



# Full wwPDB X-ray Structure Validation Report ⓘ

May 11, 2026 – 01:24 PM JST

PDB ID : 9LDU / pdb\_00009ldu  
Title : Crystal structure of HCoV 229E main protease in complex with Oridonin  
Authors : Zeng, P.; Li, J.  
Deposited on : 2025-01-06  
Resolution : 1.94 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

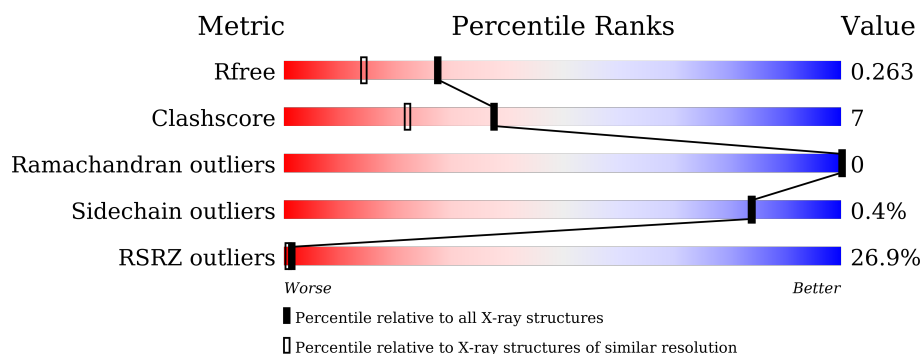
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	299	<div> <div>26%</div> <div>83%</div> <div>13%</div> <div>.</div> </div>
1	B	299	<div> <div>26%</div> <div>84%</div> <div>14%</div> <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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ODN	A	401	-	-	X	-

## 2 Entry composition [i](#)

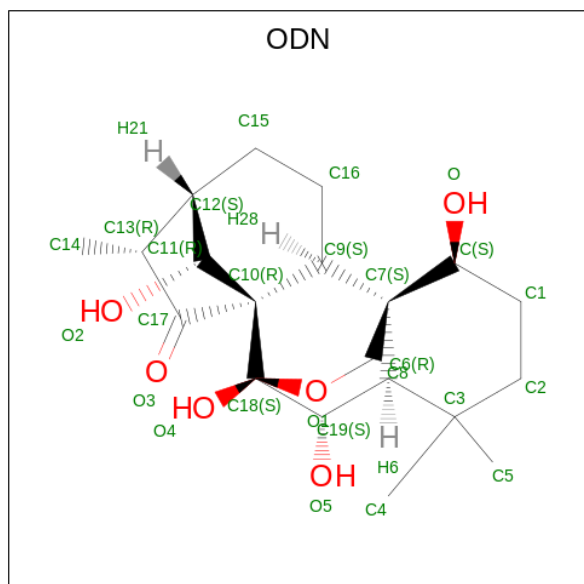
There are 3 unique types of molecules in this entry. The entry contains 4647 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2200	1397	377	408	18			
1	B	294	Total	C	N	O	S	0	0	0
			2254	1431	387	418	18			

- Molecule 2 is (1beta,6beta,7beta,8alpha,9beta,10alpha,13alpha,14R,16beta)-1,6,7,14-tetrahydroxy-7,20-epoxykauran-15-one (CCD ID: ODN) (formula:  $C_{20}H_{30}O_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			26	20	6		

