



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:02 AM UTC

PDB ID : 1ER8 / pdb_00001er8
Title : THE ACTIVE SITE OF ASPARTIC PROTEINASES
Authors : Hemmings, A.M.; Veerapandian, B.; Szelke, M.; Cooper, J.B.; Blundell, T.L.
Deposited on : 1989-10-16
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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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

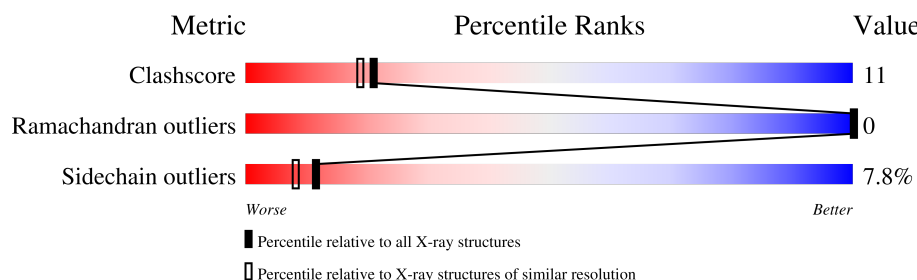
1 Overall quality at a glance

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	I	8	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2529 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 a protein called H-77.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	8	Total	C	N	O	0	0	0
			73	52	12	9			

- Molecule 3 is water.

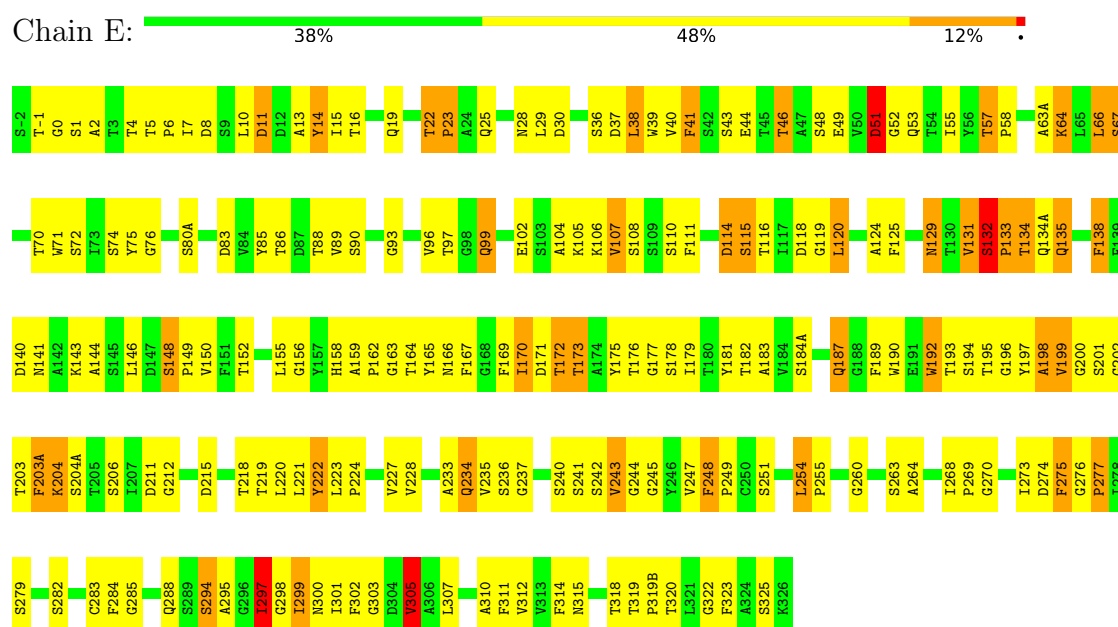
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	67	Total	O	0	0
			67	67		

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: Endothiapepsin



• Molecule 2: H-77



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	43.20 Å 75.70 Å 42.90 Å 90.00° 97.10° 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	unknown	Depositor
R, R_{free}	0.170 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2529	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: DHI

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	1.99	76/2445 (3.1%)	3.00	277/3345 (8.3%)
2	I	2.69	4/66 (6.1%)	2.16	3/87 (3.4%)
All	All	2.01	80/2511 (3.2%)	2.99	280/3432 (8.2%)

