



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:28 PM GMT

PDB ID : 1AY6  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

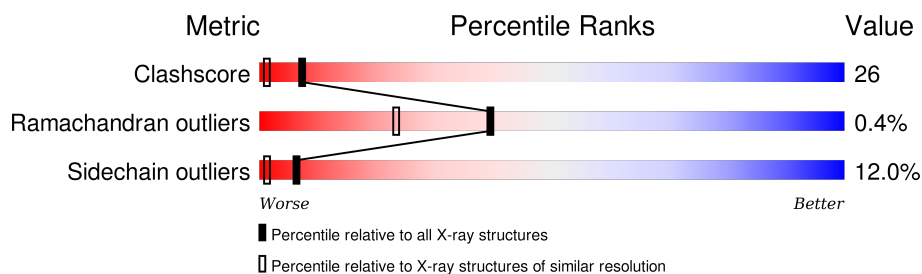
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	36	
2	H	259	
3	I	13	

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	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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			

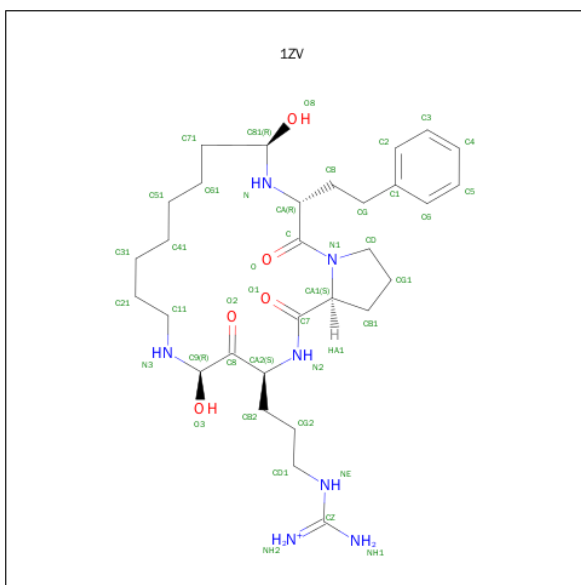
- Molecule 3 is a protein called HIRUGEN.

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-1,6-(2-PHENYLETHYL)ICOSAHYDRO-1H-PYRROLO[1,2-D][1,4,7,11]TETRAAZACYCLONONADecin-3-yl}propyl)amino)methaniminium (three-letter code: 1ZV) (formula: C<sub>30</sub>H<sub>50</sub>N<sub>7</sub>O<sub>5</sub>).



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 15 15	0	0
5	H	160	Total O 160 160	0	0
5	I	1	Total O 1 1	0	0

### 3 Residue-property plots

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

Note EDS was not executed.

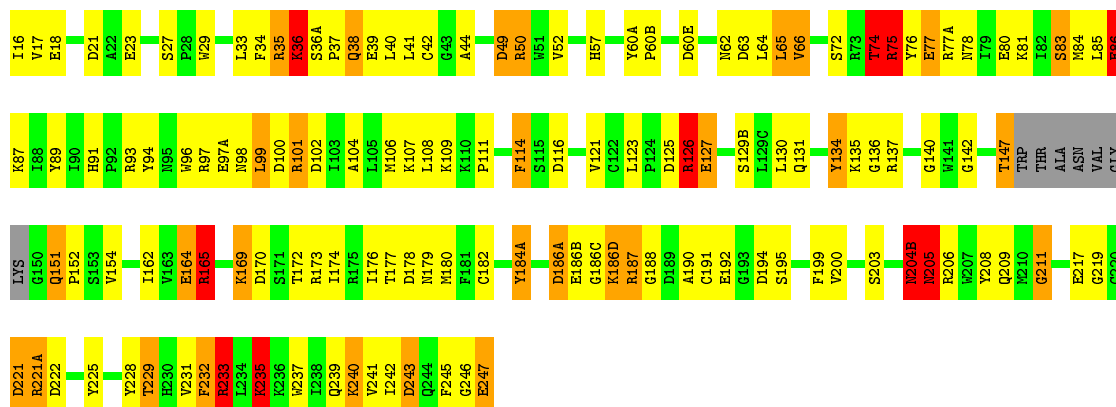
#### • Molecule 1: THROMBIN LIGHT CHAIN

Chain L: 




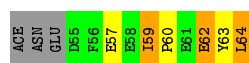
#### • Molecule 2: THROMBIN HEAVY CHAIN

Chain H: 



#### • Molecule 3: HIRUGEN

Chain I: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.08 Å   72.14 Å   72.82 Å 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 <sup>2</sup> )	31.0	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: 1ZV, TYS

