Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 12:48 am BST

PDB ID	:	4J80
Title	:	Thermus thermophilus DnaJ
Authors	:	Barends, T.R.M.; Brosi, R.W.; Steinmetz, A.; Scherer, A.; Hartmann, E.; Eschenbach, J.; Lorenz, T.; Seidel, R.; Shoeman, R.; Zimmermann, S.; Bittl, R.; Schlichting, I.; Reinstein, J.
Deposited on	:	2013-02-14
Resolution	:	2.90 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 following versions of software and data (see references ⓘ) were used in the production of this report:

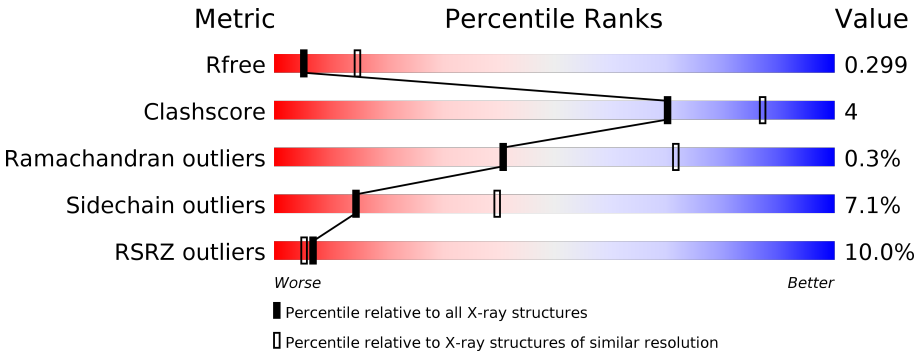
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 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	284	4% 81% 12% • 5%
1	B	284	15% 82% 13% • 5%
1	C	284	4% 81% 14% 5%
1	D	284	14% 81% 12% • 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8460 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 Chaperone protein DnaJ 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	Se	0	0	0
			2115	1348	374	387	6			
1	B	271	Total	C	N	O	Se	0	0	0
			2115	1348	374	387	6			
1	C	271	Total	C	N	O	Se	0	0	0
			2115	1348	374	387	6			
1	D	271	Total	C	N	O	Se	0	0	0
			2115	1348	374	387	6			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	MSE	LEU	ENGINEERED MUTATION	UNP Q56237
A	?	-	GLY	DELETION	UNP Q56237
A	?	-	PHE	DELETION	UNP Q56237
A	?	-	GLY	DELETION	UNP Q56237
A	?	-	ARG	DELETION	UNP Q56237
A	?	-	ARG	DELETION	UNP Q56237
A	?	-	SER	DELETION	UNP Q56237
A	?	-	ARG	DELETION	UNP Q56237
A	142	MSE	ILE	ENGINEERED MUTATION	UNP Q56237
A	173	MSE	LEU	ENGINEERED MUTATION	UNP Q56237
A	226	MSE	LEU	ENGINEERED MUTATION	UNP Q56237
A	231	GLY	LYS	ENGINEERED MUTATION	UNP Q56237
A	274	ALA	-	EXPRESSION TAG	UNP Q56237
A	275	ALA	-	EXPRESSION TAG	UNP Q56237
A	276	ALA	-	EXPRESSION TAG	UNP Q56237
A	277	LEU	-	EXPRESSION TAG	UNP Q56237
A	278	GLU	-	EXPRESSION TAG	UNP Q56237
A	279	HIS	-	EXPRESSION TAG	UNP Q56237
A	280	HIS	-	EXPRESSION TAG	UNP Q56237
A	281	HIS	-	EXPRESSION TAG	UNP Q56237
A	282	HIS	-	EXPRESSION TAG	UNP Q56237

