



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:09 PM UTC

PDB ID : 1DT3 / pdb_00001dt3
Title : THE STRUCTURAL ORIGINS OF INTERFACIAL ACTIVATION IN THERMOMYCES (HUMICOLA) LANUGINOSA LIPASE
Authors : Brozozowski, A.M.; Savage, H.
Deposited on : 2000-01-11
Resolution : 2.60 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

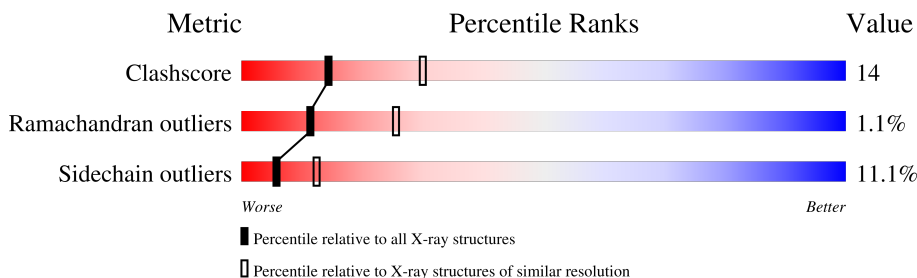
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4384 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			
1	B	269	Total	C	N	O	S	0	0	0
			2071	1303	359	403	6			

- Molecule 2 is water.

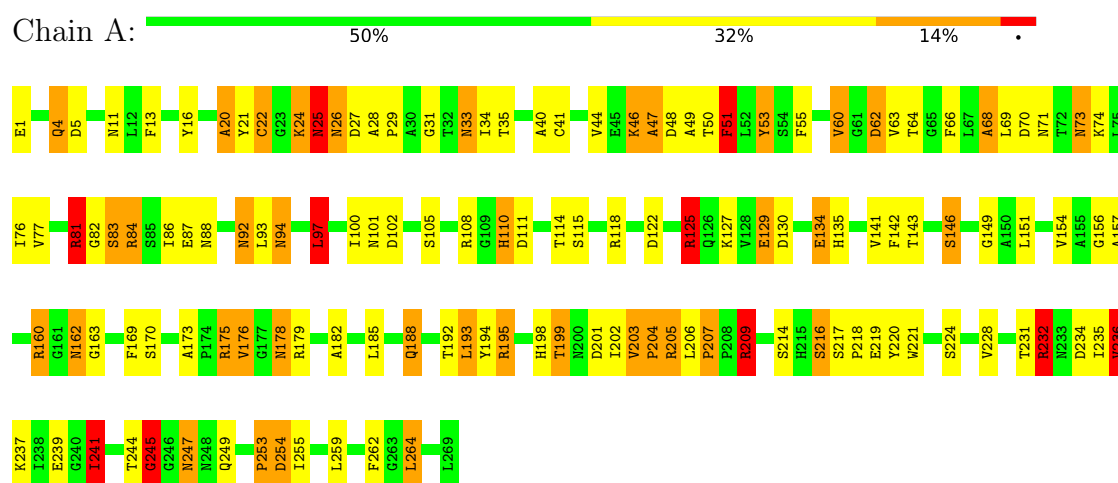
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	99	Total	O	0	0
			99	99		
2	B	143	Total	O	0	0
			143	143		

3 Residue-property plots

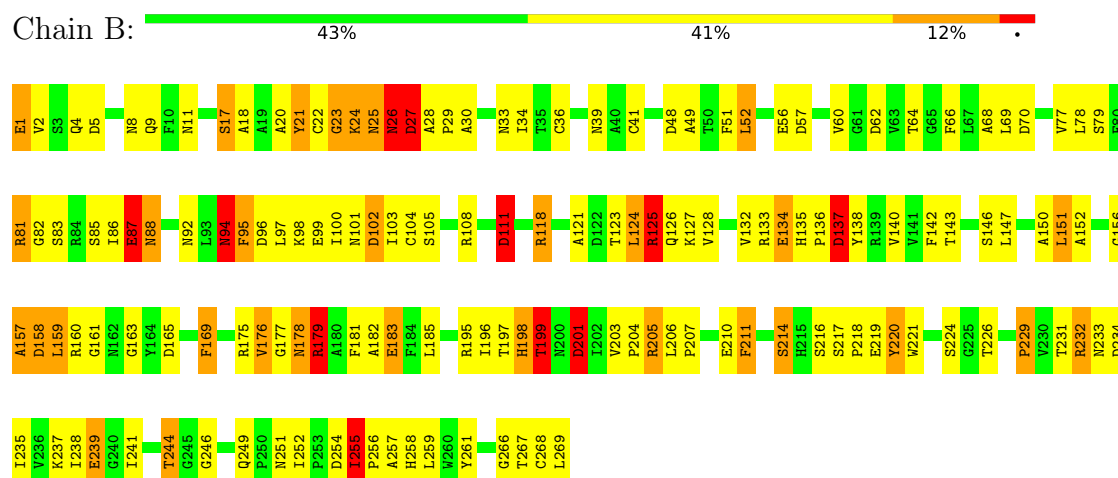
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 61	Depositor
Cell constants a, b, c, α , β , γ	139.92Å 139.92Å 80.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	99.4 (20.00-2.60)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.228 , 0.288	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4384	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.84	0/2121	2.25	111/2887 (3.8%)
1	B	0.89	1/2121 (0.0%)	2.38	121/2887 (4.2%)
All	All	0.87	1/4242 (0.0%)	2.31	232/5774 (4.0%)

