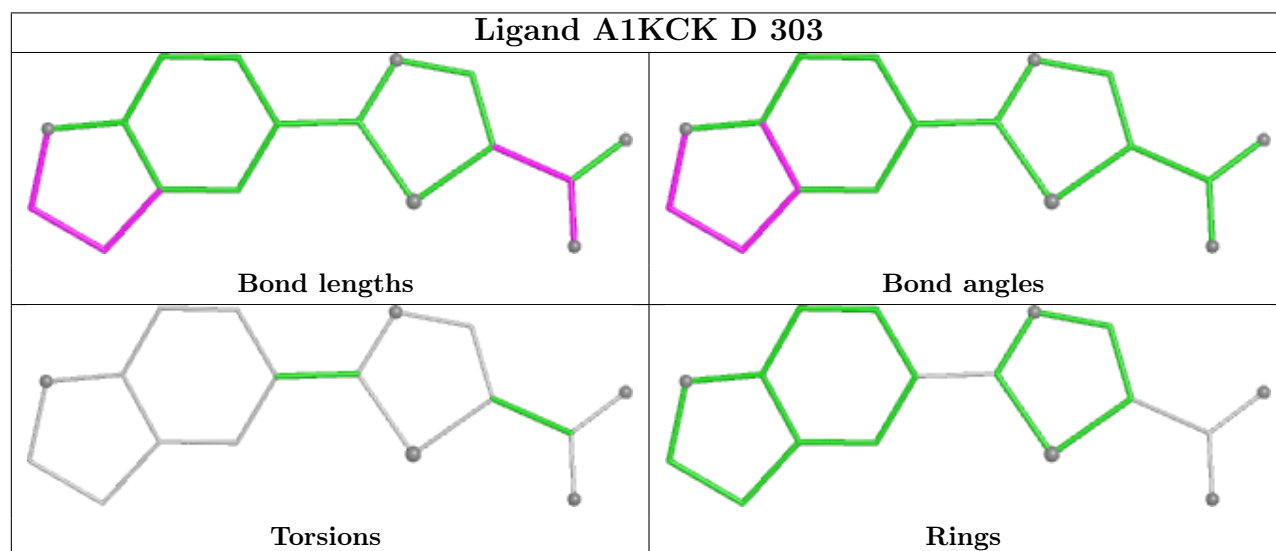
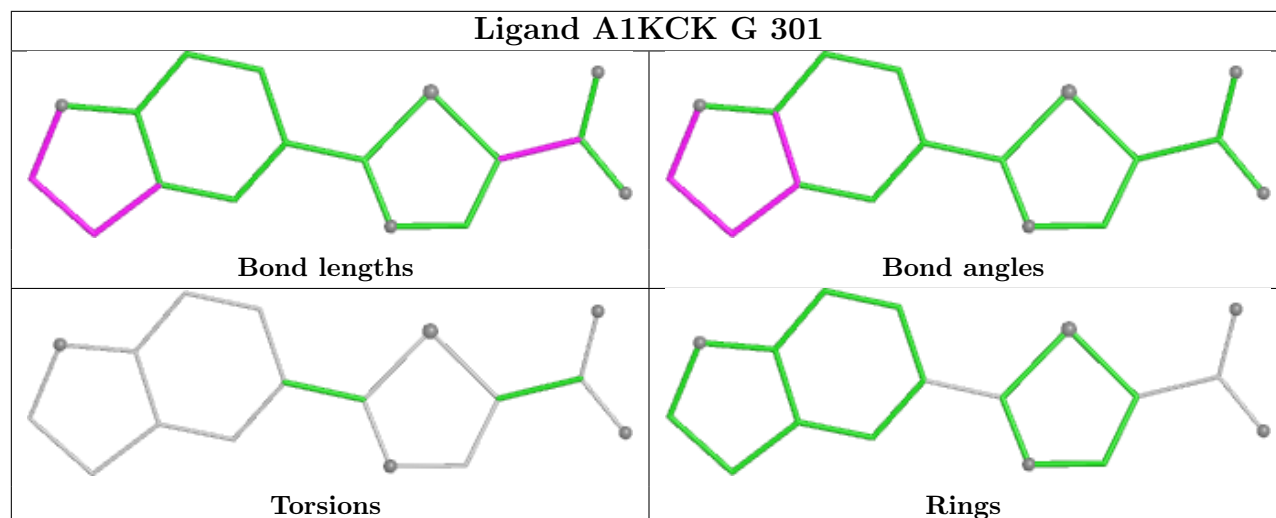
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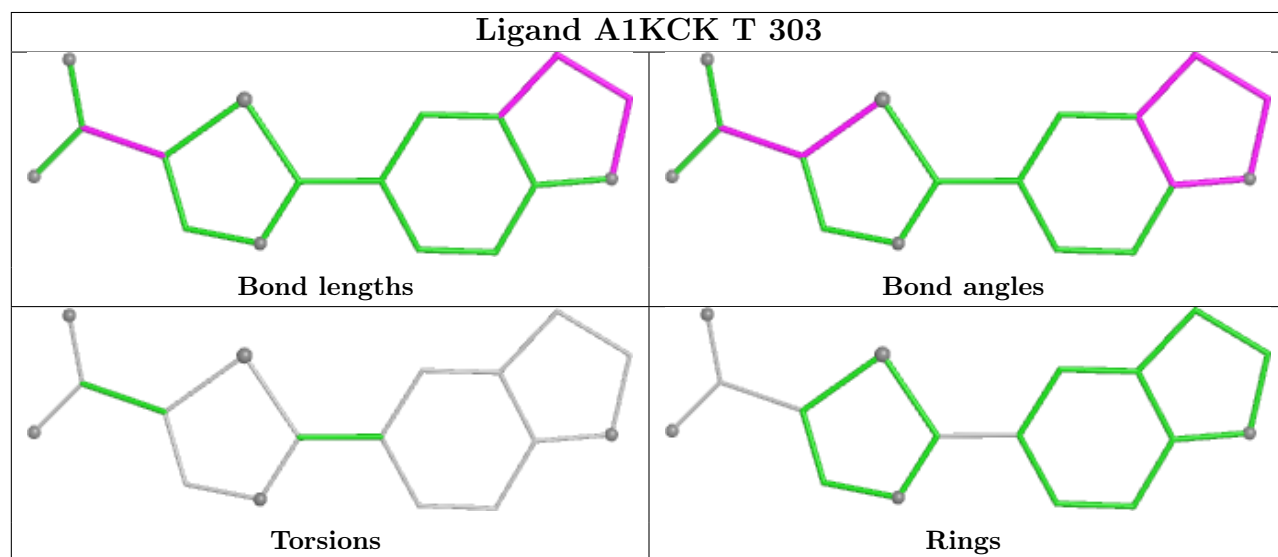
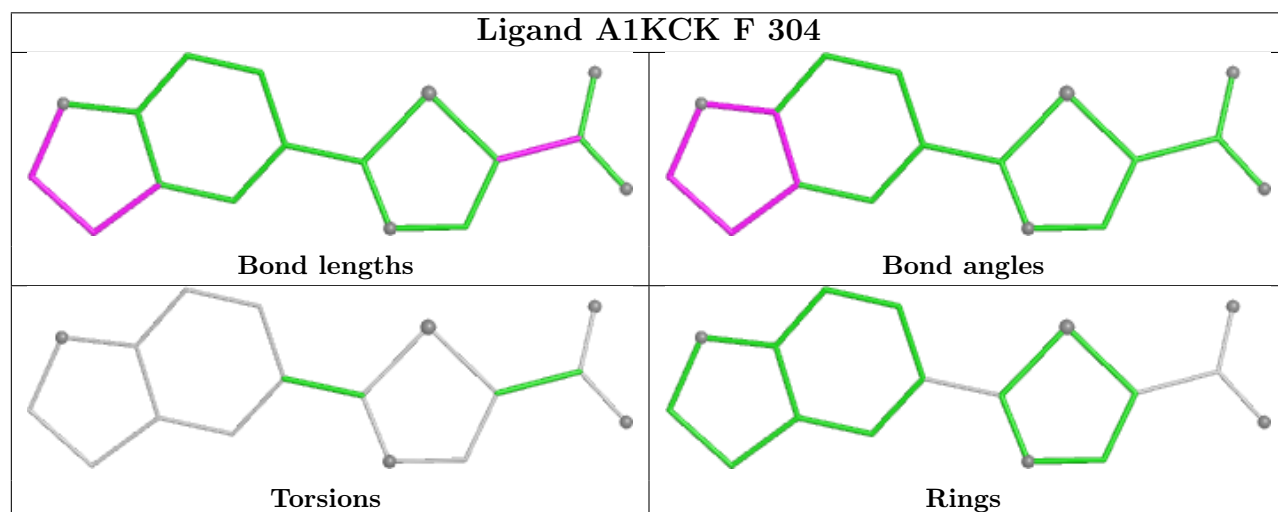
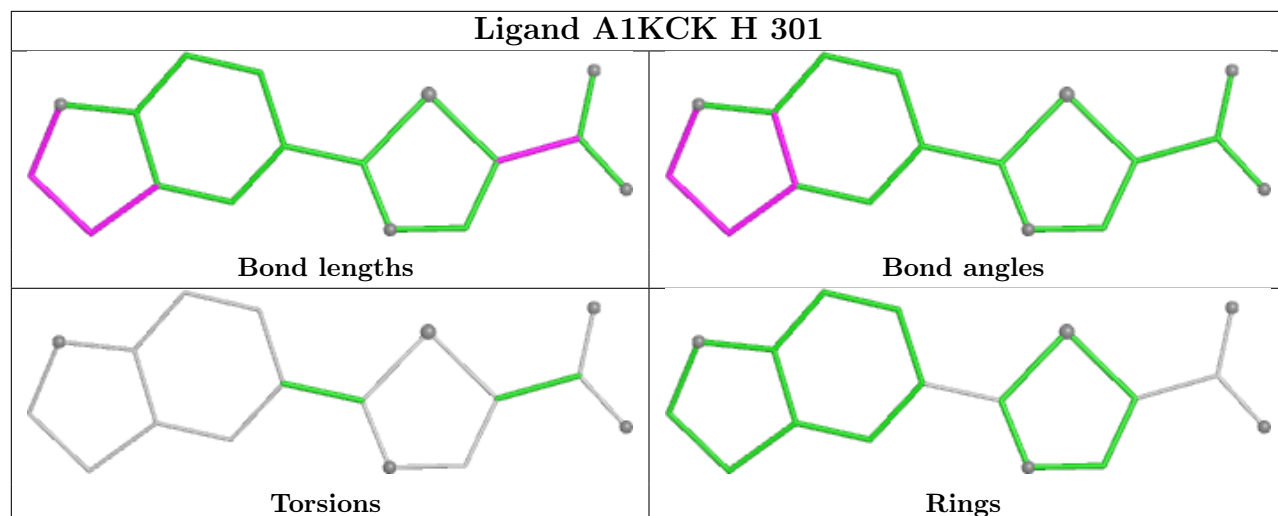


