



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:09 AM UTC

PDB ID : 1JWT / pdb_00001jwt
Title : CRYSTAL STRUCTURE OF THROMBIN IN COMPLEX WITH A NOVEL BICYCLIC LACTAM INHIBITOR
Authors : Levesque, S.; St-Denis, Y.; Bachand, B.; Preville, P.; Leblond, L.; Winocour, P.D.; Edmunds, J.J.; Rubin, J.R.; Siddiqui, M.A.
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

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>.

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

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

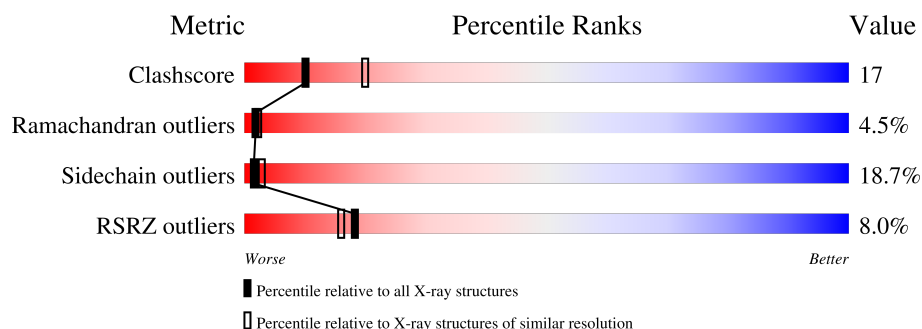
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	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.

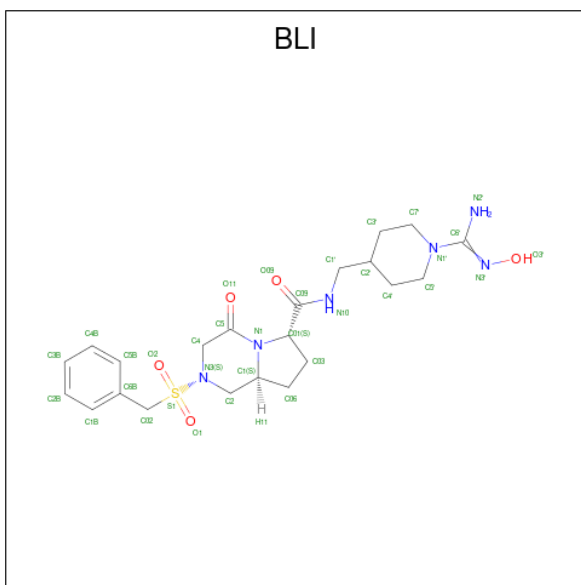
- Molecule 1 is a protein called Prothrombin.

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 (CCD ID: BLI) (formula: C₂₂H₃₂N₆O₅S).

