



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:55 AM UTC

PDB ID : 1TIB / pdb_00001tib
Title : CONFORMATIONAL LABILITY OF LIPASES OBSERVED IN THE ABSENCE OF AN OIL-WATER INTERFACE: CRYSTALLOGRAPHIC STUDIES OF ENZYMES FROM THE FUNGI HUMICOLA LANUGINOSA AND RHIZOPUS DELEMAR
Authors : Derewenda, U.; Swenson, L.; Wei, Y.; Derewenda, Z.S.
Deposited on : 1993-12-06
Resolution : 1.84 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

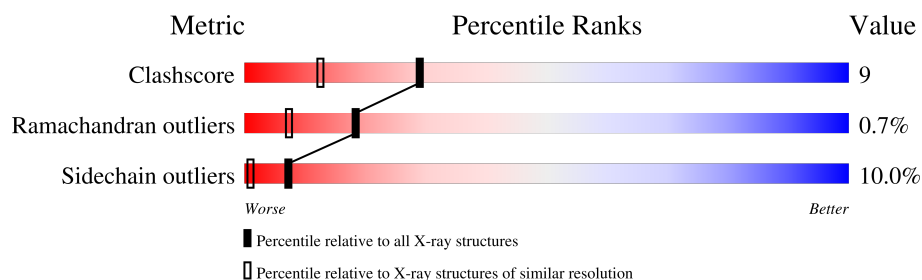
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)

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	269	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2427 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 LIPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2071	1303	359	403	6			

- Molecule 2 is water.

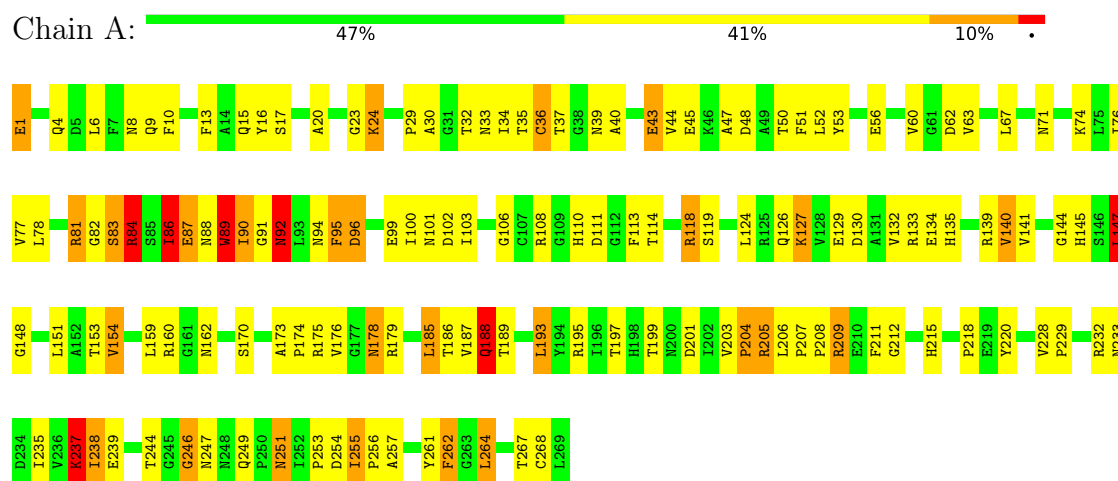
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	356	Total	O	0	0
			356	356		

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. 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: LIPASE



4 Data and refinement statistics

Xtriage (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	103.17Å 51.99Å 45.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.50 – 1.84	Depositor
% Data completeness (in resolution range)	(Not available) (7.50-1.84)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2427	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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	1.46	8/2121 (0.4%)	2.92	204/2887 (7.1%)

