



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:14 AM GMT

PDB ID : 3DU6
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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

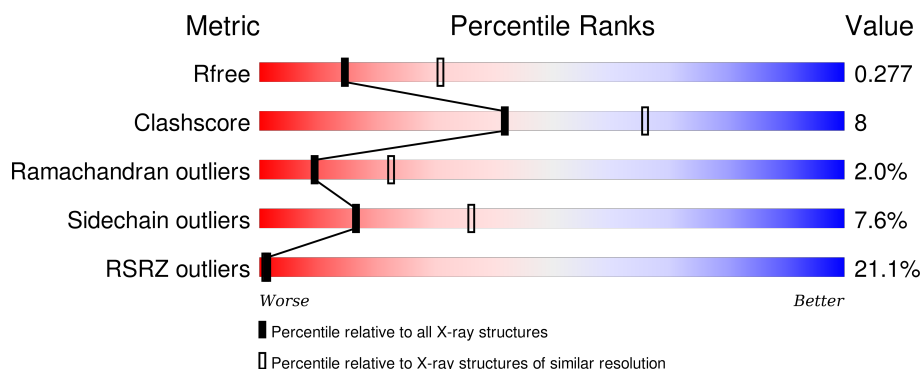
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

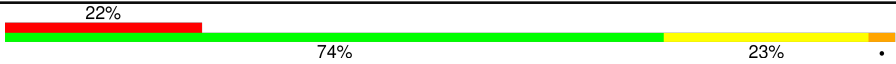

The reported resolution of this entry is 2.71 Å.

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}	91344	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	
1	B	596	

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			

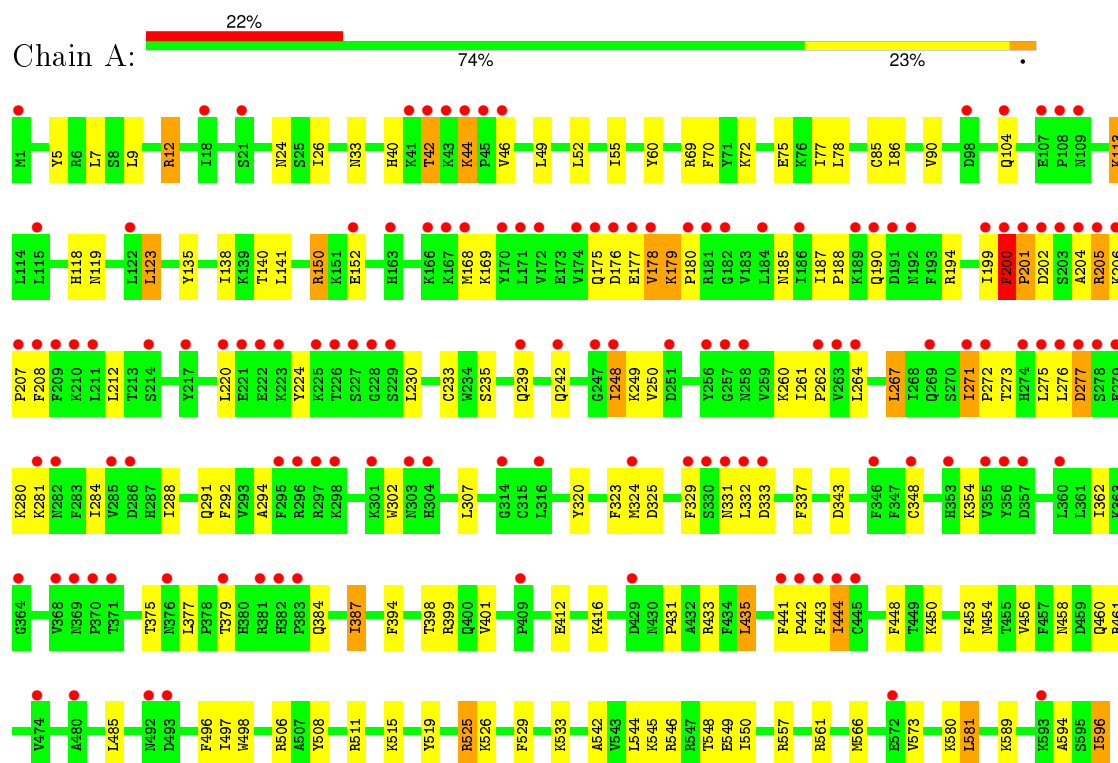
- Molecule 2 is water.

