WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:15 AM GMT

PDB ID	:	2GAJ
Title	:	Structure of Full Length Topoisomerase I from Thermotoga maritima in monoclinic crystal form
Authors	:	Hansen, G.
Deposited on	:	2006-03-09
Resolution	:	1.95 Å(reported)

The following versions of software and data (see references (i)) 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
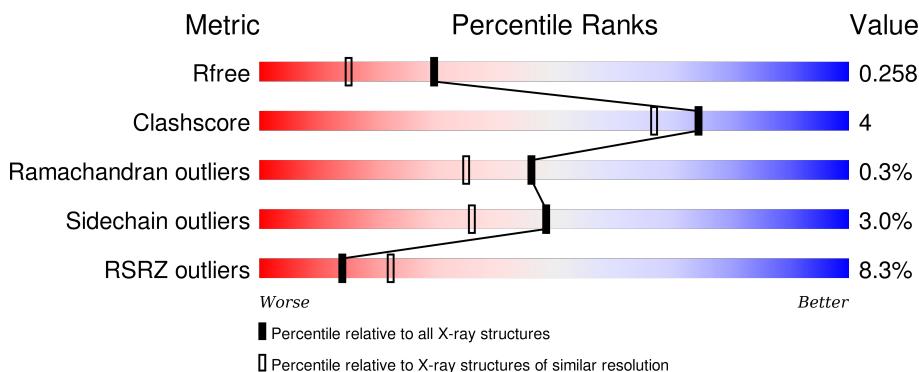
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
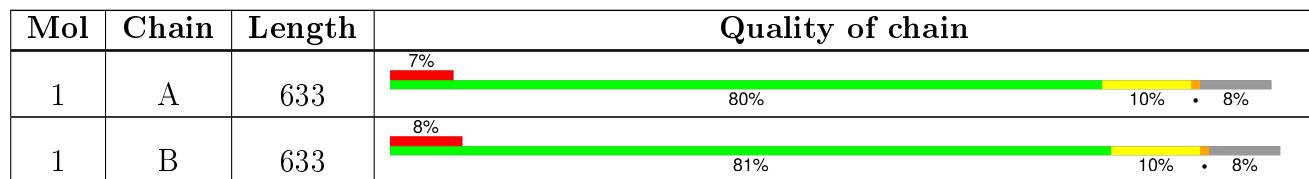
The reported resolution of this entry is 1.95 Å.

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.

