Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 09:35 pm BST

PDB ID	:	5BPT
Title	:	Atomic-resolution structures of the APC/C subunits Apc4 and the Apc5 N-terminal domain
Authors	:	Cronin, N.; Yang, J.; Zhang, Z.; Barford, D.
Deposited on	:	2015-05-28
Resolution	:	3.20 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 ①) were used in the production of this report:

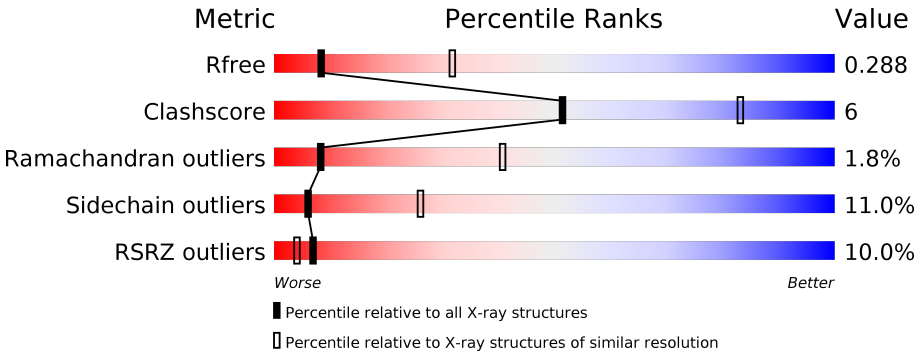
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 <=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	741	8%, 63%, 18%, 