



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:18 PM UTC

PDB ID : 1LAP / pdb_00001lap
Title : MOLECULAR STRUCTURE OF LEUCINE AMINOPEPTIDASE AT 2.7-ANGSTROMS RESOLUTION
Authors : Burley, S.K.; David, P.R.; Taylor, A.; Lipscomb, W.N.
Deposited on : 1990-08-01
Resolution : 2.70 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

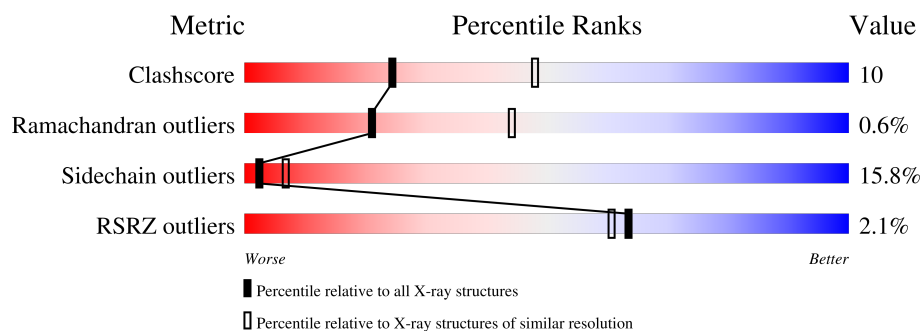
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

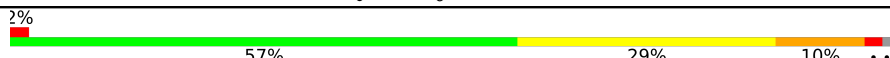
The reported resolution of this entry is 2.70 Å.

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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 $\leq 5\%$. 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.

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 4488 atoms, of which 815 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 Cytosol aminopeptidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	481	Total	C	H	N	O	S	0	0	0
			4486	2321	815	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

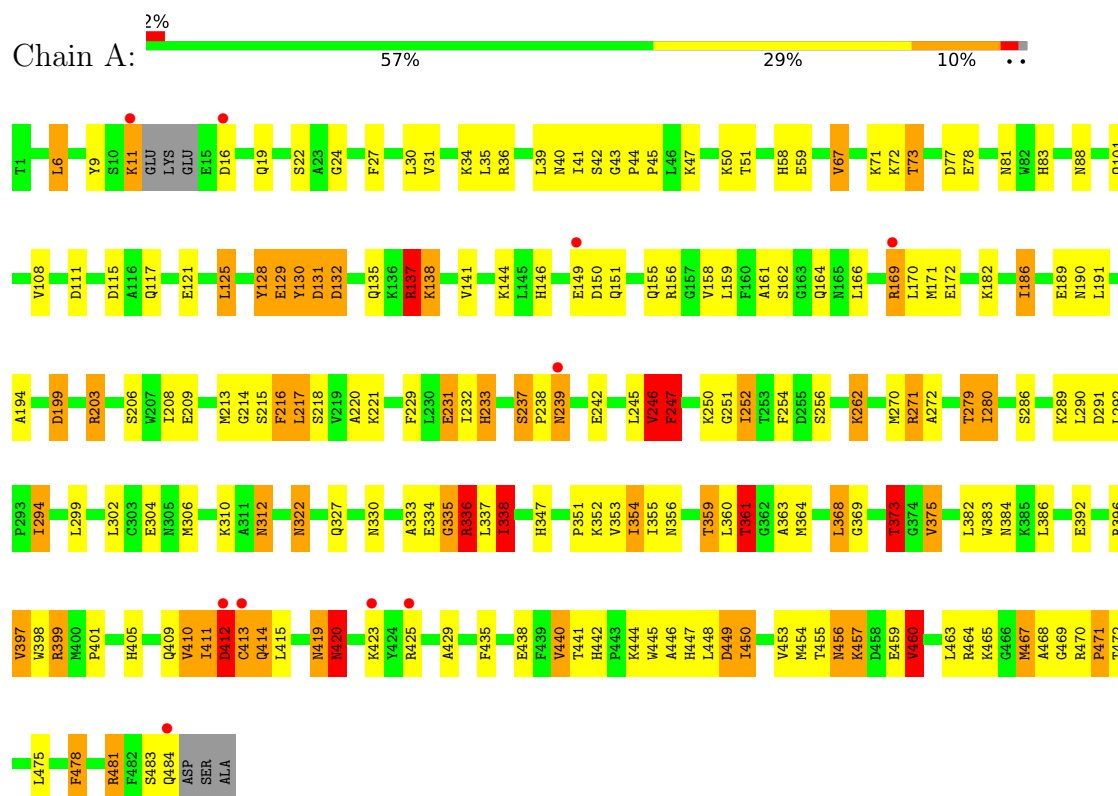
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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 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.