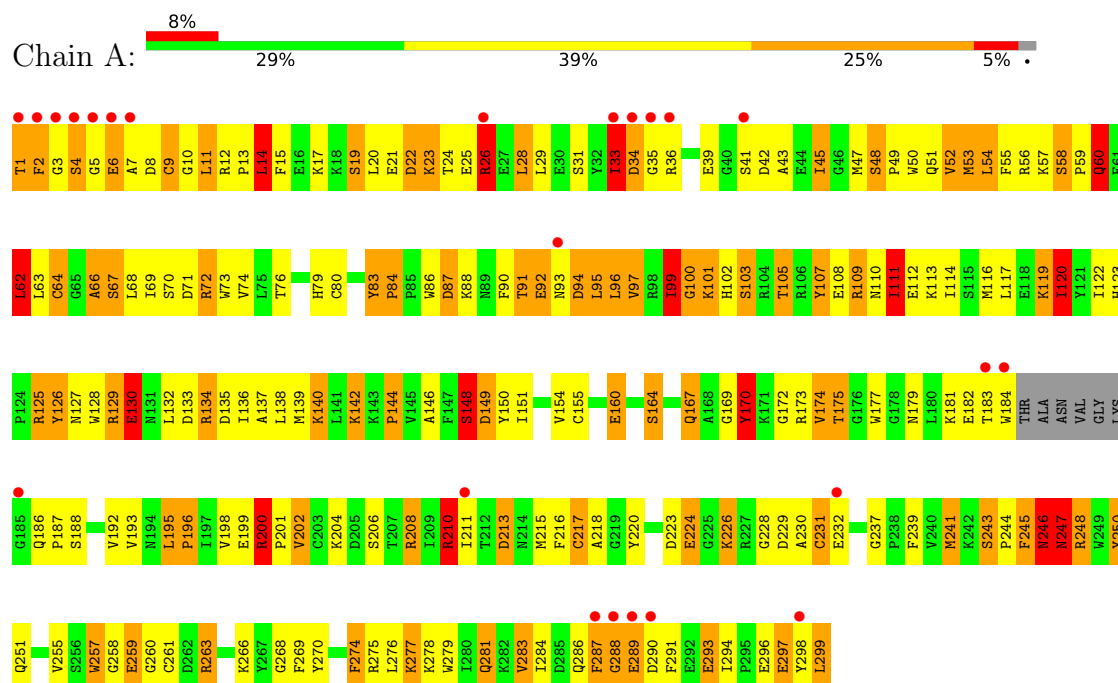


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			34	22	6	5	1		

3 Residue-property plots

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: Prothrombin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	71.54Å 72.18Å 73.41Å 90.00° 100.99° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50 25.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.4 (25.00-2.50) 90.0 (25.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.49 (at 2.50Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.182 , 0.301 0.266 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 34.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	2463	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	1.46	14/2488 (0.6%)	2.57	207/3354 (6.2%)

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

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	ASP	N-CA	6.86	1.55	1.46
1	A	34	ASP	CA-C	6.46	1.61	1.52
1	A	137	ALA	CA-C	-6.34	1.45	1.52
1	A	33	ILE	CA-C	6.07	1.60	1.52
1	A	284	ILE	CA-C	5.81	1.59	1.52
1	A	102	HIS	ND1-CE1	5.81	1.38	1.32
1	A	79	HIS	CE1-NE2	5.53	1.38	1.32
1	A	109	ARG	CA-C	-5.41	1.46	1.52
1	A	199	GLU	CA-C	5.25	1.59	1.52
1	A	79	HIS	CG-CD2	5.22	1.41	1.35
1	A	196	PRO	CA-C	-5.14	1.47	1.52
1	A	111	ILE	CA-C	5.10	1.57	1.52
1	A	224	GLU	CA-C	5.06	1.59	1.52
1	A	79	HIS	ND1-CE1	5.04	1.37	1.32

