



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:52 PM UTC

PDB ID : 1PP2 / pdb_00001pp2
Title : THE REFINED CRYSTAL STRUCTURE OF DIMERIC PHOSPHOLIPASE A2 AT 2.5 ANGSTROMS. ACCESS TO A SHIELDED CATALYTIC CENTER
Authors : Brunie, S.; Sigler, P.B.
Deposited on : 1986-03-10
Resolution : 2.50 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
Xtrriage (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

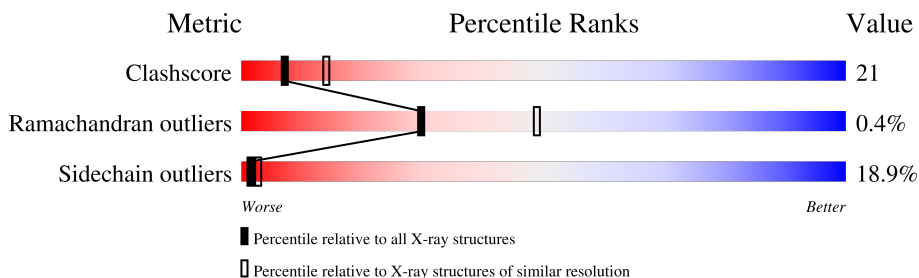
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	L	122	
1	R	122	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2029 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 CALCIUM-FREE PHOSPHOLIPASE A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	R	122	946	591	154	186	15	0	0	0
1	L	122	946	591	154	186	15	0	0	0

- Molecule 2 is water.

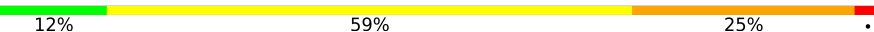
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	R	63	Total 63	O 63	0	0
2	L	74	Total 74	O 74	0	0

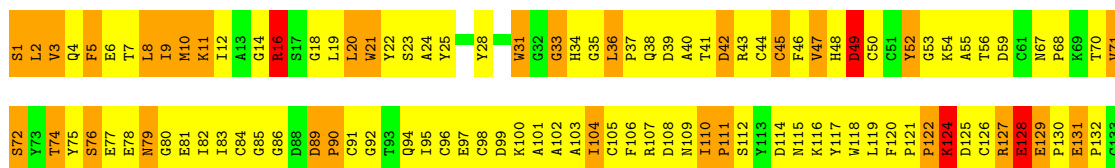
3 Residue-property plots [i](#)

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.

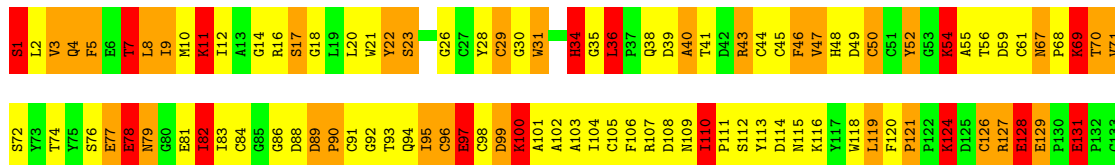
- Molecule 1: CALCIUM-FREE PHOSPHOLIPASE A2

Chain R: 



- Molecule 1: CALCIUM-FREE PHOSPHOLIPASE A2

Chain L: 



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.40Å 100.20Å 48.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.178 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2029	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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	L	1.90	12/973 (1.2%)	3.79	225/1320 (17.0%)
1	R	2.02	24/973 (2.5%)	3.82	237/1320 (18.0%)
All	All	1.96	36/1946 (1.8%)	3.81	462/2640 (17.5%)

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	L	0	1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	110	ILE	CA-CB	9.63	1.58	1.54
1	R	110	ILE	CA-CB	8.75	1.59	1.53
1	R	85	GLY	N-CA	8.09	1.54	1.45
1	R	128	GLU	N-CA	7.73	1.56	1.46
1	R	86	GLY	N-CA	-7.44	1.37	1.45
1	R	108	ASP	C-N	-7.34	1.21	1.34
1	R	96	CYS	C-O	7.23	1.32	1.24
1	L	45	CYS	C-N	-7.19	1.24	1.33
1	L	99	ASP	N-CA	7.07	1.54	1.46
1	R	105	CYS	C-O	7.04	1.32	1.24
1	R	28	TYR	CA-CB	6.93	1.64	1.53
1	R	43	ARG	CD-NE	6.69	1.55	1.46
1	R	38	GLN	C-N	-6.22	1.26	1.33
1	L	116	LYS	N-CA	6.18	1.54	1.46
1	R	128	GLU	C-O	6.01	1.30	1.23
1	R	75	TYR	N-CA	6.01	1.53	1.45
1	R	42	ASP	C-O	-5.91	1.17	1.24
1	R	43	ARG	CZ-NH2	5.89	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	40	ALA	N-CA	5.74	1.53	1.46
1	L	69	LYS	CA-CB	-5.71	1.44	1.53
1	R	48	HIS	CA-CB	5.67	1.62	1.53
1	L	121	PRO	C-O	-5.60	1.18	1.24
1	L	35	GLY	N-CA	5.54	1.52	1.45
1	R	40	ALA	C-N	-5.35	1.27	1.33
1	L	46	PHE	CA-CB	5.34	1.61	1.53
1	L	56	THR	CB-OG1	5.31	1.52	1.43
1	L	98	CYS	CA-C	5.25	1.59	1.52
1	R	22	TYR	CA-CB	5.24	1.62	1.54
1	R	83	ILE	N-CA	-5.23	1.40	1.46
1	R	120	PHE	C-O	-5.22	1.18	1.24
1	R	40	ALA	C-O	-5.18	1.18	1.24
1	R	72	SER	C-O	5.17	1.30	1.24
1	L	92	GLY	C-O	5.12	1.30	1.23
1	R	3	VAL	C-N	-5.11	1.26	1.33
1	L	46	PHE	N-CA	-5.10	1.40	1.46
1	R	117	TYR	N-CA	5.00	1.52	1.46

