



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2017 – 11:27 PM EST

PDB ID : 1ER8
Title : THE ACTIVE SITE OF ASPARTIC PROTEINASES
Authors : Hemmings, A.M.; Veerapandian, B.; Szelke, M.; Cooper, J.B.; Blundell, T.L.
Deposited on : unknown
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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

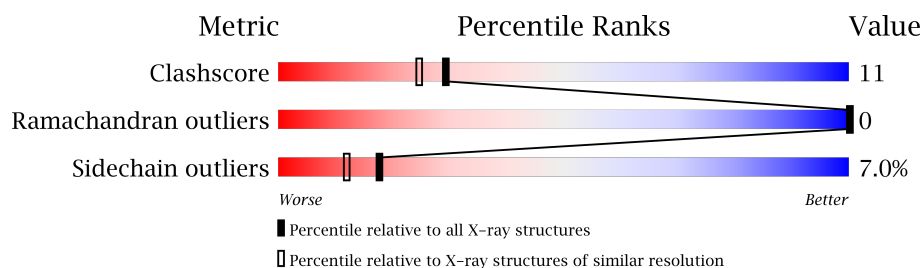
1 Overall quality at a glance

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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	330	 52% 37% 10% .
2	I	8	 63% 25% 13%

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.

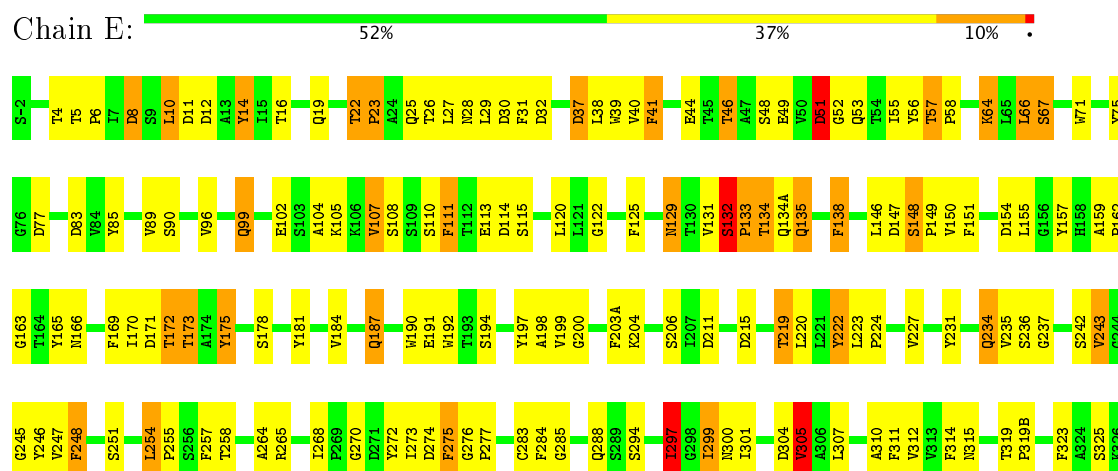
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	67	Total	O	0	0
			67	67		

3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Endothiaepsin



• 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 [i](#)

5.1 Standard geometry [i](#)

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	1.55	19/2445 (0.8%)	2.40	171/3345 (5.1%)
2	I	1.67	1/66 (1.5%)	1.73	0/87
All	All	1.55	20/2511 (0.8%)	2.39	171/3432 (5.0%)

