



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:43 AM UTC

PDB ID : 1NRR / pdb_00001nrr
Title : Crystallographic structures of Thrombin complexed with Thrombin receptor peptides: Existence of expected and novel binding modes
Authors : Tulinsky, A.; Mathews, I.I.
Deposited on : 1994-01-18
Resolution : 2.40 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

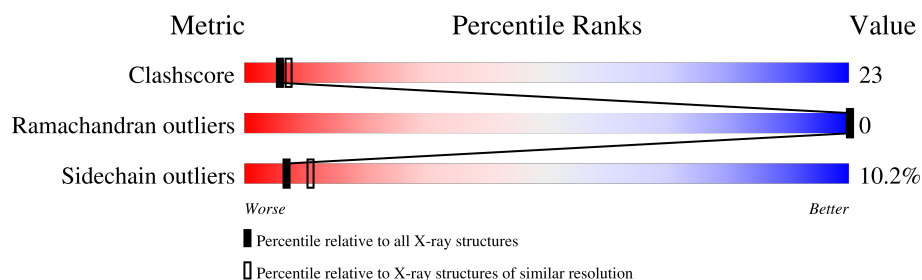
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	36	25% 44% • 28%
2	H	259	36% 42% 16% • •
3	R	18	17% 11% 72%

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
4	OG6	H	301	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2508 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 Thrombin light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	26	Total	C	N	O	S	0	0	0
			209	132	32	44	1			

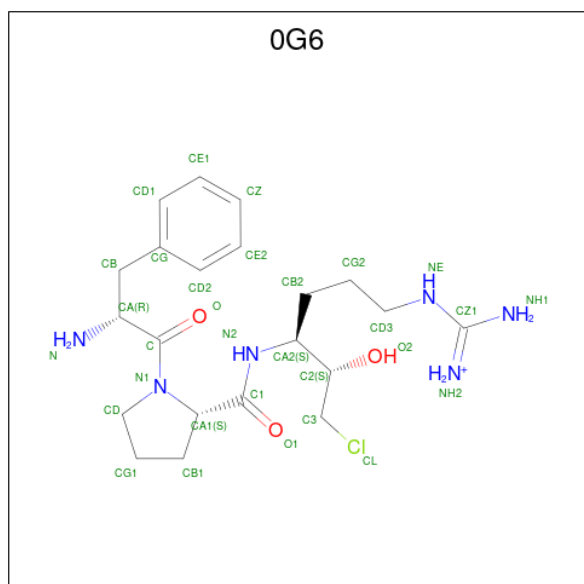
- Molecule 2 is a protein called Thrombin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	249	Total	C	N	O	S	0	0	0
			2014	1285	356	359	14			

- Molecule 3 is a protein called Proteinase-activated receptor 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	R	5	Total	C	N	O	0	0	0
			48	34	6	8			

- Molecule 4 is D-phenylalanyl-N-[(2S,3S)-6-{[amino(iminio)methyl]amino}-1-chloro-2-hydroxyhexan-3-yl]-L-prolinamide (CCD ID: 0G6) (formula: C₂₁H₃₄ClN₆O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			30	21	6	3		

- Molecule 5 is water.

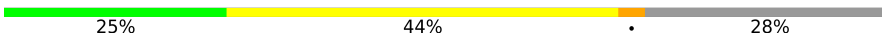
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	24	Total	O	0	0
			24	24		
5	H	180	Total	O	0	0
			180	180		
5	R	3	Total	O	0	0
			3	3		

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. 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. 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.

Note EDS was not executed.

