



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 13, 2016 – 02:14 PM EST

PDB ID : 3NMZ  
Title : Crystal structure of APC complexed with Asef  
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Deposited on : 2010-06-23  
Resolution : 3.01 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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20028442

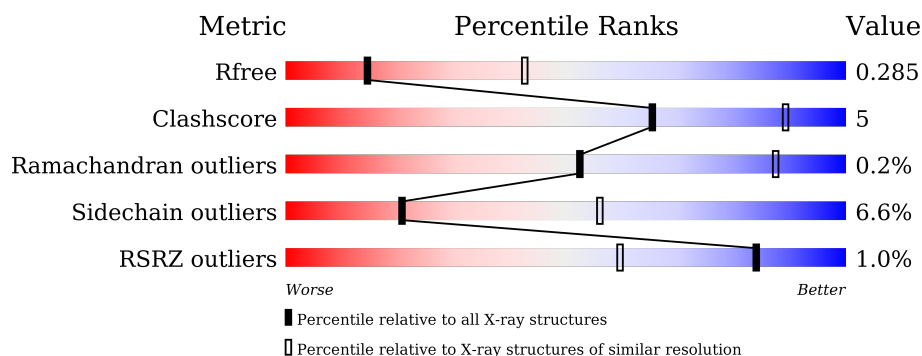
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.01 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))
$R_{free}$	91344	1773 (3.04-3.00)
Clashscore	102246	2117 (3.04-3.00)
Ramachandran outliers	100387	2050 (3.04-3.00)
Sidechain outliers	100360	2053 (3.04-3.00)
RSRZ outliers	91569	1788 (3.04-3.00)

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.

Mol	Chain	Length	Quality of chain
1	A	458	<div> <div></div> <div>76% 12% • 11%</div> </div>
1	B	458	<div> <div></div> <div>73% 14% • 13%</div> </div>
2	C	116	<div> <div></div> <div>60% 11% • 27%</div> </div>
2	D	116	<div> <div></div> <div>59% 12% • 28%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7673 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 APC variant protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	0	0
			3130	1929	576	595	30			
1	B	400	Total	C	N	O	S	0	0	0
			3088	1901	570	587	30			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	282	MET	-	EXPRESSION TAG	UNP Q4LE70
A	283	GLY	-	EXPRESSION TAG	UNP Q4LE70
A	284	SER	-	EXPRESSION TAG	UNP Q4LE70
A	285	SER	-	EXPRESSION TAG	UNP Q4LE70
A	286	HIS	-	EXPRESSION TAG	UNP Q4LE70
A	287	HIS	-	EXPRESSION TAG	UNP Q4LE70
A	288	HIS	-	EXPRESSION TAG	UNP Q4LE70
A	289	HIS	-	EXPRESSION TAG	UNP Q4LE70
A	290	HIS	-	EXPRESSION TAG	UNP Q4LE70
A	291	HIS	-	EXPRESSION TAG	UNP Q4LE70
A	292	SER	-	EXPRESSION TAG	UNP Q4LE70
A	293	SER	-	EXPRESSION TAG	UNP Q4LE70
A	294	GLY	-	EXPRESSION TAG	UNP Q4LE70
A	295	LEU	-	EXPRESSION TAG	UNP Q4LE70
A	296	VAL	-	EXPRESSION TAG	UNP Q4LE70
A	297	PRO	-	EXPRESSION TAG	UNP Q4LE70
A	298	ARG	-	EXPRESSION TAG	UNP Q4LE70
A	299	GLY	-	EXPRESSION TAG	UNP Q4LE70
A	300	SER	-	EXPRESSION TAG	UNP Q4LE70
A	301	HIS	-	EXPRESSION TAG	UNP Q4LE70
A	302	MET	-	EXPRESSION TAG	UNP Q4LE70
B	282	MET	-	EXPRESSION TAG	UNP Q4LE70
B	283	GLY	-	EXPRESSION TAG	UNP Q4LE70
B	284	SER	-	EXPRESSION TAG	UNP Q4LE70
B	285	SER	-	EXPRESSION TAG	UNP Q4LE70

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Chain	Residue	Modelled	Actual	Comment	Reference
B	286	HIS	-	EXPRESSION TAG	UNP Q4LE70
B	287	HIS	-	EXPRESSION TAG	UNP Q4LE70
B	288	HIS	-	EXPRESSION TAG	UNP Q4LE70
B	289	HIS	-	EXPRESSION TAG	UNP Q4LE70
B	290	HIS	-	EXPRESSION TAG	UNP Q4LE70
B	291	HIS	-	EXPRESSION TAG	UNP Q4LE70
B	292	SER	-	EXPRESSION TAG	UNP Q4LE70
B	293	SER	-	EXPRESSION TAG	UNP Q4LE70
B	294	GLY	-	EXPRESSION TAG	UNP Q4LE70
B	295	LEU	-	EXPRESSION TAG	UNP Q4LE70
B	296	VAL	-	EXPRESSION TAG	UNP Q4LE70
B	297	PRO	-	EXPRESSION TAG	UNP Q4LE70
B	298	ARG	-	EXPRESSION TAG	UNP Q4LE70
B	299	GLY	-	EXPRESSION TAG	UNP Q4LE70
B	300	SER	-	EXPRESSION TAG	UNP Q4LE70
B	301	HIS	-	EXPRESSION TAG	UNP Q4LE70
B	302	MET	-	EXPRESSION TAG	UNP Q4LE70

