



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:21 AM UTC

PDB ID : 1EPO / pdb_00001epo
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

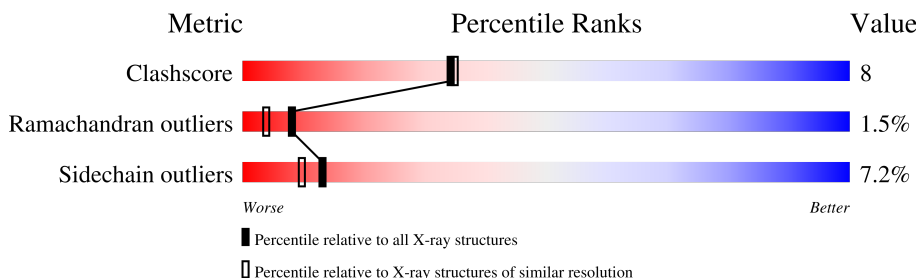
1 Overall quality at a glance

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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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 of 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](#)

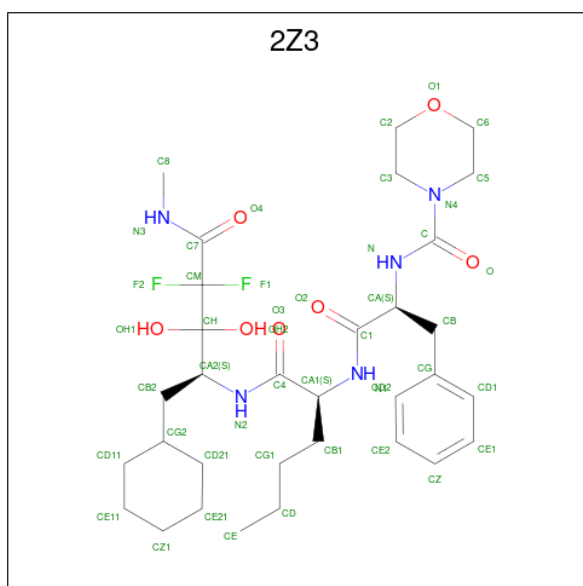
There are 3 unique types of molecules in this entry. The entry contains 2741 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	E	330	Total	C	N	O	S	0	0	0
			2389	1514	366	507	2			

- 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 (CCD ID: 2Z3) (formula: C₃₂H₄₉F₂N₅O₇).



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

- Molecule 3 is water.

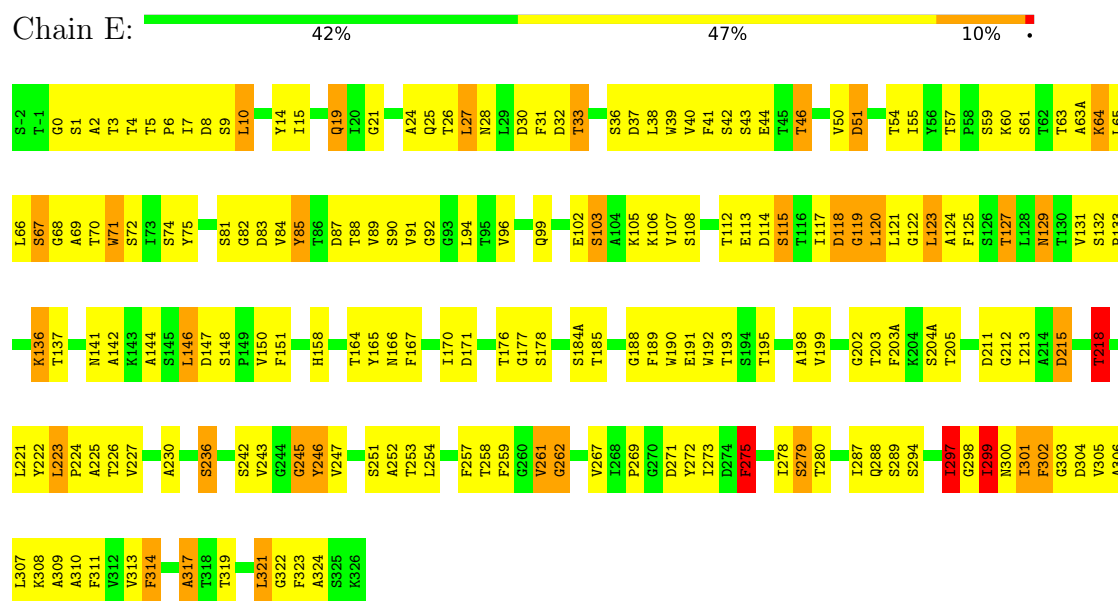
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	306	Total	O	0	0
			306	306		

3 Residue-property plots

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: ENDOTHIAPEPSIN



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	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.	Xtriage
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	2.52	146/2445 (6.0%)	2.61	207/3345 (6.2%)

