



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:17 AM UTC

PDB ID : 1BPM / pdb_00001bpm
Title : DIFFERENTIATION AND IDENTIFICATION OF THE TWO CATALYTIC METAL BINDING SITES IN BOVINE LENS LEUCINE AMINOPEPTIDASE BY X-RAY CRYSTALLOGRAPHY
Authors : Kim, H.; Lipscomb, W.N.
Deposited on : 1993-03-02
Resolution : 2.90 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

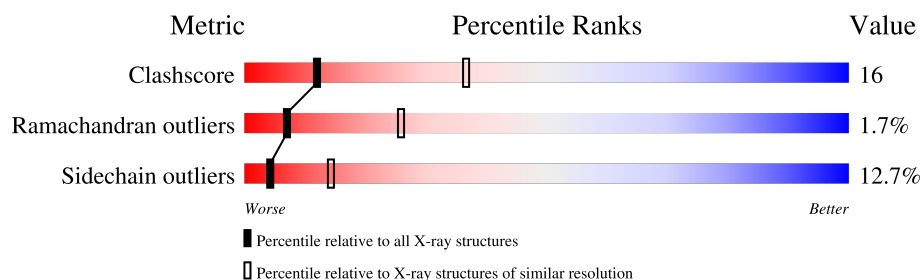
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	A	487	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3673 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	A	481	Total	C	N	O	S	0	0	0
			3671	2321	635	697	18			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	PRO	SER	conflict	UNP P00727

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

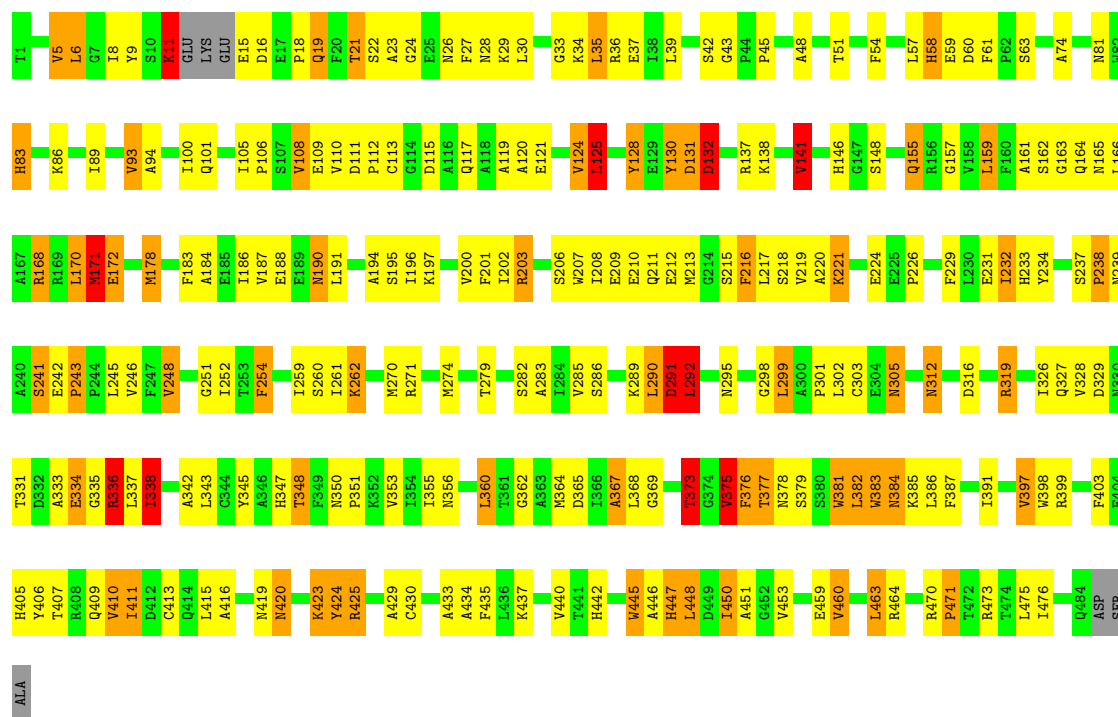
3 Residue-property plots

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: LEUCINE AMINOPEPTIDASE

Chain A: 



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	129.10Å 129.10Å 120.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.189 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3673	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: ZN, MG

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	A	1.15	20/3744 (0.5%)	2.03	115/5068 (2.3%)