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 (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	237	GLY	N-CA	9.36	1.60	1.46
1	E	6	PRO	N-CD	6.85	1.57	1.47
1	E	23	PRO	N-CD	6.60	1.57	1.47
1	E	165	TYR	CB-CG	6.59	1.61	1.51
1	E	190	TRP	NE1-CE2	-6.43	1.29	1.37
1	E	149	PRO	N-CD	6.38	1.56	1.47
1	E	19	GLN	CD-OE1	6.09	1.37	1.24
1	E	133	PRO	N-CD	5.98	1.56	1.47
1	E	319(B)	PRO	N-CD	5.98	1.56	1.47
1	E	245	GLY	N-CA	5.78	1.54	1.46
1	E	28	ASN	CG-OD1	5.71	1.36	1.24
1	E	190	TRP	CG-CD1	-5.67	1.28	1.36
1	E	122	GLY	N-CA	5.66	1.54	1.46
1	E	129	ASN	CG-OD1	5.61	1.36	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	99	GLN	CD-OE1	5.56	1.36	1.24
1	E	162	PRO	N-CD	5.41	1.55	1.47
1	E	255	PRO	N-CD	5.38	1.55	1.47
1	E	135	GLN	CD-OE1	5.30	1.35	1.24
2	I	4	HIS	CG-CD2	5.28	1.44	1.35
1	E	53	GLN	CD-OE1	5.27	1.35	1.24

