WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Oct 30, 2017 – 06:47 PM EDT

PDB ID : 3QYW
Title : Crystal structure of ERK2 in complex with an inhibitor
Authors : Gelin, M.; Pochet, S.; Hoh, F.; Pirochi, M.; Guichou, J.-F.; Ferrer, J.-L.;
Labesse, G.
Deposited on : unknown
Resolution : 1.50 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
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 : **FAILED**
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
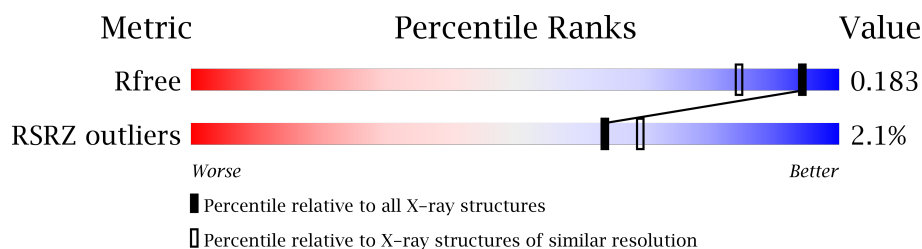Validation Pipeline (wwPDB-VP) : rb-20030345

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 1.50 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	Percentile Ranks	Value
Rfree		0.183
RSRZ outliers		2.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2279 (1.50-1.50)
RSRZ outliers	101464	2305 (1.50-1.50)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DMS	A	360	-	-	-	X
3	DMS	A	361	-	-	-	X
3	DMS	A	362	-	-	-	X
3	DMS	A	363	-	-	-	X
3	DMS	A	364	-	-	-	X
3	DMS	A	366	-	-	-	X
3	DMS	A	367	-	-	-	X
3	DMS	A	368	-	-	-	X
3	DMS	A	369	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3385 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 Mitogen-activated protein kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	341	2866	1849	484	516	17	1	24	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP P63086
A	-4	HIS	-	EXPRESSION TAG	UNP P63086
A	-3	HIS	-	EXPRESSION TAG	UNP P63086
A	-2	HIS	-	EXPRESSION TAG	UNP P63086
A	-1	HIS	-	EXPRESSION TAG	UNP P63086
A	0	HIS	-	EXPRESSION TAG	UNP P63086

- Molecule 2 is 6-(3-bromophenyl)-7H-purin-2-amine (three-letter code: 6PB) (formula: $C_{11}H_8BrN_5$).
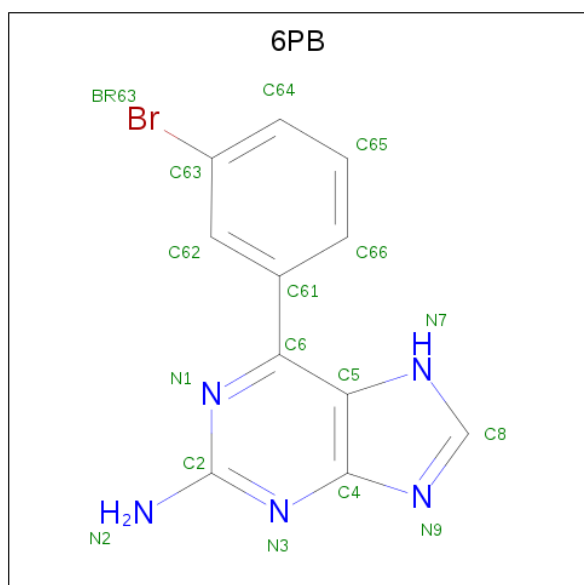
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	Br	C	N	0	0
			17	1	11	5		

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).
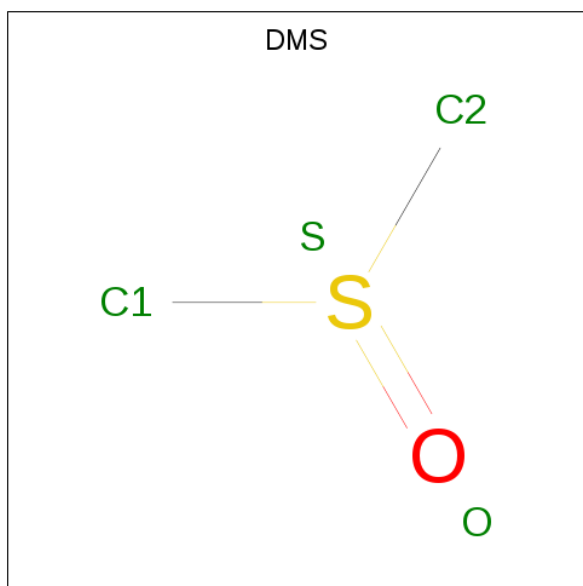
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	O 4	S 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	450	Total 457	O 457	0	7

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	49.07Å 70.25Å 60.17Å 90.00° 108.72° 90.00°	Depositor
Resolution (Å)	36.98 – 1.50 36.98 – 1.50	Depositor EDS
% Data completeness (in resolution range)	69.5 (36.98-1.50) 91.2 (36.98-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.71 (at 1.50Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.148 , 0.188 0.145 , 0.183	Depositor DCC
R_{free} test set	2818 reflections (4.99%)	DCC
Wilson B-factor (Å^2)	13.5	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 57.0	EDS
L-test for twinning [2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3385	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.99% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

1 non-standard protein/DNA/RNA residue 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	#$|Z| > 2$
1	CME	A	159	1	9,9,10	0.87	1 (11%)	6,9,11	1.33	0

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
1	CME	A	159	1	-	0/5/8/10	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	CME	CA-C	2.06	1.53	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates (i)

There are no carbohydrates in this entry.

