



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:33 PM UTC

PDB ID : 1HAH / pdb_00001hah
Title : THE ISOMORPHOUS STRUCTURES OF PRETHROMBIN2, HIRUGEN-
AND PPACK-THROMBIN: CHANGES ACCOMPANYING ACTIVATION
AND EXOSITE BINDING TO THROMBIN
Authors : Tulinsky, A.; Vijayalakshmi, J.
Deposited on : 1994-06-27
Resolution : 2.30 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

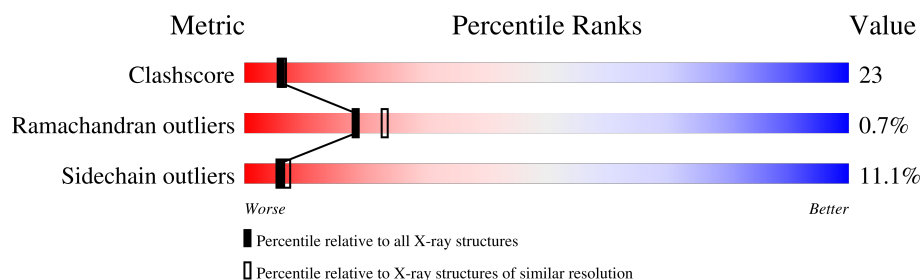
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	10	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2664 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	2	0
			2064	1315	368	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			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

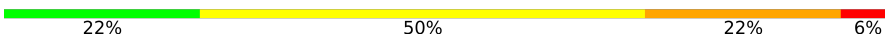
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	24	Total	O	0	0
			24	24		
5	H	178	Total	O	0	0
			178	178		
5	I	2	Total	O	0	0
			2	2		

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.

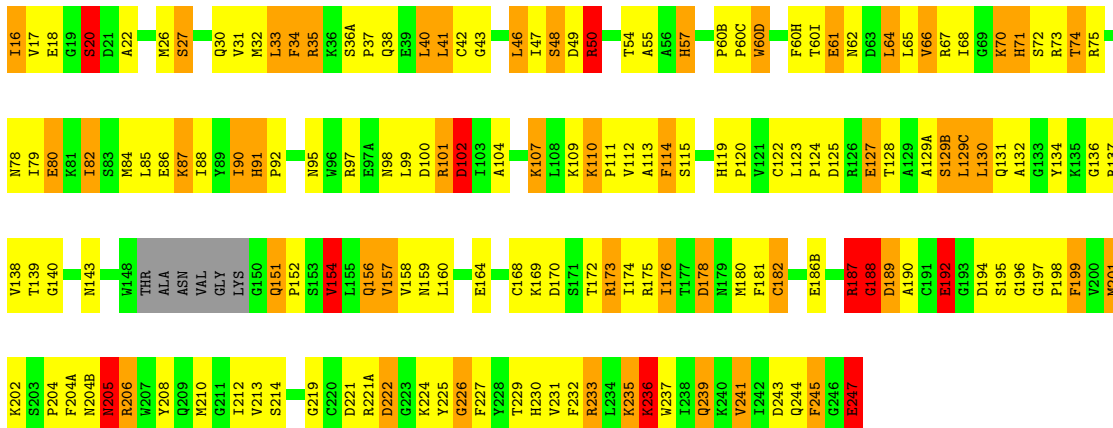
• Molecule 1: ALPHA-THROMBIN (SMALL SUBUNIT)

Chain L: 

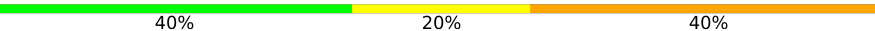


• Molecule 2: ALPHA-THROMBIN (LARGE SUBUNIT)

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	71.75Å 72.39Å 73.52Å 90.00° 101.26° 90.00°	Depositor
Resolution (Å)	7.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.114 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2664	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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, NAG

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	1.59	3/290 (1.0%)	2.88	28/384 (7.3%)
2	H	1.69	29/2129 (1.4%)	2.61	183/2874 (6.4%)
3	I	1.12	0/79	2.26	6/103 (5.8%)
All	All	1.67	32/2498 (1.3%)	2.63	217/3361 (6.5%)

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
1	L	0	3
2	H	0	9
All	All	0	12

