



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:03 pm BST

PDB ID : 1ZQU
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

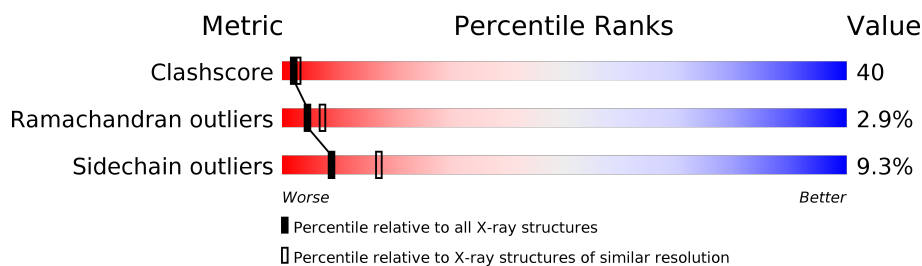
1 Overall quality at a glance

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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (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 on 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	248	

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			

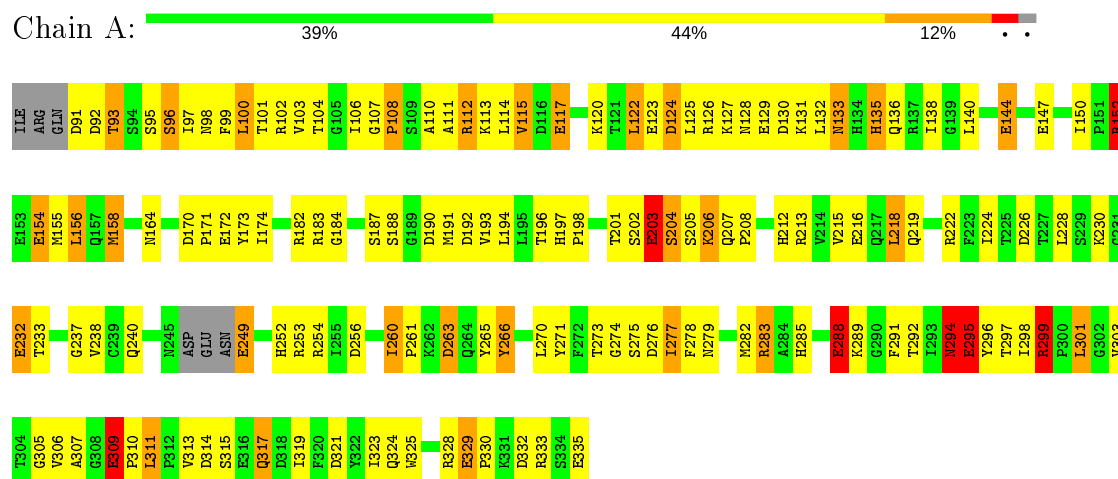
- Molecule 2 is water.

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 and DNA 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.

• 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 15.15 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.0 (20.00-2.60) 87.0 (15.15-2.15)	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)	0.28 , 124.5	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	0.88	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	1.18	14/1973 (0.7%)	1.71	40/2662 (1.5%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	GLU	CD-OE1	6.56	1.32	1.25
1	A	129	GLU	CD-OE1	6.17	1.32	1.25
1	A	147	GLU	CD-OE1	5.96	1.32	1.25
1	A	309	GLU	CD-OE1	5.92	1.32	1.25
1	A	154	GLU	CD-OE1	5.91	1.32	1.25
1	A	117	GLU	CD-OE1	5.89	1.32	1.25
1	A	203	GLU	CD-OE1	5.86	1.32	1.25
1	A	249	GLU	CD-OE1	5.72	1.31	1.25
1	A	329	GLU	CD-OE1	5.51	1.31	1.25
1	A	335	GLU	CD-OE1	5.51	1.31	1.25
1	A	295	GLU	CD-OE1	5.50	1.31	1.25
1	A	232	GLU	CD-OE1	5.43	1.31	1.25
1	A	144	GLU	CD-OE1	5.31	1.31	1.25
1	A	288	GLU	CD-OE1	5.24	1.31	1.25

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	ARG	NE-CZ-NH2	-11.46	114.57	120.30
1	A	213	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	A	253	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	A	299[A]	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	A	299[B]	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	A	192	ASP	CB-CG-OD1	-8.66	110.51	118.30
1	A	253	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	A	190	ASP	CB-CG-OD1	7.88	125.39	118.30
1	A	112	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	A	276	ASP	CB-CG-OD1	-7.50	111.55	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	ASP	CB-CG-OD1	-7.48	111.57	118.30
1	A	226	ASP	CB-CG-OD1	6.84	124.45	118.30
1	A	314	ASP	CB-CG-OD1	-6.83	112.15	118.30
1	A	152	ARG	N-CA-CB	6.82	122.87	110.60
1	A	96	SER	N-CA-CB	6.52	120.29	110.50
1	A	260	ILE	CB-CA-C	-6.51	98.57	111.60
1	A	192	ASP	CB-CG-OD2	6.27	123.95	118.30
1	A	182	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	266	TYR	CB-CG-CD1	-6.04	117.38	121.00
1	A	263	ASP	CB-CG-OD1	-5.84	113.05	118.30
1	A	299[A]	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	299[B]	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	130	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	124	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	190	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	A	226	ASP	CB-CG-OD2	-5.48	113.36	118.30
1	A	265	TYR	N-CA-CB	-5.48	100.74	110.60
1	A	321	ASP	CB-CG-OD1	-5.46	113.39	118.30
1	A	222	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	294	ASN	N-CA-CB	5.39	120.30	110.60
1	A	124	ASP	CB-CG-OD1	-5.35	113.48	118.30
1	A	263	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	256	ASP	CB-CG-OD1	-5.26	113.56	118.30
1	A	332	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	132	LEU	CB-CA-C	-5.16	100.40	110.20
1	A	218	LEU	CA-CB-CG	-5.15	103.45	115.30
1	A	276	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	131	LYS	CB-CA-C	5.13	120.67	110.40
1	A	283	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	213	ARG	CD-NE-CZ	5.02	130.62	123.60

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	154	0
2	A	105	0	0	7	0
All	All	2040	0	1868	154	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 40.

