Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:35 PM GMT

PDB ID	:	3U58
Title	:	Crystal Structure of the Tetrahymena telomerase processivity factor Teb1 AB
Authors	:	Zeng, Z.; Huang, J.; Yang, Y.; Lei, M.
Deposited on	:	2011-10-11
Resolution	:	2.61 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:

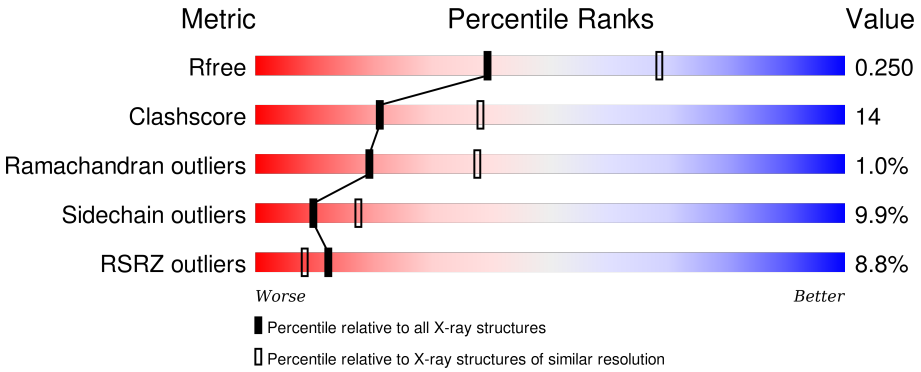
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.61 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	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

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	213	10% 65% 29% 7%
1	B	213	7% 64% 29% 6%
1	C	213	11% 69% 26%
1	D	213	8% 69% 25%
2	E	4	50% 50%

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Mol	Chain	Length	Quality of chain
2	F	4	25% 50% 25%
2	G	4	25% 75%
2	H	4	25% 75%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7378 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 Tetrahymena Teb1 AB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1759	1128	290	338	3			
1	B	210	Total	C	N	O	S	0	0	0
			1739	1118	287	331	3			
1	C	211	Total	C	N	O	S	0	0	0
			1743	1120	288	332	3			
1	D	210	Total	C	N	O	S	0	0	0
			1739	1118	287	331	3			

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*GP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	P	0	0	0
			83	40	17	23	3			
2	H	4	Total	C	N	O	P	0	0	0
			83	40	17	23	3			
2	F	4	Total	C	N	O	P	0	0	0
			83	40	17	23	3			
2	G	4	Total	C	N	O	P	0	0	0
			83	40	17	23	3			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		
3	B	20	Total	O	0	0
			20	20		
3	C	11	Total	O	0	0
			11	11		
3	D	17	Total	O	0	0
			17	17		

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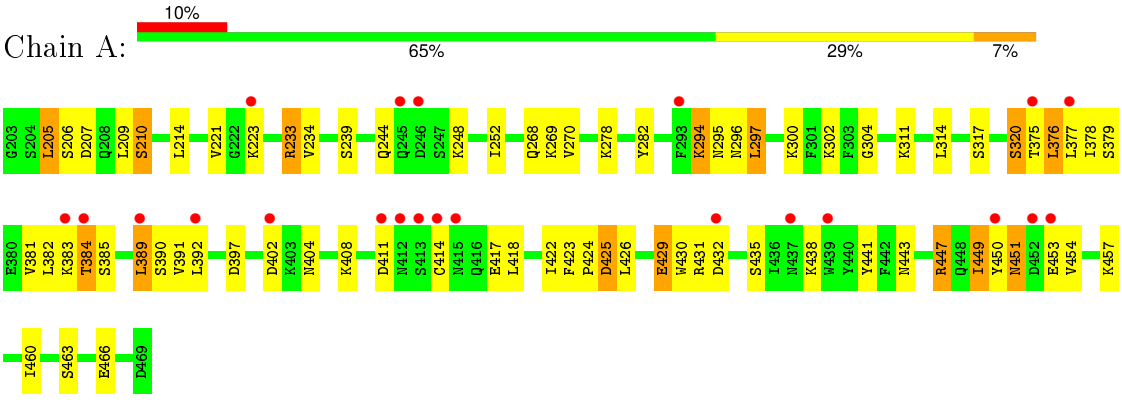
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total O 1 1	0	0
3	H	1	Total O 1 1	0	0
3	F	1	Total O 1 1	0	0

