



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:20 AM UTC

PDB ID : 1THT / pdb_00001tht
Title : STRUCTURE OF A MYRISTOYL-ACP-SPECIFIC THIOESTERASE
FROM VIBRIO HARVEYI
Authors : Lawson, D.M.; Derewenda, U.; Serre, L.; Ferri, S.; Szitter, R.; Wei, Y.;
Meighen, E.A.; Derewenda, Z.S.
Deposited on : 1994-04-19
Resolution : 2.10 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

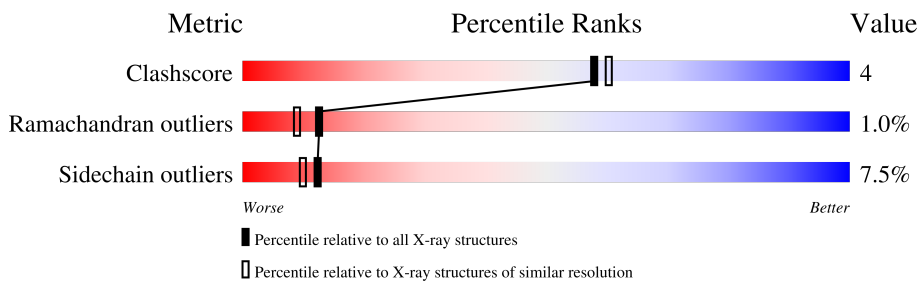
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	305	 66% 23% 7% .
1	B	305	 70% 20% 5% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4647 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 THIOESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2294	1456	383	446	9			
1	B	293	Total	C	N	O	S	0	0	0
			2298	1460	388	441	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	THR	GLU	conflict	UNP P05521
A	299	ASN	SER	conflict	UNP P05521
B	60	THR	GLU	conflict	UNP P05521
B	299	ASN	SER	conflict	UNP P05521

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	26	Total	O	0	0
			26	26		
2	B	29	Total	O	0	0
			29	29		

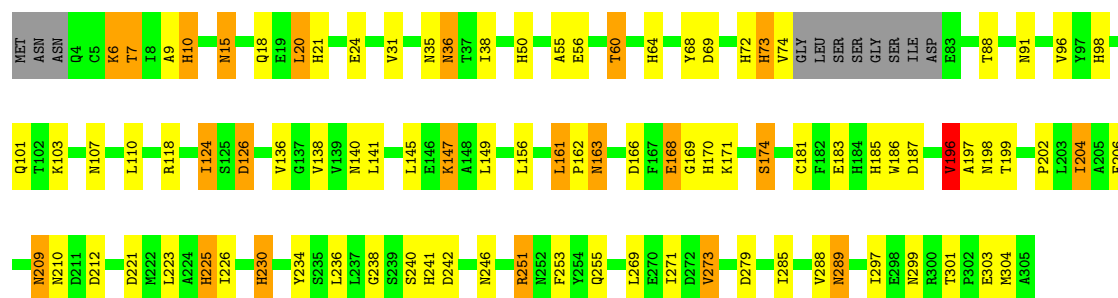
3 Residue-property plots [i](#)

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.

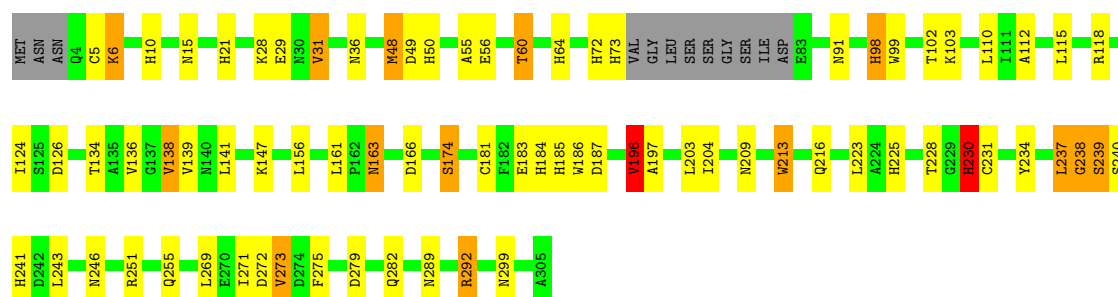
• Molecule 1: THIOESTERASE

Chain A: 



