



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 11:25 AM UTC

PDB ID : 1ZQU / pdb_00001zqu
Title : DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7), 31-KD DOMAIN;
SOAKED IN THE PRESENCE OF ARTIFICIAL MOTHER LIQUOR
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1996-04-19
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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

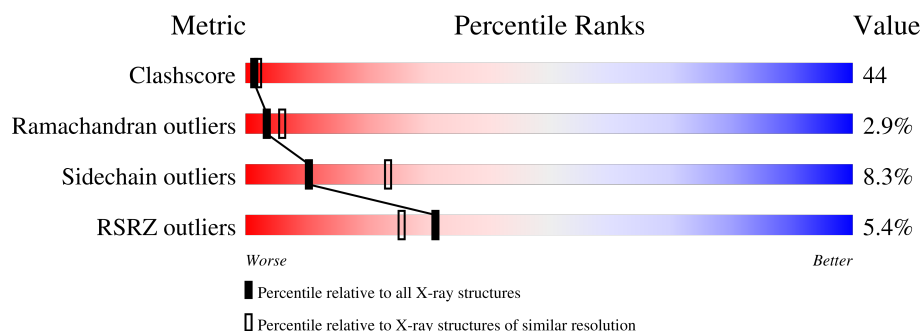
1 Overall quality at a glance

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)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	248	5% 37% 39% 20% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2040 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 BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	1	0
			1935	1218	342	367	8			

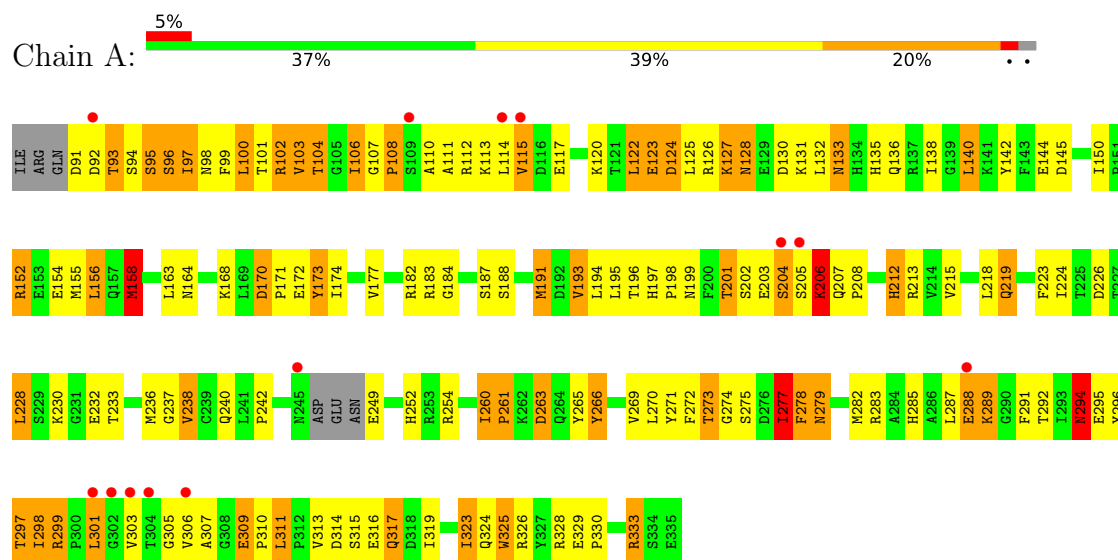
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	105	Total	O	0	0
			105	105		

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: DNA POLYMERASE BETA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	120.78Å 63.26Å 37.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.0 (20.00-2.60) 95.4 (20.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.14Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	(Not available) , (Not available) 0.196 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	12.8	Xtriage
Anisotropy	0.787	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 149.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2040	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	1.49	10/1973 (0.5%)	1.99	68/2662 (2.6%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	GLN	CA-C	-7.08	1.43	1.52
1	A	273	THR	N-CA	-6.66	1.38	1.46
1	A	238	VAL	N-CA	-6.34	1.38	1.46
1	A	201	THR	N-CA	-5.90	1.38	1.45
1	A	193	VAL	CA-CB	-5.78	1.47	1.54
1	A	261	PRO	CA-C	-5.62	1.45	1.52
1	A	269	VAL	CA-CB	-5.41	1.47	1.54
1	A	142	TYR	N-CA	-5.35	1.40	1.46
1	A	287	LEU	N-CA	-5.34	1.40	1.46
1	A	263	ASP	CG-OD1	5.08	1.35	1.25

