Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:38 PM GMT

PDB ID	:	1L8G
Title	:	Crystal structure of PTP1B complexed with 7-(1,1-Dioxo-1H-benzo[d]isothiazol-3-yloxymethyl)-2-(oxalyl-amino)-4,7-dihydro-5H-thieno[2,3-c]pyran-3-carboxylic acid
Authors	:	Iversen, L.F.; Andersen, H.S.; Moller, K.B.; Olsen, O.H.; Peters, G.H.; Branner, S.; Mortensen, S.B.; Hansen, T.K.; Lau, J.; Ge, Y.; Holsworth, D.D.; Newman, M.J.; Moller, N.P.H.
Deposited on	:	2002-03-20
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 (i) symbol.

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

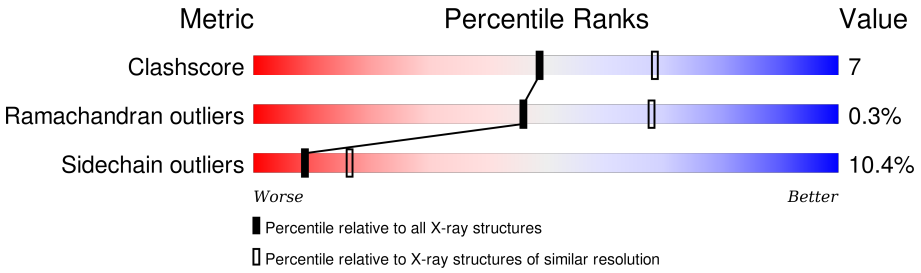
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	321	67% 18% 7% • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2593 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.

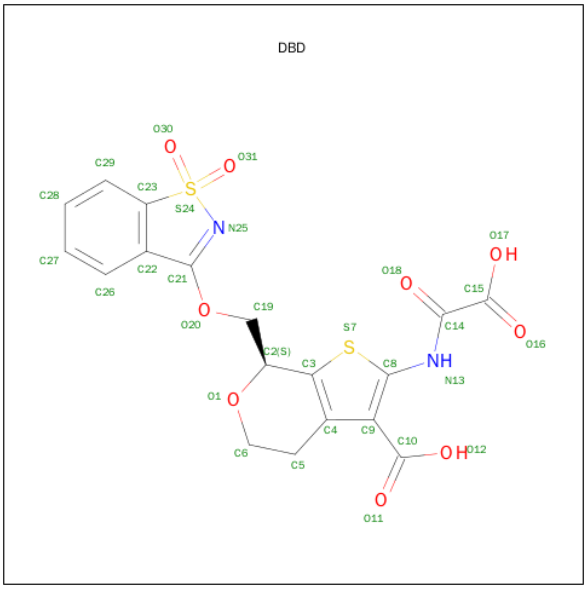
- Molecule 1 is a protein called PROTEIN-TYROSINE PHOSPHATASE, NON-RECEPTOR TYPE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	297	2426	1535	418	457	16	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	THR	SER	CONFLICT	UNP P18031
A	252	ASP	GLU	CONFLICT	UNP P18031

- Molecule 2 is 7-(1,1-DIOXO-1H-BENZO[D]ISOTHIAZOL-3-YLOXYMETHYL)-2-(OXALYL-AMINO)-4,7-DIHYDRO-5H-THIENO[2,3-C]PYRAN-3-CARBOXYLIC ACID (three-letter code: DBD) (formula: $C_{18}H_{14}N_2O_9S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	31	18	2	9	2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	136	Total O 136 136	0	0

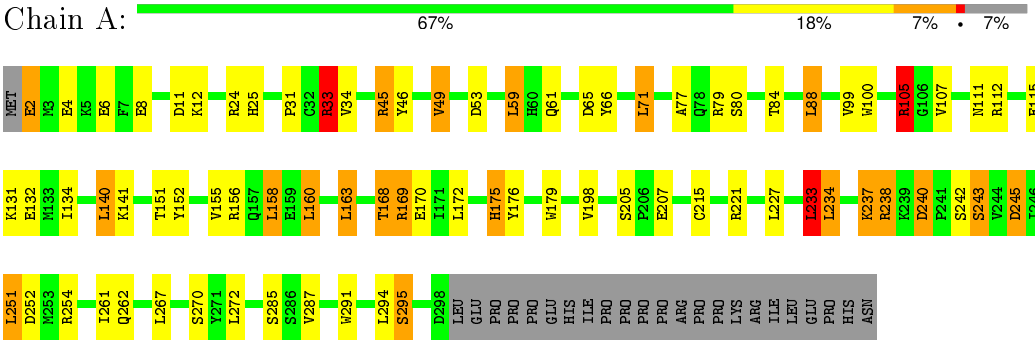
3 Residue-property plots (i)

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.

