



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:35 PM UTC

PDB ID : 1AY6 / pdb_00001ay6
Title : THROMBIN INHIBITOR FROM THEONALLA, CYCLOTHEANAMIDE-BASED MACROCYCLIC TRIPEPTIDE MOTIF
Authors : Ganesh, V.; Maryanoff, B.E.; Tulinsky, A.
Deposited on : 1997-11-14
Resolution : 1.80 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

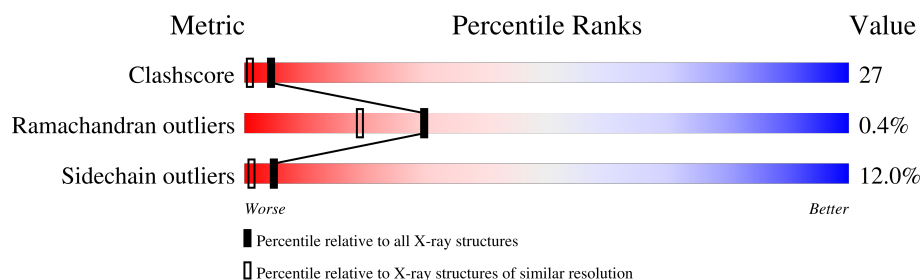
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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	19% 39% 17% 6% 19%
2	H	259	31% 47% 16% . .
3	I	13	23% 8% 38% 8% 23%

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
3	TYS	I	63	-	-	X	-
4	1ZV	H	5	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2568 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	29	Total	C	N	O	S	0	0	0
			235	147	38	49	1			

- Molecule 2 is a protein called THROMBIN HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	252	Total	C	N	O	S	0	0	0
			2030	1294	358	364	14			

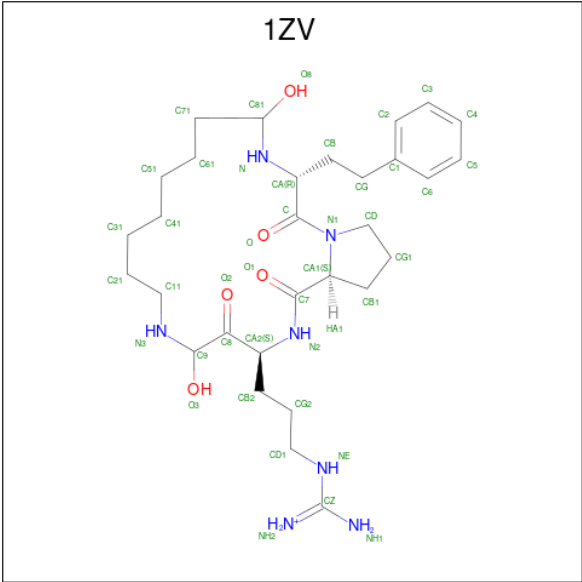
- Molecule 3 is a protein called HIRUGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	10	Total	C	N	O	S	0	0	0
			85	53	10	21	1			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	52	ACE	-	insertion	UNP P01050
I	53	ASN	-	insertion	UNP P01050
I	54	GLU	-	insertion	UNP P01050

- Molecule 4 is amino({3-[(3R,5R,14S,16S,21aR)-5,14-dihydroxy-1,4,17-trioxo-16-(2-phenylethyl)icosahydro-1H-pyrrolo[1,2-d][1,4,7,11]tetraazacyclononadecin-3-yl]propyl}amino)methaniminium (CCD ID: 1ZV) (formula: C₃₀H₅₀N₇O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			42	30	7	5		

- Molecule 5 is water.

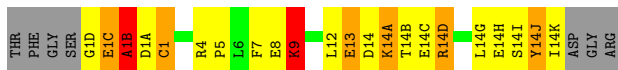
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	15	Total	O	0
			15	15	
5	H	160	Total	O	0
			160	160	
5	I	1	Total	O	0
			1	1	

3 Residue-property plots

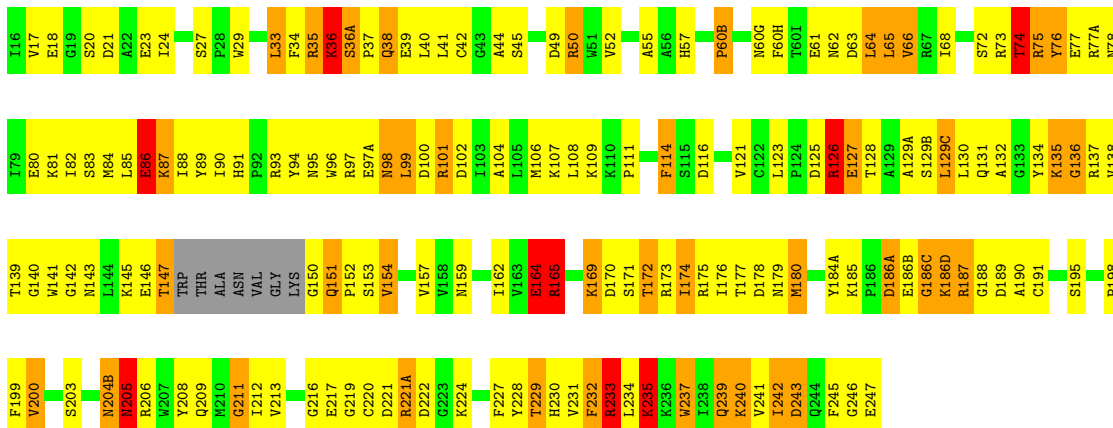
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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



• Molecule 2: THROMBIN HEAVY CHAIN



- Molecule 3: HIRUGEN



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	71.08Å 72.14Å 72.82Å 90.00° 100.80° 90.00°	Depositor
Resolution (Å)	7.00 – 1.80	Depositor
% Data completeness (in resolution range)	75.0 (7.00-1.80)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	0.12	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.166 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2568	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

