



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2020 – 12:03 PM GMT

PDB ID : 6RJ1  
Title : N-Domain P40/P90 Mycoplasma pneumoniae  
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Deposited on : 2019-04-25  
Resolution : 2.65 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](mailto: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.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
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)	:	2.14.6

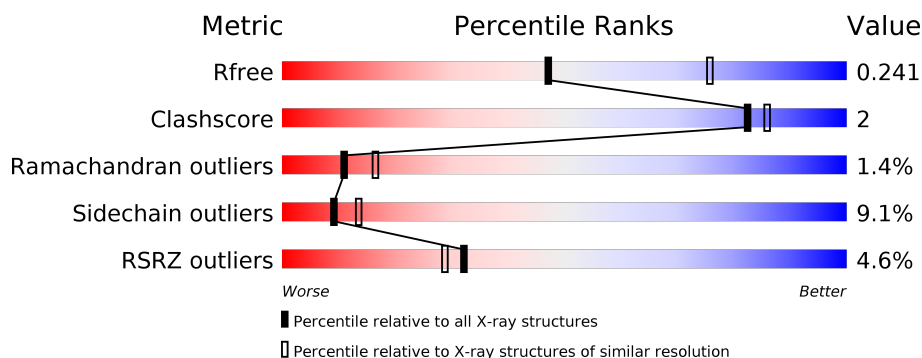
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 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	976	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>10%</div> <div>17%</div> </div> </div>
1	B	976	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>10%</div> <div>17%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12623 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 Mgp-operon protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	812	Total	C	N	O	S	0	2	0
			6292	3953	1076	1259	4			
1	B	806	Total	C	N	O	S	0	4	0
			6267	3944	1068	1251	4			

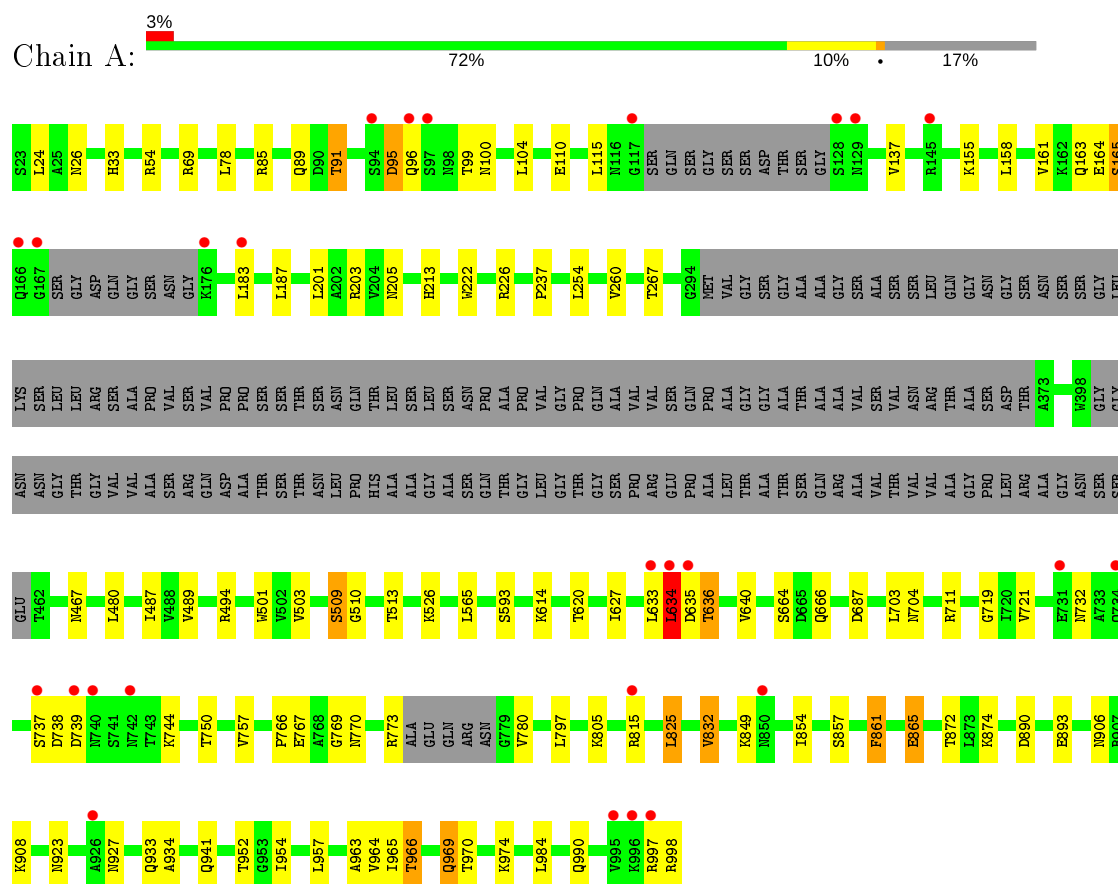
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	54	Total	O	0	0
			54	54		
2	B	10	Total	O	0	0
			10	10		

