



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:05 PM UTC

PDB ID : 3G86 / pdb_00003g86
Title : Hepatitis C virus polymerase NS5B (BK 1-570) with thiazine inhibitor
Authors : Harris, S.F.; Ghatge, M.
Deposited on : 2009-02-11
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

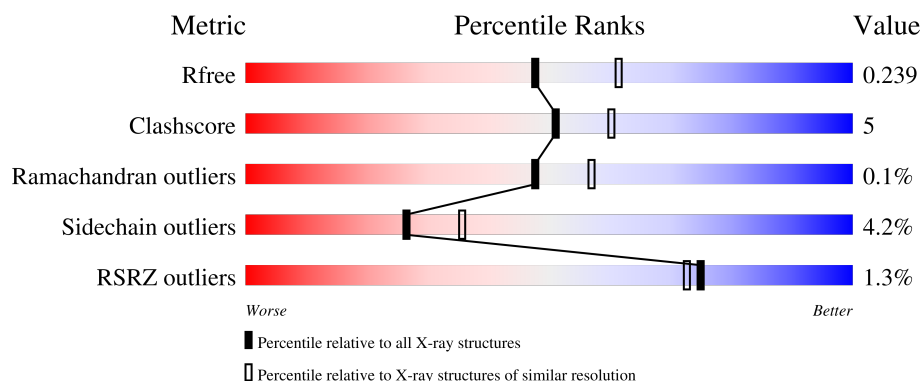
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	576	% 86% 8% • •
1	B	576	% 82% 13% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9388 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.

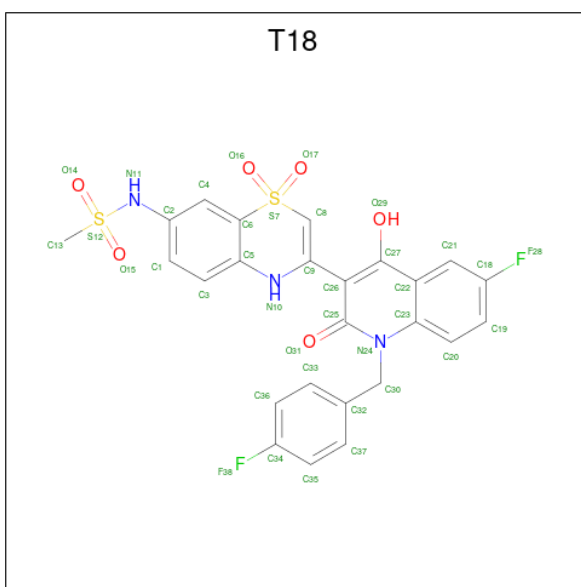
- Molecule 1 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	0	6	0
			4382	2763	776	809	34			
1	B	558	Total	C	N	O	S	0	9	0
			4414	2783	782	813	36			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	expression tag	UNP P26663
A	-4	HIS	-	expression tag	UNP P26663
A	-3	HIS	-	expression tag	UNP P26663
A	-2	HIS	-	expression tag	UNP P26663
A	-1	HIS	-	expression tag	UNP P26663
A	0	HIS	-	expression tag	UNP P26663
A	1	HIS	-	expression tag	UNP P26663
B	-5	MET	-	expression tag	UNP P26663
B	-4	HIS	-	expression tag	UNP P26663
B	-3	HIS	-	expression tag	UNP P26663
B	-2	HIS	-	expression tag	UNP P26663
B	-1	HIS	-	expression tag	UNP P26663
B	0	HIS	-	expression tag	UNP P26663
B	1	HIS	-	expression tag	UNP P26663

- Molecule 2 is N-{3-[6-fluoro-1-(4-fluorobenzyl)-4-hydroxy-2-oxo-1,2-dihydroquinolin-3-yl]-1,1-dioxido-4H-1,4-benzothiazin-7-yl}methanesulfonamide (CCD ID: T18) (formula: C₂₅H₁₉F₂N₃O₆S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			38	25	2	3	6	2		
2	B	1	Total	C	F	N	O	S	0	0
			38	25	2	3	6	2		

