



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:59 AM UTC

PDB ID : 3HAT / pdb_00003hat
Title : ACTIVE SITE MIMETIC INHIBITION OF THROMBIN
Authors : Tulinsky, A.; Mathews, I.I.
Deposited on : 1994-10-16
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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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

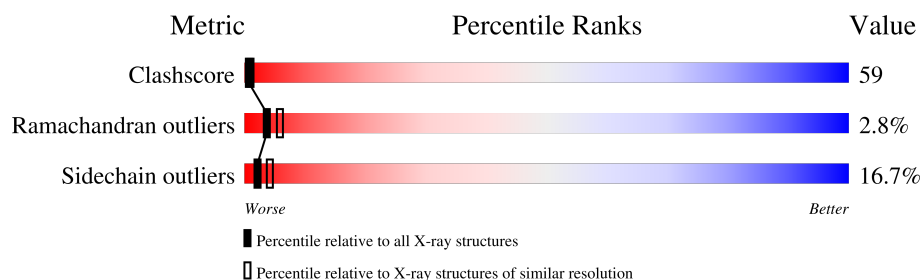
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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)

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	17% 36% 33% 14%
2	H	259	17% 47% 28% 6% .
3	I	12	17% 33% 33% 17%
4	T	4	25% 25% 25% 25%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2575 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	36	Total	C	N	O	S	0	0	0
			281	174	45	61	1			

- Molecule 2 is a protein called Thrombin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	251	Total	C	N	O	S	0	0	0
			1996	1271	355	356	14			

- Molecule 3 is a protein called Hirudin variant-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	10	Total	C	N	O	S	0	0	0
			87	56	10	20	1			

- Molecule 4 is a protein called FPAM (FIBRINOPEPTIDE A MIMIC).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	T	4	Total	C	N	O	0	0	0
			32	19	8	5			

- Molecule 5 is water.

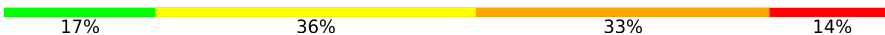
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	23	Total	O	0	0
			23	23		
5	H	146	Total	O	0	0
			146	146		
5	I	8	Total	O	0	0
			8	8		
5	T	2	Total	O	0	0
			2	2		

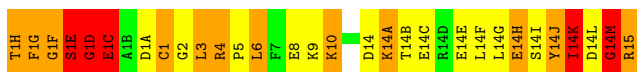
3 Residue-property plots

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.

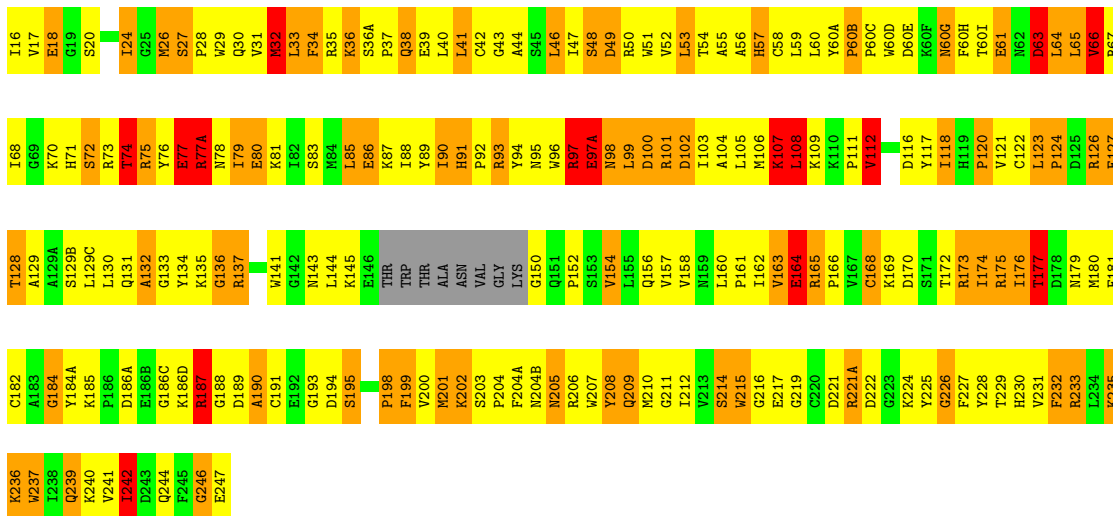
• Molecule 1: Thrombin light chain

Chain L: 



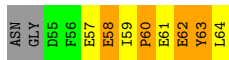
• Molecule 2: Thrombin heavy chain

Chain H: 



• Molecule 3: Hirudin variant-2

Chain I: 



• Molecule 4: FPAM (FIBRINOPEPTIDE A MIMIC)

Chain T: 



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	71.10Å 72.40Å 73.00Å 90.00° 101.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.140 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2575	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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: RNG, 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	1.43	1/284 (0.4%)	2.87	35/377 (9.3%)
2	H	1.50	10/2047 (0.5%)	2.88	208/2764 (7.5%)
3	I	1.19	0/71	3.01	7/93 (7.5%)
4	T	1.61	0/22	3.11	2/26 (7.7%)
All	All	1.49	11/2424 (0.5%)	2.88	252/3260 (7.7%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	174	ILE	CA-CB	7.17	1.62	1.54
2	H	77(A)	ARG	C-O	6.78	1.32	1.24
2	H	215	TRP	N-CA	6.65	1.53	1.46
2	H	33	LEU	N-CA	6.22	1.54	1.46
2	H	168	CYS	C-O	6.17	1.31	1.24
2	H	74	THR	CA-CB	6.02	1.63	1.53
2	H	43	GLY	N-CA	5.94	1.50	1.44
2	H	226	GLY	CA-C	5.37	1.57	1.52
2	H	102	ASP	N-CA	5.31	1.53	1.46
1	L	4	ARG	CD-NE	-5.15	1.39	1.46
2	H	97(A)	GLU	N-CA	5.05	1.52	1.46