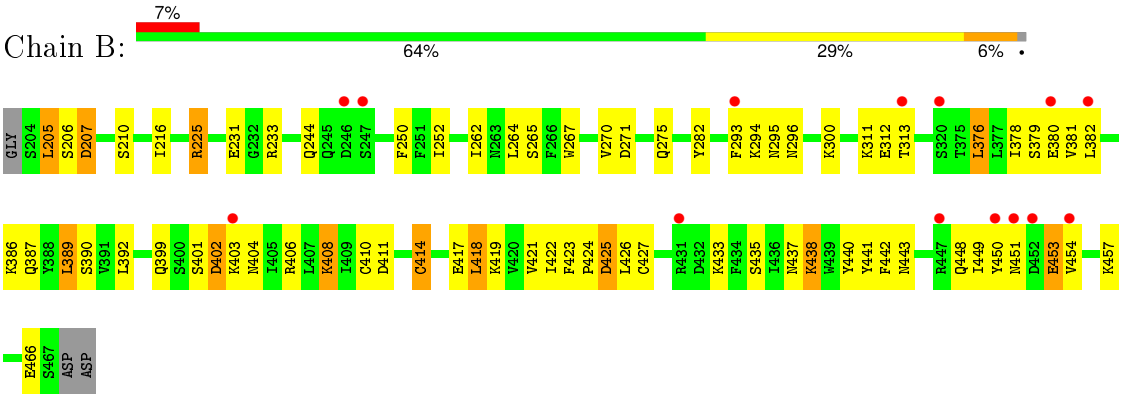
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

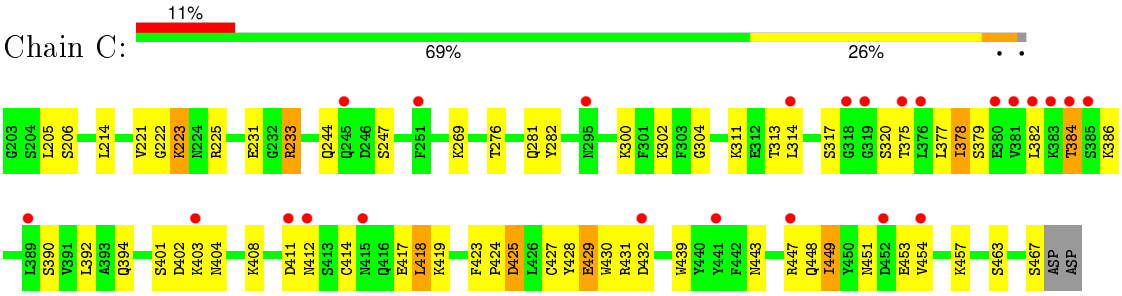
- Molecule 1: Tetrahymena Teb1 AB



- Molecule 1: Tetrahymena Teb1 AB

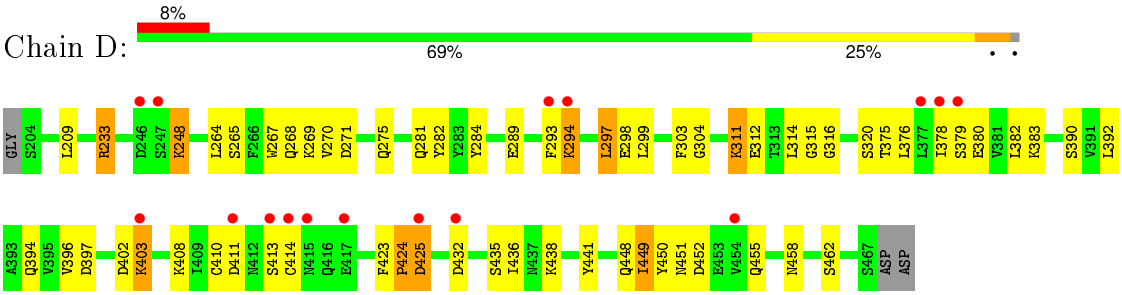


- Molecule 1: Tetrahymena Teb1 AB



- Molecule 1: Tetrahymena Teb1 AB

Chain D:



• Molecule 2: DNA (5'-D(*GP*GP*GP*T)-3')

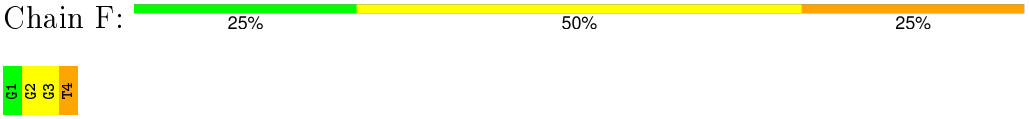
Chain E:

• Molecule 2: DNA (5'-D(*GP*GP*GP*T)-3')

Chain H:

• Molecule 2: DNA (5'-D(*GP*GP*GP*T)-3')

Chain F:



• Molecule 2: DNA (5'-D(*GP*GP*GP*T)-3')

