



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:53 PM UTC

PDB ID : 4ER4 / pdb_00004er4
Title : HIGH-RESOLUTION X-RAY ANALYSES OF RENIN INHIBITOR-
ASPARTIC PROTEINASE COMPLEXES
Authors : Foundling, S.I.; Watson, F.E.; Szelke, M.; Blundell, T.L.
Deposited on : 1991-01-05
Resolution : 2.10 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
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

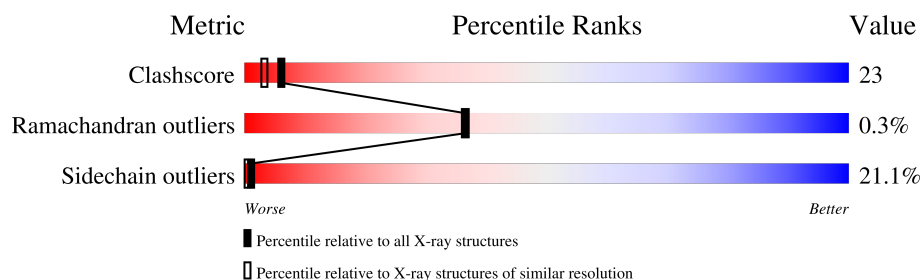
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	9	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2792 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 a protein called H-142.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	9	Total	C	N	O	0	0	1
			78	54	16	8			

- Molecule 3 is water.

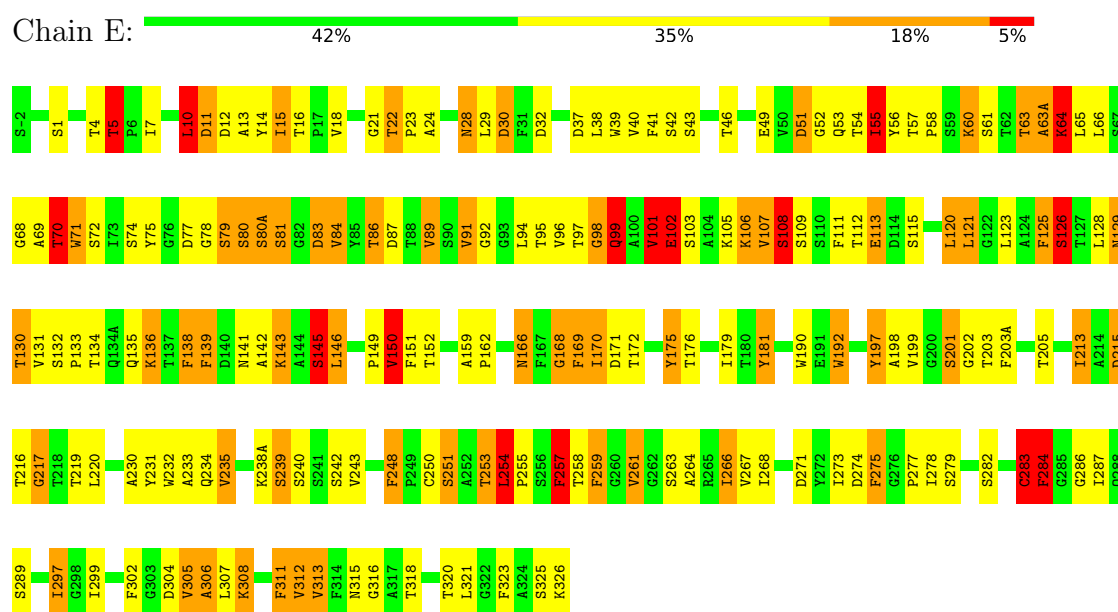
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	320	Total	O	0	0
			320	320		
3	I	5	Total	O	0	0
			5	5		

3 Residue-property plots

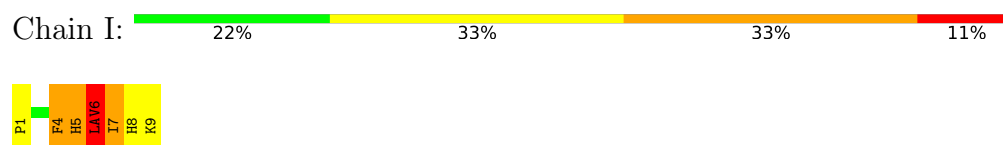
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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



