Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 09:28 AM EDT

PDB ID	:	1KTQ
Title	:	DNA POLYMERASE
Authors	:	Korolev, S.; Waksman, G.
Deposited on	:	1995-08-16
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 (i) 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 (i)) were used in the production of this report:

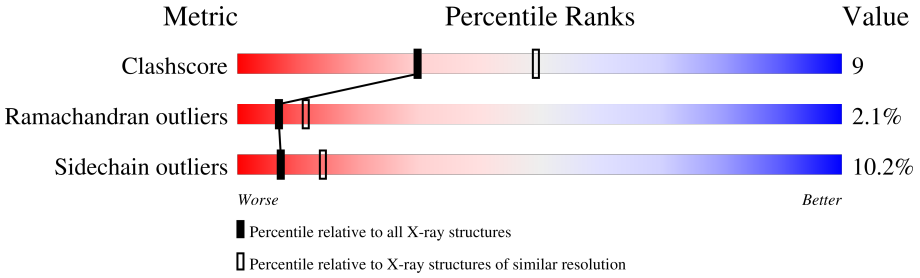
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	543	66% 27% 5% • •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6502 atoms, of which 1823 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 I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	534	5182	2698	943	761	767	13	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
2	A	440	1320	880	440	0	0

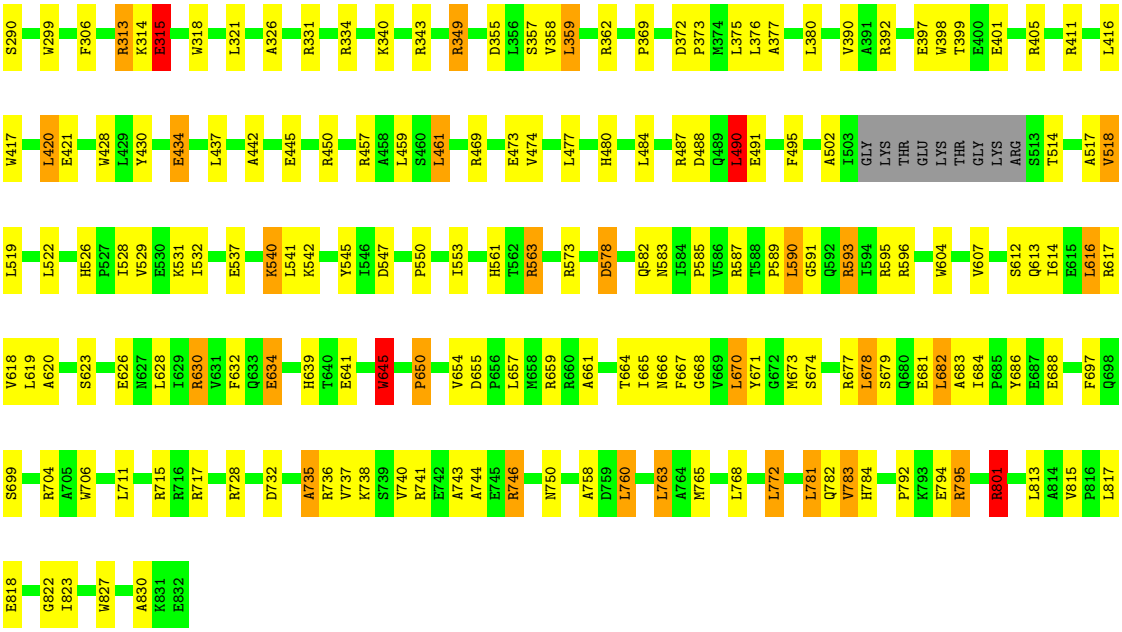
3 Residue-property plots (i)

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 I

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	109.40Å 136.80Å 45.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	90.6 (6.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.2	Depositor
R, R_{free}	0.198 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6502	wwPDB-VP
Average B, all atoms (Å^2)	31.0	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	0.78	0/4329	1.52	62/5867 (1.1%)

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	3

There are no bond length outliers.

