



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:34 PM UTC

PDB ID : 1HGT / pdb_00001hgt
Title : STRUCTURE OF THE HIRUGEN AND HIRULOG 1 COMPLEXES OF
ALPHA-THROMBIN
Authors : Tulinsky, A.; Skrzypczak-Jankun, E.
Deposited on : 1991-06-03
Resolution : 2.20 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

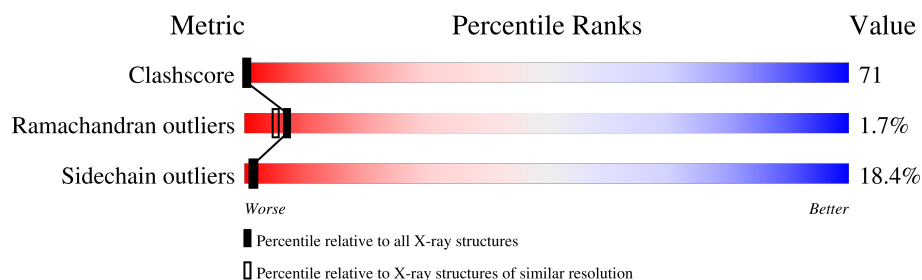
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	
2	H	259	
3	I	12	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2678 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 ALPHA-THROMBIN (SMALL SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	36	Total	C	N	O	S	0	0	0
			287	177	48	61	1			

- Molecule 2 is a protein called ALPHA-THROMBIN (LARGE SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	253	Total	C	N	O	S	0	0	0
			2053	1310	362	367	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
			95	59	10	25	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	54	GLU	GLY	conflict	UNP P09945

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	37	Total	O	0	0
			37	37		
4	H	191	Total	O	0	0
			191	191		
4	I	15	Total	O	0	0
			15	15		

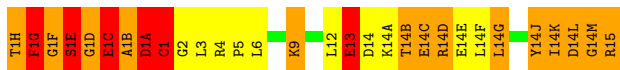
3 Residue-property plots

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.

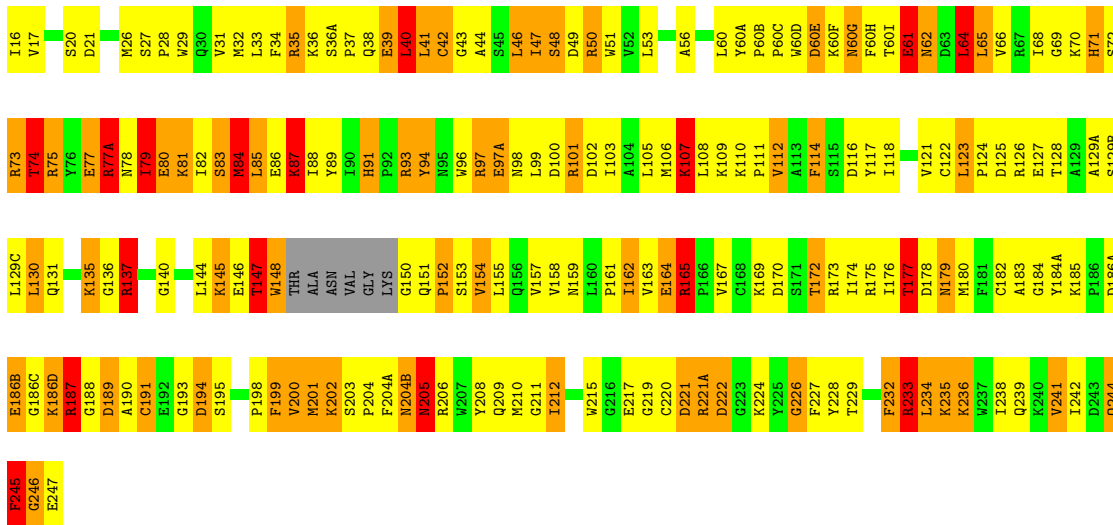
• Molecule 1: ALPHA-THROMBIN (SMALL SUBUNIT)

Chain L: 



• Molecule 2: ALPHA-THROMBIN (LARGE SUBUNIT)

Chain H: 



• Molecule 3: HIRUGEN

Chain I: 



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	70.80Å 71.80Å 72.60Å 90.00° 100.90° 90.00°	Depositor
Resolution (Å)	7.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.167 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2678	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: 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	1.55	3/290 (1.0%)	2.84	25/384 (6.5%)
2	H	1.50	5/2107 (0.2%)	2.51	152/2846 (5.3%)
3	I	1.29	0/79	2.39	5/103 (4.9%)
All	All	1.50	8/2476 (0.3%)	2.54	182/3333 (5.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	15	ARG	CD-NE	6.05	1.54	1.46
2	H	27	SER	N-CA	5.76	1.53	1.46
2	H	137	ARG	CD-NE	-5.75	1.38	1.46
2	H	78	ASN	N-CA	5.59	1.52	1.46
2	H	101	ARG	N-CA	5.22	1.54	1.46
1	L	9	LYS	C-O	5.15	1.30	1.24
2	H	107	LYS	CA-CB	-5.13	1.45	1.53
1	L	15	ARG	CZ-NH1	5.02	1.39	1.32

