



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:57 AM UTC

PDB ID : 1ATH / pdb_00001ath
Title : THE INTACT AND CLEAVED HUMAN ANTITHROMBIN III COMPLEX
AS A MODEL FOR SERPIN-PROTEINASE INTERACTIONS
Authors : Schreuder, H.A.; Hol, W.G.J.
Deposited on : 1993-12-14
Resolution : 3.20 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
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

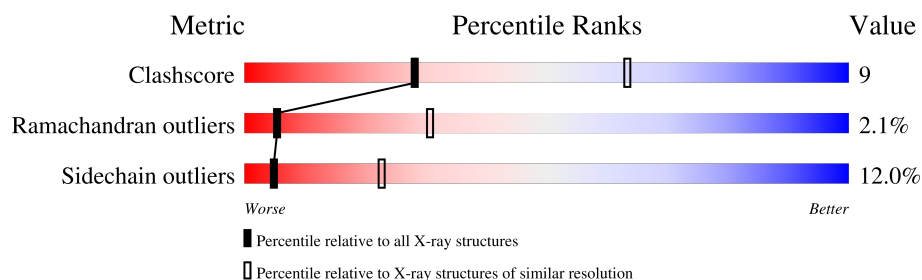
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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	A	432	
1	B	432	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6002 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 ANTITHROMBIN III.

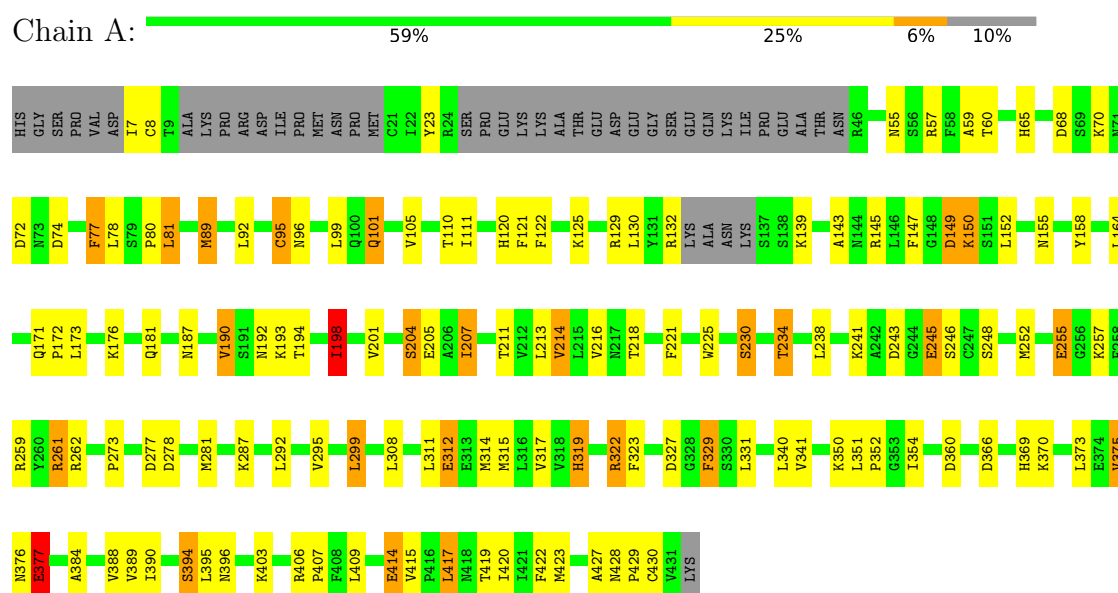
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			3110	1988	521	585	16			
1	B	362	Total	C	N	O	S	0	0	0
			2892	1857	477	542	16			

