



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:49 AM UTC

PDB ID : 1THS / pdb_00001ths
Title : STRUCTURES OF THROMBIN COMPLEXES WITH A DESIGNED AND
A NATURAL EXOSITE INHIBITOR
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Deposited on : 1993-06-16
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

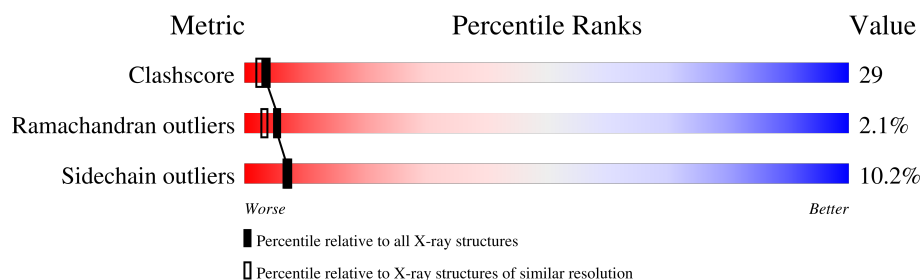
1 Overall quality at a glance

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	11	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2529 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	33	Total	C	N	O	S	0	0	0
			265	162	45	57	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
			2039	1299	360	366	14			

- Molecule 3 is a protein called SYNTHETIC INHIBITOR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	11	Total	C	N	O	0	0	1
			85	56	10	19			

- Molecule 4 is water.

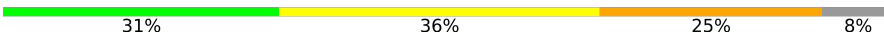
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	17	Total	O	0	0
			17	17		
4	H	123	Total	O	0	0
			123	123		

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.

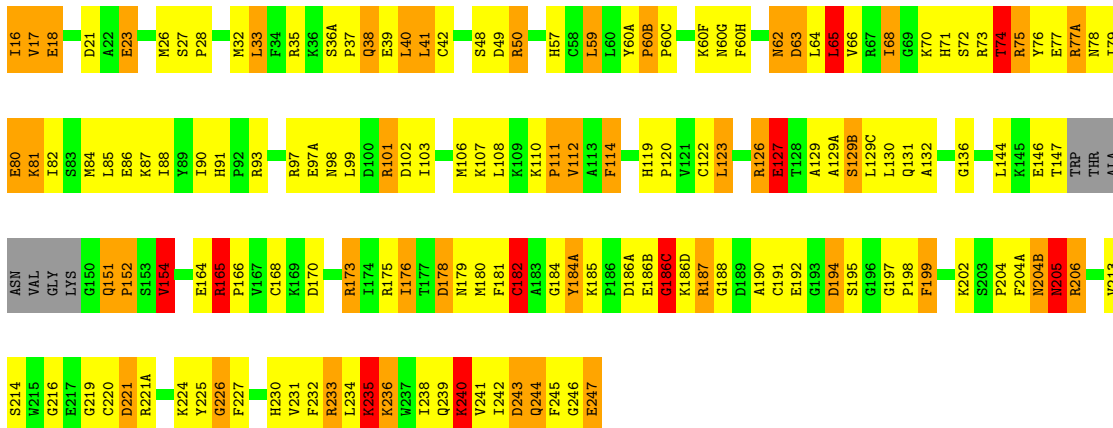
• Molecule 1: ALPHA-THROMBIN (SMALL SUBUNIT)

Chain L: 

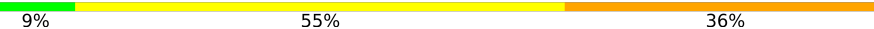


• Molecule 2: ALPHA-THROMBIN (LARGE SUBUNIT)

Chain H: 



• Molecule 3: SYNTHETIC INHIBITOR

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	72.28Å 72.73Å 73.56Å 90.00° 100.55° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.161 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2529	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: SIN, ALC

