



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:50 PM UTC

PDB ID : 1LGY / pdb_00001lgy
Title : LIPASE II FROM RHIZOPUS NIVEUS
Authors : Kohno, M.; Funatsu, J.; Mikami, B.; Kugimiya, W.; Matsuo, T.; Morita, Y.
Deposited on : 1996-05-23
Resolution : 2.20 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

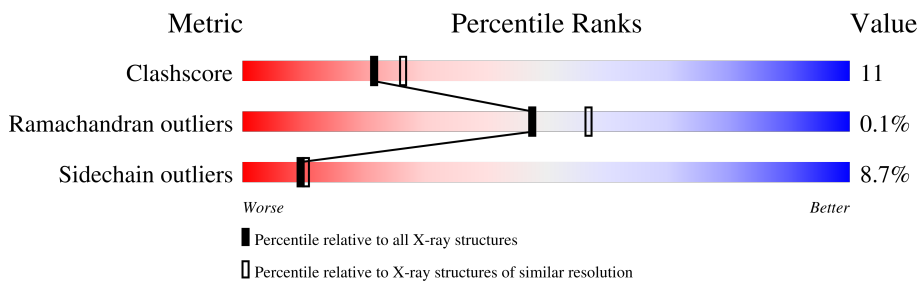
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	
1	B	269	
1	C	269	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6682 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 TRIACYLGLYCEROL LIPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2068	1326	347	388	7			
1	B	265	Total	C	N	O	S	0	0	0
			2068	1326	347	388	7			
1	C	265	Total	C	N	O	S	0	0	0
			2068	1326	347	388	7			

- Molecule 2 is water.

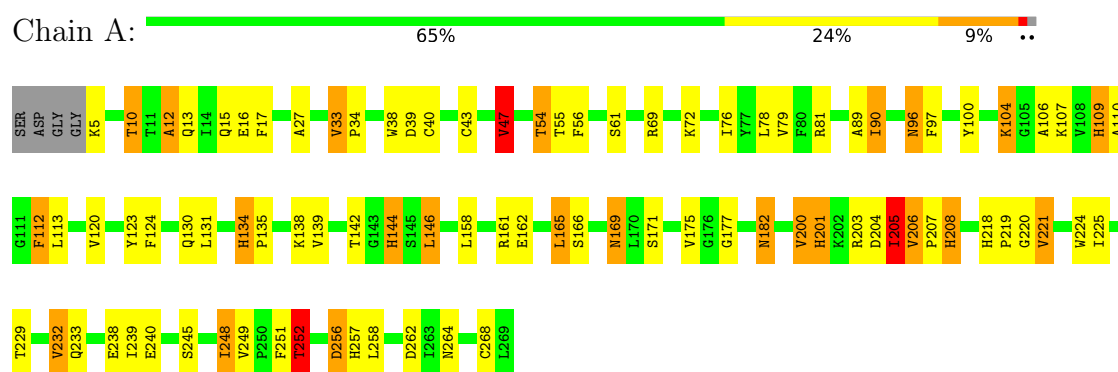
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	135	Total	O	0	0
			135	135		
2	B	157	Total	O	0	0
			157	157		
2	C	186	Total	O	0	0
			186	186		

3 Residue-property plots

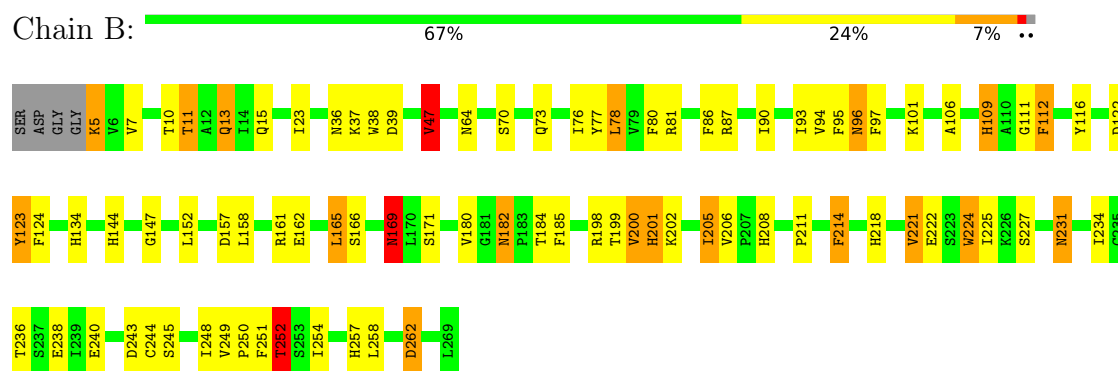
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