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	633	
1	B	633	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10305 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 DNA topoisomerase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4714	3017	799	881	17			
1	B	581	Total	C	N	O	S	0	0	0
			4714	3017	799	881	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP P46799
B	1	MET	-	INITIATING METHIONINE	UNP P46799
A	2	ALA	-	CLONING ARTIFACT	UNP P46799
B	2	ALA	-	CLONING ARTIFACT	UNP P46799
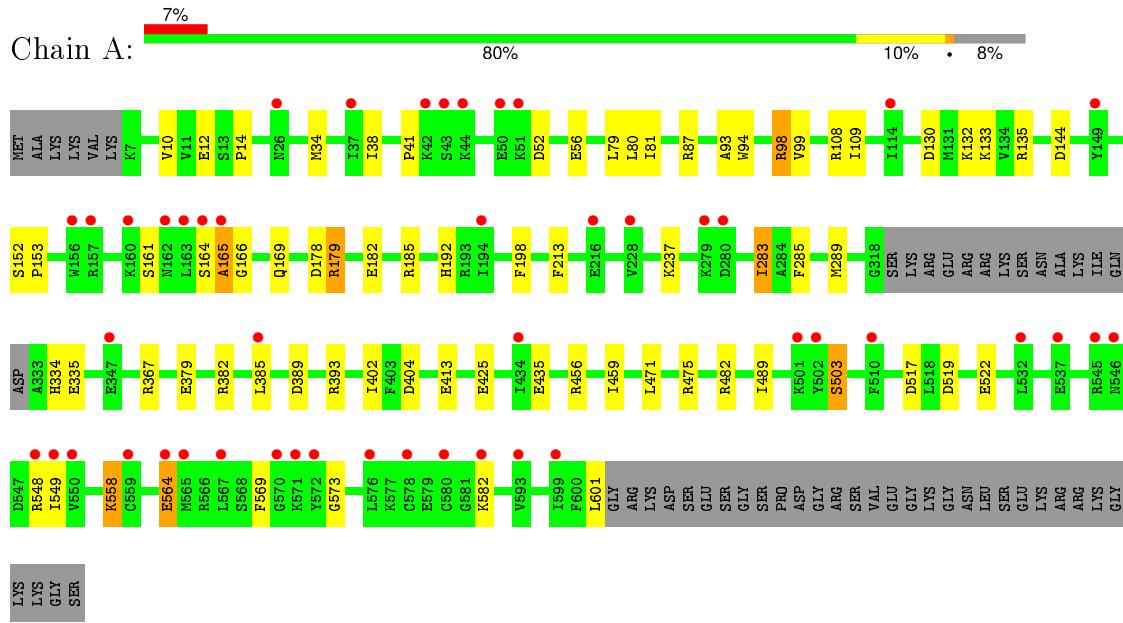
- Molecule 2 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	427	Total	O	0	0
			427	427		
2	B	450	Total	O	0	0
			450	450		
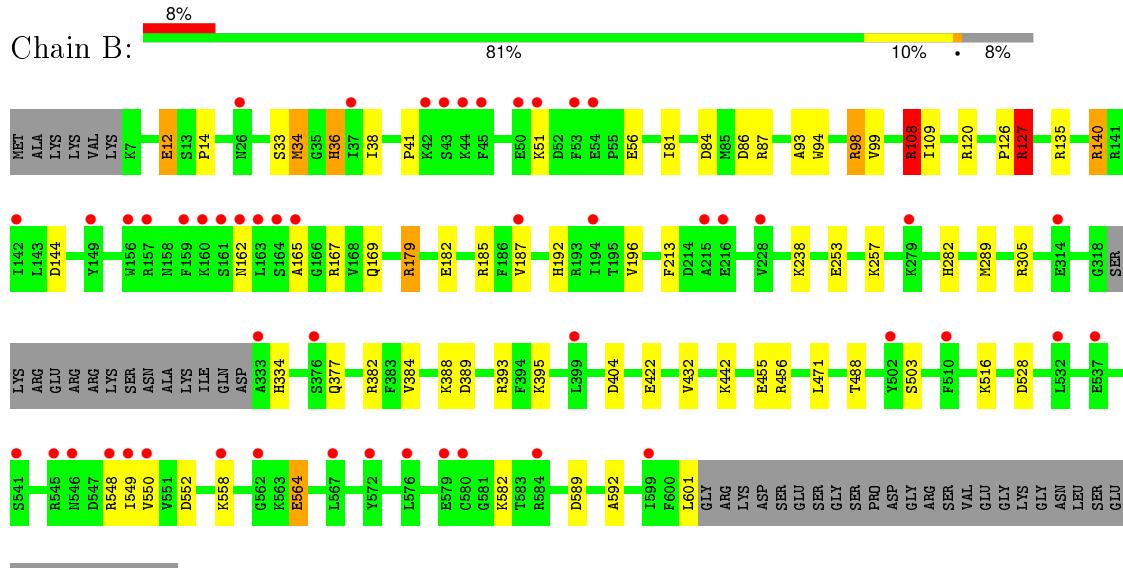
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA topoisomerase I

• Molecule 1: DNA topoisomerase I

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	45.05Å 142.71Å 127.64Å 90.00° 90.84° 90.00°	Depositor
Resolution (Å)	15.00 – 1.95 14.99 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.6 (15.00-1.95) 99.8 (14.99-1.95)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.10 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.195 , 0.246 0.209 , 0.258	Depositor DCC
R_{free} test set	5837 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	20.5	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 43.4	EDS
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
L-test for twinning[2]	$<|L|> = 0.47, <L^2> = 0.30$	Xtriage
Outliers	0 of 116577 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10305	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.74 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2655e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 (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	0.67	0/4799	1.07	23/6441 (0.4%)
1	B	0.69	0/4799	1.16	27/6441 (0.4%)
All	All	0.68	0/9598	1.12	50/12882 (0.4%)