3 Residue-property plots

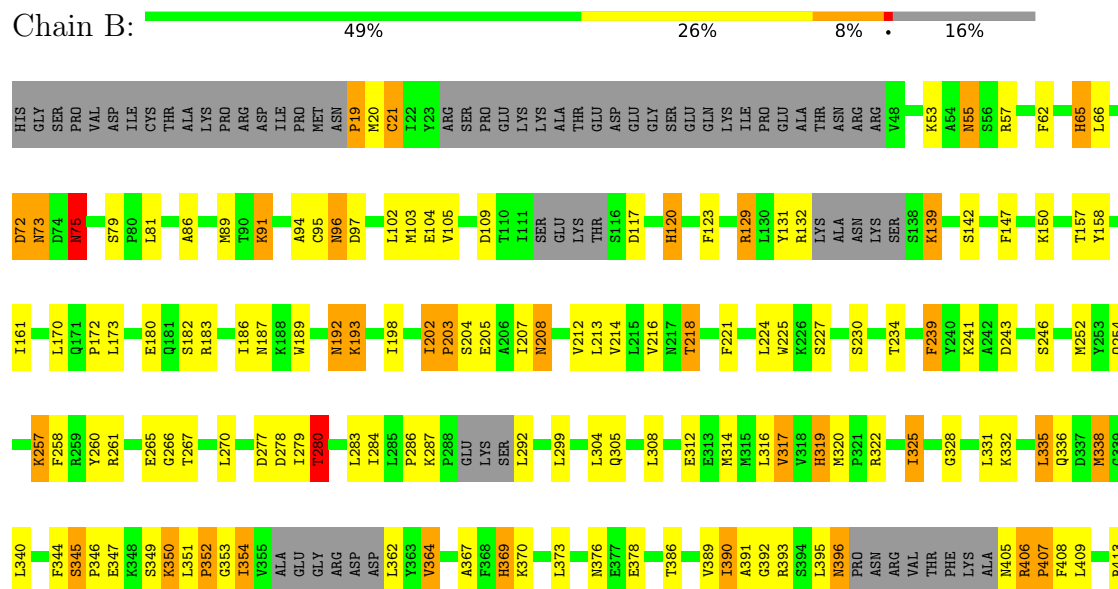
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: ANTITHROMBIN III



• Molecule 1: ANTITHROMBIN III



E414	V415	P416	L417	N418	T419	I420	R425	V426	A427	N428	P429	G430	VAL	LYS
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.95 Å 101.17 Å 69.52 Å 90.00° 105.96° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.179 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6002	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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	A	0.80	4/3169 (0.1%)	1.66	64/4275 (1.5%)
1	B	0.81	5/2946 (0.2%)	1.68	58/3972 (1.5%)
All	All	0.81	9/6115 (0.1%)	1.67	122/8247 (1.5%)

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	B	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	415	VAL	CA-CB	7.39	1.58	1.54
1	A	369	HIS	CD2-NE2	-7.09	1.30	1.37
1	A	319	HIS	CD2-NE2	-6.93	1.30	1.37
1	A	120	HIS	CD2-NE2	-6.83	1.30	1.37
1	B	319	HIS	CD2-NE2	-6.82	1.30	1.37
1	B	120	HIS	CD2-NE2	-6.81	1.30	1.37
1	B	369	HIS	CD2-NE2	-6.58	1.30	1.37
1	A	65	HIS	CD2-NE2	-6.27	1.30	1.37
1	B	65	HIS	CD2-NE2	-5.97	1.31	1.37

