



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 11:02 pm BST

PDB ID : 3U4R  
Title : Novel HCV NS5B polymerase Inhibitors: Discovery of Indole C2 Acyl sulfonamides  
Authors : Anilkumar, G.N.; Selyutin, O.; Rosenblum, S.B.; Zeng, Q.; Jiang, Y.; Chan, T.-Y.; Pu, H.; Wang, L.; Bennett, F.; Chen, K.X.; Lesburg, C.A.; Duca, J.S.; Gavalas, S.; Huang, Y.; Pinto, P.; Sannagrahi, M.; Velazquez, F.; Venkataraman, S.; Vilbubhan, B.; Agrawal, S.; Ferrari, E.; Jiang, C.-K.; Huang, H.-C.; Shih, N.-Y.; Njoroge, F.G.; Kozlowski, J.A.  
Deposited on : 2011-10-10  
Resolution : 2.00 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

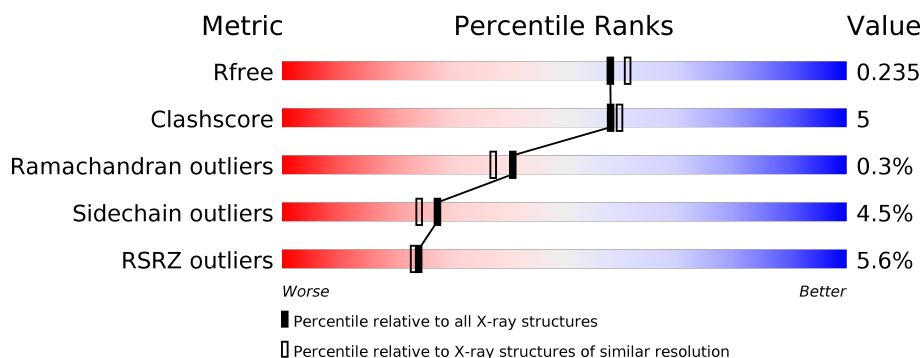
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	578	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>7% . .</div> </div> </div>
1	B	578	<div> <div>8%</div> <div> <div></div> <div>83%</div> <div>13% . .</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10100 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.

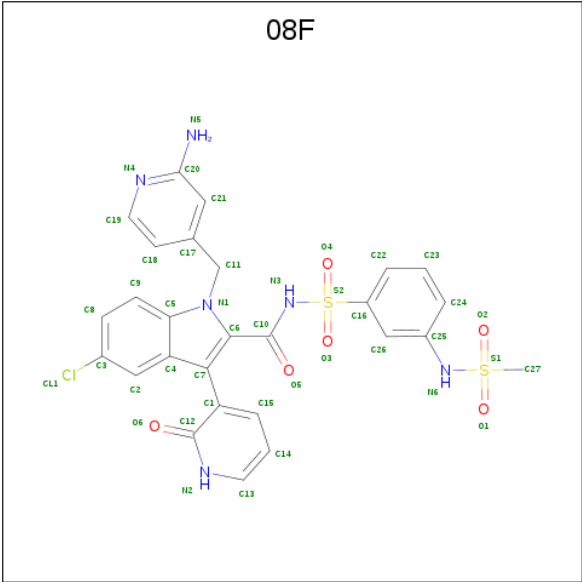
- Molecule 1 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	0	0	0
			4347	2739	769	807	32			
1	B	558	Total	C	N	O	S	0	0	0
			4347	2739	769	807	32			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	440	GLY	GLU	CONFLICT	UNP O92972
A	520	ILE	THR	CONFLICT	UNP O92972
A	571	LEU	-	EXPRESSION TAG	UNP O92972
A	572	GLU	-	EXPRESSION TAG	UNP O92972
A	573	HIS	-	EXPRESSION TAG	UNP O92972
A	574	HIS	-	EXPRESSION TAG	UNP O92972
A	575	HIS	-	EXPRESSION TAG	UNP O92972
A	576	HIS	-	EXPRESSION TAG	UNP O92972
A	577	HIS	-	EXPRESSION TAG	UNP O92972
A	578	HIS	-	EXPRESSION TAG	UNP O92972
B	440	GLY	GLU	CONFLICT	UNP O92972
B	520	ILE	THR	CONFLICT	UNP O92972
B	571	LEU	-	EXPRESSION TAG	UNP O92972
B	572	GLU	-	EXPRESSION TAG	UNP O92972
B	573	HIS	-	EXPRESSION TAG	UNP O92972
B	574	HIS	-	EXPRESSION TAG	UNP O92972
B	575	HIS	-	EXPRESSION TAG	UNP O92972
B	576	HIS	-	EXPRESSION TAG	UNP O92972
B	577	HIS	-	EXPRESSION TAG	UNP O92972
B	578	HIS	-	EXPRESSION TAG	UNP O92972