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: TYS, 1ZV

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	1.44	1/237 (0.4%)	2.82	26/315 (8.3%)
2	H	1.75	22/2082 (1.1%)	2.74	196/2812 (7.0%)
3	I	1.01	0/69	2.45	5/89 (5.6%)
All	All	1.70	23/2388 (1.0%)	2.74	227/3216 (7.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	211	GLY	N-CA	10.31	1.55	1.45
2	H	78	ASN	N-CA	9.21	1.56	1.46
2	H	200	VAL	N-CA	8.31	1.55	1.46
2	H	137	ARG	NE-CZ	6.99	1.40	1.33
2	H	159	ASN	C-N	-6.90	1.25	1.33
2	H	97	ARG	CD-NE	6.65	1.55	1.46
2	H	198	PRO	CA-CB	6.24	1.60	1.54
2	H	190	ALA	CA-C	6.24	1.61	1.53
2	H	129(C)	LEU	C-N	-6.04	1.26	1.33
2	H	224	LYS	CA-C	5.69	1.59	1.52
2	H	230	HIS	N-CA	5.59	1.53	1.46
2	H	190	ALA	C-N	-5.57	1.26	1.33
2	H	80	GLU	C-O	5.54	1.30	1.23
2	H	173	ARG	NE-CZ	5.43	1.39	1.33
2	H	24	ILE	CA-CB	5.38	1.59	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	55	ALA	N-CA	5.29	1.52	1.46
1	L	12	LEU	CA-C	5.23	1.58	1.52
2	H	136	GLY	CA-C	5.21	1.58	1.52
2	H	77(A)	ARG	C-O	5.15	1.30	1.24
2	H	172	THR	CA-CB	5.15	1.63	1.53
2	H	74	THR	CA-CB	5.12	1.61	1.53
2	H	33	LEU	CA-C	5.09	1.59	1.52
2	H	77(A)	ARG	N-CA	-5.03	1.39	1.46

