



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 09:01 AM UTC

PDB ID : 1J37 / pdb_00001j37
Title : Crystal Structure of Drosophila AnCE
Authors : Kim, H.M.; Shin, D.R.; Yoo, O.J.; Lee, H.; Lee, J.-O.
Deposited on : 2003-01-20
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

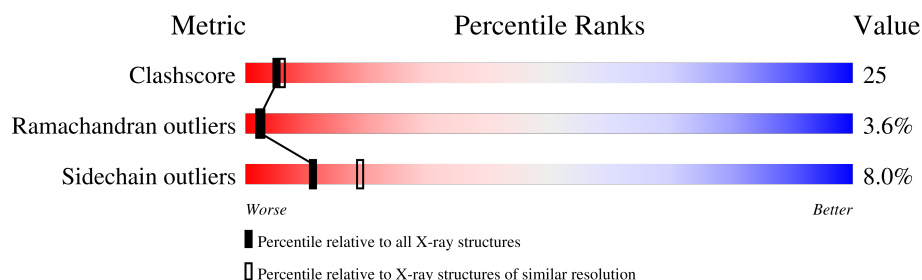
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	607	 52% 37% 8% ..
1	B	607	 53% 37% 8% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9830 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 angiotensin converting enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	598	Total	C	N	O	S	154	0	0
			4900	3135	819	926	20			
1	B	598	Total	C	N	O	S	154	0	0
			4900	3135	819	926	20			

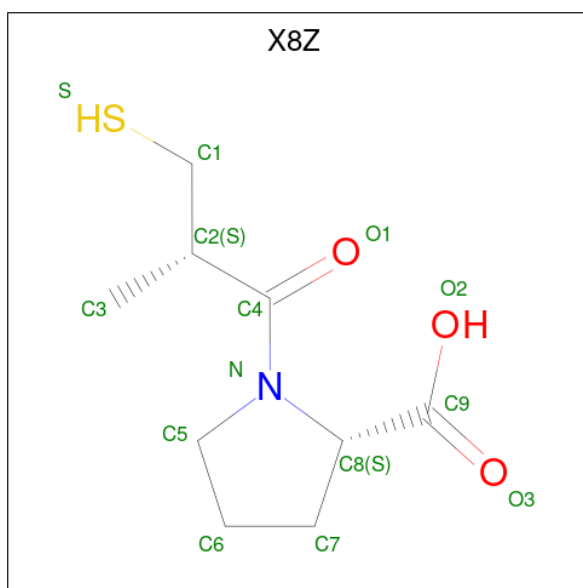
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	ARG	GLY	conflict	UNP Q10714
A	53	ALA	ASN	conflict	UNP Q10714
A	607	ILE	THR	conflict	UNP Q10714
A	616	HIS	-	expression tag	UNP Q10714
A	617	HIS	-	expression tag	UNP Q10714
A	618	HIS	-	expression tag	UNP Q10714
A	619	HIS	-	expression tag	UNP Q10714
A	620	HIS	-	expression tag	UNP Q10714
B	51	ARG	GLY	conflict	UNP Q10714
B	53	ALA	ASN	conflict	UNP Q10714
B	607	ILE	THR	conflict	UNP Q10714
B	616	HIS	-	expression tag	UNP Q10714
B	617	HIS	-	expression tag	UNP Q10714
B	618	HIS	-	expression tag	UNP Q10714
B	619	HIS	-	expression tag	UNP Q10714
B	620	HIS	-	expression tag	UNP Q10714

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is L-CAPTOPRIL (CCD ID: X8Z) (formula: $C_9H_{15}NO_3S$).