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	ASN	OD1-CG-ND2	-9.52	113.08	122.60
1	A	234	THR	N-CA-C	-8.46	94.21	108.26
1	B	73	ASN	CB-CG-ND2	8.44	129.06	116.40
1	B	117	ASP	CA-CB-CG	8.14	120.74	112.60
1	A	155	ASN	OD1-CG-ND2	-7.81	114.79	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	ASN	CA-CB-CG	7.80	120.40	112.60
1	A	394	SER	N-CA-C	-7.60	96.84	109.07
1	B	21	CYS	N-CA-C	7.44	126.65	110.80
1	A	150	LYS	N-CA-C	-7.30	95.24	110.80
1	A	278	ASP	CA-CB-CG	7.28	119.88	112.60
1	B	391	ALA	N-CA-C	7.08	120.47	112.97
1	A	243	ASP	O-C-N	6.99	132.22	123.14
1	A	245	GLU	N-CA-C	6.95	120.08	110.35
1	A	428	ASN	OD1-CG-ND2	-6.90	115.70	122.60
1	B	390	ILE	CA-C-O	-6.87	112.19	120.78
1	B	75	ASN	CB-CG-ND2	6.83	126.64	116.40
1	B	104	GLU	CA-CB-CG	6.83	127.75	114.10
1	A	299	LEU	O-C-N	-6.66	113.73	122.59
1	A	248	SER	N-CA-C	6.66	119.58	108.20
1	B	75	ASN	OD1-CG-ND2	-6.64	115.96	122.60
1	B	415	VAL	CA-C-O	-6.60	114.27	118.69
1	A	120	HIS	CB-CG-CD2	-6.59	122.63	131.20
1	B	369	HIS	CB-CG-CD2	-6.54	122.69	131.20
1	A	287	LYS	CA-C-O	-6.53	113.91	119.59
1	B	408	PHE	CA-CB-CG	6.49	120.29	113.80
1	B	390	ILE	O-C-N	-6.46	114.50	122.57
1	B	65	HIS	CB-CG-CD2	-6.41	122.87	131.20
1	B	396	ASN	CA-CB-CG	6.39	118.99	112.60
1	B	420	ILE	N-CA-C	-6.37	100.43	108.84
1	B	418	ASN	CA-CB-CG	6.33	118.93	112.60
1	B	120	HIS	CB-CG-CD2	-6.32	122.98	131.20
1	A	149	ASP	CA-C-O	6.27	129.48	120.51
1	B	338	MET	N-CA-C	-6.27	105.12	112.89
1	B	345	SER	CA-C-N	6.21	126.40	119.32
1	B	345	SER	C-N-CA	6.21	126.40	119.32
1	B	415	VAL	CB-CA-C	-6.17	105.92	114.00
1	A	322	ARG	N-CA-C	-6.14	99.65	109.96
1	A	384	ALA	N-CA-C	-6.13	99.91	109.72
1	B	280	THR	N-CA-CB	-6.08	100.22	111.53
1	A	248	SER	CA-C-O	6.07	126.85	120.54
1	A	149	ASP	CA-CB-CG	6.02	118.62	112.60
1	A	369	HIS	CB-CG-CD2	-6.01	123.39	131.20
1	B	198	ILE	N-CA-C	-6.00	98.37	107.73
1	A	225	TRP	CB-CG-CD1	-5.97	117.95	126.90
1	B	192	ASN	OD1-CG-ND2	-5.93	116.67	122.60
1	B	75	ASN	CA-CB-CG	5.86	118.46	112.60
1	A	225	TRP	CG-CD2-CE3	5.83	139.73	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	TYR	N-CA-C	-5.82	104.63	110.97
1	A	70	LYS	N-CA-C	5.82	119.04	109.85
1	B	62	PHE	N-CA-C	-5.82	104.86	111.14
1	B	79	SER	CA-C-N	5.80	125.01	118.97
1	B	79	SER	C-N-CA	5.80	125.01	118.97
1	A	130	LEU	N-CA-C	5.78	117.58	111.28
1	B	55	ASN	OD1-CG-ND2	-5.77	116.83	122.60
1	A	155	ASN	CB-CG-ND2	5.77	125.05	116.40
1	A	329	PHE	CA-CB-CG	5.76	119.56	113.80
1	B	396	ASN	OD1-CG-ND2	-5.75	116.86	122.60
1	A	246	SER	N-CA-C	-5.71	100.40	109.76
1	B	239	PHE	N-CA-C	-5.68	99.26	108.52
1	A	77	PHE	CA-CB-CG	-5.68	108.12	113.80
1	A	414	GLU	N-CA-C	-5.67	98.51	108.20
