



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:54 PM UTC

PDB ID : 9KGS / pdb\_00009kgs  
Title : Discovery of an orally bioavailable reversible covalent SARS-CoV-2 Mpro inhibitor with pan-coronavirus activity  
Authors : Baburajendran, N.  
Deposited on : 2024-11-09  
Resolution : 2.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

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

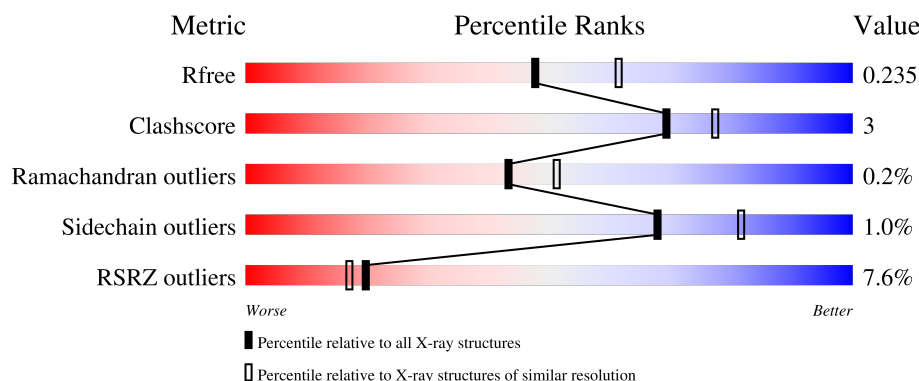
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	311	<div> <div>8%</div> <div>87%</div> <div>10%</div> <div>.</div> </div>
1	B	311	<div> <div>6%</div> <div>87%</div> <div>9%</div> <div>.</div> </div>
2	C	4	<div> <div>75%</div> <div>25%</div> </div>
2	D	4	<div> <div>100%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4941 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 3C-like proteinase nsp5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	300	Total	C	N	O	S	0	0	0
			2296	1453	390	431	22			
1	A	302	Total	C	N	O	S	0	0	0
			2320	1471	391	436	22			

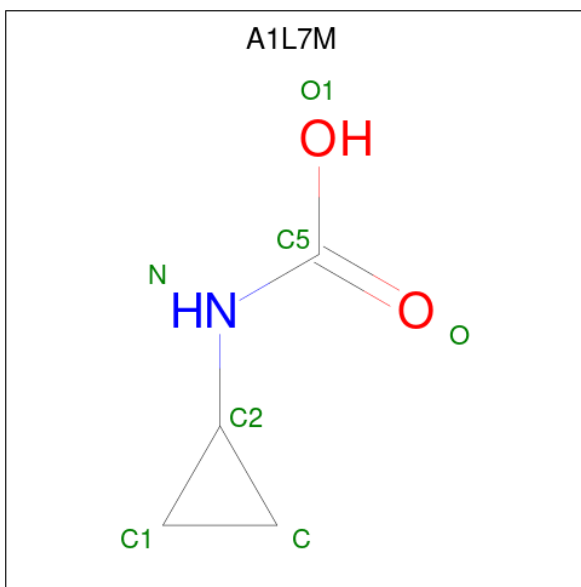
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP P0DTD1
B	-3	PRO	-	expression tag	UNP P0DTD1
B	-2	LEU	-	expression tag	UNP P0DTD1
B	-1	GLY	-	expression tag	UNP P0DTD1
B	0	SER	-	expression tag	UNP P0DTD1
A	-4	GLY	-	expression tag	UNP P0DTD1
A	-3	PRO	-	expression tag	UNP P0DTD1
A	-2	LEU	-	expression tag	UNP P0DTD1
A	-1	GLY	-	expression tag	UNP P0DTD1
A	0	SER	-	expression tag	UNP P0DTD1

- Molecule 2 is a protein called (S)-2-((R)-2-cyclopentyl-N-methyl-2-pivalamidoacetamido)-N-((S)-1-imino-3-((S)-2-oxopiperidin-3-yl)propan-2-yl)pentanamide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			35	26	4	5			
2	D	4	Total	C	N	O	0	0	0
			35	26	4	5			

