



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:15 PM UTC

PDB ID : 3DU6 / pdb_00003du6
Title : Structure of the catalytic subunit of telomerase, TERT
Authors : Skordalakes, E.
Deposited on : 2008-07-16
Resolution : 2.71 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

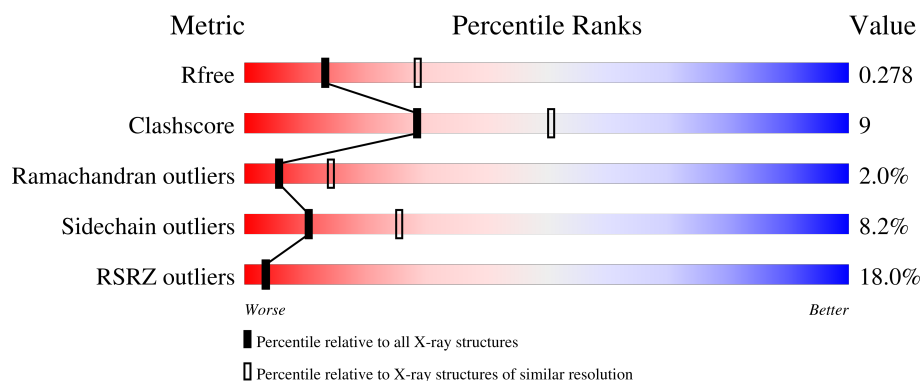
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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))
R_{free}	180053	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	596	14% 72% 23% .
1	B	596	21% 76% 20% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10319 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 Telomerase reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	0	0
			4982	3266	852	842	22			
1	B	596	Total	C	N	O	S	0	0	0
			4982	3266	852	842	22			

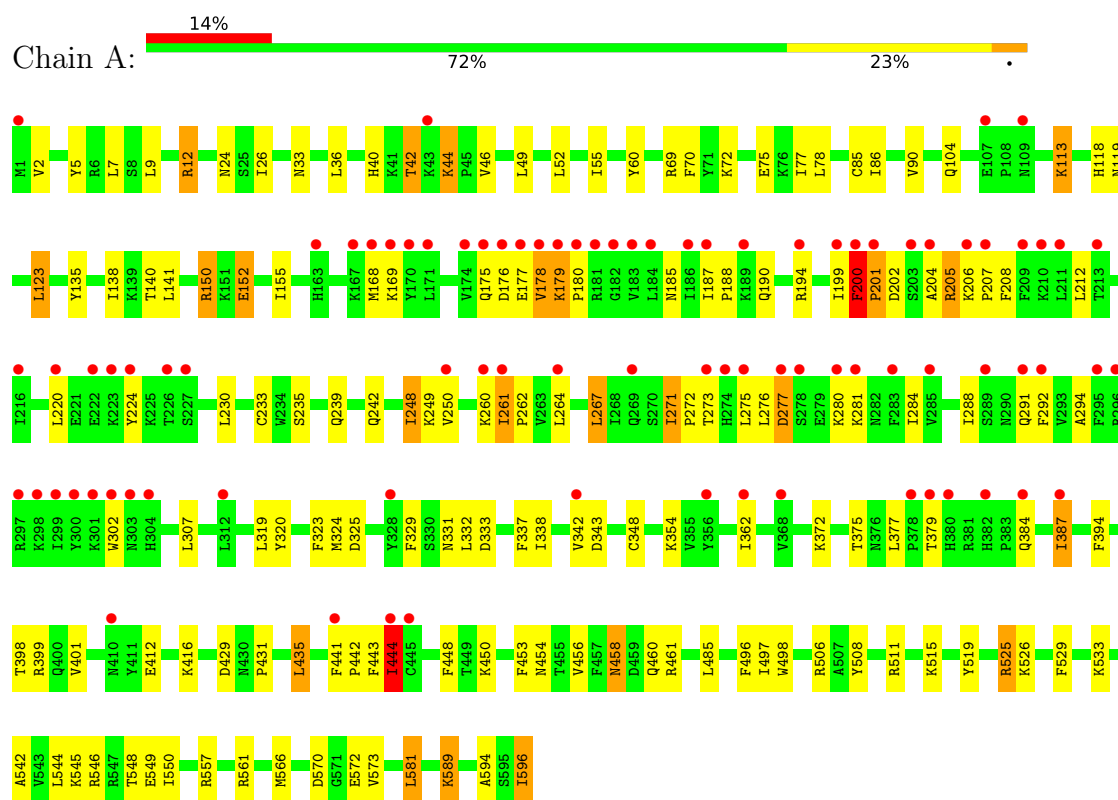
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	180	Total	O	0	0
			180	180		
2	B	175	Total	O	0	0
			175	175		