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	1.28	0/237	2.85	20/315 (6.3%)
2	H	1.34	6/2082 (0.3%)	2.53	119/2812 (4.2%)
3	I	1.03	0/69	2.03	1/89 (1.1%)
All	All	1.32	6/2388 (0.3%)	2.55	140/3216 (4.4%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	77	GLU	CD-OE2	-7.68	1.17	1.25
2	H	211	GLY	N-CA	6.38	1.55	1.46
2	H	137	ARG	NE-CZ	5.92	1.40	1.33
2	H	97	ARG	CD-NE	5.36	1.55	1.46
2	H	78	ASN	N-CA	5.24	1.56	1.46
2	H	228	TYR	CG-CD1	5.04	1.45	1.39

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	233	ARG	NE-CZ-NH1	25.72	133.16	120.30
2	H	206	ARG	NE-CZ-NH1	20.98	130.79	120.30
2	H	93	ARG	CD-NE-CZ	20.51	152.32	123.60
2	H	101	ARG	NE-CZ-NH2	-20.07	110.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	206	ARG	NE-CZ-NH2	-19.10	110.75	120.30
2	H	233	ARG	NE-CZ-NH2	-16.08	112.26	120.30
2	H	126	ARG	NE-CZ-NH1	16.04	128.32	120.30
2	H	126	ARG	NE-CZ-NH2	-15.82	112.39	120.30
2	H	93	ARG	NE-CZ-NH1	-15.17	112.72	120.30
1	L	14(D)	ARG	NE-CZ-NH2	-13.84	113.38	120.30
2	H	101	ARG	NE-CZ-NH1	13.37	126.99	120.30
2	H	77(A)	ARG	NE-CZ-NH2	-13.35	113.62	120.30
2	H	35	ARG	NE-CZ-NH2	-13.33	113.64	120.30
2	H	125	ASP	CB-CG-OD2	12.97	129.97	118.30
1	L	14(D)	ARG	NE-CZ-NH1	12.87	126.73	120.30
1	L	1(A)	ASP	CB-CG-OD1	-12.60	106.96	118.30
2	H	173	ARG	NE-CZ-NH2	12.10	126.35	120.30
2	H	97	ARG	CD-NE-CZ	-11.82	107.05	123.60
2	H	221(A)	ARG	NE-CZ-NH1	-11.80	114.40	120.30
2	H	137	ARG	NE-CZ-NH1	-11.46	114.57	120.30
2	H	194	ASP	CB-CG-OD2	11.31	128.48	118.30
2	H	35	ARG	NE-CZ-NH1	11.23	125.92	120.30
2	H	125	ASP	CB-CG-OD1	-11.21	108.21	118.30
1	L	4	ARG	NE-CZ-NH2	11.13	125.87	120.30
2	H	205	ASN	CB-CA-C	9.63	129.67	110.40
1	L	14(D)	ARG	N-CA-CB	9.61	127.90	110.60
2	H	187	ARG	NE-CZ-NH2	-9.44	115.58	120.30
2	H	225	TYR	CB-CG-CD1	-9.28	115.43	121.00
2	H	205	ASN	N-CA-CB	-9.25	93.96	110.60
2	H	97	ARG	CB-CG-CD	9.20	135.51	111.60
2	H	170	ASP	CB-CG-OD2	-9.00	110.20	118.30
2	H	205	ASN	CB-CG-OD1	-8.85	103.89	121.60
2	H	173	ARG	CG-CD-NE	8.68	130.02	111.80
1	L	1(C)	GLU	OE1-CD-OE2	8.57	133.58	123.30
2	H	97(A)	GLU	CA-CB-CG	8.21	131.47	113.40
2	H	49	ASP	CB-CG-OD2	8.12	125.60	118.30
2	H	154	VAL	CA-CB-CG1	8.04	122.95	110.90
1	L	14(J)	TYR	CB-CG-CD2	8.02	125.81	121.00