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	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	LYS	CD-CE	16.89	2.03	1.52
1	A	24	LYS	CD-CE	7.22	1.74	1.52
1	A	209	ARG	CD-NE	6.63	1.55	1.46
1	A	179	ARG	CD-NE	5.76	1.54	1.46
1	A	127	LYS	CB-CG	5.54	1.69	1.52
1	A	187	VAL	N-CA	5.24	1.53	1.46
1	A	90	ILE	N-CA	5.23	1.53	1.46
1	A	203	VAL	C-O	5.05	1.28	1.24

All (204) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	ARG	CD-NE-CZ	36.88	176.03	124.40
1	A	84	ARG	NE-CZ-NH1	24.86	146.35	121.50
1	A	84	ARG	NE-CZ-NH2	-22.12	99.29	119.20
1	A	89	TRP	N-CA-CB	17.02	135.90	110.53
1	A	92	ASN	OD1-CG-ND2	-13.66	108.94	122.60
1	A	89	TRP	N-CA-C	-13.42	96.87	113.38
1	A	127	LYS	CB-CG-CD	-13.19	80.96	111.30
1	A	262	PHE	CA-C-N	13.08	142.05	120.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	PHE	C-N-CA	13.08	142.05	120.86
1	A	89	TRP	CA-C-O	-12.73	104.64	119.15
1	A	127	LYS	CB-CA-C	12.56	131.64	110.79
1	A	127	LYS	N-CA-CB	-12.42	91.86	110.12
1	A	89	TRP	CA-CB-CG	11.41	135.28	113.60
1	A	187	VAL	CA-CB-CG2	11.36	129.72	110.40
1	A	126	GLN	CA-C-N	10.98	134.99	120.28
1	A	126	GLN	C-N-CA	10.98	134.99	120.28
1	A	187	VAL	CB-CA-C	10.80	129.75	112.26
1	A	90	ILE	CA-C-N	10.62	133.42	120.14
1	A	90	ILE	C-N-CA	10.62	133.42	120.14
1	A	126	GLN	CA-C-O	10.28	131.90	120.90
1	A	62	ASP	CA-CB-CG	10.11	122.71	112.60
1	A	215	HIS	CA-CB-CG	9.54	123.33	113.80
1	A	154	VAL	CA-C-O	-8.89	111.19	120.71
1	A	92	ASN	CA-CB-CG	8.85	121.45	112.60
1	A	145	HIS	CA-CB-CG	8.79	122.59	113.80
1	A	262	PHE	O-C-N	-8.68	111.05	122.59
1	A	47	ALA	CA-C-N	8.27	134.10	122.36
1	A	47	ALA	C-N-CA	8.27	134.10	122.36
1	A	77	VAL	O-C-N	8.26	131.95	123.20
1	A	127	LYS	CG-CD-CE	-8.23	92.37	111.30
1	A	94	ASN	CA-CB-CG	8.13	120.73	112.60
1	A	229	PRO	CA-C-O	-8.05	112.16	121.34
1	A	87	GLU	CA-C-N	7.99	132.45	120.31
1	A	87	GLU	C-N-CA	7.99	132.45	120.31
1	A	99	GLU	CB-CG-CD	7.96	126.14	112.60
1	A	188	GLN	CA-CB-CG	7.93	129.95	114.10
1	A	13	PHE	CA-CB-CG	-7.92	105.88	113.80
1	A	257	ALA	CA-C-N	7.92	132.34	120.31
1	A	257	ALA	C-N-CA	7.92	132.34	120.31
1	A	256	PRO	CA-C-N	7.87	131.61	120.28
1	A	256	PRO	C-N-CA	7.87	131.61	120.28
1	A	108	ARG	CD-NE-CZ	7.83	135.36	124.40
1	A	52	LEU	N-CA-C	-7.81	102.29	112.68
1	A	47	ALA	CA-C-O	7.71	129.07	119.05
1	A	126	GLN	O-C-N	-7.67	114.12	122.09
