Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2024 – 03:11 PM EST

PDB ID	:	2POL
Title	:	THREE-DIMENSIONAL STRUCTURE OF THE BETA SUBUNIT OF ESCHERICHIA 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:

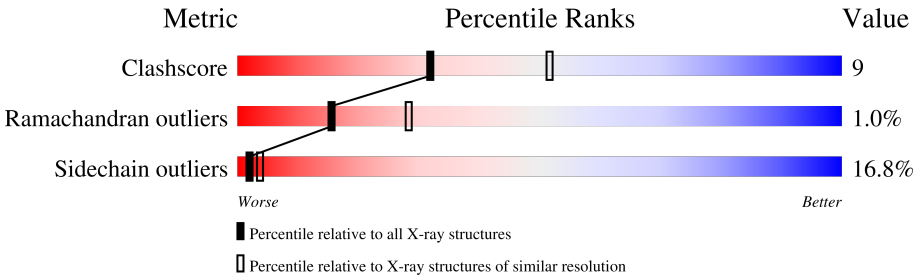
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	366	63% 25% 10% .
1	B	366	64% 25% 10% .

2 Entry composition (i)

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		

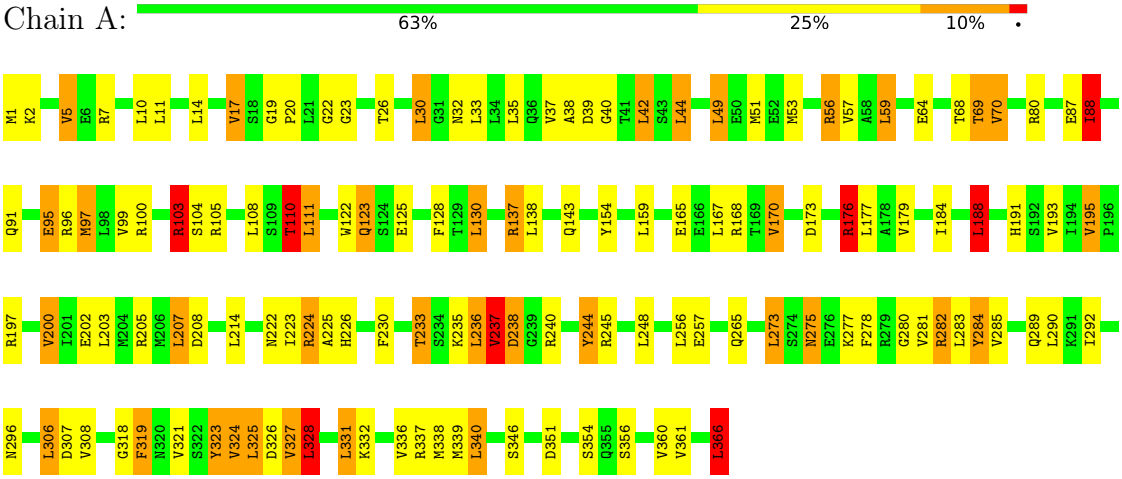
3 Residue-property plots (i)

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.

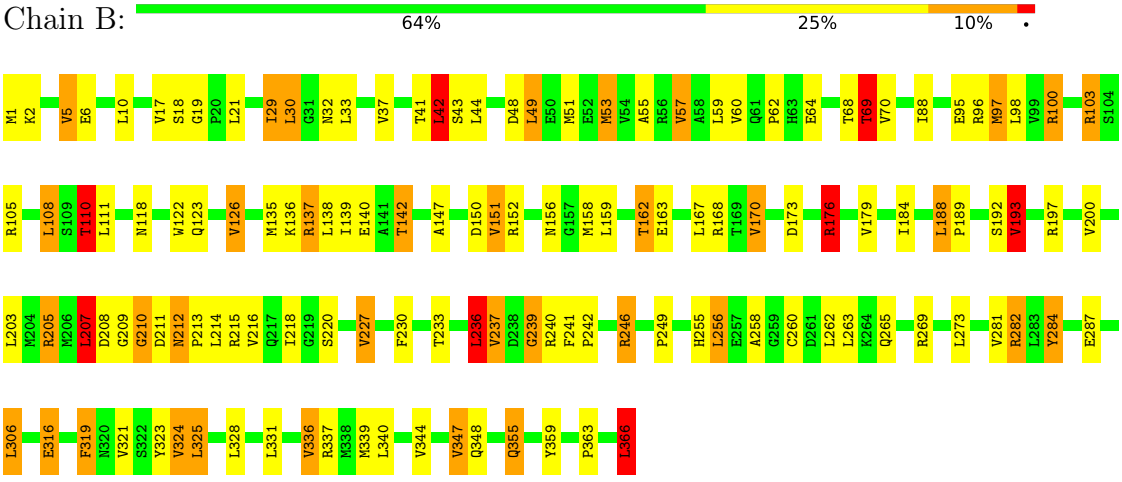
• Molecule 1: DNA POLYMERASE III (BETA SUBUNIT)

