



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:49 AM UTC

PDB ID : 1BLL / pdb_00001bll
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

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

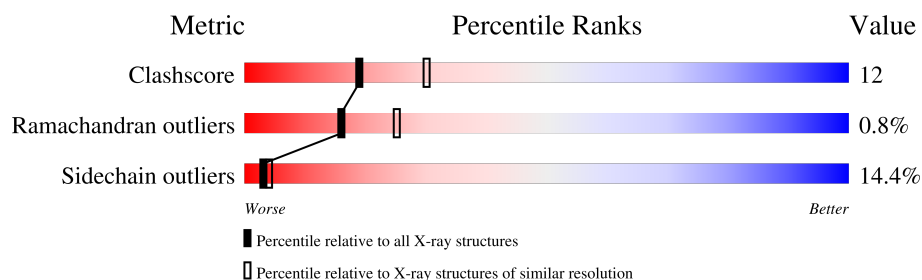
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (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 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	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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is water.

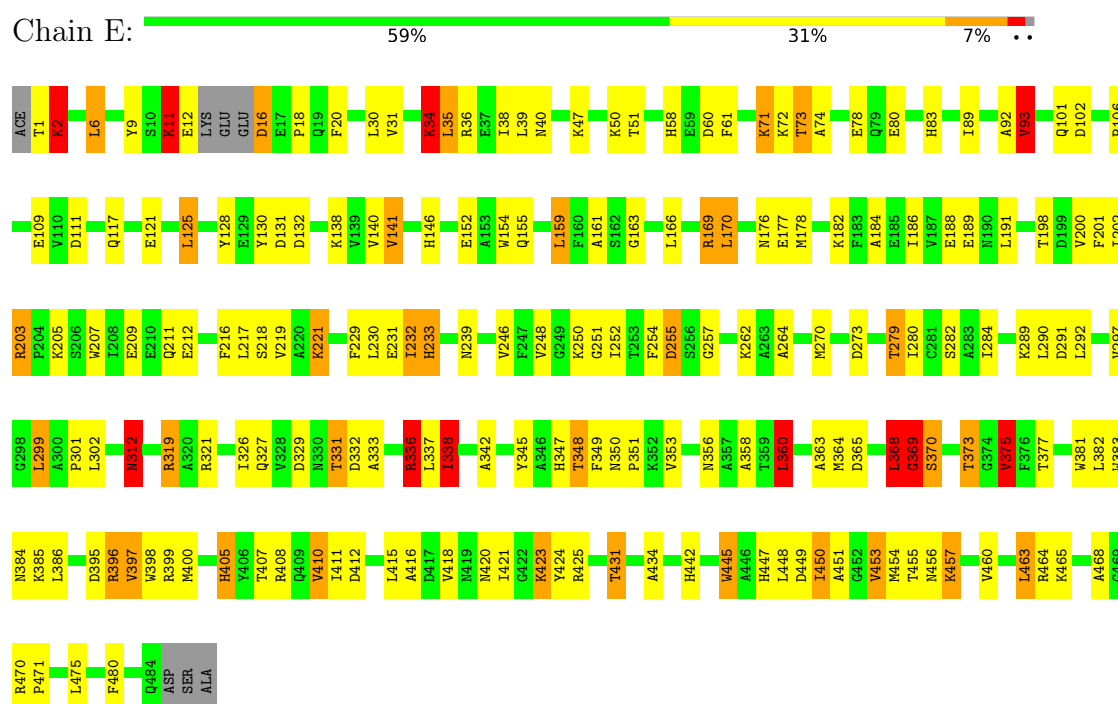
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	131	Total	O	0	0
			131	131		
4	I	1	Total	O	0	0
			1	1		

3 Residue-property plots [i](#)

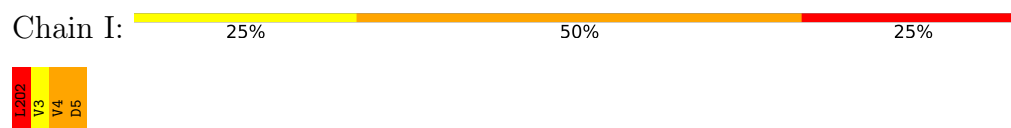
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: 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, α , β , γ	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 ²)	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: L2O, ZN

