



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 05:07 am BST

PDB ID : 1ANT
Title : BIOLOGICAL IMPLICATIONS OF A 3 ANGSTROMS STRUCTURE OF DIMERIC ANTITHROMBIN
Authors : Carrell, R.W.; Stein, P.E.; Fermi, G.; Wardell, M.R.
Deposited on : 1994-02-28
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

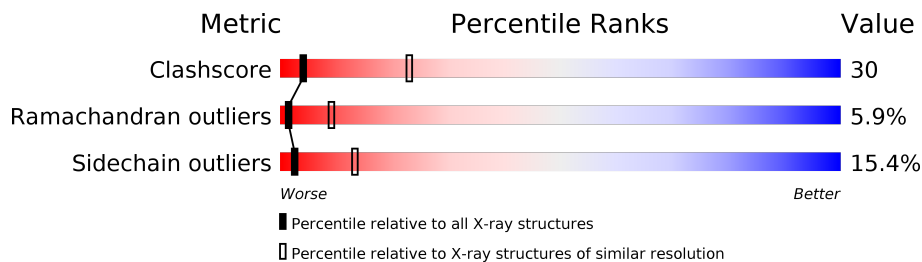
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 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	I	432	
1	L	432	

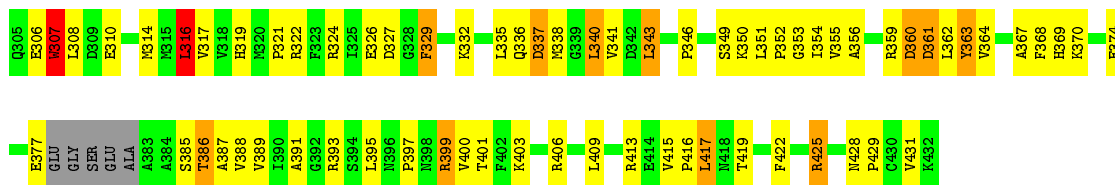
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6371 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	392	Total 3139	C 2003	N 526	O 593	S 17	0	0	0
1	I	402	Total 3232	C 2063	N 548	O 604	S 17	0	0	0



4 Data and refinement statistics

Xtrriage (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	70.06Å 101.52Å 90.45Å 90.00° 105.90° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.214 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6371	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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	I	0.64	0/3295	0.90	4/4441 (0.1%)
1	L	0.62	0/3199	0.91	6/4312 (0.1%)
All	All	0.63	0/6494	0.90	10/8753 (0.1%)

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	I	0	2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	I	283	LEU	CA-CB-CG	8.26	134.30	115.30
1	I	138	SER	N-CA-C	-6.85	92.51	111.00
1	L	210	LEU	CA-CB-CG	6.46	130.15	115.30
1	I	316	LEU	CA-CB-CG	6.04	129.19	115.30
1	L	316	LEU	CA-CB-CG	5.71	128.43	115.30
1	I	307	TRP	CA-CB-CG	5.50	124.15	113.70
1	L	21	CYS	N-CA-C	5.29	125.28	111.00
1	L	111	ILE	N-CA-C	-5.20	96.95	111.00
1	L	407	PRO	N-CA-C	5.18	125.58	112.10
1	L	315	MET	N-CA-C	-5.08	97.27	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	253	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	I	260	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	I	3232	0	3249	175	0
1	L	3139	0	3141	211	0
All	All	6371	0	6390	380	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 30.

