



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:56 am BST

PDB ID : 1EPO
Title : ENDOTHIA ASPARTIC PROTEINASE (ENDOTHIAPEPSIN) COM-
PLEXED WITH CP-81,282 (MOR PHE NLE CHF NME)
Authors : Veerapandian, B.; Cooper, J.B.; Blundell, T.L.
Deposited on : 1994-07-27
Resolution : 2.00 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (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) : 2.11

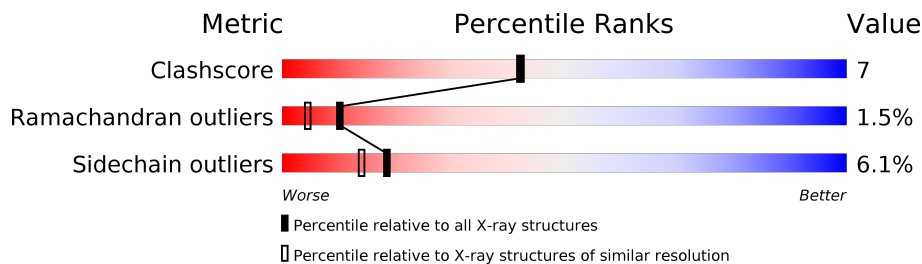
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 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	330	

2 Entry composition [i](#)

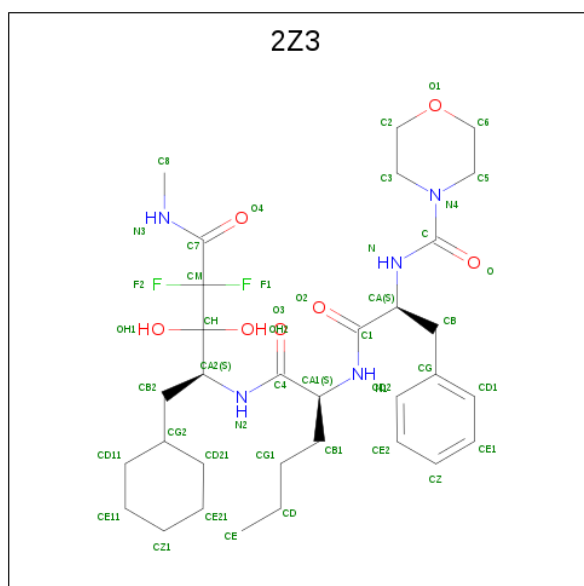
There are 3 unique types of molecules in this entry. The entry contains 2741 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ENDOTHIAPEPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	330	2389	1514	366	507	2	0	0	0

- Molecule 2 is N-(morpholin-4-ylcarbonyl)-L-phenylalanyl-N-[(1R)-1-(cyclohexylmethyl)-3,3-difluoro-2,2-dihydroxy-4-(methylamino)-4-oxobutyl]-L-norleucinamide (three-letter code: 2Z3) (formula: C₃₂H₄₉F₂N₅O₇).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	E	1	46	32	2	5	7	0	0

- Molecule 3 is water.

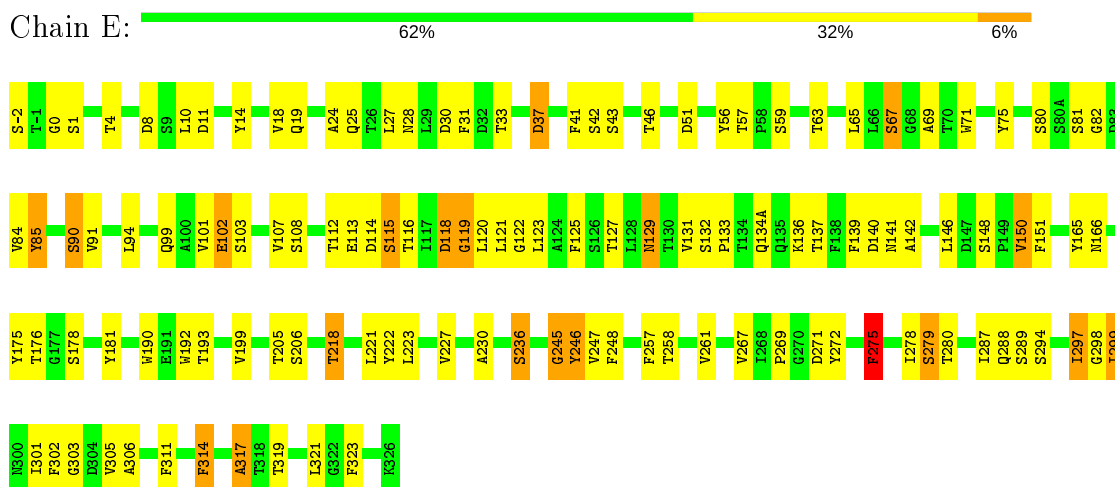
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	306	Total	O	0	0
			306	306		

