



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:20 AM UTC

PDB ID : 1DTE / pdb_00001dte
Title : THE STRUCTURAL ORIGINS OF INTERFACIAL ACTIVATION IN THERMOMYCES (HUMICOLA) LANUGINOSA LIPASE
Authors : Brozozowski, A.M.; Savage, H.
Deposited on : 2000-01-12
Resolution : 2.35 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

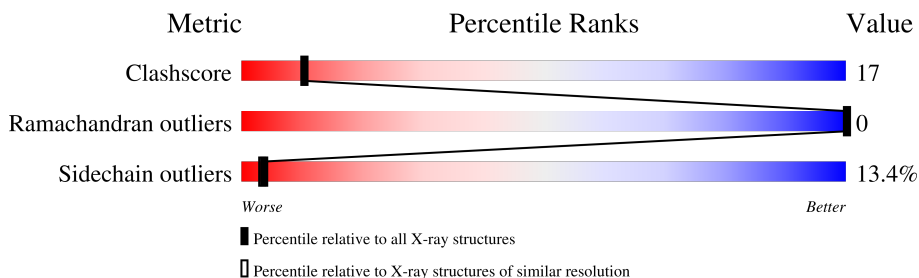
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)

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	 41% 40% 15% •
1	B	269	 36% 45% 16% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4428 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	9	0	0
			2071	1303	359	403	6			
1	B	269	Total	C	N	O	S	9	0	0
			2071	1303	359	403	6			

- Molecule 2 is water.

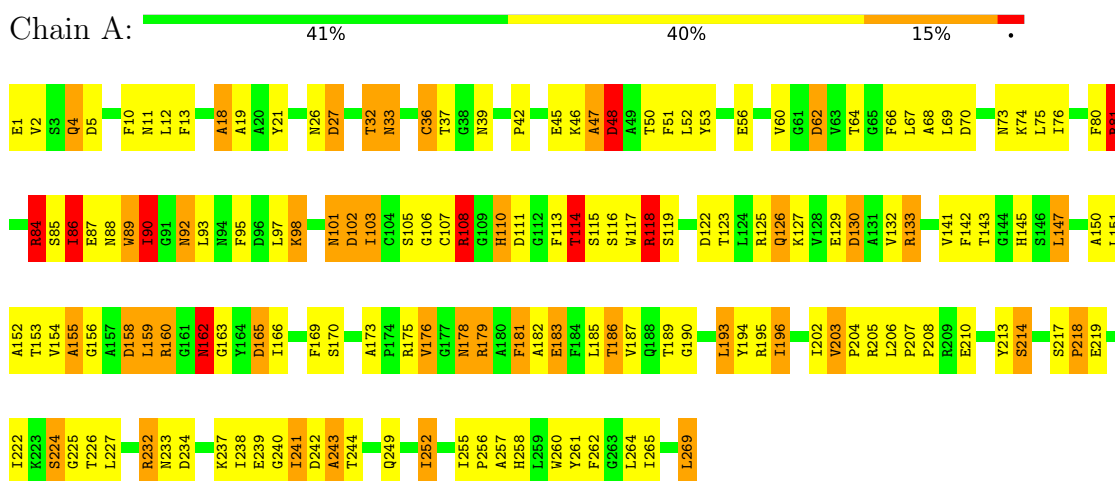
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	122	Total	O	10	0
			122	122		
2	B	164	Total	O	45	0
			164	164		

3 Residue-property plots

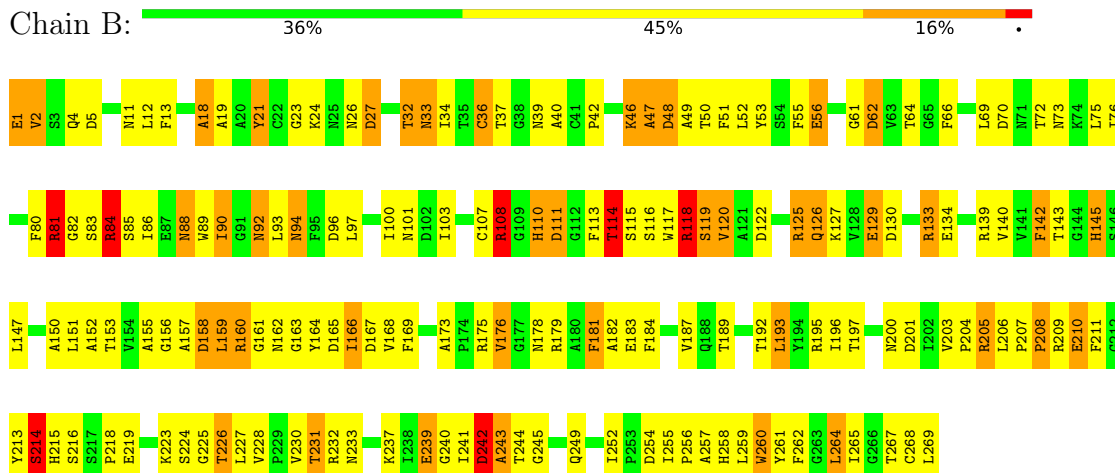
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• 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 2	Depositor
Cell constants a, b, c, α , β , γ	96.13Å 71.10Å 82.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35	Depositor
% Data completeness (in resolution range)	88.9 (20.00-2.35)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.263 , 0.352	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4428	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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	1.13	2/2121 (0.1%)	2.69	183/2887 (6.3%)
1	B	1.15	6/2121 (0.3%)	2.74	206/2887 (7.1%)
All	All	1.14	8/4242 (0.2%)	2.72	389/5774 (6.7%)

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	B	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	GLU	C-N	18.09	1.58	1.33
1	B	1	GLU	C-N	15.79	1.54	1.33
1	B	18	ALA	C-O	6.28	1.31	1.24
1	B	245	GLY	N-CA	6.14	1.53	1.45
1	B	225	GLY	C-O	-6.06	1.16	1.23
1	A	163	GLY	C-N	-5.58	1.26	1.33
1	B	241	ILE	C-O	-5.42	1.18	1.24
1	B	219	GLU	N-CA	5.01	1.52	1.46

