



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:21 PM GMT

PDB ID : 1JWT  
Title : CRYSTAL STRUCTURE OF THROMBIN IN COMPLEX WITH A NOVEL BICYCLIC LACTAM INHIBITOR  
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Deposited on : 2001-09-05  
Resolution : 2.50 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

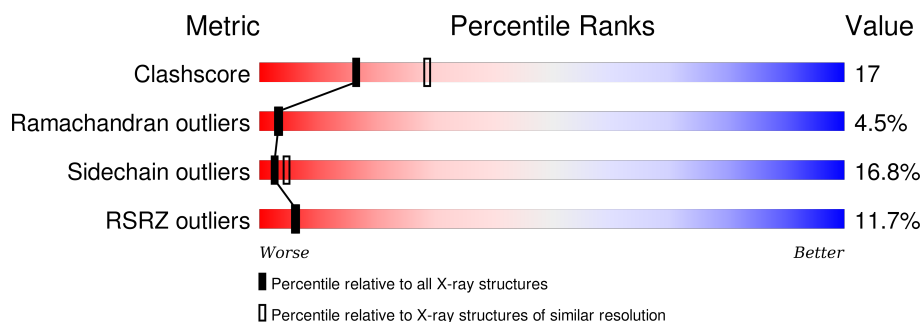
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	305	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2463 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.

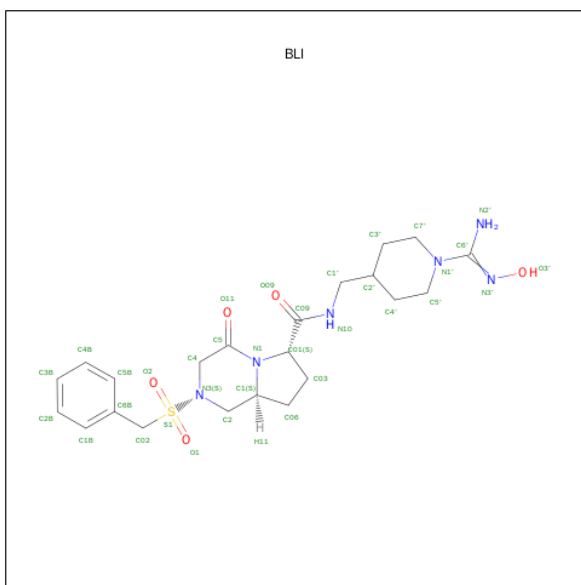
- Molecule 1 is a protein called Prothrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	299	2429	1546	420	448	15	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	ASP	-	CLONING ARTIFACT	UNP P00734
A	291	PHE	-	CLONING ARTIFACT	UNP P00734
A	292	GLU	-	CLONING ARTIFACT	UNP P00734
A	293	GLU	-	CLONING ARTIFACT	UNP P00734
A	294	ILE	-	CLONING ARTIFACT	UNP P00734
A	295	PRO	-	CLONING ARTIFACT	UNP P00734
A	296	GLU	-	CLONING ARTIFACT	UNP P00734
A	297	GLU	-	CLONING ARTIFACT	UNP P00734
A	298	TYR	-	CLONING ARTIFACT	UNP P00734
A	299	LEU	-	CLONING ARTIFACT	UNP P00734

- Molecule 2 is 4-OXO-2-PHENYLMETHANESULFONYL-OCTAHYDRO-PYRROLO[1,2-A]PYRAZINE-6-CARBOXYLIC ACID [1-(N-HYDROXYCARBAMIMIDOYL)-PIPERIDI N-4-YLMETHYL]-AMIDE (three-letter code: BLI) (formula: C<sub>22</sub>H<sub>32</sub>N<sub>6</sub>O<sub>5</sub>S).

