Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:25 pm BST

PDB ID	:	4LMO
Title	:	Structure of a vertebrate RNA binding domain of telomerase (TRBD)
Authors	:	Harkisheimer, M.; Mason, M.; Shuvaeva, E.; Skordalakes, E.
Deposited on	:	2013-07-10
Resolution	:	2.37 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 following versions of software and data (see references ①) were used in the production of this report:

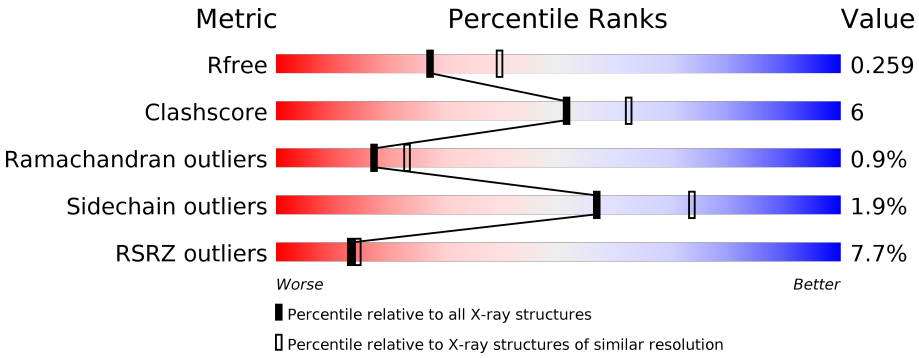
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 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 <=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	254	6% 88% 11%
1	B	254	9% 86% 12%
1	C	254	7% 82% 15%
1	D	254	8% 84% 15%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8456 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	251	Total	C	N	O	S	0	0	0
			2078	1348	383	336	11			
1	B	251	Total	C	N	O	S	0	0	0
			2078	1348	383	336	11			
1	C	251	Total	C	N	O	S	0	0	0
			2078	1348	383	336	11			
1	D	251	Total	C	N	O	S	0	0	0
			2078	1348	383	336	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	SER	-	EXPRESSION TAG	UNP Q4KTA7
A	292	ASN	-	EXPRESSION TAG	UNP Q4KTA7
A	293	ALA	-	EXPRESSION TAG	UNP Q4KTA7
B	291	SER	-	EXPRESSION TAG	UNP Q4KTA7
B	292	ASN	-	EXPRESSION TAG	UNP Q4KTA7
B	293	ALA	-	EXPRESSION TAG	UNP Q4KTA7
C	291	SER	-	EXPRESSION TAG	UNP Q4KTA7
C	292	ASN	-	EXPRESSION TAG	UNP Q4KTA7
C	293	ALA	-	EXPRESSION TAG	UNP Q4KTA7
D	291	SER	-	EXPRESSION TAG	UNP Q4KTA7
D	292	ASN	-	EXPRESSION TAG	UNP Q4KTA7
D	293	ALA	-	EXPRESSION TAG	UNP Q4KTA7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	30	Total	O	0	0
			30	30		
2	B	37	Total	O	0	0
			37	37		

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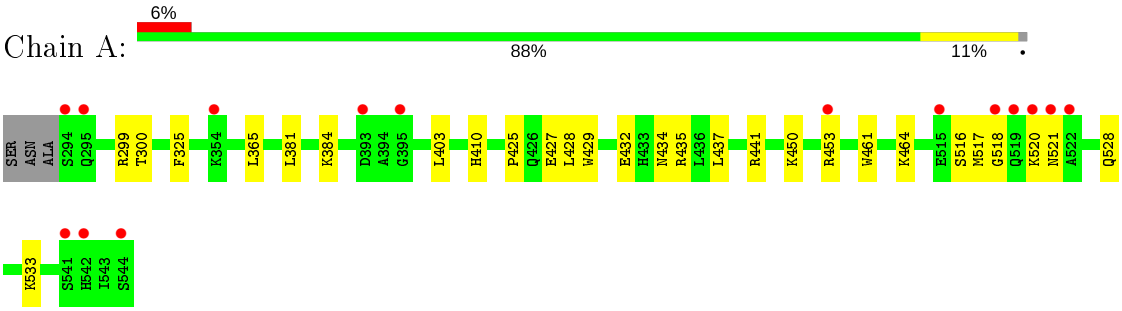
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	38	Total O 38 38	0	0
2	D	39	Total O 39 39	0	0

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 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.