• Molecule 1: Cytosol aminopeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	132.50Å 132.50Å 121.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.70 200.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70) 91.6 (200.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.169 , (Not available) 0.175 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.3	EDS
L-test for twinning ¹	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4488	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	1.16	20/3743 (0.5%)	2.08	134/5065 (2.6%)

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	A	0	5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	447	HIS	CD2-NE2	-7.49	1.29	1.37
1	A	442	HIS	CD2-NE2	-7.41	1.29	1.37
1	A	460	VAL	CA-CB	7.34	1.63	1.54
1	A	83	HIS	CD2-NE2	-7.18	1.29	1.37
1	A	186	ILE	CA-CB	6.67	1.62	1.54
1	A	405	HIS	CD2-NE2	-6.50	1.30	1.37
1	A	440	VAL	CA-CB	6.25	1.63	1.54
1	A	233	HIS	CD2-NE2	-5.92	1.31	1.37
1	A	58	HIS	CD2-NE2	-5.90	1.31	1.37
1	A	347	HIS	CD2-NE2	-5.89	1.31	1.37
1	A	373	THR	CA-CB	5.88	1.62	1.53
1	A	246	VAL	CA-CB	5.79	1.62	1.54
1	A	347	HIS	CG-ND1	-5.73	1.31	1.38
1	A	481	ARG	CA-CB	-5.71	1.44	1.53
1	A	83	HIS	CG-ND1	-5.67	1.32	1.38
1	A	450	ILE	CA-CB	5.64	1.61	1.54
1	A	146	HIS	CD2-NE2	-5.54	1.31	1.37
1	A	108	VAL	CA-CB	5.10	1.61	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	375	VAL	CA-CB	5.08	1.61	1.54
1	A	336	ARG	NE-CZ	5.03	1.38	1.33