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	168	CYS	C-O	8.22	1.33	1.24
2	H	231	VAL	CA-CB	6.89	1.63	1.54
2	H	34	PHE	N-CA	6.64	1.54	1.46
2	H	188	GLY	C-N	6.49	1.41	1.33
2	H	30	GLN	C-O	6.48	1.31	1.24
2	H	230	HIS	N-CA	6.44	1.54	1.46
2	H	182	CYS	N-CA	6.42	1.54	1.45
2	H	235	LYS	C-O	6.33	1.31	1.24
2	H	154	VAL	N-CA	6.32	1.53	1.46
2	H	172	THR	CA-CB	6.13	1.63	1.53
2	H	219	GLY	N-CA	5.97	1.55	1.45
2	H	197	GLY	N-CA	5.92	1.51	1.43
2	H	208	TYR	C-O	5.90	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	43	GLY	N-CA	5.88	1.50	1.44
1	L	15	ARG	CZ-NH1	5.83	1.41	1.32
2	H	42	CYS	C-O	5.79	1.29	1.24
2	H	67	ARG	N-CA	-5.76	1.39	1.46
2	H	107	LYS	CA-CB	-5.72	1.45	1.53
2	H	140	GLY	N-CA	5.57	1.52	1.45
2	H	134	TYR	N-CA	5.57	1.52	1.46
2	H	42	CYS	N-CA	5.49	1.52	1.46
2	H	198	PRO	CA-CB	5.47	1.60	1.54
1	L	14(D)	ARG	CZ-NH1	5.44	1.40	1.32
2	H	202	LYS	N-CA	5.43	1.52	1.46
2	H	79	ILE	C-O	5.42	1.30	1.24
2	H	127	GLU	C-O	5.42	1.31	1.24
2	H	198	PRO	N-CA	-5.17	1.41	1.47
2	H	60(I)	THR	C-N	-5.12	1.27	1.33
2	H	175	ARG	N-CA	5.09	1.52	1.46
1	L	6	LEU	N-CA	5.04	1.52	1.46
2	H	73	ARG	NE-CZ	5.04	1.38	1.33
2	H	110	LYS	N-CA	5.03	1.50	1.45

