



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 07:13 pm BST

PDB ID : 6BQJ
Title : CRYSTAL STRUCTURE OF HEPATIS C VIRUS PROTEASE (NS3)
COMPLEXED WITH TRIPEPTIDIC ACYL SULFONAMIDE INHIBITOR
(COMPOUND 16)
Authors : Klei, H.E.; Sack, J.S.
Deposited on : 2017-11-28
Resolution : 1.69 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 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

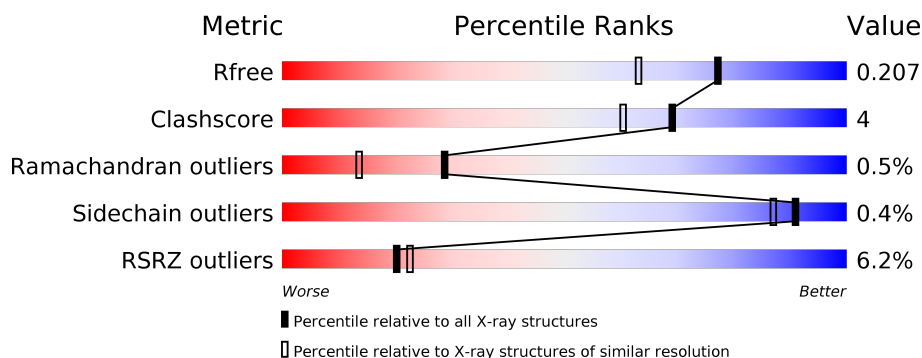
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.69 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 $\leq 5\%$. 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	219	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>7%</div> <div>11%</div> </div> </div>
1	B	219	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>5%</div> <div>11%</div> </div> </div>
1	C	219	<div> <div>9%</div> <div> <div></div> <div>88%</div> <div>6%</div> <div>5%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ACT	A	304	-	-	X	-
5	ACT	C	304	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4775 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 NS3 protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	1	0
			1391	861	251	272	7			
1	B	194	Total	C	N	O	S	0	1	0
			1390	860	253	270	7			
1	C	207	Total	C	N	O	S	0	1	0
			1485	916	270	292	7			

There are 153 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	initiating methionine	UNP A0A075D220
A	-13	LYS	-	expression tag	UNP A0A075D220
A	-12	LYS	-	expression tag	UNP A0A075D220
A	-11	LYS	-	expression tag	UNP A0A075D220
A	-10	GLY	-	expression tag	UNP A0A075D220
A	-9	SER	-	expression tag	UNP A0A075D220
A	-8	VAL	-	expression tag	UNP A0A075D220
A	-7	VAL	-	expression tag	UNP A0A075D220
A	-6	ILE	-	expression tag	UNP A0A075D220
A	-5	VAL	-	expression tag	UNP A0A075D220
A	-4	GLY	-	expression tag	UNP A0A075D220
A	-3	ARG	-	expression tag	UNP A0A075D220
A	-2	ILE	-	expression tag	UNP A0A075D220
A	-1	ASN	-	expression tag	UNP A0A075D220
A	0	LEU	-	expression tag	UNP A0A075D220
A	1	SER	-	expression tag	UNP A0A075D220
A	2	GLY	-	expression tag	UNP A0A075D220
A	3	ASP	-	expression tag	UNP A0A075D220
A	13	GLU	LEU	conflict	UNP A0A075D220
A	14	GLU	LEU	conflict	UNP A0A075D220
A	17	GLN	ILE	conflict	UNP A0A075D220
A	18	GLU	ILE	conflict	UNP A0A075D220
A	21	GLN	LEU	conflict	UNP A0A075D220

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	SER	CYS	conflict	UNP A0A075D220
A	52	LEU	CYS	conflict	UNP A0A075D220
A	72	THR	ILE	conflict	UNP A0A075D220
A	80	LYS	GLN	conflict	UNP A0A075D220
A	86	GLN	PRO	conflict	UNP A0A075D220
A	174	SER	ASN	conflict	UNP A0A075D220
A	183	ALA	-	expression tag	UNP A0A075D220
A	184	ILE	-	expression tag	UNP A0A075D220
A	185	ARG	-	expression tag	UNP A0A075D220
A	186	ALA	-	expression tag	UNP A0A075D220
A	187	PRO	-	expression tag	UNP A0A075D220
A	188	SER	-	expression tag	UNP A0A075D220
A	189	THR	-	expression tag	UNP A0A075D220
A	190	SER	-	expression tag	UNP A0A075D220
A	191	LEU	-	expression tag	UNP A0A075D220
A	192	ARG	-	expression tag	UNP A0A075D220
A	193	PRO	-	expression tag	UNP A0A075D220
A	194	HIS	-	expression tag	UNP A0A075D220
A	195	SER	-	expression tag	UNP A0A075D220
A	196	SER	-	expression tag	UNP A0A075D220
A	197	THR	-	expression tag	UNP A0A075D220
A	198	THR	-	expression tag	UNP A0A075D220
A	199	THR	-	expression tag	UNP A0A075D220
A	200	THR	-	expression tag	UNP A0A075D220
A	201	THR	-	expression tag	UNP A0A075D220
A	202	THR	-	expression tag	UNP A0A075D220
A	203	GLU	-	expression tag	UNP A0A075D220
A	204	ILE	-	expression tag	UNP A0A075D220
B	-14	MET	-	initiating methionine	UNP A0A075D220
B	-13	LYS	-	expression tag	UNP A0A075D220
B	-12	LYS	-	expression tag	UNP A0A075D220
B	-11	LYS	-	expression tag	UNP A0A075D220
B	-10	GLY	-	expression tag	UNP A0A075D220
B	-9	SER	-	expression tag	UNP A0A075D220
B	-8	VAL	-	expression tag	UNP A0A075D220
B	-7	VAL	-	expression tag	UNP A0A075D220
B	-6	ILE	-	expression tag	UNP A0A075D220
B	-5	VAL	-	expression tag	UNP A0A075D220
B	-4	GLY	-	expression tag	UNP A0A075D220
B	-3	ARG	-	expression tag	UNP A0A075D220
B	-2	ILE	-	expression tag	UNP A0A075D220
B	-1	ASN	-	expression tag	UNP A0A075D220