17%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4786 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 MGC81278 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	614	4786	3045	805	908	13	15	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

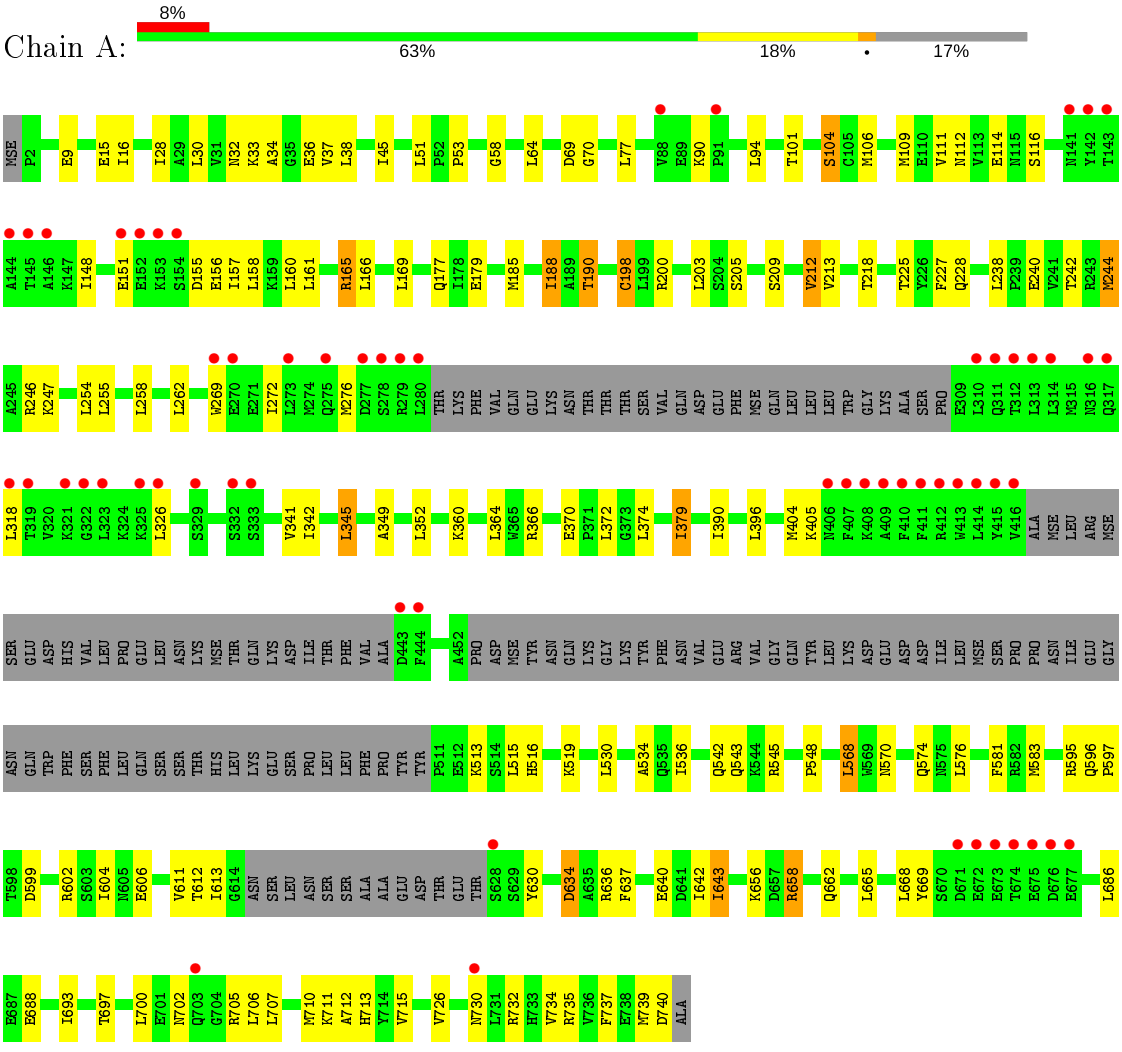
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP Q6NU36
A	312	THR	ALA	conflict	UNP Q6NU36
A	738	GLU	-	expression tag	UNP Q6NU36
A	739	MSE	-	expression tag	UNP Q6NU36
A	740	ASP	-	expression tag	UNP Q6NU36
A	741	ALA	-	expression tag	UNP Q6NU36