All (389) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	ASN	CA-CB-CG	26.94	139.54	112.60
1	A	4	GLN	OE1-CD-NE2	-20.85	101.75	122.60
1	B	244	THR	O-C-N	-16.47	104.49	122.94
1	A	92	ASN	OD1-CG-ND2	-16.07	106.53	122.60
1	B	4	GLN	OE1-CD-NE2	-15.32	107.28	122.60
1	B	92	ASN	OD1-CG-ND2	-14.49	108.11	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	160	ARG	CD-NE-CZ	13.80	143.72	124.40
1	B	73	ASN	OD1-CG-ND2	-13.73	108.87	122.60
1	B	233	ASN	OD1-CG-ND2	-13.64	108.96	122.60
1	A	92	ASN	CB-CG-ND2	13.64	136.86	116.40
1	A	233	ASN	OD1-CG-ND2	-13.26	109.34	122.60
1	B	27	ASP	CA-CB-CG	12.79	125.39	112.60
1	A	244	THR	O-C-N	-12.60	106.76	122.26
1	A	160	ARG	NH1-CZ-NH2	-12.39	103.19	119.30
1	B	210	GLU	CA-CB-CG	12.20	138.50	114.10
1	A	48	ASP	CA-CB-CG	12.18	124.78	112.60
1	A	11	ASN	OD1-CG-ND2	-12.15	110.45	122.60
1	B	47	ALA	O-C-N	-12.12	108.10	122.89
1	A	160	ARG	NE-CZ-NH1	12.09	133.59	121.50
1	B	1	GLU	O-C-N	11.91	142.05	123.00
1	B	1	GLU	CA-C-N	-11.76	104.09	122.68
1	B	1	GLU	C-N-CA	-11.76	104.09	122.68
1	B	195	ARG	CD-NE-CZ	11.57	140.60	124.40
1	B	113	PHE	CA-CB-CG	11.54	125.34	113.80
1	A	1	GLU	CA-C-N	-11.50	103.60	122.57
1	A	1	GLU	C-N-CA	-11.50	103.60	122.57
1	B	62	ASP	N-CA-C	11.48	124.34	110.91
1	A	27	ASP	CA-CB-CG	11.37	123.97	112.60
1	A	62	ASP	N-CA-C	11.24	124.07	110.91
1	B	162	ASN	CA-CB-CG	11.18	123.78	112.60
1	B	195	ARG	NE-CZ-NH1	-10.73	110.77	121.50
1	A	160	ARG	CD-NE-CZ	10.64	139.29	124.40
1	B	193	LEU	O-C-N	-10.64	111.25	123.27
1	B	237	LYS	CA-C-O	-10.41	109.44	120.58
1	B	11	ASN	OD1-CG-ND2	-10.37	112.23	122.60
1	B	181	PHE	CA-CB-CG	10.25	124.05	113.80
1	B	224	SER	CA-C-N	-10.20	111.45	122.67
1	B	224	SER	C-N-CA	-10.20	111.45	122.67
1	B	70	ASP	CA-CB-CG	10.15	122.75	112.60
1	B	81	ARG	NE-CZ-NH2	-10.14	110.07	119.20
1	B	225	GLY	O-C-N	-10.13	114.77	123.59
1	B	18	ALA	CA-C-O	10.07	131.22	120.55
1	A	181	PHE	CA-CB-CG	10.03	123.83	113.80
1	A	176	VAL	N-CA-CB	-10.00	100.43	112.33
1	B	110	HIS	CA-CB-CG	9.78	123.58	113.80
1	A	129	GLU	CA-C-O	-9.76	110.21	120.55
1	B	126	GLN	CA-CB-CG	9.60	133.30	114.10
1	B	160	ARG	NH1-CZ-NH2	-9.45	107.02	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	PHE	CA-CB-CG	9.35	123.15	113.80
1	B	175	ARG	NE-CZ-NH2	9.34	127.60	119.20
1	A	160	ARG	O-C-N	9.32	133.42	122.79
1	A	196	ILE	CA-C-O	9.32	131.24	120.71
1	B	80	PHE	CA-C-O	9.31	131.13	120.80
1	B	89	TRP	CA-C-O	9.19	130.56	120.63
1	B	73	ASN	CA-CB-CG	9.18	121.78	112.60
1	A	210	GLU	CA-CB-CG	8.94	131.98	114.10
1	A	90	ILE	CB-CA-C	8.91	124.19	112.24
1	B	201	ASP	CA-CB-CG	8.86	121.46	112.60
1	B	195	ARG	NE-CZ-NH2	8.85	127.17	119.20
1	A	175	ARG	NE-CZ-NH1	-8.79	112.71	121.50
1	B	27	ASP	N-CA-CB	-8.59	95.29	111.43
1	A	202	ILE	CA-C-N	8.51	125.60	120.24
1	A	202	ILE	C-N-CA	8.51	125.60	120.24
1	B	114	THR	O-C-N	-8.50	113.11	122.12
1	A	114	THR	N-CA-C	-8.49	102.11	111.36
1	A	237	LYS	CA-C-O	-8.48	111.02	120.60
1	B	205	ARG	CD-NE-CZ	-8.46	112.55	124.40
1	A	160	ARG	CA-C-O	-8.44	112.08	121.87
1	A	76	ILE	N-CA-CB	8.37	122.27	112.15
1	A	160	ARG	N-CA-CB	8.36	122.32	110.36
1	A	224	SER	CA-C-O	-8.36	112.47	121.99
1	B	226	THR	CA-C-O	8.34	128.72	120.88
1	A	169	PHE	CA-CB-CG	8.24	122.04	113.80
1	B	161	GLY	N-CA-C	-8.22	103.68	115.27
1	B	225	GLY	CA-C-N	8.09	135.96	121.97
1	B	225	GLY	C-N-CA	8.09	135.96	121.97
1	B	254	ASP	CA-CB-CG	8.08	120.68	112.60
1	A	51	PHE	CA-CB-CG	8.07	121.87	113.80
1	A	240	GLY	CA-C-N	8.06	133.27	121.18
1	A	240	GLY	C-N-CA	8.06	133.27	121.18
1	B	139	ARG	CA-C-O	-8.04	111.42	120.43
1	A	70	ASP	CA-CB-CG	8.02	120.62	112.60
1	B	205	ARG	CG-CD-NE	7.97	129.54	112.00
1	B	158	ASP	N-CA-C	7.95	120.02	111.36
1	A	241	ILE	CB-CG1-CD1	7.94	130.48	113.80
1	B	114	THR	N-CA-CB	-7.93	98.47	110.12
1	A	1	GLU	O-C-N	7.93	135.68	123.00
1	A	111	ASP	CA-C-O	-7.90	112.52	120.82
1	A	205	ARG	CA-C-O	7.89	128.15	119.15
1	A	243	ALA	CA-C-O	7.88	129.95	121.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	THR	CA-C-O	-7.87	112.68	121.89
1	A	163	GLY	N-CA-C	7.84	126.29	115.00
1	A	115	SER	N-CA-C	7.80	119.48	110.97
1	B	88	ASN	CA-CB-CG	7.80	120.40	112.60
1	A	90	ILE	N-CA-CB	-7.79	97.56	110.56
