



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:58 am GMT

PDB ID : 1BPN
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

<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
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) : recalc28949

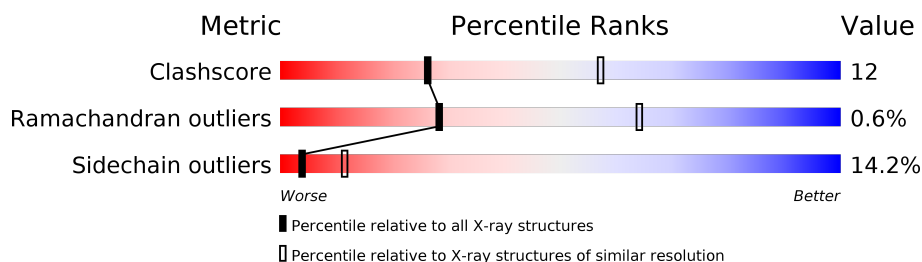
1 Overall quality at a glance

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	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (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 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	A	487	

2 Entry composition

There are 2 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 ZINC ION (three-letter code: ZN) (formula: Zn).

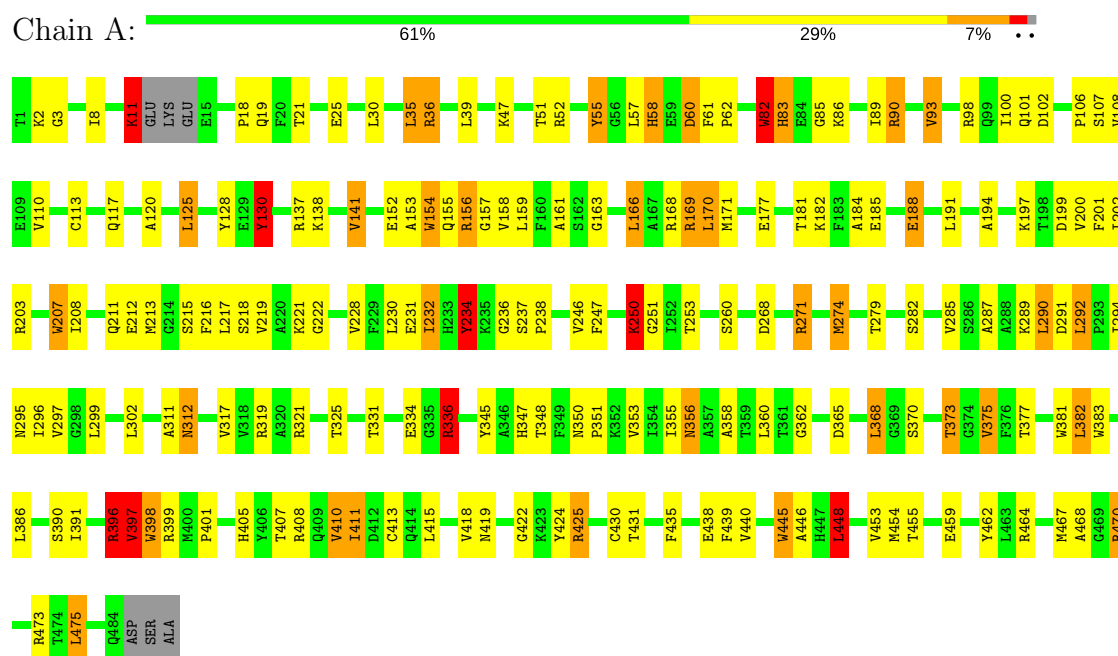
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

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 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: LEUCINE AMINOPEPTIDASE



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	129.80Å 129.80Å 120.70Å 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}	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3673	wwPDB-VP
Average B, all atoms (Å ²)	10.0	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

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	0.86	0/3744	1.68	68/5068 (1.3%)

