



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 09:21 AM GMT

PDB ID : 2XMD  
Title : G117H MUTANT OF HUMAN BUTYRYLCHOLINESTERASEIN COM-  
PLEX WITH ECHOTHIOPHATE  
Authors : Nachon, F.; Carletti, E.; Wandhammer, M.; Nicolet, Y.; Schopfer, L.M.; Mas-  
son, P.; Lockridge, O.  
Deposited on : 2010-07-27  
Resolution : 2.30 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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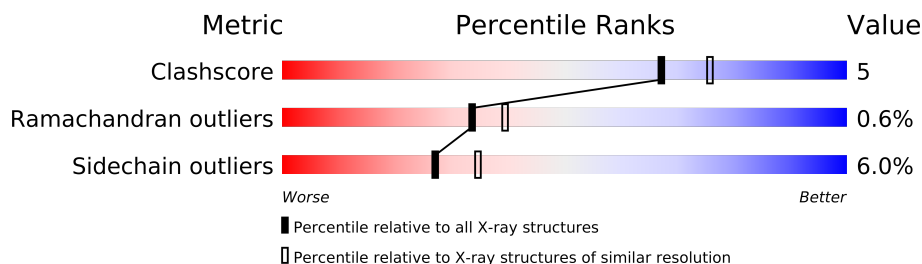
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : **FAILED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	529	

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 4705 atoms, of which 0 are hydrogen and 0 are deuterium.

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 CHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	2	0
			4222	2724	711	772	15			

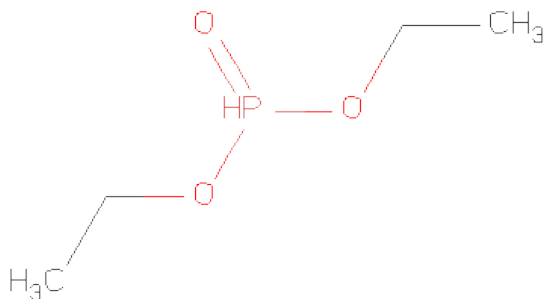
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	117	HIS	GLY	ENGINEERED MUTATION	UNP P06276
A	455	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	481	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	486	GLN	ASN	ENGINEERED MUTATION	UNP P06276

- Molecule 2 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	21	Total	X	0	0
			21	21		

- Molecule 3 is DIETHYL PHOSPHONATE (three-letter code: DEP) (formula: C<sub>4</sub>H<sub>11</sub>O<sub>3</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			8	4	3	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total Cl 4 4	0	0

- Molecule 6 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Br 1 1	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Na 2 2	0	0

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 9 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	3	Total C N O 38 22 2 14	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	117	HIS	GLY	ENGINEERED MUTATION	UNP P06276
A	455	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	481	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	486	GLN	ASN	ENGINEERED MUTATION	UNP P06276

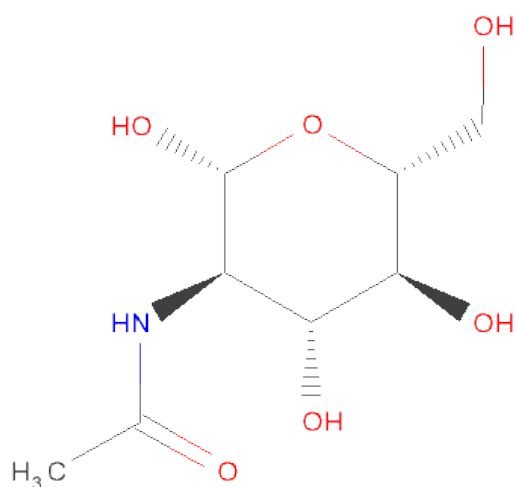
- Molecule 10 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	3	Total C N O 38 22 2 14	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	117	HIS	GLY	ENGINEERED MUTATION	UNP P06276
A	455	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	481	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	486	GLN	ASN	ENGINEERED MUTATION	UNP P06276

- Molecule 11 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	N	O	0	0
			14	8	1	5		
11	A	1	Total	C	N	O	0	0
			14	8	1	5		
11	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 12 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	3	Total	C	N	O	0	0
			38	22	2	14		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	117	HIS	GLY	ENGINEERED MUTATION	UNP P06276
A	455	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	481	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	486	GLN	ASN	ENGINEERED MUTATION	UNP P06276

- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	285	Total O 285 285	0	0

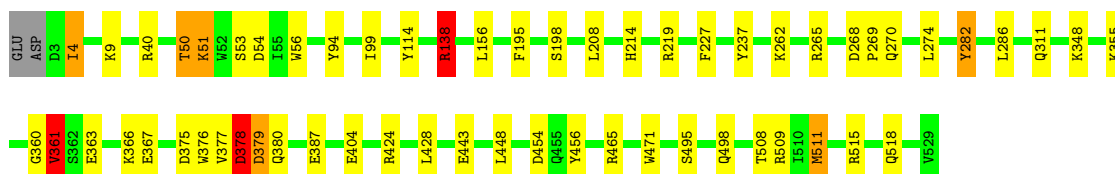
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 failed to run properly.