1	B	85	SER	CA-C-O	7.75	130.85	121.94
1	A	162	ASN	OD1-CG-ND2	-7.72	114.88	122.60
1	B	176	VAL	N-CA-CB	-7.67	103.20	112.33
1	B	111	ASP	CA-C-O	-7.66	112.43	120.55
1	A	195	ARG	NE-CZ-NH2	7.66	126.09	119.20
1	B	88	ASN	O-C-N	-7.65	113.89	122.08
1	B	233	ASN	CA-CB-CG	-7.63	104.97	112.60
1	B	209	ARG	CA-C-N	7.62	131.51	120.38
1	B	209	ARG	C-N-CA	7.62	131.51	120.38
1	B	114	THR	CB-CA-C	7.62	123.44	110.79
1	A	202	ILE	N-CA-C	7.60	118.37	110.62
1	B	160	ARG	CA-C-N	-7.59	109.80	122.25
1	B	160	ARG	C-N-CA	-7.59	109.80	122.25
1	A	203	VAL	CA-C-O	7.58	125.29	118.85
1	A	126	GLN	CA-CB-CG	7.58	129.26	114.10
1	B	258	HIS	CA-C-O	-7.57	111.72	120.20
1	A	84	ARG	NE-CZ-NH2	7.56	126.01	119.20
1	B	162	ASN	OD1-CG-ND2	-7.55	115.05	122.60
1	B	182	ALA	CA-C-N	7.55	130.25	120.44
1	B	182	ALA	C-N-CA	7.55	130.25	120.44
1	A	47	ALA	O-C-N	-7.51	112.09	122.46
1	B	175	ARG	NE-CZ-NH1	-7.51	113.99	121.50
1	B	160	ARG	CA-C-O	-7.49	113.40	121.56
1	A	156	GLY	O-C-N	-7.47	115.01	122.18
1	A	110	HIS	CA-CB-CG	7.44	121.24	113.80
1	A	142	PHE	CA-CB-CG	7.42	121.22	113.80
1	B	101	ASN	CA-CB-CG	7.40	120.00	112.60
1	B	160	ARG	NE-CZ-NH2	7.40	125.86	119.20
1	A	143	THR	CA-C-O	-7.38	113.56	121.45
1	A	196	ILE	O-C-N	-7.36	114.56	122.95
1	B	169	PHE	CA-C-N	-7.34	111.93	122.94
1	B	169	PHE	C-N-CA	-7.34	111.93	122.94
1	B	90	ILE	CB-CA-C	7.32	122.04	112.24
1	B	11	ASN	CB-CG-ND2	7.30	127.36	116.40
1	A	187	VAL	CA-C-O	7.30	125.89	118.96
1	B	152	ALA	CA-C-O	-7.29	112.75	120.63
1	A	238	ILE	CA-C-O	7.23	128.47	120.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	VAL	O-C-N	-7.21	114.95	120.07
1	A	4	GLN	CG-CD-NE2	7.18	127.17	116.40
1	A	170	SER	CA-C-O	-7.16	113.03	121.11
1	B	115	SER	N-CA-C	7.16	118.87	111.14
1	B	18	ALA	O-C-N	-7.14	114.56	122.12
1	A	114	THR	CB-CA-C	7.12	122.96	110.85
1	B	27	ASP	CB-CG-OD2	7.12	134.77	118.40
1	B	13	PHE	CA-CB-CG	-7.11	106.69	113.80
1	A	249	GLN	O-C-N	7.11	127.09	121.55
1	A	115	SER	CA-CB-OG	-7.06	96.99	111.10
1	B	142	PHE	CA-C-O	7.01	128.27	120.70
1	B	81	ARG	NH1-CZ-NH2	6.99	128.39	119.30
1	A	185	LEU	CA-C-O	-6.98	112.21	120.10
1	B	226	THR	CB-CA-C	-6.97	101.22	109.80
1	B	47	ALA	CA-C-O	-6.97	113.36	121.16
1	A	218	PRO	N-CA-CB	-6.96	94.94	102.60
1	A	175	ARG	N-CA-C	-6.96	100.69	110.50
1	A	85	SER	CA-C-O	6.93	129.91	121.94
1	A	122	ASP	CA-CB-CG	-6.92	105.68	112.60
1	A	108	ARG	CA-C-O	-6.92	113.03	121.06
1	B	2	VAL	CA-C-O	6.89	128.91	121.67
1	B	204	PRO	CA-C-N	6.87	133.14	122.49
1	B	204	PRO	C-N-CA	6.87	133.14	122.49
1	B	84	ARG	NH1-CZ-NH2	-6.86	110.39	119.30
1	A	195	ARG	CD-NE-CZ	6.82	133.95	124.40
1	A	74	LYS	O-C-N	-6.81	114.80	122.91
1	B	120	VAL	O-C-N	-6.80	115.97	122.16
1	A	132	VAL	CA-CB-CG1	6.80	121.96	110.40
1	B	120	VAL	N-CA-CB	-6.78	103.52	112.26
1	B	163	GLY	CA-C-N	6.77	133.84	121.85
1	B	163	GLY	C-N-CA	6.77	133.84	121.85
1	B	150	ALA	N-CA-C	-6.75	103.84	111.14
1	B	36	CYS	O-C-N	-6.75	115.16	123.33
1	A	84	ARG	NH1-CZ-NH2	-6.75	110.53	119.30
1	A	186	THR	CA-C-O	-6.74	112.22	119.97
1	A	11	ASN	CB-CG-ND2	6.72	126.48	116.40
1	A	225	GLY	N-CA-C	6.68	121.72	112.57
1	A	163	GLY	CA-C-N	6.61	133.18	121.75
1	A	163	GLY	C-N-CA	6.61	133.18	121.75
1	A	249	GLN	CA-C-O	-6.61	114.10	120.64
1	B	143	THR	CA-C-O	-6.59	114.21	121.33
1	A	165	ASP	CA-CB-CG	6.59	119.19	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	VAL	N-CA-CB	-6.59	106.35	110.50
1	B	175	ARG	N-CA-C	-6.58	101.23	110.50
1	A	116	SER	CA-C-O	6.57	127.93	120.90
1	A	142	PHE	CA-C-O	6.57	127.79	120.70
1	B	228	VAL	CA-C-O	-6.54	114.35	119.98
1	B	122	ASP	CA-CB-CG	-6.54	106.06	112.60
1	B	187	VAL	N-CA-CB	-6.54	105.02	112.21
1	B	51	PHE	CA-CB-CG	6.50	120.31	113.80
1	B	92	ASN	CB-CG-ND2	6.42	126.03	116.40
1	B	168	VAL	O-C-N	-6.41	116.24	123.10
1	B	163	GLY	N-CA-C	6.41	125.18	115.63
1	A	205	ARG	CD-NE-CZ	-6.41	115.43	124.40
1	A	173	ALA	CB-CA-C	6.38	117.87	108.87
1	B	214	SER	N-CA-CB	-6.34	101.34	111.43
1	A	73	ASN	CA-CB-CG	6.33	118.93	112.60
1	B	48	ASP	CA-CB-CG	6.31	118.91	112.60
1	B	196	ILE	N-CA-C	6.30	117.21	108.89
1	B	189	THR	CA-C-O	-6.24	113.97	121.89
1	A	81	ARG	NE-CZ-NH2	-6.21	113.61	119.20
