Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 02:42 AM EDT

PDB ID	:	2GAI
Title	:	Structure of Full Length Topoisomerase I from Thermotoga maritima in triclinic crystal form
Authors	:	Hansen, G.
Deposited on	:	2006-03-08
Resolution	:	1.70 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:

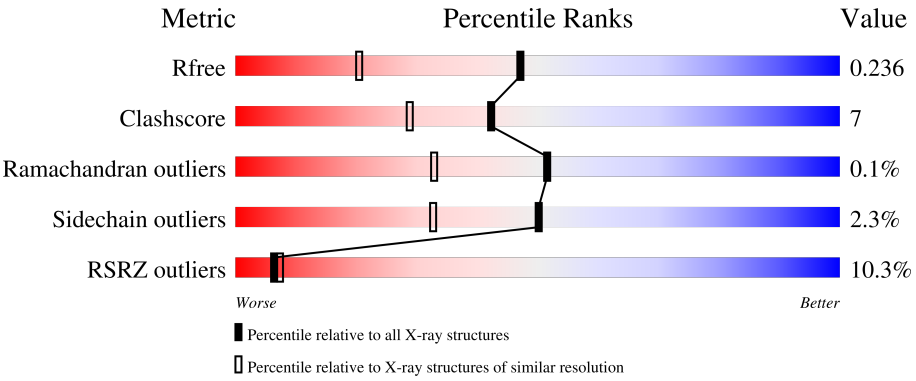
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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	10% 79% 12% • 8%
1	B	633	9% 78% 12% • 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10600 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	18	0
			4770	3059	803	891	17			
1	B	581	Total	C	N	O	S	0	20	0
			4776	3065	803	891	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.

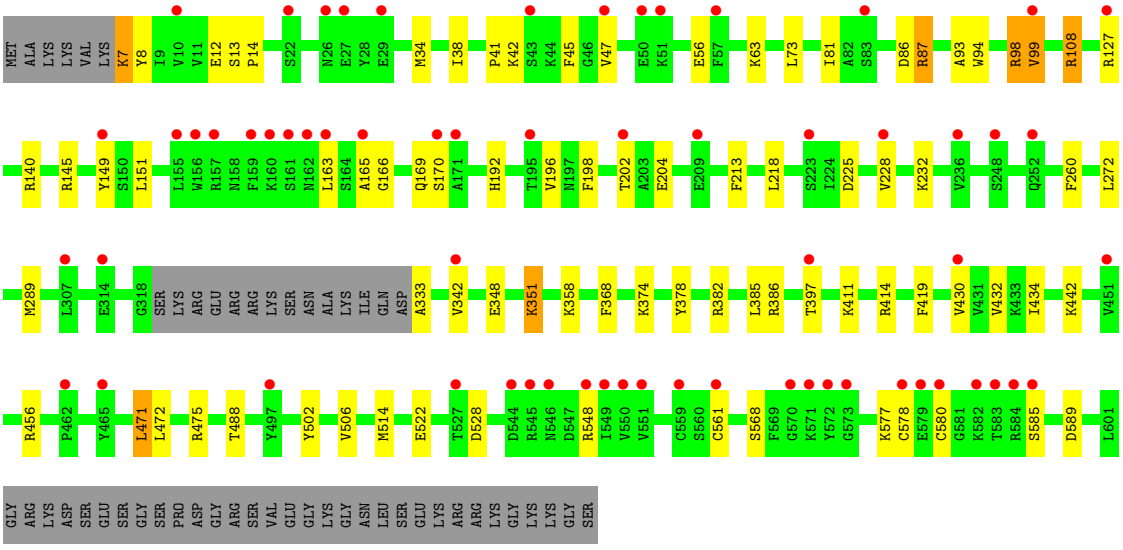
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	544	Total	O	0	0
			544	544		
2	B	510	Total	O	0	0
			510	510		

3 Residue-property plots (i)

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.

