Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 08:20 PM EDT

PDB ID	:	6C2O
Title	:	Crystal structure of HCV NS3/4A protease variant Y56H in complex with danoprevir
Authors	:	Matthew, A.N.; Schiffer, C.A.
Deposited on	:	2018-01-08
Resolution	:	1.18 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:

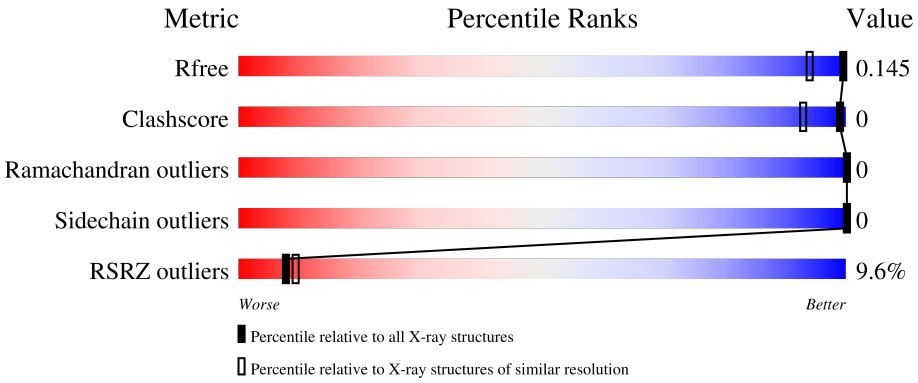
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.18 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	1123 (1.20-1.16)
Clashscore	141614	1182 (1.20-1.16)
Ramachandran outliers	138981	1134 (1.20-1.16)
Sidechain outliers	138945	1134 (1.20-1.16)
RSRZ outliers	127900	1102 (1.20-1.16)

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 <=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	198	10% 98%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3369 atoms, of which 1520 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	H	N	O	S			
1	A	198	2924	922	1424	277	293	8	0	5	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	982	HIS	-	expression tag	UNP C1KIK8
A	983	MET	-	expression tag	UNP C1KIK8
A	984	ALA	-	expression tag	UNP C1KIK8
A	985	SER	-	expression tag	UNP C1KIK8
A	986	MET	-	expression tag	UNP C1KIK8
A	987	LYS	-	expression tag	UNP C1KIK8
A	988	LYS	-	expression tag	UNP C1KIK8
A	989	LYS	-	expression tag	UNP C1KIK8
A	990	GLY	-	expression tag	UNP C1KIK8
A	991	SER	-	expression tag	UNP C1KIK8
A	992	VAL	-	expression tag	UNP C1KIK8
A	993	VAL	-	expression tag	UNP C1KIK8
A	994	ILE	-	expression tag	UNP C1KIK8
A	995	VAL	-	expression tag	UNP C1KIK8
A	996	GLY	-	expression tag	UNP C1KIK8
A	997	ARG	-	expression tag	UNP C1KIK8
A	998	ILE	-	expression tag	UNP C1KIK8
A	999	ASN	-	expression tag	UNP C1KIK8
A	1000	LEU	-	expression tag	UNP C1KIK8
A	1001	SER	-	expression tag	UNP C1KIK8
A	1002	GLY	-	expression tag	UNP C1KIK8
A	1003	ASP	-	expression tag	UNP C1KIK8
A	1013	GLU	LEU	engineered mutation	UNP C1KIK8
A	1014	GLU	LEU	engineered mutation	UNP C1KIK8
A	1017	GLN	ILE	engineered mutation	UNP C1KIK8
A	1018	GLU	ILE	engineered mutation	UNP C1KIK8
A	1021	GLN	LEU	engineered mutation	UNP C1KIK8