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

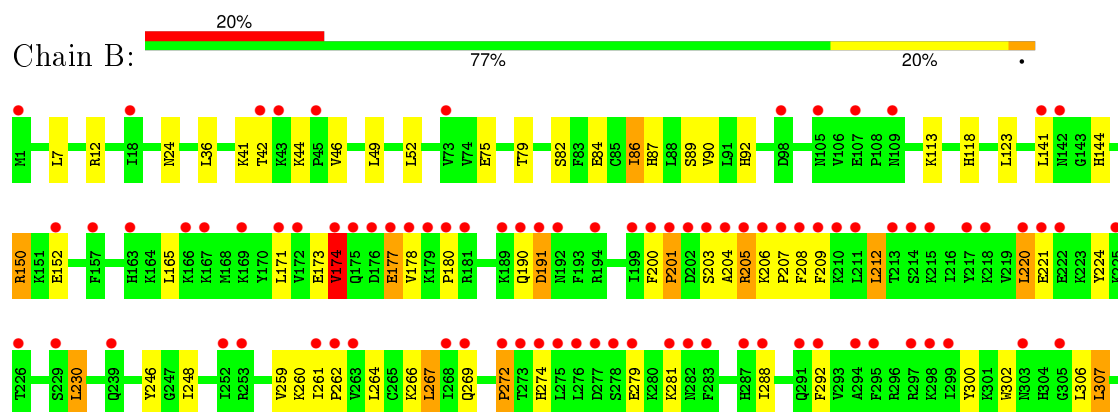
3 Residue-property plots

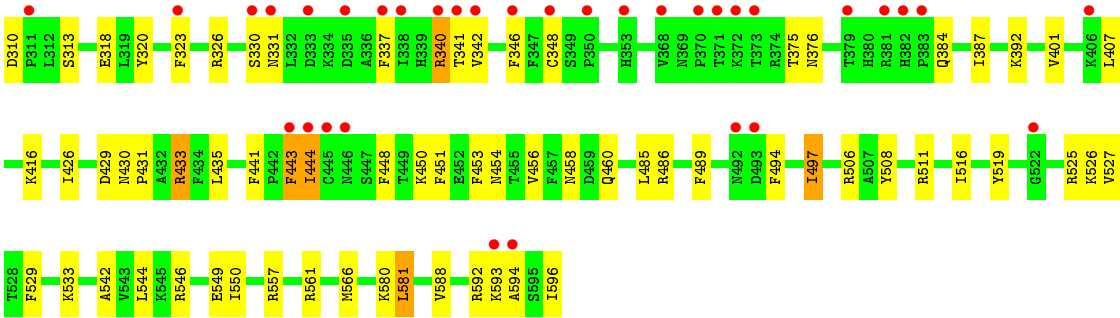
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 25.01 – 2.71	Depositor EDS
% Data completeness (in resolution range)	97.0 (20.00-2.71) 97.0 (25.01-2.71)	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 0.241 , 0.277	Depositor DCC
R_{free} test set	3016 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	15 of 59279 reflections (0.025%)	Xtriage
F_o, F_c correlation	0.93	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.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.40	0/5114	0.46	0/6893
1	B	0.40	0/5114	0.45	0/6893
All	All	0.40	0/10228	0.45	0/13786

There are no bond length outliers.

There are no bond angle outliers.

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	4982	0	5126	93	0
1	B	4982	0	5126	76	0
2	A	180	0	0	6	0
2	B	175	0	0	5	0
All	All	10319	0	10252	169	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 8.