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	5

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	ARG	NE-CZ-NH1	13.80	127.20	120.30
1	A	271	ARG	NE-CZ-NH1	11.69	126.15	120.30
1	A	321	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	A	98	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	A	52	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	A	274	MET	CG-SD-CE	-9.24	85.42	100.20
1	A	396	ARG	NE-CZ-NH2	-9.23	115.68	120.30
1	A	253	THR	CA-CB-CG2	-9.12	99.63	112.40
1	A	399	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	A	11	LYS	N-CA-C	7.96	132.50	111.00
1	A	383	TRP	CE2-CD2-CG	-7.81	101.06	107.30
1	A	381	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	A	383	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	A	90	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	A	398	TRP	CD1-CG-CD2	7.61	112.39	106.30
1	A	156	ARG	NE-CZ-NH1	7.52	124.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	TRP	CD1-CG-CD2	7.44	112.25	106.30
1	A	470	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	A	152	GLU	CA-CB-CG	7.35	129.57	113.40
1	A	207	TRP	CD1-CG-CD2	7.29	112.14	106.30
1	A	445	TRP	CD1-CG-CD2	7.10	111.98	106.30
1	A	445	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	A	381	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	A	154	TRP	CE2-CD2-CG	-7.02	101.68	107.30
1	A	321	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	A	398	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	A	137	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	A	154	TRP	CD1-CG-CD2	6.86	111.79	106.30
1	A	207	TRP	CE2-CD2-CG	-6.67	101.96	107.30
1	A	462	TYR	CB-CG-CD1	-6.54	117.08	121.00
1	A	159	LEU	CA-CB-CG	6.43	130.09	115.30
1	A	52	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	454	MET	CG-SD-CE	-6.34	90.06	100.20
1	A	396	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	A	473	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	169	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	82	TRP	CE2-CD2-CG	-6.08	102.44	107.30
1	A	397	VAL	CA-CB-CG2	-6.02	101.86	110.90
1	A	156	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	A	168	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	425	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	36	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	A	399	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	467	MET	CG-SD-CE	5.70	109.31	100.20
1	A	60	ASP	N-CA-CB	-5.68	100.37	110.60
1	A	383	TRP	CB-CG-CD1	-5.64	119.67	127.00
1	A	102	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	98	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	302	LEU	CA-CB-CG	5.58	128.13	115.30
1	A	58	HIS	CA-C-N	-5.55	104.98	117.20
1	A	425	ARG	CA-CB-CG	5.52	125.55	113.40
1	A	197	LYS	CA-CB-CG	5.47	125.44	113.40
1	A	130	TYR	CB-CG-CD1	-5.43	117.74	121.00
1	A	448	LEU	CA-CB-CG	5.36	127.62	115.30
1	A	336	ARG	CA-CB-CG	5.29	125.04	113.40
1	A	336	ARG	NH1-CZ-NH2	-5.28	113.59	119.40
1	A	381	TRP	CG-CD1-NE1	-5.28	104.82	110.10
1	A	398	TRP	CG-CD1-NE1	-5.25	104.85	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	473	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	A	55	TYR	CB-CG-CD2	-5.16	117.90	121.00
1	A	25	GLU	OE1-CD-OE2	-5.15	117.12	123.30
1	A	408	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	234	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	A	445	TRP	CG-CD2-CE3	5.06	138.46	133.90
1	A	154	TRP	CG-CD2-CE3	5.04	138.44	133.90
1	A	250	LYS	CA-CB-CG	5.04	124.49	113.40
1	A	383	TRP	CG-CD2-CE3	5.02	138.42	133.90
1	A	83	HIS	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	TYR	Sidechain
1	A	130	TYR	Sidechain
1	A	234	TYR	Sidechain
1	A	424	TYR	Sidechain
1	A	439	PHE	Sidechain