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. 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: ENDOTHIAPEPSIN



4 Data and refinement statistics

Xtrriage (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	53.70Å 73.90Å 45.80Å 90.00° 110.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2741	wwPDB-VP
Average B, all atoms (Å ²)	0.0	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:
2Z3

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	1.87	40/2445 (1.6%)	2.02	77/3345 (2.3%)

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	E	0	6

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	192	TRP	NE1-CE2	-7.10	1.28	1.37
1	E	129	ASN	CG-OD1	7.09	1.39	1.24
1	E	305	VAL	CA-C	-7.01	1.34	1.52
1	E	190	TRP	CD2-CE2	-6.85	1.33	1.41
1	E	178	SER	N-CA	6.67	1.59	1.46
1	E	206	SER	CB-OG	6.65	1.50	1.42
1	E	8	ASP	N-CA	6.44	1.59	1.46
1	E	181	TYR	CE1-CZ	6.42	1.47	1.38
1	E	258	THR	CB-OG1	6.32	1.55	1.43
1	E	288	GLN	CA-CB	-5.94	1.40	1.53
1	E	0	GLY	CA-C	5.87	1.61	1.51
1	E	141	ASN	CG-OD1	5.78	1.36	1.24
1	E	137	THR	CB-OG1	-5.77	1.31	1.43
1	E	28	ASN	CG-OD1	5.76	1.36	1.24
1	E	118	ASP	C-N	-5.75	1.22	1.33
1	E	190	TRP	CG-CD1	-5.72	1.28	1.36
1	E	298	GLY	N-CA	-5.68	1.37	1.46
1	E	59	SER	CA-CB	-5.68	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	113	GLU	C-O	5.67	1.34	1.23
1	E	289	SER	CB-OG	5.66	1.49	1.42
1	E	37	ASP	N-CA	-5.51	1.35	1.46
1	E	192	TRP	CD2-CE2	5.49	1.48	1.41
1	E	190	TRP	CD1-NE1	5.47	1.47	1.38
1	E	82	GLY	N-CA	5.45	1.54	1.46
1	E	305	VAL	C-O	5.43	1.33	1.23
1	E	119	GLY	CA-C	-5.42	1.43	1.51
1	E	245	GLY	N-CA	-5.40	1.38	1.46
1	E	303	GLY	C-O	-5.38	1.15	1.23
1	E	80	SER	CB-OG	5.38	1.49	1.42
1	E	319	THR	C-O	5.30	1.33	1.23
1	E	99	GLN	CD-OE1	5.29	1.35	1.24
1	E	108	SER	N-CA	5.28	1.56	1.46
1	E	14	TYR	C-O	5.21	1.33	1.23
1	E	18	VAL	CB-CG1	5.17	1.63	1.52
1	E	102	GLU	CD-OE1	-5.10	1.20	1.25
1	E	25	GLN	CD-OE1	5.08	1.35	1.24
1	E	90	SER	CB-OG	-5.06	1.35	1.42
1	E	-2	SER	CB-OG	5.04	1.48	1.42
1	E	122	GLY	N-CA	5.02	1.53	1.46
1	E	75	TYR	N-CA	5.00	1.56	1.46