All (207) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	ILE	N-CA-C	14.04	123.92	112.12
1	A	274	PHE	CA-CB-CG	-11.42	102.38	113.80
1	A	177	TRP	CA-C-N	-10.54	111.44	122.30
1	A	177	TRP	C-N-CA	-10.54	111.44	122.30
1	A	288	GLY	CA-C-N	10.54	140.67	121.70
1	A	288	GLY	C-N-CA	10.54	140.67	121.70
1	A	39	GLU	CA-C-N	-10.22	114.70	121.65
1	A	39	GLU	C-N-CA	-10.22	114.70	121.65
1	A	284	ILE	N-CA-C	10.10	119.91	110.42
1	A	247	ASN	CA-CB-CG	9.98	122.58	112.60
1	A	84	PRO	N-CA-C	9.96	122.85	110.70
1	A	129	ARG	CA-C-N	-9.87	106.01	122.79
1	A	129	ARG	C-N-CA	-9.87	106.01	122.79
1	A	71	ASP	N-CA-C	9.86	123.05	111.71
1	A	258	GLY	CA-C-N	-9.49	109.65	122.85
1	A	258	GLY	C-N-CA	-9.49	109.65	122.85
1	A	72	ARG	N-CA-C	9.20	124.84	111.87
1	A	93	ASN	CB-CA-C	-9.10	92.32	110.42
1	A	232	GLU	N-CA-C	9.06	123.89	110.30
1	A	274	PHE	N-CA-C	9.05	121.14	111.28
1	A	247	ASN	CB-CA-C	9.04	128.41	110.42
1	A	53	MET	CA-C-N	-8.90	111.27	122.84
1	A	53	MET	C-N-CA	-8.90	111.27	122.84
1	A	94	ASP	CA-CB-CG	-8.61	104.00	112.60
1	A	170	TYR	CA-C-N	-8.29	108.55	122.64
1	A	170	TYR	C-N-CA	-8.29	108.55	122.64
1	A	177	TRP	CB-CA-C	-8.02	98.10	111.02
1	A	293	GLU	N-CA-C	8.00	121.43	108.63
1	A	93	ASN	CA-CB-CG	-7.93	104.67	112.60
1	A	19	SER	N-CA-C	7.84	122.28	112.24
1	A	250	TYR	CA-C-N	-7.72	111.88	122.30
1	A	250	TYR	C-N-CA	-7.72	111.88	122.30
1	A	140	LYS	N-CA-C	7.65	122.49	110.17
1	A	206	SER	CA-C-O	7.42	127.62	119.24
1	A	134	ARG	N-CA-C	7.41	121.62	112.58
1	A	87	ASP	CA-CB-CG	-7.40	105.20	112.60
1	A	67	SER	N-CA-C	7.34	120.90	109.52
1	A	148	SER	CA-C-N	-7.24	108.48	121.14
1	A	148	SER	C-N-CA	-7.24	108.48	121.14
1	A	244	PRO	CA-C-O	7.21	129.10	119.00
1	A	87	ASP	N-CA-C	7.12	125.97	110.80
1	A	34	ASP	N-CA-C	7.08	125.89	110.80
1	A	213	ASP	CA-CB-CG	7.06	119.66	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	LYS	N-CA-C	7.04	119.07	110.41
1	A	199	GLU	N-CA-C	6.98	120.50	110.10
1	A	109	ARG	CA-C-N	-6.97	109.77	122.38
1	A	109	ARG	C-N-CA	-6.97	109.77	122.38
1	A	114	ILE	CA-C-N	-6.95	111.68	122.87
1	A	114	ILE	C-N-CA	-6.95	111.68	122.87
1	A	182	GLU	N-CA-C	6.95	119.50	111.02
1	A	109	ARG	N-CA-C	6.88	119.42	111.02
1	A	86	TRP	CB-CA-C	-6.69	102.58	111.74
1	A	11	LEU	CA-C-N	-6.67	111.02	120.49
1	A	11	LEU	C-N-CA	-6.67	111.02	120.49
1	A	200	ARG	N-CA-C	6.67	124.54	109.81
1	A	142	LYS	N-CA-C	6.63	119.49	111.40
1	A	120	ILE	CB-CG1-CD1	-6.63	99.88	113.80
1	A	91	THR	N-CA-C	6.60	118.23	108.60
1	A	97	VAL	N-CA-C	6.58	118.30	107.24
1	A	74	VAL	N-CA-CB	-6.58	104.84	112.34
1	A	293	GLU	CA-CB-CG	6.57	127.23	114.10
1	A	291	PHE	CA-CB-CG	-6.54	107.27	113.80
1	A	174	VAL	N-CA-C	6.52	119.08	108.97
1	A	105	THR	N-CA-CB	-6.48	101.66	110.67
1	A	64	CYS	N-CA-C	6.46	117.00	107.88
1	A	33	ILE	CA-C-N	6.37	133.70	121.54
1	A	33	ILE	C-N-CA	6.37	133.70	121.54
1	A	144	PRO	CA-C-N	-6.34	110.55	121.97
