



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:24 PM UTC

PDB ID : 1THR / pdb_00001thr
Title : STRUCTURES OF THROMBIN COMPLEXES WITH A DESIGNED AND
A NATURAL EXOSITE INHIBITOR
Authors : Qiu, X.; Yin, M.; Padmanabhan, K.P.; Krstenansky, J.L.; Tulinsky, A.
Deposited on : 1993-06-16
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
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

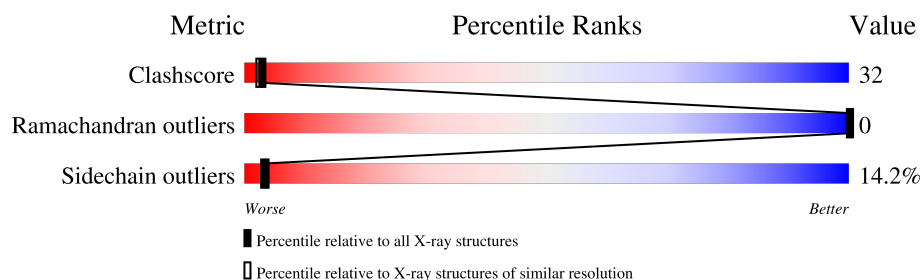
1 Overall quality at a glance

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	13	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2541 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	27	Total	C	N	O	S	0	0	1
			209	131	33	44	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	252	Total	C	N	O	S	0	0	0
			2031	1295	359	363	14			

- Molecule 3 is a protein called HIRULLIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	13	Total	C	N	O	0	0	0
			111	68	14	29			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	25	Total	O	0	0
			25	25		
4	H	160	Total	O	0	0
			160	160		
4	I	5	Total	O	0	0
			5	5		

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.

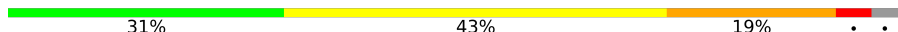
Note EDS was not executed.

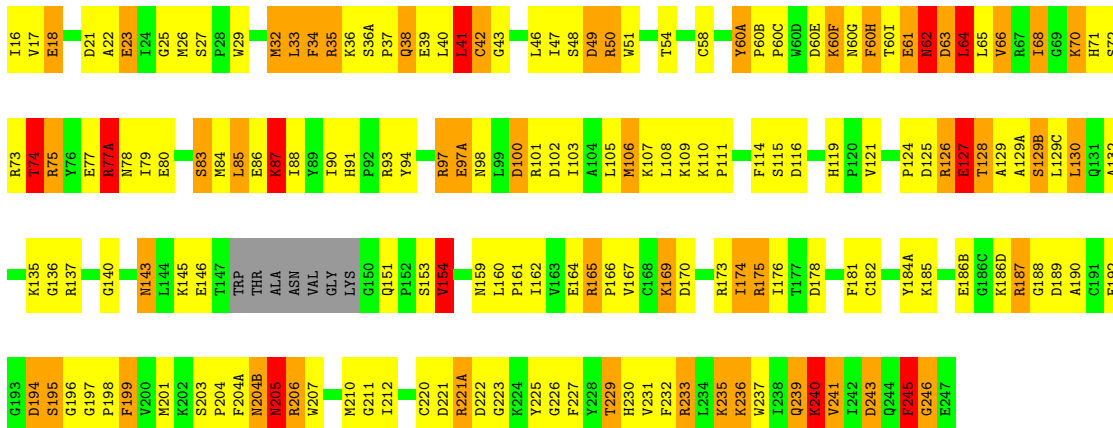
• Molecule 1: ALPHA-THROMBIN (SMALL SUBUNIT)

Chain L: 



• Molecule 2: ALPHA-THROMBIN (LARGE SUBUNIT)

Chain H: 



• Molecule 3: HIRULLIN

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	71.43Å 72.32Å 72.81Å 90.00° 100.55° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.155 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2541	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.00	0/211	2.61	18/282 (6.4%)
2	H	1.15	1/2083 (0.0%)	2.63	177/2813 (6.3%)
3	I	0.90	0/112	2.64	11/148 (7.4%)
All	All	1.13	1/2406 (0.0%)	2.63	206/3243 (6.4%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	78	ASN	N-CA	5.45	1.52	1.46

