



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 06:27 AM GMT

PDB ID : 4JSN  
Title : structure of mTORdeltaN-mLST8 complex  
Authors : Pavletich, N.P.  
Deposited on : 2013-03-22  
Resolution : 3.20 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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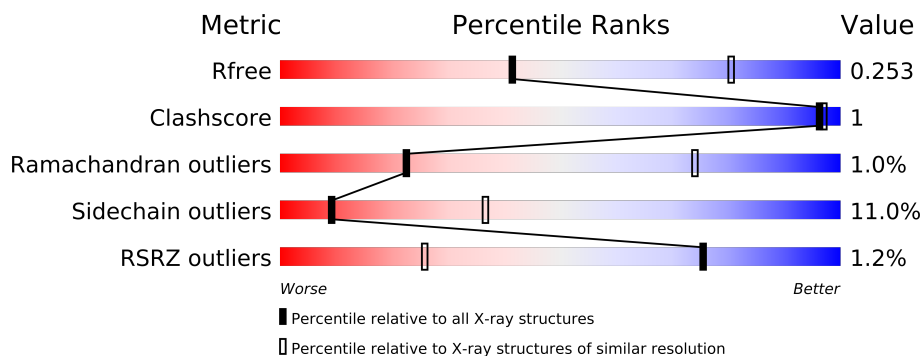
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.20 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	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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	1174	
1	B	1174	
2	C	326	
2	D	326	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22097 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.

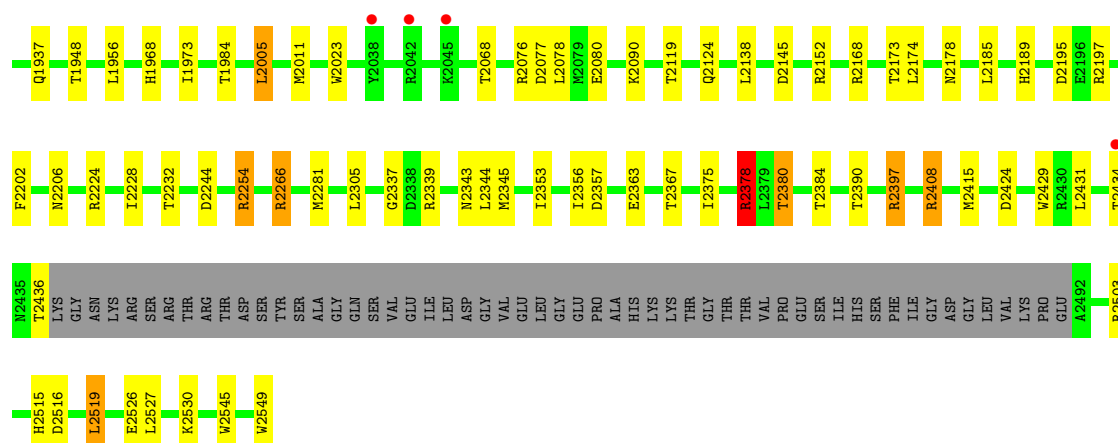
- Molecule 1 is a protein called Serine/threonine-proteinkinase mTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1058	Total	C	N	O	S	0	0	0
			8608	5472	1521	1552	63			
1	A	1054	Total	C	N	O	S	0	0	0
			8577	5451	1517	1546	63			

- Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

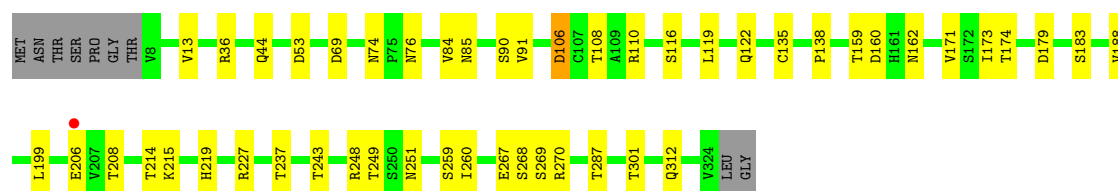
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	317	Total	C	N	O	S	0	0	0
			2456	1526	436	476	18			
2	C	317	Total	C	N	O	S	0	0	0
			2456	1526	436	476	18			