• Molecule 2: H-142



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 74.00Å 45.50Å 90.00° 109.30° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.194 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2792	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: LAV

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	1.21	17/2445 (0.7%)	2.25	147/3345 (4.4%)
2	I	1.93	2/68 (2.9%)	1.58	2/91 (2.2%)
All	All	1.24	19/2513 (0.8%)	2.23	149/3436 (4.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	9
2	I	0	2
All	All	0	11

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	5	HIS	CE1-NE2	8.06	1.40	1.32
1	E	255	PRO	N-CA	-7.10	1.39	1.46
2	I	5	HIS	ND1-CE1	7.05	1.39	1.32
1	E	55	ILE	C-N	-6.79	1.22	1.33
1	E	60	LYS	C-N	6.74	1.42	1.33
1	E	232	TRP	NE1-CE2	-6.70	1.30	1.37
1	E	5	THR	CA-C	6.46	1.58	1.52
1	E	39	TRP	NE1-CE2	-6.42	1.30	1.37
1	E	146	LEU	C-N	6.30	1.41	1.33
1	E	99	GLN	CD-OE1	5.91	1.34	1.23
1	E	5	THR	C-N	5.59	1.40	1.33
1	E	71	TRP	NE1-CE2	-5.52	1.31	1.37
1	E	190	TRP	NE1-CE2	-5.51	1.31	1.37
1	E	192	TRP	NE1-CE2	-5.48	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	28	ASN	CG-OD1	5.40	1.33	1.23
1	E	138	PHE	C-N	-5.39	1.26	1.33
1	E	234	GLN	CD-OE1	5.38	1.33	1.23
1	E	202	GLY	N-CA	5.09	1.48	1.44
1	E	139	PHE	N-CA	-5.05	1.40	1.46