Chain G:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	83.05Å 83.11Å 82.89Å 108.45° 111.59° 108.42°	Depositor
Resolution (Å)	33.58 – 2.61 39.34 – 2.61	Depositor EDS
% Data completeness (in resolution range)	94.0 (33.58-2.61) 77.6 (39.34-2.61)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.219 , 0.259 0.209 , 0.250	Depositor DCC
R_{free} test set	4903 reflections (10.09%)	DCC
Wilson B-factor (Å^2)	51.0	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 26.2	EDS
Estimated twinning fraction	0.000 for h+k+l,-l,-h 0.000 for -l,h+k+l,-k 0.429 for h+k+l,-h,-k 0.429 for -k,-l,h+k+l 0.000 for -k,h+k+l,-h 0.000 for -l,-h,h+k+l 0.000 for k,-h-k-l,l 0.000 for -h-k-l,h,l 0.000 for l,h,k 0.000 for k,l,h 0.000 for h,l,-h-k-l 0.000 for h,-h-k-l,k 0.000 for l,k,-h-k-l 0.000 for -h-k-l,k,h 0.019 for k,h,-h-k-l 0.000 for -h,-k,h+k+l 0.438 for l,-h-k-l,h 0.019 for -l,-k,-h 0.019 for -h-k-l,l,k 0.000 for h+k+l,-k,-l 0.000 for -k,-h,-l 0.018 for -h,h+k+l,-l 0.000 for -h,-l,-k	Xtriage

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[1] Intensities estimated from amplitudes.

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Property	Value	Source
L-test for twinning[2]	$< \|L\| > = 0.51, < L^2 > = 0.34$	Xtriage
Outliers	0 of 48629 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7378	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	0.38	0/1794	0.59	4/2414 (0.2%)
1	B	0.37	0/1774	0.55	2/2387 (0.1%)
1	C	0.37	0/1778	0.54	1/2392 (0.0%)
1	D	0.38	0/1774	0.57	2/2387 (0.1%)
2	E	0.62	0/93	1.00	0/143
2	F	0.70	0/93	1.29	2/143 (1.4%)
2	G	0.60	0/93	1.14	0/143
2	H	0.63	0/93	1.15	0/143
All	All	0.39	0/7492	0.61	11/10152 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	315	GLY	N-CA-C	8.19	133.56	113.10
1	C	404	ASN	N-CA-CB	-6.75	98.44	110.60
2	F	4	DT	N3-C4-O4	6.56	123.84	119.90
1	A	383	LYS	CB-CA-C	-6.22	97.96	110.40
2	F	4	DT	C5-C4-O4	-6.03	120.68	124.90
1	A	384	THR	CB-CA-C	-6.01	95.38	111.60
1	A	385	SER	N-CA-CB	-5.63	102.05	110.50
1	B	437	ASN	CB-CA-C	-5.61	99.18	110.40
1	D	316	GLY	N-CA-C	-5.46	99.45	113.10
1	B	404	ASN	N-CA-CB	-5.27	101.11	110.60
1	A	404	ASN	N-CA-CB	-5.18	101.27	110.60

