



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:22 PM GMT

PDB ID : 1J6R  
Title : Crystal structure of Activation (AdoMet binding) domain of Methionine synthase (TM0269) from *Thermotoga maritima* at 2.2 Å resolution  
Authors : Joint Center for Structural Genomics (JCSG)  
Deposited on : 2002-07-10  
Resolution : 2.30 Å (reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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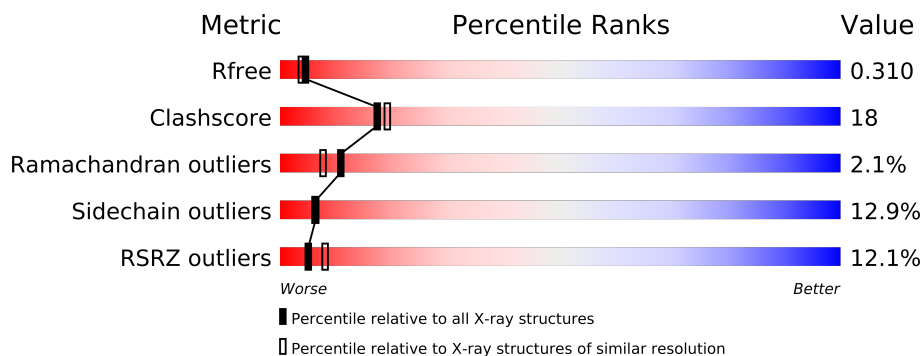
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance



The reported resolution of this entry is 2.30 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	214	
1	B	214	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3249 atoms, of which 0 are hydrogen and 0 are deuterium.

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 METHIONINE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	52	0	0
			1573	1013	261	295	4			
1	B	197	Total	C	N	O	S	110	0	0
			1573	1013	261	295	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	LEADER SEQUENCE	UNP Q9WYA6
A	-8	GLY	-	LEADER SEQUENCE	UNP Q9WYA6
A	-7	SER	-	LEADER SEQUENCE	UNP Q9WYA6
A	-6	ASP	-	LEADER SEQUENCE	UNP Q9WYA6
A	-5	LYS	-	LEADER SEQUENCE	UNP Q9WYA6
A	-4	ILE	-	LEADER SEQUENCE	UNP Q9WYA6
A	-3	HIS	-	EXPRESSION TAG	UNP Q9WYA6
A	-2	HIS	-	EXPRESSION TAG	UNP Q9WYA6
A	-1	HIS	-	EXPRESSION TAG	UNP Q9WYA6
A	0	HIS	-	EXPRESSION TAG	UNP Q9WYA6
A	1	HIS	-	EXPRESSION TAG	UNP Q9WYA6
A	2	HIS	-	EXPRESSION TAG	UNP Q9WYA6
B	-9	MET	-	LEADER SEQUENCE	UNP Q9WYA6
B	-8	GLY	-	LEADER SEQUENCE	UNP Q9WYA6
B	-7	SER	-	LEADER SEQUENCE	UNP Q9WYA6
B	-6	ASP	-	LEADER SEQUENCE	UNP Q9WYA6
B	-5	LYS	-	LEADER SEQUENCE	UNP Q9WYA6
B	-4	ILE	-	LEADER SEQUENCE	UNP Q9WYA6
B	-3	HIS	-	EXPRESSION TAG	UNP Q9WYA6
B	-2	HIS	-	EXPRESSION TAG	UNP Q9WYA6
B	-1	HIS	-	EXPRESSION TAG	UNP Q9WYA6
B	0	HIS	-	EXPRESSION TAG	UNP Q9WYA6
B	1	HIS	-	EXPRESSION TAG	UNP Q9WYA6
B	2	HIS	-	EXPRESSION TAG	UNP Q9WYA6

- Molecule 2 is water.

