



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:11 am BST

PDB ID : 5FL4  
Title : Three dimensional structure of human carbonic anhydrase IX in complex with  
5-(1-naphthalen-1-yl-1,2,3-triazol-4-yl)thiophene-2-sulfonamide  
Authors : Leitans, J.; Tars, K.; Zalubovskis, R.  
Deposited on : 2015-10-21  
Resolution : 1.82 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

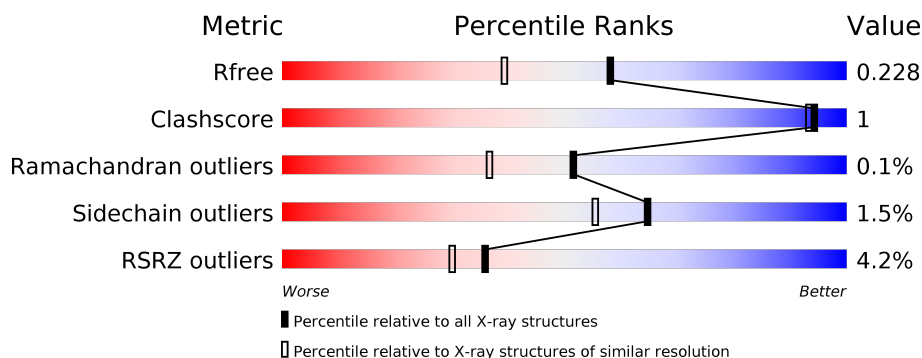
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.82 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	257	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>6%</div> </div> <div>•</div> </div>
1	B	257	<div> <div>4%</div> <div> <div></div> <div>94%</div> <div></div> </div> <div>• •</div> </div>
1	C	257	<div> <div>4%</div> <div> <div></div> <div>94%</div> <div></div> </div> <div>• •</div> </div>
1	D	257	<div> <div>6%</div> <div> <div></div> <div>96%</div> <div></div> </div> <div>• •</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ACY	C	1262	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8966 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 CARBONIC ANHYDRASE 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	1	0
			1946	1240	346	356	4			
1	B	251	Total	C	N	O	S	0	1	0
			1934	1233	342	355	4			
1	C	251	Total	C	N	O	S	0	2	0
			1945	1240	345	356	4			
1	D	251	Total	C	N	O	S	0	2	0
			1943	1240	343	356	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	GLY	-	expression tag	UNP Q16790
A	4	PRO	-	expression tag	UNP Q16790
A	42	SER	CYS	engineered mutation	UNP Q16790
B	3	GLY	-	expression tag	UNP Q16790
B	4	PRO	-	expression tag	UNP Q16790
B	42	SER	CYS	engineered mutation	UNP Q16790
C	3	GLY	-	expression tag	UNP Q16790
C	4	PRO	-	expression tag	UNP Q16790
C	42	SER	CYS	engineered mutation	UNP Q16790
D	3	GLY	-	expression tag	UNP Q16790
D	4	PRO	-	expression tag	UNP Q16790
D	42	SER	CYS	engineered mutation	UNP Q16790

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

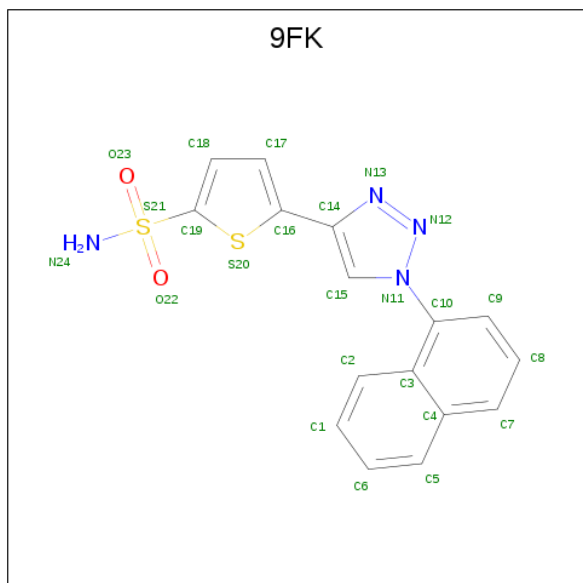
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 5-(1-naphthalen-1-yl-1,2,3-triazol-4-yl)thiophene-2-sulfonamide (three-letter code: 9FK) (formula: C<sub>16</sub>H<sub>12</sub>N<sub>4</sub>O<sub>2</sub>S<sub>2</sub>).



