Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 06:27 PM GMT

PDB ID	:	1ATH
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

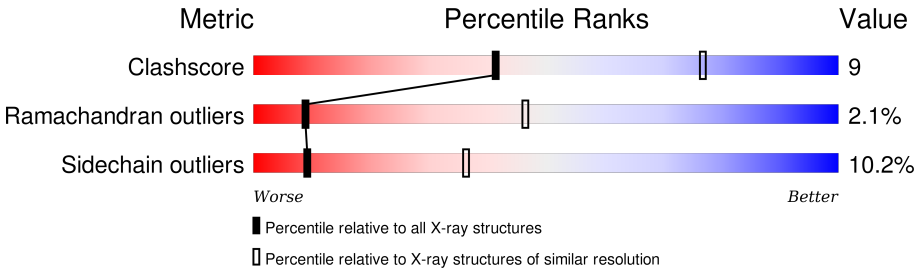
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	432	63% 22% • 10%
1	B	432	54% 25% • 16%

2 Entry composition (i)

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			

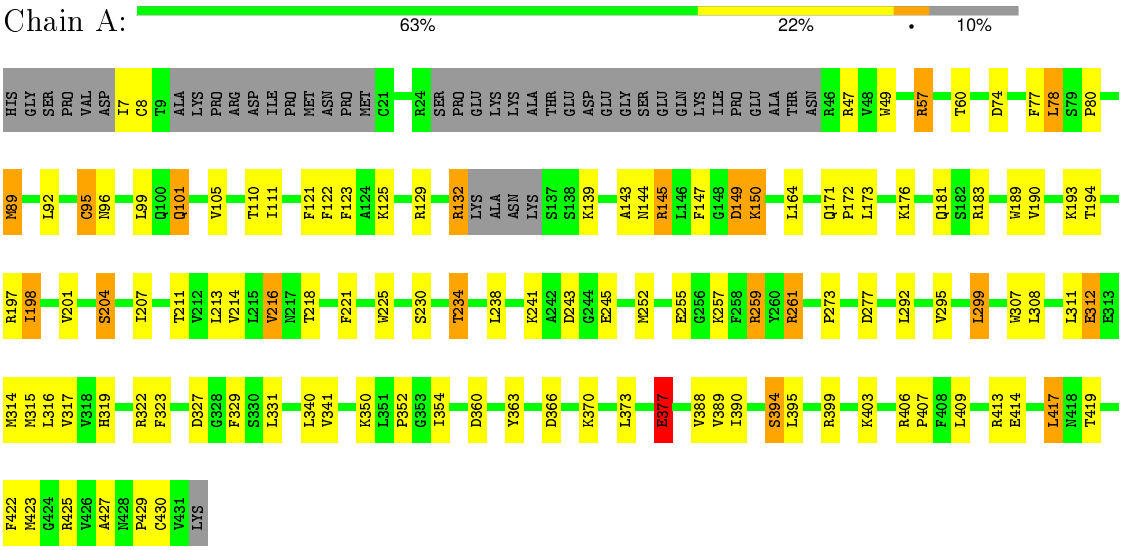
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

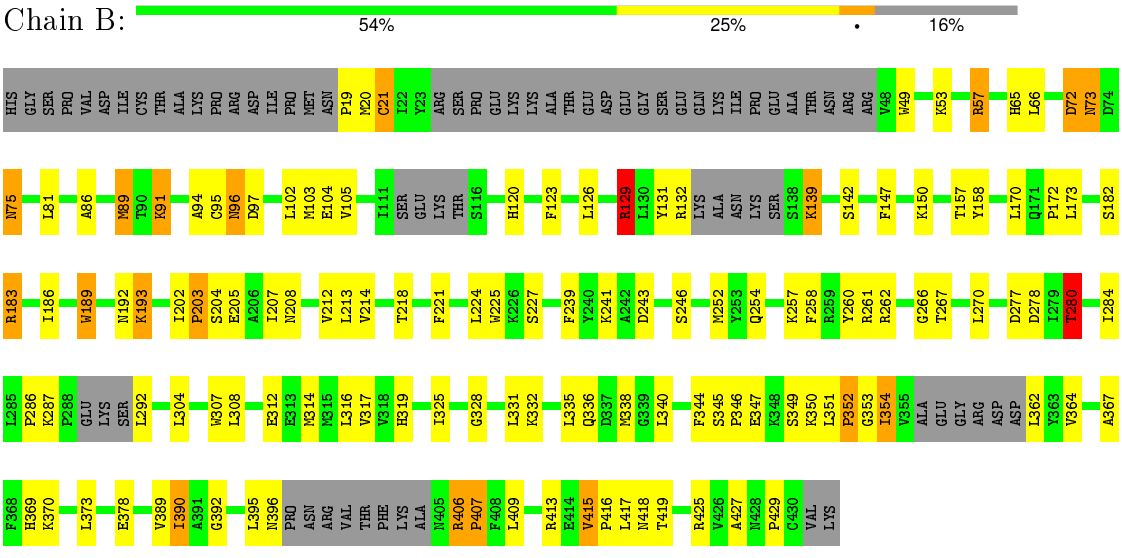
- Molecule 1: ANTITHROMBIN III

Chain A:



- Molecule 1: ANTITHROMBIN III

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.95Å 101.17Å 69.52Å 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	0.70	0/3169	1.42	37/4275 (0.9%)
1	B	0.71	1/2946 (0.0%)	1.37	27/3972 (0.7%)
All	All	0.71	1/6115 (0.0%)	1.40	64/8247 (0.8%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	189	TRP	CG-CD2	-5.14	1.34	1.43

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	189	TRP	CD1-CG-CD2	9.03	113.52	106.30
1	B	49	TRP	CD1-CG-CD2	8.49	113.09	106.30
1	A	49	TRP	CD1-CG-CD2	8.47	113.08	106.30
1	A	259	ARG	NE-CZ-NH1	8.47	124.53	120.30
1	B	225	TRP	CD1-CG-CD2	8.41	113.03	106.30
1	B	307	TRP	CD1-CG-CD2	8.30	112.94	106.30
1	A	225	TRP	CE2-CD2-CG	-8.15	100.78	107.30
1	B	225	TRP	CE2-CD2-CG	-8.12	100.80	107.30
1	A	243	ASP	CA-C-N	-8.10	100.00	116.20
1	A	307	TRP	CD1-CG-CD2	8.00	112.70	106.30
1	A	413	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	A	149	ASP	CA-C-N	-7.71	100.24	117.20
1	A	49	TRP	CE2-CD2-CG	-7.62	101.21	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	49	TRP	CE2-CD2-CG	-7.59	101.23	107.30
1	B	307	TRP	CE2-CD2-CG	-7.52	101.29	107.30
1	A	225	TRP	CD1-CG-CD2	7.50	112.30	106.30
1	A	307	TRP	CE2-CD2-CG	-7.43	101.36	107.30
1	B	390	ILE	CA-C-N	7.25	133.16	117.20
1	A	189	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	B	189	TRP	CE2-CD2-CG	-7.03	101.67	107.30
1	A	225	TRP	CB-CG-CD1	-6.96	117.95	127.00
1	B	189	TRP	CD1-CG-CD2	6.69	111.65	106.30
1	A	430	CYS	CA-CB-SG	-6.64	102.05	114.00
1	A	259	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	B	104	GLU	CA-CB-CG	6.52	127.75	113.40
1	A	225	TRP	CG-CD2-CE3	6.48	139.73	133.90
1	A	47	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	A	399	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	B	225	TRP	CB-CG-CD1	-6.30	118.80	127.00
1	B	57	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	B	225	TRP	CG-CD2-CE3	6.28	139.56	133.90
1	A	78	LEU	CA-CB-CG	6.22	129.60	115.30
1	A	234	THR	N-CA-C	-6.22	94.21	111.00
1	A	150	LYS	N-CA-C	-5.84	95.24	111.00
1	B	21	CYS	N-CA-C	5.79	126.65	111.00
1	A	189	TRP	CG-CD1-NE1	-5.73	104.37	110.10
1	A	261	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	299	LEU	CA-C-N	5.70	129.74	117.20
1	B	129	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B	89	MET	CA-CB-CG	5.64	122.88	113.30
1	A	299	LEU	O-C-N	-5.61	113.73	122.70
1	A	145	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	197	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	B	183	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	A	425	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	132	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	B	126	LEU	CA-CB-CG	5.41	127.73	115.30
1	A	57	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	A	183	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	243	ASP	O-C-N	5.31	132.22	123.20
1	B	280	THR	N-CA-CB	-5.31	100.22	110.30
1	B	49	TRP	CG-CD1-NE1	-5.29	104.81	110.10
1	B	307	TRP	CG-CD2-CE3	5.29	138.66	133.90
1	A	394	SER	N-CA-C	-5.24	96.84	111.00
1	B	73	ASN	CB-CG-ND2	5.15	129.06	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	216	VAL	CA-CB-CG2	-5.14	103.19	110.90
1	B	390	ILE	O-C-N	-5.12	114.50	122.70
1	A	406	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	101	GLN	CA-CB-CG	5.07	124.55	113.40
1	A	363	TYR	CB-CG-CD2	-5.04	117.97	121.00
1	B	49	TRP	CB-CG-CD1	-5.03	120.46	127.00
1	B	262	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	B	49	TRP	CG-CD2-CE3	5.02	138.42	133.90
1	B	307	TRP	CG-CD1-NE1	-5.02	105.08	110.10