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	1(A)	ASP	CA-CB-CG	-13.07	99.53	112.60
2	H	64	LEU	N-CA-C	12.79	129.34	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	101	ARG	NE-CZ-NH2	-11.75	108.62	119.20
2	H	137	ARG	CD-NE-CZ	11.62	140.67	124.40
1	L	12	LEU	CA-C-N	11.35	137.87	122.77
1	L	12	LEU	C-N-CA	11.35	137.87	122.77
2	H	137	ARG	NE-CZ-NH1	10.97	132.47	121.50
2	H	78	ASN	CA-CB-CG	10.91	123.52	112.60
1	L	14(D)	ARG	CD-NE-CZ	10.60	139.24	124.40
1	L	15	ARG	NH1-CZ-NH2	10.57	133.04	119.30
2	H	62	ASN	N-CA-C	9.59	121.82	111.36
2	H	82	ILE	CA-C-O	-9.46	110.41	120.53
2	H	41	LEU	CB-CA-C	9.36	125.00	109.56
2	H	34	PHE	CA-C-O	9.18	130.51	120.32
1	L	15	ARG	CD-NE-CZ	-9.15	111.59	124.40
2	H	77(A)	ARG	NE-CZ-NH2	-8.72	111.35	119.20
2	H	164	GLU	CB-CG-CD	8.70	127.39	112.60
2	H	27	SER	N-CA-CB	-8.60	99.61	110.79
2	H	74	THR	N-CA-C	8.58	124.38	112.45
2	H	71	HIS	CA-CB-CG	-8.57	105.23	113.80
2	H	187	ARG	CD-NE-CZ	-8.32	112.75	124.40
2	H	114	PHE	O-C-N	8.04	131.96	122.79
2	H	116	ASP	CA-CB-CG	8.00	120.60	112.60
1	L	15	ARG	NE-CZ-NH1	-7.92	113.58	121.50
2	H	64	LEU	N-CA-CB	-7.86	97.87	111.55
2	H	226	GLY	O-C-N	7.84	131.19	123.35
2	H	61	GLU	CA-C-N	7.81	131.38	120.29
2	H	61	GLU	C-N-CA	7.81	131.38	120.29
1	L	1(D)	GLY	CA-C-O	7.79	131.33	121.67
3	I	61	GLU	N-CA-CB	7.73	121.78	110.57
2	H	91	HIS	CA-CB-CG	-7.72	106.08	113.80
2	H	40	LEU	O-C-N	7.54	132.29	123.02
2	H	137	ARG	NE-CZ-NH2	-7.54	112.42	119.20
2	H	193	GLY	O-C-N	7.54	131.57	122.60
3	I	61	GLU	CB-CG-CD	7.49	125.33	112.60
2	H	155	LEU	CA-C-O	-7.43	112.86	120.96
2	H	60(G)	ASN	CA-CB-CG	-7.30	105.30	112.60
2	H	79	ILE	CB-CA-C	7.29	118.37	111.44
2	H	186(B)	GLU	N-CA-C	7.21	121.91	113.18
1	L	14(J)	TYR	N-CA-C	-7.20	104.51	112.72
1	L	14(C)	GLU	CA-C-O	-7.17	112.89	120.92
1	L	1(C)	GLU	CA-C-O	-7.10	110.36	120.51
1	L	1(G)	PHE	CA-CB-CG	-7.06	106.74	113.80
2	H	100	ASP	O-C-N	7.04	131.48	122.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	13	GLU	CB-CA-C	-6.92	98.98	110.19
2	H	200	VAL	O-C-N	6.90	130.28	123.03
2	H	42	CYS	N-CA-CB	-6.89	100.00	111.57
2	H	179	ASN	CA-CB-CG	-6.87	105.73	112.60
2	H	77	GLU	CA-C-O	6.84	130.69	122.41
2	H	147	THR	CA-C-O	6.79	128.36	120.75
2	H	36	LYS	CA-CB-CG	6.74	127.58	114.10
2	H	187	ARG	NE-CZ-NH2	6.74	125.27	119.20
1	L	14(G)	LEU	CB-CA-C	6.73	121.97	110.79
2	H	195	SER	O-C-N	6.73	131.18	122.97
1	L	1(D)	GLY	N-CA-C	6.67	122.95	111.47
2	H	114	PHE	CA-CB-CG	-6.67	107.13	113.80
2	H	75	ARG	NE-CZ-NH1	6.66	128.16	121.50
2	H	97	ARG	NE-CZ-NH2	-6.65	113.21	119.20
2	H	232	PHE	CA-CB-CG	-6.60	107.20	113.80
2	H	201	MET	CA-CB-CG	-6.58	100.94	114.10
2	H	233	ARG	NE-CZ-NH2	-6.57	113.28	119.20
2	H	34	PHE	CA-CB-CG	6.56	120.36	113.80
3	I	57	GLU	N-CA-C	-6.51	101.36	110.35
1	L	14(C)	GLU	CB-CA-C	-6.51	99.94	110.74
1	L	15	ARG	NE-CZ-NH2	-6.49	113.36	119.20
2	H	190	ALA	N-CA-C	-6.49	101.80	110.55
2	H	147	THR	CA-C-N	6.47	133.35	121.70
2	H	147	THR	C-N-CA	6.47	133.35	121.70
2	H	62	ASN	OD1-CG-ND2	6.45	129.05	122.60
2	H	153	SER	CA-C-N	6.44	132.92	122.69
2	H	153	SER	C-N-CA	6.44	132.92	122.69
2	H	179	ASN	OD1-CG-ND2	6.41	129.01	122.60
2	H	101	ARG	NE-CZ-NH1	6.41	127.91	121.50
2	H	77(A)	ARG	CA-C-O	-6.36	111.42	120.51
2	H	75	ARG	CB-CA-C	6.28	121.02	109.46
2	H	128	THR	CA-C-N	6.25	128.98	120.54
2	H	128	THR	C-N-CA	6.25	128.98	120.54
2	H	205	ASN	CB-CA-C	6.22	121.34	111.51
2	H	107	LYS	O-C-N	6.14	130.53	123.29
2	H	123	LEU	CB-CA-C	6.13	117.51	108.87
2	H	35	ARG	NE-CZ-NH2	-6.10	113.71	119.20
2	H	186(D)	LYS	N-CA-C	-6.08	97.84	110.80
2	H	44	ALA	O-C-N	6.03	130.60	122.59
2	H	74	THR	N-CA-CB	-6.01	101.30	110.26
3	I	61	GLU	CA-CB-CG	6.00	126.10	114.10
2	H	174	ILE	CA-C-N	5.99	131.87	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	174	ILE	C-N-CA	5.99	131.87	122.17
2	H	50	ARG	CA-CB-CG	-5.93	102.24	114.10
2	H	100	ASP	CA-C-O	-5.91	114.54	121.16
2	H	137	ARG	CG-CD-NE	5.91	125.00	112.00
2	H	110	LYS	O-C-N	5.91	128.09	122.06
2	H	135	LYS	O-C-N	5.90	130.00	123.16
2	H	48	SER	CA-C-O	-5.89	114.83	121.25