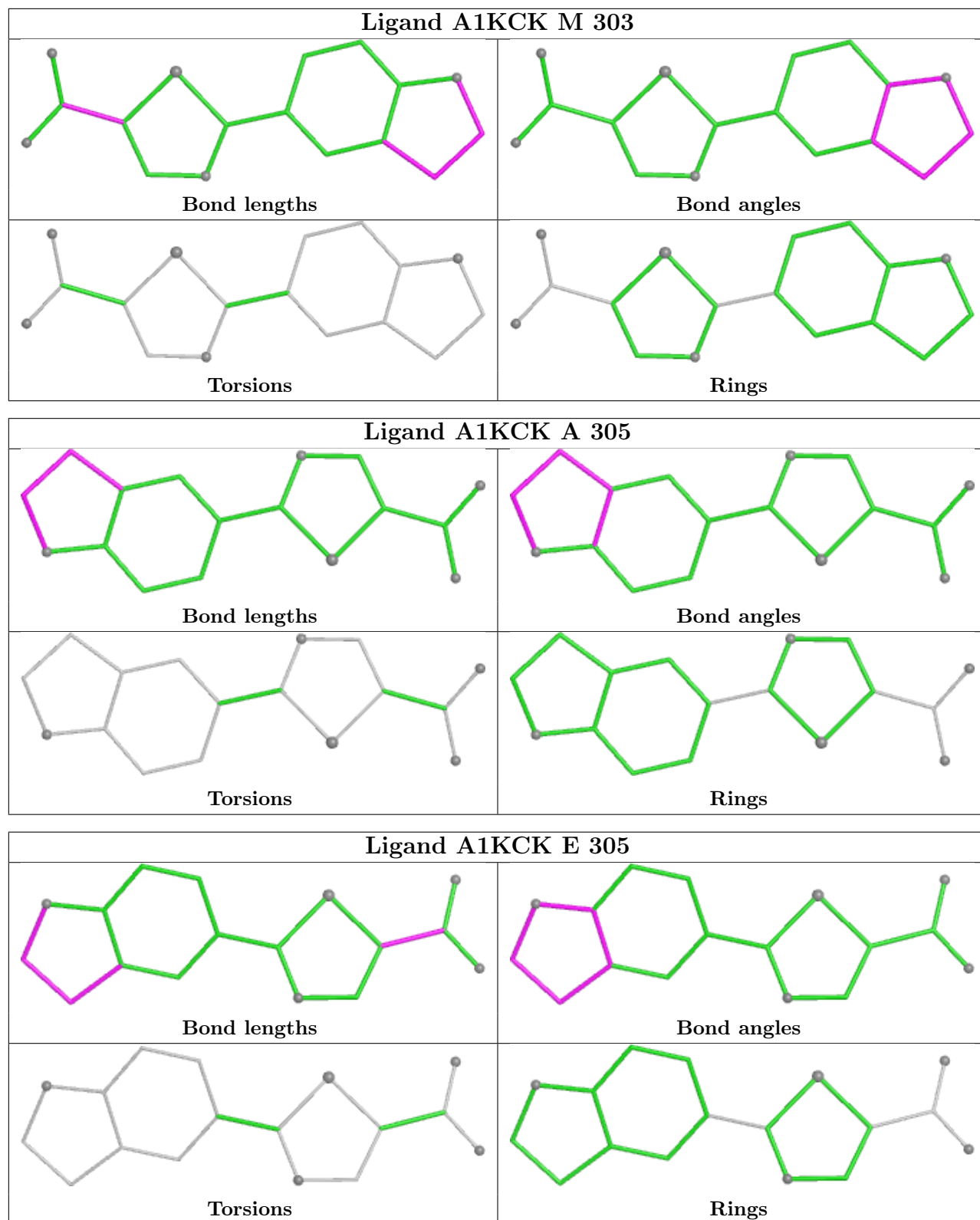
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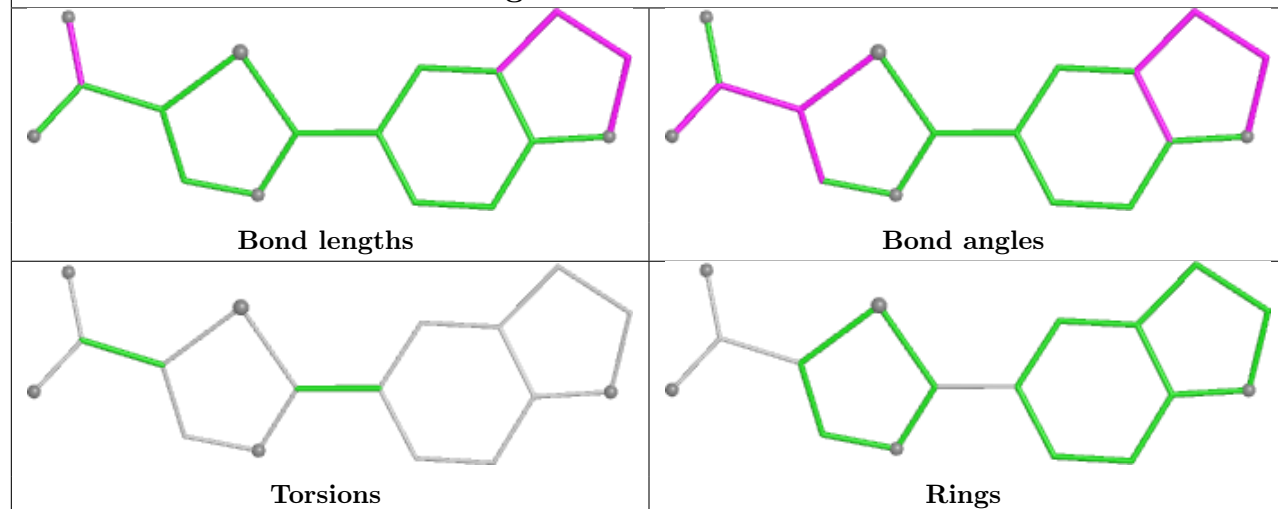




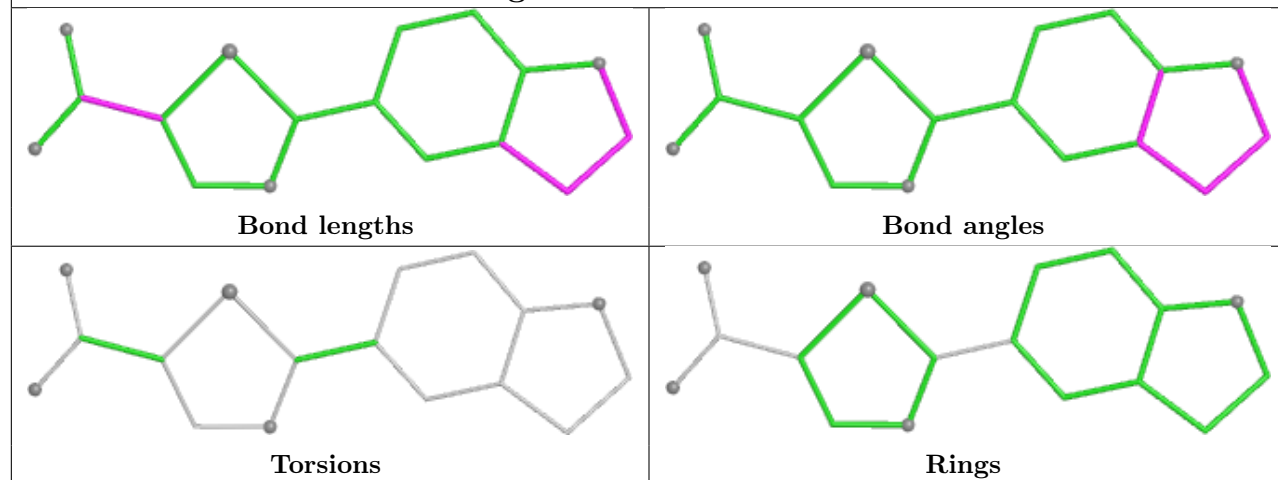




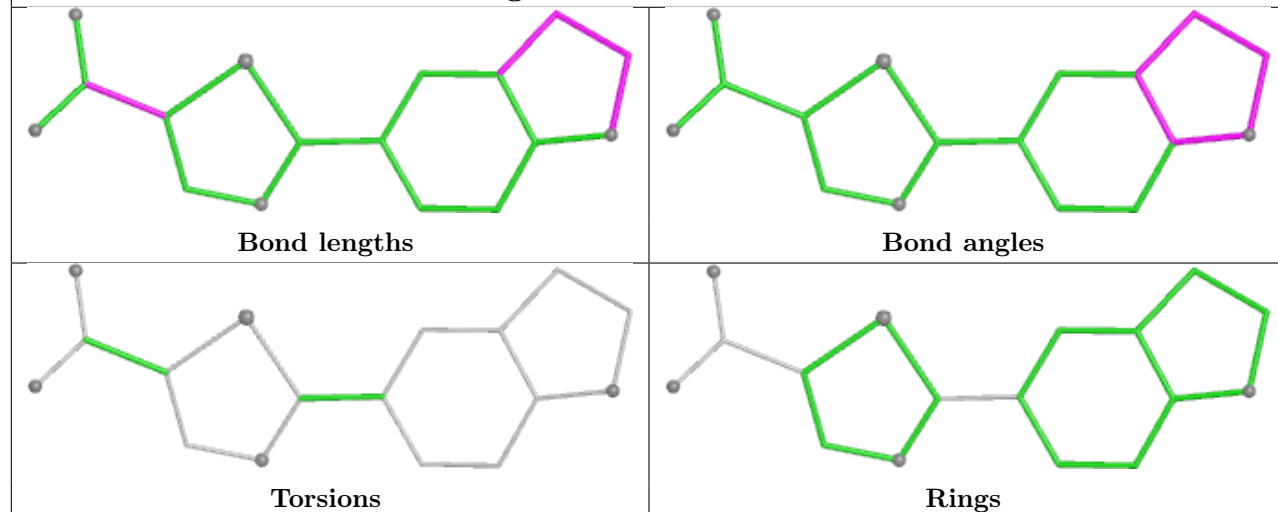
Ligand A1KCK U 302



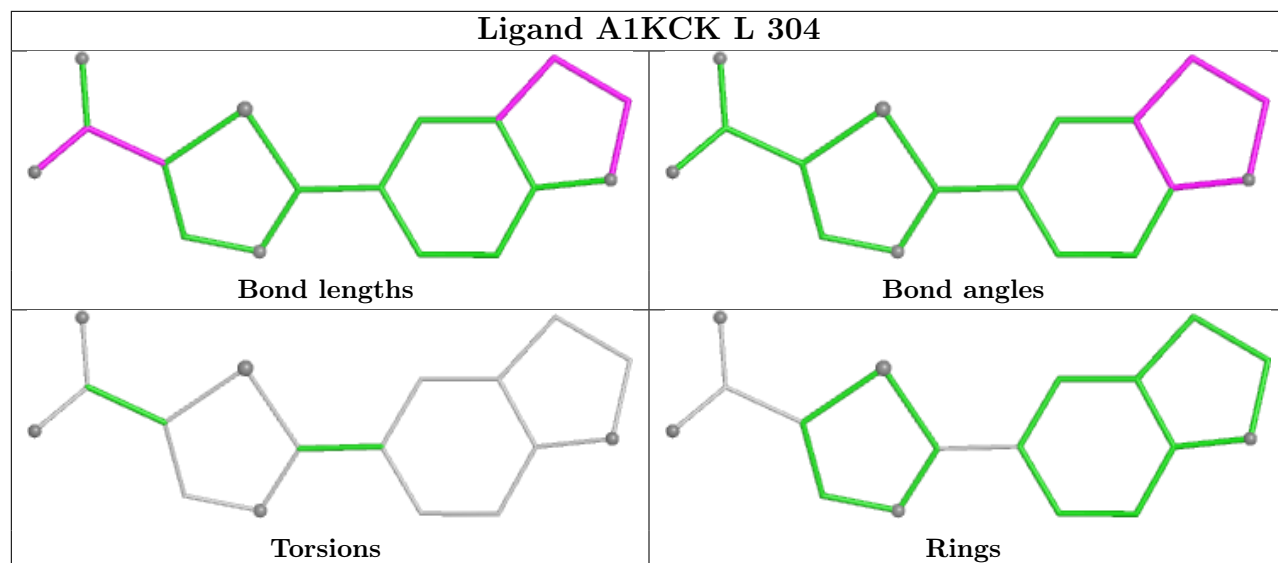
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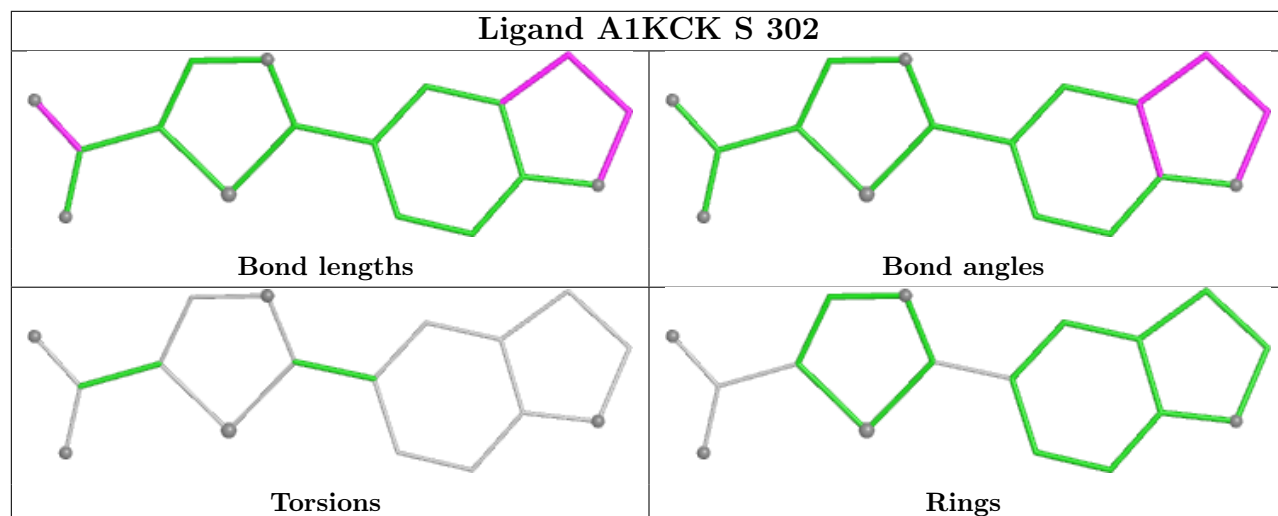
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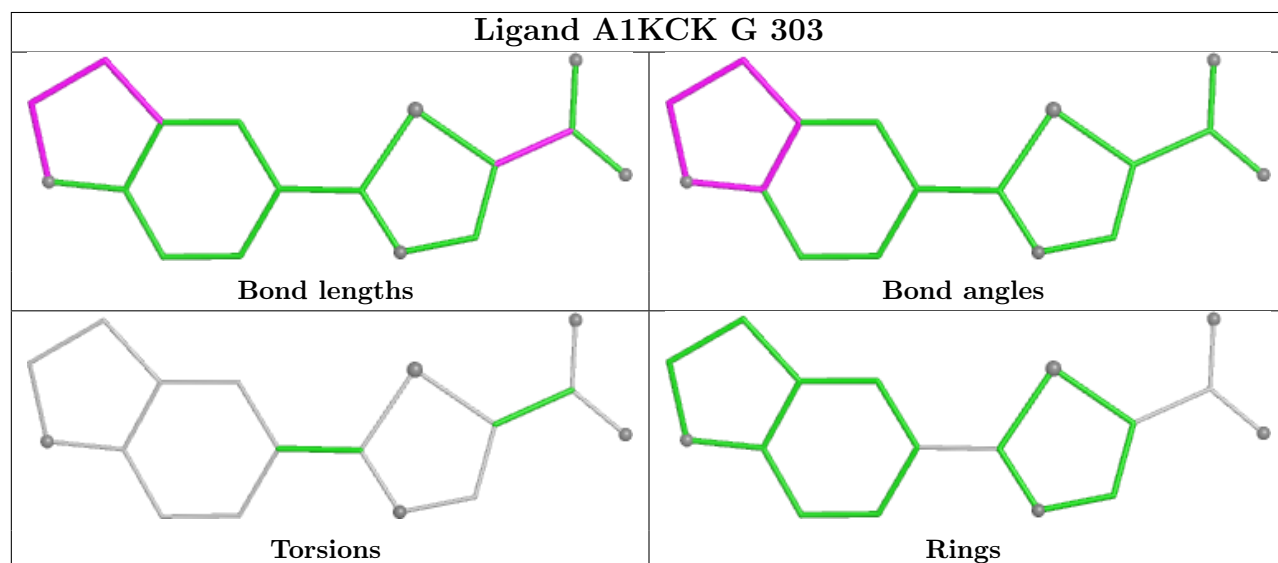
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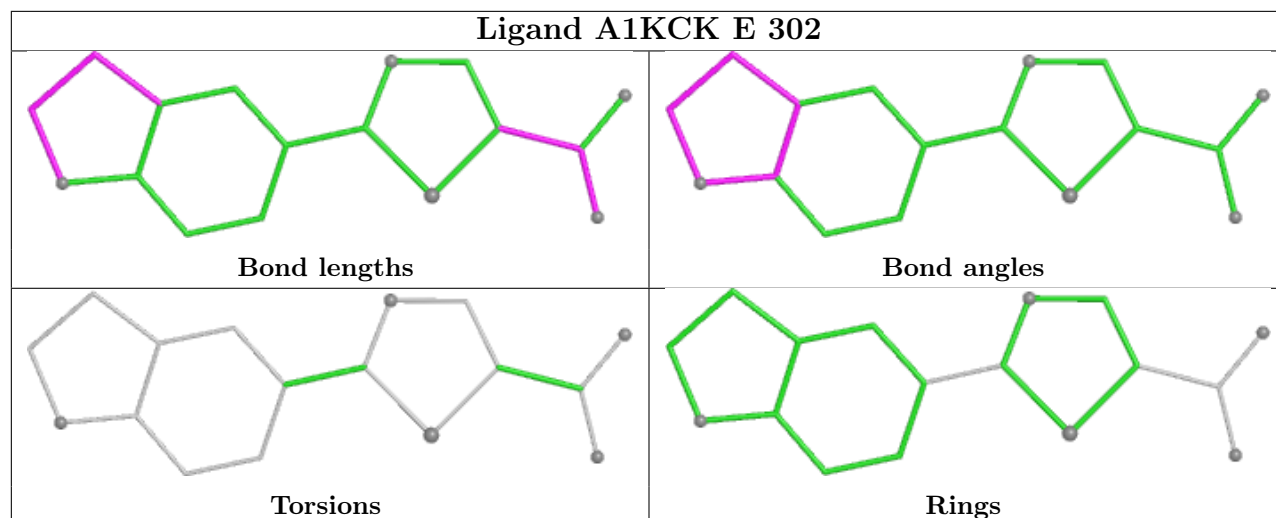