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	75	TYR	CB-CG-CD1	-15.64	111.62	121.00
1	E	151	PHE	CB-CG-CD2	-12.05	112.36	120.80
1	E	236	SER	C-N-CA	-11.54	98.06	122.30
1	E	75	TYR	CB-CG-CD2	11.40	127.84	121.00
1	E	275	PHE	CB-CG-CD1	-10.94	113.14	120.80
1	E	181	TYR	CG-CD1-CE1	-10.85	112.62	121.30
1	E	44	GLU	OE1-CD-OE2	-10.80	110.34	123.30
1	E	85	TYR	O-C-N	10.38	139.30	122.70
1	E	49	GLU	OE1-CD-OE2	-10.12	111.16	123.30
1	E	12	ASP	CB-CG-OD1	9.86	127.17	118.30
1	E	181	TYR	CB-CG-CD1	-9.48	115.31	121.00
1	E	272	TYR	CD1-CE1-CZ	9.44	128.29	119.80
1	E	30	ASP	CB-CG-OD2	9.17	126.55	118.30
1	E	254	LEU	O-C-N	9.06	138.31	121.10
1	E	151	PHE	CB-CG-CD1	9.02	127.12	120.80
1	E	215	ASP	CB-CG-OD2	8.98	126.38	118.30
1	E	197	TYR	CB-CG-CD1	-8.96	115.62	121.00
1	E	222	TYR	O-C-N	8.92	136.98	122.70
1	E	305	VAL	CG1-CB-CG2	8.77	124.93	110.90
1	E	56	TYR	CG-CD2-CE2	-8.41	114.58	121.30
1	E	319	THR	C-N-CD	8.39	146.01	128.40
1	E	211	ASP	CB-CG-OD1	-8.29	110.84	118.30
1	E	157	TYR	CB-CG-CD1	-8.23	116.06	121.00
1	E	314	PHE	CB-CG-CD1	-8.20	115.06	120.80
1	E	257	PHE	CB-CG-CD1	8.14	126.50	120.80
1	E	311	PHE	CZ-CE2-CD2	8.12	129.84	120.10
1	E	170	ILE	O-C-N	8.06	135.59	122.70
1	E	169	PHE	CG-CD2-CE2	7.99	129.59	120.80
1	E	51	ASP	CB-CG-OD2	7.94	125.45	118.30
1	E	275	PHE	CB-CG-CD2	7.91	126.34	120.80
1	E	111	PHE	CB-CG-CD2	-7.86	115.30	120.80
1	E	14	TYR	CB-CG-CD1	7.76	125.66	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	66	LEU	O-C-N	-7.75	110.31	122.70
1	E	39	TRP	CE3-CZ3-CH2	7.69	129.66	121.20
1	E	53	GLN	O-C-N	-7.65	110.47	122.70
1	E	113	GLU	OE1-CD-OE2	-7.62	114.16	123.30
1	E	41	PHE	CB-CG-CD2	7.61	126.13	120.80
1	E	323	PHE	CB-CG-CD2	-7.55	115.51	120.80
1	E	276	GLY	C-N-CD	7.49	144.12	128.40
1	E	243	VAL	CA-CB-CG1	-7.40	99.81	110.90
1	E	27	LEU	CB-CG-CD2	7.23	123.29	111.00
1	E	166	ASN	O-C-N	7.17	134.18	122.70
1	E	31	PHE	CB-CG-CD2	-7.16	115.79	120.80
1	E	148	SER	C-N-CD	7.08	143.27	128.40
1	E	254	LEU	C-N-CD	7.08	143.26	128.40
1	E	8	ASP	CB-CG-OD2	7.04	124.64	118.30
1	E	22	THR	C-N-CD	7.04	143.18	128.40
1	E	191	GLU	OE1-CD-OE2	-7.02	114.88	123.30
1	E	236	SER	O-C-N	-6.95	111.39	123.20
1	E	247	VAL	CA-CB-CG2	6.91	121.26	110.90
1	E	190	TRP	NE1-CE2-CZ2	-6.90	122.81	130.40
1	E	222	TYR	CB-CG-CD2	-6.89	116.87	121.00
1	E	96	VAL	O-C-N	-6.87	111.71	122.70
1	E	181	TYR	CD1-CG-CD2	6.87	125.46	117.90
1	E	257	PHE	CZ-CE2-CD2	-6.86	111.87	120.10
1	E	159	ALA	C-N-CD	6.84	142.77	128.40
1	E	284	PHE	CG-CD2-CE2	-6.81	113.31	120.80
1	E	310	ALA	O-C-N	6.79	133.57	122.70
1	E	305	VAL	CA-CB-CG2	6.75	121.02	110.90
1	E	56	TYR	CB-CG-CD2	-6.74	116.95	121.00
1	E	223	LEU	C-N-CD	6.71	142.49	128.40
1	E	270	GLY	O-C-N	-6.71	111.97	122.70
1	E	175	TYR	CD1-CE1-CZ	-6.67	113.79	119.80
1	E	64	LYS	CA-CB-CG	6.66	128.04	113.40
1	E	169	PHE	CB-CG-CD2	6.62	125.43	120.80
1	E	10	LEU	CB-CG-CD1	6.54	122.11	111.00
1	E	268	ILE	C-N-CD	6.52	142.09	128.40
1	E	184	VAL	CG1-CB-CG2	6.52	121.33	110.90
1	E	107	VAL	CA-CB-CG1	-6.51	101.14	110.90
1	E	248	PHE	C-N-CD	6.46	141.97	128.40
1	E	71	TRP	CE3-CZ3-CH2	6.46	128.30	121.20
1	E	265	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	E	273	ILE	CB-CG1-CD1	6.42	131.86	113.90
1	E	133	PRO	CA-N-CD	-6.37	102.58	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	300	ASN	O-C-N	6.35	132.86	122.70
1	E	175	TYR	CG-CD2-CE2	-6.33	116.24	121.30
1	E	125	PHE	O-C-N	-6.32	112.59	122.70
1	E	190	TRP	CD1-NE1-CE2	-6.32	103.31	109.00
1	E	51	ASP	OD1-CG-OD2	-6.31	111.30	123.30
1	E	96	VAL	CA-C-O	6.31	133.35	120.10
1	E	169	PHE	CD1-CG-CD2	-6.28	110.13	118.30
1	E	231	TYR	CB-CG-CD2	6.28	124.77	121.00
1	E	37	ASP	CB-CG-OD1	6.25	123.92	118.30
1	E	150	VAL	CA-CB-CG1	6.25	120.27	110.90
1	E	215	ASP	OD1-CG-OD2	-6.22	111.48	123.30