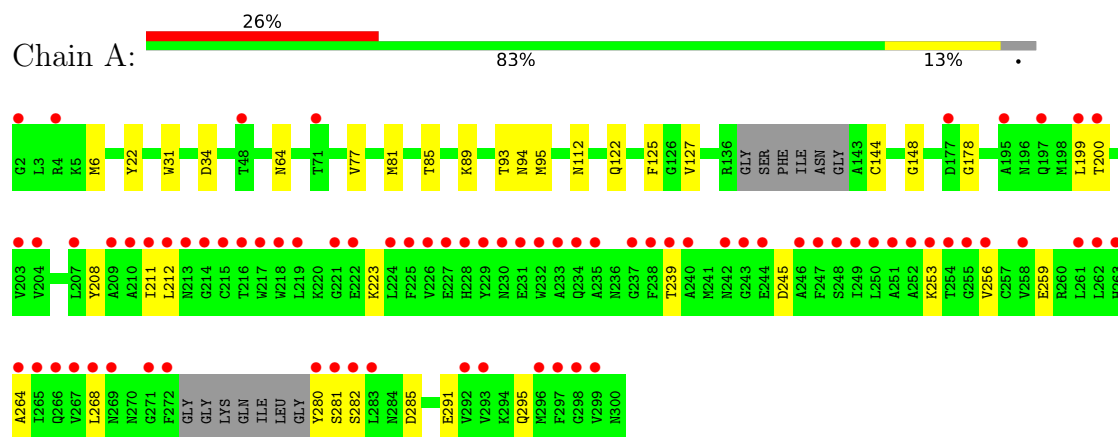
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	95	Total 95	O 95	0	0
3	B	72	Total 72	O 72	0	0

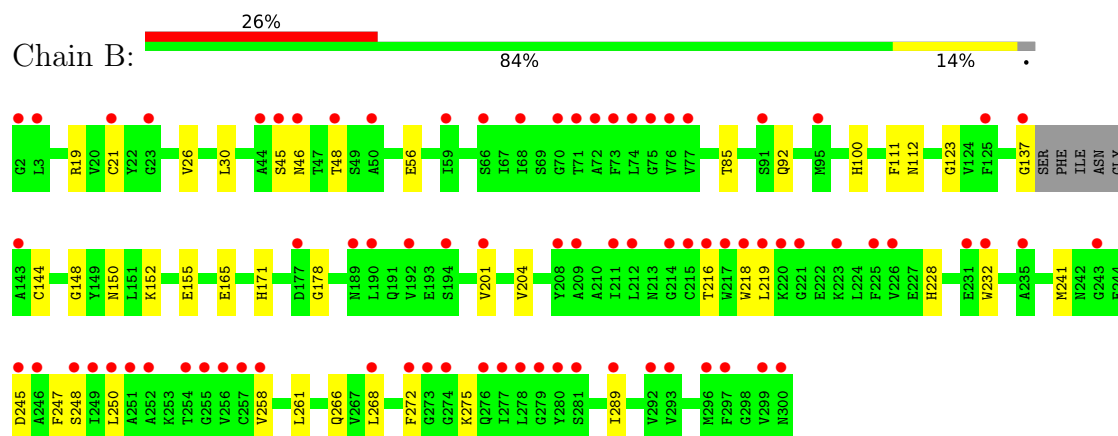
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: 3C-like proteinase



#### • Molecule 1: 3C-like proteinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.82Å 75.43Å 77.83Å 90.00° 91.08° 90.00°	Depositor
Resolution (Å)	77.82 – 1.94 77.82 – 1.94	Depositor EDS
% Data completeness (in resolution range)	98.8 (77.82-1.94) 98.8 (77.82-1.94)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.12_2829, PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.216 , 0.262 0.218 , 0.263	Depositor DCC
$R_{free}$ test set	2365 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.7	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 43.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.016 for -h,-l,-k 0.022 for h,-k,-l	Xtriage
$F_o$ , $F_c$ correlation	0.95	EDS
Total number of atoms	4647	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ODN

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	0.39	0/2248	0.56	1/3043 (0.0%)
1	B	0.32	0/2304	0.50	0/3118
All	All	0.36	0/4552	0.53	1/6161 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	ASP	N-CA-C	-5.21	105.60	111.28

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2200	0	2120	23	0
1	B	2254	0	2175	31	0
2	A	26	0	29	10	0
3	A	95	0	0	1	0
3	B	72	0	0	2	0
All	All	4647	0	4324	62	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 7.

