



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 09:25 AM BST

PDB ID : 6BQK
Title : CRYSTAL STRUCTURE OF HEPATIS C VIRUS PROTEASE (NS3)
COMPLEXED WITH TRIPEPTIDIC ACYL SULFONAMIDE INHIBITOR
(COMPOUND 18)
Authors : Klei, H.E.; Sack, J.S.
Deposited on : 2017-11-28
Resolution : 1.97 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 : 2.13.1
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) : 2.13.1

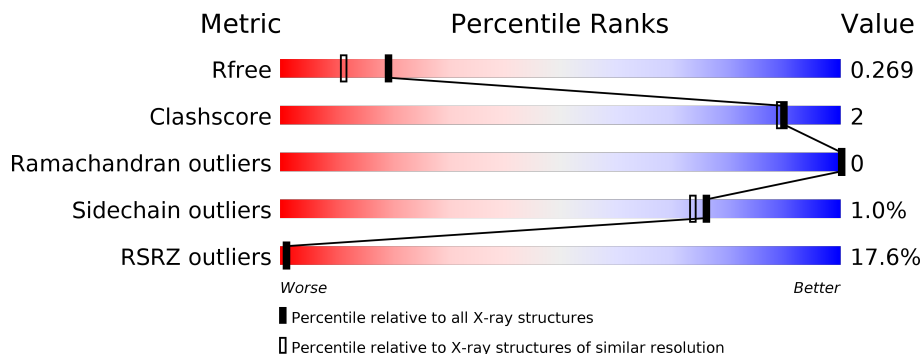
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	 15% 83% 5% 12%
1	B	219	 16% 84% 5% 12%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 3034 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
			Total	C	N	O	S			
1	A	193	1390	862	255	268	5	0	1	0
1	B	193	1389	862	255	267	5	0	0	0

There are 102 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
A	47	SER	CYS	conflict	UNP A0A075D220
A	52	LEU	CYS	conflict	UNP A0A075D220

Continued on next page...

Continued from previous page...

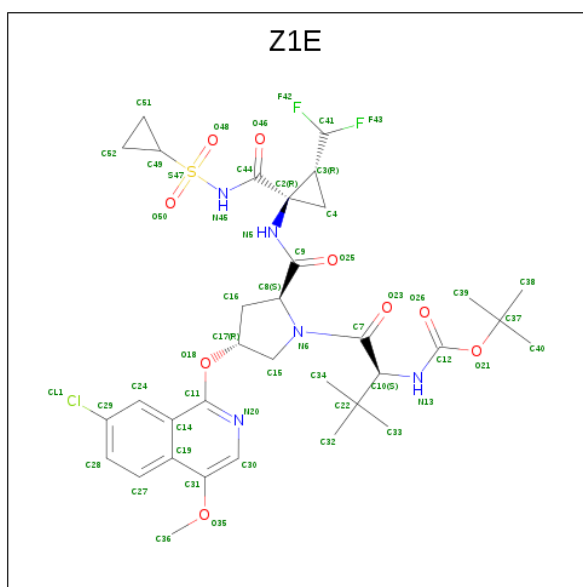
Chain	Residue	Modelled	Actual	Comment	Reference
A	72	THR	ILE	conflict	UNP A0A075D220
A	80	LYS	GLN	conflict	UNP A0A075D220
A	86	GLN	PRO	conflict	UNP A0A075D220
A	174	SER	ASN	conflict	UNP A0A075D220
A	183	ALA	-	expression tag	UNP A0A075D220
A	184	ILE	-	expression tag	UNP A0A075D220
A	185	ARG	-	expression 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
B	0	LEU	-	expression tag	UNP A0A075D220
B	1	SER	-	expression tag	UNP A0A075D220