- Molecule 2 is 1-[(2-aminopyridin-4-yl)methyl]-5-chloro-N-({3-[(methylsulfonyl)amino]phenyl}sulfonyl)-3-(2-oxo-1,2-dihydropyridin-3-yl)-1H-indole-2-carboxamide (three-letter code: 08F) (formula: C<sub>27</sub>H<sub>23</sub>ClN<sub>6</sub>O<sub>6</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			42	27	1	6	6	2		
2	B	1	Total	C	Cl	N	O	S	0	0
			42	27	1	6	6	2		

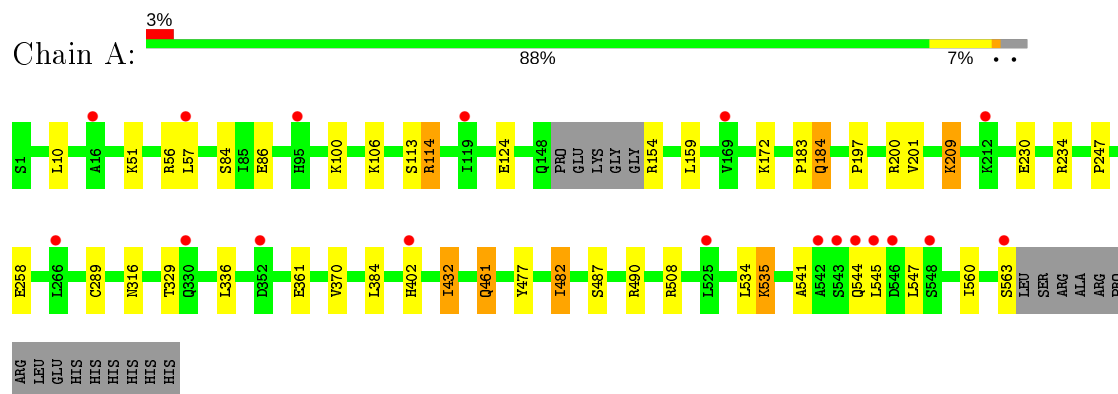
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	723	Total	O	0	0
			723	723		
3	B	599	Total	O	0	0
			599	599		

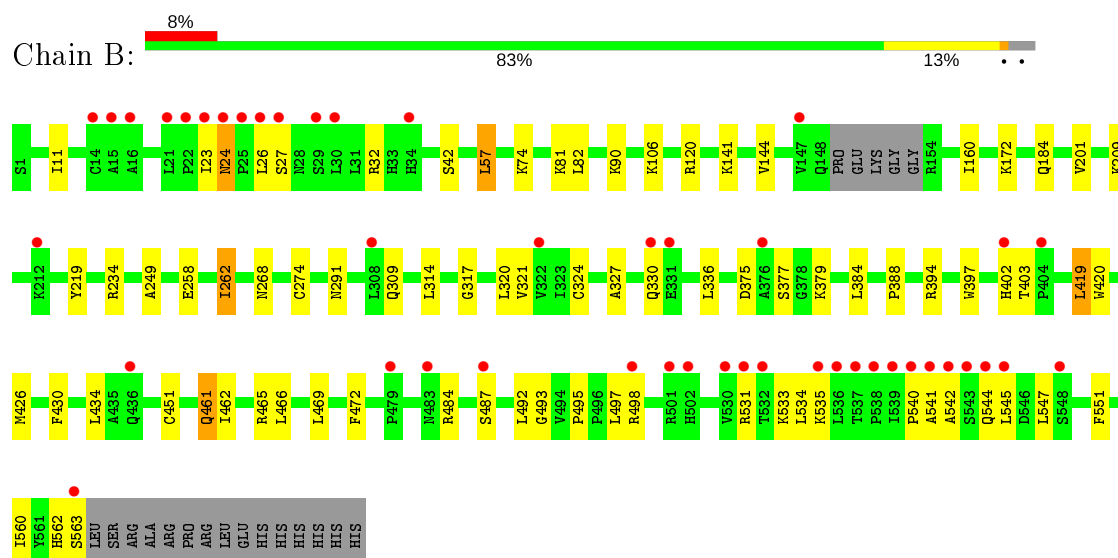
### 3 Residue-property plots [i](#)

