



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 10:25 pm GMT

PDB ID : 1RTC
Title : THE STRUCTURE OF RECOMBINANT RICIN A CHAIN AT 2.3
ANGSTROMS
Authors : Mlsna, D.; Monzingo, A.F.; Katzin, B.J.; Ernst, S.; Robertus, J.D.
Deposited on : 1992-10-29
Resolution : 2.30 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
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

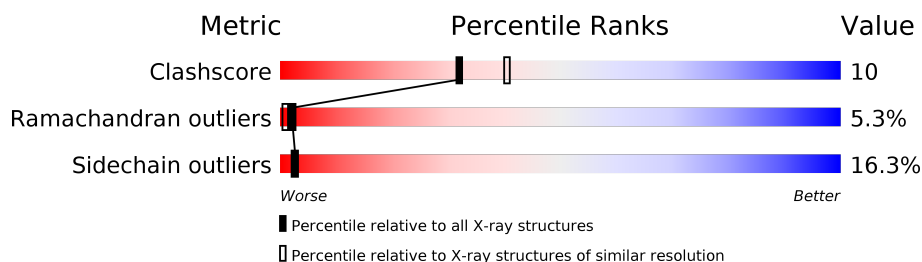
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)

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 $\leq 5\%$. 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	A	268	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2180 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 RICIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	2	0
			2132	1354	374	398	6			

- Molecule 2 is water.

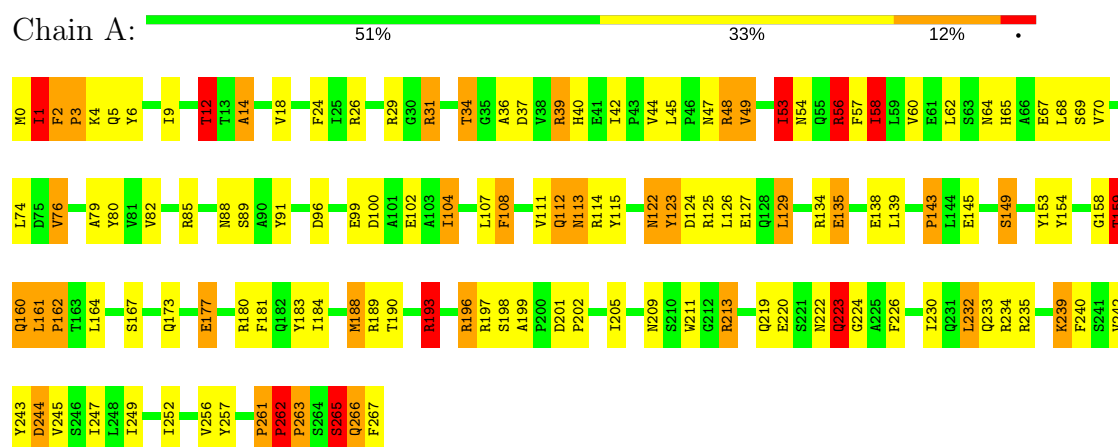
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	48	Total	O	0	0
			48	48		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 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: RICIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.60Å 68.10Å 50.20Å 90.00° 112.90° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.230 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2180	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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	1.52	3/2188 (0.1%)	2.29	107/2974 (3.6%)

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	A	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	ARG	NE-CZ	6.66	1.41	1.33
1	A	261	PRO	N-CD	-6.21	1.39	1.47
1	A	69	SER	CA-CB	-5.36	1.45	1.52