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	LEU	-	expression tag	UNP A0A075D220
B	1	SER	-	expression tag	UNP A0A075D220
B	2	GLY	-	expression tag	UNP A0A075D220
B	3	ASP	-	expression tag	UNP A0A075D220
B	13	GLU	LEU	conflict	UNP A0A075D220
B	14	GLU	LEU	conflict	UNP A0A075D220
B	17	GLN	ILE	conflict	UNP A0A075D220
B	18	GLU	ILE	conflict	UNP A0A075D220
B	21	GLN	LEU	conflict	UNP A0A075D220
B	47	SER	CYS	conflict	UNP A0A075D220
B	52	LEU	CYS	conflict	UNP A0A075D220
B	72	THR	ILE	conflict	UNP A0A075D220
B	80	LYS	GLN	conflict	UNP A0A075D220
B	86	GLN	PRO	conflict	UNP A0A075D220
B	174	SER	ASN	conflict	UNP A0A075D220
B	183	ALA	-	expression tag	UNP A0A075D220
B	184	ILE	-	expression tag	UNP A0A075D220
B	185	ARG	-	expression tag	UNP A0A075D220
B	186	ALA	-	expression tag	UNP A0A075D220
B	187	PRO	-	expression tag	UNP A0A075D220
B	188	SER	-	expression tag	UNP A0A075D220
B	189	THR	-	expression tag	UNP A0A075D220
B	190	SER	-	expression tag	UNP A0A075D220
B	191	LEU	-	expression tag	UNP A0A075D220
B	192	ARG	-	expression tag	UNP A0A075D220
B	193	PRO	-	expression tag	UNP A0A075D220
B	194	HIS	-	expression tag	UNP A0A075D220
B	195	SER	-	expression tag	UNP A0A075D220
B	196	SER	-	expression tag	UNP A0A075D220
B	197	THR	-	expression tag	UNP A0A075D220
B	198	THR	-	expression tag	UNP A0A075D220
B	199	THR	-	expression tag	UNP A0A075D220
B	200	THR	-	expression tag	UNP A0A075D220
B	201	THR	-	expression tag	UNP A0A075D220
B	202	THR	-	expression tag	UNP A0A075D220
B	203	GLU	-	expression tag	UNP A0A075D220
B	204	ILE	-	expression tag	UNP A0A075D220
C	-14	MET	-	initiating methionine	UNP A0A075D220
C	-13	LYS	-	expression tag	UNP A0A075D220
C	-12	LYS	-	expression tag	UNP A0A075D220
C	-11	LYS	-	expression tag	UNP A0A075D220
C	-10	GLY	-	expression tag	UNP A0A075D220

Continued on next page...

Continued from previous page...

