



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:49 PM UTC

PDB ID : 2POL / pdb_00002pol
Title : THREE-DIMENSIONAL STRUCTURE OF THE BETA SUBUNIT OF ES-
CHERICHIA COLI DNA POLYMERASE III HOLOENZYME: A SLIDING
DNA CLAMP
Authors : Kong, X.-P.; Kuriyan, J.
Deposited on : 1992-11-13
Resolution : 2.50 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

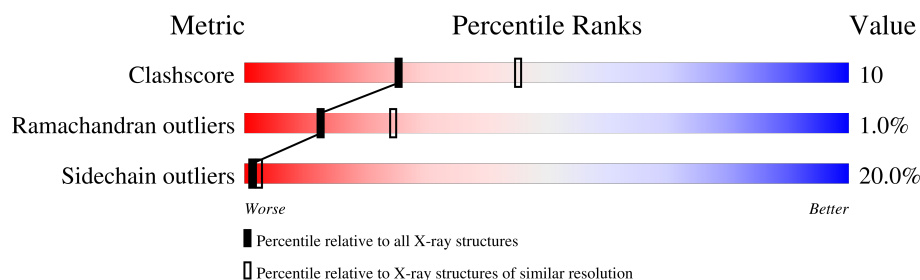
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	366	
1	B	366	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5838 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 DNA POLYMERASE III (BETA SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2844	1786	498	541	19			
1	B	366	Total	C	N	O	S	0	0	0
			2844	1786	498	541	19			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	79	Total	O	0	0
			79	79		
2	B	71	Total	O	0	0
			71	71		

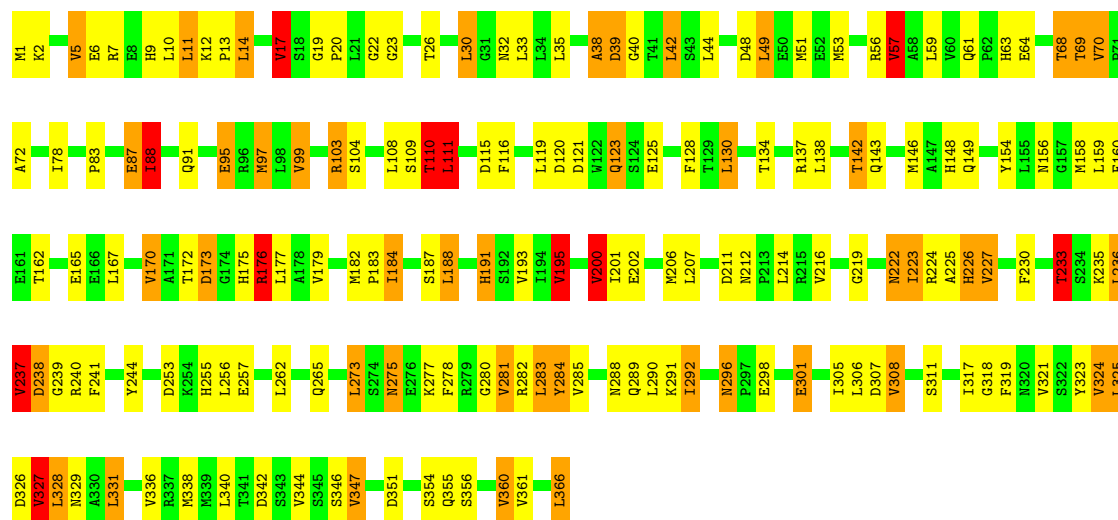
3 Residue-property plots

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.

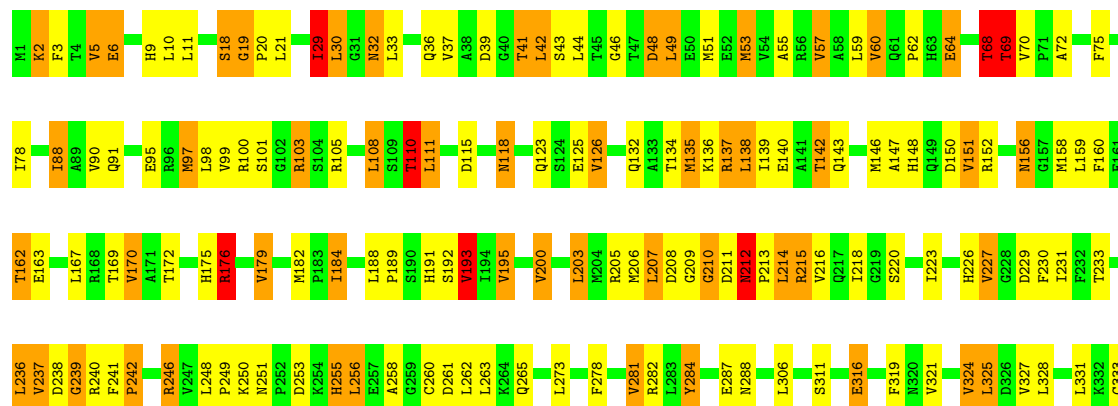
• Molecule 1: DNA POLYMERASE III (BETA SUBUNIT)