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		
3	B	1	Total	Ni	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	248	Total	O	0	0
			248	248		
4	B	266	Total	O	0	0
			266	266		

- 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, α , β , γ	85.92Å 106.17Å 126.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.97 – 2.20 48.97 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.97-2.20) 98.3 (48.97-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.190 , 0.238 0.194 , 0.239	Depositor DCC
R_{free} test set	2939 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.647	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9388	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.26 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1743e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: T18, NI

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	0.82	0/4478	0.88	1/6077 (0.0%)
1	B	0.82	1/4511 (0.0%)	0.90	1/6121 (0.0%)
All	All	0.82	1/8989 (0.0%)	0.89	2/12198 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	93	PRO	CA-C	5.56	1.54	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	321	VAL	CB-CA-C	-6.34	100.73	110.50
1	A	465	ARG	N-CA-C	5.11	116.85	111.28

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	4382	0	4394	34	0
1	B	4414	0	4423	56	0
2	A	38	0	18	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	38	0	18	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	248	0	0	6	0
4	B	266	0	0	4	0
All	All	9388	0	8853	92	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 (92) 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:A:82:LEU:HD13	1:A:249:ALA:HB2	1.55	0.89
1:A:201:VAL:HG22	1:A:384:LEU:HD22	1.61	0.82
1:B:82:LEU:HD13	1:B:249:ALA:HB2	1.64	0.79
2:A:571:T18:H8	2:A:571:T18:O29	1.89	0.73
1:B:419:LEU:C	1:B:419:LEU:HD12	2.16	0.71
1:A:119:ILE:CG2	1:A:173:MET:HE1	2.21	0.70
1:B:124:LYS:O	1:B:128:GLU:HG2	1.92	0.69
1:B:405:VAL:HG21	1:B:446:GLN:HG3	1.76	0.67
1:A:197:PRO:O	1:A:201:VAL:HG23	1.97	0.64
1:B:46:GLY:HA2	1:B:49:GLN:HE21	1.64	0.63
1:A:182[A]:LEU:C	1:A:182[A]:LEU:HD23	2.24	0.62
1:B:523:LYS:HG3	1:B:534:LEU:HD22	1.80	0.61
1:B:86:GLU:HG2	1:B:111:LEU:HD22	1.83	0.59
1:B:545:LEU:HB2	4:B:717:HOH:O	2.02	0.59
1:B:201:VAL:HG22	1:B:384:LEU:HD22	1.85	0.58
1:A:169:VAL:HG12	1:A:173:MET:HE2	1.86	0.57
1:B:306:ALA:CB	1:B:308:LEU:HD13	2.34	0.57
1:B:306:ALA:HB3	1:B:308:LEU:HD13	1.87	0.56
1:B:527:ASN:HD21	1:B:534:LEU:H	1.53	0.56
1:B:413:ILE:HD11	1:B:454:ILE:HD13	1.88	0.55
1:A:306:ALA:HB3	1:A:308:LEU:HD13	1.87	0.55
1:B:36[B]:MET:HE1	1:B:491:LYS:CG	2.37	0.55
2:B:571:T18:H8	2:B:571:T18:O29	2.05	0.55
1:A:82:LEU:CD1	1:A:249:ALA:HB2	2.34	0.54
1:B:170:CYS:HA	1:B:173:MET:HE3	1.90	0.53
1:B:503:ARG:O	1:B:507:VAL:HG23	2.09	0.53
1:B:197:PRO:O	1:B:201:VAL:HG23	2.10	0.52
1:A:336:LEU:HD12	1:A:356:PRO:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:LEU:HB2	4:A:699:HOH:O	2.09	0.52
1:B:413:ILE:CD1	1:B:454:ILE:CD1	2.88	0.51
1:B:170:CYS:HA	1:B:173:MET:CE	2.41	0.51
1:A:331:GLU:HG2	4:A:623:HOH:O	2.11	0.51
1:B:381:VAL:HG11	1:B:474:LEU:CD2	2.41	0.50