All (206) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	245	PHE	CA-C-N	-15.27	110.41	122.16
2	H	245	PHE	C-N-CA	-15.27	110.41	122.16
2	H	243	ASP	CA-CB-CG	14.02	126.62	112.60
2	H	246	GLY	O-C-N	13.32	133.26	123.14
1	L	14(J)	TYR	CA-C-O	-12.57	99.43	120.80
2	H	175	ARG	CD-NE-CZ	12.29	141.60	124.40
2	H	204(B)	ASN	CA-C-N	10.69	137.53	122.46
2	H	204(B)	ASN	C-N-CA	10.69	137.53	122.46
2	H	73	ARG	CA-C-O	10.59	131.81	120.90
2	H	232	PHE	CA-CB-CG	-10.40	103.40	113.80
2	H	239	GLN	CA-C-O	10.24	131.69	120.63
2	H	77(A)	ARG	NE-CZ-NH2	-9.80	110.38	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	165	ARG	NE-CZ-NH1	-9.80	111.70	121.50
2	H	127	GLU	CB-CG-CD	9.69	129.06	112.60
2	H	205	ASN	CB-CA-C	9.41	126.06	111.95
2	H	165	ARG	CD-NE-CZ	-9.38	111.27	124.40
2	H	78	ASN	CA-CB-CG	9.30	121.90	112.60
2	H	170	ASP	CA-CB-CG	-9.12	103.48	112.60
2	H	73	ARG	NE-CZ-NH2	8.99	127.29	119.20
2	H	159	ASN	CA-CB-CG	8.92	121.52	112.60
2	H	97	ARG	CD-NE-CZ	-8.90	111.94	124.40
2	H	35	ARG	CD-NE-CZ	-8.88	111.97	124.40
2	H	60(B)	PRO	N-CA-C	8.86	121.51	110.70
2	H	42	CYS	CA-C-N	8.76	133.92	121.30
2	H	42	CYS	C-N-CA	8.76	133.92	121.30
2	H	47	ILE	CB-CG1-CD1	8.71	132.09	113.80
2	H	231	VAL	O-C-N	8.58	130.29	121.89
2	H	165	ARG	NE-CZ-NH2	8.41	126.77	119.20
2	H	77(A)	ARG	CA-C-N	-8.31	109.24	122.79
2	H	77(A)	ARG	C-N-CA	-8.31	109.24	122.79
2	H	74	THR	OG1-CB-CG2	8.05	125.40	109.30
2	H	74	THR	N-CA-C	8.00	123.15	113.23
2	H	116	ASP	CA-CB-CG	7.94	120.54	112.60
1	L	14(A)	LYS	CA-C-O	-7.89	109.67	119.38
2	H	197	GLY	CA-C-O	7.80	130.03	122.46
2	H	97	ARG	NH1-CZ-NH2	7.76	129.39	119.30
2	H	143	ASN	OD1-CG-ND2	7.69	130.29	122.60
2	H	178	ASP	CA-C-O	-7.52	111.32	119.97
2	H	132	ALA	CA-C-O	-7.43	112.86	120.96
2	H	198	PRO	CB-CA-C	-7.35	98.67	110.21
2	H	33	LEU	CA-CB-CG	7.31	141.88	116.30
2	H	68	ILE	N-CA-C	7.21	118.99	108.53
2	H	205	ASN	CA-CB-CG	-7.14	105.46	112.60
2	H	154	VAL	N-CA-CB	-7.13	100.50	112.47
2	H	50	ARG	N-CA-CB	-7.11	100.72	110.95
3	I	59	ASP	CA-CB-CG	-7.08	105.52	112.60
2	H	75	ARG	CA-CB-CG	-7.04	100.03	114.10
2	H	186(D)	LYS	N-CA-C	-7.03	96.79	108.32
2	H	221(A)	ARG	NE-CZ-NH1	-7.00	114.50	121.50
2	H	146	GLU	CB-CG-CD	6.99	124.48	112.60
2	H	206	ARG	NE-CZ-NH2	-6.97	112.93	119.20
2	H	164	GLU	CB-CG-CD	6.91	124.35	112.60
3	I	51	ASP	CA-CB-CG	6.91	119.51	112.60
2	H	245	PHE	CA-C-O	-6.91	111.77	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	221(A)	ARG	CA-CB-CG	6.90	127.90	114.10
2	H	132	ALA	O-C-N	6.89	131.33	123.06
2	H	160	LEU	O-C-N	6.81	127.65	121.80
1	L	1(A)	ASP	N-CA-CB	-6.72	99.89	110.98
2	H	25	GLY	CA-C-N	6.72	129.83	120.29
2	H	25	GLY	C-N-CA	6.72	129.83	120.29
2	H	60(G)	ASN	OD1-CG-ND2	-6.71	115.89	122.60
2	H	115	SER	N-CA-CB	-6.71	100.64	111.24
2	H	73	ARG	CA-C-N	6.66	133.38	121.66
2	H	73	ARG	C-N-CA	6.66	133.38	121.66
1	L	8	GLU	CA-C-O	-6.59	113.82	121.07
2	H	153	SER	N-CA-CB	6.58	120.49	110.42
2	H	195	SER	CB-CA-C	6.57	120.27	109.70
1	L	14(G)	LEU	CB-CA-C	6.56	123.27	110.67