All (169) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:444:ILE:HD13	1:B:444:ILE:N	2.03	0.69
1:B:24:ASN:H	1:B:118:HIS:CE1	2.04	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: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:HE2	1:A:72:LYS:HA	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
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:84:GLU:CD	1:B:592:ARG:HH22	2.03	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:443:PHE:HD2	2:B:771:HOH:O	1.88	0.55
1:A:333:ASP:HB2	1:A:354:LYS:HD3	1.89	0.55
1:A:284:ILE:O	1:A:288:ILE:HG12	2.08	0.54
1:A:267:LEU:HD11	1:A:323:PHE:HB2	1.90	0.54
1:A:75:GLU:HG3	1:A:594:ALA: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:B:460:GLN:NE2	1:B:525:ARG:H	2.06	0.52
1:A:529:PHE:CE2	1:A:533:LYS:HD3	2.44	0.52
1:A:70:PHE:CZ	1:A:123:LEU:HD13	2.44	0.52
1:B:82:SER:HB2	1:B:144:HIS:HB3	1.91	0.52
1:A:435:LEU:HG	1:A:485:LEU:HD11	1.92	0.52
1:A:205:ARG:O	1:A:208:PHE:HB3	2.09	0.51
1:B:431:PRO:HB3	1:B:485:LEU:HD22	1.92	0.51
1:A:271:ILE:HD11	1:A:276:LEU:HB2	1.91	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ALA:O	1:A:205:ARG:HB2	2.13	0.49
1:A:387:ILE:HD13	1:A:387:ILE:H	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:443:PHE:CD2	1:B:444:ILE:HD12	2.49	0.48
1:B:204:ALA:H	1:B:209:PHE:HE2	1.62	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:A:450:LYS:HG2	1:A:519:TYR:CZ	2.50	0.47
1:B:429:ASP:C	1:B:431:PRO:HD3	2.35	0.47
1:B:529:PHE:CE2	1:B:533:LYS:HD3	2.50	0.47
1:A:5:TYR:O	1:A:85:CYS:HB3	2.14	0.47
1:A:140:THR:O	1:A:141:LEU:HB2	2.15	0.46
1:A:46:VAL:HG22	1:A:150:ARG:HH12	1.80	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:B:346:PHE:CE1	1:B:387:ILE:HG21	2.51	0.46
1:A:546:ARG:HD2	1:A:581:LEU:HD21	1.98	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: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
1:A:444:ILE:CD1	1:A:508:TYR:HE2	2.29	0.44
1:B:546:ARG:HD2	1:B:581:LEU:HD21	1.99	0.44
1:B:433:ARG:NH1	2:B:597:HOH:O	2.51	0.44
1:A:178:VAL:O	1:A:178:VAL:CG1	2.46	0.44
1:B:460:GLN:HE22	1:B:526:LYS:N	2.11	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:A:138:ILE:HD13	1:A:188:PRO:HG2	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:PHE:N	1:A:442:PRO:CD	2.82	0.43
1:B:205:ARG:HA	1:B:205:ARG:NE	2.33	0.43
1:A:273:THR:O	1:A:277:ASP:HB3	2.18	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:443:PHE:CE1	1:A:444:ILE:HG23	2.54	0.43
1:A:180:PRO:HB3	1:A:294:ALA:HB2	1.99	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:179:LYS:H	1:A:180:PRO:HD3	1.84	0.42
1:B:201:PRO:C	1:B:203:SER:H	2.23	0.42
1:B:458:ASN:HD22	1:B:458:ASN:HA	1.62	0.42
1:B:261:ILE:H	1:B:261:ILE:HD12	1.84	0.42
1:A:233:CYS:HB3	1:A:337:PHE:CE1	2.55	0.42
1:B:549:GLU:HG2	1:B:550:ILE:H	1.85	0.42
1:B:261:ILE:HG23	1:B:288:ILE:HG22	2.01	0.42
1:B:75:GLU:HG3	1:B:594:ALA:HB2	2.00	0.42
1:A:542:ALA:HB1	1:A:581:LEU:HD13	2.02	0.42
1:A:441:PHE:HB2	1:A:511:ARG:CZ	2.49	0.42
1:A:261:ILE:HB	1:A:262:PRO:HD3	2.02	0.42
1:B:426:ILE:HG12	1:B:433:ARG:CZ	2.50	0.42
1:B:174:VAL:HB	1:B:177:GLU:HG3	2.02	0.42
1:A:135:TYR:CZ	1:A:596:ILE:HB	2.55	0.41
1:A:33:ASN:HB3	1:A:55:ILE:HA	2.01	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:B:430:ASN:N	1:B:431:PRO:HD3	2.35	0.41
1:A:40:HIS:CE1	1:A:42:THR:HG23	2.55	0.41
1:B:557:ARG:HE	1:B:561:ARG:NH1	2.18	0.41
1:A:377:LEU:C	1:A:379:THR:H	2.24	0.41
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:B:596:ILE:C	2:B:698:HOH:O	2.58	0.41
1:A:78:LEU:HD22	1:A:596:ILE:HG12	2.03	0.41
1:B:407:LEU:HD13	1:B:588:VAL:HG11	2.03	0.41
1:B:230:LEU:HB3	1:B:451:PHE:HZ	1.86	0.41
1:A:387:ILE:HD13	1:A:394:PHE:O	2.20	0.41
1:A:46:VAL:HG22	1:A:150:ARG:NH1	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:GLU:HG2	1:A:589:LYS:HB2	2.03	0.40
1:B:46:VAL:HG22	1:B:150:ARG:NH1	2.31	0.40
1:B:7:LEU:HD21	1:B:86:ILE:HG23	2.02	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 [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	594/596 (100%)	547 (92%)	33 (6%)	14 (2%)	7	17
1	B	594/596 (100%)	551 (93%)	33 (6%)	10 (2%)	11	27
All	All	1188/1192 (100%)	1098 (92%)	66 (6%)	24 (2%)	9	22