All (227) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	93	ARG	CD-NE-CZ	19.94	152.32	124.40
2	H	243	ASP	CA-CB-CG	14.26	126.86	112.60
2	H	205	ASN	OD1-CG-ND2	12.99	135.59	122.60
2	H	97	ARG	CD-NE-CZ	-12.39	107.05	124.40
2	H	205	ASN	CB-CA-C	12.24	129.67	111.80
2	H	205	ASN	N-CA-CB	-12.00	93.96	111.84
2	H	233	ARG	NE-CZ-NH1	11.66	133.16	121.50
1	L	14(D)	ARG	N-CA-CB	11.37	127.90	110.28
2	H	74	THR	N-CA-C	11.35	127.26	113.41
2	H	44	ALA	O-C-N	11.23	134.72	123.04
2	H	77(A)	ARG	CA-C-N	-11.05	105.10	122.67
2	H	77(A)	ARG	C-N-CA	-11.05	105.10	122.67
1	L	1(A)	ASP	CA-CB-CG	-10.74	101.86	112.60
2	H	97	ARG	CB-CG-CD	10.53	135.51	111.30
2	H	205	ASN	CA-CB-CG	10.40	123.00	112.60
2	H	186(A)	ASP	CA-CB-CG	-10.38	102.22	112.60
2	H	74	THR	N-CA-CB	-10.26	95.49	110.47
2	H	190	ALA	N-CA-C	-10.19	96.80	110.55
2	H	77(A)	ARG	CA-C-O	-9.98	106.23	120.51
2	H	101	ARG	NE-CZ-NH2	-9.93	110.26	119.20
2	H	38	GLN	OE1-CD-NE2	9.88	132.48	122.60
2	H	154	VAL	N-CA-CB	-9.77	96.02	112.44
2	H	205	ASN	CA-C-O	9.59	132.67	121.54
2	H	206	ARG	NE-CZ-NH2	-9.39	110.75	119.20
2	H	206	ARG	NE-CZ-NH1	9.29	130.79	121.50
2	H	140	GLY	CA-C-O	9.07	131.12	121.87
2	H	78	ASN	CA-CB-CG	9.05	121.65	112.60
2	H	123	LEU	CB-CA-C	9.02	120.40	109.31
2	H	212	ILE	CA-C-O	-8.79	110.38	120.67
2	H	93	ARG	NE-CZ-NH1	-8.78	112.72	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	97(A)	GLU	CA-CB-CG	8.68	131.47	114.10
2	H	204(B)	ASN	CA-C-N	8.66	134.46	122.07
2	H	204(B)	ASN	C-N-CA	8.66	134.46	122.07
2	H	175	ARG	CA-C-N	8.54	132.78	120.91
2	H	175	ARG	C-N-CA	8.54	132.78	120.91
2	H	205	ASN	CB-CG-OD1	-8.45	103.89	120.80
2	H	36	LYS	CG-CD-CE	8.42	130.67	111.30
2	H	132	ALA	CA-C-O	-8.30	111.46	120.92
2	H	231	VAL	O-C-N	8.28	130.03	121.91
2	H	27	SER	CB-CA-C	8.20	123.32	111.27
2	H	173	ARG	CG-CD-NE	8.19	130.02	112.00
2	H	176	ILE	CA-CB-CG2	8.16	124.36	110.50
2	H	231	VAL	CA-C-O	-8.13	112.55	121.17
2	H	151	GLN	CB-CA-C	8.10	121.04	108.88
2	H	216	GLY	CA-C-O	-8.05	113.79	121.60
2	H	142	GLY	CA-C-O	7.97	132.87	122.75
2	H	173	ARG	NE-CZ-NH2	7.95	126.35	119.20
2	H	127	GLU	CB-CG-CD	7.92	126.07	112.60
2	H	27	SER	O-C-N	-7.91	114.82	121.23
1	L	14(A)	LYS	CA-C-O	-7.87	109.96	119.49
2	H	246	GLY	O-C-N	7.83	132.88	122.70
2	H	186(D)	LYS	N-CA-C	-7.79	96.76	108.99
2	H	233	ARG	NE-CZ-NH2	-7.71	112.26	119.20
2	H	52	VAL	O-C-N	7.69	131.33	123.10
2	H	126	ARG	NE-CZ-NH2	-7.57	112.39	119.20
2	H	94	TYR	CA-C-O	-7.51	112.78	120.96
2	H	127	GLU	CA-CB-CG	7.45	129.00	114.10
2	H	229	THR	CA-CB-CG2	7.44	123.15	110.50
2	H	227	PHE	CA-CB-CG	-7.41	106.39	113.80
1	L	4	ARG	NE-CZ-NH2	7.41	125.87	119.20
2	H	154	VAL	CA-CB-CG1	7.38	122.95	110.40
2	H	38	GLN	O-C-N	7.33	131.62	123.04
2	H	186(D)	LYS	O-C-N	7.32	131.60	123.33
2	H	139	THR	O-C-N	-7.29	114.81	123.27
2	H	234	LEU	CA-C-N	7.25	130.31	120.38
2	H	234	LEU	C-N-CA	7.25	130.31	120.38
2	H	221(A)	ARG	CA-C-O	-7.12	112.73	120.92
1	L	14(D)	ARG	CD-NE-CZ	-7.10	114.46	124.40
2	H	221(A)	ARG	NE-CZ-NH1	-7.10	114.40	121.50
1	L	8	GLU	O-C-N	7.10	129.47	122.09
2	H	44	ALA	CA-C-O	-7.08	113.53	121.25
1	L	14(C)	GLU	CA-C-O	-7.07	112.11	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	64	LEU	CB-CA-C	7.03	123.46	110.10
2	H	157	VAL	CA-C-O	-6.99	113.18	121.28