• Molecule 1: THIOESTERASE

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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.50Å 83.80Å 47.40Å 90.00° 97.30° 90.00°	Depositor
Resolution (Å)	8.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.227 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4647	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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	1.12	13/2344 (0.6%)	1.88	61/3190 (1.9%)
1	B	1.09	15/2347 (0.6%)	1.80	49/3191 (1.5%)
All	All	1.11	28/4691 (0.6%)	1.84	110/6381 (1.7%)

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 (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	HIS	CD2-NE2	-7.40	1.29	1.37
1	A	64	HIS	CD2-NE2	-7.15	1.29	1.37
1	B	10	HIS	CD2-NE2	-7.00	1.30	1.37
1	B	184	HIS	CD2-NE2	-6.88	1.30	1.37
1	B	21	HIS	CD2-NE2	-6.65	1.30	1.37
1	A	21	HIS	CD2-NE2	-6.55	1.30	1.37
1	A	72	HIS	CD2-NE2	-6.50	1.30	1.37
1	B	72	HIS	CD2-NE2	-6.50	1.30	1.37
1	A	10	HIS	CD2-NE2	-6.48	1.30	1.37
1	B	50	HIS	CD2-NE2	-6.31	1.30	1.37
1	B	230	HIS	CD2-NE2	-6.29	1.30	1.37
1	B	241	HIS	CD2-NE2	-6.24	1.30	1.37
1	A	230	HIS	CD2-NE2	-6.15	1.31	1.37
1	A	98	HIS	CD2-NE2	-5.90	1.31	1.37
1	B	73	HIS	CD2-NE2	-5.90	1.31	1.37
1	A	241	HIS	CD2-NE2	-5.77	1.31	1.37
1	A	50	HIS	CD2-NE2	-5.76	1.31	1.37
1	B	136	VAL	CA-CB	5.68	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	HIS	CD2-NE2	-5.58	1.31	1.37
1	A	225	HIS	CD2-NE2	-5.48	1.31	1.37
1	B	98	HIS	CD2-NE2	-5.38	1.31	1.37
1	A	73	HIS	CD2-NE2	-5.34	1.31	1.37
1	B	31	VAL	CA-CB	5.19	1.59	1.55
1	A	136	VAL	CA-CB	5.16	1.61	1.54
1	A	186	TRP	NE1-CE2	-5.14	1.31	1.37
1	B	225	HIS	CD2-NE2	-5.10	1.32	1.37
1	B	186	TRP	NE1-CE2	-5.07	1.31	1.37
1	B	10	HIS	CG-ND1	-5.06	1.32	1.38

