



wwPDB X-ray Structure Validation Summary 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 wwPDB validation summary 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>

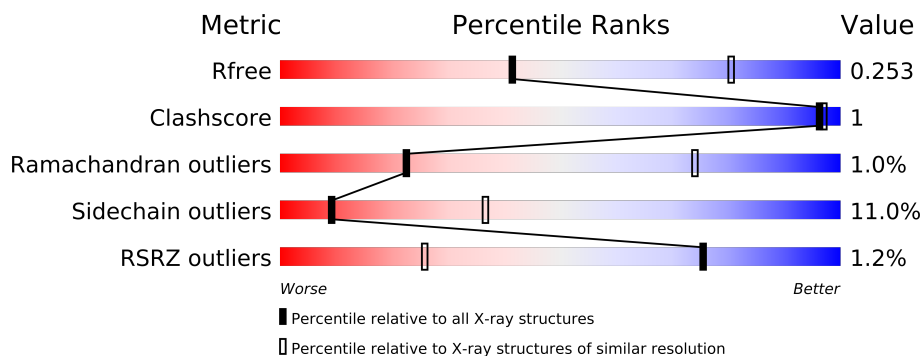
The following versions of software and data (see [references](#)) were used in the production of this report:

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 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 ≥ 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.

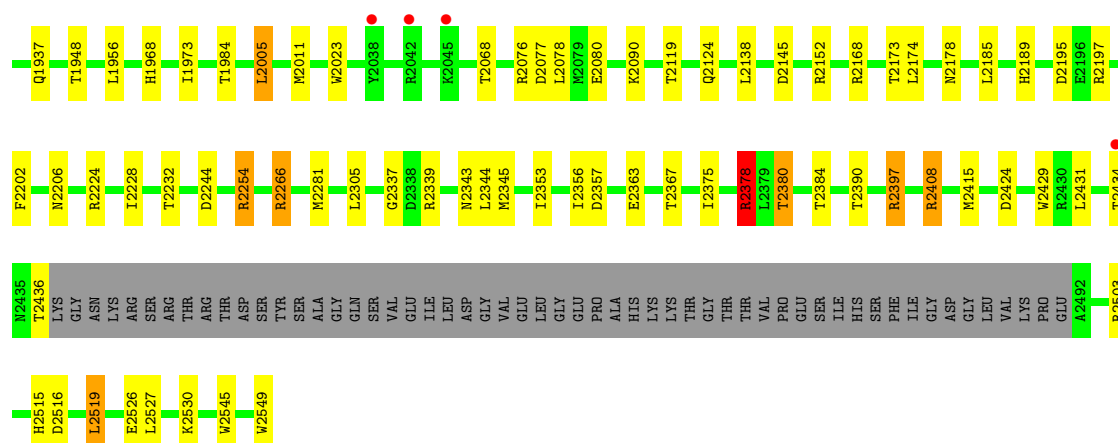
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- 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			

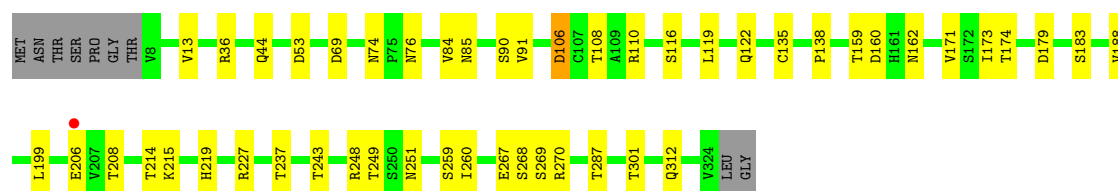
- Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

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			



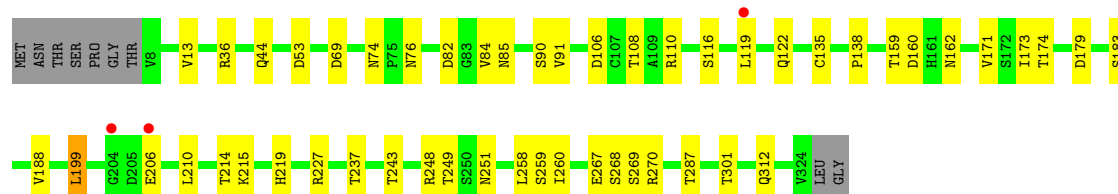
- Molecule 2: Target of rapamycin complex subunit LST8

Chain D:



- Molecule 2: Target of rapamycin complex subunit LST8

Chain C:



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	56.0	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	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 ²)	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.*

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	0.55	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.

The worst 5 of 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

There are no chirality outliers.

5 of 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	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.

The worst 5 of 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

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

5 of 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

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

5 of 264 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	214	THR
1	A	1585	ARG
2	C	171	VAL
2	D	243	THR
1	A	1419	ILE

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	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

The worst 5 of 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

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.