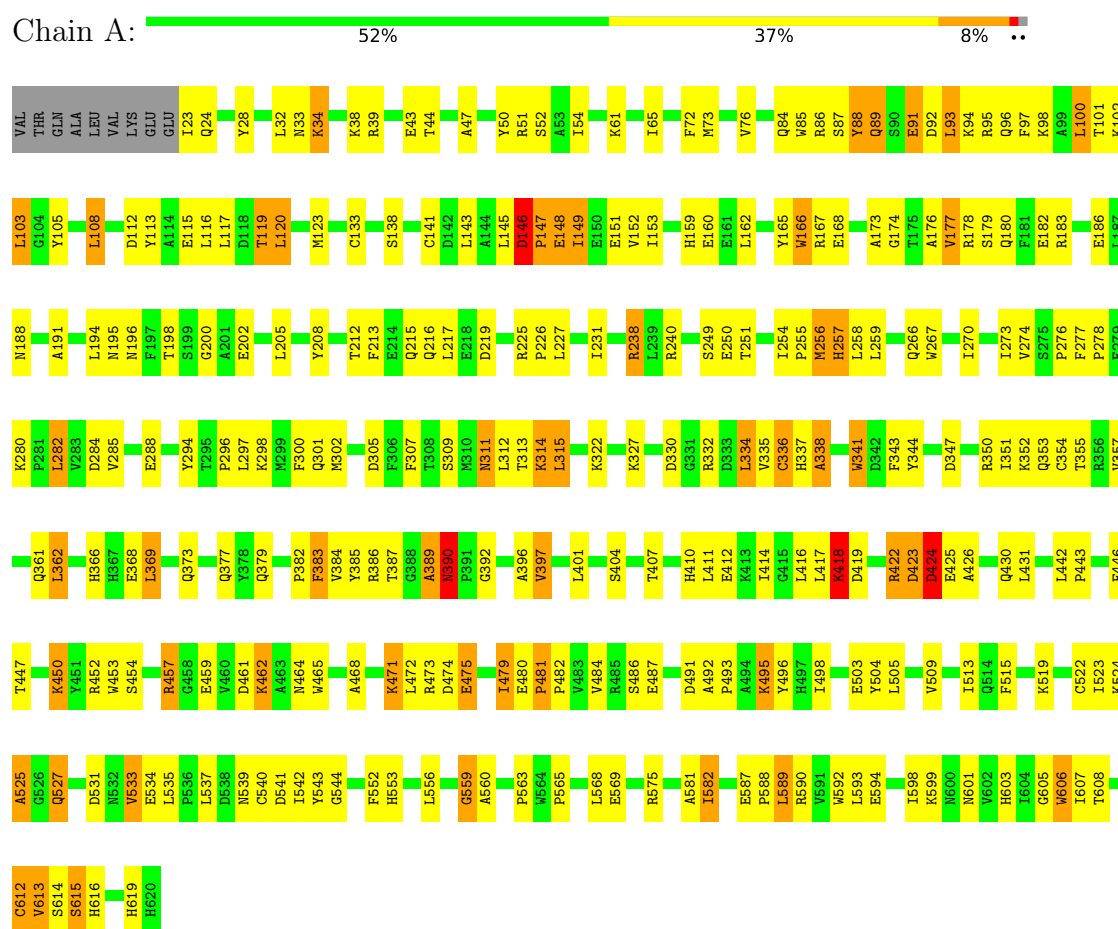
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
3	B	1	Total	C	N	O	S	0	0
			14	9	1	3	1		

3 Residue-property plots

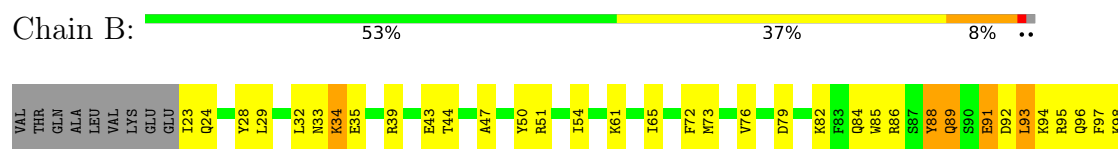
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: angiotensin converting enzyme