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	1759	0	1729	54	0
1	B	1739	0	1718	58	0
1	C	1743	0	1721	51	0
1	D	1739	0	1718	43	0
2	E	83	0	47	2	0
2	F	83	0	47	3	0
2	G	83	0	47	2	0
2	H	83	0	47	2	0
3	A	15	0	0	3	0
3	B	20	0	0	4	0
3	C	11	0	0	0	0
3	D	17	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
All	All	7378	0	7074	206	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 (206) 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:C:378:ILE:HD12	1:C:411:ASP:HB2	1.32	1.10
1:A:378:ILE:HG12	1:A:411:ASP:HB3	1.63	0.81
1:C:403:LYS:O	1:C:424:PRO:HD3	1.82	0.79
1:B:406:ARG:HH11	1:B:419:LYS:HZ3	1.30	0.79
1:D:402:ASP:O	1:D:403:LYS:HB2	1.86	0.75
1:D:423:PHE:HB3	1:D:424:PRO:HD2	1.69	0.75
1:B:406:ARG:HH11	1:B:419:LYS:NZ	1.85	0.74
1:A:376:LEU:H	1:A:376:LEU:HD12	1.51	0.74
1:C:269:LYS:HE2	1:C:304:GLY:HA2	1.71	0.73
2:F:4:DT:H2'	2:F:4:DT:OP2	1.90	0.72
1:A:397:ASP:HB3	1:A:408:LYS:HB2	1.72	0.72
1:A:384:THR:HG23	1:A:384:THR:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:424:PRO:O	1:D:425:ASP:HB2	1.91	0.71
1:C:233:ARG:HD3	1:C:282:TYR:CZ	2.25	0.71
1:B:233:ARG:HD3	1:B:282:TYR:CZ	2.26	0.71
1:A:423:PHE:HB3	1:A:424:PRO:HD2	1.72	0.70
1:C:424:PRO:O	1:C:425:ASP:HB2	1.93	0.69
1:C:378:ILE:CD1	1:C:411:ASP:HB2	2.16	0.69
1:C:378:ILE:HD13	1:C:379:SER:H	1.56	0.68
1:B:231:GLU:CD	1:B:311:LYS:HE2	2.15	0.68
1:A:389:LEU:HD13	3:A:3:HOH:O	1.94	0.67
1:D:312:GLU:OE1	2:G:1:DG:H5'	1.94	0.67
1:A:378:ILE:CG1	1:A:411:ASP:HB3	2.25	0.67
1:C:423:PHE:HB3	1:C:424:PRO:HD2	1.76	0.66
1:A:378:ILE:HG13	1:A:379:SER:N	2.09	0.66
1:B:423:PHE:HB3	1:B:424:PRO:HD2	1.78	0.66
1:B:411:ASP:OD2	1:B:414:CYS:HB2	1.96	0.65
1:A:376:LEU:HD13	1:A:381:VAL:HG22	1.78	0.65
1:A:207:ASP:O	1:A:210:SER:HB2	1.96	0.65
1:C:222:GLY:HA2	1:D:233:ARG:HH22	1.61	0.65
1:B:225:ARG:HG3	1:C:282:TYR:OH	1.97	0.64
1:A:378:ILE:HG13	1:A:379:SER:H	1.61	0.64
1:B:424:PRO:O	1:B:425:ASP:HB2	1.96	0.63
1:D:233:ARG:HD3	1:D:282:TYR:CZ	2.33	0.63
1:A:317:SER:O	1:A:320:SER:HB2	1.99	0.62
1:B:389:LEU:HD13	3:B:2:HOH:O	2.00	0.62
1:B:406:ARG:NH1	1:B:419:LYS:NZ	2.48	0.61
1:B:271:ASP:O	1:B:275:GLN:HG2	2.01	0.60
1:D:397:ASP:HB3	1:D:408:LYS:HB2	1.82	0.60
1:A:423:PHE:HE1	1:A:457:LYS:HE2	1.65	0.60
1:B:389:LEU:HB2	3:B:2:HOH:O	2.01	0.59
1:D:435:SER:HB2	1:D:438:LYS:CD	2.32	0.59
2:H:4:DT:H5'	2:H:4:DT:H6	1.66	0.59
1:A:423:PHE:CE1	1:A:457:LYS:HE2	2.38	0.58
1:A:378:ILE:CD1	1:A:411:ASP:HB3	2.34	0.58
1:C:429:GLU:HB3	1:C:430:TRP:CD1	2.39	0.58
1:C:244:GLN:HB2	1:C:247:SER:HB3	1.85	0.58
1:D:448:GLN:HG2	1:D:449:ILE:H	1.68	0.58
1:B:378:ILE:HB	1:B:411:ASP:OD2	2.03	0.57
1:B:435:SER:HB2	1:B:438:LYS:HD3	1.86	0.57
1:A:233:ARG:HD3	1:A:282:TYR:CZ	2.40	0.57
1:C:317:SER:HB2	1:C:320:SER:OG	2.05	0.57
1:C:448:GLN:OE1	1:C:457:LYS:HD3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:ILE:HD12	1:C:411:ASP:CB	2.21	0.56
1:C:424:PRO:HA	1:C:427:CYS:SG	2.45	0.56
1:A:449:ILE:HG12	1:A:454:VAL:HG12	1.88	0.56
1:B:225:ARG:HG3	1:C:282:TYR:CZ	2.40	0.56
1:B:231:GLU:OE2	1:B:311:LYS:HE2	2.06	0.56
1:C:379:SER:HB3	1:C:414:CYS:HB2	1.88	0.55
1:C:423:PHE:CB	1:C:424:PRO:HD2	2.36	0.55
1:A:381:VAL:HG21	1:A:391:VAL:HG22	1.87	0.55
2:F:2:DG:H2"	2:F:3:DG:OP1	2.07	0.55
1:D:396:VAL:O	1:D:436:ILE:HD11	2.07	0.54