2	H	159	ASN	CA-C-O	-6.94	112.70	120.54
2	H	74	THR	CA-CB-OG1	-6.93	99.20	109.60
2	H	137	ARG	NE-CZ-NH1	-6.93	114.57	121.50
2	H	98	ASN	CA-C-O	-6.90	111.97	119.08
2	H	40	LEU	O-C-N	6.85	131.05	123.04
2	H	126	ARG	NE-CZ-NH1	6.82	128.32	121.50
1	L	1	CYS	CA-C-O	6.78	128.76	121.44
2	H	179	ASN	OD1-CG-ND2	6.76	129.36	122.60
2	H	151	GLN	CA-CB-CG	-6.72	100.65	114.10
2	H	187	ARG	CD-NE-CZ	-6.72	114.99	124.40
2	H	104	ALA	O-C-N	6.64	130.84	123.33
2	H	127	GLU	CA-C-O	6.64	127.61	120.24
2	H	205	ASN	O-C-N	-6.60	113.76	122.40
2	H	61	GLU	CB-CG-CD	6.58	123.78	112.60
2	H	220	CYS	CA-C-O	-6.56	112.21	120.28
2	H	86	GLU	CG-CD-OE1	-6.54	103.35	118.40
2	H	205	ASN	CA-C-N	6.53	133.74	122.64
2	H	205	ASN	C-N-CA	6.53	133.74	122.64
2	H	186(D)	LYS	CA-C-O	-6.51	113.69	120.99
2	H	129(A)	ALA	CA-C-O	-6.51	113.65	120.55
2	H	45	SER	CA-C-O	6.50	128.60	121.06
2	H	141	TRP	CA-C-O	-6.48	112.30	119.95
2	H	213	VAL	CA-C-N	-6.47	112.86	122.56
2	H	213	VAL	C-N-CA	-6.47	112.86	122.56
1	L	14(D)	ARG	NE-CZ-NH2	-6.47	113.38	119.20
2	H	126	ARG	CA-C-N	6.45	131.61	120.58
2	H	126	ARG	C-N-CA	6.45	131.61	120.58
2	H	64	LEU	N-CA-C	6.43	118.96	109.24
2	H	74	THR	OG1-CB-CG2	6.42	122.15	109.30
1	L	1(B)	ALA	CA-C-O	6.41	129.68	120.51
2	H	173	ARG	CD-NE-CZ	-6.39	115.45	124.40
2	H	60(B)	PRO	CB-CA-C	6.39	118.71	110.92
2	H	100	ASP	CA-CB-CG	-6.38	106.22	112.60
2	H	20	SER	O-C-N	6.37	130.42	123.10
2	H	27	SER	CA-C-O	6.36	128.28	121.28
1	L	1(A)	ASP	O-C-N	6.29	132.77	122.70
2	H	84	MET	O-C-N	6.29	131.21	123.10
2	H	135	LYS	CA-C-N	6.25	128.04	122.47
2	H	135	LYS	C-N-CA	6.25	128.04	122.47
2	H	52	VAL	CA-C-O	-6.24	113.68	120.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	21	ASP	CA-C-O	-6.22	114.78	121.56
2	H	77(A)	ARG	NE-CZ-NH2	-6.20	113.62	119.20
2	H	208	TYR	O-C-N	6.19	131.27	123.23
2	H	35	ARG	NE-CZ-NH2	-6.18	113.64	119.20
2	H	239	GLN	CA-C-O	6.17	127.50	120.90
2	H	60(G)	ASN	OD1-CG-ND2	-6.16	116.44	122.60
2	H	68	ILE	CA-C-N	6.11	130.80	121.51
2	H	68	ILE	C-N-CA	6.11	130.80	121.51
2	H	229	THR	CA-CB-OG1	-6.10	100.45	109.60
2	H	245	PHE	CA-C-N	-6.10	109.45	121.41
2	H	245	PHE	C-N-CA	-6.10	109.45	121.41
2	H	35	ARG	CA-C-N	6.10	128.36	120.44
2	H	35	ARG	C-N-CA	6.10	128.36	120.44
2	H	97(A)	GLU	CA-C-N	-6.09	111.20	121.18
2	H	97(A)	GLU	C-N-CA	-6.09	111.20	121.18
2	H	212	ILE	O-C-N	6.08	129.74	123.18
2	H	66	VAL	CA-CB-CG1	6.05	120.69	110.40
2	H	173	ARG	NH1-CZ-NH2	-6.05	111.44	119.30
2	H	232	PHE	CA-CB-CG	-6.01	107.79	113.80
2	H	164	GLU	CA-C-N	5.99	129.83	120.97
2	H	164	GLU	C-N-CA	5.99	129.83	120.97
2	H	165	ARG	CA-CB-CG	5.97	126.04	114.10
2	H	165	ARG	N-CA-CB	5.96	121.35	110.08
2	H	164	GLU	CA-C-O	-5.95	114.60	121.15
2	H	38	GLN	CG-CD-NE2	-5.92	107.52	116.40
2	H	80	GLU	O-C-N	-5.91	116.28	122.96
2	H	82	ILE	O-C-N	-5.91	116.47	123.03
3	I	60	PRO	CA-C-O	5.89	127.45	121.27
2	H	146	GLU	CB-CG-CD	5.85	122.55	112.60
1	L	1(C)	GLU	CG-CD-OE2	-5.85	104.95	118.40
2	H	170	ASP	CA-C-O	-5.84	111.46	119.12
2	H	143	ASN	OD1-CG-ND2	-5.84	116.76	122.60
2	H	237	TRP	CA-C-O	-5.84	114.36	120.55
2	H	189	ASP	CA-C-N	5.83	133.57	121.32
2	H	189	ASP	C-N-CA	5.83	133.57	121.32
2	H	235	LYS	CA-CB-CG	5.82	125.73	114.10
2	H	76	TYR	N-CA-C	-5.80	99.67	108.67
