



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:50 AM UTC

PDB ID : 1A87 / pdb_00001a87
Title : COLICIN N
Authors : Vetter, I.R.; Parker, M.W.; Tucker, A.D.; Lakey, J.H.; Pattus, F.; Tsernoglou, D.
Deposited on : 1998-04-03
Resolution : 3.10 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

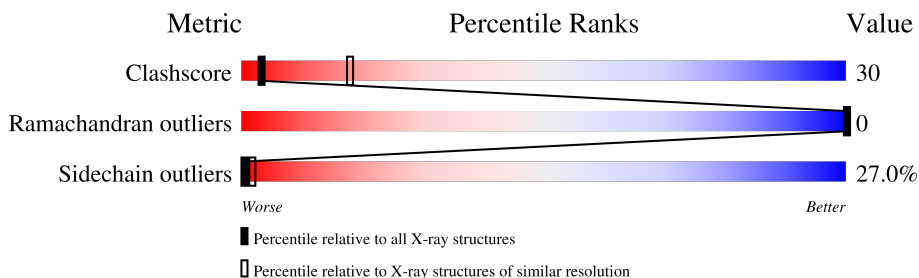
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

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	321	45% 32% 15% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2366 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 COLICIN N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2311	1478	397	430	6			

- Molecule 2 is water.

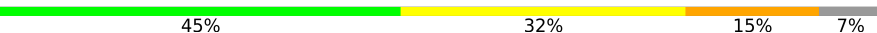
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	55	Total	O	0	0
			55	55		

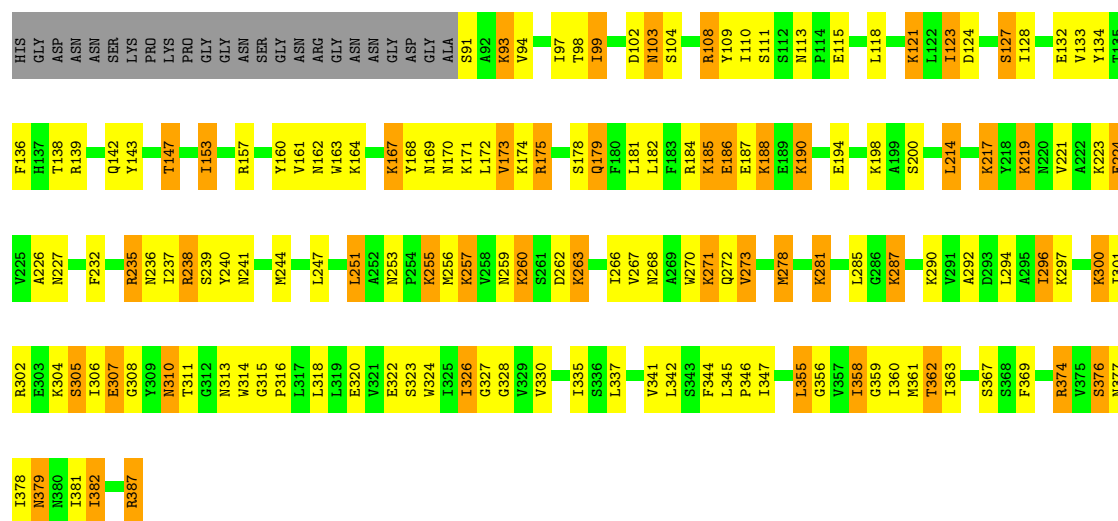
3 Residue-property plots

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: COLICIN N

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	187.30Å 187.30Å 187.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.00 – 3.10	Depositor
% Data completeness (in resolution range)	93.5 (23.00-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.173 , 0.310	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2366	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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	A	0.94	3/2348 (0.1%)	1.19	3/3162 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	387	ARG	C-OXT	7.69	1.39	1.23
1	A	241	ASN	CG-OD1	5.45	1.33	1.23
1	A	362	THR	C-N	-5.09	1.27	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	THR	CB-CA-C	-6.08	100.75	110.84
1	A	273	VAL	N-CA-C	5.15	116.23	109.58
1	A	238	ARG	N-CA-C	5.01	117.32	110.55

There are no chirality outliers.

There are no planarity outliers.

