



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:52 AM UTC

PDB ID : 1ECL / pdb_00001ecl
Title : AMINO TERMINAL 67KDA DOMAIN OF ESCHERICHIA COLI DNA TOPOISOMERASE I (RESIDUES 2-590 OF MATURE PROTEIN) CLONING ARTIFACT ADDS TWO RESIDUES TO THE AMINO-TERMINUS WHICH WERE NOT OBSERVED IN THE EXPERIMENTAL ELECTRON DENSITY (GLY-2, SER-1).
Authors : Lima, C.D.; Wang, J.C.; Mondragon, A.
Deposited on : 1995-05-05
Resolution : 1.90 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

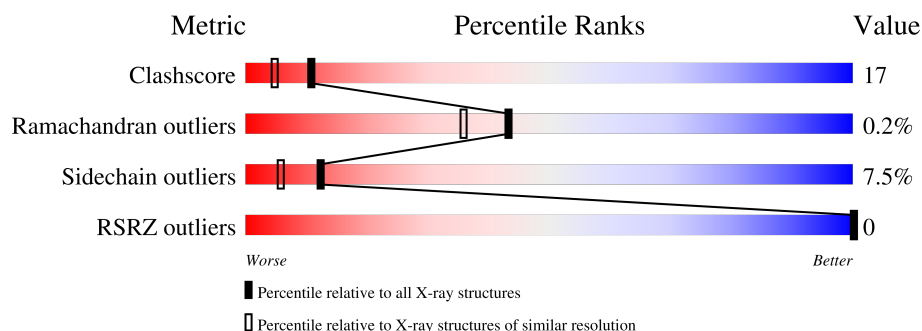
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	597	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4939 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 ESCHERICHIA COLI TOPOISOMERASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4403	2772	785	829	17			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	359	GLY	GLU	conflict	UNP P06612

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	536	Total	O	0	0
			536	536		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.19Å 77.97Å 138.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 1.90 5.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	83.4 (5.00-1.90) 78.8 (5.00-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.56 (at 1.70Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.218 , (Not available) 0.212 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	1.16 , 165.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4939	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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	1.00	5/4489 (0.1%)	1.22	33/6064 (0.5%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	MET	SD-CE	-5.77	1.65	1.79
1	A	501	ILE	CA-CB	5.34	1.60	1.54
1	A	334	MET	SD-CE	5.29	1.92	1.79
1	A	31	VAL	CA-CB	5.16	1.61	1.54
1	A	512	VAL	CA-CB	5.02	1.60	1.54

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	ILE	N-CA-C	12.17	122.03	111.56
1	A	152	ASN	N-CA-C	-8.85	100.61	111.40
1	A	478	SER	N-CA-C	-7.80	98.72	109.95
1	A	145	ASN	N-CA-C	7.58	119.63	111.36
1	A	590	ASN	N-CA-C	7.42	131.78	111.00
1	A	285	ILE	N-CA-C	-7.22	98.25	108.80
1	A	350	GLU	N-CA-C	-7.14	103.42	111.14
1	A	72	GLY	N-CA-C	-7.06	105.58	115.32
1	A	465	THR	CA-C-N	6.82	126.80	119.78
1	A	465	THR	C-N-CA	6.82	126.80	119.78
1	A	64	ARG	N-CA-C	-6.37	96.52	107.61
1	A	420	PHE	N-CA-C	6.30	120.32	110.17
1	A	112	LEU	N-CA-C	6.23	120.14	112.54
1	A	213	ALA	N-CA-C	6.19	120.69	113.20
1	A	33	HIS	N-CA-C	6.16	120.80	113.28
1	A	560	TRP	N-CA-C	6.12	118.45	111.11
1	A	34	ILE	N-CA-C	6.10	122.03	109.34
1	A	78	ASN	N-CA-C	5.98	119.67	111.54
1	A	432	ASP	N-CA-C	5.74	117.54	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	PHE	N-CA-C	5.74	118.16	110.35
1	A	7	ILE	N-CA-C	5.47	115.73	107.80
1	A	473	PRO	CA-C-N	5.44	125.45	119.90
1	A	473	PRO	C-N-CA	5.44	125.45	119.90
1	A	589	PRO	CA-C-N	5.26	131.18	121.70
1	A	589	PRO	C-N-CA	5.26	131.18	121.70
1	A	574	GLN	N-CA-C	-5.20	105.51	111.07
1	A	229	PRO	N-CA-C	-5.15	106.69	113.65
1	A	515	ARG	NE-CZ-NH2	-5.12	114.59	119.20
1	A	134	TYR	N-CA-C	5.10	118.06	109.95
1	A	581	ASP	N-CA-C	-5.10	102.74	110.39
1	A	187	ILE	CB-CA-C	-5.09	106.60	111.44
1	A	406	ALA	N-CA-C	-5.05	103.01	110.48
1	A	462	VAL	CB-CA-C	-5.01	105.79	111.55

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	4403	0	4378	146	0
2	A	536	0	0	30	0
All	All	4939	0	4378	146	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 17.

