



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2026 – 05:12 PM JST

PDB ID : 23MG / pdb\_000023mg  
Title : Crystal structure of SARS-CoV-2 main protease S144A mutant in complex with leritrelvir  
Authors : Huang, X.; Li, Q.; Yang, Z.; Zhong, N.; Xiong, X.  
Deposited on : 2026-02-11  
Resolution : 2.00 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	:	1.8.5 (274361), CSD as541be (2020)
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

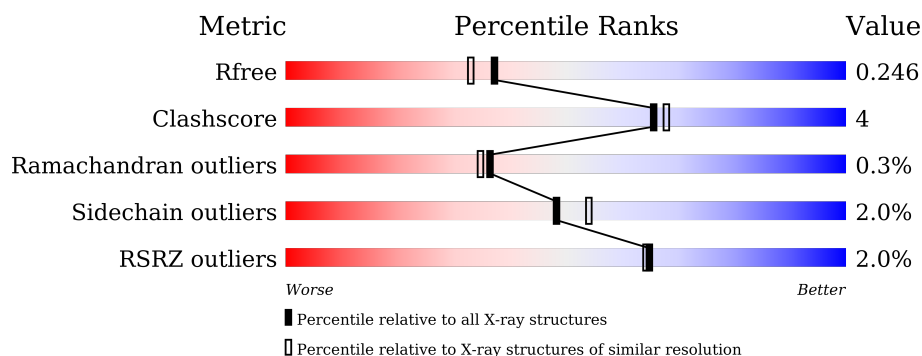
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	312	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>• •</div> </div> </div>
1	B	312	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5072 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.

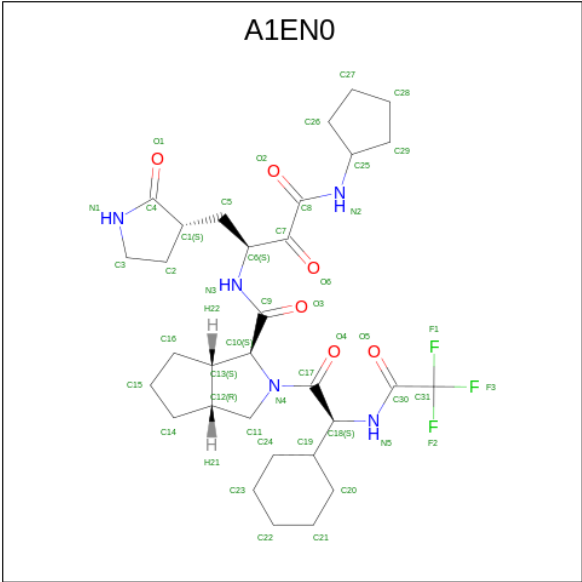
- Molecule 1 is a protein called 3C-like proteinase nsp5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2309	1461	392	435	21			
1	B	301	Total	C	N	O	S	0	1	0
			2320	1467	394	437	22			

There are 14 discrepancies between the modelled and reference sequences:

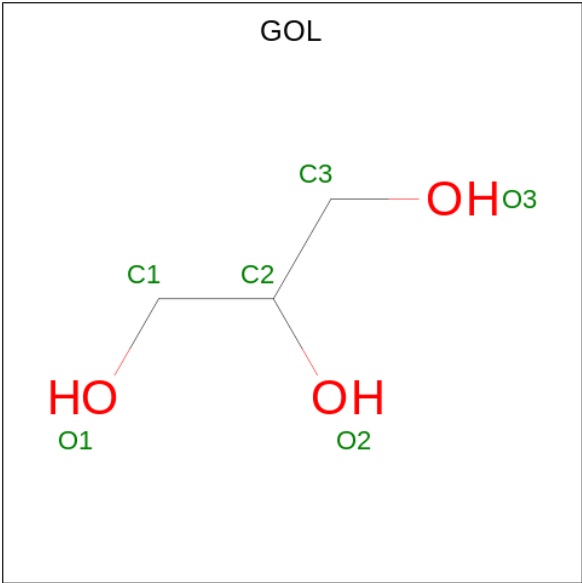
Chain	Residue	Modelled	Actual	Comment	Reference
A	144	ALA	SER	engineered mutation	UNP P0DTD1
A	307	LEU	-	expression tag	UNP P0DTD1
A	308	GLU	-	expression tag	UNP P0DTD1
A	309	VAL	-	expression tag	UNP P0DTD1
A	310	LEU	-	expression tag	UNP P0DTD1
A	311	PHE	-	expression tag	UNP P0DTD1
A	312	GLN	-	expression tag	UNP P0DTD1
B	144	ALA	SER	engineered mutation	UNP P0DTD1
B	307	LEU	-	expression tag	UNP P0DTD1
B	308	GLU	-	expression tag	UNP P0DTD1
B	309	VAL	-	expression tag	UNP P0DTD1
B	310	LEU	-	expression tag	UNP P0DTD1
B	311	PHE	-	expression tag	UNP P0DTD1
B	312	GLN	-	expression tag	UNP P0DTD1