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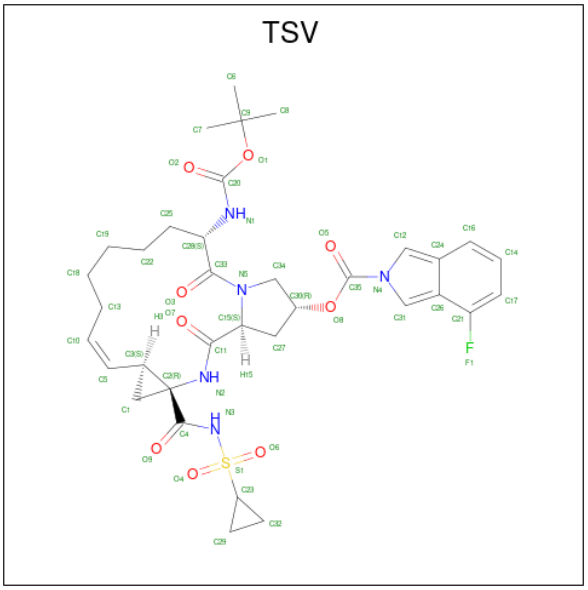
Chain	Residue	Modelled	Actual	Comment	Reference
A	1040	THR	ALA	engineered mutation	UNP C1KIK8
A	1047	SER	CYS	engineered mutation	UNP C1KIK8
A	1052	LEU	CYS	engineered mutation	UNP C1KIK8
A	1056	HIS	TYR	engineered mutation	UNP C1KIK8
A	1072	THR	ILE	engineered mutation	UNP C1KIK8
A	1086	GLN	PRO	engineered mutation	UNP C1KIK8
A	1159	SER	CYS	engineered mutation	UNP C1KIK8

- Molecule 2 is (2R,6S,12Z,13aS,14aR,16aS)-6-[(tert-butoxycarbonyl)amino]-14a-[(cyclopropylsulfonyl)carbamoyl]-5,16-dioxo-1,2,3,5,6,7,8 ,9,10,11,13a,14,14a,15,16,16a-hexadecahydrocyclopropa[e]pyrrolo[1,2-a][1,4]diazacyclopentadecin-2-yl 4-fluoro-2H-isoindole-2-carboxylate (three-letter code: TSV) (formula: $C_{35}H_{44}FN_5O_9S$) (labeled as "Ligand of Interest" by depositor).

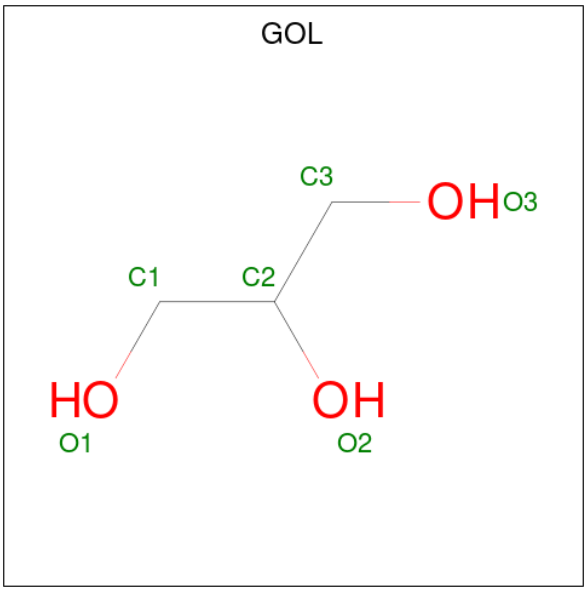


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	F	H	N	O	S	0	1
			190	70	2	88	10	18	2		

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

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	3	8	3		

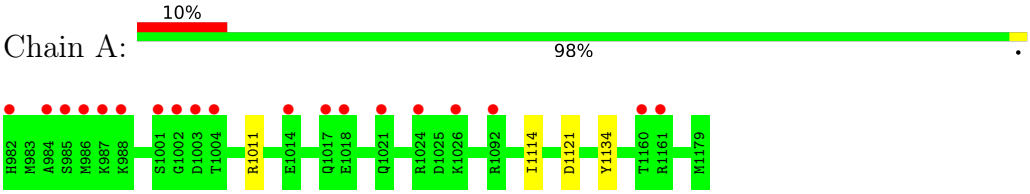
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	240	Total	O	0	0
			240	240		