All (62) 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)
2:A:401:ODN:C7	2:A:401:ODN:C8	1.77	1.62
2:A:401:ODN:C9	2:A:401:ODN:C16	1.75	1.60
2:A:401:ODN:C17	2:A:401:ODN:C10	1.84	1.41
2:A:401:ODN:C9	2:A:401:ODN:C17	2.46	0.93
2:A:401:ODN:C8	2:A:401:ODN:C	2.58	0.82
2:A:401:ODN:C8	2:A:401:ODN:C9	2.55	0.81
1:B:137:GLY:HA3	1:B:171:HIS:CD2	2.20	0.76
1:B:165:GLU:OE2	1:B:171:HIS:ND1	2.20	0.75
1:A:85:THR:HG23	1:A:178:GLY:HA2	1.78	0.66
2:A:401:ODN:C8	2:A:401:ODN:C6	2.72	0.66
2:A:401:ODN:C17	2:A:401:ODN:H28	2.26	0.65
1:B:144:CYS:SG	3:B:471:HOH:O	2.55	0.65
1:B:92:GLN:OE1	1:B:92:GLN:N	2.26	0.64
2:A:401:ODN:C7	2:A:401:ODN:C16	2.74	0.62
1:A:212:LEU:HD21	1:A:253:LYS:HG2	1.83	0.60
1:A:280:TYR:O	1:A:281:SER:HB3	2.02	0.58
1:B:241:MET:HE2	1:B:258:VAL:HG11	1.87	0.57
1:B:250:LEU:HD13	1:B:289:ILE:HD11	1.86	0.57
1:A:122:GLN:NE2	3:A:504:HOH:O	2.35	0.57
1:B:100:HIS:HA	1:B:155:GLU:HG3	1.87	0.56
1:B:19:ARG:NH1	1:B:21:CYS:SG	2.79	0.55
1:A:223:LYS:HB2	1:A:259:GLU:HB3	1.91	0.53
1:B:232:TRP:CG	1:B:266:GLN:HE21	2.27	0.51
1:B:21:CYS:SG	1:B:26:VAL:HG22	2.51	0.50
1:B:204:VAL:HG13	1:B:261:LEU:HD12	1.94	0.49
1:A:31:TRP:CD2	1:A:94:ASN:HB2	2.48	0.48
1:A:144:CYS:SG	2:A:401:ODN:H25	2.52	0.48
1:B:250:LEU:CD1	1:B:289:ILE:HD11	2.43	0.48
1:A:77:VAL:CG2	1:A:89:LYS:HG2	2.44	0.48
1:A:264:ALA:O	1:A:268:LEU:HD12	2.13	0.48
1:A:211:ILE:HD13	1:A:256:VAL:HG21	1.96	0.47
1:B:137:GLY:HA3	1:B:171:HIS:NE2	2.29	0.47
1:B:228:HIS:ND1	3:B:403:HOH:O	2.35	0.47
1:A:31:TRP:CE2	1:A:94:ASN:HB2	2.51	0.46
1:A:81:MET:HE3	1:A:81:MET:HB2	1.72	0.45
1:A:6:MET:HE3	1:B:123:GLY:HA3	1.99	0.45
1:A:200:THR:H	1:A:239:THR:HG1	1.57	0.45
1:B:111:PHE:HA	1:B:150:ASN:HD21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:PHE:CE2	1:B:289:ILE:HD13	2.52	0.44
1:A:200:THR:N	1:A:239:THR:OG1	2.29	0.44
1:B:272:PHE:HB3	1:B:275:LYS:O	2.18	0.44
1:B:232:TRP:CD1	1:B:266:GLN:HE21	2.36	0.44
1:A:34:ASP:OD2	1:A:89:LYS:NZ	2.43	0.44
1:A:93:THR:HB	1:A:95:MET:HE3	2.00	0.44
1:A:112:ASN:O	1:A:148:GLY:HA2	2.18	0.44
1:B:112:ASN:O	1:B:148:GLY:HA2	2.18	0.43
1:B:46:ASN:ND2	1:B:48:THR:OG1	2.52	0.42
1:B:216:THR:O	1:B:216:THR:OG1	2.37	0.42
1:B:218:TRP:CD1	1:B:218:TRP:H	2.36	0.42
1:B:232:TRP:CE2	1:B:266:GLN:HG3	2.54	0.42
1:A:208:TYR:O	1:A:212:LEU:HD12	2.20	0.42
1:B:245:ASP:O	1:B:248:SER:HB3	2.19	0.42
1:A:125:PHE:CD2	1:A:127:VAL:HG13	2.55	0.42
1:B:152:LYS:HE2	1:B:152:LYS:HB3	1.90	0.41
1:A:22:TYR:CE2	1:A:64:ASN:HB2	2.55	0.41
1:B:218:TRP:CZ3	1:B:219:LEU:HD13	2.56	0.41
1:B:45:SER:HG	1:B:56:GLU:CD	2.27	0.41
1:A:199:LEU:HB2	1:A:285:ASP:HB2	2.03	0.41
1:B:268:LEU:HB3	1:B:272:PHE:HE1	1.86	0.41
1:B:201:VAL:HG23	1:B:247:PHE:CE1	2.56	0.40
1:B:85:THR:HG23	1:B:178:GLY:HA2	2.02	0.40
1:A:291:GLU:O	1:A:295:GLN:HB2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	280/299 (94%)	276 (99%)	4 (1%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	290/299 (97%)	287 (99%)	3 (1%)	0	100	100
All	All	570/598 (95%)	563 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	235/245 (96%)	234 (100%)	1 (0%)	84	84
1	B	239/245 (98%)	238 (100%)	1 (0%)	84	84
All	All	474/490 (97%)	472 (100%)	2 (0%)	84	84