- Molecule 3 is cyclopropylcarbamic acid (CCD ID: A1L7M) (formula: C<sub>4</sub>H<sub>7</sub>NO<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			6	4	1	1		
3	D	1	Total	C	N	O	0	0
			6	4	1	1		

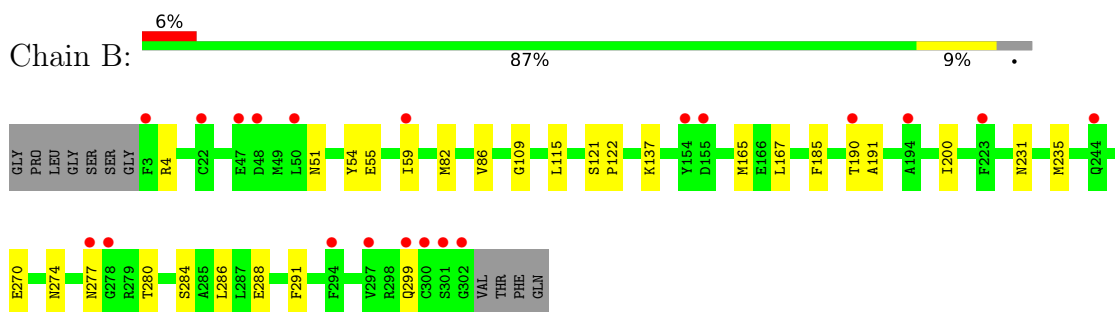
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	138	Total	O	0	0
			138	138		
4	A	102	Total	O	0	0
			102	102		
4	C	1	Total	O	0	0
			1	1		
4	D	2	Total	O	0	0
			2	2		

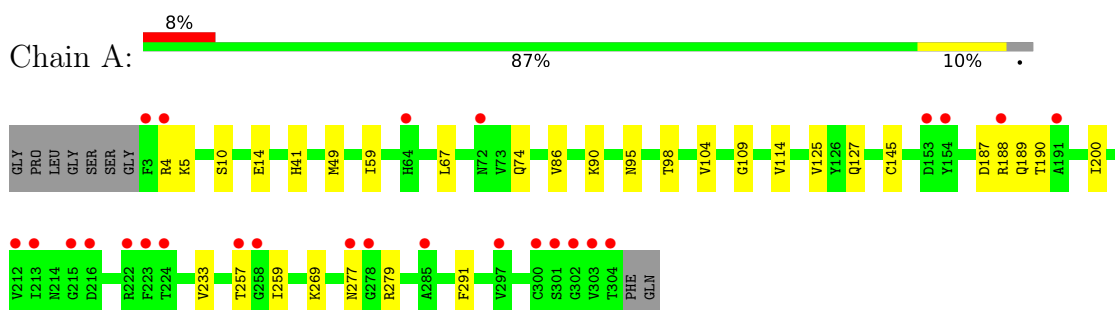
### 3 Residue-property plots

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.

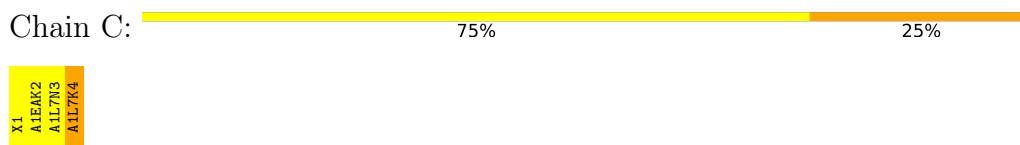
- Molecule 1: 3C-like proteinase nsp5



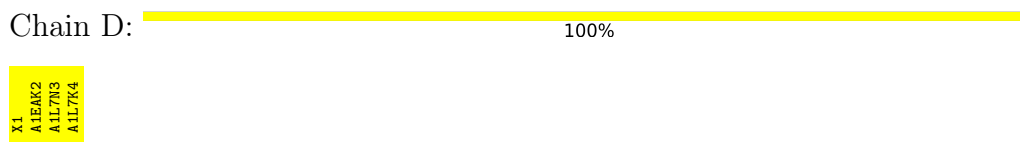
- Molecule 1: 3C-like proteinase nsp5



- Molecule 2: (S)-2-((R)-2-cyclopentyl-N-methyl-2-pivalamidoacetamido)-N-((S)-1-imino-3-((S)-2-oxopiperidin-3-yl)propan-2-yl)pentanamide



