



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:58 PM UTC

PDB ID : 3DU5 / pdb_00003du5
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

<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

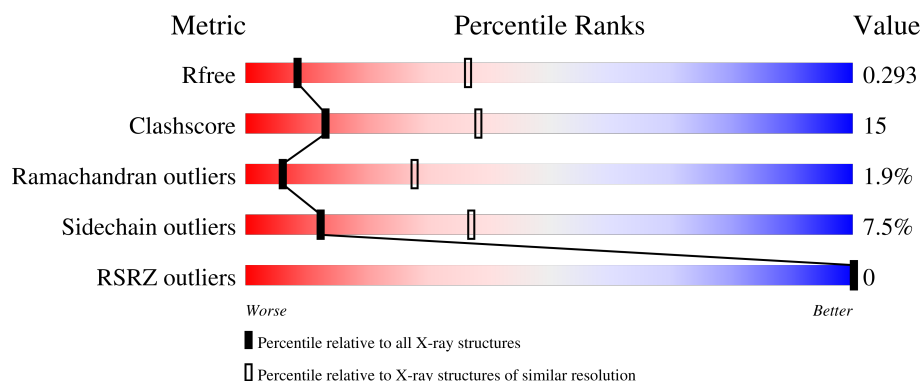
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	 66% 30% 5%
1	B	596	 64% 31% 5%

2 Entry composition

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			

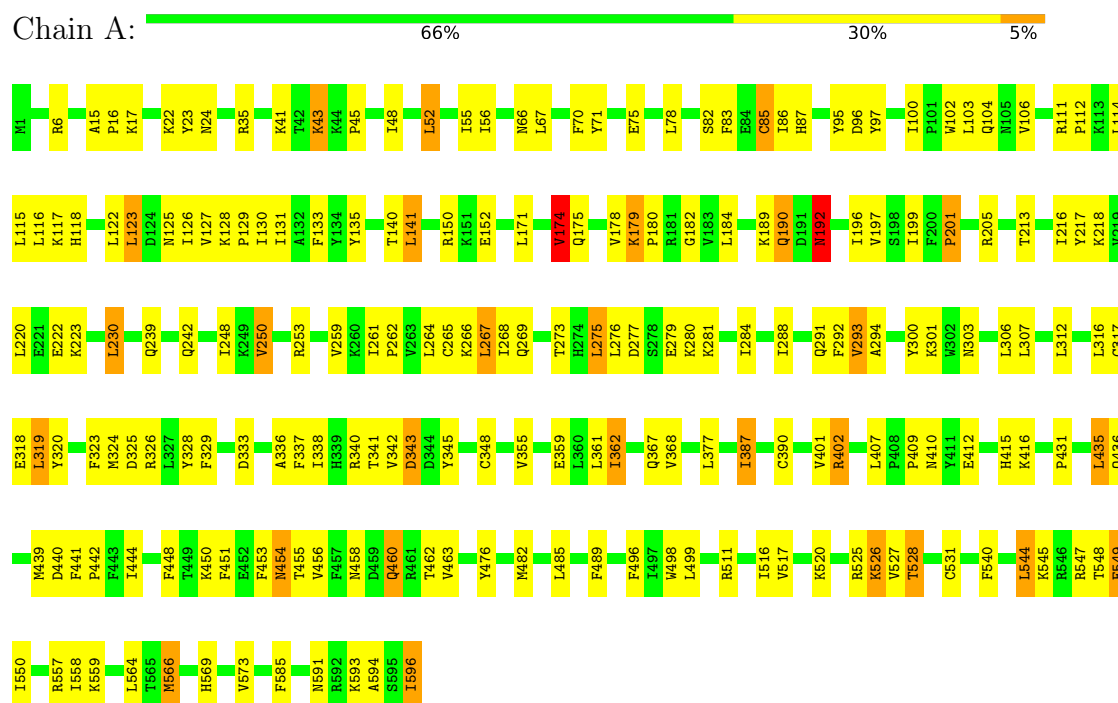
- Molecule 2 is water.