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	ASN	CA-CB-CG	-9.24	103.36	112.60
1	A	94	SER	N-CA-C	-8.44	102.03	111.82
1	A	206	LYS	CA-C-N	-8.42	113.24	122.59
1	A	206	LYS	C-N-CA	-8.42	113.24	122.59
1	A	95	SER	N-CA-C	-8.16	102.33	111.71
1	A	152	ARG	N-CA-CB	7.33	122.87	110.49
1	A	124	ASP	N-CA-C	-7.14	103.19	110.97
1	A	177	VAL	CB-CA-C	-7.10	102.37	110.96
1	A	96	SER	N-CA-CB	7.04	120.29	110.07
1	A	260	ILE	CB-CA-C	-7.03	98.57	111.36
1	A	297	THR	N-CA-C	6.96	119.50	109.14
1	A	314	ASP	CA-CB-CG	-6.83	105.77	112.60
1	A	242	PRO	CB-CA-C	-6.71	102.99	111.71
1	A	261	PRO	N-CA-CB	6.51	109.01	103.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	ASP	CA-C-N	-6.42	111.95	122.54
1	A	130	ASP	C-N-CA	-6.42	111.95	122.54
1	A	223	PHE	CA-C-N	-6.41	112.09	121.71
1	A	223	PHE	C-N-CA	-6.41	112.09	121.71
1	A	131	LYS	CB-CA-C	6.33	120.67	110.09
1	A	104	THR	N-CA-CB	6.27	119.42	109.51
1	A	266	TYR	N-CA-C	6.27	118.63	111.11
1	A	326	ARG	N-CA-C	-6.07	102.09	110.35
1	A	163	LEU	CA-C-N	-6.03	111.15	120.31
1	A	163	LEU	C-N-CA	-6.03	111.15	120.31
1	A	124	ASP	CA-CB-CG	5.97	118.57	112.60
1	A	265	TYR	N-CA-CB	-5.97	100.74	109.82
1	A	140	LEU	CA-C-O	5.96	126.83	119.97
1	A	277	ILE	O-C-N	5.95	127.74	121.91
1	A	103	VAL	CB-CA-C	-5.94	103.77	110.96
1	A	226	ASP	CA-CB-CG	5.91	118.51	112.60
1	A	128	ASN	N-CA-C	5.83	117.90	110.61
1	A	127	LYS	N-CA-C	-5.81	106.05	113.02
1	A	278	PHE	CA-CB-CG	-5.78	108.02	113.80
1	A	123	GLU	N-CA-C	-5.69	105.43	112.38
1	A	298	ILE	N-CA-CB	5.69	119.55	111.82
1	A	145	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	212	HIS	N-CA-CB	5.64	118.53	110.06
1	A	106	ILE	N-CA-CB	5.63	120.51	111.23
1	A	158	MET	CB-CA-C	5.59	119.66	110.88
1	A	199	ASN	CA-CB-CG	-5.56	107.04	112.60
1	A	191	MET	CA-C-N	-5.54	114.99	122.86
1	A	191	MET	C-N-CA	-5.54	114.99	122.86
1	A	132	LEU	CB-CA-C	-5.54	100.40	109.53
1	A	158	MET	N-CA-CB	5.53	118.03	110.01
1	A	195	LEU	N-CA-CB	-5.51	101.33	111.37
1	A	333	ARG	N-CA-C	5.51	119.01	112.72
1	A	228	LEU	N-CA-C	-5.47	104.17	112.04
1	A	94	SER	CA-C-O	5.42	126.20	119.97
1	A	173	TYR	CA-C-N	-5.41	116.48	123.19
1	A	173	TYR	C-N-CA	-5.41	116.48	123.19
1	A	294	ASN	N-CA-CB	5.36	120.30	110.76
1	A	170	ASP	CA-C-N	5.36	125.07	119.82
1	A	170	ASP	C-N-CA	5.36	125.07	119.82
1	A	325	TRP	N-CA-C	-5.35	101.05	109.50
1	A	279	ASN	O-C-N	5.34	127.64	122.09
1	A	265	TYR	N-CA-C	5.33	117.52	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	ARG	CD-NE-CZ	-5.32	116.95	124.40
1	A	266	TYR	N-CA-CB	5.32	117.86	109.94
1	A	124	ASP	N-CA-CB	5.25	117.58	109.91
1	A	323	ILE	O-C-N	5.21	126.78	122.09
1	A	289	LYS	CA-CB-CG	-5.20	103.70	114.10
1	A	272	PHE	CA-CB-CG	-5.15	108.65	113.80
1	A	213	ARG	NE-CZ-NH2	-5.15	114.57	119.20
1	A	163	LEU	N-CA-CB	5.10	118.19	110.28
1	A	131	LYS	CA-C-N	5.09	129.63	122.09
1	A	131	LYS	C-N-CA	5.09	129.63	122.09
1	A	195	LEU	CA-C-N	-5.05	114.08	122.11
1	A	195	LEU	C-N-CA	-5.05	114.08	122.11