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: RNA-directed RNA polymerase



#### • Molecule 1: RNA-directed RNA polymerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.92Å 106.68Å 134.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.92 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-2.00) 99.3 (19.92-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.01Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, $R_{free}$	0.192 , 0.237 0.191 , 0.235	Depositor DCC
$R_{free}$ test set	4337 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.0	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 58.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10100	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 08F

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	0.49	0/4441	0.64	0/6026
1	B	0.48	0/4441	0.65	0/6026
All	All	0.49	0/8882	0.65	0/12052

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4347	0	4365	34	0
1	B	4347	0	4365	47	0
2	A	42	0	23	5	0
2	B	42	0	23	9	0
3	A	723	0	0	16	0
3	B	599	0	0	9	0
All	All	10100	0	8776	85	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 5.

All (85) 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:B:24:ASN:HD21	1:B:27:SER:HB3	1.37	0.87
1:B:201:VAL:HG22	1:B:384:LEU:HG	1.61	0.81
1:B:451:CYS:HB2	3:B:805:HOH:O	1.81	0.79
1:A:461:GLN:HG2	1:A:541:ALA:HB3	1.66	0.78
1:B:291:ASN:HD22	2:B:579:08F:C27	1.96	0.77
1:B:120:ARG:HD2	3:B:846:HOH:O	1.86	0.76
2:A:579:08F:H5	2:A:579:08F:H10	1.51	0.76
1:A:477:TYR:HB2	1:A:482:ILE:HD11	1.69	0.74
1:A:230:GLU:HG2	3:A:744:HOH:O	1.91	0.70
1:B:291:ASN:HD22	2:B:579:08F:H23	1.58	0.68
1:A:201:VAL:HG22	1:A:384:LEU:HG	1.77	0.67
2:B:579:08F:H10	2:B:579:08F:H5	1.59	0.66
1:A:563:SER:O	3:A:876:HOH:O	2.13	0.65
1:B:234:ARG:HG3	1:B:262:ILE:HD11	1.77	0.65
1:B:317:GLY:HA3	2:B:579:08F:O2	1.96	0.65
1:A:114:ARG:NH1	3:A:1283:HOH:O	2.32	0.63
1:B:141:LYS:HD2	1:B:160:ILE:HD11	1.81	0.61
1:B:291:ASN:HD22	2:B:579:08F:H22	1.65	0.61
2:A:579:08F:N3	2:A:579:08F:H5	2.16	0.60
1:A:563:SER:HB2	3:A:1292:HOH:O	2.02	0.60
2:A:579:08F:H7	3:A:1144:HOH:O	2.02	0.59
1:A:247:PRO:HG3	1:B:234:ARG:NH1	2.18	0.58
1:A:535:LYS:NZ	3:A:1172:HOH:O	2.36	0.58
1:A:200:ARG:HD3	1:A:384:LEU:HD11	1.88	0.56
1:B:234:ARG:NH1	1:B:258:GLU:OE2	2.39	0.56
1:B:544:GLN:HB2	3:B:1198:HOH:O	2.05	0.55
1:B:545:LEU:HG	3:B:1311:HOH:O	2.06	0.55
1:A:201:VAL:CG2	1:A:384:LEU:HG	2.35	0.54
1:A:184:GLN:NE2	3:A:1023:HOH:O	2.41	0.54
1:B:219:TYR:HB3	1:B:320:LEU:HD23	1.91	0.53
1:A:154:ARG:NH1	3:A:698:HOH:O	2.40	0.53
1:A:508:ARG:NE	3:A:726:HOH:O	2.20	0.53
1:A:316:ASN:HB3	2:A:579:08F:H11	1.91	0.52
2:B:579:08F:N3	2:B:579:08F:H5	2.24	0.52