All (380) 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:I:198:ILE:HG23	1:I:370:LYS:HD3	1.41	1.00
1:L:190:VAL:HG21	1:L:201:VAL:HG21	1.46	0.96
1:I:108:PHE:HB3	1:I:119:ILE:HD12	1.47	0.94
1:I:132:ARG:HH11	1:I:132:ARG:HB3	1.36	0.90
1:L:406:ARG:CG	1:L:407:PRO:HD2	2.02	0.89
1:I:144:ASN:HD22	1:I:217:ASN:HB2	1.35	0.89
1:L:106:PHE:HE1	1:L:340:LEU:HD11	1.41	0.85
1:I:132:ARG:HB3	1:I:132:ARG:NH1	1.92	0.84
1:L:129:ARG:HD2	1:L:417:LEU:HD21	1.60	0.82
1:L:203:PRO:HG2	1:L:206:ALA:HB2	1.64	0.79
1:L:134:ALA:HB1	1:L:137:SER:OG	1.82	0.78
1:I:81:LEU:O	1:I:81:LEU:HD22	1.83	0.78
1:I:15:ILE:O	1:I:17:MET:SD	2.44	0.76
1:L:215:LEU:H	1:L:215:LEU:HD12	1.50	0.76
1:L:47:ARG:HG2	1:L:48:VAL:H	1.51	0.76
1:L:274:PHE:HB2	1:L:279:ILE:O	1.86	0.75
1:I:316:LEU:HB2	1:I:400:VAL:O	1.85	0.75
1:L:70:LYS:HD2	1:L:76:ILE:HG12	1.69	0.74
1:I:317:VAL:HB	1:I:401:THR:HG22	1.68	0.74
1:L:406:ARG:HD2	1:L:407:PRO:HD2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:351:LEU:HB2	1:L:362:LEU:HB3	1.70	0.73
1:I:143:ALA:O	1:I:217:ASN:HA	1.87	0.73
1:L:270:LEU:HD23	1:L:283:LEU:HD12	1.70	0.73
1:L:106:PHE:CE1	1:L:340:LEU:HD11	2.24	0.73
1:L:92:LEU:HD13	1:L:120:HIS:CE1	2.24	0.72
1:L:145:ARG:HD3	1:L:147:PHE:CZ	2.25	0.72
1:L:140:LEU:HD11	1:L:421:ILE:HD13	1.72	0.72
1:L:269:VAL:HG12	1:L:311:LEU:HD21	1.73	0.71
1:L:406:ARG:CD	1:L:407:PRO:HD2	2.20	0.71
1:I:139:LYS:HB2	1:I:222:LYS:HB2	1.72	0.70
1:L:210:LEU:HD13	1:L:391:ALA:HB1	1.74	0.70
1:L:186:ILE:O	1:L:189:TRP:HB3	1.92	0.70
1:I:141:VAL:CG1	1:I:220:TYR:HB3	2.22	0.70
1:L:331:LEU:HD11	1:L:369:HIS:HB2	1.72	0.70
1:I:146:LEU:HD13	1:I:215:LEU:HB2	1.72	0.69
1:I:130:LEU:HD13	1:I:417:LEU:HD23	1.73	0.69
1:L:316:LEU:HB2	1:I:387:ALA:O	1.92	0.69
1:I:108:PHE:HB3	1:I:119:ILE:CD1	2.23	0.68
1:L:47:ARG:HB3	1:L:47:ARG:NH1	2.08	0.68
1:L:131:TYR:CE2	1:L:142:SER:HB2	2.29	0.68
1:L:266:GLY:HA3	1:L:287:LYS:HB3	1.76	0.68
1:I:15:ILE:H	1:I:16:PRO:HD2	1.58	0.67
1:L:406:ARG:HG2	1:L:407:PRO:HD2	1.74	0.67
1:I:124:ALA:HB2	1:I:165:VAL:HG13	1.77	0.67
1:I:393:ARG:HD3	1:I:395:LEU:HD21	1.77	0.67
1:L:15:ILE:H	1:L:16:PRO:HD2	1.61	0.66
1:L:23:TYR:CE2	1:L:100:GLN:HG3	2.31	0.66
1:L:46:ARG:NH1	1:L:47:ARG:HD3	2.12	0.65
1:L:184:ALA:O	1:L:188:LYS:HD3	1.95	0.65
1:L:46:ARG:HH11	1:L:47:ARG:HD3	1.62	0.65
1:I:24:ARG:H	1:I:24:ARG:HD3	1.61	0.65
1:I:176:LYS:HG3	1:I:209:GLU:O	1.97	0.64
1:L:320:MET:CE	1:L:375:VAL:HG11	2.28	0.64
1:I:287:LYS:HB2	1:I:288:PRO:HD2	1.78	0.64
1:L:269:VAL:HG22	1:L:284:ILE:HG12	1.79	0.64
1:L:293:ALA:HB1	1:L:297:LYS:NZ	2.12	0.64
1:L:263:VAL:CG2	1:L:267:THR:HB	2.28	0.64
1:L:372:PHE:O	1:L:382:ALA:HA	1.97	0.64
1:L:321:PRO:HD3	1:I:391:ALA:O	1.98	0.64
1:I:361:ASP:O	1:I:363:TYR:HD1	1.81	0.64
1:L:260:TYR:CD1	1:L:261:ARG:N	2.66	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:346:PRO:HG3	1:I:363:TYR:CE2	2.33	0.63
1:L:219:ILE:HG22	1:L:220:TYR:N	2.13	0.63
1:L:183:ARG:HB2	1:L:207:ILE:HG13	1.80	0.62
1:L:198:ILE:HG23	1:L:370:LYS:HG2	1.81	0.62
1:L:47:ARG:HG2	1:L:48:VAL:N	2.15	0.62
1:L:431:VAL:O	1:L:432:LYS:HB2	1.99	0.62
1:I:290:LYS:H	1:I:290:LYS:HD2	1.65	0.62
1:L:261:ARG:HH21	1:L:312:GLU:HB2	1.63	0.62
1:L:139:LYS:O	1:L:221:PHE:HA	1.99	0.62
1:I:144:ASN:ND2	1:I:217:ASN:HB2	2.12	0.61
1:L:94:ALA:HA	1:L:351:LEU:HD23	1.83	0.61
1:I:170:LEU:HD23	1:I:170:LEU:H	1.66	0.61
1:L:406:ARG:HG3	1:L:406:ARG:HH11	1.65	0.61