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	E	0	6

All (146) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	305	VAL	CA-C	-14.06	1.34	1.52
1	E	178	SER	N-CA	11.30	1.59	1.45
1	E	158	HIS	CE1-NE2	10.76	1.43	1.32
1	E	8	ASP	N-CA	9.84	1.59	1.46
1	E	118	ASP	C-N	-9.39	1.22	1.33
1	E	303	GLY	C-O	-8.85	1.15	1.23
1	E	37	ASP	N-CA	-8.81	1.35	1.46
1	E	0	GLY	CA-C	8.80	1.61	1.51
1	E	108	SER	N-CA	8.75	1.56	1.45
1	E	113	GLU	C-O	8.49	1.34	1.24
1	E	129	ASN	CG-OD1	8.43	1.39	1.23
1	E	192	TRP	NE1-CE2	-8.30	1.28	1.37
1	E	120	LEU	C-N	-8.19	1.23	1.33
1	E	14	TYR	C-O	8.09	1.33	1.24
1	E	55	ILE	CA-CB	-8.09	1.44	1.54
1	E	2	ALA	CA-C	8.05	1.62	1.52
1	E	190	TRP	CA-CB	8.04	1.64	1.52
1	E	305	VAL	C-O	8.04	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	54	THR	CA-CB	-8.01	1.42	1.53
1	E	165	TYR	C-N	-7.93	1.23	1.33
1	E	203(A)	PHE	N-CA	7.85	1.55	1.46
1	E	127	THR	CA-C	-7.79	1.42	1.52
1	E	40	VAL	CA-C	-7.76	1.42	1.52
1	E	313	VAL	N-CA	7.69	1.55	1.46
1	E	258	THR	CB-OG1	7.58	1.55	1.43
1	E	137	THR	CB-OG1	-7.52	1.31	1.43
1	E	305	VAL	CA-CB	7.46	1.63	1.54
1	E	118	ASP	CA-C	7.44	1.63	1.52
1	E	198	ALA	N-CA	7.43	1.55	1.45
1	E	164	THR	N-CA	7.41	1.55	1.46
1	E	287	ILE	CA-CB	-7.36	1.44	1.54
1	E	66	LEU	N-CA	7.34	1.55	1.46
1	E	19	GLN	C-N	-7.30	1.24	1.33
1	E	119	GLY	CA-C	-7.30	1.43	1.52
1	E	87	ASP	N-CA	7.26	1.54	1.46
1	E	15	ILE	N-CA	7.22	1.54	1.46
1	E	61	SER	C-O	-7.21	1.15	1.24
1	E	75	TYR	N-CA	7.19	1.56	1.46
1	E	37	ASP	CA-CB	7.18	1.62	1.53
1	E	319	THR	C-O	7.18	1.33	1.24
1	E	257	PHE	N-CA	7.17	1.55	1.46
1	E	301	ILE	CA-CB	-7.17	1.45	1.53
1	E	83	ASP	N-CA	7.12	1.55	1.46
1	E	3	THR	C-N	7.11	1.43	1.33
1	E	106	LYS	N-CA	7.07	1.55	1.46
1	E	211	ASP	N-CA	-7.04	1.37	1.46
1	E	306	ALA	N-CA	-7.00	1.37	1.46
1	E	118	ASP	N-CA	6.96	1.55	1.46
1	E	322	GLY	CA-C	6.95	1.57	1.52
1	E	6	PRO	CA-C	-6.93	1.43	1.52
1	E	141	ASN	CG-OD1	6.91	1.36	1.23
1	E	28	ASN	CG-OD1	6.88	1.36	1.23
1	E	89	VAL	CA-C	-6.83	1.44	1.52
1	E	213	ILE	N-CA	6.80	1.54	1.46
1	E	310	ALA	N-CA	6.76	1.54	1.45
1	E	307	LEU	CA-CB	6.74	1.64	1.53
1	E	192	TRP	N-CA	6.70	1.55	1.46
1	E	107	VAL	N-CA	6.68	1.53	1.46
1	E	64	LYS	N-CA	6.67	1.54	1.46
1	E	199	VAL	CA-CB	-6.67	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	39	TRP	C-N	-6.55	1.24	1.33
1	E	190	TRP	C-N	-6.53	1.24	1.33
1	E	321	LEU	CB-CG	-6.47	1.40	1.53
1	E	15	ILE	CA-CB	-6.46	1.45	1.54
1	E	311	PHE	N-CA	6.41	1.54	1.46
1	E	4	THR	N-CA	6.36	1.53	1.45
1	E	99	GLN	CD-OE1	6.34	1.35	1.23
1	E	31	PHE	C-N	-6.30	1.24	1.33
1	E	28	ASN	N-CA	6.29	1.53	1.46
1	E	288	GLN	CA-CB	-6.27	1.40	1.54
1	E	224	PRO	CA-C	6.20	1.59	1.52