There are no chirality outliers.

There are no planarity outliers.

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	1935	0	1868	168	0
2	A	105	0	0	7	0
All	All	2040	0	1868	168	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 44.

All (168) 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:317:GLN:NE2	1:A:317:GLN:H	1.46	1.11
1:A:277:ILE:H	1:A:277:ILE:HD13	1.26	1.00
1:A:317:GLN:H	1:A:317:GLN:HE21	1.08	0.94
1:A:294:ASN:HD22	1:A:296:TYR:H	1.10	0.92
1:A:294:ASN:ND2	1:A:296:TYR:H	1.71	0.87
1:A:317:GLN:HE21	1:A:317:GLN:N	1.75	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ASN:O	1:A:283:ARG:HG2	1.81	0.81
1:A:294:ASN:ND2	1:A:297:THR:H	1.79	0.80
1:A:110:ALA:O	1:A:114:LEU:HD13	1.83	0.79
1:A:133:ASN:ND2	1:A:136:GLN:HG3	1.99	0.77
1:A:154:GLU:O	1:A:158:MET:HG2	1.86	0.76
1:A:212:HIS:CD2	1:A:230:LYS:HE3	2.20	0.75
1:A:155:MET:HA	1:A:158:MET:HG3	1.68	0.74
1:A:294:ASN:HD22	1:A:296:TYR:N	1.85	0.73
1:A:122:LEU:HD12	1:A:123:GLU:N	2.04	0.72
1:A:317:GLN:NE2	1:A:317:GLN:N	2.30	0.71
1:A:92:ASP:C	1:A:95:SER:HB3	2.15	0.71
1:A:294:ASN:HD21	1:A:297:THR:H	1.38	0.71
1:A:98:ASN:O	1:A:101:THR:HG22	1.91	0.71
1:A:278:PHE:CE2	1:A:282:MET:HE2	2.28	0.69
1:A:292:THR:HG22	1:A:301:LEU:HD11	1.74	0.69
1:A:112:ARG:O	1:A:115:VAL:HG23	1.94	0.68
1:A:123:GLU:O	1:A:127:LYS:HG2	1.95	0.66
1:A:107:GLY:O	1:A:111:ALA:N	2.28	0.66
1:A:215:VAL:O	1:A:219:GLN:HG3	1.97	0.65
1:A:100:LEU:O	1:A:103:VAL:HG23	1.97	0.64
1:A:295:GLU:H	1:A:295:GLU:CD	2.06	0.64
1:A:108:PRO:O	1:A:111:ALA:N	2.31	0.63
1:A:133:ASN:ND2	1:A:136:GLN:H	1.97	0.63
1:A:299[A]:ARG:HG3	1:A:299[A]:ARG:HH11	1.63	0.62
1:A:144:GLU:N	1:A:144:GLU:OE1	2.30	0.62
1:A:270:LEU:HD12	1:A:333:ARG:NH1	2.15	0.62
1:A:133:ASN:HD21	1:A:136:GLN:HG3	1.64	0.61
1:A:205:SER:O	1:A:206:LYS:HD3	2.00	0.61
1:A:120:LYS:N	1:A:124:ASP:OD2	2.28	0.61
1:A:328:ARG:NH2	2:A:470:HOH:O	2.32	0.61
1:A:155:MET:HA	1:A:158:MET:CG	2.30	0.60
1:A:301:LEU:N	1:A:301:LEU:HD12	2.16	0.60
1:A:208:PRO:HD2	2:A:473:HOH:O	2.01	0.60
1:A:291:PHE:CA	1:A:301:LEU:HD13	2.31	0.60
1:A:110:ALA:HA	1:A:113:LYS:HE3	1.83	0.60
1:A:297:THR:O	1:A:299[A]:ARG:NH1	2.34	0.59
1:A:92:ASP:O	1:A:95:SER:HB3	2.01	0.59
1:A:103:VAL:HB	1:A:106:ILE:CD1	2.33	0.59
1:A:197:HIS:CG	1:A:198:PRO:HD2	2.38	0.59
1:A:277:ILE:H	1:A:277:ILE:CD1	2.04	0.59
1:A:204:SER:C	1:A:206:LYS:HE2	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LYS:HG3	1:A:114:LEU:HD12	1.87	0.57
1:A:106:ILE:CG2	1:A:111:ALA:HB2	2.35	0.56
1:A:291:PHE:HA	1:A:301:LEU:HD13	1.86	0.56
1:A:133:ASN:C	1:A:133:ASN:HD22	2.12	0.56