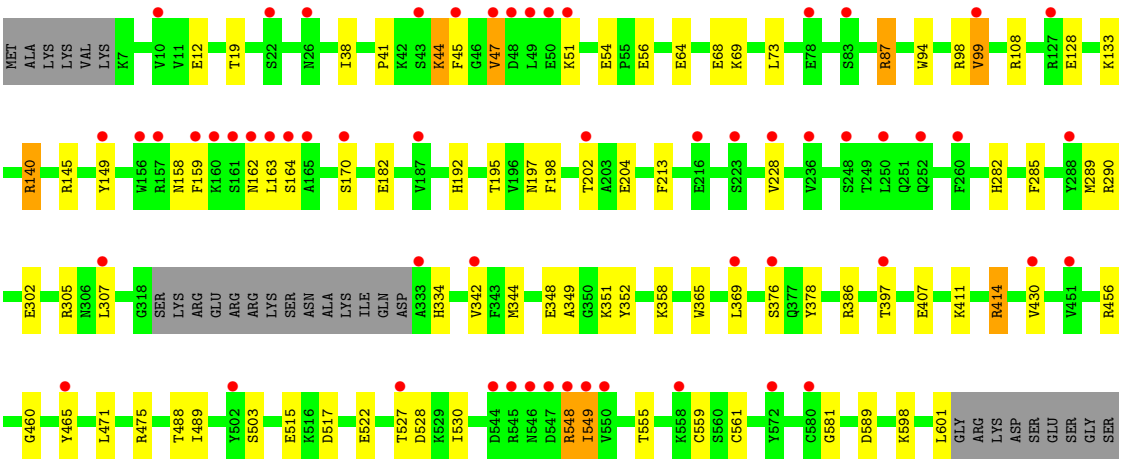
• Molecule 1: DNA topoisomerase I

Chain A:



• Molecule 1: DNA topoisomerase I

Chain B:



PRO
ASP
GLY
ARG
SER
VAL
GLU
GLY
LYS
GLY
ASN
LEU
SER
GLU
LYS
ARG
ARG
LYS
GLY
LYS
LYS
GLY
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	45.12Å 95.42Å 96.51Å 83.40° 86.15° 84.87°	Depositor
Resolution (Å)	41.56 – 1.70 41.55 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.9 (41.56-1.70) 95.9 (41.55-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.197 , 0.232 0.202 , 0.236	Depositor DCC
R_{free} test set	8387 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	20.3	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 39.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.025 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10600	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% 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	0.66	0/4927	0.90	11/6618 (0.2%)
1	B	0.67	2/4941 (0.0%)	0.90	8/6637 (0.1%)
All	All	0.66	2/9868 (0.0%)	0.90	19/13255 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	581	GLY	C-O	9.25	1.38	1.23
1	B	581	GLY	C-N	8.49	1.53	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	456	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	B	456	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	A	456	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	A	108	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	528	ASP	CB-CG-OD1	5.73	123.45	118.30
1	B	87	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	98	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	B	290	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	B	456	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	528	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	87	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	86	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	260	PHE	CB-CG-CD2	-5.43	117.00	120.80
1	B	414	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	272	LEU	CB-CG-CD1	-5.29	102.01	111.00
1	A	411	LYS	CB-CA-C	5.21	120.82	110.40
1	B	140	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	166	GLY	N-CA-C	5.11	125.86	113.10
1	B	517	ASP	CB-CG-OD1	5.02	122.82	118.30

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	4770	0	4890	60	0
1	B	4776	0	4898	73	0
2	A	544	0	0	8	0
2	B	510	0	0	10	0
All	All	10600	0	9788	133	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 7.