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 2 is N-(tert-butoxycarbonyl)-3-methyl-L-valyl-(4R)-4-[(7-chloro-4-methoxyisoquinolin-1-yl)oxy]-N-[(1R,2R)-1-[(cyclopropylsulfonyl)carbamoyl]-2-(difluoromethyl)cyclopropyl]-L-prolinamide (three-letter code: Z1E) (formula: C₃₄H₄₄ClF₂N₅O₉S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf		
			Total	C	Cl	F	N	O			S	
2	A	1	Total	52	34	1	2	5	9	1	0	0
2	B	1	Total	52	34	1	2	5	9	1	0	0

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

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

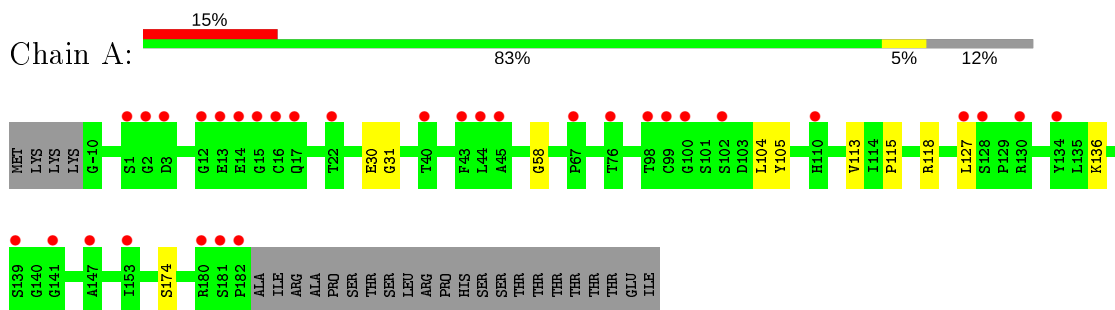
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	76	Total	76	0	0
4	B	73	Total	73	0	0

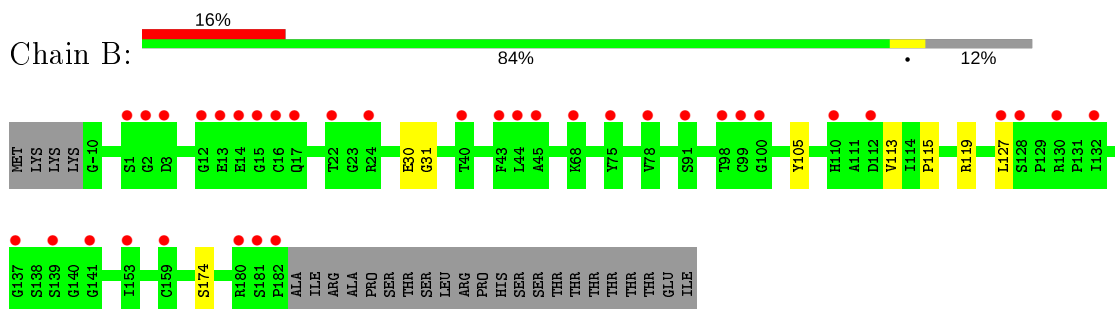
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: NS3 protease



- Molecule 1: NS3 protease



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.65Å 68.06Å 61.46Å 90.00° 109.58° 90.00°	Depositor
Resolution (Å)	23.20 – 1.97 23.00 – 1.97	Depositor EDS
% Data completeness (in resolution range)	96.2 (23.20-1.97) 96.1 (23.00-1.97)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.43 (at 1.96Å)	Xtrriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.254 , 0.267 0.256 , 0.269	Depositor DCC
R_{free} test set	1255 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	13.3	Xtrriage
Anisotropy	0.575	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3034	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.58% 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: ZN, Z1E

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	0.53	0/1420	0.71	0/1938
1	B	0.53	0/1414	0.71	0/1930
All	All	0.53	0/2834	0.71	0/3868

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	1390	0	1368	7	0
1	B	1389	0	1367	3	0
2	A	52	0	0	0	0
2	B	52	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	76	0	0	3	0
4	B	73	0	0	0	0
All	All	3034	0	2735	10	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 2.

