Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 06:24 PM GMT

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
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:

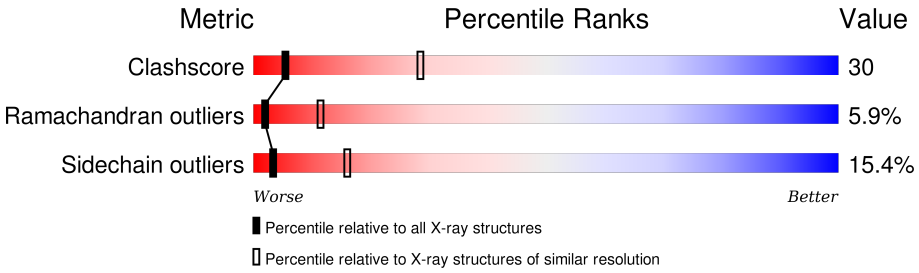
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance

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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (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. 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	I	432	44% 40% 8% • 7%
1	L	432	37% 42% 10% • 9%

2 Entry composition (i)

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
1	L	392	Total	C	N	O	S	0	0	0
			3139	2003	526	593	17			
1	I	402	Total	C	N	O	S	0	0	0
			3232	2063	548	604	17			

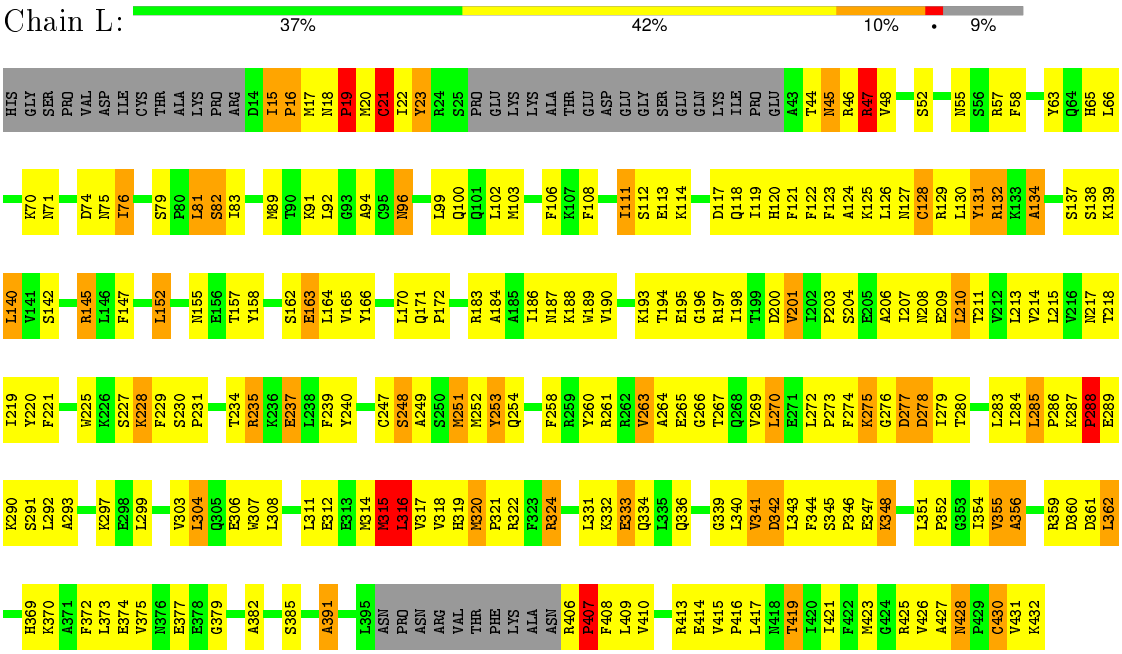
3 Residue-property plots (i)

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.