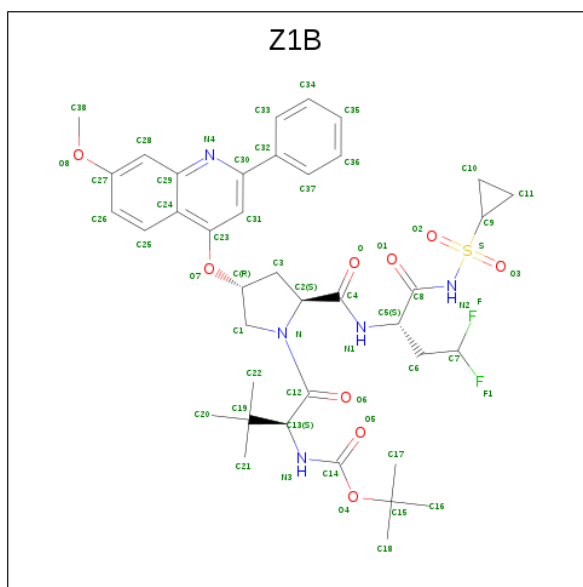
Chain	Residue	Modelled	Actual	Comment	Reference
C	-9	SER	-	expression tag	UNP A0A075D220
C	-8	VAL	-	expression tag	UNP A0A075D220
C	-7	VAL	-	expression tag	UNP A0A075D220
C	-6	ILE	-	expression tag	UNP A0A075D220
C	-5	VAL	-	expression tag	UNP A0A075D220
C	-4	GLY	-	expression tag	UNP A0A075D220
C	-3	ARG	-	expression tag	UNP A0A075D220
C	-2	ILE	-	expression tag	UNP A0A075D220
C	-1	ASN	-	expression tag	UNP A0A075D220
C	0	LEU	-	expression tag	UNP A0A075D220
C	1	SER	-	expression tag	UNP A0A075D220
C	2	GLY	-	expression tag	UNP A0A075D220
C	3	ASP	-	expression tag	UNP A0A075D220
C	13	GLU	LEU	conflict	UNP A0A075D220
C	14	GLU	LEU	conflict	UNP A0A075D220
C	17	GLN	ILE	conflict	UNP A0A075D220
C	18	GLU	ILE	conflict	UNP A0A075D220
C	21	GLN	LEU	conflict	UNP A0A075D220
C	47	SER	CYS	conflict	UNP A0A075D220
C	52	LEU	CYS	conflict	UNP A0A075D220
C	72	THR	ILE	conflict	UNP A0A075D220
C	80	LYS	GLN	conflict	UNP A0A075D220
C	86	GLN	PRO	conflict	UNP A0A075D220
C	174	SER	ASN	conflict	UNP A0A075D220
C	183	ALA	-	expression tag	UNP A0A075D220
C	184	ILE	-	expression tag	UNP A0A075D220
C	185	ARG	-	expression tag	UNP A0A075D220
C	186	ALA	-	expression tag	UNP A0A075D220
C	187	PRO	-	expression tag	UNP A0A075D220
C	188	SER	-	expression tag	UNP A0A075D220
C	189	THR	-	expression tag	UNP A0A075D220
C	190	SER	-	expression tag	UNP A0A075D220
C	191	LEU	-	expression tag	UNP A0A075D220
C	192	ARG	-	expression tag	UNP A0A075D220
C	193	PRO	-	expression tag	UNP A0A075D220
C	194	HIS	-	expression tag	UNP A0A075D220
C	195	SER	-	expression tag	UNP A0A075D220
C	196	SER	-	expression tag	UNP A0A075D220
C	197	THR	-	expression tag	UNP A0A075D220
C	198	THR	-	expression tag	UNP A0A075D220
C	199	THR	-	expression tag	UNP A0A075D220
C	200	THR	-	expression tag	UNP A0A075D220

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	201	THR	-	expression tag	UNP A0A075D220
C	202	THR	-	expression tag	UNP A0A075D220
C	203	GLU	-	expression tag	UNP A0A075D220
C	204	ILE	-	expression tag	UNP A0A075D220

- Molecule 2 is N-(tert-butoxycarbonyl)-3-methyl-L-valyl-(4R)-N-[(2S)-1-[(cyclopropylsulfonyl)amino]-4,4-difluoro-1-oxobutan-2-yl]-4-[(7-methoxy-2-phenylquinolin-4-yl)oxy]-L-proline (three-letter code: Z1B) (formula: C₃₉H₄₉F₂N₅O₉S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	6	0
			56	39	2	5	9	1		
2	B	1	Total	C	F	N	O	S	6	0
			56	39	2	5	9	1		
2	C	1	Total	C	F	N	O	S	6	0
			56	39	2	5	9	1		

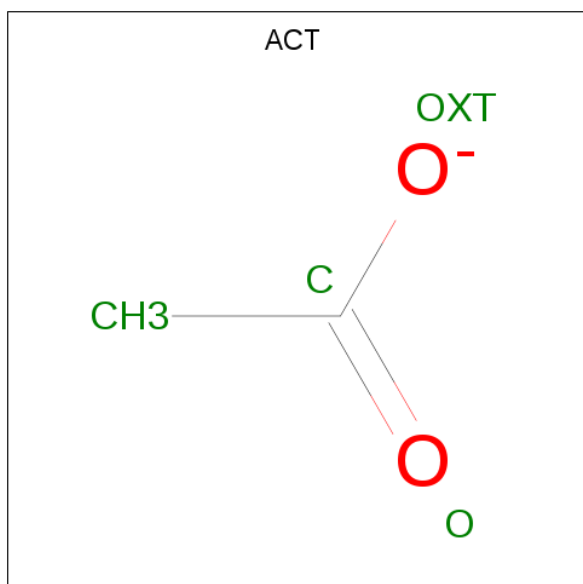
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	115	Total 115	O 115	0	0
6	B	95	Total 95	O 95	0	0
6	C	101	Total 101	O 101	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.44Å 57.47Å 89.83Å 90.00° 115.00° 90.00°	Depositor
Resolution (Å)	24.73 – 1.69 24.64 – 1.69	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.73-1.69) 99.7 (24.64-1.69)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 1.69Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.197 , 0.206 0.195 , 0.207	Depositor DCC
R_{free} test set	4582 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4775	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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 25.48 % 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 3.1475e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: ZN, CL, Z1B, ACT