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	1
2	I	0	1
All	All	0	2

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	4	HIS	CE1-NE2	10.61	1.43	1.32
1	E	245	GLY	N-CA	9.53	1.54	1.45
1	E	237	GLY	N-CA	9.47	1.60	1.44
2	I	4	HIS	ND1-CE1	9.29	1.41	1.32
1	E	158	HIS	ND1-CE1	8.46	1.41	1.32
1	E	134	THR	N-CA	8.16	1.55	1.46
2	I	4	HIS	CG-CD2	8.07	1.44	1.35
1	E	215	ASP	C-O	7.53	1.32	1.23
1	E	190	TRP	NE1-CE2	-7.51	1.29	1.37
1	E	212	GLY	N-CA	7.35	1.52	1.45
1	E	19	GLN	CD-OE1	7.26	1.37	1.23
1	E	48	SER	N-CA	7.09	1.55	1.46
1	E	273	ILE	N-CA	6.98	1.55	1.46
1	E	57	THR	C-N	6.98	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	6	PRO	N-CD	6.92	1.57	1.47
1	E	223	LEU	C-N	6.89	1.41	1.33
1	E	28	ASN	CG-OD1	6.82	1.36	1.23
1	E	0	GLY	N-CA	6.78	1.52	1.45
1	E	129	ASN	CG-OD1	6.71	1.36	1.23
1	E	99	GLN	CD-OE1	6.64	1.36	1.23
1	E	23	PRO	N-CD	6.60	1.57	1.47
1	E	311	PHE	CA-CB	6.56	1.62	1.53
1	E	179	ILE	N-CA	6.49	1.54	1.46
1	E	149	PRO	N-CD	6.45	1.56	1.47
2	I	5	LEU	C-N	6.45	1.41	1.33
1	E	135	GLN	CD-OE1	6.35	1.35	1.23
1	E	211	ASP	N-CA	6.32	1.53	1.46
1	E	53	GLN	CD-OE1	6.31	1.35	1.23
1	E	268	ILE	C-O	-6.19	1.16	1.24
1	E	297	ILE	CA-C	-6.13	1.45	1.52
1	E	276	GLY	C-N	6.07	1.40	1.33
1	E	319(B)	PRO	N-CD	6.05	1.56	1.47
1	E	124	ALA	C-O	6.01	1.30	1.23
1	E	16	THR	C-N	5.99	1.40	1.33
1	E	133	PRO	N-CD	5.98	1.56	1.47
1	E	39	TRP	C-N	-5.92	1.25	1.33
1	E	187	GLN	CD-OE1	5.89	1.34	1.23
1	E	83	ASP	C-N	-5.88	1.25	1.33
1	E	248	PHE	C-N	5.86	1.41	1.33
1	E	1	SER	CA-C	-5.86	1.45	1.52
1	E	325	SER	N-CA	5.84	1.53	1.45
1	E	268	ILE	C-N	5.83	1.41	1.33
1	E	140	ASP	C-O	-5.73	1.17	1.24
1	E	114	ASP	N-CA	5.67	1.54	1.46
1	E	182	THR	N-CA	5.66	1.53	1.45
1	E	159	ALA	C-N	5.64	1.40	1.33
1	E	221	LEU	CA-C	5.62	1.59	1.52
1	E	288	GLN	CD-OE1	5.62	1.34	1.23
1	E	72	SER	N-CA	5.61	1.52	1.46
1	E	89	VAL	N-CA	5.60	1.53	1.46
1	E	2	ALA	N-CA	5.59	1.52	1.45
1	E	106	LYS	N-CA	5.56	1.52	1.46
1	E	235	VAL	N-CA	5.56	1.53	1.46
1	E	156	GLY	N-CA	5.55	1.50	1.44
1	E	323	PHE	CA-C	5.54	1.59	1.52
1	E	158	HIS	CE1-NE2	5.54	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	25	GLN	N-CA	5.51	1.52	1.46
1	E	114	ASP	C-O	-5.49	1.17	1.23
1	E	162	PRO	N-CD	5.49	1.55	1.47
1	E	134	THR	CA-C	-5.46	1.46	1.52
1	E	7	ILE	CA-CB	-5.46	1.46	1.54
1	E	255	PRO	N-CD	5.46	1.55	1.47
1	E	158	HIS	CD2-NE2	5.45	1.43	1.37
1	E	11	ASP	C-N	-5.40	1.26	1.34
1	E	181	TYR	N-CA	5.39	1.52	1.46
1	E	170	ILE	C-N	-5.34	1.26	1.33
1	E	165	TYR	C-O	-5.32	1.17	1.24
1	E	138	PHE	N-CA	5.27	1.52	1.46
1	E	15	ILE	C-O	5.27	1.29	1.24
1	E	86	THR	C-O	-5.25	1.17	1.23
1	E	131	VAL	C-N	-5.25	1.26	1.33
1	E	170	ILE	N-CA	5.23	1.53	1.46
1	E	1	SER	N-CA	5.21	1.52	1.46
1	E	134(A)	GLN	CD-OE1	5.21	1.33	1.23
1	E	196	GLY	N-CA	5.20	1.51	1.45
1	E	294	SER	N-CA	5.18	1.52	1.46
1	E	236	SER	N-CA	5.17	1.52	1.45
1	E	192	TRP	NE1-CE2	-5.07	1.31	1.37
1	E	183	ALA	C-O	5.04	1.30	1.23
1	E	199	VAL	CA-CB	5.04	1.60	1.54