All (462) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	125	ASP	CA-CB-CG	23.81	136.41	112.60
1	L	4	GLN	OE1-CD-NE2	-17.49	105.11	122.60
1	L	16	ARG	NE-CZ-NH2	17.28	134.75	119.20
1	L	43	ARG	NE-CZ-NH1	16.65	138.15	121.50
1	L	129	GLU	CA-CB-CG	14.19	142.47	114.10
1	R	110	ILE	N-CA-CB	14.00	119.32	110.50
1	R	42	ASP	CA-CB-CG	13.60	126.20	112.60
1	R	85	GLY	CA-C-N	13.23	140.95	120.97
1	R	85	GLY	C-N-CA	13.23	140.95	120.97
1	R	67	ASN	CA-CB-CG	13.11	125.71	112.60
1	L	61	CYS	O-C-N	13.07	137.41	123.42
1	L	97	GLU	CA-CB-CG	12.87	139.84	114.10
1	L	94	GLN	CB-CG-CD	12.60	134.02	112.60
1	R	16	ARG	CD-NE-CZ	12.20	141.48	124.40
1	L	77	GLU	CA-C-O	-12.07	106.92	120.32
1	R	128	GLU	CG-CD-OE1	12.06	146.13	118.40
1	L	7	THR	CA-C-O	-11.93	106.62	120.10
1	R	124	LYS	CB-CG-CD	11.31	137.31	111.30
1	R	127	ARG	NE-CZ-NH1	11.25	132.75	121.50
1	L	38	GLN	OE1-CD-NE2	-11.24	111.36	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	99	ASP	CA-CB-CG	11.21	123.81	112.60
1	R	46	PHE	O-C-N	11.05	133.97	122.03
1	R	128	GLU	O-C-N	-11.04	109.87	123.12
1	L	4	GLN	CA-C-N	11.04	135.45	120.44
1	L	4	GLN	C-N-CA	11.04	135.45	120.44
1	L	17	SER	CA-CB-OG	10.90	132.90	111.10
1	L	16	ARG	CG-CD-NE	10.81	135.78	112.00
1	R	109	ASN	OD1-CG-ND2	-10.68	111.92	122.60
1	L	94	GLN	OE1-CD-NE2	-10.66	111.94	122.60
1	R	81	GLU	CA-C-N	10.64	136.95	123.12
1	R	81	GLU	C-N-CA	10.64	136.95	123.12
1	L	16	ARG	NH1-CZ-NH2	-10.63	105.48	119.30
1	R	55	ALA	CB-CA-C	-10.59	93.30	111.30
1	R	119	LEU	CB-CA-C	10.54	125.32	111.82
1	R	110	ILE	O-C-N	10.50	127.53	120.07
1	R	108	ASP	CA-C-O	-10.48	106.75	119.43
1	R	33	GLY	CA-C-O	10.47	130.65	119.02
1	L	50	CYS	CA-C-O	-10.45	109.47	120.55
1	R	108	ASP	CA-C-N	10.41	140.41	121.15
1	R	108	ASP	C-N-CA	10.41	140.41	121.15
1	L	43	ARG	NH1-CZ-NH2	-10.41	105.77	119.30
1	L	55	ALA	CA-C-O	-10.18	109.50	120.80
1	R	54	LYS	CA-CB-CG	10.16	134.41	114.10
1	L	94	GLN	CG-CD-NE2	10.15	131.63	116.40
1	L	45	CYS	CA-C-N	10.13	133.61	120.44
1	L	45	CYS	C-N-CA	10.13	133.61	120.44
1	R	8	LEU	O-C-N	-9.97	111.72	122.09
1	L	2	LEU	CA-C-O	-9.87	110.53	120.70
1	R	86	GLY	N-CA-C	9.77	125.01	110.75
1	L	47	VAL	N-CA-CB	9.76	127.33	110.65
1	L	52	TYR	CA-C-N	9.73	132.30	120.14
1	L	52	TYR	C-N-CA	9.73	132.30	120.14
1	R	71	VAL	CA-C-N	9.72	135.70	122.77
1	R	71	VAL	C-N-CA	9.72	135.70	122.77
1	L	78	GLU	CA-C-N	9.71	140.08	121.54
1	L	78	GLU	C-N-CA	9.71	140.08	121.54
1	R	6	GLU	CG-CD-OE1	9.62	140.54	118.40
1	L	76	SER	CA-C-O	-9.61	110.20	121.44
1	L	107	ARG	O-C-N	9.59	132.29	122.12
1	R	16	ARG	NE-CZ-NH1	9.57	131.07	121.50
1	L	129	GLU	CB-CG-CD	-9.52	96.41	112.60
1	R	124	LYS	CA-CB-CG	9.45	132.99	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	128	GLU	OE1-CD-OE2	-9.40	100.33	122.90
1	L	43	ARG	O-C-N	-9.38	111.45	122.15
1	R	54	LYS	CA-C-O	-9.37	107.12	119.11
1	L	61	CYS	CA-C-O	-9.27	111.32	121.23
1	L	16	ARG	O-C-N	9.26	133.80	123.33
1	L	11	LYS	CB-CG-CD	9.24	132.55	111.30
1	R	20	LEU	CA-C-O	-9.18	108.69	119.15
1	R	49	ASP	CB-CG-OD1	-9.13	97.40	118.40
1	R	68	PRO	CA-C-N	9.10	136.15	120.68
1	R	68	PRO	C-N-CA	9.10	136.15	120.68
1	L	119	LEU	O-C-N	-9.07	110.50	122.47
1	L	8	LEU	CA-C-N	9.04	131.95	120.56
