



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2024 – 12:40 PM EST

PDB ID : 1A87
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 : 4.02b-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) : 2.36

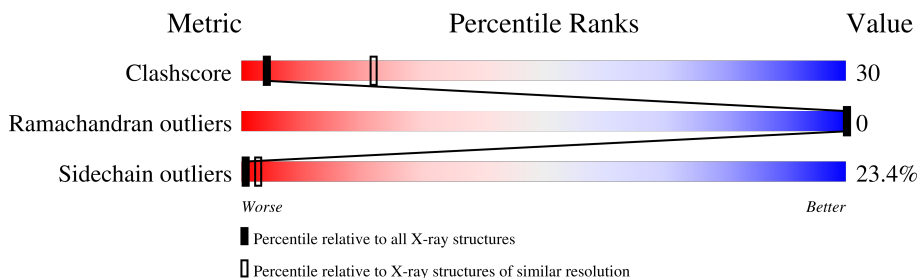
1 Overall quality at a glance

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	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (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	

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
			Total	C	N	O	S			
1	A	297	2311	1478	397	430	6	0	0	0

- Molecule 2 is water.

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

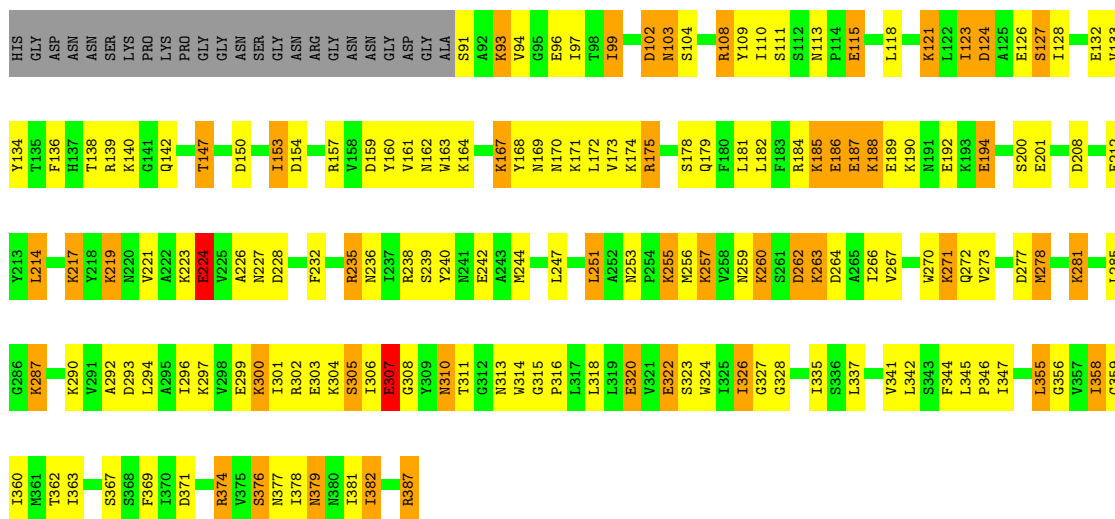
3 Residue-property plots

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

Xtrriage (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.	Xtrriage
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	0.85	18/2348 (0.8%)	1.02	22/3162 (0.7%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	387	ARG	C-OXT	8.20	1.39	1.23
1	A	303	GLU	CD-OE1	6.16	1.32	1.25
1	A	299	GLU	CD-OE1	6.01	1.32	1.25
1	A	322	GLU	CD-OE1	5.92	1.32	1.25
1	A	189	GLU	CD-OE1	5.90	1.32	1.25
1	A	186	GLU	CD-OE2	5.80	1.32	1.25
1	A	96	GLU	CD-OE1	5.79	1.32	1.25
1	A	307	GLU	CD-OE1	5.76	1.31	1.25
1	A	201	GLU	CD-OE1	5.72	1.31	1.25
1	A	242	GLU	CD-OE1	5.51	1.31	1.25
1	A	192	GLU	CD-OE2	5.48	1.31	1.25
1	A	194	GLU	CD-OE2	5.46	1.31	1.25
1	A	126	GLU	CD-OE2	5.46	1.31	1.25
1	A	224	GLU	CD-OE1	5.31	1.31	1.25
1	A	115	GLU	CD-OE1	5.30	1.31	1.25
1	A	320	GLU	CD-OE1	5.29	1.31	1.25
1	A	212	GLU	CD-OE2	5.26	1.31	1.25
1	A	187	GLU	CD-OE1	5.16	1.31	1.25