1:B:531:ARG:HG3	1:B:531:ARG:HH11	1.77	0.50
1:B:531:ARG:NH1	1:B:531:ARG:HG3	2.26	0.49
1:B:498:ARG:NH1	3:B:879:HOH:O	2.45	0.49
1:A:234:ARG:HD2	1:A:258:GLU:OE2	2.12	0.49
1:B:309:GLN:HE22	1:B:327:ALA:HB2	1.77	0.48
1:A:172:LYS:HE3	1:A:560:ILE:HD13	1.94	0.48
1:A:84:SER:OG	1:A:86:GLU:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:VAL:CG2	1:B:384:LEU:HG	2.38	0.47
1:B:268:ASN:HB3	1:B:274:CYS:SG	2.55	0.47
1:B:172:LYS:HE3	1:B:560:ILE:HD13	1.97	0.47
1:A:197:PRO:O	1:A:201:VAL:HG23	2.15	0.46
1:A:154:ARG:N	3:A:1168:HOH:O	2.47	0.46
2:A:579:08F:C11	2:A:579:08F:N3	2.79	0.46
1:B:309:GLN:O	1:B:324:CYS:HB2	2.16	0.46
1:B:465:ARG:NH2	3:B:1090:HOH:O	2.46	0.45
1:B:74:LYS:NZ	3:B:904:HOH:O	2.49	0.45
1:A:402:HIS:HB3	3:A:1187:HOH:O	2.15	0.45
1:B:426:MET:O	1:B:430:PHE:HB2	2.17	0.45
1:A:477:TYR:HB2	1:A:482:ILE:CD1	2.43	0.45
1:A:508:ARG:HH22	1:A:534:LEU:HG	1.82	0.45
1:B:291:ASN:ND2	2:B:579:08F:H22	2.30	0.45
1:A:124:GLU:HG3	3:A:867:HOH:O	2.16	0.44
1:A:361:GLU:HG2	1:A:370:VAL:O	2.17	0.44
1:B:106:LYS:HD3	3:B:714:HOH:O	2.18	0.44
1:B:462:ILE:O	1:B:466:LEU:HG	2.18	0.44
1:B:144:VAL:HB	1:B:394:ARG:HG2	1.99	0.44
1:B:375:ASP:OD1	1:B:379:LYS:HB3	2.17	0.44
1:B:82:LEU:HD13	1:B:249:ALA:HB2	2.00	0.44
1:A:461:GLN:HG2	1:A:541:ALA:CB	2.42	0.43
1:B:32:ARG:NH2	1:B:495:PRO:HG3	2.33	0.43
1:A:490:ARG:NH1	3:A:905:HOH:O	2.51	0.43
1:B:32:ARG:HD2	1:B:32:ARG:N	2.33	0.43
1:A:183:PRO:HG3	1:A:289:CYS:SG	2.59	0.43
1:B:291:ASN:ND2	2:B:579:08F:C27	2.74	0.43
1:A:247:PRO:CB	1:B:234:ARG:HH11	2.31	0.42
1:B:466:LEU:HD22	1:B:551:PHE:HE2	1.84	0.42
2:B:579:08F:C11	2:B:579:08F:N3	2.83	0.42
1:B:32:ARG:HD3	1:B:493:GLY:O	2.19	0.42
1:A:106:LYS:HD3	3:A:658:HOH:O	2.19	0.42
1:A:209:LYS:NZ	3:A:937:HOH:O	2.52	0.42
1:B:461:GLN:HB3	1:B:542:ALA:HA	2.00	0.42
1:B:57:LEU:C	3:B:869:HOH:O	2.58	0.42
1:A:247:PRO:HB3	1:B:234:ARG:HH11	1.86	0.41
1:B:388:PRO:HB3	1:B:420:TRP:CD2	2.56	0.41
1:B:314:LEU:HB3	1:B:321:VAL:HG13	2.01	0.41
1:B:419:LEU:HD21	1:B:497:LEU:HD13	2.01	0.41
1:B:144:VAL:HG21	1:B:397:TRP:CG	2.55	0.41
1:B:469:LEU:HD23	1:B:472:PHE:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:LEU:HB3	1:A:547:LEU:HG	2.03	0.40
1:A:432:ILE:HD11	3:A:1125:HOH:O	2.21	0.40
1:B:562:HIS:HB3	1:B:563:SER:H	1.76	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	554/578 (96%)	547 (99%)	7 (1%)	0	100	100
1	B	554/578 (96%)	538 (97%)	13 (2%)	3 (0%)	29	23
All	All	1108/1156 (96%)	1085 (98%)	20 (2%)	3 (0%)	41	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	535	LYS
1	B	541	ALA
1	B	540	PRO

### 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	475/492 (96%)	457 (96%)	18 (4%)	33	31
1	B	475/492 (96%)	450 (95%)	25 (5%)	22	18
All	All	950/984 (96%)	907 (96%)	43 (4%)	27	24