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	248	PHE	O-C-N	-16.25	110.34	121.88
1	E	159	ALA	O-C-N	-15.03	110.68	121.65
1	E	297	ILE	CB-CA-C	-13.81	95.71	110.62
1	E	138	PHE	CB-CA-C	-11.08	93.48	110.88
1	E	254	LEU	O-C-N	-10.88	112.07	121.31
1	E	282	SER	N-CA-C	10.70	124.15	110.24
1	E	60	LYS	O-C-N	-10.45	108.63	122.22
1	E	78	GLY	CA-C-N	9.77	134.62	120.95
1	E	78	GLY	C-N-CA	9.77	134.62	120.95
1	E	5	THR	O-C-N	-9.38	112.37	121.38
1	E	264	ALA	N-CA-C	9.15	122.61	110.53
1	E	261	VAL	CA-CB-CG1	9.14	125.94	110.40
1	E	113	GLU	CA-C-N	9.06	135.46	122.05
1	E	113	GLU	C-N-CA	9.06	135.46	122.05
1	E	311	PHE	CA-CB-CG	-8.90	104.89	113.80
1	E	175	TYR	CA-C-N	8.90	135.91	122.65
1	E	175	TYR	C-N-CA	8.90	135.91	122.65
1	E	5	THR	CB-CA-C	8.88	123.35	110.02
1	E	112	THR	CA-C-N	8.78	133.66	120.31
1	E	112	THR	C-N-CA	8.78	133.66	120.31
1	E	11	ASP	CB-CA-C	-8.76	99.02	111.80
1	E	96	VAL	CA-CB-CG2	8.52	124.89	110.40
1	E	170	ILE	CA-C-O	8.48	131.10	120.75
1	E	275	PHE	CA-CB-CG	-8.48	105.32	113.80
1	E	257	PHE	CA-C-N	8.40	133.76	122.84
1	E	257	PHE	C-N-CA	8.40	133.76	122.84
1	E	107	VAL	CA-C-O	7.97	130.12	121.67
1	E	16	THR	O-C-N	-7.94	114.32	121.39
1	E	235	VAL	O-C-N	-7.90	114.83	123.20
1	E	235	VAL	CA-C-O	7.81	128.51	120.39
1	E	150	VAL	N-CA-CB	-7.73	99.69	111.05
2	I	4	PHE	O-C-N	-7.63	113.86	123.24
1	E	287	ILE	CA-C-O	7.46	129.39	120.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	68	GLY	CA-C-N	7.41	131.32	120.95
1	E	68	GLY	C-N-CA	7.41	131.32	120.95
1	E	107	VAL	O-C-N	-7.37	115.23	122.97
1	E	168	GLY	O-C-N	-7.23	113.97	122.50
1	E	297	ILE	N-CA-CB	7.21	120.91	112.33
1	E	64	LYS	O-C-N	-7.18	114.92	123.31
1	E	70	THR	CA-C-O	-7.18	111.71	120.54
1	E	287	ILE	O-C-N	-7.13	112.28	122.76
1	E	234	GLN	CA-C-N	-7.00	113.79	123.10
1	E	234	GLN	C-N-CA	-7.00	113.79	123.10
1	E	63(A)	ALA	N-CA-C	6.87	119.46	108.41
1	E	81	SER	N-CA-C	6.77	118.83	108.07
1	E	179	ILE	CB-CA-C	-6.66	101.78	110.84
1	E	199	VAL	CA-CB-CG2	6.56	121.55	110.40
1	E	284	PHE	CA-C-N	6.53	128.37	121.45
1	E	284	PHE	C-N-CA	6.53	128.37	121.45
1	E	216	THR	CA-C-N	6.52	134.18	121.41
1	E	216	THR	C-N-CA	6.52	134.18	121.41
1	E	305	VAL	N-CA-C	6.50	117.25	110.62
2	I	4	PHE	CA-C-O	6.48	128.69	121.11
1	E	111	PHE	O-C-N	-6.47	113.81	122.23
1	E	201	SER	CA-C-N	-6.40	116.03	122.69
1	E	201	SER	C-N-CA	-6.40	116.03	122.69
1	E	146	LEU	CA-C-N	6.38	128.74	120.44
1	E	146	LEU	C-N-CA	6.38	128.74	120.44
1	E	230	ALA	CA-C-N	6.32	129.22	120.63
1	E	230	ALA	C-N-CA	6.32	129.22	120.63
1	E	125	PHE	O-C-N	6.28	130.10	123.06
1	E	169	PHE	CA-C-N	6.24	130.29	122.43
1	E	169	PHE	C-N-CA	6.24	130.29	122.43
1	E	21	GLY	O-C-N	6.23	131.31	123.02
1	E	171	ASP	CA-C-O	-6.23	113.86	121.02
1	E	24	ALA	N-CA-C	6.19	119.32	110.10
1	E	139	PHE	CA-CB-CG	-6.19	107.61	113.80
1	E	113	GLU	O-C-N	6.17	129.85	122.27
1	E	312	VAL	N-CA-C	6.16	116.73	107.80
1	E	257	PHE	CA-C-O	-6.12	113.72	120.38
1	E	83	ASP	O-C-N	-6.11	114.34	122.59
1	E	83	ASP	CA-C-O	6.08	129.55	121.46
1	E	22	THR	O-C-N	6.07	128.95	121.79
1	E	87	ASP	CA-C-O	-6.02	114.69	121.25