All (133) 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:344:MET:CE	1:B:349:ALA:HA	1.82	1.09
1:B:344:MET:HE1	1:B:349:ALA:HA	1.43	0.99
1:A:169:GLN:OE1	1:A:471:LEU:HD13	1.74	0.87
1:A:38:ILE:HD11	1:A:99[B]:VAL:HG11	1.57	0.85
1:B:192:HIS:HD2	1:B:213:PHE:H	1.21	0.84
1:B:344:MET:HE3	1:B:349:ALA:HA	1.57	0.84
1:B:334:HIS:CD2	2:B:797:HOH:O	2.29	0.83
1:B:38:ILE:HD11	1:B:99[B]:VAL:HG11	1.62	0.81
1:B:489:ILE:HD11	1:B:601:LEU:HD22	1.64	0.80
1:B:38:ILE:HD11	1:B:99[B]:VAL:CG1	2.17	0.74
1:A:165:ALA:HB3	1:A:471:LEU:HD12	1.69	0.74
1:A:471:LEU:CD2	1:A:475:ARG:HE	2.00	0.74
1:A:228[B]:VAL:HG21	1:A:386:ARG:CZ	2.19	0.72
1:A:192:HIS:HD2	1:A:213:PHE:H	1.40	0.69
1:B:19:THR:OG1	1:B:282:HIS:HD2	1.77	0.68
1:B:411:LYS:HG3	2:B:1029:HOH:O	1.94	0.68
1:A:471:LEU:HD22	1:A:475:ARG:HG2	1.76	0.66
1:B:197:ASN:OD1	1:B:202[B]:THR:HG22	1.96	0.66
1:B:344:MET:CE	1:B:349:ALA:CA	2.69	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:GLU:OE2	2:B:966:HOH:O	2.13	0.66
1:B:334:HIS:HD2	2:B:843:HOH:O	1.78	0.65
1:B:285:PHE:HE1	1:B:344:MET:CE	2.10	0.65
1:B:282:HIS:HE1	2:B:956:HOH:O	1.80	0.64
1:B:41:PRO:HB2	1:B:44:LYS:HB3	1.79	0.64
1:B:164:SER:H	1:B:475:ARG:HH12	1.44	0.64
1:B:41:PRO:HD3	1:B:56:GLU:O	1.99	0.63
1:B:460:GLY:HA3	1:B:465:TYR:CE1	2.34	0.63
1:A:45:PHE:O	1:A:145:ARG:HD2	1.99	0.62
1:A:561:CYS:SG	1:A:580:CYS:HB3	2.39	0.62
1:B:228[B]:VAL:HG21	1:B:386:ARG:CZ	2.30	0.62
1:B:334:HIS:CD2	2:B:843:HOH:O	2.53	0.61
1:B:344:MET:HE3	1:B:349:ALA:CA	2.28	0.61
1:B:198:PHE:HB3	1:B:430[B]:VAL:HG12	1.82	0.61
1:A:198:PHE:HB3	1:A:430[B]:VAL:HG12	1.81	0.61
1:B:145:ARG:HD3	1:B:149:TYR:CD1	2.35	0.60
1:A:38:ILE:HD11	1:A:99[B]:VAL:CG1	2.29	0.60
1:B:503:SER:HB2	2:B:789:HOH:O	2.00	0.60
1:A:228[B]:VAL:HG22	1:A:386:ARG:HG3	1.84	0.60
1:A:225:ASP:C	1:A:430[B]:VAL:HG22	2.22	0.60
1:B:228[B]:VAL:CG2	1:B:386:ARG:HG3	2.32	0.60
1:A:145:ARG:HD3	1:A:149:TYR:CD2	2.37	0.59
1:B:140:ARG:NH2	1:B:515:GLU:OE1	2.35	0.59
1:B:344:MET:HE1	1:B:349:ALA:CA	2.26	0.59
1:A:348:GLU:O	1:A:351:LYS:HG2	2.01	0.59
1:B:489:ILE:HD11	1:B:601:LEU:CD2	2.30	0.59