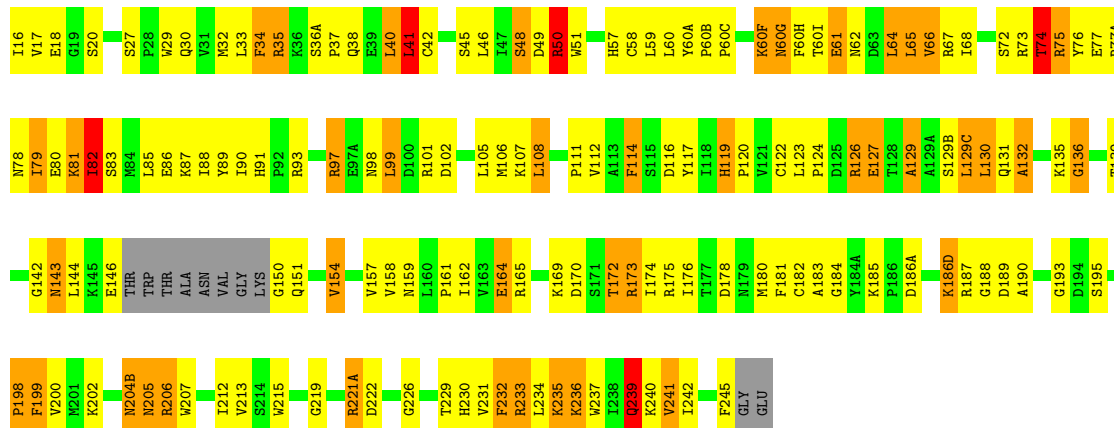
• Molecule 1: Thrombin light chain

Chain L: 



• Molecule 2: Thrombin heavy chain

Chain H: 



• Molecule 3: Proteinase-activated receptor 1

Chain R: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	71.30Å 72.20Å 72.30Å 90.00° 100.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.145 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2508	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0G6

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	L	1.08	0/211	2.36	13/281 (4.6%)
2	H	1.35	3/2066 (0.1%)	2.47	157/2792 (5.6%)
3	R	0.92	0/50	2.16	2/66 (3.0%)
All	All	1.32	3/2327 (0.1%)	2.45	172/3139 (5.5%)

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
2	H	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	102	ASP	N-CA	6.27	1.54	1.46
2	H	114	PHE	C-N	-5.66	1.26	1.33
2	H	182	CYS	N-CA	5.59	1.52	1.45