All (280) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	276	GLY	CA-C-N	-18.43	102.25	120.31
1	E	276	GLY	C-N-CA	-18.43	102.25	120.31
1	E	236	SER	CA-C-N	-16.71	98.06	122.46
1	E	236	SER	C-N-CA	-16.71	98.06	122.46
1	E	254	LEU	CA-C-N	-15.24	105.43	120.52
1	E	254	LEU	C-N-CA	-15.24	105.43	120.52
1	E	275	PHE	CA-CB-CG	-14.56	99.23	113.80
1	E	25	GLN	OE1-CD-NE2	-14.47	108.13	122.60
1	E	125	PHE	CA-CB-CG	-14.33	99.47	113.80
1	E	315	ASN	OD1-CG-ND2	-13.26	109.34	122.60
1	E	16	THR	CA-C-N	-13.05	106.31	120.14
1	E	16	THR	C-N-CA	-13.05	106.31	120.14
1	E	159	ALA	CA-C-N	-12.61	108.11	120.21
1	E	159	ALA	C-N-CA	-12.61	108.11	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	85	TYR	O-C-N	12.39	139.30	123.19
1	E	254	LEU	CA-C-O	-12.17	109.65	120.60
1	E	96	VAL	CA-C-O	11.94	133.35	120.57
1	E	170	ILE	O-C-N	11.69	135.59	123.20
1	E	223	LEU	CA-C-N	-11.31	108.83	120.03
1	E	223	LEU	C-N-CA	-11.31	108.83	120.03
1	E	248	PHE	CA-C-N	-11.09	108.67	119.76
1	E	248	PHE	C-N-CA	-11.09	108.67	119.76
1	E	134(A)	GLN	CA-C-O	-10.82	109.32	121.87
1	E	57	THR	CA-C-N	-10.60	108.85	119.56
1	E	57	THR	C-N-CA	-10.60	108.85	119.56
1	E	268	ILE	CA-C-N	-10.53	108.94	119.78
1	E	268	ILE	C-N-CA	-10.53	108.94	119.78
1	E	282	SER	CA-C-O	-10.49	109.70	121.87
1	E	22	THR	C-N-CD	10.26	143.18	120.60
1	E	66	LEU	O-C-N	-10.21	110.31	122.87
1	E	96	VAL	O-C-N	-10.20	111.71	123.03
1	E	16	THR	O-C-N	10.16	131.68	121.72
1	E	104	ALA	CA-C-O	10.11	132.31	120.58
1	E	288	GLN	CG-CD-NE2	9.96	131.34	116.40
1	E	206	SER	CA-C-O	9.91	131.99	120.49
1	E	236	SER	O-C-N	-9.72	111.39	122.86
1	E	85	TYR	CA-C-O	-9.69	110.16	121.11
1	E	270	GLY	O-C-N	-9.69	111.97	122.24
1	E	37	ASP	CA-C-N	-9.66	110.28	122.84
1	E	37	ASP	C-N-CA	-9.66	110.28	122.84
1	E	83	ASP	CA-C-O	-9.48	110.88	121.40
1	E	57	THR	CA-C-O	9.39	128.23	119.59
1	E	25	GLN	CG-CD-NE2	9.31	130.37	116.40
1	E	125	PHE	O-C-N	-9.24	112.59	122.94
1	E	222	TYR	O-C-N	9.22	136.98	122.96
1	E	53	GLN	O-C-N	-9.12	110.47	122.59
1	E	260	GLY	CA-C-O	-9.09	113.40	120.76
1	E	165	TYR	CA-C-O	-8.89	110.54	120.32
1	E	22	THR	CA-C-N	-8.86	105.74	127.00
1	E	22	THR	C-N-CA	-8.86	105.74	127.00
1	E	235	VAL	CA-C-O	8.83	129.57	120.39
1	E	166	ASN	O-C-N	8.74	134.18	123.16
1	E	274	ASP	CA-C-O	8.68	130.36	120.98
1	E	170	ILE	CA-C-O	-8.64	111.40	120.39
1	E	132	SER	C-N-CD	8.64	139.60	120.60