Ligand A1KCK S 302



Ligand A1KCK G 303





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	186/215 (86%)	0.19	13 (6%) 22 24	25, 41, 98, 118	0
1	B	188/215 (87%)	0.07	14 (7%) 20 22	16, 35, 78, 88	1 (0%)
1	C	189/215 (87%)	0.03	13 (6%) 23 24	24, 35, 78, 103	0
1	D	188/215 (87%)	0.05	9 (4%) 35 38	23, 34, 85, 118	0
1	E	189/215 (87%)	0.05	6 (3%) 50 53	24, 34, 79, 98	0
1	F	187/215 (86%)	0.09	7 (3%) 45 47	24, 37, 75, 90	0
1	G	188/215 (87%)	0.28	11 (5%) 28 30	24, 42, 95, 115	0
1	H	189/215 (87%)	0.39	17 (8%) 15 16	27, 46, 86, 117	0
1	I	187/215 (86%)	0.59	18 (9%) 13 14	33, 55, 118, 143	0
1	J	188/215 (87%)	0.75	29 (15%) 5 5	23, 59, 127, 158	1 (0%)
1	K	187/215 (86%)	0.71	26 (13%) 6 6	19, 56, 123, 151	2 (1%)
1	L	187/215 (86%)	0.01	8 (4%) 40 41	16, 34, 84, 102	1 (0%)
1	M	189/215 (87%)	0.10	8 (4%) 40 42	24, 37, 74, 102	0
1	N	187/215 (86%)	0.17	8 (4%) 40 41	24, 39, 92, 108	1 (0%)
1	O	187/215 (86%)	0.14	11 (5%) 28 30	20, 37, 90, 116	1 (0%)
1	P	187/215 (86%)	0.04	10 (5%) 32 34	14, 34, 82, 103	1 (0%)
1	Q	187/215 (86%)	0.05	11 (5%) 28 30	14, 35, 88, 109	2 (1%)
1	R	188/215 (87%)	0.06	5 (2%) 56 59	16, 37, 67, 105	1 (0%)
1	S	188/215 (87%)	0.17	10 (5%) 32 34	25, 39, 85, 112	0
1	T	187/215 (86%)	0.21	12 (6%) 25 27	16, 39, 91, 116	2 (1%)
1	U	187/215 (86%)	0.11	8 (4%) 40 41	25, 36, 83, 108	0
1	V	187/215 (86%)	0.07	7 (3%) 45 47	24, 35, 74, 101	0
All	All	4127/4730 (87%)	0.20	261 (6%) 26 27	14, 40, 90, 158	13 (0%)

