



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2020 – 02:17 PM BST

PDB ID : 6XNP
Title : Crystal Structure of Human STING CTD complex with SR-717
Authors : Chin, E.N.; Yu, C.; Wolan, D.W.; Petrassi, H.M.; Lairson, L.L.
Deposited on : 2020-07-03
Resolution : 1.77 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 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	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

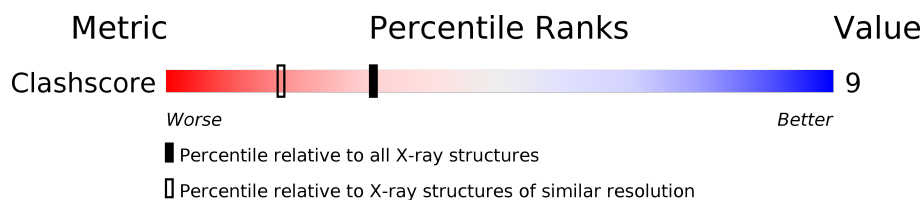
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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))
Clashscore	141614	10184 (1.80-1.76)

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 ≥ 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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	189	 77% 15% • 7%
1	B	189	 85% 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
3	GOL	B	403	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3484 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.

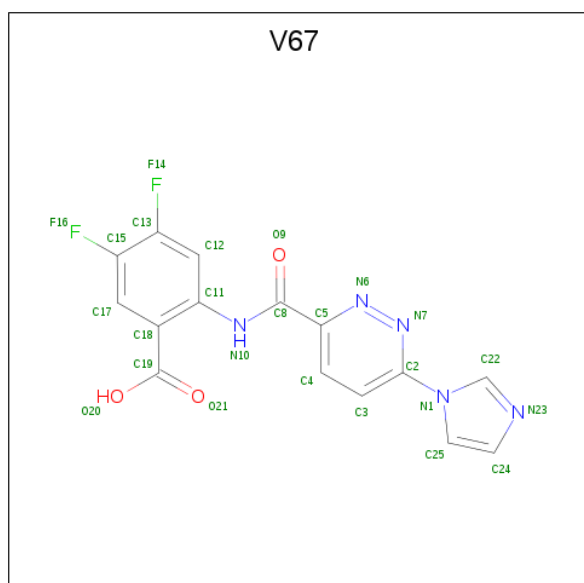
- Molecule 1 is a protein called Stimulator of interferon protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	S	0	11	0
			1523	954	273	290	6			
1	B	184	Total	C	N	O	S	0	8	0
			1542	962	276	297	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	GLY	-	expression tag	UNP A0A2R3XZB7
A	154	SER	-	expression tag	UNP A0A2R3XZB7
B	153	GLY	-	expression tag	UNP A0A2R3XZB7
B	154	SER	-	expression tag	UNP A0A2R3XZB7

- Molecule 2 is 4,5-difluoro-2-[[6-(1H-imidazol-1-yl)pyridazine-3-carbonyl]amino]benzoic acid (three-letter code: V67) (formula: C₁₅H₉F₂N₅O₃) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			25	15	2	5	3		
2	B	1	Total	C	F	N	O	0	0
			25	15	2	5	3		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

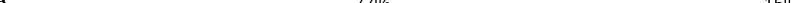


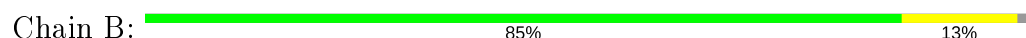
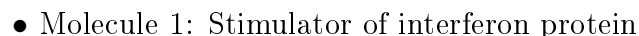
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	175	Total	O	0	0
			175	175		
5	B	178	Total	O	0	0
			178	178		

Note EDS failed to run properly.