1	B	157	ALA	CA-C-O	-6.20	113.98	120.55
1	B	90	ILE	N-CA-CB	-6.17	100.25	110.56
1	A	261	TYR	CA-CB-CG	-6.16	102.81	113.90
1	B	129	GLU	CA-C-O	-6.15	114.03	120.55
1	A	118	ARG	NH1-CZ-NH2	6.11	127.24	119.30
1	A	258	HIS	CA-C-O	-6.10	113.21	120.10
1	B	66	PHE	CA-C-N	6.09	131.58	123.00
1	B	66	PHE	C-N-CA	6.09	131.58	123.00
1	A	118	ARG	CB-CA-C	-6.08	100.34	110.68
1	B	134	GLU	CA-C-N	6.08	130.51	123.15
1	B	134	GLU	C-N-CA	6.08	130.51	123.15
1	B	159	LEU	CA-C-O	6.08	126.64	119.28
1	B	142	PHE	CA-CB-CG	6.07	119.87	113.80
1	A	233	ASN	CA-CB-CG	-6.07	106.53	112.60
1	A	60	VAL	CA-C-O	-6.07	113.70	121.40
1	B	169	PHE	CA-CB-CG	6.05	119.85	113.80
1	A	47	ALA	CA-C-O	-6.04	111.19	119.05
1	B	140	VAL	CA-C-O	-6.02	113.99	120.85
1	B	55	PHE	CA-C-O	6.00	128.02	121.06
1	B	225	GLY	N-CA-C	5.99	122.01	112.06
1	A	219	GLU	OE1-CD-OE2	-5.98	108.55	122.90
1	A	173	ALA	CA-C-N	5.97	126.31	119.92
1	A	173	ALA	C-N-CA	5.97	126.31	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	THR	CA-CB-OG1	-5.97	100.65	109.60
1	B	76	ILE	N-CA-CB	5.96	119.37	112.15
1	B	108	ARG	CA-C-O	-5.93	113.48	120.60
1	B	244	THR	N-CA-C	-5.92	101.75	110.52
1	B	175	ARG	CA-C-N	-5.92	115.56	122.14
1	B	175	ARG	C-N-CA	-5.92	115.56	122.14
1	A	179	ARG	CA-C-O	-5.91	114.16	120.42
1	B	13	PHE	CB-CA-C	5.88	120.85	110.85
1	A	86	ILE	N-CA-C	-5.88	104.78	110.42
1	B	237	LYS	O-C-N	5.87	129.97	122.93
1	B	240	GLY	CA-C-O	5.85	127.98	121.31
1	A	114	THR	N-CA-CB	-5.84	101.52	110.16
1	B	94	ASN	OD1-CG-ND2	5.83	128.43	122.60
1	A	95	PHE	N-CA-C	5.83	120.01	113.02
1	A	116	SER	CA-CB-OG	5.82	122.75	111.10
1	A	21	TYR	CD1-CG-CD2	-5.82	109.37	118.10
1	B	88	ASN	CA-C-O	5.81	127.46	121.07
1	B	32	THR	CA-CB-OG1	-5.80	100.89	109.60
1	A	89	TRP	N-CA-C	5.80	118.35	111.33
1	B	173	ALA	CA-C-N	5.79	126.12	119.92
1	B	173	ALA	C-N-CA	5.79	126.12	119.92
1	B	242	ASP	OD1-CG-OD2	-5.79	109.01	122.90
1	B	19	ALA	CA-C-N	5.78	131.84	121.66
1	B	19	ALA	C-N-CA	5.78	131.84	121.66
1	B	21	TYR	CD1-CG-CD2	-5.78	109.43	118.10
1	B	239	GLU	N-CA-C	5.76	119.64	109.96
1	B	262	PHE	N-CA-CB	5.76	120.22	110.49
1	A	155	ALA	O-C-N	5.75	128.71	122.15
1	B	159	LEU	O-C-N	-5.74	114.44	122.37
1	B	160	ARG	O-C-N	5.74	129.63	122.86
1	A	45	GLU	CA-C-O	5.73	126.63	120.55
1	A	101	ASN	CA-CB-CG	5.73	118.33	112.60
1	A	11	ASN	CA-C-O	-5.73	114.81	120.82
1	B	203	VAL	N-CA-C	5.73	120.91	112.61
1	B	143	THR	O-C-N	5.71	129.76	123.25
1	A	262	PHE	N-CA-CB	5.69	120.10	110.49
1	B	84	ARG	CD-NE-CZ	5.68	132.35	124.40
1	B	205	ARG	NE-CZ-NH1	-5.67	115.83	121.50
1	B	114	THR	N-CA-C	-5.65	105.12	111.28
1	A	12	LEU	N-CA-CB	5.62	118.16	110.01
1	A	187	VAL	N-CA-CB	-5.62	106.03	112.21
1	A	202	ILE	O-C-N	-5.62	116.42	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	160	ARG	NE-CZ-NH1	5.62	127.12	121.50
1	B	240	GLY	CA-C-N	5.62	129.60	121.18
1	B	240	GLY	C-N-CA	5.62	129.60	121.18
1	B	261	TYR	CA-CB-CG	-5.61	103.80	113.90
1	B	119	SER	CA-CB-OG	-5.60	99.89	111.10
1	A	36	CYS	O-C-N	-5.59	116.57	123.33
1	B	215	HIS	CA-C-O	5.57	126.61	120.71
1	B	48	ASP	CB-CA-C	5.57	120.06	110.77
1	A	150	ALA	N-CA-C	-5.55	105.15	111.14
1	A	147	LEU	CA-C-O	5.55	126.35	119.97
1	B	2	VAL	O-C-N	-5.54	116.89	123.04
1	B	167	ASP	CA-C-N	-5.54	115.24	122.94
1	B	167	ASP	C-N-CA	-5.54	115.24	122.94
1	A	18	ALA	O-C-N	-5.54	116.25	122.12
1	A	238	ILE	O-C-N	-5.53	115.67	122.97
1	A	218	PRO	N-CD-CG	-5.52	97.18	103.80
1	B	101	ASN	CA-C-N	5.51	128.43	120.38
1	B	101	ASN	C-N-CA	5.51	128.43	120.38
1	B	139	ARG	O-C-N	5.51	129.47	123.13
1	B	11	ASN	CA-C-O	-5.50	115.04	120.82
1	B	192	THR	CA-C-N	-5.50	115.13	122.72
1	B	192	THR	C-N-CA	-5.50	115.13	122.72
1	A	183	GLU	O-C-N	-5.50	116.15	122.09
1	B	110	HIS	CA-C-N	5.49	127.64	120.28
1	B	110	HIS	C-N-CA	5.49	127.64	120.28
1	A	106	GLY	O-C-N	-5.48	115.21	122.28
1	B	126	GLN	CB-CG-CD	5.48	121.92	112.60
1	A	258	HIS	N-CA-C	5.48	118.01	111.71
1	B	62	ASP	N-CA-CB	-5.48	102.44	111.53
1	A	12	LEU	CB-CA-C	-5.47	102.30	110.88
1	A	13	PHE	CA-CB-CG	-5.47	108.33	113.80
1	B	83	SER	N-CA-CB	5.46	117.99	109.97
1	B	245	GLY	CA-C-O	5.46	124.78	119.27
1	A	85	SER	N-CA-C	5.45	117.56	110.53
1	B	216	SER	CA-C-O	-5.45	115.68	121.94