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	GLU	N-CA-C	16.19	135.12	114.56
1	A	291	ASP	CA-CB-CG	-11.70	100.90	112.60
1	A	129	GLU	CB-CA-C	-11.27	91.55	109.13
1	A	396	ARG	N-CA-C	10.60	124.53	110.53
1	A	129	GLU	CA-C-O	-9.92	107.24	118.55
1	A	111	ASP	CA-CB-CG	9.68	122.28	112.60
1	A	397	VAL	N-CA-CB	-9.44	94.46	111.93
1	A	470	ARG	NE-CZ-NH2	9.34	127.61	119.20
1	A	137	ARG	CD-NE-CZ	-9.20	111.52	124.40
1	A	129	GLU	CB-CG-CD	9.09	128.05	112.60
1	A	359	THR	N-CA-C	-8.88	96.29	109.62
1	A	137	ARG	CG-CD-NE	8.56	130.83	112.00
1	A	419	ASN	OD1-CG-ND2	-8.32	114.28	122.60
1	A	81	ASN	OD1-CG-ND2	-8.26	114.34	122.60
1	A	81	ASN	CB-CG-ND2	8.26	128.79	116.40
1	A	410	VAL	N-CA-CB	-8.18	103.21	112.21
1	A	137	ARG	NE-CZ-NH1	-8.09	113.41	121.50
1	A	338	ILE	CA-CB-CG1	-8.07	96.68	110.40
1	A	397	VAL	CB-CA-C	7.92	123.36	110.69
1	A	399	ARG	NE-CZ-NH2	7.80	126.22	119.20
1	A	199	ASP	CA-CB-CG	7.74	120.34	112.60
1	A	247	PHE	CA-CB-CG	7.55	121.36	113.80
1	A	137	ARG	NE-CZ-NH2	7.52	125.97	119.20
1	A	361	THR	N-CA-CB	-7.43	98.33	110.81
1	A	336	ARG	NE-CZ-NH2	7.35	125.81	119.20
1	A	338	ILE	CA-CB-CG2	7.28	122.87	110.50
1	A	412	ASP	O-C-N	-7.10	113.14	122.59
1	A	449	ASP	CA-C-N	7.05	132.49	121.35
1	A	449	ASP	C-N-CA	7.05	132.49	121.35
1	A	456	ASN	CA-CB-CG	-6.85	105.75	112.60
1	A	40	ASN	OD1-CG-ND2	-6.83	115.77	122.60
1	A	456	ASN	OD1-CG-ND2	-6.75	115.85	122.60
1	A	149	GLU	N-CA-C	6.74	118.71	111.36
1	A	470	ARG	NE-CZ-NH1	-6.73	114.77	121.50
1	A	130	TYR	CA-CB-CG	-6.71	101.82	113.90
1	A	132	ASP	N-CA-C	6.67	122.38	111.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	420	ASN	CA-CB-CG	6.57	119.17	112.60
1	A	19	GLN	N-CA-C	6.42	120.35	110.20
1	A	88	ASN	OD1-CG-ND2	-6.40	116.20	122.60
1	A	306	MET	O-C-N	-6.39	115.65	121.66
1	A	291	ASP	N-CA-C	6.36	119.95	111.30
1	A	338	ILE	N-CA-CB	-6.32	101.10	110.58
1	A	44	PRO	O-C-N	-6.30	118.19	121.15
1	A	271	ARG	N-CA-C	-6.27	104.50	111.71
1	A	441	THR	N-CA-C	-6.26	104.27	112.41
1	A	155	GLN	OE1-CD-NE2	-6.26	116.34	122.60
1	A	425	ARG	CB-CG-CD	-6.26	96.91	111.30
1	A	384	ASN	CA-CB-CG	-6.23	106.37	112.60
1	A	220	ALA	N-CA-C	6.21	118.05	111.28
1	A	336	ARG	NH1-CZ-NH2	-6.05	111.44	119.30
1	A	401	PRO	N-CA-C	6.03	121.63	111.32
1	A	356	ASN	OD1-CG-ND2	-6.02	116.58	122.60
1	A	43	GLY	CA-C-N	5.98	123.97	119.66
1	A	43	GLY	C-N-CA	5.98	123.97	119.66
1	A	304	GLU	O-C-N	-5.98	115.63	123.16
1	A	151	GLN	CA-CB-CG	5.95	125.99	114.10
1	A	150	ASP	CA-CB-CG	-5.91	106.69	112.60
1	A	67	VAL	N-CA-C	5.89	116.61	108.12
1	A	131	ASP	CA-CB-CG	5.88	118.47	112.60
1	A	468	ALA	N-CA-C	5.88	120.61	113.38
1	A	396	ARG	NE-CZ-NH1	-5.87	115.63	121.50
1	A	158	VAL	O-C-N	5.86	127.80	121.94
1	A	221	LYS	CG-CD-CE	-5.84	97.86	111.30
1	A	419	ASN	CB-CG-ND2	5.84	125.16	116.40
1	A	304	GLU	N-CA-CB	-5.83	101.52	110.85
1	A	246	VAL	O-C-N	5.83	129.47	123.18
1	A	203	ARG	CB-CG-CD	5.78	124.60	111.30