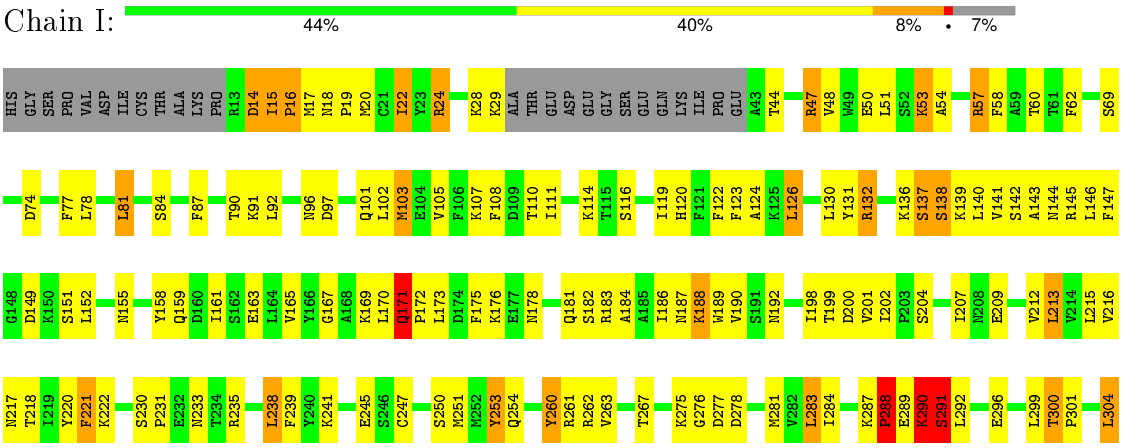
- Molecule 1: ANTITHROMBIN

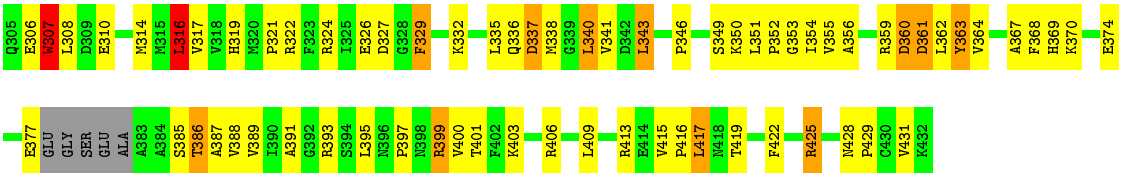
Chain L:



- Molecule 1: ANTITHROMBIN

Chain I:




Q305
E306
M307
L308
D309
E310
M314
M315
L316
V317
Y318
H319
M320
P321
R322
F323
R324
I325
E326
D327
G328
F329
K332
L335
Q336
D337
M338
G339
L340
V341
D342
L343
P346
S349
K350
L351
P352
G353
I354
V355
A356
R359
D360
D361
L362
Y363
V364
A367
F368
H369
K370
E374
E377
GLU
GLY
SER
GLU
ALA
A383
A384
S385
T386
A387
V388
V389
I390
A391
G392
R393
S394
L395
N396
P397
N398
R399
V400
T401
F402
K403
R406
L409
R413
E414
V415
P416
L417
N418
T419
F422
R425
N428
P429
C430
V431
K432