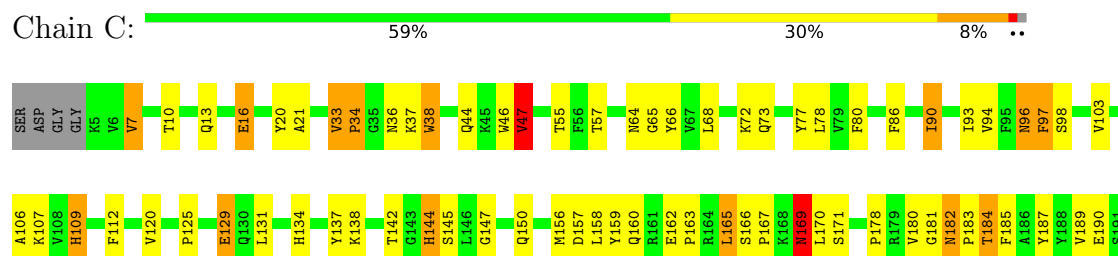
• Molecule 1: TRIACYLGLYCEROL LIPASE

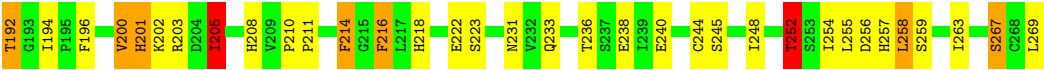


• Molecule 1: TRIACYLGLYCEROL LIPASE



• Molecule 1: TRIACYLGLYCEROL LIPASE





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	83.70Å 83.70Å 137.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, R_{free}	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6682	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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	1.23	17/2122 (0.8%)	1.88	48/2889 (1.7%)
1	B	1.15	12/2122 (0.6%)	1.89	54/2889 (1.9%)
1	C	1.08	11/2122 (0.5%)	1.87	52/2889 (1.8%)
All	All	1.16	40/6366 (0.6%)	1.88	154/8667 (1.8%)

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	B	0	1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	HIS	CD2-NE2	-8.66	1.28	1.37
1	A	201	HIS	CD2-NE2	-8.45	1.28	1.37
1	A	109	HIS	CD2-NE2	-7.67	1.29	1.37
1	B	134	HIS	CD2-NE2	-7.55	1.29	1.37
1	C	144	HIS	CD2-NE2	-7.28	1.29	1.37
1	A	218	HIS	CG-ND1	-7.21	1.30	1.38
1	A	120	VAL	CA-CB	7.18	1.63	1.54
1	A	144	HIS	CD2-NE2	-7.01	1.30	1.37
1	B	109	HIS	CD2-NE2	-6.87	1.30	1.37
1	C	218	HIS	CD2-NE2	-6.79	1.30	1.37
1	A	134	HIS	CD2-NE2	-6.75	1.30	1.37
1	A	47	VAL	CA-CB	6.62	1.62	1.54
1	A	33	VAL	CA-CB	6.61	1.59	1.54
1	A	221	VAL	CA-CB	6.59	1.62	1.54
1	C	109	HIS	CD2-NE2	-6.41	1.30	1.37
1	B	257	HIS	CD2-NE2	-6.29	1.30	1.37
1	C	208	HIS	CD2-NE2	-6.27	1.30	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	47	VAL	CA-CB	6.25	1.62	1.54
1	A	257	HIS	CG-ND1	-6.23	1.31	1.38
1	A	144	HIS	CG-ND1	-6.17	1.31	1.38
1	A	208	HIS	CD2-NE2	-6.15	1.31	1.37
1	C	257	HIS	CD2-NE2	-6.09	1.31	1.37
1	C	201	HIS	CD2-NE2	-6.08	1.31	1.37
1	C	200	VAL	CA-CB	6.06	1.63	1.54
1	B	218	HIS	CD2-NE2	-6.01	1.31	1.37
1	B	208	HIS	CD2-NE2	-5.98	1.31	1.37
1	A	257	HIS	CD2-NE2	-5.91	1.31	1.37
1	B	109	HIS	CG-ND1	-5.89	1.31	1.38
1	C	134	HIS	CD2-NE2	-5.87	1.31	1.37
1	B	201	HIS	CD2-NE2	-5.83	1.31	1.37
1	B	144	HIS	CD2-NE2	-5.81	1.31	1.37
1	A	201	HIS	CG-ND1	-5.74	1.31	1.38
1	B	47	VAL	CA-CB	5.55	1.61	1.54
1	B	221	VAL	CA-CB	5.41	1.60	1.54
1	A	134	HIS	CG-ND1	-5.38	1.32	1.38
1	A	233	GLN	CA-CB	-5.31	1.45	1.53
1	C	218	HIS	CG-ND1	-5.23	1.32	1.38
1	C	257	HIS	CG-ND1	-5.15	1.32	1.38
1	B	257	HIS	CG-ND1	-5.09	1.32	1.38
1	B	134	HIS	CG-ND1	-5.04	1.32	1.38