All (146) 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:302:LYS:HD3	1:A:302:LYS:H	1.26	1.00
1:A:516:ARG:HD3	2:A:603:HOH:O	1.64	0.97
1:A:334:MET:SD	1:A:373:VAL:HG23	2.07	0.93
1:A:28:LYS:HE2	1:A:99:LEU:HD11	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ASN:HA	2:A:962:HOH:O	1.79	0.83
1:A:580:LYS:HB3	1:A:584:GLU:HG3	1.59	0.83
1:A:410:SER:HB3	1:A:425:ARG:NH2	1.97	0.79
1:A:539:ASN:HD22	1:A:542:PHE:H	1.28	0.78
1:A:3:LYS:HD3	1:A:26:VAL:HG23	1.65	0.77
1:A:13:LYS:HG3	1:A:313:GLU:HG2	1.65	0.77
1:A:164:ALA:HA	2:A:1028:HOH:O	1.85	0.74
1:A:189:ARG:HH11	1:A:189:ARG:HG3	1.53	0.73
1:A:197:GLN:HG2	1:A:503:THR:HG21	1.69	0.73
1:A:396:ARG:HD3	2:A:663:HOH:O	1.87	0.73
1:A:189:ARG:HH11	1:A:189:ARG:CG	2.01	0.72
1:A:240:HIS:HB2	1:A:421:ARG:HB3	1.74	0.70
1:A:145:ASN:O	1:A:149:GLN:HG3	1.92	0.70
1:A:35:ARG:HE	1:A:122:HIS:HD2	1.39	0.70
1:A:548:ASN:O	1:A:552:GLN:HG3	1.93	0.69
1:A:346:LYS:HD3	1:A:346:LYS:H	1.57	0.69
1:A:423:LYS:HE3	2:A:1018:HOH:O	1.92	0.68
1:A:521:LYS:N	1:A:521:LYS:HE3	2.08	0.68
1:A:220:TRP:CZ2	1:A:251:LYS:HG2	2.32	0.65
1:A:410:SER:HB3	1:A:425:ARG:HH22	1.60	0.65
1:A:35:ARG:HE	1:A:122:HIS:CD2	2.15	0.65
1:A:250:ASN:ND2	1:A:253:GLN:H	1.94	0.65
1:A:263:LYS:HE3	2:A:645:HOH:O	1.95	0.64
1:A:277:THR:HG22	1:A:407:LYS:HD2	1.79	0.64
1:A:521:LYS:H	1:A:521:LYS:CE	2.12	0.63
1:A:152:ASN:O	1:A:154:PRO:HD3	1.98	0.63
1:A:34:ILE:HD11	1:A:92:VAL:HG11	1.81	0.63
1:A:478:SER:HB3	1:A:516:ARG:HH11	1.64	0.63
1:A:302:LYS:H	1:A:302:LYS:CD	2.08	0.62
1:A:197:GLN:HG2	1:A:503:THR:CG2	2.29	0.62
1:A:381:LYS:HG3	1:A:382:ASP:N	2.15	0.62
1:A:527:THR:O	1:A:531:GLU:HG3	2.00	0.61
1:A:34:ILE:CD1	1:A:92:VAL:HG11	2.30	0.61
1:A:302:LYS:HD3	1:A:302:LYS:N	2.07	0.61
1:A:3:LYS:HD3	1:A:26:VAL:CG2	2.30	0.61
1:A:273:ASP:HB3	2:A:632:HOH:O	1.99	0.61
1:A:434:TRP:O	1:A:437:VAL:HG22	2.01	0.60
1:A:189:ARG:HG3	1:A:189:ARG:NH1	2.17	0.60
1:A:407:LYS:HE3	2:A:1019:HOH:O	2.01	0.59
1:A:299:PHE:CE2	1:A:307:MET:HE1	2.38	0.59
1:A:98:GLN:O	1:A:101:GLU:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:THR:OG1	1:A:425:ARG:NH1	2.37	0.57
1:A:122:HIS:HE1	2:A:708:HOH:O	1.86	0.57
1:A:202:ARG:O	1:A:206:GLU:HG3	2.05	0.57
1:A:184:TRP:HB3	1:A:189:ARG:NE	2.20	0.56
1:A:220:TRP:CH2	1:A:251:LYS:HG2	2.41	0.56
1:A:382:ASP:HB2	1:A:383:MET:HE2	1.87	0.55
1:A:167:ALA:HB3	2:A:1028:HOH:O	2.06	0.55
1:A:521:LYS:HE3	1:A:521:LYS:H	1.70	0.55
1:A:392:GLN:HG3	2:A:979:HOH:O	2.07	0.54
1:A:533:ASN:HD21	1:A:587:MET:HA	1.72	0.54
1:A:250:ASN:HD21	1:A:253:GLN:H	1.54	0.54
1:A:345:LYS:HG2	2:A:1058:HOH:O	2.07	0.54
1:A:184:TRP:HB3	1:A:189:ARG:CZ	2.38	0.53
1:A:533:ASN:ND2	1:A:587:MET:HA	2.23	0.53
1:A:349:PRO:HB2	1:A:351:SER:O	2.08	0.53
1:A:4:ALA:HB1	1:A:107:TYR:HE1	1.74	0.53
1:A:279:LYS:HE2	2:A:1105:HOH:O	2.07	0.53
1:A:287:SER:O	1:A:291:GLN:HG3	2.09	0.53
1:A:296:ARG:NE	1:A:296:ARG:HA	2.24	0.53
1:A:4:ALA:HB1	1:A:107:TYR:CE1	2.44	0.52
1:A:346:LYS:H	1:A:346:LYS:CD	2.21	0.52
1:A:536:GLU:HG3	1:A:542:PHE:CD2	2.45	0.52
1:A:583:GLU:H	1:A:583:GLU:CD	2.17	0.51
1:A:374:ASN:ND2	2:A:909:HOH:O	2.43	0.51
1:A:552:GLN:NE2	2:A:676:HOH:O	2.44	0.51
1:A:535:ARG:HD2	2:A:1124:HOH:O	2.09	0.51
1:A:16:THR:HG22	1:A:142:ILE:CG2	2.42	0.50
1:A:580:LYS:HB3	1:A:584:GLU:CG	2.38	0.50
1:A:63:GLU:CG	1:A:64:ARG:N	2.75	0.49
1:A:513:GLU:HG3	1:A:518:TYR:CE1	2.48	0.49