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	1.31	0/267	2.61	18/353 (5.1%)
2	H	1.46	6/2091 (0.3%)	2.57	167/2823 (5.9%)
3	I	1.09	0/68	3.08	7/93 (7.5%)
All	All	1.43	6/2426 (0.2%)	2.59	192/3269 (5.9%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	27	SER	N-CA	7.04	1.54	1.46
2	H	78	ASN	N-CA	6.10	1.53	1.46
2	H	101	ARG	NE-CZ	5.64	1.39	1.33
2	H	198	PRO	CA-CB	5.45	1.60	1.53
2	H	220	CYS	C-N	-5.09	1.26	1.33
2	H	182	CYS	N-CA	5.03	1.52	1.45

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	243	ASP	CA-CB-CG	23.38	135.97	112.60
2	H	187	ARG	CD-NE-CZ	18.43	150.20	124.40
1	L	15	ARG	CD-NE-CZ	14.68	144.95	124.40
3	I	62	GLU	CB-CG-CD	13.50	135.55	112.60
2	H	62	ASN	CA-CB-CG	-12.38	100.22	112.60
2	H	78	ASN	CA-CB-CG	12.30	124.90	112.60
2	H	77(A)	ARG	CA-C-O	-11.67	103.82	120.51
2	H	233	ARG	NE-CZ-NH1	10.82	132.32	121.50
2	H	187	ARG	NE-CZ-NH1	10.79	132.29	121.50
1	L	14(J)	TYR	N-CA-C	-10.57	101.76	112.97
2	H	123	LEU	CB-CA-C	10.31	121.99	109.31
2	H	97	ARG	CD-NE-CZ	-9.93	110.50	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	132	ALA	CA-C-O	-9.82	110.35	121.15
2	H	233	ARG	CD-NE-CZ	9.77	138.08	124.40
2	H	27	SER	N-CA-CB	-9.66	99.11	111.09
1	L	1(A)	ASP	N-CA-C	-9.52	100.60	112.88
2	H	93	ARG	CD-NE-CZ	9.46	137.64	124.40
3	I	62	GLU	N-CA-CB	9.17	120.62	110.35
2	H	226	GLY	O-C-N	9.11	132.46	123.35
2	H	246	GLY	CA-C-N	9.07	138.03	121.70
2	H	246	GLY	C-N-CA	9.07	138.03	121.70
2	H	38	GLN	CA-C-O	-9.05	111.03	120.80
2	H	64	LEU	N-CA-C	9.00	124.11	109.72
2	H	62	ASN	OD1-CG-ND2	8.69	131.29	122.60
1	L	14(E)	GLU	CB-CG-CD	8.60	127.21	112.60
2	H	245	PHE	CA-C-O	-8.57	109.83	119.95
3	I	61	GLU	CA-CB-CG	8.53	131.16	114.10
2	H	77	GLU	CB-CG-CD	8.52	127.09	112.60
2	H	101	ARG	CD-NE-CZ	-8.49	112.52	124.40
1	L	14(A)	LYS	CA-C-O	-8.48	109.23	119.49
2	H	27	SER	CB-CA-C	8.46	125.11	111.15
2	H	192	GLU	CB-CG-CD	8.29	126.69	112.60
2	H	186(C)	GLY	C-N-CA	8.27	142.38	121.70
2	H	129(A)	ALA	CA-C-O	-8.09	112.51	121.00
2	H	220	CYS	CA-C-O	-8.07	111.38	120.66
2	H	75	ARG	CA-CB-CG	-7.95	98.21	114.10
2	H	65	LEU	CA-C-N	7.82	132.91	122.90
2	H	65	LEU	C-N-CA	7.82	132.91	122.90
3	I	56	TYR	N-CA-CB	7.78	123.73	110.50
2	H	173	ARG	NE-CZ-NH1	7.72	129.22	121.50
2	H	187	ARG	NE-CZ-NH2	-7.70	112.27	119.20
2	H	192	GLU	CB-CA-C	7.58	120.60	110.06
2	H	235	LYS	N-CA-C	7.58	119.54	111.28
2	H	151	GLN	CB-CA-C	7.51	119.05	108.76
2	H	204(B)	ASN	CA-C-N	7.33	133.03	122.40
2	H	204(B)	ASN	C-N-CA	7.33	133.03	122.40
2	H	244	GLN	CB-CG-CD	7.32	125.05	112.60
2	H	204(B)	ASN	OD1-CG-ND2	7.27	129.87	122.60
1	L	14(B)	THR	CA-C-O	-7.19	111.50	119.34
2	H	240	LYS	CA-C-O	-7.16	113.48	121.00
2	H	175	ARG	NE-CZ-NH2	7.16	125.64	119.20
2	H	181	PHE	CA-CB-CG	7.14	120.94	113.80
2	H	38	GLN	O-C-N	7.13	132.84	123.07
2	H	84	MET	CB-CA-C	7.12	122.40	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	74	THR	N-CA-C	7.11	122.21	112.90