1:B:508:ARG:HE	1:B:530:VAL:HG11	1.77	0.50
1:A:321:VAL:HG22	1:A:365:SER:HB2	1.93	0.50
1:A:465:ARG:NH2	1:A:545:LEU:O	2.45	0.50
1:A:14[B]:CYS:SG	1:A:139:MET:HE1	2.51	0.49
1:A:306:ALA:CB	1:A:308:LEU:HD13	2.42	0.49
1:B:419:LEU:C	1:B:419:LEU:CD1	2.85	0.48
1:B:112:SER:O	1:B:116:VAL:HG23	2.14	0.47
1:A:381:VAL:HG21	1:A:474:LEU:HD21	1.95	0.47
1:B:413:ILE:CD1	1:B:454:ILE:HD13	2.44	0.47
1:A:170:CYS:HA	1:A:173:MET:HE3	1.98	0.46
1:B:100:LYS:HG3	4:B:767:HOH:O	2.16	0.46
1:B:85:VAL:HG21	1:B:120:HIS:NE2	2.31	0.46
1:B:22:PRO:HG2	1:B:401:ARG:HG3	1.97	0.45
1:B:336:LEU:HD12	1:B:356:PRO:HD3	1.99	0.45
1:B:52:VAL:HG12	1:B:223[B]:CYS:SG	2.56	0.45
1:B:523:LYS:HD3	1:B:524:TYR:CE1	2.51	0.45
1:B:217:PHE:CD1	1:B:336:LEU:HD21	2.52	0.45
1:B:91:LEU:HB2	1:B:172:LYS:HD3	2.00	0.45
1:B:144:VAL:HB	1:B:394:ARG:HG2	1.99	0.44
1:B:227:THR:HB	1:B:347[A]:SER:O	2.18	0.44
1:A:48:ARG:HG3	1:A:159:LEU:HD22	1.99	0.44
1:A:413:ILE:CD1	1:A:454:ILE:HD12	2.48	0.44
1:B:217:PHE:CE1	1:B:336:LEU:HD21	2.53	0.44
1:A:77:THR:O	1:B:24:ASN:HB2	2.17	0.44
1:A:223[B]:CYS:SG	4:A:701:HOH:O	2.30	0.44
1:B:413:ILE:HD11	1:B:454:ILE:CD1	2.48	0.44
1:B:515:GLY:HA2	1:B:519:ALA:HB2	2.00	0.44
1:B:182[A]:LEU:C	1:B:182[A]:LEU:HD23	2.42	0.43
1:A:542:ALA:C	4:A:699:HOH:O	2.61	0.43
2:A:571:T18:O29	2:A:571:T18:C8	2.63	0.43
1:B:83:LEU:HB2	1:B:173:MET:HA	2.01	0.43
1:A:461:GLN:H	1:A:461:GLN:HE21	1.66	0.43
1:A:461:GLN:NE2	4:A:789:HOH:O	2.51	0.42
1:B:36[B]:MET:HE1	1:B:491:LYS:HG3	2.01	0.42
1:B:466:LEU:HD22	1:B:551:PHE:HE2	1.83	0.42
1:B:419:LEU:HD12	1:B:420:TRP:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:PRO:HG2	1:A:499:VAL:HG23	2.02	0.42
1:B:187:MET:HE2	1:B:293:LEU:HD23	2.01	0.42
1:A:172:LYS:HE3	1:A:560:ILE:HD13	2.00	0.42
1:B:321:VAL:HG22	1:B:365:SER:CB	2.50	0.42
1:B:82:LEU:CD1	1:B:249:ALA:HB2	2.45	0.42
1:B:321:VAL:HG22	1:B:365:SER:HB2	2.02	0.42
1:B:423:MET:HE1	1:B:497:LEU:HB3	2.02	0.42
1:B:227:THR:HB	1:B:347[B]:SER:O	2.20	0.41
1:B:465:ARG:NH2	1:B:545:LEU:O	2.53	0.41
1:A:416:ALA:N	1:A:417:PRO:CD	2.83	0.41
1:B:268:ASN:HB3	1:B:274[A]:CYS:SG	2.60	0.41
1:A:46:GLY:HA2	1:A:49:GLN:NE2	2.36	0.41
1:B:119:ILE:HD13	1:B:169:VAL:HG11	2.03	0.41
1:A:455:GLU:HB3	4:A:613:HOH:O	2.20	0.41
1:A:527:ASN:HD21	1:A:534:LEU:H	1.69	0.41
1:B:215:MET:HE3	1:B:324:CYS:SG	2.61	0.41
1:B:405:VAL:HG22	1:B:445:CYS:HA	2.03	0.41
1:A:187:MET:SD	1:A:292:THR:HG22	2.61	0.41
1:A:461:GLN:HA	1:A:542:ALA:HB2	2.03	0.41
1:A:419:LEU:C	1:A:419:LEU:HD12	2.45	0.41
1:B:74:LYS:NZ	4:B:708:HOH:O	2.53	0.40
1:B:542:ALA:C	4:B:717:HOH:O	2.64	0.40
1:A:531:LYS:HG2	1:A:532:THR:N	2.37	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	559/576 (97%)	548 (98%)	9 (2%)	2 (0%)	30 34
1	B	563/576 (98%)	549 (98%)	14 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1122/1152 (97%)	1097 (98%)	23 (2%)	2 (0%)	48 51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	347[A]	SER
1	A	347[B]	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	481/491 (98%)	455 (95%)	26 (5%)	20 25
1	B	485/491 (99%)	469 (97%)	16 (3%)	33 45
All	All	966/982 (98%)	924 (96%)	42 (4%)	26 35

