



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:05 AM UTC

PDB ID : 3APP / pdb_00003app
Title : STRUCTURE AND REFINEMENT OF PENICILLOPEPSIN AT 1.8
ANGSTROMS RESOLUTION
Authors : Sielecki, A.R.; James, M.N.G.
Deposited on : 1990-11-27
Resolution : 1.80 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
Xtrriage (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

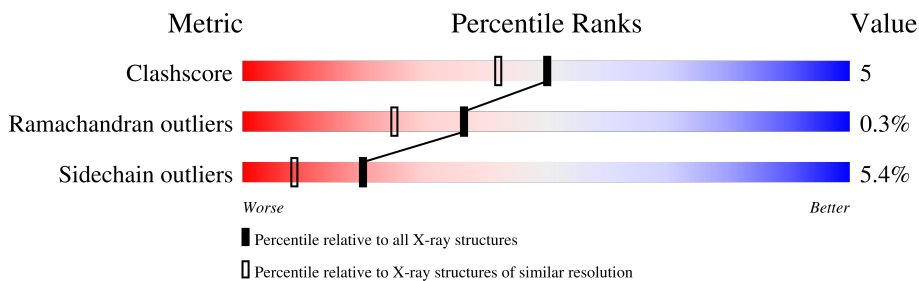
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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	323	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2684 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 PENICILLOPEPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	323	2366	1479	377	508	2	0	0	0

- Molecule 2 is water.

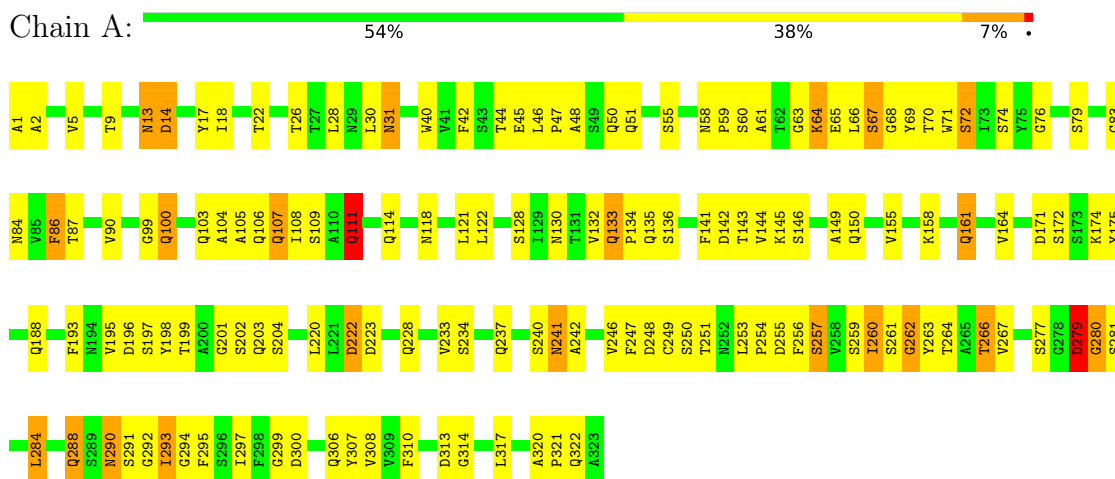
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	318	Total	O	0	0
			318	318		

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: PENICILLOPEPSIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	97.37Å 46.64Å 65.47Å 90.00° 115.40° 90.00°	Depositor
Resolution (Å)	8.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.126 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2684	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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	1.22	1/2420 (0.0%)	2.04	75/3304 (2.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	314	GLY	N-CA	5.24	1.51	1.44