1	E	108	SER	N-CA-CB	-5.99	101.35	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	39	TRP	CD2-CE2-CZ2	5.98	128.38	122.40
1	E	91	VAL	CA-CB-CG2	5.95	120.52	110.40
1	E	312	VAL	CA-CB-CG2	5.93	120.47	110.40
1	E	145	SER	CA-C-O	5.91	126.22	119.18
1	E	170	ILE	O-C-N	-5.91	115.44	122.77
1	E	149	PRO	CB-CA-C	-5.88	105.10	113.09
1	E	215	ASP	O-C-N	-5.87	115.63	123.14
1	E	30	ASP	CA-C-N	5.85	130.71	121.99
1	E	30	ASP	C-N-CA	5.85	130.71	121.99
1	E	89	VAL	CA-CB-CG2	5.84	120.33	110.40
1	E	95	THR	N-CA-CB	5.80	119.62	110.23
1	E	92	GLY	CA-C-N	-5.78	114.42	122.86
1	E	92	GLY	C-N-CA	-5.78	114.42	122.86
1	E	243	VAL	CA-CB-CG2	5.77	120.21	110.40
1	E	101	VAL	CA-CB-CG2	5.76	120.20	110.40
1	E	231	TYR	O-C-N	5.76	128.25	122.03
1	E	308	LYS	CA-C-N	5.75	132.76	122.06
1	E	308	LYS	C-N-CA	5.75	132.76	122.06
1	E	39	TRP	CA-C-N	-5.75	115.22	123.03
1	E	39	TRP	C-N-CA	-5.75	115.22	123.03
1	E	205	THR	CA-C-O	-5.74	114.39	121.11
1	E	235	VAL	CA-CB-CG2	5.70	120.09	110.40
1	E	264	ALA	O-C-N	-5.64	116.36	122.79
1	E	217	GLY	O-C-N	5.62	130.00	122.70
1	E	1	SER	CA-C-N	-5.61	115.08	122.99
1	E	1	SER	C-N-CA	-5.61	115.08	122.99
1	E	304	ASP	CA-C-N	5.57	128.10	120.46
1	E	304	ASP	C-N-CA	5.57	128.10	120.46
1	E	162	PRO	CB-CA-C	-5.55	102.54	110.75
1	E	233	ALA	N-CA-C	-5.54	106.02	112.89
1	E	217	GLY	CA-C-N	5.54	130.64	123.00
1	E	217	GLY	C-N-CA	5.54	130.64	123.00
1	E	267	VAL	CB-CA-C	-5.49	104.66	111.08
1	E	166	ASN	O-C-N	-5.48	116.25	123.21
1	E	70	THR	N-CA-CB	-5.46	101.26	111.13
1	E	162	PRO	O-C-N	5.45	129.58	123.04
1	E	318	THR	O-C-N	5.42	128.56	122.22
1	E	242	SER	N-CA-CB	5.42	119.64	110.49
1	E	84	VAL	CA-CB-CG2	5.41	119.60	110.40
1	E	108	SER	CA-C-N	5.38	131.82	121.54
1	E	108	SER	C-N-CA	5.38	131.82	121.54
1	E	111	PHE	CA-C-O	5.36	126.19	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	213	ILE	CA-C-O	5.36	128.96	121.51
1	E	168	GLY	CA-C-O	5.32	124.92	119.01
1	E	239	SER	CA-C-O	-5.30	114.55	120.54
1	E	83	ASP	N-CA-C	5.29	118.33	109.96
1	E	259	PHE	CA-CB-CG	-5.27	108.53	113.80
1	E	257	PHE	CA-CB-CG	-5.27	108.53	113.80
1	E	97	THR	N-CA-CB	-5.25	102.77	110.85
1	E	30	ASP	CA-C-O	-5.25	114.38	120.62
1	E	126	SER	N-CA-C	5.25	119.43	113.19
1	E	32	ASP	N-CA-CB	-5.23	101.79	110.47
1	E	312	VAL	CA-C-O	5.23	126.12	120.53
1	E	123	LEU	N-CA-C	-5.20	104.98	113.19
1	E	261	VAL	CB-CA-C	5.17	117.57	111.32
1	E	106	LYS	O-C-N	-5.16	117.20	123.29
1	E	255	PRO	CB-CA-C	-5.14	103.50	110.60
1	E	306	ALA	CA-C-O	5.13	125.20	119.41
1	E	63	THR	O-C-N	5.10	130.87	122.70
1	E	234	GLN	N-CA-CB	5.10	118.68	110.42
1	E	102	GLU	CA-CB-CG	-5.08	103.94	114.10
1	E	101	VAL	CA-C-N	-5.08	115.03	122.19
1	E	101	VAL	C-N-CA	-5.08	115.03	122.19
1	E	5	THR	N-CA-CB	-5.07	99.12	110.27
1	E	40	VAL	CB-CA-C	-5.06	102.57	110.52
1	E	250	CYS	N-CA-C	5.06	117.53	111.71
1	E	283	CYS	CA-C-O	-5.05	115.41	121.11
1	E	64	LYS	CA-C-N	5.05	128.27	121.05
1	E	64	LYS	C-N-CA	5.05	128.27	121.05
1	E	10	LEU	N-CA-CB	5.03	119.42	111.17
1	E	115	SER	O-C-N	-5.03	115.08	122.43
1	E	289	SER	O-C-N	-5.03	116.75	122.89
1	E	96	VAL	N-CA-CB	5.01	119.40	111.99
1	E	171	ASP	O-C-N	5.00	129.29	122.48

