



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:06 pm BST

PDB ID : 1BLL  
Title : X-RAY CRYSTALLOGRAPHIC DETERMINATION OF THE STRUCTURE OF BOVINE LENS LEUCINE AMINOPEPTIDASE COMPLEXED WITH AMASTATIN: FORMULATION OF A CATALYTIC MECHANISM FEATURING A GEM-DIOLATE TRANSITION STATE  
Authors : Kim, H.; Lipscomb, W.N.  
Deposited on : 1993-03-02  
Resolution : 2.40 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

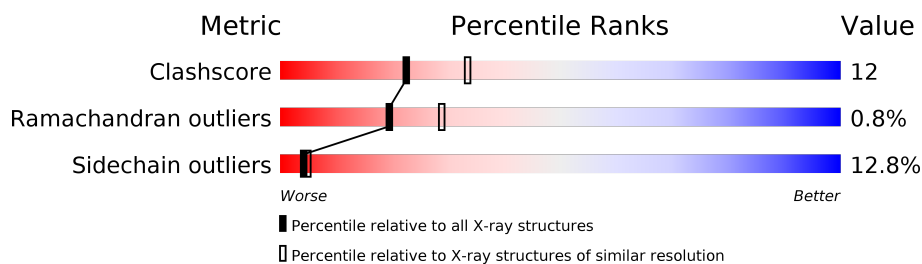
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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  $\geq 3$ , 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	488	
2	I	4	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3838 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 LEUCINE AMINOPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	481	Total	C	N	O	S	0	0	0
			3671	2321	635	697	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	ACE	-	ACETYLATION	UNP P00727
E	45	PRO	SER	CONFLICT	UNP P00727

- Molecule 2 is a protein called AMASTATIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	4	Total	C	N	O	0	0	0
			33	21	4	8			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	2	Total	Zn	0	0
			2	2		

- Molecule 4 is water.

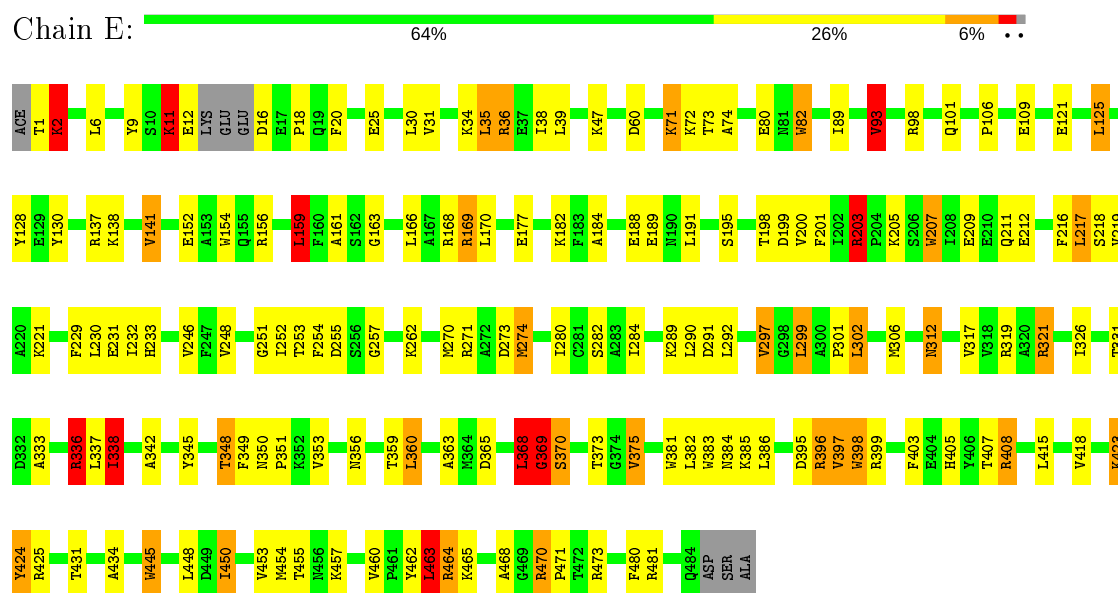
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	131	Total	O	0	0
			131	131		
4	I	1	Total	O	0	0
			1	1		