1	B	225	TRP	CG-CD2-CE3	5.66	139.56	133.90
1	A	187	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	B	322	ARG	N-CA-C	-5.64	100.61	109.25
1	A	262	ARG	CA-CB-CG	-5.64	102.83	114.10
1	A	243	ASP	CA-C-O	5.60	127.31	120.25
1	B	393	ARG	N-CA-C	5.59	118.58	110.42
1	B	386	THR	N-CA-C	-5.57	99.95	109.24
1	B	319	HIS	CB-CG-CD2	-5.56	123.98	131.20
1	A	149	ASP	O-C-N	5.53	129.94	122.59
1	A	72	ASP	N-CA-C	5.50	118.78	111.75
1	A	205	GLU	N-CA-C	5.47	118.00	111.71
1	A	192	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	B	187	ASN	OD1-CG-ND2	-5.44	117.16	122.60
1	A	351	LEU	CA-C-N	5.44	125.52	119.32
1	A	351	LEU	C-N-CA	5.44	125.52	119.32
1	B	376	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	B	225	TRP	CB-CG-CD1	-5.40	118.80	126.90
1	B	305	GLN	OE1-CD-NE2	-5.40	117.20	122.60
1	A	101	GLN	OE1-CD-NE2	-5.38	117.22	122.60
1	A	430	CYS	CA-CB-SG	-5.37	102.05	114.40
1	B	104	GLU	N-CA-CB	-5.36	102.28	110.33
1	B	299	LEU	N-CA-C	5.36	116.98	108.67
1	A	243	ASP	CA-CB-CG	-5.36	107.24	112.60
1	A	81	LEU	CA-C-O	-5.35	115.20	120.82
1	A	225	TRP	CE2-CD2-CG	-5.35	100.78	107.20
1	B	405	ASN	OD1-CG-ND2	-5.34	117.25	122.60
1	B	225	TRP	CE2-CD2-CG	-5.33	100.80	107.20
1	B	364	VAL	N-CA-C	-5.32	100.78	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	ASP	CA-CB-CG	5.31	117.91	112.60
1	B	208	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	B	109	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	319	HIS	CB-CG-CD2	-5.28	124.33	131.20
1	B	234	THR	N-CA-C	-5.27	100.72	109.46
1	B	230	SER	CA-C-N	5.24	124.75	119.19
1	B	230	SER	C-N-CA	5.24	124.75	119.19
1	A	101	GLN	CA-CB-CG	5.23	124.55	114.10
1	A	406	ARG	O-C-N	-5.22	118.37	121.71
1	B	279	ILE	N-CA-C	-5.22	100.96	108.53
1	A	415	VAL	CA-C-N	5.21	124.66	119.24
1	A	415	VAL	C-N-CA	5.21	124.66	119.24
1	B	19	PRO	CA-N-CD	-5.18	104.75	112.00
1	A	55	ASN	OD1-CG-ND2	-5.17	117.42	122.60
1	A	234	THR	CB-CA-C	5.16	118.08	110.14
1	A	198	ILE	CA-C-O	5.15	127.22	120.78
1	B	161	ILE	N-CA-C	-5.13	105.71	110.53
1	A	65	HIS	CA-CB-CG	5.12	118.92	113.80
1	A	120	HIS	CB-CG-ND1	5.12	130.37	122.70
1	A	190	VAL	CA-C-O	-5.12	115.82	121.29
1	A	376	ASN	OD1-CG-ND2	-5.09	117.51	122.60
1	A	230	SER	CA-C-N	5.09	125.38	119.47
1	A	230	SER	C-N-CA	5.09	125.38	119.47
1	A	377	GLU	N-CA-C	5.08	121.63	110.80
1	B	120	HIS	CB-CG-ND1	5.07	130.31	122.70
1	A	255	GLU	N-CA-C	-5.07	101.14	109.40
1	B	202	ILE	CA-C-N	5.06	126.17	119.84
1	B	202	ILE	C-N-CA	5.06	126.17	119.84
1	A	376	ASN	CB-CG-ND2	5.04	123.96	116.40
1	A	261	ARG	CB-CG-CD	5.03	122.88	111.30
1	A	214	VAL	O-C-N	-5.03	117.62	123.00
1	A	396	ASN	OD1-CG-ND2	-5.03	117.57	122.60
1	A	23	TYR	N-CA-C	-5.02	101.97	109.95

