



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:15 PM UTC

PDB ID : 5ER1 / pdb_00005er1
Title : A rational approach to the design of antihypertensives. X-ray studies of complexes between aspartic proteinases and aminoalcohol renin inhibitors
Authors : Cooper, J.B.; Foundling, S.I.; Blundell, T.L.
Deposited on : 1990-11-07
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

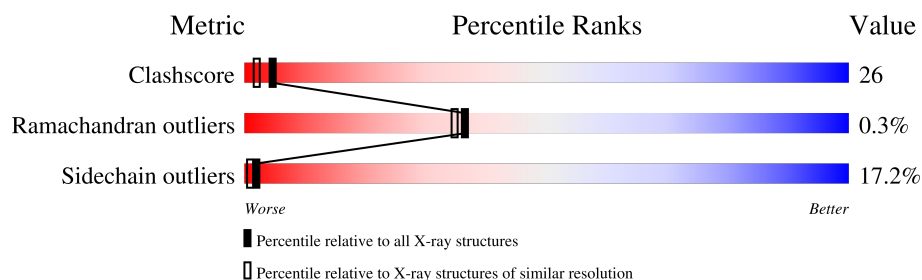
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

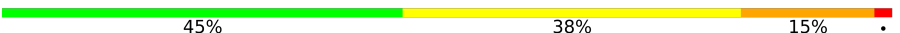
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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	

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
2	0HT	E	327	-	-	X	-

2 Entry composition [i](#)

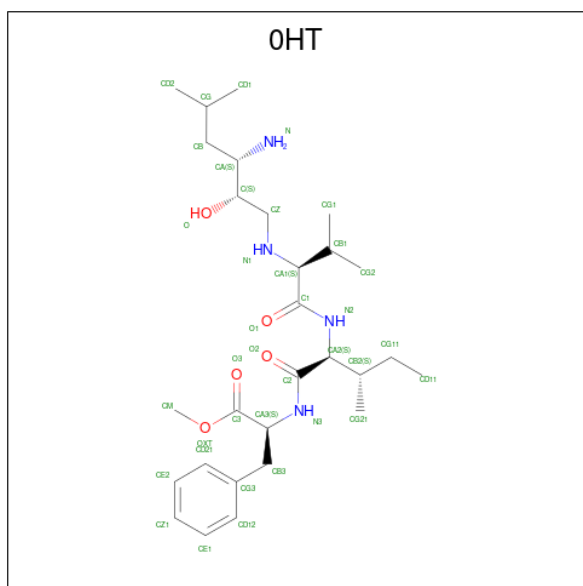
There are 3 unique types of molecules in this entry. The entry contains 2756 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ENDOTHAPEPSIN.

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 methyl N-[(2S,3S)-3-amino-2-hydroxy-5-methylhexyl]-L-valyl-L-isoleucyl-L-phenylalaninate (CCD ID: 0HT) (formula: C₂₈H₄₈N₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	N	O	0	0
			37	28	4	5		

- Molecule 3 is water.

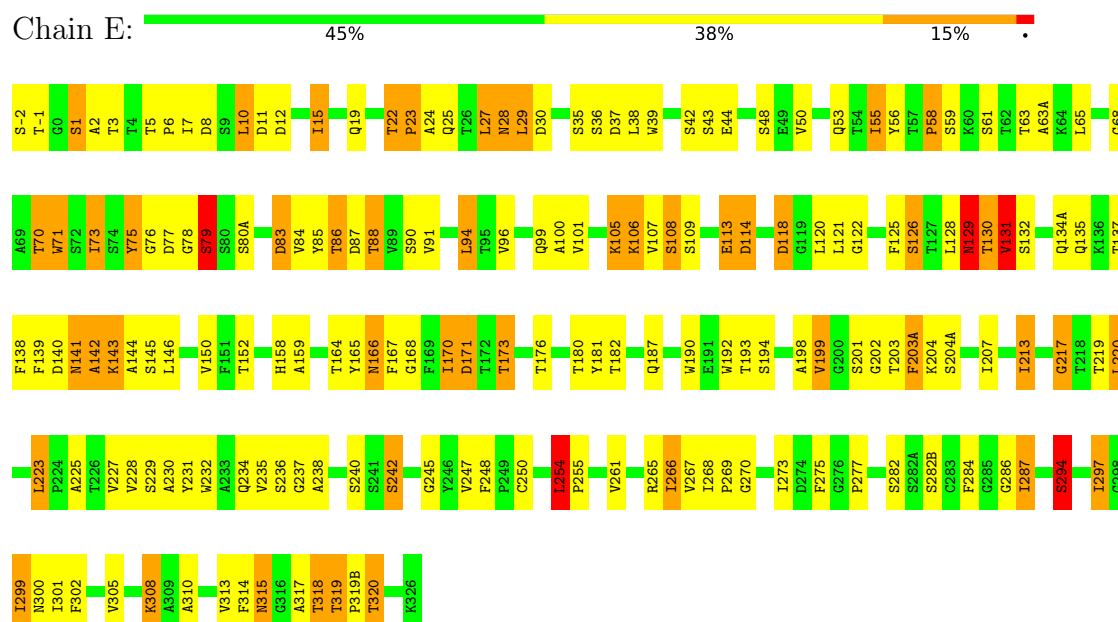
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	330	Total	O	0	0
			330	330		

