



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:52 am BST

PDB ID : 3GOR
Title : Crystal structure of putative metal-dependent hydrolase APC36150
Authors : Cooper, D.R.; Grelewski, K.; Derewenda, Z.S.; Integrated Center for Structure and Function Innovation (ISFI)
Deposited on : 2009-03-19
Resolution : 2.51 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

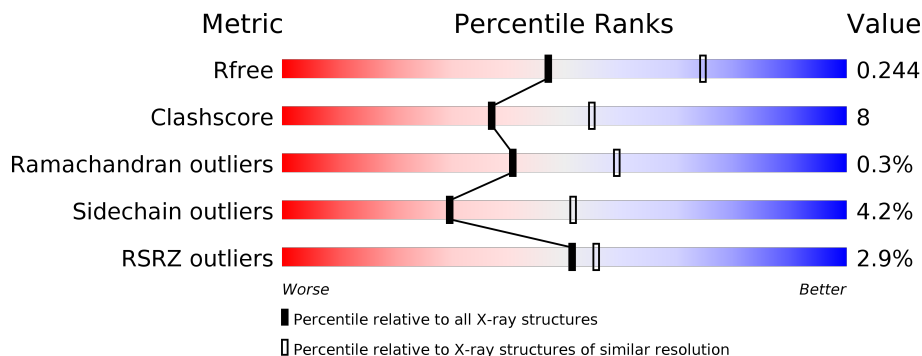
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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 respectively. 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	157	
1	B	157	
1	C	157	
1	D	157	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5133 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 Putative metal-dependent hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	157	1282	815	222	237	8	0	0	0
1	B	157	1282	815	222	237	8	0	0	0
1	C	155	1267	807	217	235	8	0	0	0
1	D	151	1240	792	212	229	7	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	PDB 3GOR
A	-1	ASN	-	EXPRESSION TAG	PDB 3GOR
A	0	ALA	-	EXPRESSION TAG	PDB 3GOR
B	-2	SER	-	EXPRESSION TAG	PDB 3GOR
B	-1	ASN	-	EXPRESSION TAG	PDB 3GOR
B	0	ALA	-	EXPRESSION TAG	PDB 3GOR
C	-2	SER	-	EXPRESSION TAG	PDB 3GOR
C	-1	ASN	-	EXPRESSION TAG	PDB 3GOR
C	0	ALA	-	EXPRESSION TAG	PDB 3GOR
D	-2	SER	-	EXPRESSION TAG	PDB 3GOR
D	-1	ASN	-	EXPRESSION TAG	PDB 3GOR
D	0	ALA	-	EXPRESSION TAG	PDB 3GOR

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ni	0	0
			1	1		
2	A	1	Total	Ni	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Ni 1 1	0	0
2	C	1	Total Ni 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	19	Total O 19 19	0	0
3	B	13	Total O 13 13	0	0
3	C	11	Total O 11 11	0	0
3	D	15	Total O 15 15	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.48Å 71.47Å 123.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.62 – 2.51 35.62 – 2.51	Depositor EDS
% Data completeness (in resolution range)	92.7 (35.62-2.51) 93.8 (35.62-2.51)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.14 (at 2.51Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.186 , 0.247 0.183 , 0.244	Depositor DCC
R_{free} test set	1028 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtrriage
Anisotropy	0.681	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.020 for k,h,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5133	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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:
NI

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	0.36	0/1306	0.50	0/1748
1	B	0.35	0/1306	0.51	0/1748
1	C	0.36	0/1291	0.47	0/1729
1	D	0.35	0/1265	0.49	0/1696
All	All	0.36	0/5168	0.49	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	1282	0	1253	27	1
1	B	1282	0	1253	25	1
1	C	1267	0	1237	16	0
1	D	1240	0	1209	15	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	19	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	13	0	0	0	0
3	C	11	0	0	0	0
3	D	15	0	0	1	0
All	All	5133	0	4952	78	1

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.