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	158	TYR	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	A	3110	0	3101	49	0
1	B	2892	0	2879	61	0
All	All	6002	0	5980	107	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 9.

All (107) 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:A:241:LYS:HD2	1:A:245:GLU:HB3	1.66	0.76
1:A:388:VAL:HG22	1:B:317:VAL:HB	1.73	0.70
1:A:281:MET:HE1	1:A:375:VAL:HG21	1.74	0.69
1:A:198:ILE:HG23	1:A:370:LYS:HD3	1.73	0.69
1:B:139:LYS:O	1:B:221:PHE:HA	1.95	0.66
1:A:255:GLU:HG2	1:A:317:VAL:HG22	1.76	0.66
1:A:407:PRO:HB3	1:A:427:ALA:HA	1.78	0.66
1:B:239:PHE:HZ	1:B:406:ARG:HG3	1.63	0.62
1:A:292:LEU:HD11	1:A:409:LEU:HG	1.81	0.62
1:B:415:VAL:HG23	1:B:416:PRO:HD3	1.83	0.61
1:B:406:ARG:HB3	1:B:407:PRO:HD3	1.83	0.61
1:B:208:ASN:ND2	1:B:392:GLY:HA2	2.16	0.61
1:B:239:PHE:CZ	1:B:406:ARG:HG3	2.36	0.60
1:A:139:LYS:O	1:A:221:PHE:HA	2.02	0.60
1:A:230:SER:HB2	1:A:388:VAL:HB	1.84	0.59
1:A:261:ARG:HB3	1:A:311:LEU:HD23	1.86	0.58
1:B:53:LYS:NZ	1:B:57:ARG:HH22	2.01	0.58
1:B:267:THR:HG22	1:B:286:PRO:HA	1.86	0.58
1:B:224:LEU:HD22	1:B:378:GLU:HG2	1.87	0.57
1:B:283:LEU:HD11	1:B:320:MET:HE2	1.87	0.57
1:B:212:VAL:HG21	1:B:362:LEU:HD21	1.87	0.56
1:B:260:TYR:CD1	1:B:316:LEU:HD21	2.39	0.56
1:A:390:ILE:HA	1:B:319:HIS:HB2	1.86	0.56
1:B:241:LYS:HE3	1:B:243:ASP:HB2	1.88	0.56
1:B:150:LYS:HG3	1:B:172:PRO:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:LEU:HB3	1:B:335:LEU:HD22	1.89	0.55
1:B:214:VAL:HG22	1:B:389:VAL:HG22	1.89	0.54
1:B:336:GLN:HA	1:B:340:LEU:O	2.08	0.54
1:B:354:ILE:HD13	1:B:362:LEU:HD13	1.88	0.54
1:A:111:ILE:HG21	1:A:122:PHE:HE2	1.73	0.53
1:A:389:VAL:HG11	1:B:270:LEU:HD22	1.90	0.53
1:A:315:MET:HG2	1:A:395:LEU:HD11	1.90	0.53
1:B:75:ASN:HB3	1:B:427:ALA:H	1.73	0.53
1:B:284:ILE:HB	1:B:409:LEU:HB2	1.90	0.53
1:A:323:PHE:HE1	1:A:373:LEU:HD23	1.74	0.52
1:A:95:CYS:SG	1:A:352:PRO:HG2	2.49	0.52
1:B:65:HIS:CE1	1:B:338:MET:HG2	2.45	0.52
1:A:59:ALA:HB1	1:A:423:MET:HE1	1.90	0.52
1:B:331:LEU:HB2	1:B:367:ALA:HB3	1.92	0.52
1:A:420:ILE:HG21	1:A:423:MET:HE2	1.92	0.51
1:B:147:PHE:HB3	1:B:173:LEU:HD23	1.92	0.51
1:B:292:LEU:HD11	1:B:407:PRO:HD2	1.92	0.50
1:B:192:ASN:HD22	1:B:193:LYS:NZ	2.10	0.50
1:B:96:ASN:HB2	1:B:350:LYS:HG2	1.94	0.50
1:A:57:ARG:HE	1:A:110:THR:HG21	1.77	0.49
1:A:149:ASP:HB3	1:A:173:LEU:O	2.13	0.49
1:B:86:ALA:HA	1:B:89:MET:HE2	1.94	0.49
1:A:143:ALA:HB3	1:A:218:THR:HG22	1.95	0.48
1:B:53:LYS:HZ2	1:B:57:ARG:HH22	1.63	0.47
1:B:208:ASN:HD22	1:B:392:GLY:HA2	1.79	0.47