1:A:152:ARG:NH2	1:A:184:GLY:HA2	2.20	0.56
1:A:260:ILE:HG22	1:A:261:PRO:O	2.06	0.56
1:A:93:THR:C	1:A:96:SER:H	2.13	0.56
1:A:150:ILE:O	1:A:188:SER:N	2.33	0.56
1:A:315:SER:HB2	1:A:317:GLN:HE22	1.71	0.56
1:A:97:ILE:HD11	1:A:112:ARG:HG2	1.89	0.55
1:A:204:SER:CA	1:A:206:LYS:HE2	2.38	0.54
1:A:218:LEU:HB3	1:A:224:ILE:HG13	1.90	0.53
1:A:193:VAL:C	1:A:194:LEU:HD12	2.34	0.53
1:A:292:THR:HG22	1:A:301:LEU:CD1	2.38	0.53
1:A:174:ILE:HB	1:A:196:THR:HG22	1.91	0.53
1:A:140:LEU:O	1:A:140:LEU:HG	2.09	0.53
1:A:114:LEU:HD12	1:A:114:LEU:N	2.22	0.52
1:A:138:ILE:HB	1:A:228:LEU:CD2	2.39	0.52
1:A:294:ASN:ND2	1:A:296:TYR:N	2.50	0.52
1:A:315:SER:HB2	1:A:317:GLN:NE2	2.24	0.52
1:A:113:LYS:O	1:A:117:GLU:HG2	2.09	0.52
1:A:155:MET:HE2	1:A:188:SER:CB	2.40	0.52
1:A:197:HIS:ND1	1:A:198:PRO:HD2	2.26	0.51
1:A:329:GLU:HB3	1:A:330:PRO:HD2	1.92	0.51
1:A:271:TYR:CG	1:A:295:GLU:HB3	2.46	0.51
1:A:274:GLY:HA2	1:A:279:ASN:OD1	2.11	0.51
1:A:103:VAL:HB	1:A:106:ILE:HD12	1.93	0.50
1:A:158:MET:HB2	1:A:191:MET:HE1	1.92	0.50
1:A:270:LEU:HD21	1:A:282:MET:CE	2.40	0.50
1:A:277:ILE:HG12	1:A:278:PHE:H	1.77	0.50
1:A:122:LEU:HD12	1:A:122:LEU:C	2.36	0.50
1:A:207:GLN:N	1:A:208:PRO:HD3	2.27	0.50
1:A:108:PRO:O	1:A:112:ARG:N	2.35	0.50
1:A:138:ILE:HB	1:A:228:LEU:HD23	1.93	0.50
1:A:155:MET:HE2	1:A:188:SER:HB2	1.94	0.50
1:A:91:ASP:C	1:A:93:THR:H	2.19	0.49
1:A:270:LEU:HD12	1:A:333:ARG:HH12	1.76	0.49
1:A:330:PRO:HA	1:A:333:ARG:HG3	1.94	0.49
1:A:113:LYS:HG3	1:A:114:LEU:CD1	2.43	0.49
1:A:317:GLN:H	1:A:317:GLN:CD	2.15	0.48
1:A:93:THR:O	1:A:96:SER:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:VAL:CG1	1:A:252:HIS:HB3	2.44	0.48
1:A:299[B]:ARG:HG2	1:A:310:PRO:N	2.27	0.48
1:A:323:ILE:C	1:A:324:GLN:HG2	2.37	0.48
1:A:303:VAL:C	1:A:305:GLY:H	2.22	0.48
1:A:155:MET:SD	1:A:158:MET:HE2	2.54	0.47
1:A:156:LEU:HD12	1:A:156:LEU:HA	1.78	0.47
1:A:133:ASN:H	1:A:136:GLN:NE2	2.13	0.47
1:A:170:ASP:HA	1:A:171:PRO:HD3	1.68	0.47
1:A:218:LEU:HD23	1:A:218:LEU:HA	1.72	0.47
1:A:232:GLU:HG3	1:A:233:THR:HG23	1.97	0.47
1:A:298:ILE:HG23	1:A:298:ILE:O	2.14	0.47
1:A:275:SER:OG	1:A:277:ILE:HG12	2.16	0.46
1:A:294:ASN:HD22	1:A:294:ASN:C	2.23	0.46
1:A:305:GLY:O	1:A:307:ALA:N	2.49	0.46
1:A:103:VAL:O	1:A:106:ILE:N	2.47	0.46
1:A:278:PHE:CE2	1:A:282:MET:CE	2.98	0.46
1:A:292:THR:N	1:A:301:LEU:HD11	2.31	0.46
1:A:97:ILE:CD1	1:A:112:ARG:HG2	2.45	0.46
1:A:263:ASP:OD1	1:A:263:ASP:N	2.44	0.45
1:A:277:ILE:HD13	1:A:277:ILE:N	2.11	0.45
1:A:249:GLU:HG3	2:A:455:HOH:O	2.15	0.45
1:A:103:VAL:HB	1:A:106:ILE:HD13	1.99	0.45
1:A:114:LEU:N	1:A:114:LEU:CD1	2.80	0.45