1	B	66	PHE	CA-C-O	5.42	127.07	121.28
1	A	208	PRO	CA-C-O	5.41	129.94	122.31
1	B	11	ASN	CA-CB-CG	-5.41	107.19	112.60
1	A	158	ASP	N-CA-C	5.40	116.98	111.14
1	B	18	ALA	N-CA-C	-5.39	105.40	111.28
1	A	105	SER	CA-CB-OG	-5.39	100.33	111.10
1	B	153	THR	O-C-N	5.38	128.68	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	HIS	CA-CB-CG	5.37	119.17	113.80
1	A	98	LYS	CB-CG-CD	5.36	123.64	111.30
1	A	73	ASN	OD1-CG-ND2	-5.36	117.24	122.60
1	A	141	VAL	CA-C-O	5.32	126.00	120.36
1	A	178	ASN	CA-CB-CG	-5.32	107.28	112.60
1	A	159	LEU	CB-CA-C	5.32	119.58	110.01
1	A	204	PRO	CA-C-O	5.32	126.01	118.99
1	A	130	ASP	O-C-N	-5.31	115.74	122.27
1	A	145	HIS	CA-CB-CG	5.31	119.11	113.80
1	A	182	ALA	CA-C-N	5.31	127.66	120.44
1	A	182	ALA	C-N-CA	5.31	127.66	120.44
1	B	76	ILE	CA-C-N	-5.30	116.25	122.93
1	B	76	ILE	C-N-CA	-5.30	116.25	122.93
1	B	62	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	122	ASP	CA-C-O	-5.29	114.83	121.02
1	A	183	GLU	CA-C-O	5.29	126.15	120.70
1	A	232	ARG	CD-NE-CZ	5.29	131.80	124.40
1	B	165	ASP	CA-C-O	-5.28	115.40	121.47
1	A	186	THR	CA-CB-OG1	-5.28	101.68	109.60
1	B	219	GLU	OE1-CD-OE2	-5.27	110.25	122.90
1	A	27	ASP	CB-CG-OD2	5.27	130.52	118.40
1	A	252	ILE	N-CA-C	-5.26	103.17	108.96
1	A	260	TRP	CE2-CD2-CE3	5.26	124.06	118.80
1	A	32	THR	CA-CB-OG1	-5.25	101.72	109.60
1	B	89	TRP	N-CA-C	5.24	117.68	111.33
1	B	237	LYS	CA-C-N	5.22	129.76	122.93
1	B	237	LYS	C-N-CA	5.22	129.76	122.93
1	A	187	VAL	O-C-N	-5.21	116.98	122.25
1	B	84	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	A	185	LEU	O-C-N	5.21	128.31	122.22
1	B	4	GLN	CG-CD-OE1	5.21	131.21	120.80
1	A	154	VAL	CA-C-N	-5.20	112.90	120.29
1	A	154	VAL	C-N-CA	-5.20	112.90	120.29
1	B	244	THR	CA-C-O	-5.20	115.58	121.72
1	A	66	PHE	CA-C-O	5.19	126.83	121.28
1	B	219	GLU	CG-CD-OE2	5.19	130.34	118.40
1	A	222	ILE	CA-C-O	-5.19	114.93	120.85
1	A	152	ALA	CA-C-O	-5.18	115.03	120.63
1	A	196	ILE	N-CA-C	5.18	116.04	108.58
1	A	166	ILE	CA-C-N	-5.18	113.21	122.07
1	A	166	ILE	C-N-CA	-5.18	113.21	122.07
1	B	260	TRP	CA-C-O	5.18	127.09	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	243	ALA	CA-C-O	5.18	126.84	121.15
1	B	5	ASP	CA-CB-CG	-5.17	107.43	112.60
1	B	184	PHE	CB-CA-C	-5.17	102.77	110.88
1	B	81	ARG	CB-CG-CD	-5.16	99.43	111.30
1	A	225	GLY	CA-C-N	5.16	128.65	121.02
1	A	225	GLY	C-N-CA	5.16	128.65	121.02
1	A	210	GLU	CB-CG-CD	5.16	121.37	112.60
1	A	80	PHE	CA-CB-CG	-5.15	108.65	113.80
1	B	125	ARG	NE-CZ-NH1	5.14	126.64	121.50
1	A	175	ARG	CA-C-N	-5.14	116.44	122.14
1	A	175	ARG	C-N-CA	-5.14	116.44	122.14
1	B	73	ASN	CB-CG-OD1	5.13	131.07	120.80
1	A	176	VAL	CB-CA-C	5.12	116.15	110.62
1	B	142	PHE	O-C-N	-5.12	116.58	123.23
1	A	4	GLN	CG-CD-OE1	5.11	131.03	120.80
1	B	111	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	160	ARG	CA-C-N	-5.10	112.87	121.85
1	A	160	ARG	C-N-CA	-5.10	112.87	121.85
1	B	225	GLY	CA-C-O	5.10	127.69	121.88
1	B	118	ARG	CB-CA-C	-5.08	102.04	110.68
1	A	89	TRP	CA-C-N	5.08	128.67	120.55
1	A	89	TRP	C-N-CA	5.08	128.67	120.55
1	B	27	ASP	CB-CG-OD1	-5.08	106.72	118.40
1	A	142	PHE	CA-C-N	-5.07	113.55	121.87
1	A	142	PHE	C-N-CA	-5.07	113.55	121.87
1	B	23	GLY	CA-C-N	5.07	127.58	120.28
1	B	23	GLY	C-N-CA	5.07	127.58	120.28
1	B	166	ILE	CA-C-N	-5.07	113.41	122.07
1	B	166	ILE	C-N-CA	-5.07	113.41	122.07
1	B	231	THR	N-CA-CB	5.06	119.48	111.43
1	B	243	ALA	O-C-N	-5.06	116.79	122.97
1	A	178	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	A	5	ASP	CA-C-O	5.05	125.78	120.42
1	A	153	THR	CA-C-O	5.05	125.77	120.42
1	A	175	ARG	NH1-CZ-NH2	5.05	125.86	119.30
1	B	197	THR	CA-C-N	-5.05	115.88	123.00
1	B	197	THR	C-N-CA	-5.05	115.88	123.00
1	A	68	ALA	N-CA-C	5.05	117.83	109.85
1	B	89	TRP	O-C-N	-5.04	116.78	122.12
1	B	85	SER	O-C-N	-5.04	116.45	122.65
1	B	208	PRO	CA-C-O	5.03	129.40	122.31
1	B	249	GLN	O-C-N	5.03	125.47	121.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	ILE	N-CA-C	-5.02	98.74	106.72
1	A	75	LEU	O-C-N	5.02	129.41	123.24
1	A	162	ASN	O-C-N	-5.01	116.33	122.34
1	A	103	ILE	CA-C-N	-5.01	113.18	121.89
1	A	103	ILE	C-N-CA	-5.01	113.18	121.89