1	E	235	VAL	N-CA-CB	-8.60	100.46	111.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	273	ILE	CB-CG1-CD1	8.60	131.86	113.80
1	E	203(A)	PHE	CA-C-O	-8.60	110.89	120.69
1	E	310	ALA	O-C-N	8.42	133.57	122.96
1	E	319	THR	C-N-CD	8.39	146.01	128.40
1	E	29	LEU	O-C-N	-8.38	113.67	123.06
1	E	51	ASP	CA-CB-CG	-8.34	104.26	112.60
1	E	159	ALA	O-C-N	8.19	128.22	121.83
1	E	300	ASN	O-C-N	8.18	132.86	122.89
1	E	254	LEU	O-C-N	8.11	138.31	121.77
1	E	134(A)	GLN	O-C-N	7.97	131.88	122.79
1	E	176	THR	CA-C-O	-7.81	112.32	121.46
2	I	7	VAL	CA-C-O	-7.78	112.91	121.23
1	E	319(B)	PRO	O-C-N	-7.77	113.80	123.21
1	E	325	SER	CA-C-O	7.74	130.85	121.87
1	E	284	PHE	O-C-N	-7.70	114.22	123.16
1	E	40	VAL	O-C-N	-7.66	114.27	123.00
1	E	264	ALA	CA-C-O	7.65	131.61	121.89
1	E	163	GLY	O-C-N	-7.61	112.81	122.70
1	E	53	GLN	CA-C-O	7.53	131.28	120.51
1	E	234	GLN	CA-C-N	-7.45	113.19	123.10
1	E	234	GLN	C-N-CA	-7.45	113.19	123.10
1	E	264	ALA	O-C-N	-7.38	114.28	122.84
1	E	155	LEU	O-C-N	-7.35	114.65	122.96
1	E	171	ASP	CA-C-O	7.35	128.91	120.60
1	E	169	PHE	CA-C-N	-7.35	113.33	123.10
1	E	169	PHE	C-N-CA	-7.35	113.33	123.10
1	E	183	ALA	CA-C-O	7.34	129.91	121.47
1	E	66	LEU	CA-C-O	7.34	128.76	120.84
1	E	319(B)	PRO	CA-C-O	7.32	131.14	122.13
1	E	222	TYR	CA-C-O	-7.29	111.39	120.57
1	E	285	GLY	CA-C-O	7.26	130.68	121.53
1	E	198	ALA	CA-C-N	7.24	132.16	122.90
1	E	198	ALA	C-N-CA	7.24	132.16	122.90
1	E	1	SER	CA-C-O	-7.22	111.40	120.28
1	E	200	GLY	CA-C-N	7.22	134.63	122.65
1	E	200	GLY	C-N-CA	7.22	134.63	122.65
2	I	3	PHE	CA-CB-CG	-7.18	106.62	113.80
1	E	67	SER	CA-C-N	-7.12	109.86	122.97
1	E	67	SER	C-N-CA	-7.12	109.86	122.97
1	E	51	ASP	O-C-N	7.09	132.02	122.59
1	E	38	LEU	CA-C-O	-7.08	113.18	120.54
1	E	102	GLU	O-C-N	7.07	131.26	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	90	SER	O-C-N	7.06	131.71	123.30
1	E	300	ASN	CA-C-O	-7.06	113.25	121.16
1	E	148	SER	O-C-N	7.05	129.25	122.06
1	E	148	SER	CA-C-N	-7.03	104.88	120.56
1	E	148	SER	C-N-CA	-7.03	104.88	120.56
1	E	314	PHE	CA-CB-CG	-7.03	106.77	113.80
1	E	279	SER	O-C-N	-7.02	114.84	123.33
1	E	43	SER	N-CA-C	-6.98	104.64	113.01
1	E	64	LYS	CA-CB-CG	6.97	128.04	114.10
1	E	273	ILE	O-C-N	-6.96	114.05	122.12
1	E	71	TRP	O-C-N	-6.89	115.28	123.27
1	E	83	ASP	O-C-N	6.87	131.92	122.78
1	E	212	GLY	CA-C-N	6.81	131.63	123.19
1	E	212	GLY	C-N-CA	6.81	131.63	123.19
1	E	13	ALA	CA-C-O	-6.75	114.01	121.23
1	E	297	ILE	CA-CB-CG2	6.73	121.94	110.50