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
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

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Mol	Chain	Res	Type
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 [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	552/552 (100%)	510 (92%)	42 (8%)	16	36
1	B	552/552 (100%)	510 (92%)	42 (8%)	16	36
All	All	1104/1104 (100%)	1020 (92%)	84 (8%)	16	36

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	26	ILE
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

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Mol	Chain	Res	Type
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	324	MET
1	A	343	ASP
1	A	362	ILE
1	A	384	GLN
1	A	387	ILE
1	A	433	ARG
1	A	435	LEU
1	A	497	ILE
1	A	506	ARG
1	A	525	ARG
1	A	544	LEU
1	A	566	MET
1	A	580	LYS
1	A	581	LEU
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	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

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Mol	Chain	Res	Type
1	B	152	GLU
1	B	174	VAL
1	B	191	ASP
1	B	212	LEU
1	B	220	LEU
1	B	221	GLU
1	B	230	LEU
1	B	260	LYS
1	B	267	LEU
1	B	279	GLU
1	B	292	PHE
1	B	307	LEU
1	B	340	ARG
1	B	342	VAL
1	B	384	GLN
1	B	392	LYS
1	B	416	LYS
1	B	433	ARG
1	B	435	LEU
1	B	443	PHE
1	B	444	ILE
1	B	486	ARG
1	B	497	ILE
1	B	506	ARG
1	B	544	LEU
1	B	566	MET
1	B	580	LYS
1	B	581	LEU
1	B	593	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	92	HIS
1	A	118	HIS
1	A	119	ASN
1	A	185	ASN
1	A	242	GLN
1	A	384	GLN
1	A	454	ASN
1	A	458	ASN

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Mol	Chain	Res	Type
1	A	460	GLN
1	B	92	HIS
1	B	118	HIS
1	B	119	ASN
1	B	185	ASN
1	B	258	ASN
1	B	269	GLN
1	B	304	HIS
1	B	454	ASN
1	B	458	ASN
1	B	460	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

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%)	1.32	131 (21%)  	22, 40, 100, 115	0
1	B	596/596 (100%)	1.31	121 (20%)  	23, 40, 113, 126	0
All	All	1192/1192 (100%)	1.31	252 (21%)  	22, 40, 106, 126	0

All (252) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	VAL	14.0
1	A	211	LEU	12.1
1	B	177	GLU	10.7
1	A	175	GLN	10.4
1	A	177	GLU	9.5
1	B	178	VAL	9.2
1	A	203	SER	9.2
1	A	190	GLN	8.1
1	B	221	GLU	8.1
1	A	277	ASP	7.8
1	B	204	ALA	7.8
1	A	382	HIS	7.7
1	B	175	GLN	7.7
1	B	203	SER	7.1
1	A	205	ARG	7.0
1	B	205	ARG	7.0
1	A	222	GLU	6.9
1	A	43	LYS	6.9
1	A	204	ALA	6.8
1	B	211	LEU	6.8
1	B	1	MET	6.7
1	A	163	HIS	6.7
1	A	226	THR	6.6
1	B	202	ASP	6.5

