



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:01 PM GMT

PDB ID : 1DPO
Title : STRUCTURE OF RAT TRYPSIN
Authors : Stroud, R.M.
Deposited on : 1997-03-31
Resolution : 1.59 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

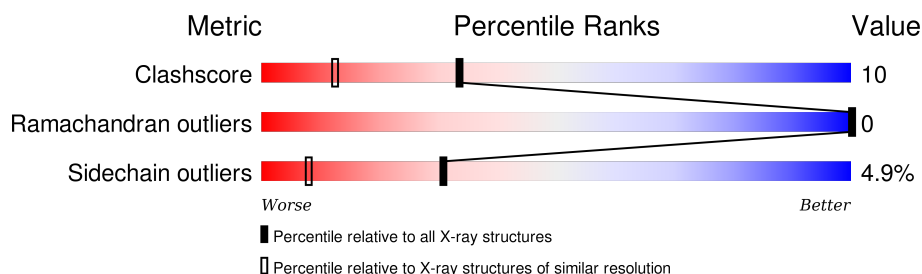
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.59 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	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)

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	223	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 1926 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 TRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	2	0
			1671	1045	285	326	15			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	CYS	SER	ENGINEERED	UNP P00763

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

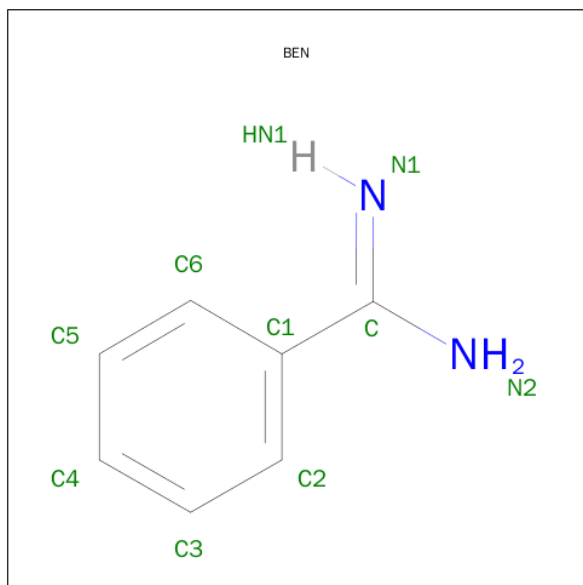
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is BENZAMIDINE (three-letter code: BEN) (formula: C₇H₈N₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 9 7 2	0	0
4	A	1	Total C N 9 7 2	0	0
4	A	1	Total C N 9 7 2	0	0

- Molecule 5 is water.

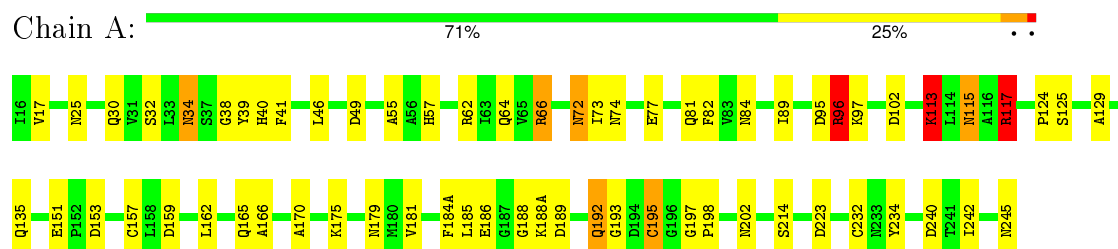
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	217	Total O 217 217	0	0

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: TRYPSIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	123.12Å 123.12Å 123.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 1.59	Depositor
% Data completeness (in resolution range)	97.0 (12.00-1.59)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.174 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1926	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, BEN, SO4

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	1.34	3/1715 (0.2%)	2.41	58/2337 (2.5%)

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	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	GLU	CD-OE2	6.54	1.32	1.25
1	A	195	CYS	CB-SG	5.23	1.91	1.82
1	A	66	ARG	CZ-NH2	5.12	1.39	1.33