Chain A: 



• Molecule 1: DNA POLYMERASE III (BETA SUBUNIT)

Chain B: 



V336	R337	M338	M339	L340	T341	D342
V347	Q348	Q355	V360	V361	M362	P363
M364	R365	L366				

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	80.61Å 68.35Å 82.35Å 90.00° 114.26° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.184 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5838	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.34	17/2893 (0.6%)	2.08	106/3915 (2.7%)
1	B	1.31	19/2893 (0.7%)	2.14	111/3915 (2.8%)
All	All	1.33	36/5786 (0.6%)	2.11	217/7830 (2.8%)

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	A	0	1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88	ILE	CA-CB	12.95	1.69	1.54
1	B	170	VAL	CA-CB	8.82	1.67	1.54
1	A	237	VAL	CA-CB	8.78	1.66	1.54
1	B	324	VAL	CA-CB	8.09	1.65	1.54
1	A	200	VAL	CA-CB	7.81	1.65	1.54
1	B	60	VAL	CA-CB	7.17	1.63	1.54
1	B	237	VAL	CA-CB	6.98	1.66	1.54
1	A	233	THR	CA-CB	6.97	1.65	1.53
1	B	360	VAL	CA-CB	6.73	1.63	1.54
1	A	175	HIS	CD2-NE2	-6.66	1.30	1.37
1	B	88	ILE	CA-CB	6.53	1.62	1.54
1	B	195	VAL	CA-CB	6.50	1.62	1.54
1	B	9	HIS	CD2-NE2	-6.45	1.30	1.37
1	A	327	VAL	CA-CB	6.44	1.62	1.54
1	A	191	HIS	CD2-NE2	-6.41	1.30	1.37
1	B	226	HIS	CD2-NE2	-6.20	1.31	1.37
1	A	9	HIS	CD2-NE2	-6.10	1.31	1.37
1	A	148	HIS	CD2-NE2	-5.99	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	148	HIS	CD2-NE2	-5.98	1.31	1.37
1	B	90	VAL	CA-CB	-5.98	1.47	1.54
1	B	191	HIS	CD2-NE2	-5.96	1.31	1.37
1	B	200	VAL	CA-CB	5.80	1.62	1.54
1	B	91	GLN	CA-CB	-5.69	1.44	1.53
1	B	175	HIS	CD2-NE2	-5.63	1.31	1.37
1	A	63	HIS	CD2-NE2	-5.52	1.31	1.37
1	A	255	HIS	CD2-NE2	-5.41	1.31	1.37
1	A	344	VAL	CA-CB	5.34	1.61	1.54
1	A	57	VAL	CA-CB	5.33	1.61	1.54
1	B	191	HIS	CG-ND1	-5.33	1.32	1.38
1	A	191	HIS	CG-ND1	-5.23	1.32	1.38
1	B	231	ILE	CA-CB	-5.23	1.47	1.54
1	A	347	VAL	CA-CB	5.18	1.63	1.55
1	A	195	VAL	CA-CB	5.11	1.60	1.54
1	B	255	HIS	CD2-NE2	-5.05	1.32	1.37
1	A	226	HIS	CD2-NE2	-5.03	1.32	1.37
1	B	99	VAL	CA-CB	-5.03	1.48	1.54