1:B:158:ASN:HD21	1:B:548:ARG:HA	1.67	0.58
1:A:169:GLN:HG3	1:A:472:LEU:HD21	1.84	0.58
1:A:382:ARG:HG2	1:A:397[A]:THR:HG22	1.85	0.58
1:A:342[A]:VAL:HG11	1:A:368:PHE:HE2	1.69	0.57
1:A:561:CYS:CB	1:A:580:CYS:HG	2.16	0.57
1:B:69:LYS:HE3	1:B:73:LEU:HD21	1.87	0.56
1:B:285:PHE:HE1	1:B:344:MET:HE3	1.71	0.56
1:B:228[B]:VAL:HG23	1:B:386:ARG:CG	2.36	0.56
1:A:488:THR:HB	1:A:589:ASP:HA	1.87	0.56
1:B:192:HIS:HD2	1:B:213:PHE:N	2.00	0.55
1:A:7:LYS:N	2:A:1147:HOH:O	2.39	0.55
1:A:228[B]:VAL:CG2	1:A:386:ARG:HG3	2.37	0.55
1:B:159:PHE:CZ	1:B:549:ILE:CD1	2.89	0.55
1:A:165:ALA:HB3	1:A:471:LEU:CD1	2.37	0.55
1:A:163:LEU:HD11	1:A:170[B]:SER:OG	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:VAL:HG12	1:A:432:VAL:HG22	1.90	0.54
1:A:87:ARG:NE	1:A:522:GLU:OE1	2.30	0.54
1:B:87:ARG:NE	1:B:522:GLU:OE1	2.23	0.54
1:B:192:HIS:CD2	1:B:213:PHE:H	2.12	0.53
1:B:51:LYS:O	1:B:54:GLU:HG2	2.08	0.53
1:B:228[B]:VAL:HG23	1:B:386:ARG:HG3	1.90	0.53
1:A:561:CYS:SG	1:A:580:CYS:CB	2.97	0.52
1:A:38:ILE:CD1	1:A:99[B]:VAL:HG11	2.36	0.52
1:A:198:PHE:CZ	1:A:385:LEU:HD11	2.44	0.52
1:A:561:CYS:HG	1:A:580:CYS:CB	2.23	0.52
1:B:163:LEU:HD11	1:B:170[B]:SER:OG	2.09	0.52
1:B:64:GLU:O	1:B:68:GLU:HG2	2.10	0.51
1:A:41:PRO:HD3	1:A:56:GLU:O	2.11	0.51
1:A:348:GLU:O	1:A:351:LYS:HE2	2.10	0.51
1:A:81:ILE:HG21	1:A:93:ALA:HA	1.93	0.51
1:B:164:SER:N	1:B:475:ARG:HH12	2.08	0.50
1:B:488:THR:HB	1:B:589:ASP:HA	1.95	0.49
1:A:192:HIS:CD2	1:A:213:PHE:H	2.27	0.48
1:A:506:VAL:O	2:A:871:HOH:O	2.19	0.48
1:A:8:TYR:CE1	1:A:73:LEU:HD22	2.48	0.48
1:B:45:PHE:CE1	1:B:145:ARG:HG3	2.47	0.48
1:A:165:ALA:CB	1:A:471:LEU:HD12	2.41	0.48
1:B:94:TRP:CE2	1:B:98:ARG:HD2	2.48	0.48
1:B:527[A]:THR:OG1	2:B:1105:HOH:O	2.14	0.47
1:B:342[A]:VAL:HG12	1:B:369[A]:LEU:HD21	1.96	0.47
1:B:128:GLU:HG3	2:B:706:HOH:O	2.14	0.47
1:A:202[A]:THR:HG22	2:A:810:HOH:O	2.14	0.47
1:A:333:ALA:HB3	2:A:971:HOH:O	2.15	0.47
1:A:471:LEU:HD21	1:A:475:ARG:HE	1.76	0.47
1:A:358:LYS:HG3	2:A:692:HOH:O	2.15	0.46
1:B:285:PHE:HE1	1:B:344:MET:HE2	1.80	0.46
1:B:195:THR:HG22	1:B:204:GLU:CD	2.35	0.46