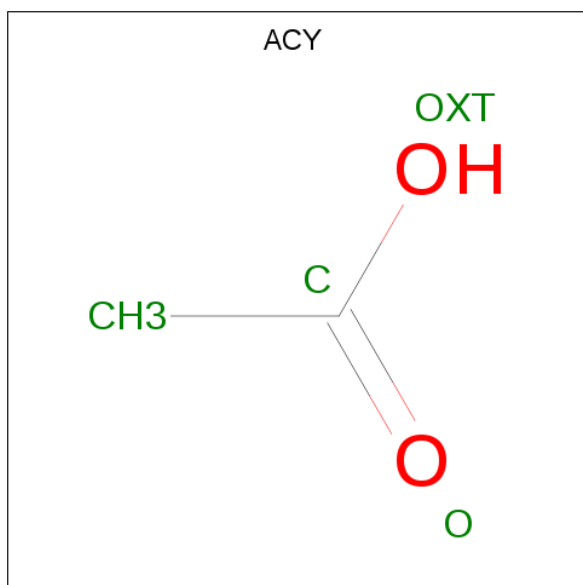
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			24	16	4	2	2		
3	B	1	Total	C	N	O	S	0	0
			24	16	4	2	2		
3	C	1	Total	C	N	O	S	0	0
			24	16	4	2	2		
3	D	1	Total	C	N	O	S	0	0
			24	16	4	2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	352	Total O 352 352	0	0
6	B	280	Total O 280 280	0	0
6	C	226	Total O 226 226	0	0
6	D	192	Total O 192 192	0	0

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

These plots are drawn for all protein, RNA and DNA 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: CARBONIC ANHYDRASE 9

Chain A: 



#### • Molecule 1: CARBONIC ANHYDRASE 9

Chain B: 



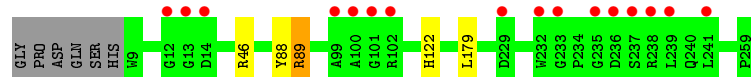
#### • Molecule 1: CARBONIC ANHYDRASE 9

Chain C: 



#### • Molecule 1: CARBONIC ANHYDRASE 9

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.29Å 152.29Å 172.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	61.56 – 1.82 57.38 – 1.82	Depositor EDS
% Data completeness (in resolution range)	100.0 (61.56-1.82) 100.0 (57.38-1.82)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.190 , 0.224 0.198 , 0.228	Depositor DCC
$R_{free}$ test set	6944 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.2	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8966	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, ACY, 9FK

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	0.58	0/2007	0.72	1/2741 (0.0%)
1	B	0.54	0/1995	0.72	2/2728 (0.1%)
1	C	0.50	0/2009	0.70	1/2745 (0.0%)
1	D	0.47	0/2007	0.68	0/2742
All	All	0.53	0/8018	0.70	4/10956 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	163	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	27	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	86	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	86	ARG	NE-CZ-NH1	5.16	122.88	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	1946	0	1897	6	0
1	B	1934	0	1876	3	0
1	C	1945	0	1896	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1943	0	1890	5	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	0	11	1	0
3	B	24	0	12	0	0
3	C	24	0	12	0	0
3	D	24	0	12	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	1	0
4	D	6	0	8	0	0
5	A	8	0	6	0	0
5	B	4	0	3	0	0
5	C	12	0	9	3	0
6	A	352	0	0	1	0
6	B	280	0	0	1	1
6	C	226	0	0	1	0
6	D	192	0	0	0	0
All	All	8966	0	7656	20	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (20) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89[A]:ARG:HH11	1:D:89[A]:ARG:HG2	1.04	1.14
1:D:89[A]:ARG:HH11	1:D:89[A]:ARG:CG	1.68	1.03
1:D:89[A]:ARG:NH1	1:D:89[A]:ARG:HG2	1.74	0.93
5:C:1262:ACY:H2	6:C:2202:HOH:O	1.95	0.66
1:D:89[A]:ARG:NH1	1:D:89[A]:ARG:CG	2.41	0.60
1:C:196:GLU:OE2	5:C:1262:ACY:H3	2.01	0.60
1:A:88:TYR:HB3	1:A:122:HIS:HB3	1.92	0.52
1:D:88:TYR:HB3	1:D:122:HIS:HB3	1.94	0.49
1:C:88:TYR:HB3	1:C:122:HIS:HB3	1.95	0.48
1:C:207:GLY:N	5:C:1262:ACY:H1	2.30	0.47
1:C:129:ARG:NH2	1:C:131[B]:ASP:OD2	2.49	0.46
1:A:55:LEU:HD21	1:A:78:LEU:HD11	1.99	0.45
1:A:48:LEU:HD11	1:A:211:THR:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:HIS:NE2	1:A:229[A]:ASP:OD2	2.50	0.44
6:A:2061:HOH:O	1:B:27:ARG:HD3	2.16	0.43
1:A:134:LEU:HD11	3:A:269:9FK:C1	2.50	0.42
1:B:61:LEU:HD13	1:B:178:GLY:HA2	2.01	0.42
1:C:92:GLN:HE22	4:C:271:GOL:H32	1.84	0.41
1:A:14:ASP:HB3	1:A:15:PRO:HA	2.03	0.41
1:B:159:GLN:NE2	6:B:2207:HOH:O	2.48	0.41