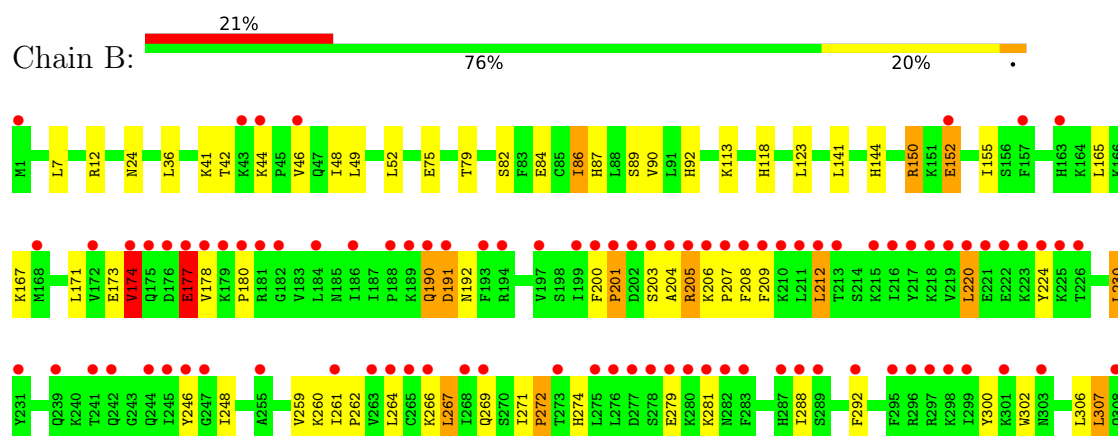
3 Residue-property plots [i](#)

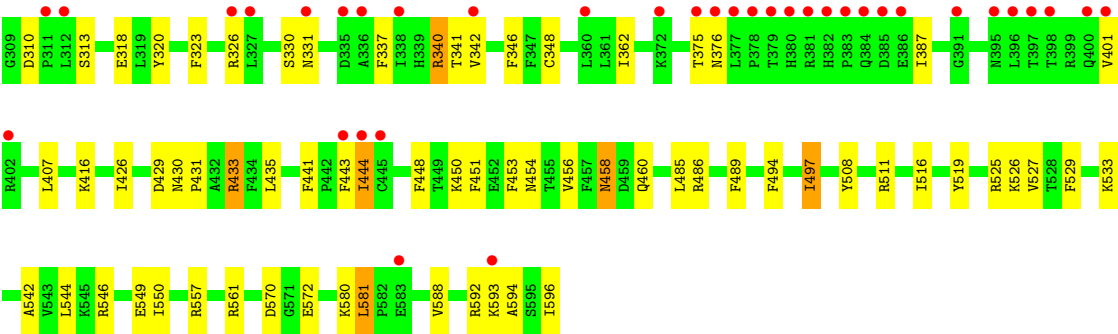
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Telomerase reverse transcriptase



• Molecule 1: Telomerase reverse transcriptase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.04Å 122.66Å 212.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.71 20.00 – 2.71	Depositor EDS
% Data completeness (in resolution range)	97.0 (20.00-2.71) 96.7 (20.00-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.238 , 0.278 0.242 , 0.278	Depositor DCC
R_{free} test set	3023 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 76.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10319	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.69 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0687e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [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	0.49	1/5114 (0.0%)	0.74	1/6893 (0.0%)
1	B	0.49	1/5114 (0.0%)	0.72	0/6893
All	All	0.49	2/10228 (0.0%)	0.73	1/13786 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	177	GLU	C-N	6.46	1.42	1.33
1	A	261	ILE	CA-CB	5.21	1.57	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	VAL	N-CA-C	5.52	114.69	106.85

There are no chirality outliers.

There are no planarity outliers.

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	4982	0	5126	97	0
1	B	4982	0	5126	80	0
2	A	180	0	0	6	0
2	B	175	0	0	5	0
All	All	10319	0	10252	177	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 9.

