



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2026 – 05:45 PM JST

PDB ID : 23LZ / pdb\_000023lz  
Title : Crystal structure of SARS-CoV-2 main protease G143S mutant in complex with leritrelvir  
Authors : Huang, X.; Li, Q.; Yang, Z.; Zhong, N.; Xiong, X.  
Deposited on : 2026-02-11  
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](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

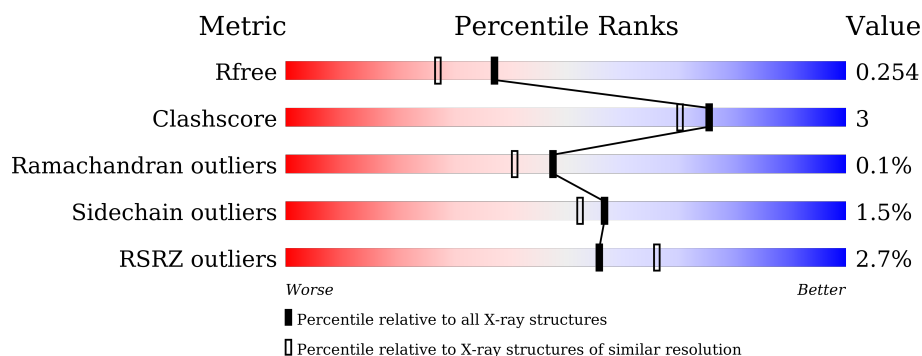
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	306	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
1	B	306	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>10%</div> </div> </div>
1	C	306	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
1	D	306	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	405	-	-	X	-
2	GOL	B	405	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10063 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	306	Total	C	N	O	S	0	0	0
			2369	1500	402	445	22			
1	B	306	Total	C	N	O	S	0	1	0
			2372	1502	402	445	23			
1	C	306	Total	C	N	O	S	0	2	0
			2375	1504	402	446	23			
1	D	306	Total	C	N	O	S	0	1	0
			2372	1502	402	445	23			

There are 4 discrepancies between the modelled and reference sequences:

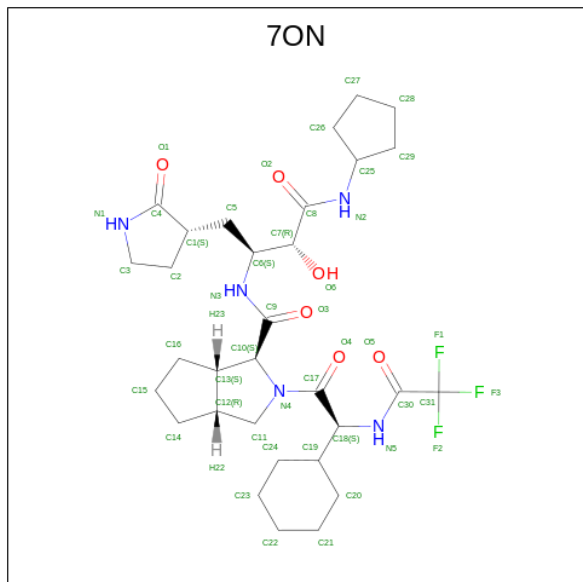
Chain	Residue	Modelled	Actual	Comment	Reference
A	143	SER	GLY	engineered mutation	UNP P0DTD1
B	143	SER	GLY	engineered mutation	UNP P0DTD1
C	143	SER	GLY	engineered mutation	UNP P0DTD1
D	143	SER	GLY	engineered mutation	UNP P0DTD1

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 3 is Leritrelvir bound form (CCD ID: 7ON) (formula:  $C_{31}H_{46}F_3N_5O_6$ ) (labeled as "Ligand of Interest" by depositor).



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

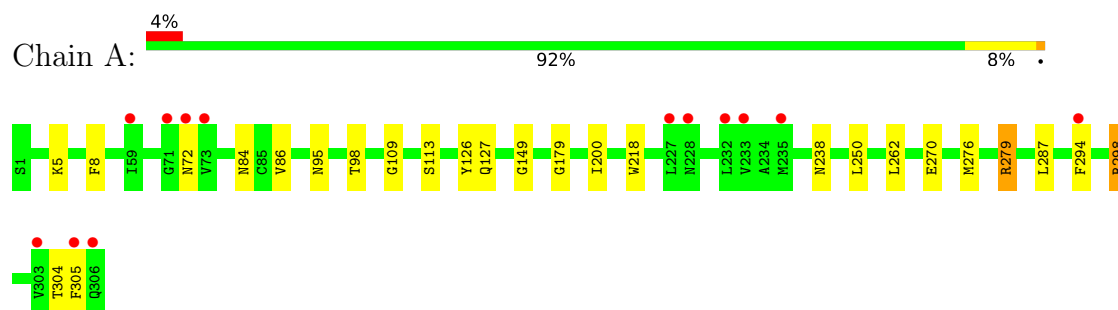
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	86	Total	O	0	0
			86	86		
4	B	57	Total	O	0	0
			57	57		
4	C	79	Total	O	0	0
			79	79		
4	D	89	Total	O	0	0
			89	89		

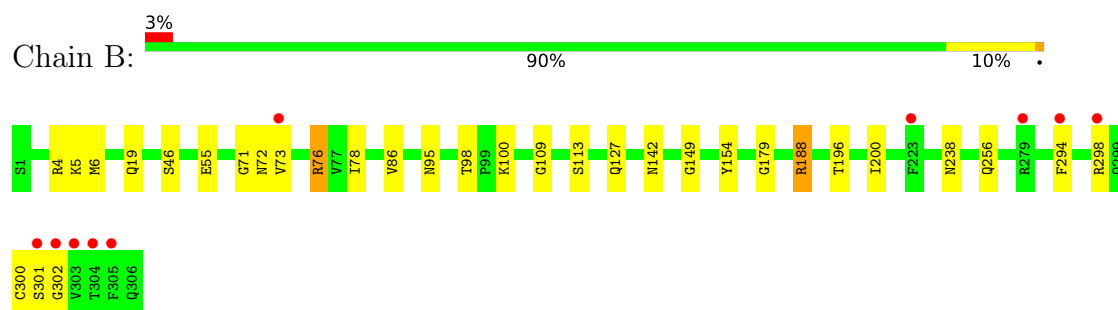
### 3 Residue-property plots [i](#)

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.