1	E	271	ASP	CA-CB	6.20	1.63	1.53
1	E	4	THR	CA-C	6.20	1.60	1.52
1	E	113	GLU	CA-C	-6.18	1.44	1.52
1	E	33	THR	CA-CB	-6.16	1.43	1.53
1	E	184(A)	SER	C-O	6.16	1.31	1.24
1	E	191	GLU	CA-C	-6.11	1.45	1.52
1	E	82	GLY	N-CA	6.11	1.54	1.45
1	E	71	TRP	N-CA	6.11	1.53	1.45
1	E	25	GLN	CD-OE1	6.09	1.35	1.23
1	E	184(A)	SER	CA-C	-6.05	1.45	1.52
1	E	122	GLY	C-O	6.05	1.29	1.23
1	E	178	SER	CA-C	-6.03	1.45	1.52
1	E	99	GLN	C-O	-6.02	1.16	1.23
1	E	289	SER	N-CA	6.02	1.53	1.45
1	E	176	THR	C-N	-6.02	1.24	1.33
1	E	308	LYS	CA-C	-5.99	1.44	1.52
1	E	222	TYR	CA-C	-5.96	1.45	1.52
1	E	129	ASN	N-CA	5.93	1.53	1.46
1	E	9	SER	N-CA	5.91	1.53	1.46
1	E	300	ASN	CG-OD1	5.87	1.34	1.23
1	E	72	SER	C-O	-5.87	1.16	1.24
1	E	19	GLN	CD-OE1	5.83	1.34	1.23
1	E	146	LEU	CA-C	-5.82	1.45	1.52
1	E	122	GLY	N-CA	5.81	1.53	1.45
1	E	261	VAL	C-O	-5.80	1.17	1.24
1	E	30	ASP	C-N	-5.78	1.25	1.33
1	E	193	THR	CA-CB	5.78	1.62	1.53
1	E	125	PHE	CA-C	-5.78	1.45	1.52
1	E	254	LEU	C-N	5.75	1.40	1.33
1	E	230	ALA	CA-CB	-5.75	1.44	1.53
1	E	69	ALA	N-CA	5.73	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	305	VAL	N-CA	5.69	1.53	1.46
1	E	0	GLY	C-N	-5.68	1.26	1.33
1	E	246	TYR	CA-CB	-5.66	1.44	1.53
1	E	324	ALA	N-CA	5.66	1.53	1.45
1	E	165	TYR	CA-CB	-5.64	1.45	1.53
1	E	245	GLY	C-O	-5.62	1.16	1.23
1	E	188	GLY	CA-C	5.61	1.59	1.51
1	E	115	SER	CA-C	-5.59	1.44	1.52
1	E	41	PHE	C-O	5.56	1.30	1.23
1	E	112	THR	CB-OG1	-5.52	1.34	1.43
1	E	262	GLY	N-CA	5.51	1.53	1.45
1	E	267	VAL	N-CA	5.50	1.53	1.46
1	E	70	THR	CB-OG1	5.50	1.52	1.43
1	E	324	ALA	CA-C	5.50	1.59	1.52
1	E	3	THR	C-O	-5.50	1.17	1.24
1	E	36	SER	CA-C	-5.49	1.46	1.52
1	E	297	ILE	N-CA	5.49	1.52	1.45
1	E	304	ASP	CA-CB	5.49	1.61	1.53
1	E	71	TRP	C-O	-5.44	1.17	1.23
1	E	6	PRO	N-CA	5.40	1.53	1.47
1	E	31	PHE	N-CA	-5.36	1.39	1.46
1	E	247	VAL	CA-CB	-5.33	1.46	1.54
1	E	254	LEU	CA-C	-5.32	1.46	1.53
1	E	59	SER	CA-CB	-5.32	1.44	1.53
1	E	83	ASP	CA-C	-5.32	1.45	1.52
1	E	171	ASP	N-CA	5.31	1.53	1.46
1	E	254	LEU	N-CA	5.29	1.54	1.46
1	E	124	ALA	N-CA	5.28	1.53	1.46
1	E	123	LEU	C-N	5.27	1.41	1.33
1	E	170	ILE	N-CA	5.27	1.52	1.46
1	E	251	SER	CA-C	-5.26	1.45	1.52
1	E	243	VAL	CA-CB	5.26	1.61	1.54
1	E	92	GLY	N-CA	5.24	1.52	1.45
1	E	99	GLN	C-N	5.21	1.41	1.33
1	E	198	ALA	C-O	5.18	1.30	1.23
1	E	245	GLY	N-CA	-5.12	1.38	1.45
1	E	212	GLY	CA-C	-5.12	1.46	1.52
1	E	245	GLY	CA-C	5.10	1.59	1.51
1	E	42	SER	C-O	5.09	1.30	1.23
1	E	3	THR	N-CA	5.07	1.52	1.46
1	E	223	LEU	CA-C	-5.07	1.46	1.52
1	E	298	GLY	N-CA	-5.04	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	125	PHE	C-O	5.02	1.30	1.23
1	E	88	THR	CA-C	5.01	1.59	1.52