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	1(A)	ASP	CA-CB-CG	-12.67	99.93	112.60
2	H	170	ASP	CA-CB-CG	-11.61	100.99	112.60
2	H	232	PHE	CA-CB-CG	-11.27	102.53	113.80
2	H	205	ASN	CA-CB-CG	-10.43	102.17	112.60
2	H	206	ARG	NE-CZ-NH2	-10.31	109.92	119.20
2	H	206	ARG	NE-CZ-NH1	9.81	131.31	121.50
2	H	132	ALA	CA-C-O	-9.66	110.57	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	27	SER	CB-CA-C	9.36	125.03	111.27
2	H	30	GLN	OE1-CD-NE2	-9.30	113.30	122.60
2	H	202	LYS	CA-C-O	-8.79	110.95	120.36
2	H	60(G)	ASN	OD1-CG-ND2	-8.64	113.96	122.60
2	H	231	VAL	O-C-N	8.26	129.89	121.87
2	H	74	THR	OG1-CB-CG2	8.24	125.78	109.30
2	H	222	ASP	CA-C-O	-8.20	112.17	121.19
2	H	233	ARG	NE-CZ-NH2	-8.18	111.84	119.20
2	H	74	THR	N-CA-CB	-8.13	98.14	110.33
2	H	60(G)	ASN	CB-CG-ND2	8.00	128.40	116.40
2	H	129	ALA	CA-C-O	7.92	128.95	120.55
2	H	91	HIS	CA-CB-CG	-7.84	105.96	113.80
2	H	132	ALA	O-C-N	7.73	132.38	122.87
2	H	101	ARG	NE-CZ-NH2	-7.70	112.27	119.20
2	H	119	HIS	CB-CA-C	7.64	120.86	109.63
2	H	154	VAL	CA-C-O	-7.62	113.67	121.67
2	H	176	ILE	CA-CB-CG2	7.61	123.44	110.50
2	H	64	LEU	N-CA-C	7.58	120.93	109.41
2	H	74	THR	N-CA-C	7.56	122.81	112.90
2	H	165	ARG	O-C-N	7.46	127.45	120.51
2	H	48	SER	O-C-N	7.45	130.96	122.99
2	H	27	SER	N-CA-CB	-7.39	101.18	110.79
2	H	159	ASN	OD1-CG-ND2	7.38	129.99	122.60
1	L	14(E)	GLU	CB-CG-CD	7.31	125.02	112.60
2	H	82	ILE	CB-CG1-CD1	7.29	129.12	113.80
2	H	240	LYS	CA-C-O	-7.25	113.21	120.82
2	H	198	PRO	CB-CA-C	-7.23	100.66	110.85
3	R	53	GLU	CA-CB-CG	7.17	128.45	114.10
2	H	34	PHE	CA-C-O	7.13	128.06	120.36
2	H	190	ALA	N-CA-C	-7.13	100.51	110.35
2	H	184	GLY	CA-C-O	7.12	132.96	120.57
2	H	239	GLN	O-C-N	7.08	129.46	122.09
2	H	189	ASP	CA-CB-CG	7.03	119.63	112.60
2	H	77	GLU	CA-C-O	6.94	129.35	121.58
2	H	90	ILE	CB-CG1-CD1	6.94	128.37	113.80
2	H	66	VAL	N-CA-CB	-6.92	101.85	111.41
2	H	234	LEU	CA-C-N	6.92	129.86	120.38
2	H	234	LEU	C-N-CA	6.92	129.86	120.38
2	H	60(F)	LYS	CA-C-O	6.91	127.96	120.43
2	H	154	VAL	N-CA-CB	-6.91	100.84	112.44
1	L	14(A)	LYS	CA-C-O	-6.84	111.22	119.49
2	H	207	TRP	CA-C-O	-6.83	112.90	120.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	175	ARG	NE-CZ-NH2	6.83	125.35	119.20
2	H	131	GLN	O-C-N	6.79	131.60	123.24
2	H	75	ARG	CG-CD-NE	6.79	126.94	112.00
2	H	123	LEU	N-CA-CB	6.76	120.33	110.32
2	H	73	ARG	NE-CZ-NH2	6.74	125.27	119.20
2	H	245	PHE	CA-C-O	-6.72	109.37	120.80
2	H	221(A)	ARG	NE-CZ-NH2	6.72	125.25	119.20
2	H	80	GLU	CA-C-N	6.71	132.44	122.99
2	H	80	GLU	C-N-CA	6.71	132.44	122.99
2	H	93	ARG	NE-CZ-NH1	6.66	128.16	121.50
3	R	53	GLU	CA-C-O	6.63	126.43	119.80
2	H	101	ARG	NE-CZ-NH1	6.61	128.11	121.50
2	H	124	PRO	CA-C-O	6.59	129.72	121.67
2	H	126	ARG	CD-NE-CZ	6.59	133.63	124.40
2	H	60(G)	ASN	CA-C-O	-6.55	113.75	120.63
2	H	78	ASN	CA-C-N	6.51	129.35	122.97
2	H	78	ASN	C-N-CA	6.51	129.35	122.97
2	H	213	VAL	CA-C-O	6.47	128.87	120.78
2	H	91	HIS	CA-C-O	6.46	125.14	119.71
2	H	130	LEU	N-CA-CB	-6.40	101.94	110.57
2	H	62	ASN	CA-CB-CG	-6.39	106.21	112.60
2	H	186(A)	ASP	CA-C-O	-6.37	113.80	120.55
2	H	142	GLY	CA-C-O	6.34	130.80	122.75
2	H	97	ARG	NE-CZ-NH2	-6.33	113.50	119.20
2	H	212	ILE	CA-C-O	-6.33	113.65	120.36
2	H	82	ILE	N-CA-CB	6.33	119.85	111.25
2	H	229	THR	CA-CB-OG1	-6.31	100.13	109.60
2	H	154	VAL	O-C-N	6.26	129.98	123.04
2	H	221(A)	ARG	CA-CB-CG	6.17	126.44	114.10
2	H	186(D)	LYS	N-CA-C	-6.09	98.68	108.55
2	H	108	LEU	CA-C-O	-6.09	114.11	121.05
1	L	4	ARG	NE-CZ-NH2	6.06	124.65	119.20
2	H	66	VAL	CB-CA-C	6.04	119.57	110.63
2	H	64	LEU	N-CA-CB	-6.03	101.84	111.43
1	L	6	LEU	CA-C-O	-6.02	112.00	119.28
2	H	175	ARG	CD-NE-CZ	-6.00	116.00	124.40
