Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2026 – 04:12 pm GMT

PDB ID	:	32DW / pdb_000032dw
Title	:	RAD52 N-terminal domain in complex with compound FORX-12-027
Authors	:	Bocquet, N.; Powell, A.J.; Barker, I.A.
Deposited on	:	2026-07-07
Resolution	:	2.30 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 (i) 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 (i)) were used in the production of this report:

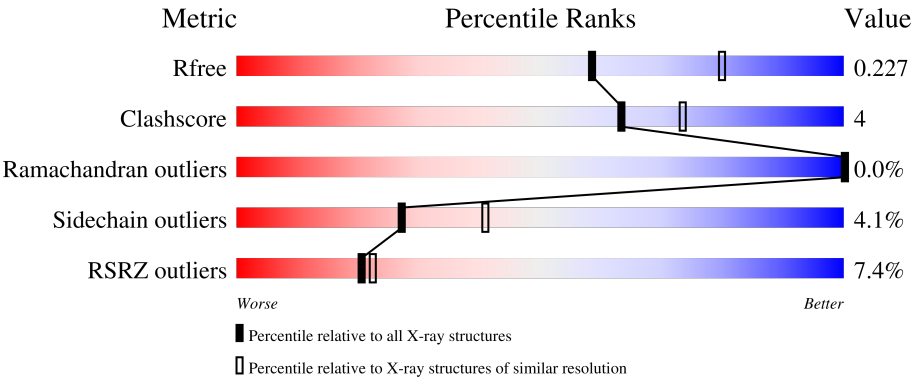
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 <=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% 76% 7% • 13%
1	B	215	4% 80% 7% • 13%
1	C	215	7% 79% 9% 12%
1	D	215	4% 78% 9% 13%
1	E	215	4% 76% 10% • 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	215	7% 79% 6% • 13%
1	G	215	5% 74% 10% •• 13%
1	H	215	12% 80% 7% • 12%
1	I	215	8% 75% 8% • 13%
1	J	215	15% 74% 9% •• 13%
1	K	215	9% 73% 11% •• 13%
1	L	215	6% 77% 9% 13%
1	M	215	7% 79% 7% • 12%
1	N	215	6% 77% 8% •• 13%
1	O	215	6% 77% 9% 13%
1	P	215	5% 78% 8% • 13%
1	Q	215	7% 74% 10% • 13%
1	R	215	5% 78% 8% • 13%
1	S	215	4% 80% 5% • 13%
1	T	215	6% 78% 7% • 13%
1	U	215	7% 77% 7% •• 13%
1	V	215	6% 78% 7% • 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	M	303	-	-	X	-
2	EDO	T	303	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 34912 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	2	0
			1494	933	270	283	8			
1	C	189	Total	C	N	O	S	0	2	0
			1497	932	272	284	9			
1	D	188	Total	C	N	O	S	0	2	0
			1492	928	273	282	9			
1	E	189	Total	C	N	O	S	0	1	0
			1489	928	270	282	9			
1	F	187	Total	C	N	O	S	0	3	0
			1492	930	271	283	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	4	0
			1502	936	272	285	9			
1	L	187	Total	C	N	O	S	0	2	0
			1484	924	270	282	8			
1	M	189	Total	C	N	O	S	0	1	0
			1489	930	269	281	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			

Continued on next page...

Continued from previous page...

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	1	0
			1482	924	269	281	8			
1	T	187	Total	C	N	O	S	0	1	0
			1480	925	267	280	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

Continued on next page...

Continued from previous page...

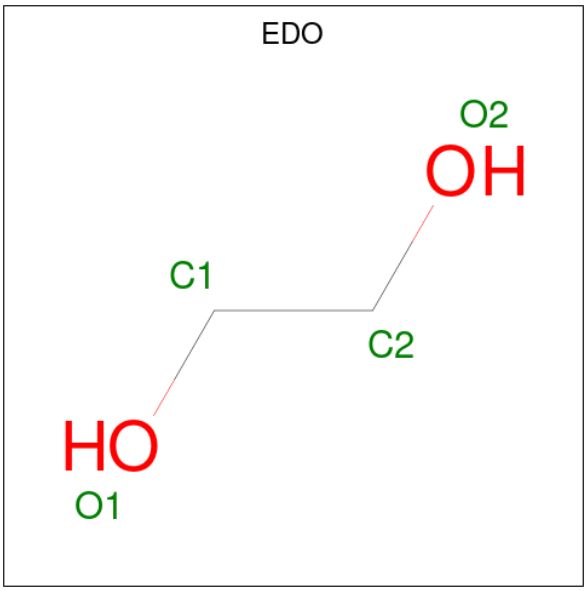
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	expression tag	UNP P43351
F	102	ALA	LYS	engineered mutation	UNP P43351
F	133	ALA	LYS	engineered mutation	UNP P43351
G	-2	GLY	-	expression tag	UNP P43351
G	-1	SER	-	expression tag	UNP P43351
G	0	HIS	-	expression tag	UNP P43351
G	102	ALA	LYS	engineered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

Continued on next page...

Continued from previous page...

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: $C_2H_6O_2$).



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	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	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	C	1	Total	C	O	0	0
			4	2	2		
2	C	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	D	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

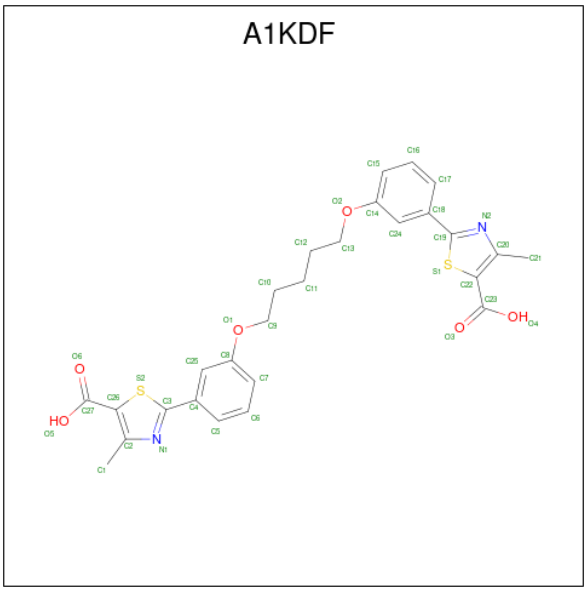
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0
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	L	1	Total C O 4 2 2	0	0
2	M	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	O	1	Total C O 4 2 2	0	0
2	P	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	P	1	Total	C	O	0	0
			4	2	2		
2	P	1	Total	C	O	0	0
			4	2	2		
2	Q	1	Total	C	O	0	0
			4	2	2		
2	Q	1	Total	C	O	0	0
			4	2	2		
2	R	1	Total	C	O	0	0
			4	2	2		
2	R	1	Total	C	O	0	0
			4	2	2		
2	S	1	Total	C	O	0	0
			4	2	2		
2	S	1	Total	C	O	0	0
			4	2	2		
2	S	1	Total	C	O	0	0
			4	2	2		
2	T	1	Total	C	O	0	0
			4	2	2		
2	T	1	Total	C	O	0	0
			4	2	2		
2	U	1	Total	C	O	0	0
			4	2	2		
2	U	1	Total	C	O	0	0
			4	2	2		
2	U	1	Total	C	O	0	0
			4	2	2		
2	V	1	Total	C	O	0	0
			4	2	2		
2	V	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is 2-[3-[5-[3-(5-carboxy-4-methyl-1,3-thiazol-2-yl)phenoxy]pentoxy]phenyl]-4-methyl-1,3-thiazole-5-carboxylic acid (CCD ID: A1KDF) (formula: $C_{27}H_{26}N_2O_6S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			37	27	2	6	2		
3	B	1	Total	C	N	O	S	0	0
			37	27	2	6	2		
3	C	1	Total	C	N	O	S	0	0
			37	27	2	6	2		
3	D	1	Total	C	N	O	S	0	0
			37	27	2	6	2		
3	E	1	Total	C	N	O	S	0	0
			37	27	2	6	2		
3	E	1	Total	C	N	O	S	0	0
			37	27	2	6	2		
3	G	1	Total	C	N	O	S	0	0
			37	27	2	6	2		
3	H	1	Total	C	N	O	S	0	0
			37	27	2	6	2		
3	I	1	Total	C	N	O	S	0	0
			37	27	2	6	2		
3	I	1	Total	C	N	O	S	0	0
			37	27	2	6	2		
3	K	1	Total	C	N	O	S	0	0
			37	27	2	6	2		
3	L	1	Total	C	N	O	S	0	0
			37	27	2	6	2		
3	M	1	Total	C	N	O	S	0	0
			37	27	2	6	2		
3	N	1	Total	C	N	O	S	0	0
			37	27	2	6	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	O	1	Total	C	N	O	S	0	0
			37	27	2	6	2		
3	P	1	Total	C	N	O	S	0	0
			37	27	2	6	2		
3	Q	1	Total	C	N	O	S	0	0
			37	27	2	6	2		
3	R	1	Total	C	N	O	S	0	0
			37	27	2	6	2		
3	S	1	Total	C	N	O	S	0	0
			37	27	2	6	2		
3	T	1	Total	C	N	O	S	0	0
			37	27	2	6	2		
3	U	1	Total	C	N	O	S	0	0
			37	27	2	6	2		
3	U	1	Total	C	N	O	S	0	0
			37	27	2	6	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	2	Total	Mg	0	0
			2	2		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		
4	G	1	Total	Mg	0	0
			1	1		
4	J	1	Total	Mg	0	0
			1	1		
4	L	2	Total	Mg	0	0
			2	2		
4	M	1	Total	Mg	0	0
			1	1		
4	N	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	O	1	Total Mg 1 1	0	0
4	Q	1	Total Mg 1 1	0	0
4	R	2	Total Mg 2 2	0	0
4	T	2	Total Mg 2 2	0	0
4	U	1	Total Mg 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Cl 2 2	0	0
5	B	2	Total Cl 2 2	0	0
5	C	1	Total Cl 1 1	0	0
5	D	2	Total Cl 2 2	0	0
5	E	1	Total Cl 1 1	0	0
5	F	2	Total Cl 2 2	0	0
5	G	2	Total Cl 2 2	0	0
5	H	1	Total Cl 1 1	0	0
5	J	1	Total Cl 1 1	0	0
5	L	1	Total Cl 1 1	0	0
5	M	3	Total Cl 3 3	0	0
5	N	2	Total Cl 2 2	0	0
5	O	2	Total Cl 2 2	0	0
5	P	2	Total Cl 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Q	2	Total Cl 2 2	0	0
5	R	2	Total Cl 2 2	0	0
5	S	1	Total Cl 1 1	0	0
5	T	3	Total Cl 3 3	0	0
5	U	2	Total Cl 2 2	0	0
5	V	2	Total Cl 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	44	Total O 44 44	0	0
6	B	68	Total O 68 68	0	0
6	C	77	Total O 77 77	0	0
6	D	73	Total O 73 73	0	0
6	E	77	Total O 77 77	0	0
6	F	59	Total O 59 59	0	0
6	G	51	Total O 51 51	0	0
6	H	42	Total O 42 42	0	0
6	I	31	Total O 31 31	0	0
6	J	21	Total O 21 21	0	0
6	K	31	Total O 31 31	0	0
6	L	61	Total O 61 61	0	0
6	M	58	Total O 58 58	0	0

Continued on next page...

Continued from previous page...

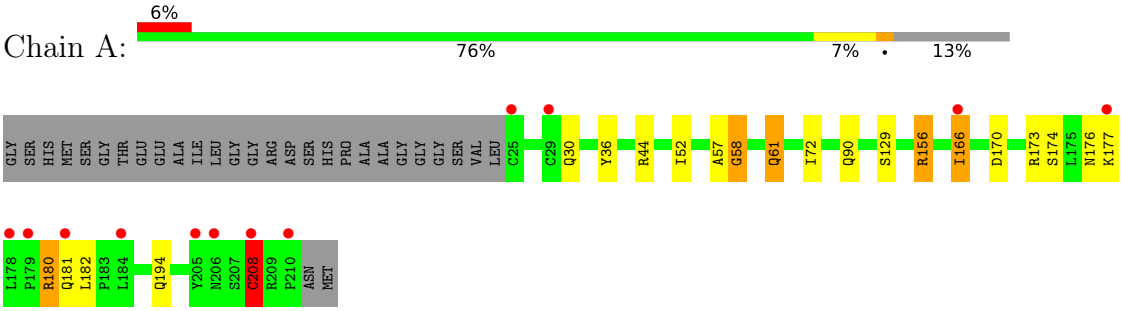
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	N	53	Total O 53 53	0	0
6	O	54	Total O 54 54	0	0
6	P	80	Total O 80 80	0	0
6	Q	85	Total O 85 85	0	0
6	R	56	Total O 56 56	0	0
6	S	46	Total O 46 46	0	0
6	T	54	Total O 54 54	0	0
6	U	63	Total O 63 63	0	0
6	V	65	Total O 65 65	0	0

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.

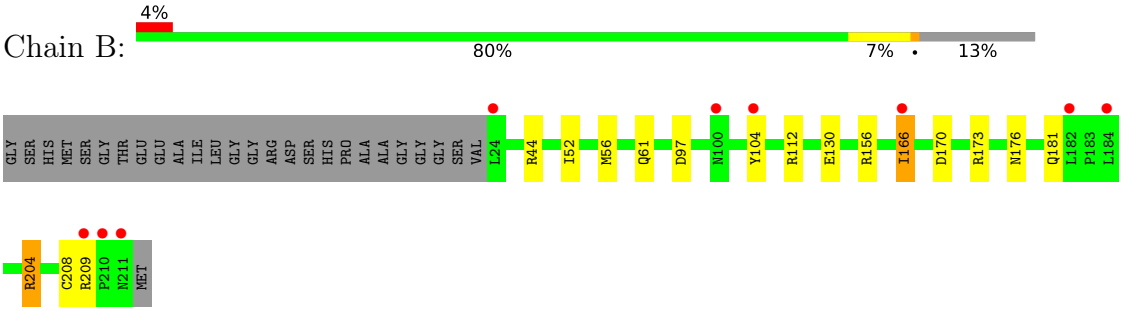
• Molecule 1: DNA repair protein RAD52 homolog

Chain A:



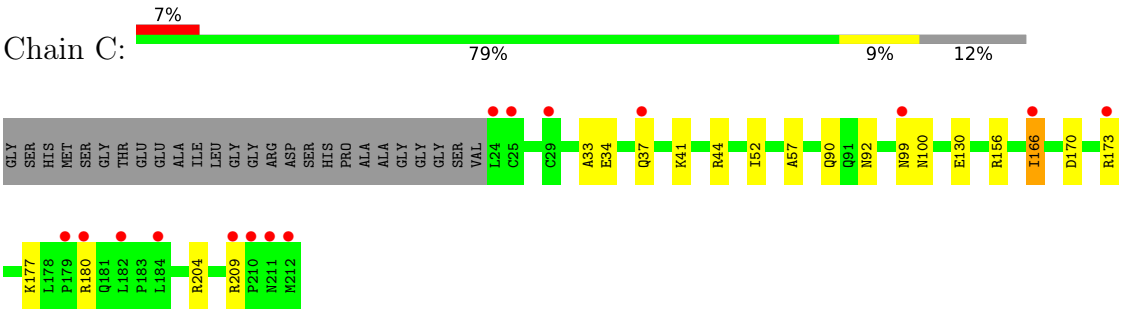
• Molecule 1: DNA repair protein RAD52 homolog

Chain B:



• Molecule 1: DNA repair protein RAD52 homolog

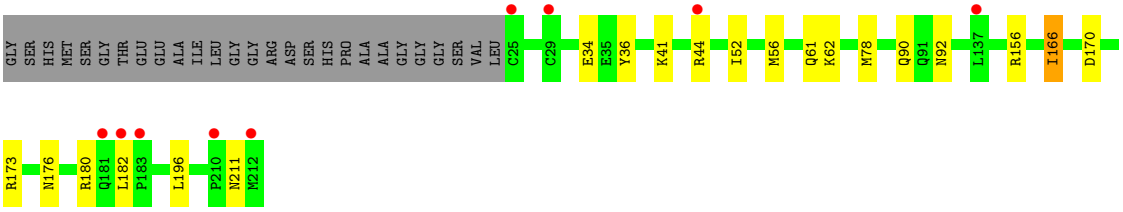
Chain C:



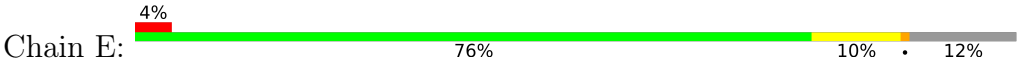
• Molecule 1: DNA repair protein RAD52 homolog

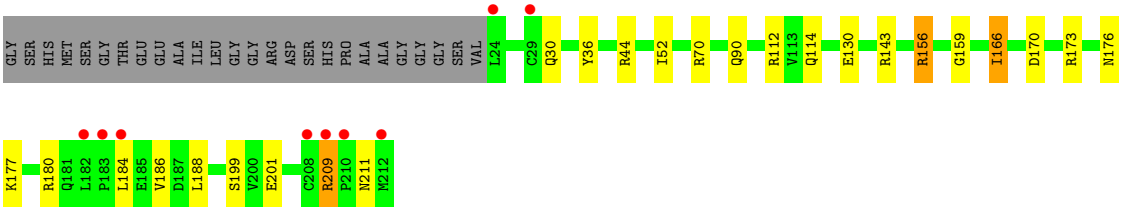
Chain D:



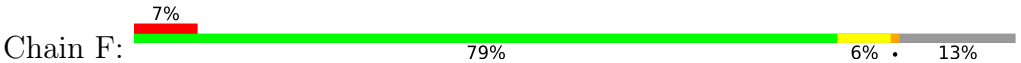


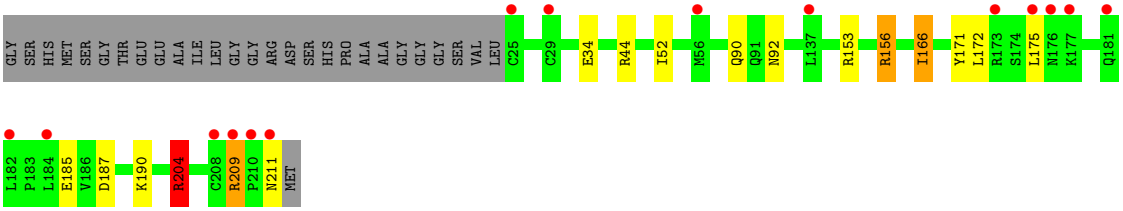
• Molecule 1: DNA repair protein RAD52 homolog





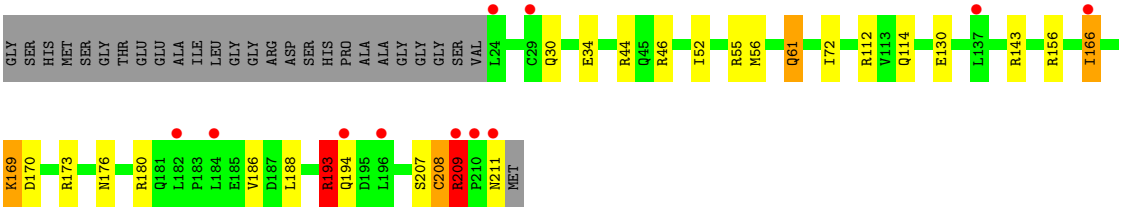
• Molecule 1: DNA repair protein RAD52 homolog



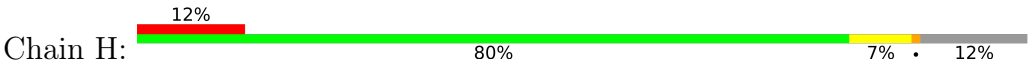


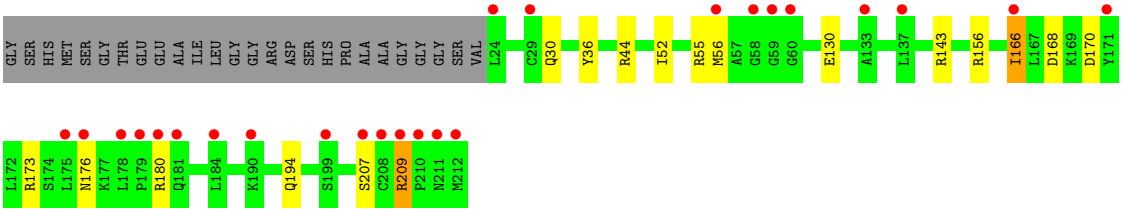
• Molecule 1: DNA repair protein RAD52 homolog





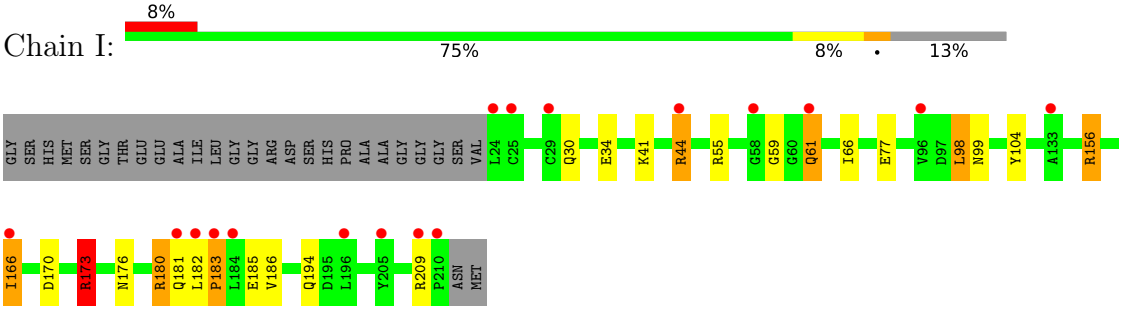
• Molecule 1: DNA repair protein RAD52 homolog





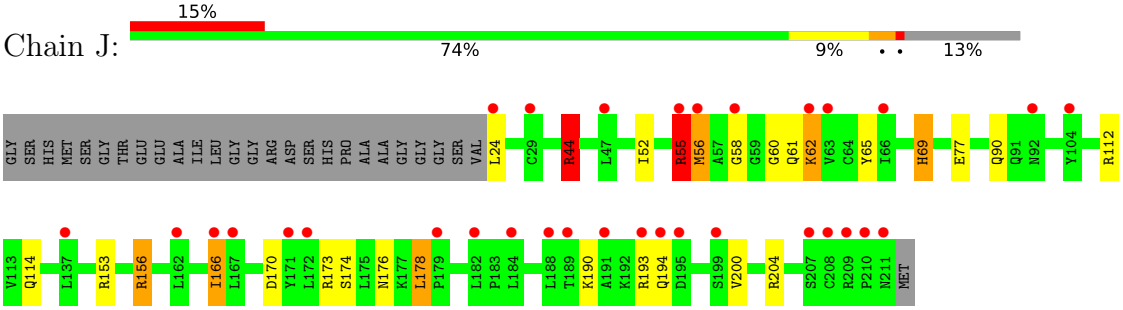
• Molecule 1: DNA repair protein RAD52 homolog

Chain I:



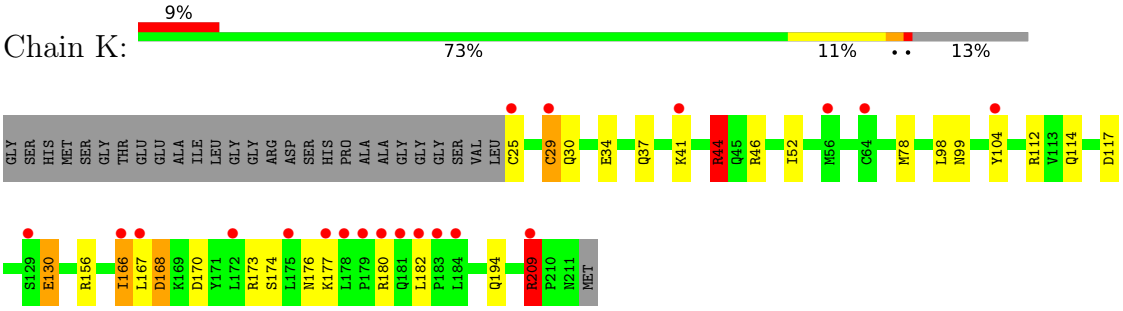
• Molecule 1: DNA repair protein RAD52 homolog

Chain J:



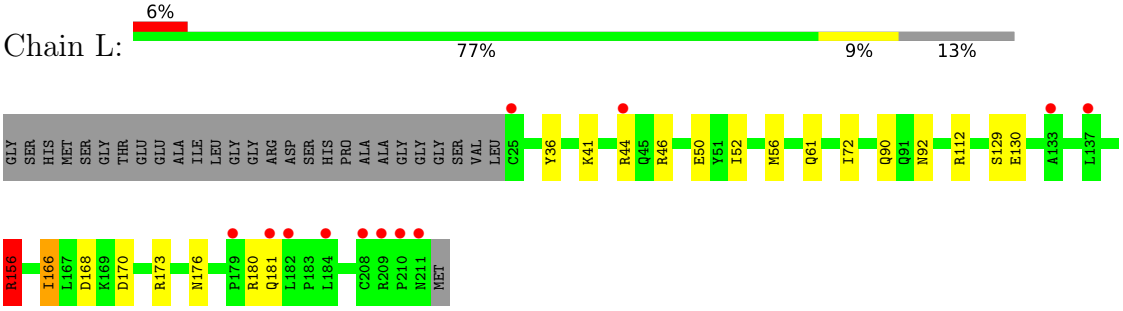
• Molecule 1: DNA repair protein RAD52 homolog

Chain K:



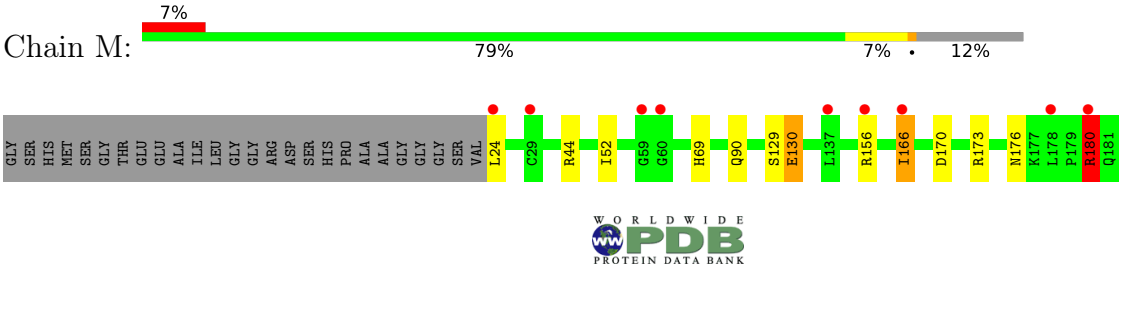
• Molecule 1: DNA repair protein RAD52 homolog

Chain L:



• Molecule 1: DNA repair protein RAD52 homolog

Chain M:

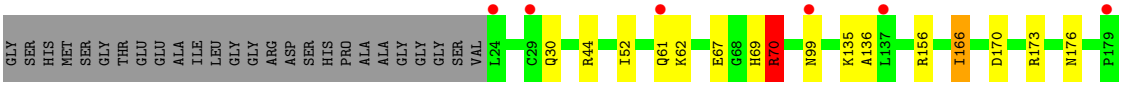


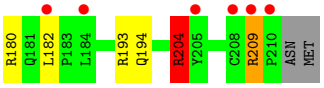


• Molecule 1: DNA repair protein RAD52 homolog

Chain N:



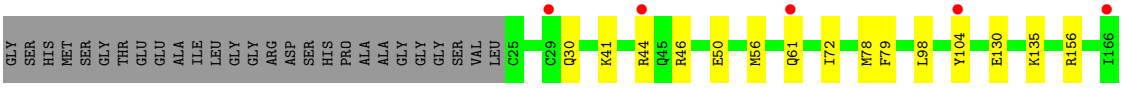


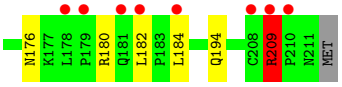


• Molecule 1: DNA repair protein RAD52 homolog

Chain O:



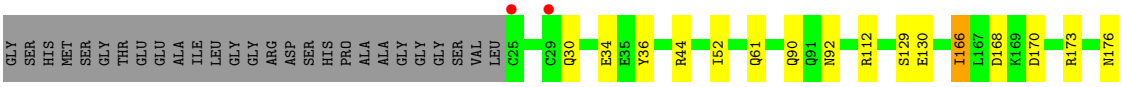


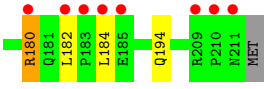


• Molecule 1: DNA repair protein RAD52 homolog

Chain P:



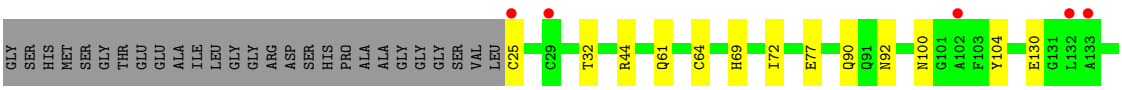


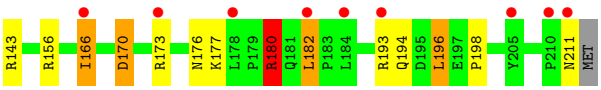


• Molecule 1: DNA repair protein RAD52 homolog

Chain Q:

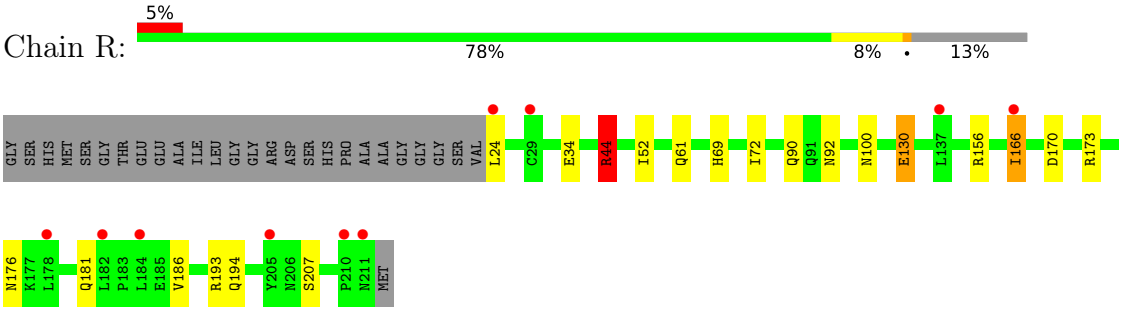






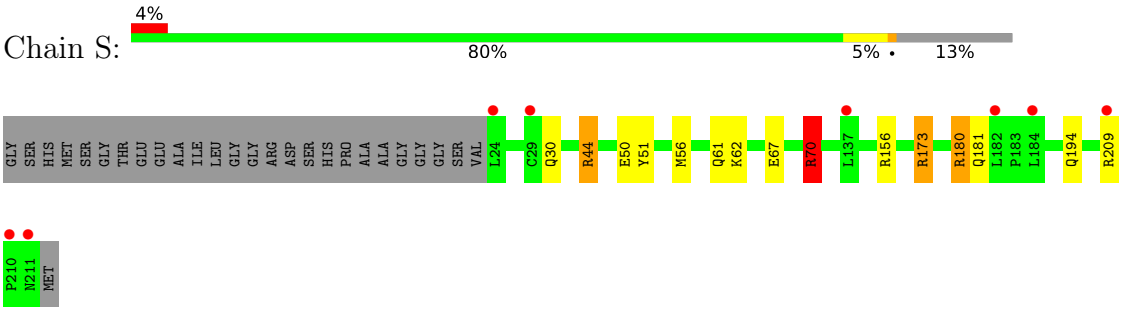
• Molecule 1: DNA repair protein RAD52 homolog

Chain R:



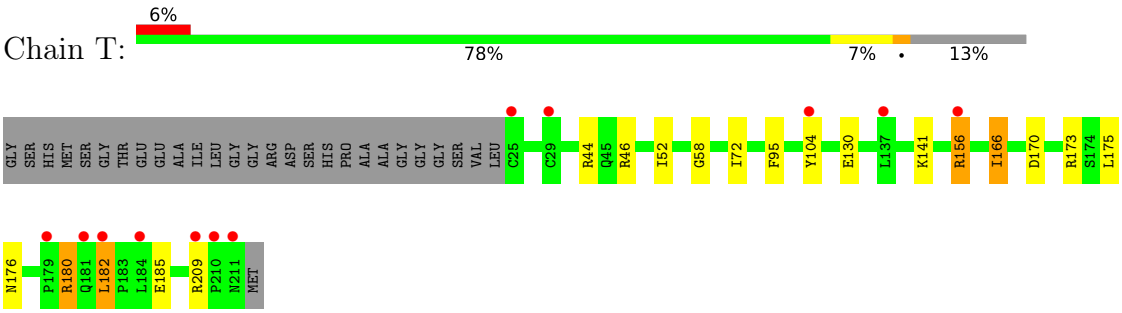
• Molecule 1: DNA repair protein RAD52 homolog

Chain S:



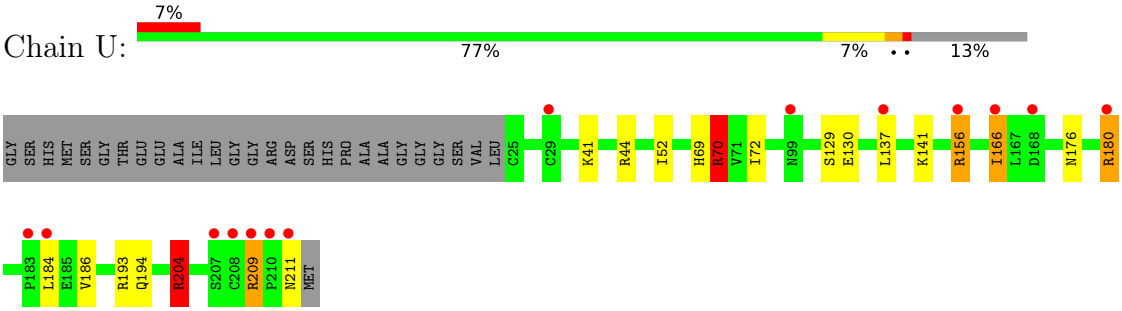
• Molecule 1: DNA repair protein RAD52 homolog

Chain T:



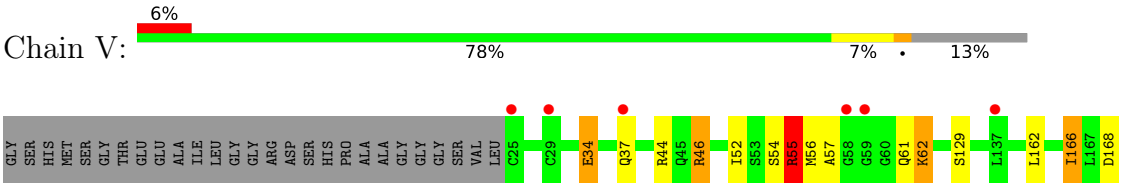
• Molecule 1: DNA repair protein RAD52 homolog

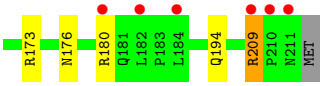
Chain U:



• Molecule 1: DNA repair protein RAD52 homolog

Chain V:




R173
N176
R180
Q181
L182
P183
L184
Q194
R209
P210
N211
MET

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	144.68Å 147.23Å 250.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.42 – 2.30 34.42 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.42-2.30) 100.0 (34.42-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.182 , 0.213 0.201 , 0.227	Depositor DCC
R_{free} test set	15179 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	47.8	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 72.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	34912	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, EDO, CL, A1KDF

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.72	0/1485	1.07	5/1999 (0.3%)
1	B	0.81	3/1520 (0.2%)	1.13	7/2047 (0.3%)
1	C	0.75	0/1522	1.09	6/2049 (0.3%)
1	D	0.73	0/1517	1.05	2/2041 (0.1%)
1	E	0.76	0/1514	1.05	5/2038 (0.2%)
1	F	0.74	0/1517	1.10	8/2043 (0.4%)
1	G	0.77	1/1495 (0.1%)	1.38	11/2013 (0.5%)
1	H	0.71	0/1506	1.05	6/2027 (0.3%)
1	I	0.71	0/1487	1.04	2/2002 (0.1%)
1	J	0.73	0/1506	1.09	6/2028 (0.3%)
1	K	0.72	0/1528	1.07	7/2058 (0.3%)
1	L	0.72	0/1509	1.07	4/2032 (0.2%)
1	M	0.74	0/1514	1.03	3/2038 (0.1%)
1	N	0.73	0/1498	1.08	6/2017 (0.3%)
1	O	0.75	0/1506	1.03	2/2028 (0.1%)
1	P	0.76	1/1501 (0.1%)	1.04	4/2021 (0.2%)
1	Q	0.77	1/1514 (0.1%)	1.13	8/2039 (0.4%)
1	R	0.74	0/1506	1.09	9/2028 (0.4%)
1	S	0.71	0/1507	1.09	6/2029 (0.3%)
1	T	0.69	0/1506	0.99	2/2028 (0.1%)
1	U	0.71	0/1493	1.08	6/2010 (0.3%)
1	V	0.78	1/1493 (0.1%)	1.17	11/2010 (0.5%)
All	All	0.74	7/33144 (0.0%)	1.09	126/44625 (0.3%)

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	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	3
1	E	0	4
1	F	0	3
1	G	0	9
1	H	0	4
1	I	0	5
1	J	0	4
1	K	0	6
1	L	0	3
1	M	0	4
1	N	0	4
1	O	0	4
1	P	0	1
1	Q	0	3
1	R	0	2
1	S	0	4
1	T	0	4
1	U	0	6
1	V	0	5
All	All	0	83

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	54	SER	C-N	-9.70	1.21	1.33
1	B	209	ARG	C-N	-9.65	1.21	1.33
1	G	208	CYS	C-N	-8.76	1.22	1.33
1	B	208	CYS	C-N	8.19	1.56	1.33
1	P	112	ARG	NE-CZ	5.76	1.39	1.33
1	Q	69	HIS	CG-CD2	-5.35	1.29	1.35
1	B	112	ARG	NE-CZ	5.34	1.39	1.33

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	209	ARG	CA-C-N	-20.77	99.95	120.52
1	G	209	ARG	C-N-CA	-20.77	99.95	120.52
1	G	209	ARG	O-C-N	13.53	137.74	121.10
1	G	208	CYS	CA-C-N	13.38	144.87	122.65
1	G	208	CYS	C-N-CA	13.38	144.87	122.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	208	CYS	O-C-N	-10.44	108.07	121.74
1	N	70	ARG	NE-CZ-NH1	-9.88	111.62	121.50
1	V	55	ARG	O-C-N	-9.39	111.80	123.17
1	U	70	ARG	NE-CZ-NH1	-9.20	112.30	121.50
1	A	208	CYS	CA-C-N	-8.62	107.44	123.55
1	A	208	CYS	C-N-CA	-8.62	107.44	123.55
1	V	62	LYS	CA-C-N	-8.53	111.76	123.10
1	V	62	LYS	C-N-CA	-8.53	111.76	123.10
1	L	156	ARG	NE-CZ-NH1	-8.52	112.98	121.50
1	B	181	GLN	CB-CA-C	7.54	122.65	110.29
1	I	183	PRO	N-CA-C	-7.49	102.76	113.47
1	R	181	GLN	CB-CA-C	7.49	122.73	110.22
1	Q	156	ARG	NE-CZ-NH1	7.41	128.91	121.50
1	S	56	MET	CG-SD-CE	7.41	117.21	100.90
1	L	156	ARG	NE-CZ-NH2	7.35	125.81	119.20
1	V	55	ARG	CA-C-N	7.25	132.41	122.19
1	V	55	ARG	C-N-CA	7.25	132.41	122.19
1	F	204	ARG	CD-NE-CZ	7.15	134.42	124.40
1	V	44	ARG	CG-CD-NE	-7.12	96.34	112.00
1	V	46	ARG	CA-CB-CG	7.08	128.26	114.10
1	B	181	GLN	N-CA-CB	-7.03	98.42	109.87
1	B	44	ARG	CG-CD-NE	-7.01	96.57	112.00
1	Q	180	ARG	CG-CD-NE	6.99	127.38	112.00
1	C	156	ARG	NE-CZ-NH2	-6.89	113.00	119.20
1	C	44	ARG	CG-CD-NE	-6.88	96.87	112.00
1	H	44	ARG	CG-CD-NE	-6.87	96.90	112.00
1	Q	44	ARG	CG-CD-NE	-6.73	97.19	112.00
1	T	44	ARG	CG-CD-NE	-6.67	97.33	112.00
1	M	204	ARG	NE-CZ-NH2	6.67	125.20	119.20
1	N	44	ARG	CG-CD-NE	-6.66	97.36	112.00
1	E	44	ARG	CG-CD-NE	-6.65	97.38	112.00
1	R	44	ARG	CB-CG-CD	6.63	126.56	111.30
1	H	156	ARG	NE-CZ-NH2	-6.63	113.24	119.20
1	P	44	ARG	CG-CD-NE	-6.55	97.58	112.00
1	J	44	ARG	CB-CA-C	-6.49	98.20	110.67
1	A	44	ARG	CG-CD-NE	-6.48	97.74	112.00
1	F	44	ARG	CG-CD-NE	-6.42	97.88	112.00
1	B	209	ARG	O-C-N	-6.32	113.61	121.64
1	K	156	ARG	NE-CZ-NH2	-6.31	113.52	119.20
1	S	156	ARG	CD-NE-CZ	6.26	133.16	124.40
1	G	193	ARG	CB-CG-CD	6.21	125.59	111.30
1	H	44	ARG	CB-CA-C	-6.21	97.32	110.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	V	44	ARG	CB-CA-C	-6.17	97.42	110.31
1	R	44	ARG	CB-CA-C	-6.17	97.42	110.31
1	U	44	ARG	CG-CD-NE	-6.16	98.45	112.00
1	F	204	ARG	NH1-CZ-NH2	6.12	127.25	119.30
1	Q	156	ARG	CD-NE-CZ	-6.10	115.86	124.40
1	R	181	GLN	N-CA-CB	-6.10	99.92	110.17
1	M	130	GLU	CB-CG-CD	6.08	122.94	112.60
1	S	70	ARG	NE-CZ-NH2	6.08	124.67	119.20
1	K	44	ARG	CB-CG-CD	6.08	125.27	111.30
1	B	204	ARG	CD-NE-CZ	6.07	132.89	124.40
1	E	44	ARG	CB-CA-C	-6.06	97.65	110.31
1	S	44	ARG	CB-CA-C	-6.02	97.74	110.31
1	F	44	ARG	CB-CA-C	-6.01	97.75	110.31
1	P	44	ARG	CB-CA-C	-6.00	97.77	110.31
1	Q	44	ARG	CB-CA-C	-6.00	97.77	110.31
1	C	180	ARG	CB-CG-CD	5.96	125.02	111.30
1	T	44	ARG	CB-CA-C	-5.96	97.85	110.31
1	B	44	ARG	CB-CA-C	-5.94	97.90	110.31
1	C	180	ARG	CA-CB-CG	5.94	125.97	114.10
1	A	44	ARG	CB-CA-C	-5.92	97.93	110.31
1	C	44	ARG	CB-CA-C	-5.92	97.93	110.31
1	L	156	ARG	CG-CD-NE	5.90	124.98	112.00
1	E	177	LYS	CG-CD-CE	5.89	124.85	111.30
1	U	44	ARG	CB-CA-C	-5.86	98.06	110.31
1	N	44	ARG	CB-CA-C	-5.85	98.08	110.31
1	K	44	ARG	CB-CA-C	-5.84	98.10	110.31
1	Q	170	ASP	CA-CB-CG	5.83	118.43	112.60
1	G	209	ARG	CG-CD-NE	5.82	124.80	112.00
1	K	209	ARG	CB-CA-C	5.80	117.79	109.26
1	Q	156	ARG	CB-CG-CD	-5.72	98.14	111.30
1	U	69	HIS	CB-CG-CD2	-5.71	123.78	131.20
1	H	168	ASP	CA-CB-CG	5.69	118.29	112.60
1	U	204	ARG	CD-NE-CZ	5.61	132.25	124.40
1	F	44	ARG	CD-NE-CZ	5.61	132.25	124.40
1	K	34	GLU	CB-CG-CD	5.61	122.13	112.60
1	N	156	ARG	NE-CZ-NH1	-5.59	115.91	121.50
1	G	130	GLU	CB-CG-CD	5.58	122.09	112.60
1	R	130	GLU	CB-CG-CD	5.55	122.04	112.60
1	G	169	LYS	CG-CD-CE	5.54	124.05	111.30
1	I	34	GLU	CB-CG-CD	5.53	122.00	112.60
1	F	187	ASP	CA-CB-CG	5.49	118.09	112.60
1	J	156	ARG	NE-CZ-NH2	-5.42	114.32	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	204	ARG	NE-CZ-NH1	-5.41	116.09	121.50
1	E	159	GLY	N-CA-C	5.40	117.90	110.56
1	H	156	ARG	NH1-CZ-NH2	5.38	126.29	119.30
1	G	209	ARG	C-N-CD	5.36	146.99	125.00
1	S	70	ARG	NE-CZ-NH1	-5.35	116.15	121.50
1	J	44	ARG	CB-CG-CD	5.34	123.58	111.30
1	B	209	ARG	CB-CA-C	5.33	117.11	109.11
1	K	156	ARG	NH1-CZ-NH2	5.33	126.23	119.30
1	R	69	HIS	CB-CG-CD2	-5.27	124.36	131.20
1	Q	182	LEU	CB-CG-CD1	5.26	126.47	110.70
1	J	69	HIS	CB-CG-CD2	-5.25	124.37	131.20
1	D	41	LYS	CG-CD-CE	5.24	123.36	111.30
1	S	44	ARG	CB-CG-CD	5.24	123.36	111.30
1	O	135	LYS	CG-CD-CE	5.23	123.32	111.30
1	N	69	HIS	CB-CG-CD2	-5.22	124.41	131.20
1	R	34	GLU	CB-CG-CD	5.21	121.46	112.60
1	J	153	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	P	34	GLU	CB-CG-CD	5.19	121.42	112.60
1	U	41	LYS	CG-CD-CE	5.18	123.22	111.30
1	C	34	GLU	CB-CG-CD	5.18	121.40	112.60
1	A	58	GLY	N-CA-C	-5.17	100.92	113.18
1	V	34	GLU	CB-CG-CD	5.15	121.36	112.60
1	F	190	LYS	CB-CG-CD	5.15	123.15	111.30
1	N	204	ARG	CD-NE-CZ	5.14	131.60	124.40
1	D	34	GLU	CB-CG-CD	5.13	121.32	112.60
1	H	130	GLU	CB-CG-CD	5.10	121.28	112.60
1	O	50	GLU	CB-CG-CD	5.09	121.26	112.60
1	M	69	HIS	CB-CG-CD2	-5.09	124.58	131.20
1	J	90	GLN	CG-CD-NE2	-5.09	108.77	116.40
1	R	44	ARG	CD-NE-CZ	5.08	131.51	124.40
1	E	44	ARG	CD-NE-CZ	5.07	131.50	124.40
1	R	69	HIS	CB-CG-ND1	5.07	130.31	122.70
1	P	168	ASP	CA-CB-CG	5.06	117.66	112.60
1	L	168	ASP	CA-CB-CG	5.06	117.66	112.60
1	V	56	MET	CG-SD-CE	5.06	112.02	100.90
1	K	168	ASP	CA-CB-CG	5.05	117.65	112.60
1	V	168	ASP	CA-CB-CG	5.03	117.63	112.60

There are no chirality outliers.

All (83) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	ARG	Sidechain
1	A	180	ARG	Sidechain
1	A	208	CYS	Mainchain
1	B	156	ARG	Sidechain
1	C	57	ALA	Peptide
1	D	156[A]	ARG	Sidechain
1	D	180	ARG	Sidechain
1	D	44	ARG	Sidechain
1	E	143	ARG	Sidechain
1	E	156	ARG	Sidechain
1	E	180	ARG	Sidechain
1	E	209	ARG	Sidechain
1	F	156	ARG	Sidechain
1	F	204	ARG	Sidechain
1	F	209	ARG	Sidechain
1	G	143	ARG	Sidechain
1	G	156	ARG	Sidechain
1	G	180	ARG	Sidechain
1	G	193	ARG	Sidechain
1	G	208	CYS	Mainchain
1	G	209	ARG	Sidechain
1	G	44	ARG	Sidechain
1	G	46	ARG	Sidechain
1	G	55	ARG	Sidechain
1	H	143	ARG	Sidechain
1	H	180	ARG	Sidechain
1	H	209	ARG	Sidechain
1	H	55	ARG	Sidechain
1	I	156	ARG	Sidechain
1	I	173	ARG	Sidechain
1	I	180	ARG	Sidechain
1	I	44	ARG	Sidechain
1	I	55	ARG	Sidechain
1	J	156	ARG	Sidechain
1	J	193	ARG	Sidechain
1	J	44	ARG	Sidechain
1	J	55	ARG	Sidechain
1	K	180	ARG	Sidechain
1	K	209	ARG	Sidechain
1	K	29[A]	CYS	Mainchain
1	K	29[B]	CYS	Mainchain
1	K	44	ARG	Sidechain
1	K	46	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	L	156	ARG	Sidechain
1	L	180	ARG	Sidechain
1	L	46	ARG	Sidechain
1	M	156	ARG	Sidechain
1	M	180	ARG	Sidechain
1	M	209	ARG	Sidechain
1	M	44	ARG	Sidechain
1	N	193	ARG	Sidechain
1	N	204	ARG	Sidechain
1	N	209	ARG	Sidechain
1	N	70	ARG	Sidechain
1	O	156	ARG	Sidechain
1	O	180	ARG	Sidechain
1	O	209	ARG	Sidechain
1	O	46	ARG	Sidechain
1	P	180	ARG	Sidechain
1	Q	143	ARG	Sidechain
1	Q	180	ARG	Sidechain
1	Q	193	ARG	Sidechain
1	R	156	ARG	Sidechain
1	R	44	ARG	Sidechain
1	S	173	ARG	Sidechain
1	S	209	ARG	Sidechain
1	S	44	ARG	Sidechain
1	S	70	ARG	Sidechain
1	T	156	ARG	Sidechain
1	T	180	ARG	Sidechain
1	T	209	ARG	Sidechain
1	T	46	ARG	Sidechain
1	U	156	ARG	Sidechain
1	U	180	ARG	Sidechain
1	U	193	ARG	Sidechain
1	U	204	ARG	Sidechain
1	U	209	ARG	Sidechain
1	U	70	ARG	Sidechain
1	V	173	ARG	Sidechain
1	V	180	ARG	Sidechain
1	V	209	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	14	0
1	B	1494	0	1460	11	0
1	C	1497	0	1464	12	0
1	D	1492	0	1460	13	0
1	E	1489	0	1459	15	0
1	F	1492	0	1463	21	0
1	G	1470	0	1435	15	0
1	H	1481	0	1454	7	0
1	I	1462	0	1430	16	0
1	J	1481	0	1450	15	0
1	K	1502	0	1465	26	0
1	L	1484	0	1453	20	0
1	M	1489	0	1464	11	0
1	N	1473	0	1444	12	0
1	O	1480	0	1451	14	0
1	P	1476	0	1448	9	0
1	Q	1488	0	1456	21	0
1	R	1481	0	1450	16	0
1	S	1482	0	1452	6	0
1	T	1480	0	1451	15	0
1	U	1468	0	1443	12	0
1	V	1468	0	1443	5	0
2	A	16	0	24	2	0
2	B	16	0	24	1	0
2	C	16	0	24	2	0
2	D	8	0	11	3	0
2	E	16	0	24	4	0
2	F	8	0	12	0	0
2	G	8	0	11	0	0
2	H	4	0	6	0	0
2	I	8	0	12	0	0
2	J	4	0	6	0	0
2	K	4	0	6	0	0
2	L	8	0	12	4	0
2	M	8	0	12	5	0
2	N	4	0	5	0	0
2	O	8	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	12	0	18	2	0
2	Q	8	0	12	0	0
2	R	8	0	12	2	0
2	S	12	0	18	1	0
2	T	8	0	12	5	0
2	U	12	0	18	3	0
2	V	8	0	12	1	0
3	A	37	0	0	0	0
3	B	37	0	0	0	0
3	C	37	0	0	0	0
3	D	37	0	0	0	0
3	E	74	0	0	0	0
3	G	37	0	0	1	0
3	H	37	0	0	0	0
3	I	74	0	0	0	0
3	K	37	0	0	0	0
3	L	37	0	0	1	0
3	M	37	0	0	0	0
3	N	37	0	0	0	0
3	O	37	0	0	0	0
3	P	37	0	0	0	0
3	Q	37	0	0	0	0
3	R	37	0	0	1	0
3	S	37	0	0	0	0
3	T	37	0	0	0	0
3	U	74	0	0	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
4	L	2	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	Q	1	0	0	0	0
4	R	2	0	0	0	0
4	T	2	0	0	0	0
4	U	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
5	E	1	0	0	0	0
5	F	2	0	0	0	0
5	G	2	0	0	0	0
5	H	1	0	0	0	0
5	J	1	0	0	0	0
5	L	1	0	0	0	0
5	M	3	0	0	0	0
5	N	2	0	0	0	0
5	O	2	0	0	0	0
5	P	2	0	0	0	0
5	Q	2	0	0	0	0
5	R	2	0	0	0	0
5	S	1	0	0	0	0
5	T	3	0	0	0	0
5	U	2	0	0	0	0
5	V	2	0	0	0	0
6	A	44	0	0	0	0
6	B	68	0	0	2	0
6	C	77	0	0	1	0
6	D	73	0	0	2	0
6	E	77	0	0	2	0
6	F	59	0	0	1	0
6	G	51	0	0	1	0
6	H	42	0	0	2	0
6	I	31	0	0	0	0
6	J	21	0	0	0	0
6	K	31	0	0	0	0
6	L	61	0	0	2	0
6	M	58	0	0	4	0
6	N	53	0	0	1	0
6	O	54	0	0	0	0
6	P	80	0	0	2	0
6	Q	85	0	0	2	0
6	R	56	0	0	4	0
6	S	46	0	0	3	0
6	T	54	0	0	2	0
6	U	63	0	0	7	0
6	V	65	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	34912	0	32235	261	0

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

All (261) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:78:MET:HE3	1:K:78:MET:HA	1.28	1.14
1:I:66:ILE:HD11	1:I:166:ILE:HD11	1.36	1.08
1:F:171:TYR:CE1	1:F:175:LEU:HD21	1.92	1.04
1:M:130:GLU:H	2:M:303:EDO:H11	1.23	1.02
1:F:171:TYR:CZ	1:F:175:LEU:HD21	1.96	1.00
1:R:90:GLN:HE21	1:R:92[B]:ASN:HD21	1.17	0.93
1:A:58:GLY:O	1:A:61:GLN:NE2	2.02	0.92
1:D:90:GLN:NE2	1:D:92[B]:ASN:OD1	2.04	0.90
1:S:173:ARG:NH1	6:S:401:HOH:O	2.04	0.88
1:I:66:ILE:CD1	1:I:166:ILE:HD11	2.04	0.86
1:R:130:GLU:H	2:R:303:EDO:H22	1.44	0.81
1:E:130:GLU:H	2:E:303:EDO:H22	1.44	0.81
1:F:171:TYR:CE2	1:F:175:LEU:HD11	2.15	0.80
1:N:99[A]:ASN:ND2	6:N:401:HOH:O	1.92	0.79
1:M:130:GLU:N	2:M:303:EDO:H11	1.98	0.79
1:E:112:ARG:HH22	1:E:114:GLN:HE21	1.31	0.77
1:G:112:ARG:HH22	1:G:114:GLN:HE21	1.31	0.77
1:R:90:GLN:NE2	1:R:92[B]:ASN:HD21	1.83	0.76
1:K:104[A]:TYR:HE1	1:K:130:GLU:OE2	1.69	0.74
1:C:100:ASN:O	1:O:98:LEU:HD23	1.86	0.74
1:Q:104[A]:TYR:CD1	1:Q:130:GLU:HG2	2.22	0.74
1:K:78:MET:HA	1:K:78:MET:CE	2.15	0.73
1:I:41:LYS:HA	1:I:44:ARG:HE	1.54	0.73
1:K:104[A]:TYR:CE1	1:K:130:GLU:OE2	2.41	0.73
1:J:112:ARG:HH12	1:J:114:GLN:HE21	1.37	0.72
1:B:104[A]:TYR:CD1	1:B:130:GLU:HG2	2.25	0.71
1:K:78:MET:HE3	1:K:78:MET:CA	2.17	0.71
1:F:211:ASN:HD21	1:G:207:SER:HA	1.55	0.70
1:Q:104[A]:TYR:HD1	1:Q:130:GLU:HG2	1.57	0.70
1:J:174:SER:O	1:J:178:LEU:HD13	1.92	0.69
1:J:200:VAL:HG21	1:K:78:MET:HE1	1.76	0.68
1:O:104[A]:TYR:CD1	1:O:130:GLU:HG2	2.29	0.68
1:R:90:GLN:HE21	1:R:92[B]:ASN:ND2	1.91	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:196:LEU:HD13	1:Q:198:PRO:HG3	1.76	0.67
1:F:204:ARG:HD2	1:H:36:TYR:OH	1.94	0.67
1:D:90:GLN:HA	2:D:303:EDO:H22	1.76	0.67
1:K:112:ARG:HH22	1:K:114:GLN:HE21	1.41	0.67
1:L:72:ILE:HD11	6:M:419:HOH:O	1.94	0.67
1:A:72:ILE:HD11	6:B:428:HOH:O	1.94	0.67
1:O:104[A]:TYR:HD1	1:O:130:GLU:HG2	1.60	0.67
1:B:204:ARG:HD2	1:D:36:TYR:OH	1.95	0.67
1:J:77:GLU:OE1	1:K:44:ARG:HD3	1.95	0.67
6:R:401:HOH:O	1:S:30:GLN:HG3	1.95	0.67
1:A:30:GLN:OE1	1:K:29[A]:CYS:SG	2.54	0.66
1:I:66:ILE:CG1	1:I:166:ILE:HD11	2.26	0.66
1:L:36:TYR:OH	1:U:204:ARG:HD2	1.94	0.66
1:Q:100:ASN:OD1	6:Q:401:HOH:O	2.15	0.65
1:A:129:SER:HA	2:A:301:EDO:H12	1.79	0.65
1:A:36:TYR:OH	1:J:204:ARG:HD2	1.98	0.64
1:E:211:ASN:HD21	1:G:34:GLU:H	1.45	0.64
1:L:90:GLN:HA	2:L:301:EDO:H12	1.79	0.63
1:B:104[A]:TYR:HD1	1:B:130:GLU:HG2	1.61	0.63
1:Q:211:ASN:HD21	1:R:207:SER:HA	1.62	0.63
1:U:130:GLU:H	2:U:304:EDO:H22	1.63	0.63
1:M:52:ILE:HD12	1:M:166:ILE:HD11	1.81	0.62
1:T:141:LYS:HE3	2:T:303:EDO:C2	2.30	0.62
1:U:129:SER:HA	2:U:304:EDO:H21	1.82	0.62
1:E:188:LEU:CD1	1:F:175:LEU:HD23	2.30	0.61
1:M:129:SER:HA	2:M:303:EDO:H11	1.82	0.60
1:T:52:ILE:HD12	1:T:166:ILE:HD11	1.83	0.59
1:F:171:TYR:O	1:F:175:LEU:HG	2.02	0.59
6:M:401:HOH:O	1:N:30:GLN:HG3	2.01	0.59
1:T:72:ILE:HD12	6:U:449:HOH:O	2.03	0.58
1:M:90:GLN:HA	2:M:302:EDO:H12	1.86	0.58
1:L:129:SER:HA	2:L:302:EDO:H22	1.86	0.58
1:C:204:ARG:HD2	1:E:36:TYR:OH	2.02	0.58
1:U:137:LEU:HB3	6:U:454:HOH:O	2.03	0.58
1:L:130:GLU:H	2:L:302:EDO:H21	1.69	0.57
1:E:201:GLU:OE1	6:E:401:HOH:O	2.17	0.57
1:Q:196:LEU:CD1	1:Q:198:PRO:HG3	2.34	0.57
1:M:129:SER:HA	2:M:303:EDO:C1	2.35	0.57
1:P:52:ILE:HD12	1:P:166:ILE:HD12	1.87	0.57
1:T:141:LYS:HE3	2:T:303:EDO:H21	1.86	0.57
1:D:90:GLN:HE21	1:D:92[B]:ASN:CG	2.12	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:435:HOH:O	2:E:306:EDO:H12	2.04	0.56
1:E:52:ILE:HD12	1:E:166:ILE:HD12	1.87	0.56
1:E:70:ARG:HH11	2:E:306:EDO:H11	1.70	0.56
1:A:57:ALA:O	1:A:58:GLY:C	2.48	0.56
1:Q:77:GLU:OE2	1:R:44:ARG:HD3	2.05	0.56
1:Q:104[A]:TYR:HE1	1:Q:130:GLU:OE2	1.87	0.56
1:K:98:LEU:HD23	1:R:100:ASN:O	2.05	0.56
1:Q:90:GLN:HE21	1:Q:92[A]:ASN:HD21	1.52	0.56
1:P:90:GLN:NE2	1:P:92[B]:ASN:HD21	2.05	0.55
1:N:204:ARG:HD2	1:P:36:TYR:OH	2.07	0.55
1:S:67:GLU:OE1	1:S:70:ARG:NH1	2.39	0.55
1:I:170:ASP:HA	1:I:173:ARG:HD2	1.86	0.55
1:D:211:ASN:HD21	1:F:34:GLU:H	1.54	0.55
1:L:72:ILE:CD1	6:M:419:HOH:O	2.54	0.55
1:D:90:GLN:HA	2:D:303:EDO:C2	2.37	0.54
1:F:172:LEU:HA	1:F:175:LEU:HD12	1.89	0.54
1:P:129:SER:HA	2:P:303:EDO:H21	1.88	0.54
1:K:52:ILE:HD12	1:K:166:ILE:HD12	1.88	0.54
1:D:52:ILE:HD12	1:D:166:ILE:HD12	1.87	0.54
1:F:52:ILE:HD12	1:F:166:ILE:HD12	1.89	0.54
1:R:72:ILE:HD11	6:S:409:HOH:O	2.08	0.54
1:V:129:SER:HA	2:V:302:EDO:H21	1.90	0.54
1:A:52:ILE:HD12	1:A:166:ILE:HD12	1.89	0.54
1:K:166:ILE:HG22	1:K:167:LEU:HD22	1.90	0.54
1:C:177:LYS:NZ	6:C:401:HOH:O	2.31	0.53
1:Q:90:GLN:HE21	1:Q:92[A]:ASN:ND2	2.06	0.53
1:U:211:ASN:ND2	6:U:402:HOH:O	2.42	0.53
1:E:211:ASN:ND2	1:G:34:GLU:H	2.06	0.53
1:V:52:ILE:HD12	1:V:166:ILE:HD12	1.91	0.53
1:B:104[A]:TYR:HE1	1:B:130:GLU:OE2	1.92	0.53
1:T:141:LYS:CE	2:T:303:EDO:H21	2.39	0.53
1:A:72:ILE:CD1	6:B:428:HOH:O	2.52	0.53
1:K:37:GLN:NE2	1:K:41:LYS:HG3	2.24	0.52
1:L:52:ILE:HD12	1:L:166:ILE:HD12	1.91	0.52
1:Q:170:ASP:OD1	1:Q:173:ARG:NH2	2.43	0.52
1:C:130:GLU:H	2:C:302:EDO:H11	1.74	0.52
1:G:188:LEU:O	1:G:193:ARG:NH2	2.43	0.52
1:K:104[A]:TYR:HD1	1:K:130:GLU:HB3	1.74	0.52
1:K:174:SER:HA	1:K:177:LYS:HD2	1.92	0.52
1:O:41:LYS:HA	1:O:44:ARG:HH21	1.75	0.52
1:E:188:LEU:HD11	1:F:175:LEU:HD23	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:72:ILE:HD11	6:P:429:HOH:O	2.09	0.52
1:B:104[A]:TYR:CE1	1:B:130:GLU:OE2	2.64	0.51
1:U:141:LYS:HE3	2:U:304:EDO:H12	1.92	0.51
1:I:98:LEU:C	1:I:98:LEU:CD2	2.84	0.51
1:J:52:ILE:HD12	1:J:166:ILE:HD12	1.92	0.51
1:N:52:ILE:HD12	1:N:166:ILE:HD12	1.92	0.51
1:P:90:GLN:HE21	1:P:92[B]:ASN:HD21	1.58	0.51
1:G:52:ILE:HD12	1:G:166:ILE:HD12	1.93	0.51
1:O:209:ARG:HD2	1:Q:32:THR:HA	1.91	0.51
1:L:36:TYR:OH	1:U:204:ARG:CD	2.59	0.51
1:Q:104[A]:TYR:CE1	1:Q:130:GLU:OE2	2.64	0.50
1:R:193:ARG:HH11	1:S:181:GLN:HE22	1.59	0.50
1:H:52:ILE:HD12	1:H:166:ILE:HD12	1.94	0.50
1:O:72:ILE:CD1	6:P:429:HOH:O	2.59	0.50
1:B:52:ILE:HD12	1:B:166:ILE:HD12	1.94	0.50
1:C:52:ILE:HD12	1:C:166:ILE:HD12	1.94	0.50
1:K:112:ARG:HH22	1:K:114:GLN:NE2	2.09	0.50
1:J:112:ARG:HH12	1:J:114:GLN:NE2	2.08	0.49
1:F:90:GLN:HE21	1:F:92[B]:ASN:CG	2.20	0.49
1:F:153:ARG:HA	1:F:156:ARG:HD3	1.93	0.49
6:G:410:HOH:O	1:H:30:GLN:HG3	2.12	0.49
1:K:182:LEU:HD23	1:K:182:LEU:H	1.78	0.49
1:O:104[A]:TYR:CE1	1:O:130:GLU:OE2	2.66	0.49
6:F:440:HOH:O	1:G:30:GLN:HG3	2.11	0.49
1:R:130:GLU:N	2:R:303:EDO:H22	2.20	0.49
1:L:90:GLN:HE21	1:L:92[A]:ASN:HD21	1.61	0.48
6:T:406:HOH:O	1:V:34:GLU:HG2	2.12	0.48
1:A:174:SER:HA	1:A:177:LYS:HD2	1.95	0.48
1:P:170:ASP:OD1	1:P:173:ARG:NH2	2.45	0.48
1:C:170:ASP:OD1	1:C:173:ARG:NH2	2.47	0.48
1:E:188:LEU:HD13	1:F:175:LEU:HD23	1.95	0.48
1:R:52:ILE:HD12	1:R:166:ILE:HD12	1.96	0.48
1:R:61:GLN:OE1	3:R:301:A1KDF:C9	2.62	0.48
1:G:72:ILE:HD11	6:H:414:HOH:O	2.12	0.48
1:D:170:ASP:OD1	1:D:173:ARG:NH2	2.47	0.48
1:K:170:ASP:OD1	1:K:173:ARG:NH2	2.47	0.48
1:Q:90:GLN:HE21	1:Q:92[A]:ASN:CG	2.22	0.48
1:V:55:ARG:NH1	1:V:57:ALA:HB2	2.28	0.48
2:D:303:EDO:H11	6:E:406:HOH:O	2.14	0.47
1:J:69:HIS:CD2	1:K:168:ASP:HB2	2.49	0.47
1:T:72:ILE:CD1	6:U:418:HOH:O	2.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:72:ILE:HD11	6:U:418:HOH:O	2.14	0.47
1:T:104[B]:TYR:CE1	6:T:405:HOH:O	2.67	0.47
1:G:112:ARG:HH22	1:G:114:GLN:NE2	2.07	0.47
1:Q:64:CYS:HB3	1:Q:166:ILE:HD11	1.95	0.47
1:L:50:GLU:HG3	1:L:181:GLN:HE22	1.79	0.47
1:L:36:TYR:CZ	1:U:204:ARG:HD3	2.50	0.47
1:A:170:ASP:OD1	1:A:173:ARG:NH2	2.47	0.47
1:J:56:MET:HG3	1:J:60:GLY:HA2	1.97	0.47
1:N:170:ASP:OD1	1:N:173:ARG:NH2	2.48	0.47
1:T:52:ILE:HG13	1:T:175:LEU:HD21	1.96	0.47
1:L:90:GLN:HE21	1:L:92[A]:ASN:ND2	2.12	0.47
1:L:90:GLN:HE21	1:L:92[A]:ASN:CG	2.22	0.47
1:L:130:GLU:H	2:L:302:EDO:C2	2.26	0.47
1:F:211:ASN:ND2	1:G:207:SER:HA	2.28	0.47
1:I:98:LEU:C	1:I:98:LEU:HD23	2.40	0.47
1:M:189:THR:HG23	1:M:190:LYS:HG3	1.97	0.47
1:U:52:ILE:HD12	1:U:166:ILE:HD12	1.95	0.47
1:A:61:GLN:HE21	1:A:61:GLN:HB2	1.49	0.47
1:B:97:ASP:HB3	2:B:302:EDO:H21	1.97	0.47
1:G:209:ARG:HD2	1:I:30:GLN:OE1	2.15	0.47
1:R:24:LEU:O	6:R:401:HOH:O	2.20	0.46
1:N:67:GLU:OE1	1:N:70:ARG:NH1	2.48	0.46
1:R:170:ASP:OD1	1:R:173:ARG:NH2	2.48	0.46
1:G:170:ASP:OD1	1:G:173:ARG:NH2	2.48	0.46
1:J:62:LYS:HB3	1:J:62:LYS:HE3	1.61	0.46
1:L:112:ARG:NE	6:L:401:HOH:O	2.33	0.46
1:L:170:ASP:OD1	1:L:173:ARG:NH2	2.48	0.46
1:N:204:ARG:NH2	1:O:78:MET:O	2.40	0.46
1:T:141:LYS:HE3	2:T:303:EDO:H22	1.97	0.46
1:G:72:ILE:CD1	6:H:414:HOH:O	2.64	0.46
1:S:180:ARG:HA	1:S:180:ARG:HD3	1.67	0.46
1:B:170:ASP:OD1	1:B:173:ARG:NH2	2.49	0.46
1:Q:196:LEU:HD13	1:Q:198:PRO:CG	2.45	0.46
1:M:170:ASP:OD1	1:M:173:ARG:NH2	2.48	0.46
1:F:171:TYR:CZ	1:F:175:LEU:HD11	2.51	0.45
1:T:170:ASP:OD1	1:T:173:ARG:NH2	2.48	0.45
1:H:170:ASP:OD1	1:H:173:ARG:NH2	2.49	0.45
1:B:204:ARG:CD	1:D:36:TYR:OH	2.64	0.45
1:F:204:ARG:CD	1:H:36:TYR:CZ	2.99	0.45
1:I:181:GLN:HG2	1:I:183:PRO:HD3	1.98	0.45
1:P:90:GLN:HE21	1:P:92[B]:ASN:ND2	2.14	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:36:TYR:CZ	1:U:204:ARG:CD	3.00	0.45
1:K:37:GLN:HE22	1:K:41:LYS:HG3	1.82	0.44
1:C:209:ARG:NH1	1:E:30:GLN:O	2.50	0.44
1:F:171:TYR:CE1	1:F:175:LEU:CD2	2.82	0.44
1:I:59:GLY:HA3	1:I:61:GLN:HE21	1.82	0.44
1:K:99[B]:ASN:HB2	1:K:104[B]:TYR:CE1	2.53	0.44
1:T:72:ILE:CD1	6:U:449:HOH:O	2.63	0.44
1:B:204:ARG:CD	1:D:36:TYR:CZ	3.01	0.44
1:L:173:ARG:HG3	6:L:424:HOH:O	2.18	0.44
1:M:24:LEU:O	6:M:401:HOH:O	2.21	0.44
1:Q:90:GLN:NE2	1:Q:92[A]:ASN:HD21	2.16	0.44
1:F:90:GLN:NE2	1:F:92[B]:ASN:HD21	2.16	0.43
1:I:98:LEU:HD23	1:I:99:ASN:N	2.33	0.43
1:K:167:LEU:HD22	1:K:167:LEU:N	2.32	0.43
1:N:182:LEU:HD23	1:N:182:LEU:H	1.82	0.43
1:R:72:ILE:CD1	6:S:409:HOH:O	2.65	0.43
6:D:418:HOH:O	1:E:30:GLN:HG3	2.17	0.43
1:J:24:LEU:HA	1:K:30:GLN:OE1	2.19	0.43
1:J:200:VAL:HG21	1:K:78:MET:CE	2.46	0.43
1:U:70:ARG:NH2	6:U:401:HOH:O	2.28	0.43
1:B:204:ARG:HD3	1:D:36:TYR:CZ	2.54	0.43
1:C:37:GLN:OE1	1:C:41:LYS:HD3	2.19	0.43
1:F:90:GLN:HE21	1:F:92[B]:ASN:ND2	2.16	0.43
1:S:51:TYR:CE1	2:S:303:EDO:H21	2.53	0.43
1:C:52:ILE:O	2:C:304:EDO:H12	2.20	0.42
1:M:209:ARG:HH11	1:O:30:GLN:HB3	1.84	0.42
1:K:29[A]:CYS:O	1:K:117:ASP:HA	2.19	0.42
1:Q:72:ILE:CD1	6:R:421:HOH:O	2.67	0.42
1:Q:177:LYS:HD2	6:Q:484:HOH:O	2.19	0.42
1:E:170:ASP:OD1	1:E:173:ARG:NH2	2.49	0.42
1:I:66:ILE:HG13	1:I:166:ILE:CD1	2.49	0.42
1:J:55:ARG:HG2	1:J:65:TYR:CE1	2.54	0.42
1:G:211:ASN:OD1	1:H:207:SER:HA	2.18	0.42
1:N:204:ARG:CD	1:P:36:TYR:OH	2.66	0.42
1:D:90:GLN:NE2	1:D:92[B]:ASN:CG	2.72	0.42
1:I:77:GLU:OE2	1:J:44:ARG:HD3	2.20	0.42
1:P:130:GLU:H	2:P:303:EDO:C2	2.33	0.41
1:A:90:GLN:HA	2:A:302:EDO:C2	2.50	0.41
1:N:136:ALA:H	1:O:104[A]:TYR:HH	1.59	0.41
1:E:90:GLN:HA	2:E:304:EDO:C2	2.51	0.41
1:A:208:CYS:HB2	1:C:33:ALA:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:204:ARG:HD3	1:H:36:TYR:CZ	2.55	0.41
1:I:99:ASN:HB3	1:I:104:TYR:HE2	1.84	0.41
1:T:95:PHE:HE2	1:T:104[B]:TYR:CD1	2.38	0.41
1:G:61:GLN:OE1	3:G:301:A1KDF:C10	2.68	0.41
1:N:204:ARG:NH2	1:O:79:PHE:HA	2.36	0.41
1:L:41:LYS:HA	1:L:44:ARG:HE	1.85	0.41
1:L:156:ARG:NH1	3:L:303:A1KDF:O6	2.53	0.41
1:N:135:LYS:N	1:O:104[A]:TYR:OH	2.53	0.41
1:C:204:ARG:NH2	1:D:78:MET:O	2.46	0.40
1:I:182:LEU:HD12	1:I:182:LEU:HA	1.90	0.40
1:J:170:ASP:OD1	1:J:173:ARG:NH2	2.48	0.40
1:O:209:ARG:H	1:O:209:ARG:HG3	1.49	0.40
1:C:90:GLN:HE21	1:C:92[B]:ASN:CG	2.29	0.40
1:I:183:PRO:O	1:I:185:GLU:HG3	2.21	0.40
1:A:181:GLN:H	1:A:181:GLN:HG3	1.76	0.40
1:K:78:MET:CE	1:K:78:MET:CA	2.90	0.40
1:T:130:GLU:O	2:T:303:EDO:H12	2.20	0.40
1:T:182:LEU:HD13	1:T:182:LEU:HA	1.91	0.40
1:U:72:ILE:HD12	6:V:455:HOH:O	2.22	0.40
1:M:180:ARG:HA	1:M:180:ARG:HD3	1.64	0.40
1:Q:72:ILE:HD11	6:R:421:HOH:O	2.21	0.40
1:Q:211:ASN:ND2	1:R:207:SER:HA	2.32	0.40
1:V:55:ARG:HH12	1:V:57:ALA:HB2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	184/215 (86%)	183 (100%)	1 (0%)	0	100	100
1	B	188/215 (87%)	188 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	189/215 (88%)	189 (100%)	0	0	100	100
1	D	188/215 (87%)	187 (100%)	1 (0%)	0	100	100
1	E	188/215 (87%)	188 (100%)	0	0	100	100
1	F	188/215 (87%)	187 (100%)	1 (0%)	0	100	100
1	G	186/215 (86%)	185 (100%)	1 (0%)	0	100	100
1	H	187/215 (87%)	186 (100%)	1 (0%)	0	100	100
1	I	185/215 (86%)	184 (100%)	1 (0%)	0	100	100
1	J	187/215 (87%)	185 (99%)	1 (0%)	1 (0%)	24	31
1	K	189/215 (88%)	187 (99%)	2 (1%)	0	100	100
1	L	187/215 (87%)	186 (100%)	1 (0%)	0	100	100
1	M	188/215 (87%)	188 (100%)	0	0	100	100
1	N	186/215 (86%)	185 (100%)	1 (0%)	0	100	100
1	O	186/215 (86%)	185 (100%)	1 (0%)	0	100	100
1	P	186/215 (86%)	186 (100%)	0	0	100	100
1	Q	187/215 (87%)	186 (100%)	1 (0%)	0	100	100
1	R	187/215 (87%)	187 (100%)	0	0	100	100
1	S	187/215 (87%)	186 (100%)	1 (0%)	0	100	100
1	T	186/215 (86%)	185 (100%)	0	1 (0%)	24	31
1	U	185/215 (86%)	185 (100%)	0	0	100	100
1	V	185/215 (86%)	184 (100%)	1 (0%)	0	100	100
All	All	4109/4730 (87%)	4092 (100%)	15 (0%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	58	GLY
1	T	58	GLY