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	282	SER
1	B	30	LEU

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

Mol	Chain	Res	Type
1	A	55	HIS
1	A	153	ASN
1	A	266	GLN
1	B	46	ASN

### 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](#)

1 ligand is 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	ODN	A	401	1	28,30,30	6.26	13 (46%)	40,54,54	4.44	14 (35%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	ODN	C10-C17	15.09	1.84	1.51
2	A	401	ODN	C8-C7	14.57	1.77	1.53
2	A	401	ODN	C16-C9	13.16	1.75	1.53
2	A	401	ODN	O1-C8	11.80	1.60	1.43
2	A	401	ODN	C13-C17	-10.00	1.34	1.51
2	A	401	ODN	C14-C13	9.39	1.73	1.53
2	A	401	ODN	C13-C12	-7.32	1.40	1.53
2	A	401	ODN	C16-C15	5.68	1.67	1.52
2	A	401	ODN	C12-C11	-4.15	1.47	1.54
2	A	401	ODN	C10-C9	-3.54	1.53	1.58
2	A	401	ODN	C3-C6	3.20	1.61	1.56
2	A	401	ODN	C7-C6	2.90	1.61	1.56
2	A	401	ODN	C6-C19	-2.69	1.50	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	ODN	C11-C10-C17	-17.78	79.24	100.12
2	A	401	ODN	C10-C17-C13	11.57	117.91	105.13
2	A	401	ODN	O3-C17-C10	-7.48	115.95	127.16
2	A	401	ODN	C9-C10-C17	-7.44	93.12	106.88
2	A	401	ODN	O1-C18-C19	6.94	112.75	105.52
2	A	401	ODN	C8-C7-C	-6.70	101.50	111.23
2	A	401	ODN	C8-O1-C18	-6.52	107.72	113.59
2	A	401	ODN	O5-C19-C6	-4.41	104.47	111.98
2	A	401	ODN	C18-C19-C6	4.24	112.52	109.59
2	A	401	ODN	C8-C7-C9	-3.78	100.00	107.69
2	A	401	ODN	C7-C6-C19	2.78	111.63	109.09
2	A	401	ODN	O5-C19-C18	-2.53	109.30	112.91
2	A	401	ODN	C3-C6-C19	-2.35	110.61	113.79
2	A	401	ODN	O4-C18-O1	2.09	111.85	107.23

There are no chirality outliers.