Chain A:



• Molecule 1: DNA POLYMERASE III (BETA SUBUNIT)

Chain B:



4 Data and refinement statistics (i)

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 (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	1.01	3/2893 (0.1%)	1.82	60/3915 (1.5%)
1	B	1.01	3/2893 (0.1%)	1.88	63/3915 (1.6%)
All	All	1.01	6/5786 (0.1%)	1.85	123/7830 (1.6%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88	ILE	CA-CB	6.43	1.69	1.54
1	B	170	VAL	CA-CB	6.16	1.67	1.54
1	B	237	VAL	CA-CB	5.33	1.66	1.54
1	A	237	VAL	CA-CB	5.33	1.66	1.54
1	B	324	VAL	CA-CB	5.24	1.65	1.54
1	A	200	VAL	CA-CB	5.02	1.65	1.54

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	176	ARG	NE-CZ-NH2	-20.82	109.89	120.30
1	B	246	ARG	NE-CZ-NH2	-15.21	112.69	120.30
1	A	176	ARG	NE-CZ-NH1	15.14	127.87	120.30
1	B	246	ARG	NE-CZ-NH1	13.83	127.22	120.30
1	B	152	ARG	NE-CZ-NH1	13.77	127.18	120.30
1	A	176	ARG	NE-CZ-NH2	-13.64	113.48	120.30
1	B	176	ARG	NE-CZ-NH1	12.85	126.72	120.30
1	A	96	ARG	NE-CZ-NH1	11.39	126.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	152	ARG	NE-CZ-NH2	-11.11	114.75	120.30
1	A	168	ARG	NE-CZ-NH1	10.93	125.77	120.30
1	B	336	VAL	CG1-CB-CG2	-10.11	94.72	110.90
1	B	96	ARG	NE-CZ-NH1	10.01	125.31	120.30
1	B	168	ARG	NE-CZ-NH1	10.01	125.30	120.30
1	A	100	ARG	NE-CZ-NH1	9.96	125.28	120.30
1	A	7	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	A	96	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	A	238	ASP	CA-C-N	8.86	133.91	116.20
1	A	361	VAL	CG1-CB-CG2	-8.68	97.02	110.90
1	A	56	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	B	97	MET	CG-SD-CE	-8.19	87.09	100.20
1	B	256	LEU	CA-CB-CG	8.19	134.14	115.30
1	A	245	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	A	244	TYR	CB-CG-CD1	-8.14	116.11	121.00
1	A	137	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	A	97	MET	CG-SD-CE	-8.02	87.36	100.20
1	B	100	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	A	188	LEU	CA-CB-CG	7.44	132.41	115.30
1	B	359	TYR	CB-CG-CD2	-7.32	116.61	121.00
1	B	331	LEU	CA-CB-CG	7.30	132.09	115.30
1	A	122	TRP	CD1-CG-CD2	7.29	112.13	106.30
1	A	306	LEU	CA-CB-CG	7.29	132.07	115.30
1	B	284	TYR	CB-CG-CD2	-7.07	116.76	121.00
1	B	44	LEU	CA-CB-CG	7.03	131.46	115.30
1	B	366	LEU	CA-CB-CG	7.00	131.41	115.30
1	A	103	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	A	337	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	A	44	LEU	CA-CB-CG	6.84	131.04	115.30
1	A	366	LEU	CA-CB-CG	6.82	130.97	115.30
1	A	100	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	284	TYR	CB-CG-CD2	-6.72	116.97	121.00
1	A	340	LEU	CA-CB-CG	6.71	130.74	115.30
1	A	80	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	122	TRP	CE2-CD2-CG	-6.67	101.97	107.30
1	B	108	LEU	CA-CB-CG	6.63	130.55	115.30
1	B	197	ARG	NE-CZ-NH2	6.61	123.60	120.30
1	B	347	VAL	CG1-CB-CG2	-6.59	100.36	110.90
1	A	110	THR	N-CA-CB	-6.56	97.83	110.30
1	A	17	VAL	N-CA-CB	-6.50	97.19	111.50
1	B	323	TYR	CB-CG-CD1	-6.50	117.10	121.00
1	B	122	TRP	CE2-CD2-CG	-6.49	102.11	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	269	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	338	MET	CA-CB-CG	6.45	124.27	113.30
1	B	142	THR	N-CA-CB	-6.45	98.04	110.30