1	A	144	PRO	C-N-CA	-6.34	110.55	121.97
1	A	286	GLN	N-CA-C	6.33	119.47	111.69
1	A	169	GLY	CA-C-O	6.29	125.04	119.56
1	A	90	PHE	N-CA-C	6.26	118.11	110.41
1	A	107	TYR	CA-C-O	6.25	127.73	120.98
1	A	48	SER	N-CA-C	6.24	119.78	109.79
1	A	204	LYS	N-CA-C	6.24	118.88	111.33
1	A	266	LYS	CA-C-O	6.24	127.44	120.70
1	A	217	CYS	CA-C-N	-6.24	112.10	122.21
1	A	217	CYS	C-N-CA	-6.24	112.10	122.21
1	A	246	ASN	CA-C-O	6.20	127.13	120.24
1	A	50	TRP	N-CA-C	6.20	118.84	111.71
1	A	96	LEU	CA-C-N	-6.20	114.56	123.11
1	A	96	LEU	C-N-CA	-6.20	114.56	123.11
1	A	100	GLY	CA-C-O	6.18	126.07	119.03
1	A	43	ALA	N-CA-C	6.17	120.12	110.32
1	A	105	THR	CA-C-O	6.16	125.56	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	PHE	CA-C-N	-6.16	110.05	120.58
1	A	245	PHE	C-N-CA	-6.16	110.05	120.58
1	A	289	GLU	CA-CB-CG	6.16	126.42	114.10
1	A	60	GLN	CA-C-N	-6.16	111.88	123.27
1	A	60	GLN	C-N-CA	-6.16	111.88	123.27
1	A	113	LYS	CA-C-N	-6.16	114.88	123.13
1	A	113	LYS	C-N-CA	-6.16	114.88	123.13
1	A	175	THR	CA-C-O	6.16	127.99	120.60
1	A	6	GLU	CA-C-N	-6.16	112.07	120.44
1	A	6	GLU	C-N-CA	-6.16	112.07	120.44
1	A	154	VAL	CA-C-N	-6.13	112.65	121.42
1	A	154	VAL	C-N-CA	-6.13	112.65	121.42
1	A	62	LEU	CA-C-N	-6.09	111.72	122.26
1	A	62	LEU	C-N-CA	-6.09	111.72	122.26
1	A	202	VAL	N-CA-C	6.08	121.99	109.34
1	A	47	MET	N-CA-C	6.05	119.93	112.54
1	A	260	GLY	CA-C-N	-6.05	114.46	122.99
1	A	260	GLY	C-N-CA	-6.05	114.46	122.99
1	A	261	CYS	N-CA-C	5.95	118.59	108.90
1	A	246	ASN	N-CA-CB	5.94	119.05	110.20
1	A	244	PRO	CB-CA-C	5.93	120.34	111.68
1	A	10	GLY	N-CA-C	5.93	123.24	115.47
1	A	51	GLN	N-CA-C	5.92	118.78	109.96
1	A	45	ILE	CA-C-N	-5.92	112.79	122.20
1	A	45	ILE	C-N-CA	-5.92	112.79	122.20
1	A	83	TYR	CA-CB-CG	-5.91	103.27	113.90
1	A	196	PRO	CA-C-O	-5.91	114.75	122.19
1	A	251	GLN	CA-C-N	-5.90	112.88	122.26
1	A	251	GLN	C-N-CA	-5.90	112.88	122.26
1	A	223	ASP	N-CA-CB	5.89	118.55	110.01
1	A	74	VAL	CA-CB-CG1	5.88	120.40	110.40
1	A	290	ASP	CA-CB-CG	-5.88	106.72	112.60
1	A	284	ILE	N-CA-CB	-5.88	104.01	110.65
1	A	257	TRP	N-CA-C	5.86	118.09	109.24
1	A	243	SER	N-CA-C	5.84	119.79	109.58
1	A	193	VAL	CA-C-N	-5.75	114.94	123.11
1	A	193	VAL	C-N-CA	-5.75	114.94	123.11
1	A	216	PHE	CA-C-N	-5.74	113.59	122.59
1	A	216	PHE	C-N-CA	-5.74	113.59	122.59
1	A	52	VAL	N-CA-C	5.69	117.79	108.97
1	A	170	TYR	N-CA-C	5.66	119.14	110.20
1	A	179	ASN	N-CA-C	5.66	118.27	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	ARG	N-CA-C	5.64	117.92	108.23
1	A	49	PRO	N-CA-C	5.63	121.36	113.53
1	A	80	CYS	O-C-N	5.63	128.09	122.12
1	A	133	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	224	GLU	N-CA-C	5.61	122.75	110.80
1	A	187	PRO	CA-C-N	-5.60	111.34	121.14
1	A	187	PRO	C-N-CA	-5.60	111.34	121.14
1	A	291	PHE	N-CA-C	5.57	118.55	110.42
1	A	110	ASN	N-CA-C	5.56	120.06	113.16
1	A	95	LEU	N-CA-C	5.56	118.69	109.46