All (252) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	126	ARG	CD-NE-CZ	18.93	150.90	124.40
2	H	135	LYS	CA-C-N	13.37	133.05	121.82
2	H	135	LYS	C-N-CA	13.37	133.05	121.82
2	H	173	ARG	NE-CZ-NH2	13.03	130.92	119.20
2	H	77(A)	ARG	CD-NE-CZ	12.96	142.54	124.40
2	H	75	ARG	CD-NE-CZ	12.52	141.93	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	157	VAL	CA-C-O	-12.47	108.57	121.67
2	H	230	HIS	CA-CB-CG	12.34	126.14	113.80
2	H	233	ARG	CD-NE-CZ	12.22	141.50	124.40
2	H	33	LEU	CB-CA-C	12.12	130.18	110.78
2	H	77(A)	ARG	NE-CZ-NH2	-11.81	108.57	119.20
2	H	74	THR	N-CA-C	11.44	128.35	112.45
2	H	75	ARG	NE-CZ-NH1	11.23	132.73	121.50
2	H	60(G)	ASN	OD1-CG-ND2	-10.86	111.74	122.60
2	H	85	LEU	O-C-N	10.38	135.11	122.86
2	H	78	ASN	CA-CB-CG	10.22	122.83	112.60
2	H	77(A)	ARG	CA-C-N	-9.94	104.40	122.38
2	H	77(A)	ARG	C-N-CA	-9.94	104.40	122.38
2	H	173	ARG	NE-CZ-NH1	-9.79	111.71	121.50
3	I	60	PRO	CB-CA-C	9.44	123.63	111.64
2	H	164	GLU	CB-CG-CD	9.40	128.59	112.60
2	H	26	MET	CA-C-N	9.36	133.15	122.85
2	H	26	MET	C-N-CA	9.36	133.15	122.85
2	H	193	GLY	CA-C-N	9.35	134.52	120.31
2	H	193	GLY	C-N-CA	9.35	134.52	120.31
2	H	75	ARG	NH1-CZ-NH2	-9.34	107.16	119.30
1	L	15	ARG	CD-NE-CZ	9.19	137.26	124.40
2	H	232	PHE	CA-CB-CG	-9.17	104.63	113.80
2	H	77(A)	ARG	CA-C-O	-9.16	107.41	120.51
1	L	14(K)	ILE	CA-C-O	9.00	132.03	120.78
1	L	14	ASP	CA-CB-CG	9.00	121.60	112.60
2	H	128	THR	N-CA-C	-8.96	101.46	111.14
1	L	14(K)	ILE	CB-CA-C	8.94	125.95	111.29
2	H	18	GLU	CB-CA-C	-8.91	99.08	111.73
2	H	59	LEU	CA-C-N	8.91	135.52	123.05
2	H	59	LEU	C-N-CA	8.91	135.52	123.05
2	H	73	ARG	CD-NE-CZ	8.90	136.86	124.40
2	H	207	TRP	O-C-N	8.83	133.28	123.22
2	H	67	ARG	CD-NE-CZ	8.64	136.50	124.40
2	H	102	ASP	CA-CB-CG	8.64	121.24	112.60
2	H	39	GLU	CB-CG-CD	8.62	127.26	112.60
1	L	4	ARG	NE-CZ-NH1	8.55	130.05	121.50
2	H	38	GLN	OE1-CD-NE2	-8.42	114.18	122.60
1	L	14(J)	TYR	N-CA-C	-8.37	103.19	113.15
2	H	201	MET	CA-C-O	-8.34	110.60	120.60
2	H	198	PRO	CB-CA-C	-8.33	97.13	110.21
3	I	60	PRO	CA-C-O	8.31	130.38	121.32
2	H	63	ASP	CA-C-O	-8.29	109.32	119.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	205	ASN	CA-CB-CG	7.98	120.58	112.60
2	H	190	ALA	N-CA-C	-7.96	99.36	110.35
2	H	34	PHE	CA-C-O	7.95	128.95	120.36
1	L	1(A)	ASP	N-CA-C	-7.91	103.19	112.92
2	H	67	ARG	NE-CZ-NH2	7.88	126.29	119.20
2	H	68	ILE	N-CA-C	7.84	119.58	108.36
2	H	221(A)	ARG	NE-CZ-NH1	7.82	129.32	121.50
1	L	1(G)	PHE	N-CA-C	-7.76	98.12	110.14
1	L	14(A)	LYS	CA-CB-CG	7.75	129.59	114.10
2	H	157	VAL	O-C-N	7.73	131.62	123.04
2	H	173	ARG	CG-CD-NE	7.70	128.94	112.00
2	H	233	ARG	NE-CZ-NH1	7.64	129.14	121.50
2	H	95	ASN	OD1-CG-ND2	-7.54	115.06	122.60
2	H	66	VAL	N-CA-CB	-7.53	101.97	111.46
3	I	60	PRO	CA-C-N	7.52	132.63	120.60
3	I	60	PRO	C-N-CA	7.52	132.63	120.60
2	H	74	THR	OG1-CB-CG2	7.50	124.31	109.30
2	H	74	THR	CA-CB-OG1	-7.50	98.35	109.60
2	H	91	HIS	CA-CB-CG	-7.48	106.32	113.80
2	H	24	ILE	CA-C-N	7.44	133.72	120.77
2	H	24	ILE	C-N-CA	7.44	133.72	120.77
2	H	64	LEU	O-C-N	7.42	132.79	123.15
2	H	165	ARG	NE-CZ-NH2	7.41	125.87	119.20
2	H	163	VAL	CA-C-O	7.38	129.13	120.72
2	H	201	MET	O-C-N	7.37	132.25	123.33
2	H	98	ASN	CA-C-O	-7.31	110.85	119.48
2	H	85	LEU	CA-C-O	-7.31	113.60	121.56
2	H	116	ASP	CA-CB-CG	7.25	119.85	112.60
1	L	4	ARG	CG-CD-NE	7.24	127.92	112.00
2	H	63	ASP	O-C-N	7.21	132.64	122.41
2	H	203	SER	CA-C-O	7.20	126.17	119.76
2	H	154	VAL	N-CA-CB	-7.19	100.39	112.47
2	H	165	ARG	CD-NE-CZ	7.17	134.43	124.40
2	H	231	VAL	CB-CA-C	7.16	121.42	112.04
2	H	187	ARG	NE-CZ-NH2	-7.16	112.76	119.20