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	179	ARG	NE-CZ-NH2	-25.81	107.40	120.30
1	B	179	ARG	NE-CZ-NH1	18.68	129.64	120.30
1	A	456	ARG	NE-CZ-NH2	-11.42	114.59	120.30
1	B	127	ARG	NE-CZ-NH1	10.76	125.68	120.30
1	B	86	ASP	CB-CG-OD1	10.51	127.76	118.30
1	A	519	ASP	CB-CG-OD1	10.44	127.69	118.30
1	B	86	ASP	CB-CG-OD2	-10.25	109.07	118.30
1	B	127	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	A	456	ARG	NE-CZ-NH1	8.47	124.54	120.30
1	A	98	ARG	NE-CZ-NH2	-8.31	116.14	120.30
1	B	404	ASP	CB-CG-OD1	8.23	125.71	118.30
1	B	179	ARG	CG-CD-NE	-8.10	94.79	111.80
1	B	179	ARG	CD-NE-CZ	8.00	134.80	123.60
1	B	404	ASP	CB-CG-OD2	-7.89	111.20	118.30
1	A	393	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	A	367	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	A	179	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	A	144	ASP	CB-CG-OD1	6.86	124.48	118.30
1	A	519	ASP	CB-CG-OD2	-6.78	112.19	118.30
1	B	185	ARG	NE-CZ-NH2	-6.73	116.93	120.30
1	B	98	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	B	84	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	A	404	ASP	CB-CG-OD2	-6.56	112.40	118.30
1	A	475	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	B	135	ARG	NE-CZ-NH1	6.36	123.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	A	178	ASP	CB-CG-OD1	6.30	123.97	118.30
1	B	389	ASP	CB-CG-OD1	6.30	123.97	118.30
1	A	482	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	B	382	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	B	140	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	B	305	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	130	ASP	CB-CG-OD1	6.09	123.78	118.30
1	B	305	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	A	389	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	517	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	135	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	482	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	B	528	ASP	CB-CG-OD1	5.64	123.37	118.30
1	B	140	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	12	GLU	CA-CB-CG	5.62	125.76	113.40
1	A	185	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	B	456	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	120	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	87	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	404	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	335	GLU	OE1-CD-OE2	5.36	129.74	123.30
1	B	144	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	382	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	108	ARG	NE-CZ-NH1	5.12	122.86	120.30

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	4714	0	4821	35	0
1	B	4714	0	4821	42	0
2	A	427	0	0	7	0
2	B	450	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10305	0	9642	77	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 4.