2	H	61	GLU	CB-CG-CD	6.49	123.63	112.60
2	H	124	PRO	CB-CA-C	-6.45	102.54	110.98
2	H	187	ARG	NE-CZ-NH1	6.42	127.92	121.50
2	H	62	ASN	CA-CB-CG	-6.37	106.23	112.60
2	H	60(F)	LYS	N-CA-CB	6.34	120.77	110.43
2	H	181	PHE	CB-CA-C	6.34	123.45	109.94
2	H	140	GLY	CA-C-O	6.32	128.32	121.87
2	H	74	THR	N-CA-CB	-6.32	100.58	110.44
2	H	60(A)	TYR	CA-CB-CG	-6.27	102.61	113.90
2	H	190	ALA	N-CA-C	-6.27	102.08	110.55
2	H	43	GLY	N-CA-C	-6.21	103.08	112.89
2	H	66	VAL	CB-CA-C	6.20	120.07	110.83
2	H	77(A)	ARG	NE-CZ-NH1	6.18	127.68	121.50
2	H	33	LEU	O-C-N	6.16	130.24	123.22
2	H	23	GLU	CB-CG-CD	6.15	123.06	112.60
3	I	57	LEU	N-CA-C	-6.15	105.87	113.19
3	I	51	ASP	CA-C-N	6.11	129.43	120.82
3	I	51	ASP	C-N-CA	6.11	129.43	120.82
2	H	231	VAL	CA-C-O	-6.08	114.72	121.05
2	H	207	TRP	N-CA-CB	6.08	120.20	110.16
3	I	55	PHE	O-C-N	6.08	131.05	123.15
3	I	52	PHE	CA-CB-CG	-6.07	107.73	113.80
2	H	34	PHE	N-CA-C	6.05	118.27	108.41
2	H	221(A)	ARG	NE-CZ-NH2	6.05	124.64	119.20
1	L	12	LEU	CA-C-O	-6.04	114.33	121.16
2	H	27	SER	N-CA-CB	-6.04	101.44	110.99
2	H	42	CYS	O-C-N	-6.04	115.77	122.72
2	H	240	LYS	N-CA-CB	-6.03	100.65	109.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	60(H)	PHE	CA-CB-CG	-6.02	107.78	113.80
2	H	176	ILE	CA-C-O	-5.99	114.82	121.23
1	L	14(J)	TYR	CA-C-N	5.97	130.35	117.20
2	H	206	ARG	NE-CZ-NH1	5.95	127.45	121.50
2	H	41	LEU	CB-CA-C	5.93	120.65	110.86
2	H	21	ASP	CA-C-O	-5.92	114.01	120.81
2	H	73	ARG	NE-CZ-NH1	-5.92	115.58	121.50
1	L	11	SER	CB-CA-C	5.91	120.12	111.73
2	H	165	ARG	CA-C-N	5.91	125.39	119.24
2	H	165	ARG	C-N-CA	5.91	125.39	119.24
2	H	97	ARG	NE-CZ-NH1	-5.91	115.59	121.50
2	H	90	ILE	CB-CG1-CD1	5.89	126.18	113.80
2	H	167	VAL	N-CA-CB	-5.87	102.56	110.54
2	H	165	ARG	CB-CG-CD	5.86	124.79	111.30
2	H	229	THR	CA-CB-OG1	-5.86	100.81	109.60
2	H	77	GLU	C-N-CA	5.86	136.34	121.70
2	H	77	GLU	CB-CG-CD	5.86	122.55	112.60
2	H	77(A)	ARG	CA-C-O	-5.84	112.15	120.51
2	H	80	GLU	CG-CD-OE2	-5.84	104.96	118.40
2	H	70	LYS	N-CA-C	5.84	119.12	110.48
2	H	80	GLU	CG-CD-OE1	5.81	131.76	118.40
2	H	74	THR	CA-CB-OG1	-5.80	100.89	109.60
2	H	220	CYS	CA-C-O	-5.78	113.90	120.32
2	H	127	GLU	CA-CB-CG	5.77	125.63	114.10
2	H	233	ARG	CD-NE-CZ	5.76	132.47	124.40
2	H	204	PRO	N-CA-C	-5.76	106.50	114.27
2	H	18	GLU	CA-C-O	-5.71	113.73	120.81
2	H	98	ASN	CA-C-O	-5.71	113.15	119.78
2	H	137	ARG	NE-CZ-NH1	-5.71	115.79	121.50
2	H	22	ALA	CA-C-N	5.71	130.86	121.39
2	H	22	ALA	C-N-CA	5.71	130.86	121.39
2	H	66	VAL	N-CA-CB	-5.70	103.50	111.25
2	H	68	ILE	O-C-N	-5.70	117.33	123.14
2	H	204(A)	PHE	CA-C-O	-5.69	113.19	120.31
2	H	49	ASP	CA-CB-CG	-5.67	106.93	112.60
2	H	129(B)	SER	CA-C-O	-5.67	112.28	119.31
2	H	199	PHE	CB-CA-C	5.67	120.02	110.79
2	H	18	GLU	CB-CA-C	-5.66	102.56	111.51
1	L	14(C)	GLU	CA-C-O	-5.64	113.73	120.10
2	H	33	LEU	CB-CA-C	5.63	119.31	110.19
2	H	164	GLU	CA-CB-CG	5.62	125.33	114.10
2	H	129(A)	ALA	CA-C-O	-5.60	114.94	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	245	PHE	CA-CB-CG	5.59	119.39	113.80
