Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:22 PM GMT

PDB ID	:	3TSZ
Title	:	crystal structure of PDZ3-SH3-GUK core module from human ZO-1 in complex with 12mer peptide from human JAM-A cytoplasmic tail
Authors	:	Nomme, J.; Lavie, A.
Deposited on	:	2011-09-13
Resolution	:	2.50 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:

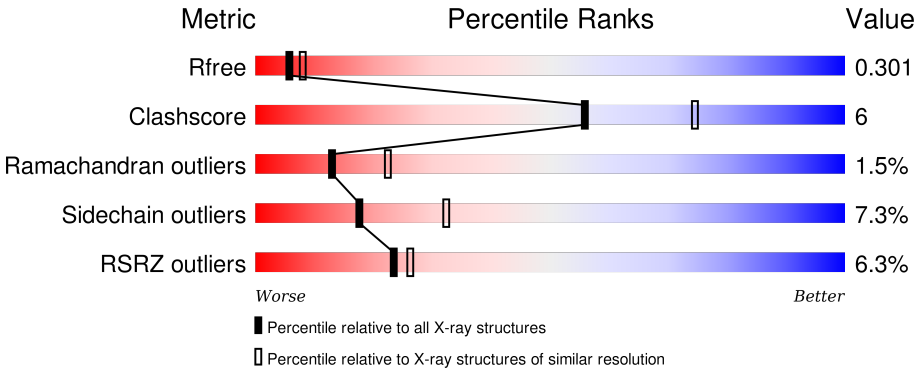
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 <=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	391	6%, 71%, 14%, •, 13%
2	B	12	50%, 33%, 17%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2849 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 Tight junction protein ZO-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2729	1729	489	506	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	413	GLY	-	EXPRESSION TAG	UNP Q07157
A	414	SER	-	EXPRESSION TAG	UNP Q07157
A	415	HIS	-	EXPRESSION TAG	UNP Q07157
A	416	MET	-	EXPRESSION TAG	UNP Q07157

- Molecule 2 is a protein called Junctional adhesion molecule A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	10	Total	C	N	O	0	0	0
			80	52	11	17			

- Molecule 3 is water.

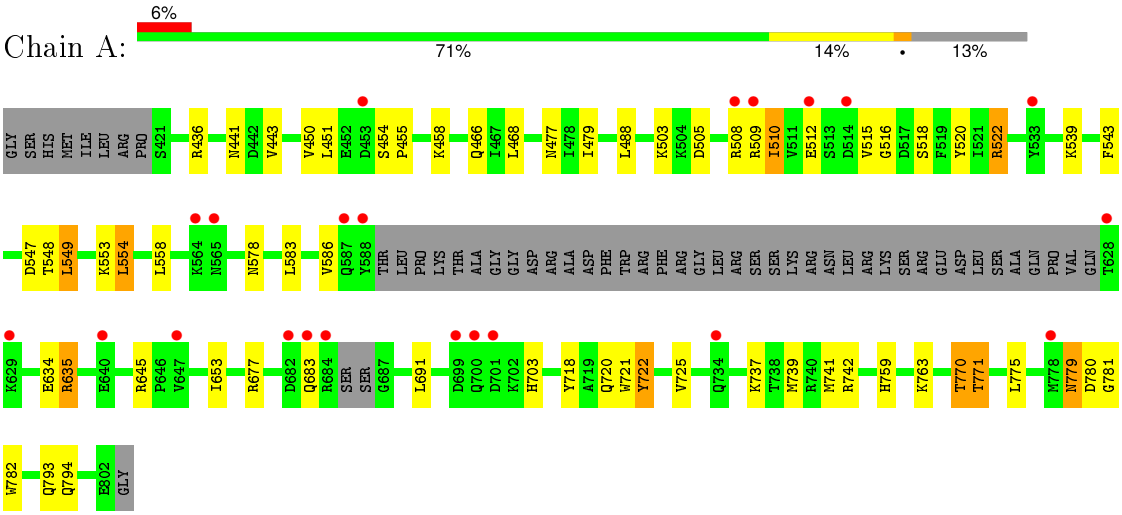
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	40	Total	O	0	0
			40	40		

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: Tight junction protein ZO-1

Chain A:



- Molecule 2: Junctional adhesion molecule A

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.50Å 49.70Å 91.80Å 90.00° 101.10° 90.00°	Depositor
Resolution (Å)	90.08 – 2.50 28.20 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.2 (90.08-2.50) 96.2 (28.20-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.240 , 0.309 0.233 , 0.301	Depositor DCC
R_{free} test set	1520 reflections (11.21%)	DCC
Wilson B-factor (Å^2)	54.4	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 28.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 15077 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	2849	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.38	0/2778	0.56	0/3748
2	B	0.53	0/81	0.59	0/107
All	All	0.38	0/2859	0.56	0/3855

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	2729	0	2739	35	0
2	B	80	0	70	2	0
3	A	40	0	0	1	0
All	All	2849	0	2809	35	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 6.