All (77) 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:489:ILE:HD11	1:A:601:LEU:HD21	1.56	0.86
1:A:80:LEU:HD13	1:A:109:ILE:HD11	1.58	0.84
1:A:413:GLU:O	2:A:892:HOH:O	1.96	0.82
1:A:334:HIS:HD2	2:A:729:HOH:O	1.65	0.80
1:B:192:HIS:HD2	1:B:213:PHE:H	1.31	0.77
1:A:334:HIS:CD2	2:A:729:HOH:O	2.37	0.77
1:B:253:GLU:OE1	1:B:257:LYS:HE2	1.88	0.73
1:B:94:TRP:CE2	1:B:98:ARG:HD2	2.25	0.71
1:B:14:PRO:HG3	1:B:34:MET:HE1	1.73	0.70
1:A:80:LEU:HB3	1:A:109:ILE:HD12	1.73	0.70
1:B:187:VAL:O	2:B:1009:HOH:O	2.10	0.69
1:B:282:HIS:HE1	2:B:802:HOH:O	1.78	0.66
1:A:41:PRO:HD3	1:A:56:GLU:O	1.98	0.62
1:A:169:GLN:NE2	1:A:471:LEU:HD21	2.14	0.62
1:B:94:TRP:CZ2	1:B:98:ARG:HD2	2.37	0.60
1:B:592:ALA:HB2	1:B:601:LEU:HD23	1.84	0.60
1:A:379:GLU:HG3	1:A:402:ILE:HD11	1.84	0.59
1:A:10:VAL:CG2	1:A:79:LEU:HD11	2.32	0.59
1:A:192:HIS:HD2	1:A:213:PHE:H	1.50	0.58
1:B:14:PRO:HG3	1:B:34:MET:CE	2.35	0.56
1:A:334:HIS:CD2	2:A:1024:HOH:O	2.57	0.55
1:B:41:PRO:HD3	1:B:56:GLU:O	2.07	0.55
1:B:38:ILE:HD11	1:B:99:VAL:HG11	1.89	0.55
1:B:140:ARG:HD2	2:B:761:HOH:O	2.06	0.54
1:B:167:ARG:HD3	2:B:635:HOH:O	2.08	0.54
1:A:165:ALA:HB2	1:A:471:LEU:HD13	1.90	0.54
1:B:127:ARG:HG3	1:B:127:ARG:HH11	1.73	0.53
1:B:34:MET:CA	1:B:34:MET:HE3	2.39	0.52
1:A:425:GLU:OE2	2:A:847:HOH:O	2.19	0.51
1:B:81:ILE:HG21	1:B:93:ALA:HA	1.92	0.50
1:B:516:LYS:HG2	2:B:907:HOH:O	2.11	0.50
1:B:34:MET:HA	1:B:34:MET:HE3	1.91	0.50
1:B:552:ASP:OD2	2:B:945:HOH:O	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:GLU:OE2	1:B:442:LYS:NZ	2.40	0.50
1:B:282:HIS:CE1	2:B:802:HOH:O	2.59	0.49
1:A:94:TRP:CE2	1:A:98:ARG:HD2	2.49	0.48
1:B:169:GLN:NE2	1:B:471:LEU:CD2	2.77	0.48
1:B:334:HIS:HD2	2:B:661:HOH:O	1.97	0.47
1:B:14:PRO:HD3	1:B:34:MET:CE	2.44	0.47
1:B:388:LYS:NZ	2:B:972:HOH:O	2.25	0.47
1:A:80:LEU:HD13	1:A:109:ILE:CD1	2.38	0.47
1:A:94:TRP:CZ2	1:A:98:ARG:HD2	2.50	0.47
1:B:238:LYS:HG2	1:B:377:GLN:HG2	1.96	0.47
1:A:14:PRO:HG3	1:A:34:MET:SD	2.55	0.47
1:A:165:ALA:CB	1:A:471:LEU:HD13	2.43	0.47
1:A:198:PHE:CZ	1:A:385:LEU:HD11	2.49	0.47
1:A:38:ILE:HD11	1:A:99:VAL:CG1	2.46	0.46
1:A:152:SER:N	1:A:153:PRO:CD	2.80	0.45
1:B:488:THR:HB	1:B:589:ASP:HA	1.98	0.45
1:B:384:VAL:HG22	1:B:395:LYS:HG2	1.97	0.45
1:A:237:LYS:NZ	2:A:943:HOH:O	2.49	0.44
1:B:34:MET:CE	1:B:34:MET:HA	2.47	0.44
1:B:165:ALA:HB3	1:B:471:LEU:HD13	1.99	0.44
1:B:33:SER:C	1:B:34:MET:HG2	2.39	0.43
1:A:179:ARG:NH1	1:A:182:GLU:OE1	2.51	0.43
1:B:558:LYS:HE3	1:B:564:GLU:HB3	2.01	0.43
1:A:132:LYS:HE2	2:A:866:HOH:O	2.18	0.43
1:A:569:PHE:CE1	1:A:573:GLY:HA2	2.53	0.43
1:A:38:ILE:HD11	1:A:99:VAL:HG11	2.01	0.43
1:A:558:LYS:NZ	1:A:564:GLU:HB2	2.33	0.43
1:B:108:ARG:HD2	1:B:127:ARG:NH1	2.35	0.42
1:B:282:HIS:HD2	2:B:678:HOH:O	2.03	0.42
1:B:109:ILE:CD1	1:B:126:PRO:HB3	2.50	0.42
1:B:196:VAL:HG12	1:B:432:VAL:HG22	2.00	0.42
1:B:282:HIS:CD2	2:B:678:HOH:O	2.73	0.42
1:B:38:ILE:HD11	1:B:99:VAL:CG1	2.48	0.42
1:A:164:SER:C	1:A:166:GLY:H	2.22	0.41
1:B:169:GLN:NE2	1:B:471:LEU:HD21	2.35	0.41
1:A:81:ILE:HG21	1:A:93:ALA:HA	2.02	0.41
1:A:283:ILE:HD11	1:A:285:PHE:CZ	2.54	0.41
1:A:80:LEU:HB3	1:A:109:ILE:CD1	2.47	0.41
1:B:34:MET:CE	1:B:34:MET:CA	2.98	0.41
1:B:36:HIS:CD2	2:B:942:HOH:O	2.74	0.41
1:A:459:ILE:HA	1:A:459:ILE:HD13	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:LYS:HG3	2:B:932:HOH:O	2.21	0.40
1:A:10:VAL:HG22	1:A:79:LEU:HD11	2.04	0.40
1:A:87:ARG:NE	1:A:522:GLU:OE1	2.45	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	577/633 (91%)	561 (97%)	14 (2%)	2 (0%)	46	35
1	B	577/633 (91%)	562 (97%)	14 (2%)	1 (0%)	52	43
All	All	1154/1266 (91%)	1123 (97%)	28 (2%)	3 (0%)	46	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	550	VAL
1	A	503	SER
1	A	165	ALA

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	519/562 (92%)	505 (97%)	14 (3%)	52	41
1	B	519/562 (92%)	502 (97%)	17 (3%)	45	32
All	All	1038/1124 (92%)	1007 (97%)	31 (3%)	48	36