- Molecule 2 is (3 {S},3 {a} {S},6 {a} {R})-2-[(2 {S})-2-cyclohexyl-2-[2,2,2-tris(fluoranyl)ethanoylamino]ethanoyl]- {N}-[(2 {S})-4-(cyclopentylamino)-3,4-bis(oxidanylidene)-1-[(3 {S})-2-oxidanylidene-pyrrolidin-3-yl]butan-2-yl]-3,3 {a},4,5,6,6 {a}-hexahydro-1 {H}-cyclopenta[c]pyrrole-3-carboxamide (CCD ID: A1EN0) (formula: C<sub>31</sub>H<sub>44</sub>F<sub>3</sub>N<sub>5</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			45	31	3	5	6		
2	B	1	Total	C	F	N	O	0	0
			45	31	3	5	6		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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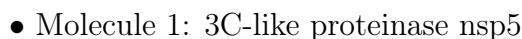
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	111	Total O 111 111	0	0
4	B	128	Total O 128 128	0	0



- Molecule 1: 3C-like proteinase nsp5



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.58Å 107.06Å 54.32Å 90.00° 102.91° 90.00°	Depositor
Resolution (Å)	53.53 – 2.00 53.53 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.5 (53.53-2.00) 91.5 (53.53-2.00)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, $R_{free}$	0.184 , 0.239 0.191 , 0.246	Depositor DCC
$R_{free}$ test set	1714 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.0	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 42.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5072	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% 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: A1EN0, GOL

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	0.61	0/2360	1.01	4/3211 (0.1%)
1	B	0.63	0/2371	1.04	4/3225 (0.1%)
All	All	0.62	0/4731	1.03	8/6436 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	216	ASP	CA-CB-CG	6.15	118.75	112.60
1	A	153	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	21	THR	CA-CB-OG1	-5.36	101.56	109.60
1	B	21	THR	CA-CB-OG1	-5.32	101.63	109.60
1	A	127	GLN	N-CA-CB	-5.24	101.87	110.41
1	B	280	THR	CA-CB-OG1	-5.21	101.78	109.60
1	A	187	ASP	CA-CB-CG	5.19	117.79	112.60
1	B	289	ASP	CA-CB-CG	5.09	117.69	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	B	217	ARG	Sidechain

## 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	2309	0	2243	13	0
1	B	2320	0	2255	22	0
2	A	45	0	0	0	0
2	B	45	0	0	0	0
3	A	48	0	64	3	0
3	B	66	0	88	5	0
4	A	111	0	0	5	0
4	B	128	0	0	6	0
All	All	5072	0	4650	36	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.