2	H	158	VAL	CA-C-N	5.89	130.60	122.77
2	H	158	VAL	C-N-CA	5.89	130.60	122.77
1	L	1	CYS	CA-C-O	5.88	127.62	121.15
2	H	233	ARG	CB-CA-C	-5.88	99.76	110.63
1	L	14(C)	GLU	CA-CB-CG	5.87	125.84	114.10
2	H	204(B)	ASN	CA-C-N	5.87	130.91	122.40
2	H	204(B)	ASN	C-N-CA	5.87	130.91	122.40
2	H	205	ASN	CA-C-N	5.85	132.58	122.64
2	H	205	ASN	C-N-CA	5.85	132.58	122.64
2	H	80	GLU	CA-C-O	5.84	128.19	121.47
2	H	125	ASP	N-CA-C	-5.84	101.88	110.52
2	H	221	ASP	CA-CB-CG	-5.84	106.76	112.60
1	L	2	GLY	O-C-N	5.84	128.96	122.31
2	H	97(A)	GLU	N-CA-C	5.83	119.94	112.12
2	H	145	LYS	O-C-N	5.81	130.11	123.31
2	H	140	GLY	CA-C-O	5.79	127.29	121.62
2	H	43	GLY	N-CA-C	-5.74	103.82	112.60
2	H	152	PRO	CA-C-O	-5.74	114.73	122.08
2	H	62	ASN	CA-CB-CG	-5.74	106.86	112.60
2	H	60	LEU	N-CA-CB	-5.73	101.71	110.65
2	H	153	SER	N-CA-C	-5.71	106.48	113.50
1	L	1(E)	SER	C-N-CA	5.70	134.27	122.30
2	H	87	LYS	N-CA-C	5.69	117.93	108.99
2	H	186(D)	LYS	O-C-N	5.68	130.15	122.59
2	H	75	ARG	CA-C-O	5.67	127.99	121.47
2	H	189	ASP	CA-CB-CG	5.67	118.27	112.60
2	H	60(E)	ASP	CA-CB-CG	-5.66	106.94	112.60
2	H	206	ARG	NE-CZ-NH1	5.65	127.15	121.50
2	H	47	ILE	CA-C-O	5.63	124.31	118.96
2	H	155	LEU	O-C-N	5.58	129.75	123.06
2	H	186(D)	LYS	CA-C-O	-5.57	112.54	120.51
2	H	129(C)	LEU	N-CA-C	5.56	120.19	113.41
2	H	75	ARG	NE-CZ-NH2	-5.55	114.20	119.20
2	H	93	ARG	NE-CZ-NH2	5.53	124.18	119.20
2	H	36	LYS	N-CA-C	-5.51	104.96	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	172	THR	N-CA-CB	-5.49	102.73	111.62
2	H	74	THR	OG1-CB-CG2	5.46	120.22	109.30
2	H	117	TYR	O-C-N	5.44	128.82	122.24
2	H	212	ILE	N-CA-CB	5.43	119.45	111.52
2	H	34	PHE	CA-C-N	5.43	129.06	121.24
2	H	34	PHE	C-N-CA	5.43	129.06	121.24
2	H	60(E)	ASP	CB-CA-C	-5.41	102.53	111.36
2	H	151	GLN	O-C-N	5.41	126.58	121.38
2	H	165	ARG	CD-NE-CZ	-5.41	116.83	124.40
2	H	173	ARG	CD-NE-CZ	5.39	131.95	124.40
2	H	191	CYS	CB-CA-C	5.39	124.78	111.95
2	H	235	LYS	CA-C-N	-5.39	113.05	120.28
2	H	235	LYS	C-N-CA	-5.39	113.05	120.28
2	H	170	ASP	CA-CB-CG	-5.39	107.21	112.60
1	L	14(K)	ILE	CB-CA-C	5.38	120.11	111.29
1	L	14(C)	GLU	CB-CG-CD	5.35	121.69	112.60
2	H	74	THR	CA-CB-OG1	-5.34	101.58	109.60
2	H	110	LYS	CB-CA-C	-5.33	101.72	109.45
1	L	9	LYS	N-CA-C	5.33	117.84	111.71
2	H	194	ASP	CA-C-N	5.33	128.41	120.90
2	H	194	ASP	C-N-CA	5.33	128.41	120.90
2	H	222	ASP	CA-CB-CG	-5.32	107.28	112.60
2	H	100	ASP	N-CA-C	-5.31	102.42	110.28
2	H	215	TRP	CA-C-O	5.31	127.01	121.38
2	H	199	PHE	CA-C-O	5.31	126.75	120.70
2	H	234	LEU	CA-C-N	5.30	127.33	120.44
2	H	234	LEU	C-N-CA	5.30	127.33	120.44
2	H	44	ALA	CA-C-O	-5.29	112.94	120.51
2	H	162	ILE	N-CA-C	-5.28	102.70	109.30
2	H	151	GLN	CG-CD-NE2	-5.26	108.51	116.40
2	H	172	THR	CA-C-N	5.25	130.91	121.66
2	H	172	THR	C-N-CA	5.25	130.91	121.66
2	H	40	LEU	CA-C-N	-5.24	112.46	122.53
2	H	40	LEU	C-N-CA	-5.24	112.46	122.53
2	H	114	PHE	CA-C-O	-5.22	115.81	121.87
2	H	62	ASN	O-C-N	5.22	128.10	122.15
2	H	77(A)	ARG	CA-C-N	-5.21	114.31	122.49
2	H	77(A)	ARG	C-N-CA	-5.21	114.31	122.49
2	H	80	GLU	CB-CG-CD	5.17	121.39	112.60
3	I	57	GLU	CA-CB-CG	5.16	124.43	114.10
2	H	177	THR	CA-CB-OG1	-5.16	101.87	109.60
2	H	60	LEU	N-CA-C	5.15	116.81	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	94	TYR	CA-C-O	-5.14	115.06	120.92
2	H	84	MET	O-C-N	5.13	129.73	123.21
2	H	246	GLY	O-C-N	5.13	129.37	122.70
2	H	244	GLN	CB-CG-CD	5.12	121.31	112.60
2	H	212	ILE	O-C-N	5.12	128.73	123.20
2	H	206	ARG	O-C-N	5.10	128.96	123.10
2	H	151	GLN	OE1-CD-NE2	5.07	127.67	122.60
2	H	80	GLU	CA-CB-CG	5.07	124.23	114.10
1	L	14(B)	THR	CA-C-O	-5.06	113.31	119.03
2	H	221(A)	ARG	NE-CZ-NH2	-5.04	114.66	119.20
2	H	107	LYS	N-CA-C	-5.02	100.98	109.07
2	H	245	PHE	CA-CB-CG	5.02	118.82	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	233	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	287	0	278	71	2
2	H	2053	0	2020	278	2
3	I	95	0	73	29	0
4	H	191	0	0	30	0
4	I	15	0	0	4	0
4	L	37	0	0	8	0
All	All	2678	0	2371	339	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 71.