2	H	154	VAL	N-CA-CB	-7.07	100.59	112.47
2	H	232	PHE	CA-CB-CG	-7.04	106.75	113.80
2	H	205	ASN	CB-CA-C	6.95	122.48	111.51
2	H	42	CYS	CA-C-N	6.91	131.25	121.30
2	H	42	CYS	C-N-CA	6.91	131.25	121.30
2	H	110	LYS	O-C-N	6.90	126.78	121.88
2	H	247	GLU	CB-CG-CD	6.90	124.33	112.60
2	H	233	ARG	NE-CZ-NH2	-6.89	113.00	119.20
2	H	23	GLU	CB-CG-CD	6.84	124.23	112.60
2	H	74	THR	CA-CB-OG1	-6.82	99.36	109.60
2	H	93	ARG	NE-CZ-NH1	6.80	128.30	121.50
2	H	187	ARG	N-CA-C	6.79	117.01	108.45
2	H	80	GLU	CG-CD-OE1	6.79	134.01	118.40
1	L	14(K)	ILE	CB-CA-C	6.78	122.40	111.29
2	H	205	ASN	CA-C-N	6.75	132.71	122.65
2	H	205	ASN	C-N-CA	6.75	132.71	122.65
2	H	74	THR	N-CA-CB	-6.66	100.33	110.33
2	H	102	ASP	CA-C-O	-6.54	114.49	122.41
2	H	77(A)	ARG	N-CA-CB	6.54	121.54	110.49
3	I	62	GLU	CB-CA-C	-6.51	102.44	112.07
1	L	1(A)	ASP	CA-C-O	6.50	127.27	119.59
2	H	40	LEU	N-CA-CB	6.50	120.46	109.87
2	H	197	GLY	CA-C-O	6.47	129.04	122.38
2	H	119	HIS	O-C-N	-6.47	116.79	121.84
2	H	62	ASN	O-C-N	6.39	129.70	122.22
2	H	132	ALA	O-C-N	6.39	130.77	122.97
2	H	146	GLU	N-CA-CB	6.37	119.48	110.12
2	H	38	GLN	N-CA-C	-6.36	100.77	110.30
2	H	63	ASP	O-C-N	6.34	131.21	122.46
2	H	234	LEU	CB-CA-C	6.33	121.22	111.02
2	H	48	SER	CA-C-O	-6.31	114.38	120.94
2	H	73	ARG	CA-C-N	6.25	133.03	121.52
2	H	73	ARG	C-N-CA	6.25	133.03	121.52
2	H	93	ARG	NE-CZ-NH2	-6.24	113.59	119.20
2	H	154	VAL	CA-C-N	6.21	129.93	121.05
2	H	154	VAL	C-N-CA	6.21	129.93	121.05
2	H	129(B)	SER	CA-C-O	-6.16	111.67	119.31
2	H	179	ASN	CA-CB-CG	-6.10	106.50	112.60
2	H	184	GLY	CA-C-O	6.10	128.15	122.05
2	H	173	ARG	NH1-CZ-NH2	-6.05	111.43	119.30
2	H	119	HIS	CB-CA-C	6.04	118.52	109.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	164	GLU	CB-CG-CD	5.98	122.77	112.60
2	H	127	GLU	CA-CB-CG	5.98	126.06	114.10
2	H	198	PRO	N-CA-C	5.97	121.64	111.68
2	H	114	PHE	O-C-N	5.95	129.91	122.65
1	L	14(J)	TYR	CA-C-O	5.95	127.77	119.80
2	H	66	VAL	CA-C-N	5.94	131.38	123.00
2	H	66	VAL	C-N-CA	5.94	131.38	123.00
2	H	194	ASP	CA-CB-CG	-5.94	106.66	112.60
2	H	198	PRO	CB-CA-C	-5.93	102.15	110.63
1	L	14(J)	TYR	CA-C-N	-5.93	104.16	117.20
2	H	164	GLU	CA-C-N	5.93	129.74	120.97
2	H	164	GLU	C-N-CA	5.93	129.74	120.97
2	H	231	VAL	CA-C-O	-5.92	114.79	120.95
2	H	59	LEU	O-C-N	5.92	130.30	122.36
2	H	97	ARG	N-CA-CB	5.92	119.34	110.22
2	H	247	GLU	CA-CB-CG	5.88	125.86	114.10
2	H	190	ALA	N-CA-C	-5.84	102.67	110.55
2	H	23	GLU	N-CA-C	-5.82	103.02	110.53
2	H	213	VAL	O-C-N	5.82	128.89	122.66
2	H	76	TYR	CA-C-O	-5.79	113.72	120.62
2	H	26	MET	O-C-N	5.79	128.75	122.15
3	I	57	GLU	O-C-N	5.77	127.24	121.30
2	H	219	GLY	N-CA-C	-5.73	102.39	112.77
2	H	192	GLU	CG-CD-OE2	5.73	131.58	118.40
2	H	114	PHE	CA-CB-CG	-5.71	108.09	113.80
2	H	225	TYR	CA-C-O	5.71	127.85	121.40
2	H	206	ARG	NE-CZ-NH1	5.65	127.15	121.50
2	H	245	PHE	N-CA-C	5.64	119.47	112.59