All (207) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	41	PHE	CA-CB-CG	12.68	126.48	113.80
1	E	314	PHE	CA-CB-CG	-11.75	102.05	113.80
1	E	190	TRP	CA-C-N	10.72	138.38	121.66
1	E	190	TRP	C-N-CA	10.72	138.38	121.66
1	E	113	GLU	O-C-N	-10.49	111.00	122.12
1	E	305	VAL	N-CA-C	10.28	122.34	110.62
1	E	305	VAL	O-C-N	-9.75	112.33	121.89
1	E	165	TYR	CA-C-N	9.62	136.28	123.00
1	E	165	TYR	C-N-CA	9.62	136.28	123.00
1	E	297	ILE	N-CA-C	-9.55	104.17	111.90
1	E	236	SER	O-C-N	-9.48	109.98	122.59
1	E	202	GLY	CA-C-N	9.40	134.15	120.90
1	E	202	GLY	C-N-CA	9.40	134.15	120.90
1	E	42	SER	O-C-N	-8.70	112.00	122.96
1	E	275	PHE	N-CA-CB	8.66	125.13	110.49
1	E	190	TRP	O-C-N	8.64	133.79	122.38
1	E	37	ASP	N-CA-C	8.43	122.47	108.73
1	E	297	ILE	CB-CA-C	-8.06	103.56	111.30
1	E	254	LEU	CA-C-O	7.95	126.86	120.19
1	E	4	THR	CA-CB-OG1	7.81	121.31	109.60
1	E	302	PHE	CA-CB-CG	-7.77	106.03	113.80
1	E	113	GLU	N-CA-C	7.75	120.71	111.33
1	E	288	GLN	OE1-CD-NE2	-7.68	114.92	122.60
1	E	30	ASP	CA-C-N	7.57	135.99	121.54
1	E	30	ASP	C-N-CA	7.57	135.99	121.54
1	E	257	PHE	CA-CB-CG	-7.55	106.25	113.80
1	E	190	TRP	CB-CG-CD2	-7.55	116.23	126.80
1	E	222	TYR	CA-C-O	-7.52	112.05	120.32
1	E	74	SER	CA-C-N	-7.36	109.91	123.01
1	E	74	SER	C-N-CA	-7.36	109.91	123.01
1	E	177	GLY	CA-C-N	-7.33	110.50	122.81
1	E	177	GLY	C-N-CA	-7.33	110.50	122.81
1	E	10	LEU	CA-C-O	-7.30	110.81	119.35
1	E	226	THR	N-CA-C	7.28	119.84	111.11
1	E	176	THR	CA-C-N	7.25	131.81	120.00
1	E	176	THR	C-N-CA	7.25	131.81	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	190	TRP	CA-C-O	-7.24	113.64	122.41
1	E	258	THR	OG1-CB-CG2	-7.22	94.86	109.30
1	E	309	ALA	CA-C-N	-7.21	110.82	122.36
1	E	309	ALA	C-N-CA	-7.21	110.82	122.36
1	E	31	PHE	N-CA-CB	7.16	122.60	110.49
1	E	211	ASP	CA-C-N	-7.09	112.95	122.03
1	E	211	ASP	C-N-CA	-7.09	112.95	122.03
1	E	195	THR	N-CA-C	7.07	121.73	113.18
1	E	107	VAL	CA-C-N	-7.02	108.18	121.66
1	E	107	VAL	C-N-CA	-7.02	108.18	121.66
1	E	287	ILE	CA-CB-CG1	7.01	122.33	110.40
1	E	87	ASP	CA-C-O	-7.00	113.78	121.28
1	E	218	THR	CB-CA-C	6.99	122.35	109.70
1	E	190	TRP	CB-CA-C	-6.96	100.69	111.83
1	E	190	TRP	CB-CG-CD1	6.95	137.33	126.90
1	E	108	SER	CA-C-N	6.94	129.58	120.28
1	E	108	SER	C-N-CA	6.94	129.58	120.28
1	E	112	THR	CA-CB-OG1	6.94	120.00	109.60
1	E	271	ASP	CA-CB-CG	-6.93	105.67	112.60
1	E	25	GLN	OE1-CD-NE2	-6.92	115.68	122.60
1	E	27	LEU	CA-C-N	-6.84	113.47	123.05
1	E	27	LEU	C-N-CA	-6.84	113.47	123.05
1	E	125	PHE	O-C-N	-6.80	114.99	123.01
1	E	37	ASP	CA-CB-CG	-6.79	105.81	112.60
1	E	69	ALA	CB-CA-C	6.79	121.00	109.53
1	E	246	TYR	N-CA-CB	6.76	121.92	110.49
1	E	115	SER	O-C-N	-6.75	114.51	122.20
1	E	267	VAL	CA-CB-CG2	6.72	121.82	110.40
1	E	141	ASN	OD1-CG-ND2	-6.71	115.89	122.60
1	E	247	VAL	CA-CB-CG2	6.61	121.63	110.40
1	E	306	ALA	O-C-N	-6.56	114.67	122.15
1	E	297	ILE	CA-C-N	6.55	133.91	122.05