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Chain	Residue	Modelled	Actual	Comment	Reference
A	283	HIS	-	EXPRESSION TAG	UNP Q56237
A	284	HIS	-	EXPRESSION TAG	UNP Q56237
B	57	MSE	LEU	ENGINEERED MUTATION	UNP Q56237
B	?	-	GLY	DELETION	UNP Q56237
B	?	-	PHE	DELETION	UNP Q56237
B	?	-	GLY	DELETION	UNP Q56237
B	?	-	ARG	DELETION	UNP Q56237
B	?	-	ARG	DELETION	UNP Q56237
B	?	-	SER	DELETION	UNP Q56237
B	?	-	ARG	DELETION	UNP Q56237
B	142	MSE	ILE	ENGINEERED MUTATION	UNP Q56237
B	173	MSE	LEU	ENGINEERED MUTATION	UNP Q56237
B	226	MSE	LEU	ENGINEERED MUTATION	UNP Q56237
B	231	GLY	LYS	ENGINEERED MUTATION	UNP Q56237
B	274	ALA	-	EXPRESSION TAG	UNP Q56237
B	275	ALA	-	EXPRESSION TAG	UNP Q56237
B	276	ALA	-	EXPRESSION TAG	UNP Q56237
B	277	LEU	-	EXPRESSION TAG	UNP Q56237
B	278	GLU	-	EXPRESSION TAG	UNP Q56237
B	279	HIS	-	EXPRESSION TAG	UNP Q56237
B	280	HIS	-	EXPRESSION TAG	UNP Q56237
B	281	HIS	-	EXPRESSION TAG	UNP Q56237
B	282	HIS	-	EXPRESSION TAG	UNP Q56237
B	283	HIS	-	EXPRESSION TAG	UNP Q56237
B	284	HIS	-	EXPRESSION TAG	UNP Q56237
C	57	MSE	LEU	ENGINEERED MUTATION	UNP Q56237
C	?	-	GLY	DELETION	UNP Q56237
C	?	-	PHE	DELETION	UNP Q56237
C	?	-	GLY	DELETION	UNP Q56237
C	?	-	ARG	DELETION	UNP Q56237
C	?	-	ARG	DELETION	UNP Q56237
C	?	-	SER	DELETION	UNP Q56237
C	?	-	ARG	DELETION	UNP Q56237
C	142	MSE	ILE	ENGINEERED MUTATION	UNP Q56237
C	173	MSE	LEU	ENGINEERED MUTATION	UNP Q56237
C	226	MSE	LEU	ENGINEERED MUTATION	UNP Q56237
C	231	GLY	LYS	ENGINEERED MUTATION	UNP Q56237
C	274	ALA	-	EXPRESSION TAG	UNP Q56237
C	275	ALA	-	EXPRESSION TAG	UNP Q56237
C	276	ALA	-	EXPRESSION TAG	UNP Q56237
C	277	LEU	-	EXPRESSION TAG	UNP Q56237
C	278	GLU	-	EXPRESSION TAG	UNP Q56237