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	ASN	OD1-CG-ND2	-10.42	112.18	122.60
1	A	161	GLN	N-CA-CB	8.66	122.81	110.77
1	A	83	GLY	O-C-N	7.93	130.38	123.80
1	A	300	ASP	O-C-N	7.90	130.50	122.12
1	A	30	LEU	O-C-N	7.75	133.10	123.10
1	A	14	ASP	CA-CB-CG	7.75	120.35	112.60
1	A	317	LEU	CA-C-O	-7.71	112.03	120.36
1	A	313	ASP	CA-C-O	-7.67	112.37	120.58
1	A	300	ASP	CA-C-O	-7.67	112.35	120.63
1	A	122	LEU	CA-C-N	7.53	128.41	120.43
1	A	122	LEU	C-N-CA	7.53	128.41	120.43
1	A	161	GLN	O-C-N	7.43	127.62	121.83
1	A	17	TYR	CA-C-O	-7.13	112.67	120.30
1	A	267	VAL	O-C-N	7.11	125.85	121.37
1	A	262	GLY	CA-C-O	6.95	126.70	119.27
1	A	111	GLN	CA-C-O	-6.90	112.31	120.10
1	A	55	SER	N-CA-C	-6.76	98.24	109.46
1	A	288	GLN	OE1-CD-NE2	6.67	129.28	122.60
1	A	130	ASN	CA-CB-CG	-6.67	105.93	112.60
1	A	150	GLN	O-C-N	6.54	128.81	121.94
1	A	246	VAL	O-C-N	6.51	130.27	123.04
1	A	58	ASN	CB-CA-C	6.44	116.89	110.33
1	A	105	ALA	O-C-N	6.33	130.48	123.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	GLN	CA-C-O	-6.26	114.15	121.16
1	A	9	THR	O-C-N	6.23	127.36	121.38
1	A	164	VAL	O-C-N	6.15	129.97	123.02
1	A	320	ALA	CB-CA-C	6.09	118.26	110.22
1	A	307	TYR	N-CA-C	-6.08	99.28	109.07
1	A	297	ILE	CA-C-O	-6.07	113.56	120.66
1	A	222	ASP	CA-C-O	-6.02	115.17	121.55
1	A	9	THR	CA-C-O	-5.97	114.12	119.86
1	A	267	VAL	CA-C-O	-5.97	114.71	119.25
1	A	31	ASN	CA-C-O	-5.96	113.76	120.43
1	A	30	LEU	CA-C-O	-5.90	114.42	121.56
1	A	280	GLY	CA-C-N	5.70	132.42	121.54
1	A	280	GLY	C-N-CA	5.70	132.42	121.54
1	A	308	VAL	O-C-N	5.70	129.41	123.26
1	A	197	SER	N-CA-CB	-5.69	102.70	111.46
1	A	31	ASN	CB-CA-C	5.65	119.66	110.22
1	A	141	PHE	O-C-N	5.65	127.89	122.07
1	A	42	PHE	N-CA-C	-5.61	102.09	110.23
1	A	2	ALA	CA-C-O	5.61	127.67	121.56
1	A	299	GLY	CA-C-O	5.60	128.52	122.47
1	A	13	ASN	OD1-CG-ND2	5.59	128.19	122.60
1	A	266	THR	O-C-N	5.56	129.85	123.29
1	A	150	GLN	CA-C-O	-5.56	114.03	120.03
1	A	22	THR	CA-CB-OG1	-5.55	101.27	109.60
1	A	84	ASN	CA-C-N	-5.50	114.80	122.71
1	A	84	ASN	C-N-CA	-5.50	114.80	122.71
1	A	247	PHE	CA-C-O	5.48	127.19	121.38
1	A	114	GLN	CA-C-O	-5.47	112.88	119.49
1	A	67	SER	CB-CA-C	5.42	118.36	109.90
1	A	241	ASN	O-C-N	5.42	127.65	122.07
1	A	314	GLY	N-CA-C	-5.41	101.30	112.34
1	A	320	ALA	N-CA-C	-5.41	103.35	108.22
1	A	86	PHE	CA-CB-CG	-5.35	108.45	113.80
1	A	317	LEU	O-C-N	5.29	129.60	123.30
1	A	5	VAL	CA-C-O	-5.29	114.84	120.39
1	A	262	GLY	N-CA-C	5.28	120.97	114.69
1	A	171	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	260	ILE	O-C-N	5.26	128.62	122.99
1	A	26	THR	CA-C-O	-5.25	114.70	120.43
1	A	284	LEU	O-C-N	5.24	129.24	123.16
1	A	237	GLN	CB-CG-CD	5.24	121.51	112.60
1	A	109	SER	CA-C-N	5.18	127.47	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^o)	Ideal(^o)
1	A	109	SER	C-N-CA	5.18	127.47	120.38
1	A	42	PHE	CA-C-O	-5.15	115.52	121.19
1	A	279	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	90	VAL	O-C-N	5.13	128.64	123.20
1	A	114	GLN	CB-CG-CD	5.10	121.27	112.60
1	A	257	SER	CA-CB-OG	-5.10	100.90	111.10
1	A	317	LEU	CA-C-N	-5.08	117.68	122.66
1	A	317	LEU	C-N-CA	-5.08	117.68	122.66
1	A	290	ASN	N-CA-C	-5.05	106.96	113.02
1	A	193	PHE	CA-CB-CG	5.03	118.83	113.80

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	2366	0	2183	24	333
2	A	318	0	0	4	24
All	All	2684	0	2183	24	334

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 5.

All (24) 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:280:GLY:CA	2:A:523:HOH:O	2.07	1.02
1:A:280:GLY:HA3	2:A:523:HOH:O	1.63	0.95
1:A:233:VAL:HG13	1:A:251:THR:HG21	1.70	0.74
1:A:280:GLY:HA2	2:A:523:HOH:O	1.76	0.73
1:A:79:SER:HB3	1:A:111:GLN:HG3	1.79	0.65
1:A:188:GLN:NE2	2:A:522:HOH:O	2.27	0.65
1:A:79:SER:HB3	1:A:111:GLN:CG	2.27	0.64
1:A:106:GLN:C	1:A:107:GLN:HG2	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:GLN:C	1:A:322:GLN:HG3	2.34	0.52
1:A:203:GLN:OE1	1:A:228:GLN:HG3	2.12	0.49
1:A:40:TRP:NE1	1:A:121:LEU:HD12	2.28	0.48
1:A:172:SER:HA	1:A:175:TYR:CE1	2.49	0.47
1:A:40:TRP:HE1	1:A:121:LEU:HD12	1.80	0.47
1:A:40:TRP:HA	1:A:103:GLN:O	2.15	0.46
1:A:1:ALA:HB1	1:A:149:ALA:HA	1.98	0.46
1:A:242:ALA:HB1	1:A:277:SER:HB2	1.98	0.45
1:A:242:ALA:CB	1:A:277:SER:HB2	2.47	0.45
1:A:155:VAL:HG12	1:A:310:PHE:HE1	1.82	0.44
1:A:71:TRP:CE2	1:A:103:GLN:HB3	2.52	0.44
1:A:31:ASN:HB3	1:A:121:LEU:HD23	2.00	0.43
1:A:220:LEU:HA	1:A:288:GLN:O	2.19	0.43
1:A:13:ASN:O	1:A:14:ASP:HB2	2.20	0.41
1:A:79:SER:HB3	1:A:111:GLN:CD	2.45	0.41
1:A:253:LEU:HA	1:A:254:PRO:HD3	1.91	0.40

