Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:13 AM GMT

PDB ID	:	3DU5
Title	:	Structure of the catalytic subunit of telomerase, TERT
Authors	:	Skordalakes, E.
Deposited on	:	2008-07-16
Resolution	:	3.25 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

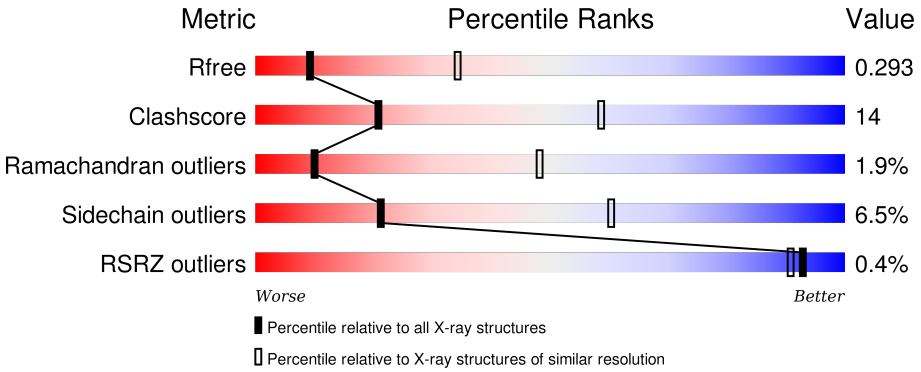
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.25 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	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

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 <=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	67% 29% .
1	B	596	% 65% 31% .

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10041 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.

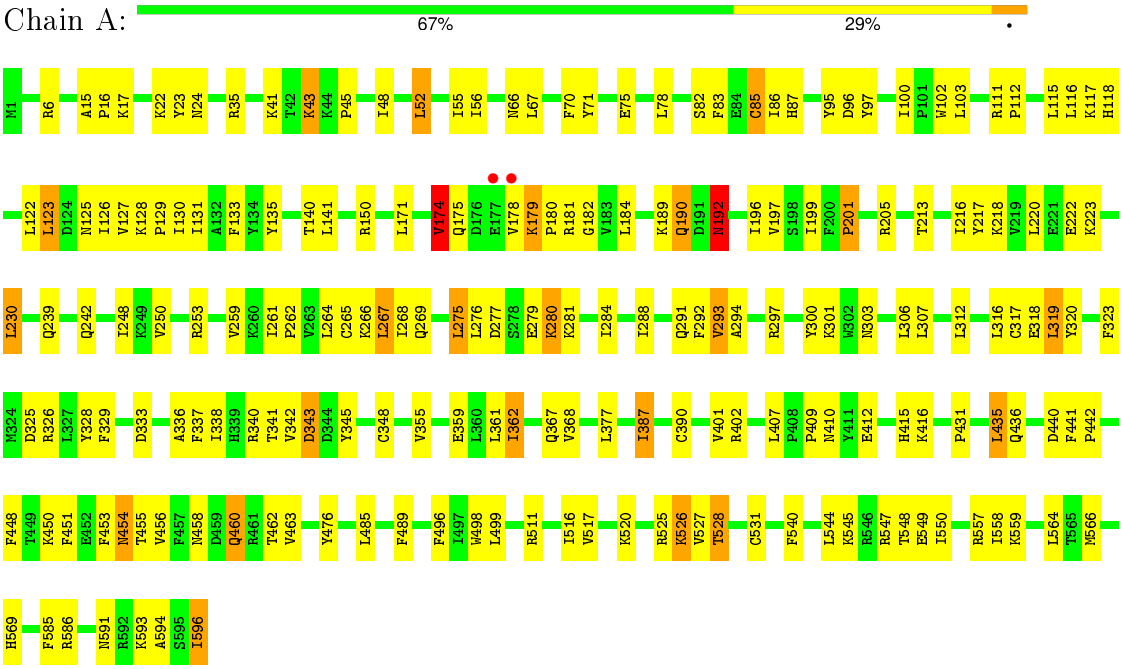
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	45	Total	O	0	0
			45	45		
2	B	32	Total	O	0	0
			32	32		

3 Residue-property plots (i)

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.