1:A:95:GLU:O	1:A:99:LEU:HG	2.13	0.48
1:A:407:LYS:HB3	1:A:430:ARG:NH1	2.28	0.48
1:A:400:ALA:HB2	1:A:437:VAL:HG21	1.94	0.48
1:A:407:LYS:CB	1:A:430:ARG:HD2	2.44	0.48
1:A:521:LYS:H	1:A:521:LYS:NZ	2.11	0.48
1:A:114:ARG:HH22	1:A:551:ASP:HA	1.79	0.48
1:A:382:ASP:HB3	2:A:702:HOH:O	2.13	0.48
1:A:381:LYS:HG3	1:A:382:ASP:H	1.77	0.47
1:A:282:ALA:HB1	1:A:283:PRO:HD2	1.96	0.47
1:A:187:ILE:HD11	1:A:529:ARG:HG3	1.96	0.47
1:A:13:LYS:O	1:A:17:ILE:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LYS:HE2	1:A:212:LYS:HB2	1.69	0.47
1:A:354:GLN:HB2	2:A:1075:HOH:O	2.14	0.46
1:A:493:ARG:HA	1:A:493:ARG:HD2	1.71	0.46
1:A:36:ASP:OD1	1:A:169:ARG:NH1	2.49	0.46
1:A:37:LEU:HB3	1:A:38:PRO:HD2	1.97	0.46
1:A:34:ILE:HG12	2:A:940:HOH:O	2.16	0.46
1:A:121:TRP:CD1	2:A:1072:HOH:O	2.68	0.46
1:A:91:LYS:HE2	2:A:943:HOH:O	2.15	0.46
1:A:16:THR:HG22	1:A:142:ILE:HG21	1.98	0.46
1:A:306:MET:HE2	1:A:310:ARG:HE	1.81	0.45
1:A:413:LEU:O	1:A:423:LYS:HD3	2.16	0.45
1:A:35:ARG:HD3	1:A:126:VAL:HG22	1.97	0.45
1:A:228:THR:HB	1:A:229:PRO:CD	2.46	0.45
1:A:181:PRO:HA	1:A:184:TRP:CE3	2.52	0.45
1:A:410:SER:CB	1:A:425:ARG:HH22	2.27	0.45
1:A:103:ALA:O	1:A:133:ARG:NH2	2.40	0.45
1:A:533:ASN:ND2	2:A:686:HOH:O	2.49	0.45
1:A:484:LYS:NZ	2:A:1056:HOH:O	2.48	0.45
1:A:512:VAL:HA	1:A:516:ARG:O	2.17	0.44
1:A:403:MET:SD	1:A:437:VAL:HG13	2.57	0.44
1:A:187:ILE:O	1:A:188:ALA:HB2	2.18	0.44
1:A:407:LYS:HB3	1:A:430:ARG:HH11	1.83	0.44
1:A:236:LEU:HD23	1:A:424:ALA:HB2	1.99	0.44
1:A:570:ASP:HB2	2:A:1040:HOH:O	2.18	0.44
1:A:269:LEU:O	1:A:455:LYS:HD2	2.17	0.43
1:A:8:VAL:O	1:A:29:SER:HA	2.18	0.43
1:A:93:VAL:HG13	1:A:126:VAL:CG1	2.47	0.43
1:A:229:PRO:HD2	2:A:809:HOH:O	2.18	0.43
1:A:169:ARG:HE	1:A:169:ARG:HB2	1.35	0.43
1:A:254:THR:O	1:A:258:VAL:HG23	2.19	0.43
1:A:189:ARG:N	1:A:189:ARG:HD2	2.34	0.43
1:A:533:ASN:HB3	1:A:578:ALA:HB2	2.00	0.43
1:A:30:SER:HB2	1:A:34:ILE:HD11	2.00	0.43
1:A:93:VAL:HG13	1:A:126:VAL:HG12	2.00	0.43
1:A:220:TRP:CZ2	1:A:251:LYS:CG	3.00	0.43
1:A:306:MET:HG2	2:A:772:HOH:O	2.18	0.43
1:A:380:LEU:HD11	1:A:391:TYR:CG	2.53	0.43
1:A:407:LYS:HB2	1:A:430:ARG:HD2	2.01	0.43
1:A:180:SER:HB2	1:A:181:PRO:HD3	2.01	0.42
1:A:306:MET:HE2	1:A:310:ARG:NE	2.33	0.42
1:A:68:VAL:HG12	2:A:679:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:GLY:N	1:A:102:LYS:O	2.53	0.42
1:A:309:GLN:NE2	2:A:1065:HOH:O	2.52	0.42
1:A:279:LYS:NZ	2:A:1118:HOH:O	2.52	0.42
1:A:35:ARG:HD3	1:A:126:VAL:CG2	2.50	0.42
1:A:228:THR:OG1	1:A:232:GLU:HB2	2.20	0.42
1:A:454:ASN:O	1:A:457:ASP:HB2	2.19	0.42
1:A:465:THR:HA	1:A:466:PRO:HD3	1.86	0.42
1:A:521:LYS:N	1:A:521:LYS:CE	2.75	0.42
1:A:194:GLY:HA3	1:A:197:GLN:HB2	2.01	0.41
1:A:228:THR:HB	1:A:229:PRO:HD2	2.02	0.41
1:A:432:ASP:OD1	1:A:433:GLY:N	2.53	0.41
1:A:319:TYR:CE1	1:A:320:MET:HE2	2.56	0.41
1:A:182:LEU:HD21	1:A:578:ALA:HB1	2.03	0.41
1:A:250:ASN:HD22	1:A:250:ASN:C	2.28	0.41
1:A:171:MET:HE2	1:A:171:MET:HB3	1.85	0.41
1:A:488:LYS:HE3	1:A:488:LYS:HB2	1.43	0.41
1:A:515:ARG:NH2	2:A:754:HOH:O	2.38	0.41
1:A:13:LYS:HG3	1:A:313:GLU:CG	2.42	0.40
1:A:13:LYS:CG	1:A:313:GLU:HG2	2.44	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	544/597 (91%)	526 (97%)	17 (3%)	1 (0%)	43	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	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	468/505 (93%)	433 (92%)	35 (8%)	12 6