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	0.54	0/1421	0.66	0/1942
1	B	0.52	0/1417	0.66	0/1935
1	C	0.51	0/1516	0.65	0/2072
All	All	0.52	0/4354	0.66	0/5949

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 [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	1391	0	1353	12	0
1	B	1390	0	1360	10	0
1	C	1485	0	1453	12	0
2	A	56	0	0	0	0
2	B	56	0	0	0	0
2	C	56	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	8	0	6	2	0
5	B	4	0	3	1	0
5	C	12	0	9	3	0
6	A	115	0	0	0	0
6	B	95	0	0	1	0
6	C	101	0	0	0	0
All	All	4775	0	4184	32	0

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

The worst 5 of 32 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:119:ARG:O	1:B:15:GLY:HA2	1.86	0.75
1:C:-3:ARG:HE	1:C:8:GLN:NE2	1.87	0.72
1:C:42:THR:HG21	1:C:109:ARG:HH22	1.56	0.69
1:A:114:ILE:HD11	1:A:134:TYR:HE2	1.63	0.63
1:A:42:THR:HG21	1:A:109:ARG:HH22	1.64	0.62

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	193/219 (88%)	187 (97%)	4 (2%)	2 (1%)	15 4
1	B	193/219 (88%)	189 (98%)	4 (2%)	0	100 100
1	C	204/219 (93%)	201 (98%)	2 (1%)	1 (0%)	29 13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	590/657 (90%)	577 (98%)	10 (2%)	3 (0%)	29	13

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	C	191	LEU
1	A	3	ASP

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	147/181 (81%)	146 (99%)	1 (1%)	84	77
1	B	146/181 (81%)	146 (100%)	0	100	100
1	C	160/181 (88%)	159 (99%)	1 (1%)	86	80
All	All	453/543 (83%)	451 (100%)	2 (0%)	91	87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	C	190	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	C	41	GLN
1	B	41	GLN
1	A	27	ASN
1	C	8	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 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 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	Z1B	A	301	-	57,60,60	0.69	2 (3%)	77,90,90	0.65	0
2	Z1B	B	301	-	57,60,60	0.74	2 (3%)	77,90,90	0.65	0
5	ACT	C	306	-	1,3,3	3.99	1 (100%)	0,3,3	0.00	-
5	ACT	C	305	-	1,3,3	4.97	1 (100%)	0,3,3	0.00	-
5	ACT	B	304	-	1,3,3	4.43	1 (100%)	0,3,3	0.00	-
5	ACT	C	304	-	1,3,3	2.54	1 (100%)	0,3,3	0.00	-
5	ACT	A	304	-	1,3,3	6.62	1 (100%)	0,3,3	0.00	-
2	Z1B	C	301	-	57,60,60	0.74	2 (3%)	77,90,90	0.64	0
5	ACT	A	305	-	1,3,3	6.18	1 (100%)	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
2	Z1B	A	301	-	-	10/58/74/74	0/5/5/5
2	Z1B	B	301	-	-	6/58/74/74	0/5/5/5
2	Z1B	C	301	-	-	7/58/74/74	0/5/5/5

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	304	ACT	CH3-C	6.62	1.57	1.48
5	A	305	ACT	CH3-C	6.18	1.56	1.48
5	C	305	ACT	CH3-C	4.97	1.55	1.48
5	B	304	ACT	CH3-C	4.43	1.54	1.48
5	C	306	ACT	CH3-C	3.99	1.53	1.48

There are no bond angle outliers.

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	Z1B	C6-C5-C8-N2
2	A	301	Z1B	C5-C8-N2-S
2	A	301	Z1B	O1-C8-N2-S
2	A	301	Z1B	C8-N2-S-O2
2	A	301	Z1B	C8-N2-S-O3