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	ARG	CD-NE-CZ	34.95	172.53	123.60
1	A	117	ARG	NE-CZ-NH1	25.64	133.12	120.30
1	A	62	ARG	NE-CZ-NH2	-20.66	109.97	120.30
1	A	96	ARG	NE-CZ-NH1	14.50	127.55	120.30
1	A	113	LYS	CA-CB-CG	14.25	144.75	113.40
1	A	117	ARG	NE-CZ-NH2	-13.29	113.66	120.30
1	A	66	ARG	NE-CZ-NH1	13.17	126.89	120.30
1	A	175	LYS	CD-CE-NZ	12.64	140.77	111.70
1	A	175	LYS	CG-CD-CE	11.68	146.95	111.90
1	A	62	ARG	CG-CD-NE	-11.37	87.93	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	TYR	CB-CG-CD1	-10.79	114.53	121.00
1	A	96	ARG	CB-CG-CD	10.19	138.09	111.60
1	A	95	ASP	CB-CG-OD2	-10.13	109.18	118.30
1	A	41	PHE	CB-CG-CD1	-9.97	113.82	120.80
1	A	62	ARG	CD-NE-CZ	-9.36	110.49	123.60
1	A	95	ASP	CB-CG-OD1	9.31	126.67	118.30
1	A	39	TYR	CB-CG-CD2	8.94	126.36	121.00
1	A	49	ASP	CB-CG-OD1	8.49	125.94	118.30
1	A	153	ASP	CB-CG-OD2	-8.21	110.91	118.30
1	A	62	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	A	82	PHE	CB-CG-CD1	7.44	126.01	120.80
1	A	186	GLU	OE1-CD-OE2	7.36	132.13	123.30
1	A	175	LYS	CA-CB-CG	7.17	129.18	113.40
1	A	186	GLU	CG-CD-OE2	-7.04	104.23	118.30
1	A	245	ASN	CA-C-O	-7.00	105.41	120.10
1	A	240	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	A	96	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	202	ASN	OD1-CG-ND2	-6.52	106.91	121.90
1	A	184(A)	PHE	CB-CG-CD1	-6.50	116.25	120.80
1	A	96	ARG	CD-NE-CZ	-6.44	114.58	123.60
1	A	125	SER	CB-CA-C	6.39	122.24	110.10
1	A	242	ILE	O-C-N	6.30	132.78	122.70
1	A	202	ASN	CB-CG-OD1	6.29	134.17	121.60
1	A	223	ASP	CB-CG-OD1	-6.26	112.67	118.30
1	A	89	ILE	O-C-N	6.24	132.69	122.70
1	A	96	ARG	CA-CB-CG	6.19	127.01	113.40
1	A	151	GLU	OE1-CD-OE2	6.16	130.69	123.30
1	A	170	ALA	CB-CA-C	-6.04	101.04	110.10
1	A	81	GLN	N-CA-CB	5.94	121.30	110.60
1	A	62	ARG	NH1-CZ-NH2	5.91	125.90	119.40
1	A	82	PHE	CB-CG-CD2	-5.78	116.76	120.80
1	A	179	ASN	OD1-CG-ND2	5.66	134.91	121.90
1	A	117	ARG	NH1-CZ-NH2	-5.63	113.21	119.40
1	A	159	ASP	O-C-N	-5.51	113.89	122.70
1	A	197	GLY	O-C-N	5.43	131.43	121.10
1	A	234	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	A	84	ASN	CB-CG-ND2	5.34	129.53	116.70
1	A	77	GLU	OE1-CD-OE2	5.27	129.62	123.30
1	A	46	LEU	CB-CG-CD2	-5.23	102.11	111.00
1	A	245	ASN	CA-CB-CG	-5.16	102.06	113.40
1	A	189	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	73	ILE	CA-C-O	-5.07	109.45	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	CYS	N-CA-CB	-5.06	101.49	110.60
1	A	159	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	166	ALA	CA-C-O	-5.04	109.52	120.10
1	A	188	GLY	CA-C-O	-5.03	111.55	120.60
1	A	55	ALA	CB-CA-C	-5.01	102.59	110.10
1	A	185	LEU	CB-CG-CD1	-5.01	102.49	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	96	ARG	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	1671	0	1611	34	0
2	A	1	0	0	0	0
3	A	10	0	0	0	0
4	A	27	0	21	0	0
5	A	217	0	0	4	3
All	All	1926	0	1632	34	3