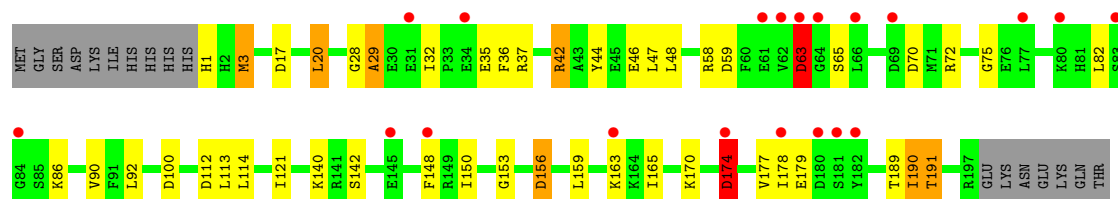
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	42	Total 42	O 42	0	0
2	B	61	Total 61	O 61	0	0

### 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.

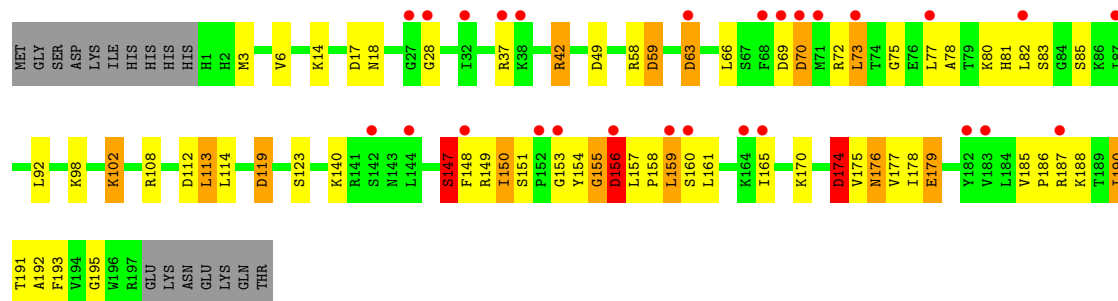
#### • Molecule 1: METHIONINE SYNTHASE

Chain A: 



#### • Molecule 1: METHIONINE SYNTHASE

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.40Å 60.74Å 81.57Å 90.00° 99.97° 90.00°	Depositor
Resolution (Å)	36.22 – 2.30 36.22 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (36.22-2.30) 99.6 (36.22-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.251 , 0.290 0.279 , 0.310	Depositor DCC
$R_{free}$ test set	1308 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.4	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 37.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 38947 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3249	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.67	0/1603	0.78	7/2159 (0.3%)
1	B	0.74	0/1603	0.92	9/2159 (0.4%)
All	All	0.70	0/3206	0.85	16/4318 (0.4%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	ASP	CB-CG-OD2	8.22	125.70	118.30
1	B	59	ASP	CB-CG-OD2	8.15	125.64	118.30
1	B	17	ASP	CB-CG-OD2	6.88	124.49	118.30
1	B	112	ASP	CB-CG-OD2	6.50	124.16	118.30
1	B	178	ILE	C-N-CA	6.25	137.32	121.70
1	A	112	ASP	CB-CG-OD2	5.91	123.61	118.30
1	B	174	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	174	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	179	GLU	N-CA-C	5.58	126.06	111.00
1	A	100	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	59	ASP	CB-CG-OD2	5.44	123.20	118.30
1	B	156	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	63	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	70	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	17	ASP	CB-CG-OD2	5.15	122.93	118.30
1	B	63	ASP	CB-CG-OD2	5.05	122.85	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1573	0	1601	27	0
1	B	1573	0	1601	78	0
2	A	42	0	0	4	0
2	B	61	0	0	26	0
All	All	3249	0	3202	105	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