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14[A]	CYS
1	A	14[B]	CYS
1	A	47	LEU
1	A	51	LYS
1	A	57	LEU
1	A	82	LEU
1	A	128	GLU
1	A	159	LEU
1	A	182[A]	LEU
1	A	182[B]	LEU
1	A	201	VAL
1	A	212	LYS
1	A	308	LEU
1	A	321	VAL
1	A	377	SER
1	A	381	VAL

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Mol	Chain	Res	Type
1	A	384	LEU
1	A	419	LEU
1	A	431	SER
1	A	439	LEU
1	A	454	ILE
1	A	461	GLN
1	A	473	SER
1	A	531	LYS
1	A	543	SER
1	A	547	LEU
1	B	51	LYS
1	B	112	SER
1	B	159	LEU
1	B	160	ILE
1	B	201	VAL
1	B	308	LEU
1	B	321	VAL
1	B	381	VAL
1	B	384	LEU
1	B	405	VAL
1	B	419	LEU
1	B	439	LEU
1	B	469	LEU
1	B	492	LEU
1	B	543	SER
1	B	547	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	49	GLN
1	A	330	GLN
1	A	446	GLN
1	A	461	GLN
1	A	527	ASN
1	B	49	GLN
1	B	446	GLN
1	B	527	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
2	T18	A	571	-	42,42,42	1.33	4 (9%)	58,65,65	1.74	13 (22%)
2	T18	B	571	-	42,42,42	1.48	4 (9%)	58,65,65	1.83	14 (24%)

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	T18	A	571	-	-	0/9/28/28	0/4/5/5
2	T18	B	571	-	-	2/9/28/28	0/4/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	571	T18	C8-S7	5.03	1.77	1.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	571	T18	C8-S7	4.92	1.77	1.71
2	B	571	T18	O16-S7	-3.87	1.40	1.44
2	B	571	T18	C9-N10	3.76	1.39	1.35
2	A	571	T18	C9-N10	3.21	1.39	1.35
2	A	571	T18	C13-S12	3.02	1.82	1.75
2	A	571	T18	S12-N11	2.65	1.66	1.63
2	B	571	T18	C13-S12	2.43	1.81	1.75