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	51	LYS
1	A	56	ARG
1	A	57	LEU
1	A	100	LYS
1	A	113	SER
1	A	114	ARG
1	A	159	LEU
1	A	184	GLN
1	A	209	LYS
1	A	329	THR
1	A	336	LEU
1	A	432	ILE
1	A	461	GLN
1	A	482	ILE
1	A	487	SER
1	A	535	LYS
1	A	544	GLN
1	B	11	ILE
1	B	23	ILE
1	B	24	ASN
1	B	26	LEU
1	B	42	SER
1	B	57	LEU
1	B	81	LYS
1	B	90	LYS
1	B	184	GLN
1	B	209	LYS
1	B	262	ILE
1	B	330	GLN
1	B	336	LEU
1	B	377	SER

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Mol	Chain	Res	Type
1	B	402	HIS
1	B	403	THR
1	B	419	LEU
1	B	434	LEU
1	B	461	GLN
1	B	484	ARG
1	B	487	SER
1	B	492	LEU
1	B	533	LYS
1	B	534	LEU
1	B	547	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	291	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	08F	B	579	-	41,46,46	2.12	10 (24%)	56,69,69	1.45	8 (14%)
2	08F	A	579	-	41,46,46	2.19	7 (17%)	56,69,69	1.44	8 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	08F	B	579	-	-	4/24/28/28	0/5/5/5
2	08F	A	579	-	-	2/24/28/28	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	579	08F	S1-N6	8.98	1.75	1.63
2	B	579	08F	S1-N6	8.36	1.74	1.63
2	A	579	08F	C12-N2	5.00	1.41	1.33
2	B	579	08F	C12-N2	4.83	1.41	1.33
2	B	579	08F	C14-C15	3.93	1.47	1.38
2	A	579	08F	C14-C15	3.84	1.47	1.38
2	A	579	08F	C12-C1	3.78	1.53	1.43
2	B	579	08F	C12-C1	3.74	1.53	1.43
2	A	579	08F	C7-C4	-2.69	1.40	1.47
2	B	579	08F	C7-C4	-2.46	1.41	1.47
2	B	579	08F	C9-C8	2.31	1.41	1.36
2	B	579	08F	S2-N3	2.28	1.69	1.64
2	A	579	08F	C9-C8	2.17	1.41	1.36
2	B	579	08F	C8-C3	2.04	1.41	1.38
2	A	579	08F	C8-C3	2.04	1.41	1.38
2	B	579	08F	O3-S2	2.02	1.45	1.43
2	B	579	08F	C2-C3	2.00	1.40	1.36

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	579	08F	O4-S2-C16	-4.20	102.79	107.97
2	B	579	08F	O4-S2-C16	-3.95	103.10	107.97
2	B	579	08F	O4-S2-O3	3.78	124.19	119.55
2	A	579	08F	O3-S2-C16	-3.43	103.74	107.97
2	A	579	08F	O4-S2-O3	3.38	123.71	119.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	579	08F	O3-S2-C16	-3.27	103.94	107.97
2	A	579	08F	O2-S1-C27	-3.16	103.21	108.28
2	B	579	08F	C13-N2-C12	2.91	123.39	116.43
2	A	579	08F	C13-N2-C12	2.89	123.35	116.43
2	B	579	08F	C15-C1-C7	2.89	125.34	119.41
2	A	579	08F	C15-C1-C7	2.87	125.32	119.41
2	B	579	08F	O2-S1-C27	-2.74	103.87	108.28
2	A	579	08F	C17-C11-N1	2.63	116.71	112.63
2	B	579	08F	O1-S1-N6	2.55	112.29	107.10
2	B	579	08F	C17-C21-C20	2.53	119.89	117.97
2	A	579	08F	C17-C21-C20	2.03	119.51	117.97

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	579	08F	C25-N6-S1-O2
2	B	579	08F	C25-N6-S1-C27
2	A	579	08F	N1-C11-C17-C21
2	B	579	08F	N1-C11-C17-C21
2	A	579	08F	N1-C11-C17-C18
2	B	579	08F	N1-C11-C17-C18

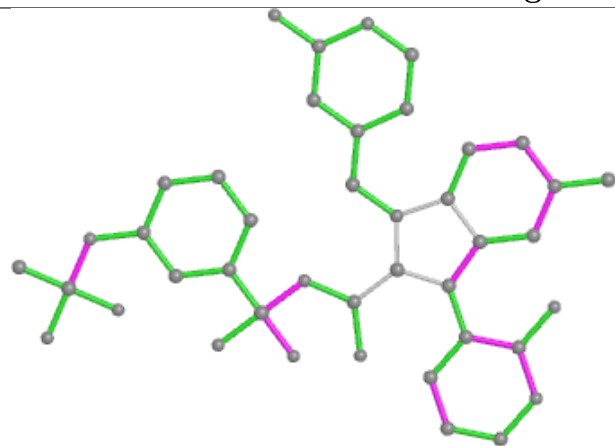
There are no ring outliers.