1:I:187:ASN:OD1	1:I:201:VAL:HG12	2.01	0.60
1:L:234:THR:HG23	1:L:251:MET:O	2.01	0.60
1:L:304:LEU:HD22	1:L:304:LEU:O	2.01	0.60
1:L:293:ALA:HB1	1:L:297:LYS:HZ1	1.66	0.60
1:I:140:LEU:HD23	1:I:221:PHE:HB2	1.84	0.59
1:L:183:ARG:HD2	1:L:203:PRO:O	2.02	0.59
1:L:248:SER:O	1:L:430:CYS:HB3	2.02	0.59
1:L:406:ARG:CB	1:L:407:PRO:HD2	2.31	0.59
1:L:102:LEU:HD23	1:L:340:LEU:HD22	1.84	0.59
1:I:261:ARG:HG3	1:I:262:ARG:N	2.15	0.59
1:L:373:LEU:HD12	1:L:374:GLU:H	1.68	0.59
1:I:152:LEU:HD22	1:I:356:ALA:HB2	1.84	0.59
1:L:52:SER:HB2	1:L:419:THR:HG23	1.84	0.59
1:I:340:LEU:CD2	1:I:343:LEU:HB2	2.32	0.58
1:I:91:LYS:HE2	1:I:120:HIS:CE1	2.38	0.58
1:I:152:LEU:HD22	1:I:356:ALA:CB	2.33	0.58
1:L:106:PHE:HB2	1:L:108:PHE:CE2	2.39	0.58
1:L:17:MET:O	1:L:19:PRO:HD3	2.03	0.58
1:L:83:ILE:HG12	1:L:331:LEU:HD21	1.85	0.58
1:L:89:MET:HB3	1:L:166:TYR:CD2	2.39	0.57
1:I:212:VAL:HG13	1:I:213:LEU:H	1.69	0.57
1:I:239:PHE:CE2	1:I:429:PRO:HD3	2.39	0.57
1:I:263:VAL:HG22	1:I:267:THR:O	2.05	0.57
1:L:308:LEU:HD22	1:L:413:ARG:NH1	2.19	0.57
1:L:112:SER:O	1:L:114:LYS:HD2	2.03	0.57
1:L:52:SER:O	1:L:55:ASN:HB2	2.05	0.57
1:I:50:GLU:OE1	1:I:111:ILE:HG23	2.05	0.56
1:L:82:SER:HB2	1:L:217:ASN:ND2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:101:GLN:O	1:I:105:VAL:HG23	2.04	0.56
1:I:126:LEU:HD11	1:I:419:THR:HG21	1.87	0.56
1:L:20:MET:CE	1:L:352:PRO:HB2	2.35	0.56
1:I:263:VAL:HG23	1:I:267:THR:HB	1.87	0.56
1:I:152:LEU:HD13	1:I:354:ILE:HG21	1.87	0.56
1:L:183:ARG:NE	1:L:204:SER:HA	2.20	0.56
1:I:29:LYS:HG3	1:I:110:THR:HG23	1.87	0.56
1:I:184:ALA:O	1:I:188:LYS:HG2	2.06	0.56
1:I:143:ALA:HB3	1:I:218:THR:HG22	1.88	0.56
1:L:314:MET:HG3	1:L:315:MET:N	2.21	0.55
1:I:395:LEU:HD12	1:I:399:ARG:HH12	1.72	0.55
1:L:15:ILE:H	1:L:16:PRO:CD	2.18	0.55
1:I:349:SER:OG	1:I:363:TYR:HB3	2.07	0.55
1:I:350:LYS:C	1:I:352:PRO:HD3	2.27	0.55
1:L:218:THR:HG22	1:L:385:SER:OG	2.06	0.55
1:L:121:PHE:O	1:L:124:ALA:HB3	2.06	0.55
1:L:183:ARG:CZ	1:L:204:SER:HA	2.37	0.55
1:I:304:LEU:O	1:I:307:TRP:HB2	2.07	0.55
1:L:127:ASN:O	1:L:131:TYR:HD1	1.90	0.55
1:I:51:LEU:HD22	1:I:122:PHE:CB	2.37	0.54
1:I:250:SER:HB2	1:I:322:ARG:HD3	1.89	0.54
1:L:163:GLU:O	1:L:163:GLU:HG2	2.08	0.54
1:L:332:LYS:NZ	1:L:344:PHE:HB3	2.23	0.54
1:L:103:MET:SD	1:L:108:PHE:CB	2.96	0.54
1:L:273:PRO:HA	1:L:280:THR:HG22	1.89	0.54
1:L:162:SER:O	1:L:164:LEU:N	2.41	0.53
1:I:149:ASP:HA	1:I:173:LEU:O	2.08	0.53
1:L:215:LEU:N	1:L:215:LEU:HD12	2.23	0.53
1:L:253:TYR:HB2	1:L:319:HIS:CD2	2.43	0.53
1:I:260:TYR:CG	1:I:261:ARG:N	2.77	0.53
1:I:169:LYS:NZ	1:I:171:GLN:HG2	2.24	0.53
1:L:91:LYS:HE2	1:L:120:HIS:CE1	2.43	0.53
1:L:125:LYS:HA	1:L:128:CYS:HB2	1.89	0.53
1:L:351:LEU:N	1:L:352:PRO:HD3	2.23	0.53
1:L:91:LYS:NZ	1:L:120:HIS:NE2	2.55	0.53
1:L:229:PHE:HD2	1:L:252:MET:SD	2.32	0.53
1:L:263:VAL:HG23	1:L:267:THR:HB	1.89	0.53
1:L:248:SER:C	1:L:430:CYS:HB3	2.29	0.53
1:L:415:VAL:HB	1:L:416:PRO:HD3	1.90	0.52
1:I:250:SER:HB3	1:I:322:ARG:HD2	1.92	0.52
1:I:102:LEU:HD21	1:I:343:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:17:MET:SD	1:I:17:MET:N	2.82	0.52
1:I:51:LEU:HD22	1:I:122:PHE:HB3	1.92	0.52
1:L:91:LYS:CE	1:L:120:HIS:CE1	2.92	0.52
1:L:63:TYR:HB2	1:L:423:MET:CE	2.40	0.52
1:L:355:VAL:HG22	1:L:355:VAL:O	2.10	0.51
1:L:406:ARG:HD2	1:L:407:PRO:CD	2.38	0.51
1:L:427:ALA:O	1:L:428:ASN:HB2	2.11	0.51
1:I:169:LYS:HG2	1:I:170:LEU:N	2.26	0.51
1:I:24:ARG:NE	1:I:24:ARG:O	2.43	0.51