All (10) 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:115:PRO:HB2	1:A:127:LEU:HD12	1.87	0.57
1:B:115:PRO:HB2	1:B:127:LEU:HD22	1.87	0.56
1:A:105:TYR:HB3	1:A:113:VAL:HG12	1.91	0.53
1:B:105:TYR:HB3	1:B:113:VAL:HG12	1.91	0.52
1:A:136:LYS:HB3	4:A:471:HOH:O	2.12	0.49
1:A:58:GLY:HA3	4:A:452:HOH:O	2.17	0.44
1:B:30:GLU:HG3	1:B:31:GLY:N	2.33	0.43
1:A:30:GLU:HG3	1:A:31:GLY:N	2.34	0.43
1:A:58:GLY:CA	4:A:452:HOH:O	2.66	0.42
1:A:104:LEU:HD11	1:A:118:ARG:HG3	2.02	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	192/219 (88%)	188 (98%)	4 (2%)	0	100	100
1	B	191/219 (87%)	188 (98%)	3 (2%)	0	100	100
All	All	383/438 (87%)	376 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	147/181 (81%)	146 (99%)	1 (1%)	84	83
1	B	146/181 (81%)	144 (99%)	2 (1%)	67	62
All	All	293/362 (81%)	290 (99%)	3 (1%)	76	73

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	SER
1	B	119	ARG
1	B	174	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-1	ASN
1	A	110	HIS

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](#)

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	Z1E	B	301	-	49,56,56	0.40	0	72,88,88	0.66	0
2	Z1E	A	301	-	49,56,56	0.39	0	72,88,88	0.66	0

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	Z1E	B	301	-	-	5/57/81/81	0/5/5/5
2	Z1E	A	301	-	-	7/57/81/81	0/5/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

