



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:55 PM GMT

PDB ID : 1PPL  
Title : CRYSTALLOGRAPHIC ANALYSIS OF TRANSITION-STATE MIMICS  
BOUND TO PENICILLOPEPSIN: PHOSPHORUS-CONTAININGPEP-  
TIDE ANALOGUES  
Authors : Fraser, M.E.; James, M.N.G.  
Deposited on : 1992-06-01  
Resolution : 1.70 Å(reported)

This is a full wwPDB validation 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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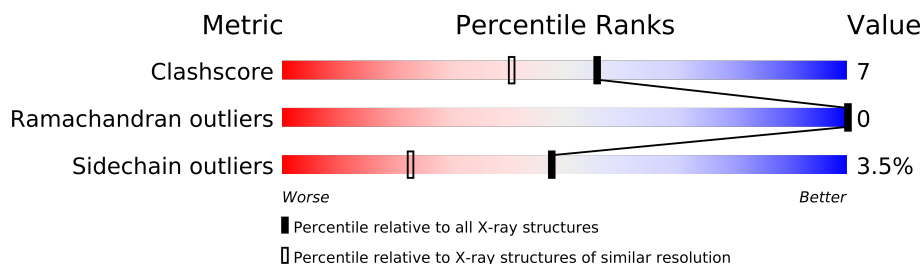
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
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 1.70 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	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)

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 was not executed.

Mol	Chain	Length	Quality of chain
1	E	323	

## 2 Entry composition i

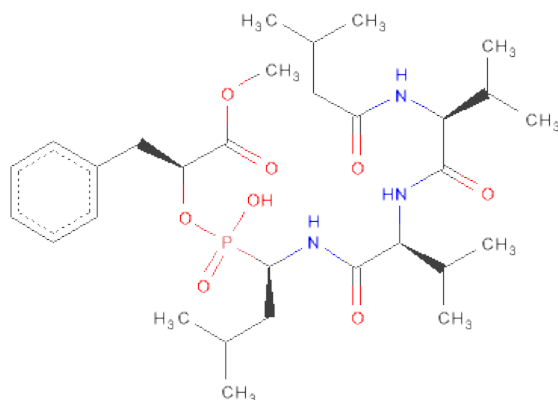
There are 6 unique types of molecules in this entry. The entry contains 2713 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PENICILLOPEPSIN.

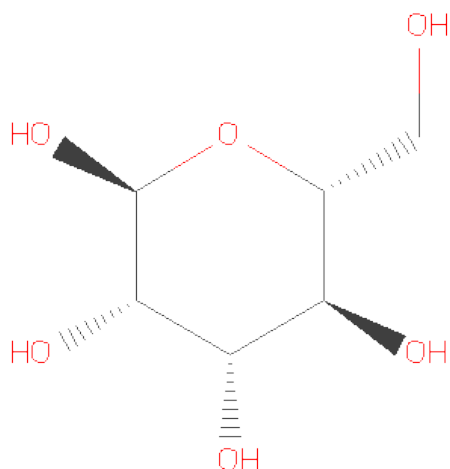
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	323	2370	1480	378	510	2	0	2	0

- Molecule 2 is N-(3-METHYLBUTANOYL)-L-VALYL-N-{(1S)-1-[(R)-[(1R)-1-BENZYL-2-METHOXY-2-OXOETHOXY](HYDROXY)PHOSPHORYL]-3-METHYLBUTYL}-L-VAL INAMIDE (three-letter code: 1Z7) (formula: C<sub>30</sub>H<sub>50</sub>N<sub>3</sub>O<sub>8</sub>P).



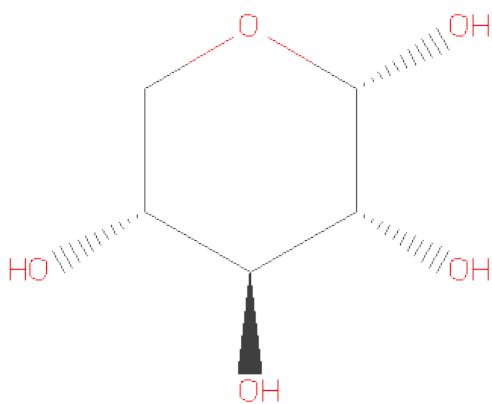
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	E	1	42	30	3	8	1	0	0