All (261) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	24	LEU	5.5
1	G	24	LEU	5.5
1	L	184	LEU	5.4
1	H	24	LEU	5.2
1	J	24	LEU	5.1
1	L	210	PRO	5.0
1	G	210	PRO	4.6
1	I	24	LEU	4.5
1	K	179	PRO	4.5
1	R	24	LEU	4.4
1	K	178	LEU	4.4
1	I	210	PRO	4.3
1	M	184	LEU	4.3
1	T	184	LEU	4.3
1	N	182	LEU	4.3
1	C	24	LEU	4.2
1	Q	184	LEU	4.2
1	H	210	PRO	4.2
1	S	210	PRO	4.2
1	H	184	LEU	4.2
1	I	183	PRO	4.2
1	S	184	LEU	4.1
1	V	184	LEU	4.1
1	N	24	LEU	4.1
1	Q	182	LEU	4.1
1	S	24	LEU	4.1
1	K	177	LYS	4.1
1	Q	25	CYS	4.0
1	A	210	PRO	4.0
1	M	24	LEU	4.0
1	U	211	ASN	4.0
1	A	25	CYS	4.0
1	D	182	LEU	3.9
1	P	182	LEU	3.9
1	K	175	LEU	3.9
1	F	25	CYS	3.8
1	K	184	LEU	3.8
1	T	104[A]	TYR	3.7
1	A	184	LEU	3.7
1	F	182	LEU	3.7
1	G	211	ASN	3.6
1	O	211	ASN	3.6
1	S	182	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	184	LEU	3.6
1	D	184	LEU	3.6
1	E	184	LEU	3.6
1	K	183	PRO	3.6
1	B	25	CYS	3.6
1	I	209	ARG	3.5
1	P	211	ASN	3.5
1	B	210	PRO	3.5
1	K	180	ARG	3.5
1	K	211	ASN	3.5
1	G	182	LEU	3.4
1	P	184	LEU	3.4
1	K	25	CYS	3.4
1	J	210	PRO	3.4
1	P	183	PRO	3.4
1	U	184	LEU	3.4
1	M	209	ARG	3.4
1	T	210	PRO	3.4
1	B	211	ASN	3.3
1	D	212	MET	3.3
1	F	29	CYS	3.3
1	I	184	LEU	3.3
1	G	209	ARG	3.3
1	I	182	LEU	3.3
1	O	184	LEU	3.3
1	J	184	LEU	3.2
1	K	182	LEU	3.2
1	E	24	LEU	3.2
1	J	166	ILE	3.2
1	V	29	CYS	3.2
1	D	183	PRO	3.1
1	J	102	ALA	3.1
1	A	57	ALA	3.1
1	I	175	LEU	3.1
1	G	104	TYR	3.1
1	B	179	PRO	3.1
1	U	180	ARG	3.1
1	H	166	ILE	3.1
1	O	182	LEU	3.0
1	H	181	GLN	3.0
1	V	104	TYR	3.0
1	C	210	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	J	208	CYS	3.0
1	J	182	LEU	3.0
1	H	209	ARG	3.0
1	R	211	ASN	3.0
1	H	208	CYS	3.0
1	K	60	GLY	3.0
1	I	179	PRO	3.0
1	O	58	GLY	2.9
1	I	104	TYR	2.9
1	V	211	ASN	2.9
1	J	63	VAL	2.9
1	T	186	VAL	2.9
1	K	104	TYR	2.9
1	H	212	MET	2.9
1	T	211	ASN	2.9
1	H	182	LEU	2.8
1	J	56	MET	2.8
1	D	29	CYS	2.8
1	L	25	CYS	2.8
1	P	29	CYS	2.8
1	O	179	PRO	2.8
1	T	209	ARG	2.8
1	C	58	GLY	2.8
1	R	29	CYS	2.8
1	M	210	PRO	2.8
1	O	210	PRO	2.8
1	P	30	GLN	2.8
1	K	57	ALA	2.8
1	K	210	PRO	2.8
1	M	29	CYS	2.8
1	S	58	GLY	2.8
1	J	171	TYR	2.8
1	D	25	CYS	2.8
1	O	29	CYS	2.8
1	C	211	ASN	2.7
1	K	176	ASN	2.7
1	Q	178	LEU	2.7
1	E	183	PRO	2.7
1	L	183	PRO	2.7
1	N	210	PRO	2.7
1	R	210	PRO	2.7
1	C	212	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	178	LEU	2.7
1	V	210	PRO	2.7
1	B	29	CYS	2.7
1	J	199	SER	2.7
1	J	172	LEU	2.7
1	A	209	ARG	2.7
1	J	167	LEU	2.6
1	K	167	LEU	2.6
1	K	188	LEU	2.6
1	S	211	ASN	2.6
1	H	207	SER	2.6
1	A	29	CYS	2.6
1	Q	210	PRO	2.6
1	J	209	ARG	2.6
1	O	104[A]	TYR	2.6
1	J	58	GLY	2.6
1	K	181	GLN	2.6
1	P	58	GLY	2.6
1	F	211	ASN	2.6
1	J	133	ALA	2.6
1	O	209	ARG	2.6
1	G	167	LEU	2.6
1	G	184	LEU	2.6
1	I	188	LEU	2.6
1	J	207	SER	2.6
1	A	186	VAL	2.5
1	N	58	GLY	2.5
1	K	209	ARG	2.5
1	B	57	ALA	2.5
1	P	210	PRO	2.5
1	T	182	LEU	2.5
1	E	212	MET	2.5
1	G	166	ILE	2.5
1	E	210	PRO	2.5
1	A	58	GLY	2.5
1	L	211	ASN	2.5
1	O	176	ASN	2.5
1	R	209	ARG	2.5
1	D	58	GLY	2.5
1	T	58	GLY	2.5
1	I	29	CYS	2.4
1	H	190	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	178	LEU	2.4
1	C	180	ARG	2.4
1	B	100	ASN	2.4
1	J	211	ASN	2.4
1	K	99	ASN	2.4
1	B	104[A]	TYR	2.4
1	C	57	ALA	2.4
1	B	58	GLY	2.4
1	J	131	GLY	2.4
1	K	56	MET	2.4
1	P	209	ARG	2.4
1	F	104	TYR	2.4
1	C	182	LEU	2.4
1	L	182	LEU	2.4
1	M	182	LEU	2.4
1	T	167	LEU	2.4
1	G	56	MET	2.4
1	H	183	PRO	2.4
1	I	181	GLN	2.3
1	P	167	LEU	2.3
1	Q	211	ASN	2.3
1	F	210	PRO	2.3
1	T	189	THR	2.3
1	J	99	ASN	2.3
1	M	211	ASN	2.3
1	K	166	ILE	2.3
1	S	166	ILE	2.3
1	J	179	PRO	2.3
1	K	172	LEU	2.3
1	B	177	LYS	2.3
1	L	179	PRO	2.3
1	Q	29	CYS	2.3
1	S	209	ARG	2.3
1	U	210	PRO	2.2
1	A	60	GLY	2.2
1	C	29	CYS	2.2
1	Q	60	GLY	2.2
1	B	184	LEU	2.2
1	O	178	LEU	2.2
1	I	174	SER	2.2
1	L	209	ARG	2.2
1	N	209	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	Q	180	ARG	2.2
1	M	212	MET	2.2
1	J	60	GLY	2.2
1	G	29	CYS	2.2
1	A	178	LEU	2.2
1	E	182	LEU	2.2
1	H	175	LEU	2.2
1	K	37	GLN	2.2
1	Q	181	GLN	2.2
1	J	104	TYR	2.2
1	C	166	ILE	2.2
1	N	183	PRO	2.2
1	K	58	GLY	2.2
1	H	29	CYS	2.2
1	T	25	CYS	2.2
1	S	179	PRO	2.1
1	A	166	ILE	2.1
1	U	173	ARG	2.1
1	C	179	PRO	2.1
1	D	210	PRO	2.1
1	B	30	GLN	2.1
1	F	166	ILE	2.1
1	J	59	GLY	2.1
1	N	131	GLY	2.1
1	J	57	ALA	2.1
1	A	182	LEU	2.1
1	I	132	LEU	2.1
1	I	196	LEU	2.1
1	J	177	LYS	2.1
1	A	56	MET	2.1
1	H	56	MET	2.1
1	N	60	GLY	2.1
1	U	166	ILE	2.1
1	U	174	SER	2.1
1	H	211	ASN	2.1
1	C	183	PRO	2.1
1	K	131	GLY	2.1
1	V	58	GLY	2.1
1	I	62	LYS	2.1
1	I	166	ILE	2.1
1	H	57	ALA	2.1
1	U	209	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	49	PRO	2.0
1	D	104	TYR	2.0
1	B	56	MET	2.0
1	V	25	CYS	2.0
1	S	177	LYS	2.0
1	J	183	PRO	2.0
1	T	131	GLY	2.0
1	Q	104[A]	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	A1KCK	T	303	17/17	0.70	0.20	54,75,92,93	0
3	A1KCK	C	303	17/17	0.73	0.19	48,54,75,76	0
3	A1KCK	A	304	17/17	0.73	0.19	48,58,71,72	0
3	A1KCK	S	303	17/17	0.74	0.18	56,66,74,77	0
3	A1KCK	H	303	17/17	0.76	0.18	57,80,86,87	0
3	A1KCK	I	303	17/17	0.76	0.17	70,101,106,106	0
3	A1KCK	K	301	17/17	0.77	0.18	62,86,108,108	0
3	A1KCK	V	305	17/17	0.77	0.19	53,60,75,79	0
5	CL	F	306	1/1	0.77	0.26	65,65,65,65	0
2	EDO	E	303	4/4	0.78	0.16	48,52,54,59	0
3	A1KCK	E	305	17/17	0.78	0.18	48,62,72,74	0
3	A1KCK	F	304	17/17	0.78	0.17	54,68,74,75	0
3	A1KCK	L	302	17/17	0.78	0.18	51,65,79,83	0
5	CL	G	305	1/1	0.78	0.23	73,73,73,73	0
5	CL	T	305	1/1	0.78	0.27	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	A	302	4/4	0.79	0.19	42,44,51,53	0
2	EDO	A	301	4/4	0.80	0.17	57,59,59,61	0
5	CL	O	306	1/1	0.80	0.25	71,71,71,71	0
3	A1KCK	P	303	17/17	0.80	0.19	59,65,81,81	0
5	CL	U	304	1/1	0.80	0.24	67,67,67,67	0
3	A1KCK	U	302	17/17	0.82	0.15	52,74,86,86	0
5	CL	Q	305	1/1	0.82	0.22	77,77,77,77	0
5	CL	B	307	1/1	0.83	0.19	66,66,66,66	0
5	CL	R	305	1/1	0.83	0.20	71,71,71,71	0
2	EDO	H	302	4/4	0.84	0.19	54,61,62,70	0
3	A1KCK	N	303	17/17	0.84	0.18	51,75,86,88	0
3	A1KCK	K	304	17/17	0.84	0.14	56,63,71,73	0
3	A1KCK	R	303	17/17	0.85	0.15	52,58,63,68	0
5	CL	E	306	1/1	0.85	0.19	66,66,66,66	0
4	MG	I	304	1/1	0.85	0.15	78,78,78,78	0
3	A1KCK	K	302	17/17	0.86	0.14	55,83,104,105	0
3	A1KCK	D	303	17/17	0.86	0.15	46,63,71,73	0
3	A1KCK	J	301	17/17	0.86	0.14	64,92,113,114	0
5	CL	R	304	1/1	0.86	0.17	66,66,66,66	0
3	A1KCK	M	303	17/17	0.86	0.15	48,68,81,81	0
3	A1KCK	I	301	17/17	0.86	0.14	61,79,98,98	0
5	CL	G	304	1/1	0.86	0.20	75,75,75,75	0
4	MG	B	304	1/1	0.87	0.17	69,69,69,69	0
5	CL	C	306	1/1	0.87	0.15	61,61,61,61	0
2	EDO	O	301	4/4	0.87	0.13	37,42,44,45	0
5	CL	B	306	1/1	0.87	0.16	70,70,70,70	0
5	CL	U	305	1/1	0.88	0.17	70,70,70,70	0
4	MG	C	304	1/1	0.89	0.11	50,50,50,50	0
5	CL	S	305	1/1	0.89	0.18	78,78,78,78	0
3	A1KCK	V	304	17/17	0.89	0.12	41,54,72,73	0
3	A1KCK	A	306	17/17	0.89	0.14	44,64,90,92	0
2	EDO	B	301	4/4	0.89	0.17	59,60,62,68	0
3	A1KCK	O	303	17/17	0.90	0.12	49,62,65,66	0
3	A1KCK	P	302	17/17	0.90	0.13	46,62,78,79	0
2	EDO	C	302	4/4	0.90	0.12	43,45,47,48	0
2	EDO	F	303	4/4	0.90	0.13	47,50,51,54	0
2	EDO	Q	301	4/4	0.90	0.12	39,45,48,51	0
3	A1KCK	D	301	17/17	0.90	0.12	37,52,70,71	0
2	EDO	V	303	4/4	0.90	0.14	64,65,68,69	0
3	A1KCK	N	301	17/17	0.90	0.13	45,62,74,74	0
3	A1KCK	E	302	17/17	0.90	0.12	38,57,75,76	0
3	A1KCK	T	302	17/17	0.91	0.11	44,56,71,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	E	301	4/4	0.91	0.14	56,60,63,67	0
3	A1KCK	G	301	17/17	0.91	0.13	41,62,85,85	0
4	MG	V	307	1/1	0.91	0.10	51,51,51,51	0
3	A1KCK	S	302	17/17	0.91	0.11	41,52,61,62	0
2	EDO	D	302	4/4	0.91	0.12	40,42,44,47	0
5	CL	P	304	1/1	0.91	0.15	69,69,69,69	0
3	A1KCK	Q	302	17/17	0.92	0.12	39,53,65,66	0
3	A1KCK	O	302	17/17	0.92	0.11	40,55,74,75	0
4	MG	O	304	1/1	0.92	0.09	62,62,62,62	0
5	CL	S	304	1/1	0.92	0.12	75,75,75,75	0
4	MG	V	306	1/1	0.92	0.11	66,66,66,66	0
2	EDO	V	301	4/4	0.92	0.11	41,45,45,51	0
3	A1KCK	F	301	17/17	0.92	0.11	43,55,74,77	0
2	EDO	R	301	4/4	0.92	0.11	42,44,46,50	0
3	A1KCK	B	303	17/17	0.93	0.09	38,41,43,48	0
3	A1KCK	Q	303	17/17	0.93	0.10	41,42,46,47	0
3	A1KCK	L	304	17/17	0.93	0.11	43,45,46,49	0
5	CL	N	304	1/1	0.93	0.14	79,79,79,79	0
2	EDO	L	301	4/4	0.93	0.09	42,49,50,53	0
4	MG	O	305	1/1	0.93	0.10	51,51,51,51	0
4	MG	T	304	1/1	0.93	0.09	52,52,52,52	0
2	EDO	U	301	4/4	0.93	0.10	40,45,48,50	0
2	EDO	M	301	4/4	0.93	0.10	42,45,47,52	0
2	EDO	V	302	4/4	0.93	0.11	54,54,55,58	0
2	EDO	G	302	4/4	0.93	0.14	47,52,55,64	0
5	CL	C	305	1/1	0.93	0.14	71,71,71,71	0
5	CL	U	303	1/1	0.93	0.21	77,77,77,77	0
2	EDO	P	301	4/4	0.93	0.10	36,40,42,45	0
2	EDO	K	303	4/4	0.93	0.12	48,49,52,58	0
2	EDO	I	302	4/4	0.94	0.11	49,50,52,54	0
5	CL	B	305	1/1	0.94	0.13	68,68,68,68	0
3	A1KCK	C	301	17/17	0.94	0.09	38,41,47,48	0
2	EDO	A	303	4/4	0.94	0.10	42,44,45,51	0
3	A1KCK	G	303	17/17	0.94	0.09	48,55,58,59	0
3	A1KCK	L	303	17/17	0.94	0.09	38,56,72,72	0
3	A1KCK	H	301	17/17	0.94	0.09	43,56,64,65	0
2	EDO	B	302	4/4	0.94	0.09	41,44,45,48	0
2	EDO	F	302	4/4	0.94	0.10	50,50,50,56	0
2	EDO	S	301	4/4	0.94	0.10	39,43,46,51	0
2	EDO	T	301	4/4	0.94	0.09	41,47,50,55	0
2	EDO	N	302	4/4	0.95	0.11	42,44,46,51	0
2	EDO	J	302	4/4	0.95	0.09	49,51,51,55	0

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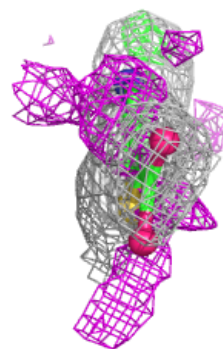
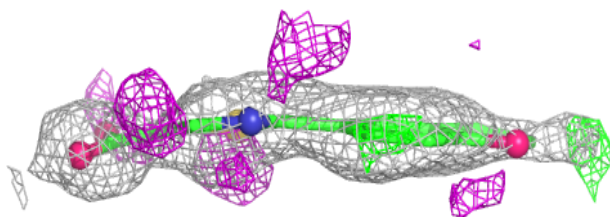
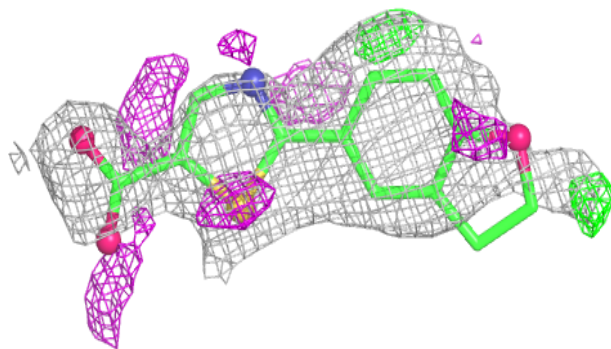
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	A1KCK	M	302	17/17	0.95	0.08	36,43,52,52	0
4	MG	M	304	1/1	0.95	0.08	66,66,66,66	0
3	A1KCK	A	305	17/17	0.95	0.08	37,43,52,53	0
5	CL	D	304	1/1	0.96	0.12	69,69,69,69	0
2	EDO	E	304	4/4	0.96	0.08	40,45,46,50	0
5	CL	L	305	1/1	0.96	0.20	69,69,69,69	0
5	CL	F	305	1/1	0.96	0.14	67,67,67,67	0
3	A1KCK	R	302	17/17	0.96	0.07	35,42,53,54	0
5	CL	Q	304	1/1	0.97	0.14	67,67,67,67	0
5	CL	P	305	1/1	0.97	0.11	69,69,69,69	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.

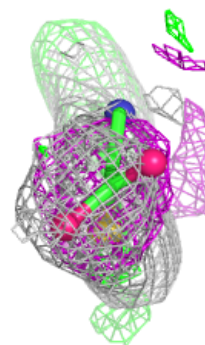
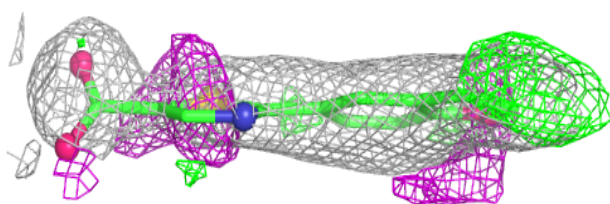
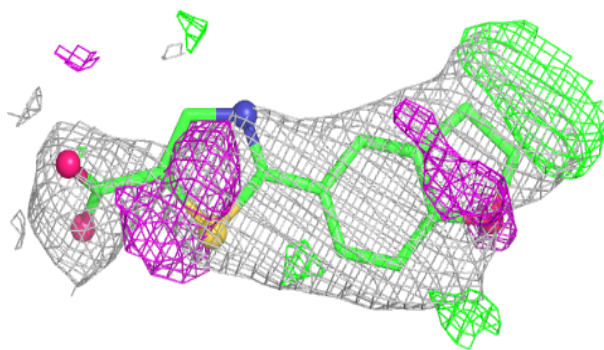
Electron density around A1KCK T 303:

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

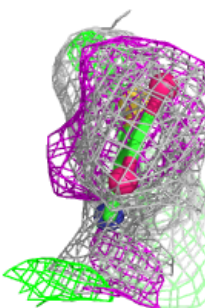
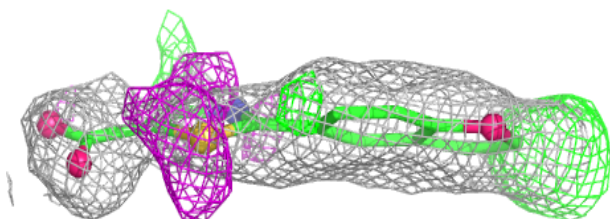
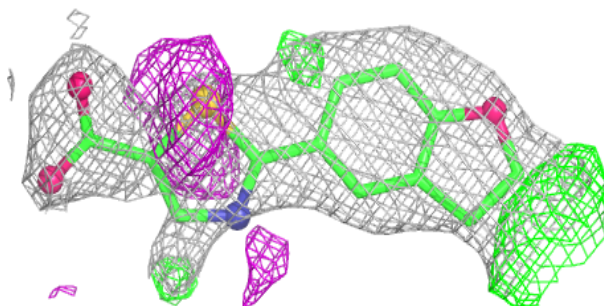