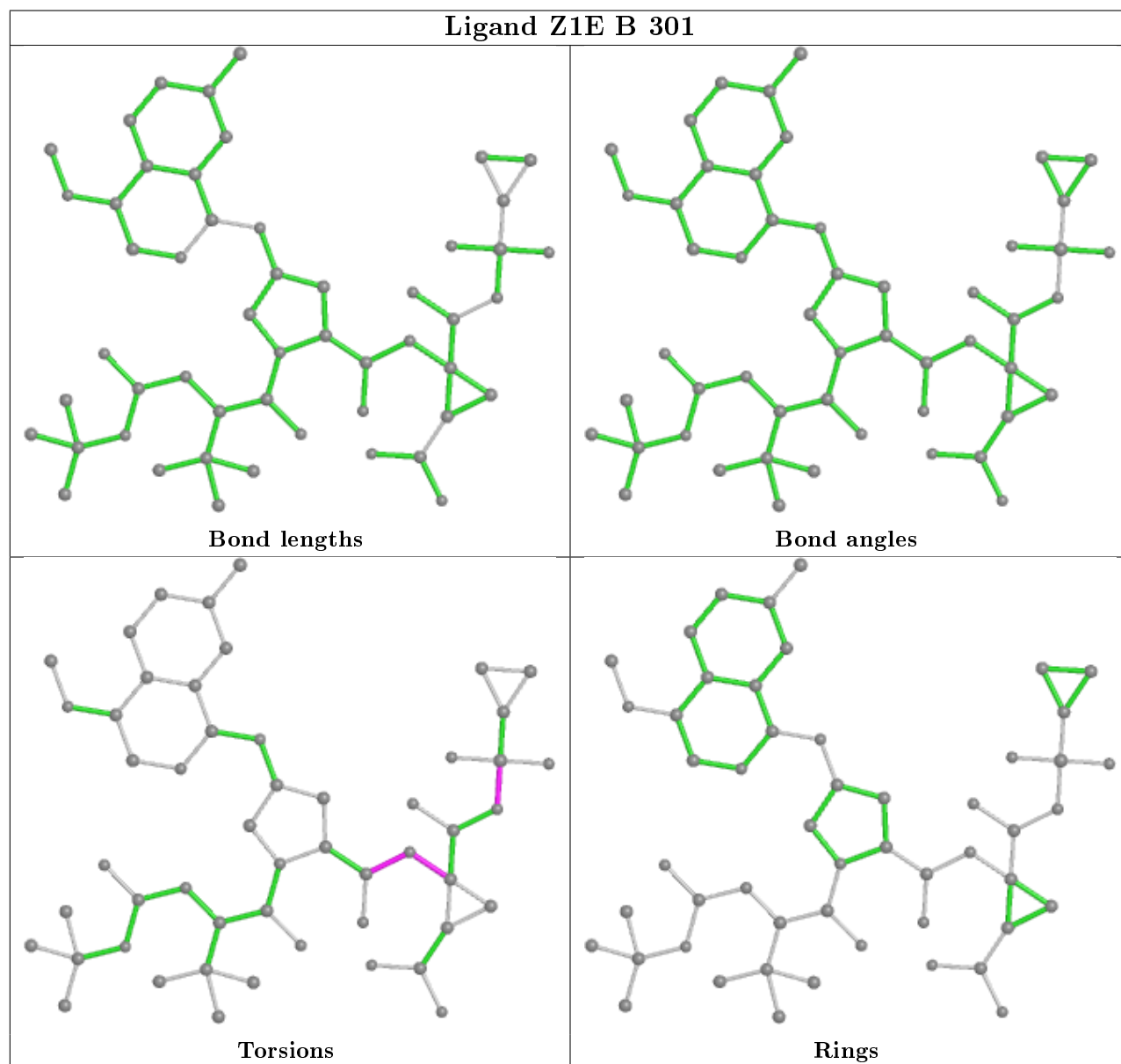
Mol	Chain	Res	Type	Atoms
2	B	301	Z1E	C3-C2-N5-C9
2	B	301	Z1E	C4-C2-N5-C9
2	B	301	Z1E	C44-N45-S47-C49
2	A	301	Z1E	C3-C2-N5-C9
2	A	301	Z1E	C4-C2-N5-C9
2	A	301	Z1E	C44-N45-S47-C49
2	A	301	Z1E	C52-C49-S47-O50
2	B	301	Z1E	O25-C9-N5-C2
2	A	301	Z1E	O25-C9-N5-C2
2	A	301	Z1E	C8-C9-N5-C2
2	B	301	Z1E	C8-C9-N5-C2
2	A	301	Z1E	C51-C49-S47-O48