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

- Molecule 1: MGC81278 protein

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	90.47Å 90.47Å 115.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.71 – 3.20 48.71 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.71-3.20) 100.0 (48.71-3.20)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 3.19Å)	Xtriage
Refinement program	BUSTER-TNT 2.10.1, BUSTER 2.11.4	Depositor
R, R_{free}	0.223 , 0.265 0.242 , 0.288	Depositor DCC
R_{free} test set	1016 reflections (6.59%)	wwPDB-VP
Wilson B-factor (Å^2)	90.0	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 74.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4786	wwPDB-VP
Average B, all atoms (Å^2)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.39	0/4856	0.64	0/6556

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	4786	0	4755	53	0
All	All	4786	0	4755	53	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 6.

All (53) 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:225:THR:HG22	1:A:548:PRO:HA	1.77	0.66
1:A:104:SER:HB3	1:A:198:CYS:O	2.00	0.61
1:A:106:MSE:HE2	1:A:169:LEU:HD11	1.85	0.59
1:A:576:LEU:HD12	1:A:595:ARG:HB2	1.85	0.59
1:A:16:ILE:H	1:A:732:ARG:HD2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ILE:HD13	1:A:734:VAL:HG13	1.85	0.58
1:A:111:VAL:HG23	1:A:165:ARG:HD2	1.86	0.58
1:A:15:GLU:HA	1:A:732:ARG:HG3	1.86	0.57
1:A:637:PHE:HA	1:A:643:ILE:HG22	1.87	0.56
1:A:658:ARG:HH21	1:A:737:PHE:HB2	1.71	0.55
1:A:583:MSE:HE1	1:A:686:LEU:HB3	1.89	0.54
1:A:36:GLU:HB3	1:A:53:PRO:HD3	1.91	0.52
1:A:212:VAL:HG13	1:A:227:PHE:HB2	1.92	0.52
1:A:254:LEU:O	1:A:255:LEU:HB3	2.10	0.52
1:A:341:VAL:HA	1:A:345:LEU:HB2	1.93	0.51
1:A:613:ILE:HD11	1:A:700:LEU:HD21	1.92	0.51
1:A:360:LYS:HB2	1:A:379:ILE:HD11	1.92	0.50
1:A:597:PRO:HD3	1:A:604:ILE:HB	1.94	0.50
1:A:166:LEU:HB2	1:A:242:THR:HG23	1.94	0.50
1:A:581:PHE:HE2	1:A:583:MSE:HE3	1.78	0.49
1:A:200:ARG:HB2	1:A:213:VAL:HB	1.95	0.49
1:A:656:LYS:HG3	1:A:711:LYS:HA	1.95	0.48
1:A:244:MSE:HE2	1:A:374:LEU:HB2	1.95	0.47
1:A:366:ARG:HA	1:A:370:GLU:HB2	1.97	0.47
1:A:612:THR:HB	1:A:697:THR:HG22	1.97	0.47
1:A:634:ASP:HB2	1:A:713:HIS:O	2.14	0.47
1:A:516:HIS:HA	1:A:519:LYS:HE2	1.96	0.46
1:A:396:LEU:HD22	1:A:515:LEU:HD22	1.99	0.45
1:A:205:SER:H	1:A:570:ASN:HD21	1.63	0.45
1:A:244:MSE:HE2	1:A:374:LEU:HD13	1.99	0.45
1:A:148:ILE:HG23	1:A:156:GLU:HB2	1.99	0.44
1:A:710:MSE:HE1	1:A:726:VAL:HB	1.99	0.44
1:A:269:TRP:HA	1:A:272:ILE:HD12	1.99	0.44
1:A:37:VAL:HG21	1:A:64:LEU:HD21	1.99	0.44
1:A:581:PHE:CE2	1:A:583:MSE:HE3	2.53	0.43
1:A:349:ALA:HB3	1:A:390:ILE:HD12	2.00	0.43
1:A:255:LEU:H	1:A:258:LEU:HD13	1.84	0.43
1:A:599:ASP:HB3	1:A:602:ARG:HD3	2.01	0.43
1:A:101:THR:HG21	1:A:177:GLN:HB3	2.00	0.43
1:A:366:ARG:O	1:A:370:GLU:HB3	2.19	0.42
1:A:188:ILE:O	1:A:534:ALA:HA	2.19	0.42
1:A:244:MSE:HE3	1:A:372:LEU:HB3	2.02	0.42
1:A:161:LEU:HG	1:A:185:MSE:HE1	2.02	0.41
1:A:200:ARG:HB3	1:A:568:LEU:HD12	2.02	0.41
1:A:179:GLU:HG2	1:A:190:THR:HG23	2.03	0.41
1:A:642:ILE:HG22	1:A:662:GLN:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ILE:HD12	1:A:158:LEU:HG	2.03	0.41
1:A:9:GLU:HG3	1:A:735:ARG:HG3	2.01	0.41
1:A:228:GLN:HB3	1:A:545:ARG:HB2	2.03	0.41
1:A:32:ASN:C	1:A:34:ALA:H	2.25	0.41
1:A:94:LEU:HD22	1:A:156:GLU:HB3	2.02	0.40
1:A:262:LEU:HD11	1:A:515:LEU:HD21	2.04	0.40
1:A:58:GLY:HA3	1:A:77:LEU:HD13	2.03	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	604/741 (82%)	558 (92%)	35 (6%)	11 (2%)	8 41

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	SER
1	A	640	GLU
1	A	712	ALA
1	A	70	GLY
1	A	630	TYR
1	A	705	ARG
1	A	198	CYS
1	A	668	LEU
1	A	33	LYS
1	A	151	GLU
1	A	669	TYR

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	526/648 (81%)	468 (89%)	58 (11%)	6 26