2	H	103	ILE	CA-C-O	-5.56	115.46	121.19
2	H	205	ASN	CA-C-O	5.56	128.53	122.03
1	L	7	PHE	CA-C-O	-5.55	112.57	120.51
2	H	66	VAL	CA-CB-CG1	5.55	119.84	110.40
2	H	49	ASP	CB-CG-OD2	5.55	131.17	118.40
2	H	178	ASP	O-C-N	5.55	129.09	122.27
2	H	64	LEU	N-CA-C	5.52	117.58	109.24
2	H	227	PHE	CA-C-N	5.50	131.19	122.62
2	H	227	PHE	C-N-CA	5.50	131.19	122.62
1	L	14(I)	SER	CA-C-O	5.50	126.12	119.31
1	L	14(H)	GLU	CB-CG-CD	5.47	121.89	112.60
2	H	42	CYS	CA-C-O	5.44	126.77	121.05
2	H	212	ILE	CA-C-O	-5.43	114.74	120.39
2	H	130	LEU	CA-C-O	-5.42	115.80	122.36
1	L	14	ASP	CB-CA-C	5.42	120.79	109.68
2	H	151	GLN	CB-CA-C	5.41	115.86	109.47
2	H	143	ASN	CB-CG-ND2	-5.40	108.29	116.40
1	L	8	GLU	O-C-N	5.40	127.86	122.08
2	H	126	ARG	CD-NE-CZ	-5.40	116.84	124.40
2	H	175	ARG	NE-CZ-NH2	-5.38	114.35	119.20
2	H	33	LEU	N-CA-C	-5.38	99.96	108.73
2	H	38	GLN	N-CA-C	-5.38	101.21	109.76
1	L	12	LEU	O-C-N	5.35	129.90	123.16
2	H	63	ASP	O-C-N	5.34	130.23	122.43
2	H	173	ARG	N-CA-C	-5.33	106.45	113.17
1	L	14(C)	GLU	CG-CD-OE1	-5.32	106.16	118.40
2	H	97(A)	GLU	N-CA-CB	-5.32	101.50	110.49
2	H	178	ASP	N-CA-CB	5.30	118.49	110.28
2	H	196	GLY	N-CA-C	-5.30	108.32	115.21
3	I	62	GLN	CB-CG-CD	-5.29	103.60	112.60
2	H	87	LYS	CB-CA-C	-5.27	101.23	109.72
2	H	97(A)	GLU	CA-C-N	-5.26	113.35	122.14
2	H	97(A)	GLU	C-N-CA	-5.26	113.35	122.14
2	H	63	ASP	CA-C-N	-5.24	113.72	122.21
2	H	63	ASP	C-N-CA	-5.24	113.72	122.21
2	H	128	THR	O-C-N	5.24	128.13	122.15
2	H	54	THR	CA-CB-CG2	5.24	119.41	110.50
2	H	174	ILE	O-C-N	5.24	128.90	122.72
2	H	87	LYS	N-CA-C	5.23	116.36	108.46
3	I	55	PHE	N-CA-C	-5.21	101.45	109.52
2	H	143	ASN	CA-C-O	5.21	126.88	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	145	LYS	O-C-N	5.21	129.50	123.41
2	H	60(E)	ASP	CA-C-O	-5.20	115.51	121.54
2	H	223	GLY	N-CA-C	-5.18	107.84	115.30
2	H	106	MET	CA-C-N	5.17	129.28	122.30
2	H	106	MET	C-N-CA	5.17	129.28	122.30
2	H	194	ASP	CA-CB-CG	-5.17	107.43	112.60
2	H	85	LEU	O-C-N	5.14	129.20	123.19
2	H	206	ARG	CD-NE-CZ	5.13	131.59	124.40
2	H	225	TYR	CA-C-N	-5.12	116.02	121.45
2	H	225	TYR	C-N-CA	-5.12	116.02	121.45
2	H	176	ILE	CA-CB-CG2	5.12	119.20	110.50
2	H	205	ASN	CB-CG-ND2	-5.12	108.73	116.40
2	H	63	ASP	CA-C-O	-5.11	112.57	119.11
2	H	119	HIS	CA-C-O	5.10	124.23	119.13
2	H	78	ASN	CA-C-N	5.09	131.13	121.97
2	H	78	ASN	C-N-CA	5.09	131.13	121.97
3	I	57	LEU	CB-CA-C	5.09	120.14	110.27
2	H	102	ASP	CA-CB-CG	-5.08	107.52	112.60
1	L	14(H)	GLU	CA-C-O	-5.07	113.14	119.38
2	H	102	ASP	CA-C-O	-5.06	116.28	122.41
2	H	100	ASP	O-C-N	5.06	129.06	122.89
2	H	153	SER	N-CA-C	-5.05	106.80	113.12
3	I	51	ASP	N-CA-CB	-5.03	101.99	110.49
2	H	77(A)	ARG	N-CA-CB	5.02	118.97	110.49
1	L	8	GLU	N-CA-CB	5.02	117.44	109.82
2	H	175	ARG	CA-C-O	5.01	126.26	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	77(A)	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	209	0	203	12	0
2	H	2031	0	2000	130	0
3	I	111	0	87	14	0
4	H	160	0	0	9	0
4	I	5	0	0	1	0
4	L	25	0	0	3	0
All	All	2541	0	2290	148	0