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	A	3671	0	3669	86	0
2	A	2	0	0	0	0
All	All	3673	0	3669	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:A:336:ARG:HH11	1:A:336:ARG:H	1.34	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:CYS:SG	1:A:419:ASN:HB2	2.28	0.73
1:A:250:LYS:HG2	1:A:358:ALA:HB1	1.73	0.69
1:A:290:LEU:HB3	1:A:292:LEU:HD13	1.76	0.68
1:A:171:MET:HA	1:A:274:MET:SD	2.36	0.66
1:A:100:ILE:HG21	1:A:108:VAL:HB	1.77	0.65
1:A:373:THR:HG22	1:A:453:VAL:HG11	1.80	0.64
1:A:191:LEU:HD22	1:A:232:ILE:HG13	1.83	0.60
1:A:106:PRO:O	1:A:141:VAL:HA	2.02	0.59
1:A:218:SER:HB2	1:A:312:ASN:ND2	2.17	0.59
1:A:120:ALA:HB3	1:A:157:GLY:HA3	1.84	0.59
1:A:3:GLY:HA3	1:A:100:ILE:HD12	1.85	0.59
1:A:234:TYR:HD2	1:A:296:ILE:HD12	1.67	0.58
1:A:218:SER:HB2	1:A:312:ASN:HD21	1.68	0.58
1:A:21:THR:HG21	1:A:113:CYS:HA	1.88	0.56
1:A:382:LEU:HD13	1:A:446:ALA:HB2	1.87	0.56
1:A:201:PHE:HB2	1:A:231:GLU:HB3	1.86	0.56
1:A:58:HIS:HB3	1:A:61:PHE:HB2	1.86	0.55
1:A:163:GLY:O	1:A:282:SER:HB3	2.06	0.55
1:A:101:GLN:HE22	1:A:464:ARG:HH22	1.55	0.55
1:A:184:ALA:HB1	1:A:202:ILE:HG12	1.87	0.55
1:A:212:GLU:HB3	1:A:319:ARG:HH12	1.72	0.55
1:A:125:LEU:HD13	1:A:161:ALA:HB1	1.87	0.54
1:A:375:VAL:HB	1:A:448:LEU:HD22	1.88	0.54
1:A:8:ILE:HG13	1:A:19:GLN:O	2.08	0.54
1:A:247:PHE:HA	1:A:355:ILE:O	2.08	0.54
1:A:18:PRO:HG2	1:A:36:ARG:HH22	1.73	0.53
1:A:218:SER:O	1:A:221:LYS:HG2	2.09	0.53
1:A:468:ALA:HB1	1:A:470:ARG:HG3	1.91	0.52
1:A:213:MET:O	1:A:217:LEU:HB2	2.10	0.52
1:A:362:GLY:O	1:A:365:ASP:HB3	2.10	0.52
1:A:166:LEU:O	1:A:170:LEU:HB2	2.09	0.51
1:A:207:TRP:CH2	1:A:211:GLN:HG3	2.45	0.51
1:A:246:VAL:HG22	1:A:297:VAL:HB	1.91	0.51
1:A:345:TYR:O	1:A:348:THR:HB	2.10	0.51
1:A:177:GLU:O	1:A:182:LYS:HD2	2.11	0.51
1:A:285:VAL:HG12	1:A:289:LYS:HD3	1.93	0.51
1:A:215:SER:O	1:A:219:VAL:HG23	2.10	0.51
1:A:274:MET:O	1:A:274:MET:HE2	2.10	0.51
1:A:317:VAL:HG13	1:A:325:THR:HB	1.94	0.50
1:A:166:LEU:HD22	1:A:170:LEU:HD22	1.94	0.49
1:A:188:GLU:HB2	1:A:200:VAL:HG11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:TRP:O	1:A:211:GLN:HG2	2.13	0.49
1:A:347:HIS:HE1	1:A:440:VAL:HA	1.78	0.48
1:A:407:THR:O	1:A:411:ILE:HB	2.14	0.48
1:A:251:GLY:HA2	1:A:274:MET:HA	1.96	0.48
1:A:89:ILE:O	1:A:93:VAL:HG13	2.14	0.48
1:A:375:VAL:HG12	1:A:397:VAL:HG22	1.95	0.48
1:A:375:VAL:CG1	1:A:397:VAL:HG22	2.44	0.47
1:A:356:ASN:HD22	1:A:445:TRP:HE1	1.62	0.47
1:A:236:GLY:HA3	1:A:294:ILE:O	2.15	0.47
1:A:401:PRO:HD2	1:A:430:CYS:SG	2.56	0.46
1:A:347:HIS:CE1	1:A:440:VAL:HA	2.50	0.46
1:A:422:GLY:HA3	1:A:431:THR:HG21	1.97	0.46
1:A:181:THR:O	1:A:185:GLU:HG3	2.16	0.45
1:A:370:SER:O	1:A:470:ARG:NH2	2.50	0.45
1:A:55:TYR:HA	1:A:62:PRO:O	2.15	0.45
1:A:222:GLY:HA2	1:A:311:ALA:HA	1.99	0.45
1:A:86:LYS:O	1:A:90:ARG:HG3	2.17	0.44
1:A:353:VAL:HG12	1:A:355:ILE:HG13	1.99	0.44
1:A:117:GLN:HG3	1:A:157:GLY:CA	2.48	0.44
1:A:202:ILE:HG23	1:A:228:VAL:HG11	1.99	0.44
1:A:250:LYS:HG2	1:A:358:ALA:CB	2.46	0.44
1:A:237:SER:HA	1:A:238:PRO:HD2	1.75	0.44
1:A:440:VAL:HG11	1:A:445:TRP:CG	2.53	0.43
1:A:83:HIS:HD2	1:A:85:GLY:N	2.16	0.43
1:A:373:THR:HG23	1:A:396:ARG:O	2.18	0.43
1:A:407:THR:O	1:A:410:VAL:HG12	2.18	0.43
1:A:110:VAL:HB	1:A:154:TRP:CH2	2.53	0.43
1:A:208:ILE:CG2	1:A:217:LEU:HD13	2.50	0.42
1:A:82:TRP:HA	1:A:391:ILE:HA	2.02	0.42
1:A:101:GLN:NE2	1:A:464:ARG:HH22	2.15	0.42
1:A:153:ALA:HA	1:A:156:ARG:HE	1.85	0.42
1:A:435:PHE:O	1:A:438:GLU:HB2	2.19	0.42
1:A:247:PHE:HE2	1:A:475:LEU:HG	1.84	0.42
1:A:35:LEU:HD23	1:A:57:LEU:HD11	2.02	0.42
1:A:120:ALA:HB1	1:A:158:VAL:HG23	2.03	0.41
1:A:260:SER:HB2	1:A:331:THR:HB	2.02	0.41
1:A:287:ALA:HA	1:A:292:LEU:HD22	2.02	0.41
1:A:234:TYR:O	1:A:295:ASN:HA	2.21	0.41
1:A:368:LEU:HD21	1:A:398:TRP:HB3	2.02	0.41
1:A:101:GLN:O	1:A:101:GLN:HG2	2.20	0.41
1:A:191:LEU:O	1:A:194:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:HG	1:A:232:ILE:HD13	2.03	0.40
1:A:246:VAL:HG23	1:A:351:PRO:HB3	2.02	0.40
1:A:285:VAL:O	1:A:289:LYS:HD3	2.22	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	A	479/487 (98%)	438 (91%)	38 (8%)	3 (1%)	28 64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	130	TYR
1	A	405	HIS