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: ENDOTHAPEPSIN



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	53.50Å 73.90Å 45.70Å 90.00° 109.60° 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	PROLSQ	Depositor
R, R_{free}	0.206 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2756	wwPDB-VP
Average B, all atoms (Å ²)	0.0	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: OHT

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	1.83	55/2445 (2.2%)	2.27	152/3345 (4.5%)

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	1

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	220	LEU	N-CA	9.81	1.57	1.45
1	E	134(A)	GLN	N-CA	9.41	1.58	1.45
1	E	192	TRP	NE1-CE2	-8.43	1.28	1.37
1	E	268	ILE	N-CA	8.19	1.52	1.46
1	E	232	TRP	NE1-CE2	-7.75	1.28	1.37
1	E	75	TYR	N-CA	7.74	1.55	1.45
1	E	141	ASN	CG-OD1	7.64	1.38	1.23
1	E	122	GLY	C-O	7.43	1.31	1.23
1	E	190	TRP	NE1-CE2	-7.38	1.29	1.37
1	E	238	ALA	N-CA	7.34	1.55	1.46
1	E	118	ASP	C-N	-7.20	1.25	1.32
1	E	39	TRP	C-N	-6.99	1.25	1.33
1	E	158	HIS	ND1-CE1	6.76	1.39	1.32
1	E	39	TRP	NE1-CE2	-6.73	1.30	1.37
1	E	319	THR	N-CA	6.71	1.55	1.46
1	E	35	SER	CA-CB	-6.66	1.42	1.53
1	E	-1	THR	N-CA	6.57	1.54	1.45
1	E	317	ALA	C-N	-6.42	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	223	LEU	N-CA	6.30	1.51	1.45
1	E	28	ASN	CG-OD1	6.24	1.35	1.23
1	E	88	THR	N-CA	6.24	1.53	1.46
1	E	2	ALA	C-N	-6.17	1.24	1.33
1	E	3	THR	CA-C	-6.07	1.44	1.52
1	E	36	SER	CA-CB	-6.05	1.44	1.53
1	E	301	ILE	N-CA	5.99	1.53	1.46
1	E	201	SER	C-N	-5.91	1.26	1.33
1	E	25	GLN	CD-OE1	5.84	1.34	1.23
1	E	255	PRO	N-CA	5.81	1.53	1.47
1	E	207	ILE	CA-CB	-5.65	1.47	1.53
1	E	6	PRO	CA-CB	-5.60	1.45	1.53
1	E	265	ARG	C-N	-5.59	1.26	1.33
1	E	59	SER	CA-CB	-5.55	1.44	1.53
1	E	141	ASN	C-O	5.49	1.30	1.24
1	E	71	TRP	NE1-CE2	-5.45	1.31	1.37
1	E	245	GLY	C-N	-5.45	1.26	1.33
1	E	204	LYS	CA-CB	5.45	1.60	1.53
1	E	199	VAL	CA-CB	-5.43	1.47	1.54
1	E	134(A)	GLN	CD-OE1	5.41	1.33	1.23
1	E	235	VAL	CA-CB	5.41	1.60	1.53
1	E	235	VAL	C-N	5.38	1.40	1.33
1	E	202	GLY	N-CA	5.30	1.51	1.44
1	E	180	THR	C-O	-5.28	1.17	1.24
1	E	27	LEU	N-CA	5.23	1.52	1.45
1	E	126	SER	N-CA	-5.21	1.39	1.46
1	E	235	VAL	N-CA	5.21	1.52	1.46
1	E	166	ASN	CG-OD1	5.12	1.33	1.23
1	E	198	ALA	CA-C	5.12	1.58	1.52
1	E	318	THR	N-CA	-5.12	1.40	1.46
1	E	8	ASP	N-CA	-5.10	1.40	1.46
1	E	167	PHE	C-O	-5.09	1.18	1.24
1	E	165	TYR	C-N	-5.06	1.26	1.33
1	E	227	VAL	CA-CB	-5.05	1.48	1.54
1	E	282	SER	CA-CB	-5.03	1.45	1.53
1	E	182	THR	C-O	-5.01	1.17	1.23
1	E	106	LYS	C-O	-5.00	1.18	1.24

