



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:36 PM UTC

PDB ID : 1G3J / pdb_00001g3j
Title : CRYSTAL STRUCTURE OF THE XTCF3-CBD/BETA-CATENIN ARMADILLO REPEAT COMPLEX
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Deposited on : 2000-10-24
Resolution : 2.10 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

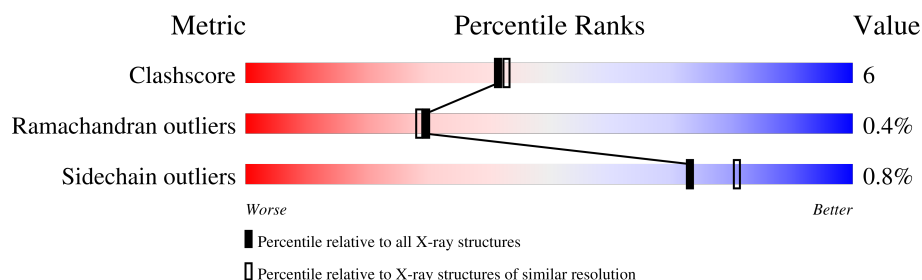
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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 of 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	532	 86% 11% .
1	C	532	 71% 11% 17%
2	B	61	 46% 16% 5% 33%
2	D	61	 46% 8% . 44%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7794 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 BETA-CATENIN ARMADILLO REPEAT REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	0	0
			3864	2435	694	709	26			
1	C	439	Total	C	N	O	S	0	0	0
			3148	1988	560	582	18			

- Molecule 2 is a protein called TCF3-CBD (CATENIN BINDING DOMAIN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	41	Total	C	N	O	0	0	0
			286	172	47	67			
2	D	34	Total	C	N	O	0	0	0
			233	143	39	51			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	180	Total	O	0	0
			180	180		
3	B	12	Total	O	0	0
			12	12		
3	C	67	Total	O	0	0
			67	67		
3	D	4	Total	O	0	0
			4	4		



MET	P2	E11	A14	R20	F24	GLY	GLU	GLN	GLU	GLU	LYS	SER	PRO	GLY	GLU	GLY	SER	ALA	GLU	GLY	D49	V49	N50	GLU	SER	GLU	ASN	HIS	SER	SER	ASP	SER	ASP	SER
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.13Å 153.25Å 188.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-2.10)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7794	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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	0.42	0/3918	0.87	2/5335 (0.0%)
1	C	0.37	0/3190	0.87	1/4356 (0.0%)
2	B	0.35	0/285	0.96	1/382 (0.3%)
2	D	0.34	0/232	0.91	2/311 (0.6%)
All	All	0.39	0/7625	0.88	6/10384 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	474	ARG	N-CA-C	7.27	121.42	111.54
2	B	2	PRO	N-CA-CB	6.42	110.06	103.00
2	D	2	PRO	N-CA-CB	6.36	109.99	103.00
1	C	474	ARG	N-CA-C	5.68	119.18	111.17
2	D	20	ARG	N-CA-C	5.60	118.30	108.56
1	A	265	HIS	N-CA-C	5.01	120.77	114.31