2	H	145	LYS	O-C-N	5.80	129.89	123.33
2	H	100	ASP	O-C-N	5.79	129.81	123.04
1	L	4	ARG	NH1-CZ-NH2	-5.78	111.79	119.30
2	H	60(G)	ASN	CB-CG-ND2	5.77	125.06	116.40
2	H	147	THR	CA-C-O	5.77	130.61	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	14(D)	ARG	CA-C-O	-5.75	113.36	119.97
2	H	138	VAL	O-C-N	5.71	129.02	123.03
2	H	128	THR	CA-C-N	5.68	127.82	120.44
2	H	128	THR	C-N-CA	5.68	127.82	120.44
2	H	174	ILE	CB-CG1-CD1	5.66	125.69	113.80
2	H	217	GLU	CB-CA-C	5.63	119.85	111.17
2	H	208	TYR	CA-C-N	-5.60	114.97	122.42
2	H	208	TYR	C-N-CA	-5.60	114.97	122.42
2	H	186(C)	GLY	N-CA-C	5.60	122.56	114.10
2	H	180	MET	CA-C-O	-5.59	114.57	121.06
2	H	139	THR	CA-CB-OG1	-5.58	101.22	109.60
2	H	86	GLU	CG-CD-OE2	5.58	131.24	118.40
1	L	14	ASP	CA-C-O	5.57	128.38	121.81
1	L	9	LYS	CA-C-O	-5.56	112.76	119.49
2	H	137	ARG	NH1-CZ-NH2	5.54	126.50	119.30
2	H	208	TYR	CA-C-O	-5.54	114.72	120.70
1	L	14(J)	TYR	N-CA-C	-5.53	103.85	111.81
2	H	171	SER	N-CA-C	-5.51	106.23	113.17
2	H	101	ARG	NE-CZ-NH1	5.49	126.99	121.50
3	I	57	GLU	CA-C-O	5.48	127.30	121.05
2	H	187	ARG	CG-CD-NE	-5.44	100.03	112.00
2	H	27	SER	N-CA-CB	-5.43	103.73	110.79
2	H	114	PHE	CB-CA-C	5.42	120.80	109.68
1	L	14(B)	THR	CA-C-O	-5.42	112.91	119.03
2	H	50	ARG	CA-CB-CG	5.40	124.90	114.10
1	L	14(D)	ARG	CB-CG-CD	5.37	123.64	111.30
2	H	116	ASP	CA-CB-CG	5.36	117.96	112.60
2	H	102	ASP	N-CA-CB	-5.36	102.86	110.58
2	H	205	ASN	N-CA-C	5.35	118.82	111.54
2	H	95	ASN	CA-C-O	-5.34	115.41	121.39
2	H	98	ASN	O-C-N	5.32	129.22	122.04
2	H	90	ILE	CA-C-N	5.31	127.87	120.65
2	H	90	ILE	C-N-CA	5.31	127.87	120.65
2	H	66	VAL	N-CA-CB	-5.30	104.04	111.25
2	H	233	ARG	NH1-CZ-NH2	-5.30	112.41	119.30
2	H	153	SER	CA-C-O	5.27	125.77	119.60
2	H	64	LEU	O-C-N	5.26	129.54	123.17
1	L	13	GLU	CA-CB-CG	5.25	124.60	114.10
1	L	9	LYS	CA-C-N	5.24	130.47	122.29
1	L	9	LYS	C-N-CA	5.24	130.47	122.29
1	L	14(D)	ARG	NE-CZ-NH1	5.23	126.73	121.50
2	H	245	PHE	CA-C-O	-5.23	113.01	119.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	232	PHE	N-CA-C	5.22	116.97	111.28
2	H	179	ASN	CB-CG-OD1	-5.22	110.36	120.80
2	H	97	ARG	CB-CA-C	-5.22	102.13	110.79
2	H	73	ARG	CA-C-O	5.21	126.30	120.82
1	L	14(A)	LYS	CA-CB-CG	5.21	124.51	114.10
2	H	77(A)	ARG	NH1-CZ-NH2	5.19	126.05	119.30
2	H	33	LEU	CB-CA-C	5.18	118.88	110.22
2	H	204(B)	ASN	OD1-CG-ND2	5.18	127.78	122.60
2	H	42	CYS	N-CA-CB	-5.16	100.88	111.87
2	H	242	ILE	O-C-N	5.16	128.65	121.84
1	L	7	PHE	CA-C-O	-5.14	113.16	120.51
3	I	57	GLU	O-C-N	-5.13	116.96	123.01
2	H	159	ASN	CA-CB-CG	-5.12	107.48	112.60
1	L	14(J)	TYR	CA-CB-CG	5.11	123.09	113.90
2	H	138	VAL	CA-C-O	-5.10	114.59	121.32
2	H	87	LYS	N-CA-CB	-5.10	103.14	111.24
2	H	78	ASN	CA-C-N	5.09	131.14	121.97
2	H	78	ASN	C-N-CA	5.09	131.14	121.97
2	H	151	GLN	OE1-CD-NE2	5.09	127.69	122.60
2	H	60(H)	PHE	CA-C-O	5.09	126.86	121.16
3	I	59	ILE	CA-CB-CG1	5.08	119.04	110.40
2	H	175	ARG	CD-NE-CZ	-5.07	117.30	124.40
2	H	82	ILE	CB-CG1-CD1	5.06	124.42	113.80
2	H	231	VAL	CA-C-N	-5.06	113.50	120.28
2	H	231	VAL	C-N-CA	-5.06	113.50	120.28
2	H	125	ASP	CB-CG-OD2	5.03	129.97	118.40
2	H	228	TYR	CA-C-O	-5.03	115.23	121.06
2	H	243	ASP	N-CA-C	-5.02	105.72	111.14
2	H	61	GLU	CA-C-O	5.00	125.85	120.55