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	A	0	6

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	373	THR	CA-CB	9.24	1.64	1.53
1	A	83	HIS	CD2-NE2	-7.60	1.29	1.37
1	A	110	VAL	CA-CB	7.51	1.64	1.54
1	A	233	HIS	CD2-NE2	-7.11	1.30	1.37
1	A	146	HIS	CD2-NE2	-6.83	1.30	1.37
1	A	447	HIS	CD2-NE2	-6.49	1.30	1.37
1	A	93	VAL	CA-CB	6.49	1.62	1.54
1	A	347	HIS	CD2-NE2	-6.44	1.30	1.37
1	A	405	HIS	CD2-NE2	-6.41	1.30	1.37
1	A	442	HIS	CG-ND1	-6.35	1.31	1.38
1	A	58	HIS	CD2-NE2	-6.32	1.30	1.37
1	A	233	HIS	CG-ND1	-6.14	1.31	1.38
1	A	336	ARG	NE-CZ	6.06	1.39	1.33
1	A	196	ILE	CA-CB	5.97	1.61	1.54
1	A	450	ILE	CA-CB	5.60	1.61	1.54
1	A	447	HIS	CG-ND1	-5.32	1.32	1.38
1	A	58	HIS	CG-ND1	-5.23	1.32	1.38
1	A	375	VAL	CA-CB	5.19	1.61	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	HIS	CG-ND1	-5.08	1.32	1.38
1	A	141	VAL	CA-CB	5.01	1.61	1.54