All (334) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:GLU:CD	1:A:260:ILE:N[3_545]	0.20	2.00
1:A:146:SER:N	1:A:250:SER:C[3_555]	0.37	1.83
1:A:65:GLU:C	1:A:262:GLY:N[3_545]	0.55	1.65
1:A:133:GLN:CA	1:A:293:ILE:CB[2_656]	0.55	1.65
1:A:107:GLN:NE2	1:A:203:GLN:CB[3_545]	0.56	1.64
1:A:144:VAL:CG2	2:A:399:HOH:O[3_555]	0.62	1.58
1:A:74:SER:CB	1:A:74:SER:CB[2_656]	0.63	1.57
1:A:99:GLY:O	1:A:280:GLY:O[3_555]	0.63	1.57
1:A:65:GLU:O	1:A:261:SER:C[3_545]	0.64	1.56
1:A:135:GLN:CA	1:A:294:GLY:CA[2_656]	0.65	1.55
1:A:106:GLN:CA	1:A:199:THR:CG2[3_545]	0.66	1.54
1:A:142:ASP:C	1:A:248:ASP:CB[3_555]	0.74	1.46
1:A:65:GLU:OE1	1:A:259:SER:C[3_545]	0.75	1.45
1:A:47:PRO:CA	1:A:254:PRO:CB[3_545]	0.80	1.40
1:A:67:SER:CA	1:A:196:ASP:OD1[3_545]	0.80	1.40
1:A:142:ASP:O	1:A:248:ASP:CB[3_555]	0.80	1.40
1:A:99:GLY:C	1:A:280:GLY:O[3_555]	0.81	1.39
1:A:106:GLN:CG	1:A:199:THR:OG1[3_545]	0.81	1.39
1:A:45:GLU:CG	1:A:257:SER:CB[3_545]	0.86	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:VAL:C	1:A:250:SER:CB[3_555]	0.86	1.34
1:A:249:CYS:O	2:A:394:HOH:O[3_445]	0.87	1.33
1:A:47:PRO:CB	1:A:254:PRO:CB[3_545]	0.90	1.30
1:A:74:SER:CA	1:A:74:SER:CB[2_656]	0.92	1.28
1:A:65:GLU:CA	1:A:263:TYR:N[3_545]	0.94	1.26
1:A:99:GLY:O	1:A:280:GLY:C[3_555]	0.94	1.26
1:A:47:PRO:C	1:A:254:PRO:CA[3_545]	0.95	1.25
1:A:65:GLU:OE1	1:A:259:SER:O[3_545]	0.95	1.25
1:A:145:LYS:C	1:A:250:SER:O[3_555]	0.95	1.25
1:A:107:GLN:CG	1:A:203:GLN:CA[3_545]	0.96	1.24
1:A:134:PRO:CB	1:A:290:ASN:CG[2_656]	0.96	1.24
1:A:51:GLN:NE2	1:A:255:ASP:CG[3_545]	0.97	1.23
1:A:142:ASP:C	1:A:248:ASP:CG[3_555]	0.97	1.23
1:A:144:VAL:O	1:A:250:SER:OG[3_555]	0.98	1.22
1:A:86:PHE:CE2	1:A:264:THR:N[3_545]	0.99	1.21
1:A:134:PRO:CB	1:A:290:ASN:ND2[2_656]	0.99	1.21
1:A:48:ALA:CB	1:A:253:LEU:O[3_545]	1.00	1.20
1:A:86:PHE:CD1	1:A:264:THR:OG1[3_545]	1.02	1.18
1:A:86:PHE:CE1	1:A:264:THR:OG1[3_545]	1.02	1.18
1:A:107:GLN:CG	1:A:203:GLN:C[3_545]	1.02	1.18
1:A:47:PRO:CB	1:A:254:PRO:CG[3_545]	1.04	1.16
1:A:106:GLN:CG	1:A:199:THR:CB[3_545]	1.04	1.16
1:A:133:GLN:C	1:A:293:ILE:N[2_656]	1.04	1.16
1:A:46:LEU:O	1:A:255:ASP:N[3_545]	1.05	1.15
1:A:67:SER:C	1:A:196:ASP:CG[3_545]	1.06	1.14
1:A:135:GLN:N	1:A:294:GLY:N[2_656]	1.06	1.14
1:A:146:SER:N	1:A:250:SER:O[3_555]	1.06	1.14
1:A:132:VAL:CG1	2:A:377:HOH:O[2_656]	1.07	1.13
1:A:67:SER:OG	2:A:358:HOH:O[3_545]	1.09	1.11
1:A:133:GLN:CG	1:A:293:ILE:CD1[2_656]	1.09	1.11
1:A:65:GLU:N	1:A:263:TYR:N[3_545]	1.11	1.09
1:A:135:GLN:CA	1:A:294:GLY:C[2_656]	1.11	1.09
1:A:47:PRO:CA	1:A:254:PRO:CA[3_545]	1.12	1.08
1:A:106:GLN:NE2	1:A:199:THR:N[3_545]	1.12	1.08
1:A:45:GLU:CG	1:A:257:SER:OG[3_545]	1.13	1.07
1:A:45:GLU:CD	1:A:257:SER:OG[3_545]	1.14	1.06
1:A:107:GLN:CD	1:A:203:GLN:CA[3_545]	1.15	1.05
1:A:107:GLN:CD	1:A:203:GLN:CB[3_545]	1.16	1.04
1:A:144:VAL:O	1:A:250:SER:CB[3_555]	1.16	1.04
