



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:40 PM UTC

PDB ID : 1LYN / pdb_00001lyn
Title : CRYSTAL STRUCTURE AND SUBUNIT DYNAMICS OF THE LYSIN DIMER: EGG ENVELOPES DISSOCIATE DIMERS, THE MONOMER IS THE ACTIVE SPECIES
Authors : Shaw, A.; Vacquier, V.D.; Stout, C.D.
Deposited on : 1995-03-03
Resolution : 2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

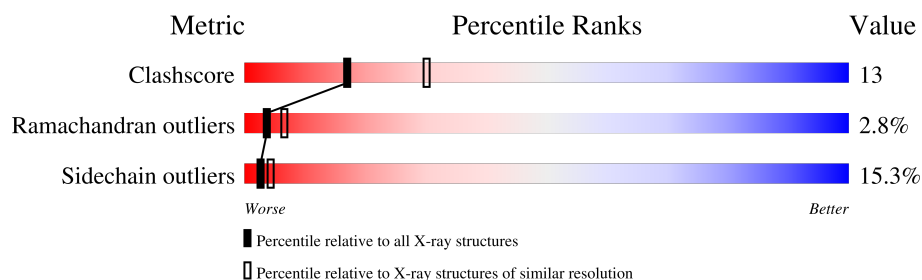
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	136	
1	B	136	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2094 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 SPERM LYSIN.

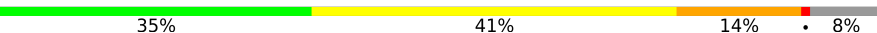
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	125	Total	C	N	O	S	0	0	0
			1047	685	185	171	6			
1	B	125	Total	C	N	O	S	0	0	0
			1047	685	185	171	6			

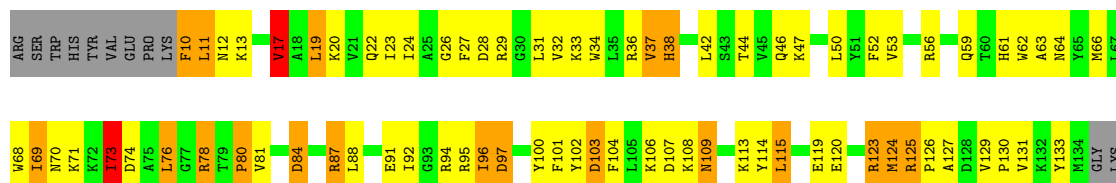
3 Residue-property plots [i](#)

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.

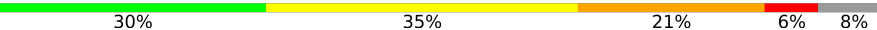
Note EDS was not executed.

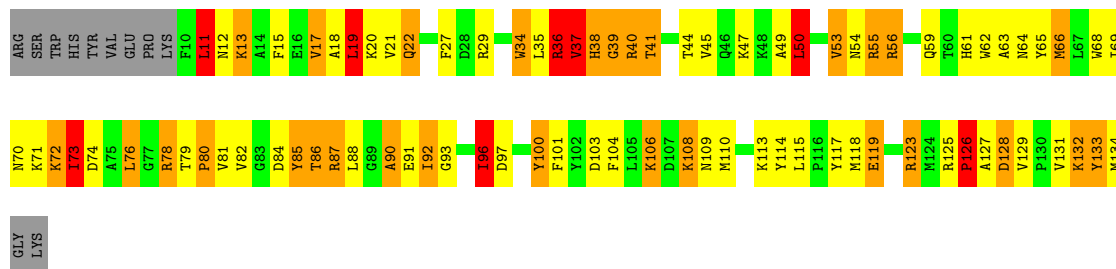
• Molecule 1: SPERM LYSIN

Chain A: 



• Molecule 1: SPERM LYSIN

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	51.20Å 47.00Å 123.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.75	Depositor
% Data completeness (in resolution range)	93.6 (8.00-2.75)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.233 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2094	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.47	6/1074 (0.6%)	2.43	81/1448 (5.6%)
1	B	1.50	13/1074 (1.2%)	2.52	97/1448 (6.7%)
All	All	1.49	19/2148 (0.9%)	2.47	178/2896 (6.1%)

