Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:38 PM GMT

PDB ID	:	1LAP
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

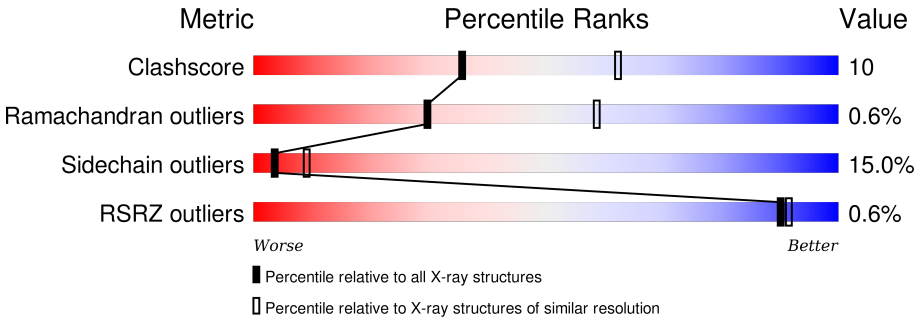
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

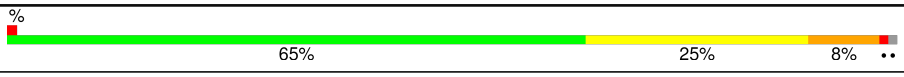
The reported resolution of this entry is 2.70 Å.

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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 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 <=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 (i)

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
			Total	C	H	N	O	S			
1	A	481	4486	2321	815	635	697	18	0	0	0

There is a discrepancy between the modelled and reference sequences:

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

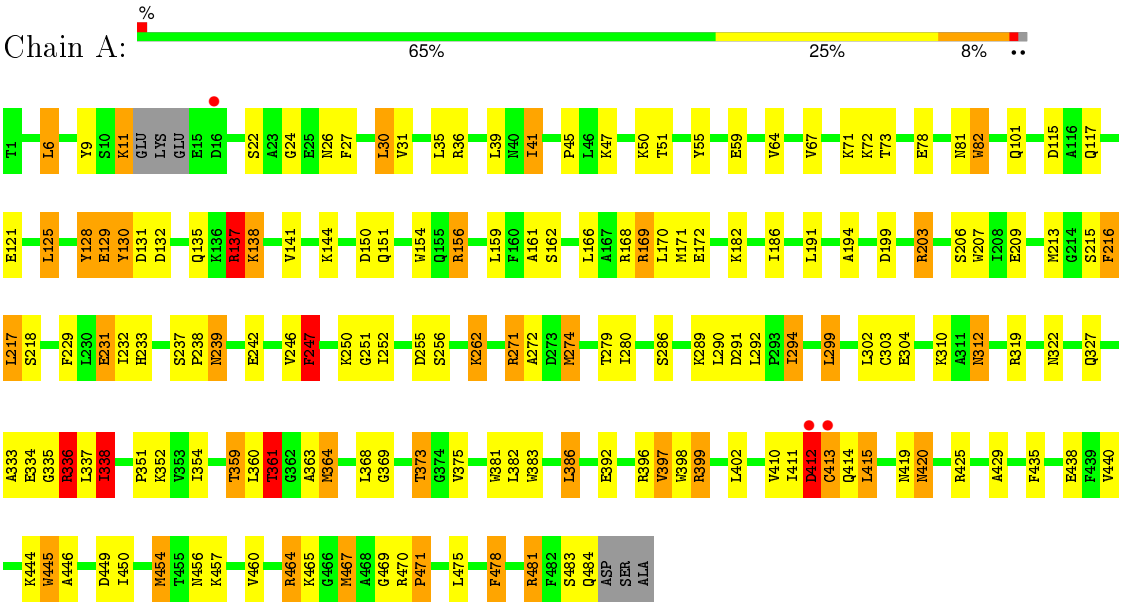
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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 errors 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 (i)

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 60.90 – 2.33	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70) 78.5 (60.90-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.169 , (Not available) 0.189 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
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 , 48.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[1]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Outliers	0 of 21709 reflections	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.*

[1]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.91	0/3743	1.75	94/5065 (1.9%)