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	571	T18	C32-C30-N24	-5.64	104.29	113.46
2	B	571	T18	C32-C30-N24	-5.08	105.20	113.46
2	A	571	T18	C30-N24-C25	4.50	121.51	116.72
2	B	571	T18	C26-C9-N10	4.34	121.22	116.09
2	B	571	T18	O15-S12-O14	-3.68	113.94	118.87
2	A	571	T18	C9-C8-S7	-3.61	120.96	123.29
2	B	571	T18	C9-C8-S7	-3.60	120.97	123.29
2	B	571	T18	O15-S12-C13	3.48	113.77	108.26
2	B	571	T18	C30-N24-C25	3.41	120.35	116.72
2	B	571	T18	O31-C25-C26	-3.28	118.16	125.16
2	B	571	T18	C13-S12-N11	-3.24	102.92	106.56
2	B	571	T18	O17-S7-C6	-3.14	104.98	108.95
2	B	571	T18	C26-C25-N24	3.13	122.50	116.89
2	A	571	T18	O15-S12-C13	3.08	113.12	108.26
2	A	571	T18	C13-S12-N11	-2.92	103.28	106.56
2	A	571	T18	C26-C25-N24	2.70	121.73	116.89
2	A	571	T18	O17-S7-O16	2.67	118.84	114.12
2	B	571	T18	C27-C26-C25	-2.65	116.87	120.39
2	A	571	T18	O17-S7-C6	-2.65	105.60	108.95
2	B	571	T18	O14-S12-C13	2.61	112.40	108.26
2	A	571	T18	C26-C9-N10	2.55	119.11	116.09
2	B	571	T18	O16-S7-C6	2.54	112.15	108.95
2	B	571	T18	C21-C22-C27	-2.52	118.56	122.08
2	A	571	T18	C21-C22-C27	-2.51	118.57	122.08
2	A	571	T18	O31-C25-C26	-2.44	119.95	125.16
2	A	571	T18	C22-C27-C26	-2.39	118.00	120.71
2	A	571	T18	C30-N24-C23	-2.10	117.74	120.04

There are no chirality outliers.

All (2) torsion outliers are listed below:

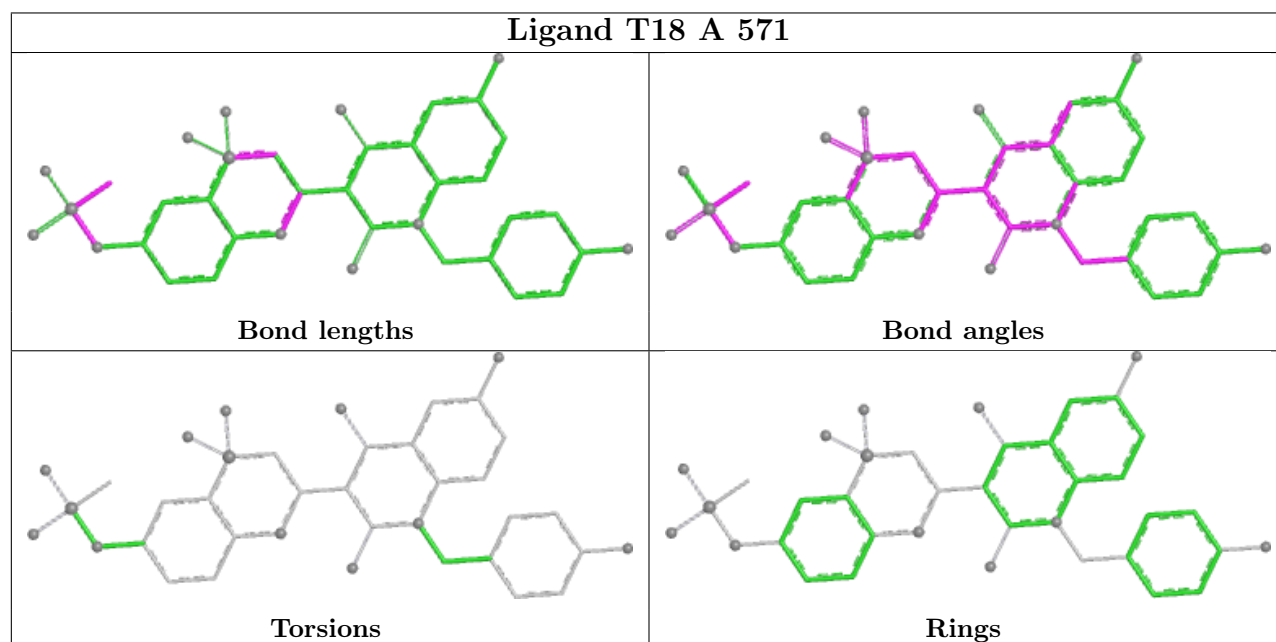
Mol	Chain	Res	Type	Atoms
2	B	571	T18	C2-N11-S12-O14
2	B	571	T18	C2-N11-S12-C13