1:A:252:MET:SD	1:A:377:GLU:N	2.88	0.47
1:A:414:GLU:OE1	1:A:417:LEU:HB2	2.15	0.47
1:B:75:ASN:HB2	1:B:325:ILE:HD11	1.96	0.47
1:B:344:PHE:HA	1:B:364:VAL:O	2.15	0.47
1:A:171:GLN:HA	1:A:172:PRO:HD2	1.82	0.47
1:B:91:LYS:NZ	1:B:120:HIS:NE2	2.63	0.47
1:A:213:LEU:HD11	1:A:354:ILE:HD13	1.97	0.46
1:B:105:VAL:HG21	1:B:340:LEU:HB2	1.96	0.46
1:B:193:LYS:HB3	1:B:218:THR:HG21	1.97	0.46
1:A:121:PHE:CE1	1:A:125:LYS:HE2	2.51	0.46
1:A:145:ARG:HD3	1:A:147:PHE:CE2	2.51	0.46
1:B:331:LEU:HD21	1:B:369:HIS:HB2	1.98	0.46
1:A:190:VAL:HG21	1:A:201:VAL:HG21	1.98	0.45
1:B:72:ASP:HA	1:B:425:ARG:NH1	2.31	0.45
1:B:91:LYS:HE3	1:B:103:MET:SD	2.56	0.45
1:A:129:ARG:HB3	1:A:417:LEU:HD21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:HIS:HB2	1:A:403:LYS:HA	1.99	0.45
1:A:145:ARG:HD3	1:A:147:PHE:CZ	2.51	0.45
1:A:257:LYS:HA	1:A:314:MET:O	2.16	0.45
1:A:96:ASN:HD22	1:A:350:LYS:HE2	1.81	0.45
1:B:345:SER:HA	1:B:346:PRO:HD3	1.74	0.45
1:B:86:ALA:O	1:B:89:MET:HB3	2.17	0.44
1:B:91:LYS:HG3	1:B:102:LEU:HD13	2.00	0.44
1:A:129:ARG:HG2	1:A:417:LEU:HD11	1.99	0.44
1:B:147:PHE:HD2	1:B:173:LEU:HD21	1.82	0.44
1:B:257:LYS:HA	1:B:314:MET:O	2.17	0.44
1:A:207:ILE:HD11	1:A:214:VAL:HG11	2.00	0.44
1:A:7:ILE:HD12	1:A:7:ILE:N	2.33	0.44
1:B:266:GLY:HA3	1:B:287:LYS:HD3	1.99	0.43
1:A:213:LEU:HD11	1:A:354:ILE:CD1	2.49	0.43
1:B:207:ILE:HD11	1:B:214:VAL:HG21	2.00	0.43
1:B:131:TYR:CE1	1:B:142:SER:HB2	2.53	0.43
1:B:241:LYS:HB2	1:B:406:ARG:HH21	1.82	0.43
1:B:328:GLY:HA2	1:B:370:LYS:HA	2.00	0.43
1:A:89:MET:O	1:A:92:LEU:HB2	2.19	0.43
1:A:7:ILE:HG12	1:A:164:LEU:HD23	2.01	0.42
1:B:202:ILE:HA	1:B:203:PRO:HD3	1.76	0.42
1:A:80:PRO:HG2	1:A:423:MET:HE3	2.01	0.42
1:A:96:ASN:ND2	1:A:350:LYS:HE2	2.35	0.42
1:A:77:PHE:CZ	1:A:422:PHE:HB3	2.55	0.42
1:A:194:THR:HG21	1:A:198:ILE:HD12	2.02	0.42
1:A:101:GLN:O	1:A:105:VAL:HG23	2.20	0.41
1:A:259:ARG:HA	1:A:312:GLU:O	2.20	0.41
1:B:95:CYS:HB2	1:B:352:PRO:HD2	2.02	0.41
1:B:280:THR:HG22	1:B:413:ARG:HG2	2.02	0.41
1:A:315:MET:CG	1:A:395:LEU:HD11	2.50	0.41
1:B:325:ILE:HG22	1:B:373:LEU:HB3	2.02	0.41
1:B:338:MET:HE2	1:B:338:MET:HB3	1.94	0.41
1:B:252:MET:O	1:B:319:HIS:HA	2.21	0.41
1:B:94:ALA:HA	1:B:351:LEU:HA	2.02	0.41
1:A:150:LYS:HG3	1:A:176:LYS:HD2	2.03	0.40
1:B:205:GLU:HB3	1:B:395:LEU:HD13	2.03	0.40
1:B:129:ARG:HB3	1:B:417:LEU:HD11	2.04	0.40
1:A:292:LEU:O	1:A:295:VAL:HB	2.21	0.40
1:B:254:GLN:OE1	1:B:258:PHE:HZ	2.04	0.40
1:A:60:THR:HG21	1:A:299:LEU:O	2.22	0.40
1:B:182:SER:O	1:B:186:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