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	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.	Xtriage
Total number of atoms	6371	wwPDB-VP
Average B, all atoms (Å^2)	56.0	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	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(^{o})	Ideal(^{o})
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:106:PHE:CE1	1:L:340:LEU:HD11	2.24	0.73
1:L:270:LEU:HD23	1:L:283:LEU:HD12	1.70	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:L:331:LEU:HD11	1:L:369:HIS:HB2	1.72	0.70
1:I:141:VAL:CG1	1:I:220:TYR:HB3	2.22	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:L:406:ARG:HG2	1:L:407:PRO:HD2	1.74	0.67
1:I:15:ILE:H	1:I:16:PRO:HD2	1.58	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:46:ARG:HH11	1:L:47:ARG:HD3	1.62	0.65
1:L:184:ALA:O	1:L:188:LYS:HD3	1.95	0.65
1:I:24:ARG:HD3	1:I:24:ARG:H	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:L:269:VAL:HG22	1:L:284:ILE:HG12	1.79	0.64
1:I:287:LYS:HB2	1:I:288:PRO:HD2	1.78	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:L:261:ARG:HH21	1:L:312:GLU:HB2	1.63	0.62
1:I:290:LYS:H	1:I:290:LYS:HD2	1.65	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:304:LEU:HD22	1:L:304:LEU:O	2.01	0.60
1:L:234:THR:HG23	1:L:251:MET:O	2.01	0.60
1:L:293:ALA:HB1	1:L:297:LYS:HZ1	1.66	0.60
1:L:183:ARG:HD2	1:L:203:PRO:O	2.02	0.59
1:I:140:LEU:HD23	1:I:221:PHE:HB2	1.84	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:152:LEU:HD22	1:I:356:ALA:CB	2.33	0.58
1:I:91:LYS:HE2	1:I:120:HIS:CE1	2.38	0.58
1:L:106:PHE:HB2	1:L:108:PHE:CE2	2.39	0.58
1:L:83:ILE:HG12	1:L:331:LEU:HD21	1.85	0.58
1:L:17:MET:O	1:L:19:PRO:HD3	2.03	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:L:308:LEU:HD22	1:L:413:ARG:NH1	2.19	0.57
1:I:263:VAL:HG22	1:I:267:THR:O	2.05	0.57
1:I:239:PHE:CE2	1:I:429:PRO:HD3	2.39	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:L:20:MET:CE	1:L:352:PRO:HB2	2.35	0.56
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:183:ARG:NE	1:L:204:SER:HA	2.20	0.56
1:I:152:LEU:HD13	1:I:354:ILE:HG21	1.87	0.56
1:I:263:VAL:HG23	1:I:267:THR:HB	1.87	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:HG2	1:L:163:GLU:O	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:L:215:LEU:N	1:L:215:LEU:HD12	2.23	0.53
1:I:149:ASP:HA	1:I:173:LEU:O	2.08	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:351:LEU:N	1:L:352:PRO:HD3	2.23	0.53
1:L:125:LYS:HA	1:L:128:CYS:HB2	1.89	0.53
1:L:91:LYS:NZ	1:L:120:HIS:NE2	2.55	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:229:PHE:HD2	1:L:252:MET:SD	2.32	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:L:91:LYS:CE	1:L:120:HIS:CE1	2.92	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:102:LEU:HD21	1:I:343:LEU:HD12	1.92	0.52
1:I:51:LEU:HD22	1:I:122:PHE:HB3	1.92	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:L:190:VAL:HG12	1:L:198:ILE:O	2.09	0.51
1:I:361:ASP:O	1:I:363:TYR:CD1	2.63	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: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:I:308:LEU:HD13	1:I:413:ARG:CZ	2.41	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:L:103:MET:SD	1:L:108:PHE:HB3	2.52	0.50
1:L:20:MET:HG2	1:L:21:CYS:SG	2.51	0.50
1:I:346:PRO:HG3	1:I:363:TYR:CD2	2.47	0.50
1:L:162:SER:C	1:L:164:LEU:H	2.15	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:L:47:ARG:HH11	1:L:47:ARG:HB3	1.75	0.49
1:I:359:ARG:O	1:I:361:ASP:N	2.45	0.49
1:I:395:LEU:HD12	1:I:399:ARG:NH1	2.27	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:L:287:LYS:HE2	1:L:290:LYS:HD2	1.94	0.49
1:I:163:GLU:O	1:I:167:GLY:HA2	2.12	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:L:20:MET:HE1	1:L:352:PRO:HB2	1.95	0.48
1:I:209:GLU:CD	1:I:209:GLU:H	2.15	0.48
1:I:122:PHE:N	1:I:122:PHE:CD1	2.78	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:L:292:LEU:HD11	1:L:409:LEU:HD13	1.95	0.48
1:I:62:PHE:HD2	1:I:338:MET:HE1	1.77	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:L:120:HIS:HB3	1:L:165:VAL:HG11	1.95	0.48
1:I:233:ASN:O	1:I:235:ARG:HG2	2.14	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:L:91:LYS:CE	1:L:120:HIS:NE2	2.77	0.47
1:I:354:ILE:O	1:I:362:LEU:HD13	2.14	0.47
1:L:229:PHE:CD1	1:L:254:GLN:OE1	2.67	0.47
1:I:48:VAL:HG13	1:I:126:LEU:HB2	1.97	0.47
1:I:22:ILE:HA	1:I:116:SER:OG	2.13	0.47
1:I:187:ASN:HB2	1:I:188:LYS:NZ	2.30	0.47
1:L:94:ALA:CA	1:L:351:LEU:HD23	2.45	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:L:254:GLN:NE2	1:L:258:PHE:HZ	2.12	0.47
1:L:138:SER:OG	1:L:276:GLY:HA3	2.14	0.47
1:I:186:ILE:HG21	1:I:202:ILE:HD11	1.96	0.47
1:L:211:THR:HA	1:L:391:ALA:O	2.15	0.47
1:I:267:THR:CG2	1:I:284:ILE:HG23	2.45	0.47
1:I:235:ARG:HG3	1:I:253:TYR:HE2	1.80	0.47
1:L:315:MET:O	1:I:386:THR:HA	2.14	0.47
1:L:207:ILE:HG22	1:L:208:ASN:N	2.30	0.47
1:L:103:MET:HA	1:L:108:PHE:HD2	1.80	0.47
1:I:363:TYR:N	1:I:363:TYR:CD1	2.83	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