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	164	THR	CA-C-N	10.12	137.49	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	164	THR	C-N-CA	10.12	137.49	123.11
1	E	245	GLY	CA-C-N	9.72	134.52	120.82
1	E	245	GLY	C-N-CA	9.72	134.52	120.82
1	E	267	VAL	CA-CB-CG2	9.06	125.81	110.40
1	E	220	LEU	CA-C-N	9.01	134.75	122.77
1	E	220	LEU	C-N-CA	9.01	134.75	122.77
1	E	94	LEU	O-C-N	8.99	133.72	122.93
1	E	213	ILE	CA-C-O	8.79	130.74	120.72
1	E	227	VAL	CA-CB-CG2	8.79	125.34	110.40
1	E	37	ASP	O-C-N	8.58	133.51	123.30
1	E	19	GLN	OE1-CD-NE2	-8.42	114.18	122.60
1	E	302	PHE	CA-CB-CG	-8.36	105.44	113.80
1	E	250	CYS	N-CA-C	-7.91	102.89	112.54
1	E	24	ALA	CA-C-N	7.81	133.15	122.77
1	E	24	ALA	C-N-CA	7.81	133.15	122.77
1	E	142	ALA	CA-C-N	7.80	136.44	121.54
1	E	142	ALA	C-N-CA	7.80	136.44	121.54
1	E	107	VAL	CA-C-N	7.26	131.72	120.75
1	E	107	VAL	C-N-CA	7.26	131.72	120.75
1	E	235	VAL	N-CA-CB	-7.22	102.58	111.67
1	E	217	GLY	CA-C-N	7.19	132.92	123.00
1	E	217	GLY	C-N-CA	7.19	132.92	123.00
1	E	213	ILE	O-C-N	-7.18	115.81	123.14
1	E	275	PHE	CG-CD2-CE2	-7.13	108.58	120.70
1	E	164	THR	CA-C-O	-7.11	112.06	120.60
1	E	137	THR	CA-C-O	-7.10	113.89	121.99
1	E	108	SER	CA-C-N	7.04	131.37	120.82
1	E	108	SER	C-N-CA	7.04	131.37	120.82
1	E	70	THR	CA-C-O	-7.02	113.13	120.99
1	E	108	SER	CA-C-O	-6.99	114.14	121.55
1	E	131	VAL	CA-C-O	-6.97	112.75	120.84
1	E	68	GLY	N-CA-C	-6.97	105.19	114.25
1	E	28	ASN	OD1-CG-ND2	-6.90	115.70	122.60
1	E	137	THR	CA-C-N	6.84	129.75	120.44
1	E	137	THR	C-N-CA	6.84	129.75	120.44
1	E	199	VAL	CA-C-N	6.83	134.80	121.41
1	E	199	VAL	C-N-CA	6.83	134.80	121.41
1	E	75	TYR	CA-C-N	6.74	128.57	120.14
1	E	75	TYR	C-N-CA	6.74	128.57	120.14
1	E	158	HIS	CA-CB-CG	-6.74	107.06	113.80
1	E	107	VAL	CA-CB-CG2	6.73	121.84	110.40
1	E	42	SER	O-C-N	6.67	131.33	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	275	PHE	CA-CB-CG	-6.53	107.27	113.80
1	E	159	ALA	N-CA-C	6.51	113.99	108.13
1	E	125	PHE	CA-C-N	6.43	129.55	120.28
1	E	125	PHE	C-N-CA	6.43	129.55	120.28
1	E	248	PHE	CA-CB-CG	-6.38	107.42	113.80
1	E	59	SER	N-CA-C	6.33	118.18	111.28