Electron density around A1KCK C 303:

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

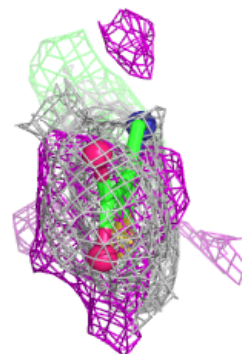
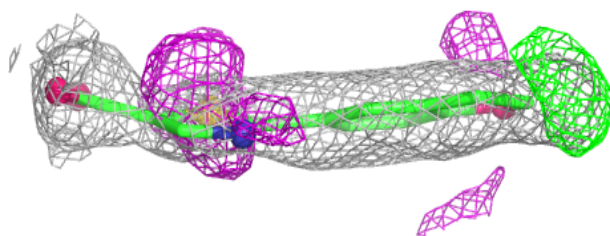
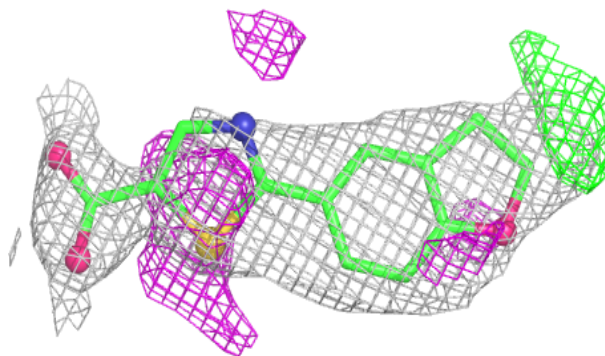
**Electron density around A1KCK A 304:**

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

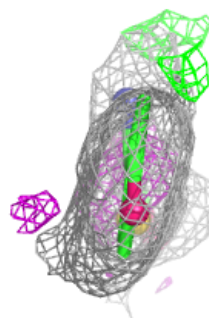
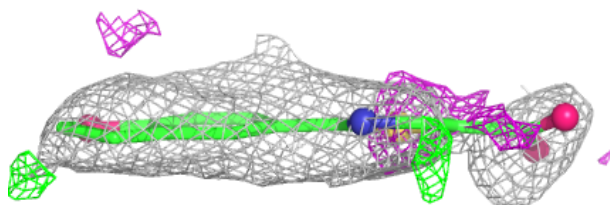
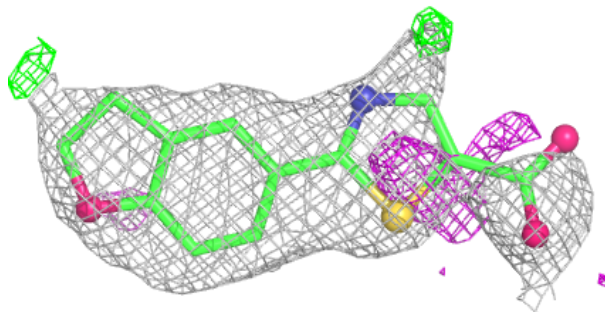


Electron density around A1KCK S 303:

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

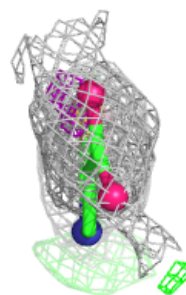
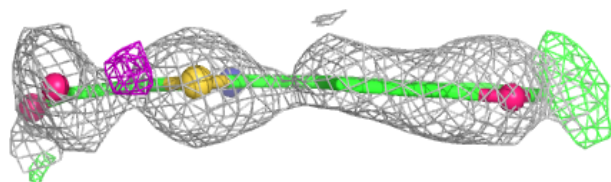
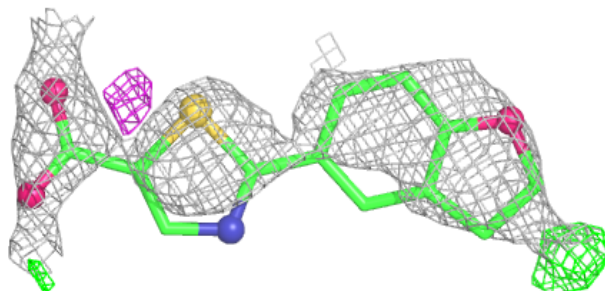
**Electron density around A1KCK H 303:**

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

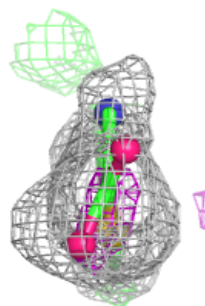
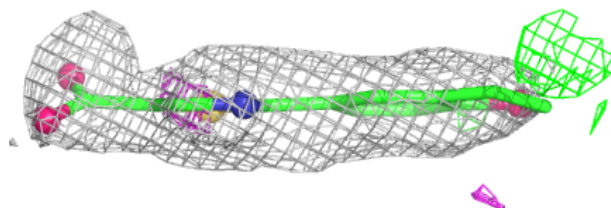
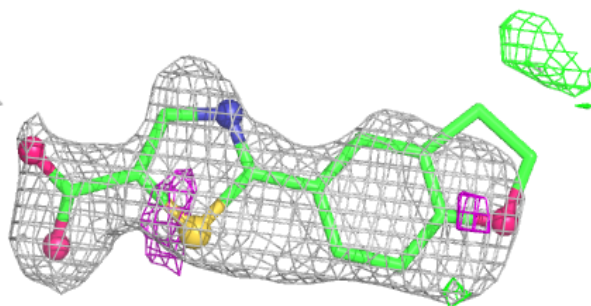


Electron density around A1KCK I 303:

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

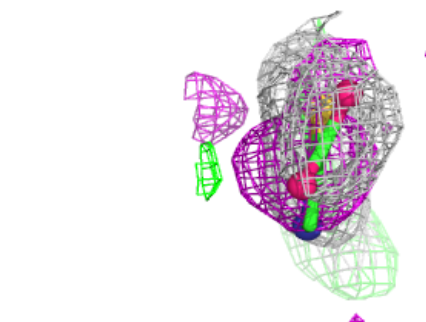
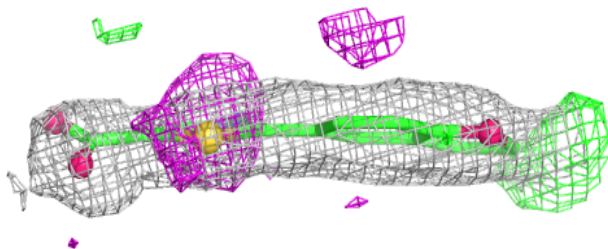
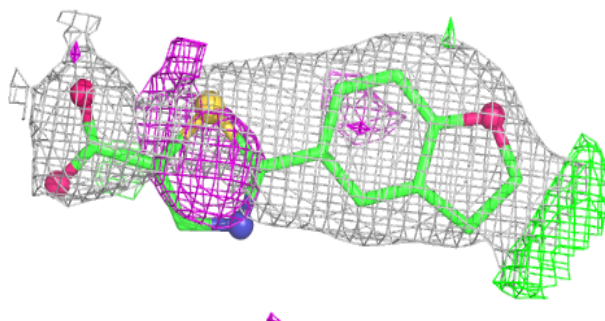
**Electron density around A1KCK K 301:**

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

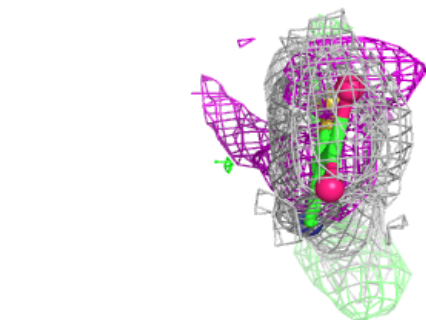
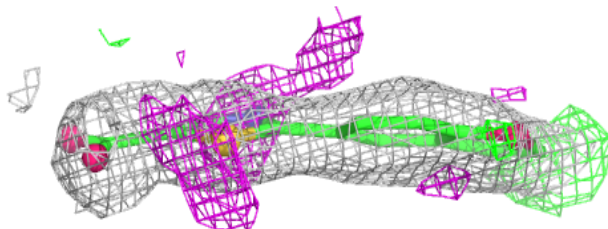
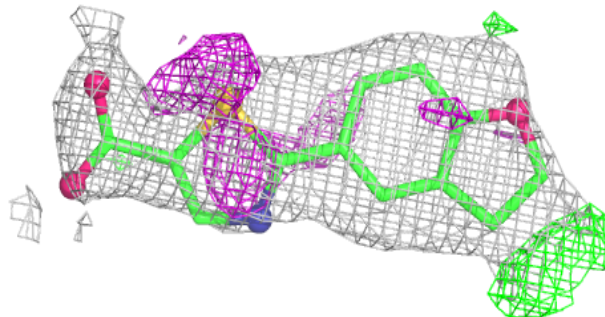


Electron density around A1KCK V 305:

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

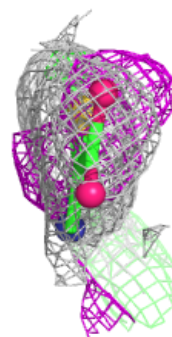
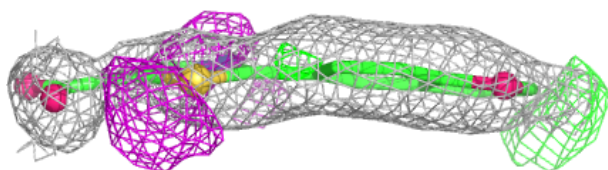
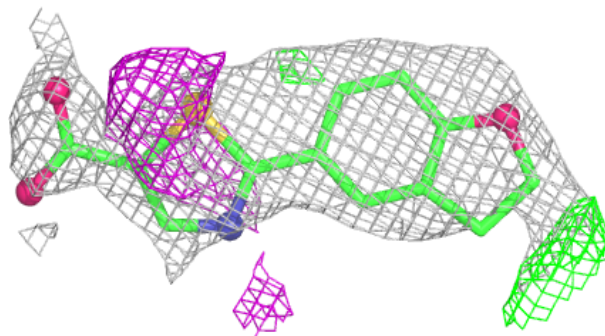
**Electron density around A1KCK E 305:**

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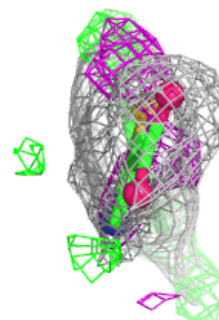
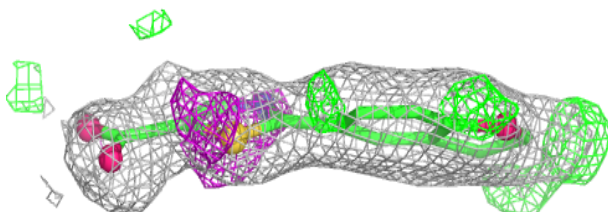
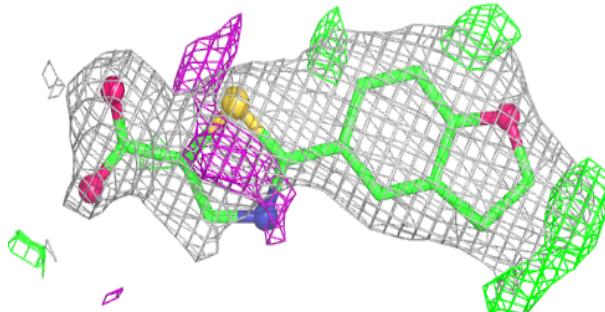


Electron density around A1KCK F 304:

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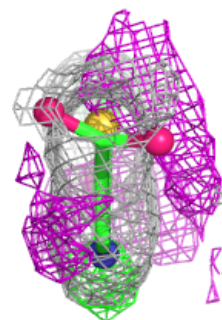
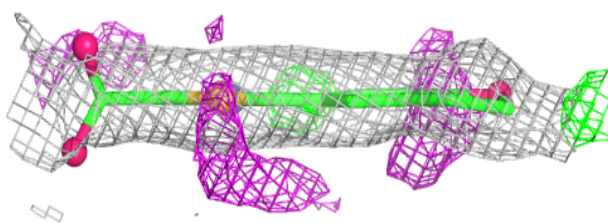
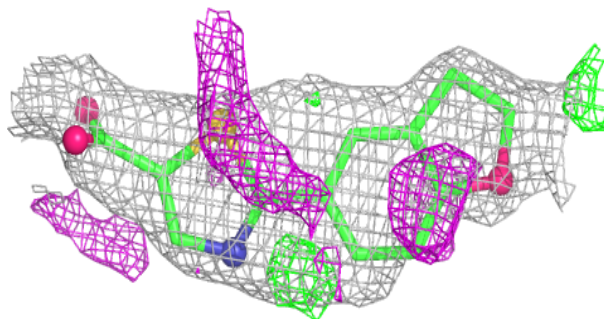
**Electron density around A1KCK L 302:**