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	2311	0	2400	143	0
2	A	55	0	0	5	0
All	All	2366	0	2400	143	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 (143) 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:103:ASN:HD22	1:A:103:ASN:H	1.11	0.94
1:A:263:LYS:HB2	1:A:263:LYS:HZ3	1.34	0.90
1:A:260:LYS:HE3	1:A:260:LYS:N	1.90	0.86
1:A:103:ASN:H	1:A:103:ASN:ND2	1.70	0.85
1:A:171:LYS:HE2	1:A:175:ARG:HG3	1.56	0.84
1:A:263:LYS:HB2	1:A:263:LYS:NZ	1.92	0.78
1:A:93:LYS:HG2	1:A:97:ILE:O	1.84	0.77
1:A:278:MET:HE1	1:A:344:PHE:HB2	1.67	0.76
1:A:345:LEU:HD12	1:A:346:PRO:HD2	1.67	0.75
1:A:108:ARG:HB2	1:A:124:ASP:OD1	1.89	0.73
1:A:247:LEU:HG	1:A:251:LEU:HD22	1.70	0.72
1:A:244:MET:CE	1:A:315:GLY:HA2	2.19	0.71
1:A:187:GLU:HA	1:A:190:LYS:NZ	2.07	0.70
1:A:301:ILE:O	1:A:305:SER:HB2	1.91	0.70
1:A:103:ASN:ND2	1:A:103:ASN:N	2.40	0.70
1:A:253:ASN:OD1	1:A:255:LYS:HG2	1.92	0.70
1:A:260:LYS:HE3	1:A:260:LYS:H	1.54	0.69
1:A:379:ASN:HA	1:A:382:ILE:HG13	1.75	0.69
1:A:118:LEU:HD12	1:A:118:LEU:N	2.08	0.68
1:A:171:LYS:HZ3	1:A:175:ARG:NE	1.91	0.68
1:A:287:LYS:H	1:A:287:LYS:CD	2.04	0.68
1:A:171:LYS:NZ	1:A:175:ARG:NE	2.42	0.67
1:A:238:ARG:HG3	1:A:369:PHE:O	1.95	0.67
1:A:257:LYS:NZ	1:A:387:ARG:HG3	2.09	0.67
1:A:187:GLU:HA	1:A:190:LYS:HZ3	1.59	0.67
1:A:292:ALA:O	1:A:297:LYS:HE2	1.94	0.67
1:A:171:LYS:HZ3	1:A:175:ARG:HE	1.43	0.66
1:A:171:LYS:CE	1:A:175:ARG:HG3	2.27	0.65
1:A:111:SER:O	1:A:121:LYS:HE3	1.97	0.65
1:A:240:TYR:CZ	1:A:244:MET:HE3	2.32	0.65
1:A:244:MET:HG2	2:A:416:HOH:O	1.97	0.65
1:A:326:ILE:HD13	1:A:327:GLY:N	2.12	0.65
1:A:310:ASN:H	1:A:310:ASN:ND2	1.96	0.63
1:A:163:TRP:O	1:A:164:LYS:HD3	2.00	0.62
1:A:240:TYR:CE2	1:A:244:MET:HE3	2.36	0.61
1:A:287:LYS:H	1:A:287:LYS:HD2	1.64	0.61
1:A:172:LEU:CD1	1:A:175:ARG:HH21	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:VAL:HG22	1:A:147:THR:HB	1.85	0.59
1:A:255:LYS:N	1:A:255:LYS:HD2	2.17	0.59
1:A:259:ASN:HB2	1:A:260:LYS:CE	2.34	0.58
1:A:296:ILE:N	1:A:296:ILE:HD13	2.18	0.58
1:A:318:LEU:HD23	1:A:318:LEU:N	2.17	0.58
1:A:244:MET:HE3	1:A:315:GLY:HA2	1.86	0.57
1:A:190:LYS:NZ	1:A:190:LYS:HB3	2.20	0.57
1:A:200:SER:HB2	1:A:226:ALA:O	2.03	0.57
1:A:163:TRP:C	1:A:164:LYS:HD3	2.30	0.56
1:A:132:GLU:CD	1:A:184:ARG:HE	2.14	0.56
1:A:147:THR:HG21	2:A:449:HOH:O	2.05	0.56
1:A:217:LYS:HB2	2:A:415:HOH:O	2.05	0.56
1:A:259:ASN:ND2	1:A:259:ASN:H	2.04	0.56
1:A:307:GLU:HA	1:A:310:ASN:HD21	1.71	0.55
1:A:97:ILE:HG22	1:A:113:ASN:HB3	1.88	0.55
1:A:118:LEU:HD21	1:A:173:VAL:HG13	1.89	0.55
1:A:127:SER:C	1:A:128:ILE:HD12	2.31	0.55
1:A:244:MET:HE1	1:A:315:GLY:HA2	1.87	0.55
1:A:257:LYS:HZ2	1:A:387:ARG:HG3	1.70	0.55
1:A:315:GLY:N	1:A:316:PRO:HD2	2.23	0.54
1:A:259:ASN:H	1:A:259:ASN:HD22	1.55	0.54
1:A:253:ASN:O	1:A:256:MET:HB2	2.08	0.54
1:A:358:ILE:HG22	1:A:359:GLY:N	2.22	0.54
1:A:255:LYS:HD2	1:A:255:LYS:H	1.74	0.53
1:A:221:VAL:O	1:A:224:GLU:HG3	2.09	0.53
1:A:259:ASN:HB2	1:A:260:LYS:HE3	1.90	0.52
1:A:99:ILE:HG23	1:A:109:TYR:HB3	1.91	0.52
1:A:356:GLY:O	1:A:360:ILE:HG12	2.09	0.52
1:A:266:ILE:HG23	1:A:358:ILE:HD11	1.92	0.52
1:A:337:LEU:O	1:A:341:VAL:HG23	2.10	0.51
1:A:97:ILE:HD12	1:A:99:ILE:CD1	2.39	0.51
1:A:171:LYS:HG2	2:A:421:HOH:O	2.11	0.51
1:A:347:ILE:HB	1:A:355:LEU:HD21	1.91	0.50
1:A:374:ARG:O	1:A:377:ASN:HB2	2.10	0.50