1	E	297	ILE	C-N-CA	6.55	133.91	122.05
1	E	14	TYR	CA-C-O	-6.50	113.34	120.30
1	E	68	GLY	CA-C-N	-6.50	112.12	121.42
1	E	68	GLY	C-N-CA	-6.50	112.12	121.42
1	E	301	ILE	N-CA-C	6.50	117.19	107.51
1	E	176	THR	OG1-CB-CG2	-6.49	96.32	109.30
1	E	199	VAL	CA-CB-CG2	6.49	121.43	110.40
1	E	57	THR	OG1-CB-CG2	-6.47	96.36	109.30
1	E	51	ASP	CB-CA-C	-6.45	101.09	111.86
1	E	261	VAL	O-C-N	-6.43	116.79	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	6	PRO	CB-CA-C	6.43	119.75	111.46
1	E	114	ASP	N-CA-CB	6.40	119.21	110.57
1	E	46	THR	N-CA-CB	6.40	119.40	109.48
1	E	0	GLY	CA-C-N	6.38	131.69	122.44
1	E	0	GLY	C-N-CA	6.38	131.69	122.44
1	E	287	ILE	CB-CA-C	6.34	118.74	110.12
1	E	129	ASN	CA-CB-CG	-6.33	106.27	112.60
1	E	123	LEU	CA-C-N	-6.32	109.47	121.54
1	E	123	LEU	C-N-CA	-6.32	109.47	121.54
1	E	147	ASP	CA-CB-CG	6.31	118.91	112.60
1	E	55	ILE	O-C-N	6.30	129.61	122.93
1	E	39	TRP	CA-C-O	-6.30	114.07	121.44
1	E	307	LEU	CA-C-O	-6.28	112.38	119.79
1	E	225	ALA	N-CA-C	-6.21	104.62	111.82
1	E	313	VAL	N-CA-CB	-6.20	103.95	111.21
1	E	25	GLN	CB-CG-CD	6.14	123.04	112.60
1	E	323	PHE	CA-C-O	6.14	127.33	120.70
1	E	275	PHE	CA-CB-CG	-6.13	107.67	113.80
1	E	271	ASP	N-CA-C	-6.11	105.32	112.89
1	E	3	THR	CA-C-N	-6.10	113.05	122.87
1	E	3	THR	C-N-CA	-6.10	113.05	122.87
1	E	144	ALA	CA-C-N	6.08	133.16	121.54
1	E	144	ALA	C-N-CA	6.08	133.16	121.54
1	E	273	ILE	CA-C-O	6.05	127.36	119.85
1	E	227	VAL	CA-CB-CG2	6.05	120.69	110.40
1	E	69	ALA	O-C-N	-6.04	115.89	123.01
1	E	167	PHE	O-C-N	-6.01	116.20	123.29
1	E	212	GLY	CA-C-N	-5.97	113.72	122.68
1	E	212	GLY	C-N-CA	-5.97	113.72	122.68
1	E	254	LEU	CA-C-N	-5.95	114.48	120.31
1	E	254	LEU	C-N-CA	-5.95	114.48	120.31
1	E	178	SER	N-CA-CB	-5.95	101.57	111.20
1	E	257	PHE	CA-C-N	5.90	130.50	122.19
1	E	257	PHE	C-N-CA	5.90	130.50	122.19
1	E	67	SER	CA-C-N	5.88	132.94	121.41
1	E	67	SER	C-N-CA	5.88	132.94	121.41
1	E	306	ALA	N-CA-C	5.85	117.73	111.36
1	E	8	ASP	CA-CB-CG	5.84	118.44	112.60
1	E	41	PHE	N-CA-CB	5.83	118.25	109.34
1	E	204(A)	SER	O-C-N	-5.79	115.31	123.01
1	E	9	SER	N-CA-C	-5.78	105.89	113.17
1	E	189	PHE	CA-CB-CG	-5.77	108.03	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	171	ASP	CA-CB-CG	-5.77	106.83	112.60
1	E	170	ILE	N-CA-CB	-5.73	104.25	111.41
1	E	107	VAL	CA-CB-CG2	5.68	120.05	110.40
1	E	28	ASN	OD1-CG-ND2	-5.67	116.93	122.60
1	E	21	GLY	CA-C-O	-5.66	116.13	122.24
1	E	75	TYR	N-CA-CB	-5.64	102.31	111.22
1	E	305	VAL	CA-C-N	5.64	128.30	120.29
1	E	305	VAL	C-N-CA	5.64	128.30	120.29
1	E	63(A)	ALA	CA-C-N	-5.62	114.84	122.77
1	E	63(A)	ALA	C-N-CA	-5.62	114.84	122.77
1	E	259	PHE	CA-CB-CG	-5.62	108.18	113.80
1	E	257	PHE	N-CA-CB	-5.62	101.08	110.80
1	E	92	GLY	CA-C-N	-5.61	115.50	123.08
1	E	92	GLY	C-N-CA	-5.61	115.50	123.08
1	E	89	VAL	CA-C-O	5.60	126.30	120.36
1	E	123	LEU	CA-C-O	5.60	126.72	119.95
1	E	7	ILE	CA-C-N	-5.59	112.73	122.84
1	E	7	ILE	C-N-CA	-5.59	112.73	122.84
