



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:56 PM GMT

PDB ID : 3U3I
Title : A RNA binding protein from Crimean-Congo hemorrhagic fever virus
Authors : Guo, Y.; Wang, W.M.; Ji, W.; Deng, M.; Sun, Y.N.; Lou, Z.Y.; Rao, Z.H.
Deposited on : 2011-10-06
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
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

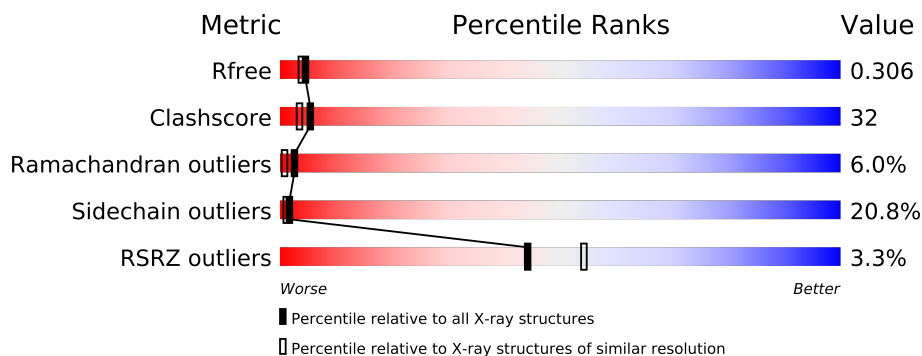
The following versions of software and data (see [references](#)) were used in the production of this report:

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 ≥ 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	482	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3995 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 Nucleocapsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	0	0
			3626	2308	615	685	18			

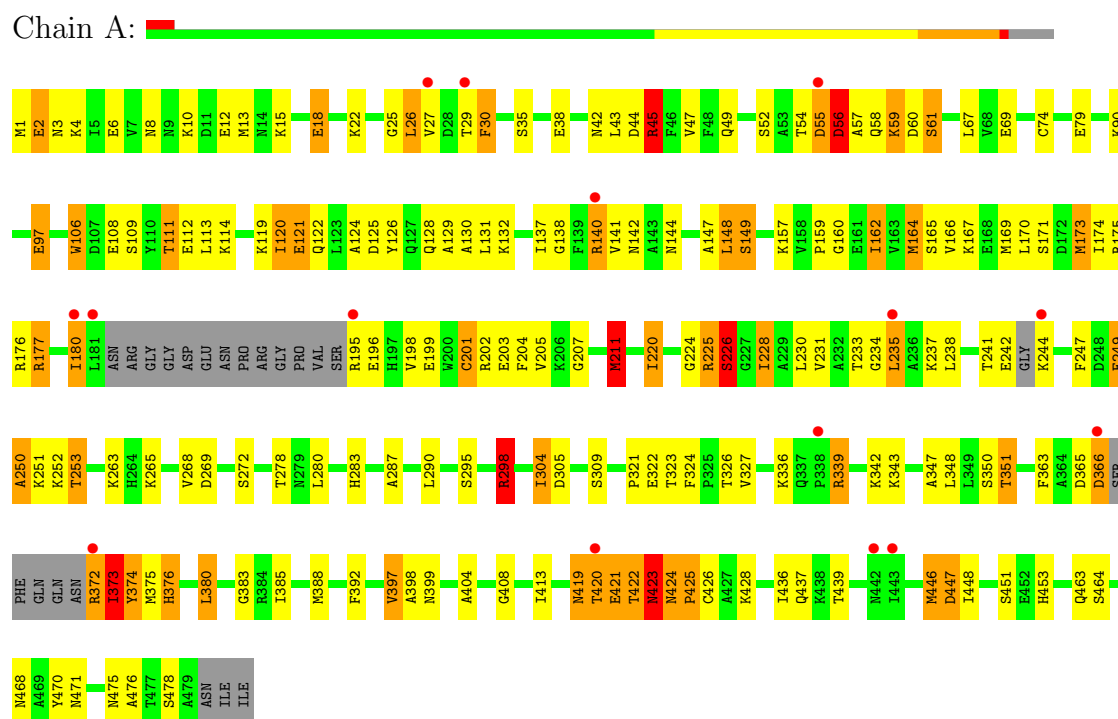
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	369	Total	O	0	0
			369	369		