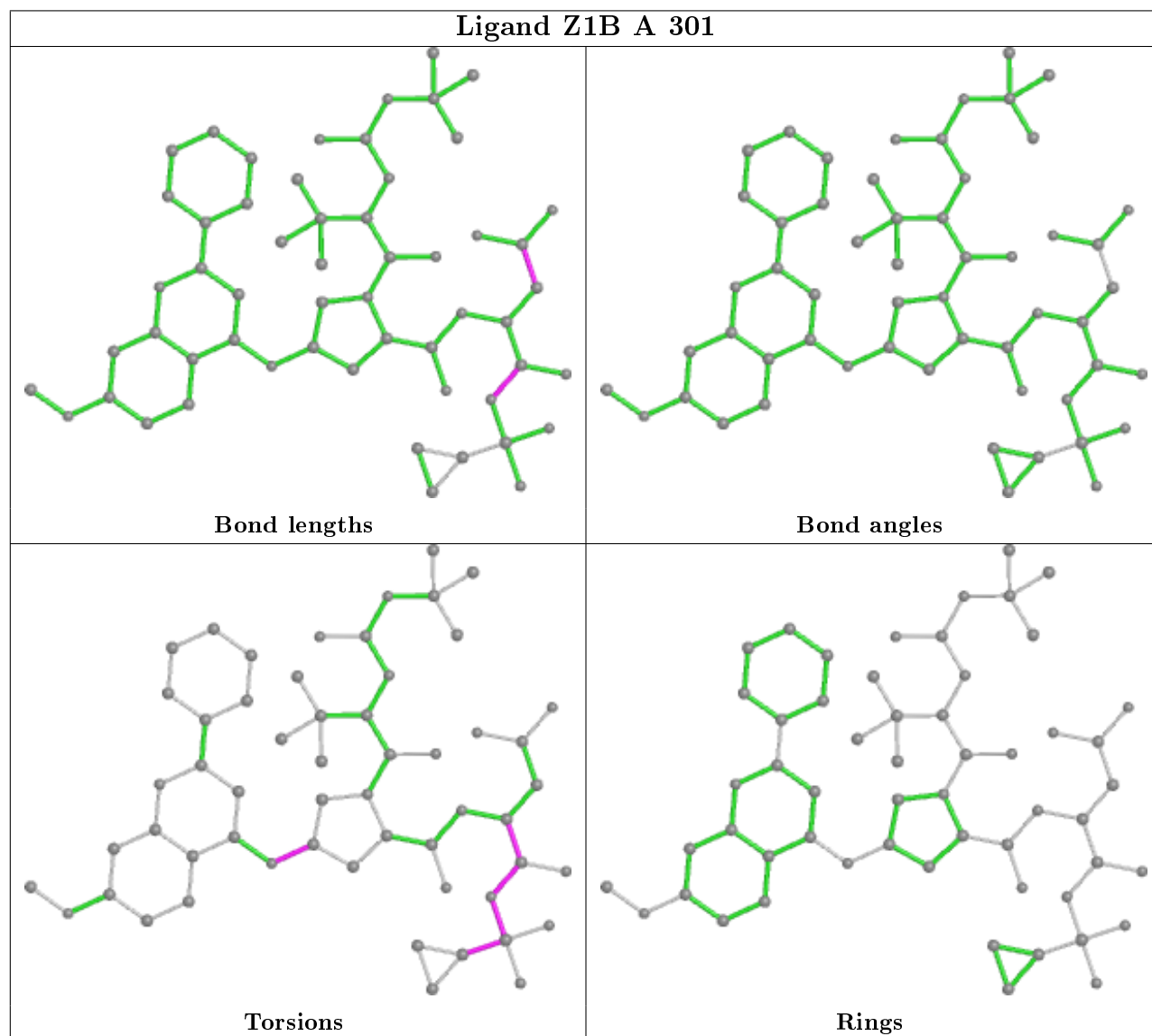
There are no ring outliers.

4 monomers are involved in 6 short contacts:

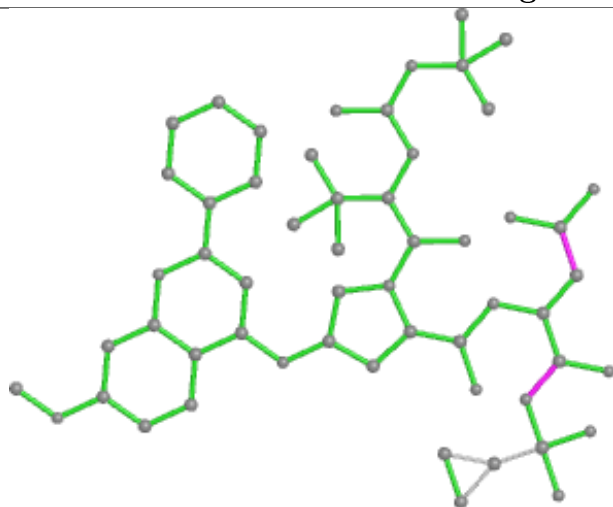
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	306	ACT	1	0
5	B	304	ACT	1	0
5	C	304	ACT	2	0
5	A	304	ACT	2	0

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

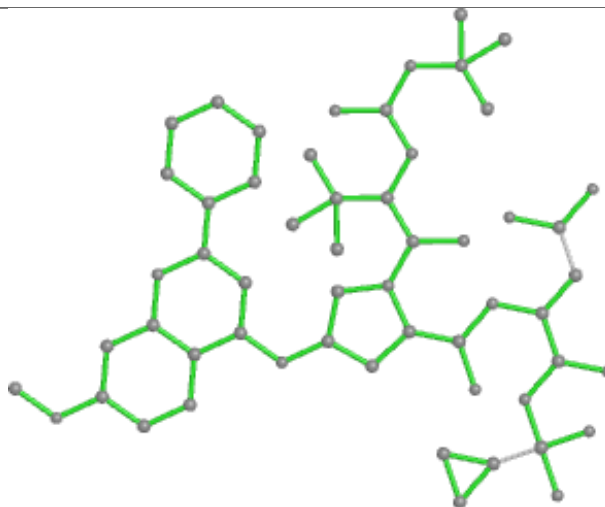
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