1	E	136	LYS	O-C-N	-5.56	116.71	122.94
1	E	26	THR	CA-C-N	-5.53	113.51	122.81
1	E	26	THR	C-N-CA	-5.53	113.51	122.81
1	E	253	THR	CA-C-O	-5.53	114.29	120.54
1	E	247	VAL	CA-C-N	5.52	134.82	121.68
1	E	247	VAL	C-N-CA	5.52	134.82	121.68
1	E	299	ILE	CA-CB-CG2	5.50	119.85	110.50
1	E	28	ASN	N-CA-CB	-5.49	101.93	110.55
1	E	85	TYR	CA-CB-CG	-5.47	104.05	113.90
1	E	188	GLY	N-CA-C	-5.45	107.75	115.43
1	E	30	ASP	CA-C-O	-5.44	114.45	120.60
1	E	118	ASP	N-CA-C	-5.42	106.35	113.17
1	E	99	GLN	CG-CD-NE2	5.42	124.52	116.40
1	E	300	ASN	N-CA-C	5.39	117.50	109.25
1	E	91	VAL	N-CA-CB	-5.35	105.67	112.15
1	E	32	ASP	CA-CB-CG	-5.34	107.26	112.60
1	E	103	SER	CB-CA-C	5.32	118.81	110.19
1	E	21	GLY	O-C-N	5.31	128.68	123.10
1	E	60	LYS	N-CA-CB	5.31	118.35	110.49
1	E	191	GLU	CA-C-N	-5.30	114.00	122.53
1	E	191	GLU	C-N-CA	-5.30	114.00	122.53
1	E	0	GLY	CA-C-O	-5.28	116.39	121.19
1	E	54	THR	CA-CB-OG1	5.28	117.52	109.60
1	E	317	ALA	CB-CA-C	5.27	120.90	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	42	SER	N-CA-C	5.25	116.97	109.14
1	E	5	THR	CA-C-N	-5.25	114.36	119.76
1	E	5	THR	C-N-CA	-5.25	114.36	119.76
1	E	57	THR	CA-C-N	-5.22	114.28	119.56
1	E	57	THR	C-N-CA	-5.22	114.28	119.56
1	E	10	LEU	N-CA-CB	-5.22	102.77	110.49
1	E	245	GLY	O-C-N	5.21	129.47	122.70
1	E	85	TYR	N-CA-CB	-5.20	102.96	110.70
1	E	192	TRP	CA-C-N	-5.19	115.49	122.86
1	E	192	TRP	C-N-CA	-5.19	115.49	122.86
1	E	193	THR	CA-CB-OG1	-5.19	101.81	109.60
1	E	171	ASP	N-CA-CB	-5.18	101.74	110.49
1	E	242	SER	CA-C-O	5.17	125.92	119.97
1	E	185	THR	CA-C-N	5.16	127.20	120.28
1	E	185	THR	C-N-CA	5.16	127.20	120.28
1	E	84	VAL	CA-C-O	-5.16	114.81	120.43
1	E	224	PRO	CA-C-N	5.15	128.14	120.31
1	E	224	PRO	C-N-CA	5.15	128.14	120.31
1	E	258	THR	O-C-N	-5.15	117.35	123.22
1	E	322	GLY	CA-C-O	-5.14	115.60	120.64
1	E	89	VAL	CA-C-N	-5.14	115.48	122.93
1	E	89	VAL	C-N-CA	-5.14	115.48	122.93
1	E	203	THR	CB-CA-C	-5.13	101.43	109.70
1	E	305	VAL	N-CA-CB	-5.13	104.06	110.47
1	E	44	GLU	CB-CG-CD	-5.12	103.89	112.60
1	E	252	ALA	N-CA-C	5.12	116.90	110.24
1	E	105	LYS	CA-C-N	-5.12	113.73	122.33
1	E	105	LYS	C-N-CA	-5.12	113.73	122.33
1	E	118	ASP	CB-CA-C	-5.11	101.56	110.09
1	E	2	ALA	CA-C-O	-5.11	114.79	120.66
1	E	4	THR	CA-CB-CG2	5.10	119.17	110.50
1	E	289	SER	CA-CB-OG	-5.09	100.92	111.10
1	E	288	GLN	CG-CD-NE2	5.08	124.02	116.40
1	E	36	SER	CA-C-N	5.08	129.52	122.77
1	E	36	SER	C-N-CA	5.08	129.52	122.77
1	E	91	VAL	CA-CB-CG2	5.06	119.00	110.40
1	E	46	THR	CA-CB-CG2	5.06	119.09	110.50
1	E	117	ILE	CA-C-N	-5.04	114.22	122.54
1	E	117	ILE	C-N-CA	-5.04	114.22	122.54
1	E	251	SER	O-C-N	-5.03	115.69	122.43
1	E	261	VAL	CA-CB-CG1	5.03	118.95	110.40
1	E	42	SER	CA-C-O	5.03	127.14	121.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	118	ASP	N-CA-CB	-5.02	103.06	110.49
1	E	215	ASP	O-C-N	-5.00	116.25	123.06
1	E	89	VAL	N-CA-CB	-5.00	104.22	111.52