1	E	8	ASP	CA-CB-CG	6.32	118.92	112.60
1	E	168	GLY	N-CA-C	-6.29	106.35	114.85
1	E	194	SER	O-C-N	-6.28	116.03	123.06
1	E	59	SER	CB-CA-C	6.24	121.16	110.79
1	E	23	PRO	CA-C-N	6.24	130.26	121.02
1	E	23	PRO	C-N-CA	6.24	130.26	121.02
1	E	121	LEU	CA-C-N	6.24	126.67	120.31
1	E	121	LEU	C-N-CA	6.24	126.67	120.31
1	E	164	THR	O-C-N	6.21	130.84	123.33
1	E	131	VAL	CA-CB-CG2	6.15	120.85	110.40
1	E	199	VAL	CA-CB-CG2	6.10	120.76	110.40
1	E	247	VAL	CA-CB-CG2	6.05	120.69	110.40
1	E	141	ASN	OD1-CG-ND2	-6.04	116.56	122.60
1	E	237	GLY	N-CA-C	-6.00	107.55	114.69
1	E	268	ILE	CB-CA-C	-5.97	104.32	110.71
1	E	5	THR	CA-C-N	-5.96	114.12	120.03
1	E	5	THR	C-N-CA	-5.96	114.12	120.03
1	E	203(A)	PHE	CA-CB-CG	5.96	119.76	113.80
1	E	213	ILE	CA-C-N	-5.94	113.00	121.50
1	E	213	ILE	C-N-CA	-5.94	113.00	121.50
1	E	234	GLN	CG-CD-NE2	5.94	125.31	116.40
1	E	22	THR	CA-CB-OG1	5.91	118.46	109.60
1	E	24	ALA	N-CA-C	5.91	118.76	109.96
1	E	79	SER	CA-C-N	5.91	131.13	122.39
1	E	79	SER	C-N-CA	5.91	131.13	122.39
1	E	91	VAL	CA-CB-CG2	5.90	120.43	110.40
1	E	294	SER	N-CA-C	-5.86	106.17	113.38
1	E	58	PRO	N-CA-C	-5.83	106.07	114.18
1	E	254	LEU	CA-C-N	-5.82	113.97	119.85
1	E	254	LEU	C-N-CA	-5.82	113.97	119.85
1	E	237	GLY	CA-C-N	-5.81	112.45	120.71
1	E	237	GLY	C-N-CA	-5.81	112.45	120.71
1	E	139	PHE	CA-CB-CG	-5.80	108.00	113.80
1	E	137	THR	O-C-N	5.80	129.72	122.65
1	E	28	ASN	CA-CB-CG	-5.78	106.82	112.60
1	E	141	ASN	N-CA-C	5.73	118.30	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	234	GLN	N-CA-CB	5.73	120.03	110.41
1	E	165	TYR	CA-C-N	5.72	131.23	122.93
1	E	165	TYR	C-N-CA	5.72	131.23	122.93
1	E	122	GLY	CA-C-O	-5.69	116.46	121.58
1	E	84	VAL	CA-CB-CG2	5.66	120.03	110.40
1	E	238	ALA	N-CA-C	-5.65	102.04	110.23
1	E	83	ASP	O-C-N	-5.62	116.11	122.68
1	E	144	ALA	O-C-N	5.61	130.33	122.36
1	E	144	ALA	N-CA-C	-5.59	105.58	112.90
1	E	207	ILE	CA-CB-CG1	5.59	119.90	110.40
1	E	318	THR	O-C-N	5.59	127.90	122.09
1	E	297	ILE	CA-C-N	-5.58	114.71	122.86
1	E	297	ILE	C-N-CA	-5.58	114.71	122.86
1	E	242	SER	N-CA-C	-5.57	104.02	112.04
1	E	101	VAL	N-CA-CB	-5.49	104.54	111.46