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	11	ASP	CB-CG-OD2	8.43	125.89	118.30
1	E	275	PHE	N-CA-CB	8.07	125.13	110.60
1	E	190	TRP	CB-CG-CD2	-7.98	116.23	126.60
1	E	190	TRP	CB-CG-CD1	7.95	137.33	127.00
1	E	139	PHE	CB-CG-CD1	7.82	126.27	120.80
1	E	236	SER	O-C-N	-7.77	109.98	123.20
1	E	113	GLU	OE1-CD-OE2	-7.39	114.43	123.30
1	E	193	THR	CA-CB-CG2	-7.36	102.10	112.40
1	E	113	GLU	O-C-N	-7.31	111.00	122.70
1	E	267	VAL	CA-CB-CG2	7.28	121.82	110.90
1	E	69	ALA	CB-CA-C	7.26	121.00	110.10
1	E	317	ALA	CB-CA-C	7.20	120.90	110.10
1	E	247	VAL	CA-CB-CG2	7.15	121.63	110.90
1	E	8	ASP	CB-CG-OD1	7.12	124.71	118.30
1	E	199	VAL	CA-CB-CG2	7.02	121.43	110.90
1	E	190	TRP	O-C-N	6.93	133.79	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	321	LEU	CB-CG-CD1	6.84	122.63	111.00
1	E	42	SER	O-C-N	-6.69	112.00	122.70
1	E	190	TRP	C-N-CA	6.67	138.38	121.70
1	E	31	PHE	N-CA-CB	6.67	122.60	110.60
1	E	258	THR	OG1-CB-CG2	-6.58	94.86	110.00
1	E	321	LEU	CB-CG-CD2	6.55	122.14	111.00
1	E	227	VAL	CA-CB-CG2	6.53	120.69	110.90
1	E	305	VAL	O-C-N	-6.48	112.33	122.70
1	E	125	PHE	CB-CG-CD1	6.36	125.25	120.80
1	E	31	PHE	CG-CD1-CE1	-6.35	113.82	120.80
1	E	246	TYR	N-CA-CB	6.29	121.92	110.60
1	E	56	TYR	CD1-CE1-CZ	-6.22	114.20	119.80
1	E	107	VAL	CA-CB-CG2	6.10	120.05	110.90
1	E	248	PHE	CB-CG-CD1	-6.07	116.55	120.80
1	E	314	PHE	CB-CG-CD2	-6.02	116.59	120.80
1	E	287	ILE	CA-CB-CG1	5.96	122.33	111.00
1	E	178	SER	N-CA-CB	-5.96	101.57	110.50
1	E	176	THR	OG1-CB-CG2	-5.95	96.32	110.00
1	E	57	THR	OG1-CB-CG2	-5.93	96.36	110.00
1	E	222	TYR	CB-CG-CD2	-5.90	117.46	121.00
1	E	246	TYR	CB-CG-CD1	-5.89	117.46	121.00
1	E	4	THR	CA-CB-OG1	5.86	121.31	109.00
1	E	139	PHE	CG-CD1-CE1	5.86	127.24	120.80
1	E	165	TYR	C-N-CA	5.83	136.28	121.70
1	E	56	TYR	CG-CD2-CE2	-5.79	116.67	121.30
1	E	14	TYR	CG-CD1-CE1	-5.75	116.70	121.30
1	E	30	ASP	C-N-CA	5.72	135.99	121.70
1	E	175	TYR	CG-CD1-CE1	-5.70	116.74	121.30
1	E	31	PHE	CZ-CE2-CD2	-5.63	113.34	120.10
1	E	30	ASP	CB-CG-OD1	5.57	123.31	118.30
1	E	56	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	E	297	ILE	C-N-CA	5.53	133.91	122.30
1	E	11	ASP	OD1-CG-OD2	-5.46	112.93	123.30
1	E	150	VAL	CA-CB-CG2	-5.45	102.73	110.90
1	E	236	SER	CA-C-N	5.44	127.09	116.20
1	E	107	VAL	C-N-CA	-5.41	108.18	121.70
1	E	91	VAL	CA-CB-CG2	5.40	119.00	110.90
1	E	317	ALA	N-CA-CB	5.39	117.64	110.10
1	E	261	VAL	CA-CB-CG1	5.37	118.95	110.90
1	E	222	TYR	CG-CD2-CE2	-5.32	117.05	121.30
1	E	31	PHE	CB-CG-CD2	-5.31	117.08	120.80
1	E	230	ALA	CB-CA-C	5.30	118.06	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	257	PHE	N-CA-CB	-5.29	101.08	110.60
1	E	288	GLN	N-CA-CB	5.26	120.07	110.60
1	E	247	VAL	C-N-CA	5.25	134.82	121.70
1	E	41	PHE	CA-CB-CG	5.24	126.48	113.90
1	E	112	THR	CA-CB-OG1	5.24	120.00	109.00
1	E	41	PHE	CB-CG-CD1	5.21	124.45	120.80
1	E	140	ASP	CB-CG-OD1	5.21	122.99	118.30
1	E	114	ASP	CB-CG-OD1	5.19	122.97	118.30
1	E	84	VAL	CA-CB-CG2	5.17	118.66	110.90
1	E	311	PHE	CB-CG-CD1	-5.14	117.20	120.80
1	E	85	TYR	CG-CD1-CE1	-5.14	117.19	121.30
1	E	116	THR	CA-CB-CG2	-5.13	105.22	112.40
1	E	115	SER	O-C-N	-5.12	114.51	122.70
1	E	175	TYR	CB-CG-CD2	-5.11	117.93	121.00
1	E	271	ASP	CB-CA-C	-5.08	100.24	110.40
1	E	67	SER	C-N-CA	5.07	132.94	122.30
1	E	323	PHE	CB-CG-CD1	5.06	124.34	120.80
1	E	101	VAL	CG1-CB-CG2	5.05	118.98	110.90
1	E	306	ALA	O-C-N	-5.02	114.67	122.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	136	LYS	Mainchain
1	E	150	VAL	Peptide
1	E	24	ALA	Peptide
1	E	245	GLY	Peptide
1	E	275	PHE	Peptide
1	E	81	SER	Peptide