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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	55.44Å 58.95Å 59.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.48 – 1.18 29.48 – 1.18	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.48-1.18) 96.3 (29.48-1.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.83 (at 1.18Å)	Xtriage
Refinement program	PHENIX 1.12-2829	Depositor
R, R_{free}	0.123 , 0.144 0.124 , 0.145	Depositor DCC
R_{free} test set	2001 reflections (3.06%)	wwPDB-VP
Wilson B-factor (Å^2)	8.8	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 48.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	3369	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.47	0/1528	0.76	3/2072 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1011	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	A	1011	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	1121	ASP	CB-CG-OD1	5.55	123.30	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1500	1424	1498	1	0
2	A	102	88	86	0	0
3	A	1	0	0	0	0
4	A	6	8	8	0	0
5	A	240	0	0	0	0
All	All	1849	1520	1592	1	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 0.

All (1) 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:1114:ILE:HD11	1:A:1134:TYR:HE2	1.83	0.43

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	201/198 (102%)	199 (99%)	2 (1%)	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	166/161 (103%)	166 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	TSV	A	1201[A]	-	50,56,56	3.56	18 (36%)	62,85,85	2.00	9 (14%)
2	TSV	A	1201[B]	-	50,56,56	3.90	27 (54%)	62,85,85	2.32	14 (22%)
4	GOL	A	1203	-	5,5,5	1.06	0	5,5,5	0.97	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	TSV	A	1201[A]	-	-	3/55/83/83	0/5/6/6
2	TSV	A	1201[B]	-	-	3/55/83/83	0/5/6/6
4	GOL	A	1203	-	-	0/4/4/4	-

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201[A]	TSV	C12-N4	13.81	1.55	1.39
2	A	1201[B]	TSV	C12-N4	13.15	1.54	1.39
2	A	1201[A]	TSV	C17-C21	10.57	1.49	1.36
2	A	1201[B]	TSV	O4-S1	9.60	1.54	1.43
2	A	1201[B]	TSV	C17-C21	7.97	1.45	1.36
2	A	1201[A]	TSV	C21-C26	7.03	1.49	1.41
2	A	1201[B]	TSV	C21-C26	6.77	1.49	1.41
2	A	1201[B]	TSV	C14-C16	6.35	1.51	1.36
2	A	1201[A]	TSV	C31-C26	6.29	1.54	1.40
2	A	1201[B]	TSV	C34-N5	5.97	1.56	1.47
2	A	1201[B]	TSV	O6-S1	5.80	1.50	1.43
2	A	1201[A]	TSV	C27-C30	-5.74	1.40	1.52
2	A	1201[A]	TSV	C14-C16	5.70	1.49	1.36
2	A	1201[A]	TSV	C14-C17	5.34	1.50	1.38
2	A	1201[B]	TSV	C27-C30	-5.17	1.41	1.52
2	A	1201[A]	TSV	C34-N5	5.02	1.55	1.47
2	A	1201[B]	TSV	C31-C26	4.87	1.51	1.40
2	A	1201[B]	TSV	C14-C17	4.77	1.49	1.38
2	A	1201[B]	TSV	O7-C11	-4.56	1.14	1.23
2	A	1201[B]	TSV	C16-C24	4.38	1.52	1.41
2	A	1201[A]	TSV	C16-C24	3.93	1.51	1.41
2	A	1201[B]	TSV	C11-N2	3.68	1.42	1.34
2	A	1201[A]	TSV	O4-S1	3.59	1.47	1.43
2	A	1201[B]	TSV	C3-C5	3.53	1.53	1.49
2	A	1201[B]	TSV	C33-N5	3.51	1.42	1.34
2	A	1201[B]	TSV	C27-C15	3.48	1.60	1.53
2	A	1201[B]	TSV	O2-C20	-3.48	1.15	1.21
2	A	1201[A]	TSV	C15-N5	-3.42	1.40	1.47
2	A	1201[B]	TSV	C31-N4	3.17	1.43	1.39
2	A	1201[B]	TSV	C15-N5	-3.12	1.40	1.47
2	A	1201[A]	TSV	C11-N2	3.04	1.40	1.34
2	A	1201[A]	TSV	C20-N1	2.96	1.42	1.34
2	A	1201[A]	TSV	C33-N5	2.94	1.41	1.34
2	A	1201[B]	TSV	O1-C9	-2.87	1.43	1.48
2	A	1201[B]	TSV	C34-C30	2.81	1.57	1.52
2	A	1201[B]	TSV	O9-C4	-2.80	1.18	1.22
2	A	1201[B]	TSV	F1-C21	-2.75	1.31	1.36
2	A	1201[B]	TSV	C20-N1	2.74	1.41	1.34
2	A	1201[B]	TSV	O8-C35	2.66	1.39	1.34
2	A	1201[B]	TSV	O3-C33	-2.57	1.17	1.22
2	A	1201[A]	TSV	O1-C9	-2.52	1.43	1.48
2	A	1201[A]	TSV	C2-N2	-2.38	1.41	1.45
2	A	1201[A]	TSV	C27-C15	2.36	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201[B]	TSV	C1-C2	2.30	1.53	1.51
2	A	1201[A]	TSV	C3-C5	2.09	1.52	1.49