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

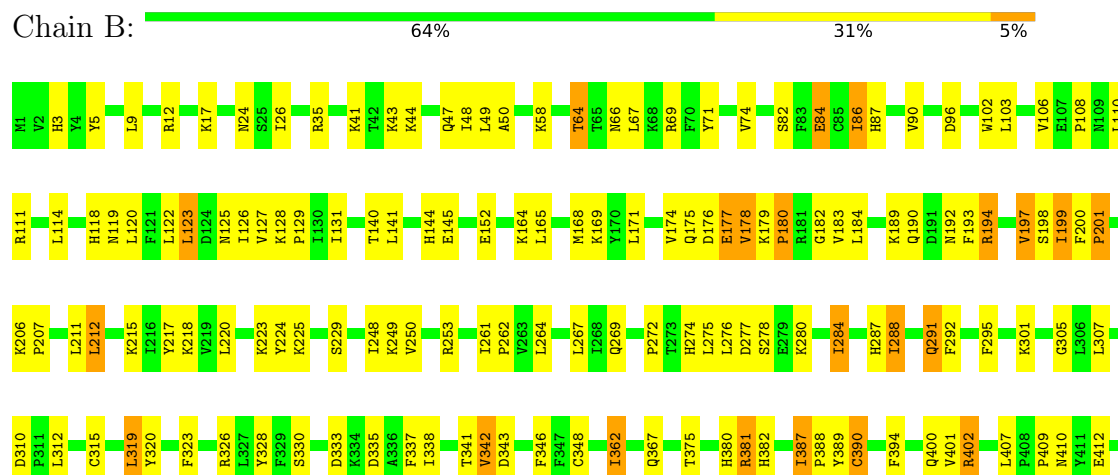
3 Residue-property plots

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



H415	K416	F417	S427	D428	P431	L435	Q436	K437	D440	F441	P442	F443	I444	S447	F448	T449	K450	F451	E452	F453	N454	T455	V456	F457	M458	D459	Q460	R461	T462	V463	M466	F467	Y476	K477	F478	M482	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

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 20.00 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-3.25) 99.6 (20.00-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ 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	1749 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 14.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.168 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	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.*

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	0.39	0/5114	0.71	0/6893
1	B	0.40	1/5114 (0.0%)	0.71	0/6893
All	All	0.40	1/10228 (0.0%)	0.71	0/13786

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	177	GLU	C-O	5.45	1.30	1.23

There are no bond angle outliers.

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	156	0
1	B	4982	0	5126	145	0
2	A	45	0	0	1	0
2	B	32	0	0	0	0
All	All	10041	0	10252	301	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 15.