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	1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	HIS	CD2-NE2	-7.75	1.29	1.37
1	A	46	GLN	CA-CB	-7.49	1.41	1.53
1	B	38	HIS	CD2-NE2	-7.29	1.29	1.37
1	B	40	ARG	CA-CB	6.84	1.65	1.53
1	B	61	HIS	CD2-NE2	-6.70	1.30	1.37
1	B	61	HIS	CG-ND1	-6.24	1.31	1.38
1	A	38	HIS	CG-ND1	-5.91	1.31	1.38
1	B	20	LYS	CA-CB	-5.81	1.44	1.53
1	A	38	HIS	CA-CB	-5.78	1.45	1.54
1	B	131	VAL	CA-CB	5.75	1.61	1.54
1	A	38	HIS	CD2-NE2	-5.74	1.31	1.37
1	B	80	PRO	CA-CB	-5.67	1.46	1.53
1	B	76	LEU	CA-CB	-5.63	1.43	1.53
1	B	126	PRO	CA-CB	-5.44	1.46	1.53
1	B	21	VAL	CA-CB	-5.42	1.47	1.54
1	A	87	ARG	NE-CZ	5.33	1.39	1.33
1	B	87	ARG	CA-CB	5.17	1.61	1.53
1	B	40	ARG	N-CA	5.16	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	87	ARG	NE-CZ	5.14	1.38	1.33