1:L:317:VAL:HB	1:I:388:VAL:HG22	1.92	0.51
1:L:410:VAL:CG2	1:L:426:VAL:HG23	2.39	0.51
1:I:361:ASP:O	1:I:363:TYR:CD1	2.63	0.51
1:L:190:VAL:HG12	1:L:198:ILE:O	2.09	0.51
1:I:91:LYS:HB2	1:I:102:LEU:HD13	1.93	0.51
1:L:278:ASP:O	1:L:415:VAL:HG23	2.11	0.51
1:I:172:PRO:O	1:I:173:LEU:HD23	2.11	0.50
1:I:169:LYS:HG2	1:I:171:GLN:H	1.76	0.50
1:L:253:TYR:HA	1:L:318:VAL:O	2.11	0.50
1:I:329:PHE:HE1	1:I:369:HIS:CD2	2.29	0.50
1:I:308:LEU:HD13	1:I:413:ARG:CZ	2.41	0.50
1:L:188:LYS:CD	1:L:188:LYS:N	2.74	0.50
1:L:333:GLU:CD	1:L:333:GLU:H	2.13	0.50
1:L:314:MET:HG3	1:L:315:MET:H	1.75	0.50
1:L:65:HIS:HB3	1:L:334:GLN:HG3	1.93	0.50
1:L:140:LEU:HD23	1:L:220:TYR:O	2.12	0.50
1:I:346:PRO:HG3	1:I:363:TYR:CD2	2.47	0.50
1:L:103:MET:SD	1:L:108:PHE:HB3	2.52	0.50
1:L:162:SER:C	1:L:164:LEU:H	2.15	0.50
1:L:20:MET:HG2	1:L:21:CYS:SG	2.51	0.50
1:L:225:TRP:CD1	1:L:379:GLY:HA2	2.47	0.50
1:I:340:LEU:HD21	1:I:343:LEU:HD12	1.94	0.50
1:L:17:MET:N	1:L:17:MET:SD	2.83	0.50
1:L:276:GLY:O	1:L:278:ASP:N	2.45	0.50
1:L:81:LEU:O	1:L:81:LEU:HD22	2.12	0.50
1:I:359:ARG:O	1:I:361:ASP:N	2.45	0.49
1:L:47:ARG:HH11	1:L:47:ARG:HB3	1.75	0.49
1:I:212:VAL:HG21	1:I:362:LEU:HD23	1.94	0.49
1:I:319:HIS:HB2	1:I:403:LYS:HA	1.93	0.49
1:I:395:LEU:HD12	1:I:399:ARG:NH1	2.27	0.49
1:I:163:GLU:O	1:I:167:GLY:HA2	2.12	0.49
1:L:287:LYS:HE2	1:L:290:LYS:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:351:LEU:N	1:I:352:PRO:HD3	2.27	0.49
1:L:155:ASN:ND2	1:L:356:ALA:HA	2.28	0.49
1:I:329:PHE:CE1	1:I:369:HIS:HD2	2.31	0.49
1:I:122:PHE:N	1:I:122:PHE:CD1	2.78	0.48
1:I:209:GLU:CD	1:I:209:GLU:H	2.15	0.48
1:L:20:MET:HE1	1:L:352:PRO:HB2	1.95	0.48
1:I:152:LEU:HA	1:I:356:ALA:CB	2.43	0.48
1:L:332:LYS:O	1:L:336:GLN:HG3	2.11	0.48
1:I:215:LEU:O	1:I:367:ALA:HA	2.14	0.48
1:I:62:PHE:HD2	1:I:338:MET:HE1	1.77	0.48
1:L:292:LEU:HD11	1:L:409:LEU:HD13	1.95	0.48
1:I:261:ARG:CG	1:I:262:ARG:N	2.77	0.48
1:L:239:PHE:HB2	1:L:249:ALA:HB2	1.94	0.48
1:I:233:ASN:O	1:I:235:ARG:HG2	2.14	0.48
1:L:120:HIS:HB3	1:L:165:VAL:HG11	1.95	0.48
1:I:103:MET:HE1	1:I:116:SER:HB3	1.96	0.48
1:L:134:ALA:HB1	1:L:137:SER:HG	1.79	0.47
1:L:342:ASP:HB2	1:L:348:LYS:NZ	2.29	0.47
1:I:198:ILE:HG23	1:I:370:LYS:CD	2.28	0.47
1:I:354:ILE:O	1:I:362:LEU:HD13	2.14	0.47
1:L:91:LYS:CE	1:L:120:HIS:NE2	2.77	0.47
1:L:229:PHE:CD1	1:L:254:GLN:OE1	2.67	0.47
1:I:22:ILE:HA	1:I:116:SER:OG	2.13	0.47
1:I:48:VAL:HG13	1:I:126:LEU:HB2	1.97	0.47
1:L:138:SER:OG	1:L:276:GLY:HA3	2.14	0.47
1:L:254:GLN:NE2	1:L:258:PHE:HZ	2.12	0.47
1:L:269:VAL:O	1:L:269:VAL:HG12	2.15	0.47
1:L:284:ILE:C	1:L:285:LEU:HD23	2.35	0.47
1:I:47:ARG:HD3	1:I:122:PHE:CE1	2.49	0.47
1:I:187:ASN:HB2	1:I:188:LYS:NZ	2.30	0.47
1:I:186:ILE:HG21	1:I:202:ILE:HD11	1.96	0.47
1:L:94:ALA:CA	1:L:351:LEU:HD23	2.45	0.47
1:I:235:ARG:HG3	1:I:253:TYR:HE2	1.80	0.47
1:I:267:THR:CG2	1:I:284:ILE:HG23	2.45	0.47
1:L:211:THR:HA	1:L:391:ALA:O	2.15	0.47
1:L:315:MET:O	1:I:386:THR:HA	2.14	0.47
1:I:213:LEU:O	1:I:213:LEU:HD12	2.15	0.47
1:I:250:SER:CB	1:I:322:ARG:HD3	2.45	0.47
1:I:363:TYR:N	1:I:363:TYR:CD1	2.83	0.47
1:L:103:MET:HA	1:L:108:PHE:HD2	1.80	0.47
1:L:207:ILE:HG22	1:L:208:ASN:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:141:VAL:HG13	1:I:220:TYR:HB3	1.95	0.46
1:I:216:VAL:HG12	1:I:368:PHE:HB2	1.95	0.46
1:I:186:ILE:HG21	1:I:202:ILE:CD1	2.45	0.46
1:I:212:VAL:HG21	1:I:362:LEU:CD2	2.45	0.46
