



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:02 pm GMT

PDB ID : 1EPW
Title : CRYSTAL STRUCTURE OF CLOSTRIDIUM NEUROTOXIN TYPE B
Authors : Swaminathan, S.; Eswaramoorthy, S.
Deposited on : 2000-03-29
Resolution : 1.90 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 : 1.7.2 (RC1), CSD as538be (2017)
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

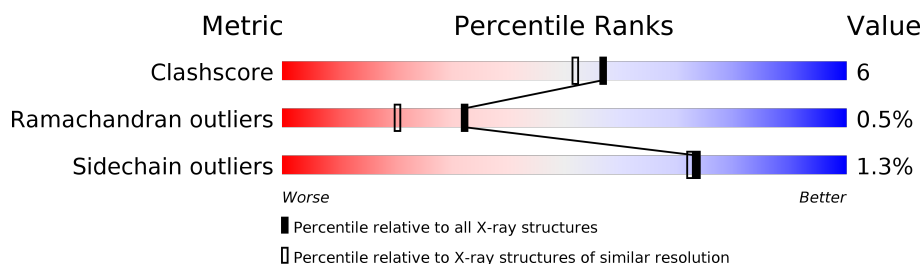
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)

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	1290	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11456 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 BOTULINUM NEUROTOXIN TYPE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1287	Total	C	N	O	S	0	0	0
			10586	6827	1704	2022	33			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	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	0	0
			5	4	1		

- Molecule 4 is water.

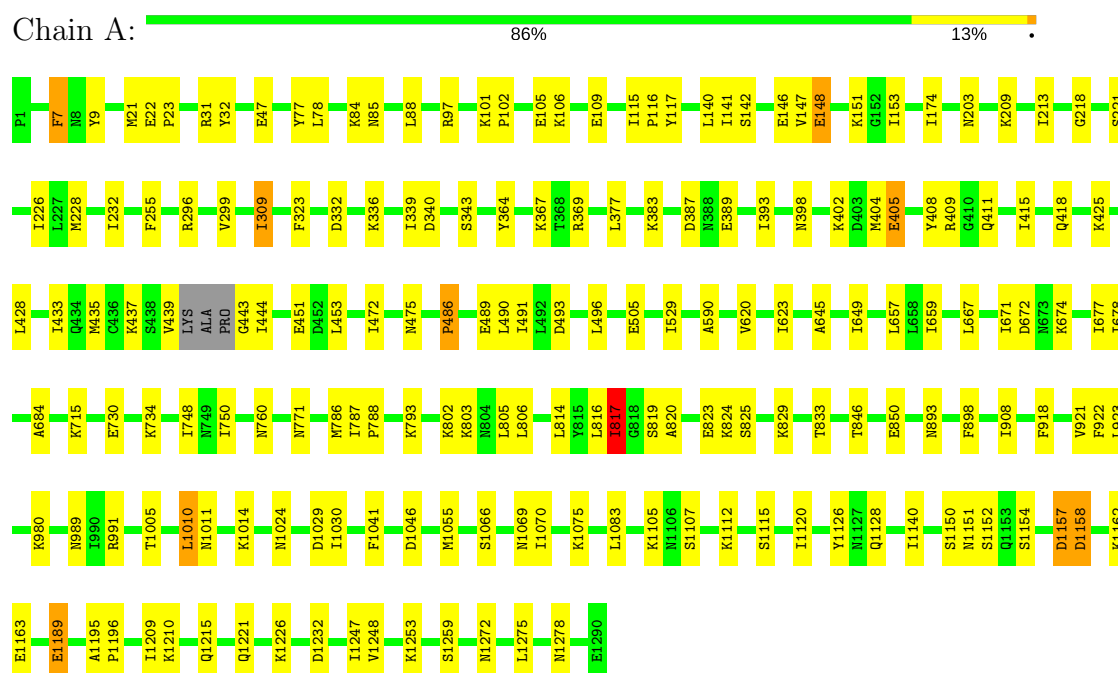
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	864	Total 864	O 864	0	0

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 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: BOTULINUM NEUROTOXIN TYPE B



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	75.82Å 123.12Å 96.23Å 90.00° 113.80° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90	Depositor
% Data completeness (in resolution range)	80.0 (50.00-1.90)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.202 , 0.233	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11456	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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: ZN, 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	0.39	0/10816	0.59	0/14611

There are no bond length outliers.