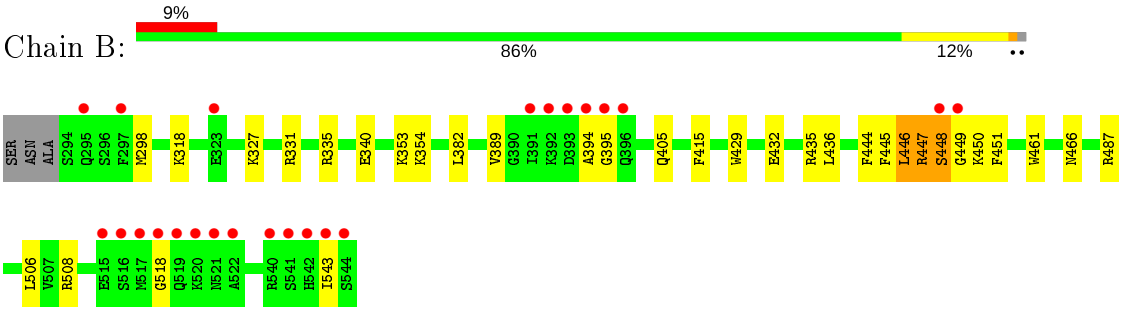
- Molecule 1: Telomerase reverse transcriptase

Chain A:



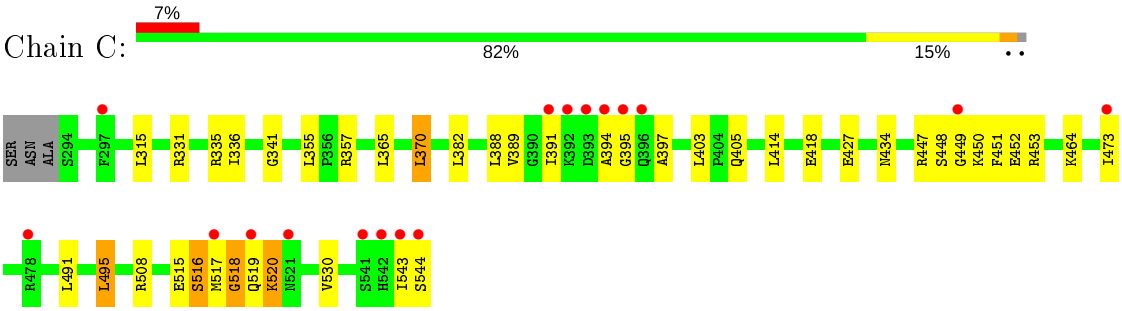
- Molecule 1: Telomerase reverse transcriptase

Chain B:



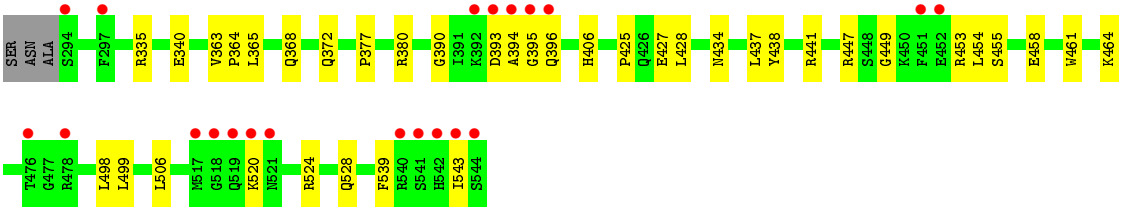
- Molecule 1: Telomerase reverse transcriptase