### 3 Residue-property plots [i](#)

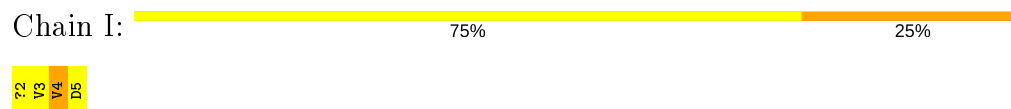
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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



#### • Molecule 2: AMASTATIN



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.30Å 130.30Å 121.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.198 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3838	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	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: ZN, L2O

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	0.81	2/3744 (0.1%)	1.60	79/5068 (1.6%)
2	I	0.65	0/22	1.88	2/28 (7.1%)
All	All	0.81	2/3766 (0.1%)	1.60	81/5096 (1.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	370	SER	CA-CB	7.88	1.64	1.52
1	E	93	VAL	CA-CB	5.09	1.65	1.54

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	470	ARG	NE-CZ-NH1	12.31	126.45	120.30
1	E	271	ARG	NE-CZ-NH1	12.03	126.32	120.30
1	E	336	ARG	NE-CZ-NH2	-11.86	114.37	120.30
1	E	336	ARG	NE-CZ-NH1	11.04	125.82	120.30
1	E	169	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	E	470	ARG	NE-CZ-NH2	-10.37	115.11	120.30
1	E	370	SER	CA-CB-OG	9.22	136.08	111.20
1	E	154	TRP	CD1-CG-CD2	9.01	113.51	106.30
1	E	168	ARG	NE-CZ-NH1	8.28	124.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	36	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	E	381	TRP	CD1-CG-CD2	8.16	112.83	106.30
1	E	207	TRP	CD1-CG-CD2	8.11	112.79	106.30
1	E	168	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	E	154	TRP	CE2-CD2-CG	-7.76	101.09	107.30
1	E	321	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	E	302	LEU	CA-CB-CG	7.68	132.96	115.30
1	E	11	LYS	N-CA-C	7.54	131.37	111.00
1	E	98	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	E	383	TRP	CD1-CG-CD2	7.46	112.27	106.30
1	E	383	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	E	381	TRP	CE2-CD2-CG	-7.38	101.40	107.30
1	E	424	TYR	CB-CG-CD2	-7.30	116.62	121.00
1	E	445	TRP	CD1-CG-CD2	7.30	112.14	106.30
1	E	398	TRP	CD1-CG-CD2	7.26	112.11	106.30
1	E	454	MET	CG-SD-CE	-7.21	88.66	100.20
1	E	445	TRP	CE2-CD2-CG	-7.09	101.63	107.30
1	E	398	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	E	450	ILE	CA-CB-CG1	-7.05	97.61	111.00
1	E	207	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	E	271	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	E	369	GLY	O-C-N	6.81	133.60	122.70
1	E	338	ILE	CA-CB-CG1	-6.80	98.08	111.00
1	E	137	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	E	383	TRP	CB-CG-CD1	-6.60	118.42	127.00
1	E	109	GLU	CA-CB-CG	-6.58	98.91	113.40
1	E	397	VAL	N-CA-CB	-6.55	97.09	111.50
1	E	450	ILE	N-CA-CB	-6.47	95.92	110.80
1	E	98	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	E	321	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	E	383	TRP	CG-CD2-CE3	6.30	139.57	133.90
1	E	381	TRP	CG-CD2-CE3	6.29	139.56	133.90
1	E	152	GLU	CA-CB-CG	6.28	127.22	113.40
1	E	396	ARG	CB-CG-CD	-6.24	95.37	111.60
1	E	82	TRP	CD1-CG-CD2	6.24	111.29	106.30
1	E	381	TRP	CB-CG-CD1	-6.24	118.89	127.00
1	E	154	TRP	CG-CD1-NE1	-6.13	103.97	110.10
1	E	156	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	E	36	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	E	445	TRP	CG-CD2-CE3	6.01	139.31	133.90
1	E	462	TYR	CB-CG-CD2	-6.00	117.40	121.00
1	E	169	ARG	CA-CB-CG	6.00	126.59	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	203	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	E	159	LEU	CA-CB-CG	5.99	129.08	115.30
1	E	368	LEU	CA-C-N	-5.98	104.24	116.20
1	E	297	VAL	CG1-CB-CG2	-5.95	101.39	110.90
1	E	450	ILE	CA-CB-CG2	5.88	122.66	110.90
1	E	464	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	E	464	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	E	381	TRP	CG-CD1-NE1	-5.76	104.34	110.10
2	I	4	VAL	CB-CA-C	-5.66	100.64	111.40
1	E	408	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	E	82	TRP	CE2-CD2-CG	-5.55	102.86	107.30
1	E	338	ILE	CA-CB-CG2	5.54	121.98	110.90
1	E	253	THR	CA-CB-CG2	-5.51	104.69	112.40
1	E	274	MET	CG-SD-CE	-5.45	91.49	100.20
1	E	336	ARG	CA-CB-CG	5.44	125.36	113.40
2	I	4	VAL	CA-CB-CG2	-5.41	102.78	110.90
1	E	217	LEU	CA-CB-CG	5.37	127.64	115.30
1	E	481	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	E	2	LYS	CA-CB-CG	5.30	125.05	113.40
1	E	473	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	E	397	VAL	CB-CA-C	5.23	121.33	111.40
1	E	207	TRP	CG-CD1-NE1	-5.22	104.88	110.10
1	E	317	VAL	CG1-CB-CG2	-5.18	102.61	110.90
1	E	25	GLU	OE1-CD-OE2	-5.18	117.09	123.30
1	E	399	ARG	CG-CD-NE	5.11	122.53	111.80
1	E	348	THR	CA-CB-CG2	5.11	119.55	112.40
1	E	399	ARG	CB-CG-CD	-5.10	98.35	111.60
1	E	463	LEU	CA-CB-CG	5.07	126.96	115.30
1	E	306	MET	CG-SD-CE	-5.03	92.16	100.20
1	E	403	PHE	CB-CG-CD2	-5.01	117.29	120.80