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	1.06	17/3744 (0.5%)	1.87	85/5068 (1.7%)
2	I	0.80	0/22	2.37	2/28 (7.1%)
All	All	1.06	17/3766 (0.5%)	1.87	87/5096 (1.7%)

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
2	I	0	1
All	All	0	7

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	93	VAL	CA-CB	8.76	1.65	1.54
1	E	405	HIS	CD2-NE2	-7.33	1.29	1.37
1	E	447	HIS	CD2-NE2	-7.09	1.30	1.37
1	E	375	VAL	CA-CB	7.02	1.63	1.54
1	E	83	HIS	CD2-NE2	-6.93	1.30	1.37
1	E	405	HIS	CG-ND1	-6.90	1.30	1.38
1	E	347	HIS	CD2-NE2	-6.78	1.30	1.37
1	E	370	SER	CA-CB	6.69	1.64	1.53
1	E	233	HIS	CD2-NE2	-6.59	1.30	1.37
1	E	146	HIS	CD2-NE2	-6.44	1.30	1.37
1	E	58	HIS	CD2-NE2	-6.34	1.30	1.37
1	E	233	HIS	CG-ND1	-5.90	1.31	1.38
1	E	442	HIS	CD2-NE2	-5.85	1.31	1.37
1	E	58	HIS	CG-ND1	-5.69	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	453	VAL	CA-CB	5.62	1.61	1.54
1	E	146	HIS	CG-ND1	-5.39	1.32	1.38
1	E	347	HIS	CG-ND1	-5.11	1.32	1.38