1:I:178:ASN:HB3	1:I:181:GLN:HB3	1.97	0.46
1:I:24:ARG:H	1:I:24:ARG:CD	2.24	0.46
1:L:91:LYS:HG2	1:L:99:LEU:HD12	1.98	0.46
1:I:212:VAL:HG13	1:I:213:LEU:N	2.30	0.46
1:L:118:GLN:O	1:L:119:ILE:C	2.54	0.46
1:I:141:VAL:HG12	1:I:220:TYR:HB3	1.97	0.46
1:I:239:PHE:HB3	1:I:247:CYS:HB3	1.97	0.46
1:I:329:PHE:HE1	1:I:369:HIS:HD2	1.64	0.46
1:L:103:MET:SD	1:L:108:PHE:HB2	2.56	0.46
1:L:269:VAL:CG1	1:L:311:LEU:HD21	2.43	0.46
1:I:340:LEU:HD21	1:I:343:LEU:HB2	1.98	0.46
1:L:263:VAL:HG22	1:L:267:THR:O	2.16	0.46
1:I:155:ASN:HB2	1:I:353:GLY:O	2.16	0.46
1:L:183:ARG:NH1	1:L:187:ASN:HD21	2.13	0.46
1:L:279:ILE:HD13	1:L:414:GLU:HG2	1.99	0.45
1:L:71:ASN:O	1:L:425:ARG:NH1	2.50	0.45
1:I:20:MET:O	1:I:20:MET:HG2	2.17	0.45
1:I:165:VAL:HG12	1:I:165:VAL:O	2.16	0.45
1:I:263:VAL:CG2	1:I:267:THR:HB	2.47	0.45
1:L:239:PHE:O	1:L:247:CYS:HB3	2.16	0.45
1:I:251:MET:SD	1:I:321:PRO:HG3	2.56	0.45
1:L:47:ARG:HB2	1:L:122:PHE:CE2	2.52	0.45
1:I:151:SER:O	1:I:356:ALA:HB1	2.16	0.45
1:I:175:PHE:HE1	1:I:207:ILE:HD13	1.82	0.45
1:I:292:LEU:HD21	1:I:425:ARG:HG2	1.99	0.45
1:L:152:LEU:HD22	1:L:355:VAL:HG21	1.98	0.45
1:L:92:LEU:HD12	1:L:92:LEU:HA	1.77	0.45
1:I:241:LYS:HZ1	1:I:428:ASN:HB2	1.82	0.44
1:L:145:ARG:HH11	1:L:145:ARG:HB2	1.83	0.44
1:I:201:VAL:HA	1:I:370:LYS:HD2	1.98	0.44
1:L:331:LEU:HD12	1:L:331:LEU:N	2.32	0.44
1:I:306:GLU:O	1:I:310:GLU:HG3	2.17	0.44
1:I:53:LYS:HA	1:I:53:LYS:HD2	1.80	0.44
1:L:189:TRP:O	1:L:193:LYS:HG2	2.17	0.44
1:L:92:LEU:HD13	1:L:120:HIS:ND1	2.31	0.44
1:I:111:ILE:HG22	1:I:114:LYS:HG2	1.98	0.44
1:L:55:ASN:O	1:L:58:PHE:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:47:ARG:HB2	1:L:122:PHE:CZ	2.53	0.44
1:L:129:ARG:HG3	1:L:132:ARG:HH21	1.83	0.44
1:I:299:LEU:O	1:I:300:THR:HG23	2.18	0.44
1:I:77:PHE:CZ	1:I:422:PHE:HB3	2.53	0.44
1:L:235:ARG:NH1	1:L:235:ARG:HB3	2.33	0.44
1:L:285:LEU:HA	1:L:286:PRO:HD3	1.77	0.44
1:L:332:LYS:HZ1	1:L:344:PHE:HB3	1.81	0.44
1:I:292:LEU:O	1:I:296:GLU:N	2.51	0.43
1:L:194:THR:O	1:L:196:GLY:N	2.51	0.43
1:L:331:LEU:HD11	1:L:369:HIS:CB	2.46	0.43
1:I:324:ARG:HA	1:I:374:GLU:HA	2.00	0.43
1:L:187:ASN:O	1:L:190:VAL:HB	2.18	0.43
1:L:324:ARG:HG3	1:L:324:ARG:O	2.15	0.43
1:L:428:ASN:O	1:L:431:VAL:HG23	2.18	0.43
1:I:57:ARG:HG3	1:I:301:PRO:HG2	2.00	0.43
1:L:131:TYR:N	1:L:131:TYR:CD1	2.86	0.43
1:L:303:VAL:O	1:L:306:GLU:N	2.52	0.43
1:L:217:ASN:CG	1:L:218:THR:N	2.71	0.43
1:L:74:ASP:O	1:L:425:ARG:HD2	2.17	0.43
1:I:386:THR:O	1:I:386:THR:HG22	2.18	0.43
1:I:190:VAL:HG11	1:I:198:ILE:HG22	2.00	0.43
1:I:288:PRO:O	1:I:290:LYS:HD2	2.19	0.43
1:I:288:PRO:O	1:I:290:LYS:CD	2.66	0.43
1:L:261:ARG:HB3	1:L:311:LEU:HD23	2.01	0.43
1:I:289:GLU:O	1:I:291:SER:N	2.52	0.43
1:L:145:ARG:HH11	1:L:145:ARG:CG	2.32	0.43
1:I:399:ARG:HD2	1:I:399:ARG:H	1.84	0.43
1:I:190:VAL:HG12	1:I:198:ILE:O	2.18	0.43
1:L:197:ARG:HG2	1:L:372:PHE:CD1	2.54	0.43
1:L:254:GLN:NE2	1:L:258:PHE:CZ	2.87	0.43
1:L:342:ASP:HB2	1:L:348:LYS:HD3	2.00	0.43
1:L:89:MET:HB3	1:L:166:TYR:CE2	2.54	0.42
1:L:229:PHE:HB2	1:L:377:GLU:HA	2.00	0.42
1:L:188:LYS:HD3	1:L:188:LYS:H	1.84	0.42
1:L:193:LYS:HZ2	1:L:193:LYS:HB3	1.84	0.42
1:L:264:ALA:O	1:L:265:GLU:HB2	2.19	0.42
1:I:182:SER:O	1:I:183:ARG:C	2.58	0.42
1:I:250:SER:CB	1:I:322:ARG:CD	2.98	0.42
1:L:171:GLN:HA	1:L:172:PRO:HD2	1.91	0.42
1:L:336:GLN:O	1:L:339:GLY:N	2.52	0.42