All (217) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	ASP	CA-CB-CG	10.93	123.53	112.60
1	A	238	ASP	CA-C-O	-10.89	109.38	120.82
1	B	11	LEU	N-CA-C	10.69	122.69	111.14
1	B	342	ASP	CA-CB-CG	10.61	123.21	112.60
1	B	176	ARG	NE-CZ-NH2	-10.34	109.89	119.20
1	B	238	ASP	CA-CB-CG	10.33	122.93	112.60
1	B	184	ILE	N-CA-CB	-10.20	100.99	112.21
1	A	351	ASP	CA-CB-CG	9.67	122.27	112.60
1	B	156	ASN	OD1-CG-ND2	-9.66	112.94	122.60
1	B	115	ASP	CA-CB-CG	9.38	121.98	112.60
1	B	6	GLU	CB-CG-CD	9.16	128.18	112.60
1	B	39	ASP	CA-CB-CG	8.90	121.50	112.60
1	B	278	PHE	CA-CB-CG	-8.67	105.13	113.80
1	B	284	TYR	N-CA-C	-8.47	95.09	108.90
1	B	238	ASP	N-CA-C	8.35	122.01	111.24
1	B	78	ILE	CA-C-O	-8.32	112.35	121.17
1	B	48	ASP	CA-CB-CG	8.29	120.89	112.60
1	B	253	ASP	CA-CB-CG	8.24	120.84	112.60
1	B	229	ASP	CA-CB-CG	8.19	120.78	112.60
1	A	72	ALA	N-CA-C	7.92	119.69	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	ASP	CA-CB-CG	7.89	120.49	112.60
1	A	292	ILE	O-C-N	-7.76	114.70	122.93
1	A	319	PHE	CA-CB-CG	7.75	121.56	113.80
1	B	355	GLN	OE1-CD-NE2	-7.66	114.94	122.60
1	A	17	VAL	N-CA-CB	-7.50	97.19	110.77
1	B	355	GLN	CG-CD-NE2	7.49	127.64	116.40
1	A	69	THR	N-CA-CB	-7.48	99.47	110.84
1	A	11	LEU	N-CA-C	7.47	119.21	111.14
1	A	238	ASP	N-CA-C	7.46	119.06	111.07
1	A	48	ASP	N-CA-C	-7.44	102.73	112.41
1	A	110	THR	N-CA-CB	-7.44	97.83	111.37
1	B	316	GLU	CB-CG-CD	7.38	125.15	112.60
1	A	115	ASP	CA-CB-CG	7.38	119.98	112.60
1	A	184	ILE	N-CA-CB	-7.37	104.11	112.21
1	B	142	THR	N-CA-CB	-7.37	98.04	110.49
1	A	241	PHE	N-CA-C	-7.33	100.41	109.65
1	B	41	THR	N-CA-C	7.31	121.49	109.06
1	B	336	VAL	CG1-CB-CG2	-7.31	94.72	110.80
1	A	327	VAL	CA-C-O	-7.25	113.17	120.85
1	B	246	ARG	NE-CZ-NH2	-7.23	112.69	119.20
1	A	212	ASN	OD1-CG-ND2	-7.22	115.38	122.60
1	B	69	THR	N-CA-CB	-7.21	99.01	110.77
1	A	78	ILE	CA-C-O	-7.16	113.58	121.17
1	B	118	ASN	CA-CB-CG	7.14	119.74	112.60
1	A	123	GLN	O-C-N	7.09	131.96	123.24
1	B	172	THR	CA-CB-OG1	-6.98	99.14	109.60
1	B	118	ASN	OD1-CG-ND2	-6.94	115.66	122.60
1	B	132	GLN	OE1-CD-NE2	-6.92	115.68	122.60
1	B	333	CYS	N-CA-C	6.90	118.98	109.18
1	B	162	THR	N-CA-CB	-6.88	99.78	110.57
1	B	179	VAL	CB-CA-C	-6.87	99.92	110.50
1	B	214	LEU	N-CA-C	-6.87	98.20	109.40
1	B	110	THR	N-CA-CB	-6.82	98.85	111.53
1	A	239	GLY	N-CA-C	6.79	120.93	110.88
1	A	111	LEU	N-CA-C	-6.78	99.73	110.10
1	A	307	ASP	O-C-N	6.77	130.94	123.22
1	B	44	LEU	N-CA-C	-6.75	97.89	108.90
1	B	265	GLN	CA-CB-CG	-6.70	100.69	114.10
1	A	308	VAL	N-CA-CB	-6.67	100.49	111.44
1	B	251	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	A	211	ASP	N-CA-C	6.63	121.45	113.23
1	A	48	ASP	CA-CB-CG	6.55	119.15	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	ILE	CB-CA-C	6.55	119.03	110.84
1	A	68	THR	CA-CB-OG1	-6.54	99.78	109.60
1	B	331	LEU	O-C-N	-6.54	113.94	122.77
1	A	87	GLU	CA-C-O	-6.46	113.67	120.58
1	A	311	SER	N-CA-C	-6.44	97.88	108.76
1	B	151	VAL	N-CA-CB	-6.41	97.60	111.05
1	B	223	ILE	N-CA-C	-6.39	98.99	108.45
1	A	176	ARG	NE-CZ-NH1	6.37	127.87	121.50
1	A	191	HIS	CB-CG-CD2	-6.37	122.92	131.20
1	A	176	ARG	NE-CZ-NH2	-6.36	113.48	119.20
1	B	111	LEU	O-C-N	-6.34	116.35	121.80