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

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	2280	32	0
2	E	46	0	49	6	0
3	E	306	0	0	1	0
All	All	2741	0	2329	36	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 8.

All (36) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:279:SER:O	1:E:280:THR:C	2.47	0.56
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:119:GLY:C	1:E:120:LEU:HD12	2.37	0.49
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: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:HD23	1:E:146:LEU:HA	1.81	0.42
1:E:38:LEU:C	1:E:38:LEU:HD23	2.45	0.42
1:E:215:ASP:OD1	1:E:215:ASP:C	2.63	0.42
1:E:269:PRO:HD2	1:E:272:TYR:CD2	2.55	0.42
1:E:223:LEU:HD23	1:E:223:LEU:HA	1.88	0.40
1:E:261:VAL:O	1:E:262:GLY:C	2.61	0.40

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	328/330 (99%)	303 (92%)	20 (6%)	5 (2%)	8	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 ⓘ

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%)	244 (93%)	19 (7%)	13	10

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	46	THR
1	E	50	VAL
1	E	51	ASP
1	E	63	THR
1	E	64	LYS
1	E	65	LEU
1	E	67	SER
1	E	96	VAL
1	E	103	SER
1	E	115	SER
1	E	121	LEU
1	E	148	SER
1	E	218	THR
1	E	221	LEU

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Mol	Chain	Res	Type
1	E	236	SER
1	E	279	SER
1	E	297	ILE
1	E	299	ILE
1	E	321	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	99	GLN
1	E	129	ASN
1	E	134(A)	GLN
1	E	141	ASN
1	E	166	ASN
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 oligosaccharides 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	-	48,48,48	2.07	13 (27%)	54,66,66	2.10	13 (24%)

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	7.13	1.47	1.40
2	E	327	2Z3	CB2-CA2	-5.32	1.48	1.52
2	E	327	2Z3	CM-C7	-4.80	1.49	1.54
2	E	327	2Z3	O2-C1	-3.24	1.17	1.23
2	E	327	2Z3	C8-N3	2.87	1.50	1.45
2	E	327	2Z3	CA2-N2	2.74	1.51	1.46
2	E	327	2Z3	C3-C2	-2.42	1.41	1.50
2	E	327	2Z3	C3-N4	-2.30	1.42	1.47
2	E	327	2Z3	O4-C7	2.27	1.26	1.22
2	E	327	2Z3	C7-N3	2.27	1.36	1.33
2	E	327	2Z3	C4-N2	-2.20	1.29	1.34
2	E	327	2Z3	CD2-CG	2.19	1.43	1.38
2	E	327	2Z3	CA-N	2.09	1.50	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	327	2Z3	O4-C7-CM	6.65	125.54	118.39
2	E	327	2Z3	O4-C7-N3	-5.13	115.95	122.80
2	E	327	2Z3	C5-N4-C3	4.38	121.62	112.68
2	E	327	2Z3	C8-N3-C7	-4.32	115.69	121.92
2	E	327	2Z3	CE11-CD11-CG2	3.74	119.94	112.08
2	E	327	2Z3	CE2-CD2-CG	-3.15	116.18	120.61
2	E	327	2Z3	CZ-CE2-CD2	3.04	123.99	120.24
2	E	327	2Z3	CZ-CE1-CD1	-2.71	116.89	120.24
2	E	327	2Z3	CG-CB-CA	-2.66	106.29	113.36
2	E	327	2Z3	O2-C1-CA	2.58	125.87	120.48
2	E	327	2Z3	CZ1-CE21-CD21	2.44	116.44	111.42
2	E	327	2Z3	CB-CA-C1	-2.40	104.16	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	327	2Z3	OH2-CH-OH1	-2.14	104.82	111.02

There are no chirality outliers.