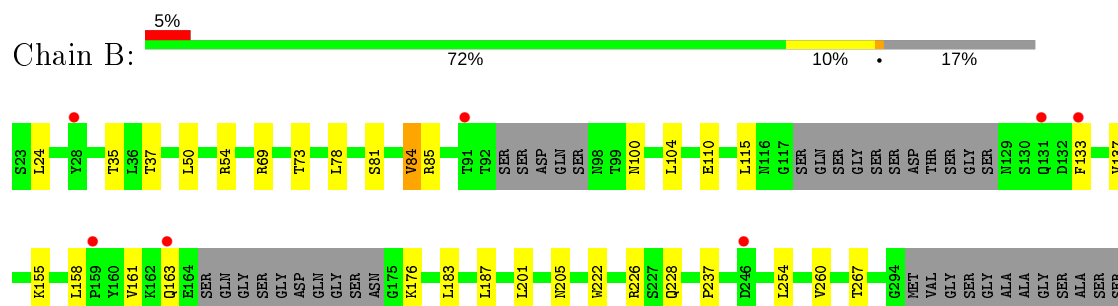
### 3 Residue-property plots

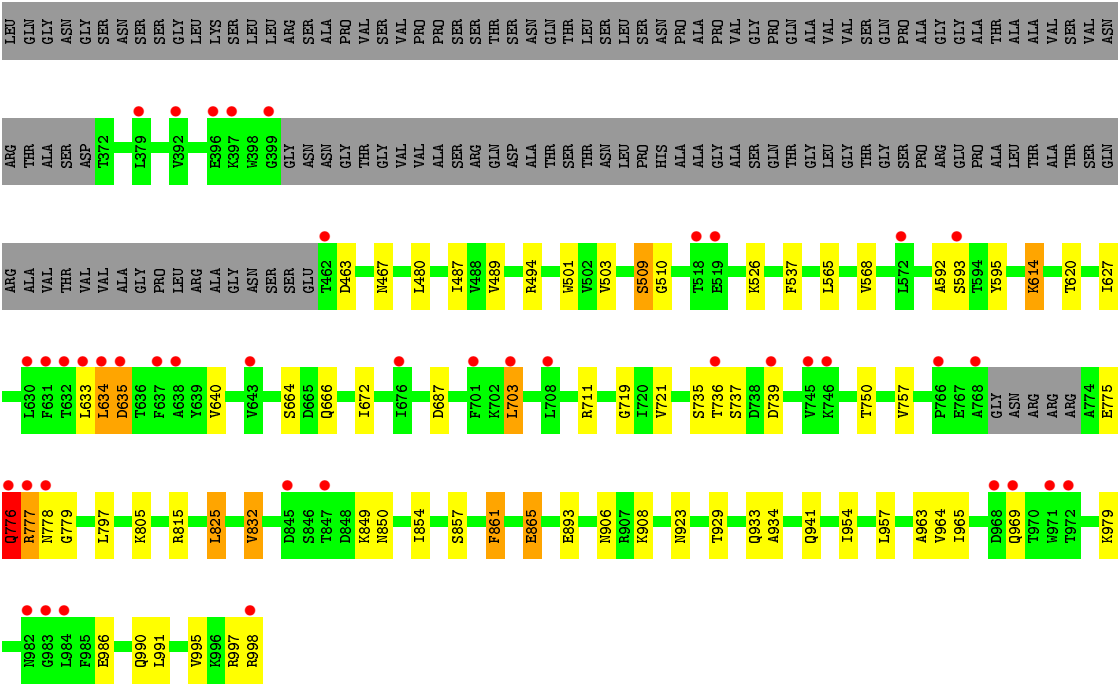
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Mgp-operon protein 3



#### • Molecule 1: Mgp-operon protein 3





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.80Å 114.43Å 165.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.53 – 2.65 82.53 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.6 (82.53-2.65) 99.6 (82.53-2.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.214 , 0.234 0.217 , 0.241	Depositor DCC
$R_{free}$ test set	2655 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.7	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 53.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12623	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.72% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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	0.40	0/6422	0.66	0/8731
1	B	0.39	0/6397	0.64	0/8698
All	All	0.40	0/12819	0.65	0/17429

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	6292	0	6117	28	0
1	B	6267	0	6091	33	0
2	A	54	0	0	1	0
2	B	10	0	0	0	0
All	All	12623	0	12208	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 2.