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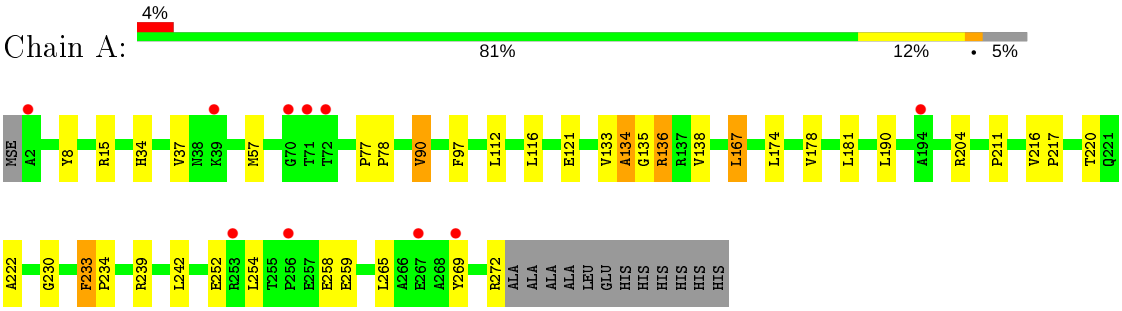
Chain	Residue	Modelled	Actual	Comment	Reference
C	279	HIS	-	EXPRESSION TAG	UNP Q56237
C	280	HIS	-	EXPRESSION TAG	UNP Q56237
C	281	HIS	-	EXPRESSION TAG	UNP Q56237
C	282	HIS	-	EXPRESSION TAG	UNP Q56237
C	283	HIS	-	EXPRESSION TAG	UNP Q56237
C	284	HIS	-	EXPRESSION TAG	UNP Q56237
D	57	MSE	LEU	ENGINEERED MUTATION	UNP Q56237
D	?	-	GLY	DELETION	UNP Q56237
D	?	-	PHE	DELETION	UNP Q56237
D	?	-	GLY	DELETION	UNP Q56237
D	?	-	ARG	DELETION	UNP Q56237
D	?	-	ARG	DELETION	UNP Q56237
D	?	-	SER	DELETION	UNP Q56237
D	?	-	ARG	DELETION	UNP Q56237
D	142	MSE	ILE	ENGINEERED MUTATION	UNP Q56237
D	173	MSE	LEU	ENGINEERED MUTATION	UNP Q56237
D	226	MSE	LEU	ENGINEERED MUTATION	UNP Q56237
D	231	GLY	LYS	ENGINEERED MUTATION	UNP Q56237
D	274	ALA	-	EXPRESSION TAG	UNP Q56237
D	275	ALA	-	EXPRESSION TAG	UNP Q56237
D	276	ALA	-	EXPRESSION TAG	UNP Q56237
D	277	LEU	-	EXPRESSION TAG	UNP Q56237
D	278	GLU	-	EXPRESSION TAG	UNP Q56237
D	279	HIS	-	EXPRESSION TAG	UNP Q56237
D	280	HIS	-	EXPRESSION TAG	UNP Q56237
D	281	HIS	-	EXPRESSION TAG	UNP Q56237
D	282	HIS	-	EXPRESSION TAG	UNP Q56237
D	283	HIS	-	EXPRESSION TAG	UNP Q56237
D	284	HIS	-	EXPRESSION TAG	UNP Q56237

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 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.

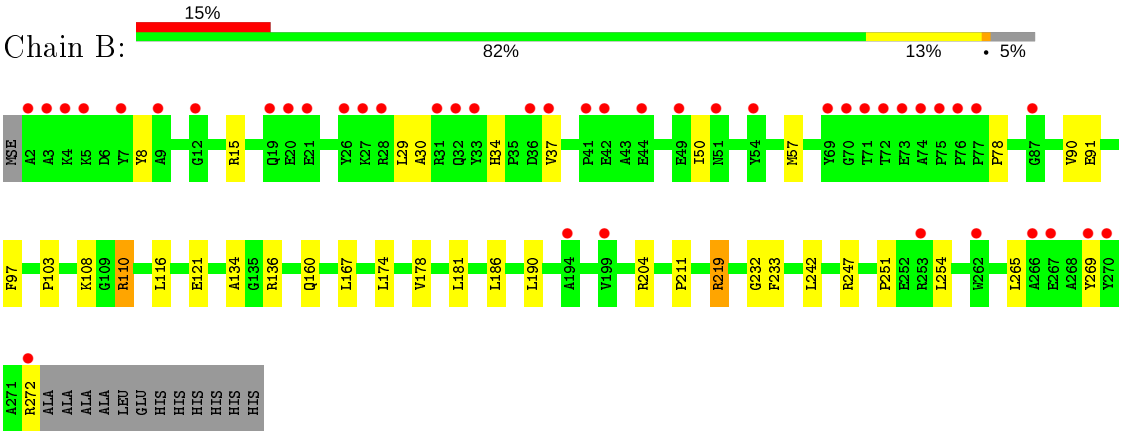
- Molecule 1: Chaperone protein DnaJ 2

Chain A:



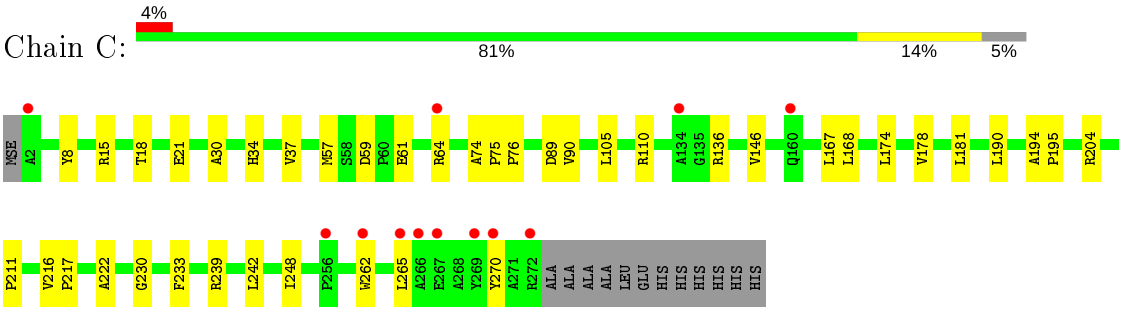
- Molecule 1: Chaperone protein DnaJ 2

Chain B:



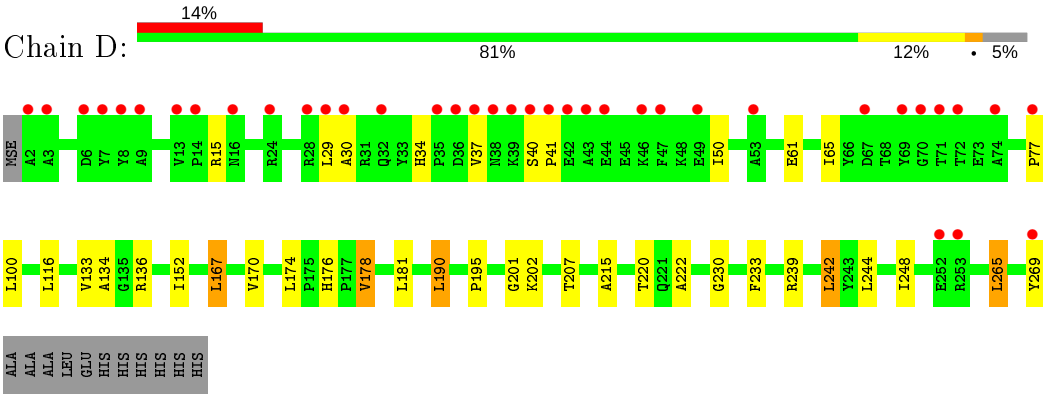
- Molecule 1: Chaperone protein DnaJ 2

Chain C:



- Molecule 1: Chaperone protein DnaJ 2

Chain D:


14%
81%
12%
5%
MSE A2 A3 D6 Y7 Y8 A9 V13 P14 R15 N16 R24 R28 L29 A30 R31 Q32 Y33 H34 P35 D36 V37 N38 K39 S40 P41 E42 A43 E44 E45 K46 F47 K48 E49 I50 A53 E61 I65 Y66 D67 T68 Y69 G70 T71 T72 E73 A74 P77 P78 E95
L100 L116 V133 A134 G135 R136 I152 L167 V170 L174 P175 H176 P177 V178 L181 L190 P195 G201 K202 T207 A215 T220 Q221 A222 G230 F233 R239 L242 Y243 L244 I248 E252 R253 L265 Y269 Y270 A271 R272 ALA
ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	102.09Å 105.00Å 130.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 19.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-2.90) 99.3 (19.98-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.43 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.265 , 0.307 0.259 , 0.299	Depositor DCC
R_{free} test set	1591 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	66.2	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 26.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8460	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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	0.32	0/2164	0.48	0/2923
1	B	0.32	0/2164	0.47	0/2923
1	C	0.32	0/2164	0.49	0/2923
1	D	0.32	0/2164	0.49	0/2923
All	All	0.32	0/8656	0.48	0/11692

There are no bond length outliers.

There are no bond angle outliers.

