



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:30 AM UTC

PDB ID : 1KTQ / pdb_00001ktq
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 ⓘ 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

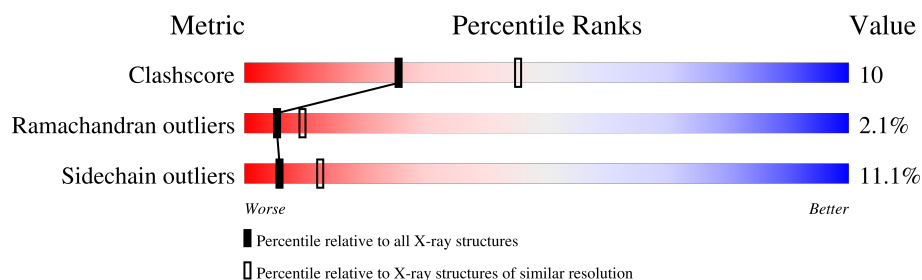
1 Overall quality at a glance

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	543	 62% 30% 6% ..

2 Entry composition

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
1	A	534	Total	C	H	N	O	S	0	0	0
			5182	2698	943	761	767	13			

- Molecule 2 is water.

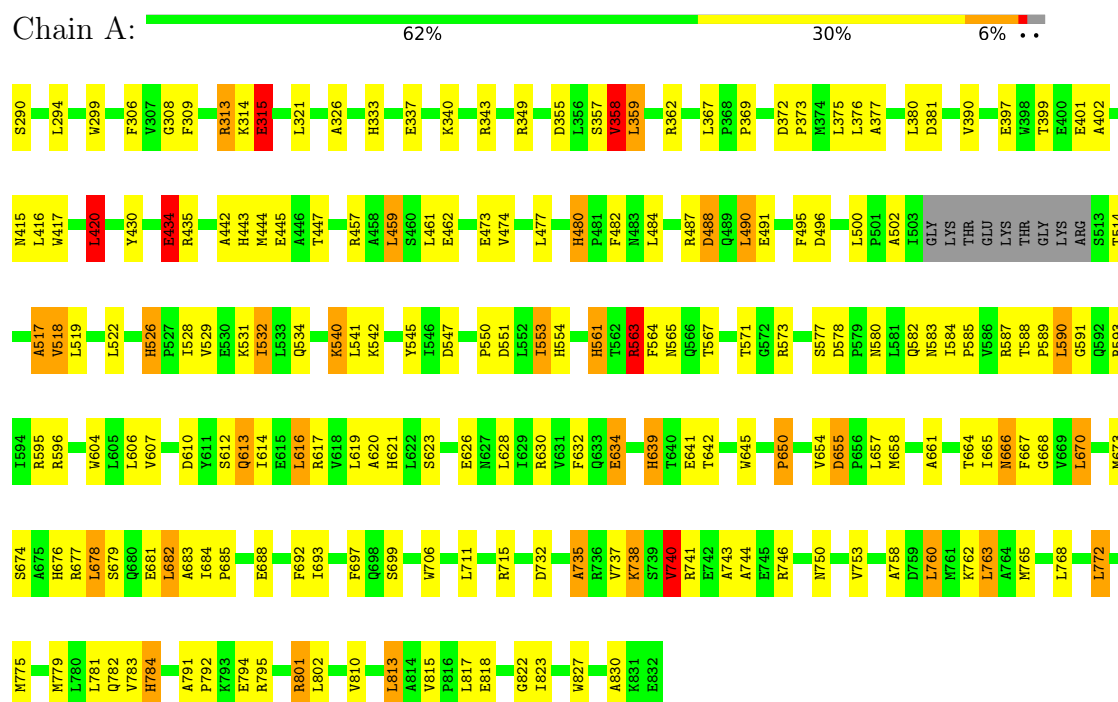
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	440	Total	H	O	0	0
			1320	880	440		

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 I



4 Data and refinement statistics

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

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	0.93	15/4329 (0.3%)	1.75	68/5867 (1.2%)