1	A	244	THR	CA-C-N	-7.63	112.77	123.08
1	A	244	THR	C-N-CA	-7.63	112.77	123.08
1	A	178	ASN	CA-C-O	7.60	129.99	122.01
1	A	132	VAL	O-C-N	-7.54	114.52	121.91
1	A	162	ASN	CA-CB-CG	7.47	120.07	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	THR	CA-CB-OG1	-7.46	98.42	109.60
1	A	179	ARG	NE-CZ-NH1	-7.45	114.05	121.50
1	A	209	ARG	NE-CZ-NH1	7.44	128.94	121.50
1	A	88	ASN	N-CA-C	7.38	120.39	111.82
1	A	111	ASP	CA-CB-CG	7.34	119.94	112.60
1	A	197	THR	CA-CB-CG2	7.26	122.84	110.50
1	A	244	THR	CA-CB-OG1	-7.12	98.92	109.60
1	A	229	PRO	O-C-N	7.09	131.62	123.03
1	A	86	ILE	CB-CA-C	-7.08	99.67	111.29
1	A	235	ILE	CA-C-O	-7.08	112.97	120.48
1	A	139	ARG	CA-C-N	-7.07	114.02	122.93
1	A	139	ARG	C-N-CA	-7.07	114.02	122.93
1	A	176	VAL	N-CA-CB	-7.07	102.59	112.35
1	A	148	GLY	CA-C-N	7.06	127.77	120.00
1	A	148	GLY	C-N-CA	7.06	127.77	120.00
1	A	170	SER	O-C-N	-7.06	114.05	123.23
1	A	159	LEU	N-CA-C	7.03	121.85	113.28
1	A	37	THR	CA-CB-OG1	-6.80	99.40	109.60
1	A	47	ALA	O-C-N	-6.80	113.08	122.46
1	A	83	SER	N-CA-CB	-6.77	100.16	110.45
1	A	88	ASN	CA-CB-CG	-6.76	105.84	112.60
1	A	254	ASP	N-CA-CB	-6.76	98.90	111.13
1	A	96	ASP	N-CA-CB	6.74	120.00	109.83
1	A	106	GLY	CA-C-O	6.70	126.40	119.10
1	A	129	GLU	CB-CG-CD	6.70	123.98	112.60
1	A	10	PHE	CA-CB-CG	6.67	120.47	113.80
1	A	140	VAL	N-CA-CB	6.67	118.99	110.99
1	A	23	GLY	CA-C-O	6.67	127.33	120.80
1	A	84	ARG	CA-CB-CG	6.66	127.41	114.10
1	A	170	SER	CA-C-N	6.64	132.77	123.07
1	A	170	SER	C-N-CA	6.64	132.77	123.07
1	A	188	GLN	CB-CG-CD	6.64	123.89	112.60
1	A	179	ARG	NH1-CZ-NH2	6.63	127.92	119.30
1	A	17	SER	CA-C-N	6.60	129.12	120.28
1	A	17	SER	C-N-CA	6.60	129.12	120.28
1	A	82	GLY	N-CA-C	-6.59	100.95	112.55
1	A	232	ARG	CA-C-N	6.52	131.76	120.68
1	A	232	ARG	C-N-CA	6.52	131.76	120.68
1	A	103	ILE	CA-C-O	-6.52	113.85	120.69
1	A	178	ASN	CA-CB-CG	6.48	119.08	112.60
1	A	30	ALA	CA-C-O	-6.44	114.72	121.55
1	A	53	TYR	CA-CB-CG	6.43	125.47	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	ASN	N-CA-CB	-6.43	100.32	110.28
1	A	130	ASP	CA-CB-CG	6.37	118.97	112.60
1	A	209	ARG	CD-NE-CZ	6.37	133.31	124.40
1	A	16	TYR	N-CA-CB	6.36	119.47	110.12
1	A	102	ASP	CA-C-N	6.35	130.19	122.63
1	A	102	ASP	C-N-CA	6.35	130.19	122.63
1	A	133	ARG	CA-C-O	-6.34	113.83	120.55