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	205	ILE	CB-CA-C	-13.35	94.12	112.14
1	A	205	ILE	CB-CA-C	-11.29	96.90	112.14
1	C	214	PHE	CA-CB-CG	-10.04	103.76	113.80
1	C	205	ILE	N-CA-CB	9.34	123.24	110.54
1	A	218	HIS	CA-CB-CG	9.21	123.02	113.80
1	A	104	LYS	CA-CB-CG	8.56	131.22	114.10
1	C	252	THR	N-CA-CB	-8.31	98.21	111.43
1	C	21	ALA	N-CA-C	-8.15	102.47	111.36
1	C	97	PHE	N-CA-C	8.15	122.12	110.14
1	B	39	ASP	CA-CB-CG	7.95	120.55	112.60
1	B	97	PHE	CA-CB-CG	7.77	121.57	113.80
1	B	205	ILE	CB-CA-C	-7.66	101.80	112.14
1	A	43	CYS	O-C-N	7.53	129.83	122.07
1	C	157	ASP	CA-CB-CG	7.43	120.03	112.60
1	C	205	ILE	CB-CG1-CD1	-7.33	98.41	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	LEU	N-CA-C	7.27	122.17	113.16
1	C	222	GLU	N-CA-C	7.22	120.03	108.41
1	A	262	ASP	N-CA-C	7.20	121.65	112.86
1	B	218	HIS	CA-CB-CG	7.14	120.94	113.80
1	B	206	VAL	CA-C-N	7.10	126.78	119.82
1	B	206	VAL	C-N-CA	7.10	126.78	119.82
1	B	38	TRP	CG-CD2-CE3	7.06	140.96	133.90
1	B	236	THR	N-CA-C	6.92	121.57	113.20
1	B	252	THR	N-CA-CB	-6.90	99.28	111.08
1	B	262	ASP	CA-CB-CG	-6.84	105.76	112.60
1	B	243	ASP	N-CA-C	6.76	120.75	112.23
1	C	218	HIS	CA-CB-CG	6.72	120.52	113.80
1	C	147	GLY	CA-C-N	6.71	127.38	120.00
1	C	147	GLY	C-N-CA	6.71	127.38	120.00
1	A	264	ASN	OD1-CG-ND2	-6.62	115.98	122.60
1	A	112	PHE	CA-CB-CG	6.61	120.41	113.80
1	A	161	ARG	NE-CZ-NH2	-6.52	113.33	119.20
1	C	109	HIS	CB-CG-CD2	-6.52	122.73	131.20
1	C	46	TRP	N-CA-C	6.45	121.22	113.23
1	A	110	ALA	N-CA-C	6.43	118.29	111.28
1	A	205	ILE	N-CA-CB	6.40	119.24	110.54
1	C	86	PHE	N-CA-C	6.38	119.05	111.33
1	A	240	GLU	N-CA-C	6.37	119.89	109.76
1	A	162	GLU	CA-C-N	6.37	126.12	119.05
1	A	162	GLU	C-N-CA	6.37	126.12	119.05
1	B	199	THR	CA-CB-OG1	-6.32	100.12	109.60
1	A	229	THR	N-CA-CB	-6.32	99.81	110.49
1	C	238	GLU	CB-CG-CD	6.29	123.29	112.60
1	B	38	TRP	CB-CG-CD1	-6.29	117.47	126.90
1	B	234	ILE	N-CA-CB	-6.28	103.86	111.21
1	A	201	HIS	CB-CG-CD2	-6.26	123.06	131.20
1	B	11	THR	N-CA-C	-6.17	104.47	111.14
1	B	224	TRP	CG-CD2-CE3	6.17	140.07	133.90
1	A	39	ASP	CA-CB-CG	6.16	118.76	112.60
1	B	95	PHE	CA-CB-CG	-6.16	107.64	113.80
1	C	21	ALA	CA-C-N	6.15	126.77	120.00
1	C	21	ALA	C-N-CA	6.15	126.77	120.00
1	B	147	GLY	N-CA-C	-6.11	105.18	113.37
1	C	231	ASN	CA-CB-CG	-6.10	106.50	112.60