1:I:90:THR:HA	1:I:158:TYR:OH	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:408:PHE:CD1	1:L:408:PHE:N	2.87	0.42
1:I:140:LEU:HA	1:I:140:LEU:HD23	1.87	0.42
1:I:145:ARG:NH1	1:I:171:GLN:HG3	2.35	0.42
1:I:230:SER:HA	1:I:231:PRO:HD3	1.91	0.42
1:L:230:SER:HA	1:L:231:PRO:HD3	1.81	0.42
1:L:158:TYR:CE2	1:L:354:ILE:HG23	2.54	0.42
1:I:136:LYS:O	1:I:138:SER:N	2.53	0.42
1:I:87:PHE:CZ	1:I:335:LEU:CD1	3.03	0.42
1:L:260:TYR:CG	1:L:261:ARG:N	2.88	0.42
1:L:287:LYS:O	1:L:288:PRO:C	2.58	0.42
1:I:122:PHE:N	1:I:122:PHE:HD1	2.16	0.41
1:I:138:SER:OG	1:I:276:GLY:HA3	2.20	0.41
1:I:199:THR:HG23	1:I:200:ASP:H	1.85	0.41
1:I:343:LEU:HD22	1:I:364:VAL:CG2	2.50	0.41
1:L:345:SER:HA	1:L:346:PRO:HD3	1.81	0.41
1:I:343:LEU:HD23	1:I:351:LEU:HD11	2.02	0.41
1:I:354:ILE:HG22	1:I:354:ILE:O	2.19	0.41
1:L:106:PHE:CB	1:L:108:PHE:CE2	3.03	0.41
1:L:47:ARG:HG2	1:L:48:VAL:HG23	2.02	0.41
1:I:131:TYR:CE1	1:I:142:SER:HB3	2.54	0.41
1:I:152:LEU:HD13	1:I:354:ILE:CG2	2.49	0.41
1:I:54:ALA:O	1:I:57:ARG:N	2.53	0.41
1:L:91:LYS:HG3	1:L:102:LEU:HD12	2.02	0.41
1:L:111:ILE:HG21	1:L:122:PHE:CE2	2.55	0.41
1:L:162:SER:C	1:L:164:LEU:N	2.73	0.41
1:L:193:LYS:HA	1:L:193:LYS:HZ3	1.84	0.41
1:L:320:MET:HE1	1:L:375:VAL:HG11	2.02	0.41
1:I:170:LEU:HG	1:I:171:GLN:N	2.35	0.41
1:I:287:LYS:O	1:I:288:PRO:C	2.58	0.41
1:I:92:LEU:HB3	1:I:158:TYR:HE1	1.86	0.41
1:I:92:LEU:HD13	1:I:120:HIS:CE1	2.55	0.41
1:L:341:VAL:HG23	1:L:342:ASP:H	1.84	0.41
1:I:47:ARG:HB3	1:I:122:PHE:CG	2.55	0.41
1:L:103:MET:O	1:L:108:PHE:N	2.47	0.41
1:L:228:LYS:HD2	1:L:228:LYS:N	2.34	0.41
1:I:131:TYR:O	1:I:132:ARG:HB3	2.20	0.41
1:L:229:PHE:HD1	1:L:254:GLN:OE1	2.02	0.41
1:L:45:ASN:ND2	1:L:45:ASN:O	2.53	0.41
1:I:15:ILE:N	1:I:16:PRO:HD2	2.29	0.41
1:I:238:LEU:HA	1:I:247:CYS:O	2.21	0.41
1:I:51:LEU:HD22	1:I:122:PHE:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:20:MET:HE2	1:L:352:PRO:HB2	2.01	0.41
1:L:79:SER:C	1:L:81:LEU:H	2.24	0.41
1:I:159:GLN:HB3	1:I:159:GLN:HE21	1.60	0.41
1:I:183:ARG:O	1:I:186:ILE:HB	2.21	0.41
1:I:198:ILE:CG2	1:I:370:LYS:HD3	2.29	0.41
1:I:415:VAL:HB	1:I:416:PRO:CD	2.50	0.41
1:I:58:PHE:CE1	1:I:62:PHE:HB2	2.56	0.41
1:L:46:ARG:O	1:L:48:VAL:N	2.54	0.41
1:L:237:GLU:HG2	1:I:393:ARG:NH1	2.35	0.41
1:I:147:PHE:CE2	1:I:186:ILE:HG23	2.56	0.41
1:I:329:PHE:CD1	1:I:329:PHE:N	2.87	0.41
1:L:240:TYR:CE2	1:I:397:PRO:HD3	2.55	0.41
1:L:57:ARG:NH1	1:L:57:ARG:HG3	2.36	0.41
1:I:92:LEU:HD21	1:I:161:ILE:HB	2.03	0.41
1:L:275:LYS:O	1:L:277:ASP:N	2.54	0.41
1:L:63:TYR:HB2	1:L:423:MET:HE1	2.01	0.41
1:I:184:ALA:C	1:I:188:LYS:HG2	2.42	0.40
1:L:82:SER:CB	1:L:217:ASN:ND2	2.84	0.40
1:L:331:LEU:N	1:L:331:LEU:CD1	2.84	0.40
1:I:336:GLN:O	1:I:337:ASP:C	2.60	0.40
1:L:272:LEU:HA	1:L:273:PRO:HD2	1.97	0.40
1:L:46:ARG:O	1:L:46:ARG:CG	2.68	0.40
1:L:66:LEU:HD12	1:L:66:LEU:HA	1.86	0.40
1:I:319:HIS:ND1	1:I:403:LYS:HG2	2.36	0.40
1:L:18:ASN:HB2	1:L:117:ASP:HB2	2.04	0.40
1:L:254:GLN:HE22	1:L:258:PHE:HZ	1.68	0.40
1:L:75:ASN:O	1:L:76:ILE:HG13	2.21	0.40
1:I:239:PHE:CE1	1:I:406:ARG:N	2.89	0.40
1:I:209:GLU:CD	1:I:209:GLU:N	2.74	0.40
1:L:152:LEU:HD22	1:L:355:VAL:CG2	2.51	0.40
1:L:188:LYS:HD3	1:L:188:LYS:N	2.36	0.40
1:L:63:TYR:HB2	1:L:423:MET:HE3	2.02	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	I	396/432 (92%)	313 (79%)	59 (15%)	24 (6%)	1	8
1	L	386/432 (89%)	305 (79%)	59 (15%)	22 (6%)	1	10
All	All	782/864 (90%)	618 (79%)	118 (15%)	46 (6%)	1	9