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:775:GLU:C	1:B:776:GLN:HG3	1.81	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:861:PHE:HB2	1:A:865:GLU:HG3	1.56	0.86
1:B:861:PHE:HB2	1:B:865:GLU:HG3	1.56	0.86
1:B:78:LEU:HB2	1:B:480:LEU:HD23	1.65	0.79
1:A:78:LEU:HB2	1:A:480:LEU:HD23	1.64	0.78
1:B:81:SER:O	1:B:84:VAL:HG23	1.85	0.77
1:A:634:LEU:HD22	1:A:635:ASP:H	1.50	0.75
1:A:155:LYS:HB3	1:A:509:SER:HB2	1.73	0.70
1:B:155:LYS:HB3	1:B:509:SER:HB2	1.73	0.70
1:B:614:LYS:HD3	1:B:849:LYS:HB3	1.79	0.64
1:B:703:LEU:H	1:B:703:LEU:HD22	1.66	0.61
1:B:537:PHE:HB3	1:B:672:ILE:HD13	1.85	0.58
1:B:775:GLU:C	1:B:776:GLN:CG	2.65	0.57
1:A:766:PRO:HG3	1:A:780:VAL:HB	1.87	0.56
1:A:95:ASP:HA	1:A:165:SER:HB3	1.89	0.54
1:B:775:GLU:O	1:B:776:GLN:HG3	2.07	0.54
1:A:872:THR:HB	1:A:890:ASP:O	2.07	0.53
1:B:719:GLY:HA3	1:B:750:THR:HG22	1.89	0.53
1:A:719:GLY:HA3	1:A:750:THR:HG22	1.90	0.52
1:A:952:THR:HB	1:A:965:ILE:HB	1.90	0.52
1:A:966:THR:HG22	1:A:974:LYS:HB3	1.92	0.52
1:B:205:ASN:HD21	1:B:687:ASP:HB2	1.75	0.52
1:A:636:THR:OG1	1:A:769:GLY:HA2	2.10	0.52
1:A:205:ASN:HD21	1:A:687:ASP:HB2	1.75	0.51
1:A:503:VAL:HG12	1:A:510:GLY:HA3	1.93	0.50
1:A:634:LEU:HD22	1:A:635:ASP:N	2.25	0.50
1:B:503:VAL:HG12	1:B:510:GLY:HA3	1.92	0.50
1:B:825:LEU:HG	1:B:832:VAL:HG13	1.96	0.48
1:B:954:ILE:HG12	1:B:964:VAL:HG22	1.96	0.48
1:B:957:LEU:HD11	1:B:963:ALA:HB2	1.96	0.48
1:A:825:LEU:HG	1:A:832:VAL:HG13	1.96	0.47
1:A:614:LYS:HD2	1:A:849:LYS:HB2	1.98	0.46
1:B:633:LEU:HG	1:B:634:LEU:HD22	1.97	0.46
1:A:489:VAL:HB	1:A:501:TRP:HB2	1.98	0.46
1:A:957:LEU:HD11	1:A:963:ALA:HB2	1.96	0.46
1:A:513:THR:HG23	1:A:732:ASN:HD22	1.82	0.45
1:B:537:PHE:CB	1:B:672:ILE:HD13	2.45	0.45
1:B:85:ARG:HG3	1:B:110:GLU:HB3	1.98	0.45
1:A:85:ARG:HG3	1:A:110:GLU:HB3	1.99	0.45
1:A:954:ILE:HG12	1:A:964:VAL:HG22	1.99	0.45
1:A:861:PHE:HB2	1:A:865:GLU:CG	2.37	0.44
1:B:778:ASN:HB3	1:B:779:GLY:H	1.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:VAL:HG22	1:B:133:PHE:O	2.18	0.44
1:A:633:LEU:C	1:A:634:LEU:HD13	2.38	0.43
1:B:222:TRP:CD2	1:B:237:PRO:HB3	2.54	0.43
1:B:777:ARG:HE	1:B:777:ARG:HB3	1.50	0.43
1:B:489:VAL:HB	1:B:501:TRP:HB2	1.98	0.43
1:B:775:GLU:O	1:B:776:GLN:CG	2.66	0.43
1:A:222:TRP:CD2	1:A:237:PRO:HB3	2.54	0.43
1:B:81:SER:O	1:B:84:VAL:CG2	2.63	0.43
1:B:854:ILE:HA	1:B:934:ALA:HB2	2.01	0.43
1:B:137:VAL:HG11	1:B:487:ILE:HG21	2.00	0.43
1:B:861:PHE:HB2	1:B:865:GLU:CG	2.37	0.42
1:A:213:HIS:HE1	2:A:1029:HOH:O	2.02	0.42
1:B:592:ALA:HB3	1:B:595:TYR:HB2	2.02	0.41
1:A:161:VAL:HG21	1:A:183:LEU:HD12	2.03	0.41
1:A:854:ILE:HA	1:A:934:ALA:HB2	2.02	0.41
1:B:991:LEU:O	1:B:995:VAL:HG23	2.21	0.41
1:B:35:THR:HA	1:B:50:LEU:O	2.21	0.40
1:A:137:VAL:HG11	1:A:487:ILE:HG21	2.02	0.40
1:B:161:VAL:HG21	1:B:183:LEU:HD12	2.03	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	802/976 (82%)	751 (94%)	37 (5%)	14 (2%)	9	13
1	B	796/976 (82%)	749 (94%)	38 (5%)	9 (1%)	14	21
All	All	1598/1952 (82%)	1500 (94%)	75 (5%)	23 (1%)	11	16

