



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 01:14 PM BST

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

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

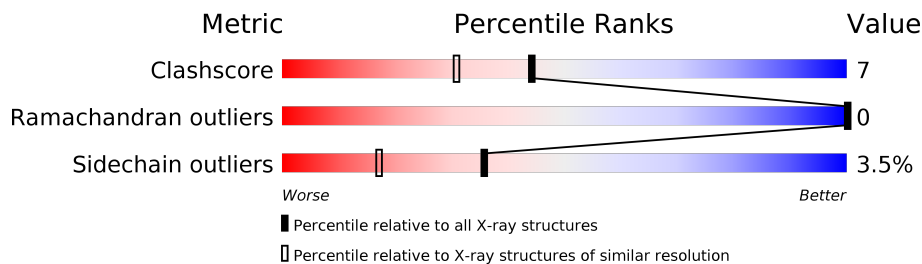
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (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 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	E	323	81% 16% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	XYS	E	330	X	-	-	-
5	SO4	E	331	-	-	X	-

## 2 Entry composition [i](#)

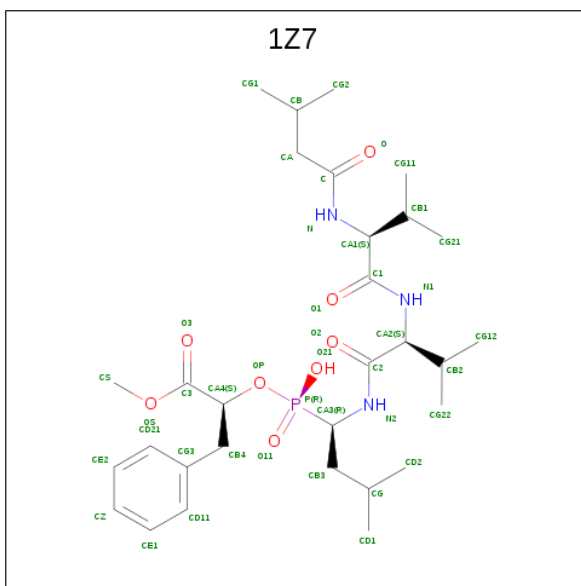
There are 6 unique types of molecules in this entry. The entry contains 2713 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PENICILLOPEPSIN.

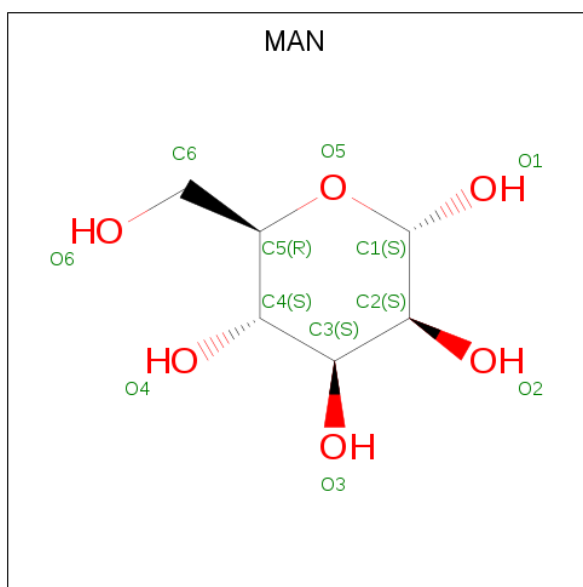
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	323	2370	1480	378	510	2	0	2	0

- Molecule 2 is N-(3-methylbutanoyl)-L-valyl-N-[(1S)-1-[(R)-[(1R)-1-benzyl-2-methoxy-2-oxoethoxy](hydroxy)phosphoryl]-3-methylbutyl]-L-valinamide (three-letter code: 1Z7) (formula: C<sub>30</sub>H<sub>50</sub>N<sub>3</sub>O<sub>8</sub>P).



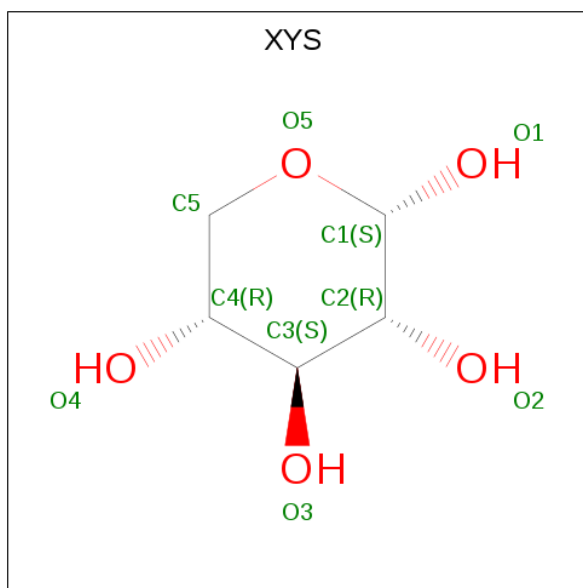
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	E	1	42	30	3	8	1	0	0

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



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

- Molecule 4 is alpha-D-xylopyranose (three-letter code: XYS) (formula: C<sub>5</sub>H<sub>10</sub>O<sub>5</sub>).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 6 is water.

