



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:47 AM GMT

PDB ID : 2IRM
Title : Crystal structure of mitogen-activated protein kinase kinase kinase 7 interacting protein 1 from *Anopheles gambiae*
Authors : Jin, X.; Bonanno, J.B.; Pelletier, L.; Freeman, J.C.; Wasserman, S.; Sauder, J.M.; Burley, S.K.; Shapiro, L.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2006-10-15
Resolution : 3.00 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
<http://wwpdb.org/validation/2016/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 : 1.7 (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

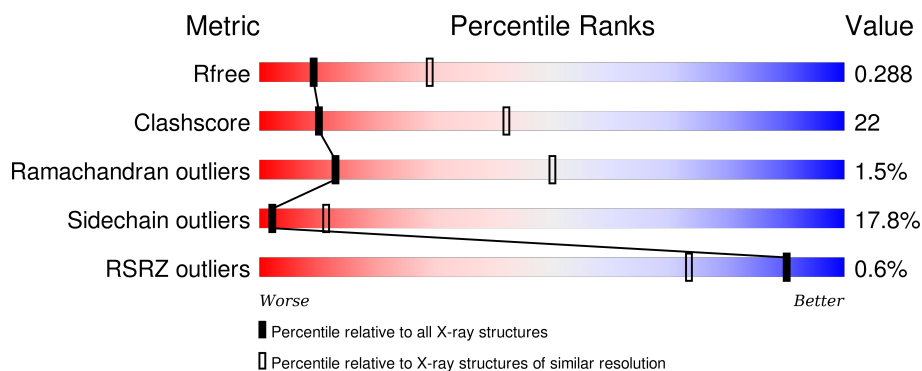
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 $\leq 5\%$. 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	358	<div> <div></div> <div>56%</div> <div>28%</div> <div>9%</div> <div>• 5%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2612 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.

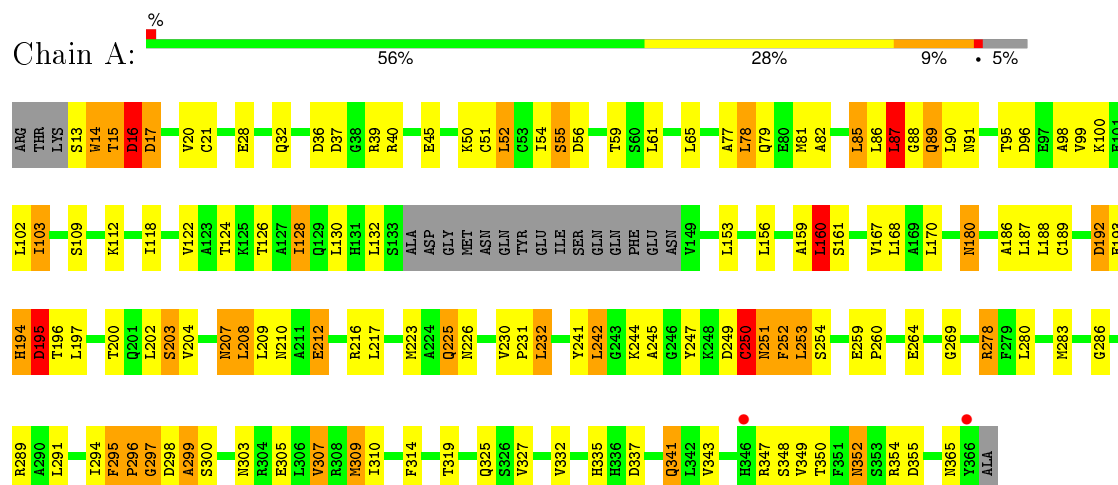
- Molecule 1 is a protein called mitogen-activated protein kinase kinase kinase 7 interacting protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2612	1624	464	507	17			