1	A	219	GLY	N-CA-C	-6.33	105.19	112.79
1	B	212	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	A	142	THR	O-C-N	-6.29	115.44	122.10
1	B	97	MET	CG-SD-CE	-6.28	87.09	100.90
1	A	361	VAL	CG1-CB-CG2	-6.26	97.02	110.80
1	A	6	GLU	N-CA-C	-6.26	99.44	109.96
1	B	69	THR	CB-CA-C	6.25	119.77	110.14
1	B	261	ASP	CA-CB-CG	6.23	118.83	112.60
1	B	193	VAL	N-CA-CB	-6.19	101.21	111.36
1	A	173	ASP	CA-CB-CG	6.18	118.78	112.60
1	A	109	SER	N-CA-C	-6.16	102.59	110.53
1	A	97	MET	CG-SD-CE	-6.15	87.36	100.90
1	B	108	LEU	N-CA-CB	-6.15	100.78	110.69
1	A	288	ASN	N-CA-C	6.15	120.11	112.24
1	B	288	ASN	OD1-CG-ND2	-6.15	116.45	122.60
1	B	242	PRO	N-CA-C	6.12	120.68	111.14
1	B	132	GLN	CG-CD-NE2	6.09	125.54	116.40
1	A	179	VAL	CB-CA-C	-6.08	101.57	110.62
1	B	134	THR	N-CA-C	-6.07	104.22	111.69
1	B	193	VAL	N-CA-C	-6.02	100.40	108.35
1	A	120	ASP	N-CA-C	6.01	118.52	110.35
1	B	210	GLY	CA-C-O	6.01	128.29	122.28
1	B	69	THR	CA-CB-OG1	-6.00	100.59	109.60
1	B	6	GLU	N-CA-C	-5.98	99.53	109.46
1	A	284	TYR	CA-C-N	-5.97	115.40	123.10
1	A	284	TYR	C-N-CA	-5.97	115.40	123.10
1	B	366	LEU	N-CA-C	-5.96	94.30	111.00
1	A	134	THR	CA-CB-OG1	-5.96	100.66	109.60
1	B	239	GLY	N-CA-C	5.92	127.22	113.18
1	A	110	THR	OG1-CB-CG2	5.91	121.11	109.30
1	B	215	ARG	CA-C-O	-5.89	113.95	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	HIS	CB-CG-CD2	-5.89	123.54	131.20
1	A	175	HIS	CB-CG-CD2	-5.84	123.60	131.20
1	A	301	GLU	CB-CG-CD	5.84	122.53	112.60
1	B	365	ARG	N-CA-C	-5.84	98.89	108.41
1	B	260	CYS	N-CA-CB	-5.83	101.54	110.16
1	B	20	PRO	N-CA-C	5.82	121.14	113.86
1	B	227	VAL	CB-CA-C	-5.82	101.09	110.28
1	A	149	GLN	N-CA-C	-5.81	97.75	107.80
1	B	281	VAL	N-CA-CB	-5.81	102.68	112.44
1	B	3	PHE	CA-CB-CG	5.78	119.58	113.80
1	B	246	ARG	NE-CZ-NH1	5.72	127.22	121.50
1	A	88	ILE	CB-CG1-CD1	-5.70	101.84	113.80
1	B	118	ASN	CB-CG-ND2	5.69	124.93	116.40
1	B	152	ARG	NE-CZ-NH1	5.68	127.18	121.50
1	A	38	ALA	N-CA-C	-5.68	99.36	108.55
1	A	172	THR	CA-C-N	5.65	133.67	121.64
1	A	172	THR	C-N-CA	5.65	133.67	121.64
1	A	296	ASN	CA-CB-CG	5.65	118.25	112.60
1	A	95	GLU	CA-CB-CG	5.64	125.38	114.10
1	B	78	ILE	N-CA-C	-5.63	105.01	110.42
1	B	255	HIS	CB-CG-ND1	5.63	131.15	122.70
1	A	317	ILE	O-C-N	-5.63	116.56	123.09
1	A	160	PHE	CA-CB-CG	-5.63	108.17	113.80
1	B	251	ASN	CA-CB-CG	5.63	118.23	112.60
1	A	195	VAL	CA-C-N	5.62	125.55	119.76
1	A	195	VAL	C-N-CA	5.62	125.55	119.76
1	B	152	ARG	N-CA-C	-5.62	98.78	108.56
1	A	253	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	305	ILE	O-C-N	-5.60	117.30	123.18
1	B	19	GLY	CA-C-N	5.60	125.22	119.56
1	B	19	GLY	C-N-CA	5.60	125.22	119.56
1	B	255	HIS	CB-CG-CD2	-5.59	123.93	131.20
1	A	354	SER	CB-CA-C	-5.59	101.54	110.14
1	B	69	THR	CA-CB-CG2	5.59	120.00	110.50
1	B	311	SER	N-CA-C	-5.58	99.33	108.76
1	B	64	GLU	CB-CA-C	5.58	116.91	109.65
1	B	53	MET	N-CA-C	-5.57	100.32	109.40
1	A	355	GLN	N-CA-C	-5.56	106.47	113.20
1	B	111	LEU	N-CA-C	-5.51	100.60	109.58
1	A	13	PRO	CA-C-N	5.51	127.66	120.28
1	A	13	PRO	C-N-CA	5.51	127.66	120.28
1	A	6	GLU	CA-C-N	5.50	127.96	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	GLU	C-N-CA	5.50	127.96	120.54
1	B	138	LEU	N-CA-CB	-5.49	102.05	110.12