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 32.

All (148) 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:240:LYS:HB3	2:H:240:LYS:NZ	1.41	1.18
2:H:26:MET:HE1	4:H:501:HOH:O	1.51	1.08
2:H:201:MET:HE3	2:H:210:MET:HG3	1.35	1.07
2:H:199:PHE:HE1	2:H:201:MET:HE2	1.21	1.02
2:H:221(A):ARG:HG3	2:H:221(A):ARG:HH11	1.21	1.02
2:H:240:LYS:HB3	2:H:240:LYS:HZ3	0.89	1.02
2:H:240:LYS:NZ	2:H:240:LYS:CB	2.26	0.95
2:H:205:ASN:HB2	4:H:670:HOH:O	1.66	0.94
1:L:14(A):LYS:HD3	2:H:23:GLU:CD	1.91	0.94
2:H:185:LYS:N	2:H:186(B):GLU:OE1	2.00	0.94
1:L:14(A):LYS:HG2	2:H:23:GLU:OE2	1.70	0.92
1:L:9:LYS:HD3	4:L:534:HOH:O	1.68	0.91
3:I:50:SER:O	3:I:52:PHE:N	2.07	0.87
2:H:201:MET:HE3	2:H:210:MET:CG	2.05	0.86
3:I:62:GLN:OXT	4:I:690:HOH:O	1.94	0.85
2:H:199:PHE:CE1	2:H:201:MET:HE2	2.11	0.85
2:H:221(A):ARG:HG3	2:H:221(A):ARG:NH1	1.89	0.85
2:H:85:LEU:HD13	2:H:106:MET:HE2	1.60	0.83
2:H:187:ARG:HD3	2:H:221:ASP:OD2	1.81	0.81
2:H:60(I):THR:OG1	2:H:62:ASN:ND2	2.18	0.76
2:H:169:LYS:HE3	4:H:766:HOH:O	1.87	0.74
2:H:201:MET:CE	2:H:210:MET:HG3	2.15	0.74
1:L:9:LYS:CD	4:L:534:HOH:O	2.30	0.74
1:L:14(D):ARG:O	1:L:14(H):GLU:HG3	1.89	0.72
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	1.97	0.71
2:H:36:LYS:O	2:H:38:GLN:HG2	1.90	0.71
2:H:204(B):ASN:HD22	2:H:205:ASN:N	1.89	0.71
2:H:126:ARG:HB2	2:H:126:ARG:NH1	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:240:LYS:HZ3	2:H:240:LYS:CB	1.85	0.71
2:H:187:ARG:NH1	2:H:221:ASP:O	2.23	0.71
2:H:85:LEU:HD13	2:H:106:MET:CE	2.21	0.69
2:H:36(A):SER:HA	2:H:37:PRO:C	2.17	0.69
2:H:199:PHE:HE1	2:H:201:MET:CE	2.01	0.68
2:H:35:ARG:HB2	2:H:41:LEU:HD13	1.75	0.68
2:H:162:ILE:HD11	2:H:199:PHE:CZ	2.28	0.68
2:H:35:ARG:NH1	2:H:39:GLU:OE2	2.24	0.67
2:H:110:LYS:HZ2	3:I:61:GLU:HG2	1.58	0.67
2:H:50:ARG:NH1	2:H:86:GLU:OE1	2.28	0.67
1:L:14(A):LYS:HD3	2:H:23:GLU:OE1	1.94	0.66
3:I:62:GLN:HA	3:I:62:GLN:OE1	1.96	0.66
3:I:50:SER:O	3:I:51:ASP:HB3	1.95	0.66
2:H:74:THR:HG22	2:H:75:ARG:HG3	1.78	0.65
3:I:50:SER:C	3:I:52:PHE:N	2.55	0.64
1:L:14(A):LYS:CG	2:H:23:GLU:OE2	2.45	0.64
2:H:84:MET:HB2	2:H:109:LYS:HG3	1.80	0.63
2:H:97:ARG:HG3	4:H:416:HOH:O	1.98	0.62
3:I:50:SER:C	3:I:52:PHE:H	2.06	0.62