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 (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	470	ARG	NE-CZ-NH2	14.61	127.61	120.30
1	A	137	ARG	NE-CZ-NH1	-13.78	113.41	120.30
1	A	399	ARG	NE-CZ-NH2	11.84	126.22	120.30
1	A	137	ARG	NE-CZ-NH2	11.34	125.97	120.30
1	A	470	ARG	NE-CZ-NH1	-11.06	114.77	120.30
1	A	336	ARG	NE-CZ-NH2	11.02	125.81	120.30
1	A	129	GLU	CB-CA-C	-9.43	91.55	110.40
1	A	396	ARG	NE-CZ-NH1	-9.35	115.63	120.30
1	A	130	TYR	CB-CG-CD2	-9.19	115.48	121.00
1	A	137	ARG	CG-CD-NE	9.06	130.83	111.80
1	A	129	GLU	N-CA-C	8.93	135.12	111.00
1	A	383	TRP	CE2-CD2-CG	-8.76	100.29	107.30
1	A	137	ARG	CD-NE-CZ	-8.63	111.52	123.60
1	A	128	TYR	CB-CG-CD1	-8.58	115.85	121.00
1	A	82	TRP	CD1-CG-CD2	8.45	113.06	106.30
1	A	207	TRP	CD1-CG-CD2	8.12	112.80	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	445	TRP	CD1-CG-CD2	8.01	112.71	106.30
1	A	397	VAL	N-CA-CB	-7.75	94.46	111.50
1	A	383	TRP	CD1-CG-CD2	7.62	112.39	106.30
1	A	338	ILE	CA-CB-CG1	-7.54	96.68	111.00
1	A	381	TRP	CD1-CG-CD2	7.51	112.31	106.30
1	A	399	ARG	NE-CZ-NH1	-7.45	116.58	120.30
1	A	207	TRP	CE2-CD2-CG	-7.44	101.34	107.30
1	A	336	ARG	NH1-CZ-NH2	-7.24	111.44	119.40
1	A	169	ARG	NE-CZ-NH2	7.13	123.86	120.30
1	A	169	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	A	271	ARG	NE-CZ-NH1	-7.07	116.77	120.30
1	A	412	ASP	CA-C-N	7.02	132.64	117.20
1	A	168	ARG	NE-CZ-NH1	-6.90	116.85	120.30
1	A	82	TRP	CE2-CD2-CG	-6.84	101.83	107.30
1	A	255	ASP	CB-CG-OD1	-6.79	112.19	118.30
1	A	398	TRP	CE2-CD2-CG	-6.75	101.90	107.30
1	A	445	TRP	CE2-CD2-CG	-6.65	101.98	107.30
1	A	203	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	A	415	LEU	CB-CG-CD2	-6.39	100.14	111.00
1	A	361	THR	N-CA-CB	-6.30	98.33	110.30
1	A	397	VAL	CB-CA-C	6.29	123.36	111.40
1	A	398	TRP	CD1-CG-CD2	6.26	111.31	106.30
1	A	55	TYR	CB-CG-CD1	-6.21	117.27	121.00
1	A	454	MET	CG-SD-CE	-6.18	90.31	100.20
1	A	381	TRP	CE2-CD2-CG	-6.17	102.36	107.30
1	A	30	LEU	CA-CB-CG	6.16	129.47	115.30
1	A	82	TRP	CG-CD1-NE1	-6.14	103.96	110.10
1	A	129	GLU	CA-C-O	-6.12	107.24	120.10
1	A	130	TYR	CA-CB-CG	-6.10	101.82	113.40
1	A	386	LEU	CA-CB-CG	6.06	129.23	115.30
1	A	156	ARG	NE-CZ-NH1	-6.05	117.27	120.30
1	A	115	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	A	402	LEU	CB-CG-CD2	-6.03	100.75	111.00
1	A	338	ILE	CA-CB-CG2	5.98	122.87	110.90
1	A	412	ASP	O-C-N	-5.97	113.14	122.70
1	A	154	TRP	CD1-CG-CD2	5.97	111.08	106.30
1	A	383	TRP	CB-CG-CD1	-5.95	119.27	127.00
1	A	319	ARG	NE-CZ-NH2	5.93	123.27	120.30
1	A	381	TRP	CG-CD1-NE1	-5.89	104.21	110.10
1	A	425	ARG	NE-CZ-NH2	5.87	123.24	120.30
1	A	398	TRP	CG-CD2-CE3	5.82	139.14	133.90
1	A	481	ARG	NE-CZ-NH2	5.79	123.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	478	PHE	CB-CG-CD2	-5.77	116.76	120.80
1	A	154	TRP	CE2-CD2-CG	-5.76	102.69	107.30
1	A	464	ARG	NE-CZ-NH1	-5.76	117.42	120.30
1	A	203	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	151	GLN	CA-CB-CG	5.72	125.99	113.40
1	A	129	GLU	OE1-CD-OE2	-5.71	116.45	123.30
1	A	454	MET	CA-CB-CG	5.69	122.98	113.30
1	A	168	ARG	NE-CZ-NH2	5.69	123.14	120.30
1	A	291	ASP	CA-CB-CG	-5.68	100.90	113.40
1	A	64	VAL	CG1-CB-CG2	-5.67	101.83	110.90
1	A	425	ARG	CB-CG-CD	-5.65	96.91	111.60
1	A	129	GLU	CA-C-N	5.57	129.45	117.20
1	A	203	ARG	NH1-CZ-NH2	-5.56	113.28	119.40
1	A	255	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	303	CYS	CA-CB-SG	5.52	123.94	114.00
1	A	396	ARG	NE-CZ-NH2	5.51	123.06	120.30
1	A	425	ARG	NE-CZ-NH1	-5.49	117.55	120.30
1	A	359	THR	N-CA-C	-5.45	96.29	111.00
1	A	216	PHE	CB-CG-CD2	-5.44	116.99	120.80
1	A	465	LYS	CA-CB-CG	5.40	125.28	113.40
1	A	383	TRP	NE1-CE2-CZ2	-5.31	124.56	130.40
1	A	41	ILE	CG1-CB-CG2	-5.29	99.75	111.40
1	A	271	ARG	NE-CZ-NH2	5.27	122.94	120.30
1	A	364	MET	CG-SD-CE	-5.25	91.80	100.20
1	A	352	LYS	CA-CB-CG	5.22	124.88	113.40
1	A	135	GLN	CA-CB-CG	5.21	124.87	113.40
1	A	398	TRP	CB-CG-CD1	-5.20	120.25	127.00
1	A	274	MET	CG-SD-CE	-5.15	91.97	100.20
1	A	129	GLU	CB-CG-CD	5.13	128.05	114.20
1	A	299	LEU	CA-CB-CG	5.13	127.10	115.30
1	A	396	ARG	CB-CG-CD	-5.10	98.33	111.60
1	A	209	GLU	CA-CB-CG	5.09	124.60	113.40
1	A	247	PHE	CB-CG-CD2	-5.05	117.27	120.80
1	A	304	GLU	N-CA-CB	-5.04	101.52	110.60
1	A	81	ASN	CB-CG-ND2	5.04	128.79	116.70
1	A	396	ARG	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	TYR	Sidechain