2	H	208	TYR	CB-CG-CD2	-7.97	116.22	121.00
2	H	74	THR	N-CA-CB	-7.80	95.49	110.30
2	H	229	THR	CA-CB-CG2	7.68	123.15	112.40
2	H	134	TYR	CD1-CE1-CZ	-7.67	112.90	119.80
2	H	21	ASP	CB-CG-OD2	-7.64	111.42	118.30
2	H	44	ALA	O-C-N	7.51	134.72	122.70
2	H	243	ASP	CB-CG-OD1	7.49	125.04	118.30
2	H	86	GLU	CG-CD-OE1	-7.47	103.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	123	LEU	CA-CB-CG	7.47	132.48	115.30
2	H	94	TYR	CB-CG-CD2	-7.28	116.63	121.00
2	H	173	ARG	NH1-CZ-NH2	-7.24	111.44	119.40
2	H	127	GLU	CA-CB-CG	7.09	129.00	113.40
2	H	100	ASP	CB-CG-OD2	-7.09	111.92	118.30
2	H	154	VAL	N-CA-CB	-7.04	96.02	111.50
2	H	247	GLU	OE1-CD-OE2	7.02	131.72	123.30
3	I	64	LEU	CB-CA-C	6.98	123.46	110.20
2	H	27	SER	CB-CA-C	6.96	123.32	110.10
1	L	4	ARG	NH1-CZ-NH2	-6.92	111.79	119.40
2	H	77(A)	ARG	CA-C-N	6.92	132.42	117.20
2	H	60(A)	TYR	CB-CG-CD2	-6.88	116.88	121.00
2	H	142	GLY	CA-C-O	6.82	132.87	120.60
2	H	221(A)	ARG	NE-CZ-NH2	6.77	123.69	120.30
2	H	176	ILE	CA-CB-CG2	6.73	124.36	110.90
1	L	1(C)	GLU	CG-CD-OE2	-6.67	104.95	118.30
2	H	77(A)	ARG	C-N-CA	-6.64	105.10	121.70
2	H	77(A)	ARG	CA-C-O	-6.60	106.23	120.10
2	H	225	TYR	CG-CD2-CE2	-6.60	116.02	121.30
2	H	184(A)	TYR	CB-CG-CD1	-6.58	117.05	121.00
2	H	165	ARG	NE-CZ-NH2	6.56	123.58	120.30
1	L	14(D)	ARG	CD-NE-CZ	-6.53	114.46	123.60
2	H	66	VAL	CA-CB-CG1	6.53	120.69	110.90
2	H	86	GLU	CG-CD-OE2	6.47	131.24	118.30
2	H	102	ASP	CB-CG-OD2	-6.47	112.48	118.30
2	H	137	ARG	NH1-CZ-NH2	6.45	126.50	119.40
2	H	217	GLU	OE1-CD-OE2	-6.45	115.57	123.30
2	H	75	ARG	NE-CZ-NH1	6.42	123.51	120.30
2	H	246	GLY	O-C-N	6.37	132.88	122.70
2	H	93	ARG	NE-CZ-NH2	6.36	123.48	120.30
2	H	233	ARG	NH1-CZ-NH2	-6.35	112.41	119.40
1	L	1(A)	ASP	O-C-N	6.29	132.77	122.70
2	H	36	LYS	CG-CD-CE	6.26	130.67	111.90
2	H	60(E)	ASP	CB-CG-OD1	-6.22	112.70	118.30
2	H	208	TYR	CZ-CE2-CD2	-6.18	114.24	119.80
2	H	187	ARG	CD-NE-CZ	-6.15	114.99	123.60
2	H	243	ASP	CA-CB-CG	6.12	126.86	113.40
2	H	245	PHE	C-N-CA	-6.12	109.45	122.30
2	H	77(A)	ARG	NH1-CZ-NH2	6.04	126.05	119.40
2	H	134	TYR	CG-CD1-CE1	6.03	126.13	121.30
2	H	74	THR	N-CA-C	6.02	127.26	111.00
2	H	205	ASN	CA-C-O	5.99	132.67	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	165	ARG	N-CA-CB	5.97	121.35	110.60