1	A	155	CYS	N-CA-C	5.54	118.95	110.20
1	A	188	SER	CA-C-O	5.54	126.17	119.31
1	A	286	GLN	CA-C-O	5.53	126.38	120.24
1	A	140	LYS	CA-C-N	-5.52	112.69	122.74
1	A	140	LYS	C-N-CA	-5.52	112.69	122.74
1	A	7	ALA	CA-C-O	5.51	126.38	120.70
1	A	42	ASP	N-CA-C	5.51	118.07	110.35
1	A	149	ASP	CA-C-O	5.49	126.11	119.31
1	A	248	ARG	N-CA-C	5.47	119.15	109.96
1	A	21	GLU	CA-C-O	-5.47	115.26	121.72
1	A	33	ILE	N-CA-C	5.45	120.67	109.34
1	A	41	SER	N-CA-C	5.45	117.56	110.53
1	A	57	LYS	N-CA-C	5.42	117.64	111.02
1	A	52	VAL	CA-CB-CG1	5.42	119.61	110.40
1	A	109	ARG	CD-NE-CZ	-5.41	116.83	124.40
1	A	164	SER	N-CA-C	5.41	119.57	112.92
1	A	26	ARG	CA-CB-CG	5.40	124.90	114.10
1	A	288	GLY	O-C-N	5.39	129.71	122.70
1	A	246	ASN	N-CA-C	5.38	118.31	111.69
1	A	186	GLN	N-CA-C	5.37	118.43	110.32
1	A	125	ARG	CA-C-N	-5.36	113.95	121.72
1	A	125	ARG	C-N-CA	-5.36	113.95	121.72
1	A	72	ARG	CB-CA-C	-5.36	102.81	111.28
1	A	297	GLU	CB-CA-C	-5.35	101.59	110.68
1	A	175	THR	CA-CB-CG2	5.35	119.59	110.50
1	A	130	GLU	CB-CG-CD	-5.34	103.52	112.60
1	A	146	ALA	N-CA-C	5.34	117.08	108.32
1	A	120	ILE	CA-CB-CG2	5.34	119.58	110.50
1	A	9	CYS	N-CA-C	5.29	117.54	110.35
1	A	195	LEU	CB-CA-C	-5.26	100.53	108.63
1	A	22	ASP	CA-C-N	-5.25	111.90	122.55
1	A	22	ASP	C-N-CA	-5.25	111.90	122.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	GLU	CB-CA-C	-5.24	101.12	111.91
1	A	297	GLU	O-C-N	5.23	127.66	122.12
1	A	125	ARG	N-CA-C	5.20	119.12	112.26
1	A	26	ARG	CD-NE-CZ	5.20	131.68	124.40
1	A	277	LYS	N-CA-C	5.19	117.61	111.33
1	A	14	LEU	N-CA-C	5.19	119.61	113.28
1	A	102	HIS	N-CA-CB	-5.18	101.73	110.49
1	A	223	ASP	N-CA-C	5.18	116.61	111.07
1	A	287	PHE	CA-CB-CG	5.17	118.97	113.80
1	A	12	ARG	N-CA-C	5.17	116.40	109.83
1	A	96	LEU	N-CA-C	5.17	117.99	109.72
1	A	281	GLN	CB-CG-CD	-5.15	103.84	112.60
1	A	183	THR	N-CA-C	5.15	116.82	109.14
1	A	289	GLU	N-CA-CB	5.14	119.25	110.50
1	A	99	ILE	N-CA-C	5.14	115.88	108.48
1	A	79	HIS	CA-C-N	-5.14	113.40	120.28
1	A	79	HIS	C-N-CA	-5.14	113.40	120.28
1	A	199	GLU	O-C-N	-5.11	116.61	122.95
1	A	259	GLU	N-CA-C	5.11	117.25	107.75
1	A	275	ARG	O-C-N	5.11	127.34	122.03
1	A	277	LYS	CA-CB-CG	-5.08	103.94	114.10
1	A	69	ILE	N-CA-C	5.08	118.53	113.71
1	A	137	ALA	CB-CA-C	-5.08	102.83	110.24
1	A	66	ALA	CA-C-N	-5.08	114.62	122.59
1	A	66	ALA	C-N-CA	-5.08	114.62	122.59
1	A	137	ALA	CA-C-N	-5.07	112.97	121.39
1	A	137	ALA	C-N-CA	-5.07	112.97	121.39
1	A	167	GLN	CA-C-O	5.07	126.67	120.99
1	A	172	GLY	CA-C-N	-5.07	113.81	122.33
1	A	172	GLY	C-N-CA	-5.07	113.81	122.33
1	A	289	GLU	CB-CG-CD	5.07	121.21	112.60
1	A	107	TYR	N-CA-C	5.05	116.91	108.23
1	A	13	PRO	CA-C-N	-5.04	112.68	122.06
1	A	13	PRO	C-N-CA	-5.04	112.68	122.06
1	A	95	LEU	CB-CA-C	-5.04	101.54	109.80
1	A	263	ARG	N-CA-C	5.03	117.94	109.95
1	A	58	SER	N-CA-C	5.02	122.22	107.37
1	A	88	LYS	CA-CB-CG	5.00	124.10	114.10