2	H	205	ASN	OD1-CG-ND2	-5.99	116.61	122.60
2	H	139	THR	CA-CB-OG1	-5.95	100.67	109.60
2	H	27	SER	CA-C-O	5.93	127.81	121.28
2	H	175	ARG	CA-C-N	5.93	131.11	121.62
2	H	175	ARG	C-N-CA	5.93	131.11	121.62
2	H	185	LYS	N-CA-C	-5.93	102.11	110.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	132	ALA	N-CA-CB	5.92	118.78	109.83
1	L	8	GLU	CA-C-N	5.91	129.01	120.38
1	L	8	GLU	C-N-CA	5.91	129.01	120.38
2	H	129(C)	LEU	CA-C-N	-5.90	113.31	122.16
2	H	129(C)	LEU	C-N-CA	-5.90	113.31	122.16
2	H	60	LEU	N-CA-C	5.88	118.32	108.02
2	H	50	ARG	CB-CA-C	-5.86	99.18	109.02
2	H	226	GLY	CA-C-O	-5.84	116.27	121.64
2	H	173	ARG	N-CA-C	-5.83	106.20	113.38
2	H	157	VAL	CA-C-O	-5.80	114.55	121.28
2	H	221(A)	ARG	NE-CZ-NH1	-5.79	115.71	121.50
1	L	14(B)	THR	CA-C-O	-5.79	113.49	119.51
2	H	35	ARG	NE-CZ-NH2	-5.78	114.00	119.20
2	H	97	ARG	NE-CZ-NH1	5.73	127.23	121.50
2	H	77	GLU	CB-CG-CD	5.72	122.32	112.60
2	H	198	PRO	O-C-N	5.71	130.25	123.06
2	H	66	VAL	CA-CB-CG1	5.70	120.09	110.40
2	H	193	GLY	CA-C-N	5.69	131.09	121.14
2	H	193	GLY	C-N-CA	5.69	131.09	121.14
2	H	182	CYS	CA-C-O	-5.64	114.86	121.46
2	H	77	GLU	CA-C-N	-5.64	104.79	117.20
2	H	230	HIS	CE1-NE2-CD2	5.63	114.63	109.00
1	L	14	ASP	N-CA-C	-5.59	103.32	110.53
2	H	102	ASP	CA-C-O	-5.55	115.69	122.41
2	H	68	ILE	N-CA-C	5.51	116.42	108.48
2	H	126	ARG	NE-CZ-NH1	5.51	127.01	121.50
2	H	73	ARG	CA-C-N	5.50	131.65	121.52
2	H	73	ARG	C-N-CA	5.50	131.65	121.52
2	H	176	ILE	CA-C-O	-5.50	114.83	121.54
2	H	41	LEU	CB-CA-C	5.50	120.61	110.88
2	H	35	ARG	CD-NE-CZ	-5.48	116.73	124.40
2	H	41	LEU	N-CA-CB	-5.47	100.48	110.27
2	H	59	LEU	O-C-N	5.42	129.28	122.19
2	H	98	ASN	N-CA-CB	-5.41	100.83	111.60
2	H	199	PHE	CB-CA-C	5.40	118.94	110.19
2	H	40	LEU	N-CA-C	-5.37	101.90	109.96
2	H	219	GLY	N-CA-C	-5.36	102.59	112.62
2	H	231	VAL	CA-C-O	-5.36	115.38	120.95
2	H	199	PHE	O-C-N	-5.34	117.13	123.22
1	L	14(D)	ARG	CA-CB-CG	5.33	124.77	114.10
2	H	204(B)	ASN	CA-CB-CG	-5.33	107.27	112.60
2	H	73	ARG	CA-C-O	5.33	126.59	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	136	GLY	N-CA-C	-5.32	103.23	112.06
2	H	181	PHE	CA-C-N	-5.31	113.89	122.81
2	H	181	PHE	C-N-CA	-5.31	113.89	122.81
1	L	3	LEU	O-C-N	5.30	129.91	123.01
2	H	230	HIS	CG-CD2-NE2	-5.26	101.94	107.20
2	H	183	ALA	CA-C-N	5.26	131.72	121.41
2	H	183	ALA	C-N-CA	5.26	131.72	121.41
2	H	61	GLU	CA-CB-CG	5.25	124.61	114.10
2	H	40	LEU	N-CA-CB	5.23	117.65	109.85
2	H	172	THR	CA-C-O	-5.23	115.65	121.51
2	H	151	GLN	CB-CA-C	5.21	115.72	109.31
2	H	174	ILE	O-C-N	5.21	128.87	122.72
2	H	77(A)	ARG	CA-C-N	-5.20	114.36	122.37
2	H	77(A)	ARG	C-N-CA	-5.20	114.36	122.37
2	H	165	ARG	CD-NE-CZ	5.18	131.65	124.40
2	H	114	PHE	CA-C-O	-5.17	115.37	121.16
2	H	198	PRO	CA-C-O	-5.17	115.28	121.48
1	L	14(B)	THR	O-C-N	5.16	130.96	122.70
2	H	42	CYS	N-CA-CB	-5.16	103.09	111.24
2	H	16	ILE	CA-C-N	5.16	129.59	123.19
2	H	16	ILE	C-N-CA	5.16	129.59	123.19
2	H	60(I)	THR	CA-C-N	5.15	128.55	120.82
2	H	60(I)	THR	C-N-CA	5.15	128.55	120.82
2	H	158	VAL	CA-C-N	5.15	129.62	122.77
2	H	158	VAL	C-N-CA	5.15	129.62	122.77
2	H	143	ASN	O-C-N	5.11	129.20	122.97
2	H	202	LYS	CA-CB-CG	-5.11	103.89	114.10
2	H	48	SER	N-CA-CB	5.10	119.31	111.24
2	H	93	ARG	CA-CB-CG	-5.09	103.91	114.10
2	H	61	GLU	CB-CG-CD	5.06	121.21	112.60
2	H	130	LEU	CA-C-O	-5.05	116.56	122.37
2	H	82	ILE	CA-C-N	-5.03	113.98	122.29
2	H	82	ILE	C-N-CA	-5.03	113.98	122.29
2	H	229	THR	OG1-CB-CG2	5.02	119.34	109.30
1	L	13	GLU	CB-CA-C	-5.02	101.05	109.48
2	H	173	ARG	N-CA-CB	5.02	118.00	110.53
2	H	91	HIS	CA-C-N	5.00	124.78	119.28
2	H	91	HIS	C-N-CA	5.00	124.78	119.28
2	H	131	GLN	CA-C-O	-5.00	115.26	121.11