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	21	CYS
1	L	47	ARG
1	L	132	ARG
1	L	195	GLU
1	L	277	ASP
1	L	288	PRO
1	L	356	ALA
1	L	407	PRO
1	I	22	ILE
1	I	107	LYS
1	I	137	SER
1	I	204	SER
1	I	288	PRO
1	I	290	LYS
1	I	291	SER
1	I	360	ASP
1	I	386	THR
1	L	15	ILE
1	L	134	ALA
1	L	289	GLU
1	L	291	SER
1	I	14	ASP
1	I	19	PRO
1	I	28	LYS
1	I	245	GLU
1	I	277	ASP
1	I	385	SER
1	I	431	VAL
1	L	19	PRO
1	L	22	ILE
1	L	163	GLU

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Mol	Chain	Res	Type
1	L	263	VAL
1	L	391	ALA
1	I	332	LYS
1	I	361	ASP
1	I	96	ASN
1	I	254	GLN
1	L	76	ILE
1	L	96	ASN
1	I	15	ILE
1	I	16	PRO
1	I	171	GLN
1	L	214	VAL
1	L	355	VAL
1	L	428	ASN
1	I	355	VAL

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	I	359/383 (94%)	306 (85%)	53 (15%)	3 14
1	L	348/383 (91%)	292 (84%)	56 (16%)	2 12
All	All	707/766 (92%)	598 (85%)	109 (15%)	2 13