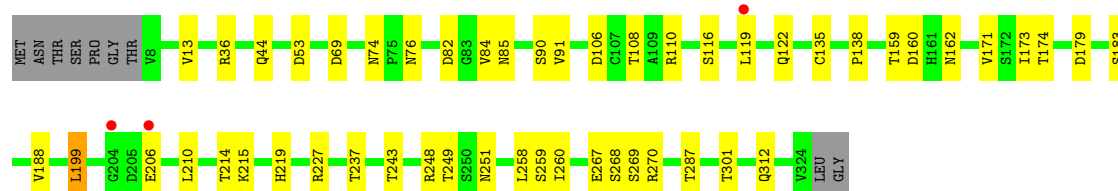
- Molecule 2: Target of rapamycin complex subunit LST8

Chain D:



- Molecule 2: Target of rapamycin complex subunit LST8

Chain C:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.40Å 163.20Å 207.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.86 – 3.20 29.84 – 3.20	Depositor EDS
% Data completeness (in resolution range)	86.6 (29.86-3.20) 86.6 (29.84-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.215 , 0.256 0.220 , 0.253	Depositor DCC
$R_{free}$ test set	1700 reflections (2.55%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.0	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 30.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 75518 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	22097	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.98 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.6294e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	0.55	0/8772	0.85	10/11872 (0.1%)
1	B	0.55	0/8805	0.85	9/11920 (0.1%)
2	C	0.55	0/2514	0.88	2/3426 (0.1%)
2	D	0.58	0/2514	0.90	0/3426
All	All	0.55	0/22605	0.86	21/30644 (0.1%)

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	2
1	B	0	2
2	C	0	1
2	D	0	1
All	All	0	6

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2378	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	B	2378	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	B	2378	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	2378	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	A	2344	LEU	CA-CB-CG	6.14	129.41	115.30
1	B	2305	LEU	CA-CB-CG	5.86	128.79	115.30
1	B	2344	LEU	CA-CB-CG	5.83	128.72	115.30
1	A	2305	LEU	CA-CB-CG	5.79	128.62	115.30
1	B	2408	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	2005	LEU	CA-CB-CG	5.42	127.77	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2005	LEU	CA-CB-CG	5.32	127.54	115.30
1	A	2254	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	A	2266	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	2174	LEU	CA-CB-CG	5.20	127.25	115.30
1	B	1445	ILE	N-CA-C	-5.17	97.05	111.00
1	B	1701	MET	CG-SD-CE	-5.10	92.04	100.20
1	B	2266	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	1907	LEU	CA-CB-CG	5.04	126.90	115.30
1	A	1599	LEU	CA-CB-CG	5.02	126.84	115.30
2	C	210	LEU	CA-CB-CG	5.01	126.81	115.30
2	C	199	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1444	GLU	Peptide
1	A	1680	ASP	Peptide
1	B	1444	GLU	Peptide
1	B	1680	ASP	Peptide
2	C	267	GLU	Peptide
2	D	267	GLU	Peptide

## 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	8577	0	0	8	1
1	B	8608	0	0	9	0
2	C	2456	0	0	4	0
2	D	2456	0	0	4	0
All	All	22097	0	0	25	1

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 1.