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	128	TYR	Sidechain
1	E	130	TYR	Sidechain
1	E	254	PHE	Sidechain
1	E	349	PHE	Sidechain
1	E	480	PHE	Sidechain
1	E	9	TYR	Sidechain

## 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	3671	0	3669	78	0
2	I	33	0	34	11	0
3	E	2	0	0	0	0
4	E	131	0	0	6	0
4	I	1	0	0	0	0
All	All	3838	0	3703	86	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 12.

All (86) 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:252:ILE:HD11	1:E:338:ILE:HD13	1.63	0.79
1:E:218:SER:HB2	1:E:312:ASN:HD21	1.47	0.79
1:E:336:ARG:H	1:E:336:ARG:HD3	1.50	0.77
1:E:336:ARG:N	1:E:336:ARG:HD3	2.00	0.75
1:E:368:LEU:HD21	1:E:398:TRP:HB3	1.72	0.70
1:E:125:LEU:HD13	1:E:161:ALA:HB1	1.74	0.69
1:E:101:GLN:NE2	1:E:464:ARG:HH22	1.91	0.69
1:E:373:THR:HG22	1:E:453:VAL:HG21	1.75	0.67
2:I:4:VAL:O	2:I:4:VAL:HG23	1.97	0.64
1:E:47:LYS:HB3	4:E:571:HOH:O	2.00	0.62
1:E:301:PRO:HG3	1:E:342:ALA:HB2	1.82	0.61
1:E:232:ILE:HG21	4:E:561:HOH:O	1.99	0.61
1:E:375:VAL:HB	1:E:448:LEU:HD22	1.81	0.61
1:E:262:LYS:HE3	1:E:270:MET:HE2	1.83	0.61
2:I:4:VAL:O	2:I:5:ASP:CB	2.48	0.60
1:E:203:ARG:HG3	1:E:229:PHE:O	2.02	0.60
1:E:255:ASP:HB3	1:E:270:MET:HE3	1.83	0.60
1:E:408:ARG:HD3	4:E:583:HOH:O	2.03	0.58
1:E:423:LYS:H	1:E:423:LYS:HD3	1.68	0.58
1:E:356:ASN:HD22	1:E:445:TRP:HE1	1.52	0.58
1:E:257:GLY:O	1:E:331:THR:HG22	2.05	0.57
1:E:273:ASP:OD1	2:I:2:L2O:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:251:GLY:HA3	1:E:302:LEU:HD13	1.88	0.55
1:E:280:ILE:O	1:E:284:ILE:HG12	2.07	0.54
1:E:373:THR:HG23	4:E:498:HOH:O	2.07	0.54
1:E:246:VAL:HG23	1:E:351:PRO:HB3	1.90	0.54
1:E:159:LEU:HG	1:E:290:LEU:HD13	1.92	0.51
1:E:365:ASP:HA	1:E:369:GLY:HA3	1.92	0.51
1:E:31:VAL:O	1:E:34:LYS:HG2	2.10	0.51
2:I:4:VAL:O	2:I:5:ASP:HB3	2.10	0.51
1:E:326:ILE:HG21	1:E:337:LEU:HD21	1.94	0.50
1:E:101:GLN:HE22	1:E:464:ARG:HH22	1.60	0.50
1:E:60:ASP:HB2	4:E:559:HOH:O	2.10	0.50
1:E:71:LYS:HE2	1:E:74:ALA:HB2	1.93	0.50
2:I:4:VAL:O	2:I:4:VAL:CG2	2.56	0.50
1:E:297:VAL:HG12	1:E:299:LEU:HD13	1.94	0.49
1:E:248:VAL:O	1:E:356:ASN:HA	2.13	0.49
1:E:101:GLN:HE22	1:E:464:ARG:HH12	1.60	0.48
2:I:2:L2O:H9	2:I:2:L2O:H3	1.59	0.48
1:E:207:TRP:CZ2	1:E:211:GLN:HG3	2.48	0.48
1:E:365:ASP:O	1:E:369:GLY:HA3	2.13	0.48