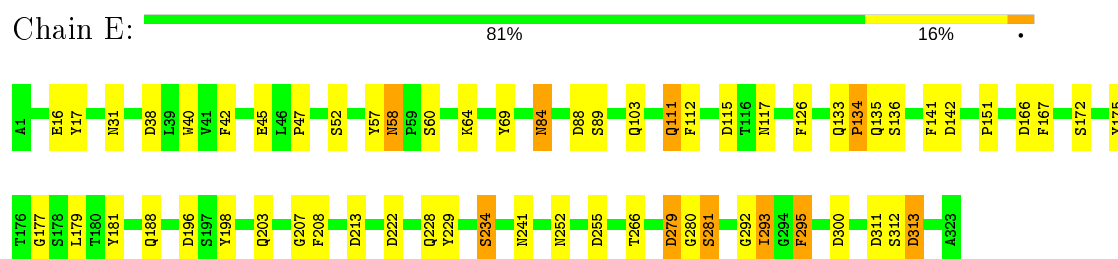
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	276	Total	O	0	0
			276	276		

### 3 Residue-property plots [i](#)

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: PENICILLOPEPSIN



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore 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.	Xtrriage
Total number of atoms	2713	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

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 Too-close contacts [\(i\)](#)

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	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

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 7.

All (31) 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)
2:E:324:1Z7:CD21	2:E:324:1Z7:HD2	0.97	1.15
2:E:324:1Z7:HD1	2:E:324:1Z7:CD11	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:HD1	2:E:324:1Z7:CE1	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:133[B]:GLN:NE2	6:E:469:HOH:O	1.99	0.45
1:E:175:TYR:OH	5:E:331:SO4:O4	2.22	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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 [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	E	323/323 (100%)	320 (99%)	3 (1%)	0	100 100

There are no Ramachandran outliers to report.

### 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	E	261/259 (101%)	252 (97%)	9 (3%)	37 18

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

Mol	Chain	Res	Type
1	E	38	ASP
1	E	47	PRO
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 [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 monosaccharides 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	-	40,42,42	1.83	9 (22%)	49,58,58	1.99	16 (32%)
4	XYS	E	330	1	9,9,10	1.29	1 (11%)	10,12,14	3.88	6 (60%)
5	SO4	E	331	-	4,4,4	0.78	0	6,6,6	0.68	0
3	MAN	E	329	1	11,11,12	0.86	0	15,15,17	1.82	6 (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
2	1Z7	E	324	-	-	3/57/57/57	0/1/1/1
4	XYS	E	330	1	4/4/3/4	-	0/1/1/1
3	MAN	E	329	1	-	0/2/19/22	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	324	1Z7	P-OP	-4.71	1.50	1.57
2	E	324	1Z7	P-CA3	-4.60	1.80	1.84
2	E	324	1Z7	P-O21	-4.47	1.46	1.56
2	E	324	1Z7	CA2-N1	3.54	1.53	1.45
2	E	324	1Z7	OS-C3	3.10	1.40	1.33
2	E	324	1Z7	O-C	2.75	1.28	1.23
4	E	330	XYS	O2-C2	-2.42	1.38	1.43
2	E	324	1Z7	CA4-C3	2.39	1.55	1.51
2	E	324	1Z7	O1-C1	2.27	1.27	1.23
2	E	324	1Z7	CB4-CA4	2.11	1.55	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	330	XYS	C5-O5-C1	8.94	125.27	111.52
2	E	324	1Z7	CA-C-N	6.79	125.23	116.33
4	E	330	XYS	O4-C4-C3	-5.21	99.70	110.14
2	E	324	1Z7	O11-P-CA3	-3.62	109.19	114.20
2	E	324	1Z7	O-C-CA	-3.53	116.33	121.50
2	E	324	1Z7	OP-CA4-CB4	3.34	113.16	107.51
4	E	330	XYS	O3-C3-C2	3.30	116.32	109.99
2	E	324	1Z7	C2-CA2-N1	-3.27	101.47	110.36
3	E	329	MAN	C6-C5-C4	3.19	120.48	113.00
2	E	324	1Z7	OP-P-O11	-3.18	109.13	115.12
4	E	330	XYS	O2-C2-C3	3.16	116.46	110.14
4	E	330	XYS	C1-C2-C3	-2.75	106.28	109.67
4	E	330	XYS	O4-C4-C5	2.73	114.74	109.15
2	E	324	1Z7	O2-C2-N2	2.70	127.92	122.93
2	E	324	1Z7	O-C-N	-2.68	118.44	122.95
2	E	324	1Z7	CA2-N1-C1	-2.65	115.14	121.89
2	E	324	1Z7	CG-CB3-CA3	2.57	120.38	114.86
3	E	329	MAN	C1-C2-C3	-2.48	106.61	109.67
3	E	329	MAN	C3-C4-C5	-2.46	105.85	110.24
2	E	324	1Z7	CB1-CA1-N	-2.44	105.40	111.43
2	E	324	1Z7	CG3-CB4-CA4	2.44	117.17	113.15
2	E	324	1Z7	OS-C3-CA4	2.29	116.17	110.93
3	E	329	MAN	O4-C4-C3	-2.26	105.12	110.35
2	E	324	1Z7	CG1-CB-CA	-2.26	102.11	111.22
2	E	324	1Z7	CD2-CG-CD1	2.21	120.71	110.51
2	E	324	1Z7	O1-C1-N1	2.17	126.95	122.93
3	E	329	MAN	O3-C3-C2	-2.12	105.92	109.99
3	E	329	MAN	O2-C2-C1	-2.12	104.81	109.15

