



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:22 AM GMT

PDB ID : 2QGX  
Title : Ubiquitin-conjugating enzyme E2Q  
Authors : Neculai, D.; Avvakumov, G.V.; Xue, S.; Walker, J.R.; Mackenzie, F.; Weigelt, J.; Sundstrom, M.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Sicheri, F.; Dhe-Paganon, S.; Structural Genomics Consortium (SGC)  
Deposited on : 2007-06-29  
Resolution : 2.56 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](mailto: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.

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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) : **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

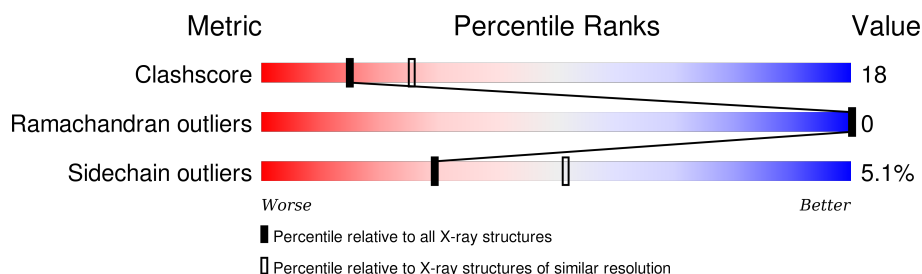
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.56 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	3729 (2.60-2.52)
Ramachandran outliers	100387	3673 (2.60-2.52)
Sidechain outliers	100360	3673 (2.60-2.52)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	169	
1	B	169	
1	C	169	
1	D	169	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5132 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 Ubiquitin-conjugating enzyme E2 Q1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	1	0
			1238	793	210	231	4			
1	B	161	Total	C	N	O	S	0	0	0
			1265	809	213	239	4			
1	C	161	Total	C	N	O	S	0	1	0
			1282	819	219	240	4			
1	D	160	Total	C	N	O	S	0	0	0
			1257	803	212	238	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q7Z7E8
B	-1	GLY	-	EXPRESSION TAG	UNP Q7Z7E8
C	-1	GLY	-	EXPRESSION TAG	UNP Q7Z7E8
D	-1	GLY	-	EXPRESSION TAG	UNP Q7Z7E8

- Molecule 2 is water.

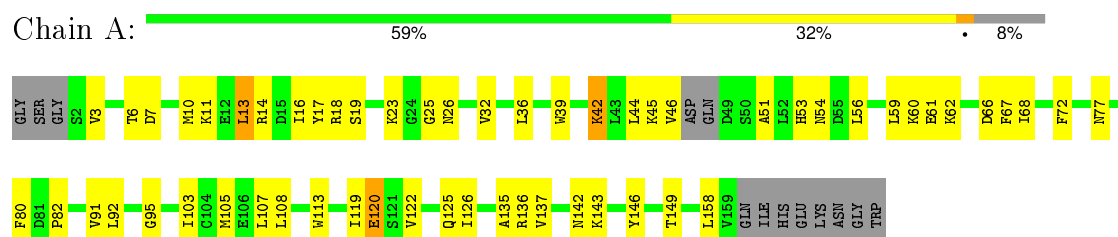
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	20	Total	O	0	0
			20	20		
2	B	20	Total	O	0	0
			20	20		
2	C	13	Total	O	0	0
			13	13		
2	D	37	Total	O	0	0
			37	37		

### 3 Residue-property plots

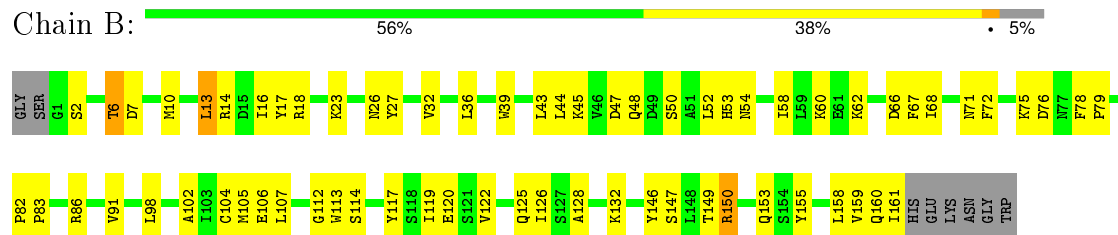
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