1	E	297	ILE	CB-CA-C	-5.49	102.30	111.29
1	E	268	ILE	N-CA-CB	-5.48	104.17	111.08
1	E	29	LEU	CA-C-N	5.46	131.01	122.17
1	E	29	LEU	C-N-CA	5.46	131.01	122.17
1	E	39	TRP	CE2-CD2-CE3	-5.45	113.35	118.80
1	E	-1	THR	CA-CB-OG1	5.45	117.77	109.60
1	E	58	PRO	CA-C-N	5.43	127.56	120.28
1	E	58	PRO	C-N-CA	5.43	127.56	120.28
1	E	192	TRP	O-C-N	-5.43	116.12	122.96
1	E	128	LEU	CA-C-O	5.41	125.09	119.14
1	E	287	ILE	CA-CB-CG2	5.39	119.66	110.50
1	E	39	TRP	CG-CD2-CE3	5.39	139.29	133.90
1	E	229	SER	O-C-N	-5.39	116.41	122.12
1	E	159	ALA	CA-C-O	5.35	124.73	120.13
1	E	230	ALA	N-CA-C	-5.33	105.55	111.36
1	E	39	TRP	CZ3-CH2-CZ2	-5.30	114.61	121.50
1	E	227	VAL	CA-C-N	5.27	127.68	120.46
1	E	227	VAL	C-N-CA	5.27	127.68	120.46
1	E	225	ALA	CA-C-N	5.26	127.28	120.44
1	E	225	ALA	C-N-CA	5.26	127.28	120.44
1	E	129	ASN	CA-C-N	5.25	131.89	122.38
1	E	129	ASN	C-N-CA	5.25	131.89	122.38
1	E	28	ASN	CB-CG-ND2	5.25	124.27	116.40
1	E	109	SER	O-C-N	5.24	128.14	122.11
1	E	318	THR	CB-CA-C	5.24	119.20	110.81
1	E	83	ASP	CA-CB-CG	5.24	117.84	112.60
1	E	273	ILE	N-CA-CB	-5.21	103.32	112.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	30	ASP	CA-C-N	5.21	128.73	121.02
1	E	30	ASP	C-N-CA	5.21	128.73	121.02
1	E	204	LYS	CA-CB-CG	-5.20	103.69	114.10
1	E	76	GLY	O-C-N	5.16	127.71	122.24
1	E	234	GLN	CB-CG-CD	-5.14	103.86	112.60
1	E	204(A)	SER	CA-C-N	5.13	131.34	121.54
1	E	204(A)	SER	C-N-CA	5.13	131.34	121.54
1	E	3	THR	CA-C-O	5.12	126.52	120.58
1	E	59	SER	CA-C-N	5.12	131.65	122.38
1	E	59	SER	C-N-CA	5.12	131.65	122.38
1	E	78	GLY	CA-C-N	5.12	127.98	120.71
1	E	78	GLY	C-N-CA	5.12	127.98	120.71
1	E	228	VAL	N-CA-C	5.11	115.84	110.62
1	E	35	SER	N-CA-CB	5.09	120.16	111.66
1	E	245	GLY	CA-C-O	-5.07	116.06	122.39
1	E	270	GLY	CA-C-N	5.07	128.01	120.31
1	E	270	GLY	C-N-CA	5.07	128.01	120.31
1	E	42	SER	N-CA-C	5.05	114.82	108.45
1	E	11	ASP	N-CA-C	-5.04	104.47	111.52
1	E	77	ASP	CA-CB-CG	5.04	117.64	112.60
1	E	168	GLY	CA-C-O	5.02	124.72	119.04
1	E	192	TRP	CA-C-N	-5.02	115.92	123.00
1	E	192	TRP	C-N-CA	-5.02	115.92	123.00
1	E	8	ASP	N-CA-CB	5.02	119.19	111.46
1	E	269	PRO	CB-CA-C	5.01	117.55	110.98