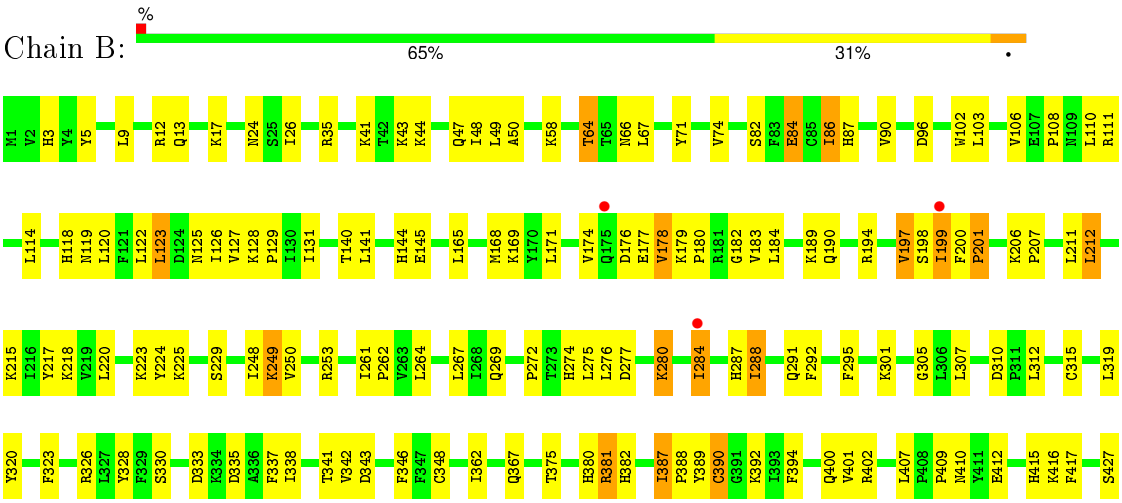
- Molecule 1: Telomerase reverse transcriptase

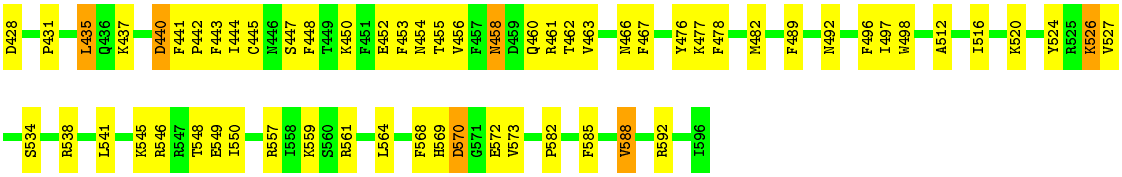
Chain A:



- Molecule 1: Telomerase reverse transcriptase

Chain B:




D428
P431
L435
Q436
K437
D440
F441
P442
F443
I444
C445
N446
S447
F448
T449
K450
F451
E452
F453
N454
T455
V456
F457
N458
D459
Q460
R461
T462
V463
N466
F467
Y476
K477
F478
N482
F489
N492
F496
I497
W498
A512
I516
K520
Y524
R525
K526
V527
S534
R538
L541
K545
R546
R547
T548
E549
I550
R557
I558
K559
S560
R561
L564
F568
H569
D570
G571
E572
V573
P582
F585
V588
R592
I596

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	199.97Å 199.97Å 96.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.25 27.08 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-3.25) 99.6 (27.08-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 3.24Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.243 , 0.297 0.240 , 0.293	Depositor DCC
R_{free} test set	1748 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	48.6	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 1.7	EDS
Estimated twinning fraction	0.168 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Outliers	0 of 34616 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	10041	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.32	0/5114	0.42	0/6893
1	B	0.33	0/5114	0.42	0/6893
All	All	0.32	0/10228	0.42	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	151	0
1	B	4982	0	5126	140	0
2	A	45	0	0	1	0
2	B	32	0	0	0	0
All	All	10041	0	10252	291	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 14.