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:2061:HOH:O	6:B:2061:HOH:O[3_555]	0.75	1.45

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	250/257 (97%)	245 (98%)	5 (2%)	0	100	100
1	B	250/257 (97%)	243 (97%)	6 (2%)	1 (0%)	34	21
1	C	251/257 (98%)	246 (98%)	5 (2%)	0	100	100
1	D	251/257 (98%)	244 (97%)	7 (3%)	0	100	100
All	All	1002/1028 (98%)	978 (98%)	23 (2%)	1 (0%)	51	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	100	ALA

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	204/210 (97%)	201 (98%)	3 (2%)	65	55
1	B	202/210 (96%)	198 (98%)	4 (2%)	55	43
1	C	204/210 (97%)	202 (99%)	2 (1%)	76	70
1	D	203/210 (97%)	199 (98%)	4 (2%)	55	43
All	All	813/840 (97%)	800 (98%)	13 (2%)	65	53

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	ASP
1	A	214	ASN
1	A	239	LEU
1	B	14	ASP
1	B	22	PRO
1	B	179	LEU
1	B	239	LEU
1	C	136	ARG
1	C	229	ASP
1	D	46	ARG
1	D	89[A]	ARG
1	D	89[B]	ARG
1	D	179	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	68	HIS
1	A	71	GLN
1	B	37	GLN
1	B	71	GLN
1	C	71	GLN

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Mol	Chain	Res	Type
1	C	159	GLN
1	C	214	ASN
1	C	247	GLN
1	D	37	GLN
1	D	71	GLN
1	D	159	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	$\# Z  > 2$
5	ACY	C	1261	-	1,3,3	1.78	0	0,3,3	0.00	-
4	GOL	C	271	-	5,5,5	0.56	0	5,5,5	1.14	0
5	ACY	C	1262	-	1,3,3	1.17	0	0,3,3	0.00	-
3	9FK	D	266	2	22,27,27	2.07	4 (18%)	21,40,40	3.10	6 (28%)
4	GOL	D	271	-	5,5,5	0.30	0	5,5,5	0.61	0
4	GOL	A	273	-	5,5,5	0.69	0	5,5,5	0.75	0
3	9FK	B	268	2	22,27,27	1.98	4 (18%)	21,40,40	2.13	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	ACY	C	1260	-	1,3,3	2.01	1 (100%)	0,3,3	0.00	-
4	GOL	B	272	-	5,5,5	0.29	0	5,5,5	0.56	0
5	ACY	B	1260	-	1,3,3	1.58	0	0,3,3	0.00	-
3	9FK	A	269	2	22,27,27	2.04	4 (18%)	21,40,40	2.34	5 (23%)
5	ACY	A	1260	-	1,3,3	1.52	0	0,3,3	0.00	-
3	9FK	C	267	2	22,27,27	2.12	5 (22%)	21,40,40	2.78	7 (33%)
5	ACY	A	1261	-	1,3,3	1.71	0	0,3,3	0.00	-

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
4	GOL	C	271	-	-	2/4/4/4	-
4	GOL	B	272	-	-	0/4/4/4	-
3	9FK	D	266	2	-	3/4/14/14	0/4/4/4
4	GOL	D	271	-	-	2/4/4/4	-
4	GOL	A	273	-	-	4/4/4/4	-
3	9FK	B	268	2	-	3/4/14/14	0/4/4/4
3	9FK	A	269	2	-	3/4/14/14	0/4/4/4
3	9FK	C	267	2	-	3/4/14/14	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	266	9FK	C19-S21	-6.57	1.66	1.76
3	C	267	9FK	C19-S21	-6.51	1.66	1.76
3	A	269	9FK	C19-S21	-6.26	1.66	1.76
3	B	268	9FK	C19-S21	-5.60	1.67	1.76
3	B	268	9FK	C3-C4	4.39	1.51	1.43
3	D	266	9FK	C3-C4	4.19	1.50	1.43
3	A	269	9FK	C3-C4	3.98	1.50	1.43
3	C	267	9FK	C3-C4	3.85	1.50	1.43
3	C	267	9FK	C10-C3	3.48	1.50	1.43
3	A	269	9FK	N13-N12	3.36	1.40	1.34
3	B	268	9FK	C10-C3	3.29	1.50	1.43
3	C	267	9FK	N13-N12	3.22	1.40	1.34
3	D	266	9FK	C10-C3	3.13	1.49	1.43
3	A	269	9FK	C10-C3	3.12	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	266	9FK	N13-N12	3.00	1.39	1.34
3	B	268	9FK	N13-N12	2.88	1.39	1.34
3	C	267	9FK	N12-N11	2.32	1.40	1.37
5	C	1260	ACY	CH3-C	2.01	1.51	1.48