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	56	TYR	Mainchain

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	103	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	37	0	48	24	0
3	E	330	0	0	17	0
All	All	2756	0	2328	123	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 26.

All (123) 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:327:OHT:CD21	2:E:327:OHT:HD21	0.97	1.15
2:E:327:OHT:HD12	2:E:327:OHT:CD11	0.97	1.10
2:E:327:OHT:CD12	2:E:327:OHT:HD14	0.97	1.09
2:E:327:OHT:CD11	2:E:327:OHT:HD11	0.97	1.04
2:E:327:OHT:CD11	2:E:327:OHT:HD13	0.97	1.04
1:E:7:ILE:HG22	1:E:15:ILE:HG12	1.49	0.95
2:E:327:OHT:CG3	2:E:327:OHT:CE2	2.43	0.93
1:E:1:SER:HB3	1:E:166:ASN:ND2	1.83	0.93
2:E:327:OHT:CG3	2:E:327:OHT:CE1	2.43	0.92
1:E:75:TYR:HD1	1:E:79:SER:HB3	1.35	0.91
1:E:217:GLY:O	2:E:327:OHT:HBA	1.73	0.88
1:E:71:TRP:HZ3	1:E:73:ILE:HD11	1.39	0.86
2:E:327:OHT:HD14	2:E:327:OHT:CE1	2.06	0.85
2:E:327:OHT:HD11	2:E:327:OHT:HD13	1.58	0.85
2:E:327:OHT:HD12	2:E:327:OHT:CG11	2.07	0.85
2:E:327:OHT:HD12	2:E:327:OHT:HD11	1.58	0.85
2:E:327:OHT:HD11	2:E:327:OHT:CG11	2.07	0.85
2:E:327:OHT:HD21	2:E:327:OHT:CG3	2.06	0.85
2:E:327:OHT:HD12	2:E:327:OHT:HD13	1.58	0.84
2:E:327:OHT:HD14	2:E:327:OHT:CG3	2.06	0.84
2:E:327:OHT:HD21	2:E:327:OHT:CE2	2.06	0.84
2:E:327:OHT:HD13	2:E:327:OHT:CG11	2.07	0.84
1:E:181:TYR:HD1	1:E:320:THR:HG23	1.43	0.82
1:E:75:TYR:CD1	1:E:79:SER:HB3	2.15	0.82
1:E:86:THR:HG22	3:E:454:HOH:O	1.82	0.80
1:E:75:TYR:HB2	1:E:79:SER:HB2	1.63	0.79
1:E:1:SER:HB3	1:E:166:ASN:HD22	1.46	0.78
1:E:299:ILE:HG12	3:E:509:HOH:O	1.84	0.77
1:E:10:LEU:N	1:E:10:LEU:HD23	1.99	0.76
1:E:315:ASN:HB2	1:E:320:THR:HG22	1.68	0.75
1:E:71:TRP:CZ3	1:E:73:ILE:HD11	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:ASP:OD2	1:E:173:THR:HB	1.91	0.71
1:E:152:THR:HG22	1:E:313:VAL:HG22	1.73	0.70
1:E:105:LYS:HB2	3:E:366:HOH:O	1.92	0.69
1:E:297:ILE:CG2	1:E:297:ILE:O	2.42	0.68
1:E:181:TYR:HD1	1:E:320:THR:CG2	2.07	0.67
1:E:181:TYR:CD1	1:E:320:THR:CG2	2.78	0.67
1:E:105:LYS:HD3	3:E:366:HOH:O	1.95	0.67
1:E:315:ASN:CB	1:E:320:THR:HG22	2.25	0.66
1:E:7:ILE:CG2	1:E:15:ILE:HG12	2.25	0.66
2:E:327:OHT:HMC1	3:E:462:HOH:O	1.95	0.65
1:E:71:TRP:HB2	1:E:130:THR:CG2	2.27	0.65
1:E:129:ASN:HD21	1:E:131:VAL:HB	1.60	0.65
1:E:113:GLU:HB2	3:E:620:HOH:O	1.95	0.65
1:E:297:ILE:O	1:E:297:ILE:HG22	1.97	0.62
1:E:1:SER:CB	1:E:166:ASN:HD22	2.12	0.61
1:E:61:SER:HB3	1:E:63(A):ALA:HB2	1.81	0.61
1:E:213:ILE:HD11	2:E:327:OHT:HG23	1.80	0.61
1:E:130:THR:O	1:E:130:THR:HG23	1.99	0.61
1:E:318:THR:O	1:E:319(B):PRO:HD3	2.01	0.61
1:E:297:ILE:HD11	3:E:433:HOH:O	2.01	0.61
1:E:220:LEU:HD22	1:E:286:GLY:HA2	1.82	0.60
1:E:143:LYS:HA	1:E:146:LEU:HD12	1.83	0.59
1:E:113:GLU:HB3	3:E:621:HOH:O	2.02	0.59
1:E:176:THR:HG23	3:E:374:HOH:O	2.04	0.58
2:E:327:OHT:HG11	2:E:327:OHT:HE1	1.84	0.57
1:E:75:TYR:HB2	1:E:79:SER:CB	2.35	0.56
1:E:297:ILE:HG23	2:E:327:OHT:HZ	1.87	0.56
1:E:94:LEU:HD21	1:E:142:ALA:CB	2.35	0.56