- Chain A:  77% 15% 7%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	33.49Å 77.63Å 135.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.04 – 1.77	Depositor
% Data completeness (in resolution range)	99.8 (39.04-1.77)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.70 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.160 , 0.202	Depositor
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.062	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3484	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: V67, GOL, EDO

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	0.80	1/1549 (0.1%)	0.95	4/2094 (0.2%)
1	B	0.75	0/1570	0.90	1/2126 (0.0%)
All	All	0.78	1/3119 (0.0%)	0.93	5/4220 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	260	GLU	CD-OE1	-5.79	1.19	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	ARG	NE-CZ-NH2	5.79	123.20	120.30
1	A	232[A]	ARG	NE-CZ-NH1	-5.47	117.57	120.30
1	A	232[B]	ARG	NE-CZ-NH1	-5.47	117.57	120.30
1	A	310	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	B	284	ARG	NE-CZ-NH2	-5.24	117.68	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	1523	0	1487	26	0
1	B	1542	0	1501	28	0
2	A	25	0	0	1	0
2	B	25	0	0	0	0
3	A	6	0	8	1	0
3	B	6	0	8	6	0
4	B	4	0	6	2	0
5	A	175	0	0	11	0
5	B	178	0	0	11	0
All	All	3484	0	3010	56	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 9.

All (56) 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:232[A]:ARG:O	1:B:235[A]:ILE:HG22	1.31	1.27
1:A:241:SER:O	1:B:235[A]:ILE:HD11	1.66	0.92
1:B:305:SER:O	3:B:403:GOL:H12	1.70	0.91
1:B:232[A]:ARG:O	1:B:235[A]:ILE:CG2	2.20	0.87
1:A:296[A]:GLU:HG2	1:A:311:LEU:HD12	1.57	0.84
1:A:223[A]:ASP:OD2	3:A:402:GOL:O1	2.01	0.79
4:B:402:EDO:H22	5:B:513:HOH:O	1.88	0.73
1:A:336:GLU:O	5:A:501:HOH:O	2.10	0.69
1:A:224:LYS:HD3	5:A:544:HOH:O	1.92	0.69
1:A:176[A]:GLN:HE21	1:A:180:ARG:HH22	1.40	0.68
3:B:403:GOL:C1	5:B:507:HOH:O	2.43	0.67
1:A:162[B]:SER:OG	1:B:267:THR:HG21	1.95	0.66
1:A:332:HIS:HE1	5:A:543:HOH:O	1.79	0.65
1:A:297[B]:ASP:OD2	5:A:502:HOH:O	2.14	0.65
1:A:272:SER:HB3	1:A:279:PHE:CD2	2.33	0.63
1:B:196:GLN:CA	1:B:196:GLN:HE21	2.10	0.63
1:B:196:GLN:HE21	1:B:196:GLN:HA	1.63	0.63
3:B:403:GOL:H12	5:B:507:HOH:O	1.98	0.63
1:A:252:GLN:NE2	5:A:503:HOH:O	2.31	0.62
1:B:197:ARG:NE	1:B:336:GLU:OE2	2.32	0.62