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	266	9FK	O23-S21-O22	-9.88	102.53	118.76
3	C	267	9FK	O23-S21-O22	-7.69	106.12	118.76
3	C	267	9FK	O23-S21-N24	6.06	116.35	107.36
3	D	266	9FK	O23-S21-N24	5.94	116.17	107.36
3	A	269	9FK	O23-S21-O22	-5.76	109.30	118.76
3	B	268	9FK	O23-S21-N24	5.70	115.81	107.36
3	A	269	9FK	O22-S21-N24	5.53	115.56	107.36
3	D	266	9FK	C16-C14-N13	-4.67	113.17	120.88
3	A	269	9FK	C16-C14-N13	-4.41	113.60	120.88
3	D	266	9FK	C8-C9-C10	4.01	125.16	117.94
3	B	268	9FK	C8-C9-C10	3.99	125.14	117.94
3	A	269	9FK	C8-C9-C10	3.82	124.83	117.94
3	C	267	9FK	C16-C14-N13	-3.81	114.58	120.88
3	B	268	9FK	C16-C14-N13	-3.73	114.71	120.88
3	C	267	9FK	O23-S21-C19	3.72	112.75	107.29
3	D	266	9FK	O23-S21-C19	3.38	112.24	107.29
3	C	267	9FK	O22-S21-C19	-3.33	102.41	107.29
3	C	267	9FK	C8-C9-C10	3.22	123.75	117.94
3	B	268	9FK	C9-C10-C3	-2.96	114.73	120.86
3	D	266	9FK	C9-C10-C3	-2.93	114.81	120.86
3	B	268	9FK	O22-S21-C19	-2.85	103.11	107.29
3	B	268	9FK	O23-S21-O22	-2.74	114.26	118.76
3	A	269	9FK	C9-C10-C3	-2.70	115.28	120.86
3	C	267	9FK	C9-C10-C3	-2.42	115.87	120.86

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	271	GOL	O1-C1-C2-O2
4	D	271	GOL	C1-C2-C3-O3
4	A	273	GOL	O1-C1-C2-C3
3	B	268	9FK	C3-C10-N11-C15
3	B	268	9FK	C3-C10-N11-N12

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Mol	Chain	Res	Type	Atoms
3	C	267	9FK	C3-C10-N11-N12
4	C	271	GOL	O1-C1-C2-C3
4	A	273	GOL	C1-C2-C3-O3
4	D	271	GOL	O2-C2-C3-O3
3	D	266	9FK	C3-C10-N11-N12
3	A	269	9FK	C3-C10-N11-N12
4	A	273	GOL	O1-C1-C2-O2
3	D	266	9FK	C9-C10-N11-C15
3	B	268	9FK	C9-C10-N11-C15
3	A	269	9FK	C9-C10-N11-C15
3	C	267	9FK	C9-C10-N11-C15
4	A	273	GOL	O2-C2-C3-O3
3	D	266	9FK	C3-C10-N11-C15
3	A	269	9FK	C3-C10-N11-C15
3	C	267	9FK	C3-C10-N11-C15

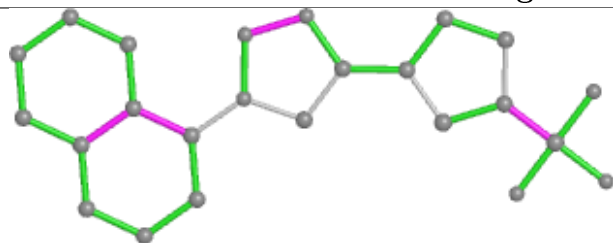
There are no ring outliers.

3 monomers are involved in 5 short contacts:

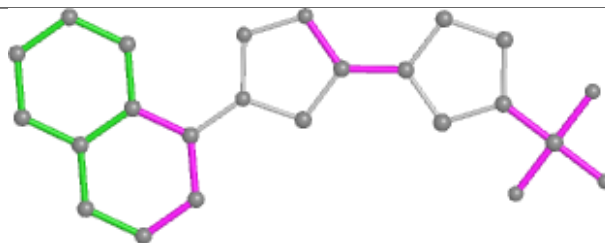
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	271	GOL	1	0
5	C	1262	ACY	3	0
3	A	269	9FK	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