All (339) 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:1(E):SER:HA	2:H:123:LEU:O	1.43	1.16
2:H:60(I):THR:CG2	2:H:62:ASN:HB2	1.75	1.15
2:H:199:PHE:CE1	2:H:201:MET:HE2	1.86	1.10
1:L:1(G):PHE:HA	2:H:123:LEU:HD12	1.32	1.10
1:L:1(H):THR:HG23	2:H:242:ILE:HD13	1.26	1.09
2:H:33:LEU:HD22	2:H:64:LEU:HD21	1.26	1.08
2:H:199:PHE:HE1	2:H:201:MET:HE2	1.11	1.07
2:H:145:LYS:HD3	2:H:148:TRP:HB3	1.30	1.07
2:H:50:ARG:NH2	2:H:108:LEU:O	1.91	1.03
1:L:1(B):ALA:HB3	4:L:645:HOH:O	1.56	1.03
2:H:199:PHE:HE1	2:H:201:MET:CE	1.71	1.03
2:H:85:LEU:HD13	2:H:106:MET:HE2	1.06	1.02
2:H:85:LEU:HD13	2:H:106:MET:CE	1.90	1.02
2:H:85:LEU:CD1	2:H:106:MET:HE2	1.90	1.01
1:L:14(J):TYR:O	1:L:14(K):ILE:HG13	1.58	1.01
2:H:33:LEU:CD2	2:H:64:LEU:HD21	1.90	1.01
3:I:61:GLU:CG	3:I:64:LEU:HB2	1.91	0.99
3:I:55:ASP:HB3	4:I:625:HOH:O	1.60	0.98
1:L:1(H):THR:HG21	2:H:242:ILE:HG21	1.45	0.98
3:I:59:ILE:HG12	3:I:64:LEU:HD21	1.44	0.98
1:L:15:ARG:HB2	2:H:204:PRO:O	1.63	0.97
2:H:50:ARG:NH2	2:H:86:GLU:OE1	1.96	0.97
2:H:74:THR:HG22	2:H:75:ARG:HG3	1.46	0.95
2:H:185:LYS:CB	2:H:186(A):ASP:OD1	2.13	0.95
1:L:14(D):ARG:HD3	4:L:901:HOH:O	1.67	0.94
2:H:148:TRP:N	2:H:148:TRP:CE3	2.35	0.93
3:I:61:GLU:HG2	3:I:64:LEU:HB2	1.51	0.92
2:H:79:ILE:HD11	4:H:662:HOH:O	1.69	0.91
3:I:59:ILE:HD11	3:I:64:LEU:HD23	1.52	0.91
3:I:59:ILE:CG1	3:I:64:LEU:HD21	2.00	0.90
2:H:61:GLU:OE1	2:H:87:LYS:HA	1.68	0.90
2:H:147:THR:HA	2:H:148:TRP:CE3	2.06	0.90
2:H:60(I):THR:HG23	2:H:62:ASN:HB2	1.50	0.89
2:H:87:LYS:HD2	2:H:88:ILE:N	1.87	0.89
3:I:59:ILE:HD11	3:I:64:LEU:CD2	2.03	0.89
1:L:9:LYS:HG2	4:L:753:HOH:O	1.72	0.89
2:H:148:TRP:N	2:H:148:TRP:HE3	1.68	0.89
2:H:147:THR:HA	2:H:148:TRP:CZ3	2.08	0.88
2:H:126:ARG:HB2	2:H:232:PHE:CZ	2.10	0.87
1:L:14(J):TYR:C	1:L:14(K):ILE:CG1	2.48	0.87
2:H:185:LYS:HB3	2:H:186(A):ASP:OD1	1.74	0.87
2:H:185:LYS:HB2	2:H:186(A):ASP:OD1	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:3:LEU:O	1:L:9:LYS:HE2	1.76	0.85
1:L:1(F):GLY:HA2	2:H:235:LYS:HZ3	1.42	0.84
2:H:162:ILE:HD11	2:H:199:PHE:CZ	2.12	0.84
2:H:165:ARG:NH2	2:H:177:THR:O	2.10	0.83
2:H:172:THR:HG21	2:H:176:ILE:HD11	1.58	0.83
1:L:1(E):SER:CA	2:H:123:LEU:O	2.27	0.82
2:H:97(A):GLU:OE1	2:H:175:ARG:NH1	2.13	0.82
1:L:1(G):PHE:O	1:L:1(D):GLY:N	2.13	0.81
2:H:51:TRP:HE1	2:H:247:GLU:H	1.29	0.80
2:H:35:ARG:O	2:H:38:GLN:HA	1.79	0.80
2:H:236:LYS:HD2	4:H:864:HOH:O	1.81	0.80
3:I:61:GLU:HG3	3:I:64:LEU:HB2	1.63	0.80
1:L:14(J):TYR:C	1:L:14(K):ILE:HG13	2.05	0.80
2:H:32:MET:HE2	2:H:40:LEU:CD1	2.12	0.79
2:H:201:MET:HE3	2:H:210:MET:HG3	1.64	0.79
1:L:1(H):THR:CG2	2:H:242:ILE:HD13	2.12	0.78
2:H:60(I):THR:HG23	2:H:62:ASN:H	1.48	0.78
2:H:185:LYS:HB2	2:H:186(B):GLU:HG3	1.65	0.77
3:I:61:GLU:HA	3:I:64:LEU:HG	1.66	0.77
2:H:130:LEU:HD23	2:H:201:MET:HE1	1.68	0.76
1:L:3:LEU:O	1:L:9:LYS:CE	2.33	0.76
2:H:87:LYS:CD	2:H:88:ILE:H	1.98	0.76
1:L:1(G):PHE:HA	2:H:123:LEU:CD1	2.15	0.75
1:L:1(H):THR:N	1:L:1(C):GLU:HA	2.01	0.75
2:H:85:LEU:CD1	2:H:106:MET:CE	2.55	0.74
2:H:41:LEU:HD13	4:H:603:HOH:O	1.86	0.74
2:H:147:THR:C	2:H:148:TRP:HE3	1.95	0.74
1:L:1(E):SER:H	2:H:235:LYS:HZ1	1.35	0.74
1:L:1(G):PHE:CA	2:H:123:LEU:HD12	2.13	0.73
1:L:15:ARG:CG	1:L:15:ARG:O	2.34	0.73
2:H:217:GLU:O	2:H:221(A):ARG:HD2	1.88	0.73
1:L:1(E):SER:H	2:H:235:LYS:NZ	1.87	0.72
1:L:1(C):GLU:N	4:L:523:HOH:O	2.21	0.72
3:I:63:TYS:HE2	3:I:63:TYS:O1	1.88	0.72
2:H:49:ASP:OD2	2:H:111:PRO:HB3	1.91	0.71
2:H:221(A):ARG:HD3	4:H:763:HOH:O	1.91	0.71
1:L:5:PRO:N	1:L:9:LYS:HD2	2.05	0.71
2:H:221(A):ARG:HG3	4:H:702:HOH:O	1.88	0.71
2:H:199:PHE:CE1	2:H:201:MET:CE	2.58	0.70
3:I:59:ILE:CD1	3:I:64:LEU:HD21	2.20	0.70
2:H:41:LEU:HB2	4:H:603:HOH:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1(C):GLU:HG3	2:H:48:SER:HA	1.74	0.70
2:H:145:LYS:CD	2:H:148:TRP:HB3	2.15	0.70