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	ASN	CA-CB-CG	-10.73	101.87	112.60
1	A	360	LEU	N-CA-C	9.98	122.11	111.03
1	A	261	ILE	N-CA-C	9.92	121.99	108.89
1	A	460	VAL	N-CA-C	-9.66	96.64	108.05
1	A	420	ASN	CA-CB-CG	9.54	122.14	112.60
1	A	11	LYS	N-CA-C	9.39	123.22	110.55
1	A	60	ASP	CA-CB-CG	8.40	121.00	112.60
1	A	327	GLN	OE1-CD-NE2	-8.02	114.58	122.60
1	A	254	PHE	CA-CB-CG	-7.96	105.84	113.80
1	A	450	ILE	N-CA-CB	-7.80	101.91	112.28
1	A	83	HIS	N-CA-C	-7.75	99.00	110.48
1	A	397	VAL	N-CA-CB	-7.57	99.03	111.45
1	A	348	THR	CA-CB-OG1	-7.54	98.30	109.60
1	A	42	SER	N-CA-C	7.50	119.09	111.07
1	A	327	GLN	CG-CD-NE2	7.46	127.60	116.40
1	A	131	ASP	CA-CB-CG	7.45	120.05	112.60
1	A	58	HIS	CA-CB-CG	-7.27	106.53	113.80
1	A	335	GLY	N-CA-C	-7.07	103.73	112.77
1	A	245	LEU	N-CA-C	-7.02	98.29	109.59
1	A	58	HIS	CA-C-O	7.01	128.72	120.66
1	A	424	TYR	N-CA-C	6.92	119.92	109.41
1	A	243	PRO	CB-CA-C	6.83	117.59	111.17
1	A	216	PHE	CA-CB-CG	6.62	120.42	113.80
1	A	292	LEU	CA-C-N	6.59	128.08	119.84
1	A	292	LEU	C-N-CA	6.59	128.08	119.84
1	A	291	ASP	O-C-N	6.58	131.34	122.59
1	A	416	ALA	N-CA-C	6.50	124.65	110.80
1	A	316	ASP	N-CA-C	6.49	120.07	109.76
1	A	35	LEU	N-CA-C	-6.47	102.72	112.04
1	A	425	ARG	CA-CB-CG	6.46	127.03	114.10
1	A	410	VAL	N-CA-CB	-6.42	99.83	110.56
1	A	109	GLU	CA-CB-CG	-6.42	101.27	114.10
1	A	384	ASN	O-C-N	6.35	128.85	122.12
1	A	146	HIS	N-CA-C	-6.35	98.85	109.07
1	A	338	ILE	N-CA-C	-6.28	104.22	110.62
1	A	224	GLU	N-CA-C	-6.26	105.28	113.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	411	ILE	N-CA-C	6.25	118.91	111.09
1	A	403	PHE	CA-CB-CG	6.24	120.04	113.80
1	A	128	TYR	N-CA-C	6.23	119.03	110.24
1	A	48	ALA	N-CA-C	6.14	119.26	110.24
1	A	286	SER	CA-C-O	-6.13	114.39	120.70
1	A	117	GLN	CB-CG-CD	6.10	122.97	112.60
1	A	336	ARG	NE-CZ-NH1	6.07	127.57	121.50
1	A	338	ILE	CA-CB-CG2	5.99	120.68	110.50
1	A	397	VAL	CB-CA-C	5.94	120.99	110.71
1	A	423	LYS	CG-CD-CE	5.93	124.94	111.30
1	A	168	ARG	NE-CZ-NH2	-5.92	113.87	119.20
1	A	172	GLU	N-CA-C	5.90	118.47	111.33
1	A	329	ASP	N-CA-C	5.89	120.20	112.89
1	A	115	ASP	CA-CB-CG	-5.88	106.72	112.60
1	A	348	THR	CA-CB-CG2	5.87	120.47	110.50
1	A	312	ASN	OD1-CG-ND2	-5.84	116.76	122.60
1	A	206	SER	N-CA-C	5.80	117.60	111.28
1	A	23	ALA	CA-C-N	5.80	126.38	119.94
1	A	23	ALA	C-N-CA	5.80	126.38	119.94
1	A	262	LYS	N-CA-C	5.79	117.81	110.33
1	A	83	HIS	CA-CB-CG	-5.78	108.02	113.80
1	A	81	ASN	CA-CB-CG	5.78	118.38	112.60
1	A	243	PRO	O-C-N	-5.78	118.44	121.15
1	A	319	ARG	N-CA-C	5.75	118.17	107.99
1	A	451	ALA	N-CA-C	5.75	119.39	112.38
1	A	89	ILE	O-C-N	5.73	127.73	121.83
1	A	190	ASN	CB-CG-ND2	5.71	124.96	116.40
1	A	29	LYS	CA-C-N	5.70	127.92	120.28
1	A	29	LYS	C-N-CA	5.70	127.92	120.28
1	A	336	ARG	CA-CB-CG	5.67	125.44	114.10
1	A	373	THR	CA-C-O	5.64	126.61	120.58
1	A	124	VAL	CA-C-O	-5.63	113.72	121.15
1	A	178	MET	N-CA-CB	-5.62	102.49	110.58
1	A	168	ARG	CA-C-O	-5.60	114.48	120.42
1	A	295	ASN	CA-CB-CG	5.60	118.20	112.60
1	A	63	SER	N-CA-C	5.59	117.76	108.20
1	A	108	VAL	O-C-N	5.58	129.14	123.00
1	A	105	ILE	CA-C-N	5.58	125.67	119.87
1	A	105	ILE	C-N-CA	5.58	125.67	119.87
1	A	171	MET	O-C-N	5.57	128.57	122.11
1	A	164	GLN	N-CA-C	-5.54	104.64	111.40
1	A	209	GLU	CA-C-N	5.53	128.24	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	GLU	C-N-CA	5.53	128.24	120.28
1	A	410	VAL	CB-CA-C	5.53	119.65	112.24
1	A	162	SER	N-CA-C	5.51	117.37	111.36
1	A	155	GLN	OE1-CD-NE2	-5.50	117.09	122.60
1	A	226	PRO	N-CA-C	5.48	117.39	110.70
1	A	261	ILE	N-CA-CB	-5.48	104.56	110.53
1	A	43	GLY	CA-C-N	5.47	126.01	120.38
1	A	43	GLY	C-N-CA	5.47	126.01	120.38
1	A	125	LEU	CA-C-O	5.45	126.52	120.63
1	A	336	ARG	CB-CG-CD	5.43	123.80	111.30
1	A	220	ALA	N-CA-C	5.39	117.91	111.71
1	A	383	TRP	CG-CD2-CE3	5.38	139.28	133.90
1	A	283	ALA	CA-C-O	-5.32	115.24	120.82
1	A	5	VAL	CA-C-O	5.29	126.85	120.66
1	A	74	ALA	CA-C-O	-5.29	115.09	120.80
1	A	445	TRP	CG-CD2-CE3	5.25	139.15	133.90
1	A	221	LYS	N-CA-C	5.25	118.78	112.38
1	A	241	SER	N-CA-C	5.23	121.95	110.80
1	A	94	ALA	O-C-N	5.21	127.64	122.12
1	A	238	PRO	CA-C-N	-5.21	115.27	122.30
1	A	238	PRO	C-N-CA	-5.21	115.27	122.30
1	A	197	LYS	CA-CB-CG	5.18	124.45	114.10
1	A	132	ASP	N-CA-C	5.17	121.82	110.80
1	A	312	ASN	CB-CG-ND2	5.12	124.08	116.40
1	A	159	LEU	CA-C-N	5.12	127.45	120.54
1	A	159	LEU	C-N-CA	5.12	127.45	120.54
1	A	442	HIS	CA-C-N	5.11	126.12	120.45
1	A	442	HIS	C-N-CA	5.11	126.12	120.45
1	A	381	TRP	O-C-N	5.11	127.33	122.07
1	A	210	GLU	CA-CB-CG	5.05	124.20	114.10
1	A	45	PRO	N-CA-C	5.05	119.24	111.57
1	A	29	LYS	O-C-N	5.04	127.46	122.12
1	A	383	TRP	CB-CG-CD1	-5.03	119.36	126.90
1	A	248	VAL	O-C-N	-5.02	117.59	122.97
1	A	221	LYS	CA-CB-CG	5.01	124.12	114.10
1	A	59	GLU	CB-CG-CD	5.01	121.11	112.60
1	A	442	HIS	N-CA-C	5.00	116.98	110.08