All (105) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:190:ILE:HG21	2:B:243:HOH:O	1.18	1.26
1:A:174:ASP:HB3	2:A:234:HOH:O	1.56	1.04
1:B:42:ARG:HA	2:B:252:HOH:O	1.66	0.94
1:B:147:SER:OG	1:B:148:PHE:N	1.98	0.92
1:B:66:LEU:HB3	1:B:73:LEU:HD22	1.54	0.88
1:B:156:ASP:CB	2:B:257:HOH:O	2.22	0.87
1:B:73:LEU:HD23	1:B:73:LEU:C	1.96	0.86
1:B:73:LEU:HD11	1:B:78:ALA:HB1	1.55	0.86
1:B:157:LEU:HB2	2:B:261:HOH:O	1.76	0.83
1:B:156:ASP:HB2	2:B:257:HOH:O	1.80	0.80
1:B:37:ARG:CD	2:B:246:HOH:O	2.32	0.78
1:B:81:HIS:CE1	2:B:236:HOH:O	2.36	0.78
1:A:1:HIS:HB3	2:A:233:HOH:O	1.85	0.77
1:B:59:ASP:O	2:B:249:HOH:O	2.06	0.73
1:B:156:ASP:HB3	2:B:257:HOH:O	1.85	0.72
1:B:66:LEU:HD13	2:B:251:HOH:O	1.90	0.72
1:B:102:LYS:NZ	2:B:256:HOH:O	2.24	0.70
1:B:156:ASP:OD1	1:B:156:ASP:N	2.22	0.70
1:B:190:ILE:CG2	2:B:243:HOH:O	1.99	0.69
1:B:3:MET:HE1	1:B:58:ARG:HD2	1.75	0.69
1:B:73:LEU:HD23	1:B:73:LEU:O	1.91	0.69
1:B:75:GLY:HA3	2:B:235:HOH:O	1.92	0.68
1:B:81:HIS:HE1	2:B:236:HOH:O	1.72	0.66
1:B:73:LEU:CD1	1:B:78:ALA:HB1	2.25	0.65
1:B:153:GLY:HA3	1:B:159:LEU:HD12	1.76	0.65
1:A:140:LYS:NZ	2:A:229:HOH:O	2.30	0.64
1:B:3:MET:CE	1:B:58:ARG:HD2	2.27	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:157:LEU:HG	1:B:161:LEU:HD12	1.81	0.63
1:B:153:GLY:HA3	1:B:159:LEU:CD1	2.30	0.62
1:B:37:ARG:HD2	2:B:246:HOH:O	1.98	0.62
1:A:177:VAL:O	1:A:179:GLU:N	2.33	0.62
1:A:3:MET:HE1	1:A:58:ARG:HB2	1.80	0.62
1:B:153:GLY:CA	1:B:159:LEU:HD12	2.28	0.61
1:B:190:ILE:HG23	1:B:191:THR:N	2.16	0.61
1:B:66:LEU:CD1	1:B:83:SER:HB3	2.30	0.61
1:B:73:LEU:HD21	1:B:78:ALA:HB1	1.81	0.61
1:A:42:ARG:O	1:A:46:GLU:HG2	2.02	0.60
1:A:3:MET:HA	1:A:3:MET:CE	2.32	0.59
1:B:98:LYS:HD2	2:B:260:HOH:O	2.03	0.58
1:B:174:ASP:CB	2:B:264:HOH:O	2.51	0.58
1:B:66:LEU:HD11	1:B:83:SER:HB3	1.86	0.57
1:B:66:LEU:CD1	2:B:251:HOH:O	2.50	0.57
1:A:163:LYS:HA	1:A:177:VAL:HG21	1.87	0.57
1:A:28:GLY:O	1:A:29:ALA:C	2.44	0.56
1:B:73:LEU:CD2	1:B:73:LEU:C	2.68	0.55
1:A:75:GLY:HA3	1:A:156:ASP:HB2	1.88	0.55
1:B:149:ARG:HH11	1:B:149:ARG:HG3	1.71	0.54
1:A:35:GLU:HG3	1:A:36:PHE:CD1	2.42	0.54
1:B:73:LEU:CG	1:B:78:ALA:HB1	2.38	0.54
1:B:66:LEU:HD21	1:B:82:LEU:C	2.29	0.54
1:B:190:ILE:CG2	1:B:191:THR:N	2.71	0.53
1:B:147:SER:HB3	1:B:195:GLY:O	2.09	0.52
1:B:158:PRO:C	1:B:160:SER:N	2.63	0.51
1:A:35:GLU:HG3	1:A:36:PHE:CE1	2.45	0.51
1:A:47:LEU:HD23	1:A:121:ILE:CG2	2.40	0.51