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	370	SER	CA-CB-OG	12.49	136.08	111.10
1	E	416	ALA	N-CA-C	9.88	123.92	109.69
1	E	11	LYS	N-CA-C	9.66	131.37	110.80
1	E	450	ILE	N-CA-CB	-9.28	95.92	111.23
1	E	410	VAL	N-CA-CB	-8.44	100.70	112.35
1	E	369	GLY	O-C-N	8.38	133.60	122.70
1	E	312	ASN	CA-CB-CG	8.30	120.90	112.60
1	E	360	LEU	N-CA-C	8.23	121.44	111.40
1	E	397	VAL	N-CA-CB	-8.02	97.09	111.93
1	E	16	ASP	CA-CB-CG	7.83	120.43	112.60
2	I	4	VAL	CB-CA-C	-7.67	100.64	111.38
1	E	109	GLU	CA-CB-CG	-7.59	98.91	114.10
1	E	450	ILE	CA-CB-CG1	-7.53	97.61	110.40
1	E	410	VAL	CB-CA-C	7.52	119.08	110.88
1	E	396	ARG	N-CA-C	7.29	120.27	110.35
1	E	338	ILE	CA-CB-CG1	-7.24	98.08	110.40
1	E	450	ILE	CA-CB-CG2	7.15	122.66	110.50
1	E	40	ASN	OD1-CG-ND2	-6.96	115.64	122.60
1	E	396	ARG	CB-CG-CD	-6.93	95.37	111.30
1	E	384	ASN	CA-CB-CG	-6.85	105.75	112.60
1	E	332	ASP	CA-CB-CG	6.76	119.36	112.60
1	E	338	ILE	CA-CB-CG2	6.75	121.98	110.50
1	E	132	ASP	N-CA-C	6.74	121.10	112.34
1	E	176	ASN	CA-CB-CG	6.65	119.25	112.60
1	E	397	VAL	CB-CA-C	6.65	121.33	110.69
1	E	152	GLU	CA-CB-CG	6.56	127.22	114.10
1	E	442	HIS	CA-C-N	6.56	127.12	120.04
1	E	442	HIS	C-N-CA	6.56	127.12	120.04
1	E	348	THR	CA-CB-OG1	-6.50	99.85	109.60
1	E	34	LYS	N-CA-C	6.47	119.15	111.71
1	E	155	GLN	OE1-CD-NE2	-6.45	116.16	122.60
1	E	50	LYS	CG-CD-CE	6.32	125.83	111.30
1	E	169	ARG	CA-CB-CG	6.25	126.59	114.10
1	E	216	PHE	CA-CB-CG	6.24	120.04	113.80
1	E	457	LYS	N-CA-C	-6.23	102.05	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	442	HIS	N-CA-C	6.22	116.75	109.60
1	E	456	ASN	OD1-CG-ND2	-6.10	116.50	122.60
1	E	329	ASP	N-CA-C	6.07	118.86	111.82
1	E	239	ASN	CA-C-O	6.04	126.82	120.36
1	E	73	THR	N-CA-C	5.68	119.83	113.02
1	E	383	TRP	CG-CD2-CE3	5.67	139.57	133.90
1	E	381	TRP	CG-CD2-CE3	5.66	139.56	133.90
1	E	383	TRP	CB-CG-CD1	-5.66	118.42	126.90
1	E	399	ARG	CB-CG-CD	-5.63	98.35	111.30
1	E	336	ARG	CA-CB-CG	5.63	125.36	114.10
1	E	368	LEU	CA-C-O	5.59	126.54	119.78
1	E	454	MET	CG-SD-CE	-5.57	88.66	100.90
1	E	431	THR	N-CA-CB	-5.56	101.93	110.16
1	E	451	ALA	N-CA-C	5.55	117.33	111.28
1	E	2	LYS	N-CA-C	5.54	118.30	109.65
1	E	400	MET	CA-C-N	5.49	125.66	119.90
1	E	400	MET	C-N-CA	5.49	125.66	119.90
1	E	2	LYS	CA-CB-CG	5.48	125.05	114.10
1	E	40	ASN	CB-CG-ND2	5.48	124.62	116.40
1	E	117	GLN	CA-CB-CG	-5.46	103.19	114.10
1	E	445	TRP	CG-CD2-CE3	5.41	139.31	133.90
1	E	412	ASP	CA-CB-CG	5.39	118.00	112.60
1	E	102	ASP	CA-CB-CG	5.38	117.98	112.60
1	E	336	ARG	NE-CZ-NH2	-5.36	114.37	119.20
1	E	291	ASP	CA-CB-CG	-5.36	107.24	112.60
1	E	381	TRP	CB-CG-CD1	-5.34	118.89	126.90
2	I	4	VAL	CA-C-O	-5.34	115.95	121.93
1	E	410	VAL	N-CA-C	-5.34	107.18	113.42
1	E	348	THR	CA-CB-CG2	5.32	119.55	110.50
1	E	203	ARG	CB-CG-CD	5.32	123.53	111.30
1	E	111	ASP	CA-CB-CG	5.31	117.91	112.60
1	E	221	LYS	N-CA-C	5.30	117.97	111.82
1	E	186	ILE	N-CA-C	-5.30	105.68	110.82
1	E	255	ASP	CA-CB-CG	5.26	117.86	112.60
1	E	279	THR	N-CA-C	5.26	117.42	111.11
1	E	358	ALA	N-CA-C	5.23	116.36	108.46
1	E	338	ILE	N-CA-CB	-5.22	102.75	110.58
1	E	450	ILE	CB-CA-C	5.20	119.81	111.29
1	E	202	ILE	N-CA-C	-5.19	98.54	109.34
1	E	450	ILE	N-CA-C	5.19	120.14	109.34
1	E	331	THR	N-CA-CB	-5.18	101.78	110.39
1	E	338	ILE	O-C-N	5.18	127.16	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	154	TRP	CE2-CD2-CG	-5.09	101.09	107.20
1	E	131	ASP	CA-CB-CG	5.08	117.69	112.60
1	E	92	ALA	CA-C-O	-5.06	115.49	120.70
1	E	319	ARG	N-CA-C	5.03	116.94	108.73
1	E	327	GLN	OE1-CD-NE2	-5.03	117.58	122.60
1	E	264	ALA	N-CA-C	5.02	116.76	111.28
1	E	377	THR	CA-CB-OG1	-5.02	102.06	109.60
1	E	420	ASN	CA-CB-CG	5.02	117.62	112.60
1	E	61	PHE	CA-C-N	5.00	124.69	119.64
1	E	61	PHE	C-N-CA	5.00	124.69	119.64

There are no chirality outliers.