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	TYR	Sidechain
1	A	130	TYR	Sidechain
1	A	254	PHE	Sidechain
1	A	406	TYR	Sidechain
1	A	424	TYR	Sidechain
1	A	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	A	3671	0	3669	115	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
All	All	3673	0	3669	115	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 16.

All (115) 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:A:171:MET:HA	1:A:274:MET:SD	2.25	0.76
1:A:120:ALA:HB3	1:A:157:GLY:HA3	1.70	0.73
1:A:373:THR:HG22	1:A:453:VAL:HG11	1.69	0.73
1:A:188:GLU:HB2	1:A:200:VAL:HG11	1.74	0.70
1:A:54:PHE:HB3	1:A:57:LEU:HD21	1.75	0.68
1:A:183:PHE:O	1:A:187:VAL:HG23	1.96	0.66
1:A:285:VAL:O	1:A:289:LYS:HD3	1.95	0.65
1:A:336:ARG:H	1:A:336:ARG:HH11	1.43	0.65
1:A:106:PRO:O	1:A:141:VAL:HA	1.97	0.65
1:A:303:CYS:SG	1:A:338:ILE:HD11	2.36	0.64
1:A:201:PHE:HB2	1:A:231:GLU:HB3	1.81	0.62
1:A:101:GLN:HE22	1:A:464:ARG:HH22	1.47	0.62
1:A:121:GLU:HA	1:A:161:ALA:HB2	1.80	0.62
1:A:409:GLN:HG2	1:A:423:LYS:HD3	1.82	0.61
1:A:232:ILE:HB	1:A:298:GLY:HA3	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LYS:HA	1:A:37:GLU:HB3	1.82	0.59
1:A:163:GLY:O	1:A:282:SER:HB3	2.02	0.59
1:A:252:ILE:HD11	1:A:338:ILE:HD13	1.84	0.59
1:A:21:THR:HG21	1:A:113:CYS:HA	1.84	0.59
1:A:121:GLU:O	1:A:125:LEU:HB2	2.02	0.59
1:A:124:VAL:HG12	1:A:165:ASN:HD21	1.68	0.58
1:A:375:VAL:CG1	1:A:397:VAL:HG22	2.34	0.57
1:A:213:MET:HE1	1:A:229:PHE:CE2	2.41	0.56
1:A:246:VAL:HG23	1:A:351:PRO:HB3	1.88	0.56
1:A:18:PRO:HG2	1:A:36:ARG:HH22	1.71	0.56
1:A:413:CYS:SG	1:A:419:ASN:HB2	2.45	0.56
1:A:373:THR:HG21	1:A:471:PRO:HB3	1.88	0.55
1:A:460:VAL:HG11	1:A:463:LEU:HD22	1.88	0.55
1:A:101:GLN:HE22	1:A:464:ARG:NH2	2.04	0.55
1:A:184:ALA:HB1	1:A:202:ILE:HG12	1.88	0.55
1:A:420:ASN:HA	1:A:435:PHE:CE2	2.42	0.55
1:A:170:LEU:HA	1:A:178:MET:HE3	1.88	0.54
1:A:252:ILE:HA	1:A:303:CYS:O	2.07	0.54
1:A:243:PRO:HB2	1:A:350:ASN:O	2.07	0.54
1:A:101:GLN:NE2	1:A:464:ARG:HH22	2.06	0.54
1:A:260:SER:HB2	1:A:331:THR:HB	1.89	0.54
1:A:368:LEU:HD21	1:A:398:TRP:HB3	1.89	0.54
1:A:299:LEU:HD21	1:A:345:TYR:HD2	1.73	0.53
1:A:11:LYS:HB3	1:A:11:LYS:HZ3	1.73	0.53
1:A:375:VAL:HG11	1:A:397:VAL:HG22	1.90	0.53
1:A:387:PHE:CZ	1:A:391:ILE:HD11	2.43	0.53
1:A:216:PHE:HE1	1:A:303:CYS:HB3	1.74	0.53
1:A:360:LEU:HD12	1:A:447:HIS:NE2	2.23	0.52
1:A:191:LEU:O	1:A:194:ALA:HB3	2.10	0.52
1:A:120:ALA:O	1:A:124:VAL:HG23	2.10	0.51
1:A:364:MET:HE2	1:A:429:ALA:CB	2.40	0.51
1:A:207:TRP:CH2	1:A:211:GLN:HG3	2.45	0.51
1:A:381:TRP:O	1:A:385:LYS:HD3	2.11	0.51
1:A:262:LYS:HE3	1:A:270:MET:HG3	1.93	0.51
1:A:6:LEU:HG	1:A:24:GLY:HA2	1.94	0.50
1:A:22:SER:O	1:A:26:ASN:HB2	2.12	0.50
1:A:125:LEU:HD13	1:A:161:ALA:HB1	1.95	0.49