2 monomers are involved in 14 short contacts:

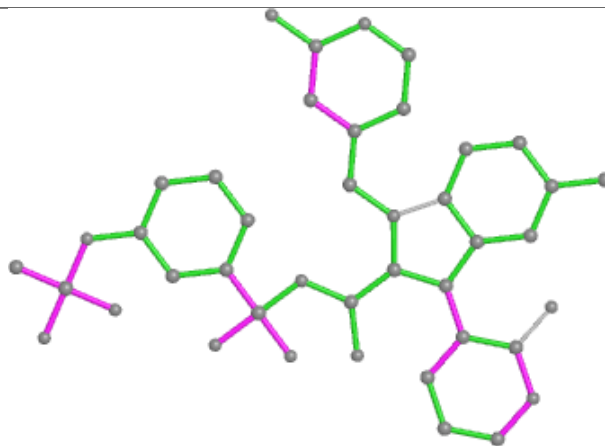
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	579	08F	9	0
2	A	579	08F	5	0

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.

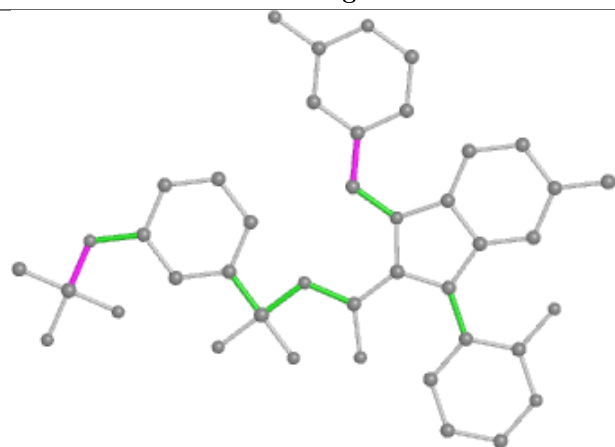
## Ligand 08F B 579



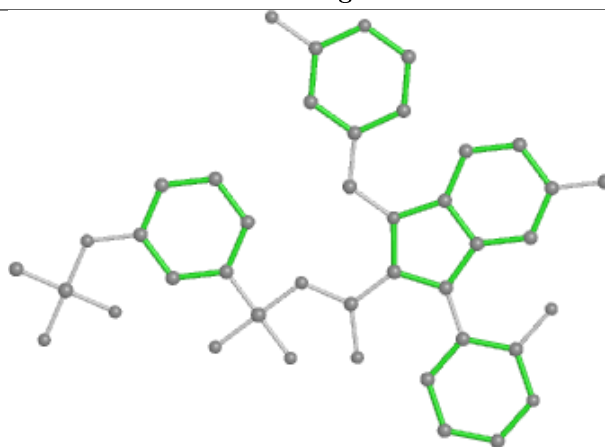
Bond lengths



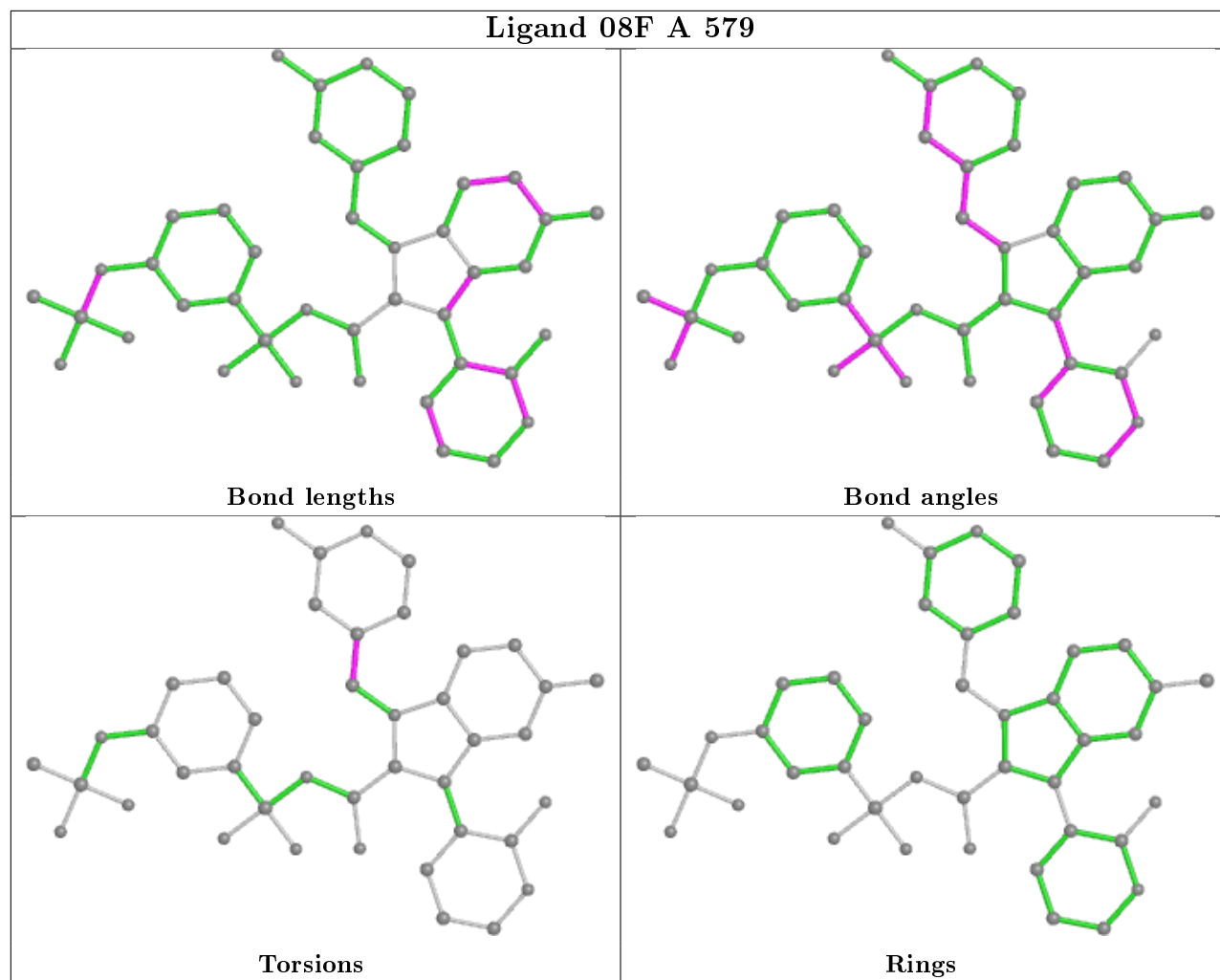
Bond angles



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	558/578 (96%)	-0.06	18 (3%)	47 46	25, 33, 54, 79	0
1	B	558/578 (96%)	0.32	45 (8%)	12 11	24, 39, 78, 108	0
All	All	1116/1156 (96%)	0.13	63 (5%)	24 23	24, 36, 64, 108	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	25	PRO	9.9
1	B	26	LEU	9.7
1	B	542	ALA	9.4
1	B	541	ALA	7.8
1	B	545	LEU	6.9
1	B	543	SER	6.4
1	B	544	GLN	6.3
1	B	563	SER	6.1
1	B	24	ASN	5.0
1	B	548	SER	5.0
1	B	27	SER	4.6
1	B	532	THR	4.5
1	B	536	LEU	4.4