1	A	383	TRP	CE2-CD2-CG	-5.76	100.29	107.20
1	A	411	ILE	N-CA-CB	-5.68	101.86	111.23
1	A	396	ARG	CB-CG-CD	-5.64	98.33	111.30
1	A	322	ASN	CA-CB-CG	5.62	118.22	112.60
1	A	135	GLN	N-CA-C	-5.61	106.27	113.23
1	A	409	GLN	CG-CD-NE2	5.61	124.81	116.40
1	A	465	LYS	CA-CB-CG	5.59	125.28	114.10
1	A	115	ASP	CA-C-O	5.58	126.49	120.63
1	A	216	PHE	CA-CB-CG	5.56	119.36	113.80
1	A	355	ILE	O-C-N	-5.52	117.30	123.26
1	A	16	ASP	CA-CB-CG	5.52	118.12	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	ILE	CB-CA-C	-5.52	103.81	110.99
1	A	399	ARG	CB-CG-CD	5.52	123.99	111.30
1	A	214	GLY	CA-C-O	-5.51	114.82	120.66
1	A	361	THR	CB-CA-C	5.51	119.29	109.65
1	A	279	THR	N-CA-CB	-5.48	102.06	110.01
1	A	409	GLN	OE1-CD-NE2	-5.48	117.12	122.60
1	A	335	GLY	CA-C-N	5.47	128.40	120.79
1	A	335	GLY	C-N-CA	5.47	128.40	120.79
1	A	470	ARG	CB-CG-CD	-5.47	98.73	111.30
1	A	164	GLN	CA-CB-CG	-5.45	103.20	114.10
1	A	409	GLN	CA-CB-CG	-5.42	103.27	114.10
1	A	478	PHE	CA-CB-CG	5.40	119.20	113.80
1	A	237	SER	CA-C-N	5.39	125.21	119.28
1	A	237	SER	C-N-CA	5.39	125.21	119.28
1	A	352	LYS	CA-CB-CG	5.39	124.88	114.10
1	A	135	GLN	CA-CB-CG	5.39	124.87	114.10
1	A	457	LYS	N-CA-C	-5.36	103.35	111.34
1	A	128	TYR	O-C-N	-5.33	116.38	122.89
1	A	280	ILE	O-C-N	-5.31	116.36	121.83
1	A	135	GLN	OE1-CD-NE2	-5.30	117.30	122.60
1	A	40	ASN	CB-CG-ND2	5.27	124.31	116.40
1	A	336	ARG	CB-CG-CD	5.27	123.42	111.30
1	A	423	LYS	N-CA-CB	-5.26	102.38	110.12
1	A	190	ASN	OD1-CG-ND2	-5.26	117.34	122.60
1	A	472	THR	N-CA-C	5.26	117.69	111.33
1	A	209	GLU	CA-CB-CG	5.25	124.60	114.10
1	A	306	MET	N-CA-C	5.25	118.06	110.14
1	A	419	ASN	CA-CB-CG	5.25	117.84	112.60
1	A	245	LEU	CA-C-N	-5.24	115.82	123.06
1	A	245	LEU	C-N-CA	-5.24	115.82	123.06
1	A	398	TRP	CG-CD2-CE3	5.24	139.14	133.90
1	A	77	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	42	SER	N-CA-C	5.22	119.37	112.89
1	A	186	ILE	CB-CA-C	-5.22	105.29	111.97
1	A	335	GLY	O-C-N	5.21	127.22	122.17
1	A	252	ILE	N-CA-C	-5.21	101.08	108.58
1	A	40	ASN	O-C-N	-5.20	116.71	122.07
1	A	158	VAL	CA-C-N	5.20	127.20	120.44
1	A	158	VAL	C-N-CA	5.20	127.20	120.44
1	A	459	GLU	N-CA-C	5.20	116.94	111.28
1	A	42	SER	CA-CB-OG	5.18	121.47	111.10
1	A	169	ARG	NE-CZ-NH2	5.18	123.86	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	ASN	OD1-CG-ND2	-5.18	117.42	122.60
1	A	73	THR	N-CA-CB	-5.14	101.39	110.39
1	A	254	PHE	CA-CB-CG	-5.13	108.67	113.80
1	A	414	GLN	CA-C-N	-5.12	112.65	121.66
1	A	414	GLN	C-N-CA	-5.12	112.65	121.66
1	A	453	VAL	N-CA-C	-5.12	106.45	111.77
1	A	149	GLU	CA-C-N	-5.11	115.51	122.87
1	A	149	GLU	C-N-CA	-5.11	115.51	122.87
1	A	189	GLU	CA-CB-CG	5.10	124.30	114.10
1	A	368	LEU	N-CA-CB	-5.10	103.85	110.88
1	A	383	TRP	CB-CG-CD1	-5.09	119.27	126.90
1	A	322	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	A	186	ILE	N-CA-CB	5.04	116.44	110.55
1	A	208	ILE	CA-C-O	-5.04	115.71	120.95