2	H	180	MET	CA-C-O	-7.13	113.30	121.58
2	H	77	GLU	CB-CG-CD	7.13	124.71	112.60
2	H	67	ARG	NH1-CZ-NH2	-7.11	110.06	119.30
2	H	170	ASP	CA-C-O	-7.07	109.86	119.12
2	H	60	LEU	N-CA-C	7.06	120.03	108.52
1	L	1(G)	PHE	O-C-N	7.05	135.19	123.20
1	L	14(K)	ILE	C-N-CA	7.05	139.33	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	165	ARG	NH1-CZ-NH2	-7.03	110.16	119.30
2	H	205	ASN	CA-C-O	-6.96	112.18	120.81
3	I	58	GLU	N-CA-CB	6.96	119.99	110.38
2	H	73	ARG	CA-C-N	6.93	136.40	121.64
2	H	73	ARG	C-N-CA	6.93	136.40	121.64
2	H	44	ALA	CA-C-O	-6.91	113.72	121.25
2	H	66	VAL	O-C-N	-6.89	115.04	123.10
2	H	174	ILE	CA-C-O	-6.88	113.87	121.23
2	H	77	GLU	CA-C-O	6.86	130.65	122.36
2	H	205	ASN	CB-CG-ND2	-6.83	106.15	116.40
2	H	136	GLY	N-CA-C	-6.82	101.19	111.14
2	H	173	ARG	CA-C-O	-6.81	111.65	119.14
2	H	123	LEU	N-CA-C	-6.76	101.55	110.07
2	H	237	TRP	N-CA-C	-6.73	103.87	111.14
2	H	126	ARG	NE-CZ-NH2	6.72	125.25	119.20
2	H	173	ARG	CD-NE-CZ	-6.71	115.01	124.40
2	H	244	GLN	N-CA-CB	6.70	121.82	110.49
2	H	199	PHE	CB-CA-C	6.68	121.68	110.79
1	L	1(G)	PHE	CB-CA-C	6.66	121.69	109.71
2	H	209	GLN	CA-C-O	-6.64	113.63	120.54
3	I	57	GLU	CA-C-O	-6.62	114.34	121.56
2	H	100	ASP	O-C-N	6.61	130.78	123.04
2	H	55	ALA	CA-C-O	-6.57	113.12	120.54
2	H	129(B)	SER	CA-C-O	-6.52	111.22	119.31
2	H	136	GLY	CA-C-O	-6.52	114.60	121.57
2	H	32	MET	CA-C-N	-6.47	114.42	122.84
2	H	32	MET	C-N-CA	-6.47	114.42	122.84
2	H	181	PHE	N-CA-CB	6.47	122.71	111.39
2	H	208	TYR	CA-C-N	-6.41	114.51	122.84
2	H	208	TYR	C-N-CA	-6.41	114.51	122.84
2	H	137	ARG	O-C-N	6.38	130.77	123.31
2	H	38	GLN	CB-CG-CD	6.36	123.41	112.60
2	H	118	ILE	CA-C-O	6.34	125.87	120.22
2	H	211	GLY	O-C-N	6.34	129.12	123.60
2	H	141	TRP	CA-CB-CG	6.31	125.60	113.60
2	H	44	ALA	O-C-N	6.31	129.60	123.04
2	H	228	TYR	N-CA-C	6.29	119.75	109.24
2	H	186(D)	LYS	CA-C-O	-6.26	113.23	120.31
2	H	80	GLU	CA-CB-CG	6.23	126.57	114.10
2	H	145	LYS	O-C-N	6.20	130.84	123.33
1	L	2	GLY	CA-C-O	-6.19	109.81	120.57
1	L	14(B)	THR	O-C-N	6.19	132.60	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	1(A)	ASP	CA-CB-CG	-6.17	106.44	112.60
2	H	187	ARG	NE-CZ-NH1	6.16	127.66	121.50
2	H	111	PRO	N-CA-CB	6.13	108.69	103.35
2	H	165	ARG	CG-CD-NE	6.12	125.46	112.00
2	H	164	GLU	CA-CB-CG	6.11	126.33	114.10
2	H	108	LEU	CB-CA-C	6.06	120.61	109.46
1	L	1(D)	GLY	CA-C-O	-6.06	110.02	120.57
2	H	102	ASP	OD1-CG-OD2	6.05	137.41	122.90
2	H	18	GLU	CA-C-O	-6.04	114.09	121.28
2	H	173	ARG	O-C-N	6.04	130.58	122.49
1	L	1(E)	SER	CB-CA-C	6.02	122.41	110.42
2	H	71	HIS	CA-C-O	6.02	129.12	120.51
2	H	97	ARG	CA-C-O	-6.02	114.50	120.70
2	H	130	LEU	CA-C-O	-6.01	115.13	122.64
2	H	27	SER	N-CA-CB	-5.99	103.01	110.79
2	H	117	TYR	N-CA-C	5.98	121.31	113.30
2	H	72	SER	O-C-N	5.97	130.18	122.89
2	H	92	PRO	CA-C-O	-5.97	110.48	119.55
2	H	199	PHE	N-CA-C	-5.95	97.46	107.99
2	H	60(E)	ASP	CA-CB-CG	-5.94	106.66	112.60
2	H	175	ARG	NH1-CZ-NH2	5.94	127.03	119.30
4	T	305	VAL	CA-C-O	-5.93	113.37	120.78
2	H	60(B)	PRO	CB-CA-C	5.93	118.15	110.92
2	H	73	ARG	CA-C-O	5.92	127.21	121.00
2	H	93	ARG	NE-CZ-NH1	-5.91	115.59	121.50
1	L	3	LEU	CA-C-O	5.88	126.76	120.46
2	H	38	GLN	N-CA-C	-5.88	100.95	109.59
2	H	120	PRO	CA-C-O	5.87	129.60	122.08
2	H	244	GLN	N-CA-C	-5.85	98.34	110.80
2	H	58	CYS	CA-C-N	5.85	129.84	121.71
2	H	58	CYS	C-N-CA	5.85	129.84	121.71
2	H	184	GLY	CA-C-O	-5.84	116.21	122.05
2	H	233	ARG	NH1-CZ-NH2	-5.81	111.74	119.30
2	H	54	THR	CA-CB-CG2	5.81	120.38	110.50
1	L	14(B)	THR	CA-C-O	-5.81	113.09	119.08
2	H	74	THR	N-CA-CB	-5.79	101.63	110.26