All (291) 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:178:VAL:HG12	1:B:179:LYS:N	1.61	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:VAL:HG11	1:B:178:VAL:CG2	1.78	1.12
1:B:178:VAL:HG12	1:B:179:LYS:H	0.97	1.10
1:A:276:LEU:HB3	1:A:280:LYS:HG2	1.29	1.07
1:B:174:VAL:HG11	1:B:178:VAL:HG21	1.40	1.01
1:B:178:VAL:CG1	1:B:179:LYS:H	1.74	0.93
1:B:174:VAL:CG1	1:B:178:VAL:HG21	2.04	0.88
1:A:401:VAL:H	1:A:458:ASN:HD21	1.22	0.88
1:B:174:VAL:HG11	1:B:178:VAL:HG23	1.53	0.87
1:A:264:LEU:HD23	1:A:288:ILE:HD13	1.56	0.87
1:B:24:ASN:H	1:B:118:HIS:HE1	1.23	0.86
1:A:75:GLU:HG3	1:A:594:ALA:HB2	1.57	0.86
1:A:264:LEU:HD13	1:A:320:TYR:HB2	1.57	0.84
1:A:184:LEU:HB3	1:A:293:VAL:HG11	1.59	0.84
1:B:401:VAL:H	1:B:458:ASN:HD21	1.24	0.82
1:A:45:PRO:HA	1:A:150:ARG:HH12	1.43	0.82
1:A:261:ILE:HD12	1:A:288:ILE:HG23	1.64	0.80
1:B:174:VAL:CG1	1:B:178:VAL:CG2	2.60	0.80
1:B:546:ARG:HH12	1:B:588:VAL:HG23	1.47	0.79
1:B:264:LEU:HD13	1:B:320:TYR:HB2	1.64	0.78
1:A:178:VAL:HG12	1:A:179:LYS:N	1.99	0.77
1:B:178:VAL:CG1	1:B:179:LYS:N	2.36	0.75
1:A:596:ILE:HD13	1:A:596:ILE:H	1.52	0.73
1:A:220:LEU:HD21	1:A:319:LEU:HA	1.70	0.73
1:B:220:LEU:HD21	1:B:319:LEU:HA	1.71	0.72
1:A:292:PHE:HD1	1:A:301:LYS:HG2	1.53	0.72
1:B:440:ASP:HB3	1:B:442:PRO:HD2	1.70	0.72
1:A:6:ARG:HA	1:A:85:CYS:HB3	1.70	0.72
1:A:178:VAL:O	1:A:179:LYS:HB2	1.89	0.72
1:A:66:ASN:HD21	1:A:96:ASP:HB3	1.55	0.72
1:B:431:PRO:HB2	1:B:496:PHE:CZ	2.25	0.71
1:B:24:ASN:H	1:B:118:HIS:CE1	2.09	0.71
1:A:440:ASP:HB3	1:A:442:PRO:HD2	1.73	0.71
1:A:24:ASN:H	1:A:118:HIS:CE1	2.09	0.69
1:A:24:ASN:H	1:A:118:HIS:HE1	1.40	0.69
1:B:165:LEU:HB3	1:B:171:LEU:HD22	1.74	0.69
1:A:441:PHE:N	1:A:442:PRO:HD2	2.10	0.67
1:A:528:THR:HG23	1:A:531:CYS:HB2	1.78	0.66
1:B:570:ASP:O	1:B:573:VAL:HG12	1.96	0.65
1:B:443:PHE:CE1	1:B:444:ILE:HG12	2.32	0.65
1:A:179:LYS:N	1:A:180:PRO:HD3	2.12	0.64
1:A:269:GLN:HE22	1:A:281:LYS:HG3	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:ILE:O	1:B:444:ILE:HG22	1.96	0.64
1:A:97:TYR:OH	1:A:112:PRO:HA	1.98	0.64
1:A:402:ARG:HD3	1:A:462:THR:HG23	1.77	0.64
1:B:249:LYS:HG3	1:B:389:TYR:HB2	1.80	0.63
1:B:402:ARG:HD3	1:B:462:THR:HG23	1.81	0.63
1:A:178:VAL:CG1	1:A:179:LYS:N	2.62	0.63
1:A:179:LYS:N	1:A:180:PRO:CD	2.62	0.62
1:B:272:PRO:HG2	1:B:275:LEU:HD12	1.83	0.61
1:A:448:PHE:HA	1:A:453:PHE:HE1	1.66	0.61
1:A:337:PHE:HB3	1:A:348:CYS:HB2	1.83	0.61
1:B:417:PHE:HB3	1:B:477:LYS:HE3	1.83	0.60
1:B:441:PHE:N	1:B:442:PRO:HD2	2.16	0.60
1:B:140:THR:O	1:B:141:LEU:HB2	2.00	0.60
1:A:189:LYS:HE2	1:A:192:ASN:HB3	1.83	0.60
1:A:333:ASP:HB3	1:A:336:ALA:HB2	1.83	0.60
1:B:337:PHE:HB3	1:B:348:CYS:HB2	1.84	0.60
1:A:549:GLU:HG2	1:A:550:ILE:HD12	1.84	0.59
1:B:450:LYS:O	1:B:454:ASN:HB3	2.02	0.59
1:B:24:ASN:ND2	1:B:102:TRP:HB2	2.17	0.59
1:A:178:VAL:HG12	1:A:179:LYS:H	1.68	0.59
1:A:171:LEU:HD22	1:A:300:TYR:HB2	1.85	0.59
1:A:178:VAL:CG1	1:A:179:LYS:H	2.16	0.58
1:B:212:LEU:HD11	1:B:284:ILE:HG12	1.84	0.58
1:A:325:ASP:O	1:A:329:PHE:HB2	2.03	0.58
1:A:516:ILE:HG21	1:A:527:VAL:HG21	1.85	0.58
1:A:450:LYS:O	1:A:454:ASN:HB3	2.04	0.58
1:B:48:ILE:HD13	1:B:131:ILE:HG12	1.85	0.57
1:B:165:LEU:HB3	1:B:171:LEU:CD2	2.34	0.57
1:A:261:ILE:HD12	1:A:288:ILE:CG2	2.35	0.57
1:B:66:ASN:HD21	1:B:96:ASP:HB3	1.70	0.57