- Molecule 2: (S)-2-((R)-2-cyclopentyl-N-methyl-2-pivalamidoacetamido)-N-((S)-1-imino-3-((S)-2-oxopiperidin-3-yl)propan-2-yl)pentanamide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.61Å 99.08Å 59.40Å 90.00° 108.48° 90.00°	Depositor
Resolution (Å)	46.56 – 2.20 46.56 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.56-2.20) 99.4 (46.56-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.81 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.195 , 0.236 0.196 , 0.235	Depositor DCC
$R_{free}$ test set	2002 reflections (6.45%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.9	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 33.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4941	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1EAK, A1L7N, PIV, A1L7K, A1L7M

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	0.12	0/2372	0.35	0/3227
1	B	0.13	0/2347	0.34	0/3195
All	All	0.12	0/4719	0.34	0/6422

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

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	2320	0	2249	18	0
1	B	2296	0	2223	16	0
2	C	35	0	9	1	0
2	D	35	0	9	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
4	A	102	0	0	0	0
4	B	138	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
All	All	4941	0	4490	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 3.

All (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:B:54:TYR:HB3	1:B:82:MET:HE1	1.83	0.60
1:B:4:ARG:O	1:B:299:GLN:NE2	2.34	0.60
1:B:109:GLY:HA2	1:B:200:ILE:HD13	1.85	0.59
1:B:165:MET:HE1	1:B:185:PHE:HB3	1.88	0.56
1:A:145:CYS:SG	2:C:4:A1L7K:O	2.64	0.54
1:B:51:ASN:N	1:B:51:ASN:OD1	2.41	0.53
1:B:288:GLU:HG2	1:B:291:PHE:CD2	2.44	0.53
1:A:257:THR:HG23	1:A:259:ILE:H	1.73	0.53
1:A:187:ASP:OD1	1:A:187:ASP:N	2.42	0.51
1:B:288:GLU:HG2	1:B:291:PHE:HD2	1.75	0.50
1:A:277:ASN:OD1	1:A:279:ARG:HD2	2.12	0.50
1:A:109:GLY:HA2	1:A:200:ILE:HD13	1.93	0.48
1:B:231:ASN:O	1:B:235:MET:HG3	2.14	0.47
1:A:5:LYS:HG2	1:A:291:PHE:CZ	2.50	0.46
1:B:4:ARG:NH1	1:A:127:GLN:O	2.43	0.46
1:B:55:GLU:O	1:B:59:ILE:HG23	2.16	0.46
1:B:280:THR:OG1	1:B:284:SER:N	2.50	0.45
1:B:270:GLU:HG2	1:B:274:ASN:OD1	2.17	0.44
1:A:41:HIS:CD2	1:A:49:MET:HE1	2.52	0.44
1:A:114:VAL:O	1:A:125:VAL:HA	2.17	0.44
1:A:95:ASN:HB3	1:A:98:THR:OG1	2.18	0.43
1:B:115:LEU:HD11	1:B:122:PRO:HB3	2.01	0.43
1:A:233:VAL:HG11	1:A:269:LYS:HG3	2.01	0.43
1:A:90:LYS:HE2	1:A:90:LYS:HB2	1.86	0.43
1:A:67:LEU:HD11	1:A:74:GLN:HG2	2.01	0.42
1:B:190:THR:HG22	1:B:191:ALA:H	1.85	0.42
1:A:59:ILE:HD12	1:A:59:ILE:HA	1.87	0.42
1:B:137:LYS:O	1:A:4:ARG:NH2	2.52	0.41
1:A:188:ARG:HB2	1:A:190:THR:HG22	2.02	0.41
1:A:10:SER:O	1:A:14:GLU:HG3	2.21	0.41
1:B:167:LEU:HD11	1:B:185:PHE:CE1	2.56	0.40
1:A:49:MET:HG3	1:A:189:GLN:HB2	2.03	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	300/311 (96%)	288 (96%)	12 (4%)	0	100	100
1	B	298/311 (96%)	291 (98%)	6 (2%)	1 (0%)	36	42
All	All	598/622 (96%)	579 (97%)	18 (3%)	1 (0%)	43	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	277	ASN