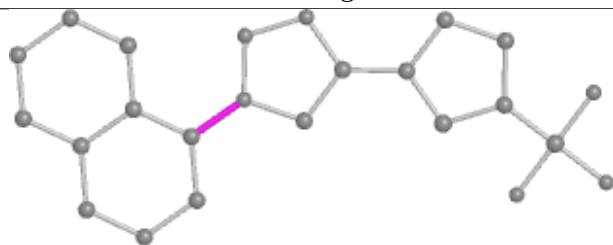
## Ligand 9FK D 266



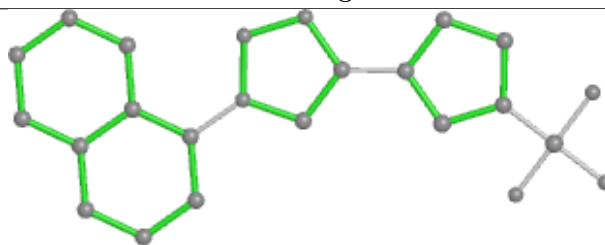
Bond lengths



Bond angles

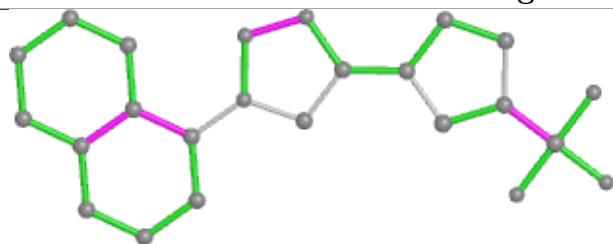


Torsions

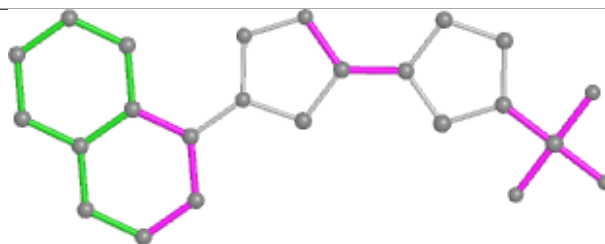


Rings

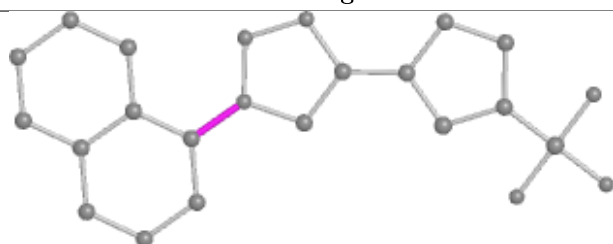
## Ligand 9FK B 268



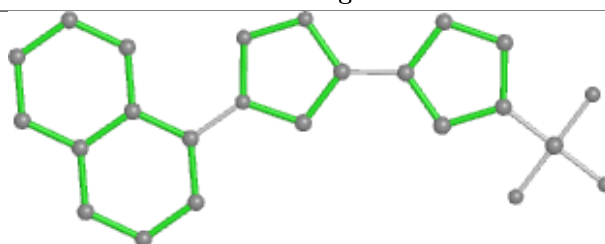
Bond lengths



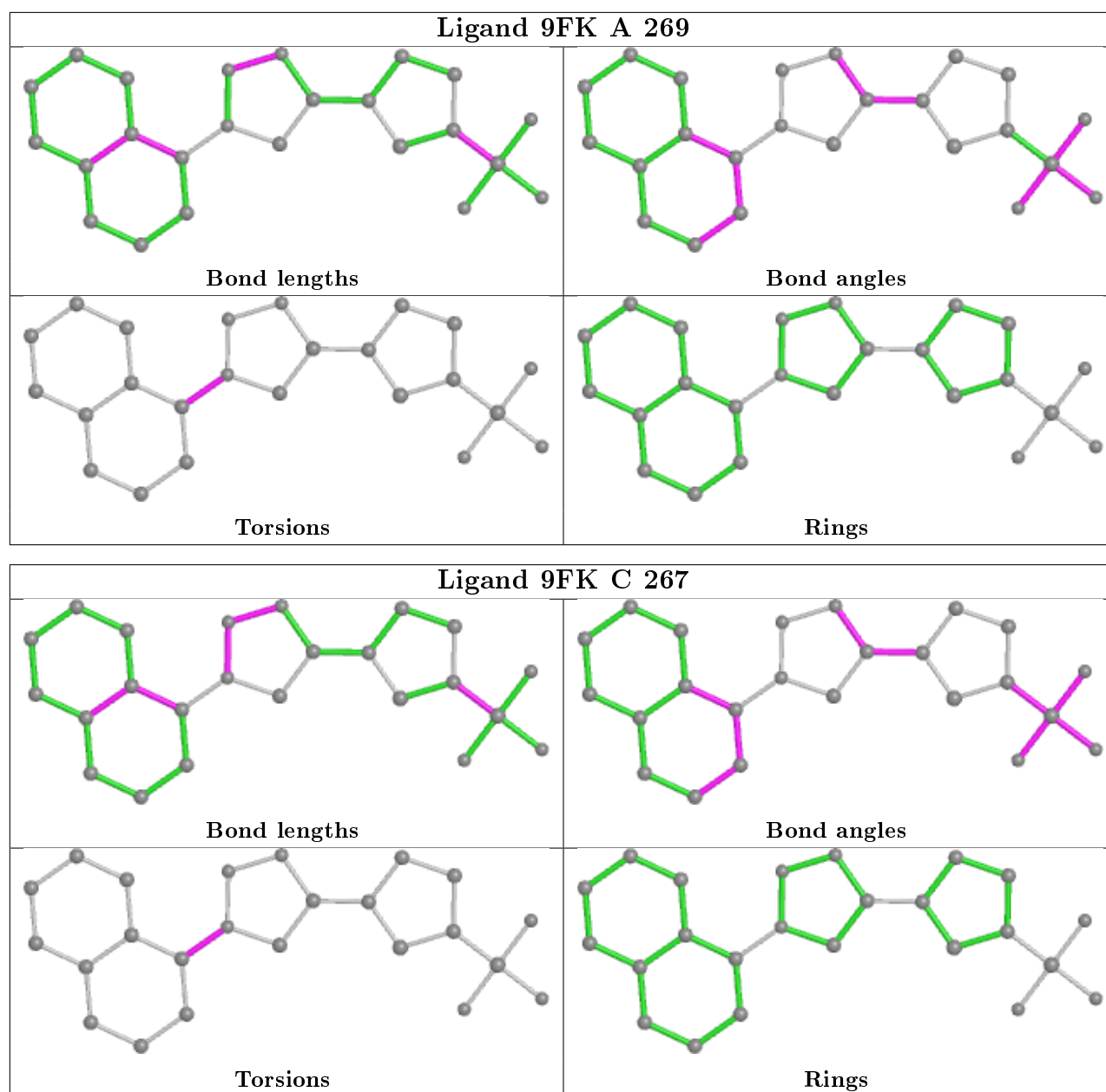
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	251/257 (97%)	-0.31	5 (1%) 65 61	15, 24, 43, 60	0
1	B	251/257 (97%)	-0.17	10 (3%) 38 32	17, 26, 53, 73	0
1	C	251/257 (97%)	-0.05	11 (4%) 34 28	20, 31, 52, 71	0
1	D	251/257 (97%)	0.10	16 (6%) 19 15	20, 34, 59, 80	0
All	All	1004/1028 (97%)	-0.11	42 (4%) 36 30	15, 29, 53, 80	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	235	GLY	5.8
1	D	232	TRP	5.5