1:A:176[A]:GLN:NE2	5:A:505:HOH:O	2.33	0.61
1:B:267:THR:HG22	1:B:271:MET:SD	2.43	0.59
1:A:232[B]:ARG:HD2	5:A:585:HOH:O	2.05	0.55
1:B:196:GLN:NE2	1:B:196:GLN:HA	2.22	0.55
1:B:235[A]:ILE:O	1:B:235[A]:ILE:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:THR:O	1:A:271:MET:HG3	2.07	0.54
1:B:305:SER:O	3:B:403:GOL:C1	2.50	0.54
1:A:310:ARG:HH21	1:A:332:HIS:HD2	1.56	0.53
4:B:402:EDO:C2	5:B:513:HOH:O	2.52	0.52
1:B:293:ARG:HD2	5:B:531:HOH:O	2.09	0.52
1:A:272:SER:HB3	1:A:279:PHE:HD2	1.72	0.51
1:A:228:GLN:NE2	5:A:511:HOH:O	2.43	0.50
1:A:241:SER:O	1:B:235[A]:ILE:CD1	2.52	0.50
1:B:267:THR:OG1	5:B:501:HOH:O	2.19	0.47
1:A:315:GLN:HG3	5:A:589:HOH:O	2.14	0.47
1:B:300:ALA:O	3:B:403:GOL:O2	2.32	0.47
1:B:316:GLU:HG2	1:B:323:PHE:CD2	2.50	0.46
1:A:232[B]:ARG:NH2	2:A:401:V67:O20	2.47	0.46
1:B:232[A]:ARG:NH1	5:B:514:HOH:O	2.48	0.45
1:B:176:GLN:HA	1:B:196:GLN:HE22	1.80	0.45
1:B:235[A]:ILE:CG2	1:B:238:ARG:HB2	2.47	0.45
1:B:175:LEU:HD22	1:B:198:LEU:HB2	1.99	0.44
1:B:226:PRO:HG2	5:B:675:HOH:O	2.17	0.44
1:A:229:THR:HA	1:A:238:ARG:O	2.18	0.43
1:B:163:TYR:HB2	1:B:264:PRO:HG2	2.00	0.43
1:B:175:LEU:CD2	1:B:198:LEU:HB2	2.49	0.42
1:A:310:ARG:NE	5:A:513:HOH:O	2.44	0.42
1:B:229:THR:HA	1:B:238:ARG:O	2.20	0.42
1:A:208:VAL:HB	1:A:266:GLN:HG2	2.02	0.41
1:B:332:HIS:HE1	5:B:511:HOH:O	2.02	0.41
1:A:285:LEU:HG	1:A:289:LYS:HE3	2.03	0.41
1:A:333:LEU:HA	1:A:333:LEU:HD23	1.95	0.41
1:B:310:ARG:NE	1:B:332:HIS:HD2	2.18	0.41
1:B:169[B]:ARG:NH2	5:B:508:HOH:O	2.41	0.40
3:B:403:GOL:C2	5:B:507:HOH:O	2.70	0.40
1:A:174:GLU:HG2	5:A:506:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
3	GOL	B	403	-	5,5,5	0.26	0	5,5,5	0.89	0
2	V67	A	401	-	25,27,27	2.06	6 (24%)	32,38,38	2.99	8 (25%)
4	EDO	B	402	-	3,3,3	0.46	0	2,2,2	0.07	0
3	GOL	A	402	-	5,5,5	0.08	0	5,5,5	0.23	0
2	V67	B	401	-	25,27,27	1.00	1 (4%)	32,38,38	2.86	5 (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	GOL	B	403	-	-	2/4/4/4	-
2	V67	A	401	-	-	0/12/16/16	0/3/3/3
4	EDO	B	402	-	-	1/1/1/1	-
3	GOL	A	402	-	-	0/4/4/4	-
2	V67	B	401	-	-	0/12/16/16	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	V67	C2-N1	-5.89	1.35	1.44
2	A	401	V67	C18-C19	4.85	1.52	1.47
2	A	401	V67	C11-N10	-3.17	1.35	1.41
2	A	401	V67	C5-C8	-2.81	1.43	1.50
2	A	401	V67	N7-N6	-2.52	1.27	1.34
2	A	401	V67	C22-N23	-2.23	1.29	1.34
2	B	401	V67	C2-N1	-2.22	1.40	1.44