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	ASP	CB-CG-OD1	-6.49	112.46	118.30
1	A	159	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	A	150	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	A	262	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	A	124	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	150	ASP	CB-CG-OD1	5.88	123.59	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	ASP	CB-CG-OD2	-5.83	113.06	118.30
1	A	208	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	A	264	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	124	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	228	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	154	ASP	CB-CG-OD1	5.64	123.37	118.30
1	A	102	ASP	CB-CG-OD1	-5.57	113.29	118.30
1	A	159	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	264	ASP	CB-CG-OD1	5.56	123.30	118.30
1	A	293	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	A	277	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	A	371	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	A	208	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	262	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	277	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	293	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2311	0	2400	139	0
2	A	55	0	0	5	0
All	All	2366	0	2400	139	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 (139) 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:260:LYS:HE3	1:A:260:LYS:N	1.90	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ASN:H	1:A:103:ASN:ND2	1.70	0.85
1:A:263:LYS:HB2	1:A:263:LYS:NZ	1.92	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:HZ3	1.47	0.79
1:A:93:LYS:HG2	1:A:97:ILE:O	1.84	0.77
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: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: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: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	0.64
1:A:240:TYR:CZ	1:A:244:MET:HE3	2.33	0.64
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:244:MET:HE3	1:A:315:GLY:HA2	1.83	0.60
1:A:172:LEU:CD1	1:A:175:ARG:HH21	2.14	0.60
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:171:LYS:HZ3	1:A:175:ARG:NE	2.01	0.58
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LYS:HZ3	1:A:175:ARG:HE	1.52	0.57
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: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:244:MET:HE1	1:A:315:GLY:HA2	1.91	0.52
1:A:356:GLY:O	1:A:360:ILE:HG12	2.09	0.52
1:A:163:TRP:C	1:A:164:LYS:HD3	2.30	0.52
1:A:132:GLU:CD	1:A:184:ARG:HE	2.14	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:127:SER:C	1:A:128:ILE:HD12	2.31	0.50
1:A:347:ILE:HB	1:A:355:LEU:HD21	1.91	0.50
1:A:171:LYS:HZ1	1:A:175:ARG:NE	2.07	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: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
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:257:LYS:HZ1	1:A:387:ARG:HG3	1.79	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:257:LYS:HZ2	1:A:387:ARG:HG3	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:171:LYS:HZ1	1:A:175:ARG:CD	2.29	0.46
1:A:244:MET:HE2	1:A:318:LEU:HD12	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:306:ILE:HG22	1:A:307:GLU:N	2.32	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: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:278:MET:CE	1:A:344:PHE:HB2	2.48	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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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 [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	252/268 (94%)	193 (77%)	59 (23%)	1 3

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	SER
1	A	93	LYS
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	140	LYS
1	A	147	THR
1	A	153	ILE
1	A	167	LYS
1	A	169	ASN
1	A	170	ASN
1	A	174	LYS
1	A	175	ARG
1	A	178	SER
1	A	181	LEU
1	A	185	LYS
1	A	188	LYS
1	A	194	GLU
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	239	SER
1	A	251	LEU
1	A	255	LYS
1	A	257	LYS
1	A	260	LYS
1	A	263	LYS
1	A	271	LYS

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Mol	Chain	Res	Type
1	A	272	GLN
1	A	278	MET
1	A	281	LYS
1	A	287	LYS
1	A	294	LEU
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	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 (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	179	GLN
1	A	191	ASN
1	A	227	ASN
1	A	248	ASN
1	A	259	ASN
1	A	310	ASN
1	A	313	ASN

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 monosaccharides 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.