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ASP	CA-CB-CG	11.11	123.71	112.60
1	B	147	LYS	CA-CB-CG	-10.29	93.51	114.10
1	B	187	ASP	N-CA-C	9.42	124.09	112.23
1	A	69	ASP	CA-CB-CG	9.36	121.96	112.60
1	A	168	GLU	O-C-N	9.12	133.71	123.04
1	A	279	ASP	CA-CB-CG	8.61	121.21	112.60
1	B	174	SER	N-CA-C	8.57	120.62	111.28
1	A	35	ASN	OD1-CG-ND2	-8.49	114.11	122.60
1	B	230	HIS	CA-CB-CG	8.37	122.17	113.80
1	B	29	GLU	N-CA-C	8.35	121.21	111.02
1	B	272	ASP	CA-CB-CG	8.29	120.89	112.60
1	B	36	ASN	OD1-CG-ND2	-8.26	114.34	122.60
1	A	98	HIS	CA-CB-CG	-8.22	105.58	113.80
1	A	103	LYS	N-CA-C	-8.15	103.33	113.20
1	B	48	MET	CG-SD-CE	-7.91	83.50	100.90
1	A	187	ASP	N-CA-C	7.67	121.89	112.23
1	A	140	ASN	OD1-CG-ND2	-7.62	114.98	122.60
1	A	73	HIS	N-CA-C	7.51	122.47	112.25
1	A	273	VAL	N-CA-CB	-7.39	100.03	112.44
1	A	36	ASN	OD1-CG-ND2	-7.32	115.28	122.60
1	A	225	HIS	CA-CB-CG	-7.27	106.53	113.80
1	B	213	TRP	N-CA-C	7.03	119.80	111.71
1	A	169	GLY	N-CA-C	-6.91	96.81	113.18
1	B	230	HIS	CB-CG-CD2	-6.90	122.23	131.20
1	B	240	SER	N-CA-C	-6.81	96.30	110.80
1	B	299	ASN	OD1-CG-ND2	-6.77	115.83	122.60
1	A	35	ASN	CB-CG-ND2	6.74	126.52	116.40
1	A	72	HIS	CB-CG-CD2	-6.69	122.50	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ASP	O-C-N	-6.66	116.12	121.65
1	B	147	LYS	CG-CD-CE	-6.66	95.98	111.30
1	A	181	CYS	CB-CA-C	-6.56	100.32	110.81
1	B	73	HIS	CB-CG-CD2	-6.54	122.70	131.20
1	B	273	VAL	N-CA-CB	-6.41	101.67	112.44
1	B	98	HIS	CB-CG-CD2	-6.39	122.89	131.20
1	B	279	ASP	CA-CB-CG	6.39	118.99	112.60
1	A	69	ASP	N-CA-C	6.38	114.87	108.75
1	A	196	VAL	N-CA-CB	-6.36	101.03	110.58
1	A	101	GLN	CA-CB-CG	-6.34	101.41	114.10
1	A	174	SER	N-CA-C	6.31	117.82	111.07
1	A	168	GLU	CA-C-O	6.31	127.88	120.69
1	A	183	GLU	CA-CB-CG	-6.16	101.77	114.10
1	A	253	PHE	CA-CB-CG	6.15	119.95	113.80
1	A	289	ASN	CA-CB-CG	6.08	118.68	112.60
1	B	50	HIS	CB-CG-CD2	-6.07	123.31	131.20
1	B	271	ILE	N-CA-C	6.07	117.99	112.29
1	A	186	TRP	CA-C-O	6.05	126.04	119.15
1	A	15	ASN	N-CA-C	5.97	123.53	110.80
1	B	238	GLY	N-CA-C	-5.97	99.02	113.18
1	A	36	ASN	CB-CG-ND2	5.97	125.35	116.40
1	B	36	ASN	CB-CG-ND2	5.90	125.25	116.40
1	B	204	ILE	N-CA-C	-5.89	99.86	108.11
1	A	209	ASN	N-CA-CB	-5.89	100.87	109.82
1	A	50	HIS	CA-CB-CG	-5.88	107.92	113.80
1	B	237	LEU	CA-CB-CG	5.87	136.85	116.30
1	A	88	THR	CA-CB-OG1	-5.83	100.85	109.60
1	B	99	TRP	CG-CD2-CE3	5.82	139.72	133.90
1	B	181	CYS	CB-CA-C	-5.82	101.13	110.79
1	B	239	SER	CA-CB-OG	5.81	122.72	111.10
1	A	140	ASN	CA-CB-CG	5.80	118.40	112.60
1	A	246	ASN	CA-CB-CG	5.77	118.37	112.60
1	B	5	CYS	CA-CB-SG	5.71	127.54	114.40
1	B	197	ALA	N-CA-C	5.69	120.76	111.37
1	A	271	ILE	N-CA-C	5.69	117.57	112.17
1	A	187	ASP	CA-CB-CG	5.68	118.28	112.60
1	B	184	HIS	CB-CG-CD2	-5.63	123.89	131.20
1	A	242	ASP	CA-CB-CG	5.61	118.21	112.60
1	B	72	HIS	CB-CG-CD2	-5.61	123.91	131.20
1	B	166	ASP	CA-CB-CG	5.59	118.19	112.60
1	B	163	ASN	N-CA-C	5.59	117.05	111.07
1	A	55	ALA	N-CA-C	-5.56	105.30	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	LYS	N-CA-C	5.54	122.61	110.80
1	A	251	ARG	NE-CZ-NH1	5.54	127.04	121.50
1	B	103	LYS	CA-CB-CG	-5.54	103.03	114.10
1	A	240	SER	O-C-N	-5.51	116.78	122.84
1	A	166	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	147	LYS	CA-CB-CG	-5.48	103.15	114.10
1	B	239	SER	CA-C-O	5.48	128.34	120.51
1	B	49	ASP	CA-CB-CG	5.42	118.02	112.60
1	B	209	ASN	O-C-N	-5.41	116.46	122.09
1	A	273	VAL	CB-CA-C	5.37	118.72	110.55
1	B	196	VAL	N-CA-CB	-5.36	101.60	110.56
1	A	91	ASN	CB-CG-ND2	5.34	124.41	116.40
1	A	168	GLU	CA-C-N	5.30	131.81	121.41
1	A	168	GLU	C-N-CA	5.30	131.81	121.41
1	B	98	HIS	CB-CG-ND1	5.30	130.65	122.70
1	B	55	ALA	N-CA-C	-5.23	105.47	111.07
1	B	183	GLU	CA-CB-CG	-5.22	103.67	114.10
1	A	7	THR	CB-CA-C	5.21	118.12	109.53
1	A	246	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	B	91	ASN	OD1-CG-ND2	-5.18	117.42	122.60
1	B	234	TYR	N-CA-C	-5.18	101.67	109.85
1	A	18	GLN	OE1-CD-NE2	-5.18	117.42	122.60
1	B	241	HIS	CB-CG-CD2	-5.17	124.48	131.20
1	A	198	ASN	CA-CB-CG	5.17	117.77	112.60
1	A	6	LYS	N-CA-C	5.13	121.72	110.80
1	B	21	HIS	CB-CG-CD2	-5.12	124.54	131.20
1	A	204	ILE	N-CA-C	-5.10	100.97	108.11
1	A	197	ALA	N-CA-C	5.10	121.66	110.80
1	A	50	HIS	CB-CG-CD2	-5.09	124.58	131.20
1	B	246	ASN	CA-CB-CG	5.08	117.68	112.60
1	B	282	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	B	216	GLN	OE1-CD-NE2	-5.05	117.55	122.60
1	A	303	GLU	N-CA-C	-5.04	100.95	109.07
1	A	170	HIS	CB-CG-CD2	-5.04	124.65	131.20
1	A	163	ASN	N-CA-C	5.03	116.76	111.28
1	A	225	HIS	CB-CG-CD2	-5.03	124.66	131.20
1	A	141	LEU	CB-CA-C	-5.01	102.79	110.81
1	A	126	ASP	N-CA-C	-5.01	107.72	113.88
1	B	139	VAL	O-C-N	-5.00	116.31	122.57
1	A	299	ASN	OD1-CG-ND2	-5.00	117.60	122.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	168	GLU	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	2294	0	2185	25	0
1	B	2298	0	2212	20	0
2	A	26	0	0	0	0
2	B	29	0	0	0	0
All	All	4647	0	4397	40	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 4.