2	H	154	VAL	CB-CA-C	5.78	119.22	110.90
2	H	242	ILE	CA-C-N	-5.75	114.60	123.17
2	H	242	ILE	C-N-CA	-5.75	114.60	123.17
2	H	53	LEU	CA-C-O	5.74	126.90	120.70
1	L	14(M)	GLY	N-CA-C	5.74	126.79	113.18
2	H	117	TYR	CA-C-N	5.71	131.41	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	117	TYR	C-N-CA	5.71	131.41	122.84
1	L	1(E)	SER	CA-CB-OG	5.71	122.53	111.10
2	H	179	ASN	CA-C-O	-5.69	112.59	119.59
2	H	181	PHE	N-CA-C	-5.67	99.80	108.76
1	L	1	CYS	CA-C-O	5.67	127.39	121.15
2	H	177	THR	CA-C-N	5.64	132.58	121.58
2	H	177	THR	C-N-CA	5.64	132.58	121.58
2	H	104	ALA	O-C-N	5.64	129.54	123.56
2	H	76	TYR	O-C-N	-5.63	115.11	122.43
2	H	107	LYS	CA-C-O	5.62	126.37	120.36
1	L	14	ASP	CA-C-O	5.62	128.39	121.87
2	H	36	LYS	CA-C-O	-5.62	115.10	121.00
1	L	14(A)	LYS	CA-C-O	-5.61	112.48	120.51
2	H	177	THR	CA-CB-OG1	-5.60	101.19	109.60
2	H	86	GLU	N-CA-C	-5.59	106.50	113.55
2	H	225	TYR	CA-CB-CG	-5.59	103.85	113.90
3	I	57	GLU	N-CA-C	-5.58	102.62	110.50
2	H	107	LYS	CA-CB-CG	5.58	125.27	114.10
2	H	128	THR	CB-CA-C	5.57	119.70	110.90
2	H	163	VAL	CA-C-N	5.57	128.67	120.82
2	H	163	VAL	C-N-CA	5.57	128.67	120.82
2	H	216	GLY	CA-C-O	-5.57	116.17	121.62
2	H	164	GLU	OE1-CD-OE2	-5.56	109.56	122.90
4	T	306	ARG	NE-CZ-NH2	5.56	124.20	119.20
2	H	49	ASP	CA-CB-CG	-5.55	107.05	112.60
2	H	29	TRP	CA-C-O	-5.54	112.58	119.18
2	H	207	TRP	CA-C-O	-5.54	114.28	120.54
2	H	97	ARG	C-N-CA	-5.50	107.94	121.70
2	H	93	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	L	14(H)	GLU	CG-CD-OE1	-5.48	105.80	118.40
2	H	76	TYR	CA-C-N	5.48	131.25	122.32
2	H	76	TYR	C-N-CA	5.48	131.25	122.32
2	H	77(A)	ARG	NE-CZ-NH1	5.47	126.97	121.50
2	H	108	LEU	O-C-N	5.46	129.13	122.96
2	H	189	ASP	CA-CB-CG	5.45	118.05	112.60
1	L	1(A)	ASP	CA-C-O	5.44	125.93	119.56
2	H	68	ILE	O-C-N	-5.44	116.99	123.03
1	L	14(H)	GLU	OE1-CD-OE2	5.42	135.91	122.90
2	H	112	VAL	O-C-N	5.40	128.66	122.93
2	H	80	GLU	CB-CG-CD	5.38	121.75	112.60
2	H	230	HIS	CA-C-O	-5.37	115.33	120.92
2	H	214	SER	N-CA-C	5.35	119.29	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	124	PRO	CB-CA-C	-5.33	103.01	110.63
2	H	27	SER	CB-CA-C	-5.29	103.50	111.27
1	L	1(A)	ASP	CA-C-N	-5.28	105.58	117.20
2	H	131	GLN	CB-CG-CD	-5.27	103.64	112.60
1	L	1(H)	THR	CA-C-N	-5.26	105.64	117.20
1	L	1(G)	PHE	CA-C-O	-5.25	115.21	121.56
1	L	6	LEU	N-CA-C	5.24	119.66	113.16
2	H	111	PRO	CA-C-N	5.24	130.40	122.91
2	H	111	PRO	C-N-CA	5.24	130.40	122.91
2	H	80	GLU	N-CA-C	5.23	117.43	110.53
2	H	132	ALA	O-C-N	5.21	129.32	122.97
2	H	38	GLN	CA-C-O	-5.20	114.55	120.58
2	H	97(A)	GLU	OE1-CD-OE2	5.18	135.34	122.90
2	H	226	GLY	N-CA-C	-5.18	102.46	111.62
2	H	27	SER	CA-C-N	5.17	124.89	119.82
2	H	27	SER	C-N-CA	5.17	124.89	119.82
2	H	179	ASN	N-CA-C	-5.16	107.15	112.93
2	H	33	LEU	N-CA-C	-5.16	99.38	108.20
1	L	1(C)	GLU	CB-CG-CD	5.16	121.36	112.60
1	L	14(H)	GLU	CA-CB-CG	-5.14	103.81	114.10
2	H	92	PRO	O-C-N	5.14	128.86	122.22
2	H	91	HIS	CA-C-O	5.14	124.03	119.71
2	H	165	ARG	CB-CG-CD	5.13	123.10	111.30
2	H	129	ALA	CB-CA-C	5.13	119.07	110.92
2	H	205	ASN	OD1-CG-ND2	5.10	127.70	122.60
2	H	176	ILE	CA-CB-CG2	5.10	119.17	110.50
1	L	14(M)	GLY	CA-C-O	5.10	129.44	120.57
2	H	101	ARG	CD-NE-CZ	-5.09	117.27	124.40
2	H	165	ARG	CA-C-N	5.09	126.20	119.84
2	H	165	ARG	C-N-CA	5.09	126.20	119.84
2	H	94	TYR	CA-CB-CG	5.09	123.06	113.90
2	H	132	ALA	CA-C-N	-5.09	111.44	121.41
2	H	132	ALA	C-N-CA	-5.09	111.44	121.41
2	H	79	ILE	CB-CA-C	5.08	119.62	111.29
2	H	199	PHE	CA-CB-CG	-5.04	108.76	113.80
2	H	102	ASP	CB-CG-OD2	-5.00	106.90	118.40