2:H:49:ASP:HB3	2:H:114:PHE:CZ	2.34	0.62
2:H:162:ILE:HD11	2:H:199:PHE:HZ	1.65	0.61
2:H:35:ARG:O	2:H:38:GLN:HA	2.01	0.60
2:H:236:LYS:N	2:H:236:LYS:HD3	2.14	0.60
1:L:14(A):LYS:CD	2:H:23:GLU:CD	2.72	0.60
2:H:126:ARG:HB3	2:H:127:GLU:OE1	2.03	0.59
2:H:64:LEU:HD12	2:H:85:LEU:HD12	1.83	0.59
2:H:61:GLU:OE2	2:H:88:ILE:N	2.33	0.59
2:H:50:ARG:HD2	2:H:108:LEU:O	2.03	0.58
2:H:62:ASN:ND2	2:H:63:ASP:OD1	2.37	0.58
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.40	0.56
3:I:56:SER:C	3:I:58:ASP:H	2.13	0.56
2:H:235:LYS:HE3	2:H:239:GLN:OE1	2.06	0.56
2:H:126:ARG:NH1	2:H:126:ARG:CB	2.68	0.56
2:H:17:VAL:O	2:H:188:GLY:HA2	2.05	0.56
2:H:77(A):ARG:HD3	4:H:444:HOH:O	2.04	0.56
2:H:51:TRP:HZ2	2:H:246:GLY:HA3	1.71	0.56
2:H:62:ASN:HD22	2:H:63:ASP:N	2.04	0.56
2:H:32:MET:HG3	2:H:40:LEU:HD12	1.88	0.56
2:H:126:ARG:CB	2:H:126:ARG:CZ	2.84	0.56
3:I:59:ASP:OD1	3:I:59:ASP:N	2.34	0.55
2:H:187:ARG:NH2	2:H:222:ASP:OD1	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:32:MET:HG3	2:H:40:LEU:CD1	2.37	0.55
2:H:110:LYS:NZ	3:I:61:GLU:HG2	2.21	0.55
2:H:205:ASN:C	2:H:205:ASN:ND2	2.63	0.55
2:H:85:LEU:HD22	2:H:106:MET:HB3	1.88	0.55
2:H:49:ASP:OD1	2:H:49:ASP:C	2.47	0.54
2:H:38:GLN:NE2	4:H:513:HOH:O	2.39	0.54
2:H:203:SER:O	2:H:205:ASN:HA	2.08	0.54
2:H:188:GLY:O	2:H:189:ASP:HB2	2.07	0.54
2:H:18:GLU:HG3	2:H:187:ARG:HG3	1.89	0.54
2:H:62:ASN:ND2	2:H:63:ASP:N	2.56	0.53
2:H:58:CYS:O	2:H:60(F):LYS:HD2	2.08	0.53
1:L:5:PRO:HA	1:L:9:LYS:HG3	1.91	0.52
2:H:50:ARG:NH1	2:H:107:LYS:HE3	2.24	0.52
2:H:71:HIS:CD2	2:H:154:VAL:HG22	2.45	0.51
2:H:16:ILE:N	2:H:194:ASP:OD2	2.44	0.51
2:H:64:LEU:HD12	2:H:85:LEU:CD1	2.40	0.51
2:H:204(B):ASN:C	2:H:204(B):ASN:ND2	2.60	0.51
2:H:126:ARG:HB2	2:H:126:ARG:HH11	1.77	0.50
2:H:85:LEU:CD1	2:H:106:MET:CE	2.89	0.49
2:H:88:ILE:CD1	2:H:106:MET:HE3	2.43	0.49
2:H:34:PHE:CZ	2:H:38:GLN:HB3	2.47	0.49
2:H:70:LYS:HE3	2:H:72:SER:O	2.13	0.49
2:H:85:LEU:CD1	2:H:106:MET:HE2	2.37	0.48
2:H:221(A):ARG:HH11	2:H:221(A):ARG:CG	1.91	0.48
1:L:12:LEU:HB3	4:L:701:HOH:O	2.12	0.48
2:H:187:ARG:HB2	2:H:221:ASP:OD1	2.13	0.48
2:H:185:LYS:HB2	2:H:186(B):GLU:HG3	1.95	0.48
2:H:125:ASP:OD1	2:H:128:THR:CB	2.62	0.48