Note EDS was not executed.

- Molecule 1: PROTEIN-TYROSINE PHOSPHATASE, NON-RECEPTOR TYPE 1

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	88.26Å 88.26Å 103.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.189 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2593	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DBD

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	1.08	8/2481 (0.3%)	1.48	33/3345 (1.0%)

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	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	GLU	CD-OE1	-7.32	1.17	1.25
1	A	242	SER	CB-OG	6.87	1.51	1.42
1	A	243	SER	CB-OG	6.28	1.50	1.42
1	A	205	SER	CB-OG	6.07	1.50	1.42
1	A	45	ARG	CZ-NH2	-5.63	1.25	1.33
1	A	237	LYS	CB-CG	5.35	1.67	1.52
1	A	285	SER	CB-OG	5.04	1.48	1.42
1	A	240	ASP	C-O	-5.02	1.13	1.23

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	152	TYR	CB-CG-CD2	7.81	125.68	121.00
1	A	243	SER	N-CA-CB	-7.64	99.05	110.50
1	A	169	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	A	168	THR	CA-CB-OG1	7.01	123.73	109.00
1	A	45	ARG	NE-CZ-NH1	6.56	123.58	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	198	VAL	CA-CB-CG2	6.06	120.00	110.90
1	A	160	LEU	CB-CG-CD2	6.02	121.23	111.00
1	A	33	ARG	NE-CZ-NH1	-5.99	117.31	120.30
1	A	84	THR	CA-CB-OG1	5.98	121.56	109.00
1	A	49	VAL	CG1-CB-CG2	5.91	120.36	110.90
1	A	243	SER	CB-CA-C	-5.90	98.90	110.10
1	A	79	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	151	THR	CB-CA-C	-5.85	95.80	111.60
1	A	107	VAL	CA-CB-CG2	5.72	119.48	110.90
1	A	163	LEU	CB-CG-CD1	5.68	120.65	111.00
1	A	249	VAL	CA-CB-CG1	5.66	119.38	110.90
1	A	158	LEU	CB-CG-CD1	5.63	120.57	111.00
1	A	238	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	152	TYR	CB-CG-CD1	-5.54	117.68	121.00
1	A	233	LEU	CB-CG-CD2	5.45	120.26	111.00
1	A	88	LEU	CB-CG-CD1	5.44	120.25	111.00
1	A	49	VAL	CA-CB-CG1	5.42	119.04	110.90
1	A	245	ASP	N-CA-CB	-5.38	100.91	110.60
1	A	25	HIS	CA-CB-CG	-5.37	104.48	113.60
1	A	249	VAL	CG1-CB-CG2	5.26	119.32	110.90
1	A	169	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	295	SER	N-CA-CB	-5.19	102.72	110.50
1	A	99	VAL	CA-CB-CG2	5.17	118.65	110.90
1	A	155	VAL	CA-CB-CG2	5.16	118.63	110.90
1	A	140	LEU	CB-CG-CD1	5.07	119.62	111.00
1	A	71	LEU	CB-CG-CD2	5.06	119.60	111.00
1	A	251	LEU	CB-CG-CD1	5.06	119.60	111.00
1	A	234	LEU	CB-CG-CD1	5.06	119.60	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ARG	Sidechain
1	A	221	ARG	Sidechain
1	A	66	TYR	Sidechain

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	2426	0	2381	35	0
2	A	31	0	12	0	0
3	A	136	0	0	0	0
All	All	2593	0	2393	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 7.