1	A	134	HIS	CA-C-N	6.06	126.58	120.04
1	A	134	HIS	C-N-CA	6.06	126.58	120.04
1	B	152	LEU	N-CA-C	-6.04	104.04	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	23	ILE	N-CA-C	-6.03	104.42	111.00
1	B	218	HIS	CB-CG-CD2	-6.02	123.38	131.20
1	C	167	PRO	N-CA-C	6.01	121.86	114.35
1	B	76	ILE	N-CA-C	-6.01	97.73	107.28
1	A	204	ASP	CA-CB-CG	6.00	118.60	112.60
1	A	218	HIS	CB-CG-CD2	-5.99	123.42	131.20
1	A	17	PHE	CA-CB-CG	5.96	119.76	113.80
1	A	218	HIS	CB-CA-C	-5.95	102.00	109.31
1	A	252	THR	N-CA-CB	-5.93	101.23	111.55
1	A	47	VAL	CA-C-N	5.93	126.34	119.47
1	A	47	VAL	C-N-CA	5.93	126.34	119.47
1	C	169	ASN	CA-CB-CG	5.91	118.51	112.60
1	B	201	HIS	CB-CG-CD2	-5.86	123.59	131.20
1	B	251	PHE	CA-CB-CG	-5.82	107.98	113.80
1	C	46	TRP	CG-CD2-CE3	5.82	139.72	133.90
1	C	171	SER	O-C-N	-5.81	116.63	123.25
1	A	12	ALA	O-C-N	5.80	128.26	122.12
1	C	252	THR	CB-CA-C	5.79	121.77	110.30
1	B	134	HIS	CB-CG-CD2	-5.79	123.68	131.20
1	B	252	THR	CB-CA-C	5.78	120.72	109.33
1	A	258	LEU	N-CA-C	5.71	120.24	113.16
1	B	240	GLU	N-CA-CB	-5.68	100.19	109.56
1	C	218	HIS	CB-CG-CD2	-5.64	123.86	131.20
1	A	97	PHE	CA-CB-CG	5.63	119.43	113.80
1	A	264	ASN	CB-CG-ND2	5.63	124.84	116.40
1	C	137	TYR	O-C-N	5.61	129.18	122.79
1	C	120	VAL	N-CA-C	5.61	116.34	110.62
1	B	77	TYR	O-C-N	-5.59	116.85	123.22
1	C	267	SER	N-CA-C	5.58	120.21	113.17
1	A	89	ALA	N-CA-C	-5.57	104.84	111.69
1	B	222	GLU	N-CA-C	5.57	117.77	109.25
1	B	169	ASN	CA-CB-CG	5.56	118.16	112.60
1	A	134	HIS	CB-CG-CD2	-5.54	124.00	131.20
1	C	134	HIS	O-C-N	-5.53	116.56	121.20
1	A	256	ASP	CA-CB-CG	5.52	118.12	112.60
1	C	192	THR	N-CA-C	-5.51	104.91	111.69
1	B	206	VAL	N-CA-C	5.48	120.72	108.88
1	A	248	ILE	CA-CB-CG2	-5.46	101.21	110.50
1	B	171	SER	N-CA-CB	-5.46	102.19	111.69
1	C	33	VAL	CA-C-O	5.46	122.78	119.94
1	B	231	ASN	CA-CB-CG	5.46	118.06	112.60
1	A	113	LEU	CA-C-O	-5.46	115.09	120.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	236	THR	N-CA-C	5.46	119.43	112.34
1	B	13	GLN	OE1-CD-NE2	-5.45	117.15	122.60
1	B	101	LYS	N-CA-C	5.45	121.86	109.81
1	B	134	HIS	N-CA-C	5.43	119.14	110.73
1	C	180	VAL	CA-C-O	-5.42	114.74	119.29
1	A	40	CYS	N-CA-CB	-5.41	102.07	110.46
1	C	38	TRP	CE2-CD2-CG	-5.38	100.74	107.20
1	A	61	SER	N-CA-C	5.38	119.53	112.92
1	B	134	HIS	CA-C-N	5.37	126.55	119.84