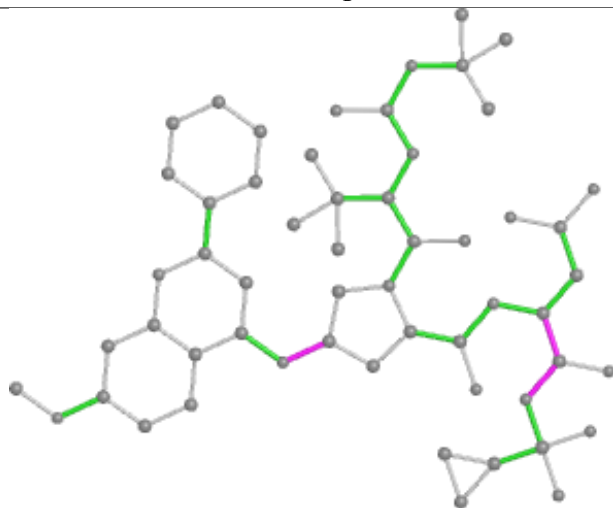
Ligand Z1B B 301



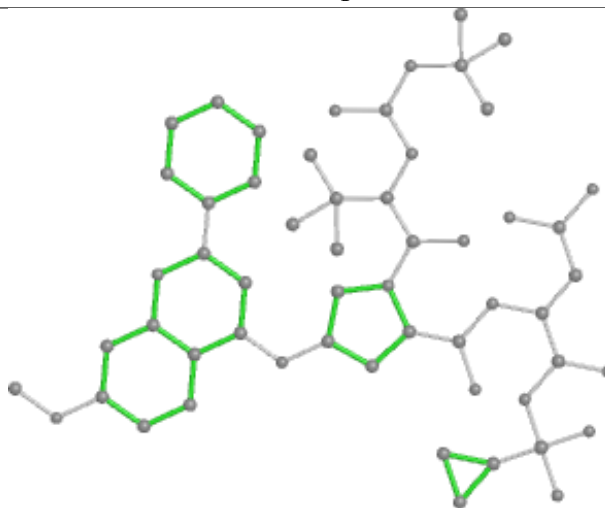
Bond lengths



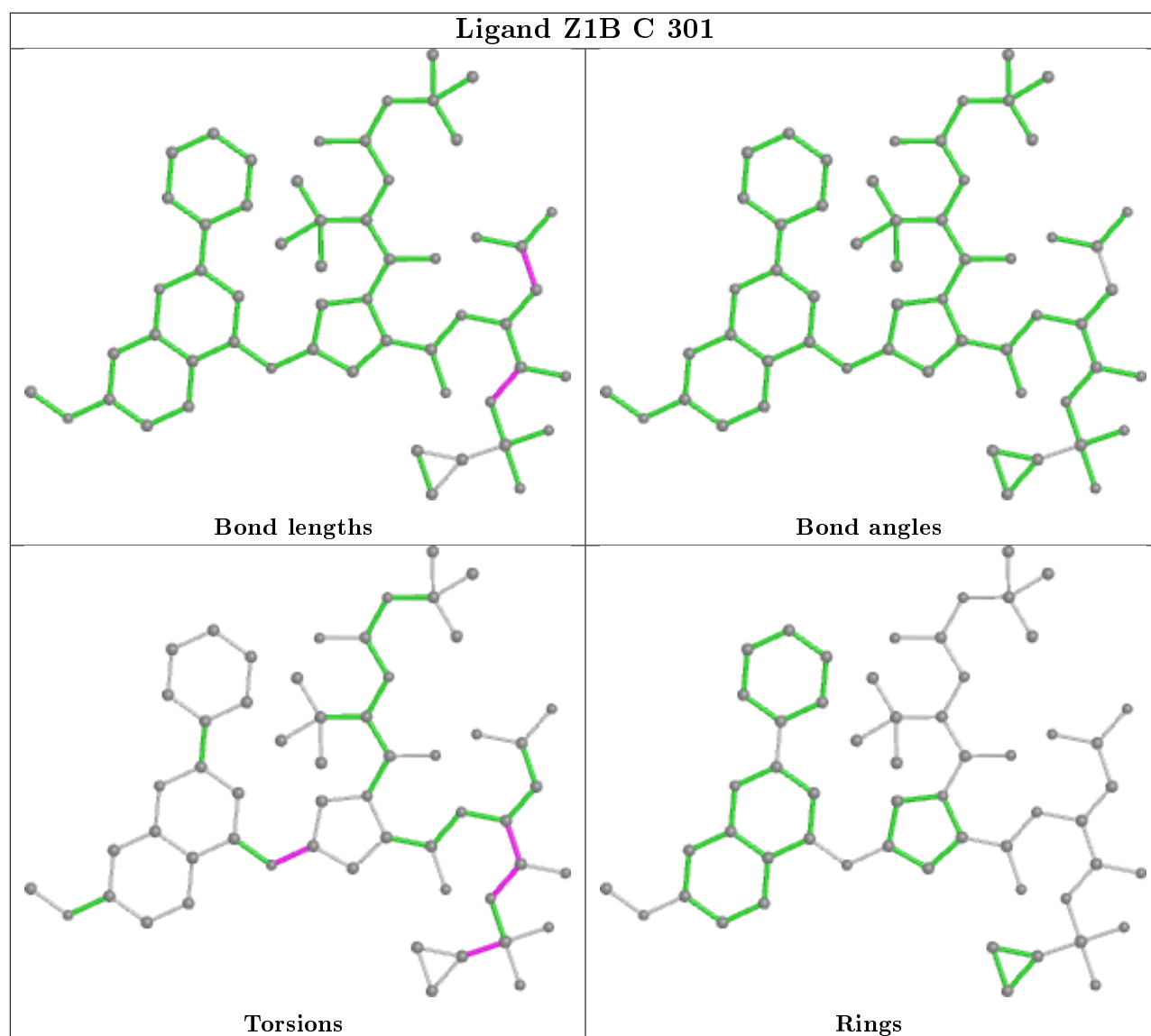
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	194/219 (88%)	0.43	13 (6%) 17 20	15, 22, 42, 70	0
1	B	194/219 (88%)	0.32	5 (2%) 56 60	16, 23, 37, 85	0
1	C	207/219 (94%)	0.57	19 (9%) 9 10	17, 25, 48, 76	0
All	All	595/657 (90%)	0.44	37 (6%) 20 23	15, 24, 45, 85	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	THR	11.9
1	A	2	GLY	9.9
1	A	1	SER	6.9
1	C	3	ASP	6.6
1	C	202	THR	6.5