1	E	169	PHE	CA-CB-CG	6.64	120.44	113.80
1	E	166	ASN	CA-C-O	-6.64	113.66	121.16
1	E	133	PRO	N-CD-CG	-6.62	95.86	103.80
1	E	201	SER	CA-C-N	6.61	128.81	122.27
1	E	201	SER	C-N-CA	6.61	128.81	122.27
1	E	76	GLY	O-C-N	6.58	129.78	122.54
1	E	39	TRP	CE3-CZ3-CH2	6.58	129.66	121.10
1	E	297	ILE	CA-C-O	6.54	128.29	121.29
1	E	36	SER	CA-CB-OG	-6.54	98.03	111.10
1	E	5	THR	CA-C-N	-6.54	113.22	119.76
1	E	5	THR	C-N-CA	-6.54	113.22	119.76
1	E	295	ALA	O-C-N	-6.53	115.19	122.12
1	E	183	ALA	O-C-N	-6.51	115.60	122.96
1	E	297	ILE	O-C-N	-6.47	115.28	121.94
1	E	305	VAL	CG1-CB-CG2	6.42	124.93	110.80
1	E	93	GLY	CA-C-O	6.42	126.14	119.01
1	E	141	ASN	CA-C-O	-6.41	113.76	120.55
1	E	75	TYR	CA-CB-CG	-6.40	102.39	113.90
1	E	273	ILE	CA-C-O	6.39	126.90	119.36
1	E	247	VAL	CA-CB-CG2	6.39	121.26	110.40
1	E	133	PRO	CA-N-CD	-6.37	102.58	111.50
1	E	297	ILE	N-CA-C	6.37	116.48	110.30
1	E	197	TYR	CA-C-O	-6.34	113.92	120.89
1	E	149	PRO	N-CA-CB	-6.33	97.43	102.36
1	E	141	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	E	310	ALA	CA-C-N	-6.27	114.27	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	310	ALA	C-N-CA	-6.27	114.27	123.05
1	E	41	PHE	CA-C-N	-6.27	112.11	122.39
1	E	41	PHE	C-N-CA	-6.27	112.11	122.39
1	E	305	VAL	CA-CB-CG2	6.25	121.02	110.40
1	E	19	GLN	OE1-CD-NE2	-6.24	116.36	122.60
1	E	243	VAL	CA-CB-CG1	-6.23	99.81	110.40
1	E	120	LEU	CA-C-N	-6.21	114.01	123.07
1	E	120	LEU	C-N-CA	-6.21	114.01	123.07
1	E	11	ASP	CA-C-O	-6.20	113.90	121.28
1	E	315	ASN	CB-CG-ND2	6.19	125.68	116.40
1	E	170	ILE	CB-CG1-CD1	6.15	126.72	113.80
1	E	14	TYR	CA-C-N	-6.14	112.35	122.67
1	E	14	TYR	C-N-CA	-6.14	112.35	122.67
1	E	29	LEU	CA-C-N	6.13	131.12	121.99
1	E	29	LEU	C-N-CA	6.13	131.12	121.99
1	E	40	VAL	CA-C-O	6.13	127.78	121.28
1	E	75	TYR	CB-CG-CD1	-6.12	111.62	120.80
1	E	70	THR	O-C-N	-6.12	115.25	122.96
1	E	235	VAL	O-C-N	-6.11	116.73	123.20
1	E	310	ALA	CA-C-O	-6.04	114.74	121.51
1	E	-1	THR	CA-C-N	-6.04	116.96	121.61
1	E	-1	THR	C-N-CA	-6.04	116.96	121.61
1	E	74	SER	CA-CB-OG	-6.04	99.03	111.10
1	E	244	GLY	CA-C-N	-6.02	113.01	121.56
1	E	244	GLY	C-N-CA	-6.02	113.01	121.56
1	E	134	THR	O-C-N	-5.99	113.11	122.70
1	E	178	SER	O-C-N	5.99	130.93	123.15
1	E	99	GLN	O-C-N	-5.95	115.61	122.93
1	E	184(A)	SER	CA-C-N	-5.93	113.16	122.65
1	E	184(A)	SER	C-N-CA	-5.93	113.16	122.65
1	E	318	THR	O-C-N	-5.86	115.36	122.22