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

All (3) torsion outliers are listed below:

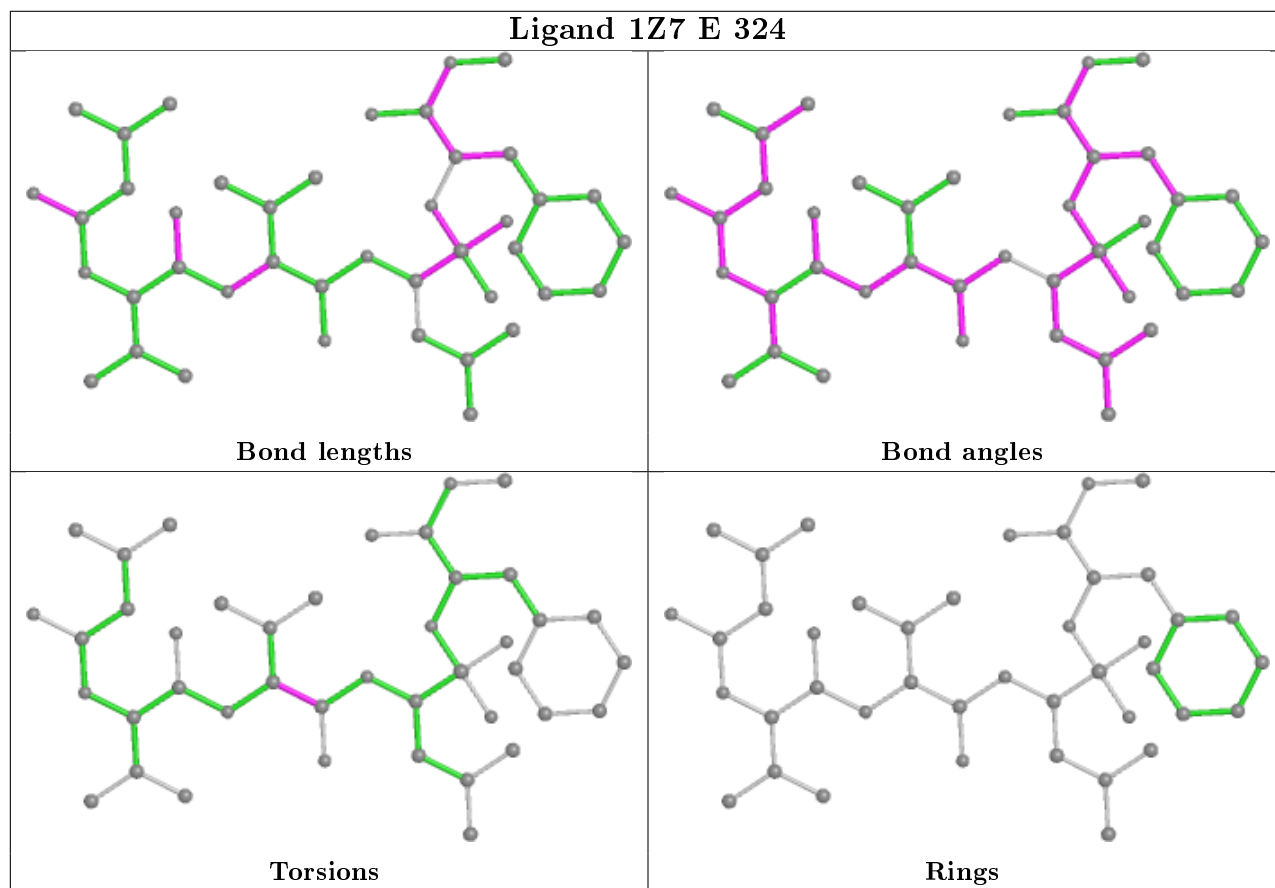
Mol	Chain	Res	Type	Atoms
2	E	324	1Z7	N2-C2-CA2-N1
2	E	324	1Z7	O2-C2-CA2-N1
2	E	324	1Z7	N2-C2-CA2-CB2

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	324	1Z7	8	0
5	E	331	SO4	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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.