1:A:146:SER:CB	1:A:251:THR:O[3_555]	1.16	1.04
1:A:48:ALA:CA	1:A:253:LEU:O[3_545]	1.17	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:GLN:CD	2:A:412:HOH:O[3_545]	1.17	1.03
1:A:65:GLU:C	1:A:262:GLY:CA[3_545]	1.17	1.03
1:A:134:PRO:CG	1:A:290:ASN:OD1[2_656]	1.18	1.02
1:A:144:VAL:C	1:A:250:SER:OG[3_555]	1.18	1.02
1:A:68:GLY:N	1:A:196:ASP:CG[3_545]	1.19	1.01
1:A:65:GLU:O	1:A:262:GLY:N[3_545]	1.20	1.00
1:A:106:GLN:NE2	1:A:198:TYR:C[3_545]	1.20	1.00
1:A:143:THR:N	1:A:248:ASP:CG[3_555]	1.20	1.00
1:A:143:THR:O	1:A:249:CYS:N[3_555]	1.20	1.00
1:A:145:LYS:N	1:A:250:SER:CB[3_555]	1.20	1.00
1:A:51:GLN:NE2	1:A:255:ASP:OD2[3_545]	1.23	0.97
1:A:65:GLU:CD	1:A:259:SER:C[3_545]	1.24	0.96
1:A:44:THR:OG1	1:A:266:THR:CG2[3_545]	1.25	0.95
1:A:47:PRO:CD	1:A:201:GLY:CA[3_545]	1.25	0.95
1:A:249:CYS:C	2:A:394:HOH:O[3_445]	1.25	0.95
1:A:50:GLN:OE1	2:A:412:HOH:O[3_545]	1.26	0.94
1:A:61:ALA:CA	1:A:321:PRO:CG[3_545]	1.27	0.93
1:A:65:GLU:OE2	1:A:260:ILE:N[3_545]	1.27	0.93
1:A:128:SER:CA	1:A:188:GLN:NE2[2_656]	1.28	0.92
1:A:107:GLN:NE2	1:A:203:GLN:CG[3_545]	1.29	0.91
1:A:128:SER:CB	1:A:188:GLN:NE2[2_656]	1.29	0.91
1:A:133:GLN:O	1:A:293:ILE:N[2_656]	1.31	0.89
1:A:70:THR:N	1:A:291:SER:O[2_656]	1.32	0.88
1:A:143:THR:N	1:A:248:ASP:OD1[3_555]	1.32	0.88
1:A:67:SER:C	1:A:196:ASP:OD2[3_545]	1.33	0.87
1:A:86:PHE:CE2	1:A:263:TYR:C[3_545]	1.33	0.87
1:A:135:GLN:C	1:A:294:GLY:CA[2_656]	1.33	0.87
1:A:65:GLU:O	1:A:261:SER:O[3_545]	1.36	0.84
1:A:67:SER:CA	1:A:196:ASP:CG[3_545]	1.36	0.84
1:A:86:PHE:CD2	1:A:264:THR:N[3_545]	1.36	0.84
1:A:48:ALA:N	1:A:254:PRO:CA[3_545]	1.39	0.81
1:A:66:LEU:N	1:A:262:GLY:CA[3_545]	1.39	0.81
1:A:106:GLN:OE1	1:A:198:TYR:O[3_545]	1.39	0.81
1:A:106:GLN:CB	1:A:199:THR:CB[3_545]	1.39	0.81
1:A:128:SER:C	1:A:188:GLN:NE2[2_656]	1.39	0.81
1:A:134:PRO:O	1:A:295:PHE:O[2_656]	1.40	0.80
1:A:65:GLU:OE1	1:A:260:ILE:N[3_545]	1.41	0.79
1:A:67:SER:N	1:A:196:ASP:OD1[3_545]	1.42	0.78
1:A:65:GLU:CG	1:A:260:ILE:N[3_545]	1.43	0.77
1:A:69:TYR:C	1:A:291:SER:O[2_656]	1.43	0.77
1:A:133:GLN:CA	1:A:293:ILE:CA[2_656]	1.45	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:THR:CG2	1:A:281:SER:O[3_555]	1.45	0.75
1:A:134:PRO:CG	1:A:290:ASN:CG[2_656]	1.46	0.74
1:A:107:GLN:CA	1:A:202:SER:C[3_545]	1.47	0.73
1:A:135:GLN:CA	1:A:294:GLY:N[2_656]	1.47	0.73
1:A:146:SER:N	1:A:251:THR:N[3_555]	1.47	0.73
1:A:255:ASP:CA	2:A:424:HOH:O[3_455]	1.47	0.73
1:A:67:SER:C	1:A:196:ASP:OD1[3_545]	1.48	0.72
1:A:100:GLN:OE1	1:A:281:SER:CB[3_555]	1.48	0.72
1:A:70:THR:CG2	2:A:444:HOH:O[3_545]	1.49	0.71
1:A:72:SER:OG	1:A:76:GLY:CA[2_656]	1.49	0.71
1:A:66:LEU:N	1:A:262:GLY:N[3_545]	1.50	0.70
1:A:99:GLY:C	1:A:280:GLY:C[3_555]	1.50	0.70
1:A:128:SER:CB	1:A:188:GLN:CD[2_656]	1.50	0.70
1:A:68:GLY:N	1:A:196:ASP:CB[3_545]	1.51	0.69
1:A:65:GLU:CA	1:A:262:GLY:C[3_545]	1.52	0.68