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

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	740	VAL	CA-CB	6.84	1.63	1.54
1	A	554	HIS	CD2-NE2	-6.81	1.30	1.37
1	A	333	HIS	CD2-NE2	-6.67	1.30	1.37
1	A	480	HIS	CD2-NE2	-6.65	1.30	1.37
1	A	676	HIS	CD2-NE2	-6.58	1.30	1.37
1	A	561	HIS	CD2-NE2	-6.48	1.30	1.37
1	A	621	HIS	CD2-NE2	-6.33	1.30	1.37
1	A	639	HIS	CD2-NE2	-6.20	1.31	1.37
1	A	526	HIS	CD2-NE2	-5.79	1.31	1.37
1	A	443	HIS	CD2-NE2	-5.78	1.31	1.37
1	A	784	HIS	CD2-NE2	-5.30	1.32	1.37
1	A	333	HIS	CG-ND1	-5.11	1.32	1.38
1	A	554	HIS	CG-ND1	-5.06	1.32	1.38
1	A	561	HIS	CG-ND1	-5.00	1.32	1.38
1	A	621	HIS	CG-ND1	-5.00	1.32	1.38

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	420	LEU	N-CA-C	10.50	126.65	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	488	ASP	CA-CB-CG	9.47	122.07	112.60
1	A	692	PHE	CA-CB-CG	-8.85	104.95	113.80
1	A	685	PRO	N-CA-C	7.90	122.90	111.13
1	A	459	LEU	N-CA-C	-7.53	103.70	113.12
1	A	737	VAL	N-CA-C	-7.22	97.03	107.78
1	A	554	HIS	CA-C-N	6.99	127.29	119.32
1	A	554	HIS	C-N-CA	6.99	127.29	119.32
1	A	738	LYS	N-CA-C	6.98	118.89	111.28
1	A	735	ALA	N-CA-C	6.89	125.47	110.80
1	A	526	HIS	CB-CG-CD2	-6.75	122.42	131.20
1	A	565	ASN	OD1-CG-ND2	-6.75	115.85	122.60
1	A	462	GLU	N-CA-C	-6.62	103.69	111.03
1	A	584	ILE	N-CA-C	-6.38	101.31	107.76
1	A	294	LEU	N-CA-C	-6.29	98.15	108.41
1	A	402	ALA	N-CA-C	6.25	118.65	111.02
1	A	554	HIS	CA-C-O	-6.25	114.65	119.46
1	A	358	VAL	CB-CA-C	-6.20	104.06	111.81
1	A	482	PHE	CA-CB-CG	6.18	119.98	113.80
1	A	358	VAL	N-CA-CB	6.17	117.34	110.62
1	A	309	PHE	CA-CB-CG	6.10	119.90	113.80
1	A	337	GLU	CA-C-N	6.00	125.21	118.97
1	A	337	GLU	C-N-CA	6.00	125.21	118.97
1	A	564	PHE	CA-CB-CG	-6.00	107.80	113.80
1	A	381	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	791	ALA	O-C-N	-5.77	117.78	121.88
1	A	313	ARG	N-CA-C	5.76	119.51	111.90
1	A	308	GLY	N-CA-C	-5.66	102.25	110.90
1	A	434	GLU	N-CA-C	5.65	117.13	110.97
1	A	588	THR	CA-C-N	5.62	125.08	119.24
1	A	588	THR	C-N-CA	5.62	125.08	119.24
1	A	417	TRP	CG-CD2-CE3	5.58	139.49	133.90
1	A	551	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	567	THR	N-CA-CB	-5.52	103.53	111.54
1	A	553	ILE	N-CA-C	-5.52	102.46	109.58
1	A	554	HIS	CB-CG-CD2	-5.51	124.04	131.20
1	A	540	LYS	CA-C-O	-5.45	115.10	120.82
1	A	580	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	A	367	LEU	CA-C-N	5.39	123.54	119.66
1	A	367	LEU	C-N-CA	5.39	123.54	119.66
1	A	782	GLN	OE1-CD-NE2	-5.34	117.26	122.60
1	A	517	ALA	N-CA-C	-5.34	99.43	110.80
1	A	299	TRP	N-CA-C	-5.31	102.48	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	496	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	613	GLN	OE1-CD-NE2	-5.26	117.34	122.60
1	A	604	TRP	CG-CD2-CE3	5.24	139.14	133.90
1	A	775	MET	N-CA-C	-5.24	106.79	114.39
1	A	693	ILE	N-CA-C	-5.22	105.40	110.42
1	A	827	TRP	CG-CD2-CE3	5.21	139.11	133.90
1	A	526	HIS	CB-CG-ND1	5.19	130.48	122.70
1	A	810	VAL	N-CA-C	5.18	116.53	110.62
1	A	563	ARG	CG-CD-NE	5.17	123.36	112.00
1	A	613	GLN	CG-CD-NE2	5.16	124.13	116.40
1	A	604	TRP	CE2-CD2-CG	-5.14	101.03	107.20
1	A	571	THR	N-CA-C	5.12	119.22	112.92
1	A	447	THR	CA-CB-OG1	-5.12	101.92	109.60
1	A	443	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	A	587	ARG	CA-CB-CG	-5.09	103.92	114.10
1	A	706	TRP	CE2-CD2-CG	-5.07	101.11	107.20
1	A	610	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	435	ARG	CA-C-N	5.06	124.67	119.05
1	A	435	ARG	C-N-CA	5.06	124.67	119.05
1	A	666	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	A	642	THR	CA-CB-OG1	-5.05	102.03	109.60
1	A	415	ASN	CA-CB-CG	5.04	117.64	112.60
1	A	417	TRP	CE2-CD2-CG	-5.03	101.16	107.20
1	A	577	SER	O-C-N	-5.01	115.99	121.76
1	A	447	THR	N-CA-CB	-5.01	102.74	110.01