1	E	273	ILE	N-CA-C	-5.85	105.05	113.07
1	E	150	VAL	CA-CB-CG1	5.81	120.27	110.40
1	E	237	GLY	O-C-N	-5.80	115.32	122.46
1	E	294	SER	N-CA-C	-5.80	105.79	112.92
1	E	192	TRP	CA-C-O	-5.79	115.26	121.45
1	E	63(A)	ALA	CA-C-N	-5.78	113.37	122.73
1	E	63(A)	ALA	C-N-CA	-5.78	113.37	122.73
1	E	120	LEU	O-C-N	5.77	130.34	123.24
1	E	29	LEU	CA-C-O	5.77	128.28	121.36
1	E	320	THR	O-C-N	5.77	130.15	123.17
1	E	118	ASP	N-CA-C	-5.75	105.92	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	234	GLN	CG-CD-OE1	-5.73	109.34	120.80
1	E	99	GLN	CG-CD-NE2	5.72	124.99	116.40
1	E	181	TYR	CG-CD1-CE1	-5.72	112.62	121.20
1	E	203	THR	CA-C-O	5.72	128.22	121.36
1	E	263	SER	CA-C-O	5.71	126.61	119.12
1	E	288	GLN	CA-C-O	-5.68	115.10	121.40
1	E	189	PHE	CA-C-O	5.67	128.58	121.66
1	E	288	GLN	OE1-CD-NE2	-5.66	116.94	122.60
1	E	30	ASP	CA-CB-CG	5.66	118.25	112.60
1	E	169	PHE	CD1-CG-CD2	-5.64	110.13	118.60
1	E	152	THR	CA-C-N	5.61	130.91	123.00
1	E	152	THR	C-N-CA	5.61	130.91	123.00
1	E	277	PRO	CA-C-O	5.61	129.07	122.12
1	E	187	GLN	OE1-CD-NE2	-5.60	117.00	122.60
1	E	39	TRP	CZ3-CH2-CZ2	-5.59	114.23	121.50
1	E	164	THR	CA-C-O	-5.58	114.73	120.99
1	E	302	PHE	CA-CB-CG	-5.58	108.22	113.80
1	E	228	VAL	CA-C-O	5.58	126.75	120.95
1	E	322	GLY	CA-C-N	-5.57	114.17	122.74
1	E	322	GLY	C-N-CA	-5.57	114.17	122.74
1	E	241	SER	CA-C-N	5.56	127.67	120.44
1	E	241	SER	C-N-CA	5.56	127.67	120.44
1	E	187	GLN	CA-C-N	5.56	133.35	121.18
1	E	187	GLN	C-N-CA	5.56	133.35	121.18
1	E	319(B)	PRO	N-CD-CG	-5.55	94.87	103.20
1	E	274	ASP	O-C-N	-5.55	115.13	122.57
1	E	71	TRP	CE3-CZ3-CH2	5.54	128.30	121.10
1	E	202	GLY	CA-C-N	-5.54	112.59	122.07
1	E	202	GLY	C-N-CA	-5.54	112.59	122.07
1	E	141	ASN	CA-CB-CG	-5.54	107.06	112.60
1	E	39	TRP	CA-C-N	-5.52	114.41	122.58
1	E	39	TRP	C-N-CA	-5.52	114.41	122.58
1	E	269	PRO	CA-C-N	-5.51	113.26	120.14
1	E	269	PRO	C-N-CA	-5.51	113.26	120.14
1	E	234	GLN	OE1-CD-NE2	5.50	128.10	122.60
1	E	311	PHE	N-CA-CB	-5.50	101.92	110.55
1	E	176	THR	CA-C-N	5.49	128.91	120.07
1	E	176	THR	C-N-CA	5.49	128.91	120.07
1	E	195	THR	CA-CB-OG1	5.48	117.82	109.60
2	I	3	PHE	CA-C-O	-5.48	114.97	121.16
1	E	311	PHE	CZ-CE2-CD2	5.47	129.84	120.00
1	E	107	VAL	CA-CB-CG1	-5.45	101.14	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	192	TRP	CA-C-N	-5.44	115.13	123.07
1	E	192	TRP	C-N-CA	-5.44	115.13	123.07
1	E	114	ASP	CA-CB-CG	-5.41	107.19	112.60
