



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2018 – 07:38 AM EDT

PDB ID : 5WJ6
Title : Crystal structure of glutaminase C in complex with inhibitor 2-phenyl-N-{5-[4-({5-[(phenylacetyl)amino]-1,3,4-thiadiazol-2-yl}amino)piperidin-1-yl]-1,3,4-thiadiazol-2-yl}acetamide (UPGL-00004)
Authors : Huang, Q.; Cerione, R.A.
Deposited on : 2017-07-21
Resolution : 2.44 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
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-20030736

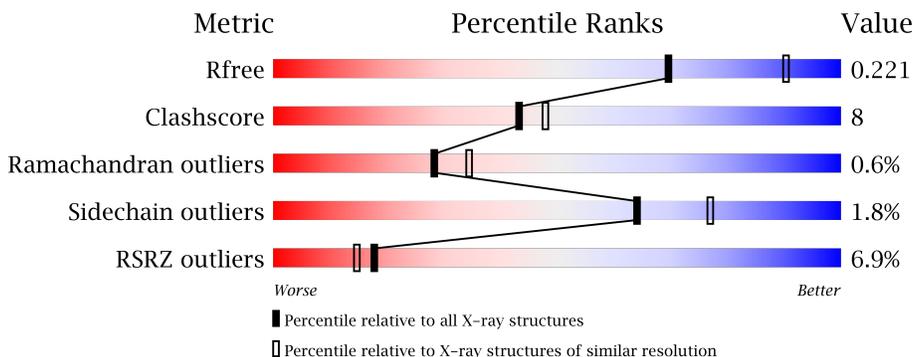
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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}	100719	1152 (2.46-2.42)
Clashscore	112137	1224 (2.46-2.42)
Ramachandran outliers	110173	1217 (2.46-2.42)
Sidechain outliers	110143	1217 (2.46-2.42)
RSRZ outliers	101464	1158 (2.46-2.42)

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 $\leq 5\%$. 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	539	 5% 65% 11% • 24%
1	C	539	 6% 63% 12% • 24%
1	D	539	 6% 65% 10% • 24%
2	B	539	 5% 64% 11% • 24%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 13503 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 Glutaminase kidney isoform, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	410	3194	2036	540	590	28	1	0	0
1	C	410	3197	2037	540	592	28	1	0	0
1	D	410	3195	2035	540	592	28	2	0	0

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	MET	-	expression tag	UNP O94925
A	61	ARG	-	expression tag	UNP O94925
A	62	GLY	-	expression tag	UNP O94925
A	63	SER	-	expression tag	UNP O94925
A	64	HIS	-	expression tag	UNP O94925
A	65	HIS	-	expression tag	UNP O94925
A	66	HIS	-	expression tag	UNP O94925
A	67	HIS	-	expression tag	UNP O94925
A	68	HIS	-	expression tag	UNP O94925
A	69	HIS	-	expression tag	UNP O94925
A	70	GLY	-	expression tag	UNP O94925
A	71	SER	-	expression tag	UNP O94925
A	268	ALA	VAL	conflict	UNP O94925
C	60	MET	-	expression tag	UNP O94925
C	61	ARG	-	expression tag	UNP O94925
C	62	GLY	-	expression tag	UNP O94925
C	63	SER	-	expression tag	UNP O94925
C	64	HIS	-	expression tag	UNP O94925
C	65	HIS	-	expression tag	UNP O94925
C	66	HIS	-	expression tag	UNP O94925
C	67	HIS	-	expression tag	UNP O94925
C	68	HIS	-	expression tag	UNP O94925
C	69	HIS	-	expression tag	UNP O94925

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Chain	Residue	Modelled	Actual	Comment	Reference
C	70	GLY	-	expression tag	UNP O94925
C	71	SER	-	expression tag	UNP O94925
C	268	ALA	VAL	conflict	UNP O94925
D	60	MET	-	expression tag	UNP O94925
D	61	ARG	-	expression tag	UNP O94925
D	62	GLY	-	expression tag	UNP O94925
D	63	SER	-	expression tag	UNP O94925
D	64	HIS	-	expression tag	UNP O94925
D	65	HIS	-	expression tag	UNP O94925
D	66	HIS	-	expression tag	UNP O94925
D	67	HIS	-	expression tag	UNP O94925
D	68	HIS	-	expression tag	UNP O94925
D	69	HIS	-	expression tag	UNP O94925
D	70	GLY	-	expression tag	UNP O94925
D	71	SER	-	expression tag	UNP O94925
D	268	ALA	VAL	conflict	UNP O94925

- Molecule 2 is a protein called Glutaminase kidney isoform, mitochondrial.