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ARG	NE-CZ-NH2	-14.10	113.25	120.30
1	A	125	ARG	NE-CZ-NH1	11.54	126.07	120.30
1	A	85	ARG	NE-CZ-NH1	10.58	125.59	120.30
1	A	180	ARG	NE-CZ-NH2	-10.29	115.16	120.30
1	A	114	ARG	NE-CZ-NH2	-10.23	115.19	120.30
1	A	161	LEU	CA-CB-CG	9.36	136.83	115.30
1	A	211	TRP	CD1-CG-CD2	9.27	113.72	106.30
1	A	31	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	A	211	TRP	CG-CD2-CE3	8.82	141.84	133.90
1	A	211	TRP	CE2-CD2-CG	-8.79	100.27	107.30
1	A	112	GLN	O-C-N	-8.51	109.09	122.70
1	A	196	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	A	12	THR	CA-CB-CG2	8.29	124.01	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	A	56	ARG	CG-CD-NE	-8.16	94.66	111.80
1	A	34	THR	CA-CB-CG2	-8.16	100.98	112.40
1	A	45	LEU	N-CA-CB	-8.12	94.17	110.40
1	A	36	ALA	N-CA-C	7.99	132.58	111.00
1	A	188	MET	CG-SD-CE	-7.96	87.47	100.20
1	A	37	ASP	N-CA-C	-7.93	89.58	111.00
1	A	53	ILE	CB-CA-C	-7.91	95.77	111.60
1	A	159	THR	CA-CB-CG2	7.87	123.42	112.40
1	A	112	GLN	CA-C-N	7.86	134.49	117.20
1	A	114	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	A	213	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	A	29	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	A	143	PRO	CA-N-CD	-7.49	101.01	111.50
1	A	159	THR	OG1-CB-CG2	-7.32	93.16	110.00
1	A	262	PRO	CA-N-CD	-7.21	101.40	111.50
1	A	242	VAL	CG1-CB-CG2	-7.18	99.42	110.90
1	A	0	MET	N-CA-C	-7.15	91.69	111.00
1	A	100	ASP	CB-CG-OD1	7.05	124.65	118.30
1	A	3	PRO	CA-N-CD	-6.78	102.01	111.50
1	A	100	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	A	158	GLY	C-N-CA	6.66	138.35	121.70
1	A	201	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	A	56	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	A	80	TYR	CB-CG-CD1	6.61	124.97	121.00
1	A	44	VAL	CG1-CB-CG2	-6.61	100.33	110.90
1	A	244	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	A	219	GLN	CA-CB-CG	-6.43	99.24	113.40
1	A	180	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	153	TYR	CB-CG-CD1	-6.29	117.23	121.00
1	A	205	ILE	CA-C-N	6.29	131.03	117.20
1	A	167	SER	O-C-N	-6.24	112.72	122.70
1	A	2	PHE	N-CA-C	6.19	127.71	111.00
1	A	6	TYR	CB-CG-CD1	-6.19	117.29	121.00
1	A	113	ASN	CB-CA-C	-6.17	98.07	110.40
1	A	220	GLU	CA-CB-CG	6.10	126.82	113.40
1	A	125	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	A	196	ARG	NH1-CZ-NH2	-6.07	112.72	119.40
1	A	104	ILE	CA-CB-CG1	-6.06	99.49	111.00
1	A	112	GLN	CB-CG-CD	6.05	127.33	111.60
1	A	161	LEU	CB-CA-C	-6.05	98.70	110.20