1:A:180:PRO:C	1:A:182:GLY:H	2.08	0.56
1:B:287:HIS:O	1:B:291:GLN:HG3	2.05	0.56
1:B:224:TYR:OH	1:B:267:LEU:HD21	2.05	0.56
1:B:199:ILE:H	1:B:199:ILE:HD13	1.70	0.56
1:B:261:ILE:HB	1:B:262:PRO:HD3	1.86	0.56
1:B:460:GLN:HE22	1:B:526:LYS:H	1.53	0.56
1:B:516:ILE:HG21	1:B:527:VAL:HG21	1.88	0.56
1:B:269:GLN:HA	1:B:280:LYS:HZ2	1.70	0.56
1:A:218:LYS:HE3	1:A:275:LEU:HD23	1.88	0.55
1:B:197:VAL:HG22	1:B:307:LEU:HD22	1.87	0.55
1:A:288:ILE:HD11	1:A:316:LEU:HD13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:TYR:CE2	1:B:315:CYS:HB3	2.42	0.55
1:B:182:GLY:HA2	1:B:198:SER:O	2.06	0.55
1:A:253:ARG:HE	1:A:367:GLN:HG2	1.72	0.55
1:A:23:TYR:HE1	1:A:117:LYS:HG2	1.71	0.55
1:A:78:LEU:HB3	1:A:596:ILE:HD11	1.89	0.55
1:A:264:LEU:CD2	1:A:288:ILE:HD13	2.34	0.54
1:B:435:LEU:HD21	1:B:478:PHE:CE1	2.41	0.54
1:B:276:LEU:HD13	1:B:280:LYS:HD3	1.88	0.54
1:B:250:VAL:HG21	1:B:362:ILE:HG21	1.90	0.54
1:A:197:VAL:HG13	1:A:307:LEU:HD22	1.89	0.54
1:B:84:GLU:OE1	1:B:592:ARG:NH2	2.40	0.54
1:A:178:VAL:C	1:A:180:PRO:HD3	2.28	0.54
1:A:292:PHE:CD1	1:A:301:LYS:HG2	2.41	0.54
1:A:441:PHE:N	1:A:442:PRO:CD	2.70	0.54
1:A:476:TYR:HE1	1:A:585:PHE:HB3	1.72	0.53
1:A:280:LYS:HD2	1:A:281:LYS:N	2.22	0.53
1:A:431:PRO:HB2	1:A:496:PHE:CZ	2.43	0.53
1:B:441:PHE:N	1:B:442:PRO:CD	2.71	0.53
1:A:123:LEU:HA	1:A:127:VAL:HB	1.90	0.53
1:B:267:LEU:HD22	1:B:319:LEU:HD11	1.89	0.53
1:B:453:PHE:HA	1:B:463:VAL:HG13	1.91	0.53
1:A:174:VAL:HG22	1:A:301:LYS:HE2	1.90	0.53
1:A:596:ILE:H	1:A:596:ILE:CD1	2.20	0.53
1:A:454:ASN:HD22	1:A:456:VAL:H	1.56	0.52
1:A:17:LYS:HA	1:A:35:ARG:NH1	2.24	0.52
1:B:12:ARG:HD3	1:B:129:PRO:HA	1.89	0.52
1:A:277:ASP:O	1:A:280:LYS:HG3	2.10	0.52
1:A:22:LYS:HD3	1:A:117:LYS:HZ1	1.74	0.52
1:B:145:GLU:HA	1:B:415:HIS:ND1	2.25	0.52
1:A:230:LEU:HB3	1:A:451:PHE:HZ	1.75	0.52
1:A:180:PRO:HB3	1:A:294:ALA:HB2	1.91	0.52
1:B:267:LEU:HD11	1:B:323:PHE:HB2	1.91	0.52
1:B:250:VAL:HG11	1:B:362:ILE:HG21	1.92	0.52
1:A:82:SER:O	1:A:83:PHE:HB2	2.10	0.51
1:A:24:ASN:N	1:A:118:HIS:HE1	2.06	0.51
1:A:197:VAL:HG11	1:A:307:LEU:HD13	1.93	0.51
1:B:41:LYS:HB3	1:B:43:LYS:HG2	1.92	0.51
1:B:253:ARG:HD3	1:B:367:GLN:HE21	1.75	0.51
1:A:250:VAL:HG21	1:A:362:ILE:HG21	1.92	0.51
1:A:276:LEU:HB3	1:A:280:LYS:CG	2.21	0.50
1:A:52:LEU:HB3	1:A:71:TYR:HE2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:HIS:HE1	1:A:489:PHE:CE2	2.30	0.50
1:A:448:PHE:HA	1:A:453:PHE:CE1	2.45	0.50
1:B:128:LYS:HB2	1:B:129:PRO:HD3	1.93	0.50
1:A:291:GLN:HB3	1:A:307:LEU:HD12	1.94	0.50
1:A:387:ILE:HD13	1:A:387:ILE:H	1.77	0.49
1:A:43:LYS:HD2	1:A:43:LYS:H	1.76	0.49
1:A:441:PHE:H	1:A:442:PRO:HD2	1.77	0.49
1:A:275:LEU:HD12	1:A:275:LEU:H	1.77	0.49
1:B:520:LYS:HD2	1:B:524:TYR:CD2	2.47	0.49
1:B:200:PHE:N	1:B:201:PRO:HA	2.28	0.49
1:A:275:LEU:O	1:A:276:LEU:HB2	2.13	0.49
1:B:122:LEU:HD23	1:B:126:ILE:HD12	1.95	0.49
1:B:125:ASN:O	1:B:129:PRO:HG2	2.13	0.49
1:B:103:LEU:HD22	1:B:111:ARG:HG2	1.95	0.49
1:A:545:LYS:O	1:A:548:THR:HG23	2.13	0.49
1:A:312:LEU:HB3	1:A:316:LEU:HD12	1.94	0.49
1:B:249:LYS:CG	1:B:389:TYR:HB2	2.42	0.48
1:B:534:SER:O	1:B:538:ARG:HG2	2.13	0.48
1:B:189:LYS:HG2	1:B:190:GLN:H	1.78	0.48
1:B:482:MET:HE1	1:B:497:ILE:HG13	1.95	0.48
1:A:328:TYR:O	1:A:361:LEU:HD21	2.12	0.48
1:B:387:ILE:HD13	1:B:394:PHE:O	2.13	0.48
1:A:70:PHE:CZ	1:A:123:LEU:HD13	2.49	0.48