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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:212:VAL:HG21	1:I:362:LEU:CD2	2.45	0.46
1:I:186:ILE:HG21	1:I:202:ILE:CD1	2.45	0.46
1:I:178:ASN:HB3	1:I:181:GLN:HB3	1.97	0.46
1:L:91:LYS:HG2	1:L:99:LEU:HD12	1.98	0.46
1:I:24:ARG:CD	1:I:24:ARG:H	2.24	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:L:263:VAL:HG22	1:L:267:THR:O	2.16	0.46
1:I:340:LEU:HD21	1:I:343:LEU:HB2	1.98	0.46
1:L:183:ARG:NH1	1:L:187:ASN:HD21	2.13	0.46
1:I:155:ASN:HB2	1:I:353:GLY:O	2.16	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:L:47:ARG:HB2	1:L:122:PHE:CE2	2.52	0.45
1:I:251:MET:SD	1:I:321:PRO:HG3	2.56	0.45
1:I:151:SER:O	1:I:356:ALA:HB1	2.16	0.45
1:L:152:LEU:HD22	1:L:355:VAL:HG21	1.98	0.45
1:I:292:LEU:HD21	1:I:425:ARG:HG2	1.99	0.45
1:I:175:PHE:HE1	1:I:207:ILE:HD13	1.82	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:L:92:LEU:HD13	1:L:120:HIS:ND1	2.31	0.44
1:L:189:TRP:O	1:L:193:LYS:HG2	2.17	0.44
1:I:53:LYS:HA	1:I:53:LYS:HD2	1.80	0.44
1:I:306:GLU:O	1:I:310:GLU:HG3	2.17	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:129:ARG:HG3	1:L:132:ARG:HH21	1.83	0.44
1:L:47:ARG:HB2	1:L:122:PHE:CZ	2.53	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:L:235:ARG:NH1	1:L:235:ARG:HB3	2.33	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:331:LEU:HD11	1:L:369:HIS:CB	2.46	0.43
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:187:ASN:O	1:L:190:VAL:HB	2.18	0.43
1:L:428:ASN:O	1:L:431:VAL:HG23	2.18	0.43
1:L:324:ARG:HG3	1:L:324:ARG:O	2.15	0.43
1:I:324:ARG:HA	1:I:374:GLU:HA	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:I:57:ARG:HG3	1:I:301:PRO:HG2	2.00	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:L:261:ARG:HB3	1:L:311:LEU:HD23	2.01	0.43
1:I:288:PRO:O	1:I:290:LYS:CD	2.66	0.43
1:L:145:ARG:HH11	1:L:145:ARG:CG	2.32	0.43
1:I:289:GLU:O	1:I:291:SER:N	2.52	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:193:LYS:HB3	1:L:193:LYS:HZ2	1.84	0.42
1:L:188:LYS:HD3	1:L:188:LYS:H	1.84	0.42
1:L:264:ALA:O	1:L:265:GLU:HB2	2.19	0.42
1:I:250:SER:CB	1:I:322:ARG:CD	2.98	0.42
1:I:182:SER:O	1:I:183:ARG:C	2.58	0.42
1:L:336:GLN:O	1:L:339:GLY:N	2.52	0.42
1:L:171:GLN:HA	1:L:172:PRO:HD2	1.91	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:N	1:L:408:PHE:CD1	2.87	0.42
1:I:145:ARG:NH1	1:I:171:GLN:HG3	2.35	0.42
1:I:140:LEU:HA	1:I:140:LEU:HD23	1.87	0.42
1:L:158:TYR:CE2	1:L:354:ILE:HG23	2.54	0.42
1:L:230:SER:HA	1:L:231:PRO:HD3	1.81	0.42
1:I:230:SER:HA	1:I:231:PRO:HD3	1.91	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:343:LEU:HD22	1:I:364:VAL:CG2	2.50	0.41
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:L:345:SER:HA	1:L:346:PRO:HD3	1.81	0.41
