



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 12:57 AM GMT

PDB ID : 1LUJ
Title : Crystal Structure of the Beta-catenin/ICAT Complex
Authors : Graham, T.A.; Clements, W.K.; Kimelman, D.; Xu, W.
Deposited on : 2002-05-22
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

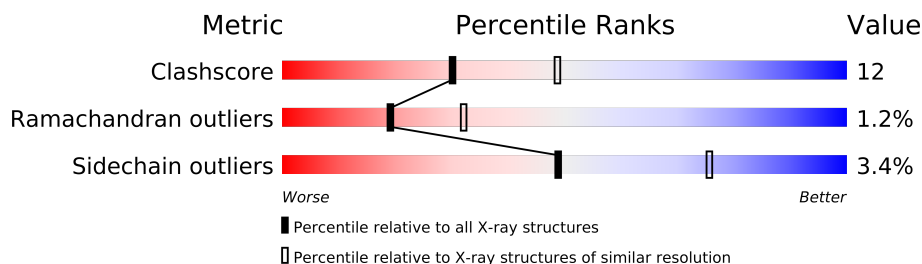
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : NOT EXECUTED
EDS : NOT EXECUTED
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	514	
2	B	75	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4216 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			3699	2331	669	673	26			

- Molecule 2 is a protein called beta-catenin-interactingprotein ICAT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	71	Total	C	N	O	S	0	0	0
			517	323	89	102	3			

There are 3 discrepancies between the modelled and reference sequences:

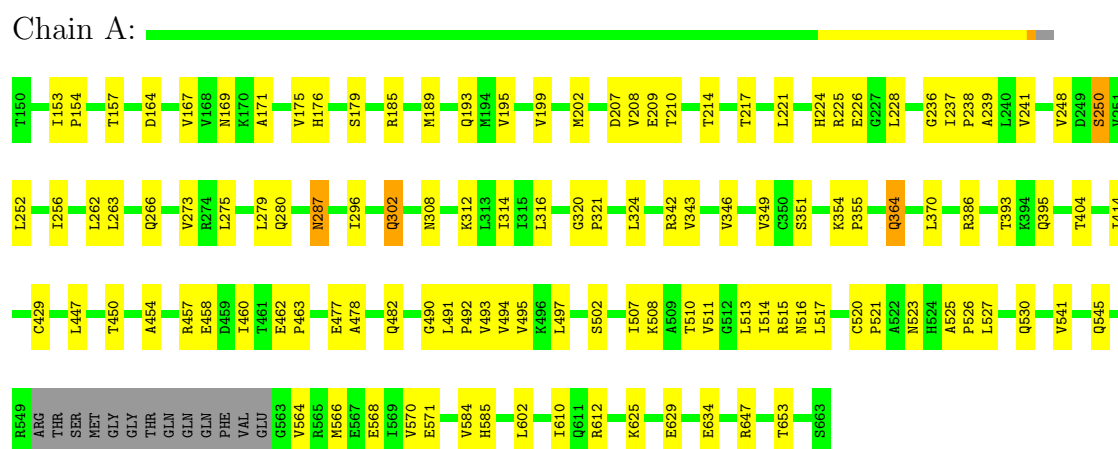
Chain	Residue	Modelled	Actual	Comment	Reference
B	8	ALA	GLY	CONFLICT	UNP Q9NSA3
B	49	SER	ASN	CONFLICT	UNP Q9NSA3
B	63	ALA	GLY	CONFLICT	UNP Q9NSA3

3 Residue-property plots

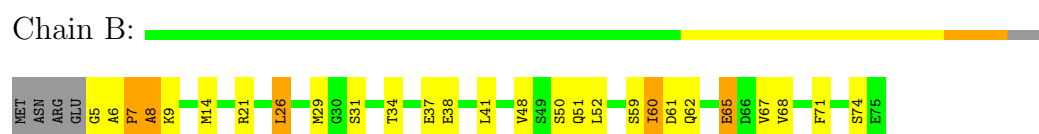
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Beta-catenin



• Molecule 2: beta-catenin-interactingprotein ICAT



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 2	Depositor
Cell constants a, b, c, α , β , γ	95.17Å 98.50Å 86.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.74 – 2.50	Depositor
% Data completeness (in resolution range)	82.8 (43.74-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.210 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4216	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

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	0.33	0/3752	0.56	0/5111
2	B	0.42	0/524	0.56	0/709
All	All	0.34	0/4276	0.56	0/5820

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3699	0	3758	85	0
2	B	517	0	477	23	0
All	All	4216	0	4235	101	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (101) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:653:THR:HG21	2:B:29:MET:HE3	1.50	0.93
2:B:8:ALA:HB3	2:B:14:MET:SD	2.12	0.90