All (36) 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:154:TYR:CB	4:A:607:HOH:O	2.47	0.62
1:A:153:ASP:O	1:A:154:TYR:CB	2.48	0.60
1:B:215:GLY:HA2	4:B:566:HOH:O	2.00	0.60
1:A:237:TYR:OH	1:A:273:GLN:HA	2.03	0.58
1:A:83:GLN:HE21	3:A:406:GOL:H31	1.72	0.55
1:B:31:TRP:CD2	1:B:95:ASN:HB2	2.41	0.55
1:B:153:ASP:O	1:B:154:TYR:CB	2.55	0.54
1:B:228:ASN:HB2	3:B:402:GOL:H32	1.91	0.53
1:B:86:VAL:HG13	1:B:179:GLY:HA2	1.91	0.52
1:A:31:TRP:CD2	1:A:95:ASN:HB2	2.45	0.52
1:B:279:ARG:HH12	3:B:407:GOL:H31	1.75	0.51
1:B:188:ARG:HG3	1:B:190:THR:HG22	1.93	0.51
1:B:217:ARG:HG3	1:B:217:ARG:HH11	1.76	0.50
1:A:83:GLN:NE2	3:A:406:GOL:H31	2.27	0.50
1:B:226:THR:HG21	3:B:402:GOL:H31	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:GLN:HG2	4:B:575:HOH:O	2.13	0.49
1:B:249:ILE:HD11	4:B:628:HOH:O	2.13	0.49
1:B:5:LYS:HD3	4:B:521:HOH:O	2.12	0.48
1:B:58:LEU:HD22	1:B:82:MET:HB2	1.96	0.48
1:B:249:ILE:CG2	1:B:293:PRO:HG2	2.46	0.46
1:B:199:THR:HG21	1:B:239:TYR:CZ	2.52	0.44
1:A:31:TRP:CE2	1:A:95:ASN:HB2	2.52	0.44
1:B:238:ASN:HB2	4:B:525:HOH:O	2.17	0.44
1:A:5:LYS:HD3	4:A:508:HOH:O	2.18	0.43
1:B:31:TRP:CE2	1:B:95:ASN:HB2	2.53	0.43
1:A:60:ARG:NH2	4:A:510:HOH:O	2.51	0.42
1:B:33:ASP:OD1	3:B:408:GOL:H31	2.20	0.42
1:B:277[B]:ASN:O	1:B:277[B]:ASN:OD1	2.37	0.42
1:A:199:THR:HG21	1:A:239:TYR:CZ	2.55	0.41
3:A:404:GOL:H11	4:A:501:HOH:O	2.21	0.41
1:B:113:SER:O	1:B:149:GLY:HA2	2.21	0.40
1:B:217:ARG:CZ	4:B:531:HOH:O	2.69	0.40
1:B:287:LEU:HG	3:B:406:GOL:H31	2.03	0.40
1:A:226:THR:HG23	1:A:229:ASP:H	1.87	0.40
1:A:64:HIS:HB2	4:A:584:HOH:O	2.21	0.40
1:A:113:SER:O	1:A:149:GLY:HA2	2.21	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	299/312 (96%)	292 (98%)	6 (2%)	1 (0%)	36	35
1	B	300/312 (96%)	291 (97%)	8 (3%)	1 (0%)	36	35
All	All	599/624 (96%)	583 (97%)	14 (2%)	2 (0%)	36	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	TYR
1	B	154	TYR

### 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	254/268 (95%)	249 (98%)	5 (2%)	48	54
1	B	256/268 (96%)	251 (98%)	5 (2%)	48	54
All	All	510/536 (95%)	500 (98%)	10 (2%)	48	54

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ILE
1	A	226	THR
1	A	228	ASN
1	A	249	ILE
1	A	298	ARG
1	B	59	ILE
1	B	123	SER
1	B	228	ASN
1	B	235	MET
1	B	249	ILE

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 [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