All (217) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	205	ASN	OD1-CG-ND2	14.56	137.16	122.60
1	L	15	ARG	NE-CZ-NH1	13.73	135.24	121.50
1	L	15	ARG	CD-NE-CZ	13.63	143.49	124.40
1	L	14(M)	GLY	CA-C-N	13.59	146.17	121.70
1	L	14(M)	GLY	C-N-CA	13.59	146.17	121.70
2	H	195	SER	CA-C-O	-13.17	107.21	121.44
2	H	205	ASN	CA-CB-CG	-11.31	101.29	112.60
1	L	15	ARG	NE-CZ-NH2	-10.39	109.85	119.20
2	H	95	ASN	OD1-CG-ND2	-10.21	112.39	122.60
2	H	27	SER	N-CA-CB	9.98	123.47	111.09
2	H	66	VAL	CA-C-N	9.87	137.48	123.07
2	H	66	VAL	C-N-CA	9.87	137.48	123.07
2	H	154	VAL	N-CA-CB	-9.70	96.15	112.44
2	H	241	VAL	N-CA-CB	9.49	121.65	110.55
2	H	190	ALA	N-CA-C	-9.43	97.82	110.55
1	L	14(J)	TYR	N-CA-C	-9.34	103.06	112.97
2	H	213	VAL	CA-C-O	9.30	132.41	120.78
1	L	1(A)	ASP	CA-CB-CG	-9.22	103.38	112.60
2	H	137	ARG	NE-CZ-NH1	-9.01	112.49	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	115	SER	CA-C-O	-8.85	111.74	120.94
2	H	60(I)	THR	CA-CB-OG1	-8.42	96.97	109.60
1	L	14(B)	THR	CA-C-O	-8.39	109.54	119.03
2	H	127	GLU	CB-CG-CD	8.36	126.81	112.60
2	H	164	GLU	CB-CG-CD	8.26	126.64	112.60
2	H	113	ALA	O-C-N	8.26	132.85	123.19
2	H	175	ARG	CA-C-N	8.11	133.88	121.71
2	H	175	ARG	C-N-CA	8.11	133.88	121.71
2	H	189	ASP	CA-CB-CG	8.10	120.70	112.60
2	H	151	GLN	CB-CA-C	8.00	118.92	109.47
2	H	170	ASP	CA-CB-CG	-7.92	104.67	112.60
2	H	232	PHE	CA-CB-CG	-7.88	105.92	113.80
2	H	60(B)	PRO	N-CA-C	7.87	120.30	110.70
2	H	54	THR	CA-C-N	7.80	132.65	121.50
2	H	54	THR	C-N-CA	7.80	132.65	121.50
2	H	197	GLY	CA-C-O	7.75	129.75	121.62
2	H	243	ASP	CA-CB-CG	7.73	120.33	112.60
2	H	27	SER	O-C-N	7.67	127.69	121.17
2	H	129(A)	ALA	CA-C-O	-7.55	112.89	120.82
2	H	192	GLU	CA-C-O	-7.54	112.74	120.96
2	H	97	ARG	NE-CZ-NH2	-7.41	112.53	119.20
2	H	233	ARG	NE-CZ-NH1	7.39	128.89	121.50
2	H	60(H)	PHE	CA-C-O	7.37	129.60	121.56
2	H	104	ALA	O-C-N	7.30	131.65	123.48
2	H	119	HIS	O-C-N	-7.25	116.19	121.84
2	H	186(B)	GLU	C-N-CA	-7.25	107.08	122.30
2	H	154	VAL	CB-CA-C	7.24	121.56	110.55
1	L	14(D)	ARG	NE-CZ-NH2	7.14	125.62	119.20
2	H	91	HIS	CA-CB-CG	-7.13	106.67	113.80
2	H	26	MET	CA-C-O	-7.12	111.78	119.97
2	H	205	ASN	CB-CG-ND2	-7.05	105.82	116.40
2	H	172	THR	CA-C-O	-7.05	113.58	121.40
2	H	197	GLY	O-C-N	-7.04	116.08	122.42
2	H	27	SER	CB-CA-C	-7.04	99.54	111.15
2	H	132	ALA	CA-C-O	-7.02	112.92	120.92
2	H	243	ASP	CB-CA-C	7.02	121.86	109.65
2	H	245	PHE	CA-CB-CG	7.01	120.81	113.80
1	L	14(D)	ARG	CD-NE-CZ	6.98	134.17	124.40
2	H	137	ARG	NE-CZ-NH2	6.96	125.46	119.20
2	H	60(I)	THR	CA-CB-CG2	6.93	122.29	110.50
2	H	60(D)	TRP	N-CA-C	-6.93	102.88	112.30
2	H	33	LEU	CB-CA-C	6.91	121.76	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	1(F)	GLY	CA-C-O	-6.91	108.55	120.57
1	L	14(E)	GLU	CB-CG-CD	6.91	124.35	112.60
2	H	229	THR	OG1-CB-CG2	6.90	123.10	109.30
2	H	40	LEU	CA-C-O	-6.86	112.62	120.58
2	H	60(D)	TRP	CA-C-O	-6.84	111.84	119.78
2	H	43	GLY	N-CA-C	-6.84	101.77	112.58
2	H	64	LEU	N-CA-C	6.83	120.65	109.85
2	H	61	GLU	CB-CG-CD	-6.78	101.07	112.60
2	H	101	ARG	NE-CZ-NH1	6.78	128.28	121.50