1	L	8	LEU	C-N-CA	9.04	131.95	120.56
1	R	108	ASP	CB-CG-OD1	9.00	139.10	118.40
1	L	81	GLU	CA-C-O	-8.96	110.38	120.32
1	L	43	ARG	CD-NE-CZ	8.90	136.86	124.40
1	L	52	TYR	CA-C-O	8.89	130.15	120.10
1	L	119	LEU	CA-C-O	8.87	131.98	120.98
1	R	120	PHE	CA-C-O	-8.87	110.64	119.24
1	R	80	GLY	CA-C-O	8.82	128.70	119.27
1	R	5	PHE	CA-CB-CG	8.80	122.60	113.80
1	R	116	LYS	CG-CD-CE	8.78	131.49	111.30
1	L	99	ASP	CA-C-N	8.77	135.13	121.19
1	L	99	ASP	C-N-CA	8.77	135.13	121.19
1	R	54	LYS	CB-CG-CD	8.68	131.25	111.30
1	R	128	GLU	CB-CA-C	8.58	123.17	109.61
1	L	97	GLU	O-C-N	-8.52	113.09	122.12
1	R	49	ASP	N-CA-CB	-8.50	97.11	110.28
1	R	115	ASN	CA-C-N	8.46	134.85	120.72
1	R	115	ASN	C-N-CA	8.46	134.85	120.72
1	R	10	MET	N-CA-CB	-8.44	97.40	110.06
1	R	94	GLN	CA-C-N	8.43	131.18	120.56
1	R	94	GLN	C-N-CA	8.43	131.18	120.56
1	L	34	HIS	O-C-N	8.41	132.09	123.26
1	R	84	CYS	O-C-N	8.36	132.40	122.96
1	R	81	GLU	CA-C-O	-8.34	111.74	121.16
1	L	115	ASN	CA-CB-CG	-8.32	104.28	112.60
1	L	94	GLN	CA-C-O	8.31	129.52	119.97
1	R	49	ASP	CA-CB-CG	-8.29	104.31	112.60
1	L	4	GLN	O-C-N	-8.29	112.08	122.27
1	L	69	LYS	CA-CB-CG	8.28	130.65	114.10
1	L	97	GLU	CA-C-O	8.27	129.56	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	97	GLU	CA-C-N	8.27	132.03	120.29
1	L	97	GLU	C-N-CA	8.27	132.03	120.29
1	R	109	ASN	CA-C-O	-8.23	110.95	119.51
1	R	119	LEU	N-CA-CB	-8.21	99.12	112.25
1	L	3	VAL	CB-CA-C	-8.20	97.84	111.29
1	R	18	GLY	N-CA-C	-8.16	102.62	112.49
1	R	46	PHE	CA-C-O	-8.16	112.50	120.90
1	R	90	PRO	O-C-N	-8.13	113.40	122.18
1	L	93	THR	CA-C-N	8.09	132.60	120.31
1	L	93	THR	C-N-CA	8.09	132.60	120.31
1	R	122	PRO	O-C-N	8.07	131.94	122.17
1	L	88	ASP	CB-CG-OD1	8.06	136.93	118.40
1	R	77	GLU	CB-CG-CD	8.00	126.19	112.60
1	R	108	ASP	CA-CB-CG	8.00	120.59	112.60
1	L	128	GLU	CA-C-O	7.97	131.04	122.03
1	R	47	VAL	CA-C-N	7.95	131.28	120.54
1	R	47	VAL	C-N-CA	7.95	131.28	120.54
1	R	124	LYS	CA-C-N	7.94	134.60	122.37
1	R	124	LYS	C-N-CA	7.94	134.60	122.37
1	L	16	ARG	CA-C-O	-7.94	112.10	120.99
1	R	43	ARG	CA-C-O	-7.87	111.21	120.10
1	R	52	TYR	O-C-N	-7.86	113.02	122.22
1	L	109	ASN	CA-C-N	7.86	127.97	120.43
1	L	109	ASN	C-N-CA	7.86	127.97	120.43
1	L	3	VAL	N-CA-CB	7.85	124.17	111.23
1	L	47	VAL	CA-CB-CG1	7.83	123.72	110.40
1	L	56	THR	CA-CB-CG2	7.83	123.81	110.50
1	L	10	MET	O-C-N	-7.78	114.05	122.07
1	L	81	GLU	CB-CG-CD	7.77	125.81	112.60
1	R	116	LYS	CA-C-N	-7.73	110.28	122.65
1	R	116	LYS	C-N-CA	-7.73	110.28	122.65
1	R	55	ALA	N-CA-CB	7.72	121.85	110.35
1	L	12	ILE	N-CA-C	7.71	119.75	111.58
1	R	109	ASN	O-C-N	7.68	132.59	122.15
1	R	72	SER	N-CA-CB	-7.67	97.91	110.42
1	L	127	ARG	CB-CG-CD	-7.66	93.67	111.30
1	R	9	ILE	CA-C-O	-7.64	113.11	121.29
1	R	97	GLU	O-C-N	-7.63	114.03	122.12
1	R	46	PHE	N-CA-C	-7.60	102.60	111.03
1	L	74	THR	CA-C-O	-7.60	112.53	121.11
1	L	89	ASP	CA-C-N	7.58	127.61	119.28
1	L	89	ASP	C-N-CA	7.58	127.61	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	44	CYS	CA-C-N	7.57	130.73	120.44
1	L	44	CYS	C-N-CA	7.57	130.73	120.44
1	L	7	THR	O-C-N	7.56	131.06	122.22
1	R	20	LEU	CB-CA-C	7.54	122.77	109.65
1	R	129	GLU	CG-CD-OE2	-7.54	101.06	118.40
1	R	12	ILE	CA-C-O	-7.54	111.64	120.83