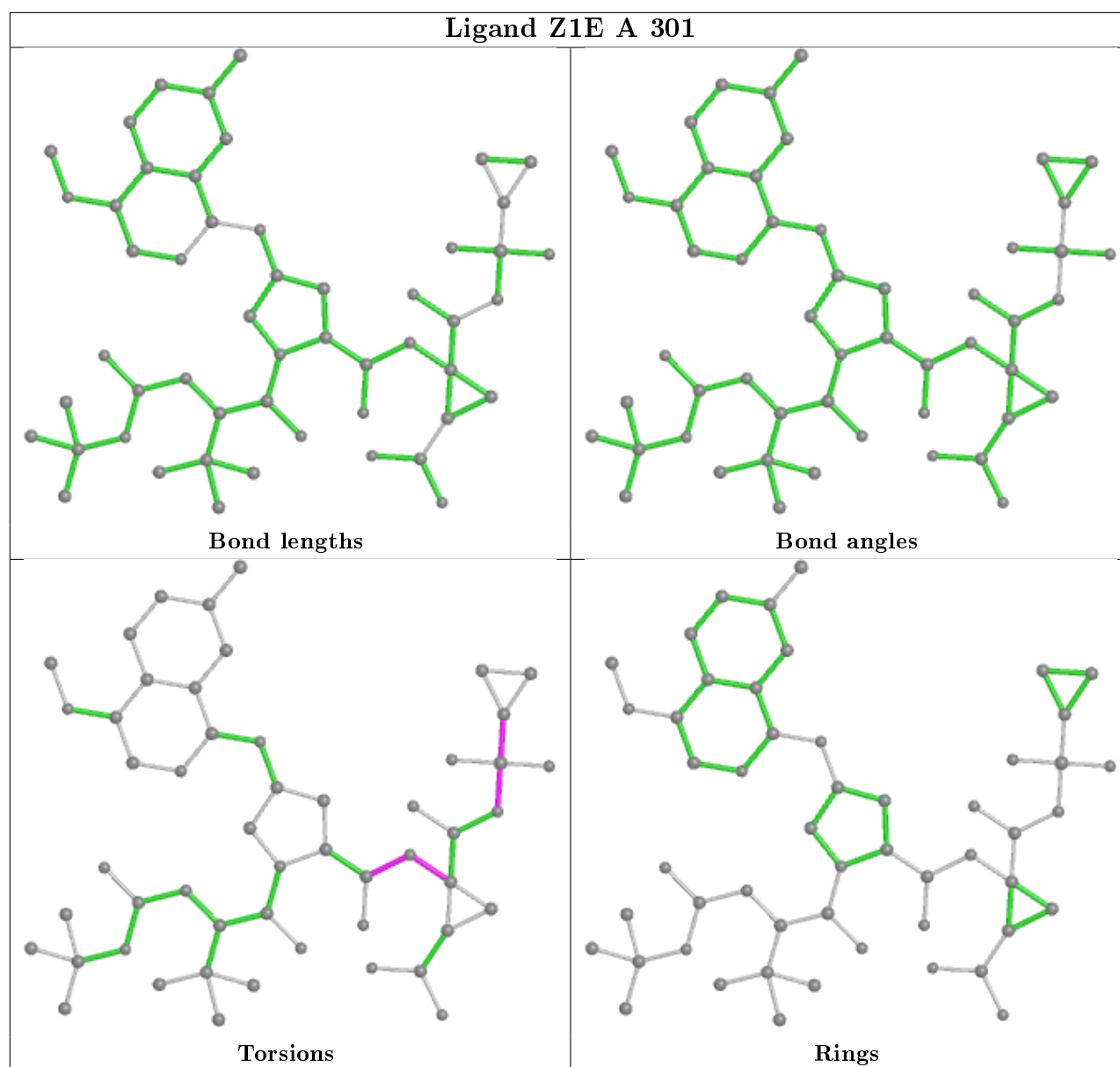
There are no ring outliers.

No monomer is involved in short contacts.

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

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	193/219 (88%)	1.23	32 (16%) 1 1	5, 18, 44, 68	0
1	B	193/219 (88%)	1.25	36 (18%) 1 1	5, 18, 46, 64	0
All	All	386/438 (88%)	1.24	68 (17%) 1 1	5, 18, 45, 68	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	99	CYS	7.3
1	B	98	THR	5.9
1	A	182	PRO	5.7
1	A	14	GLU	5.4
1	B	14	GLU	5.4
1	B	182	PRO	5.2
1	B	99	CYS	5.1
1	A	16	CYS	4.9
1	A	12	GLY	4.8
1	B	15	GLY	4.8
1	A	15	GLY	4.7
1	A	98	THR	4.6
1	A	13	GLU	4.5
1	B	128	SER	4.4
1	A	128	SER	4.1
1	A	134	TYR	3.8
1	A	127	LEU	3.8
1	B	127	LEU	3.8
1	A	40	THR	3.6
1	B	12	GLY	3.6
1	B	13	GLU	3.4
1	A	181	SER	3.3
1	A	3	ASP	3.3
1	A	2	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	180	ARG	3.3
1	B	2	GLY	3.2
1	B	3	ASP	3.2
1	B	16	CYS	3.2
1	A	17	GLN	3.1
1	A	147	ALA	3.1
1	B	43	PHE	3.0
1	B	40	THR	3.0
1	A	43	PHE	2.9
1	A	180	ARG	2.9
1	B	45	ALA	2.9
1	B	17	GLN	2.8
1	B	181	SER	2.8
1	B	110	HIS	2.8
1	B	112	ASP	2.7
1	B	139	SER	2.7
1	A	110	HIS	2.7
1	B	24	ARG	2.7
1	B	22	THR	2.6
1	B	100	GLY	2.5
1	A	1[A]	SER	2.5
1	A	44	LEU	2.5
1	B	132	ILE	2.4
1	B	1	SER	2.3
1	B	68	LYS	2.3
1	B	44	LEU	2.2
1	B	141	GLY	2.2
1	A	153	ILE	2.2
1	B	153	ILE	2.2
1	A	45	ALA	2.2
1	B	78	VAL	2.2
1	A	76	THR	2.1
1	A	100	GLY	2.1
1	A	141	GLY	2.1
1	A	22	THR	2.1
1	B	137	GLY	2.1
1	B	75	TYR	2.1
1	A	102	SER	2.1
1	A	67	PRO	2.1
1	B	159	CYS	2.0
1	B	91	SER	2.0
1	A	130	ARG	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	139	SER	2.0
1	B	130	ARG	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 monosaccharides in this entry.