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	126	ARG	Sidechain
2	H	233	ARG	Sidechain
2	H	77	GLU	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	235	0	234	28	0
2	H	2030	0	1992	88	2
3	I	85	0	64	16	1
4	H	42	0	45	2	0
5	H	160	0	0	10	1
5	I	1	0	0	0	0
5	L	15	0	0	4	0
All	All	2568	0	2335	126	2

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 27.

All (126) 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:L:14(D):ARG:NH2	1:L:14(H):GLU:OE1	1.73	1.22
1:L:14(D):ARG:HD2	5:L:461:HOH:O	1.47	1.10
2:H:81:LYS:CB	5:H:829:HOH:O	2.02	1.08
1:L:14(D):ARG:HE	1:L:14(H):GLU:HB3	1.19	1.05
1:L:14(D):ARG:CD	5:L:461:HOH:O	2.02	1.04
2:H:219:GLY:HA3	2:H:221(A):ARG:HE	1.22	1.02
2:H:187:ARG:NH2	2:H:222:ASP:OD1	1.93	1.01
2:H:162:ILE:CG2	5:H:505:HOH:O	2.09	1.00
1:L:14(D):ARG:NH2	1:L:14(H):GLU:CD	2.20	1.00
1:L:14(D):ARG:HH21	1:L:14(H):GLU:CD	1.68	0.99
2:H:50:ARG:NH1	2:H:108:LEU:O	1.95	0.98
2:H:36:LYS:O	2:H:38:GLN:HG2	1.74	0.88
2:H:35:ARG:HD3	2:H:39:GLU:OE2	1.74	0.87
1:L:14(D):ARG:HE	1:L:14(H):GLU:CB	1.88	0.85
1:L:14(D):ARG:NE	1:L:14(H):GLU:HB3	1.91	0.84
2:H:74:THR:HG22	2:H:75:ARG:HD3	1.58	0.82
2:H:50:ARG:NH1	2:H:107:LYS:HE2	1.97	0.80
2:H:85:LEU:HD13	2:H:106:MET:HE2	1.64	0.79
3:I:59:ILE:HD11	3:I:64:LEU:HD21	1.65	0.78
1:L:14(D):ARG:HG2	1:L:14(D):ARG:O	1.82	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:17:VAL:O	2:H:188:GLY:HA2	1.83	0.77
2:H:75:ARG:HD3	2:H:75:ARG:N	1.98	0.77
2:H:35:ARG:O	2:H:38:GLN:HA	1.85	0.76
1:L:1(C):GLU:HA	1:L:1:CYS:HB3	1.66	0.76
2:H:76:TYR:HB3	3:I:57:GLU:OE1	1.84	0.75
2:H:75:ARG:HH11	2:H:75:ARG:HG3	1.52	0.74
2:H:18:GLU:OE1	5:H:846:HOH:O	2.06	0.73
2:H:57:HIS:NE2	4:H:5:1ZV:O3	2.17	0.73
2:H:75:ARG:HG3	2:H:75:ARG:NH1	2.04	0.72
2:H:165:ARG:NE	5:H:844:HOH:O	1.85	0.72
2:H:165:ARG:NH1	5:H:450:HOH:O	2.22	0.72
1:L:14(D):ARG:HH21	1:L:14(H):GLU:CG	2.02	0.72
2:H:165:ARG:NH2	2:H:180:MET:O	2.23	0.72
2:H:72:SER:OG	2:H:75:ARG:HG2	1.89	0.71
3:I:60:PRO:HG2	3:I:63:TYS:HE2	1.72	0.71
2:H:162:ILE:HG22	5:H:505:HOH:O	1.83	0.71
1:L:14(D):ARG:NE	5:L:461:HOH:O	2.19	0.70
1:L:14(D):ARG:HH21	1:L:14(H):GLU:CB	2.03	0.70
3:I:59:ILE:HD11	3:I:64:LEU:CD2	2.22	0.70
1:L:14(A):LYS:HG2	2:H:23:GLU:OE2	1.93	0.69
2:H:74:THR:CG2	2:H:75:ARG:HD3	2.23	0.69
2:H:219:GLY:HA3	2:H:221(A):ARG:NE	2.04	0.68
3:I:59:ILE:HD13	3:I:63:TYS:HB3	1.74	0.67
2:H:49:ASP:OD2	2:H:111:PRO:HB3	1.95	0.66
2:H:130:LEU:HD23	2:H:162:ILE:HD13	1.77	0.65
1:L:1(B):ALA:H	1:L:1:CYS:H	1.46	0.64
2:H:162:ILE:HG23	5:H:505:HOH:O	1.87	0.64
2:H:76:TYR:N	3:I:57:GLU:OE1	2.29	0.64
1:L:14(D):ARG:CZ	1:L:14(H):GLU:OE1	2.47	0.62
1:L:14(K):ILE:C	1:L:14(K):ILE:HD12	2.22	0.61
2:H:35:ARG:CD	2:H:39:GLU:OE2	2.47	0.61
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	2.08	0.61
2:H:186(A):ASP:OD1	2:H:186(A):ASP:N	2.31	0.60
2:H:36(A):SER:HA	2:H:37:PRO:C	2.26	0.60
2:H:187:ARG:NH1	2:H:221:ASP:O	2.32	0.59
2:H:50:ARG:HH11	2:H:107:LYS:HE2	1.66	0.58
2:H:86:GLU:HG3	2:H:109:LYS:HA	1.86	0.58
2:H:74:THR:HG22	2:H:75:ARG:CD	2.29	0.58
2:H:187:ARG:HD3	2:H:221:ASP:OD2	2.04	0.58
2:H:232:PHE:O	2:H:235:LYS:HB2	2.04	0.57
2:H:87:LYS:HG3	2:H:89:TYR:CE1	2.40	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:75:ARG:N	2:H:75:ARG:CD	2.56	0.56
2:H:165:ARG:NH2	2:H:177:THR:O	2.40	0.54
2:H:195:SER:CB	4:H:5:1ZV:O3	2.55	0.54
1:L:1(D):GLY:HA3	2:H:114:PHE:HE2	1.73	0.54
2:H:164:GLU:H	2:H:164:GLU:CD	2.14	0.54
3:I:60:PRO:O	3:I:63:TYS:N	2.39	0.53
2:H:204(B):ASN:HD22	2:H:205:ASN:N	2.07	0.53
1:L:14(K):ILE:C	1:L:14(K):ILE:CD1	2.82	0.52
2:H:150:GLY:C	2:H:151:GLN:HG3	2.29	0.52
2:H:130:LEU:HD23	2:H:162:ILE:CD1	2.40	0.52
2:H:237:TRP:O	2:H:240:LYS:HB3	2.10	0.51
3:I:60:PRO:HB2	3:I:62:GLU:CD	2.35	0.51
2:H:242:ILE:HG23	2:H:247:GLU:CB	2.41	0.51
3:I:60:PRO:HG2	3:I:63:TYS:CE2	2.40	0.50
2:H:135:LYS:NZ	5:H:862:HOH:O	2.45	0.50
2:H:165:ARG:O	2:H:169:LYS:HD2	2.13	0.49
2:H:62:ASN:ND2	2:H:63:ASP:OD1	2.45	0.49
1:L:14(J):TYR:C	1:L:14(K):ILE:HD12	2.38	0.49
2:H:184(A):TYR:HA	2:H:186(B):GLU:OE1	2.12	0.49
2:H:35:ARG:HB3	2:H:39:GLU:HG2	1.94	0.49
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.48	0.48
2:H:200:VAL:HG12	2:H:209:GLN:HA	1.94	0.48
2:H:211:GLY:HA2	2:H:229:THR:O	2.13	0.48
2:H:76:TYR:CB	3:I:57:GLU:OE1	2.57	0.48
2:H:49:ASP:O	2:H:111:PRO:HA	2.14	0.48
2:H:242:ILE:HG23	2:H:247:GLU:HB2	1.96	0.47
2:H:178:ASP:O	2:H:233:ARG:HD2	2.14	0.47
2:H:91:HIS:CE1	2:H:101:ARG:HD3	2.50	0.47
2:H:240:LYS:HB2	2:H:240:LYS:HE2	1.43	0.47
3:I:62:GLU:OE1	3:I:63:TYS:CE2	2.63	0.47
2:H:247:GLU:O	2:H:247:GLU:CD	2.58	0.47
2:H:35:ARG:HD2	2:H:41:LEU:HD21	1.97	0.46
1:L:14(A):LYS:HG2	2:H:23:GLU:CD	2.40	0.46
2:H:151:GLN:HA	2:H:152:PRO:HD3	1.85	0.45
1:L:14(D):ARG:CZ	5:L:461:HOH:O	2.61	0.45
2:H:130:LEU:HD23	2:H:130:LEU:HA	1.69	0.45
2:H:204(B):ASN:C	2:H:204(B):ASN:ND2	2.72	0.45
2:H:131:GLN:O	2:H:134:TYR:HB2	2.17	0.45
2:H:186(C):GLY:O	2:H:186(D):LYS:HG3	2.17	0.45
1:L:14(I):SER:C	1:L:14(K):ILE:H	2.26	0.44
2:H:34:PHE:CZ	2:H:38:GLN:HB3	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:203:SER:O	2:H:205:ASN:HA	2.18	0.44
2:H:87:LYS:NZ	2:H:88:ILE:O	2.39	0.43
2:H:165:ARG:CZ	5:H:844:HOH:O	2.50	0.43
3:I:60:PRO:O	3:I:61:GLU:C	2.61	0.43
3:I:60:PRO:C	3:I:62:GLU:N	2.73	0.43
1:L:14(D):ARG:NH2	1:L:14(H):GLU:CB	2.79	0.43
2:H:98:ASN:O	2:H:99:LEU:HB2	2.19	0.43
3:I:62:GLU:OE1	3:I:63:TYS:CZ	2.67	0.42
2:H:165:ARG:HH11	2:H:165:ARG:HD3	1.64	0.42
1:L:5:PRO:HA	1:L:9:LYS:HG3	2.01	0.42
1:L:14(D):ARG:NE	1:L:14(H):GLU:CB	2.64	0.42
2:H:60(B):PRO:HG2	2:H:96:TRP:CE2	2.54	0.41
2:H:36:LYS:HE3	5:H:819:HOH:O	2.20	0.41
2:H:36:LYS:HG3	2:H:65:LEU:HD22	2.03	0.41
2:H:17:VAL:HG11	2:H:221:ASP:CB	2.51	0.41
2:H:17:VAL:HG23	2:H:191:CYS:HB2	2.02	0.41
2:H:29:TRP:CG	2:H:121:VAL:HB	2.55	0.41
1:L:14(G):LEU:HD22	1:L:14(G):LEU:N	2.35	0.41
2:H:164:GLU:CD	2:H:185:LYS:HZ1	2.29	0.40
3:I:59:ILE:HD11	3:I:64:LEU:CG	2.51	0.40
1:L:14(J):TYR:O	1:L:14(K):ILE:HD12	2.21	0.40
2:H:186(C):GLY:C	2:H:186(D):LYS:HG3	2.47	0.40
3:I:60:PRO:O	3:I:62:GLU:N	2.54	0.40
2:H:126:ARG:HA	2:H:232:PHE:CZ	2.56	0.40