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	50	ARG	Mainchain

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	L	209	0	205	7	0
2	H	2014	0	1983	88	1
3	R	48	0	43	10	1
4	H	30	0	30	8	0
5	H	180	0	0	13	0
5	L	24	0	0	4	0
5	R	3	0	0	1	0
All	All	2508	0	2261	103	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 23.

All (103) 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)
5:H:454:HOH:O	3:R:51:LYS:HG2	1.47	1.13
3:R:51:LYS:N	3:R:51:LYS:HE2	1.66	1.11
2:H:85:LEU:CD1	2:H:106:MET:HE2	1.88	1.03
2:H:195:SER:OG	4:H:301:OG6:C3	2.06	1.02
2:H:50:ARG:NH1	2:H:107:LYS:HE2	1.85	0.91
2:H:85:LEU:HD13	2:H:106:MET:HE2	1.53	0.91
2:H:60(G):ASN:ND2	5:H:661:HOH:O	1.98	0.89
2:H:75:ARG:HB3	5:H:480:HOH:O	1.76	0.85
2:H:85:LEU:HD11	2:H:106:MET:HE2	1.59	0.83
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	1.87	0.83
2:H:232:PHE:O	2:H:235:LYS:HB2	1.80	0.81
2:H:57:HIS:CE1	4:H:301:OG6:C3	2.66	0.79
2:H:126:ARG:HB3	2:H:127:GLU:OE2	1.83	0.78
2:H:236:LYS:CE	2:H:239:GLN:HE22	1.98	0.76
2:H:236:LYS:HE2	2:H:239:GLN:HE22	1.51	0.75
2:H:195:SER:CB	4:H:301:OG6:C3	2.65	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:81:LYS:HE3	2:H:112:VAL:HG23	1.73	0.70
2:H:85:LEU:HD11	2:H:106:MET:CE	2.23	0.68
2:H:72:SER:OG	2:H:75:ARG:HG3	1.94	0.67
5:H:454:HOH:O	3:R:51:LYS:CD	2.39	0.67
2:H:34:PHE:CZ	2:H:38:GLN:HB3	2.31	0.65
2:H:236:LYS:HE2	2:H:239:GLN:NE2	2.11	0.65
2:H:50:ARG:NH1	2:H:108:LEU:O	2.30	0.64
2:H:204(B):ASN:C	2:H:204(B):ASN:ND2	2.55	0.62
2:H:35:ARG:HB2	2:H:41:LEU:HD13	1.82	0.62
2:H:236:LYS:CE	2:H:239:GLN:NE2	2.61	0.61
2:H:32:MET:HG3	2:H:40:LEU:CD1	2.30	0.61
2:H:129:ALA:O	2:H:130:LEU:HB2	2.01	0.60
2:H:143:ASN:HA	2:H:150:GLY:O	2.02	0.60
2:H:99:LEU:HD21	4:H:301:OG6:HB21	1.84	0.59
1:L:14(C):GLU:O	1:L:14(G):LEU:HD23	2.04	0.58
2:H:204(B):ASN:HD22	2:H:205:ASN:N	2.02	0.57
3:R:55:PHE:N	3:R:55:PHE:CD1	2.69	0.57
1:L:14(J):TYR:HB3	5:L:662:HOH:O	2.04	0.56
2:H:20:SER:HA	5:H:599:HOH:O	2.05	0.56
2:H:132:ALA:CB	2:H:164:GLU:HG3	2.36	0.56
2:H:146:GLU:CD	2:H:221(A):ARG:HE	2.14	0.56
2:H:17:VAL:O	2:H:188:GLY:HA2	2.06	0.55
2:H:50:ARG:NH1	2:H:86:GLU:OE1	2.31	0.55
2:H:204(B):ASN:ND2	2:H:206:ARG:H	2.04	0.54
1:L:14(J):TYR:C	5:L:493:HOH:O	2.50	0.54
2:H:204(B):ASN:HD21	2:H:206:ARG:HB2	1.71	0.54
2:H:60(F):LYS:HD3	2:H:60(H):PHE:CE2	2.41	0.54
2:H:236:LYS:N	2:H:236:LYS:HD2	2.23	0.54
2:H:76:TYR:HB3	3:R:53:GLU:HG2	1.89	0.53
2:H:204(B):ASN:ND2	2:H:206:ARG:HB2	2.24	0.52
2:H:97:ARG:HG2	2:H:97:ARG:NH1	2.25	0.51