1:A:568:SER:OG	1:A:577:LYS:HE2	2.15	0.46
1:B:559:CYS:SG	1:B:561:CYS:SG	3.14	0.46
1:A:94:TRP:CE2	1:A:98:ARG:HD2	2.50	0.46
1:B:378:TYR:CZ	1:B:414:ARG:HD2	2.51	0.46
1:A:94:TRP:CZ2	1:A:98:ARG:HD2	2.52	0.45
1:A:578:CYS:C	1:A:580:CYS:H	2.20	0.45
1:B:228[B]:VAL:HG21	1:B:386:ARG:NH1	2.31	0.45
1:B:344:MET:HE2	1:B:352:TYR:HD2	1.81	0.45
1:B:344:MET:HE2	1:B:352:TYR:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:PHE:CE2	1:B:47[B]:VAL:HG22	2.52	0.44
1:A:232:LYS:HE3	1:A:419:PHE:HD2	1.83	0.44
1:B:365:TRP:CH2	1:B:369[B]:LEU:HD22	2.53	0.44
1:A:228[B]:VAL:CG2	1:A:386:ARG:CG	2.95	0.44
1:B:307[B]:LEU:HD12	1:B:369[B]:LEU:CD1	2.47	0.44
1:B:471:LEU:C	1:B:471:LEU:HD23	2.38	0.43
1:B:158:ASN:HD22	1:B:548:ARG:NH1	2.15	0.43
1:B:358:LYS:CG	2:B:829:HOH:O	2.66	0.43
1:A:471:LEU:HD22	1:A:475:ARG:CG	2.46	0.43
1:A:38:ILE:CD1	1:A:99[B]:VAL:CG1	2.95	0.43
1:B:527[B]:THR:HG23	1:B:530:ILE:HD12	2.00	0.43
1:B:302:GLU:OE1	1:B:305:ARG:NH1	2.47	0.43
1:A:218:LEU:HD22	1:A:434:ILE:HG21	2.01	0.42
1:A:34:MET:HB2	1:A:63:LYS:HZ1	1.83	0.42
1:B:348:GLU:O	1:B:351:LYS:HG2	2.19	0.42
1:B:344:MET:CE	1:B:352:TYR:HD2	2.32	0.42
1:A:204:GLU:OE1	2:A:806:HOH:O	2.22	0.42
1:A:342[A]:VAL:HG13	2:A:738:HOH:O	2.19	0.42
1:A:378:TYR:CZ	1:A:414:ARG:HD2	2.55	0.42
1:A:514:MET:HB3	1:A:514:MET:HE2	1.78	0.41
1:B:285:PHE:CE1	1:B:344:MET:HE2	2.54	0.41
1:A:145:ARG:HD3	1:A:149:TYR:CE2	2.55	0.41
1:A:13:SER:HA	1:A:14:PRO:HD3	1.87	0.41
1:A:151:LEU:HD21	1:A:502:TYR:CZ	2.56	0.41
1:B:555:THR:O	1:B:598:LYS:HE3	2.21	0.41
1:B:69:LYS:O	1:B:73:LEU:HG	2.21	0.41
1:B:344:MET:HE3	1:B:349:ALA:CB	2.49	0.41
1:B:94:TRP:CZ2	1:B:98:ARG:HD2	2.56	0.41
1:B:376[A]:SER:OG	1:B:407:GLU:HG3	2.20	0.41
1:A:442:LYS:HD2	2:A:765:HOH:O	2.21	0.41
1:A:34:MET:HB2	1:A:63:LYS:NZ	2.35	0.40
1:B:38:ILE:CD1	1:B:99[B]:VAL:CG1	2.94	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	595/633 (94%)	584 (98%)	11 (2%)	0	100	100
1	B	597/633 (94%)	587 (98%)	9 (2%)	1 (0%)	47	30
All	All	1192/1266 (94%)	1171 (98%)	20 (2%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	44	LYS