1	L	16	ARG	CD-NE-CZ	-7.53	113.86	124.40
1	R	49	ASP	OD1-CG-OD2	7.50	140.89	122.90
1	R	67	ASN	CB-CA-C	7.50	118.77	110.15
1	L	29	CYS	O-C-N	-7.45	113.10	122.27
1	R	37	PRO	CB-CA-C	7.44	121.01	111.64
1	L	112	SER	CA-C-O	-7.44	110.81	119.59
1	L	1	SER	N-CA-CB	-7.42	97.88	110.50
1	L	98	CYS	CA-CB-SG	7.40	131.42	114.40
1	L	70	THR	CB-CA-C	7.40	121.01	109.03
1	R	106	PHE	CA-CB-CG	7.38	121.18	113.80
1	L	121	PRO	CA-C-N	7.36	129.04	119.84
1	L	121	PRO	C-N-CA	7.36	129.04	119.84
1	R	83	ILE	CA-C-N	7.34	133.58	121.39
1	R	83	ILE	C-N-CA	7.34	133.58	121.39
1	R	71	VAL	O-C-N	-7.33	114.86	122.63
1	L	18	GLY	O-C-N	7.32	129.22	122.19
1	L	127	ARG	NE-CZ-NH2	-7.30	112.63	119.20
1	R	79	ASN	N-CA-CB	-7.30	98.16	110.49
1	L	94	GLN	O-C-N	-7.29	113.30	122.27
1	R	121	PRO	N-CA-C	7.29	119.59	110.70
1	L	3	VAL	CA-CB-CG2	7.27	122.75	110.40
1	L	78	GLU	CA-C-O	7.27	128.48	119.98
1	R	119	LEU	CA-C-N	7.25	137.37	121.63
1	R	119	LEU	C-N-CA	7.25	137.37	121.63
1	L	82	ILE	CA-C-N	-7.25	113.42	123.13
1	L	82	ILE	C-N-CA	-7.25	113.42	123.13
1	L	2	LEU	N-CA-C	-7.25	103.31	111.14
1	R	131	GLU	CA-CB-CG	7.22	128.54	114.10
1	L	28	TYR	N-CA-CB	-7.22	101.40	111.00
1	L	23	SER	O-C-N	7.21	132.10	122.43
1	L	47	VAL	CA-C-O	-7.18	112.89	120.57
1	R	16	ARG	O-C-N	7.16	131.41	123.25
1	R	103	ALA	CA-C-O	-7.16	112.83	120.42
1	R	96	CYS	CA-C-N	7.13	129.83	120.28
1	R	96	CYS	C-N-CA	7.13	129.83	120.28
1	R	24	ALA	N-CA-CB	-7.12	100.98	111.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	103	ALA	CA-C-O	-7.08	112.92	120.42
1	R	45	CYS	O-C-N	-7.06	112.72	122.46
1	R	50	CYS	CA-C-N	7.04	129.94	120.65
1	R	50	CYS	C-N-CA	7.04	129.94	120.65
1	L	88	ASP	CA-C-N	-7.04	113.84	122.64
1	L	88	ASP	C-N-CA	-7.04	113.84	122.64
1	R	79	ASN	CA-CB-CG	7.03	119.63	112.60
1	L	116	LYS	CA-CB-CG	7.03	128.15	114.10
1	R	59	ASP	CA-CB-CG	7.01	119.61	112.60
1	L	114	ASP	CB-CA-C	7.01	120.93	110.14
1	R	114	ASP	CA-C-O	6.98	127.77	120.30
1	L	17	SER	O-C-N	6.96	131.23	123.01
1	L	93	THR	CA-C-O	6.96	128.15	120.63
1	L	124	LYS	CD-CE-NZ	-6.95	89.67	111.90
1	L	56	THR	N-CA-C	-6.95	104.08	114.64
1	R	49	ASP	CB-CA-C	6.94	123.99	110.67
1	R	97	GLU	CA-C-N	6.94	129.46	120.44
1	R	97	GLU	C-N-CA	6.94	129.46	120.44
1	R	115	ASN	O-C-N	-6.92	113.22	122.43
1	L	90	PRO	CA-C-N	6.89	130.79	120.31
1	L	90	PRO	C-N-CA	6.89	130.79	120.31
1	L	77	GLU	N-CA-C	-6.86	97.17	108.76
1	L	49	ASP	CA-C-O	6.85	127.68	120.42
1	L	104	ILE	CA-C-O	6.83	128.05	120.95
1	L	1	SER	CB-CA-C	-6.83	97.13	110.10
1	L	102	ALA	N-CA-C	-6.82	102.98	112.45
1	R	8	LEU	CA-C-N	6.80	129.20	120.70
1	R	8	LEU	C-N-CA	6.80	129.20	120.70
1	R	116	LYS	N-CA-C	-6.78	104.26	112.54
1	R	28	TYR	N-CA-C	6.77	121.62	112.88
1	R	110	ILE	CB-CA-C	-6.76	107.18	114.35
1	R	108	ASP	N-CA-C	6.76	121.13	113.02
1	L	102	ALA	CA-C-O	-6.75	111.76	120.00
1	L	116	LYS	CA-C-N	6.75	133.46	122.65
1	L	116	LYS	C-N-CA	6.75	133.46	122.65
1	L	101	ALA	CA-C-O	-6.75	111.33	119.49
1	L	105	CYS	N-CA-CB	6.70	119.92	109.94
1	L	39	ASP	O-C-N	6.70	130.52	122.75
1	L	120	PHE	CA-C-O	6.69	126.11	119.49
1	R	122	PRO	CB-CA-C	-6.65	101.16	112.26
1	R	83	ILE	O-C-N	-6.64	116.21	123.18
1	R	101	ALA	CA-C-N	6.63	129.06	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	101	ALA	C-N-CA	6.63	129.06	120.44