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	26
1	B	0	24
All	All	0	50

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	195	ARG	NE-CZ	-5.03	1.27	1.33

All (232) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	195	ARG	CD-NE-CZ	36.27	175.18	124.40
1	A	205	ARG	CD-NE-CZ	20.92	153.69	124.40
1	B	24	LYS	CA-C-N	15.03	145.09	121.19
1	B	24	LYS	C-N-CA	15.03	145.09	121.19
1	A	245	GLY	CA-C-N	11.74	144.42	121.41
1	A	245	GLY	C-N-CA	11.74	144.42	121.41
1	A	94	ASN	CA-CB-CG	11.62	124.22	112.60
1	A	162	ASN	OD1-CG-ND2	-11.53	111.07	122.60
1	A	209	ARG	CD-NE-CZ	11.42	140.39	124.40
1	B	138	TYR	CA-C-N	11.21	137.98	121.72
1	B	138	TYR	C-N-CA	11.21	137.98	121.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	ASN	CA-CB-CG	-10.97	101.63	112.60
1	B	229	PRO	O-C-N	-9.93	110.38	122.99
1	A	203	VAL	N-CA-CB	9.65	116.58	110.50
1	A	262	PHE	CA-C-N	9.28	135.64	120.51
1	A	262	PHE	C-N-CA	9.28	135.64	120.51
1	B	62	ASP	CA-C-N	9.02	134.01	122.37
1	B	62	ASP	C-N-CA	9.02	134.01	122.37
1	A	25	ASN	CA-CB-CG	8.98	121.58	112.60
1	A	83	SER	CA-C-O	8.98	131.22	121.16
1	B	158	ASP	N-CA-C	8.95	122.20	111.82
1	A	205	ARG	CA-C-O	8.84	129.69	119.35
1	B	158	ASP	CA-CB-CG	-8.75	103.85	112.60
1	A	201	ASP	CA-CB-CG	8.69	121.29	112.60
1	B	198	HIS	CA-C-O	8.63	129.78	120.38
1	B	137	ASP	CA-C-N	8.61	132.94	120.71
1	B	137	ASP	C-N-CA	8.61	132.94	120.71
1	A	125	ARG	NE-CZ-NH2	8.31	126.68	119.20
1	A	134	GLU	O-C-N	-8.14	112.92	122.20
1	B	104	CYS	N-CA-CB	8.11	125.19	111.57
1	A	22	CYS	N-CA-C	8.00	120.46	109.11
1	B	201	ASP	CA-CB-CG	7.90	120.50	112.60
1	A	129	GLU	OE1-CD-OE2	7.88	141.82	122.90
1	A	160	ARG	NE-CZ-NH2	7.83	126.25	119.20
1	B	178	ASN	OD1-CG-ND2	7.75	130.35	122.60
1	B	205	ARG	CD-NE-CZ	7.73	135.22	124.40
1	B	217	SER	CA-C-O	-7.72	111.73	120.46
1	B	177	GLY	N-CA-C	7.70	123.56	111.08
1	B	9	GLN	CA-CB-CG	7.58	129.27	114.10
1	B	5	ASP	N-CA-CB	7.47	120.81	109.91
1	A	254	ASP	N-CA-CB	-7.37	97.95	110.99
1	B	137	ASP	CA-CB-CG	7.37	119.97	112.60
1	B	26	ASN	CB-CA-C	7.32	122.55	110.92
1	B	27	ASP	N-CA-C	7.25	118.97	110.41
1	B	88	ASN	OD1-CG-ND2	-7.22	115.38	122.60
1	A	195	ARG	NE-CZ-NH1	-7.19	114.31	121.50
1	A	221	TRP	N-CA-C	7.18	120.38	108.96
1	B	176	VAL	N-CA-CB	-7.17	104.32	112.21
1	B	33	ASN	CB-CG-ND2	7.16	127.14	116.40
1	B	267	THR	CA-C-O	-7.15	112.23	120.31
1	A	205	ARG	CB-CG-CD	7.12	127.68	111.30
1	A	232	ARG	NE-CZ-NH2	-7.09	112.82	119.20
1	A	5	ASP	CA-CB-CG	-7.05	105.55	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	24	LYS	O-C-N	-7.04	113.23	122.59
1	B	179	ARG	N-CA-CB	7.01	121.09	110.30
1	B	125	ARG	NE-CZ-NH2	6.92	125.43	119.20
1	B	94	ASN	O-C-N	-6.90	113.92	122.68
1	B	178	ASN	N-CA-C	6.87	120.51	109.79
1	B	88	ASN	CB-CA-C	6.86	124.34	109.99
1	B	204	PRO	CA-C-N	6.84	133.09	122.49
1	B	204	PRO	C-N-CA	6.84	133.09	122.49
1	B	216	SER	O-C-N	6.80	130.95	122.65
1	A	176	VAL	CB-CA-C	6.76	122.38	111.29
1	B	87	GLU	CB-CG-CD	6.75	124.07	112.60
1	A	110	HIS	CA-C-O	6.74	128.08	120.80
1	B	151	LEU	CA-C-O	-6.71	113.30	120.42
1	A	86	ILE	N-CA-C	6.63	117.42	110.72
1	B	60	VAL	N-CA-C	6.60	117.35	110.62
1	B	176	VAL	CA-C-O	6.55	125.19	118.96
1	A	241	ILE	N-CA-CB	6.54	118.89	110.13
1	B	8	ASN	OD1-CG-ND2	-6.49	116.11	122.60
1	B	102	ASP	CA-CB-CG	6.47	119.07	112.60
1	B	147	LEU	CA-C-N	6.47	127.17	119.98