1	B	306	LEU	CA-CB-CG	6.42	130.07	115.30
1	A	319	PHE	CB-CG-CD2	-6.40	116.32	120.80
1	B	137	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	B	151	VAL	N-CA-CB	-6.32	97.60	111.50
1	B	282	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	351	ASP	CB-CG-OD1	6.22	123.90	118.30
1	B	366	LEU	N-CA-C	-6.18	94.30	111.00
1	B	60	VAL	CG1-CB-CG2	-6.17	101.03	110.90
1	A	205	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	B	344	VAL	CG1-CB-CG2	-6.16	101.05	110.90
1	B	207	LEU	CB-CG-CD2	-6.13	100.57	111.00
1	B	122	TRP	CD1-CG-CD2	6.13	111.20	106.30
1	B	168	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	B	179	VAL	CB-CA-C	-6.04	99.92	111.40
1	B	110	THR	N-CA-CB	-6.03	98.85	110.30
1	A	7	ARG	NH1-CZ-NH2	-6.02	112.77	119.40
1	B	193	VAL	CA-CB-CG2	-6.02	101.87	110.90
1	B	210	GLY	CA-C-N	-5.95	104.12	117.20
1	B	69	THR	N-CA-CB	-5.94	99.01	110.30
1	B	319	PHE	CB-CG-CD2	-5.90	116.67	120.80
1	B	284	TYR	N-CA-C	-5.89	95.09	111.00
1	A	123	GLN	O-C-N	5.79	131.96	122.70
1	B	265	GLN	CA-CB-CG	-5.78	100.69	113.40
1	B	337	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	B	137	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	56	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	103	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	69	THR	N-CA-CB	-5.70	99.47	110.30
1	B	42	LEU	CB-CG-CD1	-5.69	101.33	111.00
1	B	188	LEU	CA-CB-CG	5.68	128.36	115.30
1	B	239	GLY	N-CA-C	5.65	127.22	113.10
1	A	105	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	A	323	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	B	162	THR	N-CA-CB	-5.54	99.78	110.30
1	A	197	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	1	MET	CG-SD-CE	-5.50	91.40	100.20
1	B	331	LEU	O-C-N	-5.47	113.94	122.70
1	A	207	LEU	CA-CB-CG	5.47	127.88	115.30
1	A	95	GLU	CA-CB-CG	5.45	125.38	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	236	LEU	CA-CB-CG	5.43	127.79	115.30
1	A	248	LEU	CB-CG-CD1	-5.43	101.77	111.00
1	B	69	THR	CA-CB-CG2	5.43	120.00	112.40
1	B	227	VAL	CB-CA-C	-5.43	101.09	111.40
1	A	108	LEU	CA-CB-CG	5.37	127.65	115.30
1	A	59	LEU	CB-CG-CD2	-5.30	101.98	111.00
1	A	224	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	366	LEU	CB-CG-CD2	-5.30	101.99	111.00
1	B	173	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	240	ARG	CA-CB-CG	5.26	124.96	113.40
1	A	328	LEU	CA-CB-CG	5.23	127.33	115.30
1	B	205	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	354	SER	N-CA-CB	5.20	118.29	110.50
1	B	6	GLU	CB-CG-CD	5.18	128.18	114.20
1	A	179	VAL	CB-CA-C	-5.17	101.57	111.40
1	B	316	GLU	CA-CB-CG	5.17	124.77	113.40
1	B	151	VAL	CB-CA-C	5.16	121.21	111.40
1	B	17	VAL	CG1-CB-CG2	-5.15	102.65	110.90
1	A	307	ASP	O-C-N	5.15	130.94	122.70
1	A	324	VAL	CG1-CB-CG2	-5.15	102.66	110.90
1	B	53	MET	N-CA-CB	-5.14	101.36	110.60
1	A	68	THR	CA-CB-CG2	5.13	119.59	112.40
1	A	265	GLN	CA-CB-CG	5.11	124.65	113.40
1	A	238	ASP	CA-C-O	-5.10	109.38	120.10
1	B	287	GLU	CA-C-N	-5.10	105.98	117.20
1	A	203	LEU	CA-CB-CG	5.07	126.95	115.30
1	A	282	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	260	CYS	N-CA-CB	-5.04	101.54	110.60
1	A	339	MET	CG-SD-CE	5.03	108.24	100.20
1	A	59	LEU	CA-CB-CG	5.00	126.81	115.30
1	A	308	VAL	N-CA-CB	-5.00	100.49	111.50