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	31	VAL
1	A	33	HIS
1	A	64	ARG
1	A	67	LEU
1	A	78	ASN
1	A	80	GLU
1	A	84	GLU
1	A	85	VAL
1	A	101	GLU
1	A	130	ASP
1	A	135	SER
1	A	173	ARG
1	A	181	PRO
1	A	189	ARG
1	A	227	THR
1	A	237	GLN
1	A	250	ASN
1	A	302	LYS
1	A	320	MET
1	A	346	LYS
1	A	354	GLN
1	A	382	ASP
1	A	425	ARG
1	A	428	ILE
1	A	436	LYS
1	A	441	LEU
1	A	472	LYS
1	A	473	PRO
1	A	481	SER

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Mol	Chain	Res	Type
1	A	503	THR
1	A	521	LYS
1	A	535	ARG
1	A	581	ASP
1	A	583	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	69	ASN
1	A	78	ASN
1	A	98	GLN
1	A	122	HIS
1	A	152	ASN
1	A	165	GLN
1	A	250	ASN
1	A	309	GLN
1	A	354	GLN
1	A	374	ASN
1	A	392	GLN
1	A	454	ASN
1	A	505	GLN
1	A	533	ASN
1	A	539	ASN
1	A	548	ASN
1	A	552	GLN
1	A	590	ASN

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 oligosaccharides 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 [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	552/597 (92%)	-0.70	0 100 100	17, 29, 40, 47	0

There are no RSRZ outliers to report.

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.