All (178) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	128	ASP	CA-CB-CG	12.59	125.19	112.60
1	A	22	GLN	OE1-CD-NE2	-10.66	111.94	122.60
1	B	65	TYR	N-CA-C	-8.79	99.38	112.04
1	B	103	ASP	O-C-N	-8.74	112.18	122.15
1	B	47	LYS	N-CA-C	-8.70	101.71	111.71
1	B	101	PHE	N-CA-C	-8.68	101.40	111.03
1	A	74	ASP	CA-CB-CG	8.44	121.04	112.60
1	A	12	ASN	OD1-CG-ND2	-8.38	114.22	122.60
1	B	76	LEU	N-CA-C	8.14	122.17	111.75
1	A	12	ASN	CB-CG-ND2	8.07	128.50	116.40
1	A	133	TYR	N-CA-C	8.01	121.58	109.41
1	A	36	ARG	CA-CB-CG	8.01	130.12	114.10
1	A	125	ARG	CG-CD-NE	7.82	129.21	112.00
1	B	36	ARG	CA-CB-CG	7.77	129.65	114.10
1	B	86	THR	CB-CA-C	7.68	122.93	110.88
1	B	38	HIS	CB-CG-CD2	-7.65	121.26	131.20
1	B	68	TRP	CG-CD2-CE3	7.63	141.53	133.90
1	B	38	HIS	CB-CG-ND1	7.59	134.08	122.70
1	A	126	PRO	O-C-N	-7.48	113.64	122.24
1	B	29	ARG	N-CA-C	-7.46	103.44	112.54
1	B	21	VAL	CA-CB-CG2	-7.45	97.74	110.40
1	A	97	ASP	CA-CB-CG	-7.39	105.21	112.60
1	B	86	THR	N-CA-CB	-7.36	99.33	110.01
1	B	40	ARG	CA-CB-CG	7.33	128.75	114.10
1	B	36	ARG	O-C-N	-7.31	112.87	122.59
1	A	26	GLY	CA-C-O	-7.23	112.80	120.90
1	B	37	VAL	O-C-N	-7.21	113.55	122.57
1	B	96	ILE	CB-CG1-CD1	-7.21	98.65	113.80
1	A	123	ARG	CA-CB-CG	-7.18	99.73	114.10
1	B	71	LYS	O-C-N	-7.13	113.11	122.59
1	A	10	PHE	CA-CB-CG	-7.12	106.69	113.80
1	B	108	LYS	CG-CD-CE	6.99	127.38	111.30
1	B	11	LEU	N-CA-C	-6.97	96.89	108.32
1	B	106	LYS	CA-C-O	-6.95	113.70	121.00
1	B	34	TRP	CG-CD2-CE3	6.94	140.84	133.90
1	B	59	GLN	OE1-CD-NE2	-6.94	115.66	122.60
1	B	90	ALA	CA-C-N	6.93	129.44	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	ALA	C-N-CA	6.93	129.44	120.44
1	B	49	ALA	N-CA-C	-6.89	103.46	110.97
1	B	74	ASP	CA-CB-CG	6.88	119.48	112.60
1	B	66	MET	CG-SD-CE	-6.87	85.79	100.90
1	A	17	VAL	CA-CB-CG2	-6.74	98.94	110.40
1	A	28	ASP	CA-CB-CG	6.73	119.33	112.60
1	B	110	MET	CG-SD-CE	-6.71	86.13	100.90
1	A	24	ILE	CA-C-O	-6.68	113.36	120.64
1	B	53	VAL	N-CA-CB	-6.66	102.14	110.47
1	A	17	VAL	CA-CB-CG1	6.64	121.68	110.40
1	A	115	LEU	CA-C-N	6.57	126.81	119.32
1	A	115	LEU	C-N-CA	6.57	126.81	119.32
1	B	97	ASP	CA-C-O	6.57	129.65	120.52
1	A	109	ASN	CB-CA-C	-6.49	102.21	111.95
1	A	84	ASP	CA-CB-CG	6.48	119.08	112.60
1	B	22	GLN	OE1-CD-NE2	-6.48	116.12	122.60
1	B	63	ALA	N-CA-C	6.48	120.04	111.75
1	A	124	MET	CB-CA-C	-6.47	97.63	109.54
1	B	44	THR	N-CA-C	6.44	117.96	111.07
1	B	84	ASP	N-CA-C	-6.44	104.35	111.82
1	B	91	GLU	N-CA-C	6.43	117.95	111.07
1	B	34	TRP	CE2-CD2-CG	-6.41	99.50	107.20
1	A	103	ASP	CA-CB-CG	6.38	118.98	112.60
1	A	130	PRO	O-C-N	-6.34	115.99	123.10
1	B	114	TYR	N-CA-C	6.31	118.72	108.63
1	A	97	ASP	N-CA-C	6.30	119.08	107.99
1	A	124	MET	N-CA-CB	6.28	119.21	110.17
1	A	33	LYS	O-C-N	-6.26	115.62	122.07
1	B	133	TYR	N-CA-C	6.24	118.79	109.25
1	B	119	GLU	CA-CB-CG	-6.20	101.70	114.10
1	B	37	VAL	CG1-CB-CG2	-6.18	97.20	110.80
1	A	34	TRP	CB-CG-CD1	-6.15	117.68	126.90
1	B	87	ARG	CA-CB-CG	6.14	126.37	114.10
1	B	12	ASN	OD1-CG-ND2	-6.13	116.47	122.60
1	B	54	ASN	CB-CA-C	-6.09	101.31	110.88
1	A	64	ASN	OD1-CG-ND2	-6.07	116.53	122.60
1	B	35	LEU	CA-C-O	-6.07	114.45	120.82
1	A	56	ARG	CA-CB-CG	-6.05	101.99	114.10
1	A	46	GLN	N-CA-C	-6.05	104.98	112.90
1	B	41	THR	N-CA-CB	-6.04	99.33	110.32
1	B	125	ARG	CA-C-N	6.03	127.38	119.84
1	B	125	ARG	C-N-CA	6.03	127.38	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	59	GLN	CB-CG-CD	-6.02	102.37	112.60
1	A	34	TRP	CG-CD2-CE3	6.02	139.92	133.90
1	A	64	ASN	CB-CG-ND2	6.00	125.39	116.40
1	B	68	TRP	CE2-CD2-CG	-5.98	100.03	107.20
1	A	53	VAL	O-C-N	-5.95	115.13	122.57
1	B	64	ASN	CA-CB-CG	5.95	118.55	112.60
1	A	46	GLN	CA-CB-CG	-5.94	102.23	114.10
1	B	50	LEU	N-CA-C	5.93	118.51	111.33
1	A	17	VAL	N-CA-CB	-5.91	103.64	110.55
1	B	125	ARG	CA-CB-CG	5.90	125.90	114.10
1	B	62	TRP	CG-CD2-CE3	5.89	139.79	133.90
1	B	96	ILE	CB-CA-C	-5.87	100.38	110.30
