wwPDB X-ray Structure Validation Summary Report (i)

Sep 23, 2023 – 11:41 PM EDT

PDB ID	:	5TSR
Title	:	Crystal structure of PRL-3 phosphatase in complex with the Bateman domain of CNNM3 magnesium transporter
Authors	:	Kozlov, G.; Zhang, H.; Gehring, K.
Deposited on	:	2016-10-31
Resolution	:	3.19 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

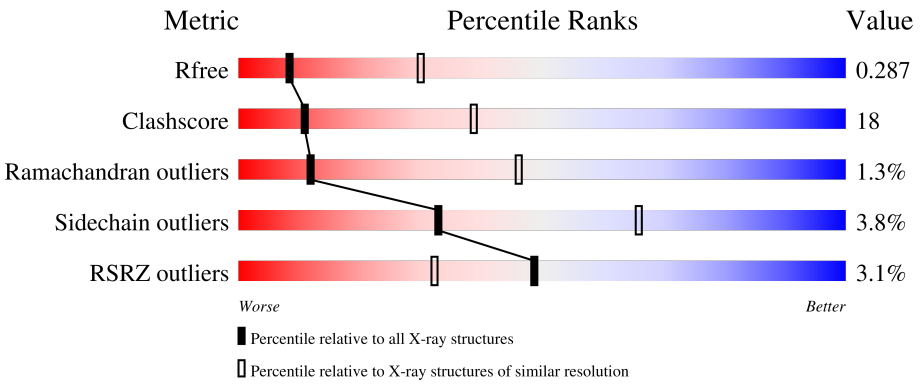
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.19 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	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	172	4% 51% 36% • • 10%
1	C	172	2% 57% 28% • • 10%
2	B	155	3% 68% 25% • •
2	D	155	2% 66% 24% • • 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4767 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 Protein tyrosine phosphatase type IVA 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	155	1216	779	213	219	5	0	0	0
1	C	154	1201	770	208	218	5	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP O75365
A	-1	SER	-	expression tag	UNP O75365
A	0	HIS	-	expression tag	UNP O75365
A	104	ALA	CYS	engineered mutation	UNP O75365
C	-2	GLY	-	expression tag	UNP O75365
C	-1	SER	-	expression tag	UNP O75365
C	0	HIS	-	expression tag	UNP O75365
C	104	ALA	CYS	engineered mutation	UNP O75365

- Molecule 2 is a protein called Metal transporter CNNM3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	149	1180	754	192	227	7	0	0	0
2	D	147	1167	747	190	223	7	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	298	GLY	-	expression tag	UNP Q8NE01
B	299	PRO	-	expression tag	UNP Q8NE01
B	300	LEU	-	expression tag	UNP Q8NE01
B	301	ASN	-	expression tag	UNP Q8NE01

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Chain	Residue	Modelled	Actual	Comment	Reference
B	302	MET	-	expression tag	UNP Q8NE01
B	303	ILE	-	expression tag	UNP Q8NE01
B	304	GLN	-	expression tag	UNP Q8NE01
B	305	GLY	-	expression tag	UNP Q8NE01
B	306	VAL	-	expression tag	UNP Q8NE01
B	307	LEU	-	expression tag	UNP Q8NE01
B	308	GLU	-	expression tag	UNP Q8NE01
D	298	GLY	-	expression tag	UNP Q8NE01
D	299	PRO	-	expression tag	UNP Q8NE01
D	300	LEU	-	expression tag	UNP Q8NE01
D	301	ASN	-	expression tag	UNP Q8NE01
D	302	MET	-	expression tag	UNP Q8NE01
D	303	ILE	-	expression tag	UNP Q8NE01
D	304	GLN	-	expression tag	UNP Q8NE01
D	305	GLY	-	expression tag	UNP Q8NE01
D	306	VAL	-	expression tag	UNP Q8NE01
D	307	LEU	-	expression tag	UNP Q8NE01
D	308	GLU	-	expression tag	UNP Q8NE01

- Molecule 3 is water.