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ILE
1	A	30	LEU
1	A	38	LEU
1	A	51	LEU
1	A	69	ASP
1	A	90	LYS
1	A	104	SER
1	A	109	MSE
1	A	112	ASN
1	A	114	GLU
1	A	155	ASP
1	A	160	LEU
1	A	165	ARG
1	A	188	ILE
1	A	190	THR
1	A	203	LEU
1	A	209	SER
1	A	212	VAL
1	A	218	THR
1	A	238	LEU
1	A	240	GLU
1	A	244	MSE
1	A	246	ARG
1	A	247	LYS
1	A	276	MSE
1	A	318	LEU
1	A	326	LEU
1	A	342	ILE
1	A	345	LEU
1	A	352	LEU

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Mol	Chain	Res	Type
1	A	364	LEU
1	A	379	ILE
1	A	404	MSE
1	A	405	LYS
1	A	513	LYS
1	A	530	LEU
1	A	536	ILE
1	A	542	GLN
1	A	543	GLN
1	A	568	LEU
1	A	574	GLN
1	A	596	GLN
1	A	606	GLU
1	A	611	VAL
1	A	634	ASP
1	A	636	ARG
1	A	643	ILE
1	A	658	ARG
1	A	665	LEU
1	A	688	GLU
1	A	693	ILE
1	A	702	ASN
1	A	706	LEU
1	A	707	LEU
1	A	715	VAL
1	A	730	ASN
1	A	739	MSE
1	A	740	ASP

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

Mol	Chain	Res	Type
1	A	40	HIS
1	A	123	ASN
1	A	316	ASN
1	A	570	ASN
1	A	577	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

There are no ligands in this entry.

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

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^{th} 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	599/741 (80%)	0.50	60 (10%) 7 4	56, 98, 191, 257	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	314	LEU	7.3
1	A	628	SER	6.9
1	A	411	PHE	6.9
1	A	317	GLN	6.7
1	A	310	LEU	5.9
1	A	674	THR	5.6
1	A	142	TYR	5.3
1	A	143	THR	5.0
1	A	443	ASP	4.8
1	A	312	THR	4.8
1	A	318	LEU	4.8
1	A	277	ASP	4.6
1	A	313	LEU	4.5
1	A	416	VAL	4.4
1	A	412	ARG	4.3
1	A	316	ASN	4.2
1	A	332	SER	4.2
1	A	415	TYR	4.1
1	A	673	GLU	4.1
1	A	273	LEU	4.1
1	A	146	ALA	4.0
1	A	322	GLY	3.7
1	A	414	LEU	3.7
1	A	280	LEU	3.6
1	A	321	LYS	3.5
1	A	410	PHE	3.5
1	A	409	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	413	TRP	3.4
1	A	278	SER	3.4
1	A	279	ARG	3.3
1	A	703	GLN	3.3
1	A	672	GLU	3.3
1	A	152	GLU	3.3
1	A	270	GLU	3.3
1	A	141	ASN	3.1
1	A	333	SER	3.0
1	A	154	SER	3.0
1	A	444	PHE	2.9
1	A	671	ASP	2.9
1	A	153	LYS	2.8
1	A	88	VAL	2.7
1	A	275	GLN	2.7
1	A	730	ASN	2.6
1	A	326	LEU	2.6
1	A	311	GLN	2.6
1	A	151	GLU	2.5
1	A	145	THR	2.5
1	A	407	PHE	2.4
1	A	408	LYS	2.3
1	A	675	GLU	2.3
1	A	319	THR	2.3
1	A	323	LEU	2.3
1	A	269	TRP	2.3
1	A	676	ASP	2.2
1	A	91	PRO	2.2
1	A	325	LYS	2.2
1	A	677	GLU	2.2
1	A	329	SER	2.1
1	A	406	ASN	2.1
1	A	144	ALA	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.