1:I:199:THR:HG23	1:I:200:ASP:H	1.85	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:354:ILE:HG22	1:I:354:ILE:O	2.19	0.41
1:I:343:LEU:HD23	1:I:351:LEU:HD11	2.02	0.41
1:I:131:TYR:CE1	1:I:142:SER:HB3	2.54	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: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:152:LEU:HD13	1:I:354:ILE:CG2	2.49	0.41
1:L:162:SER:C	1:L:164:LEU:N	2.73	0.41
1:I:54:ALA:O	1:I:57:ARG:N	2.53	0.41
1:I:287:LYS:O	1:I:288:PRO:C	2.58	0.41
1:I:170:LEU:HG	1:I:171:GLN:N	2.35	0.41
1:I:92:LEU:HD13	1:I:120:HIS:CE1	2.55	0.41
1:I:92:LEU:HB3	1:I:158:TYR:HE1	1.86	0.41
1:L:341:VAL:HG23	1:L:342:ASP:H	1.84	0.41
1:L:103:MET:O	1:L:108:PHE:N	2.47	0.41
1:I:47:ARG:HB3	1:I:122:PHE:CG	2.55	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:L:20:MET:HE2	1:L:352:PRO:HB2	2.01	0.41
1:I:238:LEU:HA	1:I:247:CYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:51:LEU:HD22	1:I:122:PHE:HB2	2.01	0.41
1:L:79:SER:C	1:L:81:LEU:H	2.24	0.41
1:I:198:ILE:CG2	1:I:370:LYS:HD3	2.29	0.41
1:L:46:ARG:O	1:L:48:VAL:N	2.54	0.41
1:I:58:PHE:CE1	1:I:62:PHE:HB2	2.56	0.41
1:I:183:ARG:O	1:I:186:ILE:HB	2.21	0.41
1:I:159:GLN:HB3	1:I:159:GLN:HE21	1.60	0.41
1:I:415:VAL:HB	1:I:416:PRO:CD	2.50	0.41
1:L:237:GLU:HG2	1:I:393:ARG:NH1	2.35	0.41
1:I:329:PHE:CD1	1:I:329:PHE:N	2.87	0.41
1:I:147:PHE:CE2	1:I:186:ILE:HG23	2.56	0.41
1:L:57:ARG:NH1	1:L:57:ARG:HG3	2.36	0.41
1:L:240:TYR:CE2	1:I:397:PRO:HD3	2.55	0.41
1:I:92:LEU:HD21	1:I:161:ILE:HB	2.03	0.41
1:L:63:TYR:HB2	1:L:423:MET:HE1	2.01	0.41
1:L:275:LYS:O	1:L:277:ASP:N	2.54	0.41
1:I:184:ALA:C	1:I:188:LYS:HG2	2.42	0.40
1:L:331:LEU:N	1:L:331:LEU:CD1	2.84	0.40
1:L:82:SER:CB	1:L:217:ASN:ND2	2.84	0.40
1:L:46:ARG:CG	1:L:46:ARG:O	2.68	0.40
1:L:272:LEU:HA	1:L:273:PRO:HD2	1.97	0.40
1:L:66:LEU:HD12	1:L:66:LEU:HA	1.86	0.40
1:I:336:GLN:O	1:I:337:ASP:C	2.60	0.40
1:L:75:ASN:O	1:L:76:ILE:HG13	2.21	0.40
1:L:254:GLN:HE22	1:L:258:PHE:HZ	1.68	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:I:239:PHE:CE1	1:I:406:ARG:N	2.89	0.40
1:L:188:LYS:HD3	1:L:188:LYS:N	2.36	0.40
1:I:209:GLU:CD	1:I:209:GLU:N	2.74	0.40
1:L:63:TYR:HB2	1:L:423:MET:HE3	2.02	0.40
1:L:152:LEU:HD22	1:L:355:VAL:CG2	2.51	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%)	2 11
1	L	386/432 (89%)	305 (79%)	59 (15%)	22 (6%)	2 12
All	All	782/864 (90%)	618 (79%)	118 (15%)	46 (6%)	2 11

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%)	4 17
1	L	348/383 (91%)	292 (84%)	56 (16%)	3 14
All	All	707/766 (92%)	598 (85%)	109 (15%)	3 16

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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.