- Molecule 2 is a protein called Rho guanine nucleotide exchange factor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	84	Total	C	N	O	S	0	0	0
			661	414	116	128	3			
2	C	85	Total	C	N	O	S	0	0	0
			667	417	117	130	3			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	161	MET	-	EXPRESSION TAG	UNP Q9NR80
D	162	GLY	-	EXPRESSION TAG	UNP Q9NR80
D	163	HIS	-	EXPRESSION TAG	UNP Q9NR80
D	164	HIS	-	EXPRESSION TAG	UNP Q9NR80
D	165	HIS	-	EXPRESSION TAG	UNP Q9NR80
D	166	HIS	-	EXPRESSION TAG	UNP Q9NR80
D	167	HIS	-	EXPRESSION TAG	UNP Q9NR80
D	168	HIS	-	EXPRESSION TAG	UNP Q9NR80
D	169	MET	-	EXPRESSION TAG	UNP Q9NR80
C	161	MET	-	EXPRESSION TAG	UNP Q9NR80
C	162	GLY	-	EXPRESSION TAG	UNP Q9NR80
C	163	HIS	-	EXPRESSION TAG	UNP Q9NR80
C	164	HIS	-	EXPRESSION TAG	UNP Q9NR80

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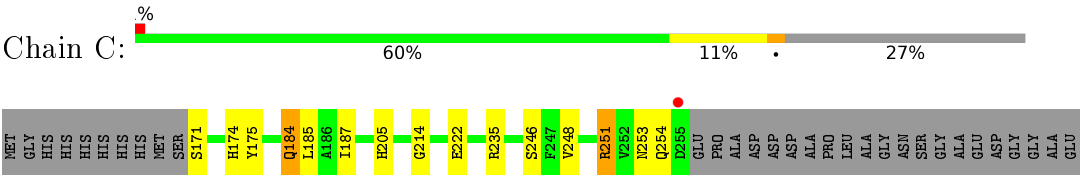
Chain	Residue	Modelled	Actual	Comment	Reference
C	165	HIS	-	EXPRESSION TAG	UNP Q9NR80
C	166	HIS	-	EXPRESSION TAG	UNP Q9NR80
C	167	HIS	-	EXPRESSION TAG	UNP Q9NR80
C	168	HIS	-	EXPRESSION TAG	UNP Q9NR80
C	169	MET	-	EXPRESSION TAG	UNP Q9NR80

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total	O	0	0
			50	50		
3	B	56	Total	O	0	0
			56	56		
3	D	11	Total	O	0	0
			11	11		
3	C	10	Total	O	0	0
			10	10		



● Molecule 2: Rho guanine nucleotide exchange factor 4



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.18Å 163.18Å 242.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.01 40.70 – 3.01	Depositor EDS
% Data completeness (in resolution range)	90.2 (50.00-3.01) 90.7 (40.70-3.01)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.62 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.249 , 0.284 0.248 , 0.285	Depositor DCC
$R_{free}$ test set	2202 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	76.2	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.298 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7673	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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](#)

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	0.27	0/3170	0.46	0/4273
1	B	0.28	0/3127	0.47	0/4214
2	C	0.32	0/686	0.50	0/933
2	D	0.30	0/680	0.47	0/925
All	All	0.28	0/7663	0.47	0/10345

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	3130	0	3160	29	0
1	B	3088	0	3112	32	0
2	C	667	0	600	8	0
2	D	661	0	595	7	0
3	A	50	0	0	1	0
3	B	56	0	0	2	0
3	C	10	0	0	0	0
3	D	11	0	0	0	0
All	All	7673	0	7467	75	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 5.

The worst 5 of 75 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:473:GLN:H	1:A:473:GLN:HE21	1.20	0.84
2:D:199:ALA:HB1	2:D:248:VAL:HG13	1.61	0.83
1:B:629:LEU:H	1:B:629:LEU:HD23	1.45	0.80
2:C:251:ARG:HD3	2:C:253:ASN:H	1.48	0.78
1:B:692:PRO:HA	1:B:695:GLN:HG2	1.68	0.75

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	400/458 (87%)	385 (96%)	14 (4%)	1 (0%)	46	82
1	B	394/458 (86%)	379 (96%)	14 (4%)	1 (0%)	46	82
2	C	83/116 (72%)	73 (88%)	10 (12%)	0	100	100
2	D	82/116 (71%)	77 (94%)	5 (6%)	0	100	100
All	All	959/1148 (84%)	914 (95%)	43 (4%)	2 (0%)	52	87

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	362	GLY
1	A	734	PRO

### 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	345/391 (88%)	326 (94%)	19 (6%)	27	64
1	B	340/391 (87%)	318 (94%)	22 (6%)	21	56
2	C	68/89 (76%)	62 (91%)	6 (9%)	12	41
2	D	67/89 (75%)	60 (90%)	7 (10%)	9	31
All	All	820/960 (85%)	766 (93%)	54 (7%)	21	56

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	407	LEU
1	B	497	LEU
2	C	184	GLN
1	B	441	PRO
1	B	473	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	427	HIS
1	B	433	GLN
2	D	173	HIS
1	B	372	ASN
1	B	388	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	406/458 (88%)	0.32	3 (0%) 89 70	56, 79, 108, 162	1 (0%)
1	B	400/458 (87%)	0.37	5 (1%) 79 52	55, 80, 128, 160	2 (0%)
2	C	85/116 (73%)	0.30	1 (1%) 81 55	62, 81, 112, 124	0
2	D	84/116 (72%)	0.35	1 (1%) 81 55	62, 82, 112, 125	0
All	All	975/1148 (84%)	0.34	10 (1%) 84 60	55, 80, 119, 162	3 (0%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	368	VAL	6.6
2	D	255	ASP	4.4
1	A	367	SER	4.1
2	C	255	ASP	3.4
1	B	436	ASN	3.2

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.