1:A:203:ARG:HD3	1:A:207:TRP:CE2	2.47	0.49
1:A:305:ASN:OD1	1:A:334:GLU:HG3	2.12	0.49
1:A:218:SER:O	1:A:221:LYS:HG2	2.13	0.48
1:A:382:LEU:HD13	1:A:446:ALA:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:VAL:HG12	1:A:355:ILE:HG13	1.95	0.48
1:A:375:VAL:HB	1:A:448:LEU:HD22	1.95	0.48
1:A:212:GLU:HB3	1:A:319:ARG:HH12	1.78	0.48
1:A:279:THR:HG21	1:A:471:PRO:HD2	1.95	0.48
1:A:356:ASN:HD22	1:A:445:TRP:HE1	1.62	0.48
1:A:83:HIS:HD2	1:A:86:LYS:H	1.62	0.47
1:A:376:PHE:CE2	1:A:430:CYS:HA	2.49	0.47
1:A:383:TRP:CZ3	1:A:397:VAL:HG13	2.50	0.47
1:A:5:VAL:O	1:A:111:ASP:HB2	2.14	0.47
1:A:132:ASP:HA	1:A:137:ARG:NH1	2.29	0.47
1:A:93:VAL:HG21	1:A:119:ALA:O	2.14	0.47
1:A:234:TYR:OH	1:A:291:ASP:HA	2.15	0.46
1:A:11:LYS:HG2	1:A:15:GLU:H	1.81	0.46
1:A:100:ILE:HG21	1:A:108:VAL:HB	1.98	0.46
1:A:237:SER:HA	1:A:238:PRO:HD2	1.53	0.46
1:A:301:PRO:HG3	1:A:342:ALA:HB2	1.97	0.45
1:A:362:GLY:O	1:A:365:ASP:HB3	2.15	0.45
1:A:28:ASN:ND2	1:A:33:GLY:HA2	2.32	0.45
1:A:251:GLY:HA3	1:A:302:LEU:HD13	1.99	0.45
1:A:248:VAL:HA	1:A:299:LEU:O	2.17	0.45
1:A:106:PRO:C	1:A:141:VAL:HA	2.42	0.45
1:A:207:TRP:O	1:A:211:GLN:HG2	2.17	0.44
1:A:407:THR:HA	1:A:434:ALA:HB1	1.99	0.44
1:A:8:ILE:HG13	1:A:19:GLN:O	2.17	0.44
1:A:326:ILE:HD13	1:A:337:LEU:HD23	1.99	0.44
1:A:208:ILE:HG23	1:A:213:MET:SD	2.57	0.44
1:A:232:ILE:HB	1:A:298:GLY:CA	2.47	0.44
1:A:343:LEU:HD13	1:A:440:VAL:HG23	1.99	0.44
1:A:259:ILE:HD13	1:A:259:ILE:HA	1.63	0.44
1:A:364:MET:O	1:A:367:ALA:HB3	2.17	0.44
1:A:373:THR:O	1:A:397:VAL:HA	2.18	0.44
1:A:290:LEU:HB3	1:A:292:LEU:HD13	2.01	0.43
1:A:83:HIS:CD2	1:A:86:LYS:H	2.37	0.43
1:A:27:PHE:HZ	1:A:58:HIS:HB2	1.84	0.43
1:A:58:HIS:HB3	1:A:61:PHE:HB2	2.01	0.43
1:A:333:ALA:HA	1:A:336:ARG:CZ	2.48	0.43
1:A:101:GLN:O	1:A:101:GLN:HG2	2.20	0.42
1:A:215:SER:OG	1:A:337:LEU:HB3	2.19	0.42
1:A:229:PHE:CZ	1:A:299:LEU:HG	2.55	0.42
1:A:131:ASP:HB3	1:A:137:ARG:HD3	2.02	0.42
1:A:375:VAL:HG12	1:A:397:VAL:HG22	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ARG:O	1:A:172:GLU:HB2	2.19	0.42
1:A:453:VAL:HB	1:A:470:ARG:HB2	2.01	0.42
1:A:111:ASP:HB3	1:A:113:CYS:SG	2.59	0.42
1:A:252:ILE:CD1	1:A:338:ILE:HD13	2.49	0.41
1:A:125:LEU:HG	1:A:463:LEU:HD11	2.02	0.41
1:A:473:ARG:HA	1:A:476:ILE:HD12	2.02	0.41
1:A:183:PHE:CE1	1:A:187:VAL:HG21	2.56	0.41
1:A:186:ILE:HG22	1:A:190:ASN:HD22	1.85	0.41
1:A:215:SER:O	1:A:219:VAL:HG23	2.21	0.41
1:A:360:LEU:HD12	1:A:447:HIS:CE1	2.56	0.41
1:A:379:SER:HB3	1:A:382:LEU:HB2	2.03	0.41
1:A:433:ALA:HB2	1:A:447:HIS:HD2	1.85	0.41
1:A:437:LYS:HB2	1:A:445:TRP:CZ3	2.56	0.41
1:A:246:VAL:CG2	1:A:351:PRO:HB3	2.50	0.40
1:A:377:THR:C	1:A:379:SER:H	2.29	0.40
1:A:111:ASP:HA	1:A:112:PRO:HD2	1.94	0.40
1:A:239:ASN:OD1	1:A:242:GLU:HG2	2.22	0.40
1:A:328:VAL:O	1:A:328:VAL:HG12	2.22	0.40