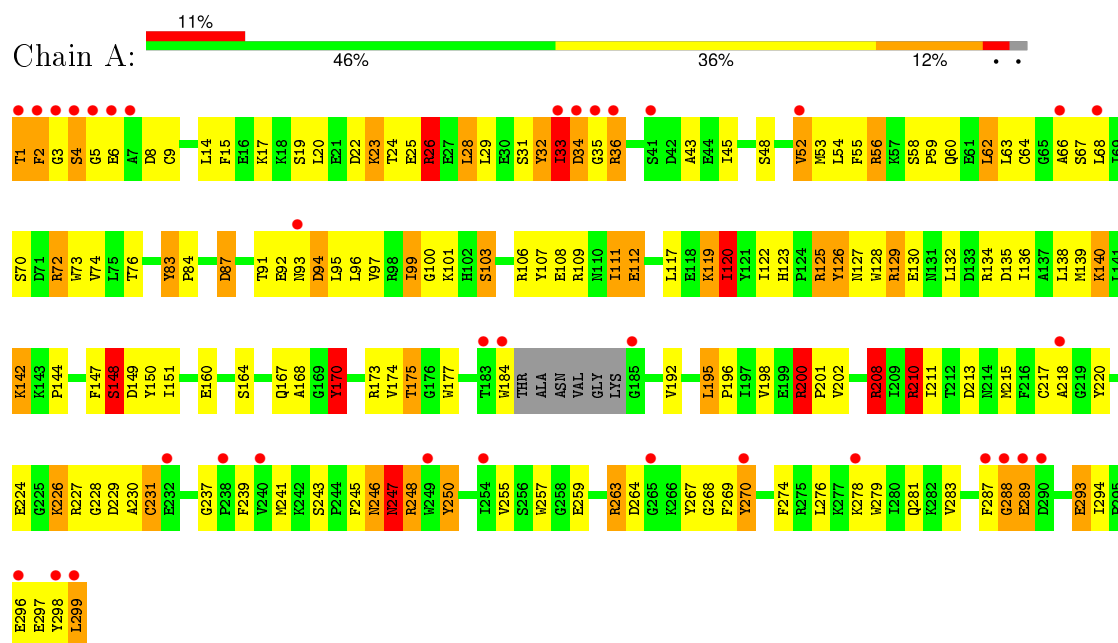


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			34	22	6	5	1		

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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Prothrombin



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.54Å 72.18Å 73.41Å 90.00° 100.99° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50 24.84 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.4 (25.00-2.50) 90.1 (24.84-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.49 (at 2.50Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.182 , 0.301 0.270 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	34.1	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 39.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 12595 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	2463	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	7.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.46% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: BLI

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	1.13	0/2488	1.90	45/3354 (1.3%)

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	A	0	19

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	36	ARG	NE-CZ-NH1	9.67	125.14	120.30
1	A	93	ASN	CB-CA-C	-9.04	92.32	110.40
1	A	247	ASN	CB-CA-C	9.01	128.41	110.40
1	A	56	ARG	NE-CZ-NH2	-8.43	116.08	120.30
1	A	200	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	A	288	GLY	C-N-CA	7.59	140.67	121.70
1	A	125	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	A	267	TYR	CB-CG-CD2	-7.40	116.56	121.00
1	A	248	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	72	ARG	NE-CZ-NH2	-6.93	116.84	120.30
1	A	147	PHE	CB-CG-CD2	-6.84	116.01	120.80
1	A	210	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	A	170	TYR	CB-CG-CD2	-6.48	117.11	121.00
1	A	250	TYR	CB-CG-CD2	-6.41	117.16	121.00
1	A	74	VAL	CA-CB-CG1	6.33	120.40	110.90
1	A	293	GLU	CA-CB-CG	6.29	127.23	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	GLU	OE1-CD-OE2	-6.28	115.76	123.30
1	A	129	ARG	C-N-CA	-6.28	106.01	121.70
1	A	208	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	A	72	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	177	TRP	CB-CA-C	-6.15	98.10	110.40
1	A	32	TYR	CB-CG-CD2	-6.09	117.35	121.00
1	A	270	TYR	CB-CG-CD2	-6.08	117.35	121.00
1	A	289	GLU	CA-CB-CG	5.92	126.42	113.40
1	A	83	TYR	CB-CG-CD1	-5.88	117.47	121.00
1	A	227	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	A	52	VAL	CA-CB-CG1	5.81	119.61	110.90
1	A	26	ARG	CD-NE-CZ	5.77	131.68	123.60
1	A	43	ALA	CB-CA-C	-5.61	101.69	110.10
1	A	142	LYS	C-N-CA	-5.61	107.69	121.70
1	A	87	ASP	N-CA-C	5.54	125.97	111.00
1	A	34	ASP	N-CA-C	5.51	125.89	111.00
1	A	83	TYR	CA-CB-CG	-5.33	103.27	113.40
1	A	263	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	148	SER	C-N-CA	-5.29	108.48	121.70
1	A	170	TYR	CG-CD2-CE2	-5.29	117.07	121.30
1	A	170	TYR	C-N-CA	-5.26	108.55	121.70
1	A	26	ARG	CA-CB-CG	5.23	124.90	113.40
1	A	177	TRP	C-N-CA	-5.17	111.44	122.30
1	A	175	THR	CA-CB-CG2	5.14	119.59	112.40
1	A	168	ALA	N-CA-CB	-5.13	102.92	110.10
1	A	72	ARG	N-CA-C	5.13	124.84	111.00
1	A	195	LEU	CB-CA-C	-5.09	100.53	110.20
1	A	200	ARG	N-CA-C	5.01	124.54	111.00
1	A	120	ILE	CB-CG1-CD1	-5.01	99.88	113.90