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
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	84	0
2	A	34	0	32	2	0
All	All	2463	0	2404	84	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 (84) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLU:HB2	1:A:9:CYS:HB3	1.69	0.74
1:A:239:PHE:HE1	1:A:241:MET:HE2	1.53	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:257:TRP:HB2	2:A:300:BLI:O11	1.97	0.65
1:A:296:GLU:HA	1:A:299:LEU:HB2	1.79	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
1:A:239:PHE:CE1	1:A:241:MET:HE2	2.33	0.64
1:A:58:SER:HA	1:A:59:PRO:C	2.25	0.61
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: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:53:MET:HE3	1:A:101:LYS:HD3	1.91	0.52
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: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:54:LEU:HD21	1:A:139:MET:HE1	1.95	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:25:GLU:O	1:A:26:ARG:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:111:ILE:HD12	1:A:111:ILE:C	2.38	0.47
1:A:243:SER:CB	1:A:250:TYR:HE2	2.28	0.46
1:A:160:GLU:H	1:A:160:GLU:CD	2.23	0.46
1:A:101:LYS:HZ3	1:A:112:GLU:CD	2.24	0.46
1:A:229:ASP:OD2	2:A:300:BLI:N2'	2.49	0.45
1:A:263:ARG:HE	1:A:263:ARG:HB3	1.60	0.45
1:A:288:GLY:O	1:A:289:GLU:HG2	2.16	0.45
1:A:2:PHE:H	1:A:2:PHE:HD1	1.64	0.45
1:A:127:ASN:HD21	1:A:130:GLU:HB3	1.79	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:210:ARG:HG3	1:A:210:ARG:O	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: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:116:MET:HE2	1:A:116:MET:HB3	1.89	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:195:LEU:HD21	1:A:228:GLY:C	2.45	0.42
1:A:8:ASP:OD2	1:A:17:LYS:NZ	2.51	0.42
1:A:92:GLU:OE1	1:A:119:LYS:HA	2.20	0.42
1:A:92:GLU:H	1:A:92:GLU:HG2	1.56	0.42
1:A:195:LEU:HD21	1:A:228:GLY:HA3	2.01	0.42
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:276:LEU:O	1:A:277:LYS:C	2.63	0.41
1:A:52:VAL:HG22	1:A:99:ILE:HG12	2.02	0.40
1:A:22:ASP:O	1:A:24:THR:N	2.54	0.40
1:A:148:SER:HB2	1:A:149:ASP:H	1.79	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	291/305 (95%)	235 (81%)	43 (15%)	13 (4%)	2 2