1	L	106	PHE	CA-C-N	6.59	129.41	120.38
1	L	106	PHE	C-N-CA	6.59	129.41	120.38
1	R	100	LYS	CA-C-N	6.58	129.00	120.44
1	R	100	LYS	C-N-CA	6.58	129.00	120.44
1	L	2	LEU	O-C-N	6.58	129.20	122.09
1	R	103	ALA	O-C-N	6.56	129.63	122.15
1	R	20	LEU	N-CA-CB	-6.55	100.78	110.53
1	R	56	THR	CA-CB-CG2	6.54	121.61	110.50
1	R	117	TYR	CB-CA-C	6.54	121.60	110.56
1	L	81	GLU	O-C-N	6.54	130.96	123.31
1	L	78	GLU	N-CA-CB	6.51	119.88	110.37
1	L	10	MET	N-CA-CB	-6.50	100.59	110.01
1	L	34	HIS	CB-CA-C	-6.48	98.47	111.17
1	R	43	ARG	O-C-N	6.46	129.78	122.22
1	L	79	ASN	CA-C-O	6.46	129.75	120.51
1	L	100	LYS	CB-CA-C	-6.46	100.11	110.84
1	L	31	TRP	CA-C-O	-6.46	111.28	120.51
1	R	54	LYS	N-CA-CB	6.45	121.24	110.41
1	R	121	PRO	CA-C-N	6.43	126.93	119.47
1	R	121	PRO	C-N-CA	6.43	126.93	119.47
1	R	131	GLU	CA-C-O	-6.42	114.82	120.60
1	R	16	ARG	NE-CZ-NH2	-6.38	113.46	119.20
1	L	119	LEU	CB-CA-C	6.38	120.31	111.63
1	R	97	GLU	CA-C-O	6.37	127.30	120.55
1	L	49	ASP	OD1-CG-OD2	6.35	138.15	122.90
1	L	29	CYS	CA-C-N	6.33	133.81	121.41
1	L	29	CYS	C-N-CA	6.33	133.81	121.41
1	L	41	THR	O-C-N	-6.32	115.42	122.12
1	L	22	TYR	N-CA-CB	-6.31	101.16	111.01
1	R	126	CYS	CA-C-N	6.30	129.89	120.31
1	R	126	CYS	C-N-CA	6.30	129.89	120.31
1	L	108	ASP	CA-C-O	-6.30	111.69	119.18
1	L	99	ASP	CB-CA-C	6.29	120.69	110.95
1	L	10	MET	CB-CA-C	6.27	120.73	110.88
1	R	59	ASP	CA-C-O	-6.27	112.22	119.56
1	R	102	ALA	N-CA-CB	6.26	119.09	110.01
1	R	48	HIS	CA-CB-CG	-6.24	107.56	113.80
1	R	127	ARG	NE-CZ-NH2	-6.23	113.59	119.20
1	L	36	LEU	CA-C-O	-6.23	111.95	119.67
1	L	102	ALA	O-C-N	6.21	131.41	122.28
1	L	36	LEU	CB-CA-C	6.20	116.79	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	34	HIS	CE1-NE2-CD2	6.18	115.18	109.00
1	R	92	GLY	CA-C-N	6.18	128.84	120.44
1	R	92	GLY	C-N-CA	6.18	128.84	120.44
1	L	89	ASP	CB-CG-OD1	6.17	132.58	118.40
1	L	113	TYR	CA-CB-CG	6.17	125.00	113.90
1	R	115	ASN	OD1-CG-ND2	-6.16	116.44	122.60
1	L	44	CYS	CA-C-O	6.16	127.28	120.63
1	R	22	TYR	CA-C-O	-6.15	112.08	119.03
1	R	54	LYS	N-CA-C	-6.15	105.74	113.18
1	R	71	VAL	CA-CB-CG2	6.14	120.85	110.40
1	R	25	TYR	O-C-N	6.14	130.21	123.27
1	L	48	HIS	O-C-N	6.13	129.14	122.15
1	L	104	ILE	CA-C-N	6.12	128.80	120.54
1	L	104	ILE	C-N-CA	6.12	128.80	120.54
1	L	38	GLN	CG-CD-OE1	6.11	133.02	120.80
1	R	2	LEU	N-CA-CB	6.11	119.04	109.94
1	R	48	HIS	CA-C-O	6.07	127.39	120.90
1	R	109	ASN	N-CA-C	-6.06	103.39	112.54
1	L	46	PHE	CB-CA-C	6.05	120.39	110.88
1	R	34	HIS	CA-C-O	6.03	127.84	120.60
1	R	116	LYS	CA-CB-CG	6.03	126.15	114.10
1	R	40	ALA	N-CA-C	-6.03	104.40	110.97
1	R	18	GLY	CA-C-O	-6.02	114.16	120.90
1	L	116	LYS	CB-CA-C	5.99	122.50	109.99
1	L	5	PHE	N-CA-C	-5.98	104.69	111.14
1	R	33	GLY	O-C-N	-5.98	114.80	122.39
1	R	55	ALA	CA-C-O	-5.97	114.71	120.92
1	R	108	ASP	CB-CG-OD2	-5.97	104.66	118.40
1	R	37	PRO	N-CA-C	-5.97	101.84	111.03
1	R	8	LEU	CA-C-O	5.96	127.28	120.90
1	R	129	GLU	CG-CD-OE1	5.96	132.10	118.40
1	R	10	MET	CA-C-O	5.95	127.06	120.63
1	R	97	GLU	OE1-CD-OE2	-5.95	108.62	122.90
1	R	4	GLN	CA-C-N	5.94	129.05	120.79
1	R	4	GLN	C-N-CA	5.94	129.05	120.79
1	R	44	CYS	N-CA-CB	5.93	118.83	110.12