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 (34) 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:162[B]:LEU:HD21	1:A:181:VAL:CG2	1.36	1.51
1:A:162[B]:LEU:CD2	1:A:181:VAL:CG2	2.15	1.24
1:A:162[B]:LEU:CD2	1:A:181:VAL:HG21	1.79	1.02
1:A:57:HIS:NE2	1:A:195:CYS:HB3	1.80	0.97
1:A:162[B]:LEU:CD2	1:A:181:VAL:HG22	1.90	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ASN:HD22	1:A:74:ASN:H	1.26	0.83
1:A:162[B]:LEU:HD21	1:A:181:VAL:HG21	0.82	0.82
1:A:25:ASN:HD22	1:A:117:ARG:NH1	1.79	0.80
1:A:135:GLN:NE2	5:A:459:HOH:O	2.15	0.80
1:A:34:ASN:ND2	1:A:38:GLY:H	1.82	0.77
1:A:25:ASN:HD22	1:A:117:ARG:HH11	1.29	0.76
1:A:72:ASN:ND2	1:A:74:ASN:H	1.85	0.75
1:A:64:GLN:HE21	1:A:66:ARG:HE	1.38	0.71
1:A:64:GLN:NE2	1:A:66:ARG:HE	1.92	0.68
1:A:115:ASN:HD22	1:A:117:ARG:H	1.45	0.64
1:A:64:GLN:HE22	1:A:66:ARG:HH21	1.45	0.63
1:A:32:SER:OG	1:A:40:HIS:HD2	1.82	0.62
1:A:57:HIS:NE2	1:A:195:CYS:CB	2.64	0.56
1:A:115:ASN:ND2	1:A:117:ARG:H	2.02	0.56
1:A:162[B]:LEU:HD13	5:A:359:HOH:O	2.06	0.55
1:A:115:ASN:C	1:A:115:ASN:HD22	2.10	0.55
1:A:162[B]:LEU:HD23	1:A:181:VAL:HG22	1.88	0.52
1:A:72:ASN:C	1:A:72:ASN:HD22	2.14	0.51
1:A:40:HIS:HE1	1:A:193:GLY:O	1.98	0.47
1:A:57:HIS:HE1	1:A:214:SER:HA	1.79	0.47
1:A:195:CYS:SG	5:A:354:HOH:O	2.23	0.46
1:A:192:GLN:H	1:A:192:GLN:NE2	2.13	0.46
1:A:57:HIS:ND1	1:A:102:ASP:OD2	2.42	0.45
1:A:30:GLN:HE22	1:A:198:PRO:HD2	1.82	0.44
1:A:57:HIS:CD2	5:A:354:HOH:O	2.71	0.43
1:A:17:VAL:O	1:A:188(A):LYS:HA	2.20	0.42
1:A:124:PRO:HG2	1:A:232:CYS:HA	2.03	0.41
1:A:129:ALA:HB3	1:A:162[A]:LEU:HD11	2.03	0.41
1:A:113:LYS:HE2	1:A:113:LYS:HB3	1.69	0.40

All (3) 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)
5:A:404:HOH:O	5:A:404:HOH:O[4_566]	1.98	0.22
5:A:399:HOH:O	5:A:402:HOH:O[3_556]	2.04	0.16
5:A:323:HOH:O	5:A:323:HOH:O[2_565]	2.17	0.03

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	223/223 (100%)	219 (98%)	4 (2%)	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	187/185 (101%)	178 (95%)	9 (5%)	31	8

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	72	ASN
1	A	96	ARG
1	A	97	LYS
1	A	113	LYS
1	A	115	ASN
1	A	117	ARG
1	A	165	GLN
1	A	192	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	25	ASN
1	A	30	GLN
1	A	34	ASN
1	A	40	HIS
1	A	50	GLN
1	A	64	GLN
1	A	72	ASN
1	A	84	ASN
1	A	93	ASN
1	A	101	ASN
1	A	115	ASN
1	A	135	GLN
1	A	165	GLN
1	A	192	GLN
1	A	210	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](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BEN	A	247	-	9,9,9	1.95	3 (33%)	9,11,11	2.65	6 (66%)
4	BEN	A	248	-	9,9,9	1.99	3 (33%)	9,11,11	1.51	2 (22%)
4	BEN	A	249	-	9,9,9	2.24	2 (22%)	9,11,11	2.40	4 (44%)
3	SO4	A	250	-	4,4,4	0.73	0	6,6,6	0.82	0
3	SO4	A	251	-	4,4,4	1.10	0	6,6,6	0.77	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BEN	A	247	-	-	0/4/4/4	0/1/1/1
4	BEN	A	248	-	-	0/4/4/4	0/1/1/1
4	BEN	A	249	-	-	0/4/4/4	0/1/1/1
3	SO4	A	250	-	-	0/0/0/0	0/0/0/0
3	SO4	A	251	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	249	BEN	C1-C	-4.90	1.39	1.47
4	A	248	BEN	C1-C	-3.78	1.41	1.47
4	A	247	BEN	C1-C	-3.28	1.42	1.47
4	A	247	BEN	C5-C4	2.09	1.43	1.38
4	A	248	BEN	C4-C3	2.20	1.43	1.38
4	A	247	BEN	C5-C6	2.40	1.43	1.38
4	A	248	BEN	C3-C2	2.52	1.44	1.38
4	A	249	BEN	C4-C3	2.87	1.45	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	249	BEN	C2-C1-C	-4.63	114.81	120.67
4	A	247	BEN	C3-C2-C1	-3.48	115.96	120.33
4	A	247	BEN	C5-C4-C3	-3.18	114.34	119.93
4	A	249	BEN	C4-C3-C2	-3.03	115.75	120.19
4	A	249	BEN	C5-C6-C1	-2.57	117.10	120.33
4	A	247	BEN	C6-C1-C	-2.08	118.04	120.67
4	A	248	BEN	C6-C1-C2	-2.04	115.57	118.60
4	A	247	BEN	C6-C1-C2	2.23	121.92	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	248	BEN	C5-C6-C1	2.58	123.58	120.33
4	A	247	BEN	C1-C-N2	2.98	122.87	118.11
4	A	249	BEN	C6-C1-C2	3.49	123.79	118.60
4	A	247	BEN	C4-C3-C2	4.33	126.52	120.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 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.