1	A	145	GLU	CB-CA-C	-6.04	98.32	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	VAL	CG1-CB-CG2	-5.96	101.37	110.90
1	A	58	ILE	CG1-CB-CG2	-5.93	98.36	111.40
1	A	149	SER	CA-CB-OG	-5.89	95.30	111.20
1	A	29	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	A	39	ARG	NH1-CZ-NH2	-5.88	112.93	119.40
1	A	193	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	2	PHE	CB-CG-CD2	-5.85	116.70	120.80
1	A	26	ARG	CA-CB-CG	-5.85	100.54	113.40
1	A	48	ARG	CD-NE-CZ	5.82	131.75	123.60
1	A	14	ALA	CA-C-O	-5.80	107.91	120.10
1	A	0	MET	CA-C-N	5.76	129.88	117.20
1	A	164	LEU	CA-CB-CG	5.76	128.55	115.30
1	A	235	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	14	ALA	CB-CA-C	-5.71	101.53	110.10
1	A	1	ILE	CA-C-N	5.71	129.76	117.20
1	A	240	PHE	CA-C-N	5.70	129.74	117.20
1	A	164	LEU	O-C-N	-5.70	113.59	122.70
1	A	45	LEU	CB-CA-C	5.63	120.90	110.20
1	A	265	SER	O-C-N	-5.61	113.73	122.70
1	A	24	PHE	CB-CG-CD2	-5.59	116.88	120.80
1	A	125	ARG	CB-CG-CD	5.55	126.04	111.60
1	A	104	ILE	CA-CB-CG2	5.53	121.96	110.90
1	A	74	LEU	O-C-N	-5.51	113.89	122.70
1	A	243	TYR	CB-CG-CD1	-5.50	117.70	121.00
1	A	3	PRO	N-CA-C	5.50	126.40	112.10
1	A	183	TYR	CG-CD1-CE1	-5.45	116.94	121.30
1	A	223	GLN	CA-C-N	-5.45	105.31	116.20
1	A	45	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	211	TRP	CA-C-N	5.40	127.01	116.20
1	A	12	THR	CA-CB-OG1	-5.38	97.69	109.00
1	A	114	ARG	CB-CG-CD	-5.38	97.60	111.60
1	A	65	HIS	CB-CA-C	-5.31	99.78	110.40
1	A	196	ARG	O-C-N	-5.31	114.20	122.70
1	A	244	ASP	N-CA-CB	-5.28	101.10	110.60
1	A	34	THR	N-CA-CB	-5.26	100.30	110.30
1	A	256	VAL	O-C-N	-5.25	114.29	122.70
1	A	124	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	82	VAL	CG1-CB-CG2	-5.23	102.53	110.90
1	A	14	ALA	CA-C-N	5.22	126.65	116.20
1	A	108	PHE	N-CA-C	-5.22	96.92	111.00
1	A	193	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	112	GLN	N-CA-C	-5.18	97.00	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	ASN	N-CA-CB	5.18	119.93	110.60
1	A	68	LEU	CA-CB-CG	5.18	127.21	115.30
1	A	76	VAL	N-CA-CB	-5.17	100.12	111.50
1	A	88	ASN	CA-C-O	-5.14	109.30	120.10
1	A	76	VAL	CB-CA-C	5.12	121.13	111.40
1	A	193	ARG	CD-NE-CZ	5.11	130.75	123.60
1	A	85	ARG	NH1-CZ-NH2	-5.08	113.81	119.40
1	A	190	THR	CA-CB-CG2	5.08	119.51	112.40
1	A	2	PHE	N-CA-CB	-5.07	101.48	110.60
1	A	257	TYR	CG-CD2-CE2	5.06	125.35	121.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	ILE	Peptide
1	A	115	TYR	Sidechain
1	A	223	GLN	Mainchain
1	A	56	ARG	Sidechain
1	A	91	TYR	Sidechain

