



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:36 AM GMT

PDB ID : 2NGR
Title : TRANSITION STATE COMPLEX FOR GTP HYDROLYSIS BY CDC42:
COMPARISONS OF THE HIGH RESOLUTION STRUCTURES FOR
CDC42 BOUND TO THE ACTIVE AND CATALYTICALLY COMPROMISED
FORMS OF THE CDC42-GAP.
Authors : Nassar, N.; Hoffman, G.; Clardy, J.; Cerione, R.
Deposited on : 1998-07-31
Resolution : 1.90 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
<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 (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

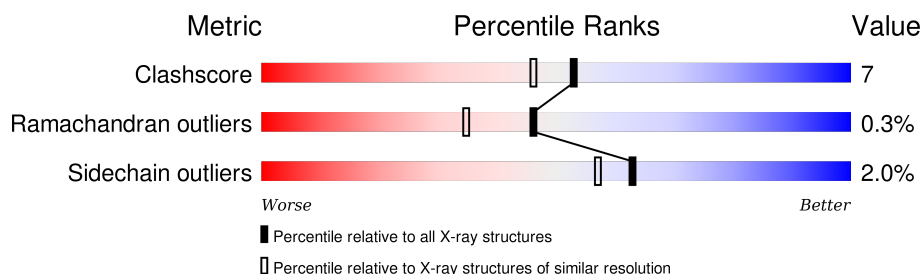
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	191	 85% 15%
2	B	234	 66% 17% 16%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3205 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 PROTEIN (GTP BINDING PROTEIN (G25K)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	0	0
			1494	960	242	284	8			

- Molecule 2 is a protein called PROTEIN (GTPASE ACTIVATING PROTEIN (RHG)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	196	Total	C	N	O	S	0	0	0
			1577	1021	264	290	2			

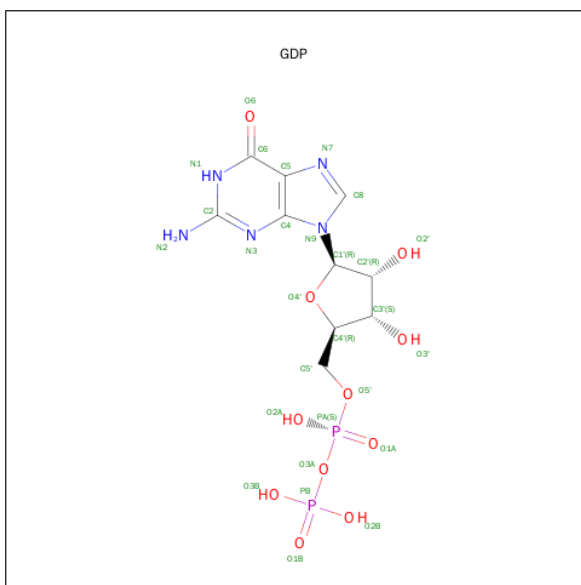
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	305	ALA	ARG	MUTATION	UNP Q07960

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

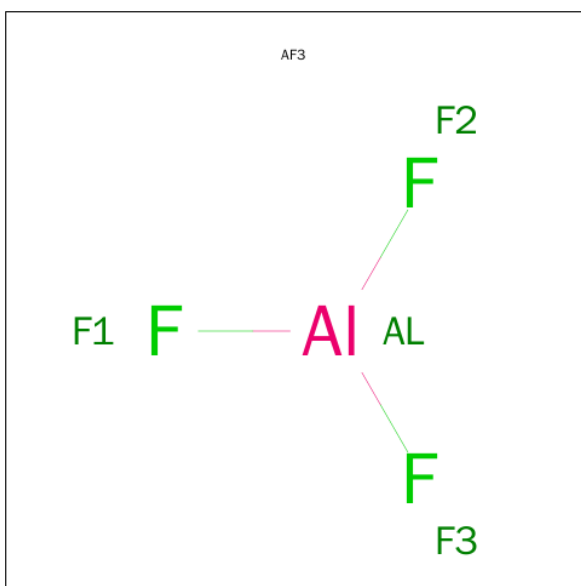
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 5 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Al	F	0	0
			4	1	3		

- Molecule 6 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	65	Total 65	O 65	0	0
6	B	36	Total 36	O 36	0	0

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.

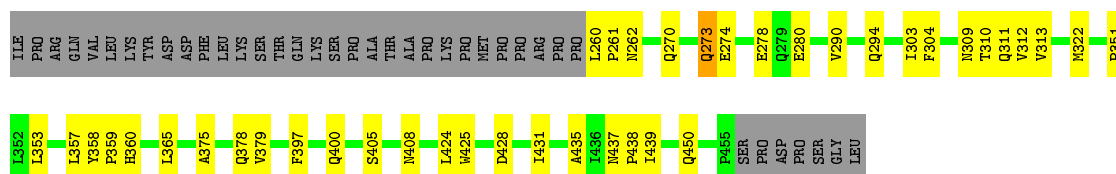
- Molecule 1: PROTEIN (GTP BINDING PROTEIN (G25K))

Chain A: 



- Molecule 2: PROTEIN (GTPASE ACTIVATING PROTEIN (RHG))

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.82Å 67.69Å 131.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.00 – 1.90	Depositor
% Data completeness (in resolution range)	99.5 (22.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.253 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3205	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, AF3

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	0.35	0/1527	0.61	0/2076
2	B	0.36	0/1615	0.55	0/2207
All	All	0.35	0/3142	0.58	0/4283

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

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	1494	0	1521	16	0
2	B	1577	0	1582	25	0
3	A	1	0	0	0	0
4	A	28	0	12	0	0
5	A	4	0	0	0	0
6	A	65	0	0	0	0
6	B	36	0	0	0	0
All	All	3205	0	3115	41	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 7.