All (35) 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:635:ARG:HH21	1:A:635:ARG:HG2	1.38	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:ARG:HH21	1:A:635:ARG:CG	1.91	0.84
1:A:779:ASN:HD22	1:A:781:GLY:H	1.28	0.79
1:A:645:ARG:H	1:A:794:GLN:HE22	1.35	0.73
1:A:677:ARG:HD2	1:A:683:GLN:HA	1.75	0.69
1:A:508:ARG:HD2	1:A:509:ARG:HH21	1.58	0.67
1:A:779:ASN:ND2	1:A:781:GLY:H	1.94	0.63
1:A:635:ARG:NH2	1:A:635:ARG:HG2	2.07	0.62
1:A:770:THR:HG23	1:A:793:GLN:NE2	2.16	0.61
1:A:509:ARG:HA	1:A:512:GLU:HG2	1.83	0.60
1:A:703:HIS:HE1	1:A:794:GLN:HE21	1.52	0.57
1:A:725:VAL:H	1:A:770:THR:HB	1.70	0.57
1:A:443:VAL:HG21	1:A:510:ILE:HD11	1.85	0.57
1:A:441:ASN:HD21	1:A:518:SER:H	1.52	0.57
1:A:645:ARG:H	1:A:794:GLN:NE2	2.04	0.54
1:A:770:THR:CG2	1:A:793:GLN:NE2	2.71	0.53
1:A:547:ASP:HB3	1:A:558:LEU:HB3	1.90	0.53
1:A:451:LEU:HD22	2:B:426:LEU:HD21	1.91	0.52
1:A:443:VAL:CG2	1:A:510:ILE:HD11	2.40	0.51
1:A:780:ASP:HA	1:A:782:TRP:CD1	2.48	0.49
1:A:454:SER:HB2	1:A:455:PRO:HD2	1.96	0.47
1:A:718:TYR:C	1:A:720:GLN:H	2.19	0.46
1:A:441:ASN:ND2	1:A:518:SER:H	2.14	0.46
1:A:770:THR:HG22	1:A:771:THR:HG22	1.96	0.45
1:A:554:LEU:HA	3:A:14:HOH:O	2.17	0.45
1:A:466:GLN:HE21	1:A:503:LYS:HD2	1.83	0.44
1:A:522:ARG:HB3	1:A:634:GLU:HG2	2.00	0.43
1:A:739:MET:HG2	1:A:742:ARG:HH22	1.83	0.42
1:A:549:LEU:HD22	1:A:553:LYS:O	2.20	0.42
1:A:520:TYR:HA	1:A:543:PHE:O	2.20	0.42
1:A:479:ILE:HD12	1:A:548:THR:HG21	2.01	0.41
1:A:721:TRP:O	1:A:722:TYR:C	2.59	0.41
1:A:653:ILE:HG22	1:A:653:ILE:O	2.21	0.41
1:A:436:ARG:HG2	2:B:424:SER:O	2.21	0.40
1:A:737:LYS:O	1:A:741:MET:HG2	2.21	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	335/391 (86%)	310 (92%)	21 (6%)	4 (1%)	16 29
2	B	8/12 (67%)	6 (75%)	1 (12%)	1 (12%)	0 0
All	All	343/403 (85%)	316 (92%)	22 (6%)	5 (2%)	13 22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	515	VAL
2	B	422	THR
1	A	586	VAL
1	A	516	GLY
1	A	722	TYR

5.3.2 Protein sidechains (i)

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	292/338 (86%)	271 (93%)	21 (7%)	18 33
2	B	9/11 (82%)	8 (89%)	1 (11%)	8 14
All	All	301/349 (86%)	279 (93%)	22 (7%)	17 32

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	450	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	458	LYS
1	A	468	LEU
1	A	477	ASN
1	A	488	LEU
1	A	505	ASP
1	A	510	ILE
1	A	522	ARG
1	A	539	LYS
1	A	549	LEU
1	A	554	LEU
1	A	578	ASN
1	A	583	LEU
1	A	635	ARG
1	A	691	LEU
1	A	759	HIS
1	A	763	LYS
1	A	770	THR
1	A	771	THR
1	A	775	LEU
1	A	779	ASN
2	B	427	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	441	ASN
1	A	466	GLN
1	A	472	ASN
1	A	477	ASN
1	A	551	ASN
1	A	578	ASN
1	A	587	GLN
1	A	711	ASN
1	A	764	ASN
1	A	774	ASN
1	A	779	ASN
1	A	793	GLN
1	A	794	GLN
1	A	796	GLN
2	B	421	GLN

5.3.3 RNA

There are no RNA molecules 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^{th} 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	341/391 (87%)	0.44	22 (6%) 22 25	32, 53, 81, 99	0
2	B	10/12 (83%)	0.36	0 100 100	56, 67, 104, 124	0
All	All	351/403 (87%)	0.44	22 (6%) 23 26	32, 54, 81, 124	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	588	TYR	4.9
1	A	508	ARG	4.6
1	A	682	ASP	4.1
1	A	509	ARG	4.0
1	A	514	ASP	3.2
1	A	701	ASP	3.2
1	A	533	TYR	3.2
1	A	628	THR	3.1
1	A	683	GLN	3.1
1	A	778	MET	2.8
1	A	587	GLN	2.8
1	A	684	ARG	2.8
1	A	699	ASP	2.6
1	A	640	GLU	2.5
1	A	734	GLN	2.5
1	A	453	ASP	2.4
1	A	629	LYS	2.4
1	A	564	LYS	2.3
1	A	512	GLU	2.2
1	A	565	ASN	2.1
1	A	700	GLN	2.1
1	A	647	VAL	2.1

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.