All (78) 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:1:MSE:HE2	1:B:5:LYS:HB3	1.57	0.86
1:A:153:ARG:HB2	1:A:153:ARG:HH11	1.42	0.82
1:D:72:GLU:HB3	3:D:168:HOH:O	1.92	0.68
1:C:75:GLU:HB3	1:C:81:LEU:HD13	1.75	0.68
1:C:108:THR:HA	1:C:113:THR:N	2.09	0.67
1:A:108:THR:HA	1:A:113:THR:N	2.11	0.66
1:C:108:THR:HA	1:C:113:THR:H	1.60	0.66
1:B:108:THR:HA	1:B:113:THR:N	2.12	0.65
1:D:108:THR:HA	1:D:113:THR:N	2.12	0.64
1:A:108:THR:HA	1:A:113:THR:H	1.63	0.64
1:A:-2:SER:O	1:A:-1:ASN:HB2	1.97	0.64
1:D:108:THR:HA	1:D:113:THR:H	1.64	0.63
1:B:108:THR:HA	1:B:113:THR:H	1.63	0.62
1:A:68:ARG:NH1	1:A:110:ILE:HG23	2.15	0.61
1:B:75:GLU:HB3	1:B:81:LEU:HD13	1.81	0.61
1:B:68:ARG:NH1	1:B:110:ILE:HG23	2.16	0.60
1:C:68:ARG:NH1	1:C:110:ILE:HG23	2.16	0.60
1:A:75:GLU:HB3	1:A:81:LEU:HD13	1.81	0.60
1:D:68:ARG:NH1	1:D:110:ILE:HG23	2.17	0.59
1:C:108:THR:O	1:C:112:GLY:HA2	2.03	0.59
1:B:152:LYS:O	1:B:154:GLY:N	2.36	0.58
1:D:75:GLU:HB3	1:D:81:LEU:HD13	1.86	0.57
1:D:75:GLU:O	1:D:76:THR:HB	2.05	0.56
1:A:108:THR:O	1:A:112:GLY:HA2	2.06	0.55
1:B:108:THR:O	1:B:112:GLY:HA2	2.07	0.55
1:D:108:THR:O	1:D:112:GLY:HA2	2.06	0.55
1:B:75:GLU:O	1:B:76:THR:HB	2.07	0.55
1:C:75:GLU:O	1:C:76:THR:HB	2.07	0.55
1:A:133:GLY:O	1:B:134:GLN:HG2	2.08	0.54
1:D:68:ARG:HH12	1:D:110:ILE:HG23	1.72	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ARG:HH12	1:A:110:ILE:HG23	1.71	0.53
1:B:152:LYS:C	1:B:154:GLY:H	2.10	0.53
1:A:140:ARG:HH21	1:B:37:THR:HB	1.74	0.53
1:A:75:GLU:O	1:A:76:THR:HB	2.08	0.51
1:A:75:GLU:HB2	3:A:167:HOH:O	2.10	0.51
1:B:153:ARG:HH11	1:B:153:ARG:HA	1.75	0.51
1:A:74:PRO:HD2	3:A:167:HOH:O	2.09	0.51
1:B:68:ARG:HH12	1:B:110:ILE:HG23	1.75	0.50
1:C:68:ARG:HH12	1:C:110:ILE:HG23	1.74	0.50
1:B:1:MSE:HE2	1:B:5:LYS:CB	2.37	0.50
1:A:1:MSE:O	1:A:2:SER:C	2.50	0.49
1:C:73:GLU:HA	1:C:74:PRO:HD3	1.69	0.49
1:A:50:PHE:HB3	1:A:71:ILE:HD12	1.96	0.48
1:A:-2:SER:O	1:A:-1:ASN:CB	2.62	0.47
1:A:73:GLU:HA	1:A:74:PRO:HD3	1.66	0.47
1:A:153:ARG:CB	1:A:153:ARG:HH11	2.22	0.46
1:A:140:ARG:HH21	1:B:37:THR:CB	2.27	0.46
1:B:55:PHE:CG	1:B:124:ALA:HB2	2.51	0.46
1:D:73:GLU:HA	1:D:74:PRO:HD3	1.68	0.46
1:D:50:PHE:HB3	1:D:71:ILE:HD12	1.96	0.45
1:B:50:PHE:HB3	1:B:71:ILE:HD12	1.98	0.45
1:B:73:GLU:HA	1:B:74:PRO:HD3	1.68	0.44
1:B:152:LYS:C	1:B:154:GLY:N	2.71	0.44
1:C:55:PHE:CG	1:C:124:ALA:HB2	2.53	0.44
1:A:134:GLN:HG2	1:B:133:GLY:O	2.19	0.43
1:C:78:LEU:HD23	1:C:78:LEU:HA	1.84	0.43
1:A:45:ALA:O	1:A:49:LEU:HG	2.19	0.42
1:A:31:ASP:HA	1:A:40:THR:HB	2.01	0.42
1:D:78:LEU:HA	1:D:78:LEU:HD23	1.84	0.42
1:B:45:ALA:O	1:B:49:LEU:HG	2.20	0.42
1:D:45:ALA:O	1:D:49:LEU:HG	2.20	0.42
1:A:144:HIS:N	3:A:173:HOH:O	2.53	0.41
1:A:144:HIS:CE1	3:A:173:HOH:O	2.74	0.41
1:A:5:LYS:HE2	1:A:5:LYS:HB2	1.88	0.41
1:B:147:LEU:HA	1:B:148:PRO:HD3	1.89	0.41
1:D:115:MSE:HB2	1:D:115:MSE:HE3	1.94	0.41
1:A:115:MSE:HE3	1:A:115:MSE:HB2	1.94	0.41
1:C:121:LEU:HA	1:C:121:LEU:HD23	1.91	0.41
1:C:30:TYR:CD2	1:C:42:LYS:HD2	2.56	0.41
1:B:30:TYR:CD2	1:B:42:LYS:HD2	2.56	0.41
1:C:5:LYS:HB2	1:C:5:LYS:HE2	1.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:PHE:HB3	1:C:71:ILE:HD12	2.02	0.41
1:B:33:LYS:HA	1:B:34:PRO:HD3	1.93	0.40
1:C:140:ARG:HH21	1:D:37:THR:HB	1.85	0.40
1:B:63:ASP:HB3	1:B:66:LEU:HD22	2.03	0.40
1:D:55:PHE:CG	1:D:124:ALA:HB2	2.56	0.40
1:A:1:MSE:HB2	1:A:1:MSE:HE3	1.68	0.40
1:C:115:MSE:HB2	1:C:115:MSE:HE3	1.94	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLU:OE2	1:B:141:GLY:O[3_556]	2.13	0.07