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: Nucleocapsid protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.34Å 67.90Å 131.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.64 – 2.30 43.64 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.1 (43.64-2.30) 89.3 (43.64-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.62 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.224 , 0.257 0.254 , 0.306	Depositor DCC
R_{free} test set	1081 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.697	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 49.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 22493 reflections (0.009%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3995	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 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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	0.94	6/3699 (0.2%)	0.96	5/4989 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	GLU	CG-CD	5.96	1.60	1.51
1	A	74	CYS	CB-SG	-5.64	1.72	1.81
1	A	404	ALA	CA-CB	5.61	1.64	1.52
1	A	464	SER	C-O	5.36	1.33	1.23
1	A	124	ALA	CA-CB	5.19	1.63	1.52
1	A	392	PHE	CD1-CE1	5.10	1.49	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	VAL	N-CA-C	-5.46	96.25	111.00
1	A	269	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	A	348	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	298	ARG	N-CA-CB	-5.26	101.14	110.60
1	A	408	GLY	N-CA-C	5.06	125.76	113.10

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	3626	0	37	119	0
2	A	369	0	0	8	0
All	All	3995	0	37	119	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 32.

All (119) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:157:LYS:CG	1:A:420:THR:CG2	2.04	1.36
1:A:29:THR:CG2	1:A:30:PHE:CE2	2.14	1.30
1:A:157:LYS:CB	1:A:420:THR:CG2	2.15	1.24
1:A:1:MET:CA	1:A:2:GLU:CB	2.22	1.15
1:A:424:ASN:OD1	1:A:428:LYS:HD2	1.49	1.12
1:A:148:LEU:CA	1:A:149:SER:CB	2.30	1.09
1:A:26:LEU:CD2	1:A:26:LEU:N	2.12	1.05
1:A:29:THR:CG2	1:A:30:PHE:CD2	2.47	0.98
1:A:475:ASN:ND2	1:A:476:ALA:N	2.11	0.98
1:A:26:LEU:HD22	1:A:26:LEU:N	1.78	0.98
1:A:228:ILE:CG1	1:A:283:HIS:CE1	2.50	0.94
1:A:373:ILE:CG1	1:A:374:TYR:N	2.30	0.92
1:A:424:ASN:N	1:A:425:PRO:CD	2.34	0.90
1:A:30:PHE:CD2	1:A:30:PHE:N	2.36	0.90
1:A:26:LEU:HD23	1:A:26:LEU:N	1.90	0.84
1:A:58:GLN:N	1:A:59:LYS:CB	2.44	0.81
1:A:421:GLU:O	1:A:422:THR:OG1	1.98	0.80
1:A:25:GLY:C	1:A:26:LEU:HD22	2.02	0.80
1:A:419:ASN:ND2	1:A:419:ASN:N	2.30	0.80
1:A:29:THR:CB	1:A:30:PHE:CD2	2.68	0.77
1:A:58:GLN:CG	1:A:61:SER:N	2.50	0.74
1:A:4:LYS:CE	1:A:398:ALA:O	2.36	0.74
1:A:29:THR:CB	1:A:30:PHE:CE2	2.73	0.72
1:A:45:ARG:NH1	1:A:45:ARG:CG	2.52	0.71
1:A:225:ARG:O	1:A:226:SER:CB	2.39	0.70
1:A:475:ASN:CG	1:A:476:ALA:N	2.44	0.70
1:A:251:LYS:NZ	2:A:627:HOH:O	2.25	0.69
1:A:420:THR:O	1:A:421:GLU:CB	2.40	0.68
1:A:375:MET:O	1:A:376:HIS:CB	2.42	0.68
1:A:164:MET:CE	1:A:164:MET:CA	2.72	0.67
1:A:148:LEU:CB	1:A:149:SER:CB	2.73	0.67
1:A:58:GLN:CA	1:A:59:LYS:CB	2.74	0.66
1:A:169:MET:O	1:A:173:MET:CG	2.44	0.65
1:A:55:ASP:O	1:A:57:ALA:N	2.30	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:424:ASN:OD1	1:A:428:LYS:CD	2.38	0.64
1:A:56:ASP:OD1	1:A:56:ASP:N	2.30	0.64
1:A:298:ARG:NH1	1:A:298:ARG:CG	2.62	0.62
1:A:58:GLN:CG	1:A:61:SER:CB	2.77	0.62
1:A:424:ASN:N	1:A:424:ASN:ND2	2.49	0.61
1:A:58:GLN:CA	1:A:60:ASP:N	2.65	0.60