All (40) 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:185:HIS:HE1	1:B:156:LEU:O	1.56	0.86
1:B:289:ASN:HA	1:B:292:ARG:HD3	1.57	0.84
1:A:156:LEU:O	1:B:185:HIS:HE1	1.66	0.78
1:B:48:MET:HE1	1:B:243:LEU:HB2	1.75	0.69
1:A:185:HIS:CE1	1:B:156:LEU:O	2.45	0.65
1:A:9:ALA:HB1	1:A:297:ILE:HD12	1.83	0.60
1:B:237:LEU:HD12	1:B:238:GLY:H	1.67	0.59
1:B:237:LEU:HD12	1:B:238:GLY:N	2.22	0.55
1:A:20:LEU:HD21	1:A:96:VAL:HG22	1.87	0.55
1:B:228:THR:HB	1:B:230:HIS:CE1	2.43	0.54
1:A:196:VAL:HG13	1:A:226:ILE:HG12	1.90	0.53
1:B:118:ARG:HB2	1:B:138:VAL:HG22	1.90	0.53
1:A:7:THR:HA	1:A:24:GLU:O	2.10	0.52
1:A:161:LEU:HG	1:A:174:SER:HB3	1.94	0.50
1:A:124:ILE:HD12	1:A:199:THR:HG21	1.94	0.50
1:A:285:ILE:O	1:A:289:ASN:HB2	2.12	0.50
1:A:145:LEU:O	1:A:149:LEU:HG	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LYS:HD3	1:A:212:ASP:O	2.12	0.49
1:A:36:ASN:OD1	1:A:107:ASN:HB3	2.14	0.48
1:A:10:HIS:HE1	1:A:24:GLU:OE1	1.98	0.46
1:B:124:ILE:HD11	1:B:196:VAL:HG22	1.98	0.46
1:B:255:GLN:HG3	1:B:275:PHE:CZ	2.51	0.45
1:B:112:ALA:O	1:B:134:THR:HA	2.17	0.45
1:A:202:PRO:HG3	1:A:230:HIS:CE1	2.54	0.43
1:B:213:TRP:CD1	1:B:213:TRP:N	2.87	0.43
1:A:221:ASP:O	1:A:225:HIS:ND1	2.49	0.42
1:A:118:ARG:HB2	1:A:138:VAL:CG2	2.49	0.42
1:A:156:LEU:C	1:B:185:HIS:HE1	2.25	0.42
1:A:68:TYR:CG	1:A:96:VAL:HG21	2.55	0.42
1:A:161:LEU:HA	1:A:162:PRO:HD2	1.88	0.42
1:A:185:HIS:CE1	1:B:156:LEU:C	2.98	0.42
1:B:115:LEU:HD12	1:B:115:LEU:HA	1.82	0.41
1:A:209:ASN:HB2	1:A:236:LEU:O	2.21	0.41
1:B:28:LYS:O	1:B:31:VAL:HG22	2.19	0.41
1:A:206:PHE:HA	1:A:234:TYR:O	2.19	0.41
1:B:98:HIS:O	1:B:102:THR:HG23	2.20	0.41
1:B:56:GLU:O	1:B:60:THR:HB	2.21	0.41
1:B:203:LEU:O	1:B:231:CYS:HA	2.20	0.40
1:A:56:GLU:O	1:A:60:THR:HB	2.22	0.40
1:A:171:LYS:HB2	1:A:171:LYS:HE3	1.89	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	290/305 (95%)	273 (94%)	14 (5%)	3 (1%)	12	9
1	B	289/305 (95%)	276 (96%)	10 (4%)	3 (1%)	12	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	579/610 (95%)	549 (95%)	24 (4%)	6 (1%)	12 9