1:A:132:GLU:OE1	1:A:184:ARG:NE	2.42	0.50
1:A:221:VAL:HA	1:A:224:GLU:HG3	1.93	0.49
1:A:244:MET:HE2	1:A:318:LEU:HD12	1.95	0.48
1:A:287:LYS:HD2	1:A:287:LYS:N	2.28	0.48
1:A:115:GLU:O	1:A:115:GLU:HG2	2.12	0.48
1:A:256:MET:HG2	1:A:382:ILE:HG21	1.94	0.48
1:A:307:GLU:O	1:A:311:THR:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LEU:HB3	1:A:168:TYR:HE2	1.78	0.48
1:A:376:SER:OG	1:A:377:ASN:N	2.47	0.47
1:A:255:LYS:H	1:A:255:LYS:CD	2.27	0.47
1:A:190:LYS:HZ3	1:A:190:LYS:HB3	1.79	0.47
1:A:267:VAL:O	1:A:271:LYS:HG3	2.15	0.47
1:A:138:THR:OG1	1:A:142:GLN:HG2	2.14	0.47
1:A:102:ASP:OD1	1:A:104:SER:OG	2.33	0.46
1:A:287:LYS:HA	1:A:290:LYS:HD3	1.97	0.46
1:A:308:GLY:HA3	1:A:314:TRP:CZ3	2.51	0.46
1:A:160:TYR:CD1	1:A:167:LYS:HG2	2.51	0.46
1:A:313:ASN:ND2	1:A:316:PRO:HD3	2.31	0.46
1:A:214:LEU:HD12	1:A:214:LEU:HA	1.62	0.46
1:A:310:ASN:ND2	1:A:310:ASN:N	2.58	0.46
1:A:358:ILE:HD12	1:A:358:ILE:HA	1.65	0.46
1:A:157:ARG:HG3	1:A:157:ARG:HH11	1.81	0.45
1:A:128:ILE:CD1	1:A:128:ILE:N	2.79	0.45
1:A:273:VAL:HB	1:A:302:ARG:HD3	1.98	0.45
1:A:285:LEU:HD23	1:A:285:LEU:HA	1.78	0.45
1:A:300:LYS:O	1:A:304:LYS:HG3	2.16	0.45
1:A:251:LEU:HD11	1:A:361:MET:HE1	1.98	0.45
1:A:118:LEU:N	1:A:118:LEU:CD1	2.79	0.45
1:A:235:ARG:HD3	1:A:235:ARG:H	1.82	0.45
1:A:315:GLY:N	1:A:316:PRO:CD	2.78	0.45
1:A:270:TRP:HE3	1:A:302:ARG:HG3	1.81	0.45
1:A:320:GLU:HA	1:A:320:GLU:OE1	2.17	0.45
1:A:97:ILE:HD12	1:A:99:ILE:HD13	1.98	0.45
1:A:171:LYS:C	1:A:171:LYS:HD3	2.42	0.45
1:A:304:LYS:NZ	2:A:481:HOH:O	2.48	0.44
1:A:184:ARG:O	1:A:188:LYS:HG2	2.18	0.44
1:A:132:GLU:OE1	1:A:134:TYR:OH	2.30	0.44
1:A:185:LYS:NZ	1:A:185:LYS:CB	2.79	0.44
1:A:94:VAL:HG12	1:A:179:GLN:HB2	2.00	0.44
1:A:102:ASP:HB3	1:A:108:ARG:HG2	1.99	0.44
1:A:374:ARG:HD3	1:A:374:ARG:HA	1.62	0.43
1:A:278:MET:HE1	1:A:344:PHE:CB	2.45	0.43
1:A:153:ILE:O	1:A:153:ILE:HG13	2.19	0.43
1:A:251:LEU:HD12	1:A:251:LEU:HA	1.72	0.43
1:A:257:LYS:HZ1	1:A:387:ARG:HG3	1.84	0.43
1:A:281:LYS:HE3	1:A:281:LYS:HB2	1.49	0.43
1:A:235:ARG:HD3	1:A:235:ARG:N	2.34	0.42
1:A:240:TYR:CE2	1:A:244:MET:CE	3.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ARG:HG3	1:A:157:ARG:NH1	2.35	0.42
1:A:310:ASN:N	1:A:310:ASN:HD22	2.16	0.42
1:A:118:LEU:HD13	1:A:136:PHE:CE2	2.54	0.42
1:A:143:TYR:C	1:A:143:TYR:CD1	2.97	0.42
1:A:182:LEU:O	1:A:186:GLU:HG3	2.19	0.42
1:A:97:ILE:HD12	1:A:99:ILE:HD11	2.01	0.42
1:A:219:LYS:O	1:A:223:LYS:HG3	2.20	0.41
1:A:301:ILE:HD11	1:A:324:TRP:CH2	2.56	0.41
1:A:378:ILE:O	1:A:381:ILE:HG13	2.20	0.41
1:A:102:ASP:CG	1:A:104:SER:HG	2.29	0.41
1:A:171:LYS:HZ1	1:A:175:ARG:NE	2.18	0.41
1:A:306:ILE:HG22	1:A:307:GLU:N	2.32	0.41
1:A:102:ASP:HB3	1:A:108:ARG:CG	2.50	0.41
1:A:270:TRP:O	1:A:273:VAL:HB	2.20	0.41
1:A:310:ASN:H	1:A:310:ASN:HD22	1.69	0.41
1:A:256:MET:HG2	1:A:382:ILE:HD12	2.03	0.40
1:A:161:VAL:O	1:A:162:ASN:HB2	2.21	0.40
1:A:235:ARG:N	1:A:235:ARG:CD	2.84	0.40
1:A:262:ASP:O	1:A:266:ILE:HG13	2.22	0.40
1:A:342:LEU:HD13	1:A:362:THR:HA	2.02	0.40
1:A:94:VAL:CG1	1:A:179:GLN:HB2	2.51	0.40
1:A:244:MET:CE	1:A:318:LEU:HD12	2.51	0.40
1:A:123:ILE:HD13	1:A:136:PHE:CD2	2.56	0.40
1:A:127:SER:O	1:A:328:GLY:HA2	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	295/321 (92%)	275 (93%)	20 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	252/268 (94%)	184 (73%)	68 (27%)	0 2