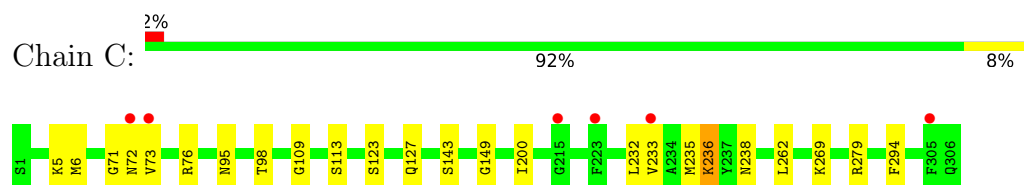
- Molecule 1: 3C-like proteinase nsp5



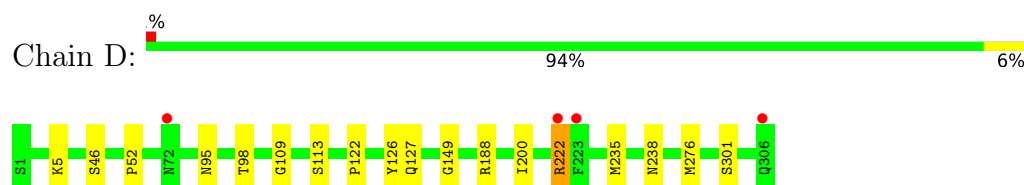
- Molecule 1: 3C-like proteinase nsp5



- Molecule 1: 3C-like proteinase nsp5



- Molecule 1: 3C-like proteinase nsp5



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.39Å 207.65Å 104.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.60 – 1.97 73.60 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.8 (73.60-1.97) 99.8 (73.60-1.97)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, $R_{free}$	0.205 , 0.247 0.204 , 0.254	Depositor DCC
$R_{free}$ test set	5227 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.3	Xtriage
Anisotropy	2.363	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10063	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.18% 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: GOL, 7ON

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	0/2422	1.00	2/3292 (0.1%)
1	B	0.62	0/2428	1.03	6/3300 (0.2%)
1	C	0.61	0/2434	1.00	2/3308 (0.1%)
1	D	0.61	0/2428	0.99	1/3300 (0.0%)
All	All	0.61	0/9712	1.01	11/13200 (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
1	C	0	2
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	ARG	CG-CD-NE	-7.87	94.69	112.00
1	D	127	GLN	N-CA-CB	-6.67	99.51	110.52
1	B	300	CYS	CB-CA-C	-6.27	99.79	110.88
1	C	127	GLN	N-CA-CB	-5.93	100.73	110.52
1	A	127	GLN	N-CA-CB	-5.72	101.07	110.52
1	B	127	GLN	N-CA-CB	-5.62	101.25	110.52
1	C	294	PHE	CA-CB-CG	5.53	119.33	113.80
1	A	298	ARG	CA-CB-CG	5.33	124.76	114.10
1	B	19	GLN	N-CA-CB	-5.31	101.78	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	294	PHE	CA-CB-CG	5.20	119.00	113.80
1	B	196	THR	CA-CB-OG1	-5.14	101.89	109.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	188	ARG	Sidechain
1	C	279	ARG	Sidechain
1	C	76	ARG	Sidechain
1	D	222	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	2369	0	2315	17	1
1	B	2372	0	2320	20	0
1	C	2375	0	2325	16	0
1	D	2372	0	2320	10	0
2	A	30	0	40	4	0
2	B	30	0	40	12	0
2	C	18	0	24	1	0
2	D	6	0	8	1	0
3	A	45	0	0	0	0
3	B	45	0	0	0	0
3	C	45	0	0	1	0
3	D	45	0	0	0	0
4	A	86	0	0	2	0
4	B	57	0	0	0	0
4	C	79	0	0	2	0
4	D	89	0	0	1	0
All	All	10063	0	9392	57	1

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 (57) 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:D:301:SER:O	4:D:501:HOH:O	1.81	0.98
2:B:405:GOL:H32	1:D:5:LYS:HD2	1.60	0.83
1:B:154:TYR:O	2:B:404:GOL:H11	1.90	0.71
1:A:84:ASN:OD1	2:A:405:GOL:H32	1.92	0.70
1:B:142:ASN:O	2:B:403:GOL:O1	2.08	0.69
1:B:4:ARG:HA	2:B:405:GOL:O1	1.93	0.67
1:B:298:ARG:HD3	2:B:406:GOL:C3	2.25	0.66
1:B:72:ASN:HB2	1:C:72:ASN:HA	1.80	0.63
1:D:46:SER:HB3	2:D:401:GOL:H32	1.79	0.63
1:A:84:ASN:HB3	2:A:405:GOL:H31	1.81	0.62
1:B:298:ARG:HD3	2:B:406:GOL:H31	1.81	0.62
1:B:72:ASN:HB3	1:C:71:GLY:O	2.02	0.60
1:B:72:ASN:CB	1:C:72:ASN:HA	2.33	0.58
1:B:6:MET:HE2	1:D:126:TYR:CE2	2.38	0.58
1:C:262:LEU:HG	4:C:553:HOH:O	2.04	0.57
1:B:154:TYR:O	2:B:404:GOL:C1	2.54	0.54
1:A:218:TRP:CE3	1:A:279:ARG:CZ	2.92	0.53
1:C:143:SER:HA	3:C:403:7ON:C26	2.39	0.52
2:B:404:GOL:H32	1:D:122:PRO:O	2.10	0.52
1:A:250:LEU:HA	4:A:536:HOH:O	2.09	0.52
1:C:109:GLY:HA2	1:C:200:ILE:HD13	1.90	0.52
1:A:109:GLY:HA2	1:A:200:ILE:HD13	1.91	0.51
1:A:84:ASN:OD1	2:A:405:GOL:C3	2.59	0.51
1:B:109:GLY:HA2	1:B:200:ILE:HD13	1.93	0.50
1:A:84:ASN:CB	2:A:405:GOL:H31	2.41	0.50
1:D:109:GLY:HA2	1:D:200:ILE:HD13	1.93	0.50
1:C:5:LYS:HD3	4:C:503:HOH:O	2.11	0.49
1:A:126:TYR:CE2	1:C:6:MET:HE2	2.48	0.49
1:B:5:LYS:HB2	2:B:405:GOL:H12	1.95	0.47
1:A:5:LYS:HG2	2:C:404:GOL:H32	1.96	0.47
1:C:232:LEU:HA	1:C:235:MET:HE2	1.97	0.46
1:B:5:LYS:H	2:B:405:GOL:C1	2.29	0.46
1:A:294:PHE:CD2	4:A:562:HOH:O	2.68	0.46
1:B:46:SER:HA	2:B:401:GOL:H12	1.98	0.45
1:C:95:ASN:HB3	1:C:98:THR:OG1	2.16	0.45
1:D:52:PRO:O	1:D:188:ARG:NH2	2.41	0.45
1:A:95:ASN:HB3	1:A:98:THR:OG1	2.17	0.45
1:B:256:GLN:OE1	1:B:301:SER:HB2	2.17	0.45
2:B:405:GOL:C3	1:D:5:LYS:HD2	2.39	0.44
1:B:95:ASN:HB3	1:B:98:THR:OG1	2.18	0.44
1:A:262:LEU:HD23	1:A:262:LEU:HA	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:ASN:HB3	1:D:98:THR:OG1	2.18	0.43
1:B:113:SER:O	1:B:149:GLY:HA2	2.19	0.43
1:B:71:GLY:O	1:B:72:ASN:HB2	2.19	0.43
1:C:113:SER:O	1:C:149:GLY:HA2	2.19	0.42
1:D:113:SER:O	1:D:149:GLY:HA2	2.19	0.42
1:B:76:ARG:HD3	1:B:78:ILE:HG22	2.01	0.42
1:C:235:MET:HG3	1:C:236:LYS:N	2.34	0.42
1:C:233:VAL:HG21	1:C:269:LYS:HD2	2.02	0.41
1:A:8:PHE:HE1	1:A:305:PHE:CZ	2.38	0.41
1:C:233:VAL:HG21	1:C:269:LYS:CD	2.50	0.41
1:B:86:VAL:HG13	1:B:179:GLY:HA2	2.03	0.41
1:A:113:SER:O	1:A:149:GLY:HA2	2.19	0.41
1:A:86:VAL:HG13	1:A:179:GLY:HA2	2.03	0.41
1:A:276:MET:HE2	1:A:287:LEU:CD2	2.51	0.41
1:C:235:MET:CG	1:C:236:LYS:N	2.84	0.41
1:A:304:THR:HG22	1:C:123:SER:HB2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ASN:O	1:A:72:ASN:ND2[2_655]	2.19	0.01