1:A:86:PHE:CZ	1:A:264:THR:CA[3_545]	1.52	0.68
1:A:100:GLN:CA	1:A:281:SER:N[3_555]	1.53	0.67
1:A:107:GLN:CD	1:A:203:GLN:C[3_545]	1.53	0.67
1:A:255:ASP:C	2:A:424:HOH:O[3_455]	1.53	0.67
1:A:87:THR:CG2	1:A:280:GLY:N[3_555]	1.54	0.66
1:A:106:GLN:CD	1:A:199:THR:N[3_545]	1.54	0.66
1:A:134:PRO:O	1:A:295:PHE:N[2_656]	1.54	0.66
1:A:107:GLN:NE2	1:A:203:GLN:CA[3_545]	1.55	0.65
1:A:68:GLY:N	1:A:196:ASP:OD2[3_545]	1.56	0.64
1:A:86:PHE:CE2	1:A:264:THR:CA[3_545]	1.56	0.64
1:A:133:GLN:CB	1:A:293:ILE:CB[2_656]	1.56	0.64
1:A:145:LYS:O	1:A:250:SER:O[3_555]	1.56	0.64
1:A:222:ASP:OD2	1:A:240:SER:OG[4_556]	1.56	0.64
1:A:64:LYS:O	1:A:262:GLY:C[3_545]	1.57	0.63
1:A:133:GLN:N	1:A:293:ILE:CB[2_656]	1.57	0.63
1:A:69:TYR:CG	1:A:292:GLY:CA[2_656]	1.58	0.62
1:A:132:VAL:O	1:A:293:ILE:O[2_656]	1.59	0.61
1:A:48:ALA:N	1:A:253:LEU:O[3_545]	1.60	0.60
1:A:132:VAL:CB	2:A:377:HOH:O[2_656]	1.60	0.60
1:A:59:PRO:CB	1:A:264:THR:CB[3_545]	1.61	0.59
1:A:51:GLN:NE2	1:A:255:ASP:OD1[3_545]	1.63	0.57
1:A:64:LYS:O	1:A:262:GLY:O[3_545]	1.63	0.57
1:A:145:LYS:C	1:A:250:SER:C[3_555]	1.63	0.57
1:A:195:VAL:CB	2:A:334:HOH:O[3_455]	1.64	0.56
1:A:45:GLU:CB	1:A:257:SER:OG[3_545]	1.65	0.55
1:A:100:GLN:OE1	1:A:281:SER:OG[3_555]	1.65	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:GLN:CD	1:A:198:TYR:C[3_545]	1.65	0.55
1:A:135:GLN:CB	1:A:294:GLY:CA[2_656]	1.65	0.55
1:A:65:GLU:OE2	1:A:260:ILE:CA[3_545]	1.66	0.54
1:A:44:THR:OG1	1:A:266:THR:CB[3_545]	1.67	0.53
1:A:67:SER:CB	2:A:358:HOH:O[3_545]	1.67	0.53
1:A:132:VAL:C	1:A:293:ILE:CG1[2_656]	1.68	0.52
1:A:134:PRO:CG	1:A:290:ASN:ND2[2_656]	1.69	0.51
1:A:106:GLN:CB	1:A:199:THR:OG1[3_545]	1.70	0.50
1:A:143:THR:OG1	1:A:281:SER:O[3_555]	1.71	0.49
1:A:144:VAL:O	1:A:250:SER:CA[3_555]	1.71	0.49
1:A:44:THR:CB	1:A:266:THR:CG2[3_545]	1.72	0.48
1:A:48:ALA:N	1:A:254:PRO:N[3_545]	1.72	0.48
1:A:128:SER:CB	1:A:188:GLN:OE1[2_656]	1.72	0.48
1:A:134:PRO:CD	1:A:290:ASN:OD1[2_656]	1.72	0.48
1:A:107:GLN:CB	1:A:203:GLN:CA[3_545]	1.73	0.47
1:A:133:GLN:N	1:A:293:ILE:CG1[2_656]	1.73	0.47
1:A:74:SER:CA	1:A:74:SER:OG[2_656]	1.74	0.46
1:A:74:SER:O	2:A:440:HOH:O[2_656]	1.74	0.46
1:A:106:GLN:CB	1:A:199:THR:CG2[3_545]	1.74	0.46
1:A:106:GLN:CG	1:A:199:THR:CA[3_545]	1.74	0.46
1:A:133:GLN:N	1:A:293:ILE:CA[2_656]	1.74	0.46
1:A:46:LEU:O	1:A:255:ASP:CA[3_545]	1.75	0.45
1:A:48:ALA:N	1:A:253:LEU:C[3_545]	1.75	0.45
1:A:59:PRO:CG	1:A:264:THR:CG2[3_545]	1.75	0.45
1:A:144:VAL:N	1:A:248:ASP:OD2[3_555]	1.75	0.45
1:A:45:GLU:OE2	1:A:257:SER:OG[3_545]	1.76	0.44
1:A:107:GLN:OE1	1:A:203:GLN:O[3_545]	1.76	0.44
1:A:142:ASP:C	1:A:248:ASP:OD1[3_555]	1.76	0.44
1:A:143:THR:N	1:A:248:ASP:CB[3_555]	1.76	0.44
1:A:51:GLN:CD	1:A:255:ASP:OD1[3_545]	1.77	0.43
1:A:65:GLU:CD	1:A:260:ILE:CA[3_545]	1.77	0.43
1:A:69:TYR:CA	1:A:291:SER:O[2_656]	1.77	0.43