2:H:144:LEU:N	2:H:150:GLY:O	2.45	0.50
2:H:49:ASP:HB3	2:H:114:PHE:CZ	2.47	0.50
2:H:237:TRP:O	2:H:241:VAL:HG13	2.12	0.49
3:R:54:PRO:C	3:R:55:PHE:CD1	2.90	0.49
2:H:35:ARG:O	2:H:38:GLN:HA	2.12	0.49
2:H:32:MET:HG3	2:H:40:LEU:HD12	1.94	0.49
2:H:34:PHE:HZ	2:H:38:GLN:HB3	1.73	0.49
2:H:51:TRP:CE2	2:H:242:ILE:HG12	2.48	0.49
1:L:14(H):GLU:OE1	5:L:665:HOH:O	2.19	0.48
2:H:60(F):LYS:HD3	2:H:60(H):PHE:HE2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:195:SER:HB2	4:H:301:OG6:C3	2.42	0.48
3:R:51:LYS:N	3:R:51:LYS:CE	2.58	0.48
2:H:18:GLU:HB2	2:H:188:GLY:HA2	1.95	0.48
2:H:79:ILE:HG23	2:H:117:TYR:CD2	2.49	0.48
1:L:1(A):ASP:HB3	5:H:462:HOH:O	2.14	0.48
2:H:146:GLU:HG3	5:H:635:HOH:O	2.14	0.48
2:H:173:ARG:HG3	5:H:411:HOH:O	2.13	0.47
2:H:49:ASP:OD2	2:H:111:PRO:HB3	2.14	0.47
2:H:60(A):TYR:CZ	2:H:60(C):PRO:HG2	2.49	0.47
2:H:195:SER:CB	4:H:301:OG6:C2	2.87	0.47
2:H:35:ARG:HB2	2:H:41:LEU:CD1	2.43	0.47
2:H:57:HIS:CE1	2:H:195:SER:OG	2.67	0.47
2:H:74:THR:OG1	3:R:51:LYS:HE3	2.15	0.47
2:H:87:LYS:HD3	2:H:88:ILE:N	2.30	0.46
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.50	0.46
2:H:130:LEU:HD23	2:H:162:ILE:CD1	2.44	0.46
5:H:454:HOH:O	3:R:51:LYS:CG	2.20	0.46
2:H:132:ALA:HB2	2:H:164:GLU:HG3	1.97	0.46
4:H:301:OG6:CD1	4:H:301:OG6:HD3	2.46	0.46
2:H:135:LYS:HA	2:H:161:PRO:HA	1.98	0.45
2:H:36(A):SER:HA	2:H:37:PRO:C	2.40	0.45
2:H:130:LEU:HD23	2:H:130:LEU:HA	1.67	0.45
2:H:164:GLU:H	2:H:164:GLU:CD	2.23	0.45
2:H:130:LEU:CD2	2:H:162:ILE:HD13	2.47	0.45
2:H:116:ASP:HB2	5:H:505:HOH:O	2.17	0.45
2:H:58:CYS:O	2:H:60(F):LYS:HD2	2.17	0.44
2:H:198:PRO:HB2	2:H:200:VAL:HG13	1.99	0.44
2:H:60(B):PRO:N	2:H:60(C):PRO:HD2	2.33	0.43
2:H:236:LYS:HE3	2:H:236:LYS:HA	2.00	0.43
2:H:97:ARG:HD2	5:H:408:HOH:O	2.18	0.43
2:H:105:LEU:HD13	2:H:241:VAL:HG22	1.99	0.43
2:H:215:TRP:CE3	4:H:301:OG6:HD2	2.53	0.43
2:H:65:LEU:HG	2:H:82:ILE:HG22	2.01	0.42
3:R:52:TYR:HB2	5:R:637:HOH:O	2.19	0.42
1:L:10:LYS:NZ	5:L:457:HOH:O	2.52	0.42
2:H:97:ARG:HG2	2:H:97:ARG:HH11	1.85	0.42
2:H:67:ARG:HG2	2:H:82:ILE:HG23	2.01	0.42
2:H:178:ASP:O	2:H:233:ARG:HD2	2.20	0.42
2:H:119:HIS:HA	2:H:120:PRO:HD3	1.95	0.42
2:H:236:LYS:CE	2:H:236:LYS:HA	2.50	0.41
2:H:46:LEU:HD11	2:H:48:SER:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:87:LYS:HD2	2:H:89:TYR:CZ	2.55	0.41
1:L:1:CYS:C	2:H:122:CYS:SG	3.04	0.41
2:H:29:TRP:O	2:H:45:SER:HA	2.21	0.41
2:H:186(D):LYS:NZ	5:H:499:HOH:O	2.48	0.41
2:H:172:THR:O	5:H:427:HOH:O	2.22	0.41