## 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	304/306 (99%)	294 (97%)	10 (3%)	0	100	100
1	B	305/306 (100%)	293 (96%)	11 (4%)	1 (0%)	36	27
1	C	306/306 (100%)	296 (97%)	10 (3%)	0	100	100
1	D	305/306 (100%)	297 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1220/1224 (100%)	1180 (97%)	39 (3%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	302	GLY

### 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	264/264 (100%)	260 (98%)	4 (2%)	57	52
1	B	265/264 (100%)	260 (98%)	5 (2%)	50	44
1	C	266/264 (101%)	263 (99%)	3 (1%)	65	61
1	D	265/264 (100%)	261 (98%)	4 (2%)	57	52
All	All	1060/1056 (100%)	1044 (98%)	16 (2%)	57	52

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	ASN
1	A	270	GLU
1	A	279	ARG
1	A	298	ARG
1	B	55	GLU
1	B	73	VAL
1	B	76	ARG
1	B	100	LYS
1	B	238	ASN
1	C	73	VAL
1	C	236	LYS
1	C	238	ASN
1	D	222	ARG
1	D	235	MET

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Mol	Chain	Res	Type
1	D	238	ASN
1	D	276	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	74	GLN
1	A	107	GLN
1	A	127	GLN
1	A	203	ASN
1	A	246	HIS
1	A	274	ASN
1	B	69	GLN
1	B	72	ASN
1	B	74	GLN
1	B	107	GLN
1	B	127	GLN
1	B	203	ASN
1	B	246	HIS
1	B	273	GLN
1	B	306	GLN
1	C	19	GLN
1	C	69	GLN
1	C	84	ASN
1	C	127	GLN
1	C	203	ASN
1	C	246	HIS
1	C	273	GLN
1	D	69	GLN
1	D	72	ASN
1	D	107	GLN
1	D	127	GLN
1	D	203	ASN
1	D	246	HIS
1	D	306	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

18 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	$\# Z  > 2$
2	GOL	B	403	-	5,5,5	0.21	0	5,5,5	0.42	0
2	GOL	C	402	-	5,5,5	0.18	0	5,5,5	0.60	0
2	GOL	A	403	-	5,5,5	0.12	0	5,5,5	0.24	0
2	GOL	A	406	-	5,5,5	0.07	0	5,5,5	0.21	0
3	7ON	B	402	1	49,49,49	1.40	3 (6%)	62,71,71	1.05	5 (8%)
2	GOL	B	405	-	5,5,5	0.13	0	5,5,5	0.67	0
2	GOL	C	404	-	5,5,5	0.21	0	5,5,5	0.43	0
2	GOL	D	401	-	5,5,5	0.13	0	5,5,5	0.52	0
3	7ON	C	403	1	49,49,49	1.38	4 (8%)	62,71,71	1.17	5 (8%)
3	7ON	A	402	1	49,49,49	1.79	4 (8%)	62,71,71	1.36	5 (8%)
2	GOL	A	405	-	5,5,5	0.11	0	5,5,5	0.51	0
2	GOL	B	406	-	5,5,5	0.06	0	5,5,5	0.29	0
3	7ON	D	402	1	49,49,49	1.27	4 (8%)	62,71,71	1.44	7 (11%)
2	GOL	C	401	-	5,5,5	0.13	0	5,5,5	0.31	0
2	GOL	A	404	-	5,5,5	0.21	0	5,5,5	0.62	0
2	GOL	B	401	-	5,5,5	0.20	0	5,5,5	0.38	0
2	GOL	B	404	-	5,5,5	0.16	0	5,5,5	0.61	0
2	GOL	A	401	-	5,5,5	0.16	0	5,5,5	0.38	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	GOL	B	403	-	-	4/4/4/4	-
2	GOL	C	402	-	-	3/4/4/4	-
2	GOL	A	403	-	-	2/4/4/4	-
2	GOL	A	406	-	-	2/4/4/4	-
3	7ON	B	402	1	-	4/46/93/93	0/5/5/5
2	GOL	B	405	-	-	4/4/4/4	-
2	GOL	C	404	-	-	4/4/4/4	-
2	GOL	D	401	-	-	4/4/4/4	-
3	7ON	C	403	1	-	6/46/93/93	0/5/5/5
3	7ON	A	402	1	-	2/46/93/93	0/5/5/5
2	GOL	A	405	-	-	4/4/4/4	-
2	GOL	B	406	-	-	4/4/4/4	-
3	7ON	D	402	1	-	3/46/93/93	0/5/5/5
2	GOL	C	401	-	-	2/4/4/4	-
2	GOL	A	404	-	-	2/4/4/4	-
2	GOL	B	401	-	-	2/4/4/4	-
2	GOL	B	404	-	-	2/4/4/4	-
2	GOL	A	401	-	-	2/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	7ON	O6-C7	-9.62	1.22	1.42
3	B	402	7ON	O6-C7	-7.93	1.26	1.42
3	C	403	7ON	O6-C7	-7.31	1.27	1.42
3	D	402	7ON	O6-C7	-6.50	1.29	1.42
3	A	402	7ON	C7-C8	-5.00	1.42	1.52
3	C	403	7ON	C7-C8	-4.09	1.44	1.52
3	A	402	7ON	C7-C6	-4.04	1.49	1.54
3	D	402	7ON	C7-C8	-3.70	1.45	1.52
3	B	402	7ON	C7-C8	-3.43	1.45	1.52
3	C	403	7ON	C4-N1	-2.85	1.30	1.33
3	D	402	7ON	C4-N1	-2.74	1.30	1.33
3	D	402	7ON	C7-C6	-2.36	1.51	1.54
3	A	402	7ON	C4-N1	-2.12	1.31	1.33
3	B	402	7ON	C4-N1	-2.03	1.31	1.33
3	C	403	7ON	C2-C3	2.01	1.56	1.53