1:A:128:SER:O	1:A:188:GLN:NE2[2_656]	1.77	0.43
1:A:135:GLN:CB	1:A:294:GLY:C[2_656]	1.77	0.43
1:A:134:PRO:N	1:A:293:ILE:N[2_656]	1.78	0.42
1:A:45:GLU:CD	1:A:257:SER:CB[3_545]	1.79	0.41
1:A:50:GLN:CG	2:A:412:HOH:O[3_545]	1.79	0.41
1:A:60:SER:O	1:A:263:TYR:OH[3_545]	1.79	0.41
1:A:60:SER:N	1:A:264:THR:O[3_545]	1.79	0.41
1:A:68:GLY:O	1:A:291:SER:CA[2_656]	1.79	0.41
1:A:107:GLN:CG	1:A:204:SER:N[3_545]	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLN:O	1:A:292:GLY:C[2_656]	1.79	0.41
1:A:135:GLN:CA	1:A:295:PHE:N[2_656]	1.79	0.41
1:A:144:VAL:C	1:A:250:SER:CA[3_555]	1.79	0.41
1:A:146:SER:CA	1:A:250:SER:C[3_555]	1.79	0.41
1:A:72:SER:CB	1:A:76:GLY:CA[2_656]	1.80	0.40
1:A:72:SER:OG	1:A:76:GLY:N[2_656]	1.80	0.40
1:A:107:GLN:C	1:A:202:SER:O[3_545]	1.80	0.40
1:A:133:GLN:CA	1:A:293:ILE:CG2[2_656]	1.80	0.40
1:A:142:ASP:O	1:A:248:ASP:CG[3_555]	1.81	0.39
1:A:50:GLN:NE2	1:A:202:SER:OG[3_545]	1.83	0.37
1:A:65:GLU:CA	1:A:262:GLY:CA[3_545]	1.83	0.37
1:A:74:SER:CB	1:A:74:SER:OG[2_656]	1.83	0.37
1:A:107:GLN:CB	1:A:203:GLN:N[3_545]	1.83	0.37
1:A:142:ASP:O	1:A:248:ASP:CA[3_555]	1.83	0.37
1:A:60:SER:O	1:A:321:PRO:CD[3_545]	1.84	0.36
1:A:86:PHE:CD2	1:A:263:TYR:C[3_545]	1.84	0.36
1:A:107:GLN:CA	1:A:202:SER:O[3_545]	1.84	0.36
1:A:146:SER:N	1:A:250:SER:CA[3_555]	1.84	0.36
1:A:146:SER:OG	1:A:249:CYS:O[3_555]	1.84	0.36
1:A:135:GLN:C	1:A:294:GLY:N[2_656]	1.85	0.35
1:A:135:GLN:N	1:A:294:GLY:CA[2_656]	1.85	0.35
1:A:146:SER:CA	1:A:250:SER:O[3_555]	1.85	0.35
1:A:69:TYR:CD2	1:A:292:GLY:CA[2_656]	1.86	0.34
1:A:291:SER:OG	2:A:444:HOH:O[4_546]	1.86	0.34
1:A:44:THR:O	1:A:255:ASP:CB[3_545]	1.87	0.33
1:A:47:PRO:CG	1:A:254:PRO:CB[3_545]	1.87	0.33
1:A:65:GLU:CB	1:A:260:ILE:O[3_545]	1.87	0.33
1:A:69:TYR:CD2	1:A:292:GLY:O[2_656]	1.87	0.33
1:A:69:TYR:CA	1:A:291:SER:C[2_656]	1.88	0.32
1:A:134:PRO:CB	1:A:290:ASN:CB[2_656]	1.88	0.32
1:A:64:LYS:C	1:A:263:TYR:N[3_545]	1.89	0.31
1:A:65:GLU:C	1:A:261:SER:C[3_545]	1.89	0.31
1:A:87:THR:CG2	1:A:279:ASP:C[3_555]	1.89	0.31
1:A:106:GLN:CB	1:A:199:THR:CA[3_545]	1.89	0.31
1:A:107:GLN:CB	1:A:202:SER:O[3_545]	1.89	0.31
1:A:107:GLN:CB	1:A:202:SER:C[3_545]	1.89	0.31
1:A:128:SER:CA	1:A:188:GLN:CD[2_656]	1.89	0.31
1:A:133:GLN:C	1:A:293:ILE:CA[2_656]	1.89	0.31
1:A:135:GLN:O	1:A:294:GLY:CA[2_656]	1.89	0.31
2:A:440:HOH:O	2:A:440:HOH:O[2_656]	1.89	0.31
1:A:46:LEU:CD2	1:A:201:GLY:O[3_545]	1.90	0.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:PRO:N	1:A:254:PRO:CB[3_545]	1.90	0.30
1:A:106:GLN:NE2	1:A:198:TYR:CA[3_545]	1.90	0.30
1:A:107:GLN:OE1	1:A:228:GLN:NE2[3_545]	1.90	0.30
1:A:134:PRO:O	1:A:295:PHE:C[2_656]	1.90	0.30
1:A:146:SER:CA	1:A:251:THR:O[3_555]	1.90	0.30
1:A:48:ALA:N	1:A:254:PRO:C[3_545]	1.91	0.29
1:A:132:VAL:O	1:A:293:ILE:CG1[2_656]	1.91	0.29
1:A:143:THR:O	1:A:249:CYS:CA[3_555]	1.91	0.29
1:A:143:THR:CB	1:A:281:SER:O[3_555]	1.91	0.29