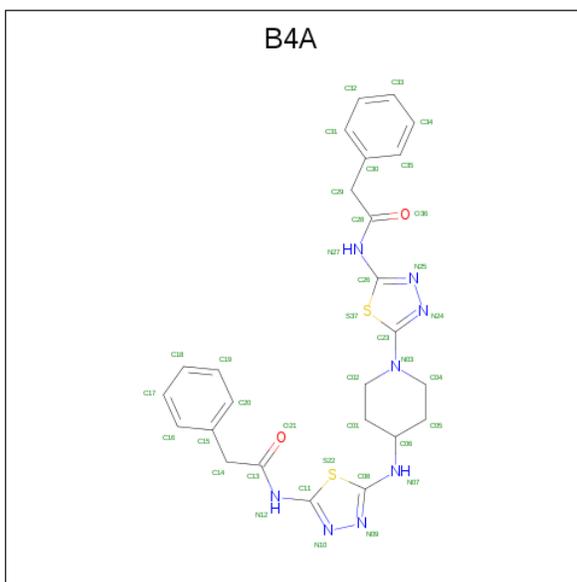
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	410	3193	2035	540	590	28	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	60	MET	-	expression tag	UNP O94925
B	61	ARG	-	expression tag	UNP O94925
B	62	GLY	-	expression tag	UNP O94925
B	63	SER	-	expression tag	UNP O94925
B	64	HIS	-	expression tag	UNP O94925
B	65	HIS	-	expression tag	UNP O94925
B	66	HIS	-	expression tag	UNP O94925
B	67	HIS	-	expression tag	UNP O94925
B	68	HIS	-	expression tag	UNP O94925
B	69	HIS	-	expression tag	UNP O94925
B	70	GLY	-	expression tag	UNP O94925
B	71	SER	-	expression tag	UNP O94925
B	205	ASN	GLN	conflict	UNP O94925
B	268	ALA	VAL	conflict	UNP O94925

- Molecule 3 is 2-phenyl-N-{5-[4-({5-[(phenylacetyl)amino]-1,3,4-thiadiazol-2-yl)amino]piperi

din-1-yl]-1,3,4-thiadiazol-2-yl}acetamide (three-letter code: B4A) (formula: C₂₅H₂₆N₈O₂S₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	N	O	S	0	0
			37	25	8	2	2		
3	C	1	Total	C	N	O	S	0	0
			37	25	8	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	138	Total	O	0	0
			138	138		
4	B	161	Total	O	0	0
			161	161		
4	C	171	Total	O	0	0
			171	171		
4	D	180	Total	O	0	0
			180	180		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.65Å 138.01Å 175.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.05 – 2.44 48.83 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.05-2.44) 99.4 (48.83-2.45)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.45Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.180 , 0.223 0.175 , 0.221	Depositor DCC
R_{free} test set	2002 reflections (2.28%)	DCC
Wilson B-factor (Å ²)	37.7	Xtrriage
Anisotropy	0.116	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13503	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.12 % 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 5.8677e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: B4A

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	0.44	0/3266	0.63	1/4408 (0.0%)
1	C	0.45	0/3269	0.60	0/4412
1	D	0.46	0/3267	0.61	0/4409
2	B	0.47	0/3265	0.61	1/4407 (0.0%)
All	All	0.45	0/13067	0.61	2/17636 (0.0%)

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	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	383	GLU	N-CA-CB	-5.36	100.95	110.60
2	B	540	LEU	CA-CB-CG	5.11	127.06	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	317	ARG	Peptide
1	C	317	ARG	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	3194	0	3170	36	0
1	C	3197	0	3172	52	0
1	D	3195	0	3165	73	0
2	B	3193	0	3168	69	0
3	A	37	0	0	0	0
3	C	37	0	0	1	0
4	A	138	0	0	2	0
4	B	161	0	0	3	0
4	C	171	0	0	4	0
4	D	180	0	0	6	0
All	All	13503	0	12675	196	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 8.