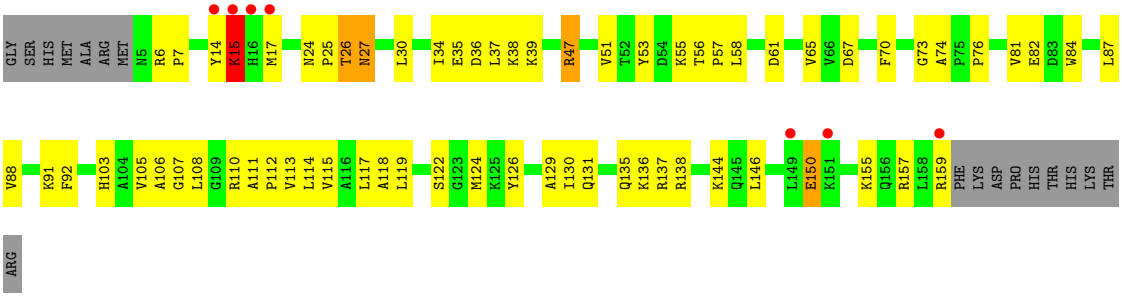
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	1	1	1	0	0
			Total	O		
3	C	1	1	1	0	0
			Total	O		
3	D	1	1	1	0	0

3 Residue-property plots (i)

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.

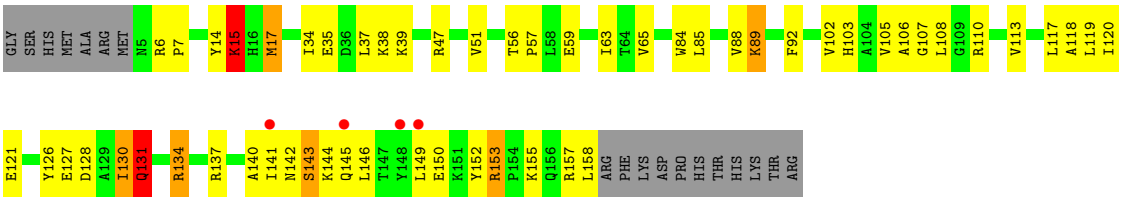
• Molecule 1: Protein tyrosine phosphatase type IVA 3

Chain A:



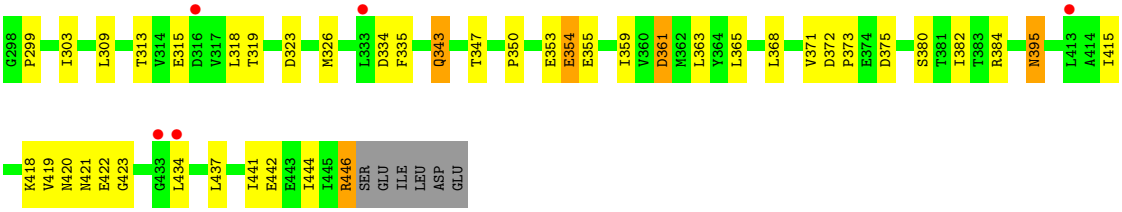
• Molecule 1: Protein tyrosine phosphatase type IVA 3

Chain C:



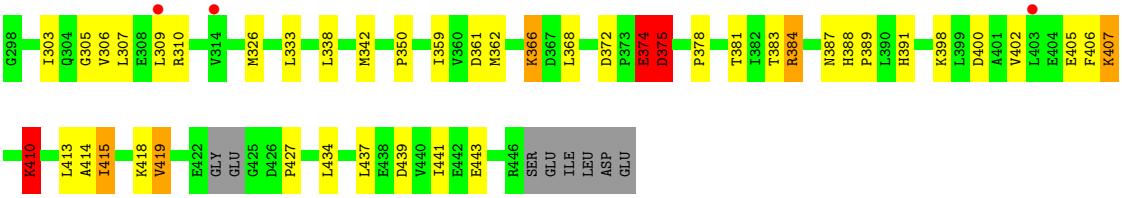
• Molecule 2: Metal transporter CNNM3

Chain B:



• Molecule 2: Metal transporter CNNM3

Chain D:


G298
I303
Q304
G305
V306
L307
E308
L309
R310
V314
M326
L333
L338
M342
P350
I359
V360
D361
M362
K366
D367
L368
D372
P373
E374
D375
P378
T381
I382
T383
R384
N387
H388
P389
L390
H391
K398
L399
D400
A401
V402
L403
E404
E405
F406
K407
K410
L413
A414
I415
K418
V419
E422
GLY
GLU
G425
D426
P427
L434
L437
E438
D439
V440
I441
E442
E443
R446
SER
GLU
ILE
LEU
ASP
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	155.34Å 125.15Å 52.04Å 90.00° 102.21° 90.00°	Depositor
Resolution (Å)	27.74 – 3.19 48.28 – 3.19	Depositor EDS
% Data completeness (in resolution range)	95.9 (27.74-3.19) 96.0 (48.28-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.239 , 0.287 0.240 , 0.287	Depositor DCC
R_{free} test set	806 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å^2)	111.9	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 78.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4767	wwPDB-VP
Average B, all atoms (Å^2)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.46	1/1244 (0.1%)	0.81	2/1690 (0.1%)
1	C	0.43	0/1229	0.77	2/1672 (0.1%)
2	B	0.36	0/1202	0.75	1/1633 (0.1%)
2	D	0.42	0/1188	0.78	3/1613 (0.2%)
All	All	0.42	1/4863 (0.0%)	0.78	8/6608 (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	C	0	2
2	D	0	2
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	GLU	CB-CG	-5.24	1.42	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	375	ASP	CB-CG-OD1	7.14	124.73	118.30
1	C	131	GLN	CA-CB-CG	7.02	128.84	113.40
2	D	307	LEU	CA-CB-CG	6.89	131.16	115.30
1	A	26	THR	N-CA-C	-6.25	94.11	111.00
1	A	15	LYS	CA-CB-CG	6.01	126.63	113.40

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	LYS	Peptide
1	A	27	ASN	Peptide
1	C	130	ILE	Peptide
1	C	15	LYS	Peptide
2	D	374	GLU	Peptide

5.2 Too-close contacts (i)

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	1216	0	1240	57	0
1	C	1201	0	1216	49	0
2	B	1180	0	1166	34	0
2	D	1167	0	1156	41	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	4767	0	4778	174	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 18.

The worst 5 of 174 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:130:ILE:HD11	1:A:146:LEU:HD21	1.32	1.10
1:C:134:ARG:HH12	1:C:141:ILE:H	1.17	0.90
1:A:124:MET:HE2	1:A:129:ALA:HA	1.57	0.87
1:A:15:LYS:HG2	1:A:17:MET:HG2	1.58	0.85
1:C:121:GLU:OE2	1:C:152:TYR:OH	1.98	0.81

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	153/172 (89%)	142 (93%)	11 (7%)	0	100	100
1	C	152/172 (88%)	140 (92%)	9 (6%)	3 (2%)	7	35
2	B	147/155 (95%)	135 (92%)	10 (7%)	2 (1%)	11	44
2	D	143/155 (92%)	133 (93%)	7 (5%)	3 (2%)	7	34
All	All	595/654 (91%)	550 (92%)	37 (6%)	8 (1%)	12	46

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	131	GLN
1	C	143	SER
2	D	374	GLU
2	D	410	LYS
2	B	375	ASP

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	131/147 (89%)	128 (98%)	3 (2%)	50	77
1	C	129/147 (88%)	123 (95%)	6 (5%)	26	60
2	B	134/142 (94%)	130 (97%)	4 (3%)	41	72
2	D	133/142 (94%)	126 (95%)	7 (5%)	22	56
All	All	527/578 (91%)	507 (96%)	20 (4%)	33	66

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	375	ASP
2	D	410	LYS
2	D	419	VAL
2	D	415	ILE
2	B	442	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	C	135	GLN
2	D	391	HIS

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	155/172 (90%)	0.36	7 (4%)	33	20	79, 112, 153, 171	0
1	C	154/172 (89%)	0.22	4 (2%)	56	40	71, 111, 145, 155	0
2	B	149/155 (96%)	0.31	5 (3%)	45	29	84, 109, 134, 146	0
2	D	147/155 (94%)	0.29	3 (2%)	65	50	81, 108, 133, 156	0
All	All	605/654 (92%)	0.29	19 (3%)	49	32	71, 110, 144, 171	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	16	HIS	5.2
1	C	145	GLN	3.4
1	A	14	TYR	2.9
2	D	403	LEU	2.8
1	C	141	ILE	2.8

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.