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 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: mitogen-activated protein kinase kinase kinase 7 interacting protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	121.77Å 73.77Å 74.51Å 90.00° 116.96° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 40.12 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.2 (20.00-3.00) 87.3 (40.12-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.218 , 0.277 0.233 , 0.288	Depositor DCC
R_{free} test set	550 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.857	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 56.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 12788 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2612	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.49% 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, 0.375 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	0.42	0/2650	0.73	13/3587 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	250	CYS	CB-CA-C	8.00	126.41	110.40
1	A	251	ASN	N-CA-CB	-7.79	96.57	110.60
1	A	15	THR	N-CA-CB	-6.39	98.15	110.30
1	A	296	PRO	CB-CA-C	5.92	126.79	112.00
1	A	307	VAL	CB-CA-C	-5.89	100.20	111.40
1	A	17	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	296	PRO	N-CA-C	-5.31	98.31	112.10
1	A	195	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	297	GLY	N-CA-C	-5.23	100.02	113.10
1	A	16	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	192	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	195	ASP	CB-CA-C	-5.15	100.11	110.40
1	A	168	LEU	CA-CB-CG	5.13	127.09	115.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	SER	Peptide
1	A	195	ASP	Peptide
1	A	249	ASP	Peptide
1	A	250	CYS	Peptide
1	A	295	PHE	Peptide
1	A	296	PRO	Peptide
1	A	87	LEU	Peptide

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	2612	0	2563	113	0
All	All	2612	0	2563	113	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 22.