- Molecule 3 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	E	1	11	6	5	0	0

- Molecule 4 is SUGAR (XYLOPYRANOSE) (three-letter code: XYS) (formula:  $C_5H_{10}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	E	1	9	5	4	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	276	Total	O	0	0
			276	276		

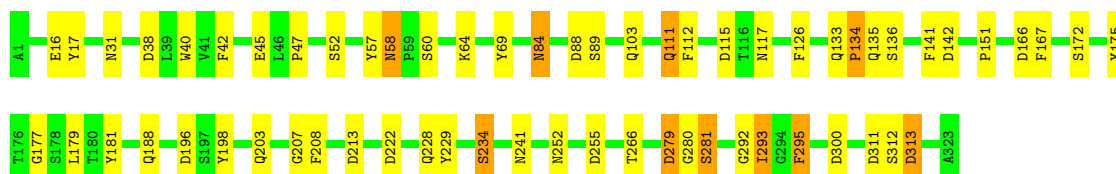
### 3 Residue-property plots

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 was not executed.

#### • Molecule 1: PENICILLOPEPSIN

Chain E: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.50Å 46.46Å 65.93Å 90.00° 115.20° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.70)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, $R_{free}$	0.148 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2713	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	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: 1Z7, XYS, SO4, MAN

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	E	1.37	4/2435 (0.2%)	1.98	52/3325 (1.6%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	16	GLU	CD-OE1	-6.13	1.19	1.25
1	E	69	TYR	CG-CD1	5.71	1.46	1.39
1	E	60	SER	CB-OG	5.23	1.49	1.42
1	E	234	SER	CB-OG	5.06	1.48	1.42

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	279	ASP	CB-CG-OD2	17.99	134.49	118.30
1	E	313	ASP	CB-CG-OD2	-15.49	104.36	118.30
1	E	255	ASP	CB-CG-OD2	12.58	129.62	118.30
1	E	311	ASP	CB-CG-OD2	-10.20	109.12	118.30
1	E	196	ASP	CB-CG-OD1	-9.56	109.70	118.30
1	E	167	PHE	CB-CG-CD1	-9.55	114.12	120.80
1	E	213	ASP	CB-CG-OD1	8.88	126.30	118.30
1	E	16	GLU	CG-CD-OE2	-8.08	102.14	118.30
1	E	16	GLU	CG-CD-OE1	7.92	134.14	118.30
1	E	313	ASP	OD1-CG-OD2	7.69	137.92	123.30
1	E	292	GLY	CA-C-O	-7.54	107.02	120.60
1	E	166	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	E	222	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	E	313	ASP	CA-CB-CG	-7.12	97.74	113.40
1	E	141	PHE	CB-CG-CD2	-7.06	115.86	120.80
1	E	88	ASP	CB-CG-OD2	6.87	124.48	118.30
1	E	57	TYR	CB-CG-CD1	-6.76	116.95	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	279	ASP	OD1-CG-OD2	-6.65	110.66	123.30
1	E	222	ASP	CB-CG-OD1	6.43	124.08	118.30
1	E	17	TYR	CB-CG-CD1	-6.30	117.22	121.00
1	E	281	SER	N-CA-CB	-6.21	101.19	110.50
1	E	266	THR	O-C-N	6.11	132.47	122.70
1	E	136	SER	O-C-N	-6.09	112.96	122.70
1	E	229	TYR	CB-CG-CD2	-6.08	117.35	121.00
1	E	58	ASN	CB-CG-OD1	-6.02	109.57	121.60
1	E	181	TYR	CB-CG-CD1	-5.91	117.45	121.00
1	E	196	ASP	OD1-CG-OD2	5.90	134.51	123.30
1	E	255	ASP	CB-CG-OD1	-5.87	113.02	118.30
1	E	142	ASP	CB-CG-OD1	5.83	123.55	118.30
1	E	234	SER	O-C-N	5.82	133.09	123.20
1	E	115	ASP	CB-CG-OD2	-5.78	113.09	118.30
1	E	300	ASP	O-C-N	5.73	131.86	122.70
1	E	89	SER	O-C-N	5.58	131.64	122.70
1	E	208	PHE	CG-CD2-CE2	5.50	126.85	120.80
1	E	207	GLY	CA-C-O	5.47	130.45	120.60
1	E	126	PHE	O-C-N	5.43	131.38	122.70
1	E	293	ILE	CA-C-N	5.42	127.04	116.20
1	E	213	ASP	N-CA-CB	-5.40	100.87	110.60
1	E	181	TYR	CB-CG-CD2	5.25	124.15	121.00
1	E	42	PHE	CB-CG-CD2	-5.23	117.14	120.80
1	E	177	GLY	O-C-N	5.22	131.06	122.70
1	E	126	PHE	CD1-CE1-CZ	5.18	126.32	120.10
1	E	280	GLY	N-CA-C	-5.17	100.17	113.10
1	E	115	ASP	N-CA-CB	-5.16	101.32	110.60
1	E	311	ASP	CB-CG-OD1	5.16	122.94	118.30
1	E	31	ASN	N-CA-CB	-5.13	101.36	110.60
1	E	295	PHE	CB-CG-CD1	-5.13	117.21	120.80
1	E	17	TYR	CD1-CG-CD2	5.11	123.52	117.90
1	E	112	PHE	CB-CG-CD2	-5.08	117.24	120.80
1	E	198	TYR	CZ-CE2-CD2	-5.04	115.26	119.80
1	E	135	GLN	O-C-N	5.02	130.73	122.70
1	E	177	GLY	CA-C-O	-5.00	111.59	120.60