5.3.2 Protein sidechains (i)

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%)	146 (95%)	7 (5%)	24	36
1	B	156/172 (91%)	152 (97%)	4 (3%)	40	59
1	C	157/172 (91%)	154 (98%)	3 (2%)	50	69
1	D	156/172 (91%)	149 (96%)	7 (4%)	24	37
1	E	156/172 (91%)	149 (96%)	7 (4%)	24	37
1	F	157/172 (91%)	154 (98%)	3 (2%)	50	69
1	G	153/172 (89%)	146 (95%)	7 (5%)	24	36
1	H	155/172 (90%)	150 (97%)	5 (3%)	34	51
1	I	152/172 (88%)	142 (93%)	10 (7%)	15	21
1	J	155/172 (90%)	146 (94%)	9 (6%)	18	26
1	K	158/172 (92%)	152 (96%)	6 (4%)	29	44
1	L	156/172 (91%)	152 (97%)	4 (3%)	40	59
1	M	156/172 (91%)	150 (96%)	6 (4%)	29	44
1	N	154/172 (90%)	147 (96%)	7 (4%)	24	37
1	O	155/172 (90%)	148 (96%)	7 (4%)	24	37
1	P	155/172 (90%)	147 (95%)	8 (5%)	21	31
1	Q	156/172 (91%)	148 (95%)	8 (5%)	21	32
1	R	155/172 (90%)	151 (97%)	4 (3%)	40	59
1	S	155/172 (90%)	149 (96%)	6 (4%)	28	43
1	T	155/172 (90%)	149 (96%)	6 (4%)	28	43
1	U	154/172 (90%)	146 (95%)	8 (5%)	21	31
1	V	154/172 (90%)	146 (95%)	8 (5%)	21	31
All	All	3413/3784 (90%)	3273 (96%)	140 (4%)	27	41

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	156	ARG
1	A	166	ILE
1	A	176	ASN
1	A	180	ARG
1	A	182	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	194	GLN
1	B	56	MET
1	B	61	GLN
1	B	166	ILE
1	B	176	ASN
1	C	99[A]	ASN
1	C	99[B]	ASN
1	C	166	ILE
1	D	56	MET
1	D	61	GLN
1	D	62	LYS
1	D	166	ILE
1	D	176	ASN
1	D	182	LEU
1	D	196	LEU
1	E	156	ARG
1	E	166	ILE
1	E	176	ASN
1	E	184	LEU
1	E	186	VAL
1	E	199	SER
1	E	209	ARG
1	F	166	ILE
1	F	185	GLU
1	F	209	ARG
1	G	56	MET
1	G	61	GLN
1	G	166	ILE
1	G	169	LYS
1	G	176	ASN
1	G	186	VAL
1	G	194	GLN
1	H	56	MET
1	H	166	ILE
1	H	176	ASN
1	H	194	GLN
1	H	209	ARG
1	I	61	GLN
1	I	98	LEU
1	I	156	ARG
1	I	166	ILE
1	I	173	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	176	ASN
1	I	180	ARG
1	I	186	VAL
1	I	194	GLN
1	I	209	ARG
1	J	55	ARG
1	J	56	MET
1	J	61	GLN
1	J	62	LYS
1	J	166	ILE
1	J	176	ASN
1	J	178	LEU
1	J	190	LYS
1	J	194	GLN
1	K	25	CYS
1	K	130	GLU
1	K	166	ILE
1	K	176	ASN
1	K	194	GLN
1	K	209	ARG
1	L	56	MET
1	L	61	GLN
1	L	166	ILE
1	L	176	ASN
1	M	166	ILE
1	M	176	ASN
1	M	180	ARG
1	M	184	LEU
1	M	194	GLN
1	M	199	SER
1	N	61	GLN
1	N	62	LYS
1	N	166	ILE
1	N	176	ASN
1	N	180	ARG
1	N	194	GLN
1	N	209	ARG
1	O	56	MET
1	O	61	GLN
1	O	176	ASN
1	O	182	LEU
1	O	184	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	194	GLN
1	O	209	ARG
1	P	30	GLN
1	P	61	GLN
1	P	166	ILE
1	P	176	ASN
1	P	180	ARG
1	P	182	LEU
1	P	184	LEU
1	P	194	GLN
1	Q	25	CYS
1	Q	61	GLN
1	Q	166	ILE
1	Q	176	ASN
1	Q	180	ARG
1	Q	182	LEU
1	Q	194	GLN
1	Q	196	LEU
1	R	166	ILE
1	R	176	ASN
1	R	186	VAL
1	R	194	GLN
1	S	50	GLU
1	S	61[A]	GLN
1	S	61[B]	GLN
1	S	62	LYS
1	S	180	ARG
1	S	194	GLN
1	T	156	ARG
1	T	166	ILE
1	T	176	ASN
1	T	180	ARG
1	T	182	LEU
1	T	185	GLU
1	U	156	ARG
1	U	166	ILE
1	U	176	ASN
1	U	180	ARG
1	U	184	LEU
1	U	186	VAL
1	U	194	GLN
1	U	209	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	V	37	GLN
1	V	61	GLN
1	V	62	LYS
1	V	162	LEU
1	V	166	ILE
1	V	176	ASN
1	V	194	GLN
1	V	209	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	61	GLN
1	A	90	GLN
1	B	28	GLN
1	B	30	GLN
1	B	211	ASN
1	C	28	GLN
1	C	30	GLN
1	C	90	GLN
1	C	194	GLN
1	D	30	GLN
1	D	61	GLN
1	D	90	GLN
1	D	211	ASN
1	E	28	GLN
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	90	GLN
1	F	211	ASN
1	G	45	GLN
1	G	114	GLN
1	H	92	ASN
1	H	99	ASN
1	H	181	GLN
1	I	28	GLN
1	I	45	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	61	GLN
1	I	69	HIS
1	I	100	ASN
1	J	90	GLN
1	J	114	GLN
1	J	181	GLN
1	K	37	GLN
1	K	61	GLN
1	K	114	GLN
1	K	206	ASN
1	L	30	GLN
1	L	45	GLN
1	L	90	GLN
1	L	181	GLN
1	L	206	ASN
1	M	45	GLN
1	M	61	GLN
1	M	92	ASN
1	M	181	GLN
1	N	30	GLN
1	N	45	GLN
1	N	181	GLN
1	P	61	GLN
1	P	90	GLN
1	Q	61	GLN
1	Q	90	GLN
1	Q	181	GLN
1	Q	194	GLN
1	Q	211	ASN
1	R	90	GLN
1	R	211	ASN
1	S	28	GLN
1	S	30	GLN
1	S	37	GLN
1	S	45	GLN
1	S	92	ASN
1	S	181	GLN
1	S	211	ASN
1	T	45	GLN
1	T	99	ASN
1	T	100	ASN
1	U	28	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	U	90	GLN
1	U	181	GLN
1	V	61	GLN
1	V	90	GLN
1	V	181	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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 129 ligands modelled in this entry, 56 are monoatomic - leaving 73 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	A1KDF	L	303	-	40,40,40	1.00	3 (7%)	53,55,55	1.58	7 (13%)
3	A1KDF	U	301	-	40,40,40	0.92	3 (7%)	53,55,55	1.98	8 (15%)
2	EDO	M	303	-	3,3,3	0.20	0	2,2,2	0.58	0
2	EDO	N	302	-	3,3,3	0.89	0	2,2,2	0.67	0
2	EDO	I	304	-	3,3,3	0.61	0	2,2,2	0.43	0
2	EDO	K	301	-	3,3,3	0.36	0	2,2,2	0.63	0
2	EDO	Q	302	-	3,3,3	0.60	0	2,2,2	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	A1KDF	C	301	-	40,40,40	0.97	2 (5%)	53,55,55	1.90	8 (15%)
3	A1KDF	E	305	-	40,40,40	0.91	3 (7%)	53,55,55	2.06	12 (22%)
2	EDO	A	304	-	3,3,3	1.72	0	2,2,2	1.58	1 (50%)
2	EDO	S	303	-	3,3,3	0.42	0	2,2,2	1.76	1 (50%)
2	EDO	S	304	-	3,3,3	0.90	0	2,2,2	0.85	0
3	A1KDF	U	303	-	40,40,40	1.09	3 (7%)	53,55,55	1.64	5 (9%)
2	EDO	H	302	-	3,3,3	0.88	0	2,2,2	0.92	0
2	EDO	U	305	-	3,3,3	0.26	0	2,2,2	0.32	0
3	A1KDF	S	301	-	40,40,40	0.94	3 (7%)	53,55,55	2.44	12 (22%)
3	A1KDF	O	301	-	40,40,40	0.85	1 (2%)	53,55,55	1.44	7 (13%)
2	EDO	A	303	-	3,3,3	0.34	0	2,2,2	0.48	0
3	A1KDF	B	301	-	40,40,40	1.08	4 (10%)	53,55,55	1.81	8 (15%)
2	EDO	C	304	-	3,3,3	0.96	0	2,2,2	1.35	0
2	EDO	P	302	-	3,3,3	0.36	0	2,2,2	0.74	0
2	EDO	I	303	-	3,3,3	0.30	0	2,2,2	1.20	0
2	EDO	L	302	-	3,3,3	0.58	0	2,2,2	0.75	0
2	EDO	P	304	-	3,3,3	0.40	0	2,2,2	0.09	0
3	A1KDF	A	305	-	40,40,40	1.03	4 (10%)	53,55,55	1.82	8 (15%)
3	A1KDF	P	301	-	40,40,40	1.14	4 (10%)	53,55,55	1.76	9 (16%)
2	EDO	G	302	-	3,3,3	0.98	0	2,2,2	1.05	0
3	A1KDF	M	301	-	40,40,40	0.79	3 (7%)	53,55,55	1.77	10 (18%)
3	A1KDF	R	301	-	40,40,40	0.84	1 (2%)	53,55,55	1.93	12 (22%)
2	EDO	R	303	-	3,3,3	0.49	0	2,2,2	0.87	0
2	EDO	D	303	-	3,3,3	0.80	0	2,2,2	1.29	0
3	A1KDF	T	301	-	40,40,40	0.82	1 (2%)	53,55,55	1.53	3 (5%)
2	EDO	S	302	-	3,3,3	0.50	0	2,2,2	0.44	0
2	EDO	B	302	-	3,3,3	0.87	0	2,2,2	0.52	0
2	EDO	A	301	-	3,3,3	0.60	0	2,2,2	0.66	0
2	EDO	C	302	-	3,3,3	0.16	0	2,2,2	0.70	0
2	EDO	D	302	-	3,3,3	0.27	0	2,2,2	0.48	0
3	A1KDF	K	302	-	40,40,40	0.93	1 (2%)	53,55,55	1.64	8 (15%)
2	EDO	U	304	-	3,3,3	0.73	0	2,2,2	1.04	0
2	EDO	T	303	-	3,3,3	0.21	0	2,2,2	0.49	0
2	EDO	M	302	-	3,3,3	0.50	0	2,2,2	0.76	0
2	EDO	O	302	-	3,3,3	0.55	0	2,2,2	1.00	0
3	A1KDF	G	301	-	40,40,40	0.91	1 (2%)	53,55,55	1.42	6 (11%)
2	EDO	G	303	-	3,3,3	0.81	0	2,2,2	0.58	0
3	A1KDF	N	301	-	40,40,40	0.91	2 (5%)	53,55,55	2.25	8 (15%)
2	EDO	E	302	-	3,3,3	0.23	0	2,2,2	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	EDO	J	301	-	3,3,3	0.46	0	2,2,2	0.49	0
3	A1KDF	Q	301	-	40,40,40	1.02	4 (10%)	53,55,55	1.65	7 (13%)
2	EDO	B	304	-	3,3,3	0.15	0	2,2,2	0.17	0
2	EDO	V	302	-	3,3,3	0.67	0	2,2,2	0.81	0
2	EDO	L	301	-	3,3,3	0.58	0	2,2,2	0.77	0
2	EDO	R	302	-	3,3,3	0.19	0	2,2,2	0.40	0
2	EDO	Q	303	-	3,3,3	0.52	0	2,2,2	0.86	0
3	A1KDF	E	301	-	40,40,40	0.89	2 (5%)	53,55,55	1.86	8 (15%)
2	EDO	O	303	-	3,3,3	0.22	0	2,2,2	0.39	0
2	EDO	C	303	-	3,3,3	0.52	0	2,2,2	1.03	0
2	EDO	B	303	-	3,3,3	0.16	0	2,2,2	0.18	0
2	EDO	E	303	-	3,3,3	0.13	0	2,2,2	0.91	0
2	EDO	T	302	-	3,3,3	0.27	0	2,2,2	0.39	0
2	EDO	U	302	-	3,3,3	0.18	0	2,2,2	0.41	0
2	EDO	V	301	-	3,3,3	0.70	0	2,2,2	0.50	0
2	EDO	C	305	-	3,3,3	0.16	0	2,2,2	1.10	0
3	A1KDF	I	302	-	40,40,40	0.93	2 (5%)	53,55,55	1.83	9 (16%)
2	EDO	A	302	-	3,3,3	0.51	0	2,2,2	1.00	0
2	EDO	F	302	-	3,3,3	0.35	0	2,2,2	1.06	0
2	EDO	B	305	-	3,3,3	0.61	0	2,2,2	0.59	0
2	EDO	P	303	-	3,3,3	0.62	0	2,2,2	0.65	0
3	A1KDF	D	301	-	40,40,40	0.98	3 (7%)	53,55,55	1.97	11 (20%)
3	A1KDF	H	301	-	40,40,40	0.96	4 (10%)	53,55,55	1.96	10 (18%)
2	EDO	E	306	-	3,3,3	0.32	0	2,2,2	0.72	0
2	EDO	F	301	-	3,3,3	0.52	0	2,2,2	0.50	0
2	EDO	E	304	-	3,3,3	0.53	0	2,2,2	0.65	0
3	A1KDF	I	301	-	40,40,40	1.03	2 (5%)	53,55,55	2.53	8 (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	A1KDF	L	303	-	-	4/26/26/26	0/4/4/4
3	A1KDF	U	301	-	-	10/26/26/26	0/4/4/4
2	EDO	M	303	-	-	1/1/1/1	-
2	EDO	N	302	-	-	1/1/1/1	-
2	EDO	I	304	-	-	0/1/1/1	-
2	EDO	K	301	-	-	1/1/1/1	-
2	EDO	Q	302	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1KDF	C	301	-	-	1/26/26/26	0/4/4/4
3	A1KDF	E	305	-	-	6/26/26/26	0/4/4/4
2	EDO	A	304	-	-	1/1/1/1	-
2	EDO	S	303	-	-	1/1/1/1	-
2	EDO	S	304	-	-	1/1/1/1	-
3	A1KDF	U	303	-	-	7/26/26/26	0/4/4/4
2	EDO	H	302	-	-	1/1/1/1	-
2	EDO	U	305	-	-	0/1/1/1	-
3	A1KDF	S	301	-	-	1/26/26/26	0/4/4/4
3	A1KDF	O	301	-	-	6/26/26/26	0/4/4/4
2	EDO	A	303	-	-	0/1/1/1	-
3	A1KDF	B	301	-	-	10/26/26/26	0/4/4/4
2	EDO	C	304	-	-	1/1/1/1	-
2	EDO	P	302	-	-	1/1/1/1	-
2	EDO	I	303	-	-	1/1/1/1	-
2	EDO	L	302	-	-	1/1/1/1	-
2	EDO	P	304	-	-	0/1/1/1	-
3	A1KDF	A	305	-	-	6/26/26/26	0/4/4/4
3	A1KDF	P	301	-	-	3/26/26/26	0/4/4/4
2	EDO	G	302	-	-	0/1/1/1	-
3	A1KDF	M	301	-	-	4/26/26/26	0/4/4/4
3	A1KDF	R	301	-	-	8/26/26/26	0/4/4/4
2	EDO	R	303	-	-	0/1/1/1	-
2	EDO	D	303	-	-	0/1/1/1	-
3	A1KDF	T	301	-	-	8/26/26/26	0/4/4/4
2	EDO	S	302	-	-	1/1/1/1	-
2	EDO	B	302	-	-	0/1/1/1	-
2	EDO	A	301	-	-	1/1/1/1	-
2	EDO	C	302	-	-	1/1/1/1	-
2	EDO	D	302	-	-	1/1/1/1	-
3	A1KDF	K	302	-	-	4/26/26/26	0/4/4/4
2	EDO	U	304	-	-	1/1/1/1	-
2	EDO	T	303	-	-	1/1/1/1	-
2	EDO	M	302	-	-	1/1/1/1	-
2	EDO	O	302	-	-	1/1/1/1	-
3	A1KDF	G	301	-	-	8/26/26/26	0/4/4/4
2	EDO	G	303	-	-	0/1/1/1	-
3	A1KDF	N	301	-	-	0/26/26/26	0/4/4/4
2	EDO	E	302	-	-	0/1/1/1	-
2	EDO	J	301	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1KDF	Q	301	-	-	7/26/26/26	0/4/4/4
2	EDO	B	304	-	-	1/1/1/1	-
2	EDO	V	302	-	-	1/1/1/1	-
2	EDO	L	301	-	-	1/1/1/1	-
2	EDO	R	302	-	-	1/1/1/1	-
2	EDO	Q	303	-	-	1/1/1/1	-
3	A1KDF	E	301	-	-	10/26/26/26	0/4/4/4
2	EDO	O	303	-	-	1/1/1/1	-
2	EDO	C	303	-	-	1/1/1/1	-
2	EDO	B	303	-	-	0/1/1/1	-
2	EDO	E	303	-	-	0/1/1/1	-
2	EDO	T	302	-	-	1/1/1/1	-
2	EDO	U	302	-	-	0/1/1/1	-
2	EDO	V	301	-	-	1/1/1/1	-
2	EDO	C	305	-	-	1/1/1/1	-
3	A1KDF	I	302	-	-	8/26/26/26	0/4/4/4
2	EDO	A	302	-	-	1/1/1/1	-
2	EDO	F	302	-	-	1/1/1/1	-
2	EDO	B	305	-	-	1/1/1/1	-
2	EDO	P	303	-	-	1/1/1/1	-
3	A1KDF	D	301	-	-	4/26/26/26	0/4/4/4
3	A1KDF	H	301	-	-	12/26/26/26	0/4/4/4
2	EDO	E	306	-	-	1/1/1/1	-
2	EDO	F	301	-	-	1/1/1/1	-
2	EDO	E	304	-	-	1/1/1/1	-
3	A1KDF	I	301	-	-	6/26/26/26	0/4/4/4

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	A1KDF	O4-C23	-3.89	1.19	1.30
3	I	301	A1KDF	C23-C22	3.79	1.55	1.48
3	U	303	A1KDF	C23-C22	3.53	1.55	1.48
3	P	301	A1KDF	O3-C23	3.53	1.32	1.22
3	P	301	A1KDF	C23-C22	3.41	1.54	1.48
3	N	301	A1KDF	O4-C23	-3.27	1.21	1.30
3	I	302	A1KDF	O5-C27	-3.26	1.21	1.30
3	L	303	A1KDF	O3-C23	3.09	1.30	1.22
3	K	302	A1KDF	O3-C23	2.94	1.30	1.22
3	Q	301	A1KDF	C27-C26	2.93	1.53	1.48
3	I	301	A1KDF	O3-C23	2.81	1.30	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	305	A1KDF	C22-C20	-2.72	1.33	1.37
3	Q	301	A1KDF	C26-C2	-2.66	1.33	1.37
3	U	301	A1KDF	O5-C27	-2.65	1.22	1.30
3	C	301	A1KDF	C22-C20	-2.63	1.33	1.37
3	A	305	A1KDF	O6-C27	2.62	1.29	1.22
3	G	301	A1KDF	C27-C26	2.62	1.53	1.48
3	O	301	A1KDF	O5-C27	-2.61	1.23	1.30
3	B	301	A1KDF	C23-C22	2.61	1.53	1.48
3	D	301	A1KDF	O5-C27	-2.61	1.23	1.30
3	S	301	A1KDF	C23-C22	2.61	1.53	1.48
3	H	301	A1KDF	O3-C23	2.56	1.29	1.22
3	H	301	A1KDF	O5-C27	-2.47	1.23	1.30
3	E	301	A1KDF	C26-C2	-2.44	1.33	1.37
3	S	301	A1KDF	C22-C20	-2.43	1.33	1.37
3	U	303	A1KDF	O5-C27	-2.40	1.23	1.30
3	Q	301	A1KDF	O6-C27	2.40	1.29	1.22
3	A	305	A1KDF	O4-C23	-2.38	1.23	1.30
3	P	301	A1KDF	O6-C27	2.36	1.28	1.22
3	L	303	A1KDF	C22-C20	-2.34	1.34	1.37
3	U	301	A1KDF	C22-C20	-2.32	1.34	1.37
3	E	305	A1KDF	C26-C2	-2.31	1.34	1.37
3	B	301	A1KDF	C22-C20	-2.27	1.34	1.37
3	P	301	A1KDF	C26-C2	-2.27	1.34	1.37
3	D	301	A1KDF	C22-C20	-2.23	1.34	1.37
3	C	301	A1KDF	O4-C23	-2.23	1.24	1.30
3	H	301	A1KDF	C23-C22	2.22	1.52	1.48
3	U	301	A1KDF	C26-C2	-2.20	1.34	1.37
3	E	301	A1KDF	C26-S2	-2.19	1.69	1.74
3	H	301	A1KDF	C22-C20	-2.18	1.34	1.37
3	S	301	A1KDF	C26-C2	-2.16	1.34	1.37
3	E	305	A1KDF	O5-C27	-2.12	1.24	1.30
3	M	301	A1KDF	C26-C2	-2.11	1.34	1.37
3	T	301	A1KDF	C26-C2	-2.10	1.34	1.37
3	L	303	A1KDF	C26-S2	-2.10	1.69	1.74
3	B	301	A1KDF	C27-C26	2.09	1.52	1.48
3	A	305	A1KDF	C20-N2	-2.08	1.33	1.38
3	M	301	A1KDF	O4-C23	-2.07	1.24	1.30
3	E	305	A1KDF	C19-S1	-2.07	1.69	1.74
3	I	302	A1KDF	O6-C27	2.05	1.28	1.22
3	N	301	A1KDF	C22-C20	-2.04	1.34	1.37
3	R	301	A1KDF	C22-C20	-2.04	1.34	1.37
3	M	301	A1KDF	C22-C20	-2.02	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	A1KDF	C26-S2	-2.02	1.70	1.74
3	U	303	A1KDF	C26-C2	-2.02	1.34	1.37
3	Q	301	A1KDF	C3-S2	-2.01	1.69	1.74