1:E:22:THR:HA	1:E:23:PRO:C	2.25	0.56
2:E:327:OHT:HE1	2:E:327:OHT:CG1	2.36	0.55
1:E:1:SER:CB	1:E:166:ASN:ND2	2.63	0.55
1:E:152:THR:OG1	1:E:166:ASN:HB2	2.06	0.55
1:E:10:LEU:N	1:E:10:LEU:CD2	2.65	0.55
1:E:131:VAL:HG11	1:E:135:GLN:HG2	1.86	0.55
1:E:1:SER:HB3	1:E:166:ASN:HD21	1.71	0.55
1:E:135:GLN:NE2	3:E:543:HOH:O	2.40	0.54
1:E:315:ASN:HB2	1:E:320:THR:O	2.08	0.54
1:E:27:LEU:HD23	1:E:118:ASP:HB3	1.90	0.53
1:E:-2:SER:HB3	3:E:573:HOH:O	2.06	0.53
1:E:150:VAL:HG21	1:E:170:ILE:HD12	1.91	0.53
1:E:28:ASN:C	1:E:29:LEU:HD23	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:ASP:C	1:E:173:THR:H	2.16	0.52
1:E:113:GLU:CB	3:E:621:HOH:O	2.57	0.52
1:E:181:TYR:CD1	1:E:320:THR:HG23	2.31	0.52
1:E:96:VAL:CG1	1:E:141:ASN:HB3	2.40	0.51
1:E:120:LEU:HD21	2:E:327:OHT:HD1A	1.92	0.51
1:E:71:TRP:HZ3	1:E:73:ILE:CD1	2.16	0.50
1:E:199:VAL:HG11	1:E:231:TYR:HA	1.93	0.50
1:E:43:SER:HB3	1:E:58:PRO:HD3	1.93	0.50
1:E:318:THR:C	1:E:319(B):PRO:HD3	2.37	0.49
1:E:126:SER:HB2	1:E:140:ASP:OD1	2.13	0.49
1:E:100:ALA:HB2	1:E:135:GLN:HE21	1.77	0.49
1:E:71:TRP:HB2	1:E:130:THR:HG22	1.96	0.48
1:E:314:PHE:CD1	1:E:314:PHE:N	2.81	0.48
1:E:94:LEU:HD21	1:E:142:ALA:HB1	1.95	0.48
1:E:220:LEU:HA	1:E:305:VAL:HG23	1.96	0.48
1:E:94:LEU:HD23	1:E:138:PHE:CZ	2.49	0.47
1:E:150:VAL:HG21	1:E:170:ILE:CD1	2.45	0.47
1:E:319:THR:O	1:E:319:THR:HG22	2.14	0.47
1:E:53:GLN:NE2	1:E:114:ASP:O	2.44	0.47
1:E:277:PRO:HA	1:E:282(B):SER:O	2.15	0.47
1:E:308:LYS:NZ	3:E:438:HOH:O	2.42	0.47
1:E:22:THR:CA	1:E:23:PRO:C	2.88	0.46
1:E:181:TYR:CD1	1:E:320:THR:HG21	2.49	0.46
1:E:242:SER:HA	3:E:545:HOH:O	2.15	0.45
1:E:113:GLU:CB	3:E:620:HOH:O	2.59	0.45
1:E:266:ILE:HG21	1:E:310:ALA:HB2	1.99	0.45
1:E:22:THR:HA	1:E:23:PRO:HA	1.77	0.45
1:E:38:LEU:C	1:E:38:LEU:HD23	2.42	0.45
1:E:220:LEU:HD11	1:E:284:PHE:HE2	1.82	0.45
1:E:94:LEU:HD21	1:E:142:ALA:HB2	1.97	0.45
1:E:44:GLU:OE1	1:E:85:TYR:HE2	2.00	0.44
1:E:96:VAL:HG11	1:E:141:ASN:HB3	1.99	0.43
1:E:187:GLN:HG2	3:E:572:HOH:O	2.18	0.43
1:E:43:SER:CB	1:E:58:PRO:HD3	2.48	0.43
1:E:220:LEU:HA	1:E:305:VAL:CG2	2.48	0.43
1:E:44:GLU:OE2	1:E:83:ASP:OD1	2.35	0.43
1:E:75:TYR:N	1:E:79:SER:O	2.45	0.42
1:E:105:LYS:CB	3:E:366:HOH:O	2.60	0.42
1:E:294:SER:CB	1:E:300:ASN:HD22	2.31	0.42
1:E:73:ILE:CD1	1:E:80(A):SER:HB3	2.49	0.42
1:E:87:ASP:OD2	1:E:88:THR:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:129:ASN:ND2	1:E:131:VAL:HB	2.30	0.42
1:E:99:GLN:NE2	1:E:138:PHE:HA	2.35	0.42
1:E:219:THR:O	1:E:305:VAL:HG23	2.19	0.42
1:E:254:LEU:HD12	1:E:254:LEU:HA	1.77	0.41
1:E:44:GLU:OE1	1:E:85:TYR:CE2	2.73	0.41
1:E:113:GLU:HG3	1:E:113:GLU:O	2.20	0.41
1:E:73:ILE:HD12	1:E:80(A):SER:HB3	2.03	0.41
1:E:131:VAL:O	1:E:131:VAL:HG12	2.14	0.41
1:E:50:VAL:HG11	1:E:55:ILE:CD1	2.51	0.41
1:E:71:TRP:CZ3	1:E:80(A):SER:HB3	2.56	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%)	314 (96%)	13 (4%)	1 (0%)	36 35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	171	ASP