### 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	255/266 (96%)	253 (99%)	2 (1%)	73	85
1	B	252/266 (95%)	249 (99%)	3 (1%)	63	78
All	All	507/532 (95%)	502 (99%)	5 (1%)	68	81

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	86	VAL
1	B	121	SER
1	B	286	LEU
1	A	86	VAL
1	A	104	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	127	GLN
1	A	72	ASN
1	A	119	ASN
1	A	180	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues 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$
2	A1EAK	D	2	2	8,9,10	3.39	4 (50%)	6,11,13	0.68	0
2	PIV	D	1	2	5,5,6	1.47	1 (20%)	7,7,9	0.65	0
2	PIV	C	1	2	5,5,6	1.50	1 (20%)	7,7,9	0.68	0
2	A1EAK	C	2	2	8,9,10	3.36	4 (50%)	6,11,13	1.16	0
2	A1L7K	D	4	2,3,1	10,12,13	5.60	8 (80%)	10,15,17	2.04	1 (10%)
2	A1L7N	C	3	2	6,7,8	0.49	0	4,7,9	1.63	1 (25%)
2	A1L7K	C	4	2,3	10,12,13	5.54	8 (80%)	10,15,17	2.74	4 (40%)
2	A1L7N	D	3	2	6,7,8	0.51	0	4,7,9	1.61	1 (25%)

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	A1EAK	D	2	2	-	2/3/13/15	0/1/1/1
2	PIV	D	1	2	-	0/3/3/6	-
2	PIV	C	1	2	-	0/3/3/6	-
2	A1EAK	C	2	2	-	2/3/13/15	0/1/1/1
2	A1L7K	D	4	2,3,1	-	1/5/17/19	0/1/1/1
2	A1L7N	C	3	2	-	2/4/7/9	-
2	A1L7K	C	4	2,3	-	0/5/17/19	0/1/1/1
2	A1L7N	D	3	2	-	2/4/7/9	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	A1L7K	CD2-NE2	14.00	1.57	1.33
2	C	4	A1L7K	CD2-NE2	13.76	1.56	1.33
2	D	2	A1EAK	C15-CB	-6.46	1.37	1.53
2	C	2	A1EAK	C15-CB	-6.29	1.38	1.53
2	C	4	A1L7K	O-C	5.74	1.41	1.20
2	D	4	A1L7K	O-C	5.61	1.41	1.20
2	C	2	A1EAK	C12-CB	5.51	1.67	1.53
2	D	2	A1EAK	C12-CB	5.42	1.67	1.53
2	D	4	A1L7K	CG-CD2	4.50	1.57	1.50
2	C	4	A1L7K	CG-CD2	4.43	1.56	1.50
2	D	4	A1L7K	CF-NE2	4.03	1.54	1.46
2	C	4	A1L7K	CF-NE2	4.03	1.54	1.46
2	D	4	A1L7K	CD1-CG	-4.00	1.42	1.53
2	C	4	A1L7K	CD1-CG	-3.93	1.43	1.53
2	D	4	A1L7K	CE1-CD1	-3.83	1.43	1.53
2	C	4	A1L7K	CE1-CD1	-3.81	1.43	1.53
2	C	4	A1L7K	CB-CG	3.61	1.61	1.53
2	D	4	A1L7K	CB-CG	3.61	1.61	1.53
2	C	2	A1EAK	C13-C12	-3.48	1.37	1.51
2	D	2	A1EAK	C13-C12	-3.42	1.37	1.51
2	C	1	PIV	CT-C	2.82	1.57	1.51
2	D	1	PIV	CT-C	2.73	1.57	1.51
2	D	2	A1EAK	C14-C15	2.25	1.61	1.51
2	C	4	A1L7K	OD2-CD2	-2.23	1.19	1.23
2	C	2	A1EAK	C14-C15	2.13	1.60	1.51
2	D	4	A1L7K	OD2-CD2	-2.08	1.19	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	A1L7K	CB-CA-C	5.74	119.82	110.99
2	D	4	A1L7K	CF-NE2-CD2	-5.04	112.14	125.79
2	C	4	A1L7K	CF-NE2-CD2	-4.60	113.33	125.79
2	C	3	A1L7N	CM-N-CA	2.68	121.71	113.70
2	D	3	A1L7N	CM-N-CA	2.64	121.61	113.70
2	C	4	A1L7K	CE1-CF-NE2	2.42	115.44	110.19
2	C	4	A1L7K	CE1-CD1-CG	2.34	115.51	111.24