1:B:82:SER:HB2	1:B:144:HIS:HB3	1.94	0.48
1:B:276:LEU:HB3	1:B:280:LYS:HG2	1.96	0.48
1:B:538:ARG:HH21	1:B:564:LEU:C	2.18	0.48
1:B:346:PHE:CZ	1:B:387:ILE:HD11	2.49	0.48
1:B:400:GLN:HE22	1:B:458:ASN:HA	1.79	0.47
1:B:269:GLN:HA	1:B:280:LYS:NZ	2.29	0.47
1:B:461:ARG:HD3	1:B:572:GLU:O	2.14	0.47
1:A:216:ILE:HD11	1:A:284:ILE:HD13	1.96	0.47
1:A:261:ILE:HG23	1:A:288:ILE:HG22	1.96	0.47
1:B:123:LEU:HA	1:B:127:VAL:HB	1.96	0.47
1:A:125:ASN:O	1:A:129:PRO:HG2	2.14	0.47
1:B:277:ASP:O	1:B:280:LYS:HE2	2.13	0.47
1:A:431:PRO:HB3	1:A:485:LEU:HD22	1.96	0.47
1:B:582:PRO:HG2	1:B:585:PHE:HD1	1.79	0.47
1:B:440:ASP:C	1:B:442:PRO:HD2	2.35	0.47
1:B:412:GLU:HB2	1:B:415:HIS:HD2	1.78	0.47
1:A:128:LYS:HB2	1:A:129:PRO:HD3	1.97	0.47
1:B:9:LEU:O	1:B:12:ARG:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:LYS:HB2	1:B:207:PRO:HD3	1.96	0.47
1:B:171:LEU:HA	1:B:301:LYS:O	2.15	0.46
1:B:183:VAL:HG12	1:B:198:SER:HB2	1.97	0.46
1:B:225:LYS:HG3	1:B:326:ARG:HG2	1.97	0.46
1:A:596:ILE:N	1:A:596:ILE:HD13	2.25	0.46
1:B:527:VAL:O	1:B:527:VAL:HG23	2.14	0.46
1:A:75:GLU:HG3	1:A:594:ALA:CB	2.35	0.46
1:B:512:ALA:O	1:B:516:ILE:HG13	2.16	0.46
1:A:125:ASN:C	1:A:129:PRO:HG2	2.36	0.46
1:B:177:GLU:O	1:B:178:VAL:CG2	2.64	0.46
1:B:443:PHE:CE1	1:B:477:LYS:HD2	2.51	0.46
1:B:284:ILE:O	1:B:288:ILE:HB	2.15	0.46
1:B:215:LYS:O	1:B:218:LYS:HB2	2.15	0.46
1:B:87:HIS:O	1:B:90:VAL:HG12	2.16	0.46
1:B:444:ILE:CG2	1:B:444:ILE:O	2.62	0.45
1:B:409:PRO:O	1:B:410:ASN:HB2	2.16	0.45
1:B:125:ASN:C	1:B:129:PRO:HG2	2.36	0.45
1:B:476:TYR:HE1	1:B:585:PHE:HB3	1.82	0.45
1:A:412:GLU:HB2	1:A:415:HIS:HD2	1.81	0.45
1:A:401:VAL:N	1:A:458:ASN:HD21	2.03	0.45
1:A:23:TYR:CE1	1:A:117:LYS:HG2	2.51	0.45
1:A:453:PHE:HA	1:A:463:VAL:HG13	1.97	0.45
1:A:100:ILE:HG21	1:A:103:LEU:HD12	1.99	0.45
1:A:559:LYS:HA	1:A:564:LEU:HD11	1.98	0.45
1:A:267:LEU:HD13	1:A:319:LEU:HD13	1.98	0.45
1:A:45:PRO:HA	1:A:150:ARG:NH1	2.21	0.45
1:A:526:LYS:HD3	1:A:569:HIS:CD2	2.51	0.45
1:A:95:TYR:CD1	1:A:115:LEU:HD21	2.52	0.45
1:B:168:MET:O	1:B:169:LYS:HB2	2.17	0.45
1:A:259:VAL:HA	1:A:320:TYR:CE2	2.52	0.45
1:B:87:HIS:HE1	1:B:489:PHE:CE2	2.35	0.45
1:B:498:TRP:CZ2	1:B:561:ARG:HD2	2.52	0.45
1:B:387:ILE:HA	1:B:388:PRO:HD3	1.90	0.45
1:A:558:ILE:HG22	1:A:564:LEU:HD21	1.98	0.45
1:A:199:ILE:HB	1:A:201:PRO:HB3	1.99	0.45
1:A:265:CYS:HA	1:A:268:ILE:HD12	1.99	0.44
1:B:559:LYS:HA	1:B:564:LEU:HD11	1.99	0.44
1:B:5:TYR:HD2	1:B:86:ILE:HD11	1.82	0.44
1:A:140:THR:O	1:A:141:LEU:HB2	2.17	0.44
1:A:56:ILE:HG12	1:A:122:LEU:HD22	1.98	0.44
1:B:3:HIS:CD2	1:B:427:SER:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:LEU:O	1:A:489:PHE:HB2	2.17	0.44
1:B:267:LEU:HD13	1:B:319:LEU:HD13	1.99	0.44
1:A:52:LEU:HD21	1:A:127:VAL:HG22	1.99	0.44
1:A:48:ILE:HG21	1:A:131:ILE:HG12	2.00	0.44
1:B:248:ILE:HG13	1:B:375:THR:HB	2.00	0.44
1:A:180:PRO:O	1:A:182:GLY:N	2.51	0.44
1:B:448:PHE:HA	1:B:453:PHE:CE1	2.53	0.44
1:B:453:PHE:HE2	1:B:467:PHE:HB2	1.83	0.44
1:A:55:ILE:HD11	1:A:130:ILE:HD12	2.00	0.44
1:B:17:LYS:HA	1:B:35:ARG:NH1	2.32	0.44
1:A:87:HIS:HE1	1:A:489:PHE:CZ	2.35	0.44
1:A:412:GLU:HB2	1:A:415:HIS:CD2	2.52	0.44
1:B:184:LEU:HB3	1:B:295:PHE:HD1	1.83	0.44
1:A:242:GLN:H	1:A:242:GLN:CD	2.21	0.44
1:B:261:ILE:HD11	1:B:305:GLY:C	2.38	0.44