1	B	134	HIS	C-N-CA	5.37	126.55	119.84
1	B	80	PHE	CA-CB-CG	5.37	119.17	113.80
1	A	220	GLY	CA-C-O	-5.36	117.40	122.39
1	A	90	ILE	N-CA-CB	-5.36	104.59	110.65
1	A	232	VAL	O-C-N	-5.34	117.27	122.99
1	B	214	PHE	CA-CB-CG	-5.34	108.46	113.80
1	B	112	PHE	CA-CB-CG	5.34	119.14	113.80
1	B	218	HIS	CB-CG-ND1	5.33	130.69	122.70
1	C	80	PHE	CA-CB-CG	5.29	119.09	113.80
1	B	38	TRP	CE2-CD2-CG	-5.28	100.86	107.20
1	C	144	HIS	CB-CG-CD2	-5.28	124.34	131.20
1	C	184	THR	O-C-N	5.28	127.71	122.12
1	B	257	HIS	CB-CG-CD2	-5.27	124.35	131.20
1	B	180	VAL	N-CA-C	5.24	116.31	111.81
1	C	240	GLU	N-CA-C	5.23	117.93	110.24
1	A	177	GLY	CA-C-N	5.22	125.20	120.03
1	A	177	GLY	C-N-CA	5.22	125.20	120.03
1	C	142	THR	N-CA-C	5.22	117.00	109.07
1	C	194	ILE	CA-C-N	5.21	125.46	119.83
1	C	194	ILE	C-N-CA	5.21	125.46	119.83
1	C	216	PHE	N-CA-C	5.21	118.31	109.76
1	B	86	PHE	N-CA-C	5.20	117.02	111.36
1	A	54	THR	CA-CB-OG1	-5.19	101.82	109.60
1	B	205	ILE	N-CA-CB	5.17	117.58	110.54
1	A	109	HIS	CB-CG-CD2	-5.17	124.48	131.20
1	C	196	PHE	CA-CB-CG	5.17	118.97	113.80
1	B	122	ASP	N-CA-C	-5.16	106.14	112.90
1	A	248	ILE	CA-CB-CG1	5.16	119.17	110.40
1	B	244	CYS	O-C-N	-5.15	115.75	122.59
1	A	206	VAL	CA-C-O	-5.14	114.48	118.85
1	B	37	LYS	O-C-N	-5.14	116.55	123.23
1	C	150	GLN	CG-CD-NE2	5.13	124.10	116.40
1	A	240	GLU	O-C-N	5.13	129.04	123.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	LEU	CD1-CG-CD2	-5.12	99.54	110.80
1	B	199	THR	CA-CB-CG2	5.11	119.19	110.50
1	C	7	VAL	CB-CA-C	-5.11	102.96	110.82
1	C	201	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	C	178	PRO	CA-C-O	-5.08	115.82	122.12
1	B	7	VAL	CB-CA-C	-5.07	104.25	111.19
1	C	258	LEU	N-CA-C	5.07	119.31	113.18
1	A	249	VAL	N-CA-CB	-5.05	104.11	110.33
1	C	16	GLU	CA-CB-CG	-5.05	103.99	114.10
1	B	73	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	C	65	GLY	O-C-N	-5.01	117.59	123.55
1	C	257	HIS	CB-CG-CD2	-5.01	124.69	131.20
1	C	46	TRP	CB-CG-CD1	-5.00	119.39	126.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	116	TYR	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	A	2068	0	2035	42	0
1	B	2068	0	2035	37	0
1	C	2068	0	2035	54	0
2	A	135	0	0	0	0
2	B	157	0	0	4	0
2	C	186	0	0	3	0
All	All	6682	0	6105	133	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 11.