1	E	80(A)	SER	O-C-N	-5.41	116.88	123.10
1	E	52	GLY	CA-C-O	-5.39	111.19	120.57
1	E	274	ASP	CA-CB-CG	5.38	117.98	112.60
1	E	53	GLN	CA-CB-CG	-5.38	103.35	114.10
1	E	171	ASP	O-C-N	-5.38	115.83	122.82
1	E	195	THR	CA-C-N	-5.34	112.63	121.12
1	E	195	THR	C-N-CA	-5.34	112.63	121.12
1	E	118	ASP	CA-C-N	-5.32	114.92	121.83
1	E	118	ASP	C-N-CA	-5.32	114.92	121.83
1	E	133	PRO	CA-C-N	-5.30	115.68	123.00
1	E	133	PRO	C-N-CA	-5.30	115.68	123.00
1	E	71	TRP	CZ3-CH2-CZ2	-5.28	114.63	121.50
1	E	189	PHE	CA-CB-CG	5.28	119.08	113.80
1	E	2	ALA	CA-C-O	5.27	127.18	121.06
1	E	298	GLY	N-CA-C	-5.27	107.73	114.37
1	E	135	GLN	CA-C-N	5.26	128.33	120.87
1	E	135	GLN	C-N-CA	5.26	128.33	120.87
1	E	249	PRO	CA-C-O	5.25	127.61	121.31
1	E	44	GLU	OE1-CD-OE2	-5.23	110.34	122.90
1	E	169	PHE	CG-CD2-CE2	5.23	129.59	120.70
1	E	0	GLY	CA-C-O	-5.22	117.03	121.57
1	E	192	TRP	O-C-N	5.21	129.09	123.10
1	E	1	SER	O-C-N	5.20	129.71	123.36
1	E	115	SER	O-C-N	5.17	129.97	122.43
1	E	125	PHE	CA-C-O	5.17	127.82	121.72
1	E	97	THR	CA-C-O	-5.16	115.20	121.28
1	E	240	SER	CA-C-O	-5.15	114.99	120.40
1	E	193	THR	CA-C-N	-5.14	112.85	121.39
1	E	193	THR	C-N-CA	-5.14	112.85	121.39
1	E	88	THR	CA-C-N	-5.13	115.30	122.75
1	E	88	THR	C-N-CA	-5.13	115.30	122.75
1	E	167	PHE	CA-C-N	-5.13	114.09	122.40
1	E	167	PHE	C-N-CA	-5.13	114.09	122.40
1	E	177	GLY	CA-C-O	-5.12	114.98	121.44
1	E	90	SER	CA-C-O	-5.12	114.83	120.36
1	E	165	TYR	CA-CB-CG	-5.12	104.68	113.90
1	E	199	VAL	N-CA-CB	-5.12	105.22	111.21
1	E	218	THR	O-C-N	-5.12	117.23	123.27
1	E	144	ALA	CA-C-N	-5.12	114.10	122.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	144	ALA	C-N-CA	-5.12	114.10	122.54
1	E	119	GLY	CA-C-O	-5.11	115.59	121.47
1	E	48	SER	N-CA-CB	-5.11	101.83	110.41
1	E	102	GLU	CA-C-O	-5.09	114.73	120.43
1	E	233	ALA	N-CA-C	-5.09	106.76	112.87
1	E	86	THR	O-C-N	-5.08	117.25	123.10
1	E	189	PHE	O-C-N	-5.08	117.30	123.03
1	E	89	VAL	CA-CB-CG2	5.07	119.02	110.40
1	E	303	GLY	CA-C-O	-5.05	117.23	122.28
1	E	49	GLU	CG-CD-OE1	5.05	130.01	118.40
1	E	143	LYS	CA-C-O	-5.05	114.17	119.97
1	E	64	LYS	CA-C-O	5.03	126.45	120.66
1	E	179	ILE	N-CA-C	-5.03	102.25	108.89
1	E	19	GLN	CG-CD-NE2	5.01	123.92	116.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	66	LEU	Mainchain
2	I	5	LEU	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	2279	53	1
2	I	73	0	72	1	0
3	E	67	0	0	1	1
All	All	2529	0	2351	53	2