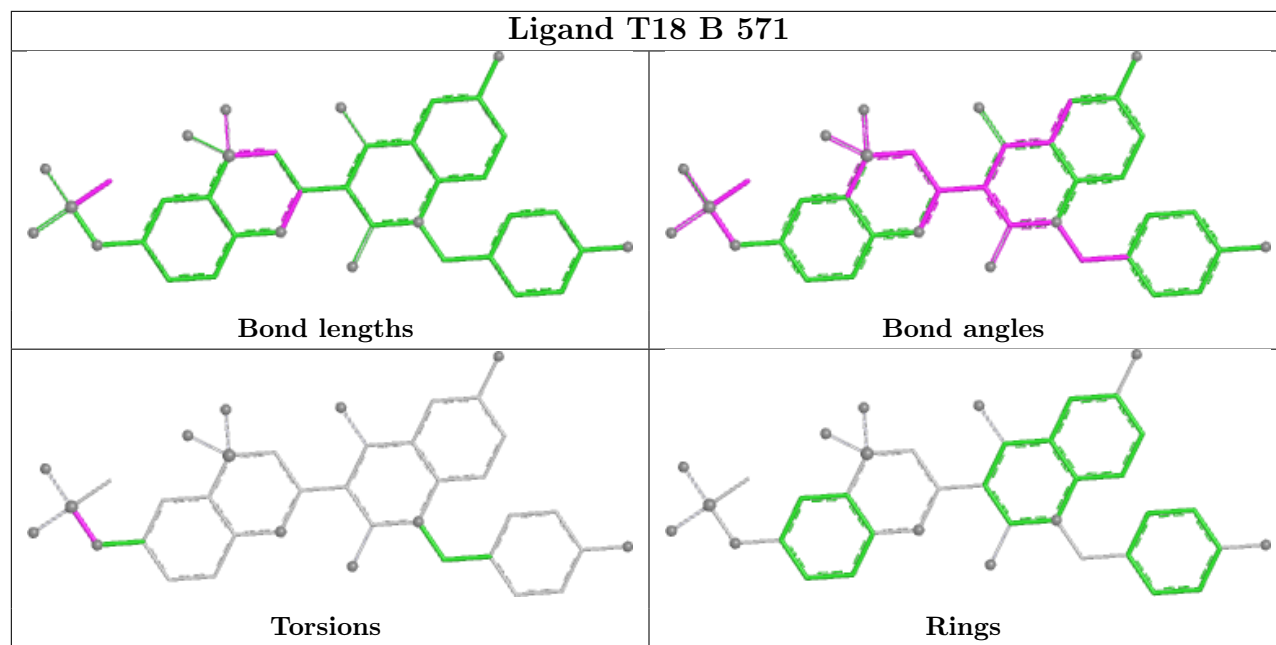
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	571	T18	2	0
2	B	571	T18	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.