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	563	ARG	NE-CZ-NH1	9.90	125.25	120.30
1	A	645	TRP	CD1-CG-CD2	9.16	113.63	106.30
1	A	318	TRP	CD1-CG-CD2	8.98	113.49	106.30
1	A	450	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	A	801	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	A	398	TRP	CD1-CG-CD2	8.34	112.97	106.30
1	A	299	TRP	CD1-CG-CD2	8.29	112.93	106.30
1	A	706	TRP	CD1-CG-CD2	8.15	112.82	106.30
1	A	604	TRP	CD1-CG-CD2	8.03	112.72	106.30
1	A	827	TRP	CD1-CG-CD2	7.94	112.65	106.30
1	A	604	TRP	CE2-CD2-CG	-7.84	101.03	107.30
1	A	428	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	A	563	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	A	706	TRP	CE2-CD2-CG	-7.73	101.11	107.30
1	A	417	TRP	CE2-CD2-CG	-7.67	101.16	107.30
1	A	645	TRP	CE2-CD2-CG	-7.61	101.21	107.30
1	A	299	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	A	313	ARG	NE-CZ-NH1	7.55	124.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	827	TRP	CE2-CD2-CG	-7.53	101.28	107.30
1	A	428	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	A	736	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	A	318	TRP	CE2-CD2-CG	-7.29	101.46	107.30
1	A	704	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	A	417	TRP	CD1-CG-CD2	7.03	111.92	106.30
1	A	334	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	A	359	LEU	CA-CB-CG	6.68	130.68	115.30
1	A	392	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	417	TRP	CG-CD2-CE3	6.21	139.49	133.90
1	A	398	TRP	CE2-CD2-CG	-6.19	102.35	107.30
1	A	645	TRP	CG-CD1-NE1	-5.99	104.11	110.10
1	A	704	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	411	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	604	TRP	CG-CD2-CE3	5.83	139.14	133.90
1	A	420	LEU	N-CA-C	5.80	126.65	111.00
1	A	827	TRP	CG-CD2-CE3	5.79	139.11	133.90
1	A	469	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	618	VAL	CG1-CB-CG2	-5.71	101.77	110.90
1	A	398	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	A	349	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	417	TRP	CB-CG-CD1	-5.59	119.73	127.00
1	A	318	TRP	CG-CD1-NE1	-5.59	104.51	110.10
1	A	450	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	A	563	ARG	CG-CD-NE	5.51	123.36	111.80
1	A	411	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	490	LEU	CA-CB-CG	5.47	127.88	115.30
1	A	746	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	331	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	735	ALA	N-CA-C	5.36	125.47	111.00
1	A	659	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	593	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	587	ARG	CA-C-N	-5.25	105.65	117.20
1	A	827	TRP	CG-CD1-NE1	-5.24	104.86	110.10
1	A	737	VAL	N-CA-C	-5.18	97.03	111.00
1	A	728	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	783	VAL	CA-CB-CG1	-5.15	103.17	110.90
1	A	795	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	630	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	461	LEU	CA-CB-CG	5.12	127.06	115.30
1	A	781	LEU	CA-CB-CG	5.09	127.02	115.30
1	A	405	ARG	NE-CZ-NH1	5.08	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	783	VAL	CB-CA-C	-5.04	101.83	111.40
1	A	717	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	290	SER	Peptide
1	A	315	GLU	Peptide
1	A	655	ASP	Peptide

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	4239	943	4273	80	0
2	A	440	880	0	17	1
All	All	4679	1823	4273	80	1