All (41) 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)
2:B:310:THR:O	2:B:313:VAL:HG22	1.93	0.68
2:B:273:GLN:HE21	2:B:273:GLN:HA	1.59	0.66
1:A:46:ILE:HD13	1:A:177:LEU:HD11	1.80	0.64
2:B:405:SER:HA	2:B:408:ASN:OD1	1.99	0.61
2:B:303:ILE:O	2:B:304:PHE:HB2	2.00	0.61
2:B:360:HIS:ND1	2:B:379:VAL:HG21	2.22	0.54
1:A:170:ASP:O	1:A:174:LEU:HG	2.07	0.53
2:B:290:VAL:O	2:B:294:GLN:HG2	2.08	0.53
2:B:353:LEU:O	2:B:357:LEU:HG	2.08	0.53
1:A:87:PRO:HA	1:A:137:ILE:HD11	1.93	0.51
2:B:358:TYR:HB3	2:B:359:PRO:HD3	1.92	0.50
1:A:61:GLN:HB3	1:A:63:ASP:OD2	2.11	0.50
1:A:180:PRO:HB3	1:A:186:ARG:HG3	1.94	0.49
1:A:11:ASP:O	1:A:14:VAL:HG22	2.13	0.48
2:B:322:MET:HE2	2:B:322:MET:HA	1.95	0.47
1:A:127:GLU:HG2	1:A:131:LYS:NZ	2.30	0.47
2:B:351:PRO:HG3	2:B:425:TRP:CE2	2.51	0.46
2:B:375:ALA:O	2:B:379:VAL:HG23	2.18	0.44
2:B:351:PRO:HB3	2:B:424:LEU:HA	1.99	0.44
1:A:133:LYS:N	1:A:133:LYS:HD2	2.33	0.44
2:B:360:HIS:CE1	2:B:379:VAL:HG21	2.53	0.44
2:B:437:ASN:HB2	2:B:438:PRO:HD3	2.00	0.43
2:B:278:GLU:HB2	2:B:280:GLU:HG3	1.99	0.43
2:B:435:ALA:C	2:B:438:PRO:HD2	2.39	0.43
2:B:435:ALA:O	2:B:439:ILE:HG13	2.17	0.43
1:A:98:VAL:HG21	1:A:149:LEU:HD13	1.99	0.43
2:B:260:LEU:HD22	2:B:322:MET:HE3	2.00	0.43
2:B:322:MET:CE	2:B:322:MET:HA	2.49	0.43
2:B:397:PHE:O	2:B:400:GLN:HB2	2.19	0.43
2:B:260:LEU:HA	2:B:261:PRO:HD3	1.86	0.43
2:B:309:ASN:HB3	2:B:312:VAL:HB	2.00	0.43
1:A:40:TYR:HB2	1:A:55:LEU:HB2	2.02	0.42
2:B:428:ASP:HB3	2:B:431:ILE:HG13	2.02	0.41
1:A:46:ILE:HD12	1:A:51:TYR:CD2	2.55	0.41
2:B:365:LEU:H	2:B:365:LEU:HD22	1.86	0.41
1:A:127:GLU:HG2	1:A:131:LYS:HZ2	1.86	0.41
1:A:98:VAL:HB	1:A:99:PRO:HD3	2.02	0.41
1:A:130:ALA:C	1:A:132:ASN:H	2.23	0.41
2:B:270:GLN:O	2:B:274:GLU:HG3	2.21	0.41
1:A:124:SER:O	1:A:128:LYS:HE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:VAL:HG12	1:A:45:MET:N	2.36	0.40

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	189/191 (99%)	181 (96%)	7 (4%)	1 (0%)	34	21
2	B	194/234 (83%)	186 (96%)	8 (4%)	0	100	100
All	All	383/425 (90%)	367 (96%)	15 (4%)	1 (0%)	46	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	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	171/171 (100%)	169 (99%)	2 (1%)	78	76
2	B	176/211 (83%)	171 (97%)	5 (3%)	51	41
All	All	347/382 (91%)	340 (98%)	7 (2%)	63	57

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	A	132	ASN
2	B	262	ASN
2	B	273	GLN
2	B	311	GLN
2	B	378	GLN
2	B	450	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	262	ASN
2	B	273	GLN
2	B	276	ASN
2	B	279	GLN
2	B	450	GLN

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
4	GDP	A	198	3,5	23,30,30	1.47	3 (13%)	30,47,47	2.32	6 (20%)
5	AF3	A	200	3,4,6	0,3,3	0.00	-	0,3,3	0.00	-

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
4	GDP	A	198	3,5	-	0/12/32/32	0/3/3/3
5	AF3	A	200	3,4,6	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	198	GDP	C8-N7	-2.71	1.29	1.34
4	A	198	GDP	O4'-C1'	2.37	1.44	1.41
4	A	198	GDP	C6-N1	3.87	1.40	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	198	GDP	C5-C6-N1	-8.75	111.63	123.59
4	A	198	GDP	O3A-PA-O5'	-2.33	96.75	102.94
4	A	198	GDP	N3-C2-N1	-2.32	123.92	127.44
4	A	198	GDP	C2'-C3'-C4'	2.11	106.95	102.61
4	A	198	GDP	O2B-PB-O1B	2.56	118.82	110.58
4	A	198	GDP	C6-N1-C2	6.57	125.05	115.94

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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