1:A:69:TYR:OH	1:A:241:ASN:ND2[3_555]	1.92	0.28
1:A:99:GLY:CA	1:A:280:GLY:O[3_555]	1.92	0.28
1:A:106:GLN:N	1:A:199:THR:CG2[3_545]	1.92	0.28
1:A:144:VAL:CA	1:A:250:SER:OG[3_555]	1.92	0.28
1:A:44:THR:OG1	1:A:266:THR:OG1[3_545]	1.93	0.27
1:A:106:GLN:CD	1:A:198:TYR:O[3_545]	1.93	0.27
1:A:107:GLN:CG	1:A:203:GLN:N[3_545]	1.93	0.27
1:A:106:GLN:O	1:A:201:GLY:O[3_545]	1.94	0.26
1:A:133:GLN:CD	1:A:293:ILE:CD1[2_656]	1.94	0.26
1:A:61:ALA:N	1:A:321:PRO:CG[3_545]	1.95	0.25
1:A:64:LYS:C	1:A:262:GLY:C[3_545]	1.95	0.25
1:A:86:PHE:CE1	1:A:264:THR:CB[3_545]	1.95	0.25
1:A:86:PHE:CE2	1:A:263:TYR:O[3_545]	1.95	0.25
1:A:87:THR:CB	1:A:280:GLY:N[3_555]	1.95	0.25
1:A:106:GLN:OE1	1:A:198:TYR:C[3_545]	1.95	0.25
1:A:69:TYR:CD2	1:A:292:GLY:C[2_656]	1.96	0.24
1:A:107:GLN:OE1	1:A:203:GLN:C[3_545]	1.96	0.24
1:A:59:PRO:C	1:A:264:THR:O[3_545]	1.97	0.23
1:A:65:GLU:CA	1:A:262:GLY:N[3_545]	1.97	0.23
1:A:104:ALA:O	2:A:378:HOH:O[3_545]	1.97	0.23
1:A:133:GLN:CG	1:A:293:ILE:CG1[2_656]	1.97	0.23
1:A:46:LEU:C	1:A:255:ASP:N[3_545]	1.98	0.22
1:A:65:GLU:CB	1:A:263:TYR:N[3_545]	1.98	0.22
1:A:132:VAL:CG2	2:A:377:HOH:O[2_656]	1.98	0.22
1:A:60:SER:CA	1:A:263:TYR:OH[3_545]	1.99	0.21
1:A:67:SER:CA	1:A:196:ASP:OD2[3_545]	1.99	0.21
1:A:135:GLN:O	1:A:294:GLY:N[2_656]	1.99	0.21
1:A:145:LYS:CA	1:A:250:SER:CB[3_555]	1.99	0.21
1:A:61:ALA:O	2:A:376:HOH:O[3_545]	2.01	0.19
1:A:136:SER:N	1:A:293:ILE:O[2_656]	2.01	0.19
1:A:47:PRO:CA	1:A:254:PRO:C[3_545]	2.02	0.18
1:A:106:GLN:CD	1:A:199:THR:OG1[3_545]	2.02	0.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:GLN:C	1:A:293:ILE:C[2_656]	2.02	0.18
1:A:65:GLU:N	1:A:263:TYR:CA[3_545]	2.03	0.17
1:A:66:LEU:C	1:A:196:ASP:OD1[3_545]	2.03	0.17
1:A:99:GLY:O	1:A:280:GLY:CA[3_555]	2.03	0.17
1:A:134:PRO:CB	1:A:290:ASN:OD1[2_656]	2.03	0.17
1:A:142:ASP:C	1:A:248:ASP:OD2[3_555]	2.03	0.17
1:A:100:GLN:CA	1:A:281:SER:CA[3_555]	2.04	0.16
1:A:107:GLN:CA	1:A:203:GLN:N[3_545]	2.04	0.16
1:A:195:VAL:CG1	2:A:334:HOH:O[3_455]	2.04	0.16
1:A:259:SER:OG	2:A:325:HOH:O[3_455]	2.04	0.16
1:A:47:PRO:C	1:A:254:PRO:CB[3_545]	2.05	0.15
1:A:74:SER:N	1:A:74:SER:OG[2_656]	2.05	0.15
1:A:86:PHE:CG	1:A:264:THR:OG1[3_545]	2.05	0.15
1:A:106:GLN:C	1:A:199:THR:CG2[3_545]	2.05	0.15
1:A:134:PRO:O	1:A:295:PHE:CA[2_656]	2.05	0.15
1:A:256:PHE:N	2:A:424:HOH:O[3_455]	2.05	0.15
1:A:291:SER:CB	2:A:444:HOH:O[4_546]	2.05	0.15
1:A:60:SER:C	1:A:263:TYR:OH[3_545]	2.06	0.14
1:A:65:GLU:N	1:A:262:GLY:C[3_545]	2.06	0.14
1:A:100:GLN:N	1:A:280:GLY:C[3_555]	2.06	0.14
1:A:100:GLN:CD	1:A:281:SER:CB[3_555]	2.06	0.14
1:A:134:PRO:CD	1:A:292:GLY:N[2_656]	2.06	0.14
1:A:135:GLN:C	1:A:293:ILE:O[2_656]	2.06	0.14
1:A:135:GLN:CB	1:A:294:GLY:O[2_656]	2.06	0.14
1:A:142:ASP:N	1:A:248:ASP:OD1[3_555]	2.06	0.14
1:A:222:ASP:CG	1:A:240:SER:OG[4_556]	2.06	0.14
1:A:65:GLU:OE2	1:A:260:ILE:CB[3_545]	2.07	0.13