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)
2:H:75:ARG:NE	3:R:53:GLU:OE1[2_555]	2.19	0.01

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	L	24/36 (67%)	23 (96%)	1 (4%)	0	100	100
2	H	245/259 (95%)	235 (96%)	10 (4%)	0	100	100
3	R	3/18 (17%)	2 (67%)	1 (33%)	0	100	100
All	All	272/313 (87%)	260 (96%)	12 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	L	23/31 (74%)	23 (100%)	0	100	100
2	H	217/225 (96%)	193 (89%)	24 (11%)	6	9
3	R	5/18 (28%)	4 (80%)	1 (20%)	1	2
All	All	245/274 (89%)	220 (90%)	25 (10%)	7	11

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	33	LEU
2	H	41	LEU
2	H	61	GLU
2	H	64	LEU
2	H	65	LEU
2	H	66	VAL
2	H	74	THR
2	H	79	ILE
2	H	81	LYS
2	H	82	ILE
2	H	83	SER
2	H	99	LEU
2	H	127	GLU
2	H	129(B)	SER
2	H	129(C)	LEU
2	H	154	VAL
2	H	164	GLU
2	H	169	LYS
2	H	180	MET
2	H	187	ARG
2	H	235	LYS
2	H	236	LYS
2	H	239	GLN
2	H	241	VAL
3	R	51	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	78	ASN
2	H	156	GLN
2	H	179	ASN
2	H	204(B)	ASN

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Mol	Chain	Res	Type
2	H	239	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 ⓘ

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	$\# Z > 2$
4	OG6	H	301	2	30,31,32	2.31	3 (10%)	37,41,42	1.58	6 (16%)

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
4	OG6	H	301	2	1/1/8/10	2/31/41/43	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	301	0G6	C3-C2	-9.49	1.24	1.51
4	H	301	0G6	O2-C2	-6.76	1.25	1.43
4	H	301	0G6	CD1-CG	2.39	1.43	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	301	0G6	NE-CZ1-NH2	-4.13	113.59	120.67
4	H	301	0G6	O2-C2-C3	3.54	120.28	109.68
4	H	301	0G6	C2-CA2-N2	2.49	115.43	110.90
4	H	301	0G6	CE2-CZ-CE1	-2.45	116.52	119.87
4	H	301	0G6	CA2-N2-C1	-2.35	119.16	123.25
4	H	301	0G6	CZ-CE2-CD2	2.17	122.91	120.24