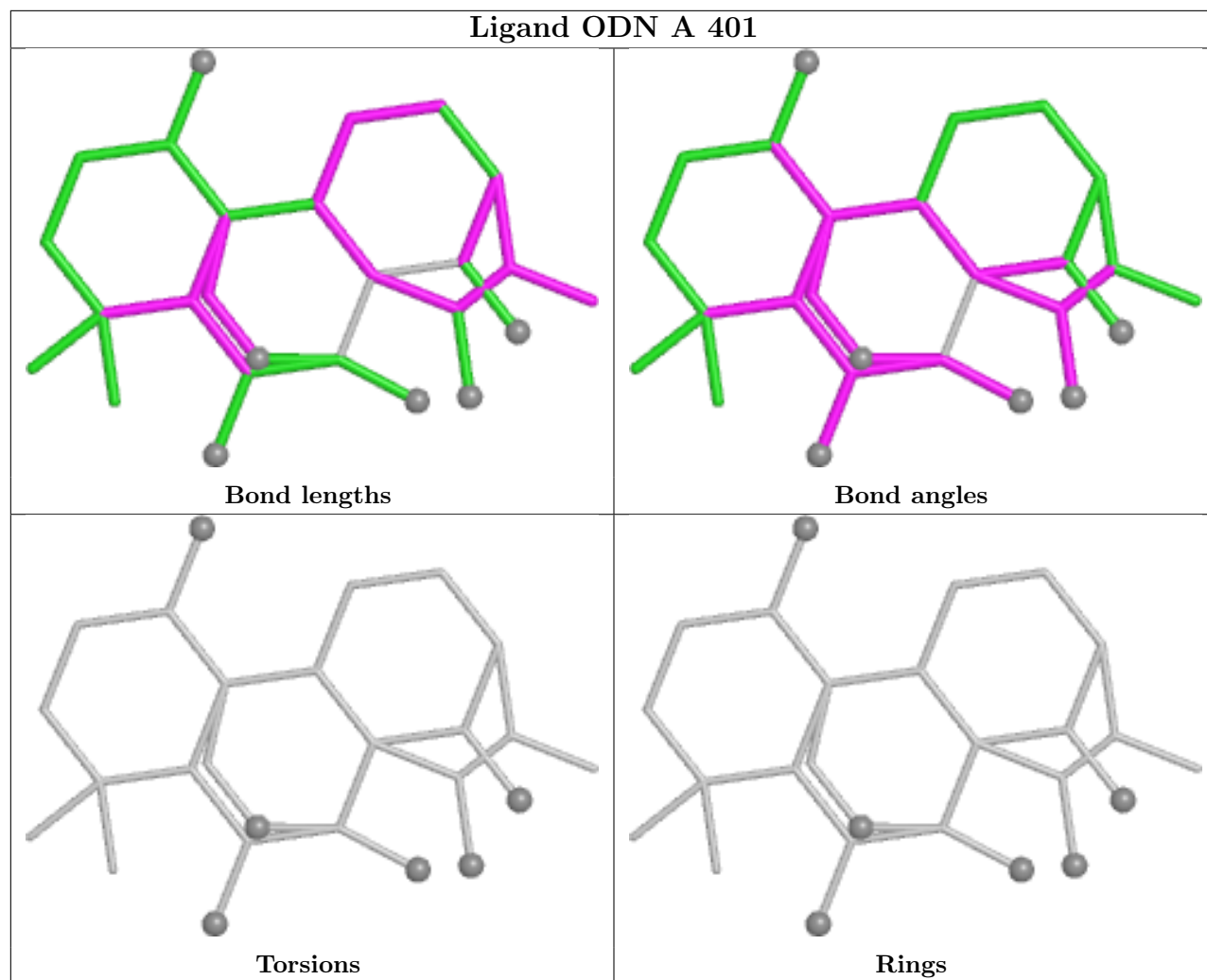
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	ODN	10	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.