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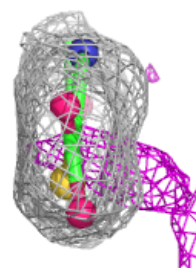
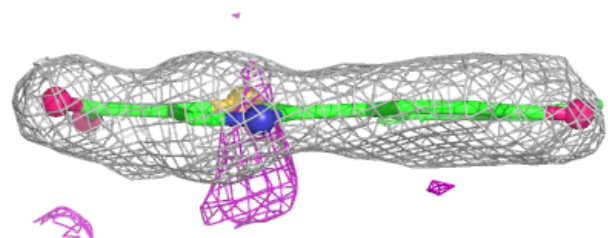
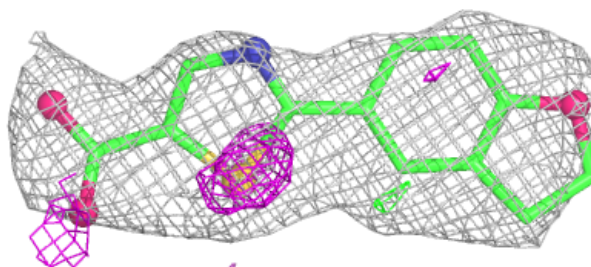


Electron density around A1KCK P 303:

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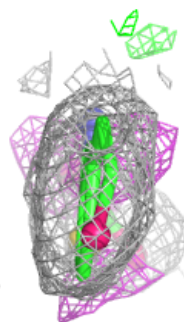
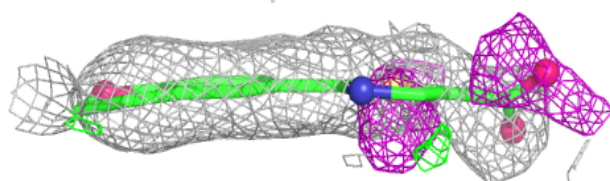
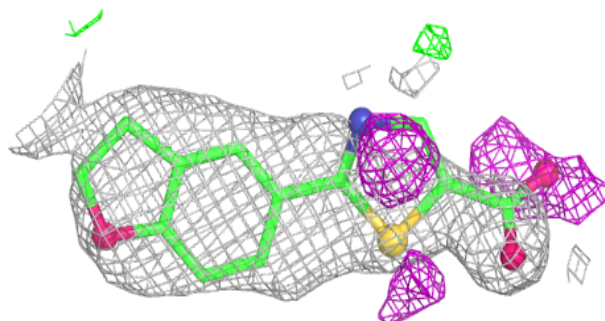
**Electron density around A1KCK U 302:**

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and green (positive)

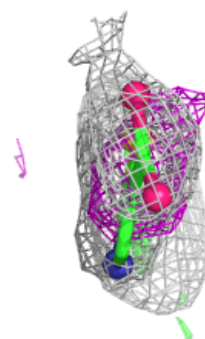
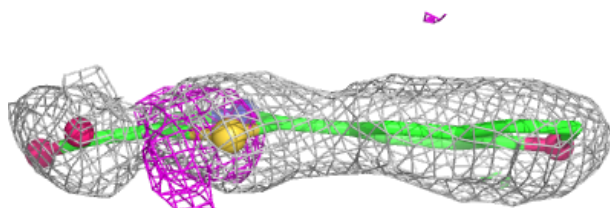
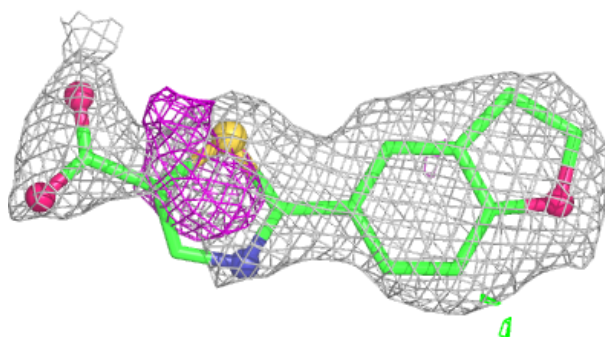


Electron density around A1KCK N 303:

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and green (positive)

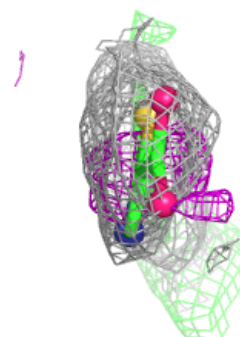
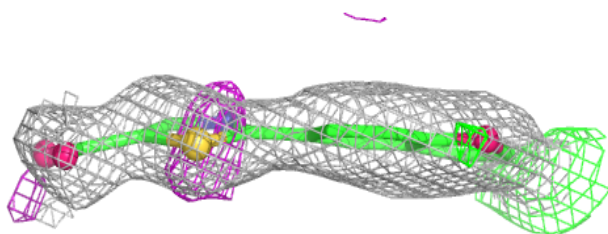
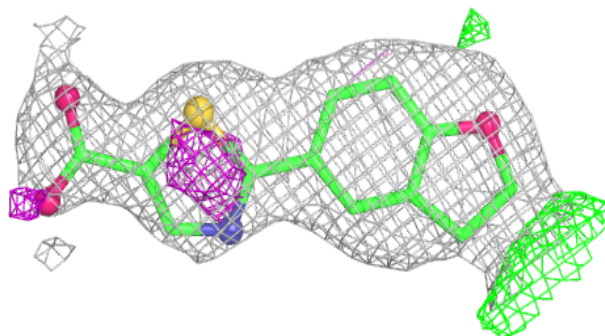
**Electron density around A1KCK K 304:**

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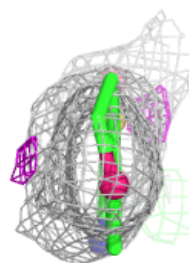
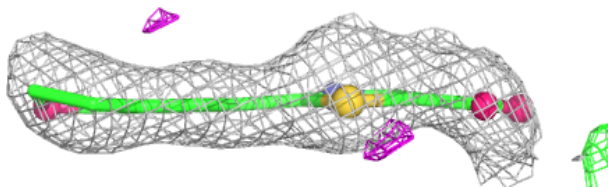
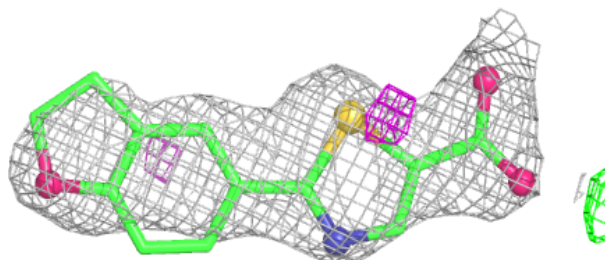


Electron density around A1KCK R 303:

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and green (positive)

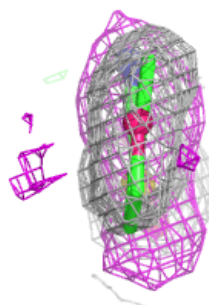
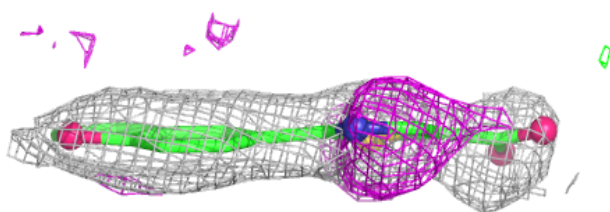
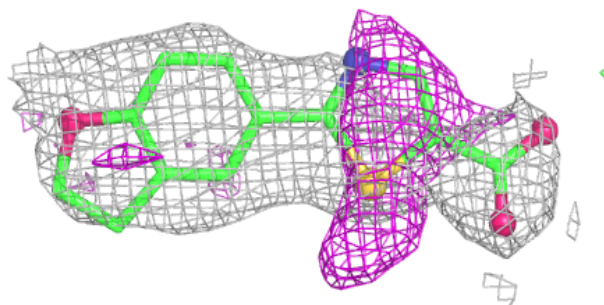
**Electron density around A1KCK K 302:**

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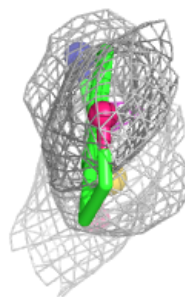
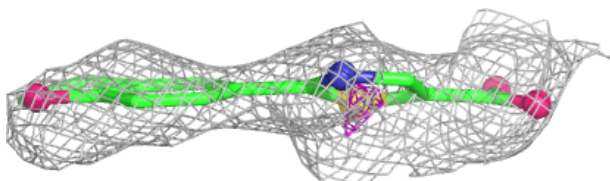
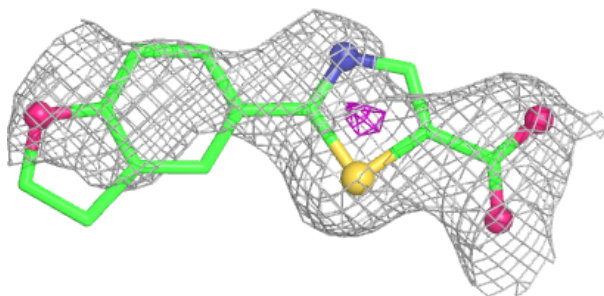


Electron density around A1KCK D 303:

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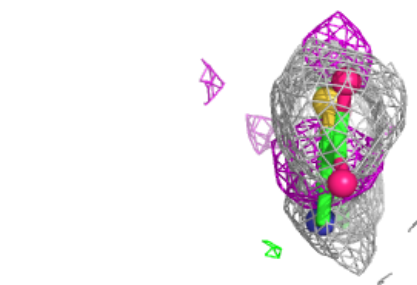
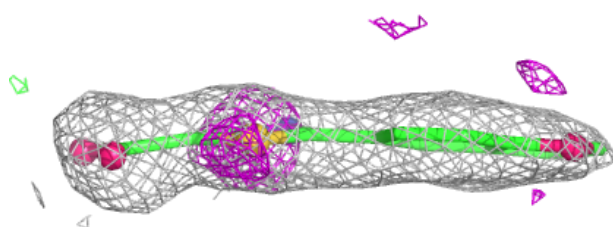
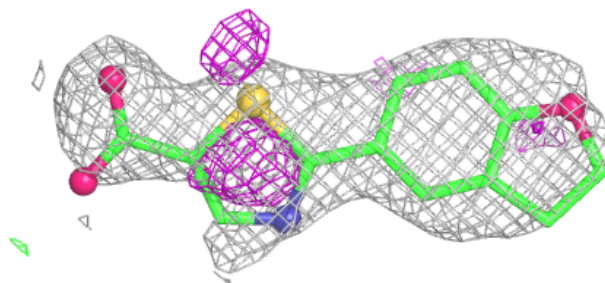
**Electron density around A1KCK J 301:**

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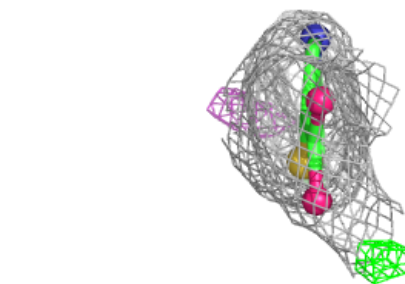
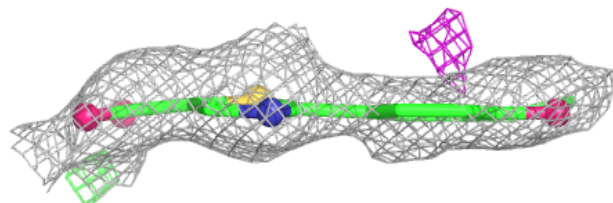
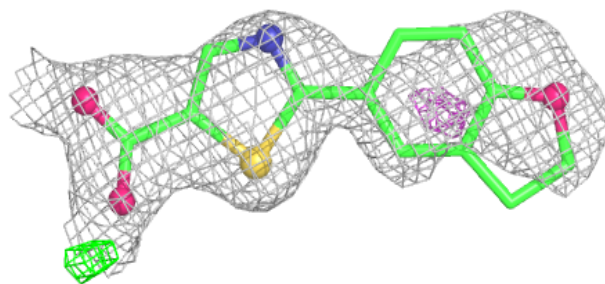


Electron density around A1KCK M 303:

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and green (positive)

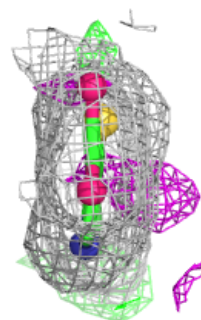
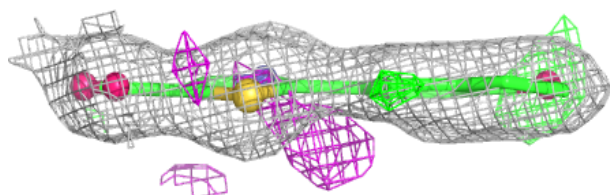
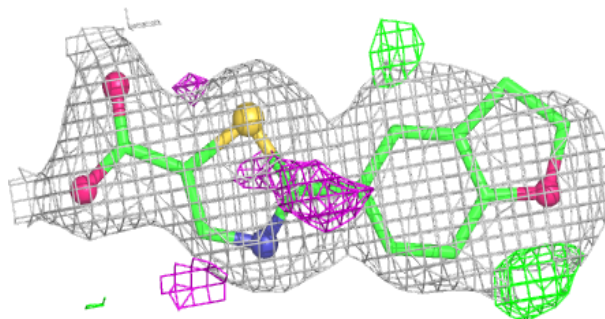
**Electron density around A1KCK I 301:**

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and green (positive)