2	H	101	ARG	NE-CZ-NH2	-6.78	113.10	119.20
2	H	157	VAL	CB-CA-C	-6.76	98.88	110.30
2	H	57	HIS	CA-CB-CG	-6.75	107.05	113.80
1	L	14(K)	ILE	CB-CA-C	6.73	122.32	111.29
2	H	50[A]	ARG	CA-C-O	-6.71	111.33	119.32
2	H	50[B]	ARG	CA-C-O	-6.71	111.33	119.32
2	H	20	SER	O-C-N	6.63	131.32	122.96
2	H	232	PHE	O-C-N	-6.60	115.12	122.12
2	H	61	GLU	N-CA-CB	-6.57	100.15	109.94
2	H	40	LEU	O-C-N	6.55	131.22	122.96
2	H	35	ARG	NE-CZ-NH2	-6.54	113.31	119.20
2	H	233	ARG	NE-CZ-NH2	-6.54	113.32	119.20
2	H	74	THR	CA-CB-OG1	-6.53	99.81	109.60
2	H	195	SER	O-C-N	6.51	131.15	122.82
2	H	66	VAL	N-CA-CB	-6.49	102.43	111.25
2	H	227	PHE	CA-CB-CG	-6.49	107.31	113.80
2	H	245	PHE	CA-C-O	-6.48	112.28	119.34
2	H	225	TYR	CA-C-N	-6.45	114.62	121.45
2	H	225	TYR	C-N-CA	-6.45	114.62	121.45
2	H	129(B)	SER	N-CA-C	6.44	119.29	111.82
2	H	206	ARG	O-C-N	6.43	130.26	123.06
2	H	115	SER	N-CA-C	-6.38	99.18	107.73
2	H	151	GLN	CA-CB-CG	-6.38	101.34	114.10
2	H	114	PHE	CA-CB-CG	-6.38	107.42	113.80
2	H	82	ILE	CA-C-O	-6.38	113.70	120.39
2	H	50[A]	ARG	CB-CA-C	-6.37	99.40	110.17
2	H	50[B]	ARG	CB-CA-C	-6.37	99.40	110.17
2	H	47	ILE	O-C-N	-6.31	116.04	122.23
2	H	175	ARG	NE-CZ-NH2	6.30	124.87	119.20
2	H	127	GLU	CA-CB-CG	6.28	126.66	114.10
2	H	241	VAL	CA-CB-CG1	6.25	121.02	110.40
2	H	175	ARG	O-C-N	-6.19	114.42	122.77
2	H	60(H)	PHE	CA-CB-CG	-6.18	107.62	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	152	PRO	N-CA-C	-6.15	102.61	111.22
2	H	178	ASP	CA-C-O	-6.14	111.82	119.38
2	H	115	SER	O-C-N	6.13	129.86	122.75
3	I	57	GLU	N-CA-CB	6.13	118.99	110.17
2	H	33	LEU	CA-C-N	-6.08	114.42	122.99
2	H	33	LEU	C-N-CA	-6.08	114.42	122.99
2	H	91	HIS	CA-C-O	6.08	124.81	119.71
2	H	125	ASP	N-CA-C	-6.08	101.00	110.42
1	L	14(K)	ILE	C-N-CA	6.04	136.79	121.70
2	H	199	PHE	N-CA-C	-6.02	98.70	108.52
2	H	102	ASP	N-CA-CB	-6.01	101.93	110.58
2	H	236	LYS	CA-C-O	-5.99	113.08	119.97
2	H	129(B)	SER	CA-C-O	-5.94	113.14	119.97
2	H	221(A)	ARG	CD-NE-CZ	5.94	132.71	124.40
2	H	99	LEU	O-C-N	-5.91	114.49	122.41
2	H	158	VAL	CA-C-O	-5.91	115.41	120.96
2	H	181	PHE	CA-C-O	-5.89	114.91	121.51
2	H	221	ASP	CA-C-O	-5.86	113.54	120.81
2	H	18	GLU	CB-CA-C	-5.84	103.44	111.73
2	H	174	ILE	CA-CB-CG2	5.84	120.43	110.50
2	H	159	ASN	CA-C-O	-5.79	114.37	120.80
2	H	205	ASN	N-CA-CB	-5.78	103.73	113.15
2	H	84	MET	O-C-N	5.76	130.42	123.16
2	H	175	ARG	NE-CZ-NH1	-5.76	115.74	121.50
2	H	62	ASN	CA-CB-CG	-5.73	106.87	112.60
2	H	235	LYS	N-CA-C	5.72	118.29	111.71
2	H	239	GLN	CA-C-O	5.72	126.83	120.82
2	H	20	SER	N-CA-CB	5.72	120.88	111.62
2	H	61	GLU	CA-C-O	5.72	127.02	120.90
1	L	15	ARG	CB-CG-CD	5.70	124.42	111.30
1	L	1(F)	GLY	O-C-N	5.70	131.81	122.70
2	H	176	ILE	CA-C-O	-5.69	114.34	121.11
1	L	14(G)	LEU	CB-CA-C	5.68	120.22	110.79
2	H	212	ILE	CA-C-O	-5.67	114.43	120.39
2	H	35	ARG	CA-C-O	5.67	127.15	120.58
2	H	192	GLU	N-CA-CB	-5.64	100.74	109.48
2	H	232	PHE	CA-C-O	5.64	126.53	120.55
2	H	124	PRO	CB-CA-C	-5.63	103.61	110.98
2	H	84	MET	CA-CB-CG	-5.62	102.86	114.10
2	H	33	LEU	N-CA-CB	-5.62	100.74	110.17
2	H	60(I)	THR	CA-C-N	5.62	128.12	120.54