2:H:87:LYS:HD2	2:H:88:ILE:H	1.53	0.69
2:H:77:GLU:HB2	2:H:80:GLU:HG2	1.73	0.69
2:H:87:LYS:CD	2:H:88:ILE:N	2.55	0.69
2:H:126:ARG:HB2	2:H:232:PHE:HZ	1.54	0.69
1:L:15:ARG:O	1:L:15:ARG:HG2	1.92	0.69
2:H:60(B):PRO:HG2	2:H:96:TRP:CD2	2.27	0.69
2:H:217:GLU:HB2	2:H:224:LYS:HD2	1.75	0.69
3:I:61:GLU:HB2	3:I:64:LEU:HD12	1.74	0.69
2:H:75:ARG:HB3	3:I:57:GLU:OE2	1.91	0.69
2:H:77(A):ARG:HD3	4:H:949:HOH:O	1.92	0.68
1:L:1(C):GLU:OE1	4:L:645:HOH:O	2.11	0.68
2:H:208:TYR:HB3	2:H:210:MET:HE3	1.75	0.68
3:I:59:ILE:CD1	3:I:64:LEU:CD2	2.71	0.68
1:L:1(C):GLU:HB2	4:L:523:HOH:O	1.92	0.68
1:L:1(B):ALA:HB2	4:L:692:HOH:O	1.95	0.67
1:L:1(A):ASP:OD2	1:L:9:LYS:NZ	2.17	0.67
1:L:4:ARG:C	1:L:9:LYS:HD2	2.20	0.67
2:H:36(A):SER:HA	2:H:37:PRO:C	2.19	0.67
2:H:105:LEU:HD12	2:H:241:VAL:CG2	2.25	0.66
2:H:60(I):THR:HG23	4:H:805:HOH:O	1.94	0.66
2:H:224:LYS:HD2	4:H:763:HOH:O	1.94	0.66
2:H:210:MET:N	2:H:210:MET:HE2	2.10	0.66
2:H:209:GLN:C	2:H:210:MET:HE2	2.21	0.66
3:I:63:TYS:O1	3:I:63:TYS:CE2	2.40	0.66
2:H:51:TRP:HZ2	2:H:246:GLY:HA3	1.59	0.65
2:H:244:GLN:NE2	2:H:245:PHE:CZ	2.65	0.65
2:H:97(A):GLU:OE1	4:H:710:HOH:O	2.14	0.65
2:H:147:THR:CA	2:H:148:TRP:CE3	2.77	0.65
1:L:14(F):LEU:HD12	2:H:135:LYS:HB3	1.77	0.65
2:H:81:LYS:HD3	2:H:118:ILE:CD1	2.26	0.65
2:H:60(D):TRP:O	2:H:60(E):ASP:HB2	1.97	0.65
2:H:179:ASN:OD1	2:H:233:ARG:HD3	1.97	0.64
1:L:1(H):THR:HA	2:H:48:SER:HB3	1.80	0.64
2:H:35:ARG:HB3	2:H:39:GLU:H	1.62	0.64
2:H:49:ASP:O	2:H:112:VAL:HG13	1.98	0.64
2:H:81:LYS:HD2	4:H:607:HOH:O	1.97	0.64
2:H:60(B):PRO:HG2	2:H:96:TRP:CE3	2.32	0.64
3:I:63:TYS:C	3:I:64:LEU:O	2.36	0.64
2:H:60(F):LYS:HG3	2:H:60(H):PHE:CE2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:33:LEU:CD2	2:H:64:LEU:CD2	2.71	0.63
2:H:74:THR:HG23	4:I:817:HOH:O	1.98	0.63
1:L:14(M):GLY:HA2	2:H:204:PRO:HB3	1.80	0.63
2:H:105:LEU:HD12	2:H:241:VAL:HG21	1.81	0.62
2:H:163:VAL:HG13	2:H:185:LYS:HE2	1.82	0.62
2:H:130:LEU:CD2	2:H:201:MET:HE1	2.28	0.62
2:H:165:ARG:NH1	4:H:833:HOH:O	2.32	0.62
1:L:1(D):GLY:CA	2:H:123:LEU:H	2.12	0.62
1:L:1(F):GLY:HA2	2:H:235:LYS:NZ	2.13	0.62
3:I:60:PRO:HB2	3:I:62:GLU:HG2	1.81	0.61
2:H:227:PHE:HE1	4:H:890:HOH:O	1.82	0.61
3:I:61:GLU:HG2	3:I:64:LEU:CB	2.27	0.61
2:H:97(A):GLU:CD	2:H:175:ARG:HH11	2.08	0.60
2:H:84:MET:CE	3:I:63:TYS:O	2.49	0.60
2:H:60(I):THR:HG21	2:H:62:ASN:HB2	1.74	0.60
2:H:187:ARG:HH21	2:H:222:ASP:CG	2.08	0.60
2:H:164:GLU:HA	4:H:782:HOH:O	2.00	0.60
2:H:69:GLY:O	2:H:79:ILE:HD11	2.03	0.59
1:L:1(E):SER:HG	2:H:208:TYR:HE1	1.50	0.59
2:H:147:THR:CA	2:H:148:TRP:HE3	2.14	0.59
1:L:1(H):THR:H2	1:L:1(C):GLU:HA	1.68	0.59
2:H:17:VAL:O	2:H:188:GLY:HA2	2.02	0.59
2:H:114:PHE:HB3	4:H:503:HOH:O	2.03	0.59
2:H:105:LEU:CD1	2:H:241:VAL:HG22	2.33	0.58
2:H:60(H):PHE:CE2	4:H:603:HOH:O	2.52	0.58
2:H:71:HIS:CD2	2:H:154:VAL:HG22	2.39	0.58
1:L:14(D):ARG:HH21	1:L:14(E):GLU:HB3	1.69	0.58
1:L:14(J):TYR:C	1:L:14(K):ILE:HG12	2.29	0.58
2:H:187:ARG:NH2	2:H:222:ASP:OD1	2.37	0.58
2:H:201:MET:HE3	2:H:210:MET:CG	2.34	0.58
3:I:61:GLU:HG2	3:I:64:LEU:C	2.29	0.58
2:H:208:TYR:HB3	2:H:210:MET:CE	2.33	0.57
2:H:236:LYS:CD	4:H:864:HOH:O	2.47	0.57
1:L:1(H):THR:HG23	2:H:242:ILE:CD1	2.18	0.57
1:L:14(J):TYR:O	1:L:14(K):ILE:CG1	2.37	0.57
3:I:60:PRO:C	3:I:62:GLU:H	2.11	0.57
2:H:87:LYS:HD3	2:H:88:ILE:H	1.68	0.57
2:H:50:ARG:HD2	2:H:111:PRO:HD3	1.86	0.57
2:H:50:ARG:CZ	2:H:108:LEU:O	2.53	0.57
3:I:61:GLU:HA	3:I:64:LEU:H	1.69	0.57
2:H:198:PRO:HB2	2:H:200:VAL:HG13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:164:GLU:OE2	4:H:760:HOH:O	2.18	0.56
2:H:97:ARG:HG3	4:H:742:HOH:O	2.05	0.56
2:H:35:ARG:HB3	2:H:39:GLU:HG3	1.88	0.56
2:H:177:THR:HG23	2:H:180:MET:HE3	1.86	0.56
2:H:182:CYS:HA	2:H:226:GLY:O	2.06	0.56
1:L:4:ARG:HG2	2:H:28:PRO:CG	2.35	0.56