1	R	132	PRO	N-CA-CB	5.92	108.50	103.35
1	L	26	GLY	CA-C-O	-5.91	114.47	122.39
1	L	67	ASN	O-C-N	5.90	126.01	121.23
1	L	4	GLN	CG-CD-OE1	5.89	132.58	120.80
1	L	69	LYS	CA-C-O	-5.89	112.67	119.14
1	L	56	THR	CB-CA-C	5.87	118.16	109.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	114	ASP	CB-CG-OD2	5.87	131.89	118.40
1	L	28	TYR	N-CA-C	5.86	122.00	114.56
1	R	129	GLU	CB-CA-C	-5.86	100.65	109.26
1	L	86	GLY	CA-C-O	5.86	126.27	122.23
1	R	39	ASP	CA-C-O	5.85	126.23	120.56
1	R	74	THR	CA-C-N	-5.83	112.76	122.21
1	R	74	THR	C-N-CA	-5.83	112.76	122.21
1	L	106	PHE	O-C-N	-5.83	115.97	122.03
1	L	50	CYS	O-C-N	5.83	128.30	122.12
1	R	85	GLY	N-CA-C	-5.80	99.63	110.66
1	L	16	ARG	N-CA-CB	5.80	122.30	111.52
1	L	110	ILE	CA-C-O	5.79	123.11	118.71
1	L	84	CYS	CA-C-O	-5.78	115.26	121.56
1	L	124	LYS	CA-C-N	5.78	132.51	122.56
1	L	124	LYS	C-N-CA	5.78	132.51	122.56
1	R	21	TRP	N-CA-C	-5.78	106.87	114.04
1	R	1	SER	CA-C-O	5.77	130.62	120.80
1	L	48	HIS	CA-C-O	-5.76	114.31	120.42
1	R	10	MET	CB-CG-SD	5.75	129.94	112.70
1	R	12	ILE	N-CA-C	5.73	116.78	111.45
1	R	34	HIS	ND1-CE1-NE2	-5.73	102.67	108.40
1	L	109	ASN	O-C-N	-5.73	115.30	122.24
1	R	125	ASP	N-CA-C	-5.73	104.86	112.94
1	R	71	VAL	CA-C-O	5.72	127.65	121.36
1	L	36	LEU	CA-C-N	5.71	126.98	119.84
1	L	36	LEU	C-N-CA	5.71	126.98	119.84
1	R	31	TRP	CA-CB-CG	5.69	124.41	113.60
1	L	9	ILE	O-C-N	-5.68	116.34	121.91
1	L	10	MET	CA-C-O	5.67	126.78	120.82
1	L	14	GLY	CA-C-O	-5.67	112.80	119.72
1	R	3	VAL	O-C-N	-5.66	116.15	121.87
1	R	111	PRO	CA-C-N	-5.66	112.83	122.56
1	R	111	PRO	C-N-CA	-5.66	112.83	122.56
1	R	83	ILE	CA-C-O	5.64	126.46	120.48
1	L	105	CYS	CA-C-N	5.64	128.10	120.65
1	L	105	CYS	C-N-CA	5.64	128.10	120.65
1	R	40	ALA	CA-C-N	5.64	128.16	120.54
1	R	40	ALA	C-N-CA	5.64	128.16	120.54
1	L	22	TYR	CB-CA-C	-5.64	100.72	109.80
1	R	44	CYS	O-C-N	5.64	128.10	122.12
1	L	95	ILE	CB-CA-C	5.61	121.30	112.16
1	R	6	GLU	OE1-CD-OE2	-5.61	109.45	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	128	GLU	N-CA-CB	-5.61	100.31	109.56
1	R	104	ILE	O-C-N	-5.58	116.09	121.90
1	L	50	CYS	CA-C-N	5.57	130.02	120.71
1	L	50	CYS	C-N-CA	5.57	130.02	120.71
1	L	131	GLU	CB-CG-CD	-5.57	103.12	112.60
1	R	42	ASP	CB-CG-OD2	5.55	131.18	118.40
1	L	69	LYS	N-CA-CB	-5.55	102.37	110.53
1	R	6	GLU	CB-CA-C	5.55	119.68	110.81
1	R	84	CYS	CA-C-O	-5.54	115.09	121.47
1	L	5	PHE	CA-C-O	-5.54	114.99	120.70
1	L	126	CYS	N-CA-CB	-5.54	103.31	111.51
1	L	49	ASP	CB-CA-C	-5.53	101.45	110.85
1	R	22	TYR	N-CA-C	5.53	122.62	113.89
1	R	98	CYS	N-CA-C	-5.53	105.16	111.07
1	R	106	PHE	N-CA-CB	5.53	118.03	110.01
1	L	79	ASN	O-C-N	-5.53	115.24	122.59
1	L	129	GLU	CB-CA-C	5.53	117.38	109.26
1	L	46	PHE	N-CA-C	-5.52	105.16	111.07
1	L	23	SER	CA-C-O	-5.52	112.59	119.38
1	R	112	SER	CA-C-O	-5.49	112.78	119.43
1	L	108	ASP	CB-CG-OD2	-5.49	105.77	118.40
1	R	8	LEU	CB-CA-C	5.48	119.58	110.81
1	L	86	GLY	O-C-N	-5.48	116.28	122.64
1	R	34	HIS	N-CA-C	5.46	118.34	109.06
1	R	52	TYR	CA-C-N	5.46	130.50	120.79
1	R	52	TYR	C-N-CA	5.46	130.50	120.79
1	R	3	VAL	CA-CB-CG2	5.45	119.67	110.40
1	L	11	LYS	N-CA-CB	5.45	117.91	110.01
1	R	117	TYR	CA-C-N	5.45	129.66	122.42