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 (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	2844	0	2861	58	0
1	B	2844	0	2861	43	0
2	A	79	0	0	0	0
2	B	71	0	0	0	0
All	All	5838	0	5722	101	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 9.

All (101) 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: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: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:A:51:MET:HE3	1:A:202:GLU:HG2	1.86	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:139:ILE:HG12	1:B:158:MET:HE1	1.90	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: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:1:MET:HE1	1:A:35:LEU:HB3	1.91	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: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:B:53:MET:HE3	1:B:230:PHE:HB3	1.93	0.51
1:B:176:ARG:O	1:B:176:ARG:HG2	2.11	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:LYS:O	1:B:140:GLU:HG3	2.16	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: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: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: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: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: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:39:ASP:CG	1:A:40:GLY:H	2.24	0.40
1:A:1:MET:HE3	1:A:37:VAL:HG23	2.03	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%)	29 48
1	B	364/366 (100%)	342 (94%)	17 (5%)	5 (1%)	11 20
All	All	728/732 (100%)	685 (94%)	36 (5%)	7 (1%)	15 28

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%)	264 (84%)	49 (16%)	2 4
1	B	313/313 (100%)	257 (82%)	56 (18%)	2 3
All	All	626/626 (100%)	521 (83%)	105 (17%)	2 4

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	11	LEU
1	A	26	THR
1	A	30	LEU
1	A	42	LEU
1	A	44	LEU
1	A	49	LEU
1	A	56	ARG
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	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	188	LEU
1	A	191	HIS
1	A	195	VAL
1	A	207	LEU
1	A	208	ASP
1	A	233	THR
1	A	236	LEU
1	A	237	VAL
1	A	238	ASP
1	A	240	ARG
1	A	257	GLU
1	A	273	LEU
1	A	275	ASN
1	A	289	GLN
1	A	306	LEU
1	A	319	PHE
1	A	325	LEU
1	A	327	VAL

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Mol	Chain	Res	Type
1	A	328	LEU
1	A	331	LEU
1	A	332	LYS
1	A	340	LEU
1	A	356	SER
1	A	366	LEU
1	B	5	VAL
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	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
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	184	ILE
1	B	188	LEU
1	B	193	VAL
1	B	200	VAL
1	B	203	LEU
1	B	205	ARG
1	B	207	LEU
1	B	211	ASP

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Mol	Chain	Res	Type
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	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	328	LEU
1	B	340	LEU
1	B	355	GLN
1	B	363	PRO
1	B	366	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	217	GLN
1	A	226	HIS
1	A	275	ASN
1	A	288	ASN
1	A	295	ASN
1	A	299	GLN
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	348	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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.