1	B	118	MET	CA-C-O	-5.86	114.21	120.42
1	A	61	HIS	CB-CG-CD2	-5.86	123.59	131.20
1	B	20	LYS	CB-CG-CD	-5.80	97.96	111.30
1	A	109	ASN	N-CA-CB	5.80	119.91	111.62
1	B	27	PHE	CA-CB-CG	5.79	119.59	113.80
1	A	133	TYR	O-C-N	5.76	130.84	122.94
1	A	26	GLY	N-CA-C	-5.75	105.53	112.49
1	B	92	ILE	CA-C-O	-5.72	114.40	120.64
1	B	73	ILE	N-CA-C	-5.72	106.24	111.67
1	A	125	ARG	CD-NE-CZ	5.68	132.36	124.40
1	A	69	ILE	CA-CB-CG1	-5.64	100.81	110.40
1	A	73	ILE	O-C-N	5.64	127.56	121.87
1	B	70	ASN	CA-CB-CG	5.63	118.23	112.60
1	B	72	LYS	CG-CD-CE	5.63	124.24	111.30
1	B	74	ASP	N-CA-C	-5.57	105.11	111.07
1	A	70	ASN	N-CA-C	5.57	117.15	111.14
1	B	91	GLU	CA-CB-CG	-5.56	102.98	114.10
1	B	123	ARG	CA-CB-CG	-5.54	103.03	114.10
1	A	12	ASN	CA-CB-CG	5.53	118.13	112.60
1	B	68	TRP	CB-CG-CD1	-5.51	118.64	126.90
1	A	96	ILE	CB-CG1-CD1	5.49	125.33	113.80
1	A	125	ARG	CA-CB-CG	-5.48	103.13	114.10
1	A	80	PRO	CA-C-N	-5.48	116.29	122.48
1	A	80	PRO	C-N-CA	-5.48	116.29	122.48
1	A	64	ASN	N-CA-C	-5.47	105.23	111.14
1	B	41	THR	N-CA-C	5.43	119.38	112.87
1	B	133	TYR	CA-C-O	5.42	126.78	120.49
1	A	109	ASN	CA-CB-CG	5.40	118.00	112.60
1	B	39	GLY	CA-C-O	-5.40	111.17	120.57
1	A	11	LEU	O-C-N	-5.39	116.61	123.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	VAL	O-C-N	-5.39	114.95	121.10
1	A	68	TRP	CB-CG-CD1	-5.39	118.82	126.90
1	A	120	GLU	CB-CG-CD	5.38	121.75	112.60
1	A	70	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	A	124	MET	CA-C-O	5.37	127.41	121.56
1	A	32	VAL	CA-C-O	-5.34	115.71	121.27
1	A	29	ARG	CA-C-O	5.33	126.07	120.42
1	A	62	TRP	CG-CD2-CE3	5.32	139.22	133.90
1	A	78	ARG	N-CA-C	5.30	117.37	110.53
1	B	85	TYR	CA-CB-CG	-5.30	104.36	113.90
1	B	108	LYS	CA-C-N	5.29	131.64	121.54
1	B	108	LYS	C-N-CA	5.29	131.64	121.54
1	B	125	ARG	N-CA-C	-5.29	102.93	109.64
1	A	34	TRP	CE2-CD2-CG	-5.28	100.86	107.20
1	B	34	TRP	N-CA-C	-5.28	105.20	111.69
1	A	10	PHE	CA-C-O	-5.26	111.85	120.80
1	A	63	ALA	N-CA-C	5.26	117.02	111.28
1	A	108	LYS	CA-C-N	5.26	129.88	122.46
1	A	108	LYS	C-N-CA	5.26	129.88	122.46
1	B	19	LEU	CB-CA-C	-5.26	102.06	110.79
1	B	100	TYR	N-CA-CB	-5.26	102.20	110.30
1	A	68	TRP	CG-CD2-CE3	5.25	139.15	133.90
1	B	17	VAL	CA-CB-CG2	-5.25	101.47	110.40
1	B	47	LYS	CA-CB-CG	5.25	124.59	114.10
1	B	54	ASN	OD1-CG-ND2	-5.25	117.35	122.60
1	A	62	TRP	CE2-CD2-CG	-5.25	100.91	107.20
1	A	76	LEU	N-CA-C	5.23	118.76	112.38
1	B	18	ALA	CA-C-O	-5.22	115.02	120.55
1	B	123	ARG	N-CA-C	5.21	117.04	111.36
1	B	68	TRP	CD1-CG-CD2	5.21	114.64	106.30
1	A	74	ASP	O-C-N	-5.21	116.70	122.07
1	B	40	ARG	CB-CG-CD	5.21	123.28	111.30
1	A	71	LYS	CB-CA-C	5.20	119.42	110.79
1	A	68	TRP	CA-C-O	-5.20	115.35	120.70
1	B	70	ASN	CB-CA-C	-5.19	102.50	110.81
1	B	62	TRP	CE2-CD2-CG	-5.19	100.97	107.20
1	B	13	LYS	CB-CG-CD	5.19	123.23	111.30
1	B	34	TRP	CD1-CG-CD2	5.18	114.59	106.30
1	A	34	TRP	CG-CD1-NE1	-5.13	103.52	110.20
1	B	134	MET	N-CA-C	-5.13	96.64	111.00
1	B	22	GLN	N-CA-C	5.12	116.94	111.36
1	A	130	PRO	CB-CA-C	5.12	117.65	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	29	ARG	CB-CG-CD	5.07	122.97	111.30
1	B	84	ASP	CA-C-N	5.07	127.34	120.44
1	B	84	ASP	C-N-CA	5.07	127.34	120.44
1	A	131	VAL	O-C-N	-5.07	117.65	122.97
1	A	94	ARG	CB-CA-C	-5.06	100.96	110.67
1	A	106	LYS	N-CA-C	5.05	116.48	111.07
1	A	20	LYS	CA-C-N	5.04	127.63	120.53
1	A	20	LYS	C-N-CA	5.04	127.63	120.53
1	B	81	VAL	N-CA-C	-5.04	101.81	108.96
1	A	97	ASP	CA-C-O	5.02	126.14	120.92
1	B	119	GLU	CB-CG-CD	5.02	121.14	112.60
1	A	27	PHE	CA-C-N	5.02	129.21	120.68
1	A	27	PHE	C-N-CA	5.02	129.21	120.68
1	A	52	PHE	CA-C-O	-5.01	115.74	121.00
1	B	68	TRP	CG-CD1-NE1	-5.00	103.69	110.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	MET	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1047	0	1072	24	0
1	B	1047	0	1072	38	0
All	All	2094	0	2144	54	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 13.