All (154) 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:HE21	1:A:317:GLN:H	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
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: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	2.27	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:92:ASP:C	1:A:95:SER:HB3	2.15	0.67
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: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:OE1	1:A:144:GLU:N	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:A:301:LEU:N	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:92:ASP:O	1:A:95:SER:HB3	2.01	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:295:GLU:H	1:A:295:GLU:CD	2.06	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: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: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: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: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:204:SER:C	1:A:206:LYS:HE2	2.30	0.52
1:A:133:ASN:HD22	1:A:133:ASN:C	2.12	0.52
1:A:197:HIS:ND1	1:A:198:PRO:HD2	2.26	0.51
1:A:93:THR:C	1:A:96:SER:H	2.13	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:270:LEU:HD21	1:A:282:MET:CE	2.40	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ILE:HG12	1:A:278:PHE:H	1.77	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:330:PRO:HA	1:A:333:ARG:HG3	1.94	0.49
1:A:270:LEU:HD12	1:A:333:ARG:HH12	1.76	0.49
1:A:113:LYS:HG3	1:A:114:LEU:CD1	2.43	0.49
1:A:193:VAL:C	1:A:194:LEU:HD12	2.34	0.48
1:A:93:THR:O	1:A:96:SER:N	2.44	0.48
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:158:MET:HB2	1:A:191:MET:HE1	1.95	0.48
1:A:156:LEU:HA	1:A:156:LEU:HD12	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:HA	1:A:218:LEU:HD23	1.72	0.47
1:A:298:ILE:O	1:A:298:ILE:HG23	2.14	0.47
1:A:232:GLU:HG3	1:A:233:THR:HG23	1.97	0.47
1:A:275:SER:OG	1:A:277:ILE:HG12	2.16	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:91:ASP:C	1:A:93:THR:H	2.19	0.46
1:A:97:ILE:CD1	1:A:112:ARG:HG2	2.45	0.46
1:A:122:LEU:C	1:A:122:LEU:HD12	2.36	0.45
1:A:263:ASP:N	1:A:263:ASP:OD1	2.44	0.45
1:A:277:ILE:N	1:A:277:ILE:HD13	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:CD1	1:A:114:LEU:N	2.80	0.45
1:A:135:HIS:CE1	1:A:228:LEU:HD13	2.52	0.45
1:A:296:TYR:HA	2:A:449:HOH:O	2.15	0.45
1:A:266:TYR:HB2	1:A:313:VAL:HG12	1.97	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:317:GLN:CD	1:A:317:GLN:H	2.15	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
1:A:323:ILE:C	1:A:324:GLN:HG2	2.37	0.43
1:A:106:ILE:HG22	1:A:111:ALA:HB2	1.98	0.43
1:A:205:SER:O	1:A:206:LYS:HB3	2.19	0.43
1:A:303:VAL:C	1:A:305:GLY:H	2.22	0.43
1:A:271:TYR:CD2	1:A:295:GLU:HB3	2.54	0.43
1:A:294:ASN:OD1	1:A:299[A]:ARG:NH2	2.51	0.43
1:A:292:THR:CG2	1:A:301:LEU:HD11	2.45	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:HG23	1:A:138:ILE:HD12	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:183:ARG:NH1	1:A:273:THR:O	2.50	0.42
1:A:294:ASN:C	1:A:294:ASN:HD22	2.23	0.41
1:A:311:LEU:HA	1:A:311:LEU:HD12	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: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:230:LYS:O	1:A:230:LYS:HG2	2.21	0.41
1:A:136:GLN:H	1:A:136:GLN:HG3	1.59	0.40
1:A:150:ILE:O	1:A:187:SER:HA	2.19	0.40
1:A:99:PHE:O	1:A:102:ARG:HB2	2.21	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:H	1:A:158:MET:HG2	1.61	0.40
1:A:183:ARG:HD2	1:A:333:ARG:HB2	2.04	0.40
1:A:201:THR:C	1:A:203:GLU:N	2.75	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

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	239/248 (96%)	205 (86%)	27 (11%)	7 (3%)	4 7

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

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%)	186 (90%)	20 (10%)	8 15

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	THR
1	A	100	LEU
1	A	115	VAL
1	A	122	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	133	ASN
1	A	135	HIS
1	A	152	ARG
1	A	156	LEU
1	A	158	MET
1	A	164	ASN
1	A	203	GLU
1	A	277	ILE
1	A	288	GLU
1	A	294	ASN
1	A	295	GLU
1	A	299[A]	ARG
1	A	299[B]	ARG
1	A	311	LEU
1	A	317	GLN
1	A	325	TRP

Some 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	157	GLN
1	A	212	HIS
1	A	217	GLN
1	A	240	GLN
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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.