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	239/263 (91%)	198 (83%)	41 (17%)	2 1

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1	SER
1	E	10	LEU
1	E	12	ASP
1	E	15	ILE
1	E	48	SER
1	E	55	ILE
1	E	63	THR
1	E	65	LEU
1	E	70	THR
1	E	73	ILE
1	E	79	SER
1	E	86	THR
1	E	90	SER
1	E	105	LYS
1	E	106	LYS
1	E	108	SER
1	E	113	GLU
1	E	114	ASP
1	E	129	ASN
1	E	130	THR
1	E	131	VAL
1	E	132	SER
1	E	143	LYS
1	E	145	SER
1	E	170	ILE
1	E	173	THR
1	E	193	THR
1	E	203	THR
1	E	203(A)	PHE
1	E	223	LEU
1	E	236	SER
1	E	240	SER
1	E	254	LEU
1	E	261	VAL
1	E	266	ILE
1	E	287	ILE
1	E	294	SER
1	E	299	ILE

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Mol	Chain	Res	Type
1	E	308	LYS
1	E	315	ASN
1	E	320	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
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 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	0HT	E	327	-	37,37,37	1.37	2 (5%)	45,49,49	1.34	6 (13%)

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	0HT	E	327	-	-	16/49/49/49	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	327	0HT	CZ-N1	-6.27	1.32	1.47
2	E	327	0HT	OXT-C3	3.75	1.42	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	327	0HT	CZ-N1-CA1	4.61	122.59	114.00
2	E	327	0HT	OXT-C3-CA3	3.35	120.00	111.49
2	E	327	0HT	CB1-CA1-C1	-2.94	104.21	111.38
2	E	327	0HT	CM-OXT-C3	-2.61	109.99	115.92
2	E	327	0HT	OXT-C3-O3	-2.47	119.03	123.85
2	E	327	0HT	CG21-CB2-CG11	-2.33	105.92	111.81

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	327	0HT	O-C-CZ-N1
2	E	327	0HT	CA-C-CZ-N1
2	E	327	0HT	C-CA-CB-CG
2	E	327	0HT	N-CA-CB-CG
2	E	327	0HT	C1-CA1-N1-CZ
2	E	327	0HT	O3-C3-OXT-CM
2	E	327	0HT	CA3-C3-OXT-CM
2	E	327	0HT	CA2-CB2-CG11-CD11
2	E	327	0HT	N3-CA3-CB3-CG3
2	E	327	0HT	CG21-CB2-CG11-CD11
2	E	327	0HT	CA3-CB3-CG3-CD12

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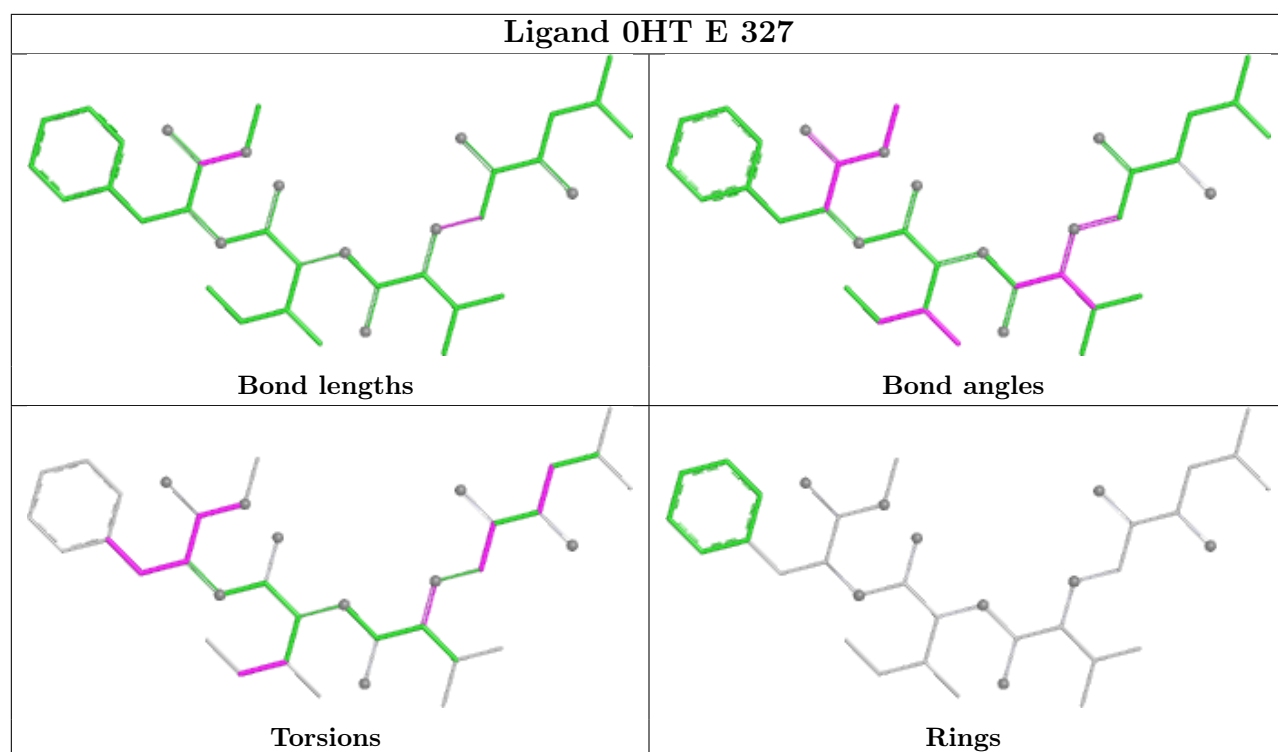
Mol	Chain	Res	Type	Atoms
2	E	327	0HT	CA3-CB3-CG3-CD21
2	E	327	0HT	CB1-CA1-N1-CZ
2	E	327	0HT	C3-CA3-CB3-CG3
2	E	327	0HT	OXT-C3-CA3-CB3
2	E	327	0HT	O3-C3-CA3-CB3

There are no ring outliers.

1 monomer is involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	327	0HT	24	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.