1:B:158:PRO:C	1:B:160:SER:H	2.14	0.51
1:B:18:ASN:HB2	2:B:242:HOH:O	2.10	0.50
1:B:174:ASP:HB2	2:B:264:HOH:O	2.11	0.50
1:A:190:ILE:HD11	2:A:236:HOH:O	2.12	0.49
1:B:191:THR:CG2	1:B:192:ALA:N	2.75	0.49
1:B:73:LEU:HD11	1:B:78:ALA:CB	2.34	0.49
1:B:73:LEU:CD2	1:B:78:ALA:HB1	2.44	0.48
1:A:20:LEU:HD21	1:A:121:ILE:HG12	1.95	0.48
1:B:119:ASP:OD1	1:B:188:LYS:HE3	2.15	0.47
1:B:154:TYR:O	1:B:155:GLY:C	2.52	0.47
1:B:37:ARG:HD3	2:B:246:HOH:O	2.05	0.47
1:B:190:ILE:HD13	2:B:243:HOH:O	2.14	0.47
1:A:165:ILE:HD13	1:A:191:THR:CG2	2.45	0.47
1:B:175:VAL:HG12	1:B:176:ASN:N	2.29	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:82:LEU:HD11	1:A:150:ILE:HD11	1.97	0.46
1:B:157:LEU:HD11	1:B:161:LEU:CD1	2.45	0.46
1:A:3:MET:HE3	1:A:3:MET:HA	1.96	0.46
1:B:119:ASP:OD1	1:B:188:LYS:CE	2.64	0.46
1:B:149:ARG:HA	1:B:193:PHE:O	2.16	0.45
1:A:47:LEU:HD23	1:A:121:ILE:HG22	1.98	0.45
1:B:153:GLY:CA	1:B:159:LEU:CD1	2.92	0.45
1:B:185:VAL:HA	1:B:186:PRO:C	2.37	0.45
1:B:191:THR:HG22	1:B:192:ALA:N	2.31	0.45
1:B:147:SER:HG	1:B:148:PHE:H	1.61	0.45
1:A:92:LEU:HD11	1:A:189:THR:CG2	2.46	0.45
1:A:3:MET:HA	1:A:3:MET:HE2	1.98	0.45
1:B:149:ARG:HG2	1:B:192:ALA:HB1	1.99	0.44
1:B:66:LEU:CB	1:B:73:LEU:HD22	2.36	0.44
1:B:175:VAL:CG1	1:B:176:ASN:N	2.80	0.44
1:A:44:TYR:CE2	1:A:48:LEU:HD11	2.53	0.44
1:A:3:MET:CE	1:A:58:ARG:HB2	2.45	0.44
1:B:165:ILE:HG22	1:B:165:ILE:O	2.17	0.44
1:A:153:GLY:HA3	1:A:159:LEU:CD1	2.49	0.43
1:B:190:ILE:CD1	2:B:208:HOH:O	2.67	0.42
1:B:69:ASP:O	1:B:70:ASP:CB	2.65	0.42
1:B:77:LEU:HD12	2:B:236:HOH:O	2.19	0.42
1:B:92:LEU:HD12	1:B:190:ILE:O	2.20	0.42
1:A:3:MET:CA	1:A:3:MET:CE	2.94	0.41
1:B:157:LEU:CD1	1:B:161:LEU:HD12	2.50	0.41
1:B:113:LEU:HA	1:B:113:LEU:HD23	1.91	0.41
1:B:157:LEU:CG	1:B:161:LEU:HD12	2.49	0.41
1:B:190:ILE:HD11	2:B:208:HOH:O	2.20	0.41
1:B:66:LEU:HD11	1:B:83:SER:CB	2.51	0.41
1:B:75:GLY:HA2	1:B:156:ASP:OD2	2.21	0.41
1:B:157:LEU:CD1	1:B:161:LEU:CD1	2.99	0.40
1:A:90:VAL:HG21	1:A:165:ILE:HG12	2.02	0.40
1:B:190:ILE:HG23	1:B:191:THR:H	1.84	0.40
1:B:150:ILE:CG2	2:B:212:HOH:O	2.69	0.40
1:B:150:ILE:HG13	1:B:150:ILE:O	2.20	0.40
1:A:42:ARG:HD3	1:A:46:GLU:OE1	2.21	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	195/214 (91%)	184 (94%)	8 (4%)	3 (2%)	15	13
1	B	195/214 (91%)	176 (90%)	14 (7%)	5 (3%)	8	5
All	All	390/428 (91%)	360 (92%)	22 (6%)	8 (2%)	11	8