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	151	PHE	Mainchain
1	E	175	TYR	Sidechain
1	E	181	TYR	Sidechain
1	E	197	TYR	Sidechain
1	E	257	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	E	259	PHE	Sidechain
1	E	284	PHE	Sidechain
1	E	311	PHE	Sidechain
1	E	60	LYS	Mainchain
2	I	6	LAV	Mainchain,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	105	3
2	I	78	0	74	12	0
3	E	320	0	0	9	8
3	I	5	0	0	1	0
All	All	2792	0	2354	109	8

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 23.

All (109) 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:145:SER:HB3	3:E:566:HOH:O	1.71	0.88
1:E:51:ASP:CG	1:E:52:GLY:N	2.30	0.86
1:E:77:ASP:OD1	1:E:79:SER:HB2	1.75	0.85
1:E:120:LEU:HD21	2:I:6:LAV:HD1A	1.62	0.81
1:E:132:SER:OG	1:E:133:PRO:HA	1.79	0.80
1:E:143:LYS:HE3	1:E:316:GLY:O	1.83	0.78
1:E:18:VAL:HG22	1:E:91:VAL:HG22	1.63	0.77
1:E:7:ILE:HG22	1:E:15:ILE:HG12	1.68	0.76
1:E:38:LEU:O	1:E:102:GLU:HG3	1.86	0.74
1:E:220:LEU:HD22	1:E:286:GLY:HA2	1.71	0.72
1:E:129:ASN:ND2	1:E:131:VAL:H	1.87	0.72
2:I:7:ILE:HG12	2:I:8:HIS:N	2.06	0.71
1:E:150:VAL:CG2	1:E:315:ASN:HA	2.21	0.70
1:E:86:THR:HG22	3:E:449:HOH:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:VAL:HG23	1:E:315:ASN:HA	1.75	0.68
1:E:7:ILE:HD13	1:E:13:ALA:HB3	1.76	0.68
1:E:70:THR:HG22	1:E:70:THR:O	1.94	0.68
1:E:10:LEU:HD13	1:E:10:LEU:H	1.61	0.65
1:E:266:ILE:HD11	1:E:323:PHE:HB3	1.80	0.64
1:E:94:LEU:HD21	1:E:142:ALA:HB1	1.80	0.63
1:E:215:ASP:OD1	2:I:6:LAV:H2	1.99	0.63
1:E:152:THR:OG1	1:E:166:ASN:HB2	1.99	0.63
1:E:66:LEU:O	1:E:69:ALA:HB3	1.98	0.62
1:E:181:TYR:HE1	1:E:313:VAL:HG11	1.64	0.62
1:E:10:LEU:HD13	1:E:10:LEU:N	2.15	0.61
1:E:5:THR:HB	3:E:338:HOH:O	2.02	0.60
1:E:7:ILE:CD1	1:E:13:ALA:HB3	2.31	0.59
1:E:12:ASP:HA	1:E:219:THR:HG23	1.83	0.59
1:E:51:ASP:CG	1:E:52:GLY:H	2.07	0.59
1:E:130:THR:O	1:E:130:THR:HG23	2.02	0.59
1:E:131:VAL:HG12	1:E:134:THR:O	2.03	0.59
1:E:46:THR:O	1:E:49:GLU:HB2	2.05	0.57
1:E:72:SER:H	1:E:130:THR:CG2	2.18	0.57
1:E:77:ASP:HB3	2:I:5:HIS:ND1	2.19	0.57
1:E:266:ILE:CD1	1:E:323:PHE:HB3	2.35	0.56
1:E:168:GLY:O	1:E:169:PHE:HB3	2.06	0.55
1:E:56:TYR:O	1:E:58:PRO:HD3	2.07	0.55
1:E:219:THR:OG1	2:I:4:PHE:N	2.39	0.55
1:E:254:LEU:CD2	1:E:274:ASP:HB2	2.37	0.55
1:E:150:VAL:HG22	1:E:315:ASN:HA	1.91	0.53
1:E:325:SER:HB2	3:E:437:HOH:O	2.09	0.53
1:E:80:SER:O	1:E:108:SER:HB2	2.09	0.53
1:E:152:THR:HA	1:E:312:VAL:O	2.10	0.52
2:I:9:LYS:N	3:I:344:HOH:O	2.42	0.51
1:E:89:VAL:HG21	1:E:99:GLN:HG2	1.92	0.51
1:E:198:ALA:HB3	1:E:258:THR:HB	1.92	0.51
1:E:22:THR:O	1:E:61:SER:HA	2.11	0.51
1:E:14:TYR:OH	1:E:308:LYS:HD2	2.11	0.51