1:E:407:THR:HA	1:E:434:ALA:HB1	1.95	0.48
1:E:191:LEU:HG	1:E:198:THR:HG21	1.96	0.47
1:E:201:PHE:HB2	1:E:231:GLU:HB3	1.96	0.47
1:E:188:GLU:HG3	1:E:200:VAL:HG21	1.97	0.47
1:E:34:LYS:HA	1:E:34:LYS:HD3	1.68	0.47
1:E:205:LYS:O	1:E:209:GLU:HG3	2.15	0.47
1:E:395:ASP:OD1	1:E:470:ARG:HD2	2.14	0.47
2:I:3:VAL:HG22	2:I:4:VAL:H	1.79	0.47
1:E:121:GLU:O	1:E:125:LEU:HB2	2.16	0.46
1:E:460:VAL:HG11	1:E:463:LEU:HD22	1.97	0.46
1:E:159:LEU:HD21	1:E:289:LYS:HB3	1.97	0.45
1:E:11:LYS:HG3	1:E:18:PRO:HD3	1.99	0.45
1:E:359:THR:O	2:I:2:L2O:H4	2.16	0.45
1:E:200:VAL:HG13	1:E:232:ILE:HD12	1.99	0.45
1:E:326:ILE:HG21	1:E:337:LEU:CD2	2.47	0.45
1:E:363:ALA:HA	2:I:5:ASP:O	2.17	0.45
1:E:163:GLY:O	1:E:282:SER:HB3	2.17	0.45
1:E:423:LYS:HE3	1:E:424:TYR:CE2	2.52	0.45
2:I:3:VAL:HG22	2:I:4:VAL:N	2.32	0.44
1:E:191:LEU:HD22	1:E:232:ILE:HG13	1.98	0.44
1:E:6:LEU:HD23	1:E:35:LEU:HD11	1.99	0.44
1:E:336:ARG:NH1	1:E:360:LEU:HD22	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:LYS:HG2	1:E:12:GLU:N	2.33	0.44
1:E:38:ILE:HA	1:E:38:ILE:HD12	1.89	0.44
2:I:2:L2O:H8	2:I:2:L2O:O	2.18	0.43
1:E:177:GLU:O	1:E:182:LYS:HG3	2.19	0.43
1:E:230:LEU:HG	1:E:232:ILE:HD13	2.00	0.43
1:E:80:GLU:HB3	1:E:396:ARG:HH21	1.83	0.43
1:E:198:THR:HA	1:E:233:HIS:O	2.19	0.43
1:E:1:THR:HB	1:E:2:LYS:HD2	2.00	0.42
1:E:20:PHE:HE2	1:E:36:ARG:HD2	1.85	0.42
1:E:184:ALA:HB1	1:E:230:LEU:HD13	2.01	0.42
1:E:106:PRO:O	1:E:141:VAL:HA	2.20	0.42
1:E:211:GLN:O	1:E:321:ARG:HG3	2.20	0.41
1:E:218:SER:O	1:E:221:LYS:HG2	2.21	0.41
1:E:345:TYR:O	1:E:348:THR:HB	2.20	0.41
1:E:356:ASN:ND2	1:E:445:TRP:HE1	2.18	0.41
1:E:457:LYS:O	1:E:465:LYS:HG2	2.21	0.41
1:E:333:ALA:HA	1:E:336:ARG:NH2	2.36	0.41
1:E:468:ALA:HB1	1:E:470:ARG:HG3	2.03	0.41
1:E:89:ILE:O	1:E:93:VAL:HG13	2.21	0.40
1:E:219:VAL:HG21	1:E:338:ILE:HD12	2.03	0.40
1:E:212:GLU:HB3	1:E:319:ARG:HH12	1.86	0.40
1:E:11:LYS:HG2	1:E:12:GLU:H	1.86	0.40
1:E:369:GLY:HA2	4:E:609:HOH:O	2.21	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	479/488 (98%)	454 (95%)	21 (4%)	4 (1%)	19	29
2	I	2/4 (50%)	2 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	481/492 (98%)	456 (95%)	21 (4%)	4 (1%)	19	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	369	GLY
1	E	370	SER
1	E	11	LYS
1	E	16	ASP