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Mol	Chain	Res	Type	RSRZ
1	B	200	PHE	6.5
1	A	200	PHE	6.2
1	A	227	SER	6.1
1	B	176	ASP	6.1
1	B	190	GLN	6.0
1	A	356	TYR	6.0
1	A	444	ILE	5.9
1	B	199	ILE	5.9
1	B	239	GLN	5.8
1	A	207	PRO	5.8
1	B	382	HIS	5.8
1	A	381	ARG	5.8
1	B	272	PRO	5.7
1	A	206	LYS	5.7
1	A	191	ASP	5.7
1	B	218	LYS	5.6
1	B	276	LEU	5.4
1	B	226	THR	5.4
1	A	371	THR	5.3
1	B	288	ILE	5.3
1	B	381	ARG	5.3
1	B	217	TYR	5.2
1	B	372	LYS	5.2
1	B	174	VAL	5.1
1	B	43	LYS	5.1
1	B	298	LYS	5.0
1	A	275	LEU	5.0
1	B	262	PRO	4.9
1	A	170	TYR	4.9
1	A	167	LYS	4.8
1	B	225	LYS	4.7
1	A	228	GLY	4.7
1	B	222	GLU	4.7
1	B	201	PRO	4.7
1	A	109	ASN	4.6
1	B	172	VAL	4.6
1	A	217	TYR	4.6
1	B	445	CYS	4.5
1	A	220	LEU	4.5
1	A	189	LYS	4.5
1	B	341	THR	4.4
1	A	176	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	208	PHE	4.4
1	B	163	HIS	4.3
1	B	278	SER	4.3
1	B	220	LEU	4.3
1	A	202	ASP	4.3
1	B	295	PHE	4.3
1	A	281	LYS	4.2
1	A	274	HIS	4.2
1	A	192	ASN	4.2
1	B	371	THR	4.2
1	B	330	SER	4.2
1	A	297	ARG	4.2
1	B	492	ASN	4.1
1	A	199	ILE	4.1
1	B	443	PHE	4.1
1	A	278	SER	4.1
1	A	286	ASP	4.0
1	A	107	GLU	4.0
1	B	45	PRO	4.0
1	A	295	PHE	4.0
1	A	201	PRO	4.0
1	A	1	MET	4.0
1	B	191	ASP	3.9
1	A	332	LEU	3.9
1	B	208	PHE	3.9
1	B	342	VAL	3.9
1	B	269	GLN	3.9
1	B	522	GLY	3.9
1	B	335	ASP	3.8
1	B	353	HIS	3.8
1	A	45	PRO	3.8
1	A	409	PRO	3.8
1	B	214	SER	3.8
1	B	277	ASP	3.7
1	A	172	VAL	3.7
1	B	273	THR	3.7
1	A	370	PRO	3.7
1	B	253	ARG	3.7
1	A	360	LEU	3.6
1	B	373	THR	3.6
1	A	42	THR	3.5
1	A	210	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	181	ARG	3.5
1	B	167	LYS	3.5
1	A	331	ASN	3.4
1	B	331	ASN	3.4
1	A	269	GLN	3.4
1	A	442	PRO	3.4
1	B	213	THR	3.4
1	A	355	VAL	3.4
1	B	109	ASN	3.4
1	B	169	LYS	3.3
1	A	263	VAL	3.3
1	B	444	ILE	3.3
1	B	446	ASN	3.3
1	B	179	LYS	3.3
1	B	207	PRO	3.3
1	B	180	PRO	3.3
1	B	107	GLU	3.3
1	A	493	ASP	3.3
1	A	152	GLU	3.2
1	A	279	GLU	3.2
1	B	338	ILE	3.2
1	B	275	LEU	3.2
1	B	274	HIS	3.2
1	A	181	ARG	3.2
1	B	297	ARG	3.2
1	A	272	PRO	3.2
1	B	283	PHE	3.2
1	A	242	GLN	3.1
1	B	593	LYS	3.1
1	B	340	ARG	3.1