1	D	235	GLY	5.1
1	B	235	GLY	4.8
1	C	236	ASP	4.6
1	D	100	ALA	4.4
1	A	235	GLY	4.2
1	B	15	PRO	4.0
1	A	236	ASP	3.6
1	B	232	TRP	3.5
1	D	12	GLY	3.4
1	D	237	SER	3.3
1	D	236	ASP	3.2
1	D	241	LEU	3.0
1	D	229	ASP	2.9
1	D	238	ARG	2.9
1	B	236	ASP	2.9
1	C	100	ALA	2.9
1	B	13	GLY	2.9
1	C	101	GLY	2.8
1	D	239	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	99	ALA	2.7
1	D	102	ARG	2.6
1	C	151	PRO	2.6
1	C	12	GLY	2.6
1	B	100	ALA	2.6
1	C	10	ARG	2.4
1	D	101	GLY	2.4
1	A	232	TRP	2.3
1	B	237	SER	2.3
1	C	232	TRP	2.3
1	B	165	GLU	2.3
1	A	13	GLY	2.2
1	C	237	SER	2.2
1	D	13	GLY	2.2
1	B	101	GLY	2.1
1	D	14	ASP	2.1
1	C	14	ASP	2.1
1	A	14	ASP	2.1
1	C	234	PRO	2.1
1	D	233	GLY	2.1
1	B	12	GLY	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ACY	A	1260	4/4	0.69	0.20	40,49,49,52	0
4	GOL	C	271	6/6	0.75	0.23	43,48,51,51	0