1	B	147	LEU	C-N-CA	6.47	127.17	119.98
1	A	31	GLY	CA-C-O	6.45	126.30	119.07
1	B	77	VAL	CA-C-O	6.42	127.13	120.39
1	B	219	GLU	CA-C-N	-6.42	114.49	122.84
1	B	219	GLU	C-N-CA	-6.42	114.49	122.84
1	B	204	PRO	CA-C-O	6.41	126.81	118.98
1	B	11	ASN	N-CA-C	6.40	118.26	111.28
1	B	216	SER	CA-C-O	-6.37	114.73	121.99
1	A	70	ASP	CA-CB-CG	6.36	118.96	112.60
1	A	236	VAL	N-CA-CB	-6.36	102.23	111.52
1	A	178	ASN	O-C-N	6.34	130.06	122.20
1	A	81	ARG	NE-CZ-NH1	6.32	127.82	121.50
1	A	135	HIS	O-C-N	-6.29	116.14	121.23
1	B	11	ASN	CA-C-O	6.28	127.21	120.55
1	B	177	GLY	CA-C-O	6.25	128.08	121.08
1	B	220	TYR	CA-C-O	-6.22	114.07	120.54
1	B	163	GLY	N-CA-C	6.18	122.16	114.37
1	B	4	GLN	OE1-CD-NE2	-6.18	116.42	122.60
1	A	234	ASP	CA-CB-CG	-6.17	106.43	112.60
1	B	257	ALA	CA-C-N	6.17	128.54	120.28
1	B	257	ALA	C-N-CA	6.17	128.54	120.28
1	B	165	ASP	CA-C-O	-6.14	114.44	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	THR	O-C-N	-6.14	114.88	123.11
1	B	103	ILE	CA-CB-CG2	6.14	120.94	110.50
1	A	264	LEU	CA-C-O	-6.13	113.93	120.92
1	A	135	HIS	CA-C-N	6.11	126.00	119.28
1	A	135	HIS	C-N-CA	6.11	126.00	119.28
1	A	217	SER	CA-C-O	-6.10	113.44	120.03
1	A	228	VAL	CA-C-O	6.07	123.50	119.38
1	B	211	PHE	N-CA-C	-6.07	105.05	112.88
1	B	137	ASP	CA-C-O	-6.06	114.45	120.82
1	B	87	GLU	CA-CB-CG	6.05	126.21	114.10
1	A	21	TYR	CB-CG-CD2	-6.04	111.74	120.80
1	B	211	PHE	N-CA-CB	6.04	120.09	110.73
1	A	241	ILE	CB-CA-C	-6.02	101.77	111.59
1	A	239	GLU	N-CA-CB	-6.02	100.59	110.52
1	A	163	GLY	CA-C-N	-6.00	113.51	122.74
1	A	163	GLY	C-N-CA	-6.00	113.51	122.74
1	A	73	ASN	OD1-CG-ND2	5.99	128.59	122.60
1	A	40	ALA	N-CA-C	5.98	117.79	111.28
1	A	231	THR	CA-CB-OG1	-5.97	100.65	109.60
1	B	255	ILE	O-C-N	-5.97	114.30	121.10
1	A	48	ASP	CA-C-O	-5.96	114.94	122.63
1	A	97	LEU	CA-C-O	5.95	128.74	121.72
1	A	77	VAL	CB-CA-C	-5.90	102.04	110.83
1	B	2	VAL	N-CA-CB	5.89	122.33	112.44
1	B	64	THR	CA-C-O	-5.88	114.23	121.11
1	A	205	ARG	N-CA-CB	-5.85	101.84	110.49
1	A	254	ASP	O-C-N	-5.83	116.84	123.48
1	B	249	GLN	CG-CD-NE2	5.82	125.13	116.40
1	A	125	ARG	CD-NE-CZ	5.80	132.52	124.40
1	B	17	SER	O-C-N	-5.80	115.14	122.27
1	B	25	ASN	CA-C-O	5.79	127.79	121.02
1	B	231	THR	CA-C-O	-5.76	114.88	121.68
1	B	25	ASN	OD1-CG-ND2	5.75	128.35	122.60
1	A	122	ASP	CA-C-O	-5.75	114.79	120.82
1	A	205	ARG	O-C-N	-5.71	115.20	122.34
1	B	232	ARG	CD-NE-CZ	-5.71	116.41	124.40
1	B	68	ALA	N-CA-C	5.71	118.86	109.85
1	A	129	GLU	CB-CG-CD	5.69	122.28	112.60
1	A	176	VAL	N-CA-CB	-5.69	101.85	111.23
1	A	47	ALA	O-C-N	-5.69	115.71	122.65
1	A	4	GLN	OE1-CD-NE2	-5.64	116.95	122.60
1	A	130	ASP	CA-C-O	-5.64	114.57	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	PHE	CA-CB-CG	5.64	119.44	113.80
1	B	22	CYS	CA-C-N	-5.63	110.36	121.41
1	B	22	CYS	C-N-CA	-5.63	110.36	121.41
1	A	26	ASN	N-CA-C	-5.62	105.14	112.23
1	A	71	ASN	CA-C-O	-5.61	111.75	119.05
1	B	244	THR	O-C-N	-5.61	115.86	123.10
1	A	160	ARG	NE-CZ-NH1	-5.60	115.90	121.50
1	A	175	ARG	NH1-CZ-NH2	5.58	126.55	119.30
1	A	205	ARG	N-CA-C	-5.57	106.15	113.17
1	B	39	ASN	OD1-CG-ND2	-5.57	117.03	122.60
1	B	111	ASP	CB-CA-C	5.55	120.83	109.67
1	B	26	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	B	159	LEU	CA-C-O	5.54	125.23	119.14
1	B	104	CYS	CA-C-N	-5.54	115.08	122.72
1	B	104	CYS	C-N-CA	-5.54	115.08	122.72