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	THR
1	A	165	SER
1	A	634	LEU
1	A	96	GLN
1	A	164	GLU
1	A	737	SER
1	A	969	GLN
1	A	997	ARG
1	B	736	THR
1	B	737	SER
1	A	467	ASN
1	A	738	ASP
1	A	770	ASN
1	B	467	ASN
1	B	735	SER
1	B	776	GLN
1	A	33[A]	HIS
1	A	33[B]	HIS
1	A	627	ILE
1	B	627	ILE
1	B	634	LEU
1	B	929	THR
1	B	635	ASP

### 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	684/800 (86%)	621 (91%)	63 (9%)	9	13
1	B	679/800 (85%)	617 (91%)	62 (9%)	9	13
All	All	1363/1600 (85%)	1238 (91%)	125 (9%)	9	13

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU

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Mol	Chain	Res	Type
1	A	26	ASN
1	A	54[A]	ARG
1	A	54[B]	ARG
1	A	69	ARG
1	A	89	GLN
1	A	91	THR
1	A	95	ASP
1	A	99	THR
1	A	100	ASN
1	A	104	LEU
1	A	115	LEU
1	A	158	LEU
1	A	163	GLN
1	A	187	LEU
1	A	201	LEU
1	A	203	ARG
1	A	226	ARG
1	A	254	LEU
1	A	260	VAL
1	A	267	THR
1	A	494	ARG
1	A	509	SER
1	A	526	LYS
1	A	565	LEU
1	A	593	SER
1	A	620	THR
1	A	634	LEU
1	A	636	THR
1	A	640	VAL
1	A	664	SER
1	A	666	GLN
1	A	703	LEU
1	A	704	ASN
1	A	711	ARG
1	A	721	VAL
1	A	739	ASP
1	A	744	LYS
1	A	757	VAL
1	A	767	GLU
1	A	773	ARG
1	A	797	LEU
1	A	805	LYS

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Mol	Chain	Res	Type
1	A	815	ARG
1	A	825	LEU
1	A	832	VAL
1	A	857	SER
1	A	861	PHE
1	A	865	GLU
1	A	874	LYS
1	A	893	GLU
1	A	906	ASN
1	A	908	LYS
1	A	923	ASN
1	A	927	ASN
1	A	933	GLN
1	A	941	GLN
1	A	966	THR
1	A	969	GLN
1	A	970	THR
1	A	984	LEU
1	A	990	GLN
1	A	998	ARG
1	B	24	LEU
1	B	37	THR
1	B	54	ARG
1	B	69	ARG
1	B	73	THR
1	B	84	VAL
1	B	100	ASN
1	B	104	LEU
1	B	115	LEU
1	B	158	LEU
1	B	163	GLN
1	B	176	LYS
1	B	187	LEU
1	B	201	LEU
1	B	226	ARG
1	B	228	GLN
1	B	254	LEU
1	B	260	VAL
1	B	267	THR
1	B	463	ASP
1	B	494[A]	ARG
1	B	494[B]	ARG