All (177) 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:B:444:ILE:HD13	1:B:444:ILE:H	1.20	1.05
1:A:24:ASN:H	1:A:118:HIS:HE1	1.05	0.97
1:B:24:ASN:H	1:B:118:HIS:HE1	1.16	0.91
1:A:401:VAL:H	1:A:458:ASN:HD21	1.20	0.89
1:A:178:VAL:O	1:A:178:VAL:HG12	1.72	0.89
1:A:177:GLU:HG2	1:A:178:VAL:H	1.39	0.87
1:A:511:ARG:HD3	2:A:715:HOH:O	1.76	0.85
1:A:200:PHE:H	1:A:201:PRO:HA	1.40	0.84
1:A:460:GLN:HE22	1:A:526:LYS:H	1.25	0.83
1:A:24:ASN:H	1:A:118:HIS:CE1	1.96	0.81
1:B:326:ARG:HA	1:B:330:SER:HB3	1.62	0.81
1:A:549:GLU:HG2	1:A:550:ILE:H	1.44	0.80
1:B:84:GLU:OE2	1:B:592:ARG:NH2	2.17	0.78
1:B:401:VAL:H	1:B:458:ASN:HD21	1.33	0.76
1:A:177:GLU:HG2	1:A:178:VAL:N	2.02	0.74
1:B:460:GLN:HE22	1:B:526:LYS:H	1.36	0.74
1:A:272:PRO:HG2	1:A:275:LEU:HD12	1.69	0.73
1:A:206:LYS:N	1:A:207:PRO:HD2	2.06	0.71
1:A:444:ILE:HD11	1:A:508:TYR:HE2	1.56	0.70
1:A:9:LEU:O	1:A:12:ARG:HB3	1.91	0.70
1:B:542:ALA:HB1	1:B:581:LEU:HD13	1.73	0.69
1:B:24:ASN:H	1:B:118:HIS:CE1	2.04	0.69
1:B:444:ILE:HD13	1:B:444:ILE:N	2.03	0.69
1:A:200:PHE:N	1:A:201:PRO:HA	2.08	0.69
1:B:454:ASN:HD22	1:B:456:VAL:H	1.41	0.69
1:A:179:LYS:N	1:A:180:PRO:HD3	2.09	0.68
1:B:220:LEU:O	1:B:224:TYR:HB2	1.94	0.68
1:A:69:ARG:HD2	2:A:774:HOH:O	1.93	0.68
1:A:549:GLU:HG2	1:A:550:ILE:N	2.09	0.67
1:A:454:ASN:HD22	1:A:456:VAL:H	1.43	0.67
1:B:46:VAL:HG22	1:B:150:ARG:HH12	1.59	0.66
1:B:84:GLU:CD	1:B:592:ARG:HH22	2.03	0.66
1:A:248:ILE:HD12	1:A:375:THR:HB	1.76	0.65
1:A:448:PHE:HA	1:A:453:PHE:HE1	1.62	0.65
1:A:72:LYS:HA	1:A:72:LYS:HE2	1.78	0.65
1:B:310:ASP:HB3	1:B:313:SER:HB2	1.79	0.65
1:B:200:PHE:N	1:B:201:PRO:HA	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:ARG:HE	1:A:561:ARG:NH1	1.97	0.63
1:A:177:GLU:CG	1:A:178:VAL:H	2.11	0.62
1:B:269:GLN:HE21	1:B:281:LYS:HB3	1.66	0.61
1:B:340:ARG:HG2	1:B:341:THR:N	2.17	0.60
1:A:461:ARG:HD2	1:A:573:VAL:HA	1.85	0.59
1:B:208:PHE:O	1:B:212:LEU:HB2	2.02	0.58
1:B:173:GLU:HA	1:B:300:TYR:HA	1.85	0.58
1:B:200:PHE:H	1:B:201:PRO:HA	1.69	0.58
1:B:549:GLU:HG2	1:B:550:ILE:N	2.19	0.58
1:A:325:ASP:HB3	2:A:722:HOH:O	2.04	0.57
1:B:444:ILE:H	1:B:444:ILE:CD1	2.03	0.57
1:A:416:LYS:HD2	2:A:700:HOH:O	2.05	0.56
1:A:337:PHE:HB3	1:A:348:CYS:HB2	1.87	0.55
1:B:220:LEU:HD11	1:B:318:GLU:HB2	1.89	0.55
1:A:333:ASP:HB2	1:A:354:LYS:HD3	1.89	0.55
1:B:443:PHE:HD2	2:B:771:HOH:O	1.88	0.55
1:A:284:ILE:O	1:A:288:ILE:HG12	2.08	0.54
1:A:75:GLU:HG3	1:A:594:ALA:HB2	1.90	0.54
1:A:267:LEU:HD11	1:A:323:PHE:HB2	1.90	0.54
1:B:527:VAL:HA	2:B:639:HOH:O	2.07	0.54
1:A:7:LEU:HD22	1:A:77:ILE:HG13	1.89	0.54
1:A:261:ILE:HG23	1:A:288:ILE:HG22	1.90	0.53
1:A:205:ARG:HB3	1:A:207:PRO:HG2	1.90	0.53