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Mol	Chain	Res	Type	Group
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	71	0
2	A	2	0	0	0	0
All	All	3673	815	3668	71	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 (71) 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: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:CG	1:A:419:ASN:HB2	2.14	0.68
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: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:454:MET:HG2	1:A:467:MET:HE2	1.83	0.59
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:272:ALA:HB3	1:A:454:MET:HE3	1.85	0.58
1:A:327:GLN:O	1:A:420:ASN:HB3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:412:ASP:O	1:A:412:ASP:CG	2.47	0.53
1:A:361:THR:HG21	1:A:429:ALA:HA	1.92	0.52
1:A:132:ASP:HA	1:A:137:ARG:HH12	1.75	0.52
1:A:131:ASP:OD2	1:A:137:ARG:NH2	2.42	0.52
1:A:361:THR:HG23	1:A:363:ALA:HB3	1.91	0.52
1:A:203:ARG:HB2	1:A:229:PHE: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:131:ASP:C	1:A:137:ARG:HH12	2.16	0.48
1:A:251:GLY:HA3	1:A:302:LEU:HD13	1.96	0.47
1:A:412:ASP:O	1:A:413:CYS:C	2.52	0.47
1:A:218:SER:HB2	1:A:312:ASN:HD21	1.79	0.47
1:A:454:MET:HG2	1:A:467:MET:CE	2.46	0.45
1:A:213:MET:O	1:A:217:LEU:HB2	2.15	0.45
1:A:101:GLN:HE21	1:A:464:ARG:HH12	1.64	0.45
1:A:71:LYS:HB3	1:A:73:THR:HG22	1.99	0.45
1:A:456:ASN:HD21	1:A:460:VAL:H	1.65	0.44
1:A:336:ARG:H	1:A:336:ARG:NH2	2.16	0.44
1:A:129:GLU:HG3	1:A:138:LYS:NZ	2.32	0.44
1:A:412:ASP:OD2	1:A:419:ASN:HB2	2.18	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:247:PHE:HB3	1:A:280:ILE:HB	2.01	0.43
1:A:27:PHE:O	1:A:31:VAL:HG22	2.18	0.43
1:A:246:VAL:CG1	1:A:351:PRO:HB3	2.49	0.43
1:A:272:ALA:HB3	1:A:454:MET:CE	2.49	0.43
1:A:121:GLU:HA	1:A:161:ALA:HB2	2.01	0.43
1:A:237:SER:HA	1:A:238:PRO:HD3	1.86	0.42
1:A:216:PHE:HA	1:A:338:ILE:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LYS:HE2	1:A:45:PRO:HG3	2.00	0.42
1:A:312:ASN:HA	1:A:312:ASN:HD22	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:481:ARG:HA	1:A:484:GLN:HG3	2.02	0.41
1:A:373:THR:HG21	1:A:471:PRO:HB3	2.03	0.41
1:A:354:ILE:O	1:A:445:TRP:HA	2.21	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 (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	477/487 (98%)	457 (96%)	17 (4%)	3 (1%)	30 59

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 (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%)	329 (85%)	58 (15%)	3 9

All (58) 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	26	ASN
1	A	30	LEU
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	82	TRP
1	A	125	LEU
1	A	137	ARG
1	A	138	LYS
1	A	141	VAL
1	A	144	LYS
1	A	150	ASP
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	262	LYS
1	A	274	MET

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) 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	305	ASN
1	A	312	ASN
1	A	322	ASN
1	A	327	GLN
1	A	456	ASN

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

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, 95^{th} 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%)	-0.70	3 (0%) 90 91	3, 14, 40, 61	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	412	ASP	4.3
1	A	413	CYS	2.5
1	A	16	ASP	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	A	489	1/1	1.00	0.07	-1.74	14,14,14,14	0
2	ZN	A	488	1/1	0.98	0.05	-4.38	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.