There are no bond angle outliers.

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	10586	0	10418	120	0
2	A	1	0	0	0	0
3	A	5	0	0	0	0
4	A	864	0	0	6	0
All	All	11456	0	10418	120	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 6.

All (120) 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:203:ASN:HD22	1:A:377:LEU:HD11	1.35	0.89
1:A:367:LYS:H	1:A:411:GLN:HE22	1.27	0.83
1:A:1066:SER:H	1:A:1069:ASN:HD22	1.33	0.76
1:A:309:ILE:HD13	1:A:309:ILE:H	1.50	0.75
1:A:659:ILE:HG22	1:A:793:LYS:HG3	1.73	0.69
1:A:1075:LYS:HE2	1:A:1215:GLN:HE22	1.57	0.69
1:A:989:ASN:ND2	1:A:991:ARG:H	1.91	0.68
1:A:590:ALA:HA	1:A:750:ILE:HD11	1.78	0.66
1:A:209:LYS:CB	1:A:218:GLY:H	2.09	0.65
1:A:1247:ILE:HG13	1:A:1248:VAL:HG23	1.78	0.64
1:A:398:ASN:HD21	1:A:411:GLN:HE21	1.45	0.63
1:A:140:LEU:HD11	1:A:147:VAL:HA	1.80	0.63
1:A:213:ILE:H	1:A:760:ASN:HD22	1.47	0.63
1:A:213:ILE:H	1:A:760:ASN:ND2	1.96	0.63
1:A:97:ARG:HA	1:A:393:ILE:HG23	1.81	0.62
1:A:1075:LYS:HE2	1:A:1215:GLN:NE2	2.15	0.61
1:A:730:GLU:HG3	1:A:734:LYS:HE3	1.82	0.60
1:A:309:ILE:CD1	1:A:309:ILE:H	2.15	0.60
1:A:106:LYS:HD3	1:A:496:LEU:HD23	1.84	0.58
1:A:309:ILE:HD13	1:A:309:ILE:N	2.18	0.58
1:A:1221:GLN:HE21	1:A:1278:ASN:HD22	1.51	0.57
1:A:332:ASP:OD2	1:A:336:LYS:HB3	2.04	0.57
1:A:715:LYS:HD2	1:A:771:ASN:OD1	2.05	0.56
1:A:296:ARG:O	1:A:299:VAL:HG12	2.05	0.56
1:A:989:ASN:HD22	1:A:991:ARG:H	1.51	0.56
1:A:142:SER:CB	1:A:148:GLU:HG3	2.36	0.55
1:A:1126:TYR:CZ	1:A:1128:GLN:HB2	2.42	0.54
1:A:47:GLU:HG2	1:A:84:LYS:HE3	1.88	0.54
1:A:1221:GLN:HE21	1:A:1278:ASN:ND2	2.05	0.54
1:A:645:ALA:HB3	1:A:649:ILE:CG2	2.38	0.53
1:A:117:TYR:HA	1:A:323:PHE:CZ	2.44	0.52
1:A:439:VAL:HB	1:A:443:GLY:HA2	1.92	0.52
1:A:425:LYS:HD3	1:A:428:LEU:HD12	1.91	0.52
1:A:748:ILE:HG22	1:A:750:ILE:HG12	1.91	0.52
1:A:472:ILE:HG21	1:A:684:ALA:HB2	1.91	0.51
1:A:486:PRO:HG2	1:A:489:GLU:HG2	1.93	0.50
1:A:141:ILE:HD11	1:A:151:LYS:HB2	1.94	0.50
1:A:1066:SER:H	1:A:1069:ASN:ND2	2.08	0.50
1:A:674:LYS:O	1:A:678:ILE:HG13	2.11	0.50
1:A:437:LYS:HD2	1:A:444:ILE:CG2	2.42	0.50
1:A:1014:LYS:HG2	1:A:1024:ASN:HD22	1.78	0.49
1:A:141:ILE:HD12	1:A:141:ILE:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1112:LYS:HD3	1:A:1115:SER:OG	2.13	0.49
1:A:409:ARG:NH1	1:A:415:ILE:HD13	2.27	0.49
1:A:101:LYS:HB2	1:A:364:TYR:CZ	2.48	0.49
1:A:402:LYS:HE3	1:A:404:MET:HG3	1.95	0.48
1:A:833:THR:HG22	1:A:921:VAL:HG21	1.94	0.48
1:A:203:ASN:ND2	1:A:377:LEU:HD11	2.15	0.48
1:A:1083:LEU:HD13	1:A:1209:ILE:CD1	2.43	0.48
1:A:825:SER:O	1:A:829:LYS:HG2	2.14	0.48
1:A:1010:LEU:HD13	1:A:1011:ASN:ND2	2.28	0.48
1:A:1162:LYS:O	1:A:1163:GLU:HB2	2.14	0.48
1:A:908:ILE:HB	1:A:1041:PHE:HB2	1.96	0.47
1:A:657:LEU:HD11	1:A:786:MET:HG2	1.97	0.47
1:A:820:ALA:O	1:A:824:LYS:HB2	2.13	0.47
1:A:435:MET:HG2	1:A:529:ILE:HD11	1.97	0.47
1:A:1107:SER:HB3	1:A:1120:ILE:CG2	2.44	0.47