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	137	ARG	Sidechain
1	A	247	PHE	Sidechain
1	A	478	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	815	3668	73	0
2	A	2	0	0	0	0
All	All	3673	815	3668	73	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 10.

All (73) 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:272:ALA:HB3	1:A:454:MET:HE3	1.55	0.88
1:A:412:ASP:CG	1:A:419:ASN:HB2	2.14	0.73
1:A:169:ARG:NH1	1:A:186:ILE:HG21	2.03	0.73
1:A:171:MET:HB3	1:A:467:MET:HG2	1.72	0.71
1:A:412:ASP:OD1	1:A:419:ASN:HB2	1.95	0.67
1:A:169:ARG:HH12	1:A:186:ILE:HG21	1.58	0.67
1:A:51:THR:HG22	1:A:67:VAL:HG12	1.77	0.66
1:A:101:GLN:NE2	1:A:464:ARG:HH12	1.94	0.66
1:A:47:LYS:HG3	1:A:50:LYS:HG3	1.79	0.64
1:A:101:GLN:HE22	1:A:464:ARG:HH22	1.46	0.63
1:A:131:ASP:O	1:A:137:ARG:NH1	2.32	0.63
1:A:454:MET:HG2	1:A:467:MET:HE2	1.81	0.62
1:A:252:ILE:HD11	1:A:338:ILE:HD13	1.82	0.61
1:A:333:ALA:HB1	1:A:336:ARG:HD2	1.83	0.60
1:A:392:GLU:HG3	1:A:481:ARG:HH11	1.67	0.59
1:A:382:LEU:HD13	1:A:446:ALA:HB2	1.85	0.58
1:A:412:ASP:CG	1:A:412:ASP:O	2.47	0.57
1:A:327:GLN:O	1:A:420:ASN:HB3	2.03	0.57
1:A:132:ASP:CA	1:A:137:ARG:HH12	2.20	0.54
1:A:172:GLU:O	1:A:271:ARG:HD2	2.08	0.54
1:A:117:GLN:NE2	1:A:156:ARG:HE	2.05	0.53
1:A:333:ALA:HB3	1:A:420:ASN:ND2	2.23	0.53
1:A:131:ASP:C	1:A:137:ARG:HH12	2.16	0.53
1:A:364:MET:HG3	1:A:449:ASP:HB3	1.91	0.53
1:A:199:ASP:HB2	1:A:233:HIS:HB2	1.90	0.53
1:A:361:THR:HG21	1:A:429:ALA:HA	1.92	0.52
1:A:412:ASP:O	1:A:413:CYS:C	2.52	0.52
1:A:131:ASP:OD2	1:A:137:ARG:NH2	2.42	0.52
1:A:132:ASP:HA	1:A:137:ARG:HH12	1.75	0.52
1:A:203:ARG:HB2	1:A:229:PHE:HB3	1.91	0.52
1:A:361:THR:HG23	1:A:363:ALA:HB3	1.91	0.52
1:A:132:ASP:HA	1:A:137:ARG:NH1	2.25	0.51
1:A:256:SER:O	1:A:262:LYS:HB2	2.11	0.51
1:A:413:CYS:SG	1:A:414:GLN:N	2.83	0.51
1:A:191:LEU:HD22	1:A:232:ILE:HG23	1.93	0.50
1:A:6:LEU:HG	1:A:24:GLY:HA2	1.94	0.49
1:A:333:ALA:HB3	1:A:420:ASN:HD21	1.77	0.49
1:A:171:MET:CE	1:A:469:GLY:HA2	2.43	0.48
1:A:9:TYR:CE2	1:A:72:LYS:HE2	2.49	0.48
1:A:251:GLY:HA3	1:A:302:LEU:HD13	1.96	0.47
1:A:218:SER:HB2	1:A:312:ASN:HD21	1.79	0.47
1:A:262:LYS:CE	1:A:270:MET:HE2	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:MET:O	1:A:217:LEU:HB2	2.15	0.45
1:A:71:LYS:HB3	1:A:73:THR:HG22	1.99	0.45
1:A:101:GLN:HE21	1:A:464:ARG:HH12	1.64	0.45
1:A:272:ALA:CB	1:A:454:MET:HE3	2.39	0.45
1:A:456:ASN:HD21	1:A:460:VAL:H	1.65	0.44
1:A:129:GLU:HG3	1:A:138:LYS:NZ	2.32	0.44
1:A:336:ARG:NH2	1:A:336:ARG:H	2.16	0.44
1:A:412:ASP:OD2	1:A:419:ASN:HB2	2.18	0.43
1:A:454:MET:HG2	1:A:467:MET:CE	2.46	0.43
1:A:121:GLU:O	1:A:125:LEU:HB2	2.18	0.43
1:A:435:PHE:O	1:A:438:GLU:HB2	2.18	0.43
1:A:27:PHE:O	1:A:31:VAL:HG22	2.18	0.43
1:A:247:PHE:HB3	1:A:280:ILE:HB	2.01	0.43
1:A:246:VAL:CG1	1:A:351:PRO:HB3	2.49	0.43
1:A:121:GLU:HA	1:A:161:ALA:HB2	2.01	0.43
1:A:129:GLU:HG3	1:A:138:LYS:HZ1	1.84	0.43
1:A:237:SER:HA	1:A:238:PRO:HD3	1.86	0.42
1:A:11:LYS:HE2	1:A:45:PRO:HG3	2.00	0.42
1:A:216:PHE:HA	1:A:338:ILE:HG13	2.01	0.42
1:A:312:ASN:HD22	1:A:312:ASN:HA	1.73	0.42
1:A:334:GLU:HA	1:A:337:LEU:HD12	2.01	0.42
1:A:450:ILE:HD12	1:A:471:PRO:HD3	2.01	0.42
1:A:286:SER:O	1:A:290:LEU:HB2	2.20	0.42
1:A:203:ARG:HD2	1:A:231:GLU:HG3	2.02	0.42
1:A:239:ASN:HB2	1:A:242:GLU:HB2	2.01	0.42
1:A:250:LYS:HE3	1:A:335:GLY:HA3	2.02	0.41
1:A:194:ALA:HB1	1:A:289:LYS:HG3	2.03	0.41
1:A:354:ILE:O	1:A:445:TRP:HA	2.21	0.41
1:A:373:THR:HG21	1:A:471:PRO:HB3	2.03	0.41
1:A:481:ARG:HA	1:A:484:GLN:HG3	2.02	0.41
1:A:294:ILE:HG12	1:A:483:SER:HB3	2.02	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	477/487 (98%)	457 (96%)	17 (4%)	3 (1%)	21	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	412	ASP
1	A	413	CYS
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%)	326 (84%)	61 (16%)	2	7