All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	7ON	C7-C8-N2	-6.09	107.86	116.25
3	D	402	7ON	C7-C8-N2	-5.61	108.52	116.25
3	C	403	7ON	C7-C8-N2	-4.98	109.39	116.25
3	D	402	7ON	O6-C7-C8	4.69	120.73	110.63
3	C	403	7ON	O6-C7-C6	3.78	119.27	108.54
3	D	402	7ON	C7-C6-N3	-3.74	102.99	110.03
3	C	403	7ON	O2-C8-C7	3.36	126.06	120.00
3	A	402	7ON	O6-C7-C6	3.33	117.99	108.54
3	B	402	7ON	C7-C6-N3	-3.20	104.01	110.03
3	D	402	7ON	O2-C8-C7	3.17	125.71	120.00
3	B	402	7ON	O6-C7-C6	3.04	117.17	108.54
3	A	402	7ON	O2-C8-C7	3.01	125.42	120.00
3	A	402	7ON	C21-C20-C19	-2.91	106.96	111.93
3	C	403	7ON	O6-C7-C8	2.84	116.75	110.63
3	D	402	7ON	C23-C24-C19	-2.55	107.59	111.93
3	A	402	7ON	O6-C7-C8	2.41	115.81	110.63
3	D	402	7ON	C24-C19-C18	2.33	114.96	111.97
3	D	402	7ON	O6-C7-C6	2.31	115.10	108.54
3	B	402	7ON	O6-C7-C8	2.28	115.55	110.63
3	B	402	7ON	O2-C8-N2	-2.21	118.84	122.93
3	B	402	7ON	C5-C6-N3	2.06	112.85	110.18
3	C	403	7ON	C29-C25-N2	2.03	115.69	112.07

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	404	GOL	C1-C2-C3-O3
2	A	405	GOL	O1-C1-C2-C3
2	A	406	GOL	O1-C1-C2-C3
2	B	401	GOL	C1-C2-C3-O3
2	B	403	GOL	O1-C1-C2-C3
2	B	403	GOL	C1-C2-C3-O3
2	B	406	GOL	O1-C1-C2-O2
2	C	404	GOL	O1-C1-C2-C3
2	C	404	GOL	C1-C2-C3-O3
3	A	402	7ON	C5-C6-C7-O6
3	A	402	7ON	N3-C6-C7-O6
3	B	402	7ON	C7-C8-N2-C25
3	B	402	7ON	O2-C8-N2-C25
3	B	402	7ON	C5-C6-C7-O6

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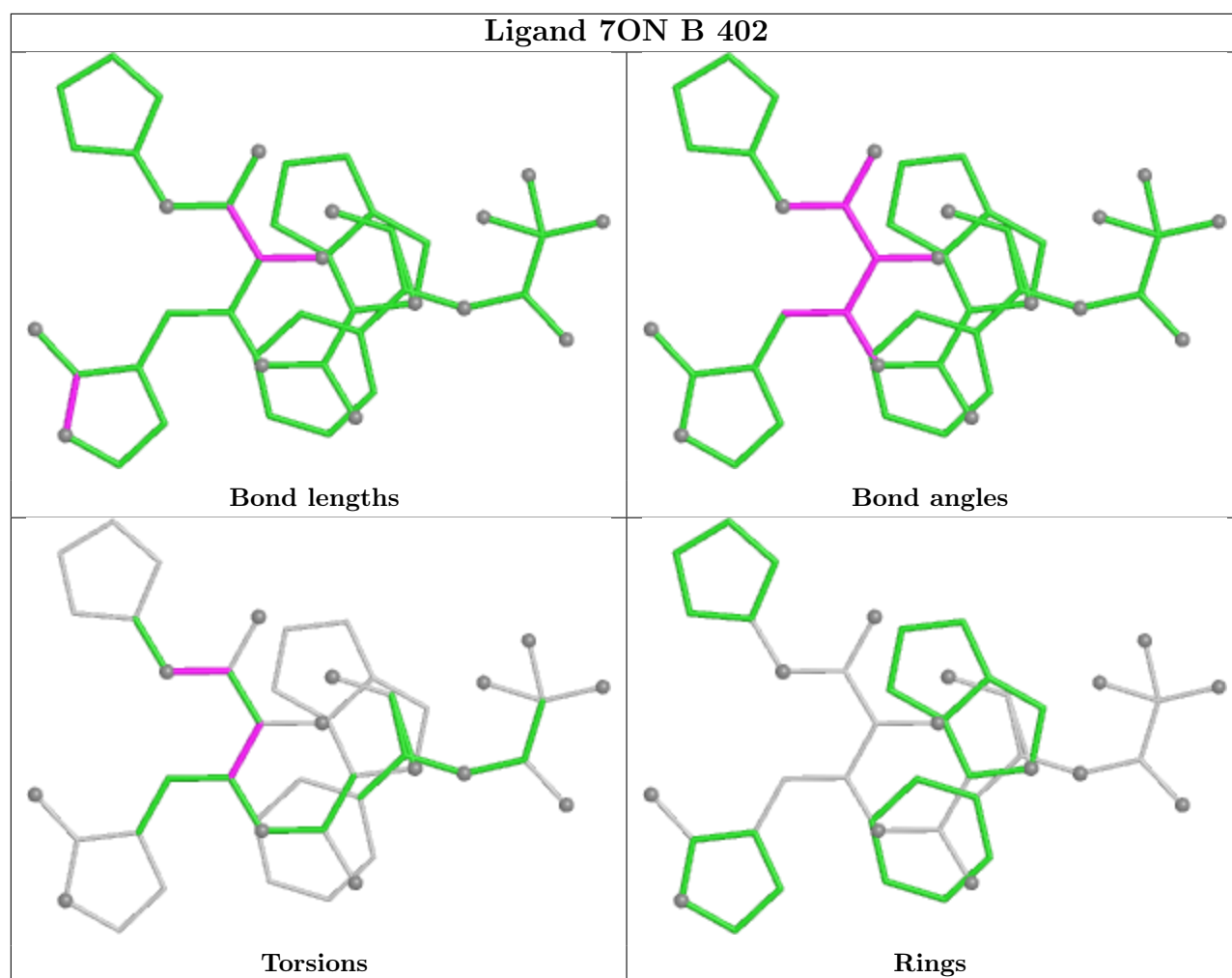
Mol	Chain	Res	Type	Atoms
3	B	402	7ON	N3-C6-C7-O6
3	C	403	7ON	C7-C8-N2-C25
3	C	403	7ON	C5-C6-C7-O6
3	C	403	7ON	N3-C6-C7-O6
3	D	402	7ON	C5-C6-C7-O6
3	D	402	7ON	N3-C6-C7-O6
3	C	403	7ON	O2-C8-N2-C25
2	A	401	GOL	O1-C1-C2-C3
2	A	403	GOL	C1-C2-C3-O3
2	A	405	GOL	C1-C2-C3-O3
2	B	404	GOL	O1-C1-C2-C3
2	B	405	GOL	O1-C1-C2-C3
2	B	405	GOL	C1-C2-C3-O3
2	B	406	GOL	O1-C1-C2-C3
2	B	406	GOL	C1-C2-C3-O3
2	C	401	GOL	C1-C2-C3-O3
2	C	402	GOL	C1-C2-C3-O3
2	D	401	GOL	C1-C2-C3-O3
2	A	404	GOL	O2-C2-C3-O3
2	A	406	GOL	O1-C1-C2-O2
2	B	403	GOL	O1-C1-C2-O2
2	B	403	GOL	O2-C2-C3-O3
2	B	406	GOL	O2-C2-C3-O3
2	B	401	GOL	O2-C2-C3-O3
2	C	404	GOL	O2-C2-C3-O3
2	A	403	GOL	O2-C2-C3-O3
2	C	401	GOL	O2-C2-C3-O3
2	C	402	GOL	O1-C1-C2-O2
2	D	401	GOL	O2-C2-C3-O3
2	C	404	GOL	O1-C1-C2-O2
2	D	401	GOL	O1-C1-C2-O2
3	C	403	7ON	O6-C7-C8-O2
3	C	403	7ON	O6-C7-C8-N2
3	D	402	7ON	C7-C8-N2-C25
2	A	405	GOL	O1-C1-C2-O2
2	B	405	GOL	O1-C1-C2-O2
2	A	401	GOL	O1-C1-C2-O2
2	A	405	GOL	O2-C2-C3-O3
2	B	405	GOL	O2-C2-C3-O3
2	D	401	GOL	O1-C1-C2-C3
2	B	404	GOL	O1-C1-C2-O2
2	C	402	GOL	O2-C2-C3-O3