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 11.

All (53) 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:107:VAL:CG1	1:E:111:PHE:HB2	2.08	0.83
1:E:297:ILE:CD1	1:E:301:ILE:HD11	2.15	0.76
1:E:107:VAL:HG11	1:E:111:PHE:HB2	1.66	0.75
1:E:129:ASN:ND2	1:E:135:GLN:H	1.86	0.74
1:E:243:VAL:O	1:E:243:VAL:HG12	1.92	0.69
1:E:192:TRP:CH2	1:E:194:SER:HB2	2.28	0.68
1:E:107:VAL:HG12	1:E:108:SER:N	2.09	0.65
1:E:38:LEU:C	1:E:38:LEU:HD23	2.22	0.65
1:E:297:ILE:HD11	1:E:301:ILE:HD11	1.78	0.64
1:E:99:GLN:NE2	1:E:138:PHE:HA	2.12	0.64
1:E:107:VAL:CG1	1:E:108:SER:N	2.59	0.63
1:E:297:ILE:HD13	1:E:301:ILE:HD11	1.81	0.63
1:E:277:PRO:HA	1:E:283:CYS:HA	1.81	0.62
1:E:120:LEU:HD21	2:I:5:LEU:HD13	1.81	0.62
1:E:107:VAL:HG11	1:E:111:PHE:CB	2.30	0.61
1:E:199:VAL:HG11	1:E:234:GLN:HG3	1.82	0.61
1:E:204:LYS:HA	1:E:204:LYS:HE2	1.85	0.57
1:E:133:PRO:HD2	1:E:134:THR:N	2.20	0.56
1:E:248:PHE:CZ	1:E:254:LEU:HD11	2.41	0.56
1:E:192:TRP:CZ3	1:E:194:SER:HB2	2.41	0.55
1:E:46:THR:HG23	1:E:105:LYS:O	2.08	0.54
1:E:133:PRO:HD2	1:E:134:THR:H	1.74	0.53
1:E:107:VAL:HG12	1:E:108:SER:O	2.11	0.51
1:E:294:SER:HA	1:E:297:ILE:HG23	1.91	0.51
1:E:220:LEU:HA	1:E:305:VAL:CG1	2.40	0.51
1:E:219:THR:HG21	1:E:275:PHE:CZ	2.45	0.51
1:E:10:LEU:O	1:E:11:ASP:HB2	2.11	0.50
1:E:297:ILE:HG12	1:E:299:ILE:O	2.12	0.50
1:E:297:ILE:HD13	1:E:301:ILE:CD1	2.44	0.48
1:E:8:ASP:HB2	3:E:366:HOH:O	2.15	0.47
1:E:4:THR:OG1	1:E:14:TYR:HB3	2.13	0.47
1:E:22:THR:HA	1:E:23:PRO:HA	1.65	0.47
1:E:22:THR:HA	1:E:23:PRO:C	2.37	0.47
1:E:172:THR:HA	1:E:175:TYR:CE1	2.50	0.47
1:E:219:THR:O	1:E:305:VAL:HG12	2.15	0.46
1:E:173:THR:O	1:E:173:THR:CG2	2.64	0.46
1:E:41:PHE:HB3	1:E:55:ILE:HG22	1.99	0.45
1:E:133:PRO:CD	1:E:134:THR:N	2.80	0.44
1:E:220:LEU:HA	1:E:305:VAL:HG11	1.99	0.44
1:E:204:LYS:HE2	1:E:204:LYS:CA	2.48	0.43
1:E:129:ASN:ND2	1:E:131:VAL:H	2.16	0.43
1:E:133:PRO:CD	1:E:134:THR:H	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:LEU:C	1:E:38:LEU:CD2	2.92	0.42
1:E:199:VAL:CG1	1:E:234:GLN:HG3	2.47	0.42
1:E:132:SER:CB	1:E:133:PRO:HA	2.49	0.42
1:E:99:GLN:HE22	1:E:138:PHE:HA	1.84	0.41
1:E:198:ALA:HB2	1:E:203(A):PHE:HA	2.03	0.41
1:E:307:LEU:HD22	1:E:312:VAL:HG21	2.02	0.41
1:E:224:PRO:HD2	1:E:227:VAL:CG2	2.51	0.41
1:E:220:LEU:HB2	1:E:222:TYR:CE2	2.56	0.40
1:E:51:ASP:OD1	1:E:115:SER:HB3	2.21	0.40
1:E:129:ASN:HD21	1:E:131:VAL:HB	1.85	0.40
1:E:57:THR:HA	1:E:58:PRO:HD3	2.02	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:392:HOH:O	3:E:393:HOH:O[1_556]	0.69	1.51
1:E:134:THR:CG2	1:E:204:LYS:NZ[2_555]	1.79	0.41

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%)	319 (97%)	9 (3%)	0	100	100
2	I	6/8 (75%)	4 (67%)	2 (33%)	0	100	100
All	All	334/338 (99%)	323 (97%)	11 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	263/263 (100%)	242 (92%)	21 (8%)	11	8
2	I	7/7 (100%)	7 (100%)	0	100	100
All	All	270/270 (100%)	249 (92%)	21 (8%)	11	8

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	46	THR
1	E	51	ASP
1	E	64	LYS
1	E	67	SER
1	E	110	SER
1	E	114	ASP
1	E	116	THR
1	E	132	SER
1	E	146	LEU
1	E	148	SER
1	E	170	ILE
1	E	172	THR
1	E	173	THR
1	E	187	GLN
1	E	204	LYS
1	E	204(A)	SER
1	E	242	SER
1	E	251	SER
1	E	297	ILE
1	E	299	ILE
1	E	305	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	99	GLN

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Mol	Chain	Res	Type
1	E	129	ASN
1	E	134(A)	GLN
1	E	141	ASN
1	E	166	ASN
1	E	300	ASN
1	E	315	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section 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.