1	A	175	ARG	NE-CZ-NH1	-5.52	115.98	121.50
1	A	146	SER	CB-CA-C	-5.51	108.63	116.34
1	B	157	ALA	N-CA-C	-5.50	105.29	111.28
1	B	150	ALA	CA-C-O	-5.49	114.61	120.42
1	B	70	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	209	ARG	O-C-N	-5.48	116.31	122.12
1	B	182	ALA	CA-C-O	5.47	126.34	120.55
1	A	232	ARG	CA-CB-CG	5.46	125.03	114.10
1	B	1	GLU	CB-CA-C	5.45	120.46	110.10
1	B	48	ASP	CA-C-O	-5.45	115.77	122.36
1	B	24	LYS	CA-C-O	5.44	128.30	120.51
1	B	8	ASN	CB-CG-ND2	5.44	124.56	116.40
1	A	22	CYS	N-CA-CB	5.44	118.64	110.11
1	A	46	LYS	CA-CB-CG	5.42	124.94	114.10
1	A	97	LEU	N-CA-CB	5.42	119.13	110.46
1	B	92	ASN	CA-CB-CG	-5.41	107.19	112.60
1	B	86	ILE	O-C-N	-5.40	116.26	121.83
1	A	62	ASP	CA-C-N	5.38	129.86	123.19
1	A	62	ASP	C-N-CA	5.38	129.86	123.19
1	B	226	THR	CA-CB-OG1	-5.37	101.54	109.60
1	B	124	LEU	CA-C-N	5.34	127.97	120.28
1	B	124	LEU	C-N-CA	5.34	127.97	120.28
1	A	151	LEU	N-CA-CB	5.33	117.96	110.12
1	A	97	LEU	CD1-CG-CD2	-5.33	99.08	110.80
1	B	83	SER	O-C-N	-5.33	116.58	122.86
1	A	188	GLN	OE1-CD-NE2	5.31	127.91	122.60
1	B	21	TYR	CA-CB-CG	5.30	123.44	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	ILE	N-CA-C	5.30	116.07	110.72
1	B	178	ASN	CB-CG-ND2	-5.29	108.46	116.40
1	A	134	GLU	CA-CB-CG	5.29	124.68	114.10
1	B	18	ALA	N-CA-CB	5.29	117.99	110.16
1	A	21	TYR	CB-CG-CD1	5.29	128.73	120.80
1	B	251	ASN	CA-C-O	-5.28	115.91	121.88
1	A	41	CYS	CA-C-N	5.28	124.78	119.19
1	A	41	CYS	C-N-CA	5.28	124.78	119.19
1	A	4	GLN	CA-C-O	5.26	126.12	120.55
1	A	92	ASN	CA-CB-CG	5.26	117.86	112.60
1	A	68	ALA	N-CA-C	5.25	118.15	109.85
1	B	205	ARG	CA-CB-CG	5.25	124.59	114.10
1	A	16	TYR	N-CA-CB	5.24	117.83	110.12
1	B	244	THR	CA-C-N	-5.24	117.21	123.08
1	B	244	THR	C-N-CA	-5.24	117.21	123.08
1	A	259	LEU	O-C-N	5.23	128.87	122.34
1	B	25	ASN	CA-CB-CG	-5.22	107.38	112.60
1	A	160	ARG	CA-C-O	-5.22	116.02	121.55
1	B	244	THR	CA-C-O	-5.21	115.25	121.56
1	B	118	ARG	CD-NE-CZ	5.20	131.68	124.40
1	B	150	ALA	N-CA-C	-5.20	105.70	111.36
1	B	30	ALA	N-CA-C	5.19	117.75	109.96
1	A	51	PHE	CB-CA-C	-5.19	99.91	109.46
1	B	52	LEU	N-CA-C	-5.18	107.02	113.55
1	A	125	ARG	NE-CZ-NH1	-5.18	116.32	121.50
1	B	214	SER	N-CA-CB	-5.18	103.23	111.62
1	A	125	ARG	CA-C-O	5.17	126.03	120.55
1	A	160	ARG	CD-NE-CZ	-5.17	117.16	124.40
1	A	203	VAL	CA-C-N	5.17	125.25	119.87
1	A	203	VAL	C-N-CA	5.17	125.25	119.87
1	B	79	SER	CB-CA-C	5.17	118.57	110.19
1	A	60	VAL	CA-C-O	-5.15	115.33	121.05
1	A	31	GLY	CA-C-N	5.14	128.17	120.87
1	A	31	GLY	C-N-CA	5.14	128.17	120.87
1	B	81	ARG	CG-CD-NE	5.14	123.30	112.00
1	B	161	GLY	CA-C-O	-5.12	113.33	119.02
1	A	11	ASN	N-CA-C	5.12	116.71	111.03
1	A	48	ASP	N-CA-C	-5.11	101.96	109.62
1	A	234	ASP	CA-C-O	-5.10	113.11	119.28
1	A	111	ASP	CA-C-N	5.09	125.61	120.00
1	A	111	ASP	C-N-CA	5.09	125.61	120.00
1	A	205	ARG	CA-CB-CG	5.09	124.29	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	THR	CA-C-N	-5.09	111.44	121.41
1	A	244	THR	C-N-CA	-5.09	111.44	121.41
1	A	255	ILE	CA-C-N	5.06	124.84	119.28
1	A	255	ILE	C-N-CA	5.06	124.84	119.28
1	A	247	ASN	OD1-CG-ND2	5.04	127.64	122.60
1	B	140	VAL	O-C-N	5.04	128.41	122.81
1	A	47	ALA	CA-C-O	5.03	127.72	121.99
1	B	232	ARG	NE-CZ-NH1	-5.02	116.48	121.50
1	B	259	LEU	CA-C-N	-5.02	115.50	123.23
1	B	259	LEU	C-N-CA	-5.02	115.50	123.23
1	B	33	ASN	CA-C-O	-5.01	114.76	120.58