1:B:424:PRO:HA	1:B:427:CYS:SG	2.48	0.54
1:B:378:ILE:HG13	1:B:411:ASP:HB3	1.90	0.54
1:C:402:ASP:HA	1:C:431:ARG:NH1	2.22	0.54
1:D:423:PHE:CB	1:D:424:PRO:HD2	2.38	0.54
1:B:392:LEU:HD13	1:B:441:TYR:CD1	2.43	0.54
1:A:384:THR:O	1:A:384:THR:CG2	2.56	0.54
2:H:2:DG:H2"	2:H:3:DG:OP1	2.08	0.53
1:C:231:GLU:CD	1:C:311:LYS:HZ2	2.11	0.53
1:A:392:LEU:HD13	1:A:441:TYR:CE1	2.44	0.53
1:D:396:VAL:C	1:D:436:ILE:HD11	2.29	0.53
1:D:269:LYS:HE2	1:D:304:GLY:HA2	1.91	0.53
1:B:408:LYS:HA	1:B:418:LEU:O	2.09	0.52
1:A:376:LEU:HD11	1:A:389:LEU:HB2	1.91	0.52
1:C:394:GLN:HB3	1:C:439:TRP:CE2	2.45	0.52
1:A:389:LEU:HB2	3:A:3:HOH:O	2.11	0.51
1:B:231:GLU:OE1	1:B:311:LYS:HE2	2.11	0.51
1:D:284:TYR:CZ	1:D:311:LYS:HE2	2.45	0.51
1:A:376:LEU:HD13	1:A:381:VAL:CG2	2.41	0.51
1:B:376:LEU:CD1	1:B:381:VAL:HG22	2.41	0.50
1:C:378:ILE:HG12	1:C:414:CYS:HB3	1.94	0.50
1:B:433:LYS:HG2	1:B:433:LYS:O	2.11	0.50
1:B:392:LEU:HD13	1:B:441:TYR:CE1	2.47	0.50
1:C:402:ASP:HA	1:C:431:ARG:HH12	1.76	0.50
2:E:2:DG:H2"	2:E:3:DG:OP1	2.11	0.50
1:B:451:ASN:H	1:B:453:GLU:CD	2.15	0.50
1:A:375:THR:HA	1:A:390:SER:O	2.12	0.49
1:B:422:ILE:HD13	1:B:422:ILE:N	2.26	0.49
1:D:403:LYS:O	1:D:424:PRO:HD3	2.12	0.49
1:D:265:SER:HB2	1:D:267:TRP:NE1	2.27	0.49
1:B:421:VAL:C	1:B:422:ILE:HD13	2.33	0.49
1:D:293:PHE:O	1:D:294:LYS:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:GLN:HG3	1:C:247:SER:HB3	1.94	0.49
1:C:375:THR:HA	1:C:390:SER:O	2.12	0.49
1:D:270:VAL:HG23	1:D:271:ASP:N	2.28	0.48
1:B:205:LEU:HD23	1:B:206:SER:H	1.77	0.48
1:A:209:LEU:HD11	1:A:314:LEU:HD11	1.94	0.48
1:A:381:VAL:HG21	1:A:391:VAL:CG2	2.44	0.48
1:A:300:LYS:HE2	2:E:2:DG:O6	2.14	0.48
2:G:2:DG:H2"	2:G:3:DG:OP1	2.13	0.48
1:B:225:ARG:CG	1:C:282:TYR:CZ	2.97	0.47
1:D:248:LYS:HB3	1:D:270:VAL:HG21	1.97	0.47
1:B:423:PHE:CD1	1:B:457:LYS:HE3	2.49	0.47
1:A:422:ILE:HG23	1:A:426:LEU:HD23	1.97	0.47
1:A:205:LEU:HD23	1:A:206:SER:N	2.30	0.47
1:A:423:PHE:HB3	1:A:424:PRO:CD	2.41	0.47
1:B:423:PHE:HB3	1:B:424:PRO:CD	2.45	0.47
1:C:205:LEU:HD23	1:C:206:SER:H	1.80	0.47
1:B:401:SER:OG	1:B:402:ASP:N	2.47	0.47
1:C:233:ARG:HD3	1:C:282:TYR:OH	2.14	0.47
1:A:392:LEU:HD13	1:A:441:TYR:CD1	2.50	0.47
1:C:384:THR:CG2	1:C:386:LYS:HG2	2.44	0.47
1:D:451:ASN:O	1:D:452:ASP:HB2	2.15	0.47
1:D:293:PHE:HB2	1:D:298:GLU:HB3	1.97	0.47
1:D:392:LEU:HD13	1:D:441:TYR:CE1	2.49	0.47
1:C:449:ILE:HG13	1:C:454:VAL:HG23	1.97	0.46
1:C:378:ILE:HD13	1:C:379:SER:N	2.28	0.46
1:B:403:LYS:O	1:B:424:PRO:HD3	2.15	0.46
1:D:209:LEU:HD11	1:D:314:LEU:HD11	1.97	0.46
1:A:443:ASN:HB2	1:A:463:SER:OG	2.16	0.46
1:A:269:LYS:HE2	1:A:304:GLY:HA2	1.98	0.46
1:B:399:GLN:HB2	1:B:406:ARG:HB2	1.98	0.46
1:B:312:GLU:O	1:B:313:THR:HB	2.15	0.46
1:B:300:LYS:HE2	2:F:2:DG:O6	2.15	0.46
1:B:422:ILE:HG23	1:B:426:LEU:HD23	1.98	0.46
1:A:278:LYS:HE3	1:A:460:ILE:O	2.16	0.46
1:C:231:GLU:OE1	1:C:311:LYS:NZ	2.48	0.46
1:B:207:ASP:O	1:B:210:SER:HB2	2.16	0.45
1:D:424:PRO:O	1:D:425:ASP:CB	2.63	0.45
1:C:419:LYS:HE3	1:C:419:LYS:HB2	1.77	0.45
1:D:264:LEU:HG	1:D:299:LEU:HB2	1.99	0.45
1:A:423:PHE:CB	1:A:424:PRO:HD2	2.44	0.45
1:B:216:ILE:HD13	1:B:262:ILE:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:ARG:H	1:B:225:ARG:HG3	1.64	0.45
1:A:423:PHE:CB	1:A:424:PRO:CD	2.95	0.45
1:B:390:SER:N	3:B:2:HOH:O	2.49	0.45