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	155/157 (99%)	151 (97%)	3 (2%)	1 (1%)	25	41
1	B	155/157 (99%)	151 (97%)	3 (2%)	1 (1%)	25	41
1	C	153/157 (98%)	150 (98%)	3 (2%)	0	100	100
1	D	149/157 (95%)	147 (99%)	2 (1%)	0	100	100
All	All	612/628 (98%)	599 (98%)	11 (2%)	2 (0%)	41	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-1	ASN
1	B	153	ARG

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	139/131 (106%)	131 (94%)	8 (6%)	20	36
1	B	139/131 (106%)	134 (96%)	5 (4%)	35	59
1	C	138/131 (105%)	134 (97%)	4 (3%)	42	67
1	D	135/131 (103%)	129 (96%)	6 (4%)	28	49
All	All	551/524 (105%)	528 (96%)	23 (4%)	30	51

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	SER
1	A	1	MSE
1	A	2	SER
1	A	19	MSE
1	A	35	THR
1	A	83	GLU
1	A	108	THR
1	A	153	ARG
1	B	19	MSE
1	B	66	LEU
1	B	83	GLU
1	B	108	THR
1	B	153	ARG
1	C	19	MSE
1	C	35	THR
1	C	83	GLU
1	C	108	THR
1	D	5	LYS
1	D	12	LEU
1	D	19	MSE
1	D	35	THR
1	D	83	GLU
1	D	108	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	130	HIS

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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

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.

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	149/157 (94%)	0.17	7 (4%) 31 34	29, 65, 109, 131	0
1	B	149/157 (94%)	0.18	2 (1%) 77 79	31, 66, 110, 130	0
1	C	147/157 (93%)	0.26	6 (4%) 37 41	29, 64, 107, 129	0
1	D	144/157 (91%)	-0.06	2 (1%) 75 78	29, 63, 104, 131	0
All	All	589/628 (93%)	0.14	17 (2%) 51 55	29, 65, 108, 131	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	154	GLY	6.6
1	A	154	GLY	3.1
1	A	110	ILE	2.9
1	A	71	ILE	2.9
1	C	111	PHE	2.8
1	A	146	ASP	2.7
1	D	98	ASP	2.6
1	C	112	GLY	2.5
1	A	73	GLU	2.5
1	B	63	ASP	2.5
1	C	64	PRO	2.3
1	C	102	ASP	2.2
1	A	111	PHE	2.2
1	A	72	GLU	2.1
1	C	110	ILE	2.1
1	C	106	ASP	2.1
1	D	65	SER	2.0

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. 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	B-factors(Å ²)	Q<0.9
2	NI	A	200	1/1	0.98	0.21	56,56,56,56	0
2	NI	B	200	1/1	0.99	0.12	37,37,37,37	0
2	NI	D	200	1/1	0.99	0.15	38,38,38,38	0
2	NI	C	200	1/1	0.99	0.20	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.