There are no chirality outliers.

All (50) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	GLU	Mainchain
1	A	154	VAL	Mainchain
1	A	156	GLY	Mainchain
1	A	170	SER	Mainchain
1	A	192	THR	Mainchain
1	A	20	ALA	Mainchain
1	A	203	VAL	Mainchain
1	A	204	PRO	Mainchain
1	A	207	PRO	Mainchain
1	A	216	SER	Mainchain
1	A	22	CYS	Mainchain
1	A	24	LYS	Mainchain
1	A	241	ILE	Mainchain
1	A	245	GLY	Mainchain
1	A	253	PRO	Mainchain
1	A	254	ASP	Mainchain
1	A	26	ASN	Mainchain
1	A	33	ASN	Mainchain
1	A	44	VAL	Mainchain
1	A	47	ALA	Mainchain
1	A	51	PHE	Mainchain
1	A	53	TYR	Mainchain
1	A	66	PHE	Mainchain
1	A	68	ALA	Mainchain
1	A	76	ILE	Mainchain
1	A	93	LEU	Mainchain

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Mol	Chain	Res	Type	Group
1	B	100	ILE	Mainchain
1	B	101	ASN	Mainchain
1	B	124	LEU	Mainchain
1	B	137	ASP	Mainchain
1	B	158	ASP	Mainchain
1	B	169	PHE	Mainchain
1	B	17	SER	Mainchain
1	B	175	ARG	Mainchain
1	B	197	THR	Mainchain
1	B	201	ASP	Mainchain
1	B	203	VAL	Mainchain
1	B	218	PRO	Mainchain
1	B	229	PRO	Mainchain
1	B	234	ASP	Mainchain
1	B	237	LYS	Mainchain
1	B	238	ILE	Mainchain
1	B	239	GLU	Mainchain
1	B	241	ILE	Mainchain
1	B	244	THR	Mainchain
1	B	255	ILE	Mainchain
1	B	268	CYS	Mainchain
1	B	34	ILE	Mainchain
1	B	41	CYS	Mainchain
1	B	94	ASN	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	58	0
1	B	2071	0	1965	57	0
2	A	99	0	0	6	0
2	B	143	0	0	4	0
All	All	4384	0	3930	114	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 14.