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	242	ASP	Mainchain

5.2 Too-close contacts [i](#)

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	65	0
1	B	2071	0	1965	72	0
2	A	122	0	0	17	1
2	B	164	0	0	24	2
All	All	4428	0	3930	137	2

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 17.

All (137) 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:259:LEU:HD23	2:B:348:HOH:O	1.70	0.91
1:B:107:CYS:HB3	1:B:181:PHE:HB2	1.58	0.86
1:B:34:ILE:HB	2:B:333:HOH:O	1.76	0.84
1:B:160:ARG:HG3	2:B:374:HOH:O	1.78	0.83
1:A:126:GLN:HG2	2:A:391:HOH:O	1.81	0.80
1:B:114:THR:HG22	2:B:334:HOH:O	1.81	0.80
1:B:166:ILE:HD12	2:B:374:HOH:O	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LEU:HD12	2:A:310:HOH:O	1.83	0.78
1:A:114:THR:HG22	2:A:313:HOH:O	1.83	0.78
1:A:110:HIS:O	1:A:114:THR:HB	1.84	0.78
1:A:126:GLN:CG	2:A:391:HOH:O	2.33	0.75
1:A:107:CYS:HB3	1:A:181:PHE:HB2	1.70	0.72
1:A:26:ASN:HB2	1:A:56:GLU:HG3	1.71	0.71
1:B:142:PHE:CZ	1:B:166:ILE:HD13	2.26	0.71
1:A:84:ARG:HH11	1:A:84:ARG:HG3	1.56	0.71
1:A:269:LEU:HD22	2:A:320:HOH:O	1.92	0.69
1:A:217:SER:HB3	2:A:324:HOH:O	1.93	0.69
1:A:102:ASP:HB3	2:A:386:HOH:O	1.92	0.68
1:A:232:ARG:HD3	2:A:297:HOH:O	1.94	0.67
1:B:166:ILE:HB	2:B:374:HOH:O	1.93	0.67
1:B:110:HIS:O	1:B:114:THR:HB	1.93	0.66
1:B:12:LEU:HD11	2:B:366:HOH:O	1.94	0.66
1:A:203:VAL:HA	2:A:310:HOH:O	1.98	0.64
1:A:206:LEU:HA	1:A:207:PRO:C	2.23	0.64
1:B:206:LEU:HA	1:B:207:PRO:C	2.24	0.62
1:A:101:ASN:HB3	2:A:387:HOH:O	2.00	0.60
1:B:166:ILE:CG1	2:B:374:HOH:O	2.49	0.60
1:B:164:TYR:HE2	1:B:166:ILE:HD11	1.66	0.59
1:A:33:ASN:N	1:A:33:ASN:HD22	2.02	0.58
1:A:84:ARG:CZ	2:A:275:HOH:O	2.51	0.58
1:A:217:SER:CB	2:A:324:HOH:O	2.49	0.58
1:B:166:ILE:CB	2:B:374:HOH:O	2.52	0.57
1:B:103:ILE:HD11	1:B:118:ARG:HH12	1.70	0.57
1:B:84:ARG:HH11	1:B:84:ARG:HG3	1.70	0.56
1:B:64:THR:HB	1:B:81:ARG:HD2	1.87	0.56
1:A:32:THR:O	1:A:50:THR:HA	2.05	0.56
1:B:26:ASN:HB2	1:B:56:GLU:HG3	1.88	0.56
1:A:214:SER:OG	1:A:242:ASP:OD2	2.20	0.55
1:B:84:ARG:CZ	2:B:287:HOH:O	2.54	0.55
1:A:162:ASN:HB3	2:A:290:HOH:O	2.06	0.55
1:B:32:THR:O	1:B:50:THR:HA	2.06	0.55
1:B:243:ALA:HB1	2:B:307:HOH:O	2.06	0.55
1:B:145:HIS:HE1	2:B:348:HOH:O	1.89	0.54
1:A:27:ASP:HB3	1:A:56:GLU:OE1	2.07	0.54
1:B:207:PRO:HG2	1:B:213:TYR:CZ	2.43	0.54
1:B:33:ASN:HD22	1:B:33:ASN:N	2.06	0.54
1:B:42:PRO:O	1:B:46:LYS:HB2	2.07	0.54
1:B:255:ILE:HB	1:B:256:PRO:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ASP:O	1:A:133:ARG:HD2	2.07	0.54
1:B:156:GLY:O	1:B:160:ARG:HD2	2.08	0.54
1:A:255:ILE:HB	1:A:256:PRO:HD3	1.90	0.53
1:B:62:ASP:CG	2:B:335:HOH:O	2.50	0.53
1:A:2:VAL:O	1:A:232:ARG:HB2	2.09	0.53
1:A:242:ASP:O	1:A:243:ALA:C	2.45	0.53
1:B:256:PRO:O	1:B:257:ALA:C	2.52	0.53
1:A:39:ASN:OD1	1:A:42:PRO:HG3	2.09	0.52
1:B:118:ARG:NH2	1:B:158:ASP:OD2	2.43	0.52
1:B:232:ARG:HD3	2:B:275:HOH:O	2.08	0.52
1:B:268:CYS:HA	2:B:289:HOH:O	2.09	0.52
1:A:64:THR:HB	1:A:81:ARG:HD2	1.92	0.51
1:B:18:ALA:HB2	1:B:265:ILE:HG13	1.92	0.51
1:B:108:ARG:HB2	1:B:178:ASN:ND2	2.26	0.51
1:A:53:TYR:CD1	1:A:127:LYS:HE3	2.46	0.51
1:A:241:ILE:HG13	2:A:324:HOH:O	2.11	0.50
1:A:84:ARG:NH1	2:A:275:HOH:O	2.43	0.50
1:B:94:ASN:ND2	1:B:96:ASP:OD2	2.44	0.50