1	A	116	PHE	CA-C-N	5.48	125.49	119.90
1	A	116	PHE	C-N-CA	5.48	125.49	119.90
1	B	68	THR	CA-CB-OG1	-5.48	101.38	109.60
1	A	110	THR	N-CA-C	-5.45	100.89	109.50
1	B	53	MET	N-CA-CB	-5.45	101.36	110.83
1	B	36	GLN	CG-CD-NE2	5.43	124.55	116.40
1	B	240	ARG	CA-CB-CG	5.43	124.96	114.10
1	B	250	LYS	N-CA-C	5.42	117.63	111.02
1	A	241	PHE	CA-C-N	5.41	125.41	119.89
1	A	241	PHE	C-N-CA	5.41	125.41	119.89
1	B	287	GLU	CA-C-O	5.41	126.92	120.70
1	B	176	ARG	N-CA-C	-5.38	100.89	109.07
1	A	255	HIS	CB-CG-CD2	-5.37	124.22	131.20
1	A	227	VAL	CB-CA-C	-5.35	103.19	110.42
1	B	355	GLN	CB-CG-CD	5.35	121.69	112.60
1	A	68	THR	CA-CB-CG2	5.35	119.59	110.50
1	A	156	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	B	72	ALA	N-CA-C	5.34	116.79	110.97
1	B	316	GLU	CA-CB-CG	5.34	124.77	114.10
1	A	329	ASN	OD1-CG-ND2	-5.33	117.27	122.60
1	B	175	HIS	CB-CG-CD2	-5.31	124.30	131.20
1	A	119	LEU	N-CA-C	-5.31	101.04	109.96
1	B	32	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	A	183	PRO	CA-C-N	5.29	128.83	122.16
1	A	183	PRO	C-N-CA	5.29	128.83	122.16
1	A	146	MET	O-C-N	-5.28	116.64	122.86
1	A	265	GLN	CA-CB-CG	5.27	124.65	114.10
1	A	17	VAL	CB-CA-C	5.26	120.79	112.26
1	A	227	VAL	N-CA-C	-5.26	99.98	107.77
1	B	125	GLU	CB-CA-C	-5.25	100.99	110.23
1	A	238	ASP	O-C-N	-5.24	116.67	122.07
1	A	123	GLN	CB-CG-CD	5.22	121.48	112.60
1	B	176	ARG	NE-CZ-NH1	5.22	126.72	121.50
1	A	291	LYS	O-C-N	-5.22	117.11	123.27
1	A	111	LEU	O-C-N	-5.22	116.51	121.57
1	A	238	ASP	CA-CB-CG	-5.21	107.39	112.60
1	B	135	MET	CA-C-O	-5.20	115.36	120.82
1	A	162	THR	O-C-N	-5.20	116.61	123.21
1	B	362	MET	CA-C-N	5.19	125.40	120.31
1	B	362	MET	C-N-CA	5.19	125.40	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	29	ILE	CB-CA-C	-5.18	101.89	111.79
1	A	61	GLN	CA-C-N	5.18	124.94	119.76
1	A	61	GLN	C-N-CA	5.18	124.94	119.76
1	B	75	PHE	N-CA-C	-5.17	105.72	111.36
1	A	222	ASN	CA-C-O	-5.14	115.77	121.33
1	B	278	PHE	N-CA-C	5.14	119.61	113.23
1	A	275	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	A	121	ASP	N-CA-C	-5.12	103.28	110.50
1	B	18	SER	CB-CA-C	-5.12	102.80	110.90
1	B	148	HIS	CA-CB-CG	5.11	118.91	113.80
1	B	184	ILE	CA-CB-CG2	5.10	119.18	110.50
1	B	256	LEU	CA-CB-CG	5.10	134.14	116.30
1	A	338	MET	CA-CB-CG	5.08	124.27	114.10
1	B	2	LYS	CA-C-O	-5.08	113.95	120.14
1	B	110	THR	OG1-CB-CG2	5.08	119.45	109.30
1	A	88	ILE	CA-CB-CG2	5.07	119.12	110.50
1	A	99	VAL	O-C-N	-5.05	117.19	123.10
1	B	46	GLY	O-C-N	-5.05	118.73	123.48
1	B	101	SER	CA-CB-OG	-5.04	101.02	111.10
1	A	187	SER	N-CA-C	-5.03	102.84	110.28
1	A	223	ILE	N-CA-C	-5.03	101.01	108.45
1	B	203	LEU	N-CA-C	-5.03	105.88	111.36
1	B	341	THR	N-CA-C	-5.03	103.38	111.02
1	A	7	ARG	NH1-CZ-NH2	-5.02	112.77	119.30
1	A	83	PRO	CA-C-N	5.02	127.90	120.82
1	A	83	PRO	C-N-CA	5.02	127.90	120.82
1	B	193	VAL	CA-CB-CG2	-5.02	101.87	110.40
1	A	56	ARG	CA-C-N	-5.01	116.57	123.14
1	A	56	ARG	C-N-CA	-5.01	116.57	123.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	284	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	2844	0	2861	60	0
1	B	2844	0	2861	50	0
2	A	79	0	0	0	0
2	B	71	0	0	0	0
All	All	5838	0	5722	110	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 10.