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 (i)

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	47	0
1	B	2892	0	2879	58	0
All	All	6002	0	5980	102	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 (102) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:331:LEU:HB3	1:B:335:LEU:HD22	1.89	0.55
1:B:336:GLN:HA	1:B:340:LEU:O	2.08	0.54
1:B:214:VAL:HG22	1:B:389:VAL:HG22	1.89	0.54
1:B:354:ILE:HD13	1:B:362:LEU:HD13	1.88	0.54
1:A:389:VAL:HG11	1:B:270:LEU:HD22	1.90	0.53
1:A:111:ILE:HG21	1:A:122:PHE:HE2	1.73	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:B:331:LEU:HB2	1:B:367:ALA:HB3	1.92	0.52
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:A:143:ALA:HB3	1:A:218:THR:HG22	1.95	0.48
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:B:75:ASN:HB2	1:B:325:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:GLU:OE1	1:A:417:LEU:HB2	2.15	0.47
1:B:344:PHE:HA	1:B:364:VAL:O	2.15	0.47
1:B:91:LYS:NZ	1:B:120:HIS:NE2	2.63	0.47
1:A:171:GLN:HA	1:A:172:PRO:HD2	1.82	0.47
1:B:105:VAL:HG21	1:B:340:LEU:HB2	1.96	0.46
1:A:213:LEU:HD11	1:A:354:ILE:HD13	1.97	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:B:331:LEU:HD21	1:B:369:HIS:HB2	1.98	0.46
1:A:145:ARG:HD3	1:A:147:PHE:CE2	2.51	0.46
1:A:190:VAL:HG21	1:A:201:VAL:HG21	1.98	0.45
1:B:91:LYS:HE3	1:B:103:MET:SD	2.56	0.45
1:B:72:ASP:HA	1:B:425:ARG:NH1	2.31	0.45
1:A:129:ARG:HB3	1:A:417:LEU:HD21	1.97	0.45
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:423:MET:HB2	1:A:423:MET:HE2	1.76	0.44
1:B:147:PHE:HD2	1:B:173:LEU:HD21	1.82	0.44
1:A:129:ARG:HG2	1:A:417:LEU:HD11	1.99	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:N	1:A:7:ILE:HD12	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:241:LYS:HB2	1:B:406:ARG:HH21	1.82	0.43
1:B:131:TYR:CE1	1:B:142:SER:HB2	2.53	0.43
1:B:328:GLY:HA2	1:B:370:LYS:HA	2.00	0.43
1:A:80:PRO:HG2	1:A:423:MET:HE3	1.99	0.43
1:A:89:MET:O	1:A:92:LEU:HB2	2.19	0.43
1:B:53:LYS:HZ2	1:B:57:ARG:HH22	1.67	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:182:SER:O	1:B:186:ILE:HG13	2.21	0.40
1:A:60:THR:HG21	1:A:299:LEU:O	2.22	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%)	15 59
1	B	348/432 (81%)	315 (90%)	23 (7%)	10 (3%)	6 36
All	All	729/864 (84%)	657 (90%)	57 (8%)	15 (2%)	9 46

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	204	SER
1	B	204	SER
1	A	377	GLU

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Mol	Chain	Res	Type
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%)	312 (91%)	32 (9%)	11 41
1	B	320/383 (84%)	284 (89%)	36 (11%)	7 31
All	All	664/766 (87%)	596 (90%)	68 (10%)	9 36

All (68) 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	89	MET
1	A	95	CYS
1	A	99	LEU
1	A	123	PHE
1	A	132	ARG
1	A	144	ASN
1	A	181	GLN
1	A	193	LYS

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Mol	Chain	Res	Type
1	A	204	SER
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	316	LEU
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	377	GLU
1	A	394	SER
1	A	417	LEU
1	A	419	THR
1	A	429	PRO
1	B	19	PRO
1	B	20	MET
1	B	21	CYS
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	183	ARG
1	B	189	TRP
1	B	193	LYS
1	B	213	LEU
1	B	227	SER

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Mol	Chain	Res	Type
1	B	246	SER
1	B	261	ARG
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	347	GLU
1	B	354	ILE
1	B	396	ASN
1	B	407	PRO
1	B	415	VAL
1	B	418	ASN
1	B	419	THR

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

Mol	Chain	Res	Type
1	A	96	ASN
1	A	369	HIS
1	B	55	ASN
1	B	192	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.