There are no ring outliers.

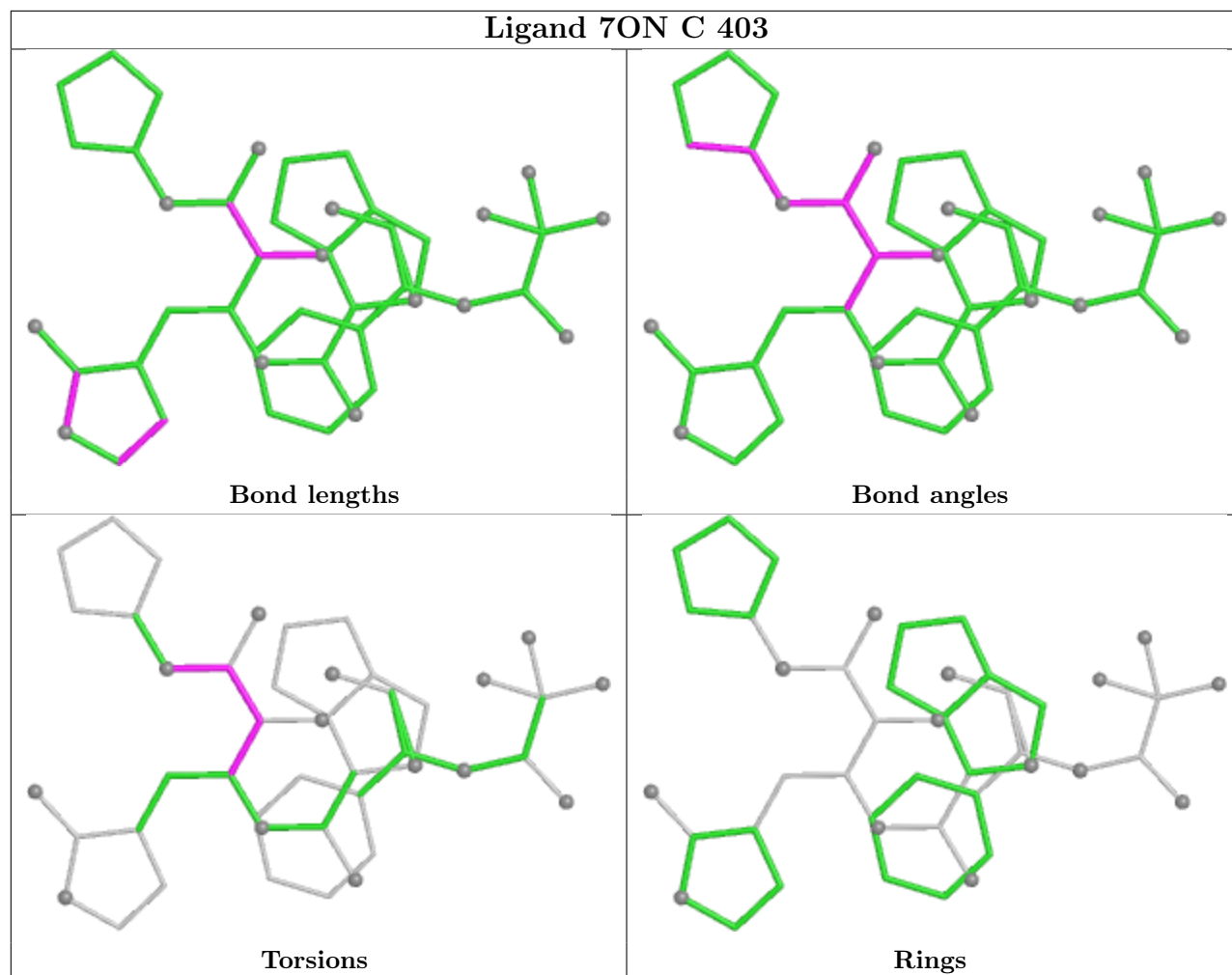
9 monomers are involved in 19 short contacts:

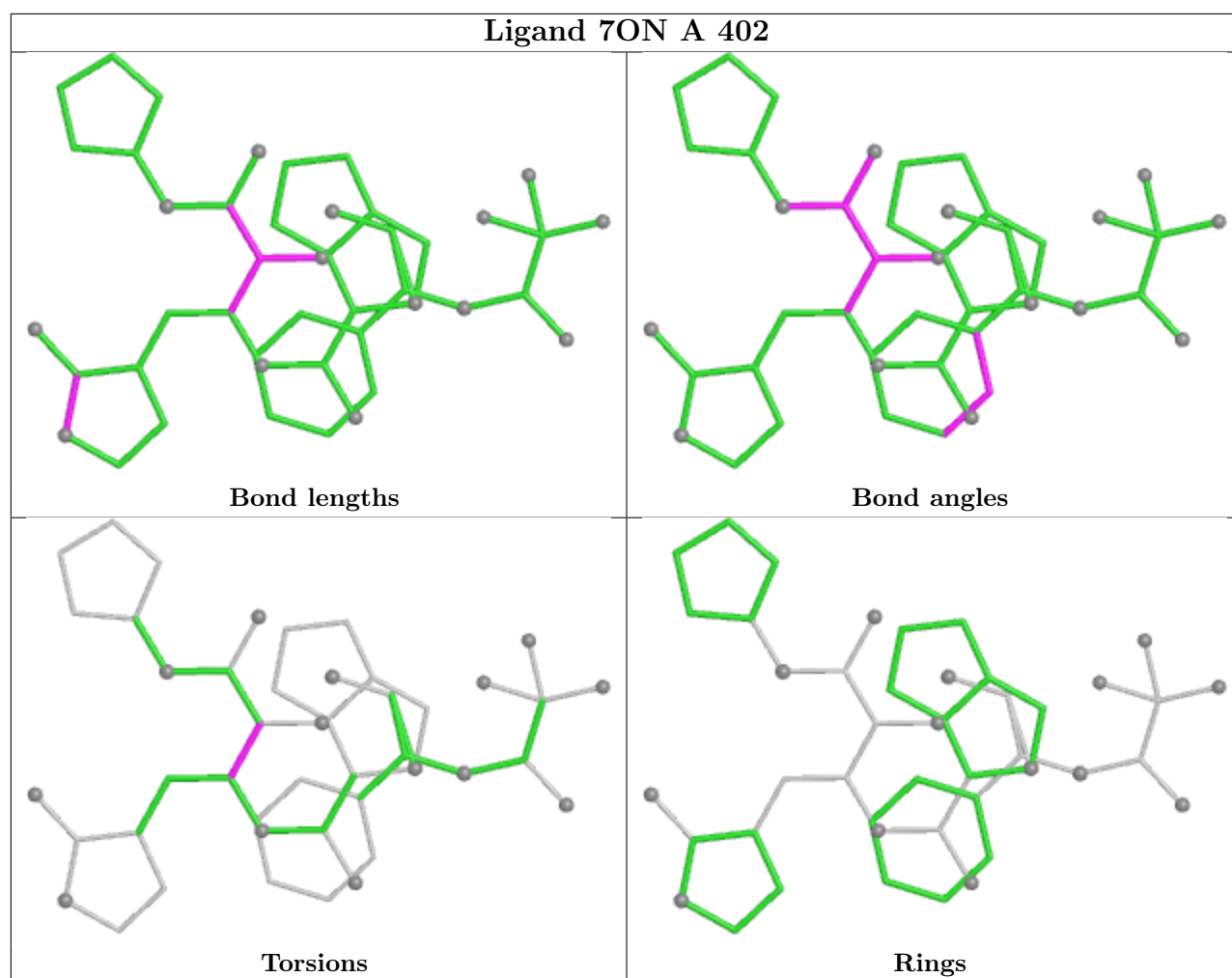
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	403	GOL	1	0
2	B	405	GOL	5	0
2	C	404	GOL	1	0
2	D	401	GOL	1	0
3	C	403	7ON	1	0
2	A	405	GOL	4	0
2	B	406	GOL	2	0
2	B	401	GOL	1	0
2	B	404	GOL	3	0

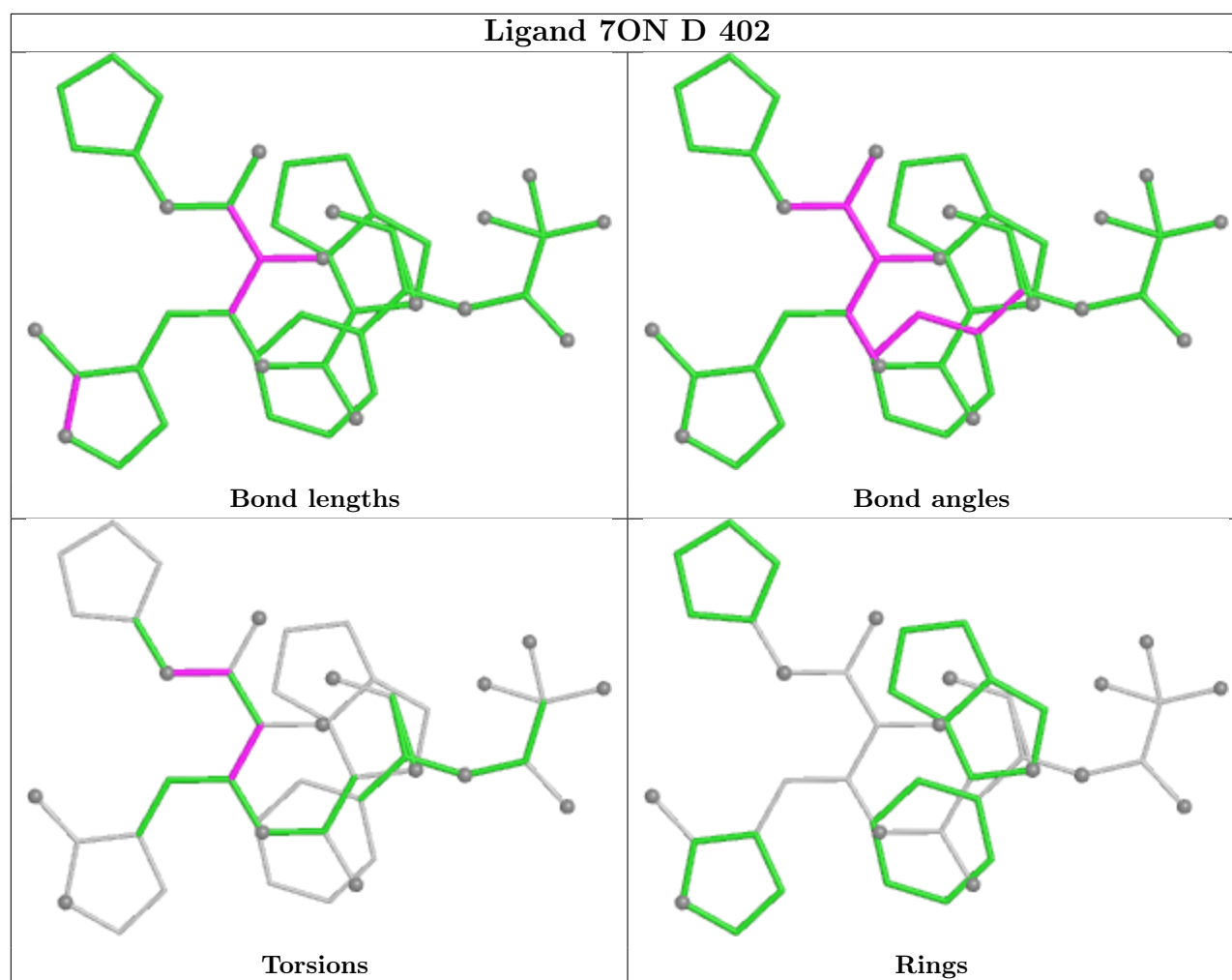
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 7ON C 403