All (301) 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: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:178:VAL:HG12	1:B:179:LYS:N	1.61	1.03
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:HG22	1:B:444:ILE:O	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:566:MET:H	1:A:566:MET:HE2	1.62	0.63
1:B:164:LYS:HG2	1:B:168:MET:HE3	1.81	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:337:PHE:HB3	1:A:348:CYS:HB2	1.83	0.61
1:A:448:PHE:HA	1:A:453:PHE:HE1	1.66	0.61
1:A:180:PRO:C	1:A:182:GLY:H	2.08	0.61
1:B:417:PHE:HB3	1:B:477:LYS:HE3	1.83	0.60
1:A:189:LYS:HE2	1:A:192:ASN:HB3	1.83	0.60
1:B:140:THR:O	1:B:141:LEU:HB2	2.00	0.60
1:B:441:PHE:N	1:B:442:PRO:HD2	2.16	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:A:178:VAL:HG12	1:A:179:LYS:H	1.68	0.59
1:B:24:ASN:ND2	1:B:102:TRP:HB2	2.17	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:A:325:ASP:O	1:A:329:PHE:HB2	2.03	0.58
1:B:212:LEU:HD11	1:B:284:ILE:HG12	1.84	0.58
1:A:516:ILE:HG21	1:A:527:VAL:HG21	1.85	0.58
1:A:178:VAL:C	1:A:180:PRO:HD3	2.28	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:B:287:HIS:O	1:B:291:GLN:HG3	2.05	0.56
1:B:199:ILE:HD13	1:B:199:ILE:H	1.70	0.56
1:B:224:TYR:OH	1:B:267:LEU:HD21	2.05	0.56
1:B:261:ILE:HB	1:B:262:PRO:HD3	1.86	0.56
1:B:269:GLN:HA	1:B:280:LYS:HZ2	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:217:TYR:CE2	1:B:315:CYS:HB3	2.42	0.55
1:A:253:ARG:HE	1:A:367:GLN:HG2	1.72	0.55
1:B:182:GLY:HA2	1:B:198:SER:O	2.06	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:250:VAL:HG21	1:B:362:ILE:HG21	1.90	0.54
1:B:276:LEU:HD13	1:B:280:LYS:HD3	1.88	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: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:A:435:LEU:HD11	1:A:482:MET:HE1	1.89	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:B:538:ARG:HH21	1:B:564:LEU:C	2.18	0.52
1:A:22:LYS:HD3	1:A:117:LYS:HZ1	1.74	0.52
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: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:440:ASP:C	1:B:442:PRO:HD2	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:125:ASN:C	1:A:129:PRO:HG2	2.36	0.51
1:A:250:VAL:HG21	1:A:362:ILE:HG21	1.92	0.51
1:A:52:LEU:HB3	1:A:71:TYR:HE2	1.76	0.50
1:A:276:LEU:HB3	1:A:280:LYS:CG	2.21	0.50
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:B:125:ASN:C	1:B:129:PRO:HG2	2.36	0.49
1:A:43:LYS:H	1:A:43:LYS:HD2	1.76	0.49
1:A:441:PHE:H	1:A:442:PRO:HD2	1.77	0.49
1:A:275:LEU:H	1:A:275:LEU:HD12	1.77	0.49
1:B:200:PHE:N	1:B:201:PRO:HA	2.28	0.49
1:B:520:LYS:HD2	1:B:524:TYR:CD2	2.47	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:A:545:LYS:O	1:A:548:THR:HG23	2.13	0.49
1:B:103:LEU:HD22	1:B:111:ARG:HG2	1.95	0.49
1:B:125:ASN:O	1:B:129:PRO:HG2	2.13	0.49
1:A:312:LEU:HB3	1:A:316:LEU:HD12	1.94	0.49
1:B:189:LYS:HG2	1:B:190:GLN:H	1.78	0.48
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:A:242:GLN:CD	1:A:242:GLN:H	2.21	0.48
1:A:328:TYR:O	1:A:361:LEU:HD21	2.12	0.48
1:B:261:ILE:HD11	1:B:305:GLY:C	2.38	0.48
1:B:328:TYR:C	1:B:330:SER:H	2.21	0.48
1:B:387:ILE:HD13	1:B:394:PHE:O	2.13	0.48
1:B:177:GLU:C	1:B:178:VAL:HG23	2.39	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:346:PHE:CZ	1:B:387:ILE:HD11	2.49	0.48
1:B:269:GLN:HA	1:B:280:LYS:NZ	2.29	0.47
1:B:400:GLN:HE22	1:B:458:ASN:HA	1.79	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:223:LYS:HZ3	1:A:326:ARG:HH12	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ASN:O	1:A:129:PRO:HG2	2.14	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:431:PRO:HB3	1:A:485:LEU:HD22	1.96	0.47
1:B:277:ASP:O	1:B:280:LYS:HE2	2.13	0.47
1:B:582:PRO:HG2	1:B:585:PHE:HD1	1.79	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
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:HD13	1:A:596:ILE:N	2.25	0.46
1:B:527:VAL:HG23	1:B:527:VAL:O	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:B:177:GLU:O	1:B:178:VAL:CG2	2.64	0.46
1:B:87:HIS:O	1:B:90:VAL:HG12	2.16	0.46
1:B:215:LYS:O	1:B:218:LYS:HB2	2.15	0.46
1:B:284:ILE:O	1:B:288:ILE:HB	2.15	0.46