All (186) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	N	301	A1KDF	C19-N2-C20	10.62	116.39	111.22
3	I	301	A1KDF	C3-N1-C2	10.05	116.11	111.22
3	U	301	A1KDF	C19-N2-C20	9.84	116.02	111.22
3	H	301	A1KDF	C19-N2-C20	9.78	115.98	111.22
3	S	301	A1KDF	C19-N2-C20	9.64	115.92	111.22
3	E	305	A1KDF	C3-N1-C2	8.55	115.38	111.22
3	S	301	A1KDF	C3-N1-C2	8.40	115.31	111.22
3	E	301	A1KDF	C19-N2-C20	8.02	115.13	111.22
3	C	301	A1KDF	C19-N2-C20	7.99	115.11	111.22
3	Q	301	A1KDF	C3-N1-C2	7.50	114.88	111.22
3	M	301	A1KDF	C19-N2-C20	7.49	114.87	111.22
3	A	305	A1KDF	C3-N1-C2	7.28	114.77	111.22
3	B	301	A1KDF	C19-N2-C20	7.26	114.76	111.22
3	C	301	A1KDF	C3-N1-C2	7.14	114.70	111.22
3	I	301	A1KDF	C20-C22-S1	-7.13	105.21	109.92
3	I	301	A1KDF	C22-S1-C19	6.87	94.66	89.68
3	U	303	A1KDF	C3-N1-C2	6.73	114.50	111.22
3	I	302	A1KDF	C3-N1-C2	6.70	114.48	111.22
3	U	301	A1KDF	C3-N1-C2	6.31	114.29	111.22
3	P	301	A1KDF	C3-N1-C2	6.21	114.25	111.22
3	L	303	A1KDF	C3-N1-C2	6.18	114.23	111.22
3	T	301	A1KDF	C19-N2-C20	6.10	114.19	111.22
3	I	301	A1KDF	C19-N2-C20	6.08	114.18	111.22
3	A	305	A1KDF	C19-N2-C20	6.04	114.16	111.22
3	R	301	A1KDF	C20-C22-S1	-6.00	105.96	109.92
3	P	301	A1KDF	C19-N2-C20	5.98	114.13	111.22
3	T	301	A1KDF	C3-N1-C2	5.95	114.12	111.22
3	D	301	A1KDF	C2-C26-S2	-5.87	106.04	109.92
3	K	302	A1KDF	C3-N1-C2	5.66	113.98	111.22
3	M	301	A1KDF	C3-N1-C2	5.64	113.97	111.22
3	E	301	A1KDF	C3-N1-C2	5.59	113.94	111.22
3	O	301	A1KDF	C19-N2-C20	5.58	113.94	111.22
3	E	305	A1KDF	C19-N2-C20	5.46	113.88	111.22
3	D	301	A1KDF	C3-N1-C2	5.46	113.88	111.22
3	N	301	A1KDF	C22-S1-C19	5.45	93.63	89.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	U	303	A1KDF	C19-N2-C20	5.35	113.82	111.22
3	R	301	A1KDF	C22-S1-C19	5.32	93.53	89.68
3	L	303	A1KDF	C19-N2-C20	5.22	113.76	111.22
3	D	301	A1KDF	C26-S2-C3	5.12	93.39	89.68
3	R	301	A1KDF	C19-N2-C20	5.07	113.69	111.22
3	N	301	A1KDF	C3-N1-C2	4.84	113.58	111.22
3	N	301	A1KDF	S1-C19-N2	-4.82	107.39	114.85
3	D	301	A1KDF	C20-C22-S1	-4.79	106.76	109.92
3	I	302	A1KDF	C19-N2-C20	4.75	113.53	111.22
3	K	302	A1KDF	C19-N2-C20	4.68	113.50	111.22
3	B	301	A1KDF	C3-N1-C2	4.62	113.47	111.22
3	E	305	A1KDF	C26-C2-N1	-4.56	111.59	114.97
3	I	301	A1KDF	C26-S2-C3	4.55	92.98	89.68
3	N	301	A1KDF	C20-C22-S1	-4.54	106.92	109.92
3	S	301	A1KDF	C26-C2-N1	-4.49	111.64	114.97
3	I	301	A1KDF	S2-C3-N1	-4.46	107.93	114.85
3	R	301	A1KDF	O2-C13-C12	-4.41	91.95	108.33
3	G	301	A1KDF	C19-N2-C20	4.41	113.36	111.22
3	S	301	A1KDF	S1-C19-N2	-4.33	108.14	114.85
3	E	305	A1KDF	C20-C22-S1	-4.20	107.15	109.92
3	B	301	A1KDF	C2-C26-S2	-4.15	107.18	109.92
3	G	301	A1KDF	C22-C20-N2	-4.05	111.97	114.97
3	I	301	A1KDF	S1-C19-N2	-4.03	108.61	114.85
3	H	301	A1KDF	C3-N1-C2	4.00	113.17	111.22
3	S	301	A1KDF	C2-C26-S2	3.98	112.56	109.92
3	H	301	A1KDF	S1-C19-N2	-3.96	108.72	114.85
3	H	301	A1KDF	C22-S1-C19	3.94	92.53	89.68
3	S	301	A1KDF	C22-S1-C19	3.91	92.52	89.68
3	Q	301	A1KDF	C26-S2-C3	3.77	92.41	89.68
3	B	301	A1KDF	C26-S2-C3	3.76	92.41	89.68
3	C	301	A1KDF	C26-S2-C3	3.76	92.40	89.68
3	S	301	A1KDF	C20-C22-S1	-3.66	107.51	109.92
3	U	303	A1KDF	O2-C13-C12	-3.62	94.87	108.33
3	O	301	A1KDF	C3-N1-C2	3.62	112.98	111.22
3	A	305	A1KDF	C20-C22-S1	-3.60	107.54	109.92
3	D	301	A1KDF	S2-C3-N1	-3.51	109.41	114.85
3	D	301	A1KDF	C22-S1-C19	3.45	92.18	89.68
3	E	301	A1KDF	C26-S2-C3	3.41	92.15	89.68
3	R	301	A1KDF	S1-C19-N2	-3.41	109.57	114.85
3	G	301	A1KDF	C26-S2-C3	-3.39	87.23	89.68
3	D	301	A1KDF	C19-N2-C20	3.35	112.85	111.22
3	I	302	A1KDF	S1-C19-N2	-3.33	109.69	114.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	N	301	A1KDF	C18-C19-S1	3.31	129.30	122.29
3	P	301	A1KDF	C2-C26-S2	-3.30	107.74	109.92
3	Q	301	A1KDF	S2-C3-N1	-3.29	109.75	114.85
3	O	301	A1KDF	C1-C2-N1	-3.28	112.73	119.38
3	L	303	A1KDF	C20-C22-S1	3.26	112.08	109.92
3	I	302	A1KDF	C24-C18-C19	3.26	125.97	120.15
3	I	302	A1KDF	C26-C2-N1	-3.25	112.56	114.97
3	C	301	A1KDF	S1-C19-N2	-3.22	109.86	114.85
3	G	301	A1KDF	C3-N1-C2	3.19	112.77	111.22
3	E	301	A1KDF	C22-C20-N2	-3.19	112.61	114.97
3	A	305	A1KDF	S2-C3-N1	-3.16	109.95	114.85
3	E	305	A1KDF	S2-C3-N1	-3.09	110.06	114.85
3	E	301	A1KDF	C22-S1-C19	3.08	91.91	89.68
3	C	301	A1KDF	S2-C3-N1	-3.07	110.09	114.85
3	L	303	A1KDF	S2-C3-N1	-3.07	110.10	114.85
3	I	302	A1KDF	C2-C26-S2	3.05	111.94	109.92
3	R	301	A1KDF	C22-C20-N2	3.02	117.20	114.97
3	B	301	A1KDF	S2-C3-N1	-3.00	110.21	114.85
3	K	302	A1KDF	C20-C22-S1	-2.98	107.95	109.92
3	B	301	A1KDF	S1-C19-N2	-2.98	110.24	114.85
3	U	303	A1KDF	S2-C3-N1	-2.97	110.25	114.85
3	T	301	A1KDF	S1-C19-N2	-2.94	110.29	114.85
3	E	305	A1KDF	C22-S1-C19	2.90	91.78	89.68
3	M	301	A1KDF	C22-C20-N2	-2.89	112.83	114.97
3	U	301	A1KDF	S1-C19-N2	-2.88	110.39	114.85
3	D	301	A1KDF	C4-C3-S2	2.85	128.33	122.29
3	E	301	A1KDF	S2-C3-N1	-2.84	110.45	114.85
3	A	305	A1KDF	S1-C19-N2	-2.81	110.50	114.85
3	E	301	A1KDF	S1-C19-N2	-2.80	110.52	114.85
3	R	301	A1KDF	C1-C2-N1	-2.78	113.74	119.38
3	P	301	A1KDF	S1-C19-N2	-2.78	110.55	114.85
3	K	302	A1KDF	S1-C19-N2	-2.74	110.60	114.85
3	B	301	A1KDF	O1-C9-C10	-2.72	98.23	108.33
3	E	305	A1KDF	S1-C19-N2	-2.71	110.66	114.85
3	L	303	A1KDF	C22-C20-N2	-2.65	113.00	114.97
3	M	301	A1KDF	C2-C26-S2	2.64	111.67	109.92
3	D	301	A1KDF	C26-C2-N1	2.62	116.90	114.97
3	M	301	A1KDF	S2-C3-N1	-2.61	110.81	114.85
3	I	301	A1KDF	C4-C3-S2	2.59	127.78	122.29
3	H	301	A1KDF	C26-C2-N1	-2.57	113.06	114.97
3	D	301	A1KDF	S1-C19-N2	-2.55	110.91	114.85
3	K	302	A1KDF	C22-S1-C19	2.53	91.51	89.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	303	A1KDF	C26-S2-C3	2.50	91.49	89.68
3	H	301	A1KDF	C20-C22-S1	-2.49	108.28	109.92
3	M	301	A1KDF	C26-C2-N1	-2.48	113.13	114.97
3	I	302	A1KDF	S2-C3-N1	-2.48	111.00	114.85
3	I	302	A1KDF	C17-C18-C19	-2.47	116.97	120.73
3	U	301	A1KDF	C26-C2-N1	-2.47	113.14	114.97
3	A	305	A1KDF	C22-S1-C19	2.46	91.47	89.68
3	S	301	A1KDF	C18-C19-S1	2.44	127.47	122.29
3	S	301	A1KDF	C21-C20-N2	-2.39	114.53	119.38
3	U	301	A1KDF	C2-C26-S2	2.39	111.50	109.92
3	G	301	A1KDF	C1-C2-N1	-2.38	114.54	119.38
3	C	301	A1KDF	C18-C19-S1	2.37	127.30	122.29
3	K	302	A1KDF	C21-C20-N2	-2.36	114.60	119.38
3	C	301	A1KDF	C2-C26-S2	-2.35	108.37	109.92
3	P	301	A1KDF	C1-C2-N1	-2.34	114.62	119.38
3	O	301	A1KDF	C22-C20-N2	-2.33	113.24	114.97
3	E	305	A1KDF	C2-C26-S2	2.32	111.46	109.92
3	P	301	A1KDF	O1-C9-C10	-2.32	99.72	108.33
3	C	301	A1KDF	C20-C22-S1	2.31	111.45	109.92
3	Q	301	A1KDF	C21-C20-N2	-2.30	114.71	119.38
3	R	301	A1KDF	C13-O2-C14	2.29	123.92	117.93
3	M	301	A1KDF	S1-C19-N2	-2.29	111.31	114.85
3	S	301	A1KDF	S2-C3-N1	-2.28	111.31	114.85
3	M	301	A1KDF	O1-C8-C7	2.28	131.13	119.94
3	P	301	A1KDF	S2-C3-N1	-2.27	111.33	114.85
3	A	305	A1KDF	C26-C2-N1	-2.27	113.29	114.97
3	H	301	A1KDF	C23-C22-S1	2.26	123.74	114.92
3	R	301	A1KDF	C2-C26-S2	-2.26	108.43	109.92
3	M	301	A1KDF	O1-C8-C25	-2.26	109.03	119.86
3	Q	301	A1KDF	O1-C9-C10	-2.24	100.00	108.33
3	H	301	A1KDF	C26-S2-C3	-2.24	88.06	89.68
3	R	301	A1KDF	C18-C19-N2	2.23	127.28	123.47
3	N	301	A1KDF	S2-C3-N1	-2.23	111.39	114.85
3	S	301	A1KDF	C24-C18-C19	2.23	124.12	120.15
3	O	301	A1KDF	C20-C22-S1	2.22	111.40	109.92
3	P	301	A1KDF	C21-C20-N2	-2.22	114.87	119.38
2	A	304	EDO	O2-C2-C1	2.21	127.79	111.91
3	U	303	A1KDF	C4-C3-S2	2.20	126.95	122.29
3	I	302	A1KDF	C22-S1-C19	2.20	91.27	89.68
3	E	305	A1KDF	C26-S2-C3	2.16	91.25	89.68
3	Q	301	A1KDF	C2-C26-S2	-2.16	108.50	109.92
3	U	301	A1KDF	C20-C22-S1	-2.16	108.50	109.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	301	A1KDF	C18-C19-S1	2.13	126.80	122.29
3	B	301	A1KDF	C26-C2-N1	2.12	116.53	114.97
3	O	301	A1KDF	S2-C3-N1	-2.12	111.58	114.85
3	G	301	A1KDF	O2-C13-C12	-2.11	100.48	108.33
3	Q	301	A1KDF	C9-O1-C8	2.10	123.42	117.93
3	O	301	A1KDF	C21-C20-C22	2.10	131.26	127.14
3	N	301	A1KDF	C23-C22-S1	2.09	123.07	114.92
3	E	305	A1KDF	O1-C8-C7	2.09	130.22	119.94
3	E	305	A1KDF	O3-C23-C22	-2.08	114.61	121.06
3	A	305	A1KDF	C23-C22-S1	2.08	123.02	114.92
3	K	302	A1KDF	S2-C3-N1	-2.08	111.64	114.85
3	D	301	A1KDF	C22-C20-N2	2.07	116.50	114.97
3	U	301	A1KDF	S2-C3-N1	-2.06	111.67	114.85
3	E	301	A1KDF	O6-C27-C26	-2.05	114.69	121.06
3	R	301	A1KDF	C26-C2-N1	2.04	116.47	114.97
3	M	301	A1KDF	C4-C25-C8	2.03	121.74	119.57
3	R	301	A1KDF	C3-N1-C2	2.03	112.21	111.22
3	L	303	A1KDF	C4-C3-S2	2.03	126.58	122.29
3	U	301	A1KDF	C4-C3-S2	2.02	126.57	122.29
3	K	302	A1KDF	O6-C27-C26	-2.02	114.79	121.06
3	P	301	A1KDF	C22-S1-C19	2.02	91.15	89.68
3	H	301	A1KDF	C2-C26-S2	2.02	111.26	109.92
3	S	301	A1KDF	O2-C14-C24	2.02	129.52	119.86
3	E	305	A1KDF	C9-O1-C8	2.01	123.19	117.93
2	S	303	EDO	O1-C1-C2	-2.01	97.42	111.91

There are no chirality outliers.

All (170) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	301	A1KDF	C20-C22-C23-O3
3	H	301	A1KDF	C20-C22-C23-O4
3	H	301	A1KDF	S1-C22-C23-O3
3	H	301	A1KDF	S1-C22-C23-O4
3	U	301	A1KDF	C20-C22-C23-O3
3	U	301	A1KDF	C20-C22-C23-O4
3	G	301	A1KDF	C10-C11-C12-C13
3	A	305	A1KDF	C24-C14-O2-C13
3	O	301	A1KDF	C25-C8-O1-C9
3	U	301	A1KDF	C25-C8-O1-C9
3	O	301	A1KDF	C7-C8-O1-C9
3	U	301	A1KDF	C7-C8-O1-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	305	A1KDF	C15-C14-O2-C13
3	R	301	A1KDF	C10-C11-C12-C13
3	I	301	A1KDF	C25-C8-O1-C9
3	I	301	A1KDF	C7-C8-O1-C9
3	R	301	A1KDF	C25-C8-O1-C9
3	G	301	A1KDF	C15-C14-O2-C13
3	I	302	A1KDF	C7-C8-O1-C9
3	I	302	A1KDF	C25-C8-O1-C9
3	R	301	A1KDF	C7-C8-O1-C9
3	U	303	A1KDF	C10-C11-C12-C13
3	G	301	A1KDF	C24-C14-O2-C13
3	R	301	A1KDF	C11-C12-C13-O2
3	U	303	A1KDF	C15-C14-O2-C13
3	T	301	A1KDF	C11-C10-C9-O1
3	M	301	A1KDF	C11-C10-C9-O1
3	T	301	A1KDF	C11-C12-C13-O2
3	U	303	A1KDF	C24-C14-O2-C13
3	E	301	A1KDF	C15-C14-O2-C13
3	H	301	A1KDF	C24-C14-O2-C13
3	I	302	A1KDF	C9-C10-C11-C12
3	E	305	A1KDF	C9-C10-C11-C12
3	H	301	A1KDF	C15-C14-O2-C13
3	I	301	A1KDF	C9-C10-C11-C12
3	K	302	A1KDF	C9-C10-C11-C12
3	O	301	A1KDF	C9-C10-C11-C12
3	B	301	A1KDF	C7-C8-O1-C9
3	Q	301	A1KDF	C7-C8-O1-C9
3	B	301	A1KDF	C10-C11-C12-C13
3	T	301	A1KDF	C10-C11-C12-C13
3	E	301	A1KDF	C24-C14-O2-C13
2	A	302	EDO	O1-C1-C2-O2
2	C	305	EDO	O1-C1-C2-O2
2	D	302	EDO	O1-C1-C2-O2
2	F	301	EDO	O1-C1-C2-O2
2	H	302	EDO	O1-C1-C2-O2
2	L	302	EDO	O1-C1-C2-O2
2	M	302	EDO	O1-C1-C2-O2
2	M	303	EDO	O1-C1-C2-O2
2	N	302	EDO	O1-C1-C2-O2
2	P	303	EDO	O1-C1-C2-O2
2	Q	303	EDO	O1-C1-C2-O2
2	R	302	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	S	302	EDO	O1-C1-C2-O2
2	T	302	EDO	O1-C1-C2-O2
2	T	303	EDO	O1-C1-C2-O2
2	V	302	EDO	O1-C1-C2-O2
3	H	301	A1KDF	C9-C10-C11-C12
3	B	301	A1KDF	C25-C8-O1-C9
3	E	301	A1KDF	C9-C10-C11-C12
3	Q	301	A1KDF	C10-C11-C12-C13
3	G	301	A1KDF	C10-C9-O1-C8
3	E	301	A1KDF	C10-C9-O1-C8
3	E	305	A1KDF	C12-C13-O2-C14
3	B	301	A1KDF	C15-C14-O2-C13
3	H	301	A1KDF	C12-C13-O2-C14
3	Q	301	A1KDF	C12-C13-O2-C14
3	Q	301	A1KDF	C25-C8-O1-C9
3	Q	301	A1KDF	C10-C9-O1-C8
3	K	302	A1KDF	C10-C9-O1-C8
3	R	301	A1KDF	C15-C14-O2-C13
3	E	301	A1KDF	C11-C12-C13-O2
3	E	305	A1KDF	C10-C11-C12-C13
3	I	301	A1KDF	C10-C11-C12-C13
3	O	301	A1KDF	C10-C11-C12-C13
3	G	301	A1KDF	C12-C13-O2-C14
3	U	303	A1KDF	C10-C9-O1-C8
3	B	301	A1KDF	C10-C9-O1-C8
3	R	301	A1KDF	C12-C13-O2-C14
3	B	301	A1KDF	C11-C10-C9-O1
3	E	305	A1KDF	C10-C9-O1-C8
3	B	301	A1KDF	C24-C14-O2-C13
3	A	305	A1KDF	C11-C10-C9-O1
3	E	301	A1KDF	C12-C13-O2-C14
3	K	302	A1KDF	C7-C8-O1-C9
3	U	301	A1KDF	C9-C10-C11-C12
3	G	301	A1KDF	C11-C10-C9-O1
2	A	301	EDO	O1-C1-C2-O2
2	C	303	EDO	O1-C1-C2-O2
2	E	304	EDO	O1-C1-C2-O2
2	Q	302	EDO	O1-C1-C2-O2
3	H	301	A1KDF	C7-C8-O1-C9
3	H	301	A1KDF	C11-C12-C13-O2
3	H	301	A1KDF	C25-C8-O1-C9
3	I	302	A1KDF	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	U	303	A1KDF	C7-C8-O1-C9
3	R	301	A1KDF	C24-C14-O2-C13
3	M	301	A1KDF	C10-C9-O1-C8
3	D	301	A1KDF	C25-C8-O1-C9
3	G	301	A1KDF	C25-C8-O1-C9
3	I	302	A1KDF	C15-C14-O2-C13
3	U	303	A1KDF	C12-C13-O2-C14
3	E	305	A1KDF	S2-C26-C27-O5
3	U	301	A1KDF	S1-C22-C23-O3
3	U	301	A1KDF	S1-C22-C23-O4
3	G	301	A1KDF	C7-C8-O1-C9
3	U	303	A1KDF	C25-C8-O1-C9
3	K	302	A1KDF	C25-C8-O1-C9
3	S	301	A1KDF	C10-C11-C12-C13
2	A	304	EDO	O1-C1-C2-O2
2	P	302	EDO	O1-C1-C2-O2
3	Q	301	A1KDF	C11-C10-C9-O1
3	I	302	A1KDF	C24-C14-O2-C13
3	L	303	A1KDF	C25-C8-O1-C9
3	A	305	A1KDF	C9-C10-C11-C12
3	T	301	A1KDF	C12-C13-O2-C14
3	U	301	A1KDF	C12-C13-O2-C14
2	U	304	EDO	O1-C1-C2-O2
3	D	301	A1KDF	C7-C8-O1-C9
3	E	301	A1KDF	C10-C11-C12-C13
3	I	302	A1KDF	C10-C9-O1-C8
3	T	301	A1KDF	C9-C10-C11-C12
3	T	301	A1KDF	C10-C9-O1-C8
3	T	301	A1KDF	S1-C22-C23-O4
3	L	303	A1KDF	C7-C8-O1-C9
3	U	301	A1KDF	C11-C12-C13-O2
3	E	301	A1KDF	C20-C22-C23-O3
3	E	305	A1KDF	C2-C26-C27-O5
2	B	304	EDO	O1-C1-C2-O2
2	C	302	EDO	O1-C1-C2-O2
2	L	301	EDO	O1-C1-C2-O2
2	O	303	EDO	O1-C1-C2-O2
2	S	303	EDO	O1-C1-C2-O2
3	D	301	A1KDF	C10-C9-O1-C8
3	I	301	A1KDF	C10-C9-O1-C8
3	Q	301	A1KDF	C9-C10-C11-C12
3	D	301	A1KDF	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	P	301	A1KDF	C9-C10-C11-C12
2	O	302	EDO	O1-C1-C2-O2
2	S	304	EDO	O1-C1-C2-O2
3	B	301	A1KDF	C9-C10-C11-C12
3	L	303	A1KDF	C10-C9-O1-C8
3	A	305	A1KDF	S2-C26-C27-O6
3	M	301	A1KDF	S2-C26-C27-O5
3	T	301	A1KDF	S1-C22-C23-O3
3	A	305	A1KDF	C12-C13-O2-C14
3	U	301	A1KDF	C10-C11-C12-C13
3	O	301	A1KDF	C12-C13-O2-C14
2	F	302	EDO	O1-C1-C2-O2
3	I	301	A1KDF	C12-C13-O2-C14
3	O	301	A1KDF	C10-C9-O1-C8
3	H	301	A1KDF	C10-C9-O1-C8
3	P	301	A1KDF	C12-C13-O2-C14
3	C	301	A1KDF	C12-C13-O2-C14
3	B	301	A1KDF	C2-C26-C27-O6
3	E	301	A1KDF	C20-C22-C23-O4
3	P	301	A1KDF	C20-C22-C23-O4
3	B	301	A1KDF	C12-C13-O2-C14
3	I	302	A1KDF	C12-C13-O2-C14
2	E	306	EDO	O1-C1-C2-O2
2	I	303	EDO	O1-C1-C2-O2
2	K	301	EDO	O1-C1-C2-O2
2	V	301	EDO	O1-C1-C2-O2
3	L	303	A1KDF	C11-C12-C13-O2
3	E	301	A1KDF	C25-C8-O1-C9
3	R	301	A1KDF	C24-C18-C19-N2
2	B	305	EDO	O1-C1-C2-O2
2	C	304	EDO	O1-C1-C2-O2
3	M	301	A1KDF	C10-C11-C12-C13

There are no ring outliers.

22 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	303	A1KDF	1	0
2	M	303	EDO	4	0
2	S	303	EDO	1	0
2	C	304	EDO	1	0
2	L	302	EDO	3	0

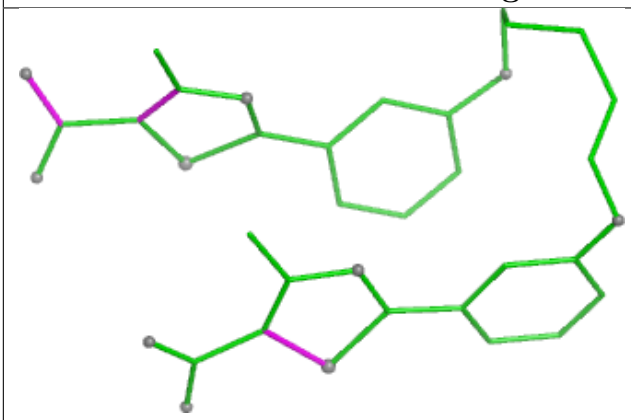
Continued on next page...

Continued from previous page...

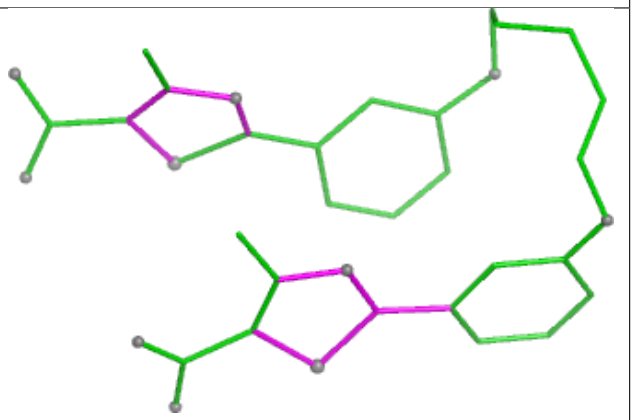
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	301	A1KDF	1	0
2	R	303	EDO	2	0
2	D	303	EDO	3	0
2	B	302	EDO	1	0
2	A	301	EDO	1	0
2	C	302	EDO	1	0
2	U	304	EDO	3	0
2	T	303	EDO	5	0
2	M	302	EDO	1	0
3	G	301	A1KDF	1	0
2	V	302	EDO	1	0
2	L	301	EDO	1	0
2	E	303	EDO	1	0
2	A	302	EDO	1	0
2	P	303	EDO	2	0
2	E	306	EDO	2	0
2	E	304	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 then 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.