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 (80) 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:358:VAL:HG22	2:A:1151:HOH:O	1.85	0.76
1:A:822:GLY:HA3	1:A:830:ALA:O	1.91	0.69
1:A:526:HIS:HB3	1:A:528:ILE:HG22	1.76	0.68
1:A:732:ASP:HB2	1:A:744:ALA:HB2	1.77	0.67
1:A:457:ARG:HH22	1:A:547:ASP:HA	1.61	0.65
1:A:442:ALA:HA	2:A:1151:HOH:O	1.99	0.62
1:A:474:VAL:HG11	1:A:484:LEU:HD21	1.83	0.60
1:A:573:ARG:HG3	1:A:758:ALA:HB2	1.85	0.58
1:A:801:ARG:HH11	1:A:801:ARG:HG3	1.68	0.57
1:A:639:HIS:HD2	1:A:666:ASN:HD22	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:MET:HA	1:A:677:ARG:HH21	1.70	0.57
1:A:620:ALA:HB3	2:A:1353:HOH:O	2.02	0.57
1:A:630:ARG:O	1:A:634:GLU:HG2	2.05	0.57
1:A:668:GLY:HA3	1:A:673:MET:SD	2.45	0.57
1:A:792:PRO:HG2	1:A:795:ARG:HG2	1.86	0.56
1:A:355:ASP:HA	1:A:358:VAL:HG23	1.88	0.56
1:A:585:PRO:O	1:A:591:GLY:HA3	2.07	0.55
1:A:607:VAL:HG22	1:A:823:ILE:HG12	1.90	0.53
1:A:380:LEU:HG	1:A:420:LEU:HD11	1.90	0.53
1:A:688:GLU:HB2	2:A:1331:HOH:O	2.08	0.53
1:A:738:LYS:NZ	1:A:741:ARG:HD3	2.23	0.53
1:A:445:GLU:O	1:A:561:HIS:HD2	1.92	0.52
1:A:616:LEU:HD13	1:A:670:LEU:HD21	1.92	0.52
1:A:813:LEU:HD22	1:A:817:LEU:HD11	1.90	0.52
1:A:768:LEU:HG	1:A:772:LEU:HD22	1.93	0.51
1:A:473:GLU:HB3	1:A:531:LYS:HD3	1.92	0.51
1:A:490:LEU:HD21	1:A:532:ILE:HD12	1.92	0.50
1:A:673:MET:SD	1:A:678:LEU:HD12	2.51	0.50
1:A:715:ARG:HD2	2:A:1333:HOH:O	2.10	0.50
1:A:815:VAL:HG11	2:A:1353:HOH:O	2.12	0.50
1:A:461:LEU:HB3	2:A:1010:HOH:O	2.12	0.50
1:A:763:LEU:HD11	2:A:1237:HOH:O	2.11	0.50
1:A:315:GLU:HB2	1:A:563:ARG:HD2	1.94	0.49
1:A:518:VAL:HG22	1:A:522:LEU:HG	1.94	0.49
1:A:540:LYS:HG2	2:A:1194:HOH:O	2.12	0.49
1:A:667:PHE:HA	1:A:670:LEU:HD12	1.94	0.49
1:A:682:LEU:O	1:A:684:ILE:HG12	2.13	0.49
1:A:550:PRO:O	1:A:553:ILE:HG12	2.14	0.48
1:A:589:PRO:O	1:A:593:ARG:HG2	2.13	0.48
1:A:495:PHE:CZ	1:A:518:VAL:HG11	2.47	0.48
1:A:620:ALA:HB2	1:A:628:LEU:HG	1.95	0.48
1:A:619:LEU:O	1:A:623:SER:HB2	2.13	0.47
1:A:377:ALA:HB2	1:A:416:LEU:HD21	1.96	0.47
1:A:578:ASP:N	2:A:1207:HOH:O	2.45	0.47
1:A:372:ASP:HB3	1:A:375:LEU:HG	1.97	0.47
1:A:617:ARG:HA	2:A:1353:HOH:O	2.15	0.47
1:A:541:LEU:HD23	1:A:590:LEU:HD12	1.97	0.47
1:A:674:SER:OG	1:A:677:ARG:HG3	2.15	0.47
1:A:390:VAL:HG11	2:A:1340:HOH:O	2.15	0.46
1:A:313:ARG:HG2	2:A:1182:HOH:O	2.15	0.46
1:A:306:PHE:HZ	1:A:349:ARG:HH21	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:THR:HG21	1:A:682:LEU:HB2	1.97	0.46
1:A:711:LEU:O	1:A:715:ARG:HG3	2.17	0.45
1:A:661:ALA:O	1:A:665:ILE:HG12	2.17	0.45
1:A:740:VAL:O	1:A:743:ALA:HB3	2.17	0.45
1:A:545:TYR:OH	1:A:583:ASN:HB2	2.18	0.44
1:A:614:ILE:HD11	1:A:760:LEU:HD23	2.00	0.44
1:A:357:SER:OG	1:A:369:PRO:HG3	2.18	0.44
1:A:430:TYR:HA	1:A:434:GLU:HB2	1.99	0.44
1:A:626:GLU:HB3	2:A:1270:HOH:O	2.17	0.44
1:A:315:GLU:CB	1:A:563:ARG:HD2	2.48	0.44
1:A:373:PRO:HA	1:A:376:LEU:HD23	1.99	0.43
1:A:487:ARG:O	1:A:491:GLU:HG3	2.18	0.43
1:A:495:PHE:HZ	1:A:518:VAL:HG11	1.81	0.43
1:A:632:PHE:HB2	1:A:815:VAL:HG13	1.99	0.43
1:A:306:PHE:O	1:A:326:ALA:HA	2.17	0.43
1:A:315:GLU:HG3	1:A:563:ARG:HD2	2.00	0.43
1:A:373:PRO:HB2	2:A:1340:HOH:O	2.19	0.43
1:A:639:HIS:HD2	1:A:666:ASN:ND2	2.17	0.43
1:A:679:SER:HB3	1:A:684:ILE:O	2.19	0.43
1:A:359:LEU:O	1:A:362:ARG:HB3	2.19	0.42
1:A:738:LYS:HZ3	1:A:741:ARG:HD3	1.83	0.42
1:A:519:LEU:HD23	1:A:529:VAL:HG13	2.01	0.42
1:A:437:LEU:HD11	1:A:765:MET:HE3	2.02	0.42
1:A:801:ARG:HG3	1:A:801:ARG:NH1	2.33	0.42
1:A:563:ARG:HH11	1:A:563:ARG:HG2	1.85	0.41
1:A:645:TRP:HB3	1:A:699:SER:OG	2.21	0.41
1:A:595:ARG:NH2	2:A:1225:HOH:O	2.54	0.41
1:A:697:PHE:HB2	2:A:1361:HOH:O	2.21	0.41
1:A:314:LYS:HB3	1:A:315:GLU:H	1.62	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1435:HOH:O	2:A:1439:HOH:H2[1_556]	1.52	0.08