All (2) 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:NH1	3:I:57:GLU:OE2[2_555]	2.06	0.14
2:H:172:THR:O	5:H:422:HOH:O[4_546]	2.10	0.10

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	L	27/36 (75%)	22 (82%)	4 (15%)	1 (4%)	2	0
2	H	248/259 (96%)	238 (96%)	10 (4%)	0	100	100
3	I	7/13 (54%)	6 (86%)	1 (14%)	0	100	100
All	All	282/308 (92%)	266 (94%)	15 (5%)	1 (0%)	30	19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	1(B)	ALA

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	L	26/31 (84%)	24 (92%)	2 (8%)	12	3
2	H	218/225 (97%)	192 (88%)	26 (12%)	5	1
3	I	7/11 (64%)	5 (71%)	2 (29%)	0	0
All	All	251/267 (94%)	221 (88%)	30 (12%)	5	1

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	9	LYS
1	L	13	GLU
2	H	33	LEU
2	H	36	LYS
2	H	36(A)	SER
2	H	64	LEU
2	H	65	LEU
2	H	66	VAL
2	H	74	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	75	ARG
2	H	83	SER
2	H	86	GLU
2	H	99	LEU
2	H	127	GLU
2	H	129(B)	SER
2	H	129(C)	LEU
2	H	147	THR
2	H	154	VAL
2	H	164	GLU
2	H	165	ARG
2	H	169	LYS
2	H	174	ILE
2	H	205	ASN
2	H	235	LYS
2	H	239	GLN
2	H	240	LYS
2	H	241	VAL
2	H	243	ASP
3	I	59	ILE
3	I	62	GLU

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	38	GLN
2	H	156	GLN
2	H	204(B)	ASN
2	H	205	ASN
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 ⓘ

1 non-standard protein/DNA/RNA residue 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
3	TYS	I	63	3	15,16,17	1.64	2 (13%)	15,22,24	1.83	5 (33%)

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
3	TYS	I	63	3	-	0/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	63	TYS	OH-CZ	-4.54	1.35	1.42
3	I	63	TYS	OH-S	3.22	1.64	1.58

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	63	TYS	CB-CG-CD1	-3.14	115.06	120.90
3	I	63	TYS	CE2-CZ-CE1	2.65	124.03	120.16
3	I	63	TYS	CD1-CE1-CZ	-2.63	116.72	119.73
3	I	63	TYS	CD2-CG-CD1	2.51	121.96	118.23
3	I	63	TYS	O3-S-O1	2.26	116.46	108.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	63	TYS	6	0

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	$\# Z > 2$
4	1ZV	H	5	2	40,44,44	2.16	6 (15%)	43,57,57	2.39	16 (37%)