- Molecule 1: angiotensin converting enzyme



V613	S614	S615	H616	H619	H620	I523	F446	Q361	V283	N188	A99
K524	A525	G526	Q527	D531	F532	T447	K450	L362	D284	L100	T101
E526	E527	Q527	D531	D533	E534	K450	Y451	H366	A191	A192	K102
D531	F532	L535	F536	L537	D538	R452	W453	E368	K193	L194	L103
H619	H620	D531	F532	L535	F536	S454	R457	L369	Y294	N195	L108
		F533	E534	L535	F536	S454	R457	Q373	T295	F197	D112
		L535	F536	L537	D538	W465	G458	Y374	P296	T198	Y113
		F536	L537	D538	N539	A468	E459	Q377	L297	S199	A114
		L537	D538	N539	C540	W465	W460	Y378	K298	G200	E115
		D541	I542	Y543	G544	A468	D461	Q379	W299	A201	L116
		F541	I542	Y543	G544	K462	K462	F300	F300	E202	L117
		D541	I542	Y543	G544	A463	A463	Q301	M302	Y208	D118
		D541	I542	Y543	G544	N464	N464	P382	M302	Y208	T119
		I542	Y543	G544		W465	W465	F383			L120
		I542	Y543	G544		A468	A468	V384			M123
		I542	Y543	G544		A468	A468	R386			C133
		I542	Y543	G544		A468	A468	T387			S138
		I542	Y543	G544		A468	A468	G388			C141
		I542	Y543	G544		A468	A468	A389			D142
		I542	Y543	G544		A468	A468	N390			L143
		I542	Y543	G544		A468	A468	P391			L145
		I542	Y543	G544		A468	A468	G392			D146
		I542	Y543	G544		A468	A468	A396			P147
		I542	Y543	G544		A468	A468	V397			E148
		I542	Y543	G544		A468	A468	L401			I149
		I542	Y543	G544		A468	A468	S404			E150
		I542	Y543	G544		A468	A468	T407			E151
		I542	Y543	G544		A468	A468	P408			V152
		I542	Y543	G544		A468	A468	K409			I153
		I542	Y543	G544		A468	A468	H410			H159
		I542	Y543	G544		A468	A468	L411			E160
		I542	Y543	G544		A468	A468	E412			E161
		I542	Y543	G544		A468	A468	K413			F161
		I542	Y543	G544		A468	A468	I414			L162
		I542	Y543	G544		A468	A468	K495			A163
		I542	Y543	G544		A468	A468	Y496			Y164
		I542	Y543	G544		A468	A468	H497			Y165
		I542	Y543	G544		A468	A468	I498			W166
		I542	Y543	G544		A468	A468	E591			R167
		I542	Y543	G544		A468	A468	W592			E168
		I542	Y543	G544		A468	A468	L593			
		I542	Y543	G544		A468	A468	E594			
		I542	Y543	G544		A468	A468	N601			A173
		I542	Y543	G544		A468	A468	F602			G174
		I542	Y543	G544		A468	A468	H603			
		I542	Y543	G544		A468	A468	I604			V177
		I542	Y543	G544		A468	A468	G605			R178
		I542	Y543	G544		A468	A468	W606			
		I542	Y543	G544		A468	A468	I607			E182
		I542	Y543	G544		A468	A468	T608			R183
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				
		I542	Y543	G544		A468	A468				

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	94.91Å 121.22Å 94.74Å 90.00° 99.39° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9830	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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: X8Z, ZN

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	0.54	0/5031	1.05	32/6814 (0.5%)
1	B	0.54	1/5031 (0.0%)	1.05	26/6814 (0.4%)
All	All	0.54	1/10062 (0.0%)	1.05	58/13628 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	119	THR	CA-CB	5.11	1.61	1.53

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	457	ARG	N-CA-C	-8.73	97.56	110.48
1	A	457	ARG	N-CA-C	-7.99	97.62	110.32
1	A	615	SER	N-CA-C	7.70	119.40	108.00
1	A	426	ALA	N-CA-C	-7.56	103.00	112.90
1	B	93	LEU	N-CA-C	-7.42	103.13	111.14

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	4900	0	4696	231	0
1	B	4900	0	4696	236	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
All	All	9830	0	9418	464	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 25.

The worst 5 of 464 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:533:VAL:HG22	1:A:534:GLU:H	1.20	1.06
1:B:533:VAL:HG22	1:B:534:GLU:H	1.21	1.04
1:B:418:LYS:HE3	1:B:418:LYS:H	1.29	0.95
1:A:347:ASP:H	1:A:379:GLN:HE22	1.14	0.91
1:A:418:LYS:HE3	1:A:418:LYS:H	1.34	0.91

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	596/607 (98%)	532 (89%)	42 (7%)	22 (4%)	2 2
1	B	596/607 (98%)	535 (90%)	40 (7%)	21 (4%)	3 2
All	All	1192/1214 (98%)	1067 (90%)	82 (7%)	43 (4%)	2 2

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	PRO
1	A	256	MET
1	A	257	HIS
1	A	423	ASP
1	A	424	ASP

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	522/530 (98%)	480 (92%)	42 (8%)	11	19
1	B	522/530 (98%)	480 (92%)	42 (8%)	11	19
All	All	1044/1060 (98%)	960 (92%)	84 (8%)	11	19

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	315	LEU
1	B	479	ILE
1	B	336	CYS
1	B	418	LYS
1	B	539	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	33	ASN
1	B	266	GLN
1	B	516	GLN
1	B	41	ASN
1	B	159	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
3	X8Z	A	801	2	14,14,14	1.06	1 (7%)	18,19,19	0.98	1 (5%)
3	X8Z	B	802	2	14,14,14	1.20	1 (7%)	18,19,19	0.99	1 (5%)

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
3	X8Z	A	801	2	-	0/14/24/24	0/1/1/1
3	X8Z	B	802	2	-	0/14/24/24	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	X8Z	O1-C4	2.93	1.27	1.22
3	A	801	X8Z	O1-C4	2.61	1.27	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	X8Z	C6-C7-C8	2.17	108.67	104.14
3	A	801	X8Z	C6-C7-C8	2.14	108.60	104.14

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 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.