All (25) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2378:ARG:NH2	1:A:2545:TRP:O	2.24	0.71
1:B:2378:ARG:NH2	1:B:2545:TRP:O	2.25	0.70
2:C:219:HIS:NE2	2:C:237:THR:CG2	2.62	0.62
2:D:219:HIS:NE2	2:D:237:THR:CG2	2.68	0.56
2:D:36:ARG:NH2	2:D:69:ASP:O	2.39	0.55
2:C:36:ARG:NH2	2:C:69:ASP:O	2.40	0.54
1:B:2197:ARG:NH1	1:B:2424:ASP:OD2	2.42	0.53
2:D:108:THR:OG1	2:D:110:ARG:NH1	2.43	0.52
2:C:108:THR:OG1	2:C:110:ARG:NH1	2.46	0.48
1:B:2380:THR:CG2	1:B:2549:TRP:C	2.83	0.47
1:B:2408:ARG:NH2	1:B:2519:LEU:O	2.48	0.46
1:A:2197:ARG:NH1	1:A:2424:ASP:OD2	2.48	0.46
1:A:2397:ARG:NH2	1:A:2526:GLU:OE1	2.50	0.45
1:A:2408:ARG:NH2	1:A:2519:LEU:O	2.51	0.44
1:A:2202:PHE:O	1:A:2206:ASN:N	2.52	0.42
1:B:2339:ARG:NH2	1:B:2356:ILE:O	2.52	0.42
2:D:106:ASP:OD1	2:D:108:THR:OG1	2.38	0.42
2:C:106:ASP:OD1	2:C:108:THR:OG1	2.38	0.42
1:A:2339:ARG:NH2	1:A:2356:ILE:O	2.53	0.41
1:A:2337:GLY:O	1:A:2339:ARG:NH1	2.54	0.41
1:B:2337:GLY:O	1:B:2339:ARG:NH1	2.54	0.41
1:A:2380:THR:CG2	1:A:2549:TRP:C	2.90	0.40
1:B:2289:HIS:O	1:B:2293:ASN:ND2	2.54	0.40
1:B:2397:ARG:NH2	1:B:2526:GLU:OE1	2.54	0.40
1:B:2202:PHE:O	1:B:2206:ASN:N	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1612:ARG:NH2	1:A:1612:ARG:NH2[2_554]	1.96	0.24

## 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	1046/1174 (89%)	967 (92%)	72 (7%)	7 (1%)	30	80
1	B	1052/1174 (90%)	967 (92%)	77 (7%)	8 (1%)	27	77
2	C	315/326 (97%)	285 (90%)	24 (8%)	6 (2%)	12	59
2	D	315/326 (97%)	284 (90%)	24 (8%)	7 (2%)	10	53
All	All	2728/3000 (91%)	2503 (92%)	197 (7%)	28 (1%)	22	74

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1630	VAL
1	B	1692	VAL
1	B	1937	GLN
2	D	74	ASN
1	A	1692	VAL
1	A	1937	GLN
2	C	74	ASN
2	D	268	SER
1	A	1630	VAL
1	A	1709	ARG
2	C	268	SER
1	B	1578	MET
1	B	1709	ARG
1	A	1578	MET
1	B	1707	SER
2	D	269	SER
1	A	1707	SER
2	C	206	GLU
2	C	269	SER
1	B	2357	ASP
2	D	76	ASN
2	D	106	ASP
2	D	138	PRO
2	D	206	GLU
1	A	2357	ASP
2	C	76	ASN
2	C	138	PRO
1	B	1682	SER

### 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	927/1024 (90%)	831 (90%)	96 (10%)	10	39
1	B	931/1024 (91%)	834 (90%)	97 (10%)	10	39
2	C	269/276 (98%)	233 (87%)	36 (13%)	6	26
2	D	269/276 (98%)	234 (87%)	35 (13%)	6	28
All	All	2396/2600 (92%)	2132 (89%)	264 (11%)	9	36

All (264) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1385	GLU
1	B	1417	ILE
1	B	1419	ILE
1	B	1420	ASN
1	B	1423	LEU
1	B	1433	LEU
1	B	1457	GLU
1	B	1480	ARG
1	B	1508	THR
1	B	1528	SER
1	B	1540	THR
1	B	1541	HIS
1	B	1559	LEU
1	B	1585	ARG
1	B	1590	MET
1	B	1593	CYS
1	B	1626	CYS
1	B	1629	ILE
1	B	1643	VAL
1	B	1655	LYS
1	B	1658	SER
1	B	1679	VAL
1	B	1683	ARG
1	B	1685	LEU
1	B	1702	LYS
1	B	1709	ARG