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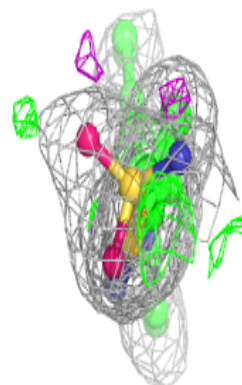
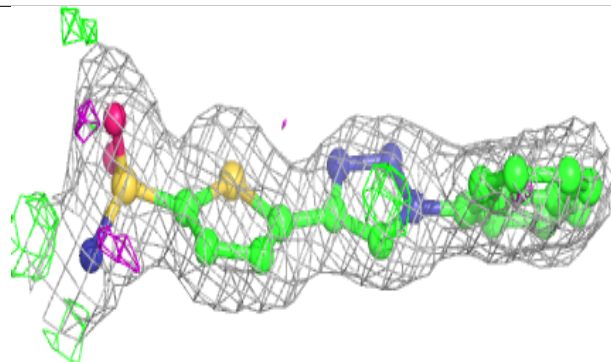
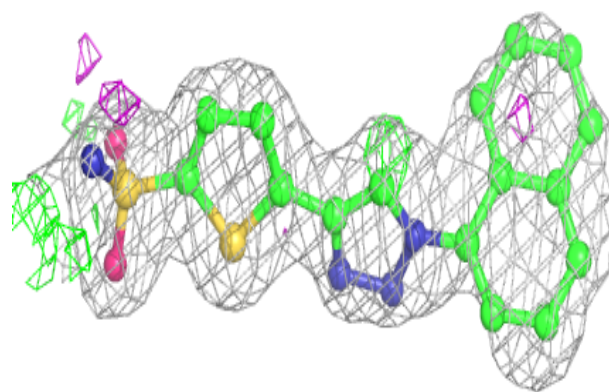
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ACY	B	1260	4/4	0.76	0.14	62,64,64,65	0
4	GOL	D	271	6/6	0.80	0.15	52,56,57,59	0
5	ACY	A	1261	4/4	0.83	0.14	40,43,45,50	0
4	GOL	A	273	6/6	0.84	0.22	32,39,41,42	0
5	ACY	C	1260	4/4	0.86	0.11	36,38,39,40	0
5	ACY	C	1261	4/4	0.86	0.19	36,39,41,42	0
5	ACY	C	1262	4/4	0.89	0.19	50,52,53,53	0
4	GOL	B	272	6/6	0.90	0.21	36,40,42,42	0
3	9FK	D	266	24/24	0.97	0.12	26,44,60,60	0
2	ZN	D	264	1/1	0.98	0.09	28,28,28,28	0
3	9FK	C	267	24/24	0.98	0.08	22,35,45,48	0
3	9FK	B	268	24/24	0.98	0.09	19,35,46,48	0
2	ZN	C	264	1/1	0.99	0.09	22,22,22,22	0
3	9FK	A	269	24/24	0.99	0.07	18,32,41,41	0
2	ZN	B	264	1/1	1.00	0.08	21,21,21,21	0
2	ZN	A	264	1/1	1.00	0.08	18,18,18,18	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.

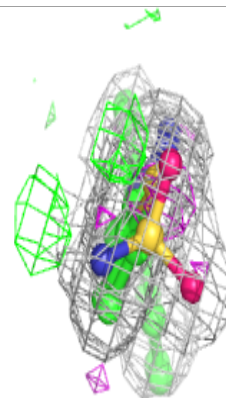
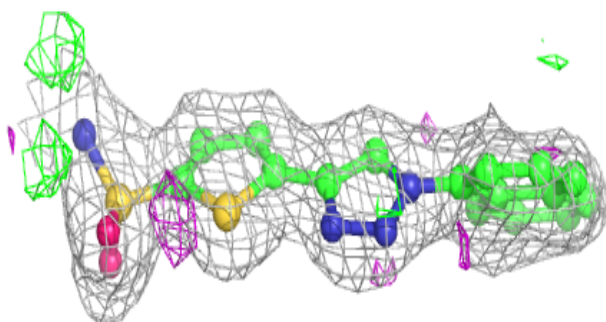
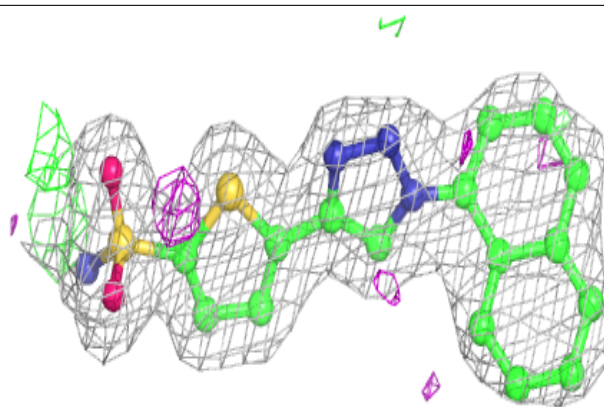
**Electron density around 9FK D 266:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