## 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	306/306 (100%)	0.17	13 (4%)	40 50	13, 28, 58, 78	2 (0%)
1	B	306/306 (100%)	0.00	10 (3%)	49 59	17, 29, 50, 62	4 (1%)
1	C	306/306 (100%)	-0.03	6 (1%)	65 74	15, 27, 45, 59	5 (1%)
1	D	306/306 (100%)	0.03	4 (1%)	75 82	15, 28, 44, 70	4 (1%)
All	All	1224/1224 (100%)	0.04	33 (2%)	56 66	13, 28, 48, 78	15 (1%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	223	PHE	6.6
1	A	72	ASN	3.8
1	A	305	PHE	3.7
1	A	232	LEU	3.5
1	A	306	GLN	3.4
1	B	294	PHE	3.4
1	A	227	LEU	3.2
1	D	72	ASN	3.1
1	B	301	SER	3.1
1	D	222	ARG	3.1
1	B	305	PHE	3.0
1	B	73	VAL	2.9
1	D	306	GLN	2.9
1	A	235	MET	2.9
1	C	305	PHE	2.9
1	A	233	VAL	2.8
1	C	223	PHE	2.8
1	B	298	ARG	2.8
1	A	73	VAL	2.8
1	B	302	GLY	2.7
1	C	233	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	294	PHE	2.6
1	C	72	ASN	2.6
1	B	223	PHE	2.5
1	C	73	VAL	2.5
1	B	303	VAL	2.4
1	A	59	ILE	2.4
1	A	228	ASN	2.4
1	C	215	GLY	2.3
1	A	303	VAL	2.1
1	B	304	THR	2.0
1	A	71	GLY	2.0
1	B	279	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 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(Å <sup>2</sup> )	Q<0.9
2	GOL	A	405	6/6	0.80	0.17	46,49,51,52	0
2	GOL	B	404	6/6	0.81	0.16	53,55,58,60	0
2	GOL	B	406	6/6	0.83	0.16	48,50,56,57	0
2	GOL	B	401	6/6	0.84	0.14	41,42,43,43	0
2	GOL	A	403	6/6	0.86	0.15	60,66,75,79	0
2	GOL	C	402	6/6	0.87	0.12	50,51,53,55	0
2	GOL	A	404	6/6	0.88	0.14	70,73,74,74	0
2	GOL	A	406	6/6	0.88	0.13	46,48,51,56	0
2	GOL	C	401	6/6	0.89	0.14	36,41,46,51	0
2	GOL	B	405	6/6	0.89	0.12	50,51,53,57	0
2	GOL	C	404	6/6	0.89	0.12	61,62,64,66	0

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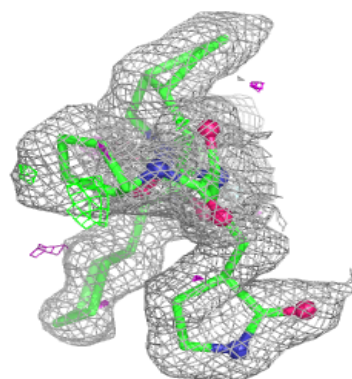
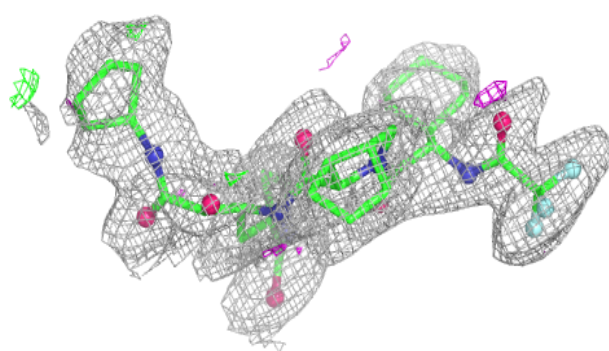
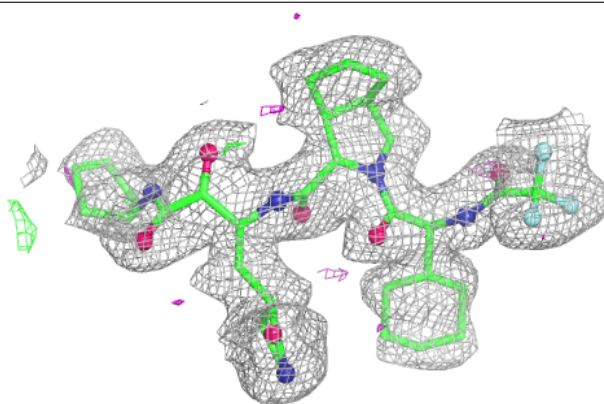
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	B	403	6/6	0.90	0.13	50,50,53,56	0
2	GOL	D	401	6/6	0.92	0.12	45,47,52,55	0
2	GOL	A	401	6/6	0.93	0.10	37,38,41,42	0
3	7ON	C	403	45/45	0.95	0.08	21,24,31,32	0
3	7ON	B	402	45/45	0.96	0.07	21,24,31,31	0
3	7ON	D	402	45/45	0.96	0.06	19,23,26,28	0
3	7ON	A	402	45/45	0.97	0.06	17,20,27,30	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.

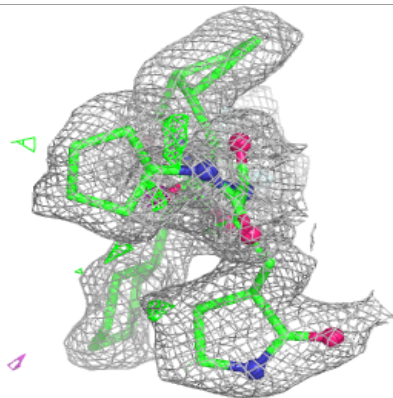
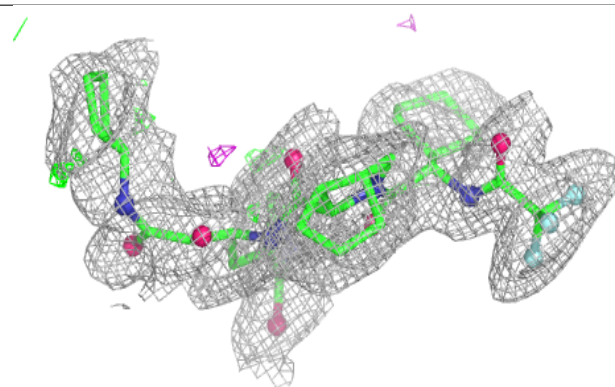
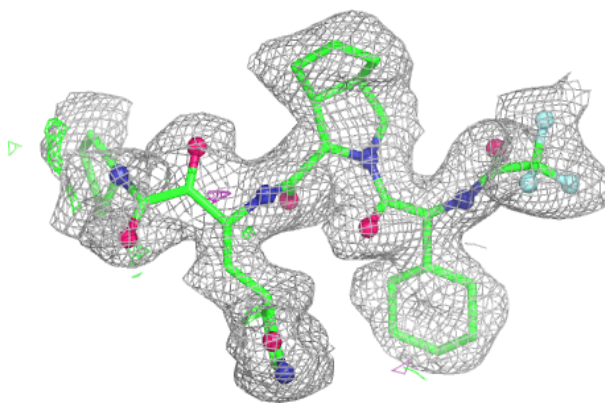
**Electron density around 7ON C 403:**