All (110) 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:206:MET:HE2	1:A:227:VAL:HG23	1.63	0.80
1:A:103:ARG:HD2	1:A:103:ARG:H	1.51	0.75
1:A:195:VAL:HG22	1:A:200:VAL:HG12	1.67	0.75
1:A:283:LEU:HG	1:A:290:LEU:HD11	1.69	0.74
1:A:1:MET:HE1	1:A:35:LEU:HB3	1.72	0.71
1:B:53:MET:HE1	1:B:230:PHE:HB3	1.72	0.70
1:B:139:ILE:HG12	1:B:158:MET:HE1	1.77	0.65
1:A:275:ASN:HD21	1:A:277:LYS:HE2	1.64	0.62
1:B:150:ASP:H	1:B:156:ASN:HD21	1.48	0.62
1:A:33:LEU:O	1:A:69:THR:HA	2.03	0.59
1:B:159:LEU:HD11	1:B:192:SER:HB3	1.85	0.58
1:A:32:ASN:HD22	1:A:69:THR:HG22	1.68	0.58
1:B:137:ARG:HG2	1:B:182:MET:HE2	1.86	0.58
1:B:68:THR:HG21	1:B:97:MET:HE3	1.87	0.57
1:A:2:LYS:HG2	1:A:91:GLN:HG3	1.86	0.56
1:B:98:LEU:HD23	1:B:100:ARG:HH12	1.69	0.56
1:A:282:ARG:HH21	1:A:366:LEU:H	1.54	0.56
1:A:177:LEU:HB3	1:A:360:VAL:HG13	1.88	0.55
1:B:135:MET:HG3	1:B:207:LEU:HD21	1.89	0.55
1:A:318:GLY:HA3	1:A:366:LEU:HD22	1.88	0.55
1:A:173:ASP:OD2	1:A:176:ARG:HD2	2.06	0.55
1:A:321:VAL:HG22	1:A:325:LEU:HD22	1.89	0.54
1:A:53:MET:CE	1:A:230:PHE:HB3	2.38	0.54
1:B:321:VAL:HG22	1:B:325:LEU:HD22	1.90	0.54
1:A:256:LEU:HD12	1:A:285:VAL:HG21	1.90	0.53
1:A:5:VAL:HG21	1:A:10:LEU:HD22	1.90	0.53
1:A:51:MET:HE3	1:A:202:GLU:HG2	1.91	0.53
1:B:282:ARG:HG2	1:B:366:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LEU:O	1:A:296:ASN:HB3	2.09	0.52
1:A:42:LEU:HB3	1:A:57:VAL:HG22	1.92	0.52
1:A:128:PHE:CD1	1:A:184:ILE:HD11	2.43	0.52
1:B:143:GLN:HB2	1:B:146:MET:HE2	1.90	0.52
1:B:263:LEU:HD23	1:B:336:VAL:HG11	1.90	0.52
1:B:69:THR:HB	1:B:111:LEU:O	2.10	0.51
1:A:10:LEU:O	1:A:14:LEU:HB2	2.11	0.51
1:B:255:HIS:CE1	1:B:339:MET:HG2	2.45	0.51
1:B:48:ASP:O	1:B:49:LEU:HB2	2.10	0.51
1:A:184:ILE:HD13	1:A:188:LEU:HD21	1.93	0.51
1:A:224:ARG:HD3	1:A:226:HIS:CE1	2.46	0.51
1:A:19:GLY:N	1:A:20:PRO:HD2	2.26	0.50
1:A:154:TYR:HA	1:A:237:VAL:HG21	1.93	0.50
1:A:331:LEU:HD23	1:A:336:VAL:HG22	1.93	0.50
1:B:284:TYR:CD2	1:B:316:GLU:HG3	2.47	0.49
1:B:53:MET:CE	1:B:230:PHE:HB3	2.42	0.49
1:B:214:LEU:HD13	1:B:227:VAL:HG22	1.94	0.49
1:A:1:MET:HA	1:A:64:GLU:O	2.13	0.49
1:B:2:LYS:HB3	1:B:64:GLU:HB3	1.94	0.49
1:B:70:VAL:HG11	1:B:97:MET:SD	2.53	0.49
1:B:208:ASP:O	1:B:210:GLY:N	2.46	0.49
1:B:258:ALA:HB3	1:B:263:LEU:HD22	1.95	0.48
1:B:33:LEU:O	1:B:69:THR:HA	2.13	0.48
1:B:158:MET:HE3	1:B:169:THR:HG21	1.95	0.48
1:A:222:ASN:HA	1:A:235:LYS:HA	1.96	0.48
1:A:321:VAL:HA	1:A:324:VAL:CG1	2.43	0.48
1:A:70:VAL:HG11	1:A:97:MET:SD	2.54	0.48
1:B:95:GLU:O	1:B:110:THR:HB	2.14	0.48
1:A:214:LEU:HD11	1:A:225:ALA:HB1	1.96	0.47
1:A:223:ILE:O	1:A:233:THR:HA	2.15	0.47
1:B:32:ASN:HD22	1:B:69:THR:HG22	1.78	0.47
1:B:249:PRO:HD2	1:B:348:GLN:HE21	1.80	0.47
1:A:88:ILE:CD1	1:A:99:VAL:HG13	2.45	0.46
1:B:103:ARG:H	1:B:103:ARG:HD2	1.80	0.46
1:B:32:ASN:HD22	1:B:69:THR:CG2	2.28	0.46
1:B:319:PHE:CZ	1:B:347:VAL:HG11	2.51	0.46
1:A:165:GLU:O	1:A:184:ILE:HG22	2.16	0.46
1:B:43:SER:HA	1:B:55:ALA:O	2.16	0.46
1:A:193:VAL:HB	1:A:236:LEU:HG	1.97	0.45
1:A:17:VAL:HG13	1:A:33:LEU:HD22	1.98	0.45
1:B:136:LYS:O	1:B:140:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ASP:CG	1:A:40:GLY:H	2.24	0.45
1:B:126:VAL:HG13	1:B:218:ILE:HB	1.99	0.45
1:A:38:ALA:O	1:A:39:ASP:HB3	2.17	0.45
1:A:30:LEU:HD21	1:A:49:LEU:HD22	1.99	0.44
1:A:235:LYS:HE3	1:A:235:LYS:HB3	1.80	0.44
1:B:42:LEU:HB3	1:B:57:VAL:HG13	2.00	0.44
1:B:18:SER:HA	1:B:21:LEU:HD22	2.00	0.44
1:B:263:LEU:HD21	1:B:338:MET:HE3	1.99	0.44
1:B:135:MET:CG	1:B:207:LEU:HD21	2.49	0.43
1:B:5:VAL:HG21	1:B:10:LEU:HD22	2.00	0.43
1:B:176:ARG:O	1:B:176:ARG:HG2	2.11	0.43
1:A:281:VAL:HG13	1:A:292:ILE:HG23	2.00	0.43
1:A:128:PHE:HB3	1:A:188:LEU:HD11	2.00	0.43
1:A:184:ILE:HD13	1:A:184:ILE:HG21	1.68	0.43
1:B:206:MET:HE2	1:B:227:VAL:HG23	2.01	0.42
1:A:95:GLU:O	1:A:110:THR:HB	2.19	0.42
1:A:323:TYR:O	1:A:327:VAL:HG13	2.19	0.42
1:B:158:MET:HE2	1:B:160:PHE:CZ	2.55	0.42
1:A:280:GLY:HA3	1:A:366:LEU:HD11	2.00	0.42
1:B:212:ASN:HA	1:B:213:PRO:HD2	1.80	0.42
1:B:150:ASP:H	1:B:156:ASN:ND2	2.16	0.42
1:A:130:LEU:HD23	1:A:130:LEU:N	2.35	0.42
1:B:263:LEU:HD12	1:B:263:LEU:HA	1.95	0.42
1:B:30:LEU:HD11	1:B:49:LEU:HD13	2.02	0.41
1:A:70:VAL:CG1	1:A:97:MET:SD	3.09	0.41
1:B:193:VAL:HG22	1:B:236:LEU:HG	2.02	0.41
1:A:176:ARG:NH2	1:A:326:ASP:OD2	2.54	0.41
1:A:10:LEU:HG	1:A:14:LEU:HD22	2.03	0.41
1:B:37:VAL:HA	1:B:41:THR:O	2.20	0.41
1:B:241:PHE:HA	1:B:242:PRO:HD2	1.82	0.41
1:A:177:LEU:HD11	1:A:244:TYR:HB2	2.02	0.41
1:A:159:LEU:HB3	1:A:170:VAL:HG13	2.03	0.41
1:B:29:ILE:HD13	1:B:29:ILE:H	1.86	0.41
1:A:346:SER:HB3	1:A:360:VAL:HG23	2.04	0.41
1:A:68:THR:HG21	1:A:97:MET:HE3	2.02	0.40
1:A:275:ASN:HD22	1:A:278:PHE:H	1.68	0.40
1:B:147:ALA:HB3	1:B:156:ASN:HD22	1.86	0.40
1:A:142:THR:OG1	1:A:158:MET:HE2	2.21	0.40
1:A:111:LEU:HD12	1:A:111:LEU:HA	1.87	0.40
1:A:184:ILE:HG21	1:A:188:LEU:HD22	2.03	0.40
1:A:324:VAL:O	1:A:328:LEU:HD22	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	364/366 (100%)	343 (94%)	19 (5%)	2 (0%)	24	43
1	B	364/366 (100%)	342 (94%)	17 (5%)	5 (1%)	9	17
All	All	728/732 (100%)	685 (94%)	36 (5%)	7 (1%)	12	24