1:E:129:ASN:HD21	1:E:131:VAL:HB	1.76	0.51
1:E:80(A):SER:O	1:E:81:SER:HB3	2.12	0.49
1:E:215:ASP:C	1:E:217:GLY:H	2.20	0.49
1:E:101:VAL:HG12	1:E:101:VAL:O	2.12	0.48
1:E:30:ASP:HB3	1:E:120:LEU:HG	1.96	0.48
1:E:51:ASP:OD1	1:E:52:GLY:N	2.41	0.48
1:E:139:PHE:O	1:E:143:LYS:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:GLN:NE2	3:E:536:HOH:O	2.45	0.48
1:E:94:LEU:HD23	1:E:138:PHE:CE2	2.48	0.48
1:E:113:GLU:HG3	3:E:611:HOH:O	2.14	0.48
1:E:75:TYR:HB2	1:E:79:SER:HB3	1.96	0.47
1:E:278:ILE:HG13	1:E:279:SER:N	2.30	0.47
1:E:143:LYS:HA	1:E:146:LEU:HD12	1.95	0.47
1:E:41:PHE:HB3	1:E:55:ILE:HD12	1.96	0.47
1:E:132:SER:HA	1:E:133:PRO:C	2.40	0.47
1:E:11:ASP:OD2	1:E:308:LYS:HE3	2.14	0.47
1:E:72:SER:H	1:E:130:THR:HG23	1.80	0.47
1:E:13:ALA:HB2	2:I:4:PHE:CD2	2.50	0.46
1:E:42:SER:C	1:E:55:ILE:HG13	2.41	0.46
1:E:71:TRP:CZ3	1:E:80(A):SER:HB3	2.51	0.46
1:E:273:ILE:HG22	1:E:273:ILE:O	2.14	0.46
1:E:77:ASP:HB3	2:I:5:HIS:HD1	1.79	0.46
1:E:106:LYS:HE2	3:E:369:HOH:O	2.16	0.46
1:E:10:LEU:N	1:E:10:LEU:CD1	2.79	0.45
1:E:94:LEU:HD21	1:E:142:ALA:CB	2.43	0.45
1:E:126:SER:OG	1:E:136:LYS:HA	2.15	0.45
1:E:192:TRP:CZ3	1:E:261:VAL:HG22	2.51	0.45
1:E:278:ILE:HG13	1:E:279:SER:H	1.82	0.45
1:E:22:THR:HA	1:E:23:PRO:HA	1.34	0.45
2:I:7:ILE:CG1	2:I:8:HIS:N	2.77	0.45
1:E:28:ASN:C	1:E:29:LEU:HD23	2.43	0.44
1:E:61:SER:HB3	1:E:63(A):ALA:HB2	1.99	0.44
1:E:128:LEU:HD13	2:I:7:ILE:HG21	1.99	0.44
1:E:307:LEU:HD22	1:E:312:VAL:HG21	1.98	0.44
1:E:313:VAL:O	1:E:313:VAL:HG12	2.16	0.44
1:E:302:PHE:CD2	1:E:302:PHE:N	2.85	0.43
1:E:266:ILE:HD11	1:E:323:PHE:CB	2.45	0.43
1:E:219:THR:O	1:E:305:VAL:HG23	2.17	0.43
1:E:77:ASP:OD1	1:E:79:SER:N	2.51	0.43
1:E:254:LEU:HD12	1:E:254:LEU:HA	1.70	0.43
1:E:41:PHE:CE2	1:E:107:VAL:HG21	2.54	0.42
1:E:201:SER:HB2	3:E:397:HOH:O	2.17	0.42
1:E:94:LEU:HD11	3:E:566:HOH:O	2.19	0.42
1:E:64:LYS:HD2	1:E:64:LYS:HA	1.39	0.42
1:E:261:VAL:HG11	1:E:323:PHE:CD1	2.54	0.42
1:E:125:PHE:O	1:E:128:LEU:HB2	2.20	0.41
1:E:220:LEU:HD11	1:E:284:PHE:HE2	1.85	0.41
1:E:86:THR:HG23	1:E:98:GLY:HA2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:7:ILE:HG12	2:I:8:HIS:H	1.85	0.41
1:E:297:ILE:HD13	1:E:297:ILE:HG21	1.70	0.41
1:E:83:ASP:HB2	1:E:84:VAL:H	1.71	0.41
1:E:275:PHE:O	2:I:1:PRO:HG3	2.21	0.41
1:E:181:TYR:CE1	1:E:313:VAL:HG11	2.51	0.41
1:E:197:TYR:HB2	1:E:257:PHE:CZ	2.56	0.41
1:E:268:ILE:HG12	1:E:306:ALA:HA	2.02	0.41
1:E:277:PRO:HA	1:E:283:CYS:HA	2.02	0.41
1:E:248:PHE:CD1	1:E:248:PHE:N	2.89	0.40
1:E:38:LEU:CD1	1:E:121:LEU:HD12	2.50	0.40
1:E:57:THR:HA	1:E:58:PRO:HD3	1.94	0.40
1:E:257:PHE:O	1:E:268:ILE:N	2.40	0.40
1:E:315:ASN:HB3	1:E:320:THR:H	1.85	0.40