There are no chirality outliers.

There are no planarity outliers.

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	281	0	267	72	3
2	H	1996	0	1955	236	3
3	I	87	0	68	9	0
4	T	32	0	34	17	0
5	H	146	0	0	19	0
5	I	8	0	0	1	0
5	L	23	0	0	4	0
5	T	2	0	0	0	0
All	All	2575	0	2324	279	3

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 59.

All (279) 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)
2:H:224:LYS:HE2	5:H:465:HOH:O	1.40	1.19
1:L:1(F):GLY:O	1:L:1(E):SER:HB3	1.46	1.14
1:L:15:ARG:NH1	2:H:204(A):PHE:O	1.83	1.08
1:L:1(H):THR:HG22	1:L:1(D):GLY:O	1.51	1.08
2:H:201:MET:CE	2:H:210:MET:HG3	1.82	1.08
2:H:240:LYS:HD2	5:H:605:HOH:O	1.56	1.03
1:L:1(D):GLY:H	2:H:123:LEU:N	1.57	1.02
2:H:165:ARG:HE	2:H:169:LYS:HZ1	1.02	1.00
2:H:60(I):THR:HG23	2:H:63:ASP:OD1	1.62	0.98
1:L:1(D):GLY:N	2:H:123:LEU:H	1.62	0.97
2:H:235:LYS:HZ1	2:H:239:GLN:NE2	1.62	0.97
2:H:201:MET:HE3	2:H:210:MET:HG3	1.44	0.97
1:L:1(D):GLY:HA3	2:H:121:VAL:O	1.66	0.95
2:H:51:TRP:HE1	2:H:247:GLU:CA	1.78	0.95
1:L:1(G):PHE:HB2	5:L:703:HOH:O	1.67	0.92
2:H:235:LYS:HZ1	2:H:239:GLN:HE22	1.18	0.92
2:H:18:GLU:HG3	2:H:187:ARG:HB2	1.52	0.91
2:H:240:LYS:CD	5:H:605:HOH:O	2.13	0.90
2:H:81:LYS:HD2	5:H:463:HOH:O	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:17:VAL:O	2:H:188:GLY:HA2	1.71	0.88
2:H:195:SER:OG	4:T:306:ARG:C	2.16	0.87
2:H:160:LEU:HG	5:H:480:HOH:O	1.74	0.87
2:H:208:TYR:HB3	2:H:210:MET:HE3	1.56	0.87
1:L:1(D):GLY:H	2:H:123:LEU:H	0.89	0.87
2:H:61:GLU:OE1	2:H:87:LYS:HA	1.75	0.86
2:H:201:MET:HE2	2:H:210:MET:HG3	1.56	0.85
1:L:15:ARG:HD2	2:H:204:PRO:O	1.76	0.84
2:H:165:ARG:NE	2:H:169:LYS:HZ1	1.75	0.84
2:H:236:LYS:H	2:H:236:LYS:HD2	1.41	0.84
1:L:1(E):SER:N	2:H:123:LEU:O	2.12	0.82
1:L:1(D):GLY:N	2:H:122:CYS:HA	1.92	0.82
2:H:236:LYS:H	2:H:236:LYS:CD	1.93	0.82
2:H:97(A):GLU:OE2	2:H:175:ARG:NH1	2.13	0.81
2:H:165:ARG:HE	2:H:169:LYS:NZ	1.77	0.81
2:H:158:VAL:HG22	5:H:480:HOH:O	1.83	0.79
1:L:1(E):SER:CA	2:H:123:LEU:O	2.31	0.79
1:L:1(H):THR:CG2	1:L:1(G):PHE:H	1.95	0.78
2:H:235:LYS:NZ	2:H:239:GLN:NE2	2.32	0.78
1:L:1(E):SER:H	2:H:123:LEU:HB2	1.48	0.77
1:L:14(J):TYR:O	1:L:14(K):ILE:HG12	1.83	0.77
2:H:74:THR:HG22	2:H:75:ARG:HD3	1.66	0.77
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	1.93	0.76
1:L:1(H):THR:HG23	1:L:1(G):PHE:N	2.00	0.76
1:L:1(F):GLY:N	2:H:235:LYS:HZ2	1.84	0.75
2:H:208:TYR:HB3	2:H:210:MET:CE	2.18	0.74
2:H:46:LEU:HD22	2:H:48:SER:O	1.86	0.74
2:H:242:ILE:O	2:H:246:GLY:HA2	1.88	0.73
2:H:75:ARG:NH2	5:H:809:HOH:O	2.22	0.72
1:L:1(F):GLY:N	2:H:235:LYS:NZ	2.37	0.72
2:H:219:GLY:HA3	2:H:221(A):ARG:HD2	1.68	0.72
1:L:1(G):PHE:CD1	2:H:239:GLN:OE1	2.42	0.72
2:H:160:LEU:CG	5:H:480:HOH:O	2.32	0.72
2:H:41:LEU:HD11	2:H:60(H):PHE:CE2	2.23	0.72
1:L:1(H):THR:CG2	1:L:1(G):PHE:N	2.53	0.72
2:H:187:ARG:HD3	2:H:221:ASP:OD2	1.90	0.71
2:H:195:SER:HB2	4:T:306:ARG:O	1.90	0.71
2:H:224:LYS:O	5:H:429:HOH:O	2.07	0.71
2:H:160:LEU:CD2	5:H:480:HOH:O	2.37	0.71
2:H:235:LYS:NZ	2:H:239:GLN:HE22	1.89	0.71
1:L:14(I):SER:C	1:L:14(K):ILE:H	1.97	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:14(E):GLU:HB2	5:L:505:HOH:O	1.89	0.70
2:H:165:ARG:NE	2:H:169:LYS:CE	2.55	0.70
2:H:87:LYS:HB3	2:H:89:TYR:CE1	2.27	0.69
3:I:61:GLU:HA	3:I:64:LEU:HD23	1.74	0.69
2:H:74:THR:HG22	2:H:75:ARG:N	2.08	0.69
1:L:1(F):GLY:CA	2:H:235:LYS:HZ2	2.06	0.68
2:H:195:SER:CB	4:T:306:ARG:O	2.41	0.68
2:H:87:LYS:HD3	2:H:88:ILE:H	1.59	0.68
1:L:1(E):SER:HA	2:H:123:LEU:N	2.09	0.67
2:H:60(I):THR:CG2	2:H:63:ASP:OD1	2.41	0.66
2:H:70:LYS:HE3	2:H:72:SER:O	1.93	0.66
2:H:201:MET:HE3	2:H:210:MET:CG	2.23	0.66
1:L:14(M):GLY:HA2	2:H:204:PRO:HB3	1.77	0.66
2:H:160:LEU:HD21	5:H:480:HOH:O	1.96	0.66
2:H:49:ASP:O	2:H:112:VAL:HG12	1.96	0.65
3:I:60:PRO:HB2	3:I:62:GLU:OE2	1.97	0.65
2:H:143:ASN:HA	2:H:150:GLY:O	1.97	0.65
2:H:35:ARG:O	2:H:38:GLN:HA	1.95	0.65
2:H:56:ALA:HB1	2:H:90:ILE:HG23	1.79	0.64
1:L:14(M):GLY:CA	2:H:204:PRO:HB3	2.27	0.64
2:H:98:ASN:OD1	2:H:98:ASN:N	2.27	0.64
2:H:195:SER:CB	4:T:306:ARG:C	2.71	0.64
2:H:70:LYS:NZ	2:H:80:GLU:OE2	2.27	0.64
3:I:60:PRO:O	3:I:63:TYS:HB3	1.98	0.63
2:H:50:ARG:HH11	2:H:107:LYS:HG3	1.63	0.63
2:H:165:ARG:NE	2:H:169:LYS:NZ	2.42	0.63
2:H:182:CYS:HA	2:H:226:GLY:O	1.98	0.63