All (7) 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
2	I	2	L2O	Mainchain

5.2 Too-close contacts [i](#)

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	80	0
2	I	33	0	29	9	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	3698	87	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 (87) 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:HD3	1:E:336:ARG:H	1.50	0.77
1:E:336:ARG:HD3	1:E:336:ARG:N	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
1:E:262:LYS:HE3	1:E:270:MET:HE2	1.80	0.63
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
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:408:ARG:HD3	4:E:583:HOH:O	2.03	0.58
1:E:423:LYS:HD3	1:E:423:LYS:H	1.68	0.58
1:E:356:ASN:HD22	1:E:445:TRP:HE1	1.52	0.58
2:I:4:VAL:O	2:I:4:VAL:HG23	1.97	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
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:364:MET:HE3	1:E:449:ASP:HB3	1.88	0.53
1:E:255:ASP:HB3	1:E:270:MET:HE3	1.91	0.52
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: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
1:E:101:GLN:HE22	1:E:464:ARG:HH22	1.60	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:34:LYS:HD3	1:E:34:LYS:HA	1.68	0.47
1:E:188:GLU:HG3	1:E:200:VAL:HG21	1.97	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
1:E:170:LEU:HA	1:E:178:MET:HE3	1.95	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:11:LYS:HZ2	1:E:11:LYS:HB3	1.81	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:6:LEU:HD23	1:E:35:LEU:HD11	1.99	0.44
1:E:191:LEU:HD22	1:E:232:ILE:HG13	1.98	0.44
1:E:336:ARG:NH1	1:E:360:LEU:HD22	2.32	0.44
1:E:11:LYS:HG2	1:E:12:GLU:N	2.33	0.44
1:E:38:ILE:HD12	1:E:38:ILE:HA	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:80:GLU:HB3	1:E:396:ARG:HH21	1.83	0.43
1:E:230:LEU:HG	1:E:232:ILE:HD13	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:ILE:O	1:E:93:VAL:HG13	2.21	0.40
1:E:212:GLU:HB3	1:E:319:ARG:HH12	1.86	0.40
1:E:219:VAL:HG21	1:E:338:ILE:HD12	2.03	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%)	16	25
2	I	2/4 (50%)	2 (100%)	0	0	100	100
All	All	481/492 (98%)	456 (95%)	21 (4%)	4 (1%)	16	25

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	387/392 (99%)	332 (86%)	55 (14%)	3	4
2	I	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	390/395 (99%)	334 (86%)	56 (14%)	3	4

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	2	LYS
1	E	6	LEU
1	E	11	LYS
1	E	30	LEU
1	E	34	LYS
1	E	35	LEU
1	E	39	LEU
1	E	51	THR
1	E	71	LYS
1	E	72	LYS
1	E	73	THR
1	E	78	GLU
1	E	93	VAL
1	E	125	LEU
1	E	138	LYS
1	E	140	VAL
1	E	141	VAL
1	E	159	LEU
1	E	166	LEU
1	E	169	ARG
1	E	170	LEU
1	E	189	GLU
1	E	217	LEU
1	E	232	ILE
1	E	250	LYS
1	E	279	THR
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

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Mol	Chain	Res	Type
1	E	373	THR
1	E	375	VAL
1	E	382	LEU
1	E	385	LYS
1	E	386	LEU
1	E	397	VAL
1	E	405	HIS
1	E	410	VAL
1	E	411	ILE
1	E	415	LEU
1	E	418	VAL
1	E	421	ILE
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
1	E	475	LEU
2	I	5	ASP

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	83	HIS
1	E	101	GLN
1	E	305	ASN
1	E	312	ASN
1	E	356	ASN
1	E	384	ASN
1	E	405	HIS

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	1.64	1 (14%)	6,11,13	1.06	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-CA	-3.97	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-CA	2.26	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	C3-C2-CA-N
2	I	2	L2O	C3-C2-CA-C6
2	I	2	L2O	C-C6-CA-N
2	I	2	L2O	O1-C6-CA-C2
2	I	2	L2O	CA-C2-C3-C4
2	I	2	L2O	CA-C2-C3-C5
2	I	2	L2O	C-C6-CA-C2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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.