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	TYR	Sidechain
1	A	108	GLU	Peptide
1	A	109	ARG	Sidechain
1	A	125	ARG	Sidechain
1	A	129	ARG	Sidechain
1	A	150	TYR	Sidechain
1	A	170	TYR	Sidechain
1	A	173	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	200	ARG	Sidechain
1	A	208	ARG	Sidechain
1	A	210	ARG	Sidechain
1	A	248	ARG	Sidechain
1	A	274	PHE	Sidechain
1	A	287	PHE	Peptide
1	A	298	TYR	Sidechain
1	A	33	ILE	Peptide
1	A	5	GLY	Peptide
1	A	64	CYS	Peptide
1	A	83	TYR	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	2429	0	2372	81	0
2	A	34	0	32	2	0
All	All	2463	0	2404	81	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 17.

All (81) 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:175:THR:HG22	1:A:192:VAL:HG12	1.65	0.77
1:A:14:LEU:HD13	1:A:149:ASP:HB3	1.66	0.76
1:A:53:MET:SD	1:A:62:LEU:HD12	2.26	0.76
1:A:6:GLU:HB2	1:A:9:CYS:HB3	1.69	0.74
1:A:29:LEU:HD12	1:A:35:GLY:HA2	1.70	0.72
1:A:138:LEU:HD13	1:A:283:VAL:HG22	1.73	0.71
1:A:296:GLU:HA	1:A:299:LEU:HB2	1.79	0.65
1:A:257:TRP:HB2	2:A:300:BLI:O11	1.97	0.65
1:A:52:VAL:HG22	1:A:99:ILE:HG23	1.78	0.65
1:A:220:TYR:CZ	1:A:226:LYS:HD2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLY:O	1:A:255:VAL:HG23	2.02	0.58
1:A:126:TYR:HE1	1:A:132:LEU:HD22	1.68	0.58
1:A:95:LEU:HD12	1:A:120:ILE:HD11	1.85	0.58
1:A:127:ASN:ND2	1:A:130:GLU:HB3	2.19	0.58
1:A:101:LYS:HE3	1:A:103:SER:O	2.03	0.57
1:A:1:THR:N	1:A:70:SER:HB3	2.19	0.57
1:A:56:ARG:O	1:A:60:GLN:HA	2.05	0.57
1:A:58:SER:HA	1:A:59:PRO:C	2.25	0.57
1:A:123:HIS:CE1	1:A:134:ARG:HD3	2.40	0.56
1:A:36:ARG:NH1	1:A:245:PHE:O	2.40	0.55
1:A:243:SER:HB2	1:A:250:TYR:HE2	1.72	0.54
1:A:53:MET:HG3	1:A:62:LEU:HD12	1.89	0.54
1:A:55:PHE:HB3	1:A:96:LEU:HB3	1.90	0.54
1:A:196:PRO:HG2	1:A:220:TYR:CD1	2.44	0.53
1:A:211:ILE:HD12	1:A:269:PHE:CE2	2.44	0.52
1:A:95:LEU:CD1	1:A:120:ILE:HD11	2.39	0.52
1:A:230:ALA:O	1:A:231:CYS:HB2	2.10	0.51
1:A:53:MET:HE3	1:A:101:LYS:HD3	1.93	0.50
1:A:53:MET:CG	1:A:62:LEU:HD12	2.41	0.50
1:A:246:ASN:O	1:A:247:ASN:HB3	2.12	0.50
1:A:167:GLN:O	1:A:170:TYR:HB2	2.12	0.49
1:A:138:LEU:HD13	1:A:283:VAL:CG2	2.41	0.49
1:A:136:ILE:HG21	1:A:276:LEU:HD13	1.93	0.49
1:A:126:TYR:CZ	1:A:128:TRP:HB3	2.48	0.49
1:A:72:ARG:HD2	1:A:144:PRO:HD3	1.94	0.49
1:A:91:THR:HG22	1:A:94:ASP:OD1	2.13	0.49