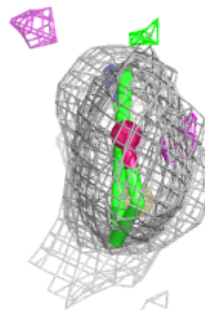
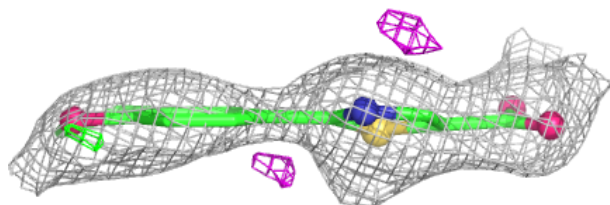
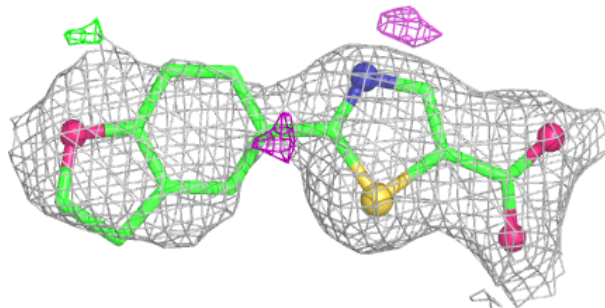


Electron density around A1KCK V 304:

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and green (positive)

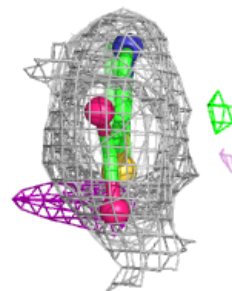
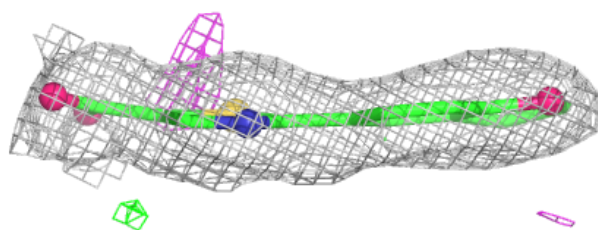
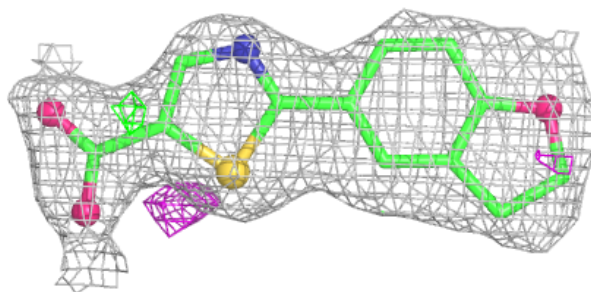
**Electron density around A1KCK A 306:**

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and green (positive)

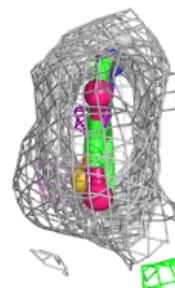
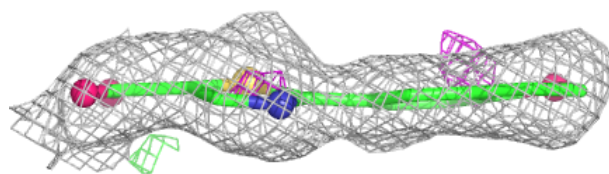
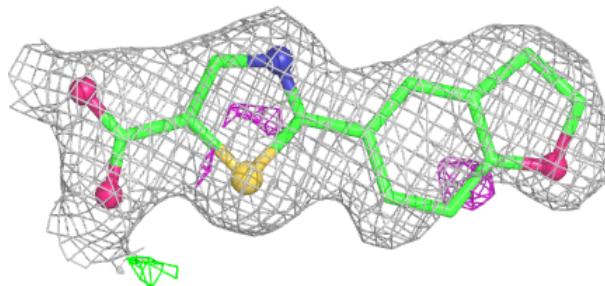


Electron density around A1KCK O 303:

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

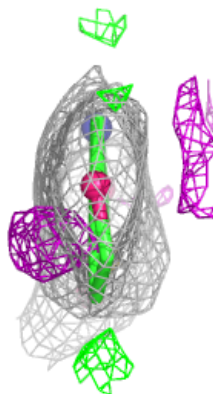
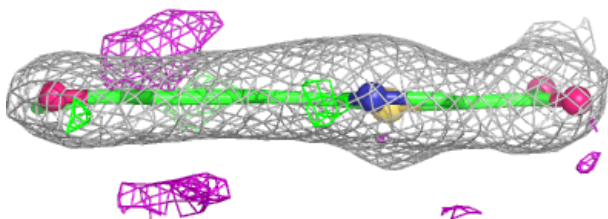
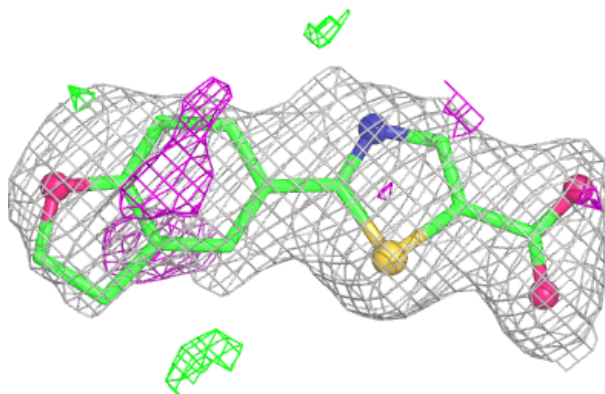
**Electron density around A1KCK P 302:**

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

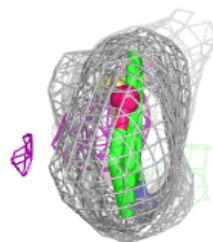
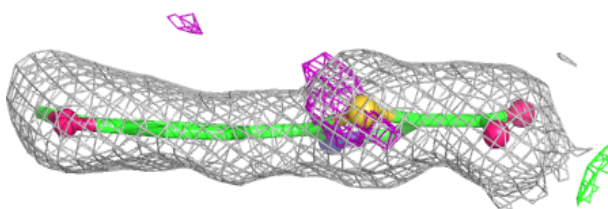
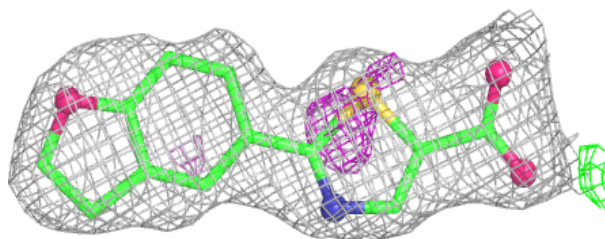


Electron density around A1KCK D 301:

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

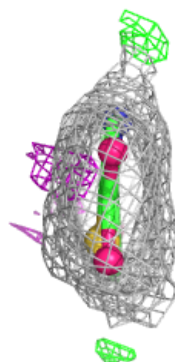
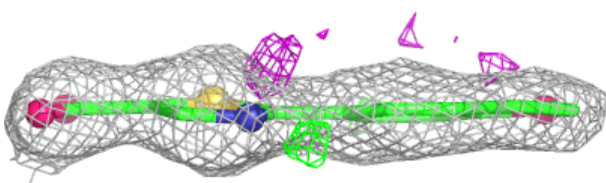
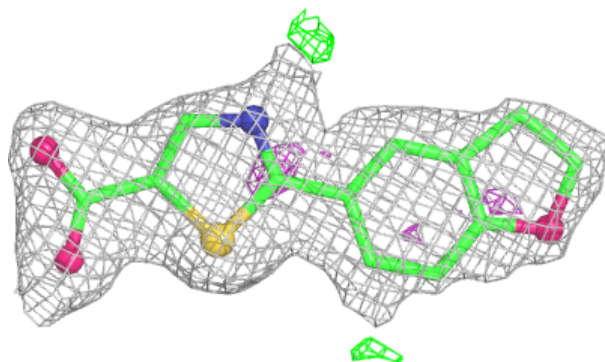
**Electron density around A1KCK N 301:**

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

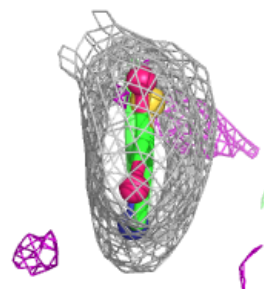
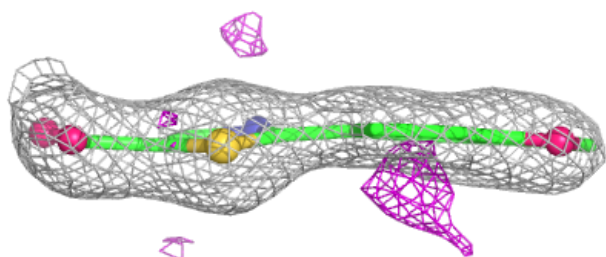
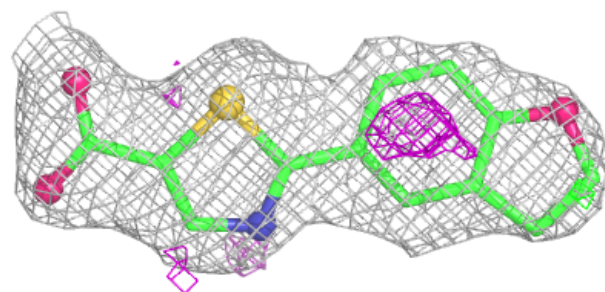


Electron density around A1KCK E 302:

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

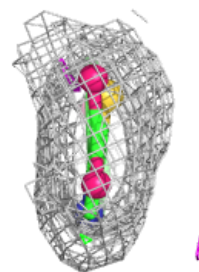
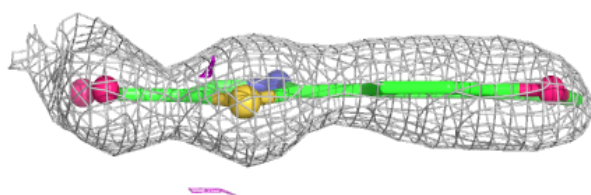
**Electron density around A1KCK T 302:**

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

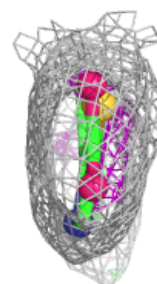
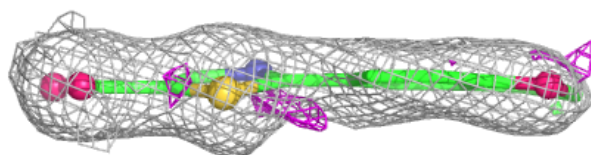
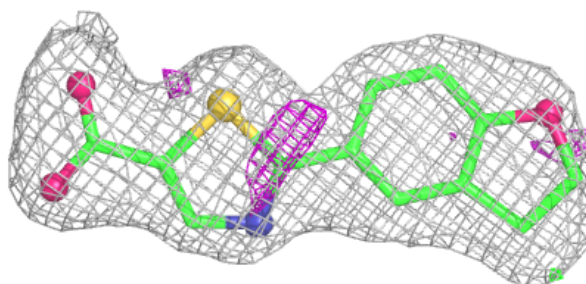


Electron density around A1KCK G 301:

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

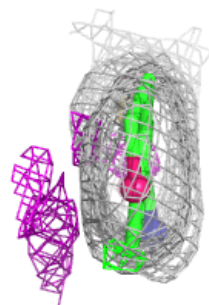
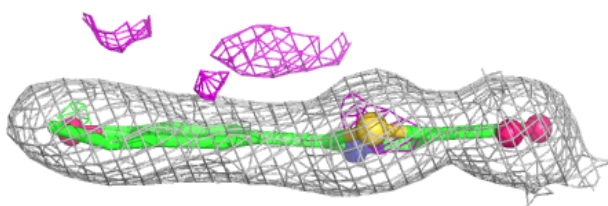
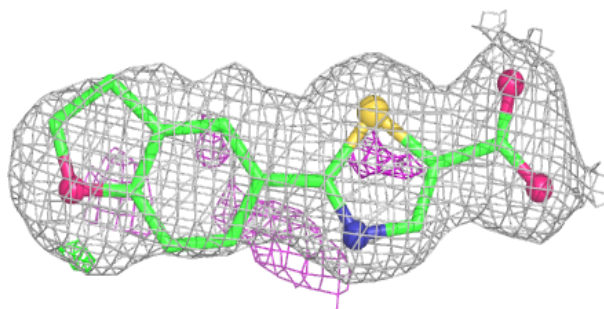
**Electron density around A1KCK S 302:**

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

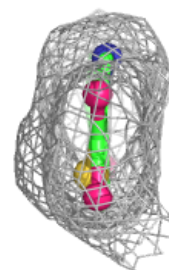
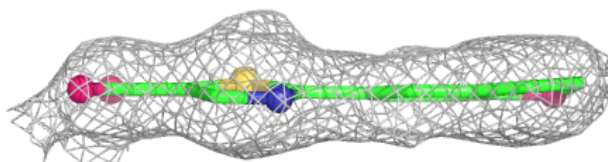
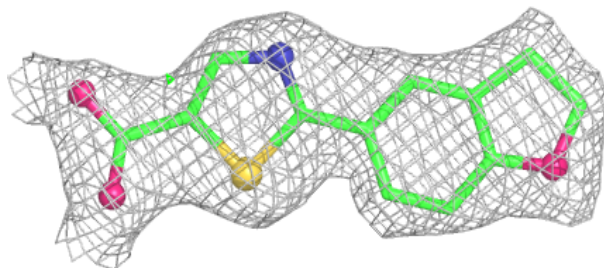