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	1ZV	H	5	2	2/2/10/14	17/46/61/61	0/2/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	5	1ZV	O2-C8	10.52	1.37	1.21
4	H	5	1ZV	O8-C81	-4.83	1.26	1.40
4	H	5	1ZV	CZ-NE	-2.76	1.28	1.33
4	H	5	1ZV	CA2-C8	2.69	1.56	1.52
4	H	5	1ZV	CA-N	2.52	1.53	1.47
4	H	5	1ZV	C81-N	-2.17	1.36	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	5	1ZV	CB-CA-C	6.79	126.58	109.75
4	H	5	1ZV	O8-C81-C71	6.20	123.92	109.17
4	H	5	1ZV	C51-C61-C71	5.20	133.20	113.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	5	1ZV	C5-C6-C1	3.59	125.65	120.61
4	H	5	1ZV	CB-CG-C1	3.26	123.95	113.22
4	H	5	1ZV	C61-C71-C81	3.25	123.09	114.13
4	H	5	1ZV	CA2-N2-C7	3.10	128.31	121.65
4	H	5	1ZV	NE-CZ-NH2	3.10	125.99	120.67
4	H	5	1ZV	C31-C21-C11	2.84	126.69	113.56
4	H	5	1ZV	C6-C1-C2	-2.70	114.22	118.23
4	H	5	1ZV	CB-CA-N	-2.64	93.58	112.17
4	H	5	1ZV	C4-C5-C6	-2.57	117.06	120.24
4	H	5	1ZV	CA1-C7-N2	2.52	122.05	116.52
4	H	5	1ZV	O-C-CA	-2.22	115.56	119.61
4	H	5	1ZV	CG2-CD1-NE	-2.13	106.22	112.20
4	H	5	1ZV	NH1-CZ-NE	-2.11	114.47	119.27

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	H	5	1ZV	C9
4	H	5	1ZV	C81

All (17) torsion outliers are listed below:

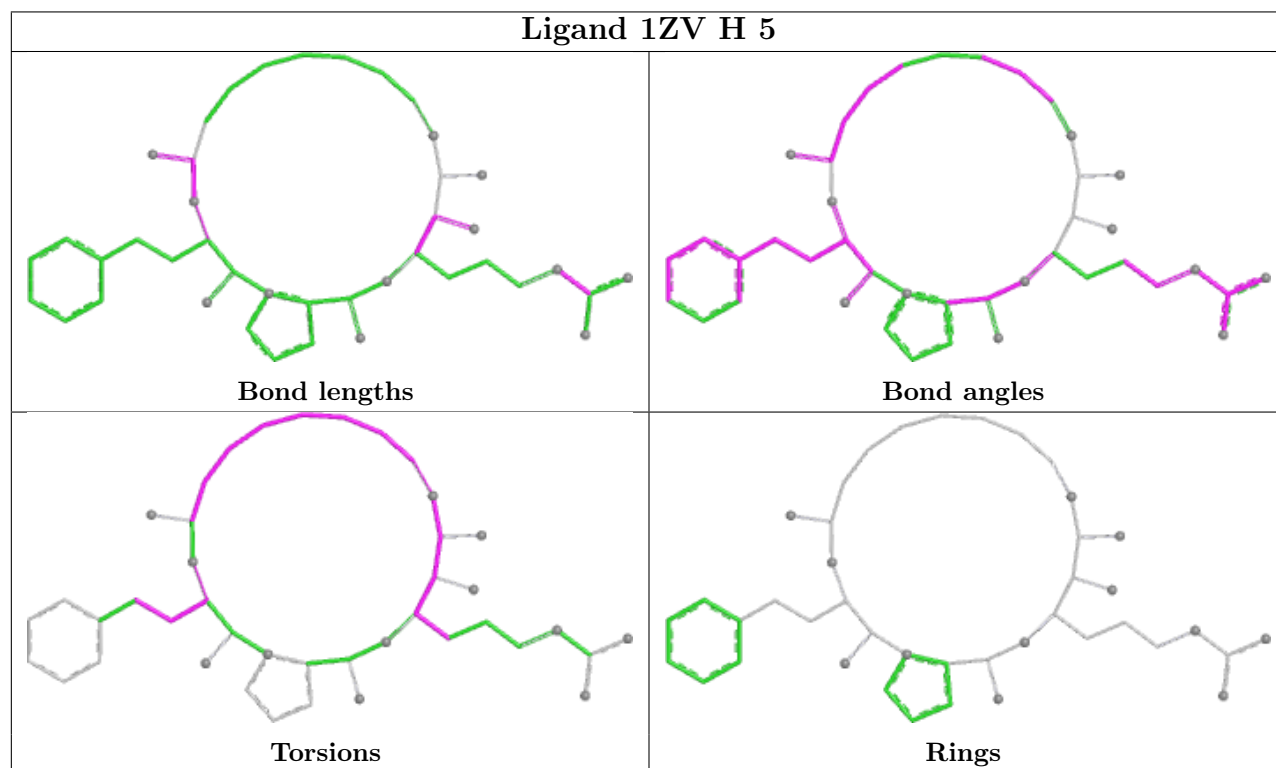
Mol	Chain	Res	Type	Atoms
4	H	5	1ZV	N-CA-CB-CG
4	H	5	1ZV	C-CA-CB-CG
4	H	5	1ZV	CA-CB-CG-C1
4	H	5	1ZV	O2-C8-C9-O3
4	H	5	1ZV	C8-C9-N3-C11
4	H	5	1ZV	N3-C11-C21-C31
4	H	5	1ZV	C41-C51-C61-C71
4	H	5	1ZV	C11-C21-C31-C41
4	H	5	1ZV	C61-C71-C81-N
4	H	5	1ZV	C31-C41-C51-C61
4	H	5	1ZV	CB-CA-N-C81
4	H	5	1ZV	C21-C31-C41-C51
4	H	5	1ZV	C21-C11-N3-C9
4	H	5	1ZV	O2-C8-CA2-CB2
4	H	5	1ZV	C51-C61-C71-C81
4	H	5	1ZV	C8-CA2-CB2-CG2
4	H	5	1ZV	O2-C8-CA2-N2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	5	1ZV	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 ⓘ

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.