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:26:LEU:HD22	2:B:31:SER:HB2	1.55	0.87
2:B:6:ALA:HB1	2:B:7:PRO:HD2	1.59	0.83
1:A:364:GLN:H	1:A:364:GLN:HE21	1.28	0.81
2:B:48:VAL:O	2:B:52:LEU:HB2	1.81	0.79
1:A:364:GLN:H	1:A:364:GLN:NE2	1.80	0.79
1:A:508:LYS:HE3	1:A:568:GLU:OE1	1.87	0.75
1:A:447:LEU:O	1:A:450:THR:HG22	1.90	0.70
1:A:612:ARG:NH1	2:B:62:GLN:HA	2.07	0.69
2:B:34:THR:HG23	2:B:37:GLU:H	1.59	0.67
1:A:185:ARG:HH11	1:A:224:HIS:CE1	2.15	0.65
1:A:263:LEU:HD21	1:A:273:VAL:HG21	1.78	0.65
2:B:5:GLY:N	2:B:50:SER:HG	1.95	0.64
1:A:490:GLY:O	1:A:494:VAL:HG23	1.97	0.64
1:A:164:ASP:O	1:A:167:VAL:HG22	1.97	0.64
1:A:564:VAL:HG13	1:A:564:VAL:O	1.98	0.63
2:B:21:ARG:HB2	2:B:51:GLN:NE2	2.13	0.63
1:A:176:HIS:O	1:A:179:SER:HB3	1.99	0.62
2:B:68:VAL:O	2:B:68:VAL:HG13	1.98	0.62
1:A:510:THR:O	1:A:514:ILE:HG12	1.99	0.62
1:A:625:LYS:O	1:A:629:GLU:HG3	2.00	0.62
1:A:478:ALA:O	1:A:482:GLN:HG3	2.00	0.62
1:A:225:ARG:NH1	1:A:266:GLN:OE1	2.32	0.61
1:A:515:ARG:HH11	1:A:516:ASN:ND2	1.99	0.61
1:A:612:ARG:HH12	2:B:62:GLN:HA	1.66	0.61
1:A:515:ARG:C	1:A:515:ARG:HD3	2.22	0.60
2:B:21:ARG:HB2	2:B:51:GLN:HE22	1.68	0.57
1:A:207:ASP:OD2	1:A:210:THR:HG23	2.04	0.57
1:A:490:GLY:O	1:A:493:VAL:HG12	2.03	0.57
1:A:185:ARG:NH1	1:A:224:HIS:CE1	2.73	0.56
1:A:202:MET:HB2	1:A:214:THR:OG1	2.05	0.56
1:A:354:LYS:HB3	1:A:355:PRO:HD3	1.88	0.56
1:A:454:ALA:O	1:A:457:ARG:HB2	2.06	0.56
1:A:653:THR:HG21	2:B:29:MET:CE	2.30	0.56
1:A:460:ILE:O	1:A:463:PRO:HD2	2.05	0.56
1:A:349:VAL:HG11	2:B:74:SER:H	1.72	0.55
1:A:320:GLY:N	1:A:321:PRO:HD2	2.22	0.55
1:A:634:GLU:O	1:A:634:GLU:HG3	2.08	0.54
1:A:237:ILE:O	1:A:241:VAL:HG23	2.08	0.54
2:B:34:THR:HG22	2:B:37:GLU:CD	2.29	0.53
1:A:458:GLU:OE2	1:A:502:SER:HA	2.09	0.53
1:A:280:GLN:NE2	1:A:314:ILE:HG21	2.24	0.52
1:A:491:LEU:HD22	1:A:527:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:515:ARG:HH11	1:A:516:ASN:HD22	1.57	0.52
1:A:447:LEU:HA	1:A:450:THR:HG22	1.91	0.51
1:A:302:GLN:HB2	1:A:343:VAL:HG22	1.91	0.51
1:A:236:GLY:O	1:A:239:ALA:HB3	2.11	0.51
1:A:279:LEU:HB2	1:A:280:GLN:NE2	2.27	0.50
2:B:34:THR:HG22	2:B:37:GLU:CG	2.42	0.49
1:A:237:ILE:HB	1:A:238:PRO:HD3	1.94	0.49
1:A:189:MET:CE	1:A:226:GLU:HB2	2.42	0.49
2:B:29:MET:HG2	2:B:60:ILE:H	1.78	0.49
2:B:7:PRO:O	2:B:8:ALA:HB2	2.13	0.49
1:A:429:CYS:SG	2:B:67:VAL:C	2.92	0.48
1:A:513:LEU:O	1:A:517:LEU:HG	2.13	0.48
1:A:525:ALA:HB3	1:A:526:PRO:HD3	1.95	0.48
1:A:185:ARG:HD2	1:A:224:HIS:HE1	1.79	0.47
1:A:414:ILE:HG23	1:A:460:ILE:HD11	1.96	0.47
1:A:153:ILE:N	1:A:154:PRO:HD2	2.30	0.47