2	H	224	LYS	CB-CA-C	5.63	120.59	109.66
2	H	170	ASP	CA-CB-CG	-5.62	106.97	112.60
2	H	179	ASN	CA-C-N	5.61	131.40	122.59
2	H	179	ASN	C-N-CA	5.61	131.40	122.59
2	H	40	LEU	O-C-N	5.55	129.85	123.02
2	H	230	HIS	CA-C-N	5.54	128.05	120.46
2	H	230	HIS	C-N-CA	5.54	128.05	120.46
2	H	73	ARG	CA-C-O	5.54	126.41	120.70
2	H	127	GLU	CB-CG-CD	5.52	121.99	112.60
1	L	13	GLU	CA-C-O	-5.52	114.74	121.36
2	H	168	CYS	N-CA-CB	5.50	117.99	110.01
1	L	5	PRO	CB-CA-C	5.48	119.63	111.85
2	H	178	ASP	N-CA-C	-5.45	105.89	112.54
2	H	42	CYS	CA-C-O	5.45	127.19	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	62	ASN	N-CA-C	5.43	117.95	111.71
2	H	184(A)	TYR	CB-CG-CD1	-5.42	112.67	120.80
2	H	242	ILE	CA-C-N	5.42	127.81	120.44
2	H	242	ILE	C-N-CA	5.42	127.81	120.44
2	H	221(A)	ARG	NE-CZ-NH2	5.39	124.06	119.20
1	L	14(M)	GLY	CA-C-N	5.38	131.39	121.70
1	L	14(M)	GLY	C-N-CA	5.38	131.39	121.70
2	H	233	ARG	CA-C-O	-5.37	112.99	119.49
2	H	199	PHE	N-CA-C	-5.37	98.49	107.99
2	H	152	PRO	N-CA-C	-5.36	101.48	111.03
2	H	114	PHE	CA-C-O	-5.32	115.92	121.99
1	L	4	ARG	CG-CD-NE	5.30	123.66	112.00
2	H	68	ILE	N-CA-C	5.26	116.06	108.48
2	H	17	VAL	CA-C-O	5.26	126.16	120.53
2	H	64	LEU	O-C-N	5.24	130.00	123.19
2	H	231	VAL	O-C-N	5.23	126.95	121.87
2	H	111	PRO	CB-CA-C	5.23	118.21	111.46
3	I	57	GLU	CB-CA-C	-5.23	101.26	109.52
2	H	221	ASP	N-CA-C	5.22	118.95	112.47
2	H	146	GLU	CB-CA-C	-5.22	102.12	110.79
2	H	16	ILE	CA-C-N	5.22	129.91	123.12
2	H	16	ILE	C-N-CA	5.22	129.91	123.12
1	L	14(A)	LYS	N-CA-CB	5.22	119.19	110.32
2	H	186(D)	LYS	CA-C-O	-5.21	113.05	120.51
1	L	14(E)	GLU	CA-CB-CG	5.21	124.52	114.10
2	H	154	VAL	CB-CA-C	5.21	118.40	110.90
2	H	97	ARG	NE-CZ-NH1	-5.20	116.30	121.50
2	H	97(A)	GLU	CA-CB-CG	5.20	124.50	114.10
2	H	107	LYS	N-CA-CB	5.20	118.89	110.42
2	H	181	PHE	O-C-N	5.20	129.20	123.33
2	H	216	GLY	CA-C-O	-5.20	115.60	121.68
2	H	39	GLU	N-CA-C	5.19	116.42	108.42
2	H	184(A)	TYR	CB-CG-CD2	5.19	128.59	120.80
2	H	74	THR	CA-CB-CG2	5.18	119.31	110.50
1	L	7	PHE	CB-CA-C	5.18	120.72	110.42
2	H	28	PRO	CA-C-O	5.17	126.00	118.86
2	H	199	PHE	CB-CA-C	5.17	119.22	110.79
2	H	77(A)	ARG	CA-C-N	-5.15	113.13	122.50
2	H	77(A)	ARG	C-N-CA	-5.15	113.13	122.50
2	H	214	SER	N-CA-C	5.13	119.16	112.13
2	H	131	GLN	CB-CG-CD	-5.12	103.90	112.60
2	H	206	ARG	NE-CZ-NH2	-5.11	114.60	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	64	LEU	N-CA-CB	-5.11	102.35	111.08
2	H	176	ILE	CA-CB-CG2	5.11	119.18	110.50
2	H	60(B)	PRO	N-CA-C	5.09	116.92	110.70
2	H	73	ARG	CD-NE-CZ	5.08	131.51	124.40
2	H	186(D)	LYS	N-CA-C	-5.07	100.00	110.80
2	H	244	GLN	OE1-CD-NE2	-5.06	117.54	122.60
2	H	165	ARG	CB-CG-CD	5.05	122.92	111.30
2	H	220	CYS	N-CA-C	-5.04	100.82	109.24
2	H	38	GLN	CB-CG-CD	5.04	121.17	112.60
2	H	18	GLU	CB-CG-CD	5.03	121.15	112.60
2	H	41	LEU	CA-C-N	5.01	131.37	122.45
2	H	41	LEU	C-N-CA	5.01	131.37	122.45