1:B:443:PHE:CE1	1:B:477:LYS:HD2	2.51	0.46
1:B:409:PRO:O	1:B:410:ASN:HB2	2.16	0.45
1:B:444:ILE:O	1:B:444:ILE:CG2	2.62	0.45
1:A:412:GLU:HB2	1:A:415:HIS:HD2	1.81	0.45
1:B:476:TYR:HE1	1:B:585:PHE:HB3	1.82	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:100:ILE:HG21	1:A:103:LEU:HD12	1.99	0.45
1:A:189:LYS:O	1:A:190:GLN:C	2.59	0.45
1:A:453:PHE:HA	1:A:463:VAL:HG13	1.97	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:95:TYR:CD1	1:A:115:LEU:HD21	2.52	0.45
1:A:526:LYS:HD3	1:A:569:HIS:CD2	2.51	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:A:199:ILE:HB	1:A:201:PRO:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:MET:HE2	1:A:439:MET:HA	1.99	0.45
1:A:558:ILE:HG22	1:A:564:LEU:HD21	1.98	0.45
1:B:387:ILE:HA	1:B:388:PRO:HD3	1.90	0.45
1:A:140:THR:O	1:A:141:LEU:HB2	2.17	0.44
1:A:265:CYS:HA	1:A:268:ILE:HD12	1.99	0.44
1:B:5:TYR:HD2	1:B:86:ILE:HD11	1.82	0.44
1:B:559:LYS:HA	1:B:564:LEU:HD11	1.99	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
1:B:277:ASP:CG	1:B:278:SER:H	2.26	0.44
1:A:485:LEU:O	1:A:489:PHE:HB2	2.17	0.44
1:A:48:ILE:HG21	1:A:131:ILE:HG12	2.00	0.44
1:A:52:LEU:HD21	1:A:127:VAL:HG22	1.99	0.44
1:B:248:ILE:HG13	1:B:375:THR:HB	2.00	0.44
1:B:267:LEU:HD13	1:B:319:LEU:HD13	1.99	0.44
1:A:55:ILE:HD11	1:A:130:ILE:HD12	2.00	0.44
1:A:180:PRO:O	1:A:182:GLY:N	2.51	0.44
1:B:17:LYS:HA	1:B:35:ARG:NH1	2.32	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: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: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:B:178:VAL:C	1:B:180:PRO:HD3	2.43	0.43
1:B:192:ASN:CG	1:B:193:PHE:H	2.25	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:B:435:LEU:HD11	1:B:482:MET:HE1	1.99	0.43
1:A:24:ASN:ND2	1:A:102:TRP:HB2	2.34	0.43
1:B:189:LYS:HD3	1:B:194:ARG:HD3	2.00	0.43
1:B:250:VAL:HG11	1:B:362:ILE:CG2	2.48	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:A:67:LEU:O	1:A:71:TYR:HD1	2.01	0.43
1:B:217:TYR:HA	1:B:220:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ALA:HA	1:A:16:PRO:HD3	1.88	0.42
1:A:104:GLN:C	1:A:106:VAL:H	2.25	0.42
1:A:342:VAL:HG23	1:A:343:ASP:H	1.84	0.42
1:A:55:ILE:HG21	1:A:126:ILE:HG21	2.01	0.42
1:B:524:TYR:HE1	1:B:527:VAL:HG22	1.84	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
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:52:LEU:HB3	1:A:71:TYR:CE2	2.54	0.42
1:A:547:ARG:HB3	1:A:550:ILE:HB	2.02	0.42
1:B:341:THR:HG21	1:B:390:CYS:SG	2.59	0.42
1:A:498:TRP:CD2	1:A:557:ARG:HD3	2.55	0.42
1:B:47:GLN:HG3	1:B:50:ALA:HB3	2.01	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:74:VAL:HG22	1:B:127:VAL:HG11	2.02	0.41
1:B:108:PRO:HA	1:B:111:ARG:HD2	2.02	0.41
1:A:268:ILE:HD11	1:A:288:ILE:HD12	2.02	0.41
1:A:409:PRO:O	1:A:410:ASN:HB2	2.20	0.41
1:B:274:HIS:CD2	1:B:274:HIS:H	2.36	0.41
1:A:180:PRO:C	1:A:182:GLY:N	2.76	0.41
1:A:213:THR:O	1:A:217:TYR:HD2	2.03	0.41
1:B:119:ASN:HD22	1:B:119:ASN:HA	1.70	0.41
1:B:549:GLU:HG2	1:B:550:ILE:H	1.85	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:248:ILE:HD13	1:A:359:GLU:HB2	2.03	0.41
1:A:250:VAL:HG11	1:A:368:VAL:HG11	2.02	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: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:67:LEU:O	1:B:71:TYR:HD1	2.04	0.41
1:B:400:GLN:NE2	1:B:458:ASN:HA	2.36	0.41
1:B:407:LEU:HD23	1:B:416:LYS:HE3	2.03	0.41
1:B:437:LYS:O	1:B:440:ASP:HB2	2.21	0.41
1:A:341:THR:HG21	1:A:390:CYS:SG	2.61	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:B:452:GLU:HB3	1:B:466:ASN:HB3	2.03	0.41
1:B:557:ARG:HD3	1:B:561:ARG:CZ	2.51	0.40
1:A:407:LEU:HD23	1:A:416:LYS:HE3	2.02	0.40
1:A:527:VAL:HG23	1:A:527:VAL:O	2.21	0.40
1:B:448:PHE:HA	1:B:453:PHE:HE1	1.85	0.40
1:A:264:LEU:CD2	1:A:288:ILE:CD1	2.99	0.40
1:B:274:HIS:C	1:B:276:LEU:H	2.27	0.40
1:A:41:LYS:HD3	1:A:133:PHE:CE1	2.57	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
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%)	10	36
1	B	594/596 (100%)	520 (88%)	59 (10%)	15 (2%)	4	22
All	All	1188/1192 (100%)	1052 (89%)	114 (10%)	22 (2%)	6	28