All (114) 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:232:ARG:HD2	2:A:272:HOH:O	1.73	0.89
1:A:1:GLU:HB2	1:A:235:ILE:O	1.81	0.80
1:A:157:ALA:HB2	1:A:185:LEU:HD21	1.68	0.74
1:A:209:ARG:HD3	2:B:330:HOH:O	1.87	0.73
1:A:28:ALA:HA	2:A:326:HOH:O	1.92	0.69
1:A:84:ARG:HB2	1:A:84:ARG:HH11	1.62	0.65
1:A:245:GLY:HA2	1:A:249:GLN:NE2	2.11	0.65
1:B:1:GLU:CD	1:B:233:ASN:HA	2.22	0.64
1:A:25:ASN:HB3	1:A:51:PHE:CZ	2.33	0.64
1:A:4:GLN:HE21	1:A:232:ARG:HG2	1.63	0.63
1:A:204:PRO:HB2	1:A:247:ASN:OD1	2.00	0.62
1:A:232:ARG:HG3	2:A:279:HOH:O	1.98	0.62
1:A:53:TYR:CD2	1:A:127:LYS:HD3	2.35	0.62
1:A:25:ASN:HB3	1:A:51:PHE:HZ	1.65	0.61
1:B:95:PHE:CD1	1:B:207:PRO:HB3	2.37	0.60
1:A:195:ARG:NH1	1:A:219:GLU:HB2	2.17	0.59
1:B:156:GLY:O	1:B:160:ARG:HD2	2.01	0.59
1:B:125:ARG:HB2	1:B:159:LEU:HD13	1.84	0.59
1:B:134:GLU:HG3	2:B:395:HOH:O	2.03	0.58
1:B:81:ARG:HD2	1:B:82:GLY:O	2.04	0.58
1:B:23:GLY:HA3	1:B:36:CYS:HA	1.86	0.57
1:B:98:LYS:HB3	1:B:111:ASP:HB2	1.87	0.56
1:B:87:GLU:OE1	1:B:88:ASN:N	2.27	0.55
1:A:175:ARG:NH2	1:A:207:PRO:O	2.37	0.55
1:A:28:ALA:HB1	1:A:29:PRO:HD2	1.88	0.54
1:B:254:ASP:OD1	1:B:256:PRO:HD2	2.08	0.54
1:B:198:HIS:NE2	1:B:224:SER:O	2.33	0.54
1:B:25:ASN:HA	1:B:51:PHE:CZ	2.44	0.53
1:A:20:ALA:O	1:A:81:ARG:HG3	2.09	0.53
1:A:245:GLY:H	1:A:249:GLN:HG3	1.74	0.53
1:A:160:ARG:NH1	1:A:188:GLN:OE1	2.40	0.52
1:A:125:ARG:HG2	1:A:125:ARG:HH11	1.75	0.52
1:A:34:ILE:HG12	1:A:51:PHE:CZ	2.45	0.52
1:A:245:GLY:HA2	1:A:249:GLN:CD	2.34	0.52
1:A:143:THR:HA	1:A:169:PHE:O	2.11	0.51
1:B:108:ARG:HG3	1:B:178:ASN:ND2	2.26	0.51
1:B:134:GLU:HB3	1:B:135:HIS:CD2	2.46	0.50
1:A:64:THR:HG21	1:A:81:ARG:NH2	2.27	0.50
1:A:220:TYR:OH	1:A:237:LYS:HE3	2.11	0.50
1:A:1:GLU:HG3	1:A:236:VAL:CG2	2.42	0.50
1:A:205:ARG:NH1	1:A:247:ASN:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LEU:HD11	1:B:69:LEU:HB2	1.94	0.49
1:A:108:ARG:HG3	1:A:178:ASN:ND2	2.28	0.49
1:B:143:THR:HA	1:B:169:PHE:O	2.13	0.49
1:B:1:GLU:HB3	1:B:235:ILE:O	2.12	0.48
1:A:33:ASN:HD22	1:A:50:THR:HG22	1.79	0.48
1:A:97:LEU:HD12	1:A:97:LEU:N	2.28	0.48
1:A:198:HIS:O	1:A:199:THR:C	2.56	0.48
1:A:108:ARG:HG3	1:A:178:ASN:HD21	1.78	0.48
1:B:23:GLY:C	1:B:25:ASN:H	2.22	0.48
1:A:253:PRO:HD3	1:B:211:PHE:HA	1.96	0.47
1:A:81:ARG:HD2	1:A:82:GLY:O	2.14	0.47
1:B:221:TRP:CE3	1:B:246:GLY:HA2	2.49	0.47
1:B:196:ILE:HA	1:B:220:TYR:O	2.14	0.47
1:A:29:PRO:HD3	2:A:326:HOH:O	2.14	0.47
1:B:26:ASN:ND2	1:B:26:ASN:H	2.12	0.47
1:B:25:ASN:OD1	1:B:66:PHE:CD2	2.68	0.47
1:B:28:ALA:HB1	1:B:29:PRO:HD2	1.96	0.46
1:B:198:HIS:O	1:B:199:THR:C	2.58	0.46
