



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2GAI / pdb_00002gai
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	:	4-5-2 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

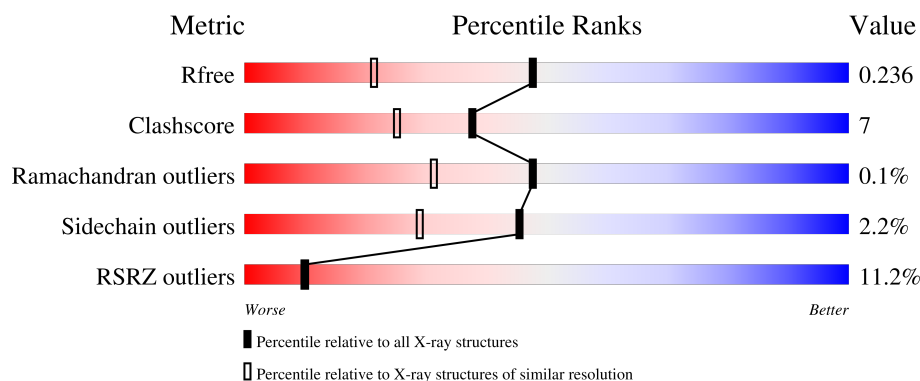
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 $\leq 5\%$. 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	633	11% 79% 12% 8%
1	B	633	9% 78% 12% 8%

2 Entry composition

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		

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

4 Data and refinement statistics

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 41.56 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.9 (41.56-1.70) 95.9 (41.56-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.79%)	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)	0.36 , 34.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

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

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	0.77	0/4927	1.06	6/6618 (0.1%)
1	B	0.78	2/4941 (0.0%)	1.06	7/6637 (0.1%)
All	All	0.77	2/9868 (0.0%)	1.06	13/13255 (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-N	14.05	1.53	1.33
1	B	581	GLY	C-O	7.66	1.38	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	411	LYS	CB-CA-C	6.83	120.82	109.89
1	B	581	GLY	O-C-N	6.66	130.03	123.31
1	A	505	VAL	N-CA-C	6.03	117.49	110.62
1	A	247	THR	O-C-N	5.63	127.87	122.07
1	B	440	LYS	CA-C-N	-5.54	114.89	120.21
1	B	440	LYS	C-N-CA	-5.54	114.89	120.21
1	A	199	ASP	N-CA-C	5.50	119.02	111.54
1	A	166	GLY	N-CA-C	5.35	125.86	113.18
1	B	455	GLU	CA-CB-CG	-5.30	103.51	114.10
1	A	455	GLU	CA-CB-CG	-5.15	103.81	114.10
1	B	162	ASN	N-CA-C	5.05	115.97	108.60
1	B	166	GLY	N-CA-C	5.00	125.04	113.18
1	B	411	LYS	CB-CA-C	5.00	118.21	109.65

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	4770	0	4890	62	0
1	B	4776	0	4898	72	0
2	A	544	0	0	8	0
2	B	510	0	0	10	0
All	All	10600	0	9788	134	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 (134) 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:HE3	1:B:349:ALA:HA	1.16	1.09
1:B:344:MET:CE	1:B:349:ALA:HA	1.82	1.09
1:B:344:MET:HE3	1:B:349:ALA:CA	1.86	1.06
1:B:285:PHE:HE1	1:B:344:MET:HE2	1.26	1.01
1:A:169:GLN:OE1	1:A:471:LEU:HD13	1.74	0.87
1:B:285:PHE:CE1	1:B:344:MET:HE2	2.09	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: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: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:344:MET:HE1	1:B:352:TYR:CD2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:MET:HE1	1:B:352:TYR:HD2	1.63	0.65
1:A:225:ASP:C	1:A:430[B]:VAL:HG22	2.22	0.64
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:514:MET:HE1	1:A:531:VAL:CG1	2.29	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: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:514:MET:HE1	1:B:531:VAL:CG1	2.31	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:285:PHE:HE1	1:B:344:MET:CE	2.10	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: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: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	2.17	0.56
1:B:69:LYS:HE3	1:B:73:LEU:HD21	1.87	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:MET:HE3	1:B:349:ALA:CB	2.36	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:B:195:THR:HG22	1:B:204:GLU:CD	2.35	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:A:578:CYS:C	1:A:580:CYS:H	2.20	0.50
1:A:514:MET:HE3	1:A:514:MET:HA	1.93	0.49
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:B:471:LEU:C	1:B:471:LEU:HD23	2.38	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: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:B:514:MET:HE3	1:B:514:MET:CA	2.46	0.46
1:A:94:TRP:CZ2	1:A:98:ARG:HD2	2.52	0.45
1:A:514:MET:HE3	1:A:514:MET:CA	2.46	0.45
1:B:228[B]:VAL:HG21	1:B:386:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:MET:HE3	1:B:514:MET:HA	1.98	0.45
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: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:B:348:GLU:O	1:B:351:LYS:HG2	2.19	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: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:344:MET:CE	1:B:352:TYR:HD2	2.32	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:94:TRP:CZ2	1:B:98:ARG:HD2	2.56	0.41
1:A:143:LEU:HD11	1:A:514:MET:HE2	2.03	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	43	28
All	All	1192/1266 (94%)	1171 (98%)	20 (2%)	1 (0%)	48	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	44	LYS

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	537/562 (96%)	520 (97%)	17 (3%)	34	17
1	B	539/562 (96%)	526 (98%)	13 (2%)	43	26
All	All	1076/1124 (96%)	1046 (97%)	30 (3%)	45	21

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	47[A]	VAL
1	A	47[B]	VAL
1	A	99[A]	VAL
1	A	99[B]	VAL
1	A	127[A]	ARG
1	A	127[B]	ARG
1	A	289	MET
1	A	351	LYS
1	A	374	LYS
1	A	471	LEU
1	A	527[A]	THR
1	A	527[B]	THR
1	A	548	ARG