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	265	0	259	41	1
2	H	2039	0	2010	123	1
3	I	85	0	74	7	0
4	H	123	0	0	5	0
4	L	17	0	0	1	0
All	All	2529	0	2343	138	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 29.

All (138) 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(D):GLY:CA	2:H:123:LEU:H	1.51	1.24
2:H:126:ARG:CB	2:H:126:ARG:HH11	1.57	1.16
1:L:1(D):GLY:N	2:H:123:LEU:H	1.45	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1(D):GLY:HA3	2:H:122:CYS:HA	1.30	1.12
1:L:1(E):SER:HB2	2:H:123:LEU:O	1.52	1.08
2:H:126:ARG:HH11	2:H:126:ARG:HB3	0.95	1.08
1:L:1(D):GLY:CA	2:H:123:LEU:N	2.18	1.07
2:H:126:ARG:HB3	2:H:126:ARG:NH1	1.71	1.06
2:H:50:ARG:NH1	2:H:86:GLU:OE1	1.92	1.01
1:L:14(J):TYR:C	1:L:14(K):ILE:HG13	1.80	1.00
1:L:1(D):GLY:HA3	2:H:122:CYS:CA	1.96	0.94
1:L:1(D):GLY:H	2:H:123:LEU:H	1.12	0.94
2:H:147:THR:HA	4:H:476:HOH:O	1.69	0.91
1:L:1(E):SER:CB	2:H:123:LEU:O	2.19	0.91
1:L:14(I):SER:C	1:L:14(K):ILE:H	1.79	0.86
2:H:87:LYS:HD3	2:H:88:ILE:H	1.39	0.85
1:L:1(D):GLY:CA	2:H:122:CYS:HA	2.07	0.83
2:H:236:LYS:HD2	2:H:239:GLN:NE2	1.92	0.83
1:L:1(D):GLY:H	2:H:123:LEU:N	1.79	0.80
2:H:49:ASP:OD2	2:H:111:PRO:HB3	1.83	0.79
2:H:50:ARG:HA	2:H:108:LEU:HD12	1.66	0.78
2:H:235:LYS:HD3	2:H:239:GLN:OE1	1.84	0.78
1:L:1(D):GLY:HA2	2:H:123:LEU:N	2.00	0.77
1:L:1(C):GLU:HG2	2:H:120:PRO:HG2	1.65	0.77
2:H:50:ARG:C	2:H:108:LEU:HD12	2.11	0.76
1:L:14(A):LYS:HE2	2:H:23:GLU:CD	2.11	0.76
2:H:65:LEU:HD21	3:I:64:ALC:HD13	1.67	0.76
1:L:14(A):LYS:HG2	2:H:23:GLU:OE2	1.87	0.74
1:L:15:ARG:HD2	2:H:204:PRO:O	1.88	0.74
2:H:35:ARG:O	2:H:38:GLN:HA	1.89	0.72
1:L:1(D):GLY:HA3	2:H:123:LEU:N	2.05	0.72
2:H:71:HIS:CD2	2:H:154:VAL:HG22	2.25	0.72
2:H:127:GLU:OE2	4:H:533:HOH:O	2.08	0.72
1:L:1(D):GLY:HA3	2:H:122:CYS:C	2.16	0.71
2:H:62:ASN:ND2	2:H:62:ASN:H	1.88	0.70
2:H:87:LYS:HD3	2:H:88:ILE:N	2.07	0.70
2:H:236:LYS:HD2	2:H:239:GLN:HE22	1.54	0.70
2:H:85:LEU:HD21	2:H:106:MET:HE2	1.74	0.68
2:H:50:ARG:CA	2:H:108:LEU:HD12	2.25	0.66
2:H:240:LYS:HD3	2:H:244:GLN:OE1	1.94	0.66
1:L:1(C):GLU:OE2	1:L:1(B):ALA:HB3	1.96	0.66
2:H:126:ARG:CB	2:H:126:ARG:NH1	2.40	0.65
2:H:187:ARG:HD3	2:H:221:ASP:OD2	1.97	0.64