### 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	387/392 (99%)	337 (87%)	50 (13%)	4	5
2	I	3/3 (100%)	3 (100%)	0	100	100
All	All	390/395 (99%)	340 (87%)	50 (13%)	4	5

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	2	LYS
1	E	11	LYS
1	E	30	LEU
1	E	35	LEU
1	E	39	LEU
1	E	71	LYS
1	E	72	LYS
1	E	73	THR
1	E	82	TRP
1	E	93	VAL
1	E	125	LEU
1	E	138	LYS
1	E	141	VAL
1	E	159	LEU

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Mol	Chain	Res	Type
1	E	166	LEU
1	E	169	ARG
1	E	170	LEU
1	E	189	GLU
1	E	195	SER
1	E	199	ASP
1	E	203	ARG
1	E	216	PHE
1	E	217	LEU
1	E	274	MET
1	E	291	ASP
1	E	292	LEU
1	E	299	LEU
1	E	312	ASN
1	E	336	ARG
1	E	338	ILE
1	E	350	ASN
1	E	353	VAL
1	E	360	LEU
1	E	368	LEU
1	E	375	VAL
1	E	382	LEU
1	E	384	ASN
1	E	385	LYS
1	E	386	LEU
1	E	397	VAL
1	E	405	HIS
1	E	415	LEU
1	E	418	VAL
1	E	423	LYS
1	E	425	ARG
1	E	431	THR
1	E	450	ILE
1	E	455	THR
1	E	463	LEU
1	E	471	PRO

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	83	HIS
1	E	101	GLN

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Mol	Chain	Res	Type
1	E	305	ASN
1	E	312	ASN
1	E	356	ASN
1	E	405	HIS
1	E	409	GLN
1	E	414	GLN

### 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	L2O	I	2	3,2	7,9,10	1.62	1 (14%)	6,11,13	1.11	1 (16%)

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	L2O	I	2	3,2	-	7/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	L2O	C2-C1	-3.93	1.46	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	2	L2O	O1-C6-C1	2.39	111.11	107.31

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	2	L2O	N-C1-C2-C3
2	I	2	L2O	C6-C1-C2-C3
2	I	2	L2O	N-C1-C6-C
2	I	2	L2O	C2-C1-C6-O1
2	I	2	L2O	C2-C1-C6-C
2	I	2	L2O	C1-C2-C3-C4
2	I	2	L2O	C1-C2-C3-C5

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	2	L2O	4	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

## 5.7 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.