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	V67	C2-N7-N6	13.33	125.85	118.45
2	A	401	V67	C2-N7-N6	12.41	125.34	118.45
2	A	401	V67	N7-C2-N1	6.55	119.22	113.49
2	B	401	V67	N7-C2-N1	5.66	118.44	113.49
2	A	401	V67	C17-C18-C11	5.11	121.79	118.46
2	A	401	V67	C25-N1-C2	4.71	130.98	125.69
2	B	401	V67	C4-C5-N6	-3.70	117.65	122.25
2	A	401	V67	C25-N1-C22	-2.61	103.78	108.50
2	B	401	V67	C17-C15-C13	-2.34	118.36	121.03
2	A	401	V67	C17-C15-C13	-2.34	118.37	121.03
2	A	401	V67	C12-C11-C18	-2.19	117.02	120.32
2	B	401	V67	C4-C5-C8	2.17	123.10	119.57
2	A	401	V67	F14-C13-C12	2.10	122.79	118.61

There are no chirality outliers.

All (3) torsion outliers are listed below:

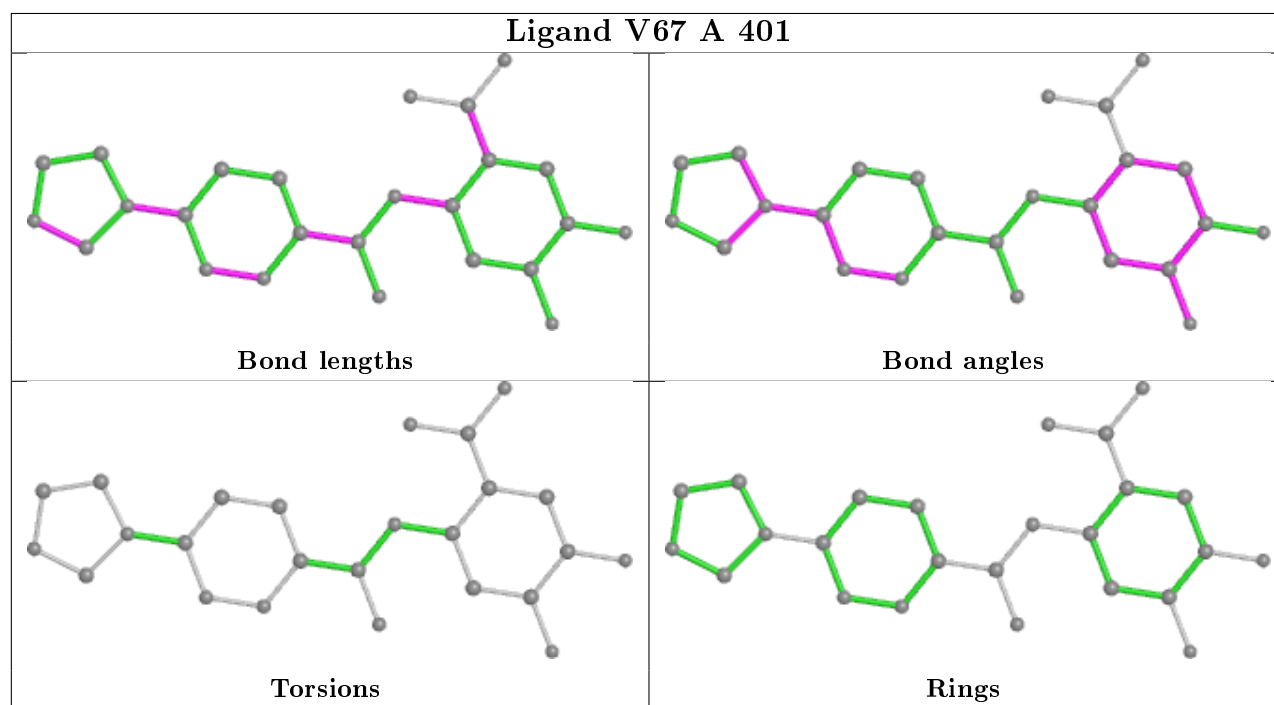
Mol	Chain	Res	Type	Atoms
3	B	403	GOL	O2-C2-C3-O3
4	B	402	EDO	O1-C1-C2-O2
3	B	403	GOL	O1-C1-C2-O2