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201[B]	TSV	O6-S1-O4	-10.57	111.31	119.24
2	A	1201[A]	TSV	C17-C21-C26	-9.06	119.96	123.48
2	A	1201[B]	TSV	C17-C21-C26	-6.93	120.78	123.48
2	A	1201[A]	TSV	O6-S1-O4	-6.51	114.36	119.24
2	A	1201[B]	TSV	C30-C34-N5	-4.94	95.85	102.62
2	A	1201[B]	TSV	C4-C2-N2	4.82	121.25	116.06
2	A	1201[A]	TSV	C4-C2-N2	4.52	120.91	116.06
2	A	1201[B]	TSV	C27-C30-C34	4.49	107.56	103.66
2	A	1201[A]	TSV	C30-C34-N5	-4.17	96.91	102.62
2	A	1201[B]	TSV	F1-C21-C17	3.59	124.69	118.29
2	A	1201[A]	TSV	C27-C30-C34	3.55	106.74	103.66
2	A	1201[A]	TSV	C12-C24-C26	3.10	111.28	104.73
2	A	1201[B]	TSV	C12-C24-C26	3.07	111.22	104.73
2	A	1201[B]	TSV	C31-C26-C24	2.98	111.02	104.73
2	A	1201[B]	TSV	C12-C24-C16	-2.96	128.90	134.80
2	A	1201[A]	TSV	C12-C24-C16	-2.94	128.94	134.80
2	A	1201[B]	TSV	F1-C21-C26	-2.91	114.51	116.90
2	A	1201[B]	TSV	O3-C33-C28	2.52	124.21	119.66
2	A	1201[A]	TSV	F1-C21-C26	2.43	118.89	116.90
2	A	1201[A]	TSV	C31-C26-C24	2.34	109.69	104.73
2	A	1201[B]	TSV	O3-C33-N5	-2.14	117.57	121.38
2	A	1201[B]	TSV	C2-C4-N3	-2.08	112.11	115.70
2	A	1201[B]	TSV	O7-C11-C15	2.03	125.68	120.63

There are no chirality outliers.