All (54) 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:B:38:HIS:HB3	1:B:106:LYS:HZ3	1.47	0.79
1:B:56:ARG:HG2	1:B:56:ARG:HH11	1.50	0.77
1:B:34:TRP:O	1:B:38:HIS:HD2	1.70	0.74
1:A:92:ILE:O	1:A:96:ILE:HG12	1.89	0.72
1:B:36:ARG:O	1:B:36:ARG:HD2	1.90	0.71
1:A:17:VAL:HG22	1:A:127:ALA:HB1	1.78	0.66
1:A:113:LYS:H	1:B:56:ARG:NH2	1.96	0.64
1:A:73:ILE:HA	1:A:76:LEU:HD23	1.80	0.62
1:B:19:LEU:HD11	1:B:85:TYR:HD1	1.66	0.60
1:B:82:VAL:O	1:B:85:TYR:HB2	2.00	0.60
1:A:19:LEU:HD21	1:A:69:ILE:HD13	1.83	0.57
1:A:119:GLU:HG3	1:A:123:ARG:HE	1.70	0.56
1:A:78:ARG:NH2	1:A:81:VAL:HG22	2.20	0.56
1:A:113:LYS:HE3	1:B:117:TYR:CE2	2.42	0.54
1:B:119:GLU:O	1:B:119:GLU:HG2	2.07	0.54
1:B:132:LYS:HE3	1:B:133:TYR:O	2.08	0.53
1:B:93:GLY:O	1:B:96:ILE:HD11	2.09	0.53
1:A:113:LYS:HE3	1:B:117:TYR:CZ	2.44	0.52
1:B:76:LEU:HD22	1:B:78:ARG:NH1	2.25	0.52
1:A:73:ILE:HA	1:A:76:LEU:CD2	2.40	0.52
1:A:113:LYS:HB3	1:B:56:ARG:HH21	1.76	0.51
1:A:31:LEU:HD13	1:A:102:TYR:CZ	2.46	0.51
1:B:38:HIS:O	1:B:106:LYS:NZ	2.44	0.51
1:A:97:ASP:OD2	1:A:100:TYR:HB2	2.09	0.51
1:A:104:PHE:HE1	1:B:100:TYR:CE2	2.29	0.50
1:A:101:PHE:HA	1:B:104:PHE:HZ	1.76	0.49
1:B:56:ARG:HG2	1:B:56:ARG:NH1	2.19	0.49
1:A:59:GLN:HE21	1:A:129:VAL:HG12	1.78	0.48
1:B:88:LEU:O	1:B:92:ILE:HG13	2.12	0.48
1:B:104:PHE:O	1:B:108:LYS:HB2	2.14	0.48
1:B:39:GLY:O	1:B:41:THR:N	2.47	0.47
1:A:101:PHE:HD1	1:B:108:LYS:HD2	1.79	0.47
1:B:119:GLU:O	1:B:123:ARG:HG3	2.14	0.46
1:B:132:LYS:HB3	1:B:132:LYS:HE2	1.80	0.46
1:B:36:ARG:O	1:B:37:VAL:HG23	2.14	0.46
1:A:37:VAL:HG12	1:A:38:HIS:CD2	2.51	0.45
1:B:69:ILE:O	1:B:73:ILE:HB	2.16	0.45
1:B:73:ILE:O	1:B:76:LEU:HB2	2.17	0.44
1:B:19:LEU:CD1	1:B:85:TYR:HD1	2.31	0.43
1:A:87:ARG:HH11	1:A:87:ARG:HG3	1.82	0.43
1:B:79:THR:HA	1:B:80:PRO:HD2	1.77	0.43
1:B:11:LEU:HD13	1:B:66:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ILE:HD11	1:B:92:ILE:HD11	2.01	0.42
1:A:42:LEU:O	1:A:47:LYS:HE2	2.20	0.41
1:B:22:GLN:HB3	1:B:90:ALA:N	2.34	0.41
1:A:91:GLU:O	1:A:95:ARG:CG	2.68	0.41
1:B:15:PHE:O	1:B:19:LEU:HD22	2.21	0.41
1:B:50:LEU:O	1:B:53:VAL:HB	2.20	0.41
1:B:113:LYS:HG3	1:B:115:LEU:HG	2.03	0.41
1:A:115:LEU:HD13	1:B:117:TYR:HB3	2.02	0.41
1:A:103:ASP:O	1:A:107:ASP:HB2	2.21	0.41
1:B:36:ARG:NH1	1:B:37:VAL:HG23	2.36	0.41
1:A:73:ILE:HD12	1:A:80:PRO:HB3	2.03	0.40
1:B:55:ARG:HH11	1:B:55:ARG:HD2	1.73	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	123/136 (90%)	116 (94%)	5 (4%)	2 (2%)	7	14
1	B	123/136 (90%)	106 (86%)	12 (10%)	5 (4%)	2	3
All	All	246/272 (90%)	222 (90%)	17 (7%)	7 (3%)	4	6