6.4 Ligands [i](#)

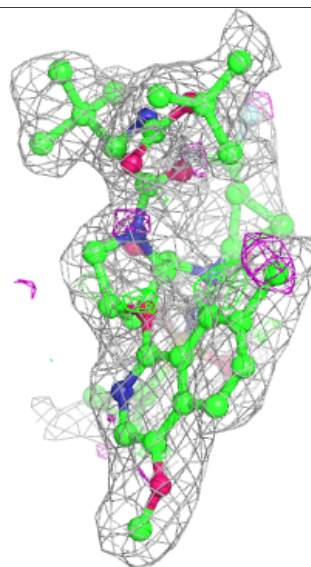
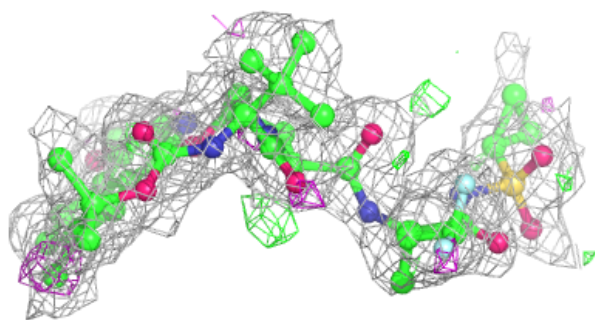
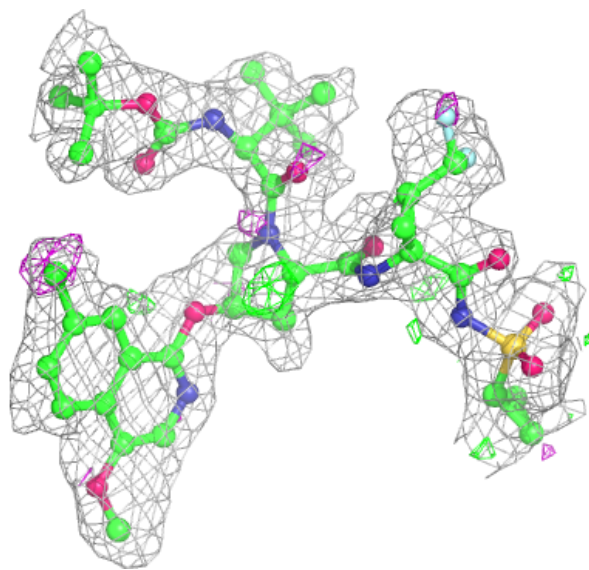
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