1:A:667:LEU:HD11	1:A:805:LEU:HD23	1.95	0.47
1:A:31:ARG:HG3	1:A:32:TYR:N	2.30	0.47
1:A:1157:ASP:O	1:A:1158:ASP:HB2	2.15	0.46
1:A:1140:ILE:HG13	4:A:1623:HOH:O	2.15	0.46
1:A:296:ARG:HG2	1:A:339:ILE:HD12	1.98	0.46
1:A:383:LYS:HD2	1:A:418:GLN:O	2.15	0.46
1:A:1005:THR:HG21	1:A:1070:ILE:HG12	1.98	0.46
1:A:31:ARG:CD	1:A:32:TYR:H	2.29	0.46
1:A:787:ILE:HB	1:A:788:PRO:HD3	1.97	0.46
1:A:387:ASP:OD1	1:A:389:GLU:HB3	2.16	0.45
1:A:9:TYR:H	1:A:85:ASN:ND2	2.15	0.45
1:A:671:ILE:O	1:A:672:ASP:HB2	2.17	0.45
1:A:1075:LYS:CE	1:A:1215:GLN:HE22	2.25	0.44
1:A:102:PRO:HB2	1:A:491:ILE:HG23	1.98	0.44
1:A:405:GLU:HG2	4:A:1464:HOH:O	2.17	0.44
1:A:22:GLU:HB2	1:A:32:TYR:CE2	2.53	0.44
1:A:228:MET:O	1:A:232:ILE:HG13	2.17	0.44
1:A:814:LEU:O	1:A:817:ILE:HG13	2.18	0.44
1:A:1189:GLU:HB3	1:A:1259:SER:HB2	2.00	0.44
1:A:174:ILE:HG13	4:A:1585:HOH:O	2.17	0.44
1:A:490:LEU:HD12	1:A:496:LEU:HD22	1.99	0.44
1:A:146:GLU:OE1	1:A:148:GLU:HG2	2.18	0.44
1:A:1083:LEU:HD13	1:A:1209:ILE:HG12	2.00	0.43
1:A:678:ILE:HG12	1:A:823:GLU:OE1	2.18	0.43
1:A:340:ASP:HB3	1:A:343:SER:OG	2.18	0.43
1:A:1195:ALA:HB1	1:A:1196:PRO:CD	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1226:LYS:HB2	1:A:1232:ASP:HB3	2.01	0.43
1:A:7:PHE:HE1	1:A:88:LEU:HD22	1.83	0.43
1:A:1152:SER:C	1:A:1154:SER:H	2.22	0.43
1:A:1105:LYS:HE2	4:A:2106:HOH:O	2.19	0.42
1:A:921:VAL:HG12	1:A:921:VAL:O	2.19	0.42
1:A:31:ARG:CG	1:A:32:TYR:N	2.81	0.42
1:A:105:GLU:O	1:A:109:GLU:HG3	2.19	0.42
1:A:367:LYS:HB2	1:A:408:TYR:CG	2.55	0.42
1:A:255:PHE:HB2	1:A:529:ILE:CD1	2.50	0.42
1:A:221:SER:HB2	1:A:226:ILE:HD11	2.02	0.42
1:A:437:LYS:HD2	1:A:444:ILE:HG23	2.02	0.42
1:A:142:SER:HB3	1:A:148:GLU:HG3	2.02	0.41
1:A:433:ILE:HG13	1:A:453:LEU:HD11	2.01	0.41
1:A:77:TYR:O	1:A:78:LEU:HB2	2.20	0.41
1:A:802:LYS:HZ2	1:A:806:LEU:HD11	1.85	0.41
1:A:846:THR:O	1:A:850:GLU:HG3	2.21	0.41
1:A:31:ARG:HD2	1:A:32:TYR:H	1.85	0.41
1:A:141:ILE:HD11	1:A:151:LYS:CB	2.50	0.41
1:A:153:ILE:HA	1:A:505:GLU:O	2.21	0.41
1:A:730:GLU:CG	1:A:734:LYS:HE3	2.50	0.41
1:A:1195:ALA:HB1	1:A:1196:PRO:HD2	2.03	0.41
1:A:1253:LYS:HD3	4:A:1817:HOH:O	2.21	0.41
1:A:677:ILE:CG2	1:A:816:LEU:HD21	2.50	0.41
1:A:1210:LYS:HE3	1:A:1210:LYS:HB3	1.91	0.41
1:A:475:ASN:HD22	1:A:475:ASN:HA	1.64	0.41
1:A:1126:TYR:OH	1:A:1128:GLN:HB2	2.21	0.40
1:A:620:VAL:CG1	1:A:623:ILE:HG13	2.51	0.40
1:A:645:ALA:HB3	1:A:649:ILE:HG23	2.02	0.40
1:A:898:PHE:CZ	1:A:1055:MET:HB3	2.56	0.40
1:A:1030:ILE:HD13	1:A:1030:ILE:HA	1.91	0.40
1:A:21:MET:O	1:A:23:PRO:HD3	2.21	0.40
1:A:115:ILE:HA	1:A:116:PRO:HD3	1.98	0.40
1:A:893:ASN:HB2	4:A:2144:HOH:O	2.21	0.40
1:A:1272:ASN:HB3	1:A:1275:LEU:HG	2.04	0.40
1:A:980:LYS:HE2	1:A:1029:ASP:HB3	2.04	0.40
1:A:989:ASN:HD21	1:A:991:ARG:HB2	1.86	0.40
1:A:9:TYR:H	1:A:85:ASN:HD22	1.68	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	1283/1290 (100%)	1227 (96%)	49 (4%)	7 (0%)	32	20