1:L:1(D):GLY:HA2	2:H:123:LEU:H	1.52	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:126:ARG:NH1	2:H:127:GLU:OE1	2.30	0.64
2:H:74:THR:HG22	2:H:75:ARG:HG3	1.80	0.63
2:H:185:LYS:HB3	2:H:186(A):ASP:OD1	1.99	0.62
2:H:186(B):GLU:O	2:H:186(C):GLY:C	2.41	0.62
1:L:1(E):SER:O	1:L:1(D):GLY:C	2.44	0.61
2:H:70:LYS:HE3	2:H:72:SER:O	2.00	0.61
2:H:144:LEU:HD11	2:H:152:PRO:CA	2.31	0.60
2:H:185:LYS:HB2	2:H:186(B):GLU:HG3	1.82	0.60
1:L:1(C):GLU:HG2	2:H:120:PRO:CG	2.30	0.60
2:H:71:HIS:CD2	2:H:154:VAL:CG2	2.85	0.60
2:H:186(B):GLU:O	2:H:186(C):GLY:O	2.20	0.60
3:I:60:PRO:C	3:I:62:GLU:N	2.57	0.60
2:H:80:GLU:C	2:H:81:LYS:HD2	2.27	0.59
3:I:63:ALA:C	3:I:65:GLU:N	2.56	0.59
1:L:1(D):GLY:HA2	2:H:123:LEU:HB2	1.84	0.59
2:H:59:LEU:HD13	2:H:88:ILE:HD13	1.84	0.58
2:H:91:HIS:CE1	2:H:101:ARG:HD3	2.38	0.58
1:L:1(D):GLY:HA2	2:H:123:LEU:CB	2.33	0.58
2:H:236:LYS:N	2:H:236:LYS:HD3	2.13	0.58
1:L:14(A):LYS:HE2	2:H:23:GLU:OE1	2.03	0.58
1:L:1(D):GLY:N	2:H:123:LEU:N	2.29	0.58
1:L:14(J):TYR:O	1:L:14(K):ILE:HG13	2.04	0.57
3:I:60:PRO:C	3:I:62:GLU:H	2.12	0.57
1:L:15:ARG:HB2	2:H:204:PRO:O	2.05	0.56
1:L:1(D):GLY:CA	2:H:122:CYS:C	2.78	0.56
2:H:60(F):LYS:HD2	2:H:60(H):PHE:HE2	1.72	0.55
2:H:178:ASP:O	2:H:233:ARG:HD2	2.06	0.55
2:H:82:ILE:HD12	3:I:59:ILE:HD13	1.89	0.55
2:H:49:ASP:OD2	2:H:111:PRO:CB	2.55	0.55
2:H:80:GLU:O	2:H:81:LYS:HD2	2.07	0.54
2:H:60(F):LYS:HD2	2:H:60(H):PHE:CE2	2.42	0.54
2:H:165:ARG:N	2:H:166:PRO:HD2	2.23	0.54
2:H:191:CYS:O	2:H:194:ASP:HB2	2.07	0.54
2:H:144:LEU:HD11	2:H:152:PRO:HA	1.89	0.54
1:L:1(E):SER:O	1:L:1(C):GLU:N	2.42	0.53
2:H:129:ALA:O	2:H:130:LEU:HB2	2.09	0.53
1:L:1(E):SER:HB3	2:H:123:LEU:O	2.09	0.52
2:H:103:ILE:HD11	2:H:238:ILE:HD11	1.91	0.52
2:H:36(A):SER:HA	2:H:37:PRO:C	2.34	0.51
2:H:85:LEU:CD2	2:H:106:MET:HE2	2.39	0.51
2:H:205:ASN:C	2:H:205:ASN:ND2	2.69	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:14(A):LYS:CG	2:H:23:GLU:OE2	2.57	0.50
2:H:21:ASP:HB3	2:H:154:VAL:CG1	2.42	0.50
1:L:1(D):GLY:CA	2:H:122:CYS:CA	2.76	0.49
2:H:17:VAL:O	2:H:18:GLU:HB2	2.12	0.49
4:L:526:HOH:O	2:H:123:LEU:HD12	2.12	0.49
2:H:68:ILE:HD12	2:H:112:VAL:HG21	1.94	0.49
2:H:57:HIS:NE2	2:H:195:SER:OG	2.45	0.49