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	SER
1	A	93	LYS
1	A	98	THR
1	A	99	ILE
1	A	103	ASN
1	A	108	ARG
1	A	110	ILE
1	A	121	LYS
1	A	123	ILE
1	A	127	SER
1	A	139	ARG
1	A	147	THR
1	A	153	ILE
1	A	167	LYS
1	A	169	ASN
1	A	170	ASN
1	A	173	VAL
1	A	174	LYS
1	A	175	ARG
1	A	178	SER
1	A	179	GLN
1	A	181	LEU
1	A	185	LYS
1	A	186	GLU
1	A	188	LYS
1	A	190	LYS
1	A	194	GLU

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Mol	Chain	Res	Type
1	A	198	LYS
1	A	214	LEU
1	A	217	LYS
1	A	219	LYS
1	A	224	GLU
1	A	227	ASN
1	A	232	PHE
1	A	235	ARG
1	A	236	ASN
1	A	237	ILE
1	A	239	SER
1	A	251	LEU
1	A	255	LYS
1	A	257	LYS
1	A	260	LYS
1	A	263	LYS
1	A	268	ASN
1	A	271	LYS
1	A	272	GLN
1	A	278	MET
1	A	281	LYS
1	A	287	LYS
1	A	294	LEU
1	A	296	ILE
1	A	300	LYS
1	A	305	SER
1	A	307	GLU
1	A	310	ASN
1	A	322	GLU
1	A	323	SER
1	A	326	ILE
1	A	330	VAL
1	A	335	ILE
1	A	355	LEU
1	A	358	ILE
1	A	363	ILE
1	A	367	SER
1	A	374	ARG
1	A	376	SER
1	A	379	ASN
1	A	382	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	142	GLN
1	A	170	ASN
1	A	179	GLN
1	A	191	ASN
1	A	227	ASN
1	A	248	ASN
1	A	268	ASN
1	A	280	ASN
1	A	310	ASN
1	A	313	ASN
1	A	379	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.