21 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	GOL	B	411	-	5,5,5	0.12	0	5,5,5	0.46	0
3	GOL	A	409	-	5,5,5	0.14	0	5,5,5	0.29	0
2	A1EN0	B	401	-	48,49,49	0.64	1 (2%)	58,71,71	0.80	2 (3%)
3	GOL	B	412	-	5,5,5	0.10	0	5,5,5	0.21	0
3	GOL	B	408	-	5,5,5	0.08	0	5,5,5	0.25	0
2	A1EN0	A	401	-	48,49,49	0.58	1 (2%)	58,71,71	0.84	3 (5%)
3	GOL	B	405	-	5,5,5	0.12	0	5,5,5	0.36	0
3	GOL	B	407	-	5,5,5	0.20	0	5,5,5	0.47	0
3	GOL	B	403	-	5,5,5	0.12	0	5,5,5	0.27	0
3	GOL	B	406	-	5,5,5	0.20	0	5,5,5	0.41	0
3	GOL	B	404	-	5,5,5	0.09	0	5,5,5	0.40	0
3	GOL	A	407	-	5,5,5	0.22	0	5,5,5	0.53	0
3	GOL	A	403	-	5,5,5	0.15	0	5,5,5	0.31	0
3	GOL	B	410	-	5,5,5	0.10	0	5,5,5	0.24	0
3	GOL	A	405	-	5,5,5	0.17	0	5,5,5	0.36	0
3	GOL	A	408	-	5,5,5	0.15	0	5,5,5	0.28	0
3	GOL	B	409	-	5,5,5	0.11	0	5,5,5	0.35	0
3	GOL	A	404	-	5,5,5	0.11	0	5,5,5	0.55	0
3	GOL	B	402	-	5,5,5	0.23	0	5,5,5	0.35	0
3	GOL	A	402	-	5,5,5	0.22	0	5,5,5	0.58	0
3	GOL	A	406	-	5,5,5	0.09	0	5,5,5	0.37	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
3	GOL	B	411	-	-	4/4/4/4	-
3	GOL	A	409	-	-	2/4/4/4	-
2	A1EN0	B	401	-	-	6/46/93/93	0/5/5/5
3	GOL	B	412	-	-	2/4/4/4	-
3	GOL	B	408	-	-	2/4/4/4	-
2	A1EN0	A	401	-	-	5/46/93/93	0/5/5/5
3	GOL	B	405	-	-	2/4/4/4	-
3	GOL	B	407	-	-	2/4/4/4	-
3	GOL	B	403	-	-	2/4/4/4	-
3	GOL	B	406	-	-	2/4/4/4	-
3	GOL	B	404	-	-	2/4/4/4	-
3	GOL	A	407	-	-	2/4/4/4	-
3	GOL	A	403	-	-	2/4/4/4	-
3	GOL	B	410	-	-	3/4/4/4	-
3	GOL	A	405	-	-	2/4/4/4	-
3	GOL	A	408	-	-	4/4/4/4	-
3	GOL	B	409	-	-	2/4/4/4	-
3	GOL	A	404	-	-	1/4/4/4	-
3	GOL	B	402	-	-	3/4/4/4	-
3	GOL	A	402	-	-	2/4/4/4	-
3	GOL	A	406	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	A1EN0	O6-C7	3.19	1.28	1.22
2	B	401	A1EN0	O6-C7	2.13	1.26	1.22

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	A1EN0	C24-C19-C20	2.64	114.09	109.44
2	A	401	A1EN0	C7-C6-N3	-2.35	106.49	109.85
2	A	401	A1EN0	C5-C1-C4	2.22	117.77	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	A1EN0	C18-N5-C30	2.12	126.07	121.30
2	B	401	A1EN0	O2-C8-N2	-2.09	119.41	123.08