## 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	286/299 (95%)	1.15	77 (26%) <b>1</b> <b>1</b>	23, 39, 87, 97	0
1	B	294/299 (98%)	1.26	79 (26%) <b>1</b> <b>1</b>	27, 46, 76, 89	0
All	All	580/598 (96%)	1.21	156 (26%) <b>1</b> <b>1</b>	23, 44, 84, 97	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	280	TYR	6.4
1	B	297	PHE	5.8
1	B	2	GLY	5.8
1	A	216	THR	5.1
1	A	229	TYR	4.7
1	A	272	PHE	4.7
1	A	225	PHE	4.6
1	B	256	VAL	4.6
1	A	265	ILE	4.5
1	A	218	TRP	4.5
1	B	245	ASP	4.3
1	A	281	SER	4.3
1	A	226	VAL	4.3
1	A	224	LEU	4.2
1	B	3	LEU	4.2
1	A	244	GLU	4.2
1	A	268	LEU	4.2
1	B	219	LEU	4.1
1	B	257	CYS	4.0
1	A	256	VAL	4.0
1	A	262	LEU	4.0
1	A	235	ALA	4.0
1	A	232	TRP	3.9
1	A	212	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	217	TRP	3.8
1	A	211	ILE	3.8
1	B	249	ILE	3.7
1	B	252	ALA	3.6
1	A	299	VAL	3.6
1	A	269	ASN	3.6
1	A	296	MET	3.5
1	B	72	ALA	3.5
1	B	48	THR	3.5
1	A	219	LEU	3.4
1	A	217	TRP	3.4
1	A	266	GLN	3.3
1	A	271	GLY	3.3
1	A	249	ILE	3.3
1	A	233	ALA	3.3
1	B	246	ALA	3.3
1	B	251	ALA	3.3
1	B	71	THR	3.2
1	A	255	GLY	3.2
1	A	214	GLY	3.2
1	A	258	VAL	3.1
1	A	2	GLY	3.1
1	A	261	LEU	3.1
1	A	263	HIS	3.1
1	B	255	GLY	3.1
1	A	297	PHE	3.1
1	A	215	CYS	3.1
1	A	210	ALA	3.1
1	A	240	ALA	3.1
1	B	50	ALA	3.1
1	A	283	LEU	3.0
1	A	71	THR	3.0
1	B	77	VAL	3.0
1	B	125	PHE	3.0
1	B	215	CYS	3.0
1	B	273	GLY	3.0
1	A	246	ALA	3.0
1	A	228	HIS	2.9
1	B	293	VAL	2.9
1	B	194	SER	2.9
1	B	218	TRP	2.9
1	A	267	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	48	THR	2.9
1	A	252	ALA	2.9
1	B	221	GLY	2.9
1	A	213	ASN	2.8
1	A	254	THR	2.8
1	B	45	SER	2.8
1	B	137	GLY	2.7
1	B	248	SER	2.7
1	A	204	VAL	2.7
1	B	281	SER	2.7
1	A	251	ALA	2.7
1	B	250	LEU	2.7
1	B	272	PHE	2.6
1	B	300	ASN	2.6
1	B	277	ILE	2.6
1	B	143	ALA	2.6
1	B	280	TYR	2.6
1	B	21	CYS	2.6
1	A	238	PHE	2.6
1	B	73	PHE	2.6
1	A	243	GLY	2.6
1	A	264	ALA	2.6
1	B	296	MET	2.6
1	B	190	LEU	2.5
1	B	278	LEU	2.5
1	B	214	GLY	2.5
1	B	74	LEU	2.5
1	B	279	GLY	2.5
1	A	247	PHE	2.5
1	B	212	LEU	2.5
1	B	189	ASN	2.5
1	B	216	THR	2.5
1	B	23	GLY	2.4
1	B	44	ALA	2.4
1	A	298	GLY	2.4
1	B	46	ASN	2.4
1	A	199	LEU	2.4
1	B	75	GLY	2.4
1	B	95	MET	2.4
1	A	207	LEU	2.4
1	B	59	ILE	2.4
1	B	276	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	221	GLY	2.4
1	B	258	VAL	2.4
1	A	250	LEU	2.3
1	B	254	THR	2.3
1	B	274	GLY	2.3
1	B	231	GLU	2.3
1	B	68	ILE	2.3
1	A	234	GLN	2.3
1	A	253	LYS	2.3
1	A	227	GLU	2.2
1	B	243	GLY	2.2
1	B	232	TRP	2.2
1	B	211	ILE	2.2
1	B	289	ILE	2.2
1	A	230	ASN	2.2
1	A	292	VAL	2.2
1	A	239	THR	2.2
1	B	70	GLY	2.2
1	A	209	ALA	2.2
1	B	220	LYS	2.2
1	B	225	PHE	2.1
1	A	197	GLN	2.1
1	B	226	VAL	2.1
1	A	4	ARG	2.1
1	A	222	GLU	2.1
1	A	195	ALA	2.1
1	B	209	ALA	2.1
1	A	177	ASP	2.1
1	A	282	SER	2.1
1	A	237	GLY	2.1
1	A	293	VAL	2.1
1	B	192	VAL	2.1
1	B	299	VAL	2.1
1	B	66	SER	2.1
1	B	91	SER	2.1
1	B	76	VAL	2.1
1	B	235	ALA	2.1
1	B	177	ASP	2.1
1	B	208	TYR	2.0
1	A	203	VAL	2.0
1	B	268	LEU	2.0
1	A	231	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	223	LYS	2.0
1	A	248	SER	2.0
1	A	200	THR	2.0
1	A	242	ASN	2.0
1	B	201	VAL	2.0
1	B	292	VAL	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](#)