1	A	301	LYS	3.1
1	A	369	ASN	3.0
1	B	209	PHE	3.0
1	A	445	CYS	3.0
1	B	279	GLU	3.0
1	B	141	LEU	3.0
1	B	152	GLU	3.0
1	B	73	VAL	3.0
1	B	368	VAL	3.0
1	A	353	HIS	2.9
1	B	287	HIS	2.9
1	A	276	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	206	LYS	2.9
1	A	239	GLN	2.9
1	A	171	LEU	2.9
1	B	281	LYS	2.9
1	B	346	PHE	2.9
1	A	593	LYS	2.9
1	A	98	ASP	2.8
1	B	98	ASP	2.8
1	B	299	ILE	2.8
1	A	221	GLU	2.8
1	A	282	ASN	2.8
1	A	324	MET	2.8
1	A	122	LEU	2.8
1	A	257	GLY	2.8
1	B	252	ILE	2.8
1	B	268	ILE	2.8
1	A	368	VAL	2.8
1	A	271	ILE	2.7
1	A	46	VAL	2.7
1	B	263	VAL	2.7
1	B	42	THR	2.7
1	A	251	ASP	2.7
1	A	184	LEU	2.7
1	B	379	THR	2.7
1	A	108	PRO	2.7
1	A	18	ILE	2.7
1	B	210	LYS	2.6
1	A	357	ASP	2.6
1	A	225	LYS	2.6
1	A	248	ILE	2.6
1	A	492	ASN	2.6
1	A	21	SER	2.6
1	A	333	ASP	2.6
1	A	364	GLY	2.6
1	A	572	GLU	2.6
1	A	346	PHE	2.6
1	B	192	ASN	2.6
1	B	194	ARG	2.6
1	A	258	ASN	2.6
1	B	348	CYS	2.6
1	A	214	SER	2.6
1	A	298	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	215	LYS	2.5
1	A	285	VAL	2.5
1	B	142	ASN	2.5
1	A	474	VAL	2.4
1	A	379	THR	2.4
1	B	323	PHE	2.4
1	A	304	HIS	2.4
1	A	182	GLY	2.4
1	B	493	ASP	2.4
1	A	314	GLY	2.4
1	A	174	VAL	2.4
1	B	18	ILE	2.4
1	A	44	LYS	2.3
1	A	443	PHE	2.3
1	A	229	SER	2.3
1	A	383	PRO	2.3
1	A	104	GLN	2.3
1	A	330	SER	2.3
1	A	480	ALA	2.3
1	B	189	LYS	2.3
1	B	333	ASP	2.3
1	A	256	TYR	2.3
1	B	261	ILE	2.3
1	B	303	ASN	2.2
1	B	229	SER	2.2
1	A	296	ARG	2.2
1	A	316	LEU	2.2
1	B	291	GLN	2.2
1	A	441	PHE	2.2
1	B	157	PHE	2.2
1	B	370	PRO	2.2
1	A	223	LYS	2.2
1	B	171	LEU	2.2
1	B	282	ASN	2.2
1	B	594	ALA	2.2
1	A	180	PRO	2.2
1	B	105	ASN	2.2
1	B	406	LYS	2.2
1	A	429	ASP	2.1
1	A	348	CYS	2.1
1	B	166	LYS	2.1
1	B	311	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	383	PRO	2.1
1	B	305	GLY	2.1
1	B	292	PHE	2.1
1	A	209	PHE	2.1
1	A	329	PHE	2.1
1	B	337	PHE	2.1
1	B	294	ALA	2.1
1	A	264	LEU	2.1
1	A	168	MET	2.1
1	A	166	LYS	2.0
1	A	186	ILE	2.0
1	B	350	PRO	2.0
1	A	247	GLY	2.0
1	A	115	LEU	2.0
1	A	303	ASN	2.0
1	A	41	LYS	2.0
1	A	262	PRO	2.0
1	A	376	ASN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.