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Mol	Chain	Res	Type
1	B	1724	MET
1	B	1734	THR
1	B	1736	ASP
1	B	1780	THR
1	B	1802	LEU
1	B	1870	THR
1	B	1872	ASP
1	B	1890	ARG
1	B	1895	SER
1	B	1896	ARG
1	B	1899	ASN
1	B	1901	GLN
1	B	1918	ASP
1	B	1932	ILE
1	B	1933	ASP
1	B	1948	THR
1	B	1956	LEU
1	B	1968	HIS
1	B	1973	ILE
1	B	1984	THR
1	B	2005	LEU
1	B	2011	MET
1	B	2023	TRP
1	B	2068	THR
1	B	2076	ARG
1	B	2077	ASP
1	B	2078	LEU
1	B	2080	GLU
1	B	2090	LYS
1	B	2119	THR
1	B	2124	GLN
1	B	2138	LEU
1	B	2145	ASP
1	B	2152	ARG
1	B	2168	ARG
1	B	2173	THR
1	B	2178	ASN
1	B	2185	LEU
1	B	2189	HIS
1	B	2195	ASP
1	B	2224	ARG
1	B	2228	ILE

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Mol	Chain	Res	Type
1	B	2232	THR
1	B	2244	ASP
1	B	2254	ARG
1	B	2260	LEU
1	B	2266	ARG
1	B	2281	MET
1	B	2343	ASN
1	B	2345	MET
1	B	2353	ILE
1	B	2363	GLU
1	B	2367	THR
1	B	2375	ILE
1	B	2378	ARG
1	B	2380	THR
1	B	2384	THR
1	B	2390	THR
1	B	2397	ARG
1	B	2408	ARG
1	B	2415	MET
1	B	2429	TRP
1	B	2431	LEU
1	B	2434	THR
1	B	2436	THR
1	B	2503	ARG
1	B	2515	HIS
1	B	2516	ASP
1	B	2519	LEU
1	B	2527	LEU
1	B	2530	LYS
2	D	13	VAL
2	D	44	GLN
2	D	53	ASP
2	D	84	VAL
2	D	85	ASN
2	D	90	SER
2	D	91	VAL
2	D	116	SER
2	D	119	LEU
2	D	122	GLN
2	D	135	CYS
2	D	159	THR
2	D	160	ASP

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Mol	Chain	Res	Type
2	D	162	ASN
2	D	171	VAL
2	D	173	ILE
2	D	174	THR
2	D	179	ASP
2	D	183	SER
2	D	188	VAL
2	D	199	LEU
2	D	208	THR
2	D	214	THR
2	D	215	LYS
2	D	227	ARG
2	D	243	THR
2	D	248	ARG
2	D	249	THR
2	D	251	ASN
2	D	259	SER
2	D	260	ILE
2	D	270	ARG
2	D	287	THR
2	D	301	THR
2	D	312	GLN
1	A	1385	GLU
1	A	1417	ILE
1	A	1419	ILE
1	A	1420	ASN
1	A	1423	LEU
1	A	1424	GLN
1	A	1433	LEU
1	A	1457	GLU
1	A	1480	ARG
1	A	1508	THR
1	A	1528	SER
1	A	1540	THR
1	A	1541	HIS
1	A	1547	ARG
1	A	1559	LEU
1	A	1585	ARG
1	A	1590	MET
1	A	1593	CYS
1	A	1626	CYS
1	A	1629	ILE

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Mol	Chain	Res	Type
1	A	1643	VAL
1	A	1679	VAL
1	A	1683	ARG
1	A	1685	LEU
1	A	1702	LYS
1	A	1709	ARG
1	A	1724	MET
1	A	1734	THR
1	A	1736	ASP
1	A	1780	THR
1	A	1802	LEU
1	A	1870	THR
1	A	1872	ASP
1	A	1890	ARG
1	A	1895	SER
1	A	1896	ARG
1	A	1899	ASN
1	A	1901	GLN
1	A	1918	ASP
1	A	1932	ILE
1	A	1933	ASP
1	A	1948	THR
1	A	1956	LEU
1	A	1968	HIS
1	A	1973	ILE
1	A	1984	THR
1	A	2005	LEU
1	A	2011	MET
1	A	2023	TRP
1	A	2068	THR
1	A	2076	ARG
1	A	2077	ASP
1	A	2078	LEU
1	A	2080	GLU
1	A	2090	LYS
1	A	2119	THR
1	A	2124	GLN
1	A	2138	LEU
1	A	2145	ASP
1	A	2152	ARG
1	A	2168	ARG
1	A	2173	THR