1:C:449:ILE:HG13	1:C:454:VAL:CG2	2.47	0.45
1:D:458:ASN:HB2	1:D:462:SER:HB2	1.99	0.45
1:D:379:SER:O	1:D:382:LEU:CD2	2.65	0.45
1:A:214:LEU:HD11	1:A:223:LYS:HE2	1.98	0.45
1:D:311:LYS:O	1:D:314:LEU:HB2	2.17	0.44
1:C:447:ARG:CZ	1:C:454:VAL:HG21	2.48	0.44
1:A:311:LYS:O	1:A:314:LEU:HB2	2.17	0.44
1:A:450:TYR:CD2	1:A:450:TYR:C	2.91	0.44
1:B:399:GLN:HG3	3:B:14:HOH:O	2.17	0.44
1:B:448:GLN:NE2	1:B:457:LYS:HD3	2.32	0.43
1:C:214:LEU:HD11	1:C:223:LYS:HE3	1.99	0.43
1:A:390:SER:N	3:A:3:HOH:O	2.51	0.43
1:D:394:GLN:HA	1:D:438:LYS:O	2.18	0.43
1:D:378:ILE:CG1	1:D:411:ASP:HB2	2.48	0.43
1:A:429:GLU:HG3	1:A:430:TRP:CD1	2.52	0.43
1:A:294:LYS:C	1:A:296:ASN:H	2.21	0.43
1:D:378:ILE:HG12	1:D:411:ASP:CG	2.38	0.43
1:A:297:LEU:HA	1:A:297:LEU:HD12	1.79	0.43
1:A:424:PRO:O	1:A:425:ASP:HB2	2.18	0.43
1:B:423:PHE:CE1	1:B:457:LYS:HE3	2.53	0.43
1:B:411:ASP:OD1	1:B:411:ASP:N	2.51	0.43
1:D:375:THR:HA	1:D:390:SER:O	2.18	0.43
1:C:233:ARG:HB2	1:C:282:TYR:CE1	2.53	0.43
1:B:311:LYS:C	1:B:312:GLU:O	2.57	0.43
1:B:265:SER:HB2	1:B:267:TRP:NE1	2.33	0.43
1:C:392:LEU:HD11	1:C:467:SER:HB2	2.01	0.43
1:C:403:LYS:HG2	1:C:428:TYR:OH	2.19	0.43
1:C:300:LYS:HE2	1:C:302:LYS:HD2	2.00	0.43
1:B:294:LYS:C	1:B:296:ASN:H	2.20	0.43
1:B:390:SER:HA	1:B:442:PHE:O	2.19	0.42
1:D:379:SER:HB3	1:D:414:CYS:SG	2.59	0.42
1:D:435:SER:HB2	1:D:438:LYS:HD2	2.00	0.42
1:B:294:LYS:O	1:B:295:ASN:HB2	2.18	0.42
1:A:248:LYS:O	1:A:270:VAL:HG21	2.19	0.42
1:A:244:GLN:HG3	1:B:387:GLN:OE1	2.19	0.42
1:D:396:VAL:HG11	1:D:410:CYS:SG	2.60	0.42
1:C:451:ASN:C	1:C:453:GLU:H	2.23	0.42
1:C:378:ILE:N	1:C:378:ILE:HD13	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:PHE:HB2	1:D:298:GLU:HG2	2.02	0.42
1:D:423:PHE:HB3	1:D:424:PRO:CD	2.45	0.42
1:A:435:SER:HB2	1:A:438:LYS:HD2	2.02	0.42
1:A:378:ILE:HD13	1:A:411:ASP:HB3	2.01	0.41
1:B:390:SER:HB3	1:B:443:ASN:HA	2.01	0.41
1:B:438:LYS:HB3	1:B:440:TYR:CE1	2.54	0.41
1:D:289:GLU:OE2	1:D:303:PHE:CE1	2.73	0.41
1:C:378:ILE:HD11	1:C:414:CYS:H	1.85	0.41
1:D:375:THR:C	1:D:376:LEU:HD12	2.41	0.41
1:A:377:LEU:O	1:A:381:VAL:HG23	2.19	0.41
1:A:389:LEU:HD21	1:A:447:ARG:HG3	2.02	0.41
1:A:234:VAL:HG22	1:A:252:ILE:HD12	2.03	0.41
1:C:379:SER:O	1:C:382:LEU:HB3	2.21	0.41
1:C:378:ILE:CG1	1:C:414:CYS:HB3	2.50	0.41
1:D:297:LEU:HA	1:D:297:LEU:HD12	1.68	0.41
1:B:250:PHE:HD2	1:B:270:VAL:HG13	1.85	0.41
1:A:375:THR:O	1:A:375:THR:HG23	2.20	0.40
1:B:225:ARG:HD2	1:C:282:TYR:CE1	2.56	0.40
1:C:424:PRO:O	1:C:425:ASP:CB	2.66	0.40
1:D:411:ASP:HB3	1:D:413:SER:H	1.85	0.40
1:D:380:GLU:O	1:D:383:LYS:N	2.52	0.40
1:A:451:ASN:C	1:A:453:GLU:N	2.73	0.40
1:D:455:GLN:O	1:D:455:GLN:HG3	2.20	0.40
1:B:406:ARG:NH1	1:B:419:LYS:HZ3	2.07	0.40
1:C:408:LYS:HA	1:C:418:LEU:O	2.22	0.40
1:A:376:LEU:HD12	1:A:390:SER:O	2.22	0.40
1:C:443:ASN:HB2	1:C:463:SER:OG	2.21	0.40
1:B:406:ARG:NH1	1:B:419:LYS:HZ1	2.16	0.40
1:B:378:ILE:HB	1:B:411:ASP:CG	2.42	0.40
1:C:384:THR:HG22	1:C:386:LYS:HG2	2.03	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	211/213 (99%)	193 (92%)	15 (7%)	3 (1%)	14	26
1	B	208/213 (98%)	189 (91%)	18 (9%)	1 (0%)	34	58
1	C	209/213 (98%)	195 (93%)	13 (6%)	1 (0%)	34	58
1	D	208/213 (98%)	193 (93%)	12 (6%)	3 (1%)	14	26
All	All	836/852 (98%)	770 (92%)	58 (7%)	8 (1%)	19	37