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1151	ASN
1	A	819	SER
1	A	922	PHE
1	A	817	ILE
1	A	923	LEU
1	A	1150	SER
1	A	486	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	1176/1189 (99%)	1161 (99%)	15 (1%)	73	72

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	148	GLU
1	A	309	ILE
1	A	369	ARG

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Mol	Chain	Res	Type
1	A	405	GLU
1	A	451	GLU
1	A	493	ASP
1	A	803	LYS
1	A	817	ILE
1	A	918	PHE
1	A	1010	LEU
1	A	1046	ASP
1	A	1157	ASP
1	A	1158	ASP
1	A	1189	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	85	ASN
1	A	143	ASN
1	A	177	GLN
1	A	178	ASN
1	A	203	ASN
1	A	411	GLN
1	A	475	ASN
1	A	605	ASN
1	A	683	ASN
1	A	689	ASN
1	A	760	ASN
1	A	764	ASN
1	A	799	ASN
1	A	828	ASN
1	A	862	ASN
1	A	873	ASN
1	A	953	ASN
1	A	989	ASN
1	A	999	ASN
1	A	1011	ASN
1	A	1024	ASN
1	A	1069	ASN
1	A	1215	GLN
1	A	1278	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	SO4	A	1292	2	4,4,4	0.25	0	6,6,6	0.09	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
3	SO4	A	1292	2	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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

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.