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	189	PRO
1	B	209	GLY
1	B	239	GLY
1	A	23	GLY
1	B	19	GLY
1	B	355	GLN
1	A	22	GLY

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	313/313 (100%)	251 (80%)	62 (20%)	1	2
1	B	313/313 (100%)	250 (80%)	63 (20%)	1	2
All	All	626/626 (100%)	501 (80%)	125 (20%)	1	2

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	11	LEU
1	A	12	LYS
1	A	14	LEU
1	A	17	VAL
1	A	26	THR
1	A	30	LEU
1	A	42	LEU
1	A	44	LEU
1	A	49	LEU
1	A	57	VAL
1	A	59	LEU
1	A	70	VAL
1	A	87	GLU
1	A	88	ILE
1	A	103	ARG
1	A	104	SER
1	A	108	LEU
1	A	110	THR
1	A	111	LEU
1	A	123	GLN
1	A	125	GLU
1	A	130	LEU
1	A	137	ARG
1	A	138	LEU
1	A	143	GLN
1	A	167	LEU
1	A	170	VAL
1	A	176	ARG
1	A	182	MET
1	A	188	LEU
1	A	191	HIS
1	A	195	VAL
1	A	200	VAL
1	A	201	ILE
1	A	207	LEU
1	A	216	VAL
1	A	233	THR
1	A	236	LEU
1	A	237	VAL
1	A	238	ASP
1	A	240	ARG