1:A:113:LYS:H	1:A:113:LYS:HD2	1.73	0.53
1:B:549:GLU:HG2	1:B:550:ILE:HG13	1.91	0.53
1:A:460:GLN:HE22	1:A:526:LYS:N	2.03	0.53
1:A:444:ILE:HD11	1:A:508:TYR:CE2	2.41	0.53
1:B:561:ARG:HD3	2:B:720:HOH:O	2.09	0.53
1:A:529:PHE:CE2	1:A:533:LYS:HD3	2.44	0.52
1:B:460:GLN:NE2	1:B:525:ARG:H	2.06	0.52
1:A:70:PHE:CZ	1:A:123:LEU:HD13	2.44	0.52
1:A:435:LEU:HG	1:A:485:LEU:HD11	1.92	0.52
1:B:82:SER:HB2	1:B:144:HIS:HB3	1.91	0.52
1:A:205:ARG:O	1:A:208:PHE:HB3	2.09	0.51
1:A:271:ILE:HD11	1:A:276:LEU:HB2	1.91	0.51
1:B:431:PRO:HB3	1:B:485:LEU:HD22	1.92	0.51
1:B:429:ASP:C	1:B:431:PRO:HD3	2.35	0.51
1:A:187:ILE:HG21	1:A:194:ARG:HH21	1.75	0.51
1:A:460:GLN:NE2	1:A:525:ARG:H	2.09	0.50
1:B:494:PHE:HD2	1:B:497:ILE:HD13	1.76	0.50
1:A:200:PHE:H	1:A:201:PRO:CA	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:PHE:HB3	1:B:348:CYS:HB2	1.93	0.50
1:B:441:PHE:HB2	1:B:511:ARG:CZ	2.42	0.50
1:A:431:PRO:HB3	1:A:485:LEU:HD22	1.93	0.50
1:A:235:SER:O	1:A:239:GLN:HG2	2.12	0.49
1:B:448:PHE:HA	1:B:453:PHE:HE1	1.77	0.49
1:B:246:TYR:HA	1:B:376:ASN:HD21	1.77	0.49
1:A:204:ALA:O	1:A:205:ARG:HB2	2.13	0.49
1:A:387:ILE:H	1:A:387:ILE:HD13	1.78	0.49
1:A:208:PHE:O	1:A:212:LEU:HB2	2.13	0.48
1:A:325:ASP:HA	1:A:329:PHE:HD1	1.78	0.48
1:A:264:LEU:HD13	1:A:320:TYR:HB2	1.96	0.48
1:A:431:PRO:HB2	1:A:496:PHE:CZ	2.47	0.48
1:B:516:ILE:HG21	1:B:527:VAL:HG21	1.93	0.48
1:B:204:ALA:H	1:B:209:PHE:HE2	1.62	0.48
1:B:443:PHE:CD2	1:B:444:ILE:HD12	2.49	0.48
1:B:450:LYS:HG2	1:B:519:TYR:CZ	2.48	0.48
1:B:262:PRO:O	1:B:266:LYS:HG2	2.14	0.48
1:A:448:PHE:HA	1:A:453:PHE:CE1	2.47	0.47
1:B:201:PRO:C	1:B:203:SER:H	2.23	0.47
1:A:450:LYS:HG2	1:A:519:TYR:CZ	2.50	0.47
1:A:5:TYR:O	1:A:85:CYS:HB3	2.14	0.47
1:B:529:PHE:CE2	1:B:533:LYS:HD3	2.50	0.47
1:A:46:VAL:HG22	1:A:150:ARG:HH12	1.80	0.46
1:A:140:THR:O	1:A:141:LEU:HB2	2.15	0.46
1:A:498:TRP:CD2	1:A:557:ARG:HD3	2.50	0.46
1:B:259:VAL:HG21	1:B:306:LEU:HD12	1.97	0.46
1:A:545:LYS:O	1:A:548:THR:HG23	2.15	0.46
1:A:377:LEU:C	1:A:379:THR:H	2.24	0.46
1:A:546:ARG:HD2	1:A:581:LEU:HD21	1.98	0.46
1:B:346:PHE:CE1	1:B:387:ILE:HG21	2.51	0.46
1:A:206:LYS:N	1:A:207:PRO:CD	2.78	0.46
1:A:42:THR:HB	1:A:44:LYS:HG2	1.98	0.46
1:B:267:LEU:HD11	1:B:323:PHE:HB2	1.98	0.46
1:B:596:ILE:C	2:B:698:HOH:O	2.58	0.46
1:A:398:THR:O	1:A:399:ARG:HB2	2.17	0.45
1:A:271:ILE:HD11	1:A:276:LEU:CB	2.46	0.45
1:A:291:GLN:HB2	1:A:302:TRP:HB3	1.99	0.45
1:A:515:LYS:HE2	2:A:721:HOH:O	2.16	0.45
1:B:89:SER:HA	1:B:92:HIS:CE1	2.52	0.45
1:B:79:THR:OG1	1:B:592:ARG:HD3	2.17	0.45
1:B:444:ILE:HD11	1:B:508:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:GLU:H	1:B:152:GLU:CD	2.23	0.44
1:A:444:ILE:CD1	1:A:508:TYR:HE2	2.29	0.44