2	H	205	ASN	OD1-CG-ND2	5.95	135.59	121.90
2	H	116	ASP	CB-CG-OD2	-5.93	112.96	118.30
2	H	140	GLY	CA-C-O	5.85	131.12	120.60
2	H	173	ARG	CD-NE-CZ	-5.82	115.45	123.60
2	H	208	TYR	CD1-CG-CD2	5.82	124.30	117.90
2	H	151	GLN	CA-CB-CG	-5.80	100.65	113.40
1	L	10	LYS	CD-CE-NZ	-5.78	98.41	111.70
2	H	165	ARG	CA-CB-CG	5.74	126.04	113.40
2	H	80	GLU	CG-CD-OE1	-5.70	106.90	118.30
2	H	179	ASN	CB-CG-OD1	-5.62	110.36	121.60
2	H	164	GLU	OE1-CD-OE2	-5.61	116.57	123.30
2	H	231	VAL	CG1-CB-CG2	-5.61	101.92	110.90
2	H	235	LYS	CA-CB-CG	5.61	125.73	113.40
2	H	187	ARG	CG-CD-NE	-5.60	100.03	111.80
1	L	14(H)	GLU	OE1-CD-OE2	5.59	130.01	123.30
2	H	205	ASN	O-C-N	-5.59	113.76	122.70
2	H	192	GLU	OE1-CD-OE2	5.58	130.00	123.30
2	H	38	GLN	O-C-N	5.58	131.62	122.70
2	H	186(D)	LYS	O-C-N	5.56	131.60	122.70
1	L	9	LYS	CA-C-N	5.52	129.34	117.20
2	H	225	TYR	CD1-CE1-CZ	-5.46	114.88	119.80
2	H	221	ASP	CB-CG-OD2	5.42	123.18	118.30
2	H	233	ARG	CD-NE-CZ	5.40	131.16	123.60
2	H	42	CYS	N-CA-CB	-5.40	100.88	110.60
2	H	52	VAL	O-C-N	5.39	131.33	122.70
1	L	14(G)	LEU	CB-CG-CD1	5.39	120.17	111.00
2	H	184(A)	TYR	CB-CG-CD2	5.38	124.23	121.00
2	H	123	LEU	CB-CA-C	5.37	120.40	110.20
2	H	208	TYR	O-C-N	5.36	131.27	122.70
2	H	83	SER	N-CA-CB	5.34	118.51	110.50
2	H	84	MET	O-C-N	5.32	131.21	122.70
2	H	151	GLN	CB-CA-C	5.32	121.04	110.40
2	H	74	THR	OG1-CB-CG2	5.28	122.15	110.00
2	H	186(D)	LYS	N-CA-C	-5.27	96.76	111.00
2	H	190	ALA	N-CA-C	-5.26	96.80	111.00
1	L	1(A)	ASP	CA-CB-CG	-5.25	101.86	113.40
2	H	50	ARG	CA-CB-CG	5.23	124.90	113.40
2	H	40	LEU	O-C-N	5.22	131.05	122.70
2	H	114	PHE	CB-CA-C	5.20	120.80	110.40
2	H	204(B)	ASN	C-N-CA	5.10	134.46	121.70
1	L	14(J)	TYR	CA-CB-CG	5.10	123.09	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	13	GLU	CA-CB-CG	5.09	124.60	113.40
2	H	104	ALA	O-C-N	5.09	130.84	122.70
2	H	186(A)	ASP	CA-CB-CG	-5.08	102.22	113.40
1	L	14(A)	LYS	CA-CB-CG	5.05	124.51	113.40
2	H	16	ILE	O-C-N	5.04	130.77	122.70
2	H	190	ALA	N-CA-CB	5.03	117.14	110.10
2	H	232	PHE	CB-CG-CD1	-5.02	117.29	120.80
2	H	187	ARG	NH1-CZ-NH2	5.01	124.91	119.40
1	L	13	GLU	OE1-CD-OE2	5.01	129.31	123.30
2	H	147	THR	CA-C-O	5.00	130.61	120.10