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	6	LYS
1	B	15	ASN
1	B	6	LYS
1	B	239	SER
1	A	238	GLY

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	248/266 (93%)	226 (91%)	22 (9%)	9 6
1	B	248/266 (93%)	233 (94%)	15 (6%)	17 15
All	All	496/532 (93%)	459 (92%)	37 (8%)	12 10

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	31	VAL
1	A	38	ILE
1	A	60	THR
1	A	73	HIS
1	A	74	VAL
1	A	110	LEU
1	A	124	ILE
1	A	126	ASP
1	A	161	LEU
1	A	163	ASN
1	A	196	VAL

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Mol	Chain	Res	Type
1	A	204	ILE
1	A	210	ASN
1	A	223	LEU
1	A	251	ARG
1	A	255	GLN
1	A	269	LEU
1	A	273	VAL
1	A	288	VAL
1	A	301	THR
1	A	304	MET
1	B	60	THR
1	B	110	LEU
1	B	126	ASP
1	B	138	VAL
1	B	141	LEU
1	B	161	LEU
1	B	163	ASN
1	B	174	SER
1	B	196	VAL
1	B	223	LEU
1	B	230	HIS
1	B	251	ARG
1	B	269	LEU
1	B	273	VAL
1	B	292	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	185	HIS
1	A	209	ASN
1	A	210	ASN
1	A	230	HIS
1	B	10	HIS
1	B	35	ASN
1	B	91	ASN
1	B	163	ASN
1	B	185	HIS
1	B	198	ASN
1	B	230	HIS
1	B	255	GLN

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.