1	A	170	SER	CA-C-O	6.33	127.53	120.70
1	A	132	VAL	CA-C-N	6.33	128.76	120.28
1	A	132	VAL	C-N-CA	6.33	128.76	120.28
1	A	36	CYS	CA-C-O	-6.30	113.90	120.70
1	A	100	ILE	CA-C-O	6.29	128.64	120.78
1	A	103	ILE	N-CA-C	-6.27	105.71	111.67
1	A	84	ARG	CB-CA-C	6.22	123.31	110.31
1	A	84	ARG	CG-CD-NE	6.21	125.66	112.00
1	A	186	THR	CA-CB-OG1	-6.15	100.38	109.60
1	A	35	THR	CA-CB-CG2	6.15	120.95	110.50
1	A	81	ARG	NE-CZ-NH2	6.13	124.72	119.20
1	A	113	PHE	CA-C-O	-6.09	114.10	120.55
1	A	144	GLY	O-C-N	6.09	130.62	122.70
1	A	256	PRO	O-C-N	-6.08	114.38	122.22
1	A	134	GLU	CB-CA-C	-6.07	98.00	110.38
1	A	159	LEU	N-CA-CB	-6.03	101.00	110.46
1	A	67	LEU	CA-C-O	-6.01	113.87	120.30
1	A	76	ILE	N-CA-CB	6.00	119.47	111.90
1	A	264	LEU	CB-CA-C	6.00	119.26	109.90
1	A	103	ILE	N-CA-CB	5.99	119.13	110.68
1	A	9	GLN	CA-C-O	5.99	126.90	120.55
1	A	195	ARG	NH1-CZ-NH2	-5.98	111.52	119.30
1	A	86	ILE	CA-C-O	-5.97	113.31	120.78
1	A	160	ARG	NE-CZ-NH1	-5.96	115.54	121.50
1	A	92	ASN	N-CA-CB	5.90	120.47	110.49
1	A	173	ALA	CA-C-O	5.89	126.24	120.23
1	A	187	VAL	CG1-CB-CG2	-5.85	97.92	110.80
1	A	84	ARG	NH1-CZ-NH2	-5.84	111.71	119.30
1	A	90	ILE	CB-CA-C	5.83	124.99	111.77
1	A	95	PHE	CA-CB-CG	5.82	119.62	113.80
1	A	101	ASN	CA-C-N	5.78	129.85	120.60
1	A	101	ASN	C-N-CA	5.78	129.85	120.60
1	A	33	ASN	O-C-N	5.76	129.81	123.01
1	A	91	GLY	CA-C-O	-5.76	114.17	120.40
1	A	110	HIS	CB-CA-C	5.75	119.27	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	ASP	CA-CB-CG	5.72	118.32	112.60
1	A	44	VAL	N-CA-C	-5.70	104.95	110.42
1	A	56	GLU	CB-CG-CD	5.68	122.25	112.60
1	A	124	LEU	CA-C-O	-5.66	114.42	120.42
1	A	23	GLY	O-C-N	-5.64	116.69	122.17
1	A	141	VAL	CA-CB-CG2	5.64	119.99	110.40
1	A	134	GLU	O-C-N	-5.63	114.78	122.33
1	A	43	GLU	CA-C-N	5.63	127.66	120.56
1	A	43	GLU	C-N-CA	5.63	127.66	120.56
1	A	118	ARG	CB-CG-CD	5.62	124.23	111.30
1	A	147	LEU	CD1-CG-CD2	5.62	123.17	110.80
1	A	9	GLN	O-C-N	-5.62	116.16	122.12
1	A	232	ARG	NE-CZ-NH2	-5.60	114.16	119.20
1	A	229	PRO	N-CA-CB	5.56	108.26	103.31
1	A	60	VAL	CA-C-O	5.55	126.51	120.57
1	A	246	GLY	N-CA-C	-5.54	100.04	113.18
1	A	153	THR	CA-C-O	-5.53	114.56	120.42
1	A	235	ILE	O-C-N	5.52	128.97	123.18
1	A	50	THR	CA-CB-CG2	5.51	119.88	110.50
1	A	267	THR	N-CA-CB	-5.51	102.29	110.61