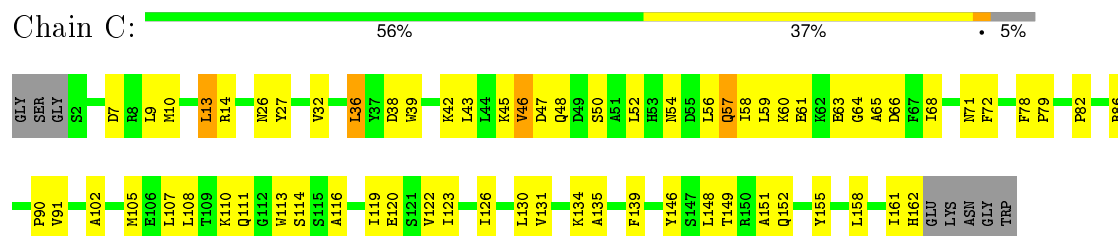
#### • Molecule 1: Ubiquitin-conjugating enzyme E2 Q1



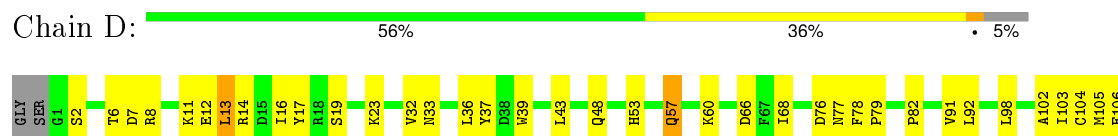
#### • Molecule 1: Ubiquitin-conjugating enzyme E2 Q1



#### • Molecule 1: Ubiquitin-conjugating enzyme E2 Q1



#### • Molecule 1: Ubiquitin-conjugating enzyme E2 Q1



L107	K110	Q111	G112	W113	S114	Y117	S118	I119	E120	S121	V122	I123	M124	Q125	I126	T129	A135	R136	A141	N142	K143	S144	Q145	Y146	S147	L148	T149	Q153	V159	Q160	I161	H162	GLU	LYS	ASN	GLY	TRP
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## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.39 Å 60.39 Å 172.82 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.72 – 2.56	Depositor
% Data completeness (in resolution range)	99.1 (38.72-2.56)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.168 , 0.208	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5132	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

## 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	0.22	0/1260	0.37	0/1697
1	B	0.22	0/1288	0.36	0/1737
1	C	0.25	0/1306	0.39	0/1761
1	D	0.22	0/1280	0.37	0/1726
All	All	0.23	0/5134	0.37	0/6921

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 [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	1238	0	1249	42	0
1	B	1265	0	1275	49	0
1	C	1282	0	1288	55	0
1	D	1257	0	1264	49	0
2	A	20	0	0	0	0
2	B	20	0	0	0	0
2	C	13	0	0	0	0
2	D	37	0	0	0	0
All	All	5132	0	5076	178	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 178 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:B:18:ARG:HA	1:B:23:LYS:HE3	1.50	0.94
1:B:60:LYS:HD3	1:B:66:ASP:HB3	1.50	0.91
1:A:42:LYS:HD3	1:A:44:LEU:HD21	1.56	0.87
1:C:52:LEU:HD22	1:C:135:ALA:HB3	1.68	0.74
1:C:105:MET:HE1	1:C:126:ILE:HA	1.68	0.74

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	153/169 (90%)	142 (93%)	11 (7%)	0	100	100
1	B	159/169 (94%)	149 (94%)	10 (6%)	0	100	100
1	C	160/169 (95%)	148 (92%)	12 (8%)	0	100	100
1	D	158/169 (94%)	152 (96%)	6 (4%)	0	100	100
All	All	630/676 (93%)	591 (94%)	39 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	136/145 (94%)	128 (94%)	8 (6%)	24	44
1	B	139/145 (96%)	132 (95%)	7 (5%)	30	52
1	C	141/145 (97%)	133 (94%)	8 (6%)	25	46
1	D	138/145 (95%)	133 (96%)	5 (4%)	42	67
All	All	554/580 (96%)	526 (95%)	28 (5%)	29	51

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	150	ARG
1	C	13	LEU
1	D	57	GLN
1	B	158	LEU
1	B	160	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	57	GLN
1	C	125	GLN
1	D	153	GLN
1	C	71	ASN
1	C	111	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 [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](#)

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

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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