2	H	60(I)	THR	C-N-CA	5.62	128.12	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	180	MET	CA-C-O	-5.61	114.56	121.06
1	L	13	GLU	CA-C-O	-5.60	114.58	120.80
2	H	114	PHE	CA-C-O	-5.59	115.39	121.87
2	H	42	CYS	N-CA-CB	-5.57	101.68	111.49
2	H	214	SER	N-CA-C	5.55	119.82	112.72
2	H	233	ARG	CD-NE-CZ	5.54	132.16	124.40
1	L	4	ARG	NE-CZ-NH2	5.52	124.17	119.20
2	H	139	THR	CA-C-N	-5.52	112.38	121.04
2	H	139	THR	C-N-CA	-5.52	112.38	121.04
2	H	55	ALA	O-C-N	-5.51	116.59	123.04
2	H	71	HIS	CA-C-O	5.51	128.39	120.51
2	H	237	TRP	N-CA-C	-5.51	105.38	111.71
2	H	99	LEU	CA-C-O	5.50	127.83	121.28
2	H	80	GLU	CG-CD-OE2	-5.48	105.80	118.40
2	H	100	ASP	N-CA-C	-5.47	101.55	110.20
2	H	18	GLU	CG-CD-OE2	-5.47	105.81	118.40
2	H	119	HIS	CB-CA-C	5.46	117.66	109.63
2	H	139	THR	CA-C-O	-5.45	115.25	121.40
2	H	187	ARG	CB-CA-C	-5.44	102.04	112.43
2	H	78	ASN	CA-CB-CG	5.44	118.04	112.60
2	H	60(I)	THR	N-CA-CB	-5.43	102.40	111.20
1	L	1(A)	ASP	N-CA-C	-5.40	106.36	113.17
2	H	22	ALA	N-CA-C	-5.40	103.41	110.53
2	H	107	LYS	CA-CB-CG	5.37	124.84	114.10
3	I	64	LEU	CB-CA-C	5.37	120.30	110.10
2	H	129(B)	SER	CB-CA-C	-5.36	100.38	110.67
1	L	1(C)	GLU	N-CA-C	5.34	122.17	110.80
1	L	14(D)	ARG	CB-CA-C	-5.34	101.88	110.74
2	H	204(A)	PHE	CA-CB-CG	-5.34	108.46	113.80
2	H	159	ASN	CA-CB-CG	-5.33	107.27	112.60
2	H	128	THR	CA-C-N	5.33	127.73	120.54
2	H	128	THR	C-N-CA	5.33	127.73	120.54
2	H	174	ILE	CB-CG1-CD1	-5.30	102.67	113.80
2	H	131	GLN	CA-C-O	-5.28	114.94	121.11
2	H	169	LYS	CA-C-O	-5.27	114.97	120.55
2	H	226	GLY	O-C-N	5.25	130.52	123.11
2	H	138	VAL	CA-C-N	-5.25	113.71	122.21
2	H	138	VAL	C-N-CA	-5.25	113.71	122.21
1	L	15	ARG	CA-CB-CG	-5.25	103.61	114.10
3	I	60	PRO	CA-C-N	5.24	129.47	120.72
3	I	60	PRO	C-N-CA	5.24	129.47	120.72
3	I	57	GLU	CA-C-N	5.24	128.15	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	57	GLU	C-N-CA	5.24	128.15	120.71
2	H	247	GLU	CG-CD-OE1	-5.23	106.36	118.40
2	H	128	THR	CA-CB-OG1	-5.22	101.77	109.60
2	H	129(B)	SER	N-CA-CB	5.21	118.36	110.28
2	H	70	LYS	N-CA-CB	5.20	118.36	110.45
2	H	205	ASN	N-CA-C	5.15	120.72	113.56
1	L	13	GLU	CB-CG-CD	5.14	121.35	112.60
2	H	187	ARG	CD-NE-CZ	5.14	131.60	124.40
2	H	97	ARG	NE-CZ-NH1	5.12	126.62	121.50
2	H	199	PHE	CA-CB-CG	-5.10	108.70	113.80
2	H	78	ASN	CB-CG-ND2	5.09	124.03	116.40
2	H	178	ASP	O-C-N	5.07	129.23	122.43
1	L	14(A)	LYS	N-CA-C	5.07	119.09	113.01
2	H	201	MET	CA-CB-CG	-5.07	103.96	114.10
2	H	196	GLY	N-CA-C	-5.07	108.98	115.42
1	L	5	PRO	CA-C-N	-5.07	114.18	122.54
1	L	5	PRO	C-N-CA	-5.07	114.18	122.54
2	H	129(C)	LEU	N-CA-CB	-5.05	103.09	110.47
2	H	198	PRO	CA-C-N	-5.05	115.97	123.05
2	H	198	PRO	C-N-CA	-5.05	115.97	123.05
1	L	4	ARG	NH1-CZ-NH2	-5.05	112.74	119.30
2	H	34	PHE	CA-CB-CG	5.04	118.84	113.80
2	H	154	VAL	CA-C-N	5.04	128.26	121.05
2	H	154	VAL	C-N-CA	5.04	128.26	121.05
2	H	156	GLN	CB-CG-CD	-5.03	104.04	112.60
2	H	48	SER	CA-C-O	-5.03	115.77	121.05
2	H	90	ILE	CB-CG1-CD1	5.03	124.35	113.80
2	H	173	ARG	CD-NE-CZ	-5.01	117.38	124.40
2	H	230	HIS	CB-CA-C	-5.01	102.40	110.77
2	H	195	SER	CA-CB-OG	-5.01	101.07	111.10