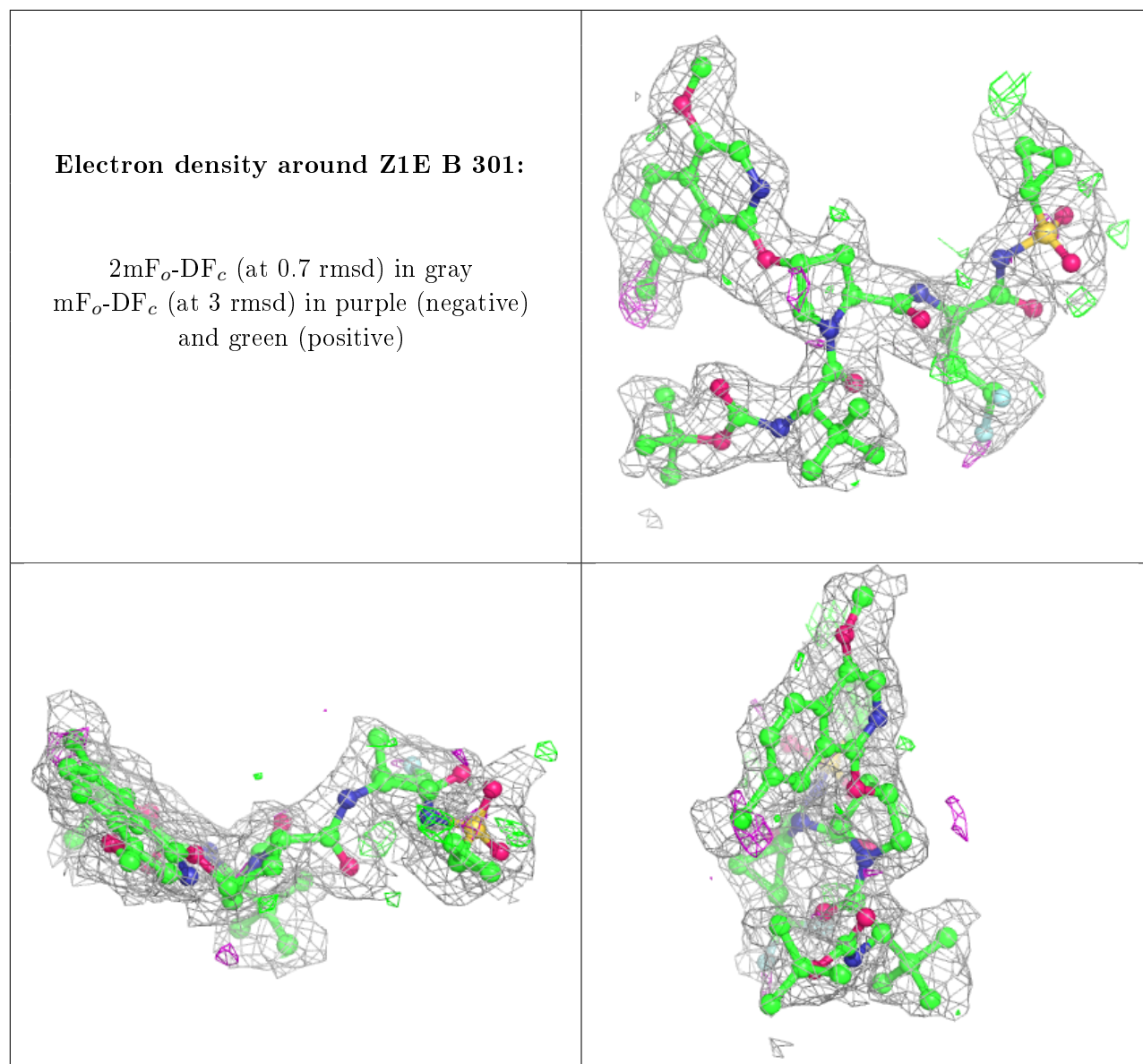
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	Z1E	A	301	52/52	0.85	0.17	9,18,30,35	0
2	Z1E	B	301	52/52	0.86	0.16	7,18,27,37	0
3	ZN	A	302	1/1	0.95	0.05	33,33,33,33	0
3	ZN	B	302	1/1	0.98	0.06	32,32,32,32	0

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 Z1E 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.