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	2115	0	2110	17	0
1	B	2115	0	2110	14	0
1	C	2115	0	2110	17	0
1	D	2115	0	2110	17	0
All	All	8460	0	8440	61	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 (61) 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:78:PRO:HG2	1:B:103:PRO:HB2	1.67	0.76
1:C:64:ARG:HH22	1:C:76:PRO:HD2	1.52	0.75
1:A:204:ARG:HH12	1:A:211:PRO:HB2	1.52	0.73
1:D:34:HIS:HB3	1:D:37:VAL:HG22	1.73	0.71
1:A:8:TYR:CE1	1:A:57:MSE:HE1	2.30	0.66
1:C:64:ARG:NH2	1:C:76:PRO:HD2	2.11	0.65
1:B:269:TYR:O	1:B:272:ARG:HG2	1.98	0.63
1:C:222:ALA:HB2	1:C:248:ILE:HG12	1.83	0.61
1:A:34:HIS:HB3	1:A:37:VAL:HG22	1.82	0.60
1:B:34:HIS:HB3	1:B:37:VAL:HG22	1.84	0.60
1:C:34:HIS:HB3	1:C:37:VAL:HG22	1.83	0.60
1:B:204:ARG:HH12	1:B:211:PRO:HB2	1.70	0.56
1:B:90:VAL:HG13	1:B:97:PHE:HE2	1.73	0.54
1:D:265:LEU:O	1:D:269:TYR:HD2	1.91	0.53
1:B:30:ALA:O	1:B:34:HIS:HB2	2.09	0.52
1:C:8:TYR:CE1	1:C:57:MSE:HE1	2.46	0.51
1:A:8:TYR:CD1	1:A:57:MSE:HE1	2.46	0.51
1:A:252:GLU:HA	1:B:219:ARG:HB3	1.94	0.49
1:D:30:ALA:O	1:D:34:HIS:HB2	2.11	0.49
1:C:270:TYR:OH	1:D:201:GLY:HA3	2.12	0.49
1:C:8:TYR:CD1	1:C:57:MSE:HE1	2.48	0.49
1:C:230:GLY:O	1:C:239:ARG:HD3	2.14	0.48
1:A:269:TYR:O	1:A:272:ARG:HG2	2.12	0.48
1:D:230:GLY:O	1:D:239:ARG:HD3	2.14	0.48
1:D:222:ALA:HB2	1:D:248:ILE:HG12	1.96	0.47
1:A:133:VAL:O	1:A:134:ALA:C	2.53	0.46
1:A:265:LEU:O	1:A:269:TYR:HD2	1.98	0.46
1:C:30:ALA:O	1:C:34:HIS:HB2	2.15	0.46
1:B:8:TYR:CE1	1:B:57:MSE:HE1	2.50	0.46
1:D:61:GLU:O	1:D:65:ILE:HG12	2.16	0.46
1:D:176:HIS:CE1	1:D:178:VAL:HG13	2.51	0.45
1:C:204:ARG:HH12	1:C:211:PRO:HB2	1.82	0.45
1:A:222:ALA:HB3	1:B:247:ARG:HH11	1.82	0.44
1:C:64:ARG:NH1	1:C:76:PRO:HG2	2.32	0.44
1:A:135:GLY:HA3	1:A:136:ARG:NH1	2.32	0.44
1:A:138:VAL:HG21	1:A:167:LEU:HD12	1.99	0.44
1:B:186:LEU:HD12	1:B:232:GLY:HA2	1.99	0.44
1:D:190:LEU:HG	1:D:244:LEU:HD13	1.98	0.44
1:B:29:LEU:HB3	1:B:50:ILE:HD13	2.00	0.44
1:A:230:GLY:O	1:A:239:ARG:HD3	2.18	0.43
1:D:133:VAL:HG11	1:D:167:LEU:HD21	2.00	0.43
1:B:265:LEU:O	1:B:269:TYR:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:TRP:CE3	1:D:195:PRO:HA	2.53	0.42
1:D:202:LYS:HE3	1:D:215:ALA:HB2	2.02	0.42
1:D:29:LEU:HB3	1:D:50:ILE:HD13	2.00	0.42
1:D:77:PRO:HA	1:D:78:PRO:HD3	1.90	0.42
1:A:216:VAL:HA	1:A:217:PRO:HD3	1.93	0.42
1:D:176:HIS:HE1	1:D:178:VAL:HG13	1.84	0.42
1:A:90:VAL:HG22	1:A:97:PHE:HE2	1.84	0.42
1:C:194:ALA:N	1:C:195:PRO:HD2	2.35	0.42
1:C:74:ALA:HA	1:C:75:PRO:HD3	1.89	0.42
1:C:59:ASP:OD1	1:C:61:GLU:HB2	2.20	0.41
1:D:207:THR:HG22	1:D:242:LEU:HD12	2.01	0.41
1:C:18:THR:OG1	1:C:21:GLU:HB2	2.20	0.41
1:A:77:PRO:HA	1:A:78:PRO:HD3	1.87	0.41
1:A:254:LEU:HD22	1:A:258:GLU:HB3	2.03	0.40
1:B:110:ARG:H	1:B:110:ARG:HG3	1.66	0.40
1:B:251:PRO:HG3	1:B:254:LEU:HD21	2.04	0.40
1:A:233:PHE:HA	1:A:234:PRO:HD3	1.92	0.40
1:C:216:VAL:HA	1:C:217:PRO:HD3	1.94	0.40
1:D:40:SER:HA	1:D:41:PRO:HD3	1.99	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	269/284 (95%)	263 (98%)	5 (2%)	1 (0%)	34 66
1	B	269/284 (95%)	259 (96%)	9 (3%)	1 (0%)	34 66
1	C	269/284 (95%)	263 (98%)	6 (2%)	0	100 100
1	D	269/284 (95%)	262 (97%)	6 (2%)	1 (0%)	34 66
All	All	1076/1136 (95%)	1047 (97%)	26 (2%)	3 (0%)	41 71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	ALA
1	B	134	ALA
1	D	134	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	217/219 (99%)	202 (93%)	15 (7%)	15	41
1	B	217/219 (99%)	201 (93%)	16 (7%)	13	38
1	C	217/219 (99%)	201 (93%)	16 (7%)	13	38
1	D	217/219 (99%)	202 (93%)	15 (7%)	15	41
All	All	868/876 (99%)	806 (93%)	62 (7%)	14	40