2:H:87:LYS:CD	2:H:88:ILE:N	2.75	0.49
3:I:60:PRO:O	3:I:62:GLU:N	2.46	0.49
2:H:85:LEU:HD11	2:H:106:MET:CE	2.42	0.49
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	2.20	0.48
2:H:98:ASN:N	2:H:98:ASN:OD1	2.44	0.48
1:L:1(C):GLU:H	1:L:1:CYS:CB	2.26	0.48
1:L:5:PRO:HA	1:L:9:LYS:HB2	1.94	0.48
2:H:205:ASN:ND2	2:H:205:ASN:O	2.47	0.48
1:L:1(C):GLU:HG3	1:L:1(B):ALA:H	1.79	0.47
2:H:184(A):TYR:HB2	4:H:509:HOH:O	2.14	0.47
2:H:32:MET:HG3	2:H:40:LEU:CD1	2.44	0.47
2:H:17:VAL:O	2:H:188:GLY:HA2	2.14	0.47
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.50	0.47
1:L:14(G):LEU:HD21	2:H:202:LYS:HD3	1.96	0.47
1:L:15:ARG:NH2	2:H:204(A):PHE:O	2.31	0.47
2:H:204(B):ASN:ND2	2:H:206:ARG:HB2	2.30	0.47
2:H:16:ILE:N	2:H:194:ASP:OD2	2.49	0.46
2:H:16:ILE:O	2:H:144:LEU:HA	2.15	0.46
2:H:182:CYS:HA	2:H:226:GLY:O	2.16	0.46
2:H:126:ARG:HH11	2:H:126:ARG:CG	2.27	0.45
2:H:185:LYS:N	2:H:186(B):GLU:OE1	2.34	0.45
2:H:205:ASN:ND2	4:H:508:HOH:O	2.49	0.45
3:I:55:SIN:O3	3:I:56:TYR:CD2	2.69	0.44
2:H:126:ARG:NH1	2:H:126:ARG:CG	2.80	0.44
2:H:144:LEU:HD21	2:H:152:PRO:HB3	1.98	0.44
2:H:114:PHE:HB3	4:H:403:HOH:O	2.18	0.44
2:H:33:LEU:HD21	2:H:106:MET:HE1	2.00	0.43
2:H:85:LEU:CD1	2:H:106:MET:CE	2.95	0.43
2:H:57:HIS:CE1	2:H:195:SER:OG	2.72	0.43
2:H:60(B):PRO:N	2:H:60(C):PRO:CD	2.82	0.42
2:H:71:HIS:NE2	2:H:154:VAL:CG2	2.82	0.42
2:H:101:ARG:HH11	2:H:101:ARG:HD2	1.59	0.42
2:H:151:GLN:HA	2:H:152:PRO:HD3	1.91	0.42
2:H:60(G):ASN:C	2:H:60(G):ASN:OD1	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:85:LEU:HD11	2:H:106:MET:HE2	2.01	0.41
2:H:176:ILE:HD12	2:H:227:PHE:CE2	2.55	0.41
2:H:165:ARG:NH2	2:H:180:MET:O	2.52	0.41
1:L:14(H):GLU:HA	1:L:14(L):ASP:HA	2.02	0.41
2:H:71:HIS:NE2	2:H:154:VAL:HG22	2.35	0.41
2:H:204(B):ASN:C	2:H:204(B):ASN:ND2	2.77	0.41
1:L:1:CYS:C	2:H:122:CYS:SG	3.04	0.41
2:H:74:THR:CG2	2:H:75:ARG:HG3	2.49	0.41
2:H:130:LEU:HD23	2:H:130:LEU:HA	1.72	0.41
2:H:50:ARG:NH1	2:H:108:LEU:O	2.54	0.40
2:H:165:ARG:N	2:H:166:PRO:CD	2.85	0.40
2:H:60(A):TYR:C	2:H:60(C):PRO:HD2	2.47	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)
1:L:14(L):ASP:O	2:H:173:ARG:NH2[4_556]	1.83	0.37