1	B	535	LYS	4.4
1	B	23	ILE	4.2
1	B	531	ARG	4.2
1	B	530	VAL	4.2
1	B	502	HIS	4.1
1	B	29	SER	4.0
1	B	537	THR	3.9
1	B	330	GLN	3.9
1	A	169	VAL	3.9
1	A	544	GLN	3.7
1	B	30	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	563	SER	3.6
1	B	14	CYS	3.5
1	A	352	ASP	3.5
1	A	548	SER	3.4
1	B	540	PRO	3.4
1	A	57	LEU	3.4
1	B	402	HIS	3.3
1	B	483	ASN	3.3
1	B	22	PRO	3.1
1	A	402	HIS	3.0
1	B	538	PRO	2.9
1	A	545	LEU	2.9
1	B	498	ARG	2.8
1	B	479	PRO	2.7
1	B	16	ALA	2.7
1	B	404	PRO	2.7
1	A	543	SER	2.7
1	A	546	ASP	2.6
1	B	487	SER	2.5
1	B	34	HIS	2.5
1	A	16	ALA	2.5
1	B	147	VAL	2.4
1	B	376	ALA	2.4
1	A	542	ALA	2.4
1	B	212	LYS	2.4
1	A	266	LEU	2.3
1	A	95	HIS	2.3
1	A	119	ILE	2.2
1	B	331	GLU	2.2
1	B	322	VAL	2.2
1	B	21	LEU	2.2
1	A	330	GLN	2.1
1	B	308	LEU	2.1
1	A	212	LYS	2.1
1	A	525	LEU	2.1
1	B	501	ARG	2.1
1	B	539	ILE	2.0
1	B	15	ALA	2.0
1	B	436	GLN	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