All (113) 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:14:TRP:CD1	1:A:79:GLN:OE1	1.92	1.22
1:A:14:TRP:HD1	1:A:79:GLN:OE1	1.27	1.16
1:A:195:ASP:HB3	1:A:196:THR:CA	1.74	1.15
1:A:252:PHE:O	1:A:252:PHE:CD2	2.04	1.11
1:A:195:ASP:CB	1:A:196:THR:HA	1.77	1.07
1:A:195:ASP:HB3	1:A:196:THR:HA	1.07	1.06
1:A:241:TYR:CZ	1:A:245:ALA:O	2.20	0.94
1:A:14:TRP:CD1	1:A:79:GLN:CD	2.44	0.89
1:A:310:ILE:HG22	1:A:327:VAL:HG21	1.54	0.89
1:A:278:ARG:HH11	1:A:278:ARG:HG3	1.37	0.88
1:A:187:LEU:HG	1:A:283:MET:HE2	1.59	0.85
1:A:250:CYS:O	1:A:254:SER:HB3	1.77	0.84
1:A:188:LEU:HB2	1:A:202:LEU:HD21	1.61	0.83
1:A:14:TRP:CD1	1:A:79:GLN:NE2	2.47	0.82
1:A:244:LYS:O	1:A:259:GLU:HG2	1.83	0.79
1:A:253:LEU:HD13	1:A:260:PRO:HG2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:VAL:O	1:A:307:VAL:HG12	1.82	0.79
1:A:187:LEU:HG	1:A:283:MET:CE	2.14	0.78
1:A:89:GLN:H	1:A:89:GLN:HE21	1.34	0.76
1:A:241:TYR:CE1	1:A:245:ALA:O	2.38	0.75
1:A:250:CYS:HB3	1:A:253:LEU:HB2	1.69	0.75
1:A:77:ALA:O	1:A:81:MET:HG3	1.89	0.73
1:A:244:LYS:O	1:A:259:GLU:CG	2.38	0.72
1:A:298:ASP:O	1:A:300:SER:N	2.24	0.70
1:A:55:SER:HB3	1:A:86:LEU:HD22	1.75	0.69
1:A:180:ASN:HD21	1:A:204:VAL:H	1.42	0.68
1:A:278:ARG:NH1	1:A:278:ARG:HG3	2.00	0.68
1:A:186:ALA:H	1:A:203:SER:HB3	1.59	0.68
1:A:232:LEU:HB2	1:A:289:ARG:HG3	1.76	0.67
1:A:208:LEU:HD11	1:A:217:LEU:HD12	1.78	0.66
1:A:252:PHE:CG	1:A:252:PHE:O	2.49	0.66
1:A:307:VAL:CG1	1:A:307:VAL:O	2.44	0.66
1:A:87:LEU:HD23	1:A:87:LEU:O	1.95	0.66
1:A:15:THR:HG21	1:A:78:LEU:HD13	1.77	0.65
1:A:194:HIS:O	1:A:195:ASP:HB2	1.99	0.62
1:A:15:THR:O	1:A:17:ASP:N	2.34	0.61
1:A:59:THR:HG21	1:A:90:LEU:HD13	1.82	0.60
1:A:294:ILE:HG13	1:A:295:PHE:CD1	2.36	0.60
1:A:82:ALA:O	1:A:86:LEU:HB2	2.01	0.59
1:A:278:ARG:CG	1:A:278:ARG:HH11	2.13	0.58
1:A:252:PHE:HD2	1:A:252:PHE:O	1.81	0.57
1:A:124:THR:O	1:A:128:ILE:HG23	2.03	0.57
1:A:250:CYS:CB	1:A:253:LEU:HB2	2.34	0.56
1:A:210:ASN:HD21	1:A:212:GLU:HG3	1.69	0.56
1:A:207:ASN:HD21	1:A:209:LEU:HB2	1.70	0.56
1:A:225:GLN:HE21	1:A:225:GLN:N	2.04	0.56
1:A:87:LEU:H	1:A:87:LEU:CD2	2.19	0.56
1:A:294:ILE:HG21	1:A:335:HIS:HA	1.88	0.55
1:A:251:ASN:O	1:A:252:PHE:HB3	2.06	0.55
1:A:52:LEU:HD12	1:A:52:LEU:H	1.70	0.55
1:A:87:LEU:H	1:A:87:LEU:HD22	1.72	0.55
1:A:210:ASN:HD21	1:A:212:GLU:CG	2.19	0.55
1:A:207:ASN:HD22	1:A:209:LEU:H	1.54	0.55
1:A:87:LEU:N	1:A:87:LEU:CD2	2.70	0.54
1:A:89:GLN:H	1:A:89:GLN:NE2	2.02	0.53
1:A:52:LEU:HD12	1:A:52:LEU:N	2.23	0.53
1:A:251:ASN:O	1:A:252:PHE:CD1	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:TRP:NE1	1:A:79:GLN:OE1	2.38	0.53
1:A:242:LEU:O	1:A:247:TYR:HA	2.09	0.52
1:A:291:LEU:O	1:A:295:PHE:HB2	2.10	0.52
1:A:251:ASN:O	1:A:252:PHE:CB	2.58	0.51
1:A:252:PHE:C	1:A:252:PHE:CD2	2.71	0.51
1:A:297:GLY:O	1:A:298:ASP:HB3	2.11	0.50
1:A:122:VAL:O	1:A:126:THR:HG22	2.11	0.50
1:A:244:LYS:O	1:A:259:GLU:CD	2.50	0.50
1:A:32:GLN:NE2	1:A:40:ARG:HD3	2.26	0.50
1:A:278:ARG:HD2	1:A:365:ASN:HB2	1.94	0.50
1:A:28:GLU:H	1:A:325:GLN:NE2	2.10	0.50
1:A:167:VAL:HG13	1:A:167:VAL:O	2.11	0.50
1:A:99:VAL:O	1:A:103:ILE:HG12	2.12	0.49
1:A:87:LEU:N	1:A:87:LEU:HD22	2.27	0.49
1:A:343:VAL:HA	1:A:347:ARG:HG2	1.95	0.49
1:A:207:ASN:C	1:A:207:ASN:HD22	2.15	0.48
1:A:100:LYS:HD2	1:A:269:GLY:HA3	1.94	0.48
1:A:21:CYS:HA	1:A:54:ILE:HD11	1.96	0.48
1:A:109:SER:HA	1:A:112:LYS:HB3	1.97	0.47
1:A:180:ASN:ND2	1:A:204:VAL:H	2.09	0.47
1:A:300:SER:HA	1:A:303:ASN:ND2	2.29	0.47
1:A:294:ILE:HG13	1:A:295:PHE:HD1	1.80	0.46
1:A:87:LEU:HD23	1:A:87:LEU:C	2.35	0.46
1:A:15:THR:O	1:A:16:ASP:C	2.55	0.45
1:A:223:MET:H	1:A:226:ASN:HD22	1.63	0.45
1:A:207:ASN:ND2	1:A:209:LEU:H	2.14	0.44
1:A:159:ALA:C	1:A:161:SER:H	2.20	0.44
1:A:153:LEU:HA	1:A:156:LEU:HD23	1.98	0.44
1:A:207:ASN:ND2	1:A:209:LEU:HB2	2.33	0.44
1:A:86:LEU:H	1:A:89:GLN:HE22	1.66	0.43
1:A:209:LEU:HD22	1:A:299:ALA:HB2	2.01	0.43
1:A:223:MET:H	1:A:226:ASN:ND2	2.16	0.43
1:A:122:VAL:HG12	1:A:160:LEU:HD22	2.00	0.43
1:A:352:ASN:HD22	1:A:352:ASN:N	2.16	0.43
1:A:225:GLN:H	1:A:225:GLN:HE21	1.65	0.43
1:A:307:VAL:HA	1:A:310:ILE:HG12	2.00	0.43
1:A:250:CYS:SG	1:A:252:PHE:CD1	3.10	0.43
1:A:15:THR:C	1:A:17:ASP:N	2.72	0.43
1:A:192:ASP:OD2	1:A:193:GLU:N	2.52	0.43
1:A:194:HIS:ND1	1:A:194:HIS:N	2.66	0.43
1:A:337:ASP:O	1:A:341:GLN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:THR:HG23	1:A:98:ALA:H	1.84	0.42
1:A:65:LEU:HD13	1:A:78:LEU:HG	2.01	0.42
1:A:286:GLY:HA2	1:A:355:ASP:HB2	2.01	0.42
1:A:187:LEU:HG	1:A:283:MET:HE1	1.97	0.42
1:A:197:LEU:HD23	1:A:197:LEU:HA	1.90	0.42
1:A:259:GLU:HA	1:A:260:PRO:HD3	1.83	0.42
1:A:118:ILE:HD13	1:A:241:TYR:HB2	2.02	0.42
1:A:85:LEU:HD22	1:A:103:ILE:HG23	2.02	0.42
1:A:297:GLY:O	1:A:298:ASP:CB	2.68	0.41
1:A:212:GLU:H	1:A:212:GLU:HG2	1.61	0.41
1:A:332:VAL:HB	1:A:354:ARG:NH1	2.36	0.41
1:A:250:CYS:SG	1:A:252:PHE:CE1	3.14	0.41
1:A:305:GLU:O	1:A:309:MET:HB2	2.21	0.41
1:A:189:CYS:HB3	1:A:197:LEU:HD22	2.04	0.40
1:A:87:LEU:N	1:A:88:GLY:HA2	2.36	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	335/358 (94%)	287 (86%)	43 (13%)	5 (2%)	13	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ASP
1	A	299	ALA
1	A	231	PRO
1	A	160	LEU
1	A	349	VAL