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	537/562 (96%)	520 (97%)	17 (3%)	39	20
1	B	539/562 (96%)	526 (98%)	13 (2%)	49	31
All	All	1076/1124 (96%)	1046 (97%)	30 (3%)	50	25

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	12	GLU
1	A	42	LYS
1	A	47[A]	VAL
1	A	47[B]	VAL
1	A	99[A]	VAL
1	A	99[B]	VAL
1	A	108	ARG
1	A	127[A]	ARG
1	A	127[B]	ARG
1	A	140	ARG

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Mol	Chain	Res	Type
1	A	289	MET
1	A	351	LYS
1	A	374	LYS
1	A	471	LEU
1	A	548	ARG
1	A	585	SER
1	B	12	GLU
1	B	47[A]	VAL
1	B	47[B]	VAL
1	B	99[A]	VAL
1	B	99[B]	VAL
1	B	108	ARG
1	B	133	LYS
1	B	162	ASN
1	B	289	MET
1	B	397[A]	THR
1	B	397[B]	THR
1	B	548	ARG
1	B	549	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	HIS
1	A	334	HIS
1	A	377	GLN
1	A	557	GLN
1	B	158	ASN
1	B	192	HIS
1	B	282	HIS
1	B	334	HIS
1	B	377	GLN
1	B	557	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 monosaccharides 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	581/633 (91%)	0.79	63 (10%) 5 6	2, 11, 26, 41	18 (3%)
1	B	581/633 (91%)	0.77	57 (9%) 7 8	2, 10, 25, 40	20 (3%)
All	All	1162/1266 (91%)	0.78	120 (10%) 6 7	2, 10, 25, 41	38 (3%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	549	ILE	9.1
1	B	228[A]	VAL	8.3
1	B	156	TRP	7.8
1	B	165	ALA	7.6
1	A	572	TYR	7.4
1	A	157	ARG	7.3
1	A	156	TRP	7.1
1	A	228[A]	VAL	6.9
1	B	99[A]	VAL	6.5
1	B	248[A]	SER	6.5
1	A	99[A]	VAL	6.1
1	B	10[A]	VAL	6.0
1	A	248[A]	SER	5.9
1	A	83[A]	SER	5.6
1	A	43	SER	5.5
1	A	10[A]	VAL	5.5
1	B	83[A]	SER	5.4
1	B	548	ARG	5.3
1	B	369[A]	LEU	5.3
1	A	160	LYS	5.2
1	A	342[A]	VAL	5.1
1	B	342[A]	VAL	5.0
1	A	170[A]	SER	5.0
1	A	165	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	163	LEU	4.9
1	B	550	VAL	4.9
1	B	157	ARG	4.8
1	A	430[A]	VAL	4.8
1	A	549	ILE	4.6
1	B	430[A]	VAL	4.6
1	A	527[A]	THR	4.4
1	A	47[A]	VAL	4.4
1	A	571	LYS	4.3
1	B	43	SER	4.3
1	A	561	CYS	4.2
1	B	170[A]	SER	4.0
1	A	584	ARG	4.0
1	B	546	ASN	3.9
1	B	545	ARG	3.9
1	A	559	CYS	3.9
1	A	127[A]	ARG	3.8
1	B	149	TYR	3.8
1	A	582	LYS	3.8
1	B	223[A]	SER	3.8
1	B	47[A]	VAL	3.8
1	B	163	LEU	3.7
1	B	162	ASN	3.7
1	A	580	CYS	3.7
1	B	202[A]	THR	3.7
1	B	547	ASP	3.6
1	B	236[A]	VAL	3.6
1	B	164	SER	3.6
1	B	376[A]	SER	3.6
1	A	573	GLY	3.6
1	B	161	SER	3.6
1	B	572	TYR	3.6
1	A	546	ASN	3.5
1	B	160	LYS	3.5
1	B	49	LEU	3.4
1	B	527[A]	THR	3.4
1	A	550	VAL	3.4
1	A	223[A]	SER	3.4
1	A	570	GLY	3.4
1	B	26	ASN	3.3
1	A	159	PHE	3.3
1	B	127[A]	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	252[A]	GLN	3.1
1	A	545	ARG	3.0
1	A	26	ASN	3.0
1	A	195[A]	THR	3.0
1	A	50	GLU	3.0
1	B	333	ALA	3.0
1	B	159	PHE	3.0
1	A	51	LYS	2.9
1	B	51	LYS	2.9
1	B	465	TYR	2.9
1	B	307[A]	LEU	2.8
1	A	585	SER	2.8
1	B	22[A]	SER	2.8
1	A	209	GLU	2.8
1	A	162	ASN	2.8
1	B	187	VAL	2.7
1	B	50	GLU	2.7
1	A	22[A]	SER	2.7
1	A	252[A]	GLN	2.7
1	B	48	ASP	2.6
1	A	579	GLU	2.6
1	A	397[A]	THR	2.5
1	B	397[A]	THR	2.5
1	A	202[A]	THR	2.5
1	A	27	GLU	2.5
1	B	558	LYS	2.5
1	A	583	THR	2.5
1	A	307[A]	LEU	2.4
1	B	502	TYR	2.4
1	B	78	GLU	2.4
1	A	544	ASP	2.4
1	B	580	CYS	2.3
1	B	544	ASP	2.3
1	A	548	ARG	2.3
1	A	551	VAL	2.3
1	B	216	GLU	2.3
1	A	57	PHE	2.2
1	A	161	SER	2.2
1	B	250	LEU	2.2
1	A	578	CYS	2.2
1	A	155	LEU	2.2
1	A	465	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	288	TYR	2.1
1	A	29	GLU	2.1
1	A	462	PRO	2.1
1	A	149	TYR	2.1
1	A	236	VAL	2.1
1	A	451	VAL	2.1
1	A	171	ALA	2.1
1	B	45	PHE	2.1
1	A	497	TYR	2.0
1	B	451	VAL	2.0
1	A	314	GLU	2.0
1	B	260	PHE	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 monosaccharides 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.