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 ⓘ

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	82	0
2	A	440	880	0	17	1
All	All	4679	1823	4273	82	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 10.

All (82) 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:655:ASP:HA	1:A:658:MET:HE3	1.74	0.69
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:444:MET:HE3	1:A:779:MET:HG2	1.78	0.64
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:738:LYS:HZ3	1:A:741:ARG:HD3	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:LYS:HA	1:A:765:MET:HE3	2.02	0.42
1:A:359:LEU:O	1:A:362:ARG:HB3	2.19	0.42
1:A:519:LEU:HD23	1:A:529:VAL:HG13	2.01	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%)	5 9

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

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Mol	Chain	Res	Type
1	A	670	LEU
1	A	650	PRO
1	A	784	HIS
1	A	502	ALA

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	433/444 (98%)	385 (89%)	48 (11%)	6 12

All (48) 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	358	VAL
1	A	359	LEU
1	A	397	GLU
1	A	399	THR
1	A	401	GLU
1	A	420	LEU
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	500	LEU
1	A	518	VAL
1	A	532	ILE
1	A	534	GLN
1	A	542	LYS
1	A	563	ARG

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Mol	Chain	Res	Type
1	A	582	GLN
1	A	590	LEU
1	A	596	ARG
1	A	606	LEU
1	A	613	GLN
1	A	616	LEU
1	A	634	GLU
1	A	641	GLU
1	A	650	PRO
1	A	678	LEU
1	A	681	GLU
1	A	682	LEU
1	A	740	VAL
1	A	746	ARG
1	A	750	ASN
1	A	753	VAL
1	A	760	LEU
1	A	763	LEU
1	A	772	LEU
1	A	781	LEU
1	A	783	VAL
1	A	794	GLU
1	A	801	ARG
1	A	802	LEU
1	A	813	LEU
1	A	818	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	443	HIS
1	A	485	ASN
1	A	534	GLN
1	A	561	HIS
1	A	639	HIS

5.3.3 RNA ⓘ

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](#)

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.