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	H	301	0G6	C2

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	301	0G6	C3-C2-CA2-N2
4	H	301	0G6	C3-C2-CA2-CB2

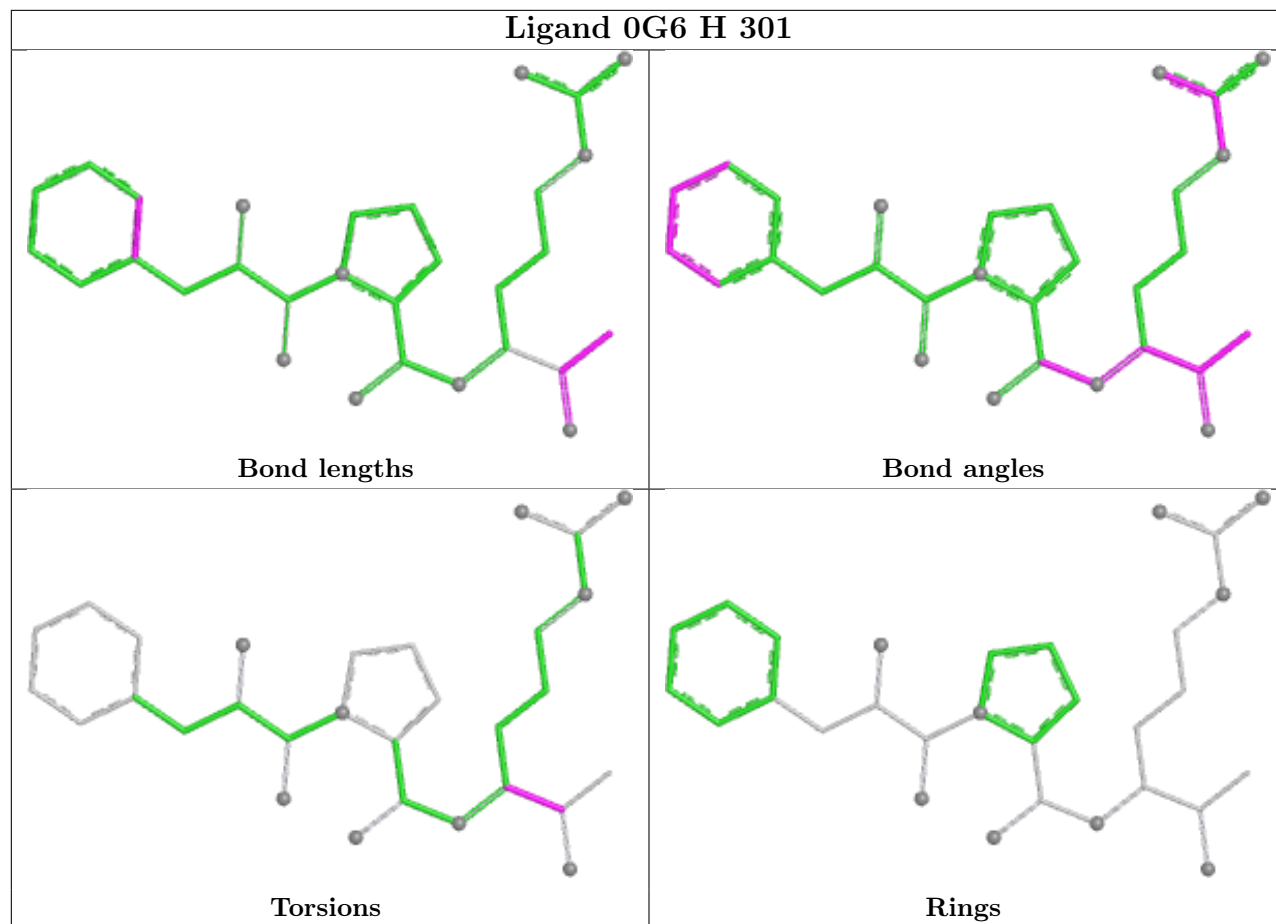
There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	301	0G6	8	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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.