1	A	201	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	135	HIS	CA-C-O	5.47	127.30	121.28
1	A	205	ARG	O-C-N	-5.47	114.83	122.37
1	A	178	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	A	203	VAL	CA-CB-CG2	-5.42	101.19	110.40
1	A	268	CYS	N-CA-C	-5.41	102.28	110.28
1	A	187	VAL	CA-CB-CG1	-5.39	101.24	110.40
1	A	17	SER	O-C-N	-5.38	116.02	122.15
1	A	24	LYS	CA-C-N	5.37	132.09	122.38
1	A	24	LYS	C-N-CA	5.37	132.09	122.38
1	A	147	LEU	CB-CG-CD2	-5.36	94.62	110.70
1	A	211	PHE	CA-CB-CG	-5.36	108.44	113.80
1	A	86	ILE	N-CA-C	5.33	120.42	109.34
1	A	91	GLY	CA-C-N	5.32	131.70	121.54
1	A	91	GLY	C-N-CA	5.32	131.70	121.54
1	A	203	VAL	CG1-CB-CG2	5.28	122.41	110.80
1	A	141	VAL	CA-C-O	5.27	125.95	120.36
1	A	4	GLN	CA-C-N	5.26	127.28	120.44
1	A	4	GLN	C-N-CA	5.26	127.28	120.44
1	A	237	LYS	CB-CG-CD	-5.26	99.20	111.30
1	A	244	THR	CA-C-O	-5.26	115.05	121.78
1	A	96	ASP	CB-CA-C	-5.24	101.03	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	A	106	GLY	CA-C-N	5.22	128.29	120.87
1	A	106	GLY	C-N-CA	5.22	128.29	120.87
1	A	151	LEU	N-CA-C	5.22	116.97	111.28
1	A	83	SER	CB-CA-C	5.22	120.14	109.76
1	A	8	ASN	CB-CG-ND2	-5.19	108.61	116.40
1	A	204	PRO	O-C-N	-5.19	114.94	122.37
1	A	176	VAL	CA-CB-CG2	5.19	119.22	110.40
1	A	175	ARG	CG-CD-NE	-5.17	100.62	112.00
1	A	208	PRO	CA-C-O	5.14	127.20	121.34
1	A	209	ARG	NE-CZ-NH2	-5.14	114.57	119.20
1	A	90	ILE	O-C-N	-5.13	115.33	122.05
1	A	179	ARG	CD-NE-CZ	-5.13	117.22	124.40
1	A	134	GLU	CA-CB-CG	5.12	124.35	114.10
1	A	185	LEU	CA-C-N	5.11	128.08	120.31
1	A	185	LEU	C-N-CA	5.11	128.08	120.31
1	A	20	ALA	CA-C-N	5.11	130.08	121.14
1	A	20	ALA	C-N-CA	5.11	130.08	121.14
1	A	185	LEU	O-C-N	-5.10	116.25	122.22
1	A	113	PHE	O-C-N	5.10	127.53	122.12
1	A	63	VAL	CA-CB-CG2	5.09	119.06	110.40
1	A	153	THR	O-C-N	5.09	127.95	122.15
1	A	174	PRO	CA-C-O	-5.07	115.59	122.08
1	A	206	LEU	O-C-N	-5.05	117.06	121.35
1	A	45	GLU	CA-C-N	5.03	127.96	120.31
1	A	45	GLU	C-N-CA	5.03	127.96	120.31
1	A	249	GLN	CG-CD-NE2	5.01	123.91	116.40
1	A	119	SER	CA-C-O	-5.01	114.44	120.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	81	ARG	Sidechain
1	A	84	ARG	Sidechain
1	A	89	TRP	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	2071	0	1965	35	0
2	A	356	0	0	10	0
All	All	2427	0	1965	35	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 9.