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	2389	0	2275	29	0
2	E	46	0	49	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	306	0	0	1	0
All	All	2741	0	2324	33	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 (33) 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:E:218:THR:HG21	1:E:301:ILE:HG21	1.18	1.14
2:E:327:2Z3:CD11	2:E:327:2Z3:HD13	0.97	1.13
2:E:327:2Z3:CD11	2:E:327:2Z3:HD12	0.97	1.09
2:E:327:2Z3:HD12	2:E:327:2Z3:CG2	1.98	0.93
2:E:327:2Z3:HD13	2:E:327:2Z3:CG2	1.98	0.91
1:E:218:THR:HG21	1:E:301:ILE:CG2	2.01	0.88
1:E:218:THR:OG1	2:E:327:2Z3:HA1	1.88	0.74
1:E:314:PHE:CD1	1:E:314:PHE:N	2.60	0.70
1:E:218:THR:CG2	1:E:301:ILE:HG21	2.11	0.64
1:E:33:THR:HG22	1:E:123:LEU:HB2	1.86	0.58
1:E:10:LEU:HD22	1:E:275:PHE:O	2.05	0.57
1:E:299:ILE:HG22	3:E:496:HOH:O	2.06	0.55
1:E:294:SER:HA	1:E:297:ILE:HD12	1.92	0.52
1:E:314:PHE:H	1:E:314:PHE:HD1	1.58	0.51
1:E:279:SER:O	1:E:280:THR:C	2.47	0.51
1:E:27:LEU:HD23	1:E:118:ASP:HB3	1.96	0.48
1:E:85:TYR:CD1	1:E:85:TYR:N	2.82	0.47
1:E:132:SER:OG	1:E:133:PRO:HA	2.13	0.47
1:E:218:THR:CG2	1:E:301:ILE:CG2	2.82	0.47
1:E:278:ILE:HG13	1:E:279:SER:N	2.30	0.47
1:E:129:ASN:ND2	1:E:131:VAL:H	2.14	0.46
1:E:1:SER:HA	1:E:166:ASN:HD22	1.80	0.46
1:E:151:PHE:CE1	1:E:314:PHE:HB2	2.52	0.45
1:E:302:PHE:N	1:E:302:PHE:CD1	2.84	0.45
1:E:71:TRP:CD1	1:E:102:GLU:HB3	2.52	0.45
1:E:94:LEU:HD21	1:E:142:ALA:HB1	1.99	0.45
1:E:119:GLY:C	1:E:120:LEU:HD12	2.37	0.44
1:E:120:LEU:HD21	2:E:327:2Z3:HD23	1.99	0.44
1:E:129:ASN:HD21	1:E:131:VAL:HG23	1.82	0.44
1:E:19:GLN:HB2	1:E:90:SER:HB2	1.99	0.44
1:E:146:LEU:HA	1:E:146:LEU:HD23	1.81	0.42
1:E:269:PRO:HD2	1:E:272:TYR:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:223:LEU:HD23	1:E:223:LEU:HA	1.88	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	E	328/330 (99%)	303 (92%)	20 (6%)	5 (2%)	10 4