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	16	PRO
1	L	19	PRO
1	L	23	TYR
1	L	44	THR
1	L	45	ASN
1	L	47	ARG
1	L	81	LEU
1	L	82	SER

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Mol	Chain	Res	Type
1	L	96	ASN
1	L	113	GLU
1	L	123	PHE
1	L	126	LEU
1	L	128	CYS
1	L	130	LEU
1	L	131	TYR
1	L	140	LEU
1	L	145	ARG
1	L	152	LEU
1	L	157	THR
1	L	170	LEU
1	L	200	ASP
1	L	201	VAL
1	L	209	GLU
1	L	213	LEU
1	L	227	SER
1	L	228	LYS
1	L	235	ARG
1	L	237	GLU
1	L	248	SER
1	L	251	MET
1	L	253	TYR
1	L	270	LEU
1	L	275	LYS
1	L	278	ASP
1	L	285	LEU
1	L	288	PRO
1	L	299	LEU
1	L	304	LEU
1	L	307	TRP
1	L	315	MET
1	L	316	LEU
1	L	320	MET
1	L	322	ARG
1	L	324	ARG
1	L	333	GLU
1	L	341	VAL
1	L	342	ASP
1	L	343	LEU
1	L	347	GLU
1	L	348	LYS

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Mol	Chain	Res	Type
1	L	359	ARG
1	L	360	ASP
1	L	361	ASP
1	L	362	LEU
1	L	419	THR
1	L	430	CYS
1	I	14	ASP
1	I	18	ASN
1	I	24	ARG
1	I	44	THR
1	I	47	ARG
1	I	53	LYS
1	I	57	ARG
1	I	60	THR
1	I	69	SER
1	I	74	ASP
1	I	78	LEU
1	I	81	LEU
1	I	84	SER
1	I	97	ASP
1	I	103	MET
1	I	123	PHE
1	I	126	LEU
1	I	132	ARG
1	I	137	SER
1	I	171	GLN
1	I	188	LYS
1	I	189	TRP
1	I	192	ASN
1	I	213	LEU
1	I	221	PHE
1	I	238	LEU
1	I	275	LYS
1	I	278	ASP
1	I	281	MET
1	I	283	LEU
1	I	288	PRO
1	I	290	LYS
1	I	291	SER
1	I	300	THR
1	I	304	LEU
1	I	307	TRP

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Mol	Chain	Res	Type
1	I	314	MET
1	I	316	LEU
1	I	326	GLU
1	I	327	ASP
1	I	329	PHE
1	I	337	ASP
1	I	340	LEU
1	I	341	VAL
1	I	343	LEU
1	I	360	ASP
1	I	363	TYR
1	I	377	GLU
1	I	389	VAL
1	I	399	ARG
1	I	409	LEU
1	I	417	LEU
1	I	425	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	45	ASN
1	L	73	ASN
1	L	127	ASN
1	L	155	ASN
1	L	159	GLN
1	L	217	ASN
1	L	254	GLN
1	L	268	GLN
1	L	319	HIS
1	I	64	GLN
1	I	96	ASN
1	I	144	ASN
1	I	268	GLN

5.3.3 RNA

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 [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.