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	A1EAK	C-CA-CB-C12
2	D	2	A1EAK	C-CA-CB-C12
2	D	2	A1EAK	C-CA-CB-C15
2	C	3	A1L7N	O-C-CA-CB
2	D	4	A1L7K	O-C-CA-CB
2	C	3	A1L7N	CA-CB-CG-CD
2	D	3	A1L7N	C-CA-CB-CG
2	D	3	A1L7N	CA-CB-CG-CD
2	C	2	A1EAK	C-CA-CB-C15

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	4	A1L7K	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 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	A1L7M	D	101	2	6,6,7	2.28	3 (50%)	6,7,9	1.66	2 (33%)
3	A1L7M	C	101	2	6,6,7	2.25	3 (50%)	6,7,9	2.55	2 (33%)

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	A1L7M	D	101	2	-	0/1/5/6	0/1/1/1
3	A1L7M	C	101	2	-	0/1/5/6	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	101	A1L7M	C5-N	4.53	1.48	1.33
3	C	101	A1L7M	C5-N	4.44	1.47	1.33
3	D	101	A1L7M	C-C2	2.06	1.53	1.48
3	C	101	A1L7M	C-C2	2.03	1.53	1.48
3	D	101	A1L7M	C1-C2	2.03	1.53	1.48
3	C	101	A1L7M	C1-C2	2.03	1.53	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	101	A1L7M	C-C2-N	-4.88	112.07	118.56
3	C	101	A1L7M	C1-C2-N	-3.83	113.47	118.56
3	D	101	A1L7M	C-C2-N	-3.22	114.27	118.56
3	D	101	A1L7M	C1-C2-N	-2.04	115.85	118.56

There are no chirality outliers.