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	317	ALA
1	E	43	SER
1	E	127	THR
1	E	205	THR
1	E	246	TYR

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	263/263 (100%)	247 (94%)	16 (6%)	18 14

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	37	ASP
1	E	46	THR
1	E	51	ASP
1	E	63	THR
1	E	65	LEU
1	E	67	SER
1	E	103	SER
1	E	115	SER
1	E	121	LEU
1	E	134(A)	GLN
1	E	148	SER
1	E	218	THR
1	E	221	LEU
1	E	236	SER
1	E	279	SER
1	E	299	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	28	ASN
1	E	99	GLN
1	E	129	ASN
1	E	134(A)	GLN
1	E	135	GLN
1	E	141	ASN
1	E	166	ASN
1	E	187	GLN
1	E	300	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	2Z3	E	327	-	46,48,48	1.90	13 (28%)	55,66,66	2.27	15 (27%)

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	2Z3	E	327	-	-	9/50/75/75	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	327	2Z3	OH1-CH	6.92	1.47	1.40
2	E	327	2Z3	CM-C7	-4.52	1.49	1.54
2	E	327	2Z3	O2-C1	-3.13	1.17	1.23
2	E	327	2Z3	C8-N3	2.87	1.50	1.45
2	E	327	2Z3	CA2-N2	2.67	1.51	1.46
2	E	327	2Z3	C3-N4	-2.32	1.42	1.47
2	E	327	2Z3	C3-C2	-2.31	1.41	1.50
2	E	327	2Z3	O4-C7	2.25	1.26	1.22
2	E	327	2Z3	C7-N3	2.24	1.36	1.33
2	E	327	2Z3	C4-N2	-2.13	1.29	1.34
2	E	327	2Z3	CA-N	2.07	1.50	1.45
2	E	327	2Z3	F1-CM	-2.04	1.28	1.35
2	E	327	2Z3	CD2-CG	2.04	1.43	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	E	327	2Z3	O4-C7-CM	9.33	125.54	118.44
2	E	327	2Z3	O4-C7-N3	-4.97	115.95	122.79
2	E	327	2Z3	C5-N4-C3	4.68	121.62	112.62
2	E	327	2Z3	C8-N3-C7	-4.23	115.69	121.95
2	E	327	2Z3	CE11-CD11-CG2	4.12	119.94	112.15
2	E	327	2Z3	CE2-CD2-CG	-2.90	116.18	120.63
2	E	327	2Z3	O2-C1-CA	2.58	125.87	120.45
2	E	327	2Z3	CG-CB-CA	-2.57	106.29	113.39
2	E	327	2Z3	CZ-CE2-CD2	2.49	123.99	120.19
2	E	327	2Z3	CZ1-CE21-CD21	2.46	116.44	111.42
2	E	327	2Z3	CB-CA-C1	-2.35	104.16	110.25
2	E	327	2Z3	CB2-CA2-N2	2.22	114.55	109.46
2	E	327	2Z3	CZ-CE1-CD1	-2.16	116.89	120.19
2	E	327	2Z3	OH2-CH-OH1	-2.09	104.82	110.89
2	E	327	2Z3	C4-CA1-N1	-2.00	105.72	111.16