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Mol	Chain	Res	Type
1	B	509	SER
1	B	526	LYS
1	B	565	LEU
1	B	568	VAL
1	B	593	SER
1	B	614	LYS
1	B	620	THR
1	B	635	ASP
1	B	640	VAL
1	B	664	SER
1	B	666	GLN
1	B	703	LEU
1	B	711	ARG
1	B	721	VAL
1	B	739	ASP
1	B	757	VAL
1	B	776	GLN
1	B	777	ARG
1	B	797	LEU
1	B	805	LYS
1	B	815	ARG
1	B	825	LEU
1	B	832	VAL
1	B	850	ASN
1	B	857	SER
1	B	861	PHE
1	B	865	GLU
1	B	893	GLU
1	B	906	ASN
1	B	908	LYS
1	B	923	ASN
1	B	933	GLN
1	B	941	GLN
1	B	965	ILE
1	B	969	GLN
1	B	979	LYS
1	B	986	GLU
1	B	990	GLN
1	B	997	ARG
1	B	998	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	732	ASN
1	A	906	ASN
1	B	205	ASN
1	B	225	GLN
1	B	734	GLN
1	B	906	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 monosaccharides 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

### 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	812/976 (83%)	0.26	26 (3%) 47 44	50, 76, 125, 169	0
1	B	806/976 (82%)	0.35	49 (6%) 21 18	55, 93, 140, 177	0
All	All	1618/1952 (82%)	0.30	75 (4%) 32 29	50, 83, 135, 177	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	167	GLY	8.4
1	B	701	PHE	8.0
1	B	778	ASN	7.8
1	B	703	LEU	7.4
1	A	996	LYS	5.9
1	A	739	ASP	5.8
1	B	968	ASP	5.5
1	A	128	SER	5.4
1	A	634	LEU	4.9
1	B	971	TRP	4.8
1	B	396	GLU	4.7
1	B	768	ALA	4.3
1	B	983	GLY	4.1
1	B	632	THR	4.0
1	B	982	ASN	3.9
1	B	631	PHE	3.6
1	A	815	ARG	3.6
1	B	131	GLN	3.5
1	A	995	VAL	3.4
1	A	97	SER	3.3
1	A	117	GLY	3.3
1	A	633	LEU	3.2
1	B	91	THR	3.1
1	B	28[A]	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	742	ASN	3.0
1	B	969	GLN	2.9
1	A	926	ALA	2.9
1	B	630	LEU	2.8
1	B	397	LYS	2.8
1	B	847	THR	2.8
1	A	740	ASN	2.7
1	B	246	ASP	2.7
1	B	736	THR	2.7
1	B	766	PRO	2.7
1	B	635	ASP	2.7
1	B	708	LEU	2.7
1	B	633	LEU	2.6
1	B	776	GLN	2.6
1	B	972	THR	2.6
1	B	133	PHE	2.5
1	B	845	ASP	2.5
1	A	997	ARG	2.4
1	B	637	PHE	2.4
1	B	572	LEU	2.4
1	B	399	GLY	2.4
1	B	643	VAL	2.4
1	B	392	VAL	2.4
1	B	777	ARG	2.4
1	B	984	LEU	2.3
1	A	176	LYS	2.3
1	A	635	ASP	2.3
1	B	634	LEU	2.3
1	A	145	ARG	2.2
1	B	638	ALA	2.2
1	B	518	THR	2.2
1	B	519	GLU	2.2
1	A	731	GLU	2.2
1	A	129	ASN	2.2
1	A	94	SER	2.1
1	A	166	GLN	2.1
1	B	998	ARG	2.1
1	B	593	SER	2.1
1	B	676	ILE	2.1
1	B	746	LYS	2.1
1	A	850	ASN	2.1
1	B	379	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	462	THR	2.1
1	B	739	ASP	2.1
1	A	734	GLN	2.0
1	A	183	LEU	2.0
1	A	96	GLN	2.0
1	A	737	SER	2.0
1	B	163	GLN	2.0
1	B	159	PRO	2.0
1	B	745	VAL	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 monosaccharides 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.