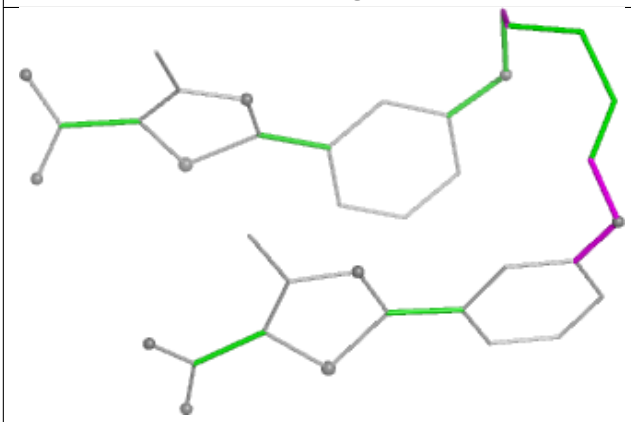
Ligand A1KDF L 303



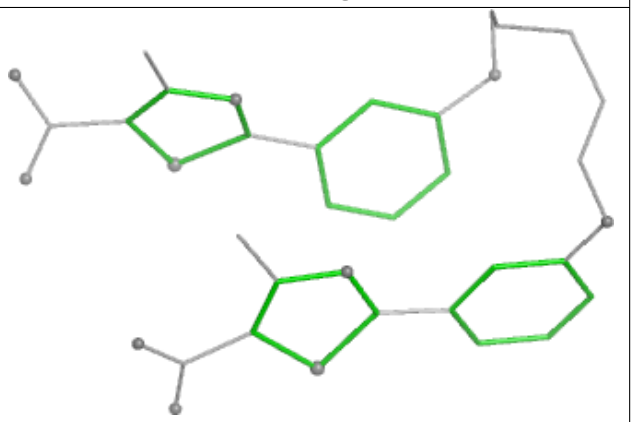
Bond lengths



Bond angles

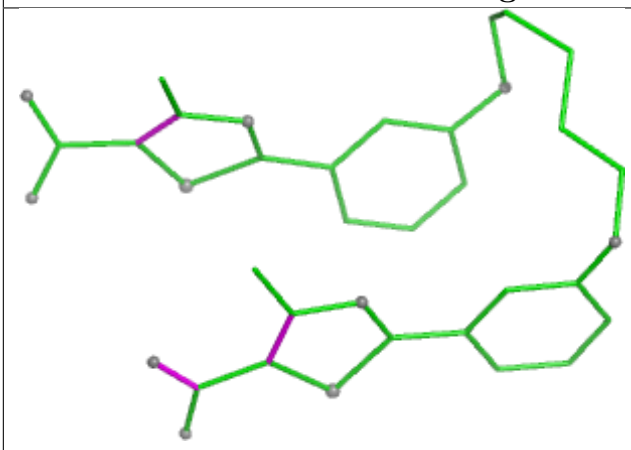


Torsions

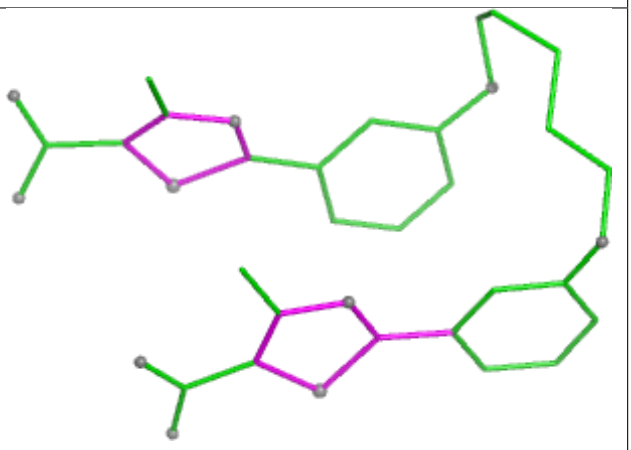


Rings

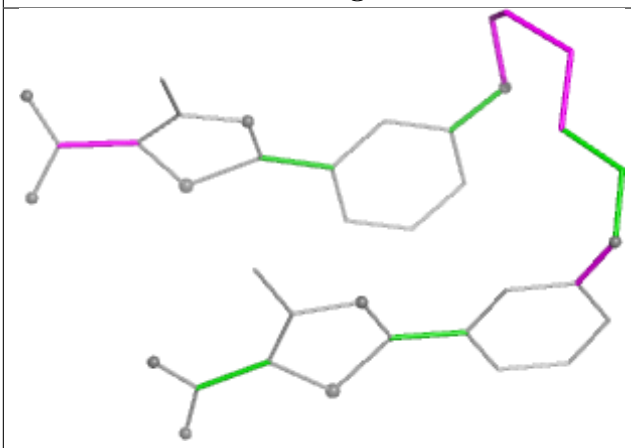
Ligand A1KDF U 301



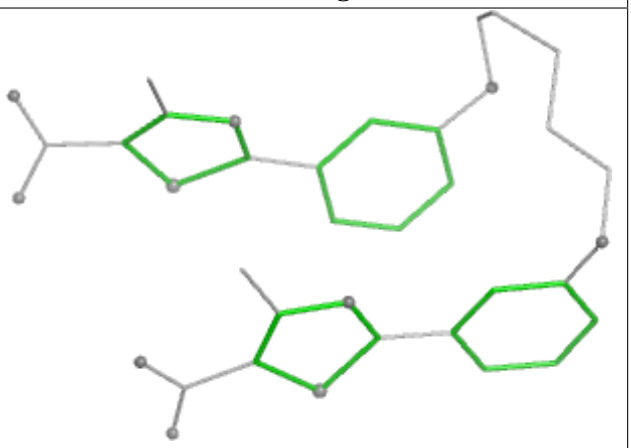
Bond lengths



Bond angles

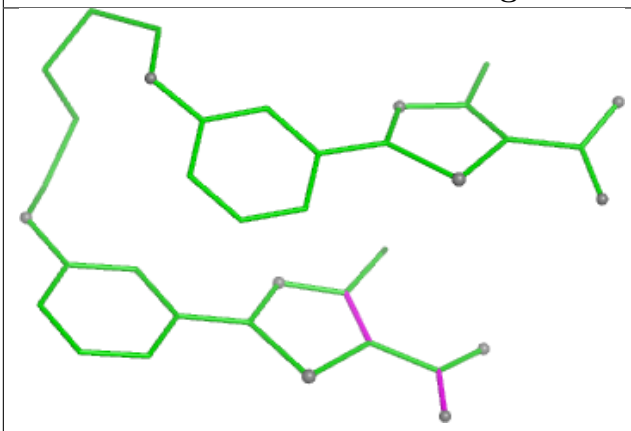


Torsions

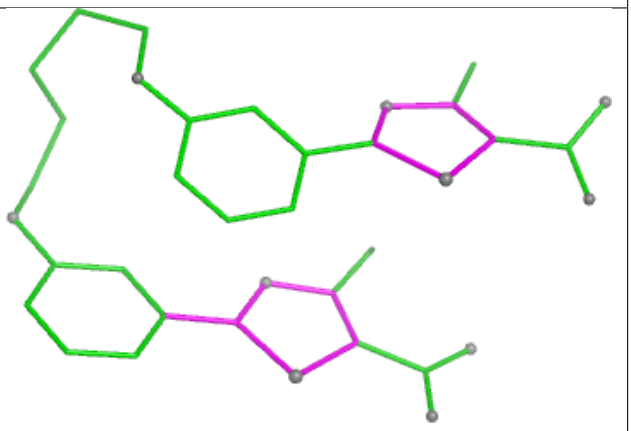


Rings

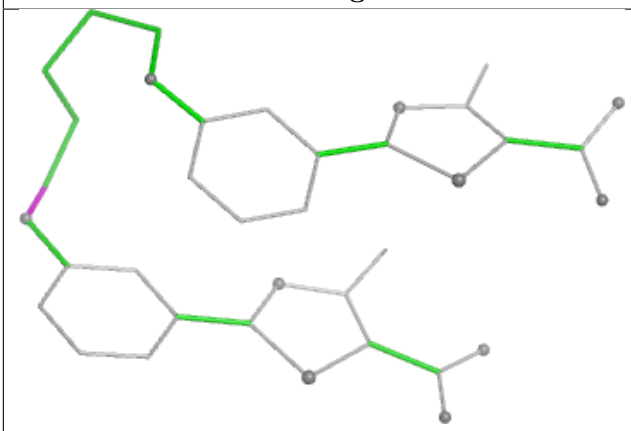
Ligand A1KDF C 301



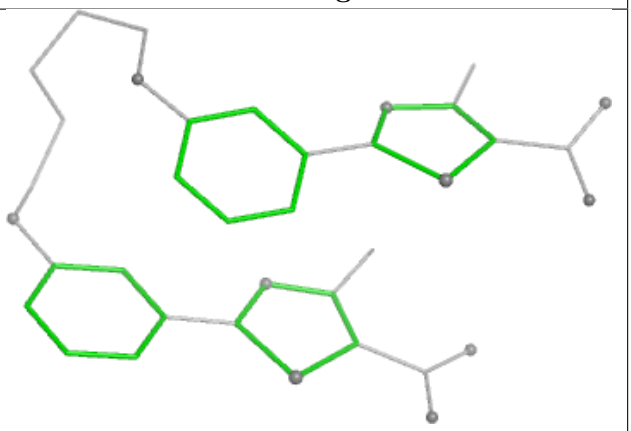
Bond lengths



Bond angles

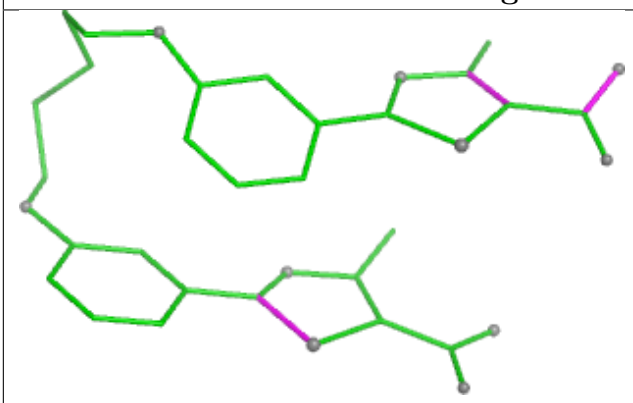


Torsions

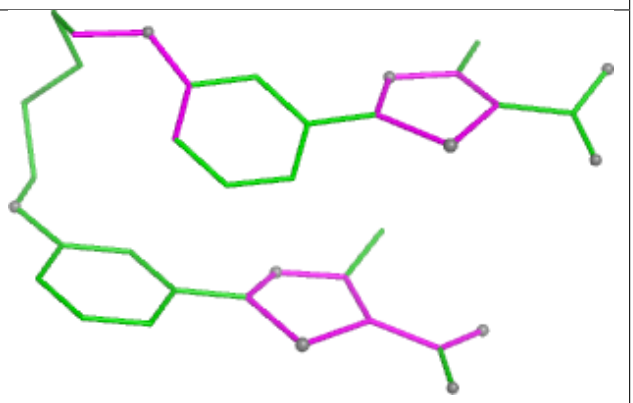


Rings

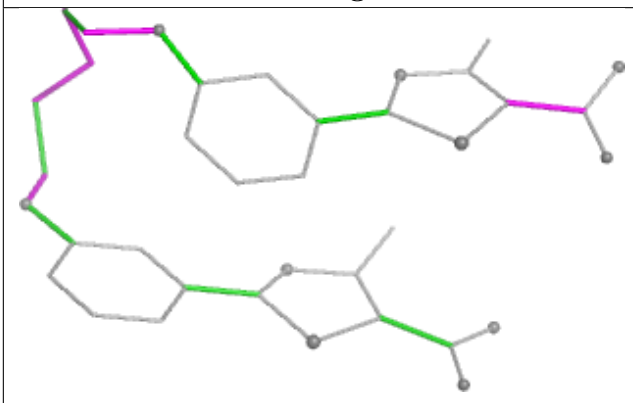
Ligand A1KDF E 305



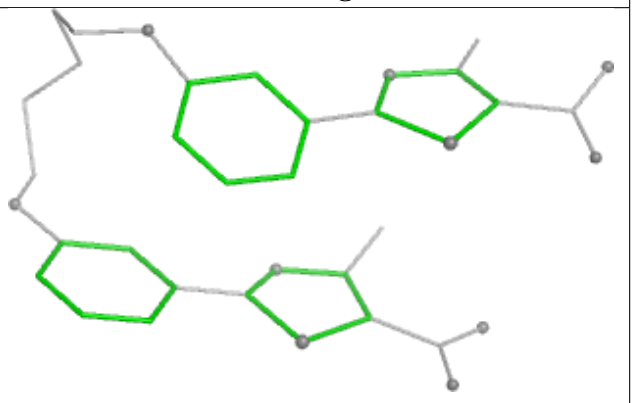
Bond lengths



Bond angles

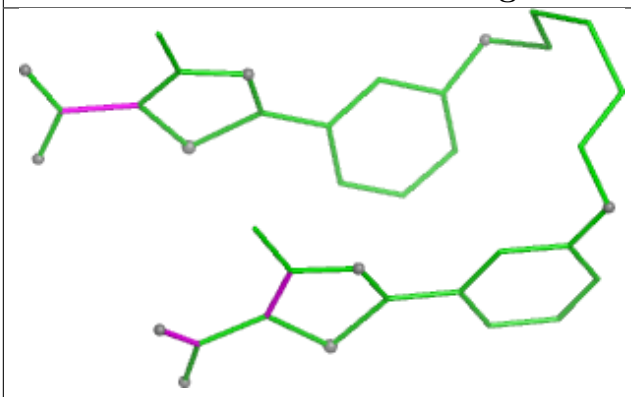


Torsions

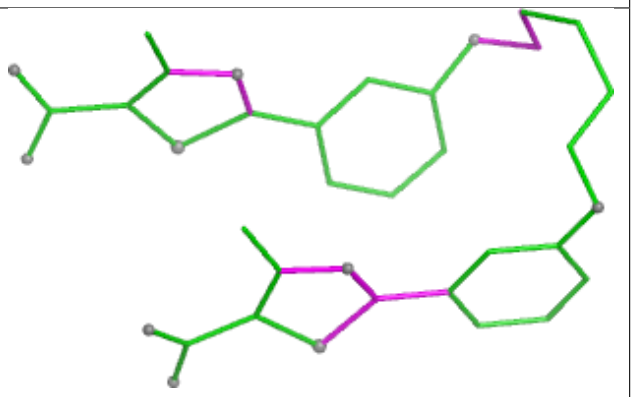


Rings

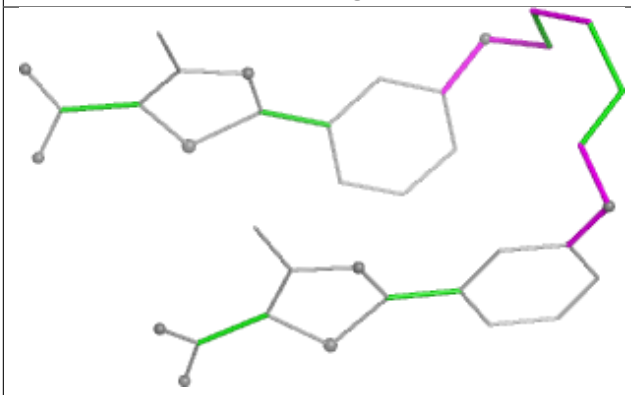
Ligand A1KDF U 303



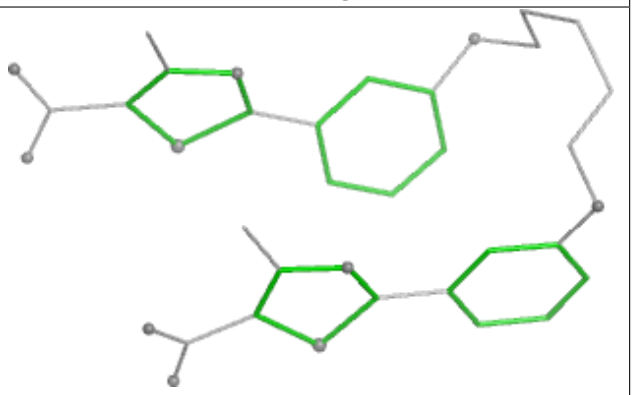
Bond lengths



Bond angles

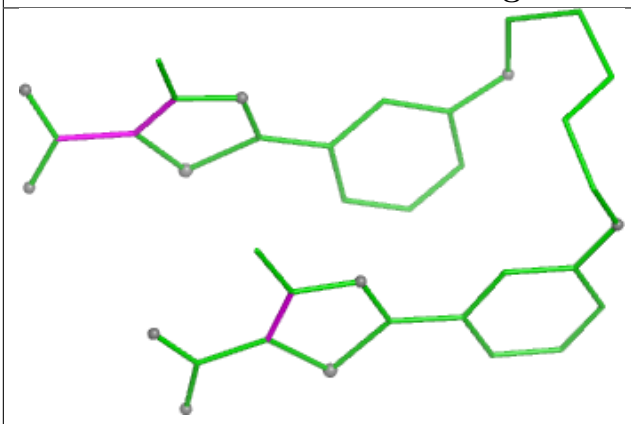


Torsions

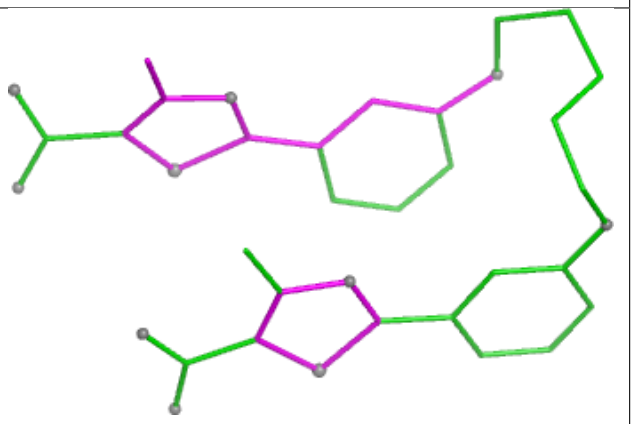


Rings

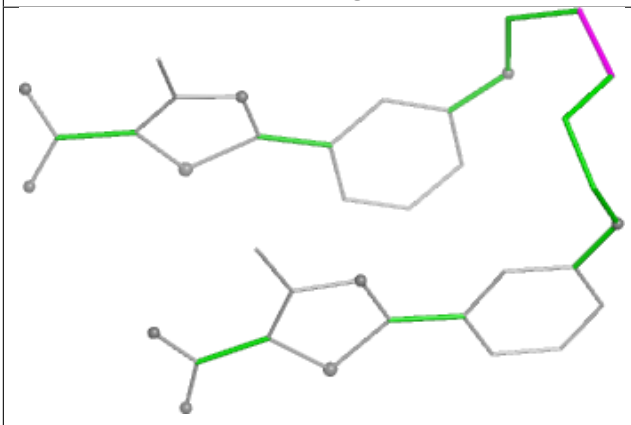
Ligand A1KDF S 301



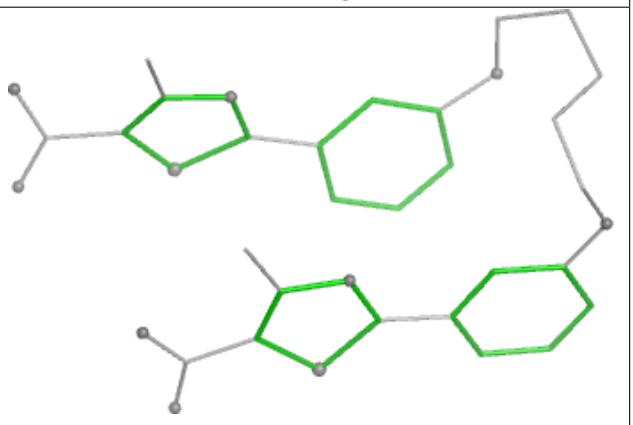
Bond lengths



Bond angles

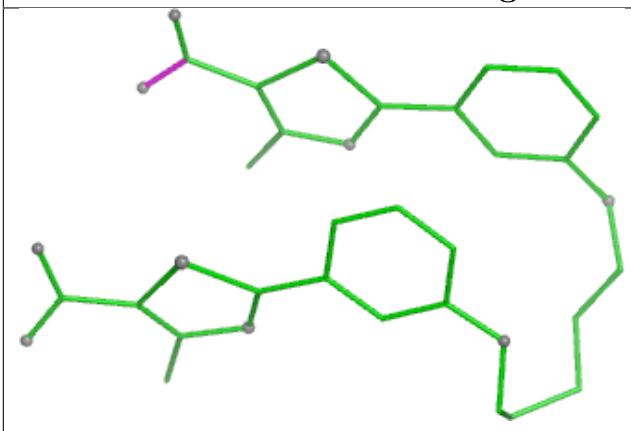


Torsions

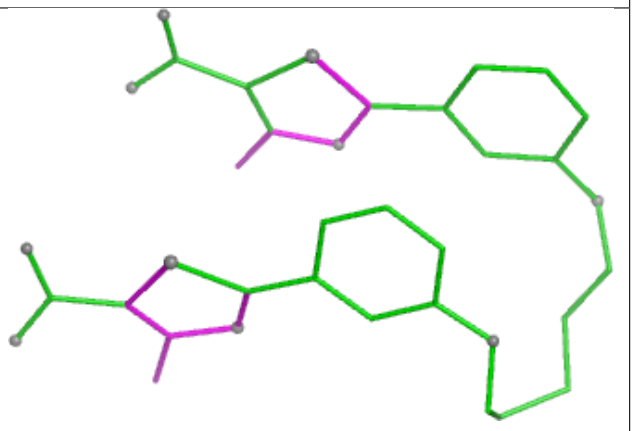


Rings

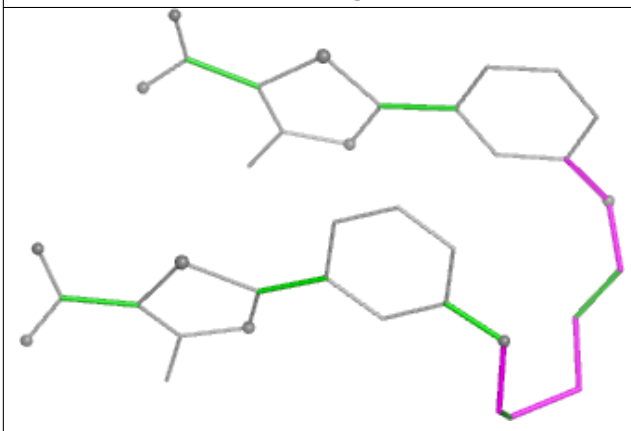
Ligand A1KDF O 301



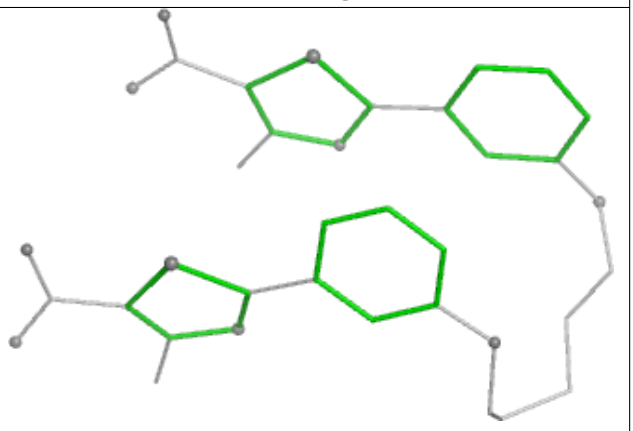
Bond lengths



Bond angles

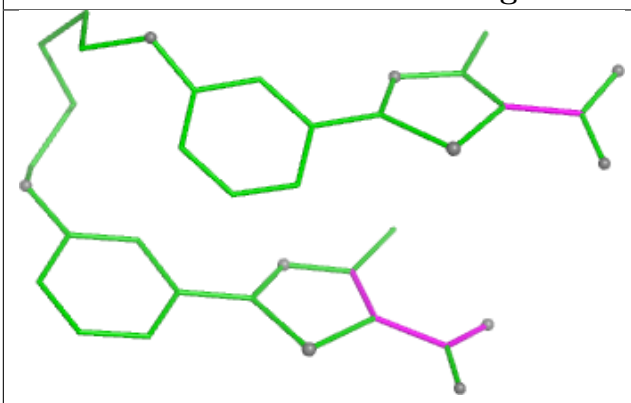


Torsions

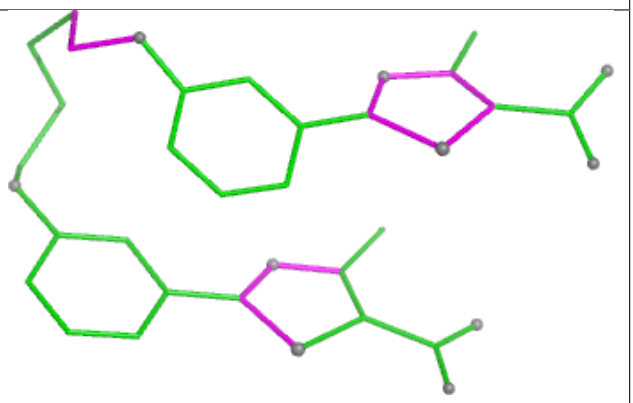


Rings

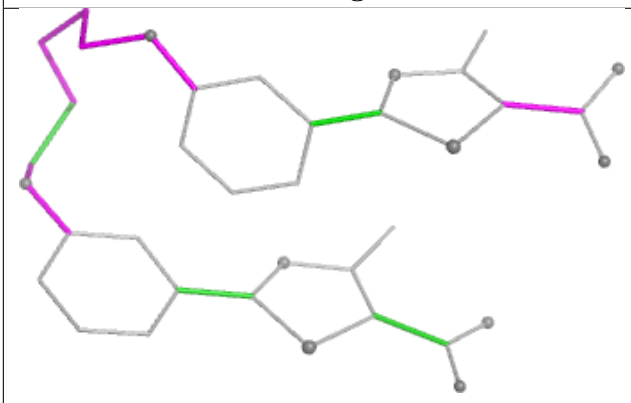
Ligand A1KDF B 301



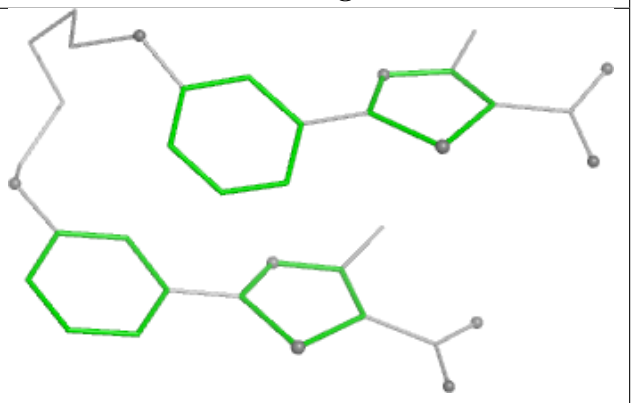
Bond lengths



Bond angles

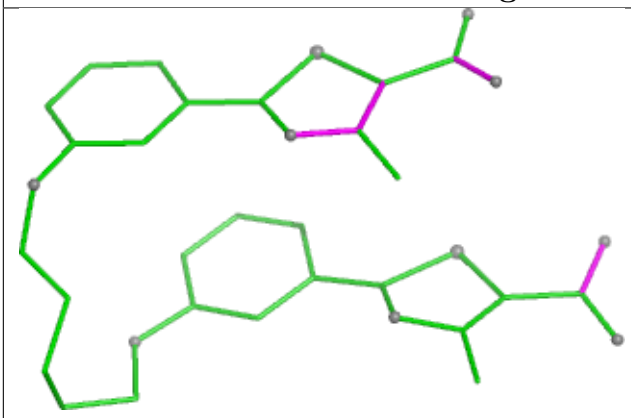


Torsions

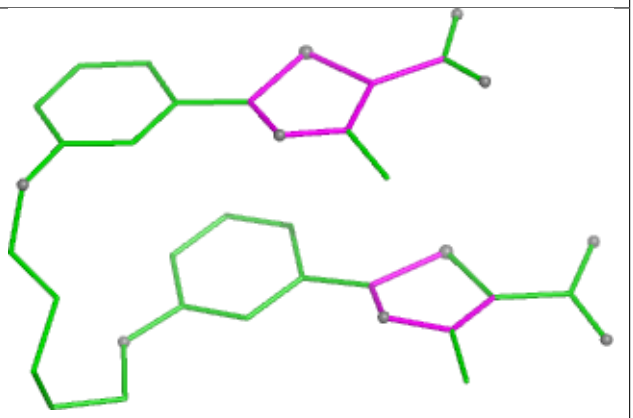


Rings

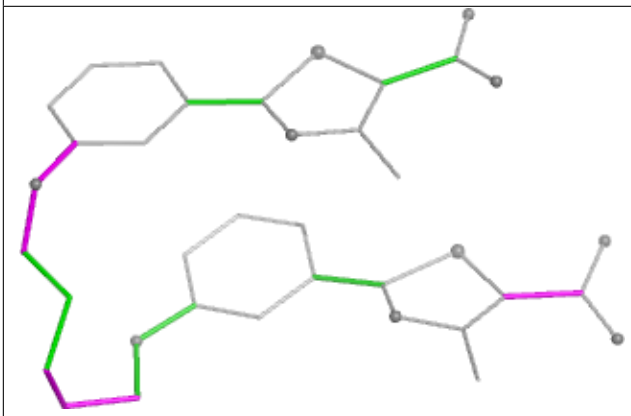
Ligand A1KDF A 305



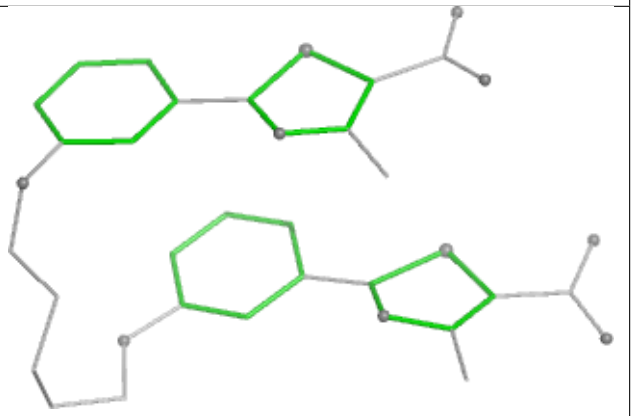
Bond lengths



Bond angles

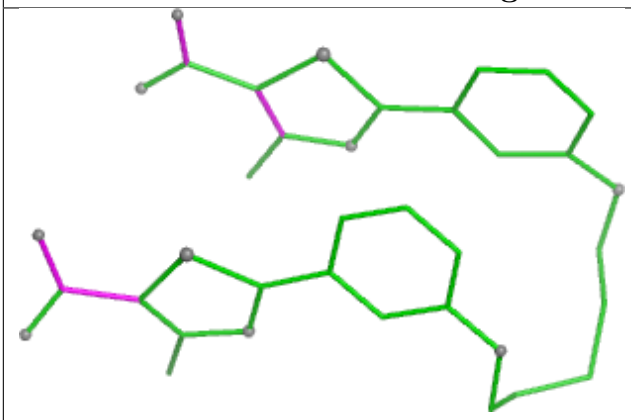


Torsions

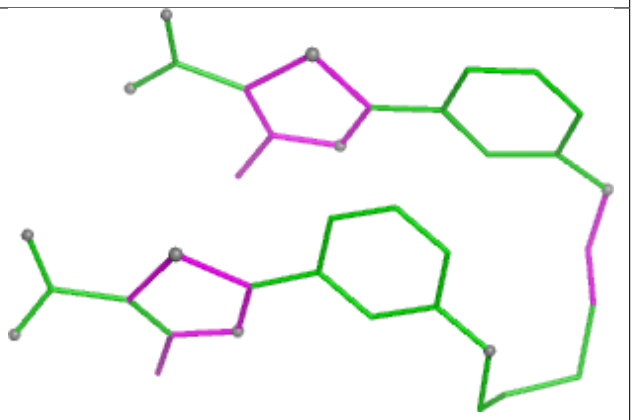


Rings

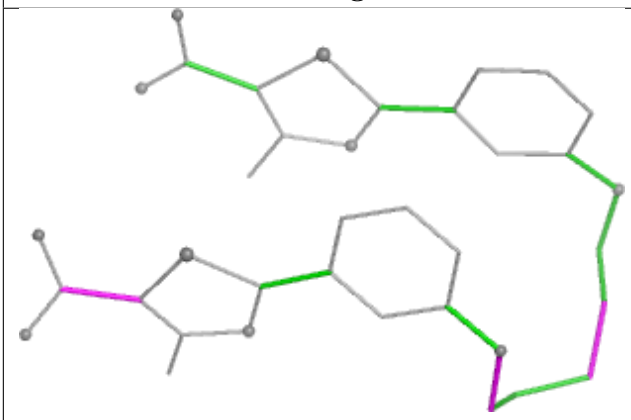
Ligand A1KDF P 301



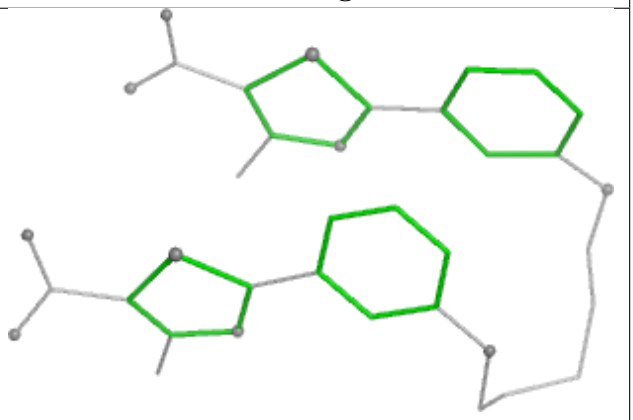
Bond lengths



Bond angles

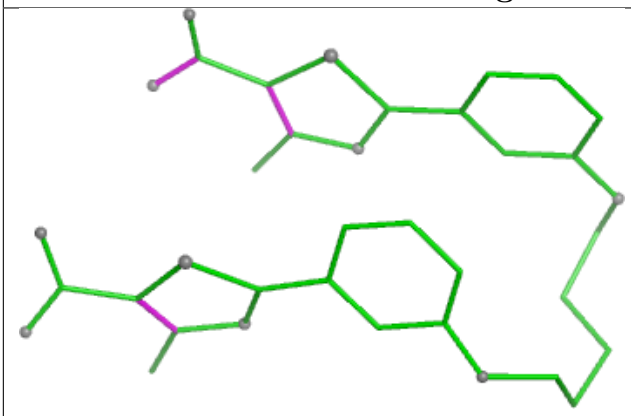


Torsions

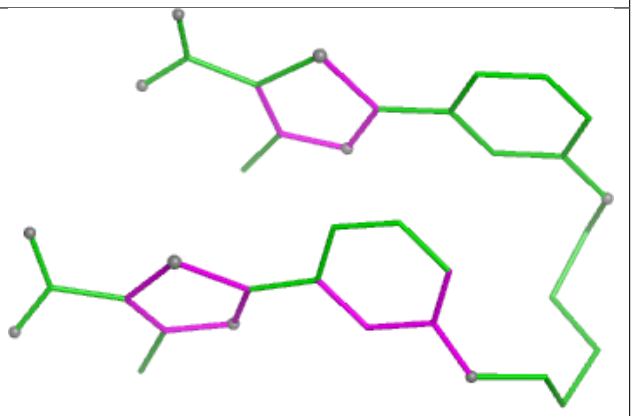


Rings

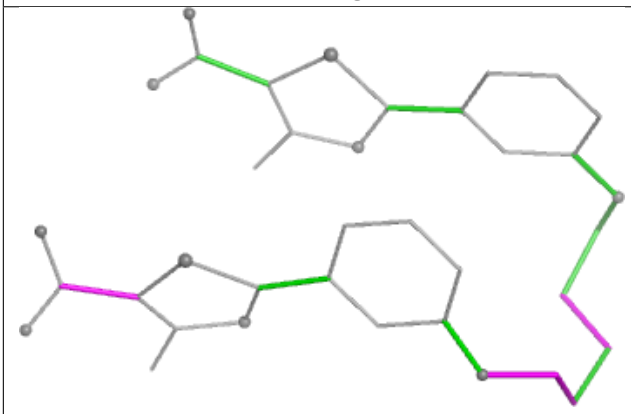
Ligand A1KDF M 301



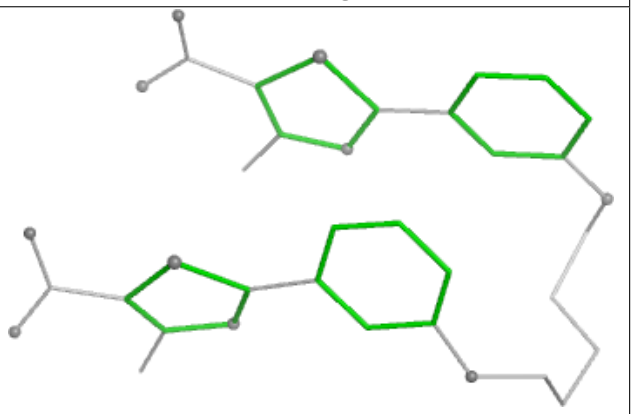
Bond lengths



Bond angles

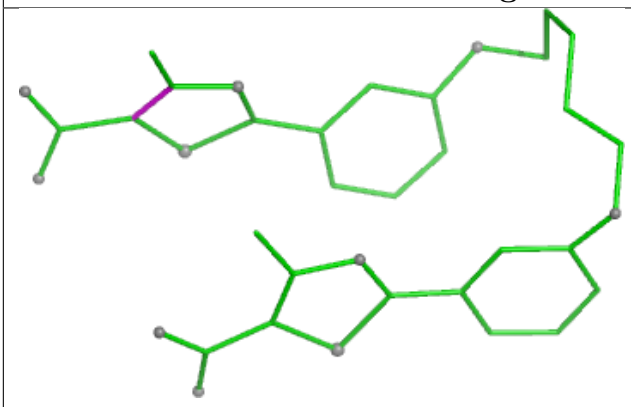


Torsions

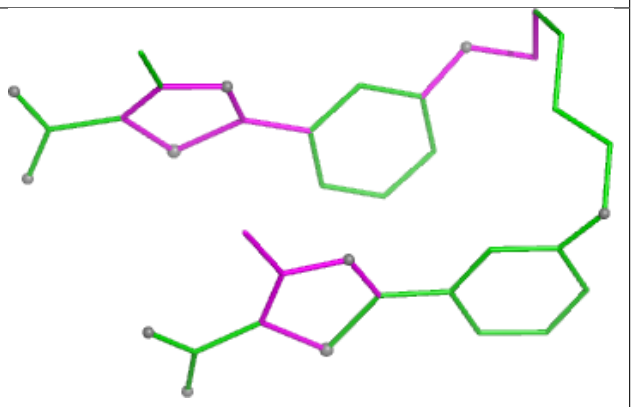


Rings

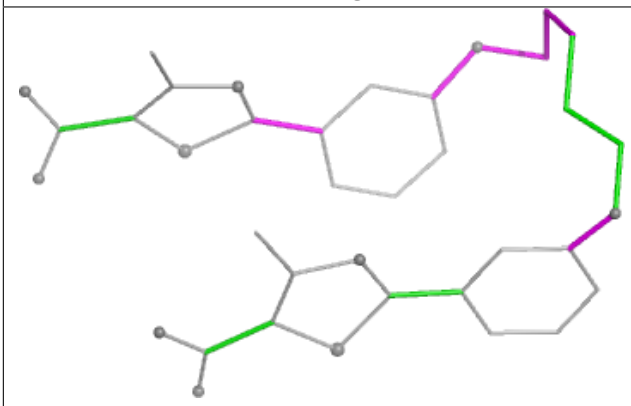
Ligand A1KDF R 301



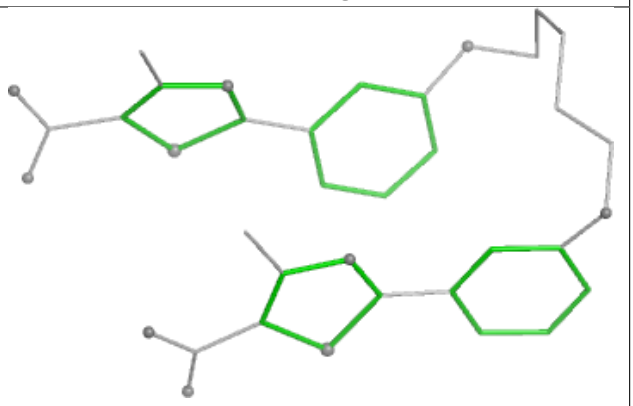
Bond lengths



Bond angles

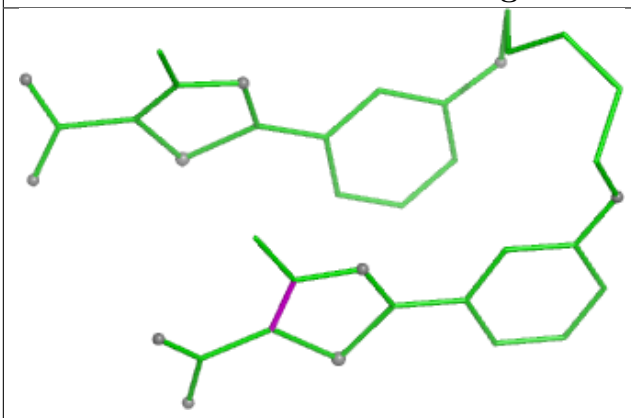


Torsions

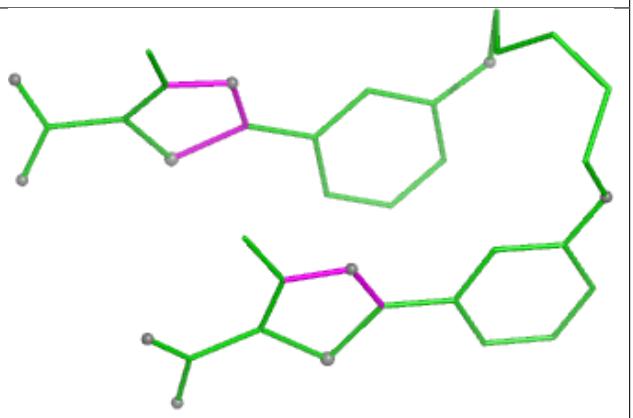


Rings

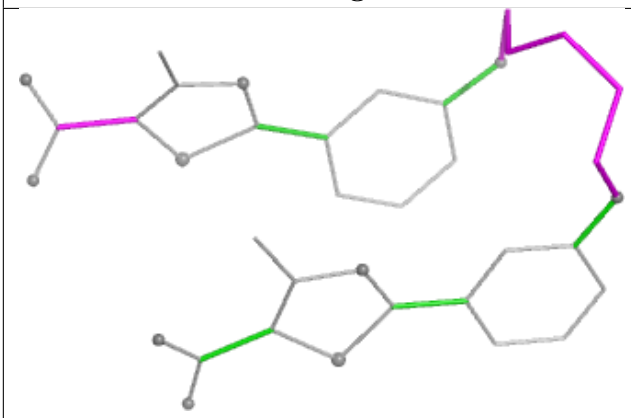
Ligand A1KDF T 301



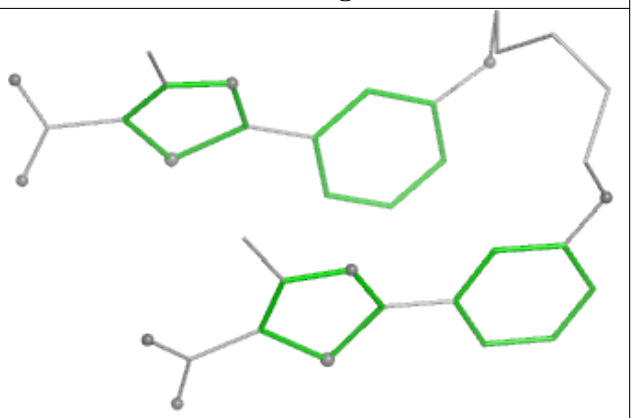
Bond lengths



Bond angles

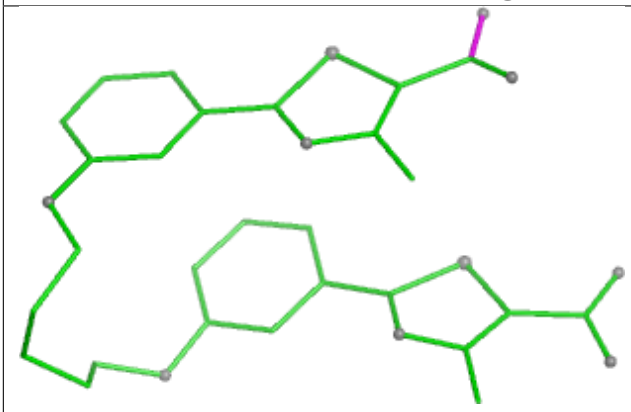


Torsions

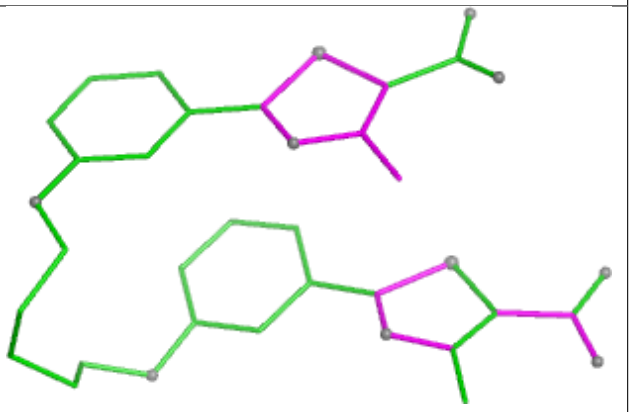


Rings

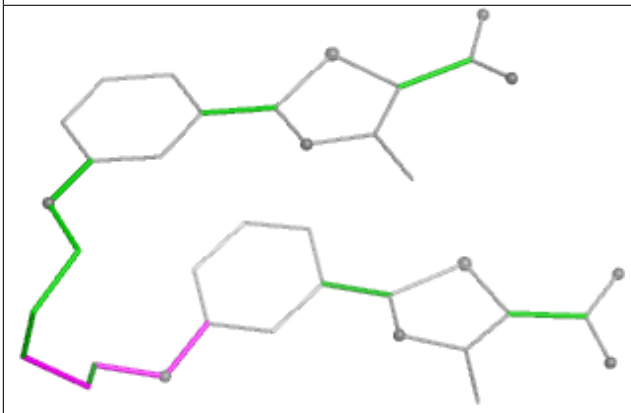
Ligand A1KDF K 302