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	327	2Z3	OH1-CH-CM-F2
2	E	327	2Z3	OH1-CH-CM-F1
2	E	327	2Z3	N2-CA2-CB2-CG2
2	E	327	2Z3	OH2-CH-CM-F2
2	E	327	2Z3	CE-CD-CG1-CB1
2	E	327	2Z3	CA2-CB2-CG2-CD21
2	E	327	2Z3	CA1-CB1-CG1-CD
2	E	327	2Z3	N2-C4-CA1-N1
2	E	327	2Z3	O3-C4-CA1-N1

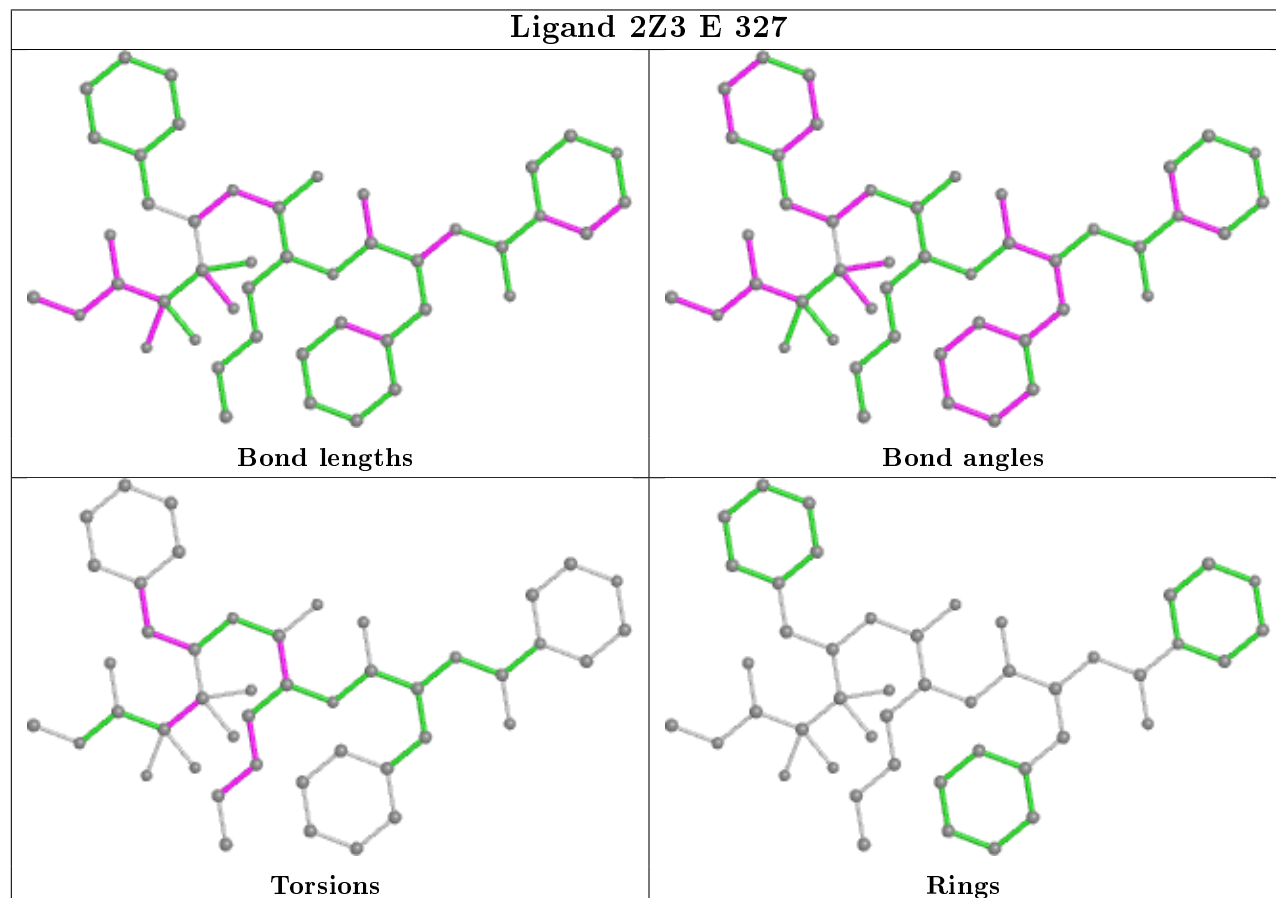
There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	327	2Z3	6	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.