1	E	163	GLY	O-C-N	-6.18	112.81	122.70
1	E	248	PHE	CZ-CE2-CD2	6.18	127.52	120.10
1	E	16	THR	C-N-CD	6.16	141.34	128.40
1	E	14	TYR	CG-CD2-CE2	6.15	126.22	121.30
1	E	39	TRP	CZ3-CH2-CZ2	-6.14	114.23	121.60
1	E	234	GLN	CG-CD-OE1	-6.13	109.34	121.60
1	E	275	PHE	CA-CB-CG	-6.11	99.23	113.90
1	E	248	PHE	CG-CD2-CE2	-6.10	114.09	120.80
1	E	288	GLN	CG-CD-NE2	6.10	131.34	116.70
1	E	125	PHE	CA-CB-CG	-6.01	99.47	113.90
1	E	134	THR	O-C-N	-5.99	113.11	122.70
1	E	25	GLN	OE1-CD-NE2	-5.99	108.13	121.90
1	E	154	ASP	CB-CG-OD2	5.98	123.68	118.30
1	E	67	SER	C-N-CA	-5.92	109.86	122.30
1	E	32	ASP	CB-CG-OD1	-5.90	112.99	118.30
1	E	274	ASP	CB-CG-OD1	5.87	123.58	118.30
1	E	197	TYR	CD1-CG-CD2	5.86	124.35	117.90
1	E	49	GLU	CG-CD-OE1	5.86	130.01	118.30
1	E	190	TRP	CH2-CZ2-CE2	-5.83	111.57	117.40
1	E	104	ALA	CA-C-O	5.81	132.31	120.10
1	E	258	THR	CA-CB-CG2	-5.81	104.26	112.40
1	E	31	PHE	CG-CD2-CE2	-5.81	114.41	120.80
1	E	71	TRP	CZ3-CH2-CZ2	-5.81	114.63	121.60
1	E	14	TYR	CD1-CE1-CZ	5.80	125.03	119.80
1	E	75	TYR	CA-CB-CG	-5.80	102.39	113.40
1	E	48	SER	N-CA-CB	-5.78	101.83	110.50
1	E	83	ASP	O-C-N	5.76	131.92	122.70
1	E	134(A)	GLN	O-C-N	5.74	131.88	122.70
1	E	25	GLN	CG-CD-NE2	5.70	130.37	116.70
1	E	206	SER	CA-C-O	5.66	131.99	120.10
1	E	31	PHE	CD1-CG-CD2	5.65	125.65	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	171	ASP	CB-CG-OD1	5.65	123.38	118.30
1	E	29	LEU	O-C-N	-5.64	113.67	122.70
1	E	219	THR	CA-CB-CG2	-5.64	104.51	112.40
1	E	90	SER	O-C-N	5.63	131.71	122.70
1	E	157	TYR	CB-CG-CD2	5.62	124.37	121.00
1	E	272	TYR	CE1-CZ-CE2	-5.61	110.82	119.80
1	E	285	GLY	CA-C-O	5.60	130.68	120.60
1	E	16	THR	O-C-N	5.57	131.68	121.10
1	E	319(B)	PRO	O-C-N	-5.56	113.80	122.70
1	E	319(B)	PRO	N-CD-CG	-5.55	94.87	103.20
1	E	297	ILE	CA-CB-CG2	5.52	121.94	110.90
1	E	138	PHE	CG-CD1-CE1	-5.51	114.74	120.80
1	E	264	ALA	CA-C-O	5.48	131.61	120.10
1	E	284	PHE	CZ-CE2-CD2	5.47	126.67	120.10
1	E	246	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	E	147	ASP	CB-CG-OD1	5.46	123.22	118.30
1	E	315	ASN	OD1-CG-ND2	-5.46	109.34	121.90
1	E	246	TYR	CZ-CE2-CD2	-5.44	114.90	119.80
1	E	5	THR	CA-CB-CG2	-5.43	104.80	112.40
1	E	257	PHE	CG-CD2-CE2	5.41	126.76	120.80
1	E	89	VAL	CA-CB-CG2	5.41	119.02	110.90
1	E	273	ILE	O-C-N	-5.41	114.05	122.70
1	E	323	PHE	CG-CD1-CE1	-5.40	114.86	120.80
1	E	102	GLU	O-C-N	5.35	131.26	122.70
1	E	197	TYR	CG-CD1-CE1	-5.35	117.02	121.30
1	E	284	PHE	CB-CG-CD1	-5.34	117.06	120.80
1	E	132	SER	C-N-CD	5.33	139.60	128.40
1	E	53	GLN	CA-C-O	5.32	131.28	120.10
1	E	83	ASP	CB-CG-OD1	5.32	123.09	118.30
1	E	247	VAL	CG1-CB-CG2	-5.30	102.42	110.90
1	E	304	ASP	CB-CG-OD1	5.29	123.06	118.30
1	E	248	PHE	CB-CG-CD2	-5.28	117.10	120.80
1	E	284	PHE	O-C-N	-5.28	114.22	123.20
1	E	311	PHE	CG-CD1-CE1	5.27	126.60	120.80
1	E	40	VAL	O-C-N	-5.27	114.27	122.70
1	E	187	GLN	C-N-CA	5.26	133.35	122.30
1	E	264	ALA	O-C-N	-5.26	114.28	122.70
1	E	30	ASP	OD1-CG-OD2	-5.24	113.34	123.30
1	E	57	THR	C-N-CD	5.24	139.41	128.40
1	E	52	GLY	CA-C-O	-5.23	111.19	120.60
1	E	51	ASP	O-C-N	5.19	132.02	123.20
1	E	51	ASP	CB-CG-OD1	5.17	122.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	200	GLY	C-N-CA	5.17	134.63	121.70
1	E	178	SER	O-C-N	5.14	130.93	122.70
1	E	134(A)	GLN	CA-C-O	-5.13	109.32	120.10
1	E	26	THR	CA-CB-CG2	-5.13	105.22	112.40
1	E	169	PHE	CB-CG-CD1	5.12	124.39	120.80
1	E	325	SER	CA-C-O	5.12	130.85	120.10
1	E	147	ASP	C-N-CA	5.08	134.40	121.70
1	E	77	ASP	CB-CG-OD1	5.08	122.87	118.30
1	E	275	PHE	CZ-CE2-CD2	-5.07	114.02	120.10
1	E	254	LEU	CB-CG-CD2	5.06	119.60	111.00
1	E	99	GLN	CG-CD-OE1	-5.05	111.50	121.60
1	E	155	LEU	O-C-N	-5.03	114.65	123.20
1	E	235	VAL	N-CA-CB	-5.02	100.46	111.50