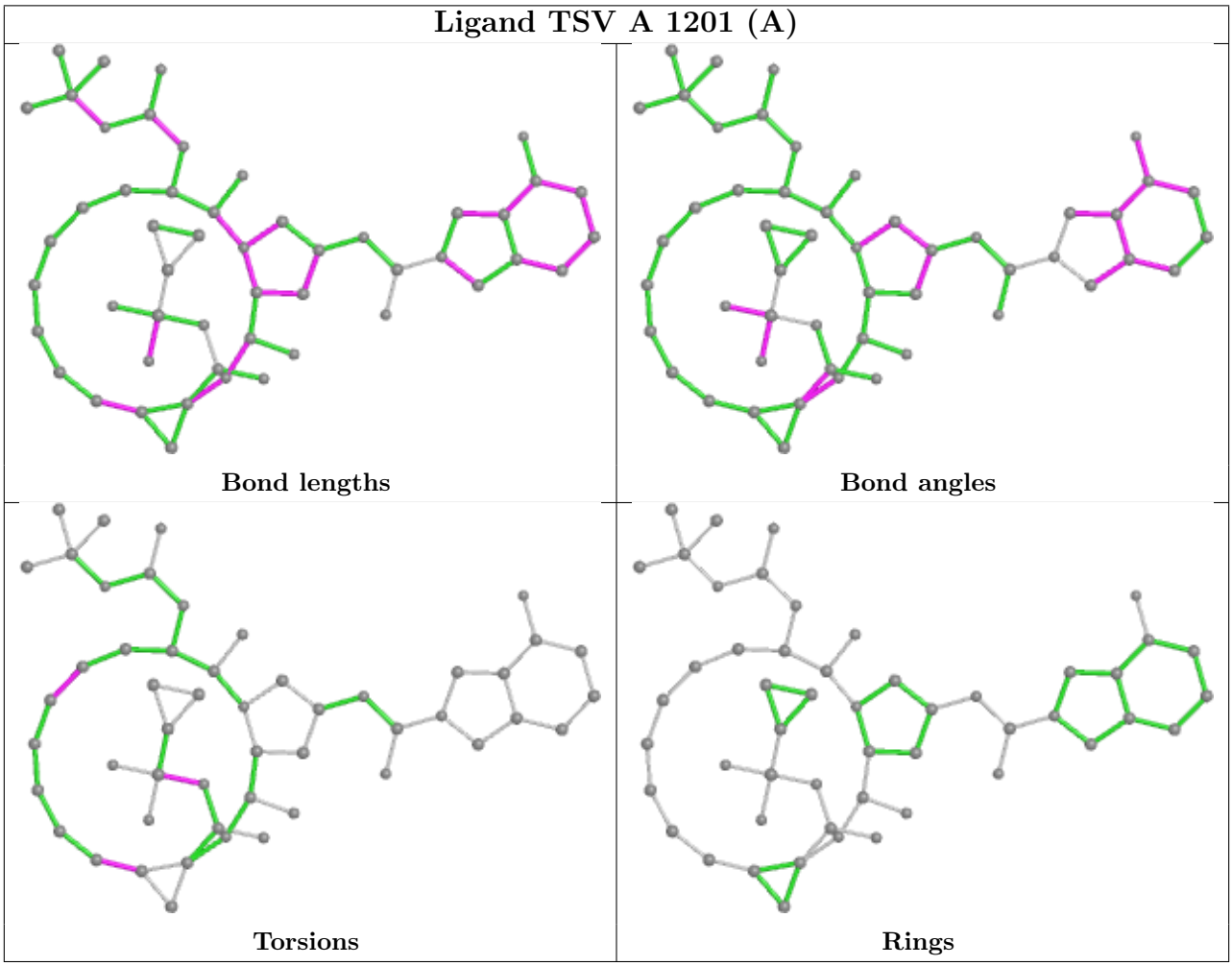
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201[A]	TSV	C4-N3-S1-C23
2	A	1201[B]	TSV	C4-N3-S1-C23
2	A	1201[A]	TSV	C18-C19-C22-C25
2	A	1201[B]	TSV	C18-C19-C22-C25
2	A	1201[A]	TSV	C2-C3-C5-C10
2	A	1201[B]	TSV	C2-C3-C5-C10