All (9) torsion outliers are listed below:

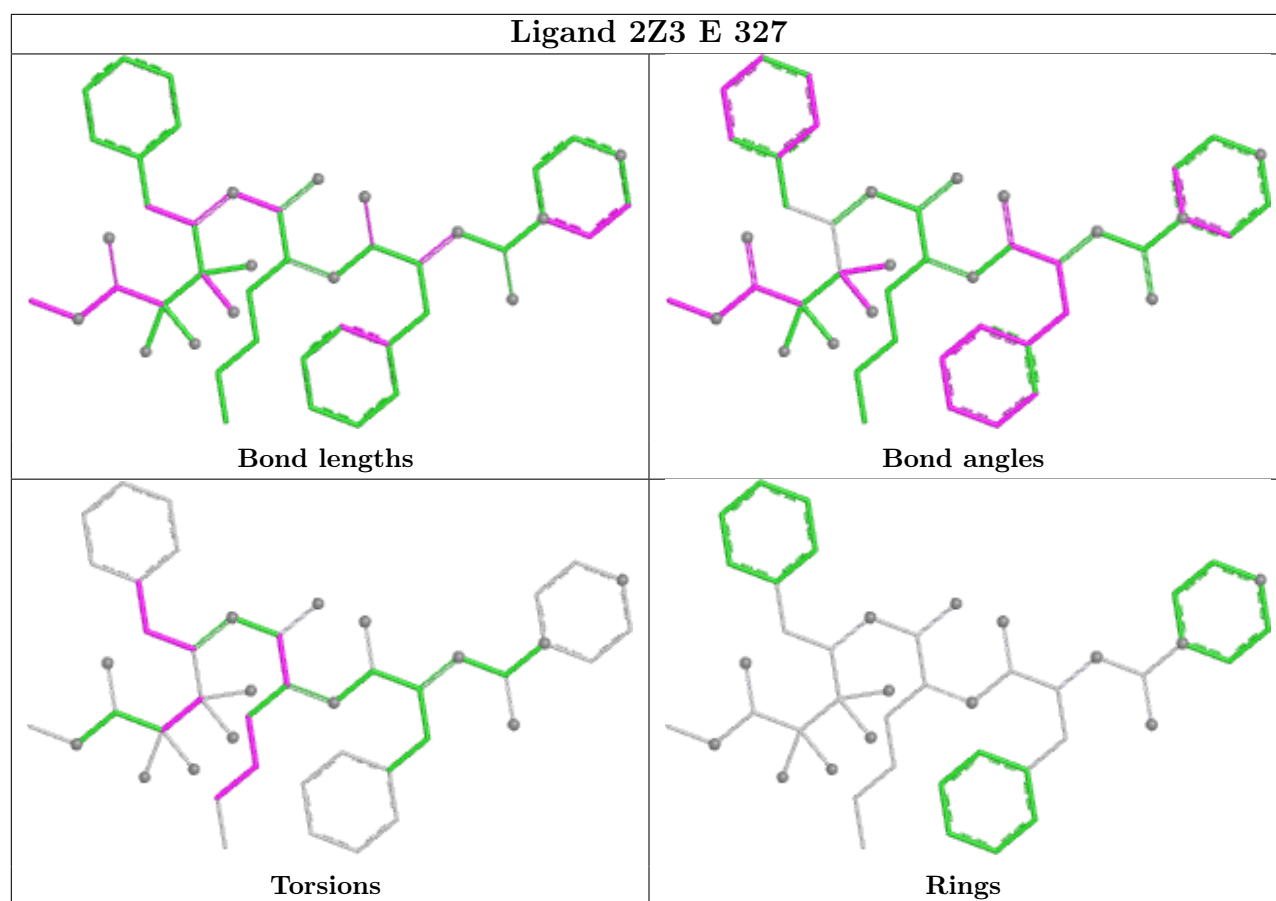
Mol	Chain	Res	Type	Atoms
2	E	327	2Z3	OH1-CH-CM-F2
2	E	327	2Z3	OH1-CH-CM-F1
2	E	327	2Z3	N2-CA2-CB2-CG2
2	E	327	2Z3	CE-CD-CG1-CB1
2	E	327	2Z3	CA2-CB2-CG2-CD21
2	E	327	2Z3	N2-C4-CA1-N1
2	E	327	2Z3	OH2-CH-CM-F2
2	E	327	2Z3	CA1-CB1-CG1-CD
2	E	327	2Z3	O3-C4-CA1-N1

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.