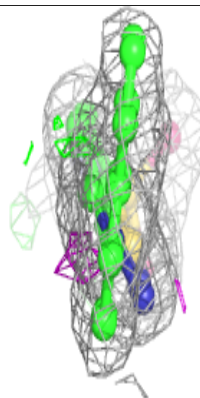
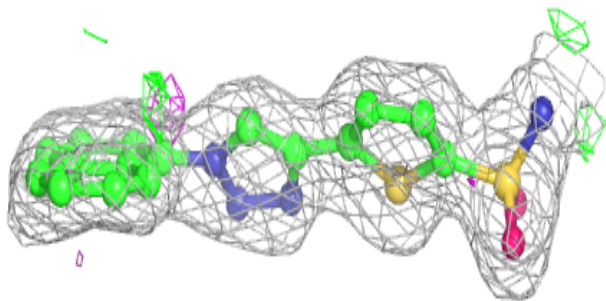
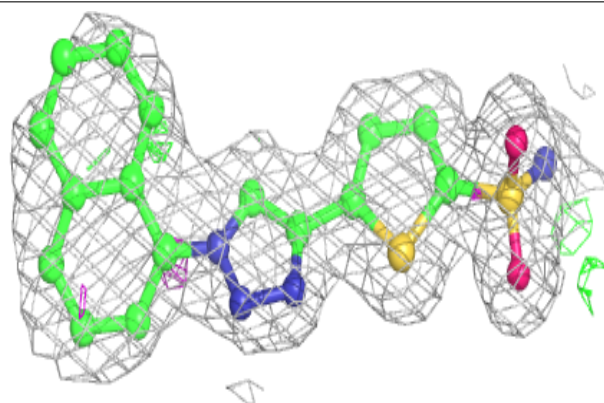


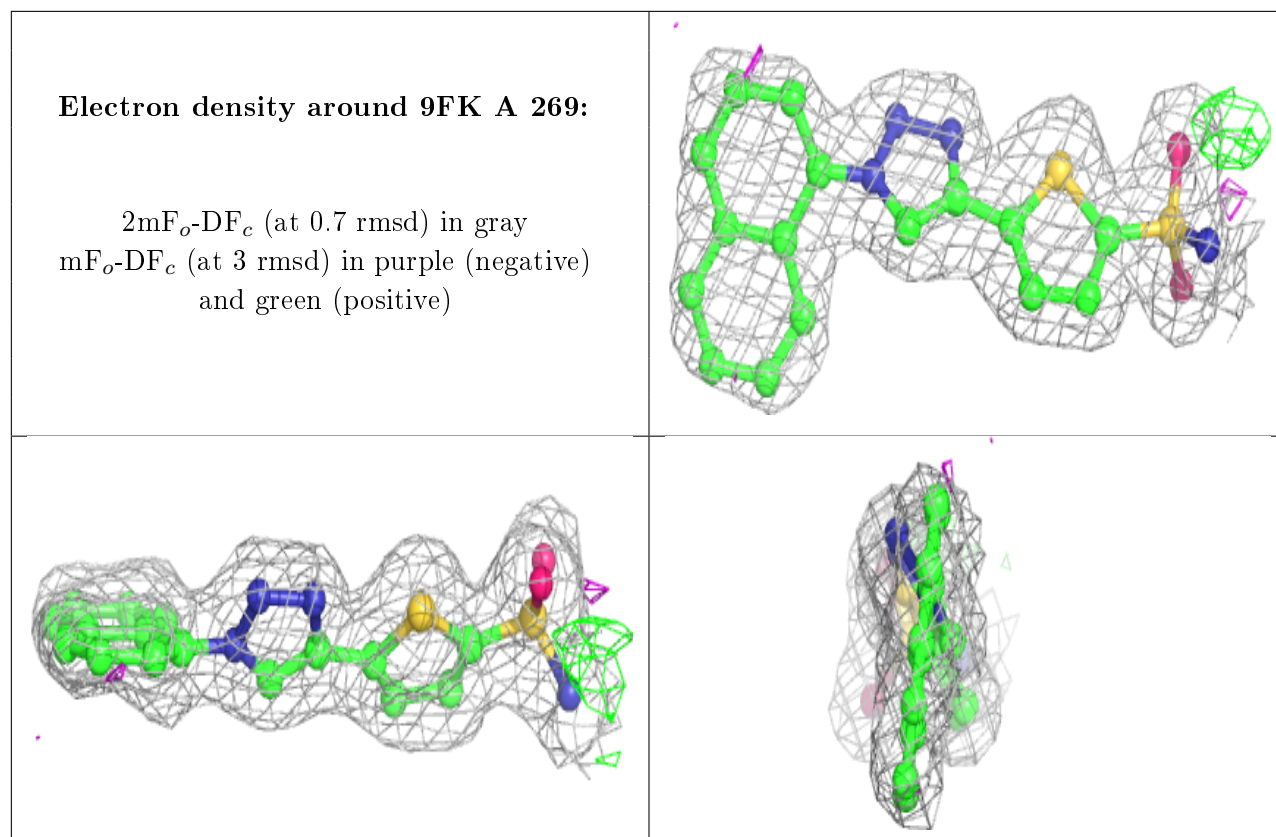
**Electron density around 9FK C 267:**

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

**Electron density around 9FK B 268:**

$2mF_o-DF_c$  (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.