All (8) 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:362:HOH:O	3:E:380:HOH:O[1_655]	1.60	0.60
3:E:508:HOH:O	3:E:546:HOH:O[2_655]	1.84	0.36
3:E:356:HOH:O	3:E:412:HOH:O[2_655]	1.89	0.31
1:E:53:GLN:O	3:E:628:HOH:O[2_655]	2.02	0.18
1:E:253:THR:OG1	3:E:576:HOH:O[1_454]	2.10	0.10
3:E:474:HOH:O	3:E:523:HOH:O[1_556]	2.11	0.09
3:E:415:HOH:O	3:E:508:HOH:O[2_645]	2.15	0.05
1:E:251:SER:OG	3:E:361:HOH:O[1_454]	2.16	0.04

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%)	311 (95%)	16 (5%)	1 (0%)	36 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	6/9 (67%)	4 (67%)	2 (33%)	0	100	100
All	All	334/339 (98%)	315 (94%)	18 (5%)	1 (0%)	36	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	98	GLY

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%)	207 (79%)	56 (21%)	1	0
2	I	7/8 (88%)	6 (86%)	1 (14%)	3	1
All	All	270/271 (100%)	213 (79%)	57 (21%)	1	0

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	4	THR
1	E	5	THR
1	E	10	LEU
1	E	15	ILE
1	E	37	ASP
1	E	43	SER
1	E	51	ASP
1	E	54	THR
1	E	55	ILE
1	E	63	THR
1	E	64	LYS
1	E	65	LEU
1	E	70	THR
1	E	74	SER
1	E	79	SER

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Mol	Chain	Res	Type
1	E	80	SER
1	E	80(A)	SER
1	E	86	THR
1	E	99	GLN
1	E	101	VAL
1	E	102	GLU
1	E	103	SER
1	E	105	LYS
1	E	108	SER
1	E	109	SER
1	E	120	LEU
1	E	121	LEU
1	E	126	SER
1	E	129	ASN
1	E	130	THR
1	E	136	LYS
1	E	141	ASN
1	E	143	LYS
1	E	145	SER
1	E	150	VAL
1	E	170	ILE
1	E	172	THR
1	E	176	THR
1	E	203	THR
1	E	203(A)	PHE
1	E	213	ILE
1	E	235	VAL
1	E	238(A)	LYS
1	E	239	SER
1	E	240	SER
1	E	251	SER
1	E	253	THR
1	E	254	LEU
1	E	263	SER
1	E	266	ILE
1	E	271	ASP
1	E	283	CYS
1	E	299	ILE
1	E	313	VAL
1	E	321	LEU
1	E	326	LYS
2	I	7	ILE

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	135	GLN
1	E	141	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	LAV	I	6	2	12,13,14	1.31	2 (16%)	12,16,18	1.97	3 (25%)

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	LAV	I	6	2	-	1/14/15/17	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	6	LAV	C1-CA	-3.50	1.49	1.53
2	I	6	LAV	C3-N1	2.04	1.51	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	6	LAV	C2-C3-C	-4.80	106.77	112.96
2	I	6	LAV	C1-N1-C3	2.70	119.02	114.00
2	I	6	LAV	CB-CA-C1	-2.18	102.98	109.38

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	6	LAV	CA-C1-N1-C3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	6	LAV	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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.