1:B:328:TYR:C	1:B:330:SER:H	2.21	0.44
1:A:340:ARG:HD3	1:A:345:TYR:CZ	2.52	0.44
1:A:97:TYR:CD1	1:A:111:ARG:HB3	2.53	0.43
1:A:264:LEU:CD2	1:A:306:LEU:HD21	2.49	0.43
1:A:460:GLN:HE22	1:A:525:ARG:H	1.66	0.43
1:A:24:ASN:ND2	1:A:102:TRP:HB2	2.34	0.43
1:B:250:VAL:HG11	1:B:362:ILE:CG2	2.48	0.43
1:B:189:LYS:HD3	1:B:194:ARG:HD3	2.00	0.43
1:B:177:GLU:C	1:B:178:VAL:HG23	2.39	0.43
1:A:264:LEU:HD23	1:A:288:ILE:CD1	2.38	0.43
1:A:267:LEU:HD11	1:A:323:PHE:HB2	1.99	0.43
1:A:517:VAL:HA	1:A:520:LYS:HG3	2.00	0.43
1:A:239:GLN:HB3	2:A:614:HOH:O	2.18	0.43
1:B:58:LYS:CE	1:B:64:THR:HG23	2.48	0.43
1:A:48:ILE:HG12	1:A:131:ILE:HA	2.00	0.43
1:B:217:TYR:HA	1:B:220:LEU:HD12	2.00	0.43
1:A:67:LEU:O	1:A:71:TYR:HD1	2.01	0.43
1:A:223:LYS:HZ3	1:A:326:ARG:HH12	1.67	0.42
1:A:342:VAL:HG23	1:A:343:ASP:H	1.84	0.42
1:A:15:ALA:HA	1:A:16:PRO:HD3	1.88	0.42
1:B:524:TYR:HE1	1:B:527:VAL:HG22	1.84	0.42
1:A:55:ILE:HG21	1:A:126:ILE:HG21	2.01	0.42
1:B:106:VAL:HG11	1:B:114:LEU:HD12	2.00	0.42
1:B:458:ASN:HA	1:B:458:ASN:HD22	1.62	0.42
1:B:541:LEU:HB3	1:B:545:LYS:HE2	2.01	0.42
1:A:184:LEU:HA	1:A:196:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:GLN:H	1:A:242:GLN:NE2	2.17	0.42
1:B:381:ARG:HB3	1:B:382:HIS:ND1	2.34	0.42
1:A:547:ARG:HB3	1:A:550:ILE:HB	2.02	0.42
1:A:52:LEU:HB3	1:A:71:TYR:CE2	2.54	0.42
1:B:341:THR:HG21	1:B:390:CYS:SG	2.59	0.42
1:B:47:GLN:HG3	1:B:50:ALA:HB3	2.01	0.42
1:A:498:TRP:CD2	1:A:557:ARG:HD3	2.55	0.42
1:B:174:VAL:HG13	1:B:178:VAL:HG21	1.98	0.42
1:B:444:ILE:HG23	1:B:447:SER:HB2	2.02	0.42
1:B:108:PRO:HA	1:B:111:ARG:HD2	2.02	0.41
1:B:74:VAL:HG22	1:B:127:VAL:HG11	2.02	0.41
1:A:268:ILE:HD11	1:A:288:ILE:HD12	2.02	0.41
1:B:274:HIS:H	1:B:274:HIS:CD2	2.36	0.41
1:A:409:PRO:O	1:A:410:ASN:HB2	2.20	0.41
1:A:213:THR:O	1:A:217:TYR:HD2	2.03	0.41
1:B:549:GLU:HG2	1:B:550:ILE:H	1.85	0.41
1:B:119:ASN:HD22	1:B:119:ASN:HA	1.70	0.41
1:B:310:ASP:OD2	1:B:312:LEU:HB2	2.21	0.41
1:A:135:TYR:CZ	1:A:596:ILE:HB	2.55	0.41
1:A:250:VAL:HG11	1:A:368:VAL:HG11	2.02	0.41
1:A:248:ILE:HD13	1:A:359:GLU:HB2	2.03	0.41
1:A:78:LEU:HD22	1:A:596:ILE:HG12	2.03	0.41
1:A:435:LEU:HG	1:A:485:LEU:HD11	2.03	0.41
1:A:333:ASP:HB3	1:A:336:ALA:CB	2.49	0.41
1:B:400:GLN:NE2	1:B:458:ASN:HA	2.36	0.41
1:B:437:LYS:O	1:B:440:ASP:HB2	2.21	0.41
1:B:67:LEU:O	1:B:71:TYR:HD1	2.04	0.41
1:B:407:LEU:HD23	1:B:416:LYS:HE3	2.03	0.41
1:A:262:PRO:O	1:A:266:LYS:HG2	2.20	0.41
1:A:540:PHE:O	1:A:544:LEU:HB2	2.21	0.41
1:B:87:HIS:HE1	1:B:489:PHE:CZ	2.39	0.41
1:B:452:GLU:HB3	1:B:466:ASN:HB3	2.03	0.41
1:A:341:THR:HG21	1:A:390:CYS:SG	2.61	0.41
1:B:557:ARG:HD3	1:B:561:ARG:CZ	2.51	0.40
1:A:189:LYS:O	1:A:190:GLN:C	2.59	0.40
1:A:527:VAL:O	1:A:527:VAL:HG23	2.21	0.40
1:B:448:PHE:HA	1:B:453:PHE:HE1	1.85	0.40
1:A:407:LEU:HD23	1:A:416:LYS:HE3	2.02	0.40
1:A:264:LEU:CD2	1:A:288:ILE:CD1	2.99	0.40
1:A:66:ASN:ND2	1:A:96:ASP:HB3	2.30	0.40
1:B:292:PHE:HD1	1:B:301:LYS:HG2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LYS:HD3	1:A:133:PHE:CE1	2.57	0.40
1:A:253:ARG:HG2	1:A:367:GLN:HE21	1.86	0.40
1:A:355:VAL:HG12	1:A:377:LEU:HD11	2.02	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%)	532 (90%)	55 (9%)	7 (1%)	16 58
1	B	594/596 (100%)	520 (88%)	59 (10%)	15 (2%)	7 40
All	All	1188/1192 (100%)	1052 (89%)	114 (10%)	22 (2%)	10 48