1:A:135:HIS:CE1	1:A:228:LEU:HD13	2.52	0.45
1:A:266:TYR:HB2	1:A:313:VAL:HG12	1.97	0.45
1:A:296:TYR:HA	2:A:449:HOH:O	2.15	0.45
1:A:237:GLY:O	1:A:254:ARG:NH1	2.50	0.44
1:A:277:ILE:HG12	1:A:278:PHE:N	2.32	0.44
1:A:291:PHE:HA	1:A:301:LEU:CD1	2.47	0.44
1:A:133:ASN:HD21	1:A:136:GLN:H	1.64	0.44
1:A:172:GLU:HG2	1:A:198:PRO:HG2	2.00	0.44
1:A:260:ILE:HG22	1:A:261:PRO:N	2.32	0.44
1:A:270:LEU:HD22	1:A:319:ILE:HD13	2.00	0.44
1:A:201:THR:C	1:A:203:GLU:H	2.25	0.44
1:A:125:LEU:O	1:A:128:ASN:N	2.40	0.44
1:A:299[A]:ARG:HG3	1:A:299[A]:ARG:NH1	2.31	0.44
1:A:126:ARG:HG2	1:A:140:LEU:HD21	1.98	0.44
1:A:330:PRO:HD2	2:A:429:HOH:O	2.17	0.44
1:A:240:GLN:NE2	1:A:252:HIS:CE1	2.86	0.44
1:A:152:ARG:NH2	1:A:184:GLY:CA	2.81	0.44
1:A:285:HIS:O	1:A:288:GLU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LYS:C	1:A:208:PRO:HD3	2.43	0.43
1:A:106:ILE:HG22	1:A:111:ALA:HB2	1.98	0.43
1:A:201:THR:C	1:A:203:GLU:N	2.75	0.43
1:A:205:SER:O	1:A:206:LYS:HB3	2.19	0.43
1:A:271:TYR:CD2	1:A:295:GLU:HB3	2.54	0.43
1:A:292:THR:CG2	1:A:301:LEU:HD11	2.45	0.43
1:A:294:ASN:OD1	1:A:299[A]:ARG:NH2	2.51	0.43
1:A:127:LYS:HA	1:A:127:LYS:HD3	1.81	0.43
1:A:183:ARG:NE	2:A:499:HOH:O	2.51	0.43
1:A:138:ILE:HD12	1:A:138:ILE:HG23	1.64	0.42
1:A:103:VAL:CG1	1:A:106:ILE:HD12	2.50	0.42
1:A:122:LEU:O	1:A:126:ARG:HG3	2.20	0.42
1:A:182:ARG:HH12	1:A:316:GLU:CD	2.27	0.42
1:A:183:ARG:NH1	1:A:273:THR:O	2.50	0.42
1:A:295:GLU:CD	1:A:295:GLU:N	2.76	0.42
1:A:311:LEU:HD12	1:A:311:LEU:HA	1.82	0.41
1:A:170:ASP:O	1:A:173:TYR:HB2	2.20	0.41
1:A:309:GLU:HG3	1:A:310:PRO:HD2	2.02	0.41
1:A:104:THR:HG22	2:A:435:HOH:O	2.20	0.41
1:A:99:PHE:CD1	1:A:99:PHE:C	2.98	0.41
1:A:127:LYS:C	1:A:128:ASN:ND2	2.79	0.41
1:A:289:LYS:NZ	1:A:324:GLN:HG3	2.36	0.41
1:A:103:VAL:CB	1:A:106:ILE:CD1	2.99	0.41
1:A:138:ILE:HD13	1:A:138:ILE:HA	1.80	0.41
1:A:183:ARG:NH1	1:A:275:SER:HA	2.36	0.41
1:A:296:TYR:C	1:A:297:THR:HG23	2.45	0.41
1:A:91:ASP:C	1:A:93:THR:N	2.78	0.41
1:A:236:MET:HE2	1:A:254:ARG:NH2	2.36	0.41
1:A:270:LEU:HD21	1:A:282:MET:HE3	2.02	0.41
1:A:136:GLN:HG3	1:A:136:GLN:H	1.59	0.40
1:A:150:ILE:O	1:A:187:SER:HA	2.19	0.40
1:A:230:LYS:O	1:A:230:LYS:HG2	2.21	0.40
1:A:99:PHE:O	1:A:102:ARG:HB2	2.21	0.40
1:A:205:SER:C	1:A:206:LYS:HD3	2.47	0.40
1:A:301:LEU:N	1:A:301:LEU:CD1	2.82	0.40
1:A:204:SER:HB3	1:A:206:LYS:HE2	2.04	0.40
1:A:158:MET:HG2	1:A:158:MET:H	1.61	0.40
1:A:183:ARG:HD2	1:A:333:ARG:HB2	2.04	0.40
1:A:270:LEU:CD1	1:A:333:ARG:NH1	2.82	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	239/248 (96%)	205 (86%)	27 (11%)	7 (3%)	3 6