All (133) 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:C:267:SER:HB3	1:C:269:LEU:HG	1.61	0.83
1:C:97:PHE:HD2	1:C:107:LYS:HB3	1.54	0.73
1:A:201:HIS:HB2	1:A:225:ILE:HD12	1.73	0.71
1:C:205:ILE:HG23	1:C:252:THR:HG23	1.72	0.71
1:C:156:MET:HE3	1:C:189:VAL:HG13	1.76	0.68
1:C:38:TRP:HZ2	1:C:47:VAL:HG13	1.58	0.67
1:A:10:THR:HG22	1:A:13:GLN:HG3	1.77	0.67
1:A:96:ASN:H	1:A:96:ASN:HD22	1.44	0.65
1:C:97:PHE:CD2	1:C:107:LYS:HB3	2.30	0.65
1:A:203:ARG:NH1	1:A:248:ILE:HB	2.12	0.64
1:A:38:TRP:HZ2	1:A:47:VAL:HG13	1.63	0.63
1:C:156:MET:SD	1:C:192:THR:HG21	2.39	0.63
1:B:10:THR:H	1:B:13:GLN:HE21	1.45	0.62
1:C:192:THR:HG22	2:C:600:HOH:O	1.99	0.61
1:C:107:LYS:H	1:C:182:ASN:ND2	1.99	0.60
1:A:169:ASN:H	1:A:169:ASN:HD22	1.49	0.59
1:B:205:ILE:HG23	1:B:252:THR:HG23	1.84	0.59
1:A:109:HIS:HD2	1:A:112:PHE:H	1.50	0.59
1:A:238:GLU:O	1:A:239:ILE:HD13	2.04	0.58
1:B:166:SER:H	1:B:169:ASN:ND2	2.02	0.58
1:B:205:ILE:HG23	1:B:252:THR:CG2	2.33	0.57
1:A:10:THR:H	1:A:13:GLN:HE21	1.53	0.56
1:C:205:ILE:HD11	1:C:254:ILE:HD13	1.87	0.56
1:C:57:THR:HG23	1:C:64:ASN:OD1	2.05	0.56
1:A:79:VAL:HG22	1:A:142:THR:HG22	1.86	0.56
1:B:96:ASN:HD22	1:B:96:ASN:H	1.53	0.54
1:C:109:HIS:HD2	1:C:112:PHE:H	1.54	0.54
1:A:165:LEU:HA	1:A:169:ASN:HD21	1.72	0.54
1:C:55:THR:HG22	1:C:66:TYR:HB3	1.90	0.54
1:B:87:ARG:HD2	2:B:645:HOH:O	2.08	0.54
1:C:10:THR:H	1:C:13:GLN:NE2	2.07	0.53
1:C:267:SER:CB	1:C:269:LEU:HG	2.36	0.53
1:C:68:LEU:HD23	1:C:77:TYR:CD1	2.44	0.53
1:A:47:VAL:O	1:A:47:VAL:HG22	2.10	0.52
1:A:200:VAL:HB	1:A:207:PRO:HG2	1.91	0.52
1:B:78:LEU:HD11	1:B:123:TYR:CD1	2.45	0.52
1:C:106:ALA:HA	1:C:184:THR:HB	1.92	0.52
1:C:125:PRO:O	1:C:129:GLU:HB2	2.10	0.52
1:A:33:VAL:HG23	1:A:55:THR:HB	1.92	0.51
1:C:210:PRO:HB2	1:C:216:PHE:CD2	2.45	0.51
1:A:107:LYS:H	1:A:182:ASN:ND2	2.07	0.51
1:B:11:THR:HG22	2:B:750:HOH:O	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:ASN:ND2	1:C:185:PHE:H	2.08	0.51
1:A:10:THR:HG23	1:A:12:ALA:HB3	1.92	0.51
1:C:107:LYS:H	1:C:182:ASN:HD21	1.59	0.51
1:A:205:ILE:HG23	1:A:252:THR:CG2	2.41	0.51
1:C:47:VAL:HB	1:C:73:GLN:HE22	1.76	0.50
1:A:38:TRP:CZ2	1:A:47:VAL:HG13	2.46	0.50
1:C:10:THR:HG22	1:C:13:GLN:NE2	2.26	0.50
1:B:5:LYS:HD3	2:B:474:HOH:O	2.11	0.50
1:C:166:SER:H	1:C:169:ASN:ND2	2.09	0.50
1:A:124:PHE:CE2	1:A:158:LEU:HD23	2.47	0.50
1:B:227:SER:O	1:B:231:ASN:HB3	2.13	0.49
1:B:10:THR:N	1:B:13:GLN:HE21	2.10	0.49
1:C:165:LEU:HA	1:C:169:ASN:HD21	1.77	0.49
1:C:201:HIS:HD2	1:C:256:ASP:O	1.96	0.49
1:B:211:PRO:HG2	1:B:214:PHE:HD2	1.78	0.49
1:C:211:PRO:HG2	1:C:214:PHE:HD2	1.77	0.49
1:C:10:THR:N	1:C:13:GLN:NE2	2.60	0.48
1:A:224:TRP:O	1:A:232:VAL:HA	2.14	0.48
1:A:10:THR:H	1:A:13:GLN:NE2	2.11	0.47
1:A:69:ARG:HD3	1:A:130:GLN:OE1	2.14	0.47
1:B:47:VAL:HG21	1:B:70:SER:HB2	1.95	0.47
1:B:78:LEU:HD11	1:B:123:TYR:CE1	2.50	0.47
1:B:205:ILE:HG12	1:B:252:THR:HG23	1.95	0.47
1:A:10:THR:HG22	1:A:13:GLN:CG	2.45	0.47
1:A:27:ALA:O	1:A:81:ARG:HD3	2.15	0.47
1:C:16:GLU:HG2	1:C:20:TYR:HE2	1.80	0.46
1:B:106:ALA:HA	1:B:184:THR:HB	1.98	0.46
1:C:159:TYR:HE2	2:C:600:HOH:O	1.98	0.46