1:B:53:TYR:CD1	1:B:127:LYS:HE3	2.46	0.50
1:B:2:VAL:O	1:B:232:ARG:HB2	2.11	0.50
1:B:84:ARG:NH1	2:B:287:HOH:O	2.45	0.50
1:A:84:ARG:HG3	1:A:84:ARG:NH1	2.20	0.50
1:B:226:THR:HG22	1:B:227:LEU:HG	1.93	0.50
1:B:214:SER:OG	1:B:242:ASP:OD2	2.21	0.50
1:A:4:GLN:HE21	1:A:232:ARG:HD2	1.77	0.49
1:A:207:PRO:HG2	1:A:213:TYR:CZ	2.47	0.49
1:B:130:ASP:O	1:B:133:ARG:HD2	2.13	0.49
1:A:193:LEU:HD12	1:A:194:TYR:N	2.27	0.49
1:A:256:PRO:O	1:A:257:ALA:C	2.55	0.49
1:B:227:LEU:H	1:B:260:TRP:CG	2.31	0.48
1:A:52:LEU:HD21	1:A:69:LEU:HB2	1.95	0.48
1:B:27:ASP:HB3	2:B:342:HOH:O	2.12	0.48
1:B:47:ALA:HB1	1:B:72:THR:HB	1.94	0.48
1:A:26:ASN:CB	1:A:56:GLU:HG3	2.43	0.48
1:B:125:ARG:O	1:B:129:GLU:HG3	2.13	0.48
1:A:108:ARG:HB2	1:A:178:ASN:ND2	2.29	0.48
1:B:230:VAL:HG12	1:B:231:THR:N	2.28	0.47
1:B:145:HIS:CE1	2:B:348:HOH:O	2.65	0.47
1:A:62:ASP:HB3	1:A:88:ASN:HD21	1.79	0.47
1:B:116:SER:O	1:B:120:VAL:HG22	2.15	0.47
1:B:62:ASP:HB3	1:B:88:ASN:HD21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ARG:CD	1:A:159:LEU:HD22	2.46	0.46
1:B:96:ASP:CG	2:B:318:HOH:O	2.58	0.46
1:A:224:SER:HB3	1:A:234:ASP:OD1	2.15	0.46
1:A:265:ILE:O	1:A:265:ILE:HG23	2.16	0.46
1:A:18:ALA:HB2	1:A:265:ILE:HG13	1.97	0.46
1:B:62:ASP:HB3	1:B:88:ASN:ND2	2.30	0.46
1:A:87:GLU:O	1:A:90:ILE:HG22	2.17	0.45
1:A:86:ILE:O	1:A:90:ILE:HB	2.16	0.45
1:A:160:ARG:HG2	1:A:190:GLY:O	2.16	0.45
1:A:165:ASP:OD1	1:A:190:GLY:HA2	2.16	0.45
1:B:164:TYR:CE2	1:B:166:ILE:HD11	2.50	0.45
1:A:89:TRP:HA	1:A:92:ASN:HD22	1.81	0.45
1:A:97:LEU:HB3	1:A:108:ARG:HG2	1.99	0.44
1:B:84:ARG:HG3	1:B:84:ARG:NH1	2.31	0.44
1:B:84:ARG:NH2	2:B:287:HOH:O	2.50	0.44
1:B:223:LYS:HD2	2:B:288:HOH:O	2.17	0.44
1:A:117:TRP:CE3	1:A:155:ALA:HB2	2.53	0.44
1:B:92:ASN:O	2:B:364:HOH:O	2.21	0.43
1:A:186:THR:HG23	1:A:217:SER:O	2.19	0.43
1:B:117:TRP:CE3	1:B:155:ALA:HB2	2.54	0.43
1:B:39:ASN:OD1	1:B:42:PRO:HG3	2.18	0.43
1:B:151:LEU:HD23	1:B:151:LEU:HA	1.86	0.43
1:B:97:LEU:HB3	1:B:108:ARG:HG2	2.00	0.43
1:A:19:ALA:HB2	1:A:36:CYS:SG	2.59	0.43
1:B:34:ILE:HG13	1:B:49:ALA:O	2.19	0.42
1:A:10:PHE:CD1	1:A:196:ILE:HD11	2.53	0.42
1:B:61:GLY:O	1:B:62:ASP:HB2	2.19	0.42
1:B:24:LYS:HA	2:B:342:HOH:O	2.19	0.42
1:A:62:ASP:HB3	1:A:88:ASN:ND2	2.35	0.42
1:B:200:ASN:HB3	2:B:340:HOH:O	2.19	0.42
1:B:52:LEU:HD21	1:B:69:LEU:HB2	2.01	0.42
1:B:125:ARG:CD	1:B:159:LEU:HD22	2.50	0.41
1:B:208:PRO:HG2	1:B:211:PHE:CD1	2.55	0.41
1:A:207:PRO:HG2	1:A:213:TYR:CE1	2.55	0.41
1:A:84:ARG:NH2	2:A:275:HOH:O	2.52	0.41
1:B:36:CYS:HB3	1:B:40:ALA:HB3	2.03	0.41
1:A:47:ALA:O	1:A:48:ASP:HB3	2.21	0.41
1:B:21:TYR:OH	1:B:82:GLY:HA3	2.21	0.41
1:A:118:ARG:NH2	1:A:158:ASP:OD2	2.54	0.41
1:A:151:LEU:HD23	1:A:151:LEU:HA	1.94	0.41
1:A:98:LYS:O	1:A:108:ARG:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ILE:HD11	1:A:118:ARG:HH12	1.86	0.40
1:B:205:ARG:HH11	1:B:205:ARG:HD2	1.27	0.40
1:A:102:ASP:HA	2:A:386:HOH:O	2.22	0.40
1:A:226:THR:HG22	1:A:227:LEU:HG	2.02	0.40
1:B:260:TRP:HE3	1:B:264:LEU:HD13	1.86	0.40
1:A:67:LEU:CD2	1:A:127:LYS:HB3	2.52	0.40
1:B:94:ASN:ND2	1:B:111:ASP:HB3	2.36	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:387:HOH:O	2:B:275:HOH:O[2_664]	2.02	0.18
2:B:300:HOH:O	2:B:329:HOH:O[3_657]	2.14	0.06