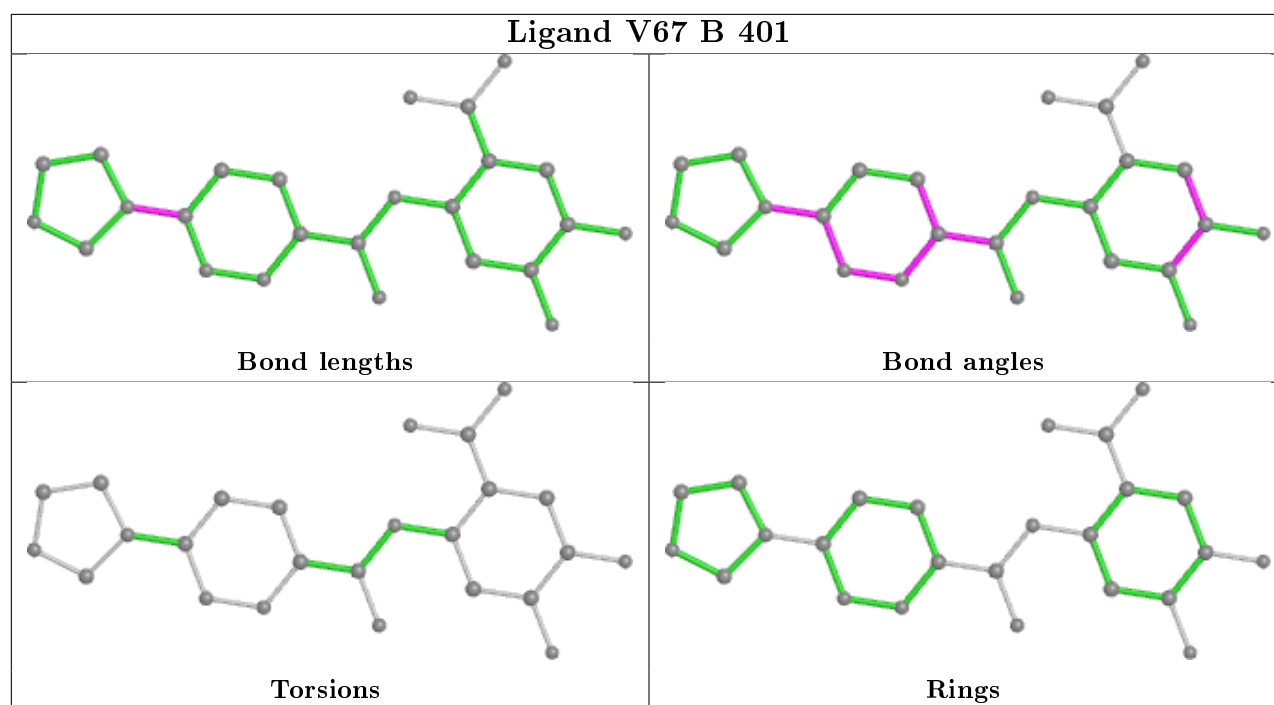
There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	403	GOL	6	0
2	A	401	V67	1	0
4	B	402	EDO	2	0
3	A	402	GOL	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

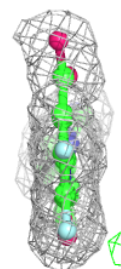
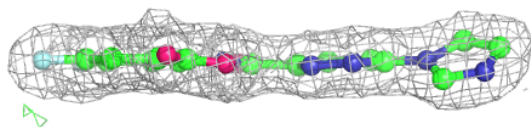
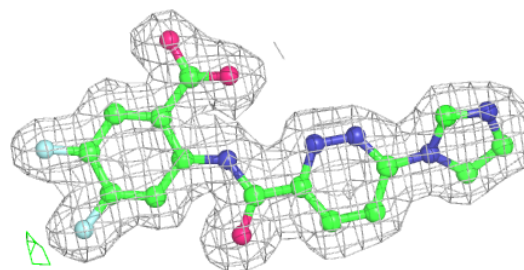
6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

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.

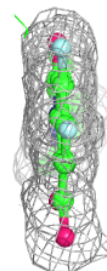
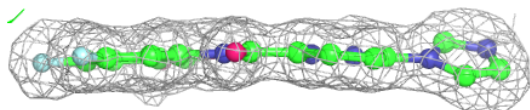
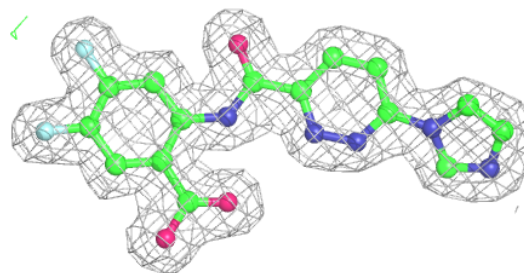
Electron density around V67 A 401:

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



Electron density around V67 B 401:

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



6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.