1:C:169:ASN:HD22	1:C:169:ASN:H	1.64	0.46
1:C:205:ILE:HD11	1:C:254:ILE:CD1	2.45	0.46
1:A:245:SER:O	1:A:248:ILE:HG13	2.15	0.46
1:C:103:VAL:HB	1:C:106:ALA:HB3	1.97	0.46
1:B:166:SER:H	1:B:169:ASN:HD21	1.63	0.46
1:B:124:PHE:CE1	1:B:158:LEU:HD23	2.50	0.46
1:B:165:LEU:HA	1:B:169:ASN:HD21	1.80	0.45
1:B:11:THR:O	1:B:15:GLN:HG3	2.16	0.45
1:A:201:HIS:HD2	1:A:256:ASP:O	1.99	0.45
1:A:56:PHE:CE2	1:A:123:TYR:HB3	2.52	0.45
1:A:205:ILE:O	1:A:208:HIS:HB2	2.16	0.45
1:B:109:HIS:HD2	1:B:112:PHE:H	1.64	0.45
1:C:131:LEU:HD11	1:C:165:LEU:CD2	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:TRP:CZ2	1:C:47:VAL:HG13	2.45	0.45
1:A:268:CYS:SG	1:A:268:CYS:O	2.74	0.44
1:C:181:GLY:O	1:C:216:PHE:HA	2.16	0.44
1:A:203:ARG:HH11	1:A:203:ARG:HG2	1.83	0.44
1:C:96:ASN:HB3	2:C:768:HOH:O	2.17	0.44
1:B:201:HIS:HB2	1:B:225:ILE:HD12	1.99	0.44
1:C:245:SER:O	1:C:248:ILE:HG13	2.18	0.44
1:B:182:ASN:ND2	1:B:185:PHE:H	2.16	0.44
1:C:159:TYR:HB2	1:C:170:LEU:HD23	2.00	0.44
1:A:76:ILE:O	1:A:139:VAL:HA	2.18	0.44
1:A:169:ASN:HD22	1:A:169:ASN:N	2.11	0.43
1:B:109:HIS:CD2	1:B:111:GLY:H	2.35	0.43
1:B:94:VAL:O	1:B:109:HIS:HE1	2.02	0.43
1:C:259:SER:HA	1:C:263:ILE:O	2.18	0.43
1:C:109:HIS:HD2	1:C:112:PHE:N	2.16	0.43
1:B:202:LYS:HG2	1:B:225:ILE:O	2.19	0.42
1:A:5:LYS:HD2	1:A:5:LYS:HA	1.75	0.42
1:B:64:ASN:HB2	1:B:81:ARG:HG3	2.02	0.42
1:A:205:ILE:HG23	1:A:252:THR:HG21	2.00	0.42
1:B:198:ARG:HD2	2:B:439:HOH:O	2.19	0.42
1:B:94:VAL:O	1:B:109:HIS:CE1	2.73	0.42
1:C:138:LYS:HB3	1:C:138:LYS:HE3	1.77	0.42
1:A:203:ARG:NH1	1:A:251:PHE:HB2	2.35	0.42
1:A:166:SER:H	1:A:169:ASN:ND2	2.18	0.41
1:B:93:ILE:HD13	1:B:93:ILE:HG21	1.83	0.41
1:B:200:VAL:O	1:B:224:TRP:HD1	2.03	0.41
1:C:90:ILE:O	1:C:93:ILE:HG22	2.19	0.41
1:B:90:ILE:HD13	1:B:90:ILE:HA	1.90	0.41
1:C:203:ARG:HB3	1:C:252:THR:HA	2.02	0.41
1:B:245:SER:O	1:B:248:ILE:HG13	2.20	0.41
1:C:47:VAL:HG22	1:C:47:VAL:O	2.21	0.41
1:A:134:HIS:HA	1:A:135:PRO:HD3	1.85	0.41
1:B:157:ASP:OD1	1:B:161:ARG:HD3	2.21	0.41
1:C:158:LEU:O	1:C:162:GLU:HB3	2.21	0.41
1:C:131:LEU:HD11	1:C:165:LEU:HD21	2.03	0.41
1:C:233:GLN:NE2	1:C:244:CYS:SG	2.91	0.41
1:A:144:HIS:HA	1:A:175:VAL:O	2.20	0.41
1:B:166:SER:N	1:B:169:ASN:HD21	2.19	0.41
1:A:76:ILE:CD1	1:A:131:LEU:HD23	2.51	0.41
1:C:33:VAL:HA	1:C:34:PRO:HA	1.89	0.41
1:C:144:HIS:CE1	1:C:145:SER:HB2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:PRO:O	1:C:187:TYR:CD2	2.74	0.41
1:C:10:THR:HG23	1:C:13:GLN:H	1.86	0.40
1:A:203:ARG:HH12	1:A:248:ILE:HB	1.84	0.40
1:A:90:ILE:HD11	1:A:206:VAL:HG22	2.03	0.40
1:B:205:ILE:HD13	1:B:205:ILE:HG21	1.86	0.40
1:A:100:TYR:HB3	1:A:106:ALA:HB3	2.04	0.40
1:B:249:VAL:HA	1:B:250:PRO:HA	1.80	0.40
1:C:94:VAL:O	1:C:109:HIS:CE1	2.74	0.40
1:C:156:MET:O	1:C:160:GLN:HG3	2.21	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	263/269 (98%)	245 (93%)	18 (7%)	0	100	100
1	B	263/269 (98%)	250 (95%)	13 (5%)	0	100	100
1	C	263/269 (98%)	242 (92%)	20 (8%)	1 (0%)	30	34
All	All	789/807 (98%)	737 (93%)	51 (6%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	202	LYS