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	31/36 (86%)	22 (71%)	6 (19%)	3 (10%)	0	0
2	H	248/259 (96%)	233 (94%)	13 (5%)	2 (1%)	16	16
3	I	7/11 (64%)	4 (57%)	2 (29%)	1 (14%)	0	0
All	All	286/306 (94%)	259 (91%)	21 (7%)	6 (2%)	5	3

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	1(D)	GLY
1	L	14(M)	GLY
2	H	186(C)	GLY
1	L	14(L)	ASP
3	I	63	ALA
2	H	77(A)	ARG

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	29/31 (94%)	28 (97%)	1 (3%)	32	44
2	H	220/225 (98%)	195 (89%)	25 (11%)	5	5
3	I	7/8 (88%)	7 (100%)	0	100	100
All	All	256/264 (97%)	230 (90%)	26 (10%)	7	7

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	9	LYS
2	H	33	LEU
2	H	41	LEU
2	H	50	ARG
2	H	63	ASP
2	H	65	LEU
2	H	74	THR
2	H	79	ILE
2	H	81	LYS
2	H	90	ILE
2	H	99	LEU
2	H	112	VAL
2	H	126	ARG
2	H	127	GLU
2	H	129(B)	SER
2	H	129(C)	LEU
2	H	154	VAL

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Mol	Chain	Res	Type
2	H	165	ARG
2	H	182	CYS
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	247	GLU

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	62	ASN
2	H	156	GLN
2	H	204(B)	ASN
2	H	205	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	ALC	I	64	3	9,11,12	0.53	0	11,13,15	2.47	2 (18%)

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	ALC	I	64	3	-	2/5/14/16	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	64	ALC	CG-CB-CA	-6.62	105.61	114.52
3	I	64	ALC	CB-CA-C	4.57	118.02	110.99

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	64	ALC	N-CA-CB-CG
3	I	64	ALC	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	64	ALC	1	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.