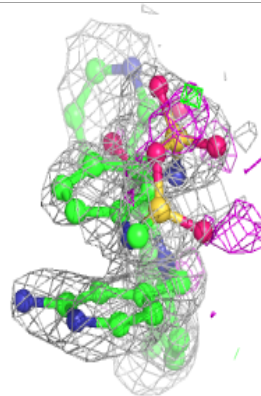
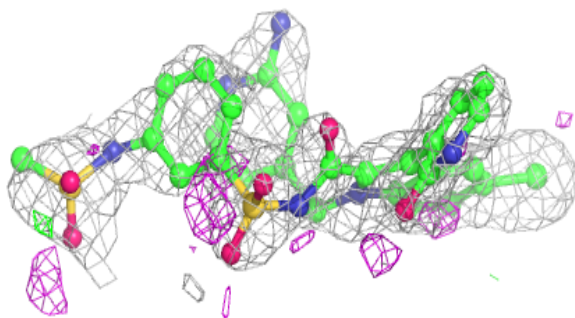
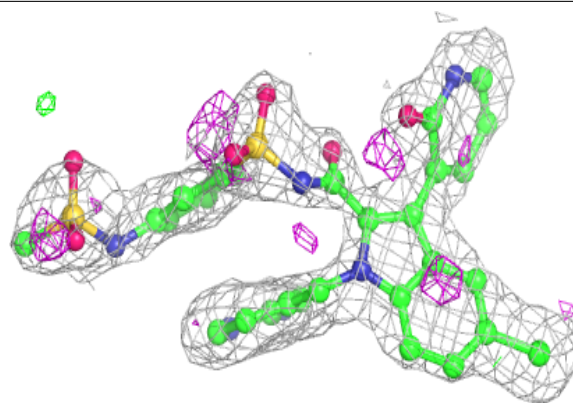
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	08F	B	579	42/42	0.86	0.26	52,57,70,74	0
2	08F	A	579	42/42	0.89	0.18	40,54,60,61	0

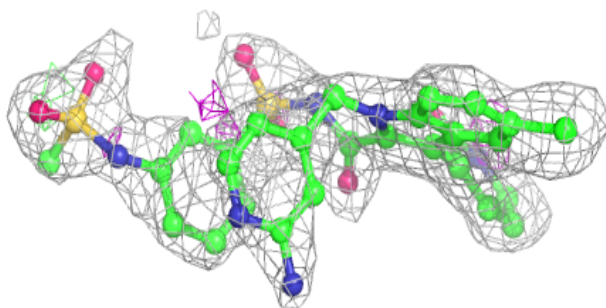
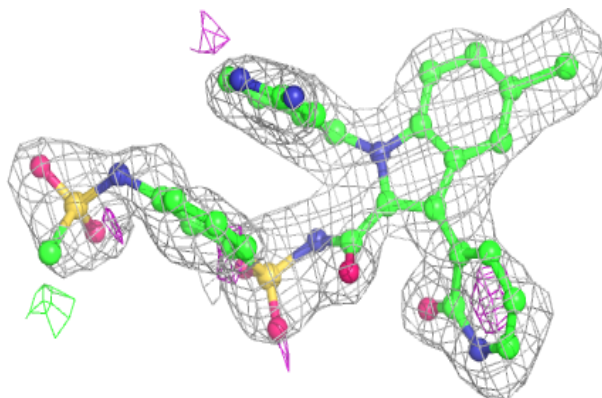
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 08F B 579:**

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

**Electron density around 08F A 579:**

$2mF_o-DF_c$  (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.