1:B:190:GLN:C	1:B:192:ASN:H	2.26	0.44
1:B:433:ARG:NH1	2:B:597:HOH:O	2.51	0.44
1:B:546:ARG:HD2	1:B:581:LEU:HD21	1.99	0.44
1:A:178:VAL:O	1:A:178:VAL:CG1	2.46	0.44
1:A:138:ILE:HD13	1:A:188:PRO:HG2	1.98	0.43
1:A:152:GLU:H	1:A:152:GLU:CD	2.26	0.43
1:B:203:SER:HB3	1:B:209:PHE:CE2	2.53	0.43
1:B:206:LYS:N	1:B:207:PRO:HD2	2.33	0.43
1:B:460:GLN:HE22	1:B:526:LYS:N	2.11	0.43
1:A:273:THR:O	1:A:277:ASP:HB3	2.18	0.43
1:A:441:PHE:N	1:A:442:PRO:CD	2.82	0.43
1:B:205:ARG:NE	1:B:205:ARG:HA	2.33	0.43
1:B:444:ILE:HD11	1:B:508:TYR:OH	2.18	0.43
1:A:220:LEU:O	1:A:224:TYR:HB2	2.19	0.43
1:A:180:PRO:HB3	1:A:294:ALA:HB2	1.99	0.43
1:A:443:PHE:CE1	1:A:444:ILE:HG23	2.54	0.43
1:B:272:PRO:HB3	1:B:274:HIS:NE2	2.33	0.43
1:A:60:TYR:OH	1:A:119:ASN:ND2	2.52	0.43
1:A:429:ASP:C	1:A:431:PRO:HD3	2.43	0.43
1:A:179:LYS:H	1:A:180:PRO:HD3	1.84	0.42
1:B:261:ILE:HD12	1:B:261:ILE:H	1.84	0.42
1:B:458:ASN:HD22	1:B:458:ASN:HA	1.62	0.42
1:A:233:CYS:HB3	1:A:337:PHE:CE1	2.55	0.42
1:B:75:GLU:HG3	1:B:594:ALA:HB2	2.00	0.42
1:B:261:ILE:HG23	1:B:288:ILE:HG22	2.01	0.42
1:B:549:GLU:HG2	1:B:550:ILE:H	1.85	0.42
1:A:337:PHE:C	1:A:338:ILE:HG13	2.45	0.42
1:A:542:ALA:HB1	1:A:581:LEU:HD13	2.02	0.42
1:A:261:ILE:HB	1:A:262:PRO:HD3	2.02	0.42
1:A:441:PHE:HB2	1:A:511:ARG:CZ	2.49	0.42
1:B:174:VAL:HB	1:B:177:GLU:HG3	2.02	0.42
1:B:426:ILE:HG12	1:B:433:ARG:CZ	2.50	0.42
1:A:33:ASN:HB3	1:A:55:ILE:HA	2.01	0.41
1:A:135:TYR:CZ	1:A:596:ILE:HB	2.55	0.41
1:B:264:LEU:HD13	1:B:320:TYR:HB2	2.01	0.41
1:A:276:LEU:HG	1:A:280:LYS:HB2	2.02	0.41
1:A:40:HIS:CE1	1:A:42:THR:HG23	2.55	0.41
1:B:430:ASN:N	1:B:431:PRO:HD3	2.35	0.41
1:B:557:ARG:HE	1:B:561:ARG:NH1	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:HIS:HE1	1:B:489:PHE:CZ	2.39	0.41
1:A:201:PRO:HB2	1:A:202:ASP:H	1.69	0.41
1:A:399:ARG:NH1	2:A:768:HOH:O	2.53	0.41
1:A:78:LEU:HD22	1:A:596:ILE:HG12	2.03	0.41
1:B:230:LEU:HB3	1:B:451:PHE:HZ	1.86	0.41
1:B:407:LEU:HD13	1:B:588:VAL:HG11	2.03	0.41
1:B:443:PHE:CD1	1:B:443:PHE:C	2.99	0.41
1:A:46:VAL:HG22	1:A:150:ARG:NH1	2.36	0.41
1:A:387:ILE:HD13	1:A:394:PHE:O	2.20	0.41
1:B:248:ILE:HG13	1:B:375:THR:HB	2.03	0.41
1:B:165:LEU:HB3	1:B:171:LEU:CD2	2.51	0.40
1:B:570:ASP:C	1:B:572:GLU:H	2.29	0.40
1:A:412:GLU:HG2	1:A:589:LYS:HB2	2.03	0.40
1:A:570:ASP:C	1:A:572:GLU:H	2.28	0.40
1:B:7:LEU:HD21	1:B:86:ILE:HG23	2.02	0.40
1:B:46:VAL:HG22	1:B:150:ARG:NH1	2.31	0.40
1:B:302:TRP:CD1	1:B:307:LEU:HG	2.57	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	594/596 (100%)	547 (92%)	33 (6%)	14 (2%)	4	11
1	B	594/596 (100%)	551 (93%)	33 (6%)	10 (2%)	7	17
All	All	1188/1192 (100%)	1098 (92%)	66 (6%)	24 (2%)	6	14