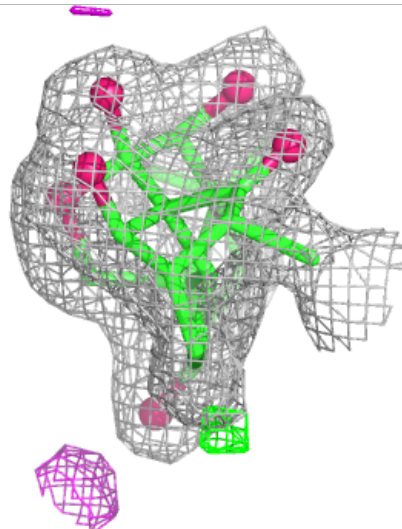
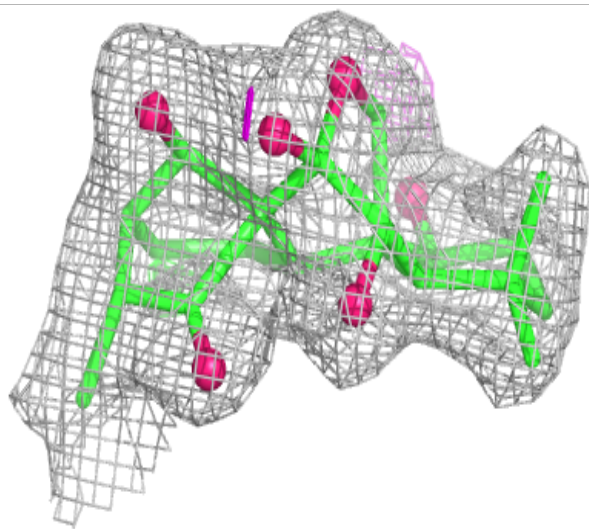
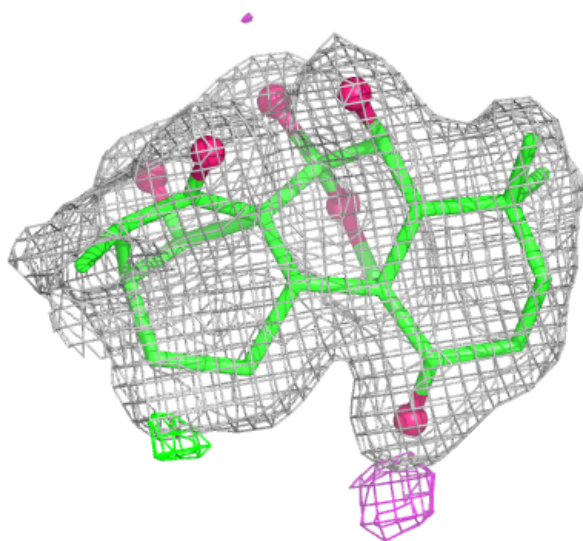
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ODN	A	401	26/26	0.88	0.10	34,39,41,42	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 ODN 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.