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 [i](#)

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%)	213 (81%)	49 (19%)	1 3

All (49) 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	11	LEU
1	A	14	LEU
1	A	19	SER
1	A	23	LYS
1	A	26	ARG
1	A	33	ILE
1	A	45	ILE
1	A	48	SER
1	A	54	LEU
1	A	60	GLN
1	A	62	LEU
1	A	63	LEU
1	A	67	SER
1	A	68	LEU
1	A	92	GLU
1	A	97	VAL
1	A	99	ILE
1	A	103	SER
1	A	105	THR
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	130	GLU
1	A	142	LYS
1	A	148	SER
1	A	160	GLU
1	A	164	SER
1	A	174	VAL
1	A	181	LYS
1	A	184	TRP
1	A	198	VAL
1	A	208	ARG
1	A	210	ARG
1	A	226	LYS
1	A	241	MET
1	A	246	ASN
1	A	247	ASN

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Mol	Chain	Res	Type
1	A	278	LYS
1	A	281	GLN
1	A	283	VAL
1	A	293	GLU
1	A	297	GLU
1	A	299	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	102	HIS
1	A	110	ASN
1	A	246	ASN
1	A	272	HIS

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 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	BLI	A	300	-	35,37,37	1.71	4 (11%)	43,53,53	1.83	11 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BLI	A	300	-	-	8/24/61/61	0/3/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	BLI	S1-N3	7.77	1.73	1.63
2	A	300	BLI	C6'-N2'	-3.49	1.27	1.34
2	A	300	BLI	O2-S1	2.27	1.45	1.43
2	A	300	BLI	C01-C09	2.25	1.58	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	BLI	C2'-C1'-N10	-4.20	105.48	112.77
2	A	300	BLI	O1-S1-C02	4.19	113.45	107.82
2	A	300	BLI	C7'-N1'-C6'	-3.31	109.40	119.17
2	A	300	BLI	O1-S1-N3	-3.20	104.16	107.28
2	A	300	BLI	O2-S1-N3	-2.89	104.46	107.28
2	A	300	BLI	C4-N3-C2	2.84	117.53	113.50
2	A	300	BLI	C02-C6B-C5B	-2.40	117.66	120.56
2	A	300	BLI	O11-C5-C4	2.39	123.50	118.26
2	A	300	BLI	C5'-N1'-C7'	2.24	117.26	112.68
2	A	300	BLI	C4'-C5'-N1'	2.21	115.00	110.66
2	A	300	BLI	C4-C5-N1	-2.20	112.41	116.77

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	BLI	C6B-C02-S1-O2
2	A	300	BLI	S1-C02-C6B-C5B
2	A	300	BLI	N10-C1'-C2'-C3'
2	A	300	BLI	N10-C1'-C2'-C4'

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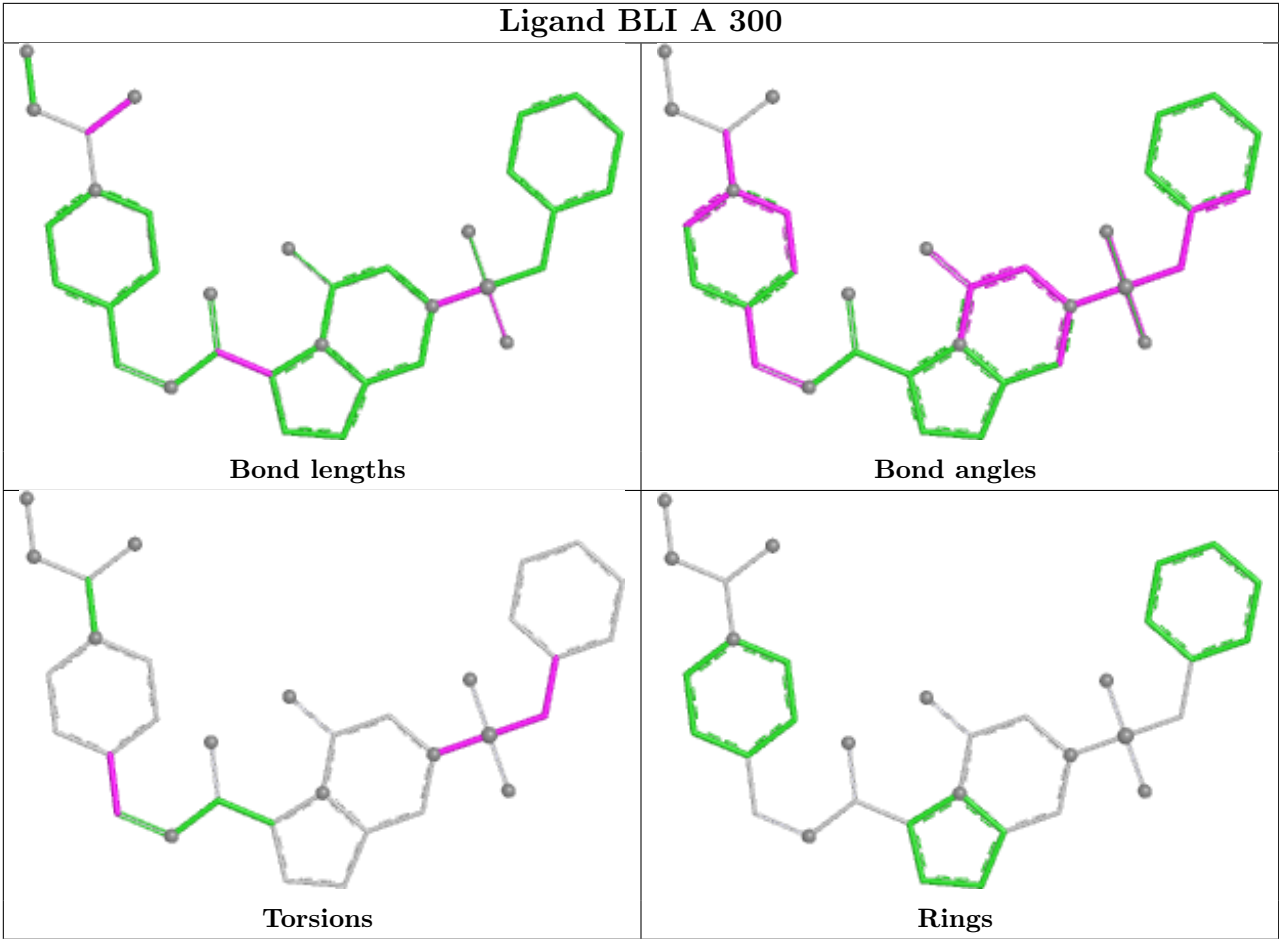
Mol	Chain	Res	Type	Atoms
2	A	300	BLI	C4-N3-S1-O2
2	A	300	BLI	C4-N3-S1-C02
2	A	300	BLI	S1-C02-C6B-C1B
2	A	300	BLI	C6B-C02-S1-N3