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	A1EN0	C7-C8-N2-C25
2	A	401	A1EN0	O2-C8-N2-C25
2	A	401	A1EN0	C5-C6-C7-O6
2	A	401	A1EN0	C6-C7-C8-N2
2	B	401	A1EN0	C7-C8-N2-C25
2	B	401	A1EN0	O2-C8-N2-C25
2	B	401	A1EN0	C5-C6-C7-O6
2	B	401	A1EN0	C6-C7-C8-N2
3	A	403	GOL	C1-C2-C3-O3
3	A	405	GOL	O1-C1-C2-C3
3	A	407	GOL	O1-C1-C2-C3
3	A	408	GOL	O1-C1-C2-C3
3	A	408	GOL	O2-C2-C3-O3
3	B	402	GOL	O2-C2-C3-O3
3	B	404	GOL	C1-C2-C3-O3
3	B	404	GOL	O2-C2-C3-O3
3	B	408	GOL	O1-C1-C2-O2
3	B	409	GOL	O1-C1-C2-O2
3	B	411	GOL	C1-C2-C3-O3
3	B	412	GOL	O1-C1-C2-C3
3	B	407	GOL	O1-C1-C2-O2
3	B	411	GOL	O2-C2-C3-O3
3	A	402	GOL	O1-C1-C2-C3
3	A	408	GOL	C1-C2-C3-O3
3	A	409	GOL	O1-C1-C2-C3
3	B	402	GOL	C1-C2-C3-O3
3	B	403	GOL	C1-C2-C3-O3