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	287/307 (94%)	236 (82%)	51 (18%)	2 11

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	TRP
1	A	20	VAL
1	A	36	ASP
1	A	37	ASP
1	A	39	ARG
1	A	45	GLU
1	A	50	LYS
1	A	51	CYS
1	A	52	LEU
1	A	55	SER
1	A	56	ASP
1	A	61	LEU
1	A	78	LEU
1	A	85	LEU
1	A	87	LEU
1	A	89	GLN
1	A	91	ASN
1	A	96	ASP
1	A	102	LEU
1	A	103	ILE
1	A	128	ILE
1	A	130	LEU
1	A	132	LEU
1	A	160	LEU
1	A	170	LEU
1	A	180	ASN
1	A	194	HIS
1	A	195	ASP
1	A	200	THR
1	A	203	SER

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Mol	Chain	Res	Type
1	A	207	ASN
1	A	208	LEU
1	A	212	GLU
1	A	216	ARG
1	A	225	GLN
1	A	230	VAL
1	A	232	LEU
1	A	242	LEU
1	A	250	CYS
1	A	252	PHE
1	A	253	LEU
1	A	264	GLU
1	A	278	ARG
1	A	280	LEU
1	A	309	MET
1	A	314	PHE
1	A	319	THR
1	A	341	GLN
1	A	348	SER
1	A	350	THR
1	A	352	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	68	HIS
1	A	79	GLN
1	A	89	GLN
1	A	172	HIS
1	A	180	ASN
1	A	207	ASN
1	A	210	ASN
1	A	225	GLN
1	A	226	ASN
1	A	272	GLN
1	A	336	HIS
1	A	352	ASN

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	339/358 (94%)	-0.22	2 (0%)	90 73	23, 48, 58, 61	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	346	HIS	2.9
1	A	366	TYR	2.1

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.