Chain C:



- Molecule 1: Telomerase reverse transcriptase

Chain D:


SER
ASN
ALA
S294
F297
R335
E340
V363
P364
L365
Q368
Q372
P377
R380
G390
I391
K392
D393
A394
G395
Q396
H406
P425
Q426
E427
L428
N434
L437
Y438
R441
R447
S448
G449
K450
F451
E452
R453
L454
S455
E458
W461
K464
T476
G477
R478
L498
L499
L506
M517
G518
Q519
K520
M521
R524
Q528
F539
R540
S541
H542
I543
S544

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.63Å 84.51Å 137.17Å 90.00° 94.31° 90.00°	Depositor
Resolution (Å)	20.00 – 2.37 44.66 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (20.00-2.37) 78.9 (44.66-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.220 , 0.259 0.220 , 0.259	Depositor DCC
R_{free} test set	2865 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	33.0	Xtriage
Anisotropy	0.574	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 34.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8456	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.51% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.46	1/2129 (0.0%)	0.50	0/2858
1	B	0.46	1/2129 (0.0%)	0.51	0/2858
1	C	0.46	0/2129	0.53	0/2858
1	D	0.46	1/2129 (0.0%)	0.50	0/2858
All	All	0.46	3/8516 (0.0%)	0.51	0/11432

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	461	TRP	CD2-CE2	5.06	1.47	1.41
1	D	461	TRP	CD2-CE2	5.03	1.47	1.41
1	B	461	TRP	CD2-CE2	5.01	1.47	1.41

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	2078	0	2140	21	0
1	B	2078	0	2140	28	0
1	C	2078	0	2140	32	0
1	D	2078	0	2140	19	0
2	A	30	0	0	0	0
2	B	37	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	38	0	0	0	0
2	D	39	0	0	0	0
All	All	8456	0	8560	95	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 6.