1:A:202:ILE:O	1:A:205:ARG:HB2	2.16	0.46
1:B:206:LEU:HA	1:B:207:PRO:C	2.39	0.46
1:B:56:GLU:O	1:B:57:ASP:HB2	2.14	0.46
1:B:20:ALA:O	1:B:81:ARG:HG3	2.16	0.46
1:A:179:ARG:O	1:A:182:ALA:HB3	2.16	0.46
1:A:1:GLU:HG3	1:A:236:VAL:HG22	1.97	0.46
1:A:49:ALA:HA	1:A:69:LEU:O	2.16	0.45
1:A:13:PHE:CE1	1:A:141:VAL:HG11	2.51	0.45
1:A:245:GLY:HA2	1:A:249:GLN:CG	2.47	0.45
1:B:24:LYS:HB3	2:B:365:HOH:O	2.17	0.45
1:A:202:ILE:HB	1:A:253:PRO:HB2	1.99	0.45
1:A:193:LEU:HD12	1:A:194:TYR:N	2.32	0.44
1:B:85:SER:HB3	1:B:87:GLU:OE1	2.17	0.44
1:B:85:SER:HB3	1:B:87:GLU:OE2	2.16	0.44
1:B:157:ALA:HB2	1:B:185:LEU:HD21	1.99	0.44
1:B:232:ARG:HH11	1:B:232:ARG:HD3	1.47	0.44
1:B:221:TRP:CD2	1:B:246:GLY:HA2	2.52	0.44
1:B:176:VAL:HG12	1:B:181:PHE:HE2	1.82	0.43
1:A:35:THR:HG21	2:A:339:HOH:O	2.17	0.43
1:B:97:LEU:HB2	2:B:408:HOH:O	2.18	0.43
1:B:133:ARG:HH11	1:B:133:ARG:HD3	1.68	0.43
1:B:198:HIS:N	1:B:261:TYR:OH	2.51	0.43
1:A:125:ARG:NH1	1:A:129:GLU:OE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:SER:O	1:A:149:GLY:N	2.49	0.43
1:B:25:ASN:HA	1:B:51:PHE:HZ	1.82	0.43
1:B:1:GLU:OE1	1:B:1:GLU:N	2.43	0.43
1:A:206:LEU:HA	1:A:207:PRO:C	2.43	0.43
1:B:179:ARG:O	1:B:183:GLU:HB2	2.19	0.43
1:B:255:ILE:HB	1:B:256:PRO:HD3	2.01	0.42
1:A:73:ASN:O	1:A:74:LYS:HB2	2.18	0.42
1:B:176:VAL:HG12	1:B:181:PHE:CE2	2.55	0.42
1:B:94:ASN:O	1:B:96:ASP:N	2.52	0.42
1:B:255:ILE:O	1:B:256:PRO:C	2.62	0.42
1:A:84:ARG:HH11	1:A:84:ARG:CB	2.28	0.42
1:A:149:GLY:HA3	1:A:173:ALA:HB2	2.01	0.42
1:A:110:HIS:O	1:A:114:THR:HB	2.20	0.42
1:B:26:ASN:O	1:B:27:ASP:OD1	2.38	0.42
1:B:1:GLU:CD	1:B:233:ASN:HD22	2.28	0.41
1:A:218:PRO:HG3	1:A:237:LYS:HE2	2.02	0.41
1:B:49:ALA:HA	1:B:69:LEU:O	2.20	0.41
1:A:1:GLU:HB3	2:A:303:HOH:O	2.19	0.41
1:B:128:VAL:O	1:B:132:VAL:HG23	2.19	0.41
1:B:151:LEU:O	1:B:152:ALA:C	2.62	0.41
1:B:269:LEU:HD23	1:B:269:LEU:HA	1.90	0.41
1:A:4:GLN:NE2	1:A:232:ARG:HG2	2.32	0.41
1:A:55:PHE:HE1	1:A:63:VAL:HG12	1.86	0.41
1:B:123:THR:O	1:B:126:GLN:HB3	2.21	0.41
1:B:133:ARG:O	1:B:136:PRO:HD3	2.20	0.41
1:A:64:THR:HG21	1:A:81:ARG:CZ	2.52	0.40
1:A:88:ASN:O	1:A:92:ASN:ND2	2.50	0.40
1:B:23:GLY:O	1:B:25:ASN:N	2.54	0.40
1:B:201:ASP:OD1	1:B:258:HIS:HB2	2.21	0.40
1:B:21:TYR:CE2	1:B:266:GLY:HA2	2.57	0.40
1:A:264:LEU:HD12	1:A:264:LEU:HA	1.87	0.40
1:B:78:LEU:HB3	1:B:142:PHE:CD1	2.56	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	267/269 (99%)	253 (95%)	12 (4%)	2 (1%)	18	38
1	B	267/269 (99%)	246 (92%)	17 (6%)	4 (2%)	8	18
All	All	534/538 (99%)	499 (93%)	29 (5%)	6 (1%)	11	25