There are no chirality outliers.

There are no planarity outliers.

## 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	E	2370	0	2182	23	0
2	E	42	0	49	8	0
3	E	11	0	10	0	0
4	E	9	0	8	0	0
5	E	5	0	0	2	0
6	E	276	0	0	6	0
All	All	2713	0	2249	31	0

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 7.

All (31) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:324:1Z7:CD21	2:E:324:1Z7:HD2	0.97	1.15
2:E:324:1Z7:CD11	2:E:324:1Z7:HD1	0.97	1.06
1:E:241:ASN:HB2	1:E:279:ASP:OD1	1.53	1.06
2:E:324:1Z7:CG3	2:E:324:1Z7:CE2	2.41	0.97
2:E:324:1Z7:CG3	2:E:324:1Z7:CE1	2.40	0.93
2:E:324:1Z7:CE2	2:E:324:1Z7:HD2	2.04	0.86
2:E:324:1Z7:CG3	2:E:324:1Z7:HD1	2.06	0.86
2:E:324:1Z7:CE1	2:E:324:1Z7:HD1	2.07	0.84
2:E:324:1Z7:CG3	2:E:324:1Z7:HD2	2.06	0.84
1:E:281:SER:O	6:E:506:HOH:O	2.10	0.69
1:E:293:ILE:HD12	1:E:295:PHE:H	1.64	0.63
1:E:188:GLN:OE1	6:E:487:HOH:O	2.16	0.63
1:E:179:LEU:N	5:E:331:SO4:O2	2.30	0.62
1:E:293:ILE:HD11	1:E:295:PHE:O	2.01	0.59
1:E:84:ASN:H	1:E:84:ASN:HD22	1.58	0.51
1:E:172:SER:HA	1:E:175:TYR:CE1	2.48	0.48
1:E:111:GLN:HB2	6:E:496:HOH:O	2.14	0.48
1:E:117:ASN:ND2	6:E:513:HOH:O	2.48	0.47
1:E:203:GLN:NE2	1:E:228:GLN:HG3	2.31	0.46
1:E:175:TYR:OH	5:E:331:SO4:O4	2.22	0.45
1:E:133[B]:GLN:NE2	6:E:469:HOH:O	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:151:PRO:HB2	1:E:312:SER:OG	2.18	0.44
1:E:40:TRP:HA	1:E:103:GLN:O	2.18	0.43
1:E:293:ILE:CD1	1:E:295:PHE:O	2.66	0.43
1:E:64:LYS:HA	1:E:64:LYS:HD3	1.78	0.43
1:E:252:ASN:ND2	6:E:570:HOH:O	2.52	0.42
1:E:133[B]:GLN:HE21	1:E:134:PRO:HA	1.85	0.42
1:E:252:ASN:HD22	1:E:252:ASN:HA	1.67	0.42
1:E:45:GLU:OE2	1:E:84:ASN:ND2	2.46	0.41

There are no symmetry-related clashes.