All (95) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:SER:CB	1:A:517:MET:HA	1.70	1.18
1:C:448:SER:HB3	1:C:452:GLU:HG3	1.27	1.15
1:B:394:ALA:CB	1:B:395:GLY:HA2	1.71	1.14
1:A:516:SER:HB3	1:A:517:MET:HA	1.18	1.10
1:C:394:ALA:H	1:C:395:GLY:HA2	0.89	1.03
1:C:394:ALA:N	1:C:395:GLY:HA2	1.73	1.01
1:B:394:ALA:HB1	1:B:395:GLY:CA	1.90	1.01
1:C:394:ALA:H	1:C:395:GLY:CA	1.76	0.98
1:B:394:ALA:HB1	1:B:395:GLY:HA2	0.95	0.95
1:B:447:ARG:C	1:B:449:GLY:HA2	1.97	0.84
1:A:516:SER:HB3	1:A:517:MET:CA	2.05	0.82
1:C:448:SER:HB3	1:C:452:GLU:CG	2.09	0.79
1:C:434:ASN:HD21	1:C:464:LYS:H	1.30	0.79
1:B:394:ALA:CB	1:B:395:GLY:CA	2.55	0.73
1:C:448:SER:CB	1:C:452:GLU:HG3	2.15	0.73
1:D:434:ASN:HD21	1:D:464:LYS:H	1.35	0.73
1:A:516:SER:HB2	1:A:517:MET:HA	1.67	0.72
1:C:357:ARG:HH12	1:C:473:ILE:HG23	1.55	0.70
1:A:516:SER:CB	1:A:517:MET:CA	2.58	0.69
1:A:434:ASN:HD21	1:A:464:LYS:H	1.42	0.68
1:C:448:SER:C	1:C:450:LYS:HA	2.18	0.64
1:B:432:GLU:CD	1:B:435:ARG:HH12	2.01	0.63
1:B:448:SER:N	1:B:449:GLY:HA2	2.13	0.62
1:A:300:THR:HG21	1:D:449:GLY:O	2.01	0.61
1:B:444:PHE:O	1:B:447:ARG:HB2	2.01	0.61
1:C:389:VAL:H	1:C:405:GLN:HE22	1.47	0.61
1:B:389:VAL:H	1:B:405:GLN:NE2	1.98	0.60
1:D:390:GLY:HA2	1:D:393:ASP:HB3	1.84	0.60
1:A:365:LEU:HD21	1:A:427:GLU:HG3	1.82	0.60
1:C:389:VAL:H	1:C:405:GLN:NE2	2.00	0.59
1:A:381:LEU:HD23	1:A:384:LYS:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:GLY:HA3	1:C:397:ALA:H	1.68	0.59
1:B:445:PHE:CD2	1:B:446:LEU:HD13	2.39	0.57
1:B:445:PHE:HD2	1:B:446:LEU:HD13	1.69	0.57
1:B:318:LYS:HE2	1:B:327:LYS:HE3	1.87	0.56
1:D:377:PRO:HB2	1:D:380:ARG:HB2	1.86	0.55
1:A:432:GLU:CD	1:A:435:ARG:HH12	2.09	0.55
1:C:336:ILE:O	1:C:341:GLY:HA2	2.06	0.55
1:C:515:GLU:O	1:C:517:MET:N	2.40	0.54
1:B:508:ARG:HH21	1:C:508:ARG:NH1	2.04	0.54
1:B:447:ARG:O	1:B:448:SER:HB2	2.08	0.54
1:A:517:MET:HB2	1:A:518:GLY:HA3	1.90	0.54
1:D:455:SER:HB3	1:D:458:GLU:HB2	1.90	0.53
1:B:331:ARG:HH12	1:B:354:LYS:HA	1.72	0.53
1:B:331:ARG:NH1	1:B:353:LYS:O	2.41	0.53
1:B:447:ARG:O	1:B:448:SER:CB	2.56	0.53
1:B:447:ARG:O	1:B:449:GLY:HA2	2.10	0.52
1:C:391:ILE:HD11	1:C:530:VAL:HG22	1.91	0.51
1:B:543:ILE:HD11	1:C:403:LEU:HD12	1.92	0.51
1:D:425:PRO:HD2	1:D:428:LEU:HD12	1.93	0.50
1:A:437:LEU:O	1:A:441:ARG:HG2	2.11	0.50