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

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Mol	Chain	Res	Type
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
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%)	506 (92%)	46 (8%)	10	34
1	B	552/552 (100%)	515 (93%)	37 (7%)	15	41
All	All	1104/1104 (100%)	1021 (92%)	83 (8%)	12	37

All (83) 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	114	LEU
1	A	116	LEU

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Mol	Chain	Res	Type
1	A	123	LEU
1	A	141	LEU
1	A	152	GLU
1	A	174	VAL
1	A	175	GLN
1	A	192	ASN
1	A	222	GLU
1	A	230	LEU
1	A	250	VAL
1	A	267	LEU
1	A	273	THR
1	A	275	LEU
1	A	279	GLU
1	A	293	VAL
1	A	303	ASN
1	A	317	CYS
1	A	318	GLU
1	A	319	LEU
1	A	324	MET
1	A	338	ILE
1	A	343	ASP
1	A	362	ILE
1	A	387	ILE
1	A	402	ARG
1	A	435	LEU
1	A	436	GLN
1	A	444	ILE
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	544	LEU
1	A	549	GLU
1	A	566	MET
1	A	573	VAL
1	A	591	ASN
1	A	593	LYS
1	A	596	ILE
1	B	26	ILE
1	B	49	LEU

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Mol	Chain	Res	Type
1	B	64	THR
1	B	69	ARG
1	B	84	GLU
1	B	86	ILE
1	B	110	LEU
1	B	120	LEU
1	B	123	LEU
1	B	152	GLU
1	B	175	GLN
1	B	194	ARG
1	B	197	VAL
1	B	199	ILE
1	B	211	LEU
1	B	212	LEU
1	B	284	ILE
1	B	288	ILE
1	B	291	GLN
1	B	319	LEU
1	B	338	ILE
1	B	342	VAL
1	B	343	ASP
1	B	362	ILE
1	B	380	HIS
1	B	387	ILE
1	B	390	CYS
1	B	402	ARG
1	B	428	ASP
1	B	435	LEU
1	B	440	ASP
1	B	455	THR
1	B	458	ASN
1	B	492	ASN
1	B	548	THR
1	B	568	PHE
1	B	588	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	92	HIS
1	A	118	HIS

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Mol	Chain	Res	Type
1	A	119	ASN
1	A	142	ASN
1	A	175	GLN
1	A	192	ASN
1	A	244	GLN
1	A	258	ASN
1	A	269	GLN
1	A	304	HIS
1	A	367	GLN
1	A	382	HIS
1	A	436	GLN
1	A	454	ASN
1	A	458	ASN
1	B	3	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	244	GLN
1	B	258	ASN
1	B	269	GLN
1	B	274	HIS
1	B	287	HIS
1	B	291	GLN
1	B	308	GLN
1	B	367	GLN
1	B	380	HIS
1	B	458	ASN
1	B	460	GLN
1	B	591	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-1.73	0 100 100	17, 32, 67, 93	0
1	B	596/596 (100%)	-1.75	0 100 100	17, 34, 70, 85	0
All	All	1192/1192 (100%)	-1.74	0 100 100	17, 34, 69, 93	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.