## 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	E	323/323 (100%)	320 (99%)	3 (1%)	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	E	261/259 (101%)	252 (97%)	9 (3%)	49	23

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

Mol	Chain	Res	Type
1	E	38	ASP
1	E	47	PRO

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Mol	Chain	Res	Type
1	E	52	SER
1	E	58	ASN
1	E	84	ASN
1	E	111	GLN
1	E	134	PRO
1	E	234	SER
1	E	313	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	13	ASN
1	E	58	ASN
1	E	84	ASN
1	E	117	ASN
1	E	150	GLN
1	E	160	GLN
1	E	194	ASN
1	E	203	GLN
1	E	228	GLN
1	E	237	GLN
1	E	238	GLN
1	E	252	ASN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands 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	$\# Z  > 2$
2	1Z7	E	324	-	42,42,42	1.69	10 (23%)	58,58,58	1.85	16 (27%)
3	MAN	E	329	1	10,11,12	1.02	1 (10%)	11,15,17	1.84	4 (36%)
4	XYS	E	330	1	8,9,10	1.30	1 (12%)	8,12,14	3.15	5 (62%)
5	SO4	E	331	-	4,4,4	1.16	0	6,6,6	0.76	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
2	1Z7	E	324	-	-	0/57/57/57	0/1/1/1
3	MAN	E	329	1	-	0/2/19/22	0/1/1/1
4	XYS	E	330	1	4/4/3/4	0/0/14/17	0/1/1/1
5	SO4	E	331	-	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	324	1Z7	P-O21	-6.22	1.46	1.56
2	E	324	1Z7	CA2-N1	3.42	1.53	1.45
2	E	324	1Z7	OS-C3	2.88	1.40	1.33
2	E	324	1Z7	O-C	2.54	1.28	1.23
4	E	330	XYS	O2-C2	-2.49	1.38	1.43
2	E	324	1Z7	CA4-C3	2.31	1.55	1.51
2	E	324	1Z7	O1-C1	2.26	1.27	1.23
2	E	324	1Z7	CB3-CA3	2.15	1.56	1.52
2	E	324	1Z7	P-CA3	-2.13	1.80	1.83
2	E	324	1Z7	C-N	-2.11	1.29	1.34
3	E	329	MAN	O5-C5	-2.06	1.41	1.45
2	E	324	1Z7	CA2-C2	2.02	1.57	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	324	1Z7	CA-C-N	7.03	125.23	116.25
4	E	330	XYS	O4-C4-C3	-5.42	99.70	110.23
4	E	330	XYS	O5-C5-C4	4.18	118.32	111.74
4	E	330	XYS	O3-C3-C2	3.49	116.32	109.94
2	E	324	1Z7	O-C-CA	-3.43	116.33	121.24
2	E	324	1Z7	OP-P-O11	-3.36	109.13	115.04
2	E	324	1Z7	C2-CA2-N1	-3.33	101.47	110.53
2	E	324	1Z7	CG-CB3-CA3	3.18	120.38	114.50
3	E	329	MAN	C6-C5-C4	3.10	120.48	113.00
2	E	324	1Z7	OP-CA4-CB4	3.03	113.16	106.94
4	E	330	XYS	O2-C2-C3	2.91	116.46	110.18
2	E	324	1Z7	O21-P-OP	2.88	115.02	105.82
4	E	330	XYS	O4-C4-C5	2.71	114.74	109.14
2	E	324	1Z7	O-C-N	-2.67	118.44	123.08
2	E	324	1Z7	O2-C2-N2	2.59	127.92	122.93
2	E	324	1Z7	CA2-N1-C1	-2.58	115.14	121.81
3	E	329	MAN	C3-C4-C5	-2.44	105.85	110.20
2	E	324	1Z7	CG3-CB4-CA4	2.43	117.17	113.20
2	E	324	1Z7	CB1-CA1-N	-2.35	105.40	111.37
3	E	329	MAN	O4-C4-C3	-2.33	105.12	110.35
2	E	324	1Z7	CG1-CB-CA	-2.20	102.11	111.22
3	E	329	MAN	O3-C3-C2	-2.19	105.92	109.94
2	E	324	1Z7	O11-P-CA3	-2.14	109.19	113.78
2	E	324	1Z7	OS-C3-CA4	2.09	116.17	111.25
2	E	324	1Z7	O1-C1-N1	2.09	126.95	122.93

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	330	XYS	C2
4	E	330	XYS	C3
4	E	330	XYS	C1
4	E	330	XYS	C4

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 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.