1:A:218:ALA:HB3	1:A:270:TYR:CE1	2.47	0.48
1:A:23:LYS:O	1:A:23:LYS:HE2	2.14	0.48
1:A:76:THR:HG21	1:A:139:MET:SD	2.52	0.48
1:A:52:VAL:HB	1:A:66:ALA:HB3	1.96	0.48
1:A:279:TRP:O	1:A:283:VAL:HG13	2.14	0.48
1:A:200:ARG:HH12	1:A:213:ASP:HA	1.79	0.48
1:A:243:SER:CB	1:A:250:TYR:HE2	2.28	0.46
1:A:229:ASP:OD2	2:A:300:BLI:N2'	2.49	0.45
1:A:288:GLY:O	1:A:289:GLU:HG2	2.16	0.45
1:A:263:ARG:HE	1:A:263:ARG:HB3	1.60	0.45
1:A:127:ASN:HD21	1:A:130:GLU:HB3	1.79	0.45
1:A:2:PHE:HD1	1:A:2:PHE:H	1.64	0.45
1:A:217:CYS:HA	1:A:268:GLY:O	2.17	0.45
1:A:218:ALA:HB3	1:A:270:TYR:HE1	1.81	0.45
1:A:239:PHE:HE1	1:A:241:MET:HE2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ARG:O	1:A:210:ARG:HG3	2.16	0.45
1:A:127:ASN:O	1:A:132:LEU:HA	2.18	0.44
1:A:55:PHE:HE1	1:A:60:GLN:HG2	1.82	0.44
1:A:243:SER:HB2	1:A:250:TYR:CE2	2.51	0.44
1:A:200:ARG:NH1	1:A:213:ASP:HA	2.33	0.44
1:A:259:GLU:O	1:A:263:ARG:HD2	2.18	0.44
1:A:25:GLU:O	1:A:26:ARG:C	2.56	0.44
1:A:76:THR:CG2	1:A:139:MET:SD	3.06	0.43
1:A:60:GLN:OE1	1:A:299:LEU:HD11	2.18	0.43
1:A:100:GLY:HA2	1:A:151:ILE:HG12	2.00	0.43
1:A:28:LEU:O	1:A:31:SER:N	2.51	0.43
1:A:84:PRO:HG2	1:A:128:TRP:CZ3	2.54	0.42
1:A:72:ARG:HD3	1:A:289:GLU:HG3	2.01	0.42
1:A:243:SER:HB3	1:A:246:ASN:ND2	2.34	0.42
1:A:200:ARG:NH2	1:A:215:MET:O	2.52	0.42
1:A:92:GLU:OE1	1:A:119:LYS:HA	2.20	0.42
1:A:8:ASP:OD2	1:A:17:LYS:NZ	2.51	0.42
1:A:111:ILE:C	1:A:111:ILE:HD12	2.38	0.42
1:A:92:GLU:H	1:A:92:GLU:HG2	1.56	0.42
1:A:239:PHE:HE1	1:A:241:MET:CE	2.33	0.42
1:A:195:LEU:HD21	1:A:228:GLY:HA3	2.01	0.42
1:A:160:GLU:H	1:A:160:GLU:CD	2.23	0.41
1:A:101:LYS:HZ3	1:A:112:GLU:CD	2.24	0.41
1:A:15:PHE:HB3	1:A:20:LEU:O	2.21	0.41
1:A:73:TRP:CZ3	1:A:140:LYS:HB3	2.55	0.41
1:A:294:ILE:HD11	1:A:299:LEU:HG	2.03	0.41
1:A:52:VAL:HG22	1:A:99:ILE:HG12	2.02	0.40
1:A:148:SER:HB2	1:A:149:ASP:H	1.79	0.40
1:A:22:ASP:O	1:A:24:THR:N	2.54	0.40
1:A:239:PHE:CE1	1:A:241:MET:HE2	2.56	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	291/305 (95%)	235 (81%)	43 (15%)	13 (4%)	3	3

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	ASP
1	A	135	ASP
1	A	201	PRO
1	A	202	VAL
1	A	224	GLU
1	A	26	ARG
1	A	247	ASN
1	A	4	SER
1	A	231	CYS
1	A	28	LEU
1	A	33	ILE
1	A	34	ASP
1	A	3	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	262/266 (98%)	218 (83%)	44 (17%)	2	4