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	101	ARG	Sidechain
2	H	102	ASP	Sidechain
2	H	16	ILE	Mainchain
2	H	160	LEU	Mainchain
2	H	173	ARG	Sidechain
2	H	187	ARG	Sidechain
2	H	188	GLY	Mainchain

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Mol	Chain	Res	Type	Group
2	H	50[A]	ARG	Sidechain
2	H	50[B]	ARG	Sidechain
1	L	14(D)	ARG	Sidechain
1	L	15	ARG	Sidechain
1	L	5	PRO	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	287	0	278	29	0
2	H	2064	0	2033	91	0
3	I	95	0	74	9	0
4	H	14	0	13	0	0
5	H	178	0	0	9	1
5	I	2	0	0	0	0
5	L	24	0	0	0	0
All	All	2664	0	2398	108	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (108) 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(F):GLY:HA2	2:H:235:LYS:HZ3	1.16	1.08
1:L:1(F):GLY:HA2	2:H:235:LYS:NZ	1.73	1.03
1:L:1(E):SER:HA	2:H:123:LEU:O	1.63	0.99
2:H:50[A]:ARG:HG2	2:H:50[A]:ARG:HH11	1.32	0.93
3:I:60:PRO:HG2	3:I:63:TYS:HE2	1.59	0.85
1:L:1(E):SER:CA	2:H:123:LEU:O	2.28	0.81
3:I:58:GLU:H	3:I:58:GLU:CD	1.86	0.81
1:L:1(D):GLY:HA3	2:H:122:CYS:HA	1.64	0.78
1:L:1(D):GLY:CA	2:H:123:LEU:H	1.98	0.76
2:H:244:GLN:HB2	5:H:595:HOH:O	1.88	0.74
2:H:36(A):SER:HA	2:H:37:PRO:C	2.15	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:14(J):TYR:O	1:L:14(K):ILE:HG13	1.88	0.72
2:H:236:LYS:HG2	5:H:509:HOH:O	1.93	0.69
1:L:1(D):GLY:N	2:H:123:LEU:H	1.91	0.69
2:H:151:GLN:OE1	5:H:581:HOH:O	2.10	0.68
1:L:14(I):SER:C	1:L:14(K):ILE:H	2.02	0.68
3:I:60:PRO:HG2	3:I:63:TYS:CE2	2.24	0.67
2:H:86:GLU:HB3	2:H:107:LYS:HG3	1.76	0.66
2:H:35:ARG:O	2:H:38:GLN:HA	1.97	0.65
3:I:60:PRO:HB2	3:I:62:GLU:CD	2.22	0.65
2:H:143:ASN:ND2	2:H:192:GLU:HB3	2.12	0.64
2:H:75[B]:ARG:NH1	3:I:57:GLU:CB	2.60	0.63
2:H:110:LYS:O	5:H:529:HOH:O	2.15	0.63
1:L:14(J):TYR:C	1:L:14(K):ILE:HG13	2.25	0.62
2:H:178:ASP:O	2:H:233:ARG:HD2	2.01	0.60
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	2.09	0.60
1:L:14(J):TYR:C	1:L:14(K):ILE:CG1	2.74	0.60
1:L:1(H):THR:O	1:L:1(H):THR:HG22	2.03	0.58
2:H:201:MET:SD	2:H:210:MET:HG3	2.42	0.58
2:H:143:ASN:ND2	2:H:192:GLU:CB	2.66	0.58
1:L:15:ARG:HB2	2:H:204:PRO:O	2.03	0.58
2:H:75[B]:ARG:NH1	3:I:57:GLU:HB3	2.19	0.58
2:H:32:MET:HG3	2:H:40:LEU:HD12	1.86	0.58
2:H:87:LYS:HD3	2:H:88:ILE:H	1.69	0.56
2:H:71:HIS:CD2	2:H:154:VAL:HG22	2.41	0.56
2:H:224:LYS:HE2	5:H:472:HOH:O	2.05	0.56
2:H:86:GLU:HB3	2:H:107:LYS:CG	2.36	0.55
2:H:91:HIS:ND1	2:H:92:PRO:HD2	2.23	0.54
2:H:75[B]:ARG:HH11	3:I:57:GLU:HB3	1.73	0.54
1:L:14:ASP:OD1	1:L:14:ASP:C	2.51	0.53
2:H:46:LEU:HD22	2:H:48:SER:O	2.08	0.52
2:H:64:LEU:HB2	2:H:85:LEU:HD12	1.91	0.52
1:L:1(F):GLY:CA	2:H:235:LYS:NZ	2.62	0.52
2:H:204(B):ASN:O	2:H:205:ASN:HB2	2.10	0.52
2:H:75[A]:ARG:NH2	5:H:520:HOH:O	2.42	0.52
2:H:72:SER:OG	2:H:75[A]:ARG:HG2	2.11	0.51