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)

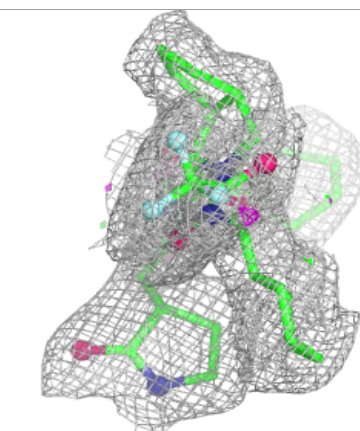
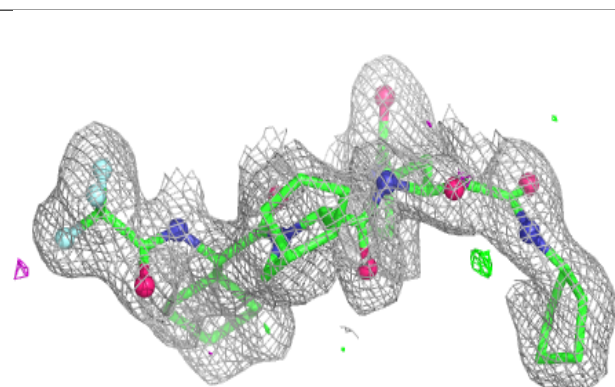
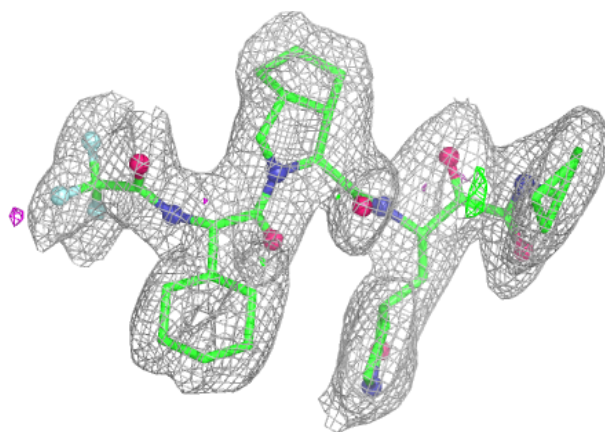


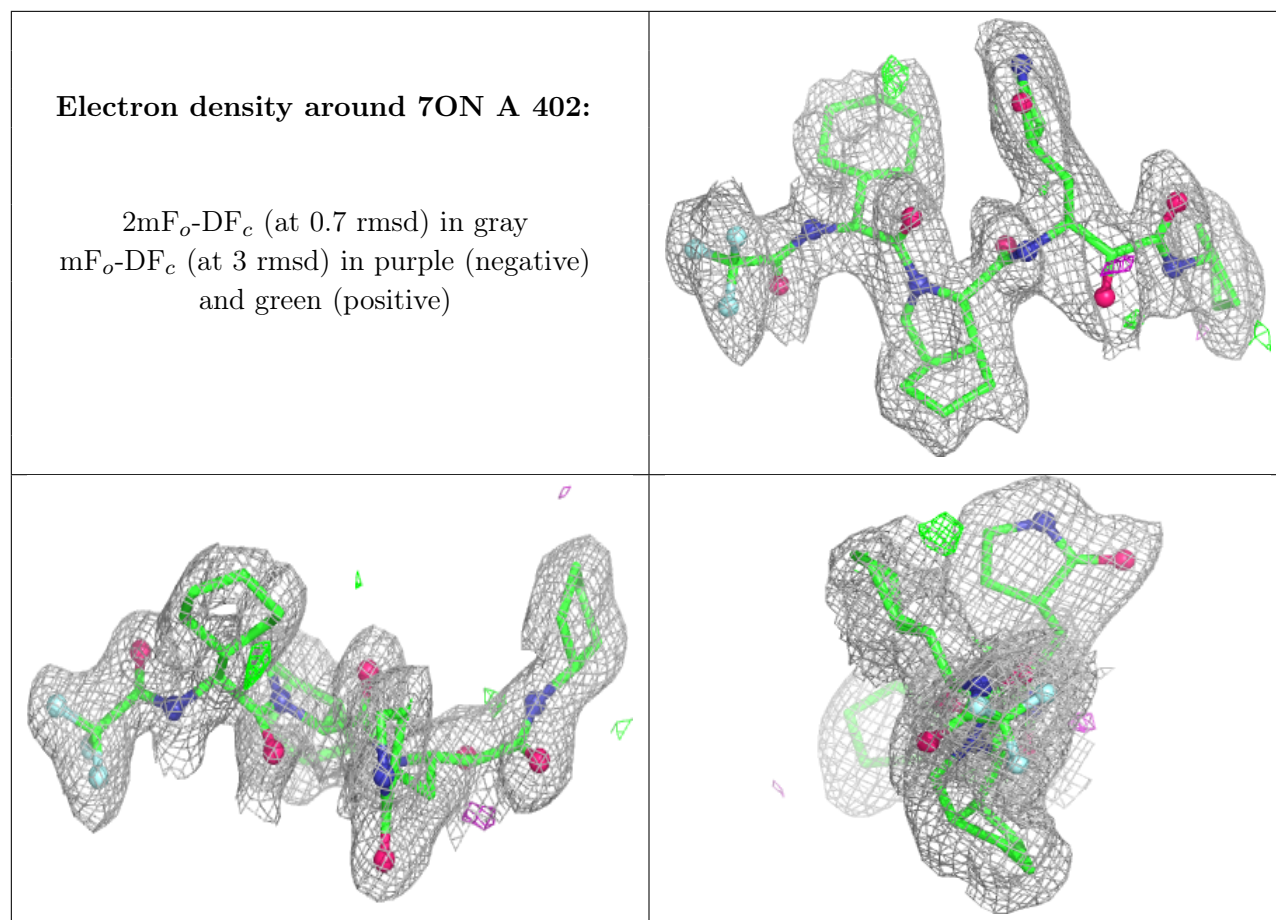
**Electron density around 7ON B 402:**

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

**Electron density around 7ON D 402:**

$2mF_o-DF_c$  (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.