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	GLN

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Mol	Chain	Res	Type
1	A	199	ILE
1	A	200	PHE
1	A	332	LEU
1	B	180	PRO
1	B	201	PRO
1	A	277	ASP
1	A	281	LYS
1	A	331	ASN
1	B	191	ASP
1	B	331	ASN
1	A	168	MET
1	A	169	LYS
1	B	177	GLU
1	B	190	GLN
1	A	178	VAL
1	A	205	ARG
1	B	205	ARG
1	A	179	LYS
1	B	272	PRO
1	A	444	ILE
1	B	174	VAL
1	B	178	VAL
1	A	201	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	552/552 (100%)	504 (91%)	48 (9%)	9	23
1	B	552/552 (100%)	510 (92%)	42 (8%)	12	29
All	All	1104/1104 (100%)	1014 (92%)	90 (8%)	10	25

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	26	ILE
1	A	36	LEU
1	A	42	THR
1	A	44	LYS
1	A	49	LEU
1	A	52	LEU
1	A	86	ILE
1	A	90	VAL
1	A	104	GLN
1	A	113	LYS
1	A	123	LEU
1	A	150	ARG
1	A	152	GLU
1	A	155	ILE
1	A	176	ASP
1	A	185	ASN
1	A	190	GLN
1	A	200	PHE
1	A	230	LEU
1	A	242	GLN
1	A	248	ILE
1	A	249	LYS
1	A	250	VAL
1	A	260	LYS
1	A	267	LEU
1	A	271	ILE
1	A	292	PHE
1	A	307	LEU
1	A	319	LEU
1	A	324	MET
1	A	342	VAL
1	A	343	ASP
1	A	362	ILE
1	A	372	LYS
1	A	384	GLN
1	A	387	ILE
1	A	435	LEU
1	A	444	ILE
1	A	458	ASN
1	A	497	ILE
1	A	506	ARG
1	A	525	ARG

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Mol	Chain	Res	Type
1	A	544	LEU
1	A	566	MET
1	A	581	LEU
1	A	589	LYS
1	A	596	ILE
1	B	12	ARG
1	B	36	LEU
1	B	41	LYS
1	B	42	THR
1	B	44	LYS
1	B	48	ILE
1	B	49	LEU
1	B	52	LEU
1	B	86	ILE
1	B	90	VAL
1	B	113	LYS
1	B	123	LEU
1	B	141	LEU
1	B	150	ARG
1	B	152	GLU
1	B	155	ILE
1	B	167	LYS
1	B	174	VAL
1	B	191	ASP
1	B	212	LEU
1	B	220	LEU
1	B	230	LEU
1	B	260	LYS
1	B	267	LEU
1	B	271	ILE
1	B	279	GLU
1	B	292	PHE
1	B	307	LEU
1	B	340	ARG
1	B	342	VAL
1	B	362	ILE
1	B	416	LYS
1	B	433	ARG
1	B	435	LEU
1	B	444	ILE
1	B	458	ASN
1	B	486	ARG