1:A:249:GLU:O	1:A:250:ALA:C	2.39	0.60
1:A:8:ASN:N	1:A:12:GLU:OE1	2.35	0.59
1:A:235:LEU:CD1	1:A:290:LEU:CB	2.80	0.59
1:A:234:GLY:CA	2:A:864:HOH:O	2.50	0.59
1:A:109:SER:O	1:A:113:LEU:CG	2.51	0.59
1:A:18:GLU:OE2	1:A:18:GLU:CA	2.49	0.59
1:A:2:GLU:CB	1:A:4:LYS:NZ	2.67	0.57
1:A:147:ALA:N	2:A:856:HOH:O	2.36	0.57
1:A:238:LEU:CD2	1:A:247:PHE:CZ	2.87	0.57
1:A:231:VAL:CG1	1:A:287:ALA:N	2.69	0.56
1:A:372:ARG:O	1:A:373:ILE:C	2.43	0.56
1:A:339:ARG:CD	1:A:339:ARG:N	2.69	0.55
1:A:3:ASN:CA	1:A:397:VAL:CG1	2.84	0.55
1:A:120:ILE:CG2	2:A:591:HOH:O	2.56	0.54
1:A:177:ARG:NH2	1:A:475:ASN:ND2	2.56	0.54
1:A:58:GLN:N	1:A:59:LYS:CG	2.71	0.54
1:A:423:ASN:C	1:A:425:PRO:CD	2.76	0.54
1:A:121:GLU:CD	1:A:121:GLU:N	2.62	0.52
1:A:419:ASN:ND2	2:A:681:HOH:O	2.42	0.52
1:A:109:SER:O	1:A:113:LEU:CB	2.58	0.52
1:A:176:ARG:NH1	1:A:446:MET:O	2.43	0.52
1:A:304:ILE:N	1:A:304:ILE:CD1	2.73	0.52
1:A:366:ASP:OD2	1:A:366:ASP:N	2.43	0.52
1:A:249:GLU:O	1:A:253:THR:CG2	2.59	0.51
1:A:385:ILE:CD1	1:A:388:MET:CE	2.89	0.51
1:A:235:LEU:C	1:A:235:LEU:CD2	2.78	0.51
1:A:126:TYR:O	1:A:130:ALA:N	2.43	0.51
1:A:97:GLU:O	1:A:97:GLU:CG	2.58	0.50
1:A:174:ILE:CG2	1:A:175:ARG:N	2.75	0.50
1:A:164:MET:O	1:A:167:LYS:N	2.45	0.50
1:A:55:ASP:C	1:A:57:ALA:N	2.65	0.49
1:A:230:LEU:O	1:A:233:THR:OG1	2.30	0.49
1:A:111:THR:OG1	1:A:112:GLU:OE2	2.30	0.49
1:A:321:PRO:O	1:A:323:THR:N	2.44	0.49
1:A:1:MET:N	1:A:2:GLU:CB	2.74	0.49
1:A:230:LEU:CD2	1:A:280:LEU:CD2	2.91	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:453:HIS:CB	2:A:803:HOH:O	2.60	0.48
1:A:363:PHE:CE1	1:A:380:LEU:CD1	2.96	0.48
1:A:422:THR:O	1:A:424:ASN:ND2	2.47	0.48
1:A:205:VAL:CG1	1:A:249:GLU:CB	2.92	0.47
1:A:422:THR:O	1:A:423:ASN:C	2.53	0.47
1:A:228:ILE:CG2	1:A:231:VAL:CG2	2.92	0.47
1:A:49:GLN:O	1:A:52:SER:CB	2.63	0.47
1:A:199:GLU:O	1:A:202:ARG:N	2.47	0.47
1:A:205:VAL:O	1:A:249:GLU:CG	2.63	0.47
1:A:383:GLY:CA	2:A:626:HOH:O	2.62	0.47
1:A:162:ILE:O	1:A:166:VAL:CG2	2.63	0.46
1:A:203:GLU:CB	1:A:211:MET:SD	3.04	0.46
1:A:204:PHE:C	1:A:204:PHE:CD2	2.89	0.46
1:A:12:GLU:O	1:A:13:MET:C	2.54	0.45
1:A:220:ILE:CG1	1:A:280:LEU:CD2	2.95	0.45
1:A:249:GLU:O	1:A:252:LYS:N	2.49	0.45
1:A:138:GLY:C	1:A:140:ARG:N	2.70	0.45
1:A:56:ASP:O	1:A:57:ALA:C	2.54	0.45
1:A:44:ASP:O	1:A:45:ARG:C	2.55	0.45
1:A:238:LEU:CD2	1:A:247:PHE:CE2	3.00	0.45
1:A:468:ASN:OD1	1:A:470:TYR:N	2.50	0.45
1:A:347:ALA:O	1:A:351:THR:CG2	2.65	0.45
1:A:79:GLU:OE2	1:A:144:ASN:ND2	2.51	0.44
1:A:244:LYS:CD	1:A:244:LYS:N	2.81	0.44
1:A:119:LYS:N	1:A:122:GLN:OE1	2.50	0.44
1:A:90:LYS:CD	2:A:785:HOH:O	2.65	0.44
1:A:174:ILE:O	1:A:177:ARG:CB	2.67	0.43
1:A:131:LEU:O	1:A:132:LYS:C	2.55	0.43
1:A:425:PRO:O	1:A:426:CYS:C	2.57	0.43
1:A:45:ARG:NH2	1:A:69:GLU:OE1	2.52	0.43
1:A:305:ASP:C	1:A:305:ASP:OD2	2.57	0.43
1:A:106:TRP:N	1:A:106:TRP:CD1	2.87	0.43
1:A:159:PRO:CD	1:A:162:ILE:CD1	2.97	0.43
1:A:324:PHE:O	1:A:327:VAL:N	2.52	0.43
1:A:235:LEU:O	1:A:235:LEU:CD2	2.67	0.42
1:A:1:MET:O	1:A:1:MET:CG	2.67	0.42
1:A:437:GLN:OE1	1:A:451:SER:OG	2.38	0.42
1:A:201:CYS:O	1:A:205:VAL:CG2	2.68	0.41
1:A:447:ASP:OD1	1:A:447:ASP:N	2.53	0.41
1:A:174:ILE:O	1:A:177:ARG:N	2.53	0.41
1:A:148:LEU:N	1:A:468:ASN:O	2.54	0.41
1:A:125:ASP:O	1:A:129:ALA:N	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:43:LEU:O	1:A:44:ASP:C	2.60	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	452/482 (94%)	360 (80%)	65 (14%)	27 (6%)	2 1