The worst 5 of 196 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:529:ASN:ND2	1:C:529:ASN:OD1	1.81	1.13
1:D:153:LYS:HE2	1:D:196:ASP:HB3	1.46	0.97
1:D:152:GLU:OE1	1:D:153:LYS:HG3	1.69	0.92
1:D:152:GLU:CD	1:D:153:LYS:HG3	1.91	0.89
2:B:317:ARG:CB	1:D:318:PHE:HE2	1.86	0.87

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	408/539 (76%)	399 (98%)	8 (2%)	1 (0%)	51	62
1	C	408/539 (76%)	399 (98%)	7 (2%)	2 (0%)	32	39
1	D	408/539 (76%)	381 (93%)	21 (5%)	6 (2%)	12	11
2	B	408/539 (76%)	400 (98%)	7 (2%)	1 (0%)	51	62
All	All	1632/2156 (76%)	1579 (97%)	43 (3%)	10 (1%)	28	34

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	191	ASP
1	D	191	ASP
1	D	316	LEU
1	D	319	ASN
1	C	191	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	353/461 (77%)	346 (98%)	7 (2%)	60	74
1	C	354/461 (77%)	351 (99%)	3 (1%)	85	90
1	D	353/461 (77%)	346 (98%)	7 (2%)	60	74
2	B	353/461 (77%)	345 (98%)	8 (2%)	56	70
All	All	1413/1844 (77%)	1388 (98%)	25 (2%)	64	77

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	259	ASP
2	B	361	PHE
1	D	361	PHE
2	B	317	ARG

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Mol	Chain	Res	Type
2	B	538	LYS

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

Mol	Chain	Res	Type
1	C	347	GLN
1	C	494	ASN
1	D	494	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
3	B4A	A	601	-	32,41,41	2.03	7 (21%)	33,55,55	2.38	9 (27%)
3	B4A	C	601	-	32,41,41	1.93	9 (28%)	33,55,55	2.50	9 (27%)

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
3	B4A	A	601	-	-	0/16/34/34	0/3/5/5
3	B4A	C	601	-	-	0/16/34/34	0/3/5/5

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	B4A	N24-N25	-2.08	1.33	1.37
3	A	601	B4A	C06-N07	-2.06	1.41	1.46
3	C	601	B4A	C01-C06	-2.03	1.46	1.51
3	C	601	B4A	C33-C34	2.04	1.43	1.38
3	A	601	B4A	C14-C13	2.16	1.56	1.51

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	B4A	C08-N07-C06	-10.24	105.34	124.10
3	A	601	B4A	C08-N07-C06	-9.58	106.53	124.10
3	C	601	B4A	C04-C05-C06	-4.33	102.55	110.41
3	A	601	B4A	C05-C06-N07	-4.31	103.17	110.55
3	A	601	B4A	C29-C30-C35	-3.80	115.41	120.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	B4A	1	0

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	410/539 (76%)	0.08	27 (6%) 19 16	24, 34, 77, 134	0
1	C	410/539 (76%)	0.04	30 (7%) 16 13	23, 33, 78, 134	1 (0%)
1	D	410/539 (76%)	0.18	31 (7%) 15 12	23, 35, 90, 170	2 (0%)
2	B	410/539 (76%)	0.15	25 (6%) 22 18	22, 34, 81, 153	0
All	All	1640/2156 (76%)	0.11	113 (6%) 18 15	22, 34, 81, 170	3 (0%)

The worst 5 of 113 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	318	PHE	8.1
1	D	546	GLY	7.8
1	C	546	GLY	7.4
1	D	192	GLY	6.9
1	A	137	PRO	6.9

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 carbohydrates in this entry.

6.4 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(\AA^2)	Q<0.9
3	B4A	A	601	37/37	0.95	0.19	-0.24	40,46,89,91	0
3	B4A	C	601	37/37	0.94	0.16	-0.52	38,47,60,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.