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	85	2
3	I	85	0	64	15	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	122	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 26.

All (122) 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
2:H:50:ARG:NH1	2:H:108:LEU:O	1.95	0.98
1:L:14(D):ARG:NH2	1:L:14(H):GLU:CD	2.20	0.95
1:L:14(D):ARG:HH21	1:L:14(H):GLU:CD	1.68	0.94
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
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
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:HG3	2:H:75:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:35:ARG:CD	2:H:39:GLU:OE2	2.47	0.61
2:H:186(A):ASP:N	2:H:186(A):ASP:OD1	2.31	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
1:L:14(K):ILE:HD12	1:L:14(K):ILE:C	2.22	0.57
2:H:87:LYS:HG3	2:H:89:TYR:CE1	2.40	0.57
2:H:85:LEU:HD13	2:H:106:MET:HE2	1.87	0.56
2:H:75:ARG:N	2:H:75:ARG:CD	2.56	0.56
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	2.08	0.56
2:H:36(A):SER:HA	2:H:37:PRO:C	2.26	0.55
2:H:195:SER:CB	4:H:5:1ZV:O3	2.55	0.54
2:H:165:ARG:NH2	2:H:177:THR:O	2.40	0.54
1:L:1(D):GLY:HA3	2:H:114:PHE:HE2	1.73	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
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
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
2:H:164:GLU:CD	2:H:164:GLU:H	2.14	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
1:L:14(K):ILE:CD1	1:L:14(K):ILE:C	2.82	0.48
2:H:49:ASP:O	2:H:111:PRO:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:I:60:PRO:HB2	3:I:62:GLU:CD	2.35	0.47
3:I:62:GLU:OE1	3:I:63:TYS:CE2	2.63	0.47
2:H:240:LYS:HE2	2:H:240:LYS:HB2	1.43	0.47
2:H:35:ARG:HD2	2:H:41:LEU:HD21	1.97	0.46
1:L:9:LYS:HZ3	1:L:9:LYS:HG3	1.71	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:85:LEU:HD13	2:H:106:MET:CE	2.46	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(J):TYR:C	1:L:14(K):ILE:HD12	2.38	0.44
2:H:34:PHE:CZ	2:H:38:GLN:HB3	2.53	0.44
2:H:203:SER:O	2:H:205:ASN:HA	2.18	0.44
2:H:165:ARG:CZ	5:H:844:HOH:O	2.50	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:247:GLU:CD	2:H:247:GLU:O	2.58	0.42
1:L:14(A):LYS:HG2	2:H:23:GLU:CD	2.40	0.42
2:H:204(B):ASN:ND2	2:H:204(B):ASN:C	2.72	0.42
3:I:60:PRO:C	3:I:62:GLU:N	2.73	0.41
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:N	1:L:14(G):LEU:HD22	2.35	0.41
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
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 [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	27/36 (75%)	22 (82%)	4 (15%)	1 (4%)	4	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%)	39	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	1(B)	ALA

### 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	26/31 (84%)	22 (85%)	4 (15%)	3	0
2	H	218/225 (97%)	194 (89%)	24 (11%)	8	1
3	I	7/11 (64%)	5 (71%)	2 (29%)	0	0
All	All	251/267 (94%)	221 (88%)	30 (12%)	6	1



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

Mol	Chain	Res	Type
1	L	1(C)	GLU
1	L	9	LYS
1	L	13	GLU
1	L	14(F)	LEU
2	H	33	LEU
2	H	36	LYS
2	H	64	LEU
2	H	65	LEU
2	H	66	VAL
2	H	74	THR
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	147	THR
2	H	165	ARG
2	H	169	LYS
2	H	174	ILE
2	H	182	CYS
2	H	204(B)	ASN
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	38	GLN
2	H	156	GLN
2	H	204(B)	ASN

### 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	1.40	1 (6%)	16,22,24	2.00	7 (43%)

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	-	0/9/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	63	TYS	OH-CZ	-4.59	1.35	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	63	TYS	CG-CB-CA	-4.52	104.01	114.21
3	I	63	TYS	CB-CG-CD1	-2.79	115.06	120.90
3	I	63	TYS	CD1-CE1-CZ	-2.40	116.72	119.74
3	I	63	TYS	O-C-CA	-2.35	119.36	125.49
3	I	63	TYS	O3-S-O1	2.10	116.46	108.56
3	I	63	TYS	CE2-CZ-CE1	2.35	124.03	120.20
3	I	63	TYS	CD2-CG-CD1	2.39	121.96	118.13

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	1ZV	H	5	2	38,44,44	2.23	3 (7%)	43,57,57	3.24	13 (30%)

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	0/43/61/61	0/2/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	5	1ZV	O8-C81	-7.72	1.26	1.40
4	H	5	1ZV	O3-C9	-3.44	1.21	1.39
4	H	5	1ZV	O2-C8	9.30	1.37	1.21

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	5	1ZV	O3-C9-C8	-13.01	87.45	110.89
4	H	5	1ZV	O2-C8-C9	-10.26	107.06	119.41
4	H	5	1ZV	C6-C1-C2	-2.44	114.22	118.13
4	H	5	1ZV	C4-C5-C6	-2.13	117.06	120.19
4	H	5	1ZV	O-C-CA	-2.13	115.56	119.59
4	H	5	1ZV	CA1-C7-N2	2.40	122.05	116.64
4	H	5	1ZV	C61-C71-C81	2.57	123.09	114.50
4	H	5	1ZV	C31-C21-C11	2.72	126.69	113.69
4	H	5	1ZV	CB-CG-C1	2.80	123.95	113.14
4	H	5	1ZV	CA2-N2-C7	2.98	128.31	121.62
4	H	5	1ZV	C5-C6-C1	3.15	125.65	120.65
4	H	5	1ZV	C51-C61-C71	5.50	133.20	113.66
4	H	5	1ZV	O8-C81-C71	6.55	123.92	109.35

All (2) chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	5	1ZV	2	0

## 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.