2:H:129(A):ALA:HB3	4:H:874:HOH:O	2.05	0.56
2:H:176:ILE:HD12	2:H:227:PHE:CE2	2.40	0.56
2:H:199:PHE:CZ	2:H:201:MET:HE2	2.40	0.56
2:H:32:MET:SD	2:H:40:LEU:HD12	2.47	0.55
2:H:107:LYS:NZ	2:H:246:GLY:HA2	2.22	0.55
2:H:31:VAL:HG12	2:H:32:MET:N	2.21	0.55
1:L:1(H):THR:HG22	1:L:1(G):PHE:N	2.22	0.55
2:H:60(I):THR:CG2	2:H:62:ASN:CB	2.67	0.54
2:H:124:PRO:HB3	2:H:210:MET:HE1	1.90	0.54
1:L:1(H):THR:CG2	2:H:242:ILE:HG21	2.29	0.54
2:H:126:ARG:HA	2:H:232:PHE:CZ	2.43	0.54
2:H:129(B):SER:O	2:H:131:GLN:NE2	2.41	0.53
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	2.16	0.53
2:H:208:TYR:CB	2:H:210:MET:HE3	2.38	0.53
2:H:46:LEU:HD22	2:H:48:SER:O	2.09	0.53
2:H:210:MET:HE2	2:H:210:MET:CA	2.39	0.53
2:H:60(I):THR:CG2	4:H:805:HOH:O	2.53	0.53
2:H:211:GLY:HA2	2:H:229:THR:O	2.09	0.53
2:H:91:HIS:CE1	2:H:101:ARG:HD3	2.44	0.53
2:H:31:VAL:CG1	2:H:32:MET:N	2.72	0.52
2:H:185:LYS:HG2	2:H:186(B):GLU:OE2	2.09	0.52
1:L:1(E):SER:N	2:H:235:LYS:HZ1	2.05	0.52
1:L:5:PRO:CA	1:L:9:LYS:HD2	2.40	0.52
3:I:59:ILE:CG1	3:I:64:LEU:CD2	2.80	0.52
2:H:32:MET:HG3	2:H:40:LEU:HD12	1.91	0.52
2:H:201:MET:CE	2:H:210:MET:HG3	2.37	0.52
1:L:14(B):THR:HA	1:L:14(D):ARG:NE	2.25	0.52
2:H:49:ASP:O	2:H:111:PRO:HA	2.10	0.51
2:H:84:MET:HE3	3:I:63:TYS:O	2.10	0.51
2:H:16:ILE:N	2:H:194:ASP:OD2	2.44	0.51
2:H:217:GLU:OE1	2:H:224:LYS:HD3	2.10	0.51
1:L:1(G):PHE:O	1:L:1(D):GLY:CA	2.59	0.51
2:H:51:TRP:CZ2	2:H:246:GLY:HA3	2.42	0.51
2:H:94:TYR:HA	2:H:101:ARG:HB2	1.91	0.51
2:H:87:LYS:NZ	2:H:88:ILE:O	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:199:PHE:HE1	2:H:201:MET:HE3	1.68	0.51
2:H:219:GLY:HA3	2:H:221(A):ARG:HD2	1.93	0.50
2:H:178:ASP:O	2:H:233:ARG:HD2	2.12	0.50
2:H:124:PRO:HG3	2:H:210:MET:CE	2.42	0.50
2:H:145:LYS:HD3	2:H:148:TRP:CB	2.21	0.49
1:L:1(D):GLY:HA3	2:H:122:CYS:HA	1.94	0.49
2:H:107:LYS:HZ2	2:H:246:GLY:HA2	1.77	0.49
1:L:14(G):LEU:HD21	2:H:202:LYS:HD2	1.94	0.49
2:H:188:GLY:O	2:H:189:ASP:HB2	2.12	0.49
2:H:162:ILE:HD11	2:H:199:PHE:HZ	1.69	0.49
2:H:204(B):ASN:HD22	2:H:205:ASN:N	2.11	0.49
2:H:32:MET:HG3	2:H:40:LEU:CD1	2.43	0.49
2:H:73:ARG:HD3	2:H:152:PRO:O	2.12	0.49
2:H:60(B):PRO:N	2:H:60(C):PRO:HD2	2.27	0.49
2:H:60(I):THR:HG22	2:H:62:ASN:HB2	1.85	0.48
2:H:122:CYS:HB2	2:H:208:TYR:CD1	2.48	0.48
2:H:126:ARG:CB	2:H:232:PHE:CZ	2.89	0.48
2:H:81:LYS:HD3	2:H:118:ILE:HD11	1.95	0.48
2:H:60(B):PRO:N	2:H:60(C):PRO:CD	2.75	0.48
2:H:164:GLU:H	2:H:164:GLU:CD	2.22	0.48
2:H:144:LEU:HD12	2:H:150:GLY:C	2.39	0.48
2:H:93:ARG:NH1	2:H:101:ARG:NH2	2.61	0.48
2:H:184:GLY:HA3	4:H:708:HOH:O	2.13	0.48
2:H:105:LEU:CD1	2:H:241:VAL:CG2	2.92	0.48
2:H:210:MET:HE2	2:H:210:MET:HA	1.96	0.47
2:H:33:LEU:HA	2:H:33:LEU:HD23	1.74	0.47
2:H:60(A):TYR:CZ	2:H:60(C):PRO:HG2	2.50	0.47
2:H:60(D):TRP:O	2:H:60(E):ASP:CB	2.63	0.47
2:H:65:LEU:HD11	2:H:84:MET:HE2	1.95	0.47
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.49	0.47
1:L:14(L):ASP:O	1:L:14(M):GLY:O	2.33	0.47
2:H:187:ARG:HB3	2:H:221:ASP:OD2	2.14	0.47
3:I:55:ASP:HA	4:I:778:HOH:O	2.14	0.47
2:H:71:HIS:NE2	2:H:154:VAL:HG22	2.30	0.46
2:H:81:LYS:HE3	4:H:547:HOH:O	2.15	0.46
2:H:51:TRP:HZ2	2:H:246:GLY:CA	2.27	0.46
2:H:73:ARG:NH2	3:I:55:ASP:OD2	2.48	0.46
1:L:5:PRO:HA	1:L:9:LYS:CD	2.45	0.46
2:H:60(B):PRO:HG2	2:H:96:TRP:CE2	2.51	0.46
2:H:89:TYR:CE2	2:H:245:PHE:CE1	3.04	0.46
2:H:124:PRO:HG3	2:H:210:MET:HE1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:177:THR:HG23	2:H:180:MET:CE	2.46	0.46
2:H:85:LEU:CD1	2:H:106:MET:HE1	2.42	0.46
2:H:79:ILE:HG13	2:H:80:GLU:N	2.31	0.46
1:L:1(C):GLU:CB	1:L:1:CYS:HB3	2.46	0.46
2:H:56:ALA:HB2	2:H:103:ILE:O	2.16	0.45
2:H:70:LYS:HE3	2:H:72:SER:O	2.16	0.45
2:H:88:ILE:HD11	2:H:106:MET:CE	2.46	0.45
2:H:64:LEU:HD22	2:H:85:LEU:HD11	1.98	0.45
2:H:203:SER:O	2:H:205:ASN:HA	2.16	0.45