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	231/233 (99%)	210 (91%)	21 (9%)	9	9
1	B	231/233 (99%)	215 (93%)	16 (7%)	14	16
1	C	231/233 (99%)	208 (90%)	23 (10%)	7	7
All	All	693/699 (99%)	633 (91%)	60 (9%)	9	10

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	15	GLN
1	A	16	GLU
1	A	34	PRO
1	A	47	VAL
1	A	54	THR
1	A	72	LYS
1	A	78	LEU
1	A	96	ASN
1	A	104	LYS
1	A	138	LYS
1	A	146	LEU
1	A	165	LEU
1	A	169	ASN
1	A	171	SER
1	A	182	ASN
1	A	200	VAL
1	A	205	ILE
1	A	219	PRO
1	A	221	VAL
1	A	252	THR
1	B	5	LYS
1	B	36	ASN
1	B	47	VAL
1	B	78	LEU
1	B	96	ASN
1	B	123	TYR
1	B	162	GLU
1	B	165	LEU
1	B	169	ASN
1	B	182	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	200	VAL
1	B	221	VAL
1	B	238	GLU
1	B	252	THR
1	B	254	ILE
1	B	262	ASP
1	C	7	VAL
1	C	34	PRO
1	C	36	ASN
1	C	37	LYS
1	C	44	GLN
1	C	47	VAL
1	C	72	LYS
1	C	78	LEU
1	C	90	ILE
1	C	96	ASN
1	C	98	SER
1	C	129	GLU
1	C	163	PRO
1	C	165	LEU
1	C	169	ASN
1	C	182	ASN
1	C	190	GLU
1	C	200	VAL
1	C	205	ILE
1	C	223	SER
1	C	252	THR
1	C	255	LEU
1	C	258	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	36	ASN
1	A	96	ASN
1	A	109	HIS
1	A	118	GLN
1	A	128	GLN
1	A	150	GLN
1	A	169	ASN
1	A	182	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	201	HIS
1	A	212	GLN
1	B	13	GLN
1	B	15	GLN
1	B	36	ASN
1	B	73	GLN
1	B	96	ASN
1	B	109	HIS
1	B	118	GLN
1	B	169	ASN
1	B	182	ASN
1	B	212	GLN
1	B	246	ASN
1	C	13	GLN
1	C	44	GLN
1	C	73	GLN
1	C	96	ASN
1	C	109	HIS
1	C	160	GLN
1	C	169	ASN
1	C	182	ASN
1	C	201	HIS

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.