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Mol	Chain	Res	Type
1	B	497	ILE
1	B	544	LEU
1	B	580	LYS
1	B	581	LEU
1	B	593	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	118	HIS
1	A	119	ASN
1	A	185	ASN
1	A	242	GLN
1	A	244	GLN
1	A	258	ASN
1	A	384	GLN
1	A	454	ASN
1	A	458	ASN
1	A	460	GLN
1	A	569	HIS
1	B	47	GLN
1	B	92	HIS
1	B	118	HIS
1	B	119	ASN
1	B	185	ASN
1	B	192	ASN
1	B	258	ASN
1	B	269	GLN
1	B	282	ASN
1	B	367	GLN
1	B	380	HIS
1	B	454	ASN
1	B	458	ASN
1	B	460	GLN
1	B	569	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

6.1 Protein, DNA and RNA chains

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	596/596 (100%)	0.73	86 (14%) 6 5	22, 40, 100, 115	0
1	B	596/596 (100%)	0.95	128 (21%) 2 2	23, 40, 113, 126	0
All	All	1192/1192 (100%)	0.84	214 (17%) 3 3	22, 40, 106, 126	0

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	VAL	12.4
1	B	177	GLU	10.9
1	A	177	GLU	10.2
1	B	178	VAL	8.6
1	B	199	ILE	7.1
1	B	174	VAL	5.9
1	A	211	LEU	5.8
1	B	276	LEU	5.7
1	B	226	THR	5.6
1	B	172	VAL	5.0
1	B	273	THR	4.9
1	B	281	LYS	4.6
1	A	203	SER	4.6
1	B	206	LYS	4.4
1	B	204	ALA	4.4
1	A	179	LYS	4.4
1	A	180	PRO	4.4
1	A	278	SER	4.3
1	A	199	ILE	4.3
1	B	1	MET	4.3
1	B	181	ARG	4.2
1	B	264	LEU	4.2
1	B	179	LYS	4.2
1	B	210	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	239	GLN	4.1
1	B	275	LEU	4.1
1	B	292	PHE	4.1
1	B	261	ILE	4.0
1	A	277	ASP	4.0
1	A	169	LYS	4.0
1	B	211	LEU	4.0
1	A	181	ARG	4.0
1	B	338	ILE	3.9
1	B	209	PHE	3.9
1	A	174	VAL	3.9
1	A	1	MET	3.9
1	B	180	PRO	3.9
1	B	377	LEU	3.8
1	B	176	ASP	3.8
1	B	379	THR	3.8
1	B	163	HIS	3.8
1	A	207	PRO	3.8
1	B	213	THR	3.8
1	A	301	LYS	3.8
1	A	175	GLN	3.7
1	B	378	PRO	3.7
1	B	219	VAL	3.7
1	B	220	LEU	3.7
1	A	292	PHE	3.7
1	B	194	ARG	3.6
1	A	182	GLY	3.6
1	B	208	PHE	3.6
1	B	443	PHE	3.5
1	B	277	ASP	3.5
1	B	298	LYS	3.5
1	B	402	ARG	3.5
1	B	225	LYS	3.4
1	B	247	GLY	3.4
1	B	385	ASP	3.4
1	B	288	ILE	3.4
1	B	376	ASN	3.4
1	A	382	HIS	3.3
1	B	207	PRO	3.2
1	B	265	CYS	3.2
1	B	400	GLN	3.2
1	A	342	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	43	LYS	3.2
1	B	222	GLU	3.2
1	B	190	GLN	3.2
1	B	289	SER	3.2
1	B	283	PHE	3.2
1	A	226	THR	3.1
1	A	444	ILE	3.1
1	B	175	GLN	3.1
1	A	109	ASN	3.1
1	B	191	ASP	3.1
1	B	188	PRO	3.1
1	A	200	PHE	3.1
1	A	170	TYR	3.1
1	A	281	LYS	3.1
1	A	227	SER	3.1
1	B	201	PRO	3.0
1	B	342	VAL	3.0
1	B	216	ILE	3.0