2:H:143:ASN:HD22	2:H:192:GLU:HB2	1.76	0.51
2:H:50[A]:ARG:HE	2:H:107:LYS:CE	2.24	0.50
2:H:74:THR:O	2:H:75[B]:ARG:NH1	2.44	0.50
2:H:49:ASP:OD2	2:H:111:PRO:HB3	2.12	0.50
1:L:1(D):GLY:HA3	2:H:122:CYS:CA	2.39	0.49
2:H:17:VAL:O	2:H:188:GLY:HA2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:87:LYS:CD	2:H:88:ILE:H	2.25	0.49
2:H:75[B]:ARG:HH12	3:I:57:GLU:N	2.10	0.49
2:H:35:ARG:HB2	2:H:41:LEU:HD13	1.94	0.48
1:L:1(H):THR:OG1	2:H:48:SER:CB	2.62	0.48
2:H:75[B]:ARG:NH1	3:I:57:GLU:HB2	2.28	0.47
1:L:14(H):GLU:HA	1:L:14(L):ASP:HA	1.95	0.47
2:H:50[B]:ARG:HD2	2:H:111:PRO:HB3	1.96	0.47
2:H:98:ASN:N	2:H:98:ASN:OD1	2.47	0.47
2:H:49:ASP:OD2	2:H:111:PRO:CB	2.63	0.47
2:H:72:SER:OG	2:H:75[B]:ARG:HG2	2.14	0.47
1:L:1(H):THR:HG21	2:H:247:GLU:OE1	2.15	0.47
2:H:87:LYS:CD	2:H:88:ILE:N	2.78	0.46
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.51	0.46
2:H:49:ASP:O	2:H:112:VAL:HG12	2.15	0.46
2:H:36(A):SER:CA	2:H:37:PRO:C	2.88	0.46
1:L:1(H):THR:OG1	2:H:48:SER:HB2	2.16	0.46
1:L:1(C):GLU:HG3	2:H:120:PRO:HG2	1.96	0.46
2:H:222:ASP:OD1	2:H:222:ASP:N	2.47	0.46
2:H:130:LEU:HD23	2:H:130:LEU:HA	1.75	0.45
2:H:182:CYS:HA	2:H:226:GLY:O	2.16	0.45
1:L:1(D):GLY:CA	5:H:442:HOH:O	2.64	0.45
2:H:61:GLU:H	2:H:61:GLU:HG2	1.03	0.45
1:L:1(B):ALA:H	1:L:1:CYS:H	1.65	0.45
2:H:50[A]:ARG:HE	2:H:107:LYS:HE2	1.80	0.45
2:H:188:GLY:O	2:H:189:ASP:HB2	2.15	0.45
1:L:1(H):THR:O	1:L:1(H):THR:CG2	2.63	0.45
2:H:32:MET:HG3	2:H:40:LEU:CD1	2.46	0.45
2:H:57:HIS:HD1	2:H:102:ASP:CG	2.25	0.45
2:H:50[A]:ARG:HG2	2:H:50[A]:ARG:NH1	2.08	0.44
1:L:4:ARG:HB2	1:L:8:GLU:OE1	2.17	0.44
2:H:50[A]:ARG:HH12	2:H:110:LYS:HA	1.83	0.44
2:H:35:ARG:HG2	5:H:464:HOH:O	2.17	0.44
2:H:64:LEU:HB2	2:H:85:LEU:CD1	2.47	0.43
1:L:1:CYS:O	2:H:206:ARG:HD3	2.18	0.43
2:H:41:LEU:HD23	2:H:64:LEU:HD21	1.99	0.43
1:L:1(D):GLY:HA2	5:H:442:HOH:O	2.20	0.42
2:H:50[A]:ARG:HH12	2:H:110:LYS:CA	2.33	0.42
2:H:244:GLN:OE1	2:H:245:PHE:CE2	2.72	0.42
2:H:60(C):PRO:O	2:H:60(D):TRP:HD1	2.02	0.42
2:H:107:LYS:HB2	2:H:107:LYS:HE3	1.64	0.41
1:L:5:PRO:O	1:L:9:LYS:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:187:ARG:HA	2:H:187:ARG:HD2	1.90	0.41
2:H:236:LYS:HG2	2:H:236:LYS:H	1.65	0.41
2:H:114:PHE:N	2:H:114:PHE:CD1	2.89	0.41
2:H:20:SER:O	2:H:156:GLN:HA	2.20	0.41
2:H:34:PHE:CZ	2:H:38:GLN:HB3	2.56	0.41
2:H:57:HIS:CD2	2:H:57:HIS:C	2.99	0.41
1:L:1(F):GLY:HA2	2:H:235:LYS:CE	2.46	0.41
2:H:16:ILE:HD13	2:H:194:ASP:OD2	2.21	0.41
2:H:74:THR:C	2:H:75[B]:ARG:NH1	2.78	0.41
2:H:70:LYS:HB3	2:H:70:LYS:HE3	1.69	0.40
2:H:87:LYS:HD2	2:H:88:ILE:N	2.36	0.40
2:H:176:ILE:HD13	2:H:176:ILE:HA	1.79	0.40
2:H:31:VAL:HG12	2:H:32:MET:N	2.37	0.40
2:H:74:THR:OG1	2:H:75[B]:ARG:CZ	2.69	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:434:HOH:O	5:H:434:HOH:O[2_555]	1.85	0.35