There are no symmetry-related clashes.

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	A	479/487 (98%)	432 (90%)	39 (8%)	8 (2%)	7	26

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	TYR
1	A	132	ASP
1	A	241	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	16	ASP
1	A	148	SER
1	A	367	ALA
1	A	378	ASN
1	A	369	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	A	387/392 (99%)	338 (87%)	49 (13%)	4 14

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	11	LYS
1	A	19	GLN
1	A	21	THR
1	A	30	LEU
1	A	35	LEU
1	A	39	LEU
1	A	51	THR
1	A	125	LEU
1	A	138	LYS
1	A	141	VAL
1	A	155	GLN
1	A	159	LEU
1	A	166	LEU
1	A	170	LEU
1	A	171	MET
1	A	195	SER
1	A	203	ARG
1	A	217	LEU
1	A	232	ILE
1	A	271	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	290	LEU
1	A	291	ASP
1	A	292	LEU
1	A	299	LEU
1	A	305	ASN
1	A	312	ASN
1	A	334	GLU
1	A	336	ARG
1	A	338	ILE
1	A	348	THR
1	A	373	THR
1	A	375	VAL
1	A	376	PHE
1	A	377	THR
1	A	382	LEU
1	A	384	ASN
1	A	386	LEU
1	A	399	ARG
1	A	410	VAL
1	A	411	ILE
1	A	415	LEU
1	A	425	ARG
1	A	448	LEU
1	A	450	ILE
1	A	459	GLU
1	A	463	LEU
1	A	471	PRO
1	A	475	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	81	ASN
1	A	83	HIS
1	A	88	ASN
1	A	101	GLN
1	A	165	ASN
1	A	190	ASN
1	A	312	ASN
1	A	347	HIS
1	A	356	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	419	ASN
1	A	447	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

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.