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	90	VAL
1	A	112	LEU
1	A	116	LEU
1	A	121	GLU
1	A	136	ARG
1	A	167	LEU
1	A	174	LEU
1	A	178	VAL
1	A	181	LEU
1	A	190	LEU
1	A	220	THR
1	A	233	PHE
1	A	242	LEU
1	A	259	GLU
1	B	15	ARG
1	B	91	GLU

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Mol	Chain	Res	Type
1	B	108	LYS
1	B	110	ARG
1	B	116	LEU
1	B	121	GLU
1	B	136	ARG
1	B	160	GLN
1	B	167	LEU
1	B	174	LEU
1	B	178	VAL
1	B	181	LEU
1	B	190	LEU
1	B	219	ARG
1	B	233	PHE
1	B	242	LEU
1	C	15	ARG
1	C	89	ASP
1	C	90	VAL
1	C	105	LEU
1	C	110	ARG
1	C	136	ARG
1	C	146	VAL
1	C	167	LEU
1	C	168	LEU
1	C	174	LEU
1	C	178	VAL
1	C	181	LEU
1	C	190	LEU
1	C	233	PHE
1	C	242	LEU
1	C	265	LEU
1	D	15	ARG
1	D	100	LEU
1	D	116	LEU
1	D	136	ARG
1	D	152	ILE
1	D	167	LEU
1	D	170	VAL
1	D	174	LEU
1	D	178	VAL
1	D	181	LEU
1	D	190	LEU
1	D	220	THR