2:H:161:PRO:HG3	2:H:184(A):TYR:CE1	2.34	0.62
1:L:14(G):LEU:HD12	1:L:14(M):GLY:HA3	1.82	0.62
3:I:60:PRO:HG2	3:I:63:TYS:HE2	1.81	0.62
1:L:1(H):THR:HG23	1:L:1(G):PHE:H	1.58	0.61
2:H:236:LYS:HD2	2:H:236:LYS:N	2.13	0.61
2:H:165:ARG:N	2:H:166:PRO:HD2	2.14	0.61
1:L:1(G):PHE:O	1:L:1(E):SER:N	2.34	0.61
2:H:100:ASP:O	2:H:101:ARG:HB2	2.01	0.61
2:H:201:MET:CE	2:H:210:MET:CG	2.71	0.61
2:H:60(B):PRO:N	2:H:60(C):PRO:HD2	2.16	0.60
1:L:1(C):GLU:N	1:L:1:CYS:HB3	2.17	0.60
2:H:17:VAL:O	2:H:18:GLU:HB2	2.01	0.60
2:H:187:ARG:NH1	2:H:221:ASP:O	2.34	0.60
1:L:1(F):GLY:HA2	2:H:235:LYS:HZ2	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:56:ALA:HB2	2:H:103:ILE:O	2.02	0.59
1:L:1(F):GLY:H	2:H:239:GLN:HE22	1.49	0.59
1:L:1(E):SER:CA	2:H:123:LEU:H	2.15	0.59
2:H:124:PRO:HB3	2:H:210:MET:HE1	1.82	0.59
2:H:187:ARG:NH2	2:H:222:ASP:OD1	2.35	0.59
2:H:60(B):PRO:O	2:H:60(C):PRO:C	2.40	0.59
2:H:86:GLU:HG3	2:H:109:LYS:HG3	1.84	0.59
2:H:57:HIS:NE2	4:T:306:ARG:OXT	2.27	0.59
2:H:239:GLN:OE1	2:H:239:GLN:HA	2.03	0.59
2:H:66:VAL:HG12	2:H:83:SER:HB2	1.85	0.58
2:H:198:PRO:HB2	2:H:200:VAL:HG13	1.83	0.58
2:H:63:ASP:OD1	2:H:63:ASP:N	2.34	0.58
2:H:208:TYR:CB	2:H:210:MET:HE3	2.30	0.58
2:H:50:ARG:HH11	2:H:107:LYS:CG	2.16	0.58
2:H:36(A):SER:HA	2:H:37:PRO:C	2.28	0.58
2:H:174:ILE:HG13	4:T:303:RNG:HG2	1.85	0.58
2:H:81:LYS:HE2	2:H:118:ILE:HD12	1.86	0.57
1:L:1(H):THR:O	1:L:1(G):PHE:HD1	1.87	0.57
1:L:1(H):THR:N	1:L:1(D):GLY:HA2	2.18	0.57
1:L:14(J):TYR:HE2	2:H:202:LYS:O	1.88	0.57
2:H:72:SER:OG	2:H:75:ARG:HG2	2.05	0.57
2:H:99:LEU:HD11	4:T:305:VAL:HB	1.86	0.57
1:L:3:LEU:HB2	1:L:9:LYS:HE2	1.87	0.56
2:H:132:ALA:HA	2:H:162:ILE:O	2.04	0.56
2:H:103:ILE:HD12	2:H:212:ILE:HD11	1.87	0.56
2:H:49:ASP:OD1	2:H:49:ASP:N	2.38	0.56
1:L:1(C):GLU:HB2	2:H:120:PRO:CG	2.36	0.56
1:L:1(E):SER:HA	2:H:123:LEU:O	2.04	0.56
2:H:36:LYS:HD2	2:H:65:LEU:HD13	1.86	0.56
2:H:53:LEU:HD11	2:H:103:ILE:HD11	1.88	0.56
2:H:81:LYS:HE2	2:H:118:ILE:CD1	2.35	0.56
2:H:20:SER:O	2:H:156:GLN:HA	2.06	0.55
2:H:191:CYS:O	2:H:194:ASP:HB2	2.05	0.55
2:H:236:LYS:CD	2:H:236:LYS:N	2.68	0.55
2:H:60(A):TYR:CZ	4:T:305:VAL:HG11	2.42	0.55
2:H:204(B):ASN:C	2:H:204(B):ASN:ND2	2.58	0.55
1:L:14(A):LYS:HG3	5:H:705:HOH:O	2.07	0.54
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.41	0.54
2:H:160:LEU:HD22	2:H:184:GLY:HA2	1.89	0.54
2:H:66:VAL:HG11	2:H:108:LEU:HD22	1.89	0.54
2:H:174:ILE:HG13	4:T:303:RNG:CG	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:158:VAL:CG2	5:H:480:HOH:O	2.46	0.54
2:H:165:ARG:HH21	2:H:169:LYS:NZ	2.06	0.54
1:L:1(E):SER:CA	2:H:123:LEU:N	2.71	0.53
1:L:1(C):GLU:CB	2:H:120:PRO:HG2	2.38	0.53
2:H:16:ILE:N	2:H:194:ASP:OD2	2.41	0.53
2:H:17:VAL:HG11	2:H:221:ASP:HB3	1.89	0.53
2:H:165:ARG:HH21	2:H:169:LYS:HZ3	1.56	0.53
2:H:42:CYS:HB3	2:H:195:SER:O	2.08	0.52
1:L:4:ARG:HB2	1:L:8:GLU:OE1	2.10	0.52
2:H:165:ARG:NH2	2:H:169:LYS:NZ	2.58	0.52
2:H:47:ILE:HD11	2:H:105:LEU:HD21	1.92	0.52
2:H:60(B):PRO:N	2:H:60(C):PRO:CD	2.72	0.52
2:H:85:LEU:CD1	2:H:106:MET:HE3	2.39	0.51
2:H:87:LYS:CD	2:H:88:ILE:H	2.21	0.51
1:L:3:LEU:CB	1:L:9:LYS:HE2	2.41	0.51
1:L:1(H):THR:H2	2:H:123:LEU:HD11	1.75	0.51
2:H:215:TRP:CE3	4:T:303:RNG:HH	2.45	0.51
1:L:1(F):GLY:CA	2:H:235:LYS:NZ	2.72	0.50
2:H:165:ARG:N	2:H:166:PRO:CD	2.74	0.50
1:L:1(D):GLY:H	2:H:122:CYS:C	2.18	0.50
1:L:1(E):SER:HA	2:H:122:CYS:HB3	1.92	0.50
2:H:100:ASP:CG	2:H:177:THR:HG21	2.36	0.50
2:H:165:ARG:CZ	2:H:169:LYS:NZ	2.74	0.50
2:H:186(A):ASP:C	2:H:186(C):GLY:N	2.69	0.50
2:H:134:TYR:N	2:H:134:TYR:HD1	2.10	0.50
2:H:164:GLU:C	2:H:166:PRO:HD2	2.37	0.49
2:H:237:TRP:HB2	5:H:937:HOH:O	2.11	0.49
2:H:165:ARG:HE	2:H:169:LYS:CE	2.22	0.49
2:H:204(B):ASN:HD22	2:H:205:ASN:N	2.09	0.49
2:H:60(G):ASN:ND2	5:H:521:HOH:O	2.38	0.49
2:H:97:ARG:HG2	2:H:97:ARG:HH11	1.78	0.49
2:H:165:ARG:O	2:H:168:CYS:HB2	2.13	0.49
1:L:1(H):THR:H1	1:L:1(D):GLY:HA2	1.78	0.48
1:L:1(E):SER:C	2:H:123:LEU:H	2.18	0.48
2:H:32:MET:HG3	2:H:40:LEU:HD12	1.96	0.48
2:H:57:HIS:HE2	4:T:306:ARG:C	2.20	0.48
5:L:756:HOH:O	2:H:26:MET:HE1	2.12	0.48
2:H:124:PRO:HG3	2:H:210:MET:CE	2.44	0.48
2:H:165:ARG:CZ	2:H:169:LYS:HZ1	2.24	0.48
1:L:4:ARG:HG2	2:H:28:PRO:CG	2.43	0.48