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Mol	Chain	Res	Type
1	A	2178	ASN
1	A	2185	LEU
1	A	2189	HIS
1	A	2195	ASP
1	A	2224	ARG
1	A	2228	ILE
1	A	2232	THR
1	A	2244	ASP
1	A	2254	ARG
1	A	2266	ARG
1	A	2281	MET
1	A	2343	ASN
1	A	2345	MET
1	A	2353	ILE
1	A	2363	GLU
1	A	2367	THR
1	A	2375	ILE
1	A	2378	ARG
1	A	2380	THR
1	A	2384	THR
1	A	2390	THR
1	A	2397	ARG
1	A	2408	ARG
1	A	2415	MET
1	A	2429	TRP
1	A	2431	LEU
1	A	2434	THR
1	A	2436	THR
1	A	2503	ARG
1	A	2515	HIS
1	A	2516	ASP
1	A	2519	LEU
1	A	2527	LEU
1	A	2530	LYS
2	C	13	VAL
2	C	44	GLN
2	C	53	ASP
2	C	82	ASP
2	C	84	VAL
2	C	85	ASN
2	C	90	SER
2	C	91	VAL

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Mol	Chain	Res	Type
2	C	116	SER
2	C	119	LEU
2	C	122	GLN
2	C	135	CYS
2	C	159	THR
2	C	160	ASP
2	C	162	ASN
2	C	171	VAL
2	C	173	ILE
2	C	174	THR
2	C	179	ASP
2	C	183	SER
2	C	188	VAL
2	C	199	LEU
2	C	214	THR
2	C	215	LYS
2	C	227	ARG
2	C	243	THR
2	C	248	ARG
2	C	249	THR
2	C	251	ASN
2	C	258	LEU
2	C	259	SER
2	C	260	ILE
2	C	270	ARG
2	C	287	THR
2	C	301	THR
2	C	312	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, 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	1054/1174 (89%)	0.02	17 (1%) 68 20	38, 86, 178, 243	0
1	B	1058/1174 (90%)	-0.13	11 (1%) 79 29	28, 72, 150, 238	0
2	C	317/326 (97%)	-0.11	3 (0%) 81 32	40, 77, 147, 222	0
2	D	317/326 (97%)	-0.27	1 (0%) 91 58	27, 52, 116, 192	0
All	All	2746/3000 (91%)	-0.09	32 (1%) 75 26	27, 74, 170, 243	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1579	ALA	4.4
1	A	1580	GLY	4.2
1	A	1559	LEU	4.1
1	B	1580	GLY	3.8
1	A	1503	LEU	3.6
1	A	2038	TYR	3.5
2	C	206	GLU	3.0
1	B	1503	LEU	3.0
1	B	2436	THR	2.9
2	C	119	LEU	2.9
1	A	2434	THR	2.9
1	A	1586	ALA	2.8
1	A	1581	GLU	2.8
1	A	1579	ALA	2.8
1	A	2042	ARG	2.6
1	B	1581	GLU	2.5
1	B	2434	THR	2.5
1	A	1469	THR	2.5
2	D	206	GLU	2.5
1	A	1499	GLU	2.5
1	A	1558	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1600	GLU	2.3
1	A	1619	TRP	2.3
1	B	2045	LYS	2.2
1	B	1469	THR	2.2
1	B	1869	VAL	2.2
1	B	1506	ASP	2.2
1	A	1531	GLU	2.2
1	A	1573	ALA	2.2
2	C	204	GLY	2.1
1	B	2435	ASN	2.1
1	A	2045	LYS	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.