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	530/543 (98%)	477 (90%)	42 (8%)	11 (2%)	7 11

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	517	ALA
1	A	683	ALA
1	A	735	ALA
1	A	514	THR
1	A	612	SER
1	A	654	VAL
1	A	657	LEU
1	A	670	LEU
1	A	650	PRO
1	A	784	HIS
1	A	502	ALA

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	433/444 (98%)	389 (90%)	44 (10%)	7 14

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	315	GLU
1	A	321	LEU
1	A	340	LYS
1	A	343	ARG
1	A	397	GLU
1	A	399	THR
1	A	401	GLU
1	A	421	GLU
1	A	434	GLU
1	A	459	LEU
1	A	477	LEU
1	A	480	HIS
1	A	488	ASP
1	A	490	LEU
1	A	518	VAL
1	A	537	GLU
1	A	540	LYS
1	A	542	LYS
1	A	578	ASP
1	A	582	GLN
1	A	590	LEU
1	A	596	ARG
1	A	613	GLN
1	A	616	LEU
1	A	634	GLU
1	A	641	GLU
1	A	645	TRP
1	A	650	PRO
1	A	671	TYR
1	A	678	LEU
1	A	681	GLU
1	A	682	LEU
1	A	686	TYR
1	A	746	ARG
1	A	750	ASN
1	A	760	LEU
1	A	763	LEU
1	A	772	LEU
1	A	781	LEU
1	A	782	GLN
1	A	783	VAL
1	A	794	GLU
1	A	801	ARG

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Mol	Chain	Res	Type
1	A	818	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	485	ASN
1	A	561	HIS
1	A	639	HIS
1	A	666	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 monosaccharides 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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.