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	179	GLU
1	A	63	ASP
1	A	178	ILE
1	B	28	GLY
1	B	147	SER
1	B	155	GLY
1	B	159	LEU
1	A	29	ALA

### 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	170/186 (91%)	152 (89%)	18 (11%)	10	10
1	B	170/186 (91%)	144 (85%)	26 (15%)	4	3
All	All	340/372 (91%)	296 (87%)	44 (13%)	6	6

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	MET

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Mol	Chain	Res	Type
1	A	20	LEU
1	A	32	ILE
1	A	37	ARG
1	A	42	ARG
1	A	63	ASP
1	A	65	SER
1	A	72	ARG
1	A	86	LYS
1	A	113	LEU
1	A	114	LEU
1	A	142	SER
1	A	148	PHE
1	A	156	ASP
1	A	170	LYS
1	A	174	ASP
1	A	190	ILE
1	A	191	THR
1	B	6	VAL
1	B	14	LYS
1	B	42	ARG
1	B	49	ASP
1	B	63	ASP
1	B	70	ASP
1	B	72	ARG
1	B	73	LEU
1	B	80	LYS
1	B	85	SER
1	B	102	LYS
1	B	108	ARG
1	B	113	LEU
1	B	114	LEU
1	B	123	SER
1	B	140	LYS
1	B	147	SER
1	B	150	ILE
1	B	151	SER
1	B	156	ASP
1	B	170	LYS
1	B	174	ASP
1	B	176	ASN
1	B	177	VAL
1	B	187	ARG

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Mol	Chain	Res	Type
1	B	190	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	197/214 (92%)	0.53	20 (10%) 7 12	19, 40, 69, 76	11 (5%)
1	B	190/214 (88%)	0.82	27 (14%) 3 6	17, 43, 68, 79	12 (6%)
All	All	387/428 (90%)	0.67	47 (12%) 5 8	17, 41, 69, 79	23 (5%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	181	SER	7.2
1	A	63	ASP	4.7
1	B	182	TYR	4.5
1	B	73	LEU	4.4
1	B	77	LEU	4.2
1	B	68	PHE	4.2
1	B	63	ASP	3.8
1	A	180	ASP	3.7
1	B	144	LEU	3.5
1	A	178	ILE	3.5
1	A	84	GLY	3.4
1	B	159	LEU	3.4
1	A	34	GLU	3.2
1	B	148	PHE	3.2
1	A	64	GLY	2.9
1	B	37	ARG	2.9
1	B	82	LEU	2.8
1	B	69	ASP	2.6
1	A	145	GLU	2.6
1	B	71	MET	2.6
1	B	87	ILE	2.5
1	B	160	SER	2.5
1	B	142	SER	2.5
1	A	83	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	28	GLY	2.4
1	B	70	ASP	2.4
1	A	163	LYS	2.4
1	B	153	GLY	2.4
1	B	27	GLY	2.3
1	A	80	LYS	2.3
1	B	187	ARG	2.2
1	B	183	VAL	2.2
1	B	164	LYS	2.2
1	B	165	ILE	2.2
1	A	31	GLU	2.2
1	A	174	ASP	2.2
1	A	61	GLU	2.2
1	A	66	LEU	2.2
1	B	156	ASP	2.2
1	A	69	ASP	2.1
1	A	77	LEU	2.1
1	B	32	ILE	2.1
1	A	148	PHE	2.1
1	A	62	VAL	2.1
1	B	38	LYS	2.1
1	B	152	PRO	2.0
1	A	182	TYR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.