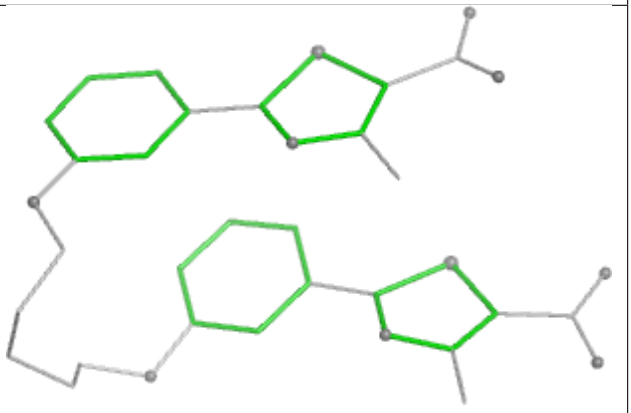
Bond lengths



Bond angles

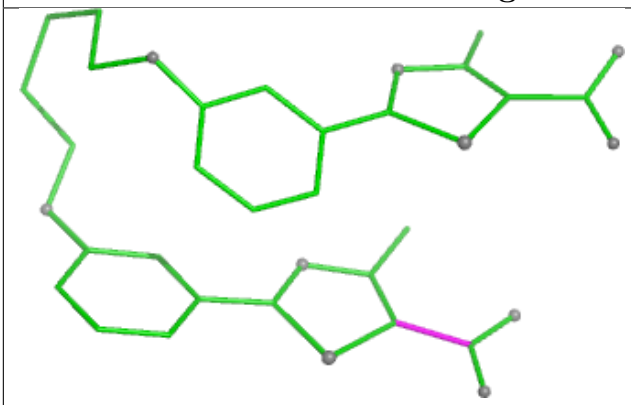


Torsions

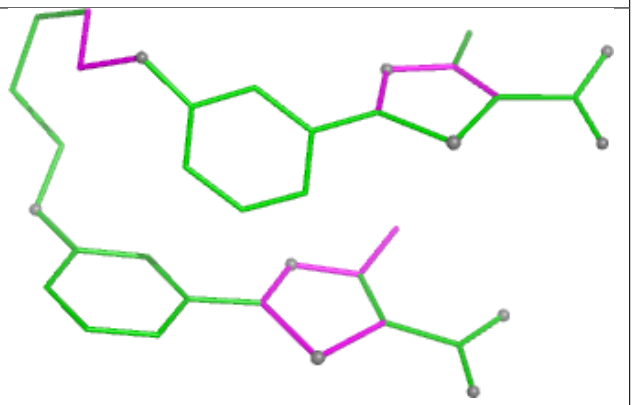


Rings

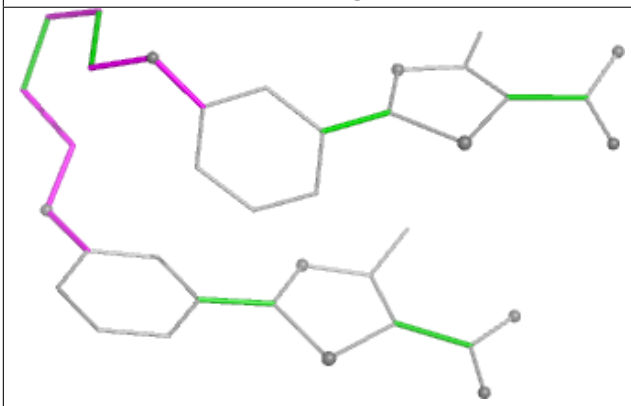
Ligand A1KDF G 301



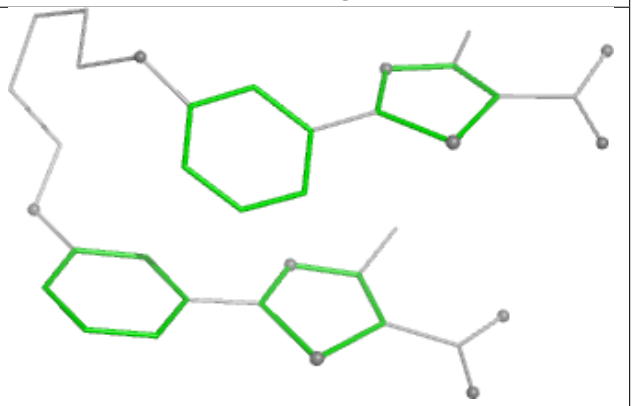
Bond lengths



Bond angles

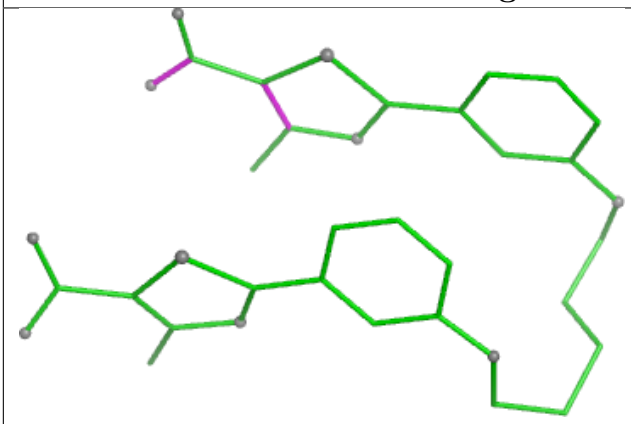


Torsions

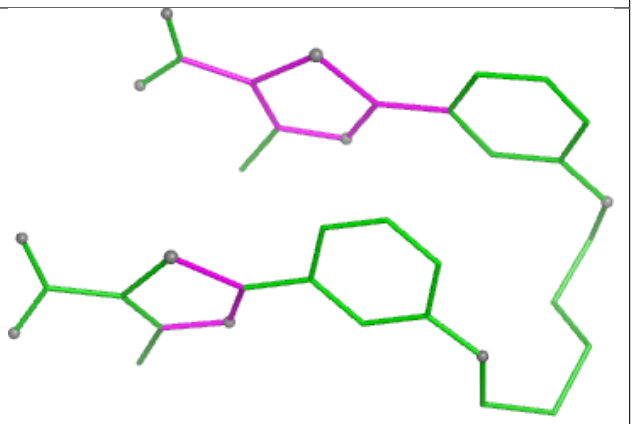


Rings

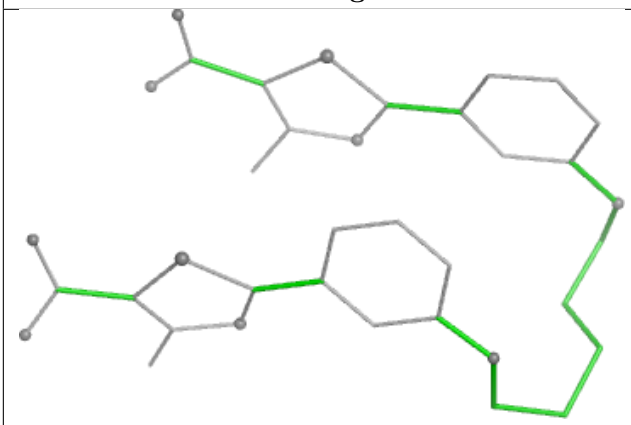
Ligand A1KDF N 301



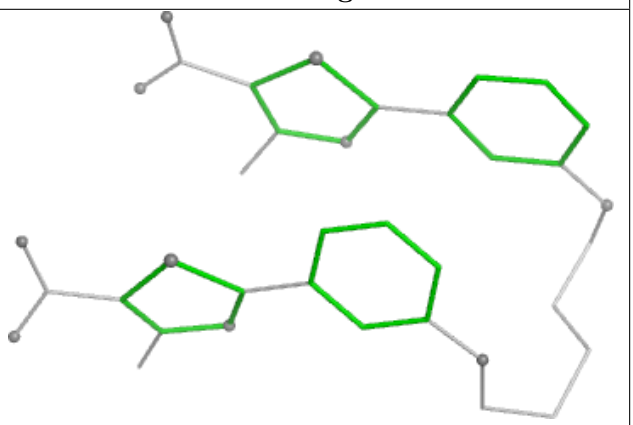
Bond lengths



Bond angles

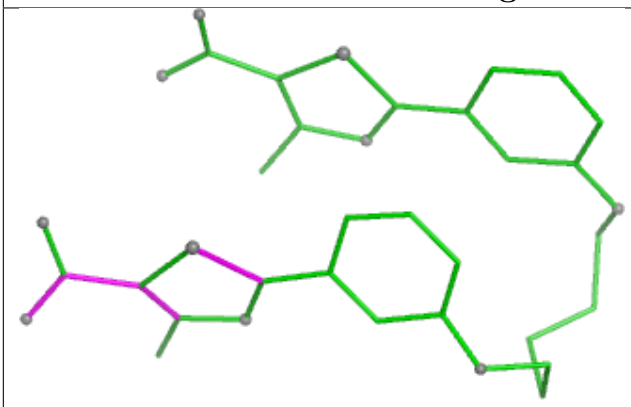


Torsions

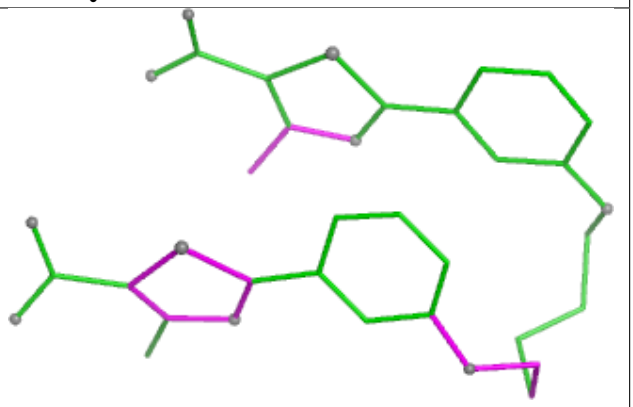


Rings

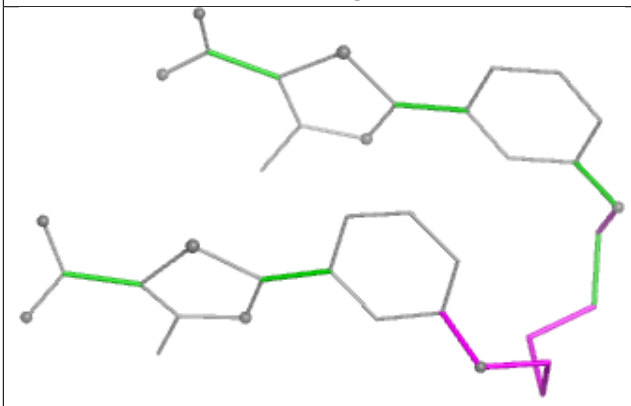
Ligand A1KDF Q 301



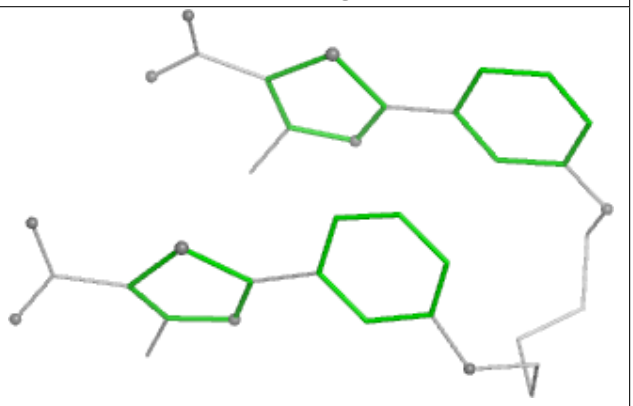
Bond lengths



Bond angles

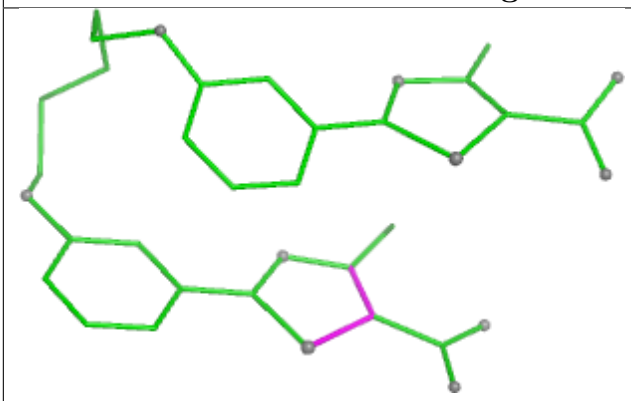


Torsions

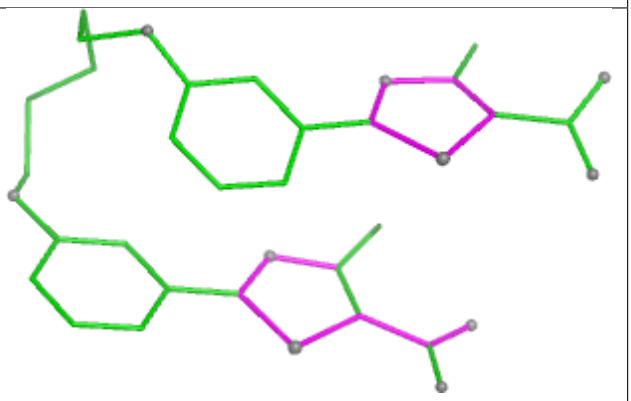


Rings

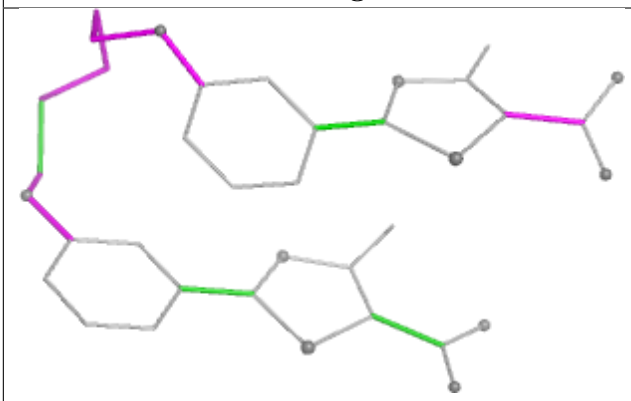
Ligand A1KDF E 301



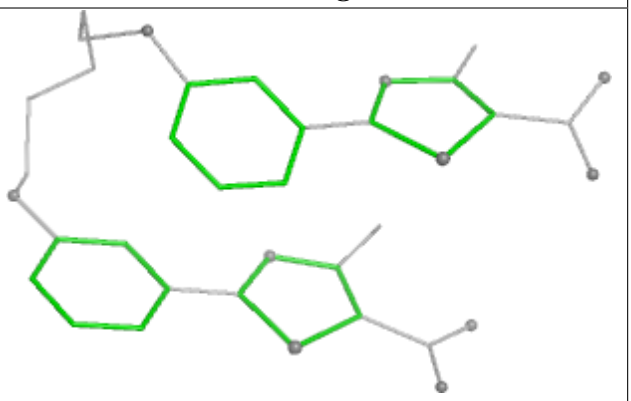
Bond lengths



Bond angles

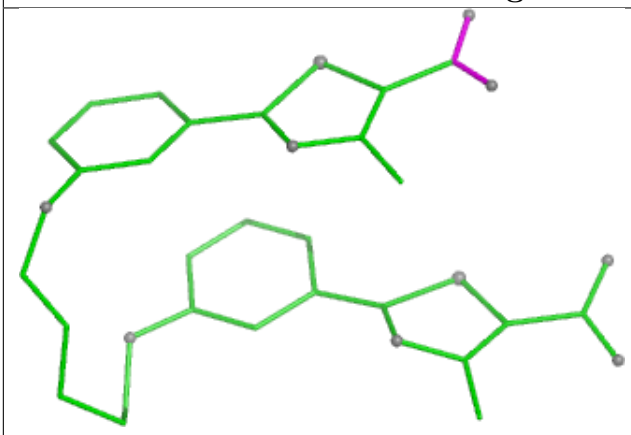


Torsions

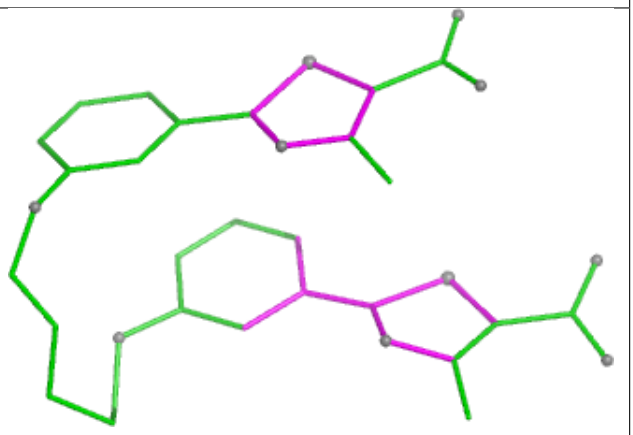


Rings

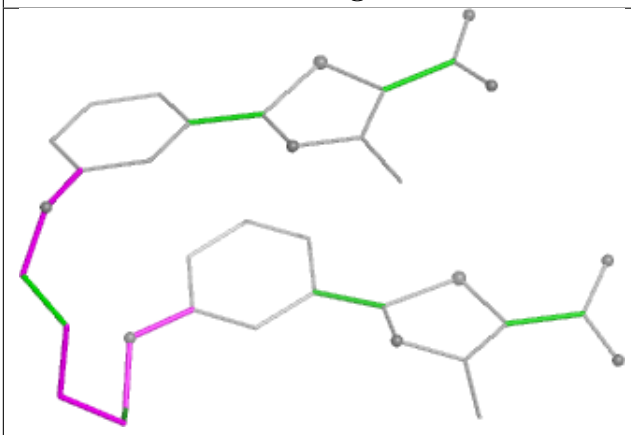
Ligand A1KDF I 302



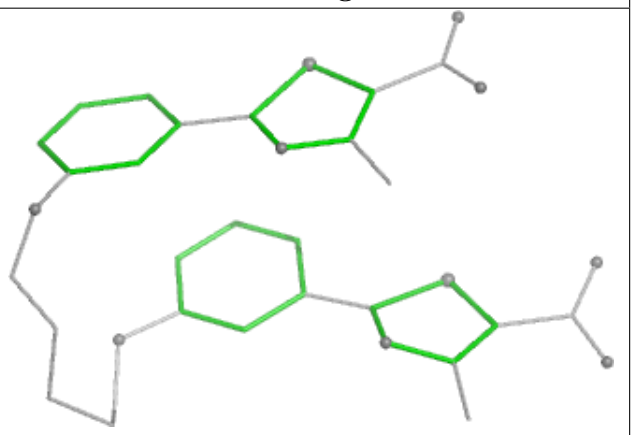
Bond lengths



Bond angles

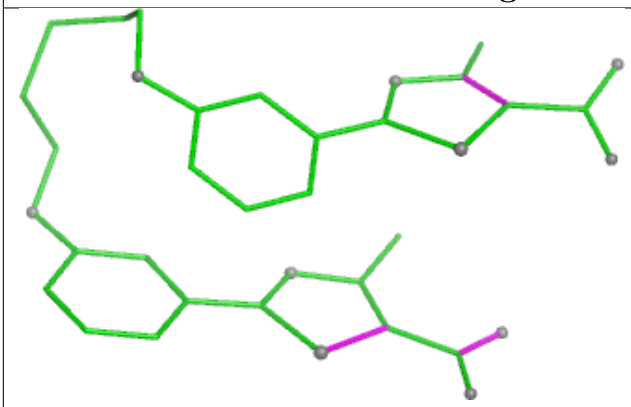


Torsions

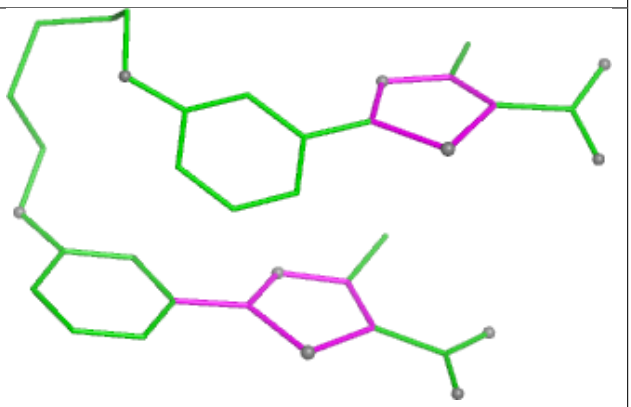


Rings

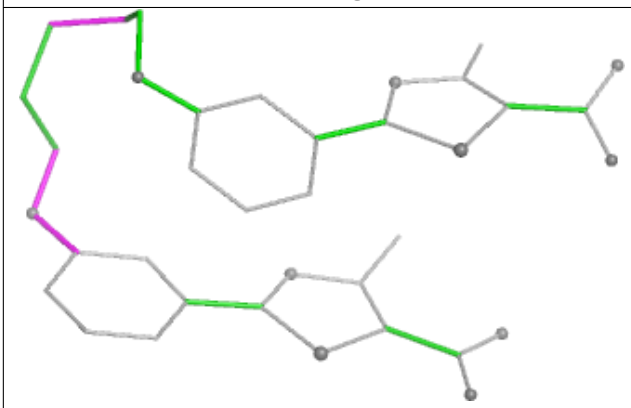
Ligand A1KDF D 301



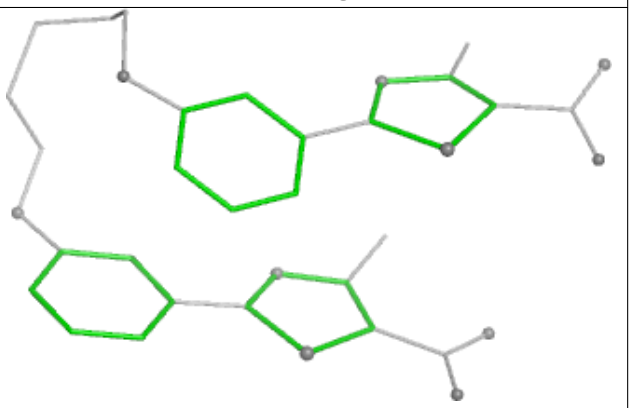
Bond lengths



Bond angles

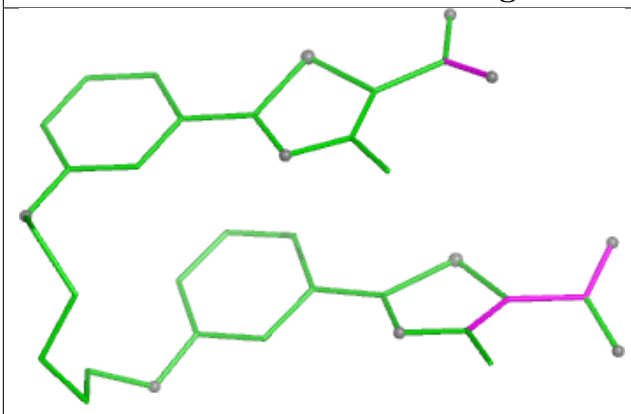


Torsions

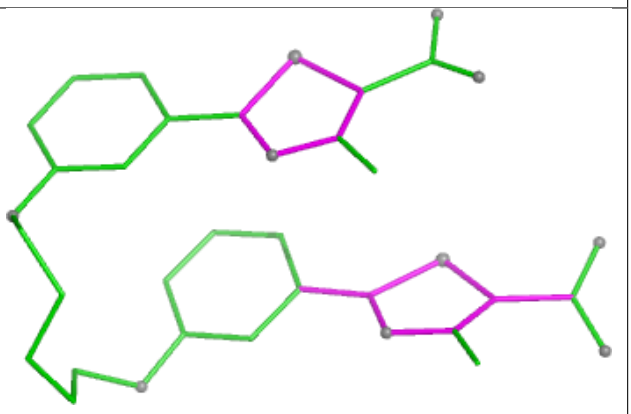


Rings

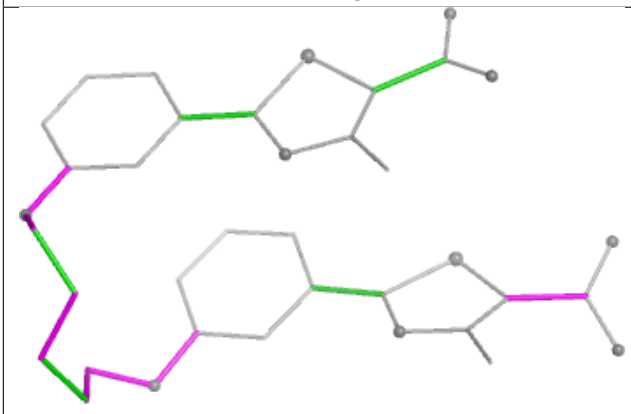
Ligand A1KDF H 301



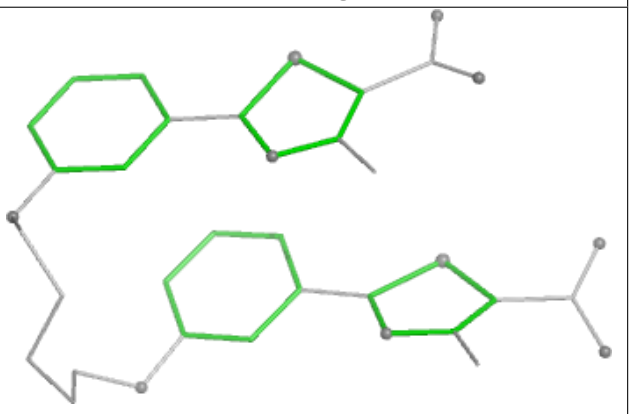
Bond lengths



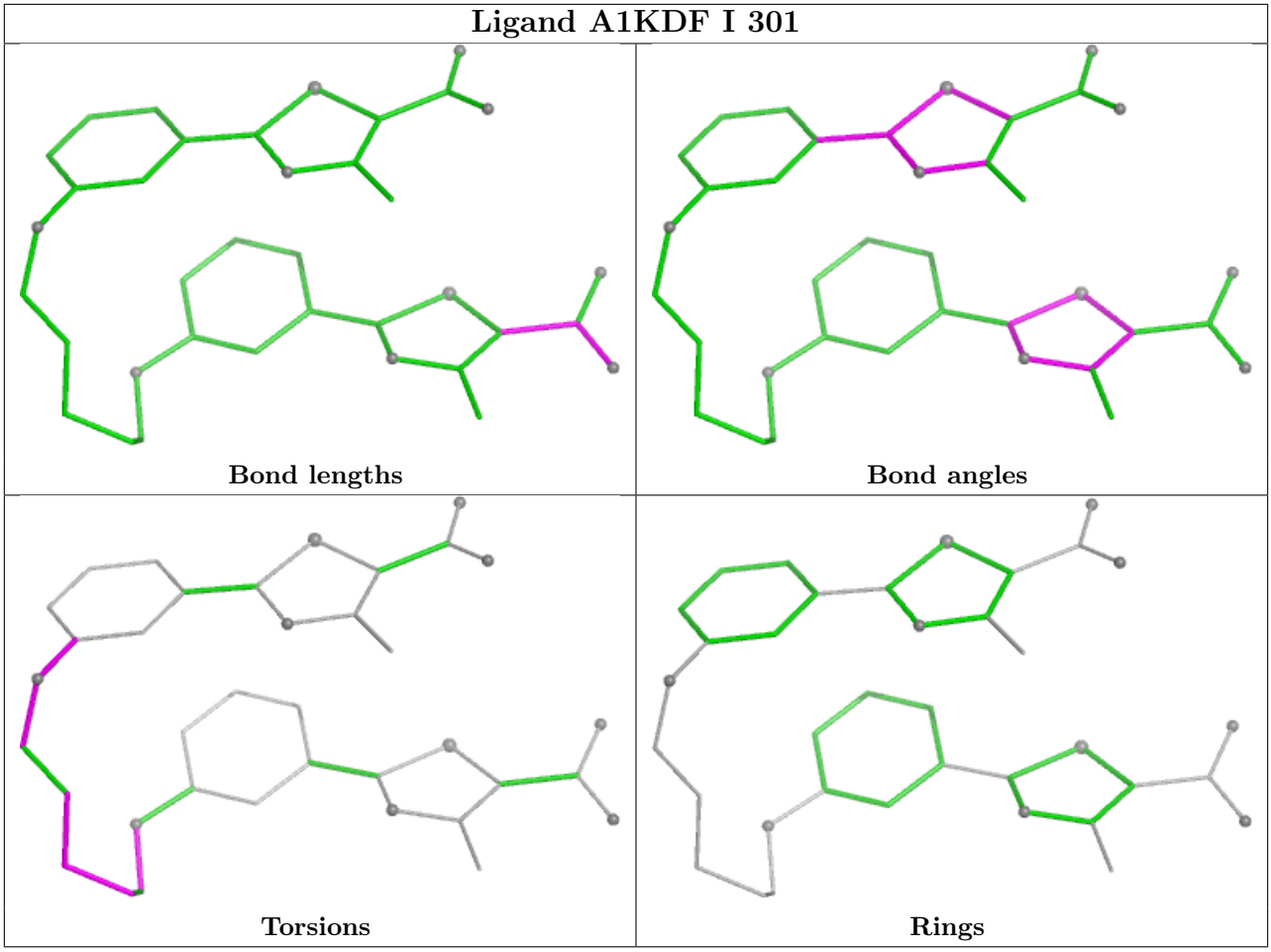
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.50	12 (6%)	25	27	59, 80, 144, 187	0
1	B	188/215 (87%)	0.42	9 (4%)	35	37	34, 72, 123, 147	2 (1%)
1	C	189/215 (87%)	0.53	15 (7%)	18	20	32, 74, 131, 171	2 (1%)
1	D	188/215 (87%)	0.35	9 (4%)	35	37	33, 73, 127, 186	2 (1%)
1	E	189/215 (87%)	0.45	9 (4%)	35	37	34, 72, 121, 158	1 (0%)
1	F	187/215 (86%)	0.50	15 (8%)	18	20	34, 73, 114, 163	3 (1%)
1	G	188/215 (87%)	0.58	11 (5%)	28	30	61, 80, 139, 192	0
1	H	189/215 (87%)	0.85	25 (13%)	7	8	65, 85, 142, 197	0
1	I	187/215 (86%)	0.98	17 (9%)	15	16	76, 99, 160, 217	0
1	J	188/215 (87%)	1.30	32 (17%)	4	5	46, 109, 204, 243	1 (0%)
1	K	187/215 (86%)	0.82	20 (10%)	11	12	35, 93, 170, 220	4 (2%)
1	L	187/215 (86%)	0.37	12 (6%)	25	27	34, 71, 126, 165	2 (1%)
1	M	189/215 (87%)	0.53	16 (8%)	16	18	38, 75, 139, 174	1 (0%)
1	N	187/215 (86%)	0.53	12 (6%)	25	27	50, 77, 130, 168	1 (0%)
1	O	187/215 (86%)	0.53	13 (6%)	22	24	40, 74, 144, 180	1 (0%)
1	P	187/215 (86%)	0.38	10 (5%)	32	34	32, 70, 128, 156	1 (0%)
1	Q	187/215 (86%)	0.49	14 (7%)	20	22	32, 72, 132, 179	2 (1%)
1	R	188/215 (87%)	0.52	10 (5%)	32	34	34, 77, 132, 175	1 (0%)
1	S	188/215 (87%)	0.51	8 (4%)	40	41	57, 83, 134, 182	1 (0%)
1	T	187/215 (86%)	0.64	12 (6%)	25	27	47, 80, 146, 185	1 (0%)
1	U	187/215 (86%)	0.55	14 (7%)	20	22	59, 77, 143, 163	0
1	V	187/215 (86%)	0.48	12 (6%)	25	27	59, 74, 120, 148	0
All	All	4127/4730 (87%)	0.58	307 (7%)	20	22	32, 79, 144, 243	26 (0%)