All (35) 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:127:LYS:CD	1:A:127:LYS:CE	2.03	1.36
1:A:205:ARG:HH22	1:A:251:ASN:HD21	1.02	0.93
1:A:1:GLU:HG2	1:A:233:ASN:HA	1.61	0.83
1:A:205:ARG:HH22	1:A:251:ASN:ND2	1.82	0.75
1:A:15:GLN:HE22	1:A:43:GLU:H	1.35	0.73
1:A:127:LYS:CE	1:A:127:LYS:CG	2.67	0.73
1:A:71:ASN:O	1:A:74:LYS:HE2	1.89	0.72
1:A:188:GLN:HE22	1:A:193:LEU:H	1.39	0.71
1:A:237:LYS:HE2	1:A:239:GLU:OE2	1.92	0.69
1:A:188:GLN:NE2	1:A:193:LEU:H	1.94	0.65
1:A:89:TRP:HE3	1:A:92:ASN:HD22	1.45	0.65
1:A:205:ARG:NH2	1:A:251:ASN:HD21	1.85	0.64
1:A:237:LYS:NZ	2:A:502:HOH:O	2.27	0.64
1:A:15:GLN:NE2	1:A:43:GLU:H	2.03	0.55
1:A:86:ILE:HD12	1:A:87:GLU:HG3	1.90	0.54
1:A:220:TYR:CE1	1:A:237:LYS:HG3	2.43	0.52
1:A:24:LYS:HG2	2:A:318:HOH:O	2.12	0.50
1:A:84:ARG:HG2	2:A:447:HOH:O	2.11	0.50
1:A:207:PRO:HG3	2:A:564:HOH:O	2.12	0.49
1:A:178:ASN:HA	1:A:212:GLY:O	2.13	0.47
1:A:204:PRO:HB2	1:A:247:ASN:ND2	2.30	0.47
1:A:261:TYR:O	1:A:262:PHE:HB2	2.16	0.46
1:A:238:ILE:HD13	1:A:246:GLY:HA3	1.99	0.44
1:A:36:CYS:HB3	1:A:40:ALA:HB3	1.99	0.44
1:A:218:PRO:HD3	2:A:465:HOH:O	2.18	0.43
1:A:147:LEU:HB2	2:A:490:HOH:O	2.18	0.43
1:A:114:THR:O	1:A:118:ARG:HG3	2.19	0.42
1:A:86:ILE:HD13	1:A:255:ILE:HG23	2.02	0.42
1:A:127:LYS:HG2	2:A:450:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:PRO:HG2	1:A:32:THR:HG21	2.01	0.41
1:A:209:ARG:HG3	2:A:282:HOH:O	2.20	0.41
1:A:209:ARG:HE	1:A:209:ARG:HB3	1.65	0.41
1:A:188:GLN:HA	2:A:368:HOH:O	2.20	0.41
1:A:34:ILE:HG12	1:A:51:PHE:CZ	2.55	0.40
1:A:39:ASN:HA	2:A:543:HOH:O	2.20	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	267/269 (99%)	255 (96%)	10 (4%)	2 (1%)	18 7

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	THR
1	A	92	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	A	220/220 (100%)	198 (90%)	22 (10%)	7 1

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	6	LEU
1	A	78	LEU
1	A	83	SER
1	A	84	ARG
1	A	86	ILE
1	A	90	ILE
1	A	95	PHE
1	A	96	ASP
1	A	140	VAL
1	A	147	LEU
1	A	154	VAL
1	A	185	LEU
1	A	188	GLN
1	A	193	LEU
1	A	228	VAL
1	A	237	LYS
1	A	238	ILE
1	A	251	ASN
1	A	253	PRO
1	A	255	ILE
1	A	264	LEU

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	15	GLN
1	A	25	ASN
1	A	92	ASN
1	A	94	ASN
1	A	135	HIS
1	A	188	GLN
1	A	233	ASN
1	A	247	ASN
1	A	248	ASN
1	A	251	ASN

5.3.3 RNA ⓘ

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.