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	A	387/392 (99%)	332 (86%)	55 (14%)	4 11

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	11	LYS
1	A	30	LEU
1	A	35	LEU
1	A	39	LEU
1	A	47	LYS
1	A	51	THR
1	A	60	ASP
1	A	82	TRP
1	A	93	VAL
1	A	107	SER
1	A	125	LEU
1	A	138	LYS
1	A	141	VAL
1	A	155	GLN
1	A	166	LEU
1	A	169	ARG
1	A	170	LEU
1	A	188	GLU
1	A	199	ASP
1	A	203	ARG
1	A	216	PHE
1	A	232	ILE
1	A	250	LYS
1	A	268	ASP
1	A	271	ARG
1	A	279	THR
1	A	290	LEU
1	A	291	ASP
1	A	292	LEU
1	A	299	LEU
1	A	312	ASN
1	A	334	GLU
1	A	336	ARG
1	A	350	ASN
1	A	356	ASN
1	A	360	LEU
1	A	368	LEU
1	A	373	THR
1	A	375	VAL
1	A	377	THR
1	A	382	LEU
1	A	386	LEU

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Mol	Chain	Res	Type
1	A	390	SER
1	A	396	ARG
1	A	397	VAL
1	A	410	VAL
1	A	411	ILE
1	A	415	LEU
1	A	418	VAL
1	A	425	ARG
1	A	448	LEU
1	A	455	THR
1	A	459	GLU
1	A	475	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	88	ASN
1	A	101	GLN
1	A	155	GLN
1	A	305	ASN
1	A	312	ASN
1	A	356	ASN
1	A	405	HIS
1	A	447	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

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.