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Mol	Chain	Res	Type
1	D	233	PHE
1	D	242	LEU
1	D	265	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	34	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	265/284 (93%)	0.07	10 (3%) 40 36	36, 64, 130, 203	0
1	B	265/284 (93%)	0.82	43 (16%) 1 1	44, 95, 236, 329	0
1	C	265/284 (93%)	0.20	12 (4%) 33 29	38, 73, 136, 200	0
1	D	265/284 (93%)	0.75	41 (15%) 2 1	37, 87, 246, 323	0
All	All	1060/1136 (93%)	0.46	106 (10%) 7 5	36, 77, 215, 329	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	72	THR	11.6
1	B	76	PRO	11.3
1	D	70	GLY	8.7
1	B	31	ARG	8.4
1	B	70	GLY	8.4
1	B	75	PRO	8.2
1	B	73	GLU	7.8
1	B	74	ALA	7.5
1	B	28	ARG	7.4
1	B	36	ASP	6.9
1	D	35	PRO	6.7
1	A	71	THR	6.7
1	D	72	THR	6.1
1	D	37	VAL	6.1
1	D	36	ASP	6.0
1	D	7	TYR	5.8
1	B	71	THR	5.5
1	B	2	ALA	5.5
1	D	71	THR	5.3
1	C	272	ARG	5.3
1	D	41	PRO	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	39	LYS	5.2
1	A	253	ARG	5.2
1	D	6	ASP	5.2
1	D	40	SER	5.0
1	D	69	TYR	4.8
1	D	9	ALA	4.7
1	D	74	ALA	4.5
1	C	269	TYR	4.5
1	B	267	GLU	4.1
1	B	42	GLU	4.1
1	D	42	GLU	4.1
1	D	8	TYR	4.1
1	C	2	ALA	4.0
1	D	3	ALA	4.0
1	A	72	THR	4.0
1	B	26	TYR	3.9
1	B	32	GLN	3.9
1	B	269	TYR	3.9
1	B	3	ALA	3.8
1	B	270	TYR	3.5
1	D	270	TYR	3.4
1	D	46	LYS	3.4
1	B	77	PRO	3.3
1	C	266	ALA	3.3
1	B	272	ARG	3.2
1	A	269	TYR	3.2
1	D	43	ALA	3.2
1	C	265	LEU	3.2
1	D	252	GLU	3.2
1	C	270	TYR	3.1
1	B	21	GLU	3.1
1	D	28	ARG	3.1
1	D	53	ALA	3.1
1	D	271	ALA	3.0
1	D	253	ARG	3.0
1	B	27	LYS	3.0
1	B	19	GLN	3.0
1	B	37	VAL	3.0
1	B	44	GLU	3.0
1	D	14	PRO	2.9
1	D	2	ALA	2.9
1	D	77	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	38	ASN	2.9
1	D	24	ARG	2.9
1	D	32	GLN	2.8
1	D	67	ASP	2.8
1	B	5	LYS	2.8
1	D	29	LEU	2.8
1	B	266	ALA	2.8
1	B	69	TYR	2.7
1	B	4	LYS	2.7
1	D	49	GLU	2.7
1	D	44	GLU	2.7
1	D	269	TYR	2.7
1	B	194	ALA	2.6
1	A	194	ALA	2.6
1	C	267	GLU	2.6
1	B	41	PRO	2.6
1	B	9	ALA	2.5
1	D	47	PHE	2.5
1	D	13	VAL	2.4
1	B	54	TYR	2.4
1	B	12	GLY	2.4
1	B	199	VAL	2.4
1	A	70	GLY	2.3
1	B	51	ASN	2.3
1	A	267	GLU	2.3
1	D	95	GLU	2.3
1	B	33	TYR	2.3
1	B	20	GLU	2.2
1	D	16	ASN	2.2
1	B	49	GLU	2.2
1	C	64	ARG	2.2
1	C	262	TRP	2.2
1	B	7	TYR	2.2
1	B	253	ARG	2.1
1	A	2	ALA	2.1
1	C	256	PRO	2.1
1	C	134	ALA	2.1
1	A	39	LYS	2.1
1	B	87	GLY	2.0
1	C	160	GLN	2.0
1	D	30	ALA	2.0
1	A	256	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	262	TRP	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.