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

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	289:GLU	C	290:ASP	N	39.02
1	A	36:ARG	C	37:ILE	N	30.95

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, 95th 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 ²)	Q<0.9
1	A	299/305 (98%)	0.68	24 (8%) 18 16	2, 5, 22, 47	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	35	GLY	10.8
1	A	5	GLY	7.6
1	A	34	ASP	5.9
1	A	4	SER	5.7
1	A	3	GLY	4.7
1	A	289	GLU	4.6
1	A	33	ILE	4.5
1	A	184	TRP	4.4
1	A	7	ALA	3.8
1	A	36	ARG	3.6
1	A	2	PHE	3.5
1	A	93	ASN	3.2
1	A	1	THR	3.0
1	A	232	GLU	3.0
1	A	185	GLY	3.0
1	A	298	TYR	2.8
1	A	41	SER	2.6
1	A	287	PHE	2.5
1	A	183	THR	2.2
1	A	6	GLU	2.2
1	A	211	ILE	2.2
1	A	288	GLY	2.1
1	A	290	ASP	2.1
1	A	26	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](#)

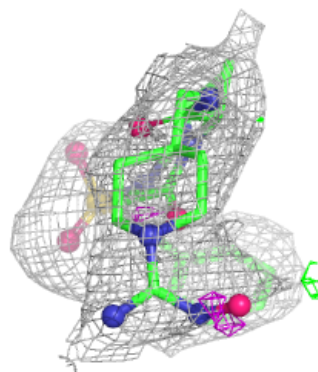
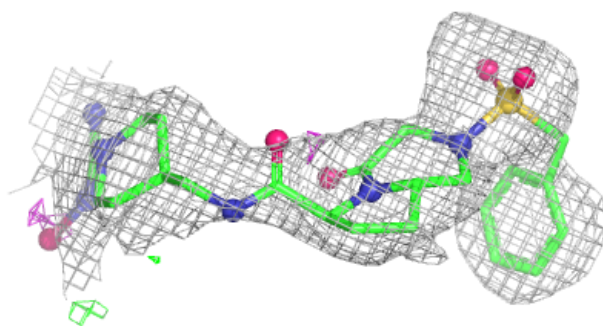
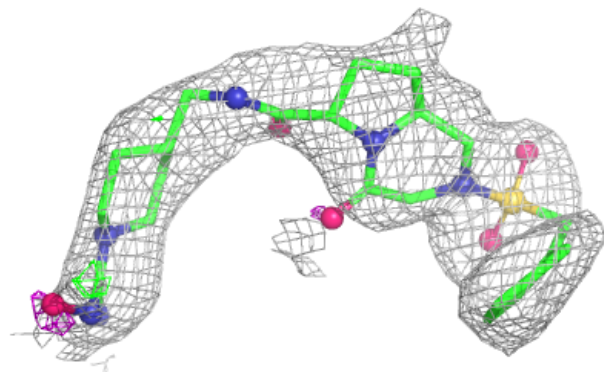
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	BLI	A	300	34/34	0.85	0.13	7,16,22,24	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 BLI A 300:

$2mF_o-DF_c$ (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.