3:I:59:ILE:O	3:I:60:PRO:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1(D):GLY:N	2:H:122:CYS:CA	2.70	0.48
2:H:195:SER:HB2	4:T:306:ARG:C	2.36	0.48
2:H:61:GLU:H	2:H:61:GLU:HG2	1.27	0.48
2:H:85:LEU:HD11	2:H:106:MET:HE3	1.95	0.47
2:H:34:PHE:HZ	2:H:38:GLN:HB3	1.79	0.47
2:H:49:ASP:O	2:H:112:VAL:CG1	2.61	0.47
2:H:97(A):GLU:CD	2:H:175:ARG:HH12	2.22	0.47
2:H:18:GLU:HG3	2:H:187:ARG:CB	2.36	0.47
2:H:34:PHE:CZ	2:H:38:GLN:HB3	2.49	0.47
2:H:176:ILE:HD12	2:H:227:PHE:CE2	2.50	0.47
1:L:5:PRO:O	1:L:9:LYS:HB2	2.15	0.47
2:H:164:GLU:CD	2:H:185:LYS:HZ1	2.22	0.47
2:H:36:LYS:O	2:H:38:GLN:HG2	2.15	0.46
1:L:14(G):LEU:O	1:L:14(L):ASP:HA	2.16	0.46
3:I:61:GLU:CD	3:I:61:GLU:H	2.23	0.46
2:H:144:LEU:HD11	2:H:152:PRO:HA	1.97	0.46
2:H:56:ALA:CB	2:H:90:ILE:HG23	2.46	0.46
2:H:74:THR:HB	5:H:902:HOH:O	2.14	0.46
2:H:161:PRO:HD3	2:H:184(A):TYR:CZ	2.50	0.46
2:H:209:GLN:C	2:H:210:MET:HE2	2.41	0.46
2:H:18:GLU:HB2	2:H:188:GLY:HA2	1.98	0.46
2:H:240:LYS:HD3	5:H:605:HOH:O	1.94	0.46
1:L:1(G):PHE:O	1:L:1(E):SER:C	2.59	0.46
2:H:70:LYS:HZ2	2:H:77:GLU:HG3	1.81	0.46
2:H:134:TYR:N	2:H:134:TYR:CD1	2.84	0.46
2:H:187:ARG:HB3	2:H:221:ASP:OD1	2.15	0.46
2:H:17:VAL:HG11	2:H:221:ASP:CB	2.46	0.46
1:L:1(C):GLU:HB2	2:H:120:PRO:HG2	1.97	0.45
1:L:14(F):LEU:O	1:L:14(I):SER:OG	2.29	0.45
2:H:165:ARG:NE	2:H:169:LYS:HE3	2.30	0.45
1:L:1(H):THR:N	2:H:123:LEU:CD1	2.80	0.45
1:L:1(D):GLY:CA	2:H:122:CYS:HA	2.46	0.44
2:H:26:MET:HE2	2:H:137:ARG:CZ	2.47	0.44
2:H:60(I):THR:CG2	2:H:63:ASP:CG	2.90	0.44
2:H:128:THR:HG23	2:H:129(C):LEU:HD12	1.98	0.44
2:H:186(A):ASP:O	2:H:186(C):GLY:N	2.50	0.44
1:L:10:LYS:NZ	5:L:817:HOH:O	2.50	0.44
2:H:57:HIS:CE1	2:H:195:SER:OG	2.71	0.44
2:H:60(B):PRO:HG2	2:H:96:TRP:CH2	2.52	0.44
2:H:195:SER:OG	4:T:306:ARG:O	2.35	0.44
1:L:1(D):GLY:H	2:H:122:CYS:CA	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:16:ILE:HD13	2:H:190:ALA:HA	2.00	0.44
2:H:217:GLU:O	2:H:221(A):ARG:HD2	2.18	0.44
2:H:165:ARG:HB3	2:H:166:PRO:HD3	1.99	0.44
2:H:41:LEU:HD22	2:H:41:LEU:HA	1.84	0.43
1:L:1(H):THR:H2	2:H:123:LEU:CD1	2.30	0.43
2:H:61:GLU:OE1	2:H:87:LYS:CA	2.55	0.43
2:H:91:HIS:CE1	2:H:101:ARG:HD2	2.54	0.43
1:L:14(A):LYS:HE3	1:L:14(A):LYS:HB2	1.68	0.43
2:H:60(A):TYR:OH	4:T:305:VAL:HG11	2.18	0.43
2:H:60(I):THR:HG23	2:H:63:ASP:CG	2.38	0.43
2:H:161:PRO:HG3	2:H:184(A):TYR:CD1	2.54	0.43
2:H:204(B):ASN:ND2	2:H:206:ARG:H	2.17	0.43
1:L:14(H):GLU:HA	1:L:14(L):ASP:HA	2.00	0.43
2:H:129(C):LEU:HD21	2:H:204:PRO:HD3	2.00	0.43
2:H:144:LEU:HD11	2:H:152:PRO:CA	2.49	0.42
2:H:60(A):TYR:C	2:H:60(C):PRO:HD2	2.44	0.42
3:I:58:GLU:HB2	5:I:426:HOH:O	2.19	0.42
3:I:64:LEU:N	3:I:64:LEU:HD22	2.33	0.42
2:H:30:GLN:HG3	2:H:31:VAL:N	2.33	0.42
2:H:81:LYS:CE	2:H:118:ILE:HD12	2.48	0.42
2:H:173:ARG:NE	5:H:733:HOH:O	2.52	0.42
3:I:63:TYS:HD1	3:I:63:TYS:HA	1.80	0.42
2:H:87:LYS:HB3	2:H:89:TYR:HE1	1.83	0.42
4:T:305:VAL:O	4:T:305:VAL:HG22	2.20	0.42
2:H:133:GLY:N	2:H:162:ILE:O	2.47	0.42
1:L:14(I):SER:C	1:L:14(K):ILE:N	2.68	0.42
2:H:60(I):THR:HG22	2:H:63:ASP:OD2	2.19	0.42
2:H:57:HIS:C	2:H:57:HIS:CD2	2.97	0.42
1:L:1(F):GLY:N	2:H:239:GLN:HE22	2.16	0.41
2:H:66:VAL:HG11	2:H:108:LEU:CD2	2.50	0.41
2:H:70:LYS:HE3	2:H:70:LYS:HB3	1.94	0.41
2:H:126:ARG:HA	2:H:232:PHE:CZ	2.55	0.41
2:H:165:ARG:CZ	2:H:169:LYS:HE2	2.50	0.41
2:H:60(D):TRP:CH2	4:T:305:VAL:HG22	2.56	0.41
2:H:242:ILE:O	2:H:246:GLY:CA	2.64	0.41
2:H:165:ARG:CZ	2:H:169:LYS:CE	2.98	0.41
2:H:236:LYS:O	2:H:240:LYS:HB3	2.20	0.41
4:T:305:VAL:O	4:T:305:VAL:CG2	2.68	0.41
1:L:1(G):PHE:HA	2:H:239:GLN:HE22	1.85	0.41
2:H:46:LEU:CD2	2:H:48:SER:O	2.64	0.41
2:H:49:ASP:HA	2:H:112:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:52:VAL:HG23	2:H:108:LEU:HD21	2.03	0.41
2:H:57:HIS:HE1	2:H:214:SER:O	2.03	0.41
2:H:102:ASP:OD2	2:H:214:SER:OG	2.34	0.41
1:L:14(C):GLU:O	1:L:14(F):LEU:HB2	2.20	0.41
1:L:15:ARG:O	1:L:15:ARG:HG3	2.21	0.41
2:H:51:TRP:NE1	2:H:247:GLU:CA	2.63	0.41
1:L:1(C):GLU:H	1:L:1(CYS):HB3	1.83	0.40
2:H:93:ARG:HH11	2:H:93:ARG:HD3	1.72	0.40
1:L:1(H):THR:C	1:L:1(G):PHE:HD1	2.30	0.40
2:H:103:ILE:HB	2:H:229:THR:HG21	2.04	0.40
2:H:127:GLU:HB3	5:H:715:HOH:O	2.21	0.40
2:H:50:ARG:HA	2:H:108:LEU:HD12	2.04	0.40
2:H:165:ARG:NH2	2:H:169:LYS:HZ3	2.18	0.40
1:L:14(J):TYR:HD2	2:H:204:PRO:HG3	1.86	0.40