1:C:449:GLY:N	1:C:450:LYS:HA	2.26	0.50
1:A:425:PRO:HD2	1:A:428:LEU:HD12	1.94	0.49
1:D:539:PHE:O	1:D:543:ILE:HG22	2.12	0.49
1:D:454:LEU:HD22	1:D:499:LEU:HD23	1.95	0.48
1:A:429:TRP:CE2	1:A:435:ARG:HG3	2.49	0.48
1:D:365:LEU:HD21	1:D:427:GLU:CG	2.44	0.48
1:D:368:GLN:HE21	1:D:372:GLN:NE2	2.12	0.48
1:C:388:LEU:HB3	1:C:391:ILE:HD13	1.95	0.48
1:A:450:LYS:HD3	1:A:453:ARG:HD2	1.97	0.47
1:C:394:ALA:N	1:C:395:GLY:CA	2.52	0.47
1:D:394:ALA:HA	1:D:395:GLY:HA3	1.77	0.46
1:A:365:LEU:HD21	1:A:427:GLU:CG	2.45	0.46
1:A:403:LEU:HD13	1:D:543:ILE:HD12	1.97	0.46
1:C:516:SER:O	1:C:517:MET:HB2	2.15	0.46
1:D:437:LEU:O	1:D:441:ARG:HG2	2.16	0.46
1:B:429:TRP:CD2	1:B:435:ARG:HG3	2.50	0.45
1:B:335:ARG:HD3	1:B:340:GLU:OE1	2.15	0.45
1:A:517:MET:H	1:A:518:GLY:HA3	1.81	0.45
1:B:389:VAL:H	1:B:405:GLN:HE22	1.62	0.45
1:C:450:LYS:HB2	1:C:451:PHE:CD2	2.51	0.45
1:C:448:SER:O	1:C:450:LYS:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:HIS:H	1:A:410:HIS:CD2	2.35	0.44
1:B:429:TRP:CE2	1:B:435:ARG:HG3	2.53	0.44
1:C:365:LEU:HD21	1:C:427:GLU:CG	2.48	0.43
1:D:438:TYR:OH	1:D:498:LEU:HB3	2.18	0.43
1:C:434:ASN:ND2	1:C:464:LYS:H	2.06	0.43
1:A:520:LYS:HA	1:A:521:ASN:HA	1.59	0.43
1:B:450:LYS:O	1:B:451:PHE:C	2.57	0.43
1:C:518:GLY:C	1:C:520:LYS:H	2.22	0.43
1:B:382:LEU:HG	1:B:415:PHE:CE1	2.53	0.43
1:D:335:ARG:HD3	1:D:340:GLU:OE1	2.19	0.43
1:C:543:ILE:O	1:C:543:ILE:HG22	2.18	0.42
1:C:491:LEU:O	1:C:495:LEU:HB2	2.19	0.42
1:C:543:ILE:HA	1:C:544:SER:HA	1.69	0.42
1:C:315:LEU:HD22	1:C:370:LEU:HD11	2.02	0.42
1:A:325:PHE:CE1	1:D:453:ARG:HG2	2.55	0.42
1:C:331:ARG:HG3	1:C:355:LEU:HD11	2.02	0.41
1:D:406:HIS:CD2	1:D:524:ARG:HD3	2.56	0.41
1:D:363:VAL:HB	1:D:364:PRO:HD3	2.01	0.41
1:C:331:ARG:O	1:C:335:ARG:HG2	2.20	0.41
1:B:445:PHE:CD2	1:B:446:LEU:CD1	3.04	0.40
1:B:448:SER:HB2	1:B:450:LYS:HG3	2.04	0.40
1:B:466:ASN:ND2	1:B:487:ARG:HH21	2.19	0.40
1:D:434:ASN:ND2	1:D:464:LYS:H	2.11	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	249/254 (98%)	237 (95%)	12 (5%)	0	100 100
1	B	249/254 (98%)	233 (94%)	14 (6%)	2 (1%)	19 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	249/254 (98%)	231 (93%)	13 (5%)	5 (2%)	7 8
1	D	249/254 (98%)	239 (96%)	8 (3%)	2 (1%)	19 27
All	All	996/1016 (98%)	940 (94%)	47 (5%)	9 (1%)	17 23