1	R	117	TYR	C-N-CA	5.45	129.66	122.42
1	R	125	ASP	OD1-CG-OD2	-5.44	109.84	122.90
1	L	55	ALA	N-CA-C	-5.43	100.85	109.76
1	R	20	LEU	CA-CB-CG	5.43	135.31	116.30
1	R	70	THR	CA-CB-OG1	-5.42	101.47	109.60
1	L	86	GLY	CA-C-N	5.42	133.15	122.31
1	L	86	GLY	C-N-CA	5.42	133.15	122.31
1	R	11	LYS	CB-CA-C	5.41	120.04	110.85
1	R	7	THR	CA-CB-OG1	-5.41	101.49	109.60
1	L	34	HIS	CA-C-O	-5.40	115.66	121.38
1	R	109	ASN	CB-CG-ND2	5.40	124.50	116.40
1	L	98	CYS	N-CA-CB	5.39	118.13	110.16
1	L	129	GLU	N-CA-C	-5.37	103.27	109.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	91	CYS	N-CA-C	-5.37	105.59	111.82
1	L	107	ARG	CA-CB-CG	5.37	124.84	114.10
1	L	54	LYS	CB-CG-CD	5.35	123.60	111.30
1	L	79	ASN	N-CA-CB	5.32	119.48	110.49
1	R	132	PRO	CA-C-O	5.31	127.72	121.56
1	L	18	GLY	N-CA-C	-5.31	106.06	112.49
1	R	86	GLY	CA-C-O	5.31	127.17	121.75
1	L	96	CYS	CA-C-N	5.31	127.66	120.38
1	L	96	CYS	C-N-CA	5.31	127.66	120.38
1	R	67	ASN	O-C-N	5.31	127.87	121.29
1	L	8	LEU	O-C-N	-5.29	115.35	122.23
1	L	99	ASP	CA-C-O	-5.28	115.46	120.90
1	R	99	ASP	CA-C-N	5.28	127.62	120.44
1	R	99	ASP	C-N-CA	5.28	127.62	120.44
1	L	43	ARG	CA-C-O	5.28	126.01	120.42
1	R	36	LEU	O-C-N	5.27	127.82	121.60
1	R	5	PHE	N-CA-C	-5.26	104.61	111.02
1	L	107	ARG	CB-CA-C	-5.26	101.74	110.68
1	L	103	ALA	CB-CA-C	5.25	119.78	110.85
1	R	91	CYS	O-C-N	-5.23	115.84	122.27
1	R	109	ASN	CA-C-N	5.21	123.52	120.24
1	R	109	ASN	C-N-CA	5.21	123.52	120.24
1	L	59	ASP	N-CA-C	5.21	119.74	113.17
1	L	108	ASP	CB-CA-C	-5.21	99.72	109.72
1	R	45	CYS	CA-C-N	5.19	127.69	120.63
1	R	45	CYS	C-N-CA	5.19	127.69	120.63
1	L	112	SER	N-CA-CB	5.19	118.77	110.73
1	R	18	GLY	O-C-N	5.18	127.17	122.19
1	R	131	GLU	CG-CD-OE2	-5.17	106.50	118.40
1	L	74	THR	CA-C-N	5.17	130.59	122.21
1	L	74	THR	C-N-CA	5.17	130.59	122.21
1	R	110	ILE	CB-CG1-CD1	5.16	124.64	113.80
1	R	127	ARG	CA-C-O	5.16	125.91	119.97
1	R	16	ARG	CB-CG-CD	-5.13	99.49	111.30
1	L	49	ASP	N-CA-C	5.13	116.95	111.36
1	L	11	LYS	O-C-N	5.13	127.35	122.07
1	R	1	SER	N-CA-C	5.12	125.35	111.00
1	R	125	ASP	CA-C-N	5.11	130.68	122.14
1	R	125	ASP	C-N-CA	5.11	130.68	122.14
1	L	109	ASN	CB-CA-C	5.11	118.81	110.17
1	L	40	ALA	CA-C-O	-5.10	115.64	121.00
1	R	45	CYS	N-CA-CB	5.10	118.71	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	75	TYR	N-CA-C	-5.08	101.56	109.24
1	R	115	ASN	CA-C-O	5.08	125.51	119.10
1	L	49	ASP	CA-C-N	5.08	127.09	120.28
1	L	49	ASP	C-N-CA	5.08	127.09	120.28
1	R	114	ASP	CA-CB-CG	5.08	117.68	112.60
1	R	89	ASP	CA-CB-CG	5.07	117.67	112.60
1	R	107	ARG	NE-CZ-NH1	-5.07	116.43	121.50
1	R	11	LYS	CD-CE-NZ	5.07	128.11	111.90
1	R	42	ASP	OD1-CG-OD2	-5.06	110.75	122.90
1	R	12	ILE	CB-CA-C	-5.06	105.29	111.92
1	L	89	ASP	OD1-CG-OD2	-5.05	110.78	122.90
1	L	23	SER	N-CA-C	-5.05	106.38	112.54
1	L	119	LEU	N-CA-CB	-5.05	104.53	112.46
1	L	88	ASP	CB-CG-OD2	-5.04	106.80	118.40
1	R	44	CYS	CA-C-O	-5.04	115.20	120.55
1	R	102	ALA	CB-CA-C	-5.04	102.96	110.88
1	L	116	LYS	N-CA-C	-5.04	106.64	112.89
1	L	46	PHE	CA-CB-CG	-5.03	108.77	113.80
1	R	70	THR	O-C-N	-5.03	116.81	122.34
1	R	46	PHE	N-CA-CB	5.02	117.26	109.98
1	L	94	GLN	CA-CB-CG	5.02	124.14	114.10
1	L	9	ILE	N-CA-C	-5.02	105.60	110.42