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	11	LYS
1	A	22	SER
1	A	30	LEU
1	A	34	LYS
1	A	35	LEU
1	A	36	ARG
1	A	39	LEU
1	A	41	ILE
1	A	59	GLU
1	A	78	GLU
1	A	125	LEU
1	A	137	ARG
1	A	138	LYS
1	A	141	VAL
1	A	144	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	159	LEU
1	A	162	SER
1	A	166	LEU
1	A	170	LEU
1	A	182	LYS
1	A	206	SER
1	A	215	SER
1	A	217	LEU
1	A	231	GLU
1	A	239	ASN
1	A	246	VAL
1	A	262	LYS
1	A	279	THR
1	A	292	LEU
1	A	294	ILE
1	A	299	LEU
1	A	310	LYS
1	A	312	ASN
1	A	322	ASN
1	A	336	ARG
1	A	338	ILE
1	A	353	VAL
1	A	359	THR
1	A	360	LEU
1	A	361	THR
1	A	368	LEU
1	A	373	THR
1	A	375	VAL
1	A	386	LEU
1	A	397	VAL
1	A	399	ARG
1	A	410	VAL
1	A	411	ILE
1	A	415	LEU
1	A	420	ASN
1	A	440	VAL
1	A	444	LYS
1	A	448	LEU
1	A	455	THR
1	A	457	LYS
1	A	460	VAL
1	A	463	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	467	MET
1	A	471	PRO
1	A	475	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	83	HIS
1	A	101	GLN
1	A	117	GLN
1	A	190	ASN
1	A	312	ASN
1	A	322	ASN
1	A	327	GLN
1	A	356	ASN
1	A	409	GLN
1	A	456	ASN

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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	481/487 (98%)	-0.20	10 (2%) 63 61	5, 15, 36, 56	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	412	ASP	6.4
1	A	413	CYS	4.2
1	A	484	GLN	3.9
1	A	16	ASP	3.1
1	A	423	LYS	3.0
1	A	149	GLU	2.8
1	A	239	ASN	2.6
1	A	11	LYS	2.6
1	A	425	ARG	2.4
1	A	169	ARG	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	488	1/1	0.99	0.10	37,37,37,37	0
2	ZN	A	489	1/1	0.99	0.04	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.