2:H:42:CYS:HB3	2:H:195:SER:O	2.15	0.47
2:H:87:LYS:HA	2:H:87:LYS:HD2	1.74	0.47
3:I:56:SER:C	3:I:58:ASP:N	2.71	0.47
2:H:143:ASN:ND2	2:H:192:GLU:HB3	2.29	0.47
2:H:165:ARG:N	2:H:166:PRO:HD2	2.30	0.47
2:H:203:SER:HB3	2:H:204(B):ASN:HD21	1.80	0.47
2:H:237:TRP:O	2:H:240:LYS:HB2	2.15	0.46
2:H:46:LEU:HD11	2:H:48:SER:O	2.16	0.46
2:H:240:LYS:CB	2:H:240:LYS:HZ2	2.26	0.46
2:H:203:SER:HB3	2:H:204(B):ASN:ND2	2.32	0.45
3:I:60:ILE:CG2	3:I:61:GLU:H	2.30	0.45
2:H:51:TRP:CZ2	2:H:246:GLY:HA3	2.52	0.45
2:H:174:ILE:HD12	2:H:174:ILE:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:36(A):SER:CA	2:H:37:PRO:C	2.88	0.44
2:H:49:ASP:O	2:H:111:PRO:HA	2.17	0.44
2:H:236:LYS:NZ	4:H:772:HOH:O	2.51	0.44
2:H:93:ARG:O	2:H:101:ARG:HD2	2.18	0.44
2:H:64:LEU:HD11	2:H:88:ILE:HD11	1.99	0.44
2:H:162:ILE:CD1	2:H:199:PHE:CZ	2.99	0.44
2:H:241:VAL:O	2:H:245:PHE:HD1	2.01	0.43
2:H:94:TYR:HA	2:H:101:ARG:HB2	2.01	0.43
2:H:129:ALA:HA	2:H:210:MET:HE1	1.99	0.43
2:H:74:THR:CG2	2:H:75:ARG:HG3	2.48	0.43
2:H:127:GLU:H	2:H:127:GLU:CD	2.26	0.43
2:H:64:LEU:HD13	2:H:106:MET:HE1	2.00	0.43
2:H:184(A):TYR:HA	2:H:186(B):GLU:OE1	2.18	0.43
2:H:100:ASP:O	2:H:101:ARG:HB2	2.18	0.43
2:H:236:LYS:O	2:H:240:LYS:HB2	2.19	0.43
2:H:23:GLU:OE2	2:H:26:MET:HE3	2.20	0.42
1:L:14(A):LYS:CD	2:H:23:GLU:OE2	2.68	0.42
2:H:97(A):GLU:OE2	2:H:175:ARG:HD3	2.19	0.42
2:H:204(B):ASN:ND2	2:H:206:ARG:H	2.17	0.42
2:H:60(H):PHE:HB3	2:H:64:LEU:HD21	2.01	0.41
3:I:60:ILE:HG22	3:I:61:GLU:H	1.86	0.41
2:H:241:VAL:HB	2:H:245:PHE:HE1	1.85	0.41
2:H:61:GLU:OE2	2:H:87:LYS:HA	2.20	0.41
2:H:129:ALA:O	2:H:130:LEU:HB2	2.21	0.41
2:H:83:SER:HB3	4:H:564:HOH:O	2.21	0.41
3:I:57:LEU:HA	3:I:60:ILE:HD12	2.02	0.41
2:H:91:HIS:CE1	2:H:101:ARG:HD3	2.55	0.41
2:H:105:LEU:HD23	2:H:105:LEU:HA	1.91	0.41
2:H:29:TRP:CG	2:H:121:VAL:HB	2.55	0.41
2:H:62:ASN:ND2	2:H:63:ASP:CG	2.79	0.41
2:H:36(A):SER:HB2	4:H:538:HOH:O	2.21	0.41
2:H:182:CYS:HA	2:H:226:GLY:O	2.21	0.41
2:H:135:LYS:HA	2:H:161:PRO:HA	2.03	0.40
2:H:165:ARG:HH11	2:H:165:ARG:HD3	1.14	0.40
1:L:14(A):LYS:HG2	1:L:14(A):LYS:H	1.64	0.40
2:H:60(A):TYR:CZ	2:H:60(C):PRO:HG2	2.57	0.40
2:H:211:GLY:HA2	2:H:229:THR:O	2.22	0.40
2:H:230:HIS:ND1	2:H:233:ARG:HG3	2.36	0.40