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	557/576 (96%)	-0.10	8 (1%) 73 71	8, 20, 35, 56	6 (1%)
1	B	558/576 (96%)	-0.16	7 (1%) 75 73	5, 19, 35, 56	9 (1%)
All	All	1115/1152 (96%)	-0.13	15 (1%) 75 73	5, 19, 35, 56	15 (1%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	542	ALA	3.7
1	B	542	ALA	3.2
1	A	95[A]	HIS	3.2
1	B	543	SER	2.7
1	A	100	LYS	2.6
1	B	95[A]	HIS	2.5
1	A	102	GLY	2.5
1	B	0	HIS	2.4
1	B	549	GLY	2.4
1	A	540	PRO	2.3
1	A	541	ALA	2.3
1	B	541	ALA	2.2
1	A	545	LEU	2.0
1	B	536	LEU	2.0
1	A	538	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

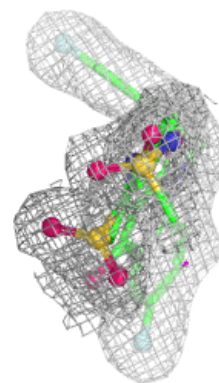
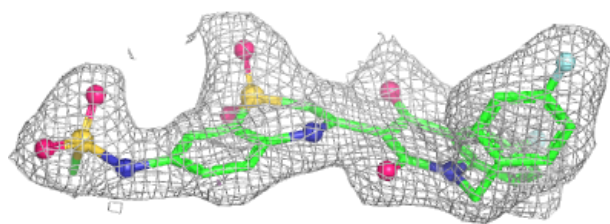
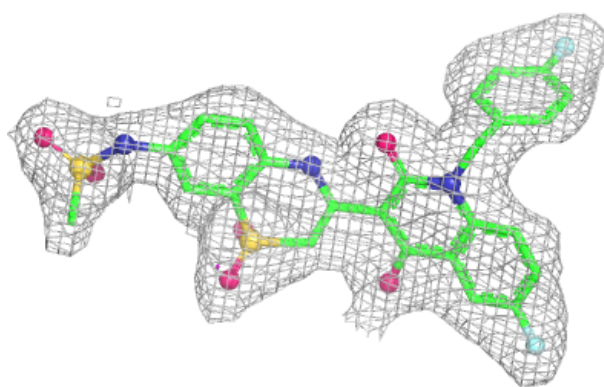
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NI	A	700	1/1	0.91	0.11	55,55,55,55	0
3	NI	B	701	1/1	0.92	0.09	60,60,60,60	0
2	T18	A	571	38/38	0.98	0.05	11,15,17,18	0
2	T18	B	571	38/38	0.98	0.05	11,14,17,18	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.

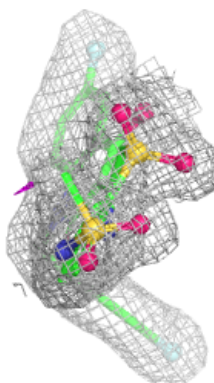
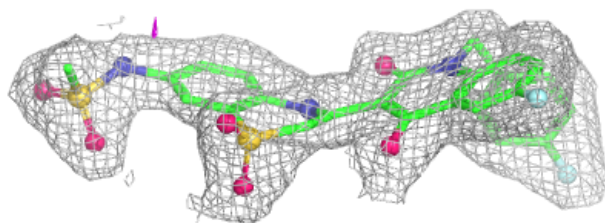
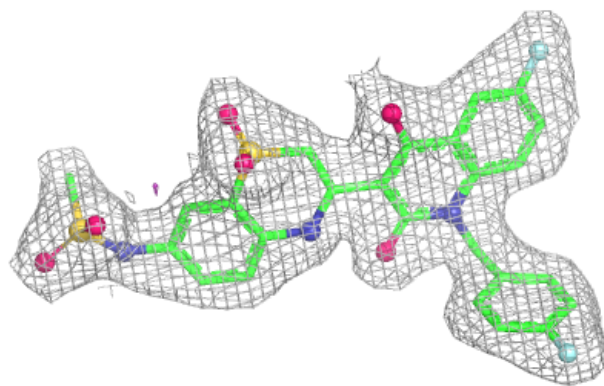
Electron density around T18 A 571:

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 T18 B 571:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.