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLU
1	A	52	ASP
1	A	108	ARG
1	A	133	LYS
1	A	161	SER
1	A	283	ILE
1	A	289	MET
1	A	435	GLU
1	A	503	SER
1	A	548	ARG
1	A	549	ILE
1	A	558	LYS
1	A	564	GLU
1	A	582	LYS
1	B	12	GLU
1	B	34	MET
1	B	36	HIS
1	B	51	LYS
1	B	108	ARG
1	B	127	ARG
1	B	162	ASN
1	B	179	ARG
1	B	289	MET
1	B	393	ARG
1	B	422	GLU
1	B	455	GLU
1	B	503	SER
1	B	548	ARG
1	B	549	ILE
1	B	564	GLU
1	B	582	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	158	ASN
1	A	192	HIS
1	A	334	HIS
1	A	523	GLN
1	A	557	GLN
1	B	26	ASN
1	B	36	HIS
1	B	158	ASN
1	B	169	GLN
1	B	192	HIS
1	B	282	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	581/633 (91%)	0.68	47 (8%)	15	23	2, 10, 24, 34	0
1	B	581/633 (91%)	0.71	50 (8%)	13	21	2, 9, 24, 36	0
All	All	1162/1266 (91%)	0.70	97 (8%)	14	22	2, 9, 24, 36	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	549	ILE	6.9
1	A	165	ALA	6.3
1	B	165	ALA	6.1
1	A	572	TYR	6.1
1	B	156	TRP	5.9
1	B	43	SER	5.4
1	A	164	SER	5.3
1	B	164	SER	5.3
1	A	156	TRP	5.3
1	A	43	SER	5.2
1	A	280	ASP	5.0
1	A	549	ILE	4.9
1	A	545	ARG	4.8
1	B	163	LEU	4.7
1	B	550	VAL	4.7
1	A	580	CYS	4.5
1	B	546	ASN	4.2
1	A	279	LYS	4.0
1	A	50	GLU	4.0
1	B	545	ARG	3.9
1	A	567	LEU	3.7
1	A	157	ARG	3.7
1	A	550	VAL	3.7
1	A	548	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	157	ARG	3.7
1	B	50	GLU	3.7
1	A	51	LYS	3.6
1	A	570	GLY	3.6
1	A	546	ASN	3.5
1	A	149	TYR	3.4
1	B	42	LYS	3.3
1	B	548	ARG	3.2
1	B	279	LYS	3.2
1	B	567	LEU	3.2
1	A	502	TYR	3.1
1	B	149	TYR	3.1
1	B	572	TYR	3.1
1	A	582	LYS	3.1
1	A	26	ASN	3.0
1	A	163	LEU	3.0
1	B	579	GLU	3.0
1	A	571	LYS	3.0
1	A	537	GLU	2.9
1	B	26	ASN	2.9
1	B	333	ALA	2.9
1	A	216	GLU	2.8
1	A	559	CYS	2.8
1	B	160	LYS	2.8
1	B	162	ASN	2.8
1	B	37	ILE	2.7
1	B	599	ILE	2.7
1	A	162	ASN	2.7
1	B	502	TYR	2.7
1	A	599	ILE	2.6
1	B	216	GLU	2.5
1	B	576	LEU	2.5
1	B	51	LYS	2.5
1	A	576	LEU	2.5
1	A	228	VAL	2.5
1	A	44	LYS	2.5
1	A	510	PHE	2.4
1	A	578	CYS	2.4
1	B	537	GLU	2.4
1	A	194	ILE	2.4
1	B	194	ILE	2.3
1	A	593	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	562	GLY	2.3
1	B	558	LYS	2.3
1	B	228	VAL	2.3
1	B	44	LYS	2.3
1	B	54	GLU	2.3
1	A	565	MET	2.3
1	B	161	SER	2.2
1	A	42	LYS	2.2
1	B	510	PHE	2.2
1	A	160	LYS	2.2
1	A	385	LEU	2.2
1	B	376	SER	2.2
1	B	215	ALA	2.1
1	A	501	LYS	2.1
1	B	142	ILE	2.1
1	B	580	CYS	2.1
1	A	532	LEU	2.1
1	A	37	ILE	2.1
1	B	53	PHE	2.1
1	B	532	LEU	2.1
1	B	314	GLU	2.1
1	B	159	PHE	2.0
1	B	584	ARG	2.0
1	B	399	LEU	2.0
1	A	564	GLU	2.0
1	B	45	PHE	2.0
1	B	187	VAL	2.0
1	B	541	SER	2.0
1	A	347	GLU	2.0
1	A	114	ILE	2.0
1	A	434	ILE	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.