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	2	PHE
1	A	4	SER
1	A	19	SER
1	A	23	LYS
1	A	26	ARG

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Mol	Chain	Res	Type
1	A	32	TYR
1	A	33	ILE
1	A	45	ILE
1	A	48	SER
1	A	54	LEU
1	A	62	LEU
1	A	63	LEU
1	A	67	SER
1	A	68	LEU
1	A	94	ASP
1	A	97	VAL
1	A	99	ILE
1	A	103	SER
1	A	106	ARG
1	A	111	ILE
1	A	117	LEU
1	A	119	LYS
1	A	120	ILE
1	A	122	ILE
1	A	126	TYR
1	A	140	LYS
1	A	142	LYS
1	A	148	SER
1	A	164	SER
1	A	174	VAL
1	A	184	TRP
1	A	198	VAL
1	A	208	ARG
1	A	210	ARG
1	A	226	LYS
1	A	246	ASN
1	A	247	ASN
1	A	264	ASP
1	A	278	LYS
1	A	281	GLN
1	A	293	GLU
1	A	297	GLU
1	A	299	LEU

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

Mol	Chain	Res	Type
1	A	102	HIS
1	A	110	ASN
1	A	127	ASN
1	A	246	ASN

### 5.3.3 RNA [i](#)

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 carbohydrates 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	BLI	A	300	-	37,37,37	1.89	7 (18%)	45,53,53	1.85	14 (31%)

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	BLI	A	300	-	-	0/24/61/61	0/3/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	BLI	C6'-N2'	-3.21	1.27	1.34
2	A	300	BLI	C02-S1	2.10	1.80	1.79
2	A	300	BLI	O2-S1	2.25	1.45	1.43
2	A	300	BLI	C01-C09	2.44	1.58	1.52
2	A	300	BLI	C6'-N1'	2.52	1.40	1.35
2	A	300	BLI	C6'-N3'	2.71	1.35	1.29
2	A	300	BLI	S1-N3	8.73	1.73	1.62

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	BLI	C2'-C1'-N10	-3.85	105.48	112.83
2	A	300	BLI	C7'-N1'-C6'	-3.65	109.40	119.40
2	A	300	BLI	O1-S1-N3	-3.18	104.16	107.20
2	A	300	BLI	C4-C5-N1	-3.01	112.41	118.06
2	A	300	BLI	O2-S1-N3	-2.86	104.46	107.20
2	A	300	BLI	C5'-C4'-C2'	-2.61	107.32	111.73
2	A	300	BLI	C02-C6B-C5B	-2.09	117.66	120.52
2	A	300	BLI	C03-C06-C1	-2.03	101.12	104.02
2	A	300	BLI	C3'-C7'-N1'	2.26	114.35	111.07
2	A	300	BLI	C4-N3-C2	2.43	117.53	113.66
2	A	300	BLI	C5'-N1'-C7'	2.54	117.26	112.56
2	A	300	BLI	O11-C5-C4	2.54	123.50	118.70
2	A	300	BLI	C4'-C5'-N1'	2.71	115.00	111.07
2	A	300	BLI	O1-S1-C02	4.36	113.45	107.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	BLI	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	299/305 (98%)	1.03	35 (11%) 6 6	2, 5, 22, 47	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	35	GLY	11.6
1	A	5	GLY	7.6
1	A	184	TRP	7.4
1	A	34	ASP	7.1
1	A	289	GLU	6.4
1	A	36	ARG	5.5
1	A	4	SER	5.2
1	A	3	GLY	4.7
1	A	1	THR	4.4
1	A	7	ALA	4.2
1	A	287	PHE	3.9
1	A	185	GLY	3.9
1	A	288	GLY	3.8
1	A	183	THR	3.7
1	A	2	PHE	3.3
1	A	33	ILE	3.1
1	A	232	GLU	2.9
1	A	6	GLU	2.9
1	A	66	ALA	2.9
1	A	299	LEU	2.8
1	A	290	ASP	2.7
1	A	238	PRO	2.7
1	A	296	GLU	2.6
1	A	93	ASN	2.4
1	A	270	TYR	2.4
1	A	298	TYR	2.4
1	A	265	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	240	VAL	2.3
1	A	249	TRP	2.2
1	A	41	SER	2.2
1	A	52	VAL	2.1
1	A	218	ALA	2.1
1	A	68	LEU	2.1
1	A	278	LYS	2.1
1	A	254	ILE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BLI	A	300	34/34	0.83	0.25	0.89	7,16,22,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.