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	3864	0	3918	48	0
1	C	3148	0	3116	42	0
2	B	286	0	238	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	233	0	203	4	0
3	A	180	0	0	4	0
3	B	12	0	0	1	0
3	C	67	0	0	1	0
3	D	4	0	0	0	0
All	All	7794	0	7475	96	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 (96) 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:C:280:GLN:HE21	1:C:280:GLN:N	1.72	0.87
1:C:280:GLN:HE21	1:C:280:GLN:H	0.89	0.87
1:A:399:GLU:HG3	1:A:437:MET:SD	2.15	0.87
1:A:363:MET:HA	1:A:363:MET:HE2	1.58	0.85
1:C:280:GLN:H	1:C:280:GLN:NE2	1.75	0.83
1:C:364:GLN:H	1:C:364:GLN:HE21	1.33	0.77
1:C:364:GLN:H	1:C:364:GLN:NE2	1.84	0.75
1:A:364:GLN:HE22	1:A:395:GLN:HE21	1.33	0.75
1:C:587:ARG:HG3	1:C:621:LEU:HD23	1.70	0.74
1:A:469:ARG:HH21	1:A:470:HIS:CE1	2.07	0.72
1:C:469:ARG:HH21	1:C:470:HIS:CE1	2.13	0.67
1:C:326:ASN:HD22	1:C:329:ARG:HH21	1.44	0.65
1:A:308:ASN:HD22	1:A:311:SER:H	1.43	0.65
1:A:287:ASN:HD22	1:A:287:ASN:H	1.45	0.64
1:A:469:ARG:HH21	1:A:470:HIS:HE1	1.46	0.63
1:C:326:ASN:ND2	1:C:329:ARG:HH21	1.98	0.62
1:C:491:LEU:HD23	1:C:526:PRO:HB2	1.81	0.61
1:A:363:MET:HE2	1:A:385:LEU:HD23	1.83	0.61
1:A:321:PRO:HB3	1:A:357:ILE:HD13	1.82	0.60
1:C:525:ALA:HB3	1:C:526:PRO:HD3	1.83	0.59
1:C:302:GLN:HB2	1:C:343:VAL:HG22	1.86	0.57
1:A:354:LYS:HG3	1:A:388:LEU:HD23	1.87	0.57
1:C:458:GLU:HA	1:C:461:THR:OG1	2.05	0.56
1:C:620:GLU:O	1:C:623:GLN:HG2	2.06	0.56
1:A:260:HIS:HD2	2:B:45:LYS:NZ	2.05	0.55
1:A:260:HIS:HE1	1:A:299:ASP:OD1	1.92	0.53
1:A:364:GLN:HE22	1:A:395:GLN:NE2	2.02	0.52
1:A:203:GLN:HG3	1:A:242:LYS:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ILE:HB	1:A:238:PRO:HD3	1.92	0.52
1:A:287:ASN:HD22	1:A:287:ASN:N	2.05	0.52
1:A:480:MET:HE2	3:A:791:HOH:O	2.10	0.52
1:C:543:ALA:HA	1:C:566:MET:HE3	1.91	0.52
1:A:363:MET:CE	1:A:385:LEU:HD23	2.40	0.52
1:A:353:ASN:O	1:A:357:ILE:HG12	2.10	0.51
2:D:11:GLU:H	2:D:11:GLU:CD	2.18	0.51
1:C:237:ILE:O	1:C:241:VAL:HG23	2.10	0.50
1:A:518:ALA:O	1:A:524:HIS:HE1	1.94	0.50
1:A:221:LEU:O	1:A:227:GLY:HA3	2.11	0.50
1:A:363:MET:HE3	1:A:388:LEU:HD13	1.93	0.50
1:A:302:GLN:OE1	2:B:27:GLN:HG2	2.11	0.49
1:C:299:ASP:O	1:C:303:ILE:HG13	2.12	0.49
1:C:292:LYS:O	1:C:296:ILE:HG12	2.13	0.49
1:A:620:GLU:O	1:A:623:GLN:HG2	2.13	0.49
1:C:654:TYR:O	1:C:658:VAL:HG23	2.12	0.49
1:C:558:GLN:HA	1:C:565:ARG:HH22	1.78	0.48
1:A:607:ILE:HA	2:B:2:PRO:O	2.13	0.48
2:B:20:ARG:HG2	3:B:351:HOH:O	2.13	0.48
1:C:414:ILE:HG13	1:C:460:ILE:HD11	1.95	0.48
1:A:543:ALA:O	1:A:547:THR:HG23	2.15	0.47
1:C:469:ARG:HH21	1:C:470:HIS:HE1	1.61	0.47
1:A:198:ILE:HD13	1:A:217:THR:HG21	1.97	0.46
1:A:480:MET:CE	1:A:484:ALA:HB2	2.45	0.46
2:D:49:VAL:HG23	2:D:50:ASN:H	1.80	0.46
2:B:27:GLN:O	2:B:29:GLU:N	2.48	0.46
1:C:541:VAL:O	1:C:545:GLN:HG3	2.15	0.45
1:C:260:HIS:HE1	1:C:299:ASP:OD2	1.99	0.45
1:A:570:VAL:O	1:A:574:THR:HG23	2.17	0.44
1:C:237:ILE:N	1:C:238:PRO:HD2	2.32	0.44
1:C:486:ARG:HG3	1:C:491:LEU:HD22	1.98	0.44
2:D:49:VAL:HG23	2:D:50:ASN:N	2.32	0.44
1:A:292:LYS:HG3	3:A:830:HOH:O	2.17	0.44
1:A:524:HIS:HD2	3:A:749:HOH:O	2.01	0.44
1:C:447:LEU:O	1:C:451:VAL:HG23	2.18	0.44
1:A:449:ARG:HH11	1:A:449:ARG:HG3	1.82	0.44
1:A:296:ILE:HD13	2:B:41:LEU:HD13	2.00	0.44
1:A:582:ARG:NH2	2:B:11:GLU:HG3	2.32	0.44
1:C:404:THR:O	1:C:408:LEU:HG	2.17	0.44
1:C:489:TYR:HB3	3:C:668:HOH:O	2.18	0.44
1:C:622:ALA:C	1:C:624:ASP:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:THR:O	1:A:431:ASN:ND2	2.45	0.43
1:A:363:MET:HE3	1:A:388:LEU:CD1	2.48	0.43
1:C:504:TRP:CZ2	1:C:566:MET:HE1	2.53	0.43
1:C:535:ARG:HA	1:C:538:GLN:HG2	2.00	0.43
1:C:227:GLY:O	1:C:231:ILE:HG13	2.19	0.43
1:A:513:LEU:O	1:A:517:LEU:HG	2.19	0.42
1:A:453:ARG:HD2	3:A:843:HOH:O	2.19	0.42
1:C:393:THR:C	1:C:394:LYS:HD2	2.44	0.42
1:C:370:LEU:HB2	1:C:404:THR:HG21	2.02	0.42
1:A:363:MET:HE1	1:A:385:LEU:HA	2.02	0.42
1:A:654:TYR:O	1:A:658:VAL:HG23	2.20	0.42
1:A:480:MET:C	1:A:480:MET:SD	3.02	0.41
1:A:627:ALA:O	1:A:631:ILE:HG13	2.20	0.41
1:C:490:GLY:O	1:C:494:VAL:HG23	2.20	0.41
1:A:490:GLY:O	1:A:494:VAL:HG23	2.20	0.41
2:B:7:GLY:HA2	2:B:17:GLU:OE2	2.21	0.41
1:A:338:TRP:O	1:A:342:ARG:HG3	2.21	0.41
1:A:425:SER:O	1:A:470:HIS:HD2	2.04	0.41
1:A:497:LEU:HD22	1:A:506:LEU:HD21	2.03	0.41
1:C:372:ASP:HA	1:C:373:PRO:HD3	1.92	0.41
1:C:515:ARG:HD3	2:D:14:ALA:HB2	2.03	0.40
1:C:263:LEU:HD21	1:C:273:VAL:HG21	2.03	0.40
1:A:458:GLU:HG2	1:A:506:LEU:HD22	2.03	0.40
1:C:528:ARG:HD3	1:C:586:ASN:OD1	2.20	0.40
1:A:609:ASN:HD22	1:A:609:ASN:HA	1.67	0.40
1:C:326:ASN:ND2	1:C:329:ARG:NH2	2.66	0.40
1:C:639:PRO:O	1:C:643:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	518/532 (97%)	514 (99%)	4 (1%)	0	100	100
1	C	435/532 (82%)	428 (98%)	7 (2%)	0	100	100
2	B	37/61 (61%)	31 (84%)	2 (5%)	4 (11%)	0	0
2	D	30/61 (49%)	29 (97%)	1 (3%)	0	100	100
All	All	1020/1186 (86%)	1002 (98%)	14 (1%)	4 (0%)	30	28