1	B	268	ILE	3.0
1	A	222	GLU	3.0
1	A	206	LYS	2.9
1	A	264	LEU	2.9
1	A	298	LYS	2.9
1	B	380	HIS	2.9
1	A	289	SER	2.9
1	B	203	SER	2.9
1	B	193	PHE	2.9
1	B	382	HIS	2.9
1	B	278	SER	2.8
1	A	302	TRP	2.8
1	B	43	LYS	2.8
1	B	186	ILE	2.8
1	A	168	MET	2.8
1	B	200	PHE	2.8
1	B	244	GLN	2.8
1	B	215	LYS	2.8
1	B	152	GLU	2.8
1	A	297	ARG	2.8
1	A	356	TYR	2.8
1	A	269	GLN	2.7
1	B	444	ILE	2.7
1	A	163	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	283	PHE	2.7
1	B	311	PRO	2.7
1	B	217	TYR	2.7
1	A	362	ILE	2.7
1	B	182	GLY	2.7
1	B	303	ASN	2.7
1	A	210	LYS	2.7
1	B	312	LEU	2.7
1	A	107	GLU	2.7
1	A	303	ASN	2.7
1	A	204	ALA	2.7
1	A	261	ILE	2.6
1	A	184	LEU	2.6
1	B	280	LYS	2.6
1	B	331	ASN	2.6
1	B	205	ARG	2.6
1	A	280	LYS	2.6
1	B	401	VAL	2.6
1	B	375	THR	2.5
1	B	384	GLN	2.6
1	A	384	GLN	2.5
1	A	312	LEU	2.5
1	B	241	THR	2.5
1	B	296	ARG	2.5
1	B	263	VAL	2.5
1	A	260	LYS	2.4
1	B	301	LYS	2.4
1	B	287	HIS	2.4
1	A	378	PRO	2.4
1	A	380	HIS	2.4
1	B	386	GLU	2.4
1	B	593	LYS	2.4
1	A	250	VAL	2.4
1	A	295	PHE	2.4
1	B	396	LEU	2.4
1	A	176	ASP	2.4
1	B	335	ASP	2.4
1	B	297	ARG	2.4
1	B	395	ASN	2.4
1	B	231	TYR	2.3
1	A	216	ILE	2.3
1	A	387	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	167	LYS	2.3
1	A	445	CYS	2.3
1	B	383	PRO	2.3
1	B	295	PHE	2.3
1	B	246	TYR	2.3
1	A	379	THR	2.3
1	B	157	PHE	2.3
1	B	266	LYS	2.3
1	A	368	VAL	2.3
1	B	197	VAL	2.3
1	A	183	VAL	2.3
1	B	46	VAL	2.3
1	B	184	LEU	2.3
1	A	186	ILE	2.2
1	A	187	ILE	2.2
1	A	274	HIS	2.2
1	B	397	THR	2.2
1	B	189	LYS	2.2
1	B	223	LYS	2.2
1	B	381	ARG	2.2
1	B	308	GLN	2.2
1	B	372	LYS	2.2
1	A	273	THR	2.2
1	B	202	ASP	2.2
1	B	391	GLY	2.2
1	B	168	MET	2.2
1	B	398	THR	2.2
1	A	194	ARG	2.2
1	B	326	ARG	2.2
1	A	300	TYR	2.2
1	B	224	TYR	2.2
1	A	285	VAL	2.2
1	B	221	GLU	2.1
1	A	291	GLN	2.1
1	B	242	GLN	2.1
1	A	171	LEU	2.1
1	A	220	LEU	2.1
1	B	336	ALA	2.1
1	A	296	ARG	2.1
1	B	218	LYS	2.1
1	A	328	TYR	2.1
1	B	360	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	304	HIS	2.1
1	A	441	PHE	2.1
1	A	189	LYS	2.1
1	A	223	LYS	2.1
1	A	201	PRO	2.1
1	B	327	LEU	2.1
1	B	282	ASN	2.1
1	B	245	ILE	2.1
1	B	269	GLN	2.1
1	A	410	ASN	2.1
1	B	445	CYS	2.1
1	B	279	GLU	2.0
1	B	583	GLU	2.0
1	B	44	LYS	2.0
1	A	275	LEU	2.0
1	A	299	ILE	2.0
1	B	299	ILE	2.0
1	A	224	TYR	2.0
1	A	209	PHE	2.0
1	B	255	ALA	2.0
1	A	213	THR	2.0
1	B	212	LEU	2.0

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.