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	A	381/432 (88%)	342 (90%)	34 (9%)	5 (1%)	9	40
1	B	348/432 (81%)	315 (90%)	23 (7%)	10 (3%)	3	24
All	All	729/864 (84%)	657 (90%)	57 (8%)	15 (2%)	5	31

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	204	SER
1	B	204	SER
1	A	377	GLU
1	B	349	SER
1	B	353	GLY
1	B	406	ARG
1	A	273	PRO
1	A	277	ASP
1	B	390	ILE
1	B	96	ASN
1	B	332	LYS
1	B	352	PRO
1	B	429	PRO
1	A	198	ILE
1	B	203	PRO

5.3.2 Protein sidechains [i](#)

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	A	344/383 (90%)	311 (90%)	33 (10%)	8	32
1	B	320/383 (84%)	273 (85%)	47 (15%)	3	16
All	All	664/766 (87%)	584 (88%)	80 (12%)	5	23

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	CYS
1	A	74	ASP
1	A	78	LEU
1	A	81	LEU
1	A	89	MET
1	A	95	CYS
1	A	99	LEU
1	A	132	ARG
1	A	152	LEU
1	A	181	GLN
1	A	193	LYS
1	A	204	SER
1	A	207	ILE
1	A	211	THR
1	A	216	VAL
1	A	234	THR
1	A	238	LEU
1	A	308	LEU
1	A	312	GLU
1	A	322	ARG
1	A	327	ASP
1	A	329	PHE
1	A	331	LEU
1	A	340	LEU
1	A	341	VAL
1	A	360	ASP
1	A	366	ASP
1	A	375	VAL
1	A	377	GLU
1	A	394	SER
1	A	417	LEU
1	A	419	THR
1	A	429	PRO
1	B	19	PRO

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Mol	Chain	Res	Type
1	B	20	MET
1	B	21	CYS
1	B	55	ASN
1	B	66	LEU
1	B	72	ASP
1	B	73	ASN
1	B	75	ASN
1	B	81	LEU
1	B	91	LYS
1	B	97	ASP
1	B	123	PHE
1	B	129	ARG
1	B	132	ARG
1	B	139	LYS
1	B	157	THR
1	B	170	LEU
1	B	180	GLU
1	B	183	ARG
1	B	189	TRP
1	B	193	LYS
1	B	213	LEU
1	B	216	VAL
1	B	218	THR
1	B	227	SER
1	B	246	SER
1	B	257	LYS
1	B	261	ARG
1	B	265	GLU
1	B	277	ASP
1	B	278	ASP
1	B	280	THR
1	B	304	LEU
1	B	308	LEU
1	B	312	GLU
1	B	317	VAL
1	B	325	ILE
1	B	335	LEU
1	B	347	GLU
1	B	350	LYS
1	B	354	ILE
1	B	396	ASN
1	B	407	PRO

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Mol	Chain	Res	Type
1	B	415	VAL
1	B	418	ASN
1	B	419	THR
1	B	428	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	336	GLN
1	A	369	HIS
1	A	396	ASN
1	B	55	ASN
1	B	73	ASN
1	B	118	GLN
1	B	192	ASN
1	B	217	ASN
1	B	268	GLN
1	B	336	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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.