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	25	GLY
2	B	51	GLU
2	B	28	GLU
2	B	26	GLU

5.3.2 Protein sidechains ⓘ

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	403/441 (91%)	402 (100%)	1 (0%)	87	93
1	C	312/441 (71%)	310 (99%)	2 (1%)	78	86
2	B	26/50 (52%)	24 (92%)	2 (8%)	12	9
2	D	21/50 (42%)	20 (95%)	1 (5%)	23	23
All	All	762/982 (78%)	756 (99%)	6 (1%)	73	81

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	287	ASN
2	B	26	GLU
2	B	27	GLN
1	C	280	GLN
1	C	364	GLN
2	D	11	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	A	165	GLN
1	A	204	ASN
1	A	220	ASN
1	A	260	HIS
1	A	287	ASN
1	A	308	ASN
1	A	322	GLN
1	A	395	GLN
1	A	440	GLN
1	A	470	HIS
1	A	482	GLN
1	A	524	HIS
1	A	530	GLN
1	A	548	GLN
1	A	594	ASN
1	A	611	GLN
1	C	260	HIS
1	C	261	ASN
1	C	280	GLN
1	C	290	ASN
1	C	302	GLN
1	C	326	ASN
1	C	364	GLN
1	C	369	HIS
1	C	395	GLN
1	C	434	ASN
1	C	440	GLN
1	C	470	HIS
1	C	482	GLN
1	C	503	HIS
1	C	530	GLN
1	C	538	GLN
1	C	545	GLN
1	C	594	ASN
1	C	611	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.