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	267/269 (99%)	252 (94%)	15 (6%)	0	100	100
1	B	267/269 (99%)	250 (94%)	17 (6%)	0	100	100
All	All	534/538 (99%)	502 (94%)	32 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	220/220 (100%)	193 (88%)	27 (12%)	4	4
1	B	220/220 (100%)	188 (86%)	32 (14%)	3	2
All	All	440/440 (100%)	381 (87%)	59 (13%)	4	3

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	37	THR
1	A	46	LYS
1	A	48	ASP
1	A	81	ARG
1	A	84	ARG
1	A	86	ILE
1	A	90	ILE
1	A	93	LEU
1	A	102	ASP
1	A	108	ARG
1	A	114	THR
1	A	118	ARG
1	A	119	SER
1	A	133	ARG
1	A	147	LEU
1	A	162	ASN
1	A	176	VAL
1	A	179	ARG
1	A	183	GLU
1	A	193	LEU
1	A	214	SER
1	A	218	PRO
1	A	239	GLU
1	A	252	ILE
1	A	264	LEU
1	A	269	LEU
1	B	1	GLU
1	B	33	ASN
1	B	37	THR
1	B	46	LYS
1	B	48	ASP
1	B	56	GLU

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Mol	Chain	Res	Type
1	B	75	LEU
1	B	81	ARG
1	B	84	ARG
1	B	86	ILE
1	B	90	ILE
1	B	93	LEU
1	B	100	ILE
1	B	108	ARG
1	B	114	THR
1	B	118	ARG
1	B	119	SER
1	B	126	GLN
1	B	133	ARG
1	B	147	LEU
1	B	176	VAL
1	B	179	ARG
1	B	183	GLU
1	B	193	LEU
1	B	210	GLU
1	B	214	SER
1	B	218	PRO
1	B	239	GLU
1	B	252	ILE
1	B	264	LEU
1	B	267	THR
1	B	269	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	11	ASN
1	A	33	ASN
1	A	92	ASN
1	A	94	ASN
1	B	4	GLN
1	B	11	ASN
1	B	25	ASN
1	B	33	ASN
1	B	73	ASN
1	B	94	ASN
1	B	198	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.