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	121	ALA
1	A	62	ASP
1	A	199	THR
1	B	199	THR
1	B	95	PHE
1	B	23	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	220/220 (100%)	192 (87%)	28 (13%)	4	9
1	B	220/220 (100%)	199 (90%)	21 (10%)	8	18
All	All	440/440 (100%)	391 (89%)	49 (11%)	6	12

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	25	ASN
1	A	27	ASP
1	A	46	LYS
1	A	60	VAL
1	A	81	ARG

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Mol	Chain	Res	Type
1	A	83	SER
1	A	84	ARG
1	A	87	GLU
1	A	94	ASN
1	A	97	LEU
1	A	100	ILE
1	A	101	ASN
1	A	102	ASP
1	A	105	SER
1	A	115	SER
1	A	118	ARG
1	A	125	ARG
1	A	162	ASN
1	A	176	VAL
1	A	193	LEU
1	A	209	ARG
1	A	214	SER
1	A	216	SER
1	A	224	SER
1	A	232	ARG
1	A	236	VAL
1	A	241	ILE
1	B	26	ASN
1	B	27	ASP
1	B	87	GLU
1	B	99	GLU
1	B	102	ASP
1	B	105	SER
1	B	111	ASP
1	B	118	ARG
1	B	125	ARG
1	B	127	LYS
1	B	134	GLU
1	B	137	ASP
1	B	146	SER
1	B	179	ARG
1	B	183	GLU
1	B	199	THR
1	B	205	ARG
1	B	210	GLU
1	B	214	SER
1	B	239	GLU

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Mol	Chain	Res	Type
1	B	252	ILE

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	4	GLN
1	A	33	ASN
1	A	88	ASN
1	A	94	ASN
1	A	162	ASN
1	B	11	ASN
1	B	25	ASN
1	B	26	ASN
1	B	135	HIS
1	B	233	ASN

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 ⓘ

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.