4.6 Ligand geometry (i)

12 ligands are 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	6PB	A	359	-	16,19,19	1.51	2 (12%)	17,27,27	1.93	4 (23%)
3	DMS	A	360	-	3,3,3	2.60	1 (33%)	3,3,3	0.41	0
3	DMS	A	361	-	3,3,3	2.62	1 (33%)	3,3,3	0.45	0
3	DMS	A	362	-	3,3,3	2.50	1 (33%)	3,3,3	0.43	0
3	DMS	A	363	-	3,3,3	2.56	1 (33%)	3,3,3	0.39	0
3	DMS	A	364	-	3,3,3	2.12	1 (33%)	3,3,3	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	DMS	A	365	-	3,3,3	2.24	1 (33%)	3,3,3	0.41	0
3	DMS	A	366	-	3,3,3	2.60	1 (33%)	3,3,3	0.28	0
3	DMS	A	367	-	3,3,3	2.62	1 (33%)	3,3,3	0.46	0
3	DMS	A	368	-	3,3,3	2.60	1 (33%)	3,3,3	0.60	0
3	DMS	A	369	-	3,3,3	2.54	1 (33%)	3,3,3	0.54	0
4	SO4	A	370	-	4,4,4	0.08	0	6,6,6	0.17	0

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	6PB	A	359	-	-	0/4/4/4	0/3/3/3
3	DMS	A	360	-	-	0/0/0/0	0/0/0/0
3	DMS	A	361	-	-	0/0/0/0	0/0/0/0
3	DMS	A	362	-	-	0/0/0/0	0/0/0/0
3	DMS	A	363	-	-	0/0/0/0	0/0/0/0
3	DMS	A	364	-	-	0/0/0/0	0/0/0/0
3	DMS	A	365	-	-	0/0/0/0	0/0/0/0
3	DMS	A	366	-	-	0/0/0/0	0/0/0/0
3	DMS	A	367	-	-	0/0/0/0	0/0/0/0
3	DMS	A	368	-	-	0/0/0/0	0/0/0/0
3	DMS	A	369	-	-	0/0/0/0	0/0/0/0
4	SO4	A	370	-	-	0/0/0/0	0/0/0/0

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	359	6PB	C6-N1	2.74	1.35	1.32
3	A	364	DMS	O-S	3.45	1.73	1.50
3	A	365	DMS	O-S	3.71	1.75	1.50
3	A	362	DMS	O-S	4.18	1.78	1.50
3	A	369	DMS	O-S	4.25	1.79	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	359	6PB	N3-C2-N1	-4.73	120.56	127.46
2	A	359	6PB	C4-C5-N7	-2.69	106.81	109.41
2	A	359	6PB	C61-C6-N1	3.33	118.59	115.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	359	6PB	C2-N3-C4	3.88	119.69	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 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(Å²)	Q<0.9
1	A	340/364 (93%)	-0.22	7 (2%)	64	69	7, 15, 30, 37	51 (15%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	GLY	4.3
1	A	329	PHE	3.4
1	A	44	LEU	2.9
1	A	336	LEU	2.7
1	A	41	TYR	2.4

5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
1	CME	A	159	10/11	0.99	0.05	-	10,14,15,17	0

5.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
3	DMS	A	368	4/4	0.80	0.27	17.09	20,21,33,40	4
3	DMS	A	360	4/4	0.91	0.21	11.67	50,50,51,52	4
3	DMS	A	364	4/4	0.89	0.23	9.61	5,9,10,11	4
3	DMS	A	363	4/4	0.95	0.12	7.06	31,31,33,33	4
3	DMS	A	367	4/4	0.92	0.13	6.67	27,49,59,65	0
3	DMS	A	369	4/4	0.92	0.16	4.05	14,32,40,53	4
3	DMS	A	366	4/4	0.81	0.21	4.02	34,34,49,51	4
3	DMS	A	362	4/4	0.96	0.20	3.80	20,21,21,22	4
3	DMS	A	361	4/4	0.92	0.12	3.28	60,60,60,61	0
2	6PB	A	359	17/17	0.99	0.06	-1.01	15,18,19,20	1
4	SO4	A	370	5/5	0.98	0.08	-	14,17,21,21	5
3	DMS	A	365	4/4	0.93	0.14	-	10,11,23,28	4

5.5 Other polymers (i)

There are no such residues in this entry.