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	34/36 (94%)	26 (76%)	6 (18%)	2 (6%)	1	0
2	H	251/259 (97%)	234 (93%)	17 (7%)	0	100	100
3	I	7/10 (70%)	7 (100%)	0	0	100	100
All	All	292/305 (96%)	267 (91%)	23 (8%)	2 (1%)	18	23

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	1(G)	PHE
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%)	30 (97%)	1 (3%)	34	51
2	H	223/225 (99%)	196 (88%)	27 (12%)	5	5
3	I	9/9 (100%)	8 (89%)	1 (11%)	6	7
All	All	263/265 (99%)	234 (89%)	29 (11%)	6	7

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	6	LEU
2	H	20	SER
2	H	27	SER
2	H	33	LEU
2	H	41	LEU
2	H	46	LEU
2	H	65	LEU
2	H	66	VAL
2	H	68	ILE
2	H	80	GLU
2	H	82	ILE
2	H	87	LYS
2	H	90	ILE
2	H	109	LYS
2	H	127	GLU
2	H	129(B)	SER
2	H	129(C)	LEU
2	H	130	LEU
2	H	154	VAL
2	H	157	VAL
2	H	187	ARG

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Mol	Chain	Res	Type
2	H	192	GLU
2	H	205	ASN
2	H	222	ASP
2	H	236	LYS
2	H	239	GLN
2	H	241	VAL
2	H	247	GLU
3	I	58	GLU

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

Mol	Chain	Res	Type
2	H	143	ASN
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	1.87	2 (13%)	15,22,24	2.12	6 (40%)

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	5.65	1.69	1.58
3	I	63	TYS	OH-CZ	-3.62	1.36	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	63	TYS	OH-S-O2	-4.32	94.40	107.56
3	I	63	TYS	CD1-CE1-CZ	-3.47	115.77	119.73
3	I	63	TYS	O2-S-O1	3.35	125.17	112.24
3	I	63	TYS	OH-CZ-CE2	-2.51	113.78	118.70
3	I	63	TYS	CE2-CZ-CE1	2.21	123.38	120.16
3	I	63	TYS	OH-CZ-CE1	2.11	122.84	118.70

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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	63	TYS	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	H	400	2	14,14,15	0.82	0	17,19,21	2.20	3 (17%)

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	NAG	H	400	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	400	NAG	C2-N2-C7	-5.46	115.59	122.90
4	H	400	NAG	O3-C3-C4	-5.44	97.56	110.38
4	H	400	NAG	O7-C7-C8	2.22	126.02	122.05

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	400	NAG	C8-C7-N2-C2
4	H	400	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.