3	B	405	GOL	C1-C2-C3-O3
3	B	407	GOL	O1-C1-C2-C3
3	B	408	GOL	O1-C1-C2-C3
3	B	409	GOL	O1-C1-C2-C3
3	B	410	GOL	O1-C1-C2-C3
3	B	410	GOL	C1-C2-C3-O3
3	B	411	GOL	O1-C1-C2-C3
3	A	403	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	405	GOL	O1-C1-C2-O2
3	A	407	GOL	O1-C1-C2-O2
3	B	405	GOL	O2-C2-C3-O3
3	B	410	GOL	O1-C1-C2-O2
3	B	412	GOL	O1-C1-C2-O2
3	B	403	GOL	O2-C2-C3-O3
2	B	401	A1EN0	C29-C25-N2-C8
3	A	402	GOL	O1-C1-C2-O2
3	B	406	GOL	O1-C1-C2-O2
3	B	411	GOL	O1-C1-C2-O2
2	B	401	A1EN0	C5-C6-C7-C8
3	B	402	GOL	O1-C1-C2-C3
3	A	409	GOL	O1-C1-C2-O2
3	B	406	GOL	O1-C1-C2-C3
3	A	408	GOL	O1-C1-C2-O2
2	A	401	A1EN0	C29-C25-N2-C8
3	A	404	GOL	O2-C2-C3-O3

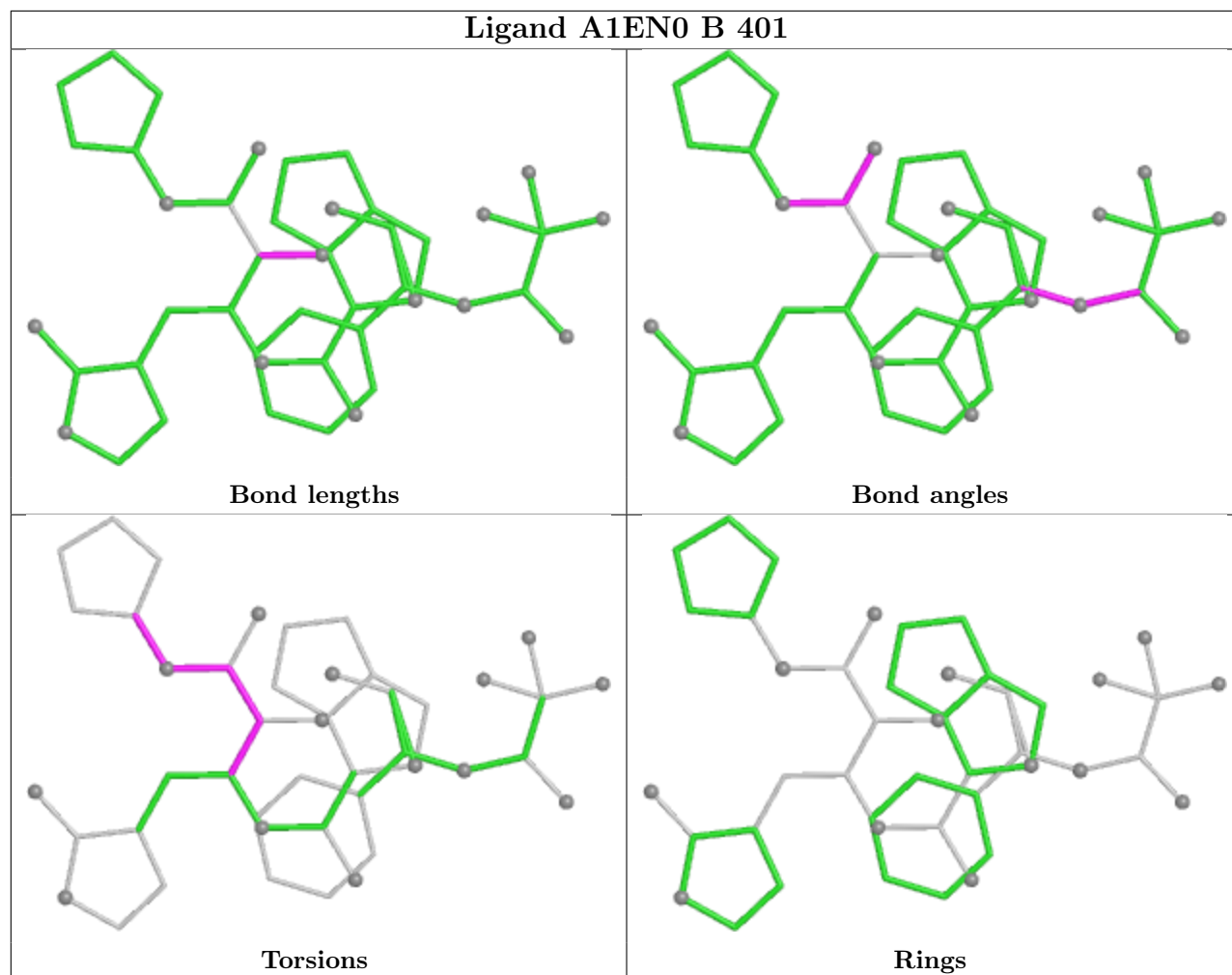
There are no ring outliers.