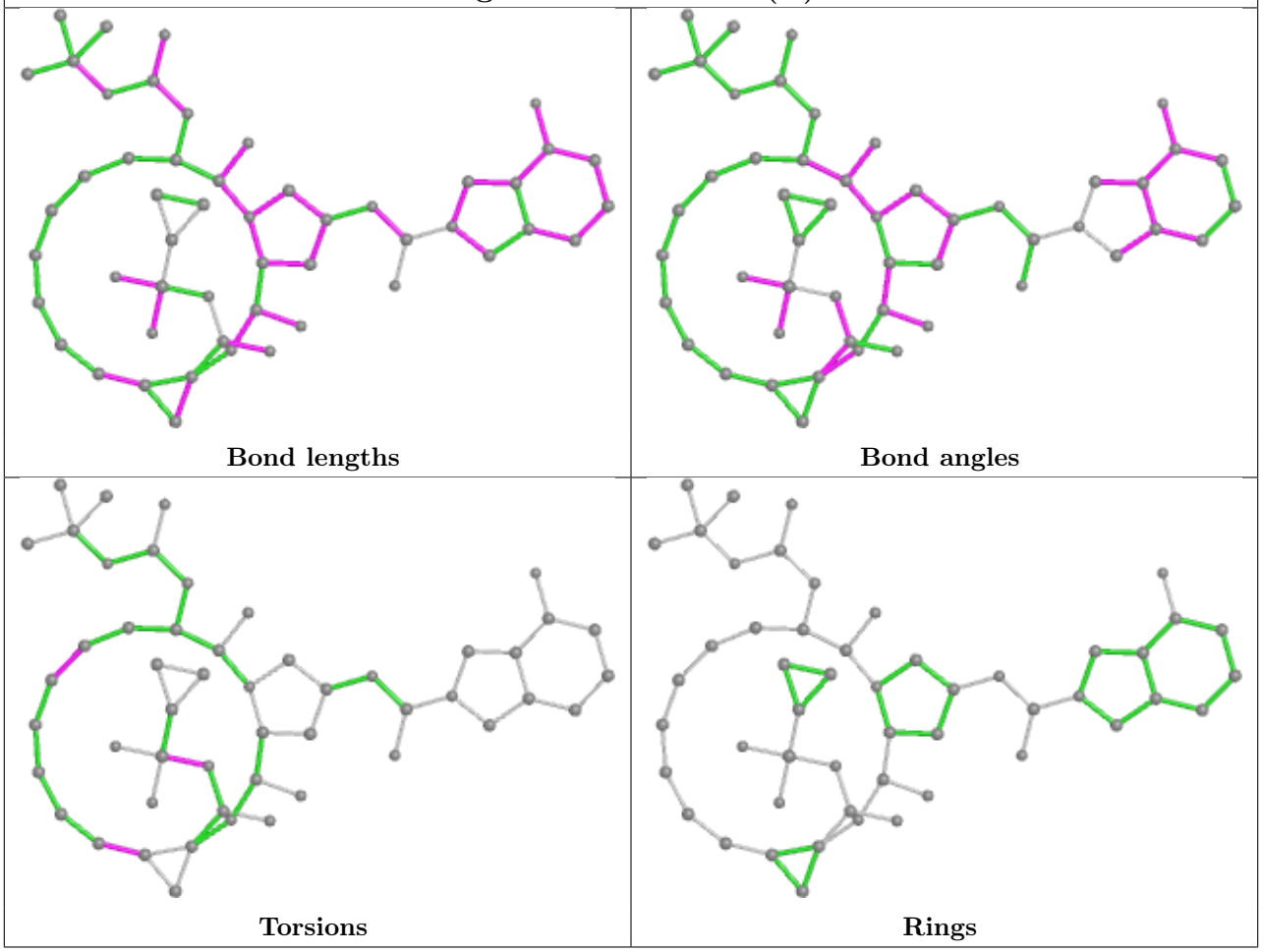
There are no ring outliers.