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Mol	Chain	Res	Type
1	A	257	GLU
1	A	262	LEU
1	A	273	LEU
1	A	281	VAL
1	A	283	LEU
1	A	289	GLN
1	A	298	GLU
1	A	301	GLU
1	A	306	LEU
1	A	308	VAL
1	A	324	VAL
1	A	325	LEU
1	A	327	VAL
1	A	328	LEU
1	A	331	LEU
1	A	340	LEU
1	A	347	VAL
1	A	356	SER
1	A	360	VAL
1	A	366	LEU
1	B	5	VAL
1	B	6	GLU
1	B	29	ILE
1	B	30	LEU
1	B	42	LEU
1	B	49	LEU
1	B	51	MET
1	B	57	VAL
1	B	59	LEU
1	B	60	VAL
1	B	62	PRO
1	B	68	THR
1	B	69	THR
1	B	88	ILE
1	B	103	ARG
1	B	105	ARG
1	B	108	LEU
1	B	110	THR
1	B	118	ASN
1	B	123	GLN
1	B	126	VAL
1	B	137	ARG

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Mol	Chain	Res	Type
1	B	138	LEU
1	B	142	THR
1	B	151	VAL
1	B	162	THR
1	B	163	GLU
1	B	167	LEU
1	B	170	VAL
1	B	176	ARG
1	B	179	VAL
1	B	184	ILE
1	B	188	LEU
1	B	193	VAL
1	B	195	VAL
1	B	200	VAL
1	B	203	LEU
1	B	205	ARG
1	B	207	LEU
1	B	211	ASP
1	B	212	ASN
1	B	215	ARG
1	B	216	VAL
1	B	220	SER
1	B	233	THR
1	B	236	LEU
1	B	237	VAL
1	B	246	ARG
1	B	248	LEU
1	B	256	LEU
1	B	262	LEU
1	B	273	LEU
1	B	281	VAL
1	B	306	LEU
1	B	324	VAL
1	B	325	LEU
1	B	327	VAL
1	B	328	LEU
1	B	340	LEU
1	B	355	GLN
1	B	360	VAL
1	B	363	PRO
1	B	366	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	91	GLN
1	A	143	GLN
1	A	191	HIS
1	A	212	ASN
1	A	217	GLN
1	A	226	HIS
1	A	275	ASN
1	A	335	ASN
1	A	348	GLN
1	B	32	ASN
1	B	36	GLN
1	B	156	ASN
1	B	217	GLN
1	B	329	ASN
1	B	335	ASN
1	B	348	GLN
1	B	355	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 ⓘ

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.