6 monomers are involved in 8 short contacts:

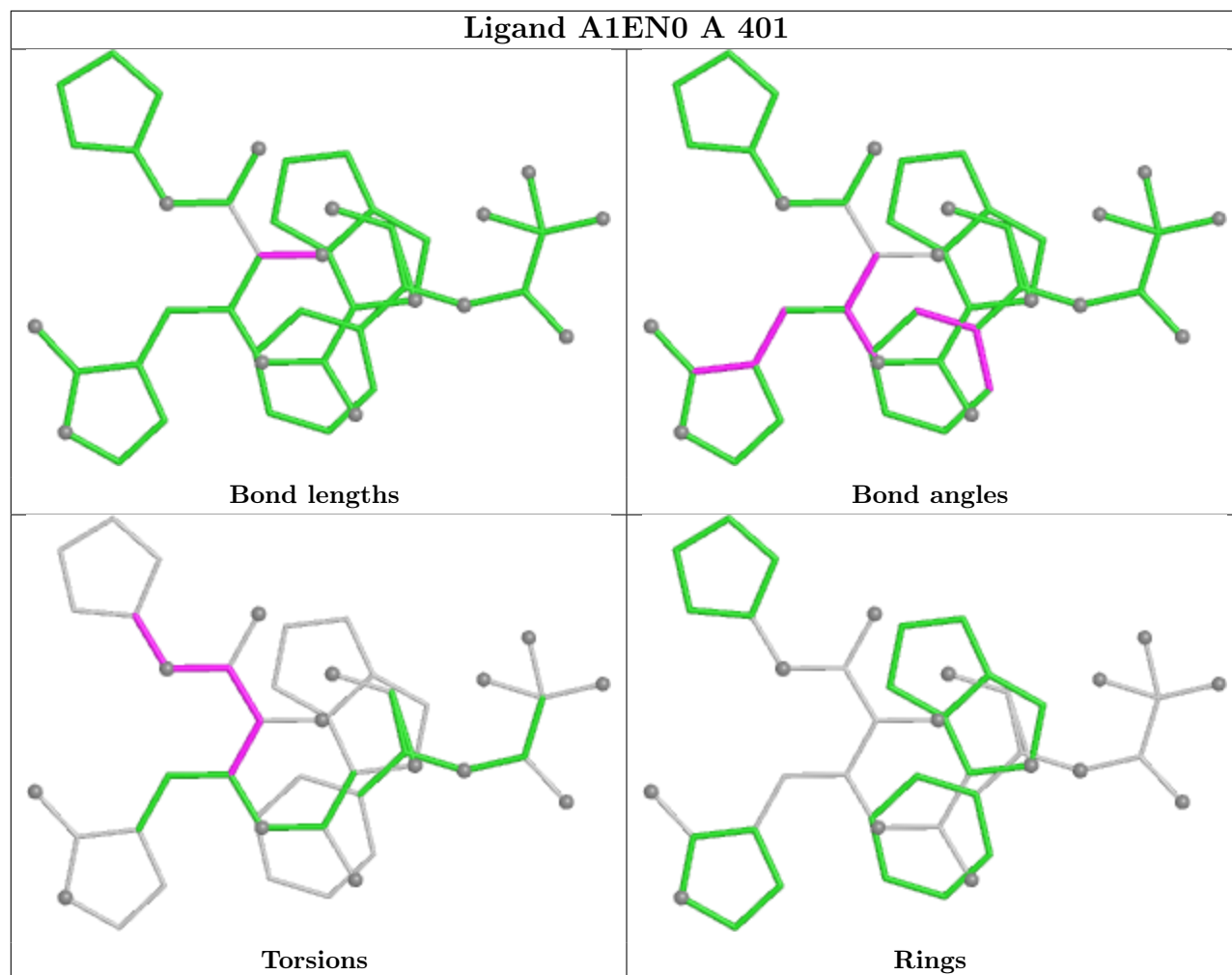
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	408	GOL	1	0
3	B	407	GOL	1	0
3	B	406	GOL	1	0
3	A	404	GOL	1	0
3	B	402	GOL	2	0
3	A	406	GOL	2	0