There are no symmetry-related clashes.

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	25/36 (69%)	23 (92%)	2 (8%)	0	100	100
2	H	248/259 (96%)	234 (94%)	14 (6%)	0	100	100
3	I	11/13 (85%)	8 (73%)	3 (27%)	0	100	100
All	All	284/308 (92%)	265 (93%)	19 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	23/31 (74%)	13 (56%)	10 (44%)	0	0
2	H	218/225 (97%)	194 (89%)	24 (11%)	6	7
3	I	13/13 (100%)	11 (85%)	2 (15%)	2	3
All	All	254/269 (94%)	218 (86%)	36 (14%)	3	3

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	14	ASP
1	L	14(A)	LYS
1	L	14(B)	THR
1	L	14(C)	GLU
1	L	14(E)	GLU

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Mol	Chain	Res	Type
1	L	14(F)	LEU
1	L	14(G)	LEU
1	L	14(H)	GLU
1	L	14(I)	SER
1	L	14(J)	TYR
2	H	32	MET
2	H	33	LEU
2	H	41	LEU
2	H	62	ASN
2	H	64	LEU
2	H	65	LEU
2	H	66	VAL
2	H	68	ILE
2	H	74	THR
2	H	79	ILE
2	H	83	SER
2	H	87	LYS
2	H	127	GLU
2	H	129(B)	SER
2	H	129(C)	LEU
2	H	154	VAL
2	H	169	LYS
2	H	205	ASN
2	H	235	LYS
2	H	236	LYS
2	H	240	LYS
2	H	241	VAL
2	H	243	ASP
2	H	245	PHE
3	I	57	LEU
3	I	62	GLN

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	62	ASN
2	H	143	ASN
2	H	156	GLN
2	H	204(B)	ASN
2	H	205	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

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.