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](#)

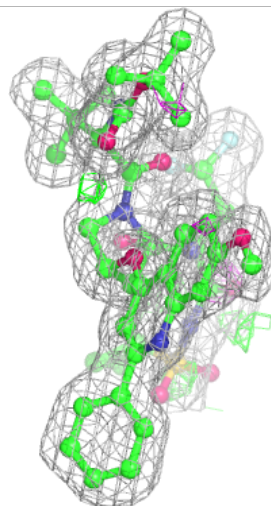
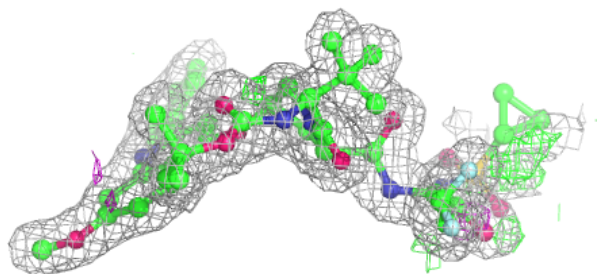
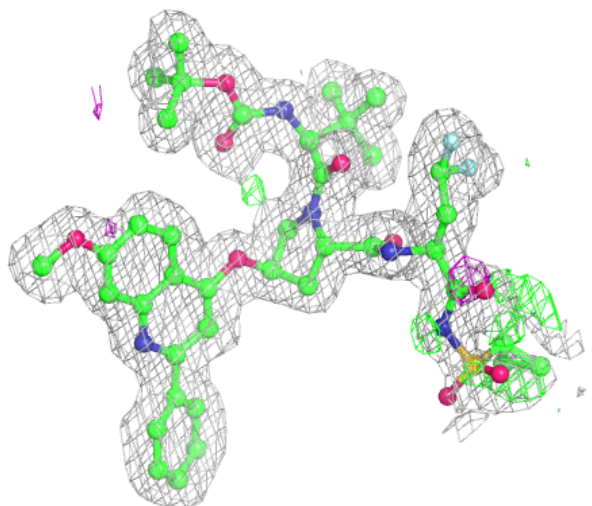
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	ACT	C	305	4/4	0.51	0.32	58,60,60,61	0
5	ACT	A	304	4/4	0.70	0.31	28,36,38,48	0
5	ACT	A	305	4/4	0.72	0.22	49,50,50,51	0
5	ACT	C	306	4/4	0.79	0.14	36,41,41,47	0
5	ACT	C	304	4/4	0.79	0.23	28,36,39,42	0
5	ACT	B	304	4/4	0.85	0.17	46,47,47,50	0
2	Z1B	C	301	56/56	0.93	0.08	17,23,29,35	6
2	Z1B	B	301	56/56	0.94	0.08	16,21,29,33	6
4	CL	C	303	1/1	0.94	0.16	43,43,43,43	0
4	CL	A	303	1/1	0.94	0.14	40,40,40,40	0
4	CL	B	303	1/1	0.95	0.14	41,41,41,41	0
2	Z1B	A	301	56/56	0.95	0.08	15,20,31,34	6
3	ZN	A	302	1/1	0.99	0.04	21,21,21,21	0
3	ZN	B	302	1/1	1.00	0.03	23,23,23,23	0
3	ZN	C	302	1/1	1.00	0.04	24,24,24,24	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.