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 then 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 TSV A 1201 (B)



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	198/198 (100%)	0.43	19 (9%) 8 9	6, 11, 27, 35	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1161	ARG	5.0
1	A	1003	ASP	4.5
1	A	1001	SER	4.0
1	A	1160	THR	3.6
1	A	982	HIS	3.3
1	A	987	LYS	3.1
1	A	1092	ARG	2.8
1	A	1017	GLN	2.8
1	A	1004	THR	2.8
1	A	986	MET	2.8
1	A	1021	GLN	2.7
1	A	985	SER	2.5
1	A	984	ALA	2.4
1	A	988	LYS	2.4
1	A	1014	GLU	2.4
1	A	1018	GLU	2.3
1	A	1002	GLY	2.3
1	A	1026	LYS	2.2
1	A	1024	ARG	2.1

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

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)

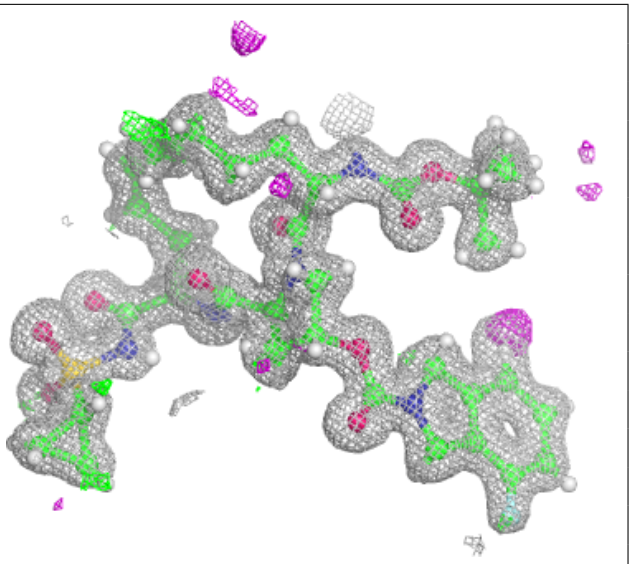
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

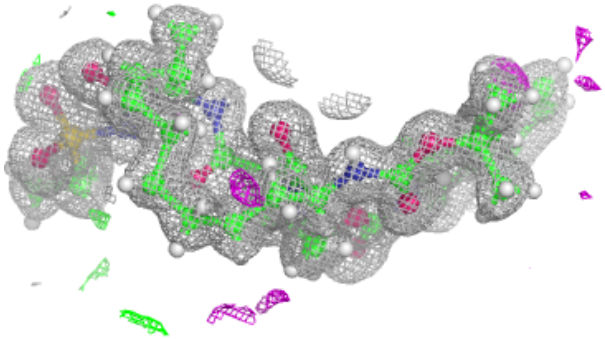
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	A	1203	6/6	0.90	0.25	27,33,39,42	0
2	TSV	A	1201[B]	51/51	0.98	0.07	6,11,16,17	95
2	TSV	A	1201[A]	51/51	0.98	0.07	5,10,18,20	0
3	ZN	A	1202	1/1	1.00	0.05	10,10,10,10	0

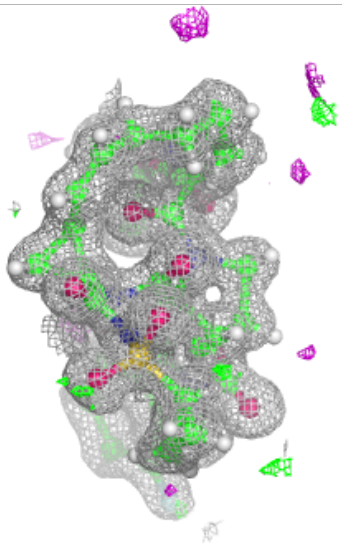
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TSV A 1201 (B):