Electron density around A1KCK Q 302:

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

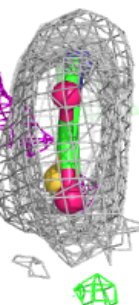
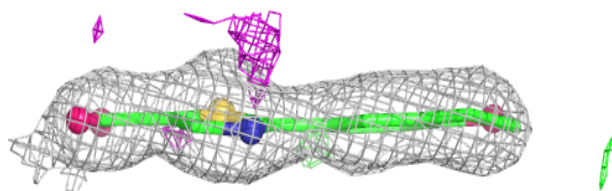
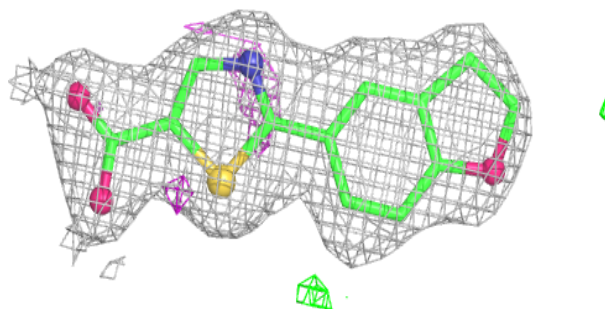
**Electron density around A1KCK O 302:**

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

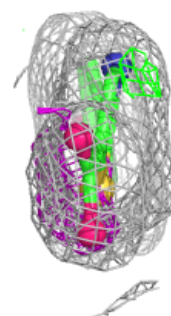
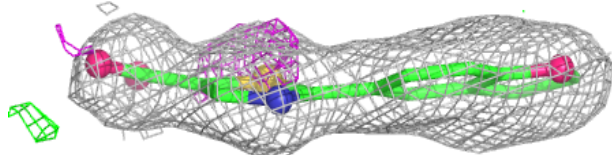
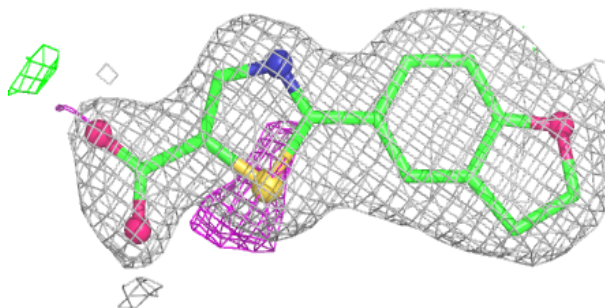


Electron density around A1KCK F 301:

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

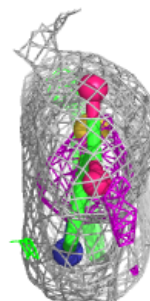
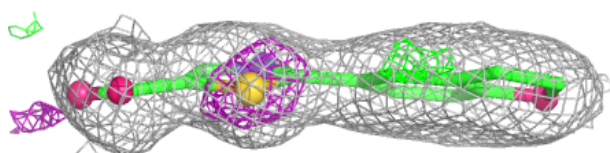
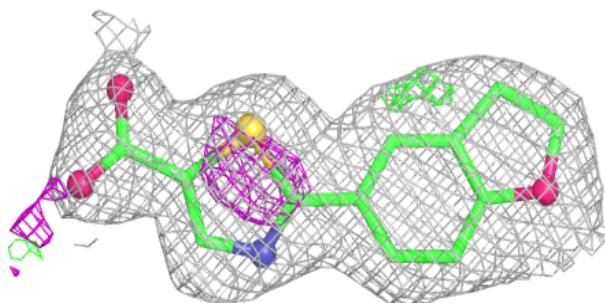
**Electron density around A1KCK B 303:**

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

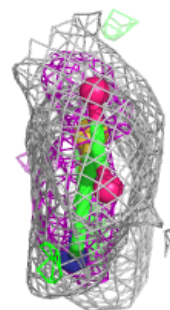
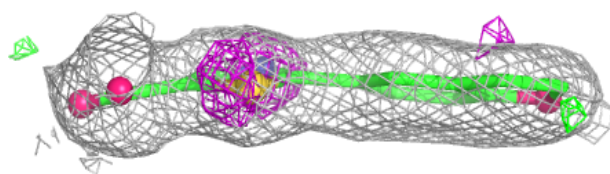
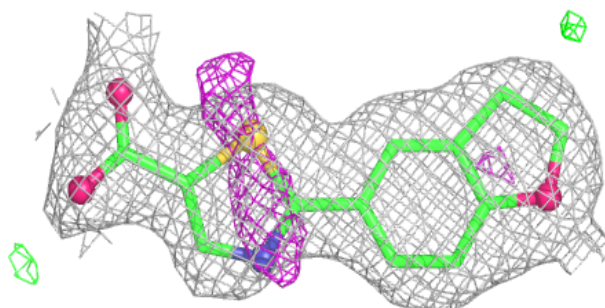


Electron density around A1KCK Q 303:

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

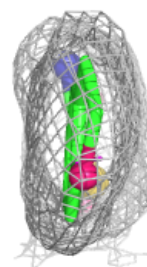
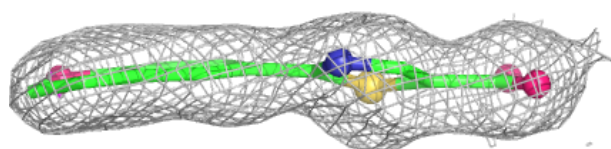
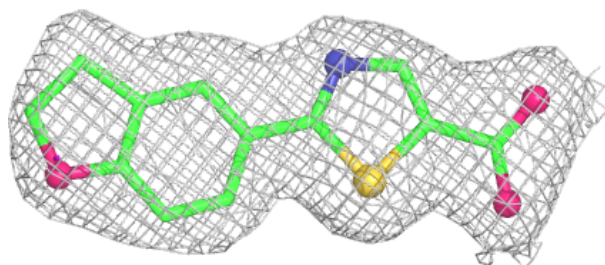
**Electron density around A1KCK L 304:**

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

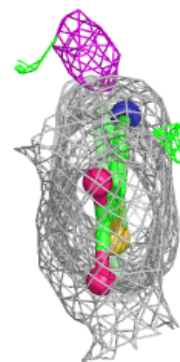
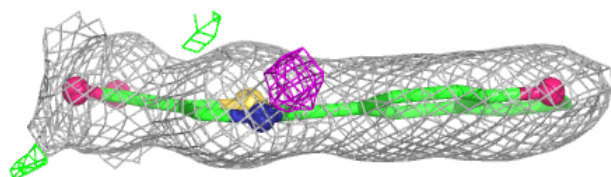
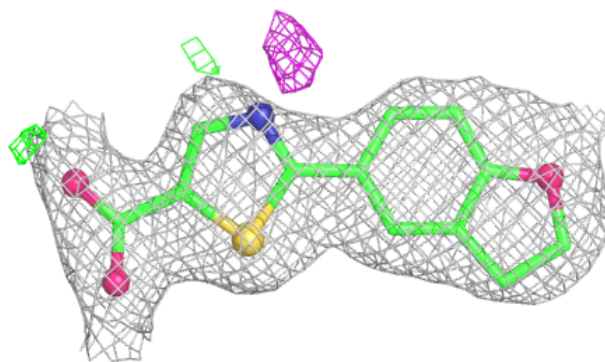


Electron density around A1KCK C 301:

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

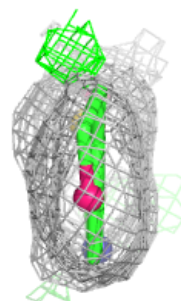
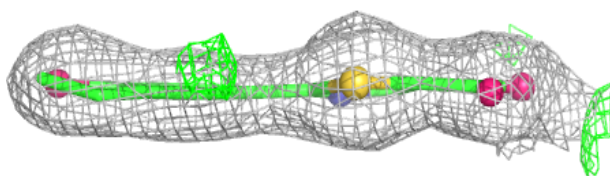
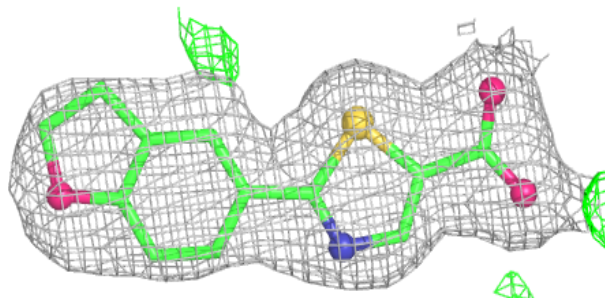
**Electron density around A1KCK G 303:**

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

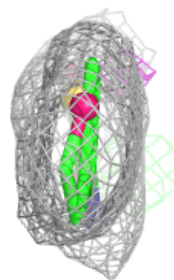
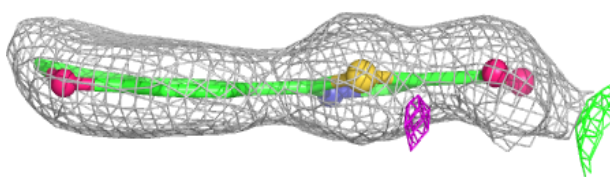
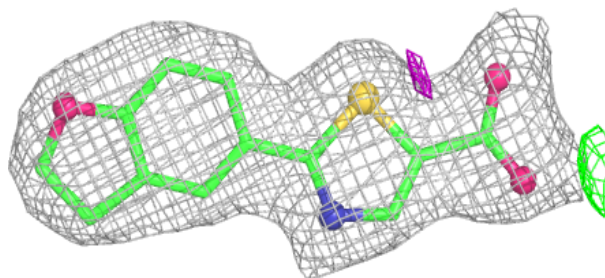


Electron density around A1KCK L 303:

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

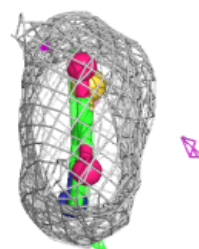
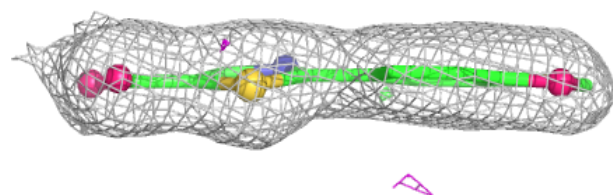
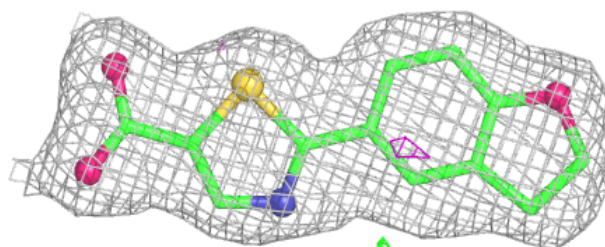
**Electron density around A1KCK H 301:**

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

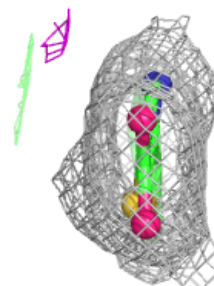
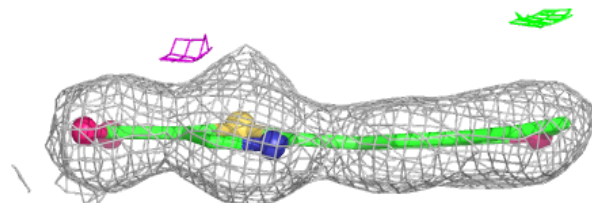
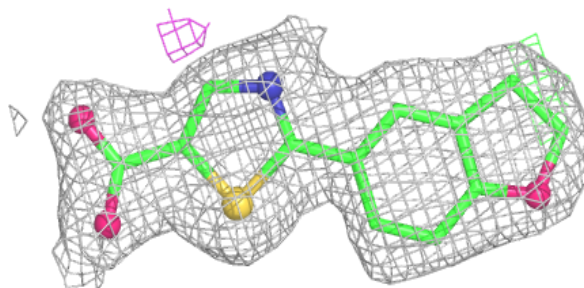


Electron density around A1KCK M 302:

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

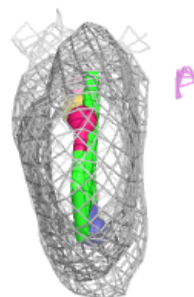
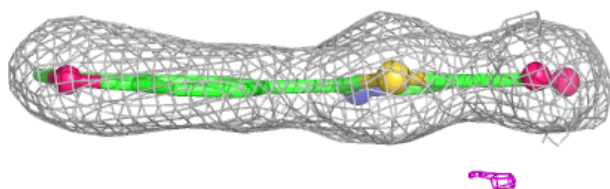
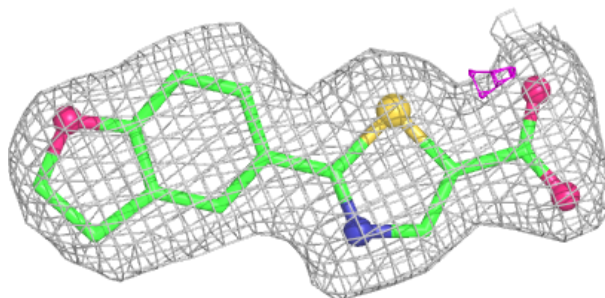
**Electron density around A1KCK A 305:**

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



Electron density around A1KCK R 302:

$2mF_o - DF_c$ (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.