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	36	ARG
1	A	114	TYR
1	B	37	VAL
1	B	40	ARG
1	A	23	ILE
1	B	127	ALA

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Mol	Chain	Res	Type
1	B	126	PRO

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	108/119 (91%)	94 (87%)	14 (13%)	4	7
1	B	108/119 (91%)	89 (82%)	19 (18%)	2	3
All	All	216/238 (91%)	183 (85%)	33 (15%)	3	4

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	PHE
1	A	11	LEU
1	A	13	LYS
1	A	17	VAL
1	A	19	LEU
1	A	37	VAL
1	A	44	THR
1	A	50	LEU
1	A	66	MET
1	A	73	ILE
1	A	84	ASP
1	A	88	LEU
1	A	109	ASN
1	A	125	ARG
1	B	11	LEU
1	B	13	LYS
1	B	17	VAL
1	B	19	LEU
1	B	36	ARG
1	B	45	VAL
1	B	50	LEU
1	B	55	ARG

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Mol	Chain	Res	Type
1	B	56	ARG
1	B	72	LYS
1	B	73	ILE
1	B	78	ARG
1	B	86	THR
1	B	87	ARG
1	B	96	ILE
1	B	109	ASN
1	B	126	PRO
1	B	128	ASP
1	B	132	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	38	HIS
1	A	59	GLN
1	A	64	ASN
1	A	70	ASN
1	A	122	ASN
1	B	38	HIS
1	B	46	GLN
1	B	61	HIS
1	B	70	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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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.