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

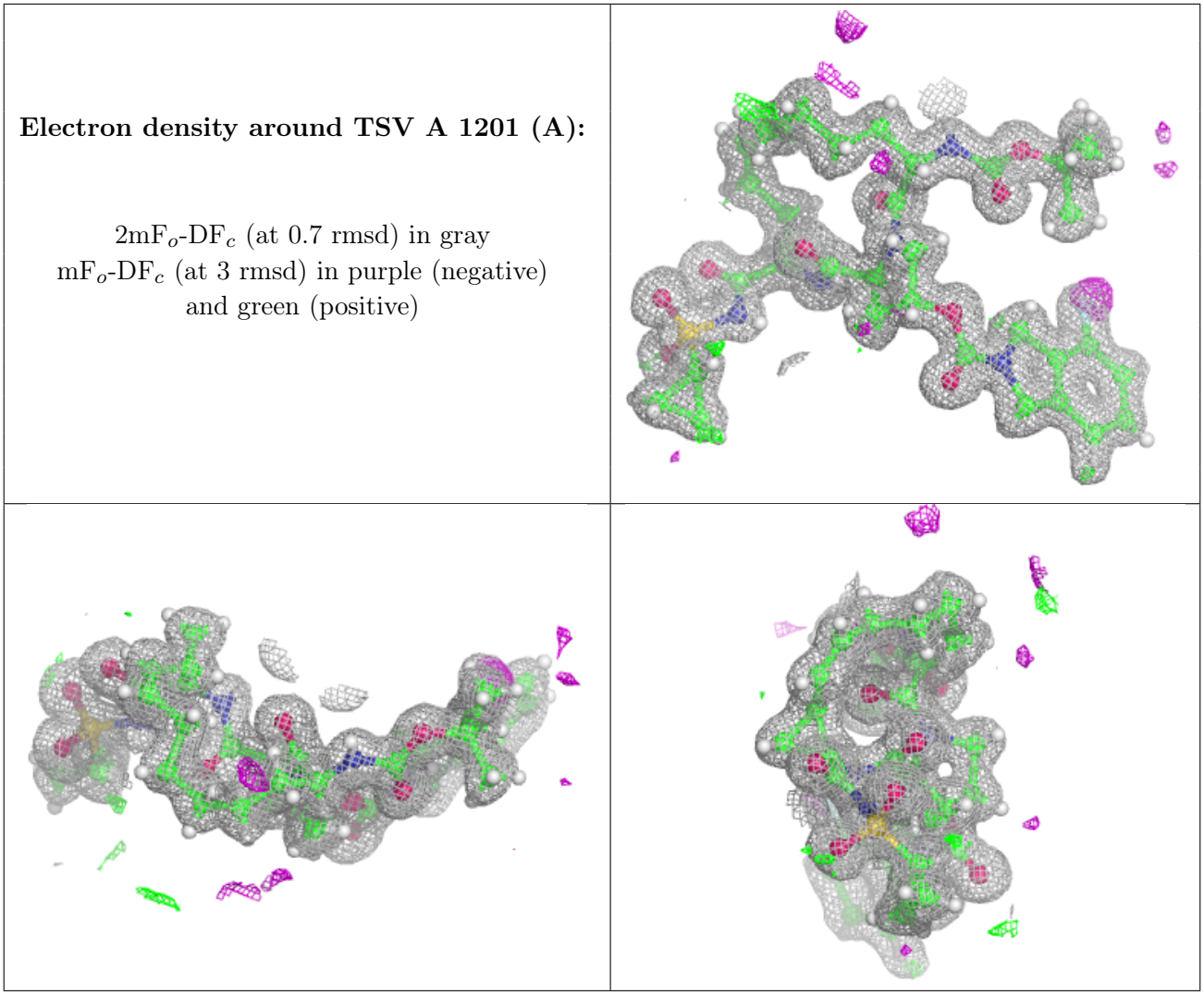






Electron density around TSV A 1201 (A):

$2mF_o$-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.