3:I:60:PRO:C	3:I:62:GLU:N	2.75	0.45
2:H:26:MET:HE2	2:H:137:ARG:CZ	2.47	0.45
2:H:244:GLN:HB3	2:H:245:PHE:CD1	2.51	0.45
2:H:97(A):GLU:OE2	2:H:175:ARG:HD3	2.16	0.45
1:L:13:GLU:HA	1:L:14(C):GLU:OE2	2.16	0.45
2:H:62:ASN:HB3	4:H:658:HOH:O	2.17	0.45
2:H:145:LYS:O	2:H:146:GLU:C	2.59	0.45
2:H:187:ARG:NH1	2:H:221:ASP:O	2.48	0.45
3:I:61:GLU:HA	3:I:64:LEU:CG	2.43	0.45
2:H:32:MET:HE2	2:H:40:LEU:HD12	1.96	0.45
2:H:61:GLU:OE1	2:H:87:LYS:HD3	2.17	0.45
2:H:61:GLU:H	2:H:61:GLU:HG2	1.20	0.45
2:H:126:ARG:HA	2:H:232:PHE:CE1	2.52	0.45
2:H:184(A):TYR:OH	2:H:186(D):LYS:NZ	2.48	0.45
1:L:1(G):PHE:O	2:H:123:LEU:HB2	2.16	0.45
2:H:74:THR:CG2	4:I:817:HOH:O	2.61	0.44
2:H:126:ARG:CA	2:H:232:PHE:CZ	3.00	0.44
2:H:32:MET:CG	2:H:40:LEU:HD12	2.47	0.44
1:L:14(J):TYR:HE2	2:H:202:LYS:O	2.00	0.44
2:H:186(B):GLU:O	2:H:186(C):GLY:C	2.60	0.44
1:L:14:ASP:OD2	2:H:137:ARG:NH2	2.42	0.44
1:L:1(H):THR:HA	2:H:47:ILE:O	2.17	0.44
1:L:14(D):ARG:HE	1:L:14(E):GLU:H	1.66	0.44
2:H:75:ARG:HA	3:I:57:GLU:HB2	2.00	0.44
1:L:1(F):GLY:CA	2:H:235:LYS:NZ	2.80	0.44
2:H:145:LYS:C	2:H:147:THR:N	2.70	0.44
1:L:1(E):SER:OG	2:H:208:TYR:HE1	2.01	0.44
2:H:236:LYS:CE	4:H:864:HOH:O	2.66	0.44
2:H:187:ARG:HD3	2:H:221:ASP:OD2	2.18	0.44
2:H:79:ILE:CD1	4:H:662:HOH:O	2.45	0.43
1:L:15:ARG:NH1	2:H:204(A):PHE:O	2.52	0.43
2:H:107:LYS:HE3	2:H:107:LYS:HB2	1.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:147:THR:HA	2:H:148:TRP:HZ3	1.74	0.43
2:H:187:ARG:NH1	2:H:221:ASP:OD2	2.51	0.43
2:H:36(A):SER:CA	2:H:37:PRO:C	2.91	0.43
1:L:1(C):GLU:CB	4:L:523:HOH:O	2.60	0.43
2:H:33:LEU:HB2	2:H:42:CYS:O	2.19	0.43
2:H:164:GLU:OE1	2:H:167:VAL:HG21	2.19	0.43
2:H:29:TRP:CG	2:H:121:VAL:HB	2.54	0.43
2:H:60(I):THR:HG23	2:H:62:ASN:CB	2.36	0.43
2:H:187:ARG:HD3	2:H:187:ARG:HH11	1.48	0.43
2:H:99:LEU:O	2:H:102:ASP:HB2	2.19	0.43
2:H:183:ALA:HB3	2:H:228:TYR:CE1	2.54	0.43
2:H:212:ILE:O	2:H:228:TYR:HA	2.19	0.43
1:L:1(H):THR:H2	1:L:1(C):GLU:CA	2.32	0.42
2:H:21:ASP:OD1	2:H:154:VAL:HG12	2.19	0.42
2:H:200:VAL:HA	2:H:208:TYR:O	2.19	0.42
2:H:179:ASN:HB3	2:H:234:LEU:HD11	2.00	0.42
2:H:201:MET:HE3	2:H:210:MET:CB	2.50	0.42
2:H:17:VAL:HG23	2:H:191:CYS:HB2	2.00	0.42
2:H:103:ILE:HD11	2:H:238:ILE:HD11	2.02	0.42
2:H:86:GLU:HB3	2:H:107:LYS:HG3	2.01	0.42
2:H:137:ARG:HD3	2:H:159:ASN:OD1	2.18	0.42
2:H:148:TRP:N	2:H:148:TRP:CD2	2.83	0.42
2:H:224:LYS:O	4:H:540:HOH:O	2.21	0.42
2:H:47:ILE:HG21	2:H:123:LEU:HD21	2.01	0.42
2:H:53:LEU:HD11	2:H:103:ILE:HD11	2.02	0.42
2:H:161:PRO:HG3	2:H:184(A):TYR:CE1	2.55	0.42
2:H:71:HIS:CD2	2:H:154:VAL:CG2	3.03	0.41
2:H:130:LEU:HD23	2:H:130:LEU:HA	1.87	0.41
2:H:217:GLU:OE1	2:H:224:LYS:CD	2.68	0.41
2:H:74:THR:CG2	2:H:75:ARG:HG3	2.33	0.41
2:H:167:VAL:H	2:H:167:VAL:HG23	1.59	0.41
1:L:14(A):LYS:HG3	4:H:846:HOH:O	2.20	0.41
2:H:98:ASN:O	2:H:99:LEU:HB2	2.19	0.41
2:H:87:LYS:HB3	2:H:89:TYR:CE1	2.55	0.41
1:L:1(B):ALA:H	1:L:1:CYS:H	1.69	0.41
2:H:182:CYS:HB3	2:H:227:PHE:CE2	2.55	0.41
2:H:96:TRP:HA	2:H:99:LEU:HD23	2.03	0.41
1:L:14(C):GLU:OE1	2:H:202:LYS:HE3	2.21	0.41
2:H:17:VAL:HG21	2:H:220:CYS:HB3	2.02	0.41
2:H:35:ARG:HB2	2:H:41:LEU:HD23	2.03	0.41
2:H:35:ARG:HD3	2:H:39:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:60(G):ASN:ND2	4:H:696:HOH:O	2.53	0.41
2:H:175:ARG:HH11	2:H:175:ARG:HD3	1.66	0.41
2:H:191:CYS:O	2:H:194:ASP:HB2	2.21	0.41
2:H:204(B):ASN:C	2:H:204(B):ASN:ND2	2.78	0.41
2:H:88:ILE:CD1	2:H:106:MET:HE3	2.51	0.41
1:L:1(D):GLY:N	2:H:123:LEU:H	2.19	0.40
2:H:199:PHE:CD1	2:H:199:PHE:C	2.99	0.40
2:H:83:SER:HB3	4:H:537:HOH:O	2.21	0.40
1:L:15:ARG:HH11	1:L:15:ARG:HD2	1.55	0.40
2:H:85:LEU:HD11	2:H:106:MET:HE1	2.03	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)
1:L:15:ARG:NH1	2:H:169:LYS:O[4_556]	2.11	0.09
1:L:15:ARG:NH1	2:H:172:THR:O[4_556]	2.13	0.07