All (3) 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)
1:L:14(L):ASP:O	2:H:173:ARG:NH1[4_556]	2.07	0.13
1:L:14(M):GLY:O	2:H:173:ARG:NH1[4_556]	2.09	0.11
1:L:15:ARG:CZ	2:H:172:THR:O[4_556]	2.18	0.02

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	34/36 (94%)	21 (62%)	7 (21%)	6 (18%)	0	0
2	H	247/259 (95%)	228 (92%)	17 (7%)	2 (1%)	16	31
3	I	7/12 (58%)	7 (100%)	0	0	100	100
4	T	2/4 (50%)	1 (50%)	1 (50%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	290/311 (93%)	257 (89%)	25 (9%)	8 (3%)	4 6

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	1(F)	GLY
1	L	1(E)	SER
1	L	1(D)	GLY
1	L	1(C)	GLU
1	L	14(M)	GLY
2	H	246	GLY
2	H	77(A)	ARG
1	L	14(K)	ILE

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	30/31 (97%)	28 (93%)	2 (7%)	15 31
2	H	212/225 (94%)	174 (82%)	38 (18%)	2 3
3	I	7/10 (70%)	6 (86%)	1 (14%)	3 6
4	T	2/2 (100%)	1 (50%)	1 (50%)	0 0
All	All	251/268 (94%)	209 (83%)	42 (17%)	2 4

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	6	LEU
1	L	10	LYS
2	H	24	ILE
2	H	27	SER
2	H	32	MET
2	H	33	LEU
2	H	41	LEU

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Mol	Chain	Res	Type
2	H	46	LEU
2	H	48	SER
2	H	57	HIS
2	H	61	GLU
2	H	63	ASP
2	H	64	LEU
2	H	65	LEU
2	H	66	VAL
2	H	74	THR
2	H	77	GLU
2	H	77(A)	ARG
2	H	79	ILE
2	H	90	ILE
2	H	97	ARG
2	H	97(A)	GLU
2	H	99	LEU
2	H	107	LYS
2	H	108	LEU
2	H	112	VAL
2	H	127	GLU
2	H	154	VAL
2	H	163	VAL
2	H	164	GLU
2	H	177	THR
2	H	187	ARG
2	H	195	SER
2	H	202	LYS
2	H	233	ARG
2	H	235	LYS
2	H	236	LYS
2	H	239	GLN
2	H	241	VAL
2	H	242	ILE
3	I	62	GLU
4	T	305	VAL

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	60(G)	ASN
2	H	156	GLN
2	H	204(B)	ASN

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Mol	Chain	Res	Type
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	2.06	2 (13%)	15,22,24	1.88	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	-	2/10/11/13	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-S	5.97	1.70	1.58
3	I	63	TYS	OH-CZ	-4.35	1.35	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	63	TYS	O2-S-O1	4.28	128.75	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	63	TYS	OH-S-O2	-2.97	98.52	107.56
3	I	63	TYS	CB-CG-CD1	-2.45	116.35	120.90
3	I	63	TYS	CD2-CG-CD1	2.21	121.52	118.23
3	I	63	TYS	CE2-CZ-CE1	2.01	123.10	120.16

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	63	TYS	CA-CB-CG-CD1
3	I	63	TYS	CA-CB-CG-CD2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.