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	LYS
1	B	178	VAL
1	B	335	ASP
1	B	381	ARG
1	A	190	GLN
1	A	201	PRO
1	A	205	ARG
1	B	176	ASP
1	B	333	ASP
1	B	526	LYS
1	B	569	HIS
1	B	570	ASP
1	B	44	LYS
1	A	526	LYS
1	B	223	LYS

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Mol	Chain	Res	Type
1	B	229	SER
1	B	456	VAL
1	A	192	ASN
1	B	342	VAL
1	A	174	VAL
1	B	180	PRO
1	B	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%)	513 (93%)	39 (7%)	18	56
1	B	552/552 (100%)	519 (94%)	33 (6%)	24	64
All	All	1104/1104 (100%)	1032 (94%)	72 (6%)	21	60

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LYS
1	A	52	LEU
1	A	85	CYS
1	A	86	ILE
1	A	116	LEU
1	A	123	LEU
1	A	174	VAL
1	A	175	GLN
1	A	181	ARG
1	A	192	ASN
1	A	222	GLU
1	A	230	LEU
1	A	267	LEU
1	A	275	LEU
1	A	279	GLU
1	A	280	LYS

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Mol	Chain	Res	Type
1	A	293	VAL
1	A	297	ARG
1	A	303	ASN
1	A	317	CYS
1	A	318	GLU
1	A	319	LEU
1	A	338	ILE
1	A	343	ASP
1	A	362	ILE
1	A	387	ILE
1	A	435	LEU
1	A	436	GLN
1	A	454	ASN
1	A	455	THR
1	A	460	GLN
1	A	499	LEU
1	A	511	ARG
1	A	528	THR
1	A	566	MET
1	A	586	ARG
1	A	591	ASN
1	A	593	LYS
1	A	596	ILE
1	B	13	GLN
1	B	26	ILE
1	B	49	LEU
1	B	64	THR
1	B	84	GLU
1	B	86	ILE
1	B	110	LEU
1	B	120	LEU
1	B	123	LEU
1	B	197	VAL
1	B	199	ILE
1	B	211	LEU
1	B	212	LEU
1	B	249	LYS
1	B	280	LYS
1	B	284	ILE
1	B	288	ILE
1	B	338	ILE
1	B	343	ASP