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	448	SER
1	C	516	SER
1	C	520	LYS
1	B	518	GLY
1	C	518	GLY
1	C	453	ARG
1	D	520	LYS
1	D	396	GLN
1	C	519	GLN

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	221/223 (99%)	218 (99%)	3 (1%)	67 81
1	B	221/223 (99%)	216 (98%)	5 (2%)	50 68
1	C	221/223 (99%)	215 (97%)	6 (3%)	44 62
1	D	221/223 (99%)	218 (99%)	3 (1%)	67 81
All	All	884/892 (99%)	867 (98%)	17 (2%)	57 73

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	299	ARG
1	A	528	GLN
1	A	533	LYS

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Mol	Chain	Res	Type
1	B	298	MET
1	B	436	LEU
1	B	446	LEU
1	B	447	ARG
1	B	506	LEU
1	C	370	LEU
1	C	382	LEU
1	C	414	LEU
1	C	418	GLU
1	C	447	ARG
1	C	495	LEU
1	D	447	ARG
1	D	506	LEU
1	D	528	GLN

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	361	ASN
1	A	368	GLN
1	A	372	GLN
1	A	405	GLN
1	A	410	HIS
1	A	433	HIS
1	A	434	ASN
1	A	467	ASN
1	B	361	ASN
1	B	368	GLN
1	B	372	GLN
1	B	405	GLN
1	B	466	ASN
1	B	542	HIS
1	C	361	ASN
1	C	368	GLN
1	C	372	GLN
1	C	405	GLN
1	C	433	HIS
1	C	434	ASN
1	C	466	ASN
1	C	542	HIS
1	D	346	ASN
1	D	361	ASN

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Mol	Chain	Res	Type
1	D	372	GLN
1	D	406	HIS
1	D	433	HIS
1	D	434	ASN
1	D	466	ASN
1	D	467	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no 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	251/254 (98%)	0.10	15 (5%) 21 24	25, 40, 87, 107	0
1	B	251/254 (98%)	0.18	24 (9%) 8 9	27, 39, 90, 119	0
1	C	251/254 (98%)	0.32	17 (6%) 17 18	27, 43, 93, 112	0
1	D	251/254 (98%)	0.30	21 (8%) 11 12	25, 42, 87, 111	0
All	All	1004/1016 (98%)	0.22	77 (7%) 13 14	25, 41, 90, 119	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	518	GLY	11.5
1	B	543	ILE	9.0
1	A	544	SER	8.4
1	C	541	SER	8.4
1	A	520	LYS	7.5
1	C	542	HIS	7.3
1	C	544	SER	7.1
1	B	542	HIS	6.5
1	D	518	GLY	6.5
1	D	541	SER	6.4
1	C	396	GLN	6.2
1	D	542	HIS	6.0
1	B	395	GLY	5.9
1	A	541	SER	5.7
1	B	521	ASN	5.7
1	C	394	ALA	5.5
1	D	544	SER	5.5
1	C	297	PHE	5.4
1	C	449	GLY	5.0
1	B	392	LYS	4.8
1	B	297	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	396	GLN	4.6
1	A	521	ASN	4.6
1	B	393	ASP	4.4
1	D	297	PHE	4.2
1	B	517	MET	4.2
1	D	395	GLY	4.2
1	D	393	ASP	4.1
1	A	294	SER	4.1
1	A	518	GLY	4.0
1	B	544	SER	4.0
1	D	517	MET	3.9
1	A	542	HIS	3.9
1	D	392	LYS	3.9
1	D	540	ARG	3.8
1	C	517	MET	3.8
1	B	519	GLN	3.5
1	C	543	ILE	3.5
1	D	519	GLN	3.5
1	A	295	GLN	3.5
1	D	543	ILE	3.4
1	C	391	ILE	3.3
1	B	540	ARG	3.3
1	C	519	GLN	3.2
1	A	393	ASP	3.2
1	D	394	ALA	3.2
1	B	394	ALA	3.1
1	B	522	ALA	3.1
1	B	323	GLU	3.1
1	D	520	LYS	2.9
1	A	395	GLY	2.9
1	C	393	ASP	2.9
1	B	449	GLY	2.7
1	B	448	SER	2.6
1	A	515	GLU	2.6
1	B	515	GLU	2.5
1	C	478	ARG	2.5
1	B	396	GLN	2.4
1	A	522	ALA	2.4
1	C	473	ILE	2.4
1	C	395	GLY	2.4
1	B	541	SER	2.4
1	C	521	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	452	GLU	2.3
1	C	392	LYS	2.2
1	A	519	GLN	2.2
1	D	478	ARG	2.2
1	B	520	LYS	2.1
1	A	354	LYS	2.1
1	D	451	PHE	2.1
1	D	294	SER	2.1
1	B	295	GLN	2.1
1	A	453	ARG	2.1
1	B	391	ILE	2.0
1	B	516	SER	2.0
1	D	521	ASN	2.0
1	D	476	THR	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 carbohydrates 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.