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:112:ARG:HH11	1:A:112:ARG:HG3	1.56	0.71
1:A:112:ARG:HH11	1:A:112:ARG:CG	2.16	0.57
1:A:8:GLU:O	1:A:12:LYS:HG3	2.07	0.54
1:A:2:GLU:HG3	1:A:4:GLU:H	1.72	0.54
1:A:227:LEU:CD1	1:A:249:VAL:HG22	2.38	0.54
1:A:134:ILE:HG13	1:A:141:LYS:HG3	1.90	0.53
1:A:105:ARG:HG2	1:A:105:ARG:HH11	1.74	0.53
1:A:31:PRO:HB2	1:A:33:ARG:NE	2.25	0.52
1:A:176:TYR:CE1	1:A:179:TRP:HB2	2.46	0.51
1:A:238:ARG:HG3	1:A:240:ASP:H	1.76	0.50
1:A:238:ARG:HD2	1:A:243:SER:OG	2.13	0.49
1:A:77:ALA:HB1	1:A:233:LEU:HD13	1.94	0.48
1:A:100:TRP:CZ3	1:A:169:ARG:HG3	2.49	0.48
1:A:245:ASP:O	1:A:249:VAL:HG13	2.14	0.47
1:A:33:ARG:HB2	1:A:33:ARG:HE	1.62	0.46
1:A:111:ASN:HD22	1:A:215:CYS:HA	1.81	0.46
1:A:45:ARG:NH2	1:A:121:CYS:HA	2.31	0.45
1:A:112:ARG:NH1	1:A:112:ARG:CG	2.78	0.45
1:A:6:GLU:OE2	1:A:247:LYS:NZ	2.46	0.45
1:A:46:TYR:HB2	1:A:49:VAL:HG13	1.99	0.44
1:A:227:LEU:HD12	1:A:249:VAL:HG22	2.00	0.44
1:A:59:LEU:HB2	1:A:65:ASP:HA	1.99	0.42
1:A:156:ARG:HH12	1:A:175:HIS:HD2	1.68	0.42
1:A:31:PRO:CB	1:A:33:ARG:HD3	2.50	0.42
1:A:59:LEU:HB3	1:A:61:GLN:HG2	2.01	0.42
1:A:24:ARG:NH2	1:A:262:GLN:O	2.53	0.42
1:A:31:PRO:HB3	1:A:33:ARG:HD3	2.02	0.42
1:A:267:LEU:O	1:A:270:SER:HB2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ARG:H	1:A:238:ARG:HG2	1.67	0.41
1:A:291:TRP:O	1:A:295:SER:HB3	2.20	0.41
1:A:34:VAL:HG13	1:A:53:ASP:OD1	2.20	0.41
1:A:156:ARG:HH12	1:A:175:HIS:CD2	2.39	0.41
1:A:176:TYR:CD1	1:A:179:TRP:HB2	2.56	0.41
1:A:115:GLU:HB2	1:A:120:LYS:HG3	2.02	0.41
1:A:2:GLU:HA	1:A:2:GLU:OE2	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	295/321 (92%)	282 (96%)	12 (4%)	1 (0%)	46 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	ILE

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	270/294 (92%)	242 (90%)	28 (10%)	9 16

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	11	ASP
1	A	33	ARG
1	A	59	LEU
1	A	71	LEU
1	A	80	SER
1	A	88	LEU
1	A	105	ARG
1	A	131	LYS
1	A	132	GLU
1	A	140	LEU
1	A	158	LEU
1	A	160	LEU
1	A	163	LEU
1	A	168	THR
1	A	172	LEU
1	A	175	HIS
1	A	207	GLU
1	A	233	LEU
1	A	234	LEU
1	A	237	LYS
1	A	249	VAL
1	A	251	LEU
1	A	252	ASP
1	A	254	ARG
1	A	272	LEU
1	A	287	VAL
1	A	294	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	21	GLN
1	A	85	GLN
1	A	111	ASN
1	A	175	HIS

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

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	DBD	A	322	-	25,34,34	2.02	7 (28%)	21,51,51	5.41	9 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DBD	A	322	-	-	0/7/42/42	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	322	DBD	C23-S24	-4.69	1.72	1.76
2	A	322	DBD	C9-C8	-3.07	1.34	1.41
2	A	322	DBD	O30-S24	-2.62	1.40	1.44
2	A	322	DBD	C19-C2	-2.56	1.49	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	322	DBD	C29-C23	3.28	1.42	1.39
2	A	322	DBD	O20-C21	3.32	1.40	1.34
2	A	322	DBD	C9-C4	3.42	1.47	1.42

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	322	DBD	C23-S24-N25	-15.07	87.31	96.76
2	A	322	DBD	C29-C23-C22	-7.66	116.40	122.74
2	A	322	DBD	C6-C5-C4	-4.41	103.66	110.62
2	A	322	DBD	C22-C21-N25	-4.32	106.37	115.48
2	A	322	DBD	O20-C21-N25	3.97	132.02	124.07
2	A	322	DBD	O31-S24-O30	4.28	122.26	115.99
2	A	322	DBD	C26-C22-C23	4.54	123.82	119.98
2	A	322	DBD	C21-N25-S24	9.41	121.82	110.16
2	A	322	DBD	C22-C23-S24	11.63	114.35	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.