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	2132	0	2104	43	0
2	A	48	0	0	4	0
All	All	2180	0	2104	43	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 10.

All (43) 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:161:LEU:HD23	2:A:299:HOH:O	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLU:HB2	2:A:292:HOH:O	1.81	0.80
1:A:143:PRO:HG3	2:A:292:HOH:O	1.84	0.75
1:A:123:TYR:O	1:A:127:GLU:HG3	1.89	0.73
1:A:161:LEU:HB2	1:A:162:PRO:HD3	1.76	0.66
1:A:122:ASN:H	1:A:122:ASN:HD22	1.46	0.64
1:A:135:GLU:O	1:A:199:ALA:HB1	2.04	0.57
1:A:129:LEU:HD23	1:A:161:LEU:HD13	1.87	0.56
1:A:122:ASN:H	1:A:122:ASN:ND2	2.03	0.56
1:A:224:GLY:O	1:A:245:VAL:HG23	2.06	0.56
1:A:159:THR:HG22	1:A:160:GLN:H	1.70	0.55
1:A:9:ILE:HD11	1:A:31:ARG:HG3	1.89	0.55
1:A:154:TYR:HD1	1:A:159:THR:HA	1.74	0.53
1:A:108:PHE:O	1:A:111:VAL:HG22	2.09	0.52
1:A:47:ASN:OD1	1:A:49:VAL:HG23	2.11	0.51
1:A:1:ILE:HG12	1:A:2:PHE:N	2.25	0.50
1:A:262:PRO:HD2	1:A:263:PRO:HD2	1.93	0.50
1:A:12:THR:HG23	1:A:14:ALA:HB3	1.93	0.49
1:A:154:TYR:CE1	1:A:159:THR:HG23	2.49	0.48
1:A:134:ARG:HH12	1:A:209:ASN:ND2	2.12	0.48
1:A:173:GLN:HA	1:A:177:GLU:HB2	1.96	0.48
1:A:226:PHE:CD2	1:A:230:ILE:HG12	2.49	0.47
1:A:202:PRO:HB3	1:A:233:GLN:NE2	2.30	0.46
1:A:134:ARG:HH22	1:A:209:ASN:HD21	1.63	0.46
1:A:60:VAL:HG12	1:A:62:LEU:HD13	1.97	0.46
1:A:129:LEU:CD2	1:A:161:LEU:HD22	2.46	0.46
1:A:139:LEU:HD13	1:A:188:MET:CE	2.46	0.46
1:A:56:ARG:O	1:A:76:VAL:HB	2.16	0.45
1:A:143:PRO:HD3	1:A:197:ARG:CZ	2.47	0.45
1:A:42:ILE:HD13	1:A:252:ILE:HG23	1.98	0.45
1:A:53:ILE:HD13	2:A:332:HOH:O	2.16	0.44
1:A:232:LEU:HA	1:A:232:LEU:HD12	1.85	0.44
1:A:202:PRO:HB3	1:A:233:GLN:HE22	1.82	0.44
1:A:154:TYR:HE1	1:A:159:THR:HG23	1.82	0.43
1:A:181:PHE:CD2	1:A:184:ILE:HD12	2.53	0.42
1:A:57:PHE:O	1:A:58:ILE:HD12	2.20	0.42
1:A:226:PHE:CE2	1:A:230:ILE:HG12	2.56	0.41
1:A:266:GLN:O	1:A:267:PHE:CD1	2.73	0.41
1:A:18:VAL:HG21	1:A:193:ARG:HG2	2.02	0.41
1:A:64:ASN:ND2	1:A:149:SER:OG	2.53	0.41
1:A:161:LEU:HB2	1:A:162:PRO:CD	2.46	0.41
1:A:249:ILE:HG21	1:A:249:ILE:HD13	1.88	0.41

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	268/268 (100%)	233 (87%)	21 (8%)	14 (5%)	2 1

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	PRO
1	A	67	GLU
1	A	159	THR
1	A	262	PRO
1	A	79	ALA
1	A	265	SER
1	A	4	LYS
1	A	160	GLN
1	A	123	TYR
1	A	40	HIS
1	A	113	ASN
1	A	1	ILE
1	A	263	PRO
1	A	261	PRO

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	229/227 (101%)	190 (83%)	39 (17%)	2 2

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ILE
1	A	5	GLN
1	A	12	THR
1	A	34	THR
1	A	39	ARG
1	A	48	ARG
1	A	53	ILE
1	A	54	ASN
1	A	56	ARG
1	A	58	ILE
1	A	70	VAL
1	A	89	SER
1	A	96	ASP
1	A	99[A]	GLU
1	A	99[B]	GLU
1	A	102	GLU
1	A	104	ILE
1	A	107	LEU
1	A	112	GLN
1	A	122	ASN
1	A	126	LEU
1	A	129	LEU
1	A	135	GLU
1	A	162	PRO
1	A	177	GLU
1	A	189	ARG
1	A	193	ARG
1	A	196	ARG
1	A	198	SER
1	A	213	ARG
1	A	222	ASN
1	A	223	GLN
1	A	232	LEU
1	A	239[A]	LYS
1	A	239[B]	LYS
1	A	244	ASP
1	A	247	ILE
1	A	265	SER

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Mol	Chain	Res	Type
1	A	266	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	55	GLN
1	A	113	ASN
1	A	122	ASN
1	A	173	GLN
1	A	182	GLN
1	A	209	ASN
1	A	223	GLN
1	A	233	GLN
1	A	266	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.