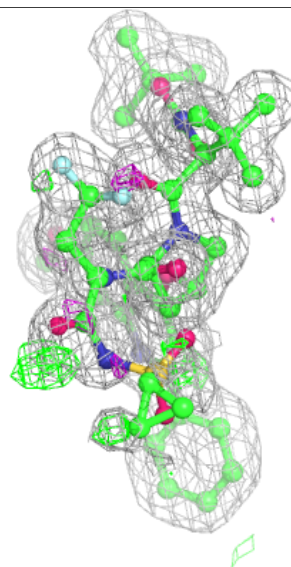
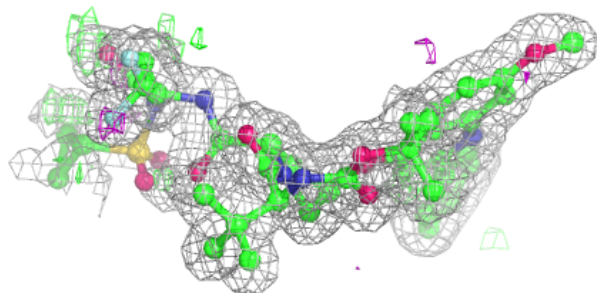
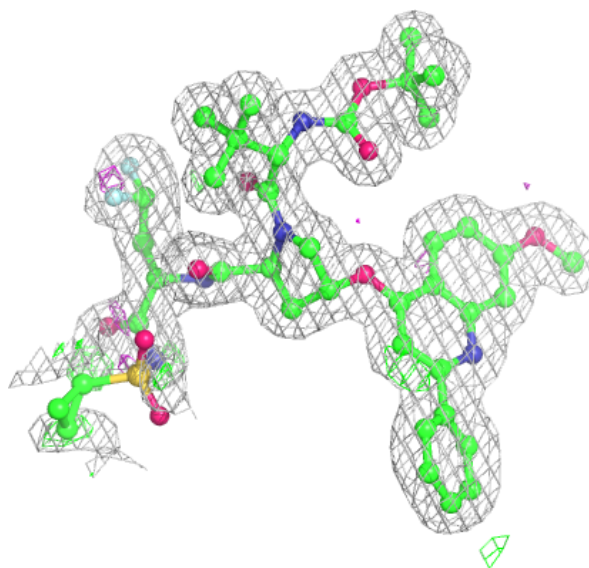
Electron density around Z1B C 301:

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



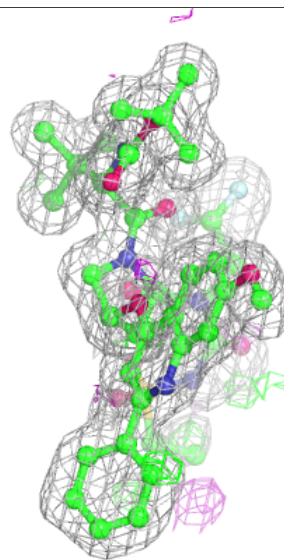
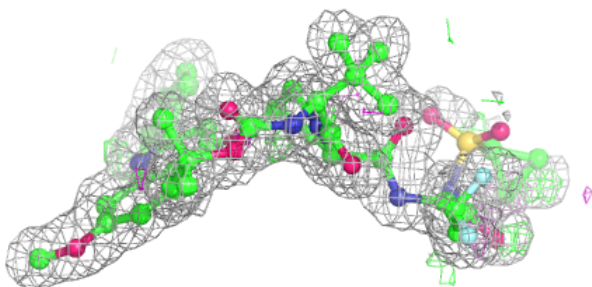
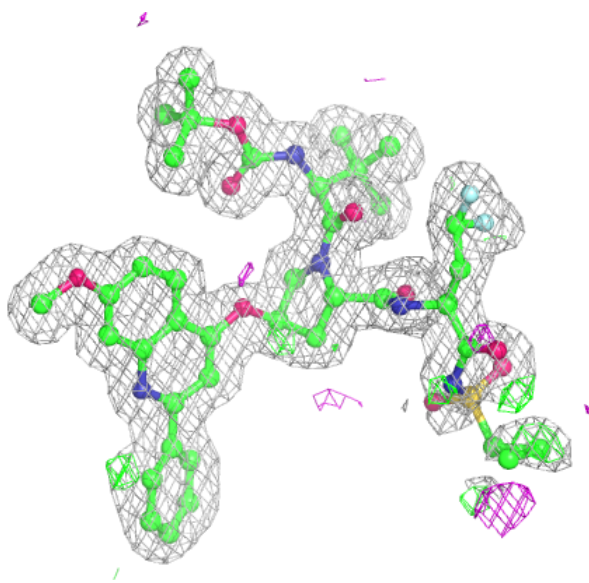
Electron density around Z1B B 301:

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



Electron density around Z1B A 301:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.