1:A:133:GLN:CB	1:A:293:ILE:CG2[2_656]	2.08	0.12
1:A:48:ALA:CB	1:A:253:LEU:C[3_545]	2.09	0.11
1:A:135:GLN:O	1:A:293:ILE:C[2_656]	2.09	0.11
1:A:46:LEU:O	1:A:255:ASP:CB[3_545]	2.10	0.10
1:A:47:PRO:C	1:A:254:PRO:N[3_545]	2.10	0.10
1:A:51:GLN:CD	1:A:255:ASP:CG[3_545]	2.10	0.10
1:A:74:SER:N	1:A:74:SER:CB[2_656]	2.10	0.10
1:A:144:VAL:CB	1:A:250:SER:OG[3_555]	2.11	0.09
1:A:48:ALA:CA	1:A:253:LEU:C[3_545]	2.12	0.08
1:A:60:SER:CB	1:A:263:TYR:OH[3_545]	2.12	0.08
1:A:65:GLU:CD	1:A:259:SER:O[3_545]	2.12	0.08
1:A:65:GLU:CG	1:A:259:SER:C[3_545]	2.12	0.08
1:A:69:TYR:CZ	1:A:241:ASN:ND2[3_555]	2.12	0.08
1:A:100:GLN:CD	1:A:281:SER:OG[3_555]	2.12	0.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLN:C	1:A:281:SER:N[3_555]	2.12	0.08
1:A:106:GLN:CD	1:A:199:THR:CA[3_545]	2.12	0.08
1:A:135:GLN:NE2	1:A:240:SER:N[3_555]	2.13	0.07
1:A:143:THR:O	1:A:248:ASP:C[3_555]	2.14	0.06
1:A:146:SER:CA	1:A:251:THR:C[3_555]	2.14	0.06
1:A:51:GLN:OE1	1:A:255:ASP:OD1[3_545]	2.15	0.05
1:A:106:GLN:CA	1:A:199:THR:CB[3_545]	2.15	0.05
1:A:107:GLN:CD	1:A:203:GLN:O[3_545]	2.15	0.05
1:A:134:PRO:C	1:A:295:PHE:N[2_656]	2.15	0.05
1:A:45:GLU:O	1:A:255:ASP:O[3_545]	2.16	0.04
1:A:47:PRO:CB	1:A:254:PRO:CA[3_545]	2.16	0.04
1:A:51:GLN:NE2	1:A:255:ASP:CB[3_545]	2.16	0.04
1:A:142:ASP:CA	1:A:248:ASP:CG[3_555]	2.16	0.04
1:A:69:TYR:CB	1:A:292:GLY:CA[2_656]	2.17	0.03
1:A:107:GLN:NE2	1:A:203:GLN:N[3_545]	2.17	0.03
1:A:107:GLN:CG	1:A:203:GLN:O[3_545]	2.17	0.03
1:A:108:ILE:N	1:A:202:SER:O[3_545]	2.17	0.03
1:A:45:GLU:CB	1:A:257:SER:CB[3_545]	2.18	0.02
1:A:47:PRO:C	1:A:254:PRO:C[3_545]	2.18	0.02
1:A:63:GLY:O	1:A:263:TYR:CD2[3_545]	2.18	0.02
1:A:86:PHE:CZ	1:A:264:THR:CB[3_545]	2.18	0.02
1:A:107:GLN:CD	1:A:203:GLN:N[3_545]	2.18	0.02
1:A:142:ASP:CA	1:A:248:ASP:CB[3_555]	2.18	0.02
1:A:100:GLN:N	1:A:280:GLY:O[3_555]	2.19	0.01
1:A:142:ASP:CA	1:A:248:ASP:OD1[3_555]	2.19	0.01
1:A:142:ASP:O	1:A:248:ASP:OD2[3_555]	2.19	0.01
1:A:146:SER:CA	1:A:251:THR:N[3_555]	2.19	0.01
1:A:146:SER:CB	1:A:251:THR:C[3_555]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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	321/323 (99%)	316 (98%)	4 (1%)	1 (0%)	36 25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	ASP

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	259/259 (100%)	245 (95%)	14 (5%)	20 8

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	28	LEU
1	A	64	LYS
1	A	72	SER
1	A	107	GLN
1	A	111	GLN
1	A	133	GLN
1	A	158	LYS
1	A	161	GLN
1	A	174	LYS
1	A	223	ASP
1	A	234	SER
1	A	284	LEU
1	A	293	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN

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Mol	Chain	Res	Type
1	A	31	ASN
1	A	50	GLN
1	A	107	GLN
1	A	114	GLN
1	A	137	GLN
1	A	150	GLN
1	A	228	GLN
1	A	306	GLN

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.