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	425	ASP
1	B	425	ASP
1	C	425	ASP
1	D	425	ASP
1	A	295	ASN
1	D	294	LYS
1	A	294	LYS
1	D	424	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	199/199 (100%)	176 (88%)	23 (12%)	7	11
1	B	197/199 (99%)	172 (87%)	25 (13%)	5	9
1	C	197/199 (99%)	179 (91%)	18 (9%)	12	22
1	D	197/199 (99%)	185 (94%)	12 (6%)	23	44
All	All	790/796 (99%)	712 (90%)	78 (10%)	10	17

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	LEU
1	A	210	SER
1	A	221	VAL
1	A	233	ARG
1	A	239	SER
1	A	268	GLN
1	A	297	LEU
1	A	302	LYS
1	A	320	SER
1	A	376	LEU
1	A	382	LEU
1	A	389	LEU
1	A	402	ASP
1	A	414	CYS
1	A	417	GLU
1	A	418	LEU
1	A	429	GLU
1	A	431	ARG
1	A	432	ASP
1	A	447	ARG
1	A	449	ILE
1	A	451	ASN
1	A	466	GLU
1	B	205	LEU
1	B	207	ASP
1	B	225	ARG
1	B	244	GLN
1	B	252	ILE
1	B	264	LEU
1	B	293	PHE
1	B	376	LEU
1	B	379	SER
1	B	380	GLU
1	B	382	LEU
1	B	386	LYS
1	B	389	LEU
1	B	402	ASP
1	B	408	LYS
1	B	410	CYS
1	B	414	CYS
1	B	417	GLU
1	B	418	LEU
1	B	438	LYS