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	LYS
1	A	309	GLU
1	A	204	SER
1	A	306	VAL
1	A	202	SER
1	A	301	LEU
1	A	108	PRO

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	206/226 (91%)	188 (91%)	18 (9%)	9 21

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	THR
1	A	97	ILE
1	A	100	LEU
1	A	115	VAL

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Mol	Chain	Res	Type
1	A	122	LEU
1	A	133	ASN
1	A	156	LEU
1	A	158	MET
1	A	164	ASN
1	A	168	LYS
1	A	277	ILE
1	A	288	GLU
1	A	294	ASN
1	A	299[A]	ARG
1	A	299[B]	ARG
1	A	311	LEU
1	A	317	GLN
1	A	325	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN
1	A	133	ASN
1	A	136	GLN
1	A	212	HIS
1	A	217	GLN
1	A	240	GLN
1	A	252	HIS
1	A	281	ASN
1	A	285	HIS
1	A	294	ASN
1	A	317	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	242/248 (97%)	0.14	13 (5%) 31 26	12, 36, 89, 100	1 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	115	VAL	3.7
1	A	303	VAL	3.3
1	A	205	SER	3.2
1	A	306	VAL	3.1
1	A	304	THR	2.9
1	A	245	ASN	2.8
1	A	288	GLU	2.4
1	A	302	GLY	2.4
1	A	114	LEU	2.3
1	A	109	SER	2.3
1	A	204	SER	2.2
1	A	92	ASP	2.2
1	A	301	LEU	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.