All (307) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	184	LEU	5.6
1	J	24	LEU	5.5
1	N	24	LEU	5.2
1	C	24	LEU	5.1
1	G	24	LEU	5.1
1	F	175	LEU	5.0
1	H	24	LEU	4.9
1	M	24	LEU	4.9
1	I	24	LEU	4.7
1	I	29	CYS	4.6
1	B	24	LEU	4.5
1	K	25	CYS	4.4
1	N	184	LEU	4.4
1	T	184	LEU	4.4
1	E	184	LEU	4.3
1	A	184	LEU	4.3
1	O	208	CYS	4.3
1	F	209	ARG	4.2
1	K	182	LEU	4.2
1	A	210	PRO	4.2
1	J	194	GLN	4.1
1	F	137[A]	LEU	4.1
1	F	210	PRO	4.1
1	B	184	LEU	4.1
1	C	184	LEU	4.1
1	M	184	LEU	4.1
1	N	210	PRO	4.1
1	Q	184	LEU	4.0
1	K	183	PRO	4.0
1	H	178	LEU	4.0
1	P	183	PRO	4.0
1	M	209	ARG	3.9
1	E	24	LEU	3.9
1	U	210	PRO	3.9
1	U	209	ARG	3.9
1	J	55	ARG	3.8
1	V	209	ARG	3.8
1	V	211	ASN	3.8
1	T	104[A]	TYR	3.8
1	K	177	LYS	3.8
1	F	208	CYS	3.8
1	K	184	LEU	3.8
1	S	24	LEU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	U	184	LEU	3.7
1	K	104[A]	TYR	3.7
1	F	182	LEU	3.6
1	T	25	CYS	3.6
1	H	56	MET	3.6
1	I	205	TYR	3.6
1	J	184	LEU	3.6
1	S	184	LEU	3.6
1	J	191	ALA	3.6
1	M	137[A]	LEU	3.6
1	H	210	PRO	3.6
1	J	137	LEU	3.5
1	P	182	LEU	3.5
1	R	24	LEU	3.5
1	R	184	LEU	3.5
1	T	29	CYS	3.5
1	E	209	ARG	3.5
1	N	209	ARG	3.5
1	J	62	LYS	3.4
1	L	184	LEU	3.4
1	M	210	PRO	3.4
1	D	29	CYS	3.4
1	J	182	LEU	3.4
1	E	212	MET	3.4
1	R	210	PRO	3.4
1	H	29	CYS	3.4
1	S	210	PRO	3.4
1	U	208	CYS	3.4
1	M	208	CYS	3.3
1	C	210	PRO	3.3
1	G	210	PRO	3.3
1	H	207	SER	3.3
1	Q	25	CYS	3.3
1	S	182	LEU	3.3
1	T	209	ARG	3.3
1	O	209	ARG	3.3
1	C	211	ASN	3.2
1	K	178	LEU	3.2
1	Q	182	LEU	3.2
1	N	205	TYR	3.2
1	H	137	LEU	3.2
1	N	182	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	T	137	LEU	3.1
1	V	184	LEU	3.1
1	H	209	ARG	3.1
1	J	29	CYS	3.1
1	O	210	PRO	3.1
1	D	44	ARG	3.1
1	I	58	GLY	3.1
1	K	180	ARG	3.1
1	J	207	SER	3.1
1	C	99[A]	ASN	3.1
1	O	184	LEU	3.1
1	T	210	PRO	3.0
1	T	182	LEU	3.0
1	G	29	CYS	3.0
1	G	194	GLN	3.0
1	V	210	PRO	3.0
1	F	25	CYS	2.9
1	H	180	ARG	2.9
1	M	211	ASN	2.9
1	I	210	PRO	2.9
1	J	47	LEU	2.9
1	L	25	CYS	2.9
1	E	210	PRO	2.9
1	L	210	PRO	2.9
1	O	29	CYS	2.9
1	H	166	ILE	2.9
1	H	58	GLY	2.9
1	Q	133	ALA	2.9
1	V	25	CYS	2.9
1	V	29	CYS	2.9
1	A	181	GLN	2.8
1	K	29[A]	CYS	2.8
1	H	59	GLY	2.8
1	C	29	CYS	2.8
1	P	180	ARG	2.8
1	L	44	ARG	2.8
1	T	211	ASN	2.8
1	B	210	PRO	2.8
1	N	137	LEU	2.8
1	F	29	CYS	2.7
1	P	29	CYS	2.7
1	E	182	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	181	GLN	2.7
1	F	176	ASN	2.7
1	F	184	LEU	2.7
1	B	166	ILE	2.7
1	J	66	ILE	2.7
1	Q	166	ILE	2.7
1	C	209	ARG	2.7
1	G	182	LEU	2.7
1	K	181	GLN	2.7
1	J	195	ASP	2.7
1	O	179	PRO	2.7
1	K	167	LEU	2.7
1	C	166	ILE	2.6
1	M	212	MET	2.6
1	L	211	ASN	2.6
1	G	209	ARG	2.6
1	J	209	ARG	2.6
1	P	209	ARG	2.6
1	R	166	ILE	2.6
1	G	137	LEU	2.6
1	I	182	LEU	2.6
1	A	177	LYS	2.6
1	A	208	CYS	2.6
1	Q	193	ARG	2.6
1	F	56	MET	2.6
1	J	179	PRO	2.6
1	K	179	PRO	2.6
1	J	166	ILE	2.6
1	P	184	LEU	2.6
1	C	180	ARG	2.6
1	J	193	ARG	2.6
1	Q	211	ASN	2.6
1	H	199	SER	2.6
1	O	104[A]	TYR	2.6
1	G	184	LEU	2.5
1	A	25	CYS	2.5
1	P	25	CYS	2.5
1	R	29	CYS	2.5
1	S	29	CYS	2.5
1	J	199	SER	2.5
1	A	205	TYR	2.5
1	K	209	ARG	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	178	LEU	2.5
1	E	208	CYS	2.5
1	A	179	PRO	2.5
1	F	177	LYS	2.5
1	L	179	PRO	2.5
1	P	210	PRO	2.5
1	O	44	ARG	2.5
1	R	205	TYR	2.5
1	T	156	ARG	2.5
1	C	182	LEU	2.5
1	L	182	LEU	2.5
1	M	182	LEU	2.5
1	U	168	ASP	2.5
1	D	210	PRO	2.5
1	F	181	GLN	2.5
1	M	166	ILE	2.4
1	D	137	LEU	2.4
1	C	212	MET	2.4
1	R	211	ASN	2.4
1	L	209	ARG	2.4
1	V	58	GLY	2.4
1	J	208	CYS	2.4
1	I	196	LEU	2.4
1	H	171	TYR	2.4
1	I	209	ARG	2.4
1	M	180	ARG	2.4
1	V	37	GLN	2.4
1	K	64	CYS	2.4
1	M	29	CYS	2.4
1	J	172	LEU	2.4
1	V	137	LEU	2.4
1	A	206	ASN	2.4
1	J	211	ASN	2.4
1	I	166	ILE	2.4
1	J	167	LEU	2.4
1	S	137	LEU	2.4
1	I	183	PRO	2.3
1	J	58	GLY	2.3
1	M	59	GLY	2.3
1	K	56	MET	2.3
1	I	44	ARG	2.3
1	U	156	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	U	180	ARG	2.3
1	Q	132	LEU	2.3
1	J	210	PRO	2.3
1	A	166	ILE	2.3
1	I	61	GLN	2.3
1	B	182	LEU	2.3
1	U	99	ASN	2.3
1	Q	210	PRO	2.3
1	K	129	SER	2.3
1	A	178	LEU	2.3
1	K	172	LEU	2.3
1	O	182	LEU	2.3
1	A	29	CYS	2.3
1	F	211	ASN	2.3
1	H	211	ASN	2.3
1	C	179	PRO	2.3
1	D	212	MET	2.3
1	J	189	THR	2.3
1	O	181	GLN	2.3
1	Q	178	LEU	2.2
1	V	182	LEU	2.2
1	L	208	CYS	2.2
1	I	133	ALA	2.2
1	Q	29	CYS	2.2
1	C	37	GLN	2.2
1	L	133	ALA	2.2
1	D	182	LEU	2.2
1	C	173	ARG	2.2
1	G	211	ASN	2.2
1	J	56	MET	2.2
1	E	29	CYS	2.2
1	P	185	GLU	2.2
1	K	41	LYS	2.2
1	Q	173	ARG	2.2
1	R	137	LEU	2.2
1	N	179	PRO	2.2
1	T	179	PRO	2.2
1	D	181	GLN	2.2
1	I	25	CYS	2.2
1	J	162	LEU	2.1
1	K	175	LEU	2.1
1	O	178	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	U	137	LEU	2.1
1	U	166	ILE	2.1
1	J	63	VAL	2.1
1	H	60	GLY	2.1
1	D	25	CYS	2.1
1	N	208	CYS	2.1
1	M	156	ARG	2.1
1	J	104	TYR	2.1
1	G	166	ILE	2.1
1	K	166	ILE	2.1
1	O	166	ILE	2.1
1	J	92[A]	ASN	2.1
1	P	211	ASN	2.1
1	U	211	ASN	2.1
1	N	61	GLN	2.1
1	B	209	ARG	2.1
1	H	190	LYS	2.1
1	Q	205	TYR	2.1
1	T	181	GLN	2.1
1	D	183	PRO	2.1
1	H	179	PRO	2.1
1	U	183	PRO	2.1
1	M	60	GLY	2.1
1	U	207	SER	2.1
1	Q	102	ALA	2.1
1	G	196	LEU	2.1
1	O	61	GLN	2.1
1	R	182	LEU	2.1
1	J	171	TYR	2.1
1	I	96	VAL	2.1
1	V	59	GLY	2.1
1	S	209	ARG	2.1
1	H	133	ALA	2.0
1	H	212	MET	2.0
1	H	208	CYS	2.0
1	L	181	GLN	2.0
1	B	100	ASN	2.0
1	B	211	ASN	2.0
1	H	176	ASN	2.0
1	N	99[A]	ASN	2.0
1	S	211	ASN	2.0
1	E	183	PRO	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	104[A]	TYR	2.0
1	F	173	ARG	2.0
1	C	25	CYS	2.0
1	H	181	GLN	2.0
1	N	29	CYS	2.0
1	U	29	CYS	2.0
1	H	175	LEU	2.0
1	I	184	LEU	2.0
1	J	188	LEU	2.0
1	L	137	LEU	2.0
1	R	178	LEU	2.0
1	V	180	ARG	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, 95^{th} 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
4	MG	U	306	1/1	0.70	0.27	96,96,96,96	0
4	MG	D	304	1/1	0.72	0.21	100,100,100,100	0
2	EDO	B	302	4/4	0.72	0.18	88,90,95,96	0
4	MG	R	304	1/1	0.73	0.23	97,97,97,97	0
2	EDO	U	304	4/4	0.77	0.18	100,105,108,114	0
2	EDO	A	304	4/4	0.77	0.24	77,78,97,98	0
5	CL	M	305	1/1	0.78	0.23	121,121,121,121	0
5	CL	F	304	1/1	0.79	0.26	120,120,120,120	0
4	MG	G	304	1/1	0.79	0.13	81,81,81,81	0
4	MG	O	304	1/1	0.80	0.19	97,97,97,97	0
5	CL	J	303	1/1	0.80	0.25	115,115,115,115	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	D	305	1/1	0.80	0.18	113,113,113,113	0
2	EDO	V	302	4/4	0.81	0.18	93,93,98,99	0
2	EDO	L	302	4/4	0.82	0.20	100,101,102,104	0
2	EDO	E	303	4/4	0.82	0.15	99,99,100,108	0
5	CL	S	305	1/1	0.82	0.22	109,109,109,109	0
5	CL	C	307	1/1	0.83	0.22	109,109,109,109	0
4	MG	J	302	1/1	0.83	0.20	104,104,104,104	0
5	CL	M	306	1/1	0.83	0.19	109,109,109,109	0
2	EDO	R	303	4/4	0.83	0.14	96,103,107,110	0
4	MG	L	305	1/1	0.84	0.14	95,95,95,95	0
2	EDO	C	305	4/4	0.85	0.16	77,92,99,104	0
5	CL	P	305	1/1	0.85	0.26	111,111,111,111	0
5	CL	R	306	1/1	0.85	0.23	116,116,116,116	0
2	EDO	G	303	4/4	0.85	0.18	88,88,91,100	0
5	CL	G	305	1/1	0.86	0.17	102,102,102,102	0
5	CL	H	303	1/1	0.86	0.19	111,111,111,111	0
4	MG	E	307	1/1	0.86	0.16	95,95,95,95	0
4	MG	F	303	1/1	0.86	0.16	100,100,100,100	0
2	EDO	C	304	4/4	0.86	0.16	68,69,70,70	0
2	EDO	A	301	4/4	0.86	0.17	92,100,100,104	0
2	EDO	S	304	4/4	0.86	0.15	72,73,74,74	0
4	MG	M	304	1/1	0.86	0.15	99,99,99,99	0
5	CL	V	303	1/1	0.86	0.21	110,110,110,110	0
5	CL	Q	305	1/1	0.87	0.22	110,110,110,110	0
2	EDO	D	302	4/4	0.87	0.16	96,97,100,112	0
4	MG	A	306	1/1	0.87	0.19	103,103,103,103	0
2	EDO	U	305	4/4	0.87	0.17	86,92,93,104	0
2	EDO	T	303	4/4	0.88	0.14	96,99,102,107	0
2	EDO	Q	302	4/4	0.88	0.17	74,75,77,81	0
2	EDO	I	303	4/4	0.88	0.18	102,105,106,109	0
5	CL	B	308	1/1	0.88	0.15	110,110,110,110	0
5	CL	B	309	1/1	0.88	0.18	104,104,104,104	0
5	CL	T	307	1/1	0.88	0.16	109,109,109,109	0
2	EDO	H	302	4/4	0.88	0.24	91,98,100,110	0
2	EDO	E	306	4/4	0.89	0.20	92,96,96,102	0
2	EDO	T	302	4/4	0.89	0.18	82,85,90,90	0
5	CL	N	305	1/1	0.89	0.19	112,112,112,112	0
5	CL	O	306	1/1	0.89	0.20	105,105,105,105	0
2	EDO	F	301	4/4	0.89	0.18	79,81,84,89	0
2	EDO	B	304	4/4	0.89	0.18	94,96,97,104	0
4	MG	R	305	1/1	0.89	0.14	92,92,92,92	0
5	CL	G	306	1/1	0.89	0.18	107,107,107,107	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	Q	303	4/4	0.89	0.20	88,93,98,104	0
2	EDO	C	302	4/4	0.89	0.18	102,103,104,104	0
4	MG	T	305	1/1	0.90	0.16	98,98,98,98	0
2	EDO	G	302	4/4	0.90	0.20	81,83,86,96	0
2	EDO	R	302	4/4	0.90	0.17	81,84,87,95	0
2	EDO	A	302	4/4	0.90	0.15	76,78,79,83	0
2	EDO	M	302	4/4	0.90	0.17	81,84,86,90	0
2	EDO	F	302	4/4	0.90	0.16	82,87,88,92	0
5	CL	E	308	1/1	0.90	0.37	30,30,30,30	0
5	CL	M	307	1/1	0.90	0.41	30,30,30,30	0
5	CL	V	304	1/1	0.90	0.18	106,106,106,106	0
2	EDO	O	302	4/4	0.91	0.17	68,80,83,85	0
2	EDO	S	302	4/4	0.91	0.15	72,76,84,91	0
5	CL	U	307	1/1	0.91	0.16	105,105,105,105	0
2	EDO	E	302	4/4	0.91	0.18	87,93,95,97	0
5	CL	R	307	1/1	0.91	0.17	100,100,100,100	0
2	EDO	L	301	4/4	0.92	0.16	74,85,86,92	0
5	CL	N	304	1/1	0.92	0.19	107,107,107,107	0
3	A1KDF	I	301	37/37	0.92	0.11	79,93,112,113	0
4	MG	L	304	1/1	0.92	0.16	95,95,95,95	0
3	A1KDF	I	302	37/37	0.92	0.12	91,106,137,138	0
2	EDO	A	303	4/4	0.92	0.14	91,93,95,96	0
4	MG	B	307	1/1	0.92	0.11	70,70,70,70	0
4	MG	C	306	1/1	0.92	0.14	84,84,84,84	0
2	EDO	C	303	4/4	0.92	0.16	73,83,83,89	0
2	EDO	N	302	4/4	0.92	0.18	74,77,84,92	0
2	EDO	K	301	4/4	0.92	0.19	86,86,87,91	0
5	CL	A	307	1/1	0.92	0.15	101,101,101,101	0
5	CL	A	308	1/1	0.92	0.18	104,104,104,104	0
4	MG	Q	304	1/1	0.93	0.13	90,90,90,90	0
2	EDO	P	303	4/4	0.93	0.13	88,92,94,99	0
2	EDO	O	303	4/4	0.93	0.15	93,100,100,107	0
3	A1KDF	K	302	37/37	0.93	0.11	91,110,147,154	0
5	CL	D	306	1/1	0.94	0.34	30,30,30,30	0
5	CL	O	305	1/1	0.94	0.13	102,102,102,102	0
2	EDO	D	303	4/4	0.94	0.16	69,78,79,83	0
4	MG	T	304	1/1	0.94	0.11	99,99,99,99	0
3	A1KDF	U	303	37/37	0.94	0.11	71,77,109,116	0
2	EDO	M	303	4/4	0.94	0.10	91,95,103,107	0
2	EDO	P	304	4/4	0.94	0.11	79,82,87,90	0
2	EDO	V	301	4/4	0.94	0.15	78,78,85,85	0
5	CL	T	306	1/1	0.94	0.18	116,116,116,116	0

Continued on next page...

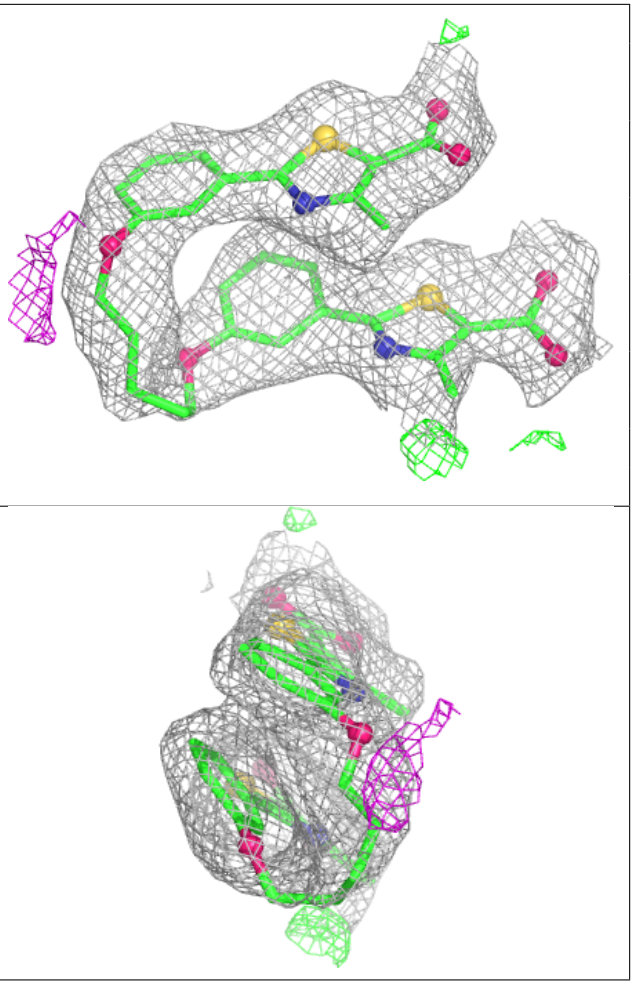
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	N	303	1/1	0.94	0.11	97,97,97,97	0
2	EDO	S	303	4/4	0.94	0.13	70,71,81,84	0
5	CL	U	308	1/1	0.94	0.36	30,30,30,30	0
2	EDO	B	305	4/4	0.94	0.14	74,76,76,83	0
2	EDO	I	304	4/4	0.94	0.12	75,81,87,87	0
3	A1KDF	E	305	37/37	0.95	0.09	66,73,101,103	0
3	A1KDF	G	301	37/37	0.95	0.09	73,78,114,117	0
3	A1KDF	H	301	37/37	0.95	0.10	74,81,109,110	0
2	EDO	J	301	4/4	0.95	0.13	85,89,92,96	0
2	EDO	B	303	4/4	0.95	0.12	82,87,94,95	0
2	EDO	E	304	4/4	0.95	0.12	74,74,76,79	0
3	A1KDF	M	301	37/37	0.95	0.09	64,74,95,101	0
5	CL	L	306	1/1	0.95	0.16	100,100,100,100	0
3	A1KDF	R	301	37/37	0.95	0.10	70,74,106,113	0
3	A1KDF	T	301	37/37	0.95	0.10	75,83,114,118	0
3	A1KDF	U	301	37/37	0.95	0.09	73,80,112,117	0
3	A1KDF	A	305	37/37	0.95	0.10	75,82,102,107	0
3	A1KDF	B	301	37/37	0.95	0.09	66,72,105,115	0
3	A1KDF	Q	301	37/37	0.96	0.09	63,69,96,97	0
5	CL	F	305	1/1	0.96	0.16	95,95,95,95	0
4	MG	B	306	1/1	0.96	0.09	87,87,87,87	0
2	EDO	U	302	4/4	0.96	0.12	79,84,84,92	0
3	A1KDF	S	301	37/37	0.96	0.08	70,76,89,92	0
5	CL	T	308	1/1	0.96	0.13	101,101,101,101	0
3	A1KDF	N	301	37/37	0.96	0.09	72,78,98,99	0
3	A1KDF	O	301	37/37	0.96	0.09	69,79,112,115	0
3	A1KDF	P	301	37/37	0.96	0.09	65,71,91,93	0
5	CL	Q	306	1/1	0.96	0.34	30,30,30,30	0
3	A1KDF	C	301	37/37	0.97	0.07	63,67,83,86	0
3	A1KDF	L	303	37/37	0.97	0.08	65,75,99,101	0
3	A1KDF	D	301	37/37	0.97	0.08	68,72,88,89	0
3	A1KDF	E	301	37/37	0.97	0.08	67,74,108,109	0
2	EDO	P	302	4/4	0.97	0.10	75,76,79,84	0
5	CL	P	306	1/1	0.97	0.34	30,30,30,30	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.

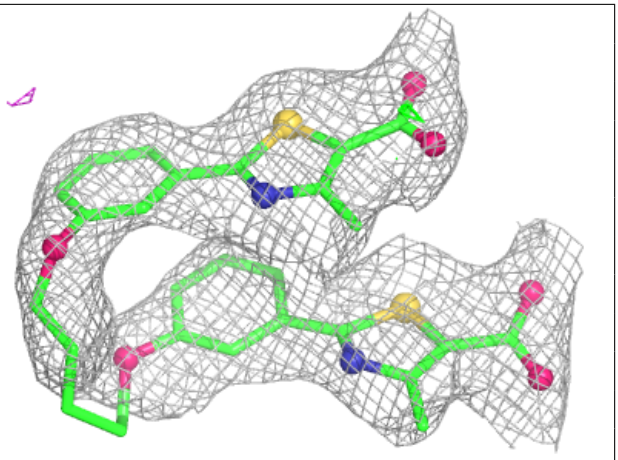
Electron density around A1KDF I 301:

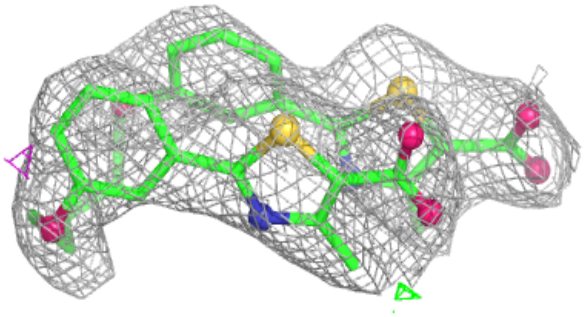
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

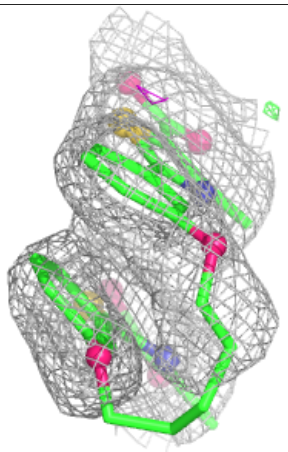


Electron density around A1KDF I 302:

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

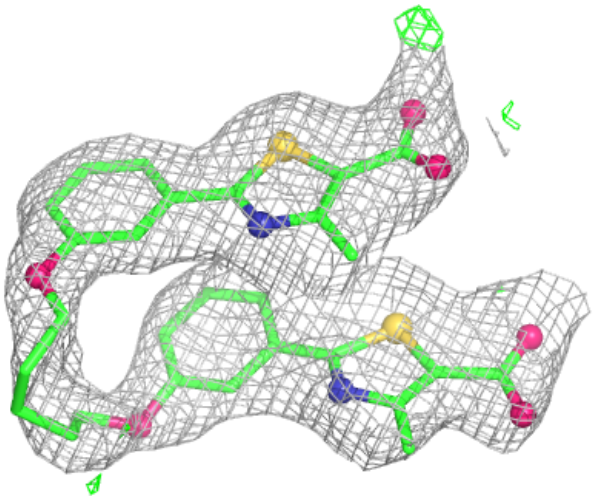


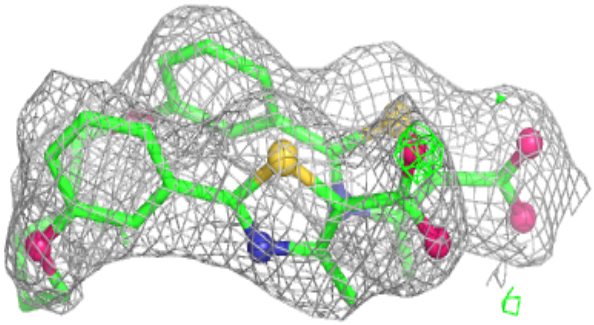


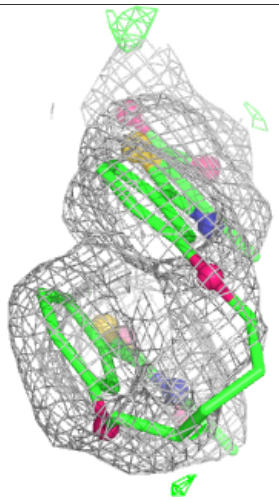


Electron density around A1KDF K 302:

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

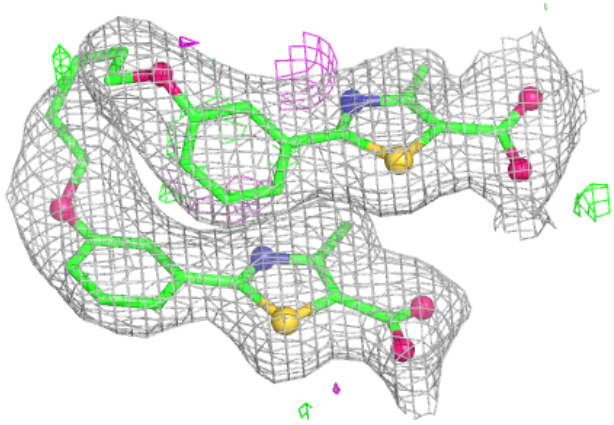


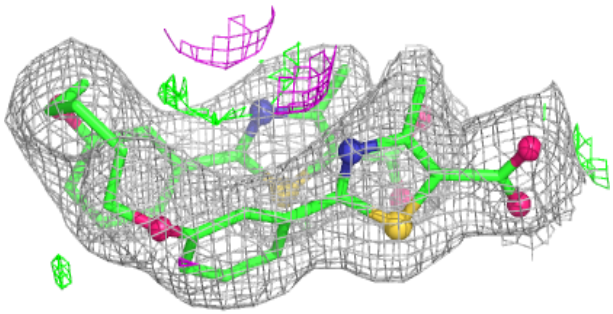


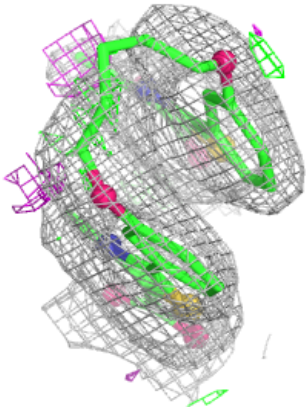


Electron density around A1KDF U 303:

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

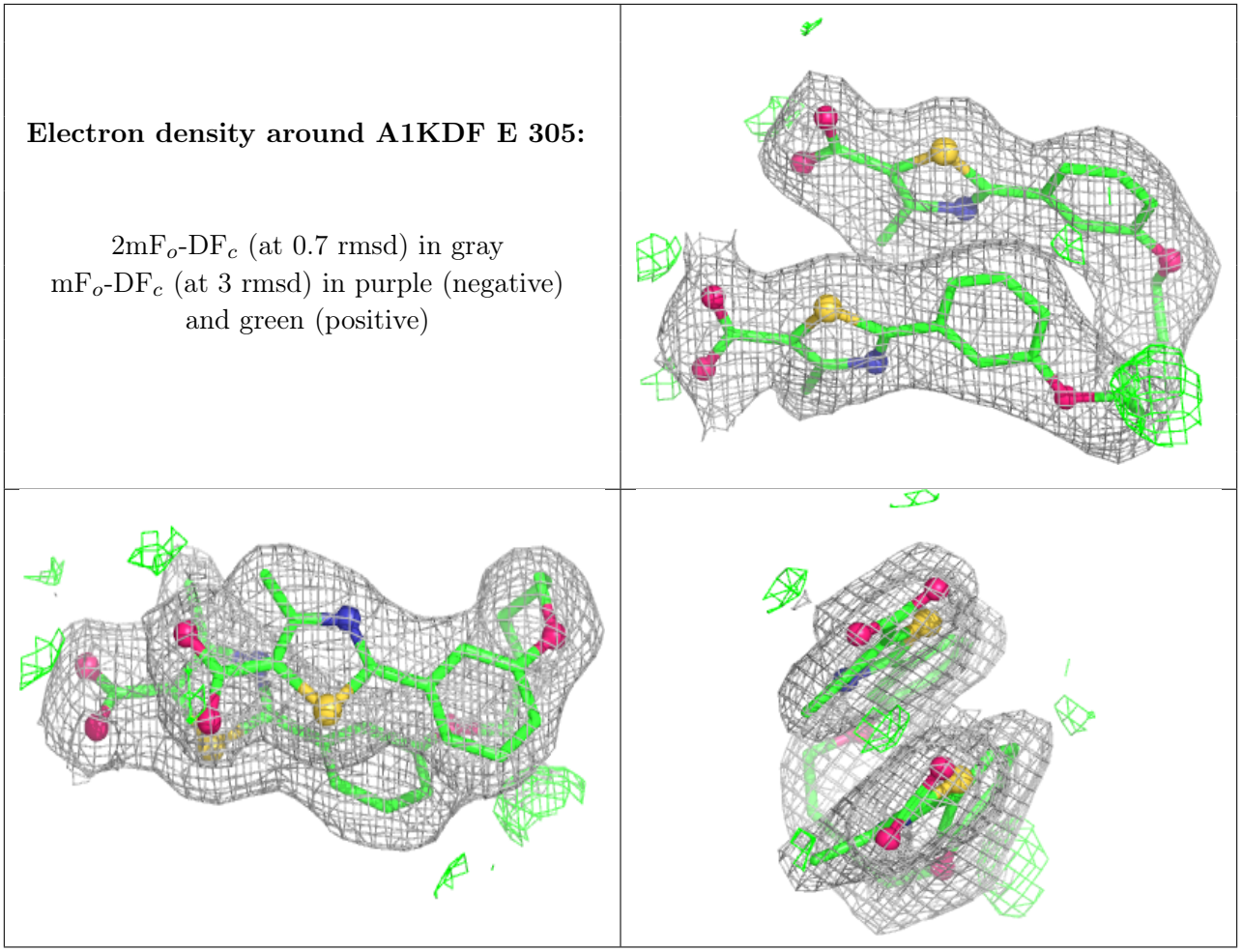






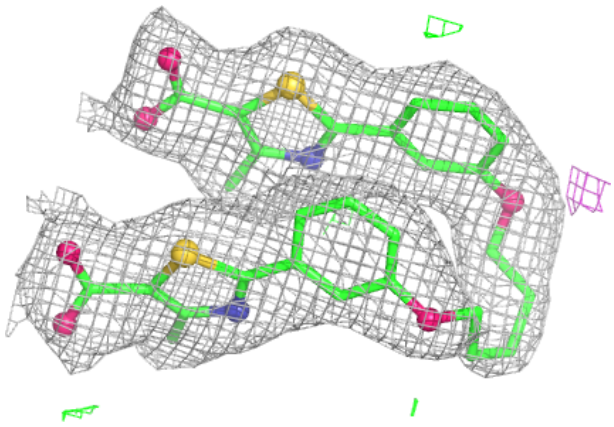
Electron density around A1KDF E 305:

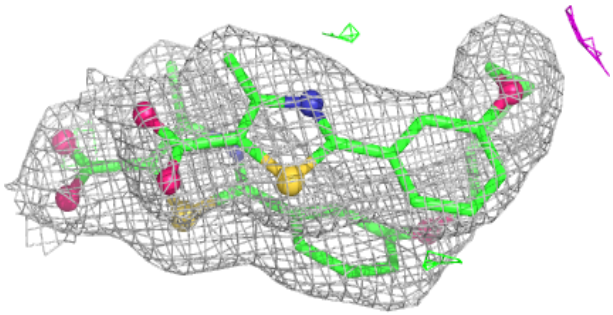
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

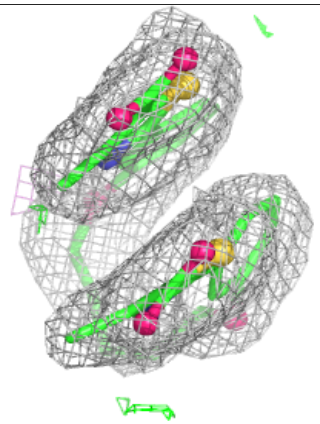


Electron density around A1KDF G 301:

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

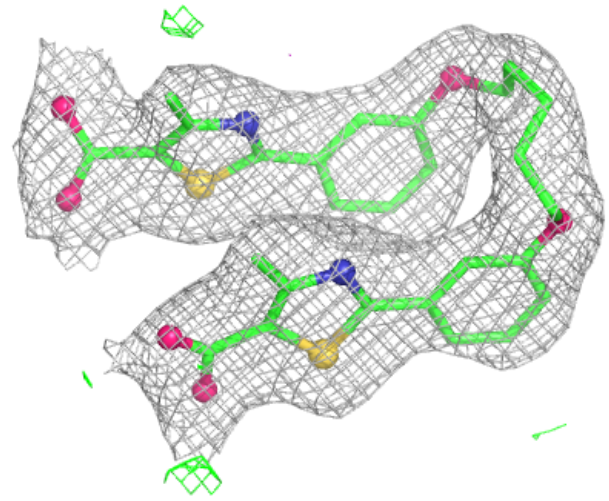


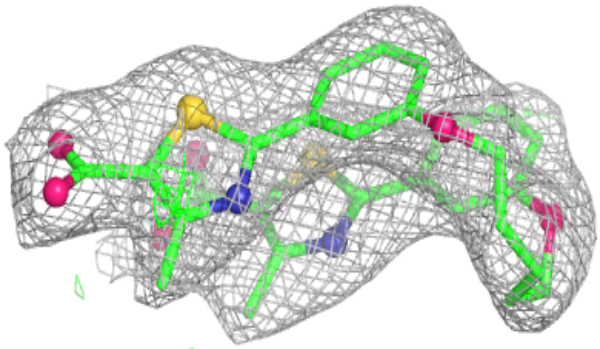


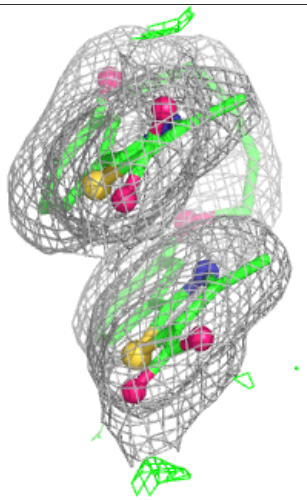


Electron density around A1KDF H 301:

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

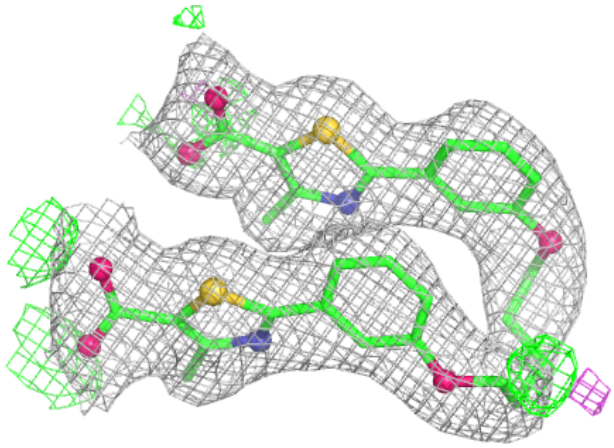


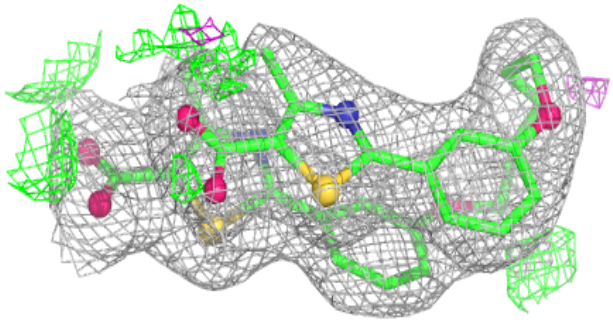


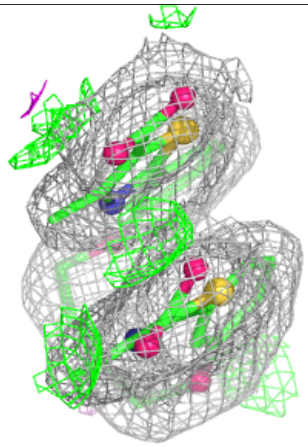


Electron density around A1KDF M 301:

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

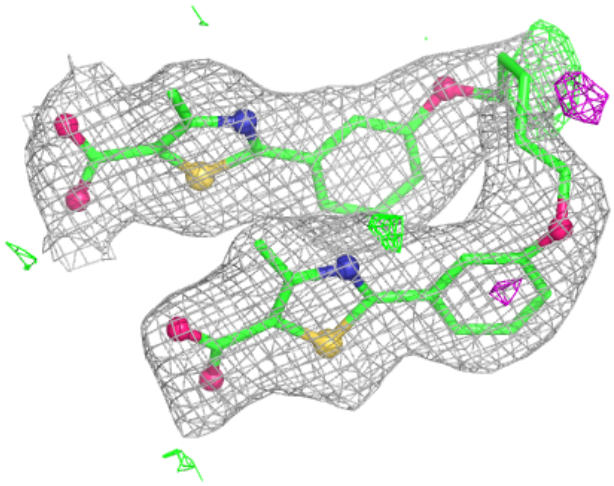


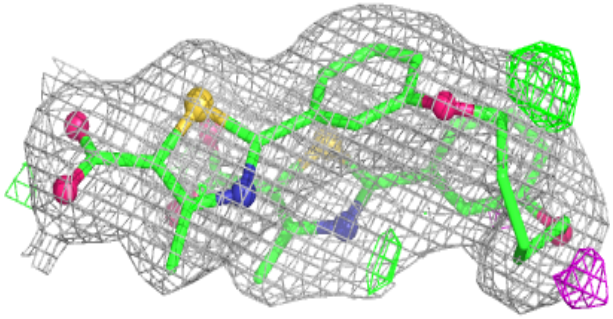


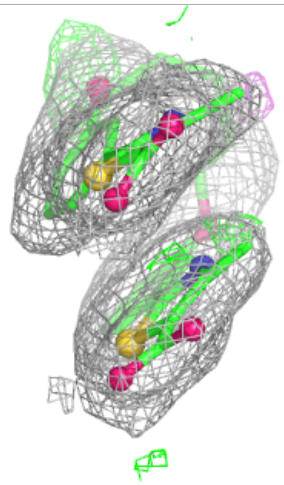


Electron density around A1KDF R 301:

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

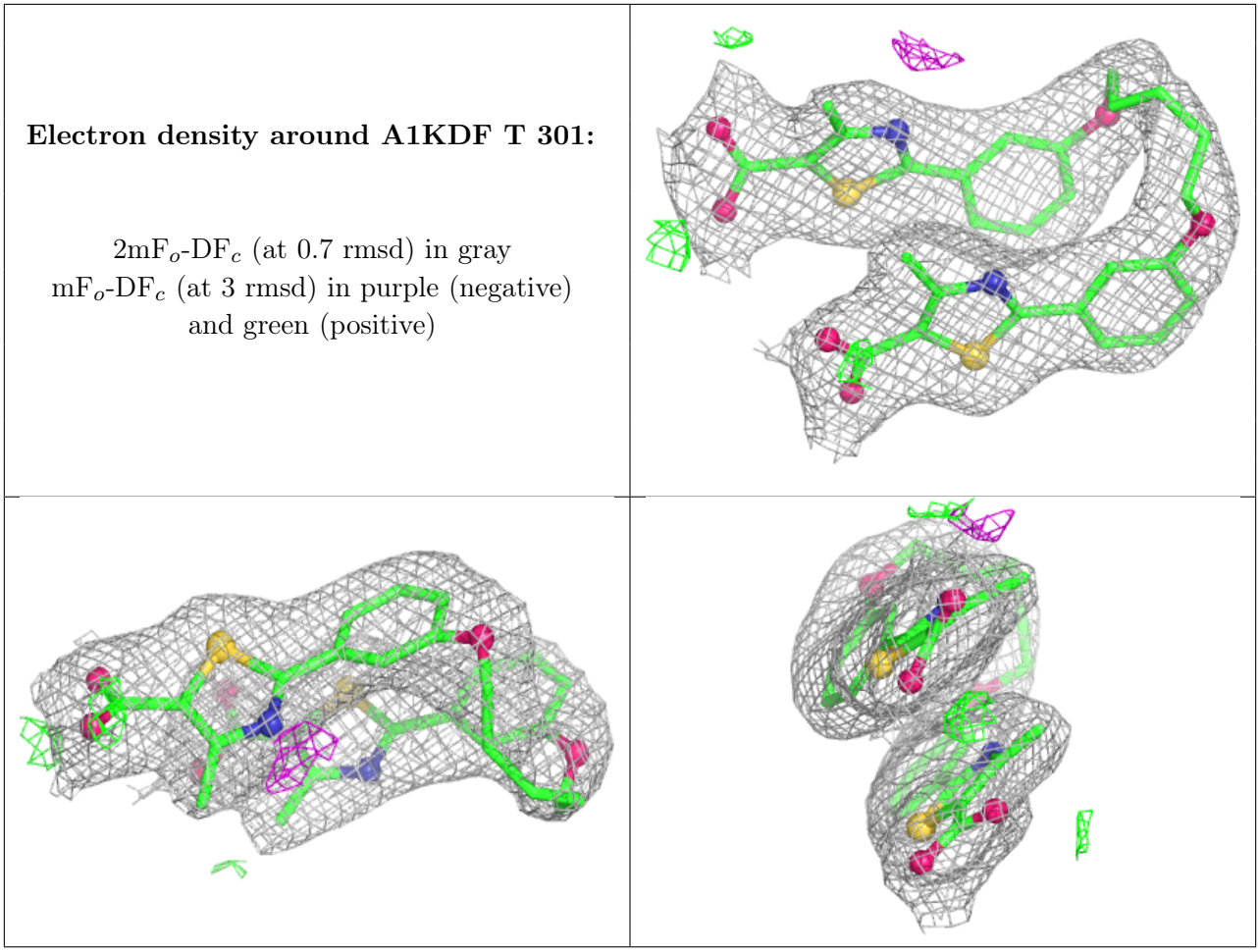






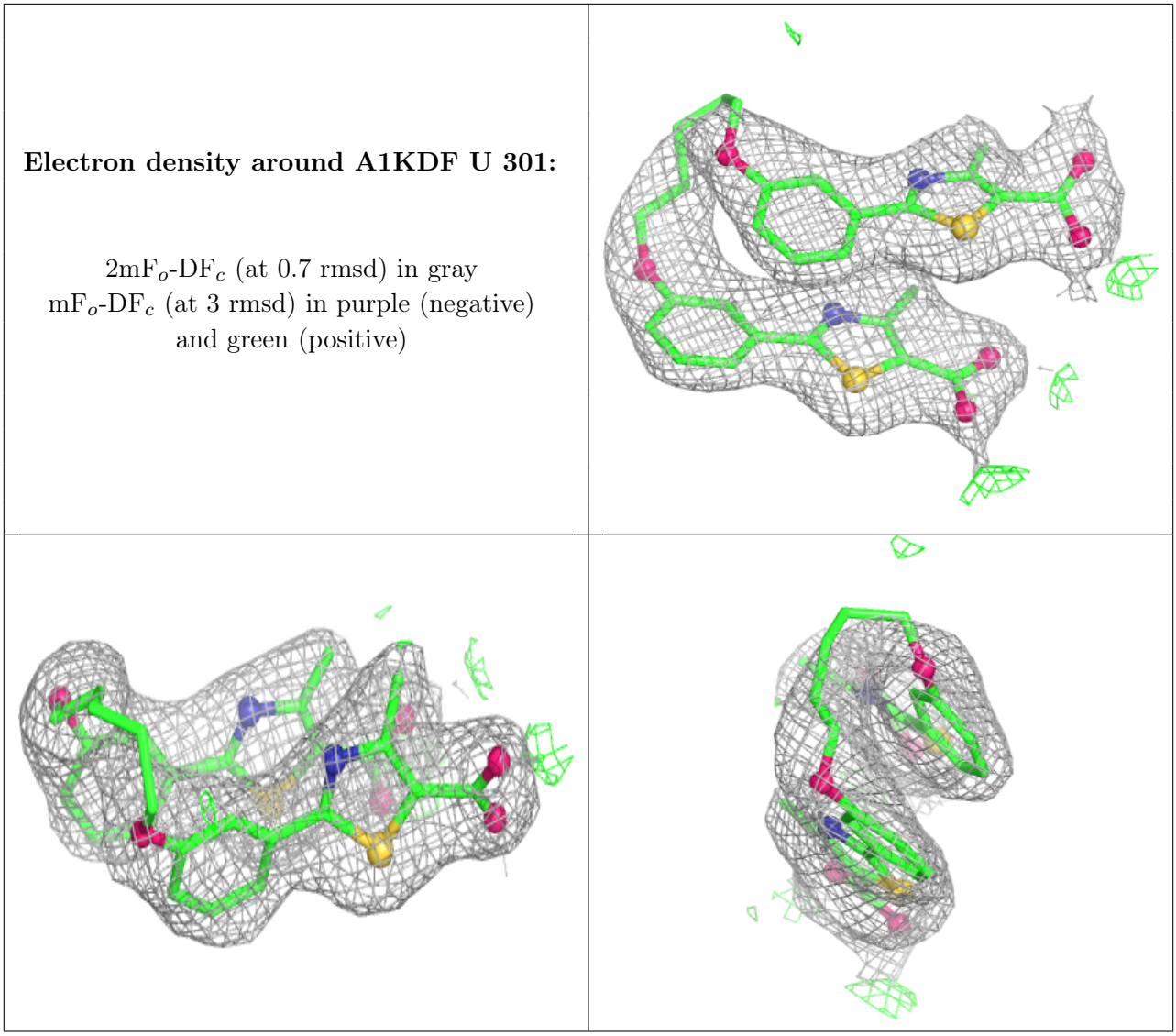
Electron density around A1KDF T 301:

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



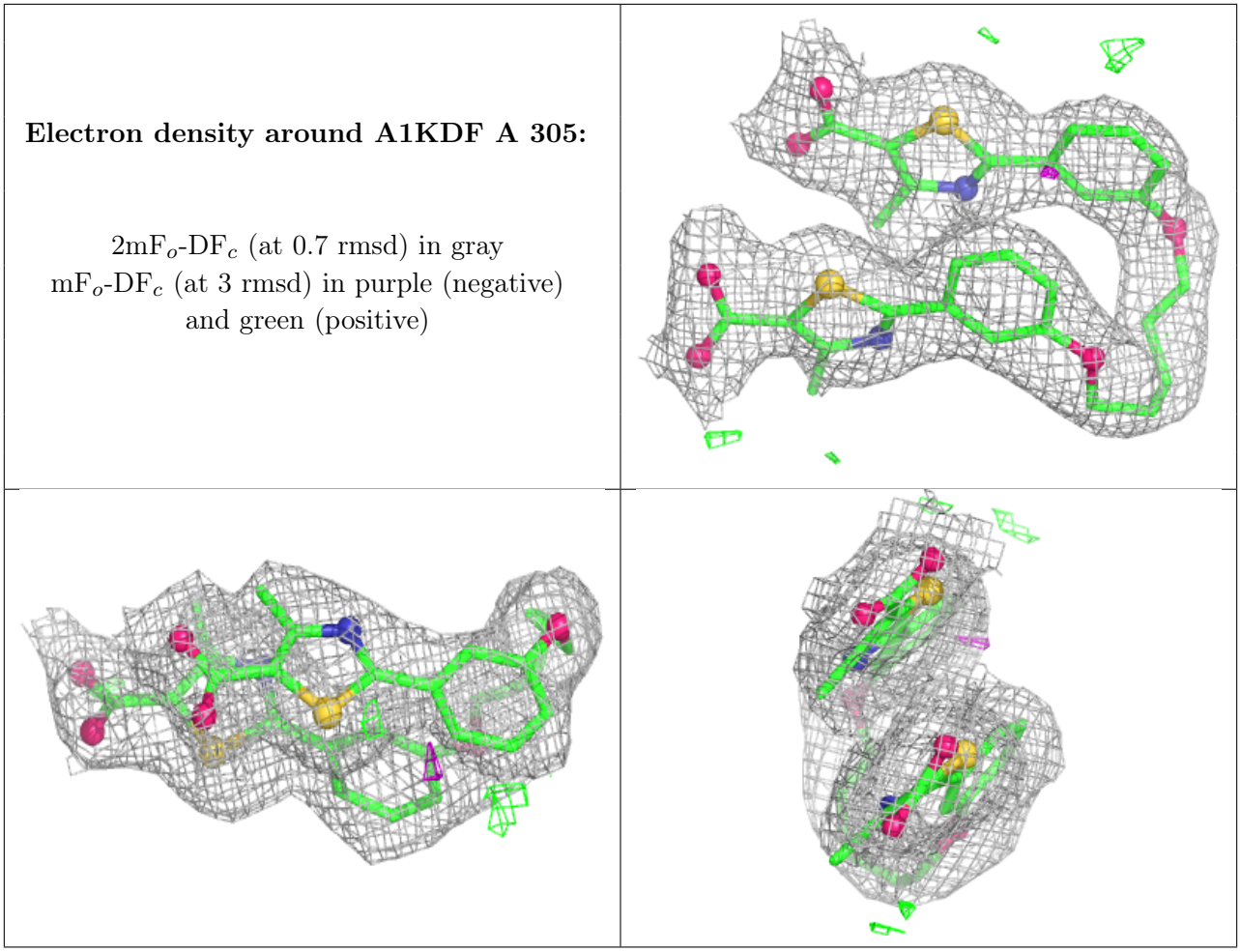
Electron density around A1KDF U 301:

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



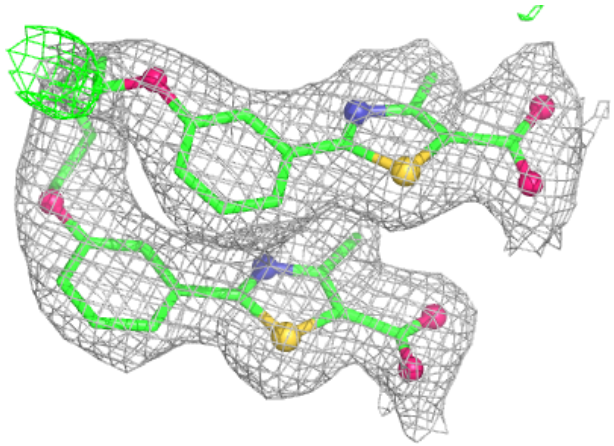
Electron density around A1KDF A 305:

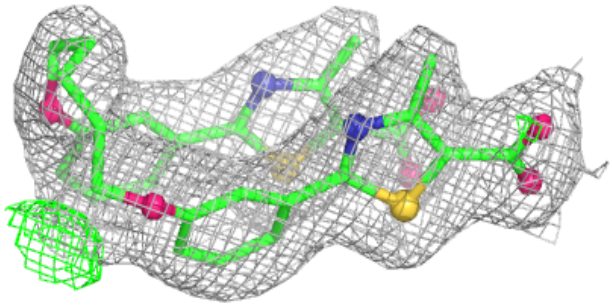
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

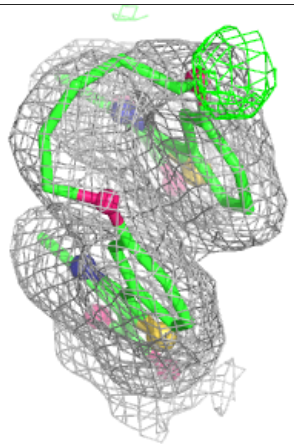


Electron density around A1KDF B 301:

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

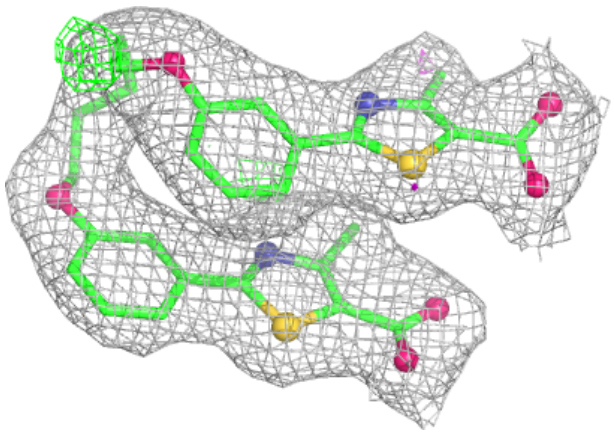


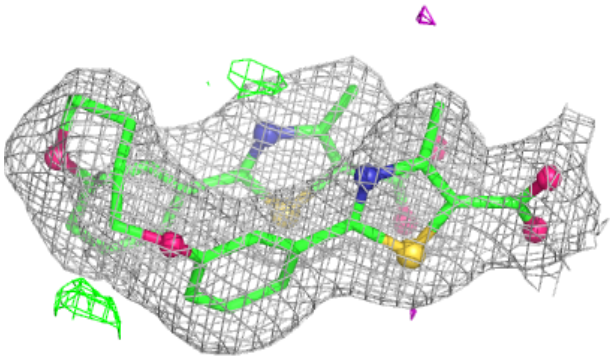


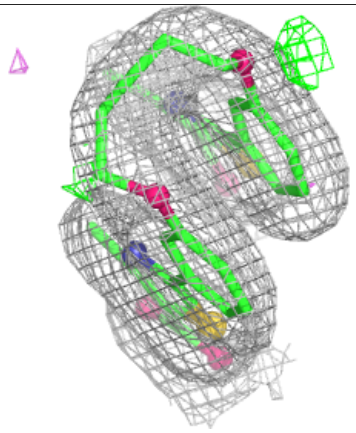


Electron density around A1KDF Q 301:

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

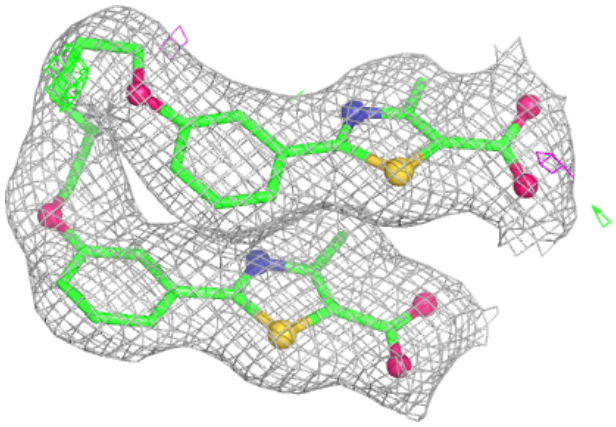


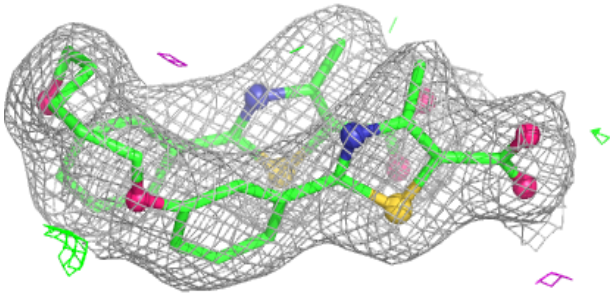


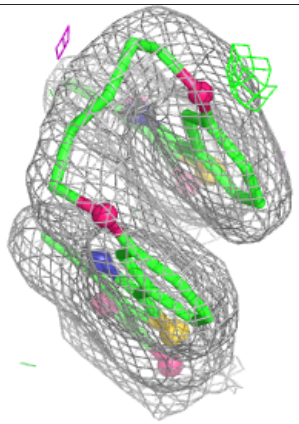


Electron density around A1KDF S 301:

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

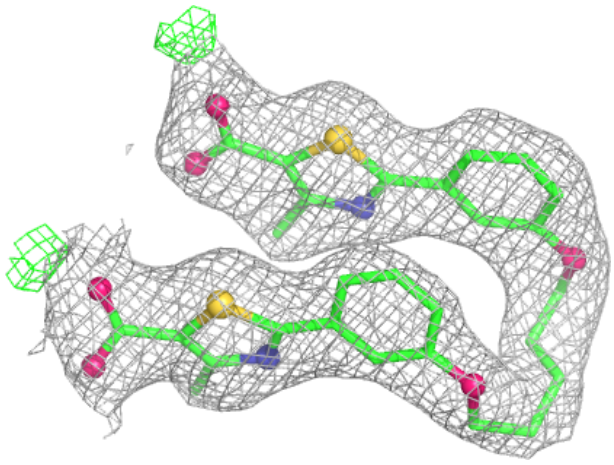


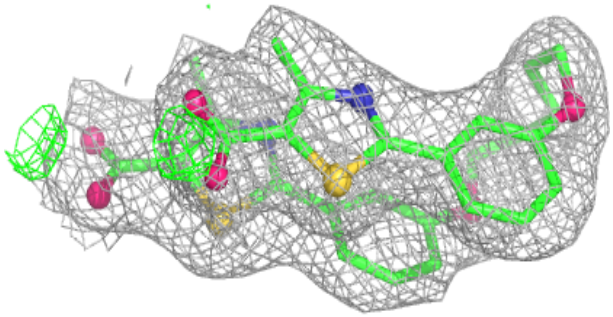


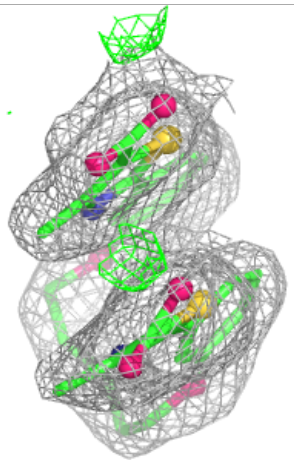


Electron density around A1KDF N 301:

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

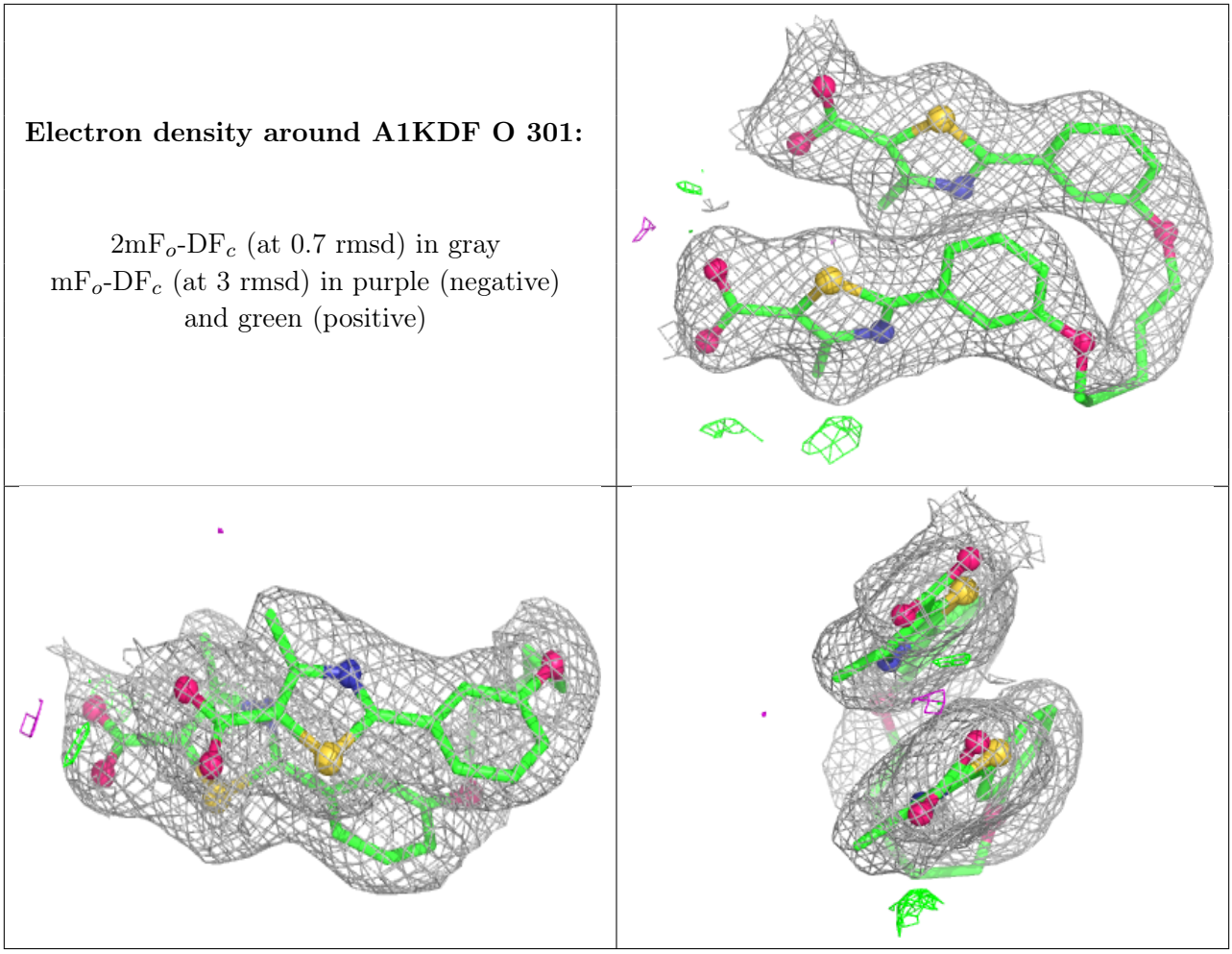






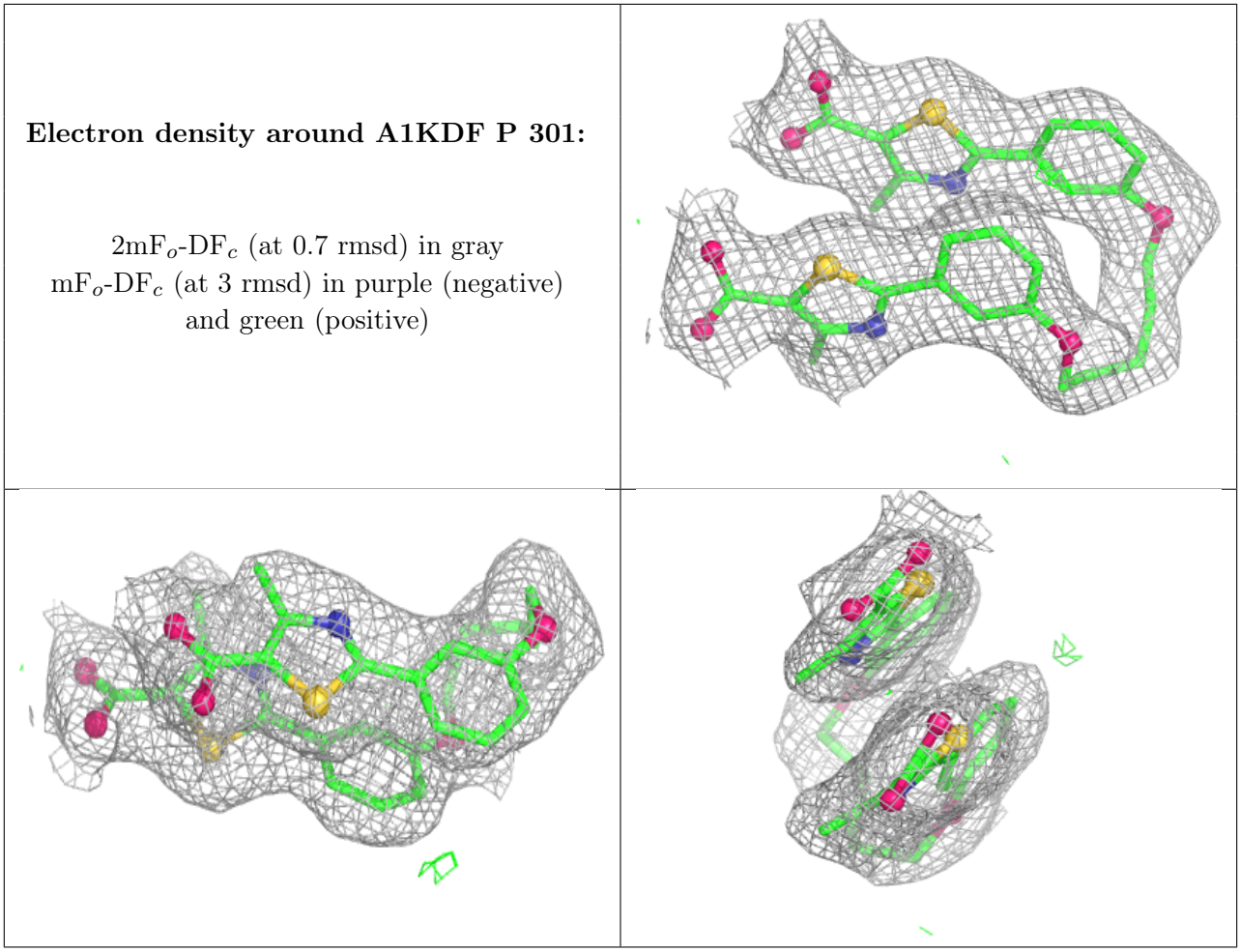
Electron density around A1KDF O 301:

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



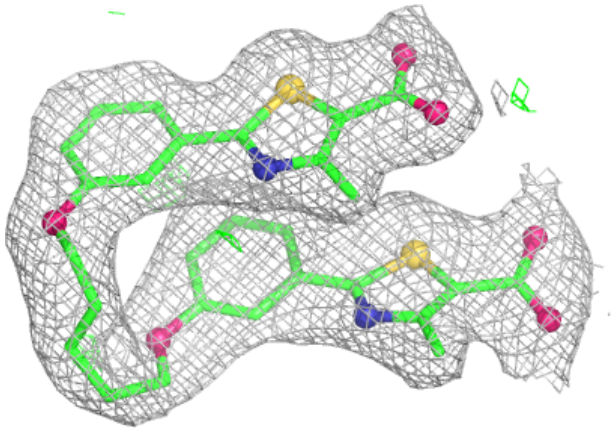
Electron density around A1KDF P 301:

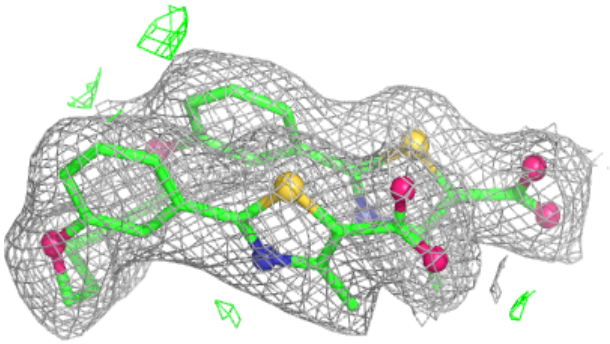
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

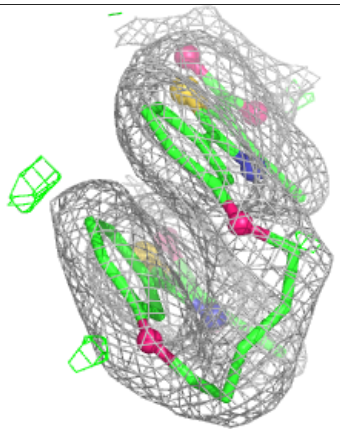


Electron density around A1KDF C 301:

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

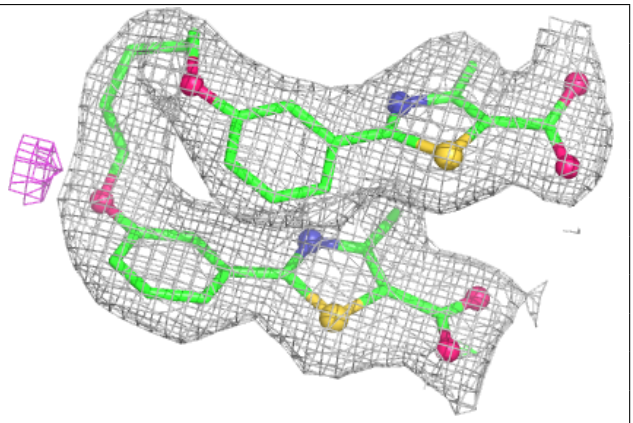


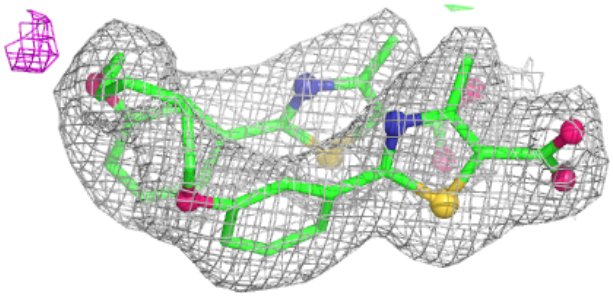


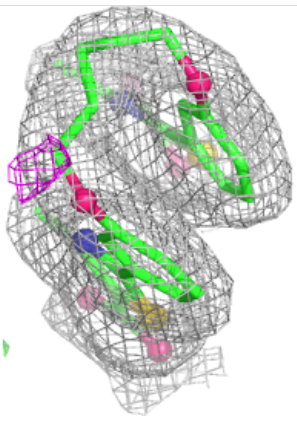


Electron density around A1KDF L 303:

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

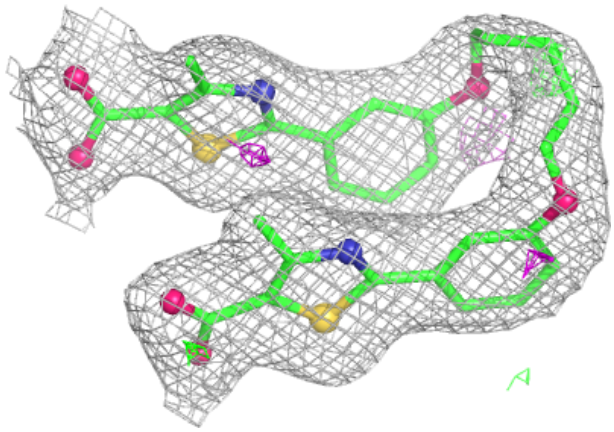


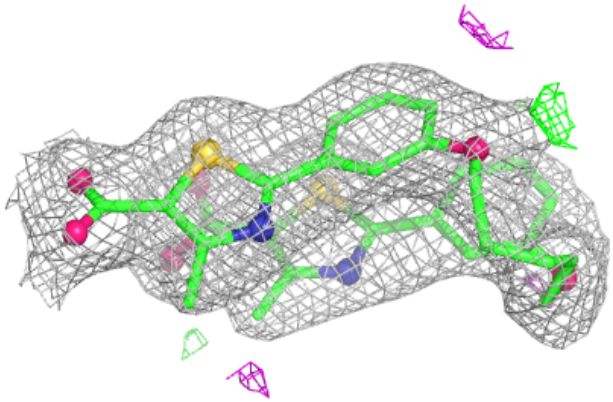


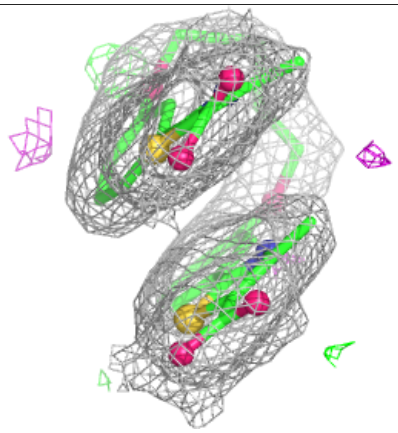


Electron density around A1KDF D 301:

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

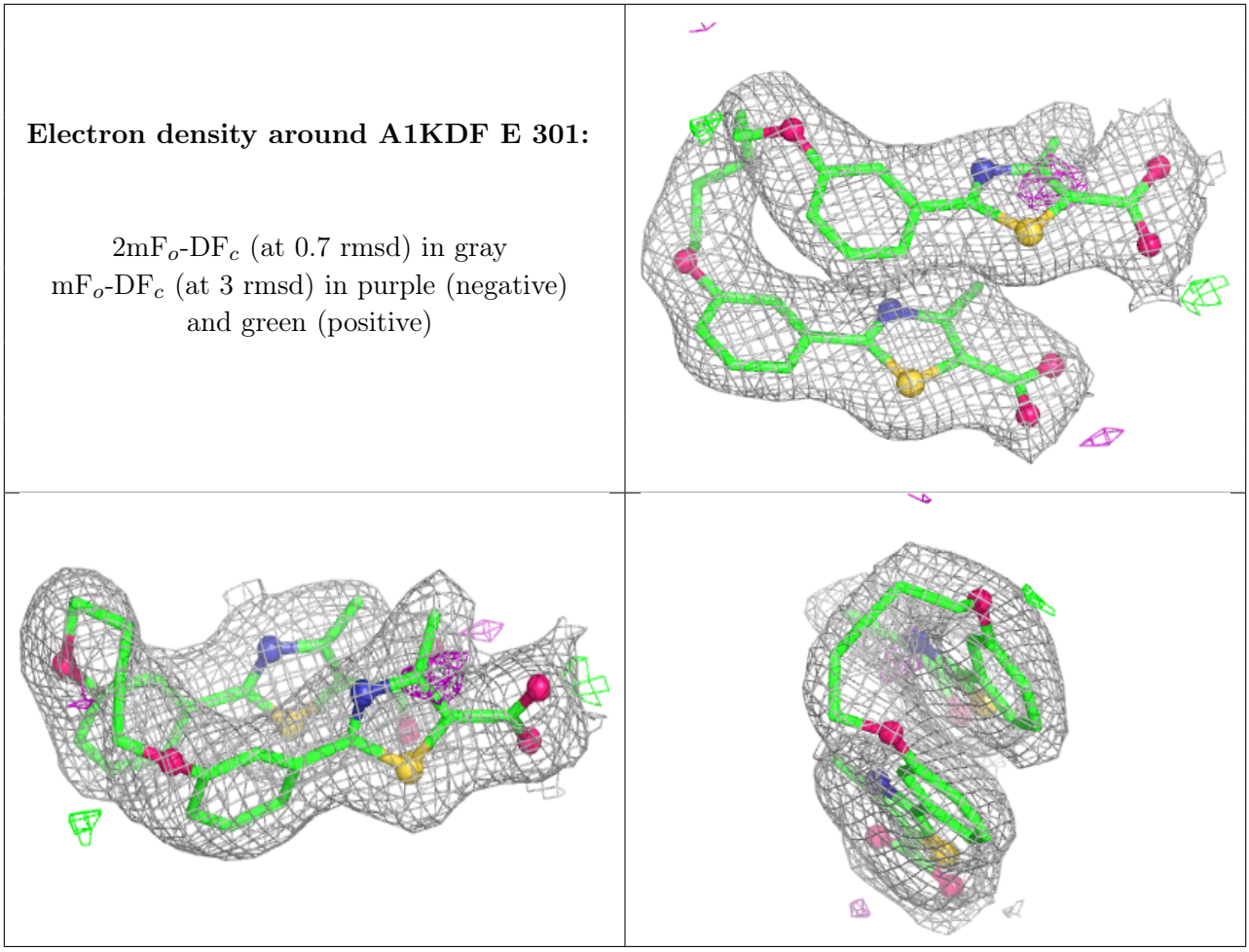






Electron density around A1KDF E 301:

$2mF_o$-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.