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Mol	Chain	Res	Type
1	A	585	SER
1	A	587	LYS
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	162	ASN
1	B	163	LEU
1	B	289	MET
1	B	397[A]	THR
1	B	397[B]	THR
1	B	413	GLU
1	B	489	ILE
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	270	GLN
1	A	282	HIS
1	A	557	GLN
1	B	158	ASN
1	B	192	HIS
1	B	282	HIS
1	B	334	HIS
1	B	557	GLN
1	B	588	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	581/633 (91%)	0.78	71 (12%) 8 8	1, 11, 26, 41	18 (3%)
1	B	581/633 (91%)	0.76	59 (10%) 12 12	1, 10, 25, 40	20 (3%)
All	All	1162/1266 (91%)	0.77	130 (11%) 10 10	1, 10, 25, 41	38 (3%)

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	228[A]	VAL	13.5
1	B	228[A]	VAL	11.3
1	B	165	ALA	8.4
1	B	342[A]	VAL	7.9
1	B	10[A]	VAL	7.7
1	A	223[A]	SER	7.6
1	A	527[A]	THR	7.4
1	B	47[A]	VAL	7.4
1	A	342[A]	VAL	7.3
1	A	430[A]	VAL	7.2
1	B	376[A]	SER	7.1
1	A	99[A]	VAL	6.9
1	B	156	TRP	6.8
1	B	99[A]	VAL	6.8
1	B	369[A]	LEU	6.7
1	A	156	TRP	6.6
1	A	47[A]	VAL	6.6
1	B	223[A]	SER	6.5
1	A	10[A]	VAL	6.4
1	B	248[A]	SER	6.3
1	B	164	SER	6.2
1	A	195[A]	THR	6.2
1	A	248[A]	SER	6.1
1	B	83[A]	SER	6.1

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Mol	Chain	Res	Type	RSRZ
1	B	22[A]	SER	6.0
1	B	236[A]	VAL	5.9
1	B	430[A]	VAL	5.9
1	B	307[A]	LEU	5.8
1	A	83[A]	SER	5.8
1	B	161	SER	5.8
1	A	22[A]	SER	5.6
1	B	397[A]	THR	5.6
1	B	170[A]	SER	5.4
1	A	165	ALA	5.4
1	B	202[A]	THR	5.2
1	B	527[A]	THR	5.2
1	A	307[A]	LEU	5.1
1	A	127[A]	ARG	5.0
1	A	572	TYR	5.0
1	A	397[A]	THR	4.9
1	A	559	CYS	4.7
1	A	170[A]	SER	4.7
1	B	162	ASN	4.6
1	A	161	SER	4.6
1	A	580	CYS	4.6
1	A	549	ILE	4.6
1	B	549	ILE	4.5
1	A	157	ARG	4.4
1	B	163	LEU	4.3
1	A	202[A]	THR	4.2
1	A	43	SER	4.1
1	A	163	LEU	4.1
1	B	252[A]	GLN	3.9
1	B	43	SER	3.9
1	B	548	ARG	3.9
1	A	550	VAL	3.8
1	B	166	GLY	3.7
1	B	333	ALA	3.7
1	A	561	CYS	3.7
1	A	160	LYS	3.6
1	B	127[A]	ARG	3.6
1	A	582	LYS	3.5
1	B	160	LYS	3.5
1	A	579	GLU	3.5
1	B	78	GLU	3.4
1	B	157	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	162	ASN	3.4
1	A	164	SER	3.4
1	B	149	TYR	3.3
1	A	570	GLY	3.2
1	A	581	GLY	3.2
1	A	585	SER	3.1
1	A	209	GLU	3.1
1	A	51	LYS	3.1
1	A	159	PHE	3.1
1	B	550	VAL	3.0
1	A	31	PHE	3.0
1	A	584	ARG	3.0
1	A	573	GLY	2.9
1	A	166	GLY	2.9
1	B	503	SER	2.9
1	B	31	PHE	2.9
1	B	545	ARG	2.9
1	A	252[A]	GLN	2.8
1	B	26	ASN	2.8
1	A	78	GLU	2.8
1	A	61	LYS	2.7
1	A	29	GLU	2.7
1	A	545	ARG	2.7
1	A	578	CYS	2.7
1	A	54	GLU	2.6
1	A	583	THR	2.6
1	B	558	LYS	2.6
1	A	27	GLU	2.5
1	A	544	ASP	2.5
1	A	57	PHE	2.5
1	A	391	LYS	2.5
1	B	559	CYS	2.4
1	B	561	CYS	2.4
1	A	155	LEU	2.4
1	A	503	SER	2.4
1	A	26	ASN	2.4
1	B	502	TYR	2.4
1	A	589	ASP	2.4
1	B	547	ASP	2.4
1	B	596	ASP	2.4
1	B	216	GLU	2.4
1	A	548	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	596	ASP	2.3
1	B	348	GLU	2.3
1	A	502	TYR	2.3
1	A	571	LYS	2.3
1	B	159	PHE	2.3
1	B	48	ASP	2.3
1	B	54	GLU	2.2
1	A	45	PHE	2.2
1	A	562	GLY	2.2
1	B	25	GLY	2.2
1	A	199	ASP	2.1
1	B	537	GLU	2.1
1	A	334	HIS	2.1
1	A	149	TYR	2.1
1	B	318	GLY	2.0
1	B	49	LEU	2.0
1	A	501	LYS	2.0
1	A	303	GLU	2.0
1	B	534	GLU	2.0
1	B	158	ASN	2.0
1	B	187	VAL	2.0
1	B	42	LYS	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 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.