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Mol	Chain	Res	Type
1	B	449	ILE
1	B	450	TYR
1	B	453	GLU
1	B	454	VAL
1	B	466	GLU
1	C	221	VAL
1	C	223	LYS
1	C	225	ARG
1	C	233	ARG
1	C	276	THR
1	C	281	GLN
1	C	313	THR
1	C	314	LEU
1	C	377	LEU
1	C	378	ILE
1	C	384	THR
1	C	401	SER
1	C	412	ASN
1	C	417	GLU
1	C	418	LEU
1	C	429	GLU
1	C	432	ASP
1	C	449	ILE
1	D	233	ARG
1	D	248	LYS
1	D	268	GLN
1	D	275	GLN
1	D	281	GLN
1	D	297	LEU
1	D	311	LYS
1	D	320	SER
1	D	403	LYS
1	D	432	ASP
1	D	449	ILE
1	D	450	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	ASN
1	B	448	GLN
1	C	461	HIS

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	213/213 (100%)	0.76	22 (10%) 9 5	32, 54, 106, 124	0
1	B	210/213 (98%)	0.66	14 (6%) 21 16	32, 54, 103, 125	0
1	C	211/213 (99%)	0.71	24 (11%) 7 4	33, 54, 105, 122	0
1	D	210/213 (98%)	0.69	16 (7%) 17 12	32, 54, 103, 129	0
2	E	4/4 (100%)	0.17	0 100 100	48, 51, 58, 70	0
2	F	4/4 (100%)	0.39	0 100 100	49, 51, 60, 75	0
2	G	4/4 (100%)	0.57	0 100 100	48, 50, 59, 70	0
2	H	4/4 (100%)	0.22	0 100 100	49, 49, 60, 74	0
All	All	860/868 (99%)	0.70	76 (8%) 12 8	32, 54, 104, 129	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	411	ASP	12.8
1	D	415	ASN	9.1
1	B	454	VAL	7.5
1	A	392	LEU	7.1
1	A	415	ASN	6.4
1	B	452	ASP	6.0
1	C	411	ASP	5.7
1	D	378	ILE	5.6
1	A	412	ASN	5.5
1	A	452	ASP	5.3
1	D	413	SER	5.2
1	D	246	ASP	4.8
1	D	294	LYS	4.6
1	B	451	ASN	4.6
1	C	452	ASP	4.6
1	C	415	ASN	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	450	TYR	4.4
1	D	432	ASP	4.2
1	C	376	LEU	4.2
1	D	414	CYS	4.1
1	D	377	LEU	4.1
1	D	379	SER	4.1
1	B	382	LEU	3.9
1	B	247	SER	3.9
1	D	247	SER	3.8
1	D	411	ASP	3.7
1	B	450	TYR	3.7
1	D	454	VAL	3.6
1	A	375	THR	3.6
1	C	412	ASN	3.6
1	A	413	SER	3.6
1	C	454	VAL	3.5
1	B	431	ARG	3.5
1	A	414	CYS	3.4
1	A	402	ASP	3.4
1	C	318	GLY	3.3
1	B	313	THR	3.2
1	A	439	TRP	3.2
1	A	384	THR	3.2
1	C	319	GLY	3.1
1	A	293	PHE	3.1
1	D	403	LYS	3.0
1	B	246	ASP	3.0
1	B	380	GLU	2.8
1	A	223	LYS	2.8
1	C	383	LYS	2.8
1	D	293	PHE	2.8
1	A	377	LEU	2.8
1	C	385	SER	2.7
1	C	389	LEU	2.7
1	A	453	GLU	2.7
1	C	384	THR	2.6
1	A	383	LYS	2.6
1	C	381	VAL	2.6
1	C	314	LEU	2.6
1	A	245	GLN	2.5
1	C	380	GLU	2.5
1	C	403	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	403	LYS	2.5
1	C	375	THR	2.5
1	D	425	ASP	2.4
1	A	246	ASP	2.4
1	C	447	ARG	2.4
1	C	382	LEU	2.3
1	C	432	ASP	2.3
1	D	417	GLU	2.3
1	C	245	GLN	2.2
1	A	432	ASP	2.2
1	B	447	ARG	2.2
1	B	320	SER	2.2
1	B	293	PHE	2.2
1	A	437	ASN	2.1
1	A	389	LEU	2.1
1	C	251	PHE	2.1
1	C	295	ASN	2.1
1	C	441	TYR	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.