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	149	SER
1	A	180	ILE
1	A	322	GLU
1	A	365	ASP
1	A	373	ILE
1	A	374	TYR
1	A	376	HIS
1	A	56	ASP
1	A	165	SER
1	A	226	SER
1	A	421	GLU
1	A	423	ASN
1	A	478	SER
1	A	164	MET
1	A	211	MET
1	A	45	ARG
1	A	47	VAL
1	A	250	ALA
1	A	425	PRO
1	A	471	ASN
1	A	6	GLU

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Mol	Chain	Res	Type
1	A	59	LYS
1	A	160	GLY
1	A	422	THR
1	A	207	GLY
1	A	224	GLY

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	389/408 (95%)	308 (79%)	81 (21%)	2 1

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	15	LYS
1	A	18	GLU
1	A	22	LYS
1	A	26	LEU
1	A	30	PHE
1	A	35	SER
1	A	38	GLU
1	A	42	ASN
1	A	45	ARG
1	A	54	THR
1	A	55	ASP
1	A	56	ASP
1	A	61	SER
1	A	67	LEU
1	A	97	GLU
1	A	106	TRP
1	A	111	THR
1	A	114	LYS
1	A	120	ILE
1	A	121	GLU
1	A	128	GLN
1	A	137	ILE

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Mol	Chain	Res	Type
1	A	140	ARG
1	A	141	VAL
1	A	142	ASN
1	A	148	LEU
1	A	162	ILE
1	A	170	LEU
1	A	171	SER
1	A	173	MET
1	A	177	ARG
1	A	180	ILE
1	A	195	ARG
1	A	196	GLU
1	A	198	VAL
1	A	201	CYS
1	A	211	MET
1	A	220	ILE
1	A	225	ARG
1	A	226	SER
1	A	228	ILE
1	A	235	LEU
1	A	237	LYS
1	A	241	THR
1	A	242	GLU
1	A	249	GLU
1	A	253	THR
1	A	263	LYS
1	A	265	LYS
1	A	268	VAL
1	A	272	SER
1	A	278	THR
1	A	295	SER
1	A	298	ARG
1	A	304	ILE
1	A	309	SER
1	A	326	THR
1	A	336	LYS
1	A	339	ARG
1	A	342	LYS
1	A	343	LYS
1	A	350	SER
1	A	351	THR
1	A	366	ASP

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Mol	Chain	Res	Type
1	A	372	ARG
1	A	373	ILE
1	A	380	LEU
1	A	397	VAL
1	A	399	ASN
1	A	413	ILE
1	A	419	ASN
1	A	420	THR
1	A	423	ASN
1	A	424	ASN
1	A	436	ILE
1	A	439	THR
1	A	446	MET
1	A	447	ASP
1	A	448	ILE
1	A	463	GLN

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, 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	460/482 (95%)	0.15	15 (3%) 44 54	25, 46, 82, 151	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	VAL	6.8
1	A	140	ARG	4.2
1	A	180	ILE	3.4
1	A	244	LYS	3.3
1	A	235	LEU	3.3
1	A	420	THR	3.1
1	A	29	THR	3.1
1	A	55	ASP	2.9
1	A	181	LEU	2.8
1	A	195	ARG	2.7
1	A	372	ARG	2.6
1	A	443	ILE	2.3
1	A	338	PRO	2.3
1	A	366	ASP	2.1
1	A	442	ASN	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.