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Mol	Chain	Res	Type
1	B	380	HIS
1	B	387	ILE
1	B	390	CYS
1	B	392	LYS
1	B	428	ASP
1	B	435	LEU
1	B	440	ASP
1	B	445	CYS
1	B	455	THR
1	B	458	ASN
1	B	492	ASN
1	B	548	THR
1	B	568	PHE
1	B	588	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	118	HIS
1	A	119	ASN
1	A	142	ASN
1	A	175	GLN
1	A	192	ASN
1	A	258	ASN
1	A	269	GLN
1	A	367	GLN
1	A	436	GLN
1	A	454	ASN
1	A	458	ASN
1	B	3	HIS
1	B	40	HIS
1	B	66	ASN
1	B	80	GLN
1	B	92	HIS
1	B	118	HIS
1	B	119	ASN
1	B	192	ASN
1	B	258	ASN
1	B	269	GLN
1	B	274	HIS
1	B	291	GLN

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Mol	Chain	Res	Type
1	B	367	GLN
1	B	380	HIS
1	B	436	GLN
1	B	454	ASN
1	B	458	ASN
1	B	460	GLN

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 carbohydrates 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

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, 95^{th} 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%)	0.01	2 (0%)	94	93	17, 32, 67, 93	0
1	B	596/596 (100%)	0.03	3 (0%)	91	88	17, 34, 70, 85	0
All	All	1192/1192 (100%)	0.02	5 (0%)	93	91	17, 34, 69, 93	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	284	ILE	3.3
1	A	178	VAL	2.9
1	A	177	GLU	2.3
1	B	175	GLN	2.3
1	B	199	ILE	2.1

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.