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%)	26 (76%)	4 (12%)	4 (12%)	0	0
2	H	249/259 (96%)	237 (95%)	11 (4%)	1 (0%)	30	34
3	I	7/12 (58%)	6 (86%)	1 (14%)	0	100	100
All	All	290/307 (94%)	269 (93%)	16 (6%)	5 (2%)	7	5

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	14(M)	GLY

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Mol	Chain	Res	Type
1	L	1(F)	GLY
1	L	1(B)	ALA
2	H	77(A)	ARG
1	L	14(L)	ASP

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	31/31 (100%)	23 (74%)	8 (26%)	0	0
2	H	221/225 (98%)	184 (83%)	37 (17%)	2	2
3	I	9/11 (82%)	6 (67%)	3 (33%)	0	0
All	All	261/267 (98%)	213 (82%)	48 (18%)	1	1

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1(H)	THR
1	L	1(G)	PHE
1	L	1(E)	SER
1	L	1(C)	GLU
1	L	1(A)	ASP
1	L	1	CYS
1	L	6	LEU
1	L	13	GLU
2	H	20	SER
2	H	39	GLU
2	H	40	LEU
2	H	46	LEU
2	H	61	GLU
2	H	64	LEU
2	H	65	LEU
2	H	66	VAL
2	H	68	ILE
2	H	73	ARG

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Mol	Chain	Res	Type
2	H	74	THR
2	H	79	ILE
2	H	81	LYS
2	H	83	SER
2	H	84	MET
2	H	85	LEU
2	H	87	LYS
2	H	107	LYS
2	H	109	LYS
2	H	112	VAL
2	H	127	GLU
2	H	130	LEU
2	H	137	ARG
2	H	147	THR
2	H	148	TRP
2	H	154	VAL
2	H	157	VAL
2	H	165	ARG
2	H	177	THR
2	H	187	ARG
2	H	202	LYS
2	H	205	ASN
2	H	233	ARG
2	H	236	LYS
2	H	239	GLN
2	H	241	VAL
2	H	245	PHE
3	I	58	GLU
3	I	59	ILE
3	I	64	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	156	GLN
2	H	204(B)	ASN
2	H	209	GLN
2	H	244	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	1.70	2 (13%)	15,22,24	1.37	1 (6%)

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	-	1/10/11/13	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	-4.71	1.49	1.58
3	I	63	TYS	OH-CZ	-3.20	1.37	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	63	TYS	CD1-CE1-CZ	-2.60	116.76	119.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	63	TYS	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	63	TYS	5	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.