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	52	1
2	I	73	0	72	1	0
3	E	67	0	0	1	1
All	All	2529	0	2351	52	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 (52) 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:HG12	1:E:243:VAL:O	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:107:VAL:CG1	1:E:108:SER:N	2.59	0.64
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: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:38:LEU:C	1:E:38:LEU:HD23	2.22	0.60
1:E:204:LYS:HE2	1:E:204:LYS:HA	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: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
1:E:199:VAL:CG1	1:E:234:GLN:HG3	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:129:ASN:HD21	1:E:131:VAL:HB	1.85	0.40
1:E:51:ASP:OD1	1:E:115:SER:HB3	2.21	0.40
1:E:57:THR:HA	1:E:58:PRO:HD3	2.02	0.40
1:E:22:THR:HA	1:E:23:PRO:C	2.37	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%)	245 (93%)	18 (7%)	18	13
2	I	7/7 (100%)	6 (86%)	1 (14%)	4	2
All	All	270/270 (100%)	251 (93%)	19 (7%)	18	12

All (19) 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	64	LYS
1	E	67	SER
1	E	110	SER
1	E	114	ASP
1	E	132	SER
1	E	146	LEU
1	E	148	SER
1	E	172	THR
1	E	173	THR
1	E	187	GLN
1	E	242	SER
1	E	251	SER
1	E	297	ILE
1	E	299	ILE
1	E	305	VAL
2	I	8	TYR

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

Mol	Chain	Res	Type
1	E	28	ASN
1	E	99	GLN
1	E	129	ASN

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Mol	Chain	Res	Type
1	E	134(A)	GLN
1	E	135	GLN
1	E	141	ASN
1	E	166	ASN
1	E	300	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.

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	DHI	I	1	2	6,10,11	1.66	1 (16%)	5,12,14	1.72	1 (20%)

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	DHI	I	1	2	-	0/4/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1	DHI	CA-C	3.36	1.54	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	I	1	DHI	O-C-CA	-3.32	115.85	125.02

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.