- Molecule 1: CHOLINESTERASE

Chain A: 





## 4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.88Å 154.88Å 127.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.15 – 2.30	Depositor
% Data completeness (in resolution range)	96.0 (28.15-2.30)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.53 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.170 , 0.214	Depositor
Wilson B-factor (Å <sup>2</sup> )	36.8	Xtriage
Anisotropy	0.205	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 33216 reflections	Xtriage
Total number of atoms	4705	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CL, DEP, NA, CA, UNX, FUC, BR, FUL, 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	1.10	4/4346 (0.1%)	0.97	14/5900 (0.2%)

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	1	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	404	GLU	CG-CD	6.25	1.61	1.51
1	A	515	ARG	CZ-NH1	5.88	1.40	1.33
1	A	114	TYR	CD1-CE1	5.37	1.47	1.39
1	A	94	TYR	CD1-CE1	5.23	1.47	1.39

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	465	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	A	515	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	A	465	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	A	424	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	A	424	ARG	NE-CZ-NH1	6.81	123.71	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	361	VAL	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	GLY	Peptide
1	A	377	VAL	Peptide
1	A	378	ASP	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4222	0	0	19	0
2	A	21	0	0	2	0
3	A	8	0	10	1	0
4	A	5	0	0	0	0
5	A	4	0	0	0	0
6	A	1	0	0	0	0
7	A	2	0	0	0	0
8	A	1	0	0	0	1
9	A	38	0	34	0	0
10	A	38	0	34	0	0
11	A	42	0	39	1	0
12	A	38	0	34	0	0
13	A	285	0	0	9	0
All	All	4705	0	151	23	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

The worst 5 of 23 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:508:THR:OG1	13:A:2263:HOH:O	1.80	0.99
1:A:99:ILE:CD1	13:A:2010:HOH:O	2.13	0.97
1:A:265:ARG:NE	13:A:2134:HOH:O	2.28	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:138:ARG:NE	13:A:2091:HOH:O	2.28	0.66
1:A:311:GLN:NE2	13:A:2154:HOH:O	2.28	0.66

All (1) 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	Distance(Å)	Clash(Å)
8:A:1537:CA:CA	8:A:1537:CA:CA[5_556]	1.55	0.65

## 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	527/529 (100%)	499 (95%)	25 (5%)	3 (1%)	33 39

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	361	VAL
1	A	379	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	455/455 (100%)	428 (94%)	27 (6%)	28 35

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	282	TYR
1	A	361	VAL
1	A	509	ARG
1	A	348	LYS
1	A	138	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

9 carbohydrates are modelled in this entry.

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	$\# Z  > 2$
9	NAG	A	1554	1,9	12,14,15	0.95	1 (8%)	15,19,21	2.21	5 (33%)
9	NAG	A	1555	9	12,14,15	0.71	0	15,19,21	2.78	4 (26%)
9	FUL	A	1556	9	9,10,11	1.22	0	10,14,16	2.10	5 (50%)
10	NAG	A	1557	1,10	12,14,15	1.08	1 (8%)	15,19,21	2.35	4 (26%)
10	FUL	A	1558	10	9,10,11	1.20	1 (11%)	10,14,16	2.54	5 (50%)
10	NAG	A	1559	10	12,14,15	0.75	0	15,19,21	2.18	3 (20%)
12	NAG	A	1563	1,12	12,14,15	0.65	0	15,19,21	2.47	5 (33%)
12	NAG	A	1564	12	12,14,15	0.75	0	15,19,21	1.63	3 (20%)
12	FUC	A	1565	12	9,10,11	0.97	0	10,14,16	1.90	4 (40%)

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
9	NAG	A	1554	1,9	-	0/6/23/26	0/1/1/1
9	NAG	A	1555	9	-	0/6/23/26	0/1/1/1
9	FUL	A	1556	9	-	0/0/17/20	0/1/1/1
10	NAG	A	1557	1,10	-	0/6/23/26	0/1/1/1
10	FUL	A	1558	10	-	0/0/17/20	0/1/1/1
10	NAG	A	1559	10	-	0/6/23/26	0/1/1/1
12	NAG	A	1563	1,12	-	0/6/23/26	0/1/1/1
12	NAG	A	1564	12	-	0/6/23/26	0/1/1/1
12	FUC	A	1565	12	-	0/0/17/20	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1558	FUL	O5-C5	-2.91	1.40	1.45
10	A	1557	NAG	C2-N2	2.54	1.49	1.46
9	A	1554	NAG	C2-N2	-2.24	1.43	1.46

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1555	NAG	C3-C2-N2	-8.84	98.31	111.76
10	A	1557	NAG	O5-C5-C6	6.73	114.04	106.98
10	A	1559	NAG	C3-C2-N2	6.16	121.14	111.76
12	A	1563	NAG	C8-C7-N2	5.13	126.14	116.11
12	A	1563	NAG	C2-N2-C7	4.83	131.19	123.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry

Of 34 ligands modelled in this entry, 21 are unknown and 8 are 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
3	DEP	A	1530	1	7,7,7	1.55	1 (14%)	7,7,7	2.63	2 (28%)
4	SO4	A	1531	-	4,4,4	0.47	0	6,6,6	0.65	0
11	NAG	A	1560	1	12,14,15	0.75	0	15,19,21	2.83	2 (13%)
11	NAG	A	1561	1	12,14,15	0.97	0	15,19,21	1.68	4 (26%)
11	NAG	A	1562	1	12,14,15	0.56	0	15,19,21	1.14	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	DEP	A	1530	1	-	0/6/6/6	0/0/0/0
4	SO4	A	1531	-	-	0/0/0/0	0/0/0/0
11	NAG	A	1560	1	-	0/6/23/26	0/1/1/1
11	NAG	A	1561	1	-	0/6/23/26	0/1/1/1
11	NAG	A	1562	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1530	DEP	P-O2	-3.50	1.52	1.58

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1560	NAG	O5-C5-C6	10.12	117.60	106.98
3	A	1530	DEP	P-O1-C1	6.10	132.73	120.01
11	A	1561	NAG	O5-C5-C4	-3.99	105.59	110.65
3	A	1530	DEP	P-O2-C3	2.68	125.59	120.01
11	A	1561	NAG	O5-C5-C6	2.39	109.49	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 failed to run properly - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.