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 A1EN0 B 401







## 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, 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	301/312 (96%)	0.11	10 (3%) 49 48	18, 30, 63, 106	0
1	B	301/312 (96%)	-0.12	2 (0%) 84 84	15, 27, 51, 74	3 (0%)
All	All	602/624 (96%)	-0.01	12 (1%) 65 64	15, 29, 57, 106	3 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	PHE	3.9
1	A	274	ASN	3.1
1	A	277	ASN	2.5
1	A	232	LEU	2.5
1	B	154	TYR	2.4
1	A	237	TYR	2.3
1	A	273	GLN	2.2
1	B	50	LEU	2.2
1	A	275	GLY	2.1
1	A	224	THR	2.1
1	A	233	VAL	2.1
1	A	234	ALA	2.1

### 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 oligosaccharides in this entry.

## 6.4 Ligands

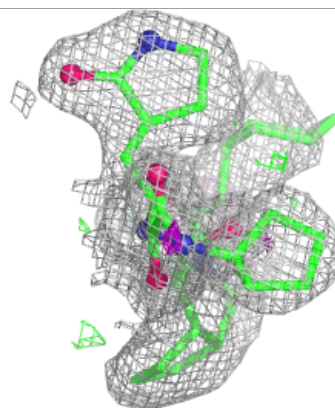
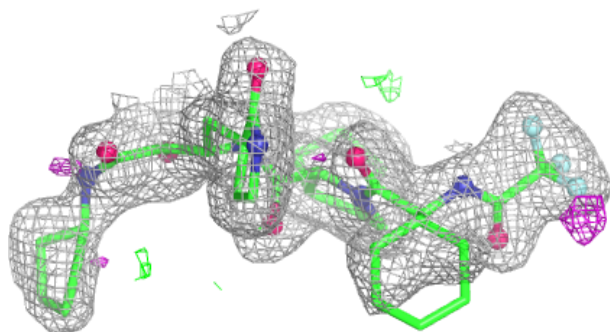
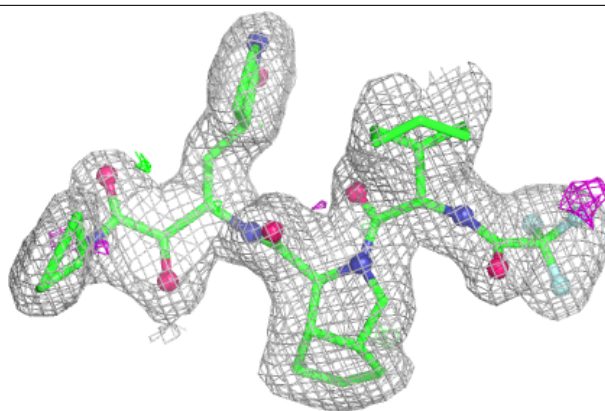
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	GOL	B	412	6/6	0.66	0.15	50,63,66,74	0
3	GOL	B	407	6/6	0.72	0.20	40,57,62,73	0
3	GOL	B	403	6/6	0.77	0.20	67,68,73,74	0
3	GOL	A	407	6/6	0.78	0.14	40,49,52,58	0
3	GOL	B	406	6/6	0.79	0.14	44,48,49,53	0
3	GOL	A	402	6/6	0.79	0.15	42,48,53,53	0
3	GOL	A	403	6/6	0.79	0.12	40,45,54,55	0
3	GOL	A	406	6/6	0.80	0.11	50,56,59,61	0
3	GOL	B	411	6/6	0.80	0.16	53,60,64,67	0
3	GOL	A	409	6/6	0.80	0.14	58,60,61,64	0
3	GOL	B	410	6/6	0.81	0.13	58,60,64,66	0
3	GOL	B	405	6/6	0.81	0.15	61,65,66,71	0
3	GOL	B	409	6/6	0.81	0.15	44,50,52,64	0
3	GOL	B	404	6/6	0.84	0.14	53,63,67,71	0
3	GOL	B	408	6/6	0.84	0.12	40,46,49,55	0
3	GOL	A	405	6/6	0.85	0.11	37,48,52,58	0
3	GOL	B	402	6/6	0.85	0.13	38,45,54,59	0
3	GOL	A	408	6/6	0.86	0.11	54,62,65,71	0
3	GOL	A	404	6/6	0.87	0.14	38,42,43,47	0
2	A1EN0	B	401	45/45	0.92	0.09	27,30,50,62	0
2	A1EN0	A	401	45/45	0.92	0.09	25,32,54,63	0

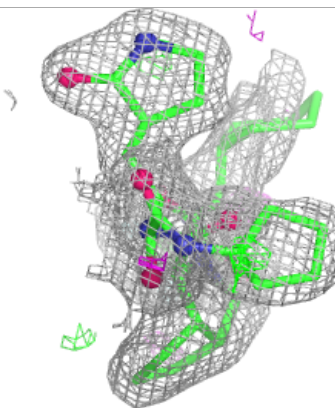
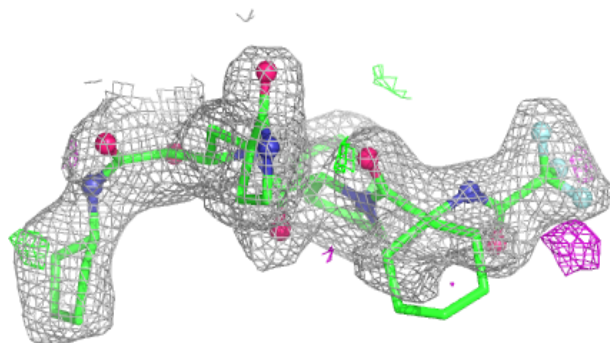
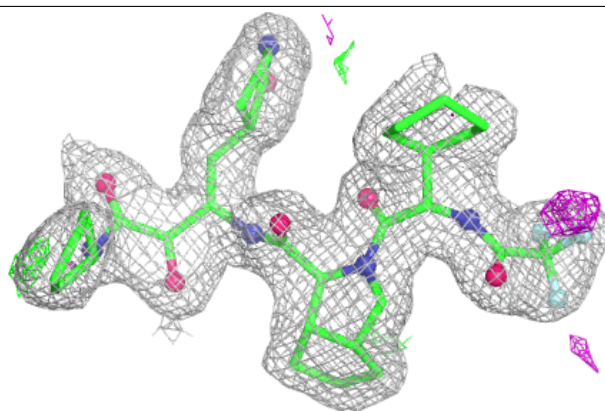
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around A1EN0 B 401:**

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

**Electron density around A1EN0 A 401:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.