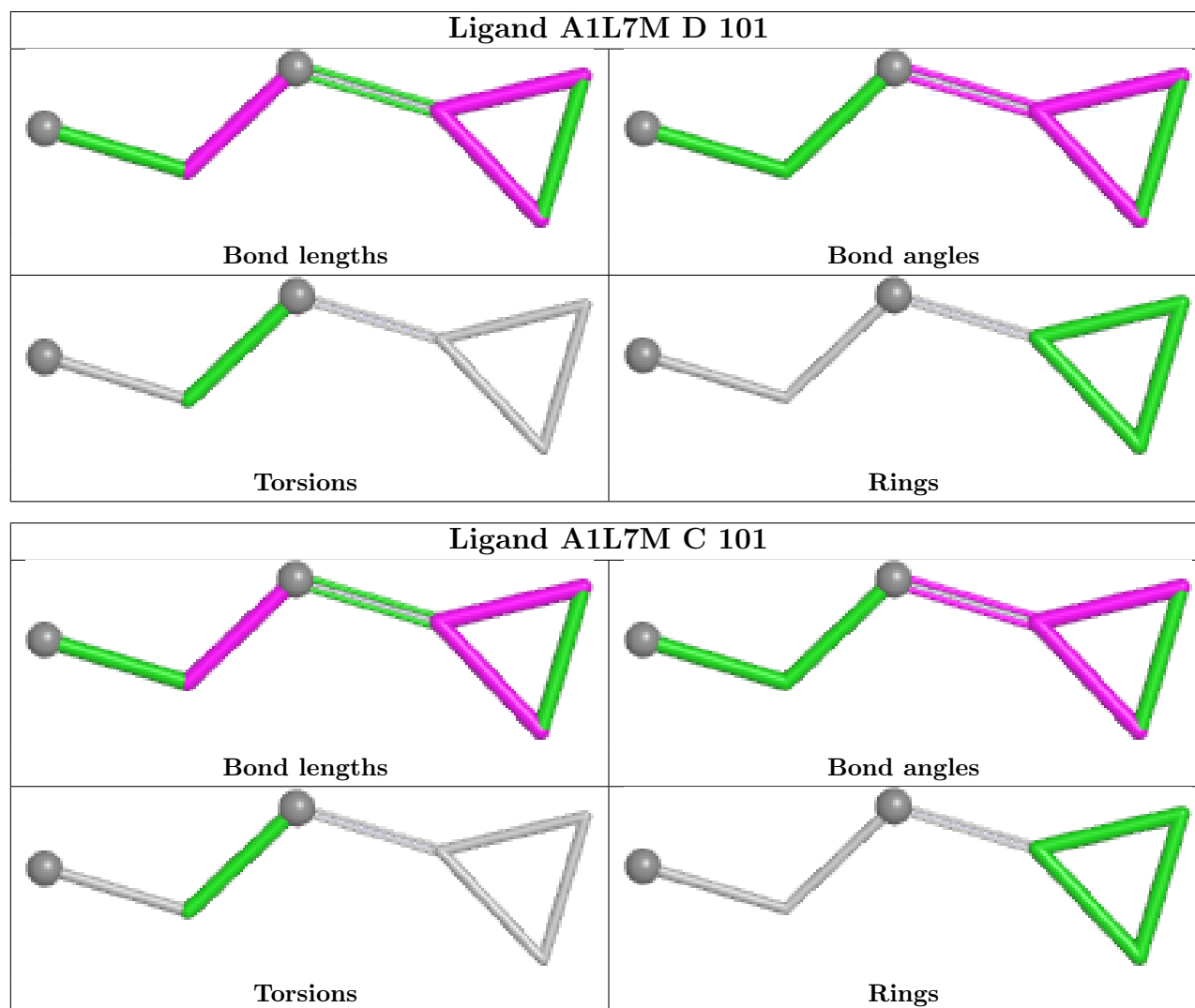
There are no torsion outliers.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	302/311 (97%)	0.39	26 (8%) 16 14	13, 27, 49, 66	0
1	B	300/311 (96%)	0.14	20 (6%) 24 21	13, 22, 47, 61	0
2	C	0/4	-	-	-	-
2	D	0/4	-	-	-	-
All	All	602/630 (95%)	0.26	46 (7%) 20 17	13, 24, 48, 66	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	PHE	6.1
1	A	301	SER	5.7
1	A	188	ARG	4.6
1	B	244	GLN	4.3
1	A	154	TYR	4.3
1	A	303	VAL	4.1
1	B	302	GLY	4.1
1	A	191	ALA	3.7
1	B	301	SER	3.5
1	A	304	THR	3.4
1	A	302	GLY	3.2
1	A	216	ASP	3.2
1	B	154	TYR	3.1
1	B	294	PHE	3.1
1	B	297	VAL	3.0
1	A	64	HIS	3.0
1	A	3	PHE	3.0
1	B	190	THR	2.9
1	B	277	ASN	2.9
1	B	155	ASP	2.8
1	A	278	GLY	2.8
1	A	277	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	300	CYS	2.7
1	A	212	VAL	2.7
1	A	213	ILE	2.6
1	A	258	GLY	2.5
1	A	72	ASN	2.4
1	A	300	CYS	2.4
1	A	222	ARG	2.3
1	B	3	PHE	2.3
1	B	47	GLU	2.3
1	A	297	VAL	2.3
1	B	48	ASP	2.3
1	B	223	PHE	2.3
1	B	194	ALA	2.3
1	B	59	ILE	2.3
1	A	257	THR	2.2
1	A	215	GLY	2.2
1	A	153	ASP	2.2
1	A	4	ARG	2.1
1	B	299	GLN	2.1
1	B	278	GLY	2.1
1	A	224	THR	2.1
1	A	285	ALA	2.1
1	B	50	LEU	2.1
1	B	22	CYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	A1L7K	C	4	12/13	0.84	0.13	19,22,27,37	0
2	A1L7N	D	3	8/9	0.86	0.15	21,25,31,38	0
2	A1EAK	C	2	9/10	0.86	0.13	23,27,33,33	0
2	PIV	D	1	6/7	0.87	0.15	33,35,37,40	0
2	A1EAK	D	2	9/10	0.89	0.10	30,32,39,40	0
2	PIV	C	1	6/7	0.90	0.10	23,23,28,28	0
2	A1L7K	D	4	12/13	0.91	0.09	19,24,27,29	0
2	A1L7N	C	3	8/9	0.92	0.11	22,25,28,28	0



## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

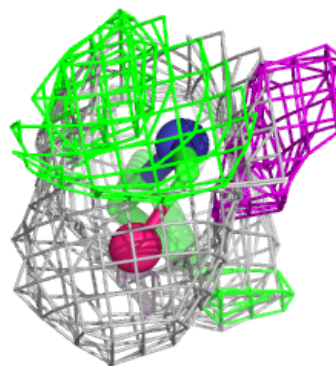
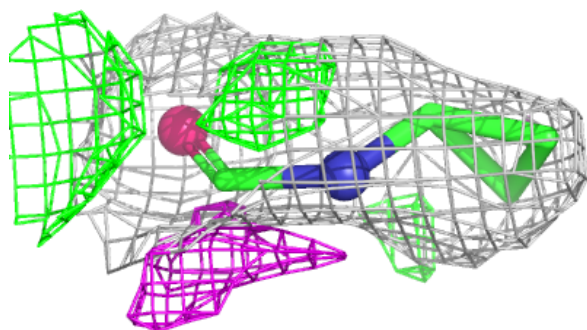
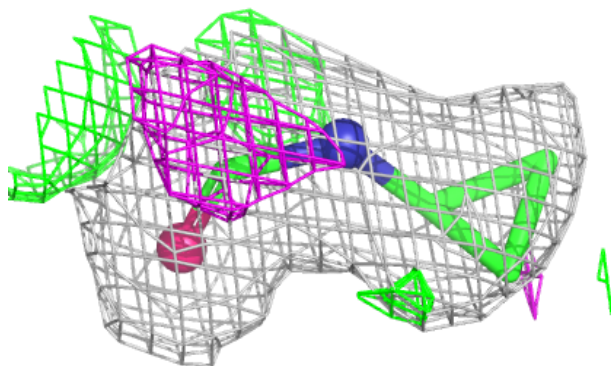
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	A1L7M	C	101	6/7	0.78	0.20	25,31,34,34	0
3	A1L7M	D	101	6/7	0.95	0.09	18,20,24,25	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.

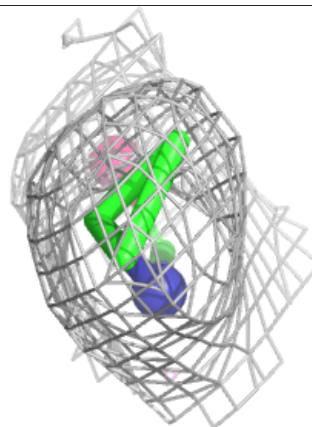
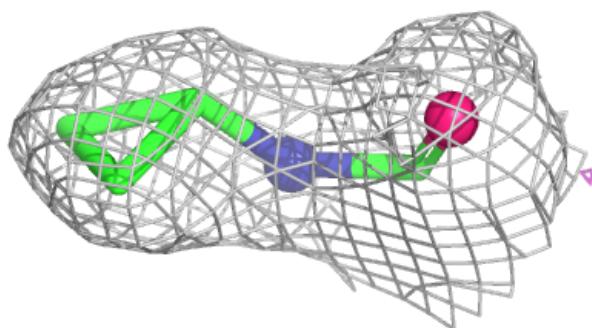
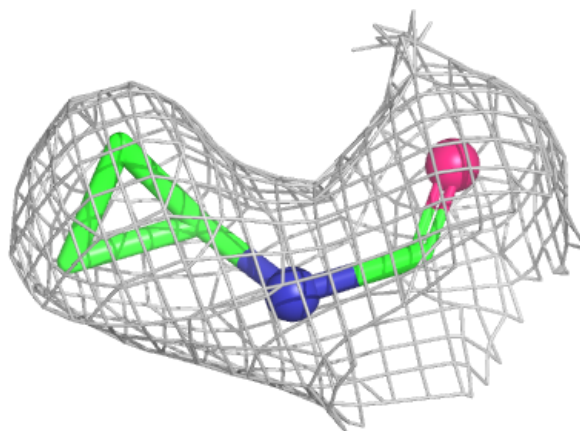
### Electron density around A1L7M C 101:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around A1L7M D 101:**

$2mF_o - DF_c$  (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.