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	127	ARG	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	L	946	0	854	56	0
1	R	946	0	853	31	0
2	L	74	0	0	2	0
2	R	63	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2029	0	1707	75	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 21.

All (75) 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:R:118:TRP:HE1	1:L:124:LYS:NZ	1.49	1.09
1:R:118:TRP:HE1	1:L:124:LYS:HZ3	1.07	1.02
1:L:36:LEU:HD12	1:L:128:GLU:HG3	1.42	1.01
1:L:11:LYS:HE3	1:L:82:ILE:HD11	1.46	0.94
1:R:53:GLY:HA2	1:L:70:THR:HG21	1.58	0.85
1:R:118:TRP:NE1	1:L:124:LYS:NZ	2.24	0.84
1:L:68:PRO:HA	1:L:95:ILE:HD13	1.61	0.83
1:R:36:LEU:N	1:R:128:GLU:OE2	2.15	0.80
1:L:124:LYS:H	1:L:124:LYS:CD	1.96	0.78
1:L:11:LYS:HE3	1:L:82:ILE:CD1	2.15	0.76
1:R:78:GLU:O	1:R:79:ASN:HB2	1.84	0.74
1:R:118:TRP:NE1	1:L:124:LYS:HZ3	1.83	0.73
1:L:68:PRO:HG3	1:L:95:ILE:HD11	1.72	0.72
1:R:89:ASP:HB2	1:R:90:PRO:HD2	1.72	0.71
1:L:36:LEU:HD12	1:L:128:GLU:CG	2.17	0.71
1:L:124:LYS:H	1:L:124:LYS:HD3	1.56	0.70
1:R:118:TRP:HE1	1:L:124:LYS:HZ1	1.37	0.70
1:L:11:LYS:CE	1:L:82:ILE:HD11	2.22	0.69
1:L:40:ALA:HA	1:L:43:ARG:HD2	1.74	0.69
1:L:121:PRO:HB3	1:L:124:LYS:HE2	1.76	0.67
1:L:5:PHE:CE2	1:L:9:ILE:HD11	2.30	0.67
1:R:49:ASP:OD1	2:R:573:HOH:O	2.14	0.65
1:L:34:HIS:HB2	1:L:126:CYS:O	1.97	0.65
1:R:118:TRP:NE1	1:L:124:LYS:HZ1	1.92	0.64
1:R:110:ILE:N	1:R:111:PRO:CD	2.61	0.63
1:L:97:GLU:OE1	1:L:100:LYS:NZ	2.33	0.62
1:L:17:SER:O	1:L:21:TRP:HB2	2.02	0.60
1:L:110:ILE:N	1:L:111:PRO:HD2	2.16	0.60
1:R:23:SER:HA	1:L:31:TRP:CE3	2.38	0.59
1:L:5:PHE:CZ	1:L:9:ILE:HD11	2.37	0.59
1:L:3:VAL:HG12	1:L:3:VAL:O	2.02	0.58
1:L:4:GLN:OE1	1:L:72:SER:HA	2.04	0.57
1:L:1:SER:N	1:L:71:VAL:O	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:36:LEU:HB2	1:R:128:GLU:OE2	2.06	0.55
1:L:124:LYS:CD	1:L:124:LYS:N	2.69	0.55
1:L:11:LYS:NZ	2:L:567:HOH:O	2.40	0.55
1:R:129:GLU:HG3	1:R:130:PRO:HD2	1.88	0.54
1:L:110:ILE:N	1:L:111:PRO:CD	2.72	0.52
1:R:45:CYS:O	1:R:49:ASP:HB2	2.10	0.51
1:R:124:LYS:O	1:R:127:ARG:HD2	2.11	0.51
1:R:31:TRP:CE3	1:L:23:SER:HA	2.46	0.51
1:L:3:VAL:O	1:L:7:THR:HG23	2.10	0.50
1:R:16:ARG:HB3	1:R:21:TRP:CD1	2.47	0.49
1:R:35:GLY:HA2	1:R:128:GLU:HB2	1.94	0.49
1:L:78:GLU:HG2	1:L:83:ILE:HD13	1.95	0.49
1:R:52:TYR:O	1:L:67:ASN:ND2	2.46	0.49
1:R:76:SER:O	1:R:82:ILE:HA	2.13	0.48
1:R:1:SER:N	1:R:71:VAL:O	2.23	0.48
1:L:50:CYS:O	1:L:54:LYS:HD2	2.14	0.48
1:L:121:PRO:CB	1:L:124:LYS:HD3	2.44	0.48
1:L:46:PHE:CZ	1:L:131:GLU:HG3	2.48	0.47
1:L:3:VAL:O	1:L:3:VAL:CG1	2.63	0.47
1:L:68:PRO:HG3	1:L:95:ILE:CD1	2.43	0.47
1:R:127:ARG:O	1:R:128:GLU:C	2.59	0.46
1:L:110:ILE:HG22	1:L:111:PRO:N	2.29	0.46
1:L:68:PRO:CA	1:L:95:ILE:HD13	2.40	0.46
1:L:70:THR:O	1:L:71:VAL:C	2.58	0.45
1:R:33:GLY:O	1:R:130:PRO:HG3	2.16	0.45
1:R:5:PHE:CE1	1:R:9:ILE:HD11	2.52	0.45
1:L:3:VAL:O	1:L:7:THR:CG2	2.65	0.44
1:L:5:PHE:O	1:L:9:ILE:HG13	2.18	0.44
1:L:1:SER:HB3	1:L:4:GLN:H	1.83	0.44
1:L:89:ASP:HA	1:L:90:PRO:HD2	1.81	0.44
1:R:14:GLY:O	1:R:16:ARG:HG3	2.17	0.44
1:R:104:ILE:HD13	1:R:104:ILE:HG21	1.83	0.43
1:L:52:TYR:OH	1:L:99:ASP:OD1	2.34	0.43
1:L:69:LYS:HE3	2:L:535:HOH:O	2.20	0.42
1:L:96:CYS:O	1:L:99:ASP:HB2	2.20	0.42
1:R:122:PRO:HG2	1:L:118:TRP:CZ2	2.55	0.41
1:R:41:THR:O	1:R:42:ASP:C	2.62	0.40
1:R:118:TRP:CE2	1:L:124:LYS:NZ	2.88	0.40
1:L:30:GLY:O	1:L:31:TRP:C	2.64	0.40
1:L:22:TYR:O	1:L:29:CYS:HB3	2.22	0.40
1:L:110:ILE:HG22	1:L:111:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:110:ILE:HB	1:L:111:PRO:HD3	2.03	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	L	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	16	31
1	R	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
All	All	240/244 (98%)	224 (93%)	15 (6%)	1 (0%)	30	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	79	ASN

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	L	103/103 (100%)	81 (79%)	22 (21%)	1	2
1	R	103/103 (100%)	86 (84%)	17 (16%)	2	4
All	All	206/206 (100%)	167 (81%)	39 (19%)	1	3

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	2	LEU
1	R	3	VAL
1	R	8	LEU
1	R	10	MET
1	R	11	LYS
1	R	16	ARG
1	R	19	LEU
1	R	20	LEU
1	R	47	VAL
1	R	49	ASP
1	R	72	SER
1	R	74	THR
1	R	76	SER
1	R	95	ILE
1	R	124	LYS
1	R	128	GLU
1	R	131	GLU
1	L	1	SER
1	L	7	THR
1	L	8	LEU
1	L	11	LYS
1	L	20	LEU
1	L	34	HIS
1	L	36	LEU
1	L	47	VAL
1	L	54	LYS
1	L	69	LYS
1	L	71	VAL
1	L	77	GLU
1	L	78	GLU
1	L	82	ILE
1	L	97	GLU
1	L	100	LYS
1	L	110	ILE
1	L	119	LEU
1	L	124	LYS
1	L	128	GLU
1	L	129	GLU
1	L	131	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

There are no ligands in this entry.

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.