1:A:202:MET:HB2	1:A:214:THR:CB	2.45	0.47
1:A:320:GLY:O	1:A:324:LEU:HG	2.14	0.47
1:A:287:ASN:H	1:A:287:ASN:HD22	1.63	0.47
1:A:584:VAL:HG13	1:A:585:HIS:N	2.29	0.47
1:A:491:LEU:HB2	1:A:492:PRO:HD3	1.96	0.47
1:A:228:LEU:HD22	1:A:262:LEU:HD23	1.96	0.47
1:A:208:VAL:HG23	1:A:209:GLU:N	2.30	0.47
1:A:495:VAL:HG21	1:A:530:GLN:HB3	1.96	0.47
1:A:462:GLU:HB3	1:A:463:PRO:HD3	1.96	0.47
1:A:179:SER:HB2	1:A:217:THR:HG23	1.96	0.46
1:A:217:THR:O	1:A:221:LEU:HG	2.16	0.46
1:A:157:THR:HG21	1:A:193:GLN:HG2	1.98	0.46
1:A:169:ASN:HA	1:A:210:THR:HG22	1.98	0.46
1:A:507:ILE:O	1:A:511:VAL:HG23	2.16	0.46
1:A:395:GLN:HB3	1:A:395:GLN:HE21	1.60	0.46
1:A:308:ASN:O	1:A:312:LYS:HG3	2.16	0.46
1:A:287:ASN:N	1:A:287:ASN:HD22	2.15	0.45
1:A:171:ALA:O	1:A:175:VAL:HG23	2.16	0.45
2:B:29:MET:HA	2:B:59:SER:CB	2.48	0.44
1:A:346:VAL:O	1:A:349:VAL:HG22	2.17	0.44
1:A:493:VAL:O	1:A:497:LEU:HG	2.18	0.44
2:B:21:ARG:CZ	2:B:51:GLN:NE2	2.80	0.44
1:A:541:VAL:O	1:A:545:GLN:HG3	2.18	0.43
1:A:566:MET:O	1:A:570:VAL:HG23	2.18	0.43
1:A:386:ARG:HG2	2:B:71:PHE:CD2	2.53	0.43
1:A:185:ARG:HH11	1:A:185:ARG:HG2	1.84	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:571:GLU:HB2	1:A:610:ILE:CD1	2.50	0.42
1:A:248:VAL:HG12	1:A:250:SER:HB3	2.02	0.42
1:A:523:ASN:C	1:A:526:PRO:HD2	2.40	0.42
1:A:316:LEU:HD12	1:A:316:LEU:O	2.20	0.42
1:A:447:LEU:C	1:A:450:THR:HG22	2.40	0.41
1:A:520:CYS:HA	1:A:521:PRO:HD2	1.88	0.41
1:A:202:MET:HB2	1:A:214:THR:HB	2.02	0.41
1:A:256:ILE:HG23	1:A:296:ILE:HG21	2.02	0.41
1:A:491:LEU:HD23	1:A:491:LEU:HA	1.89	0.41
1:A:189:MET:HE3	1:A:226:GLU:HB2	2.00	0.41
1:A:370:LEU:HB2	1:A:404:THR:HG21	2.02	0.41
1:A:571:GLU:HB2	1:A:610:ILE:HD11	2.03	0.41
1:A:195:VAL:O	1:A:199:VAL:HG23	2.21	0.41
1:A:280:GLN:NE2	1:A:280:GLN:N	2.68	0.40
2:B:68:VAL:O	2:B:68:VAL:CG1	2.69	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	497/514 (97%)	481 (97%)	14 (3%)	2 (0%)	43	66
2	B	69/75 (92%)	55 (80%)	9 (13%)	5 (7%)	2	1
All	All	566/589 (96%)	536 (95%)	23 (4%)	7 (1%)	19	32

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	60	ILE
2	B	65	GLU
1	A	250	SER
2	B	61	ASP
1	A	351	SER

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Mol	Chain	Res	Type
2	B	7	PRO
2	B	8	ALA

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	386/426 (91%)	376 (97%)	10 (3%)	59	84
2	B	49/65 (75%)	44 (90%)	5 (10%)	11	19
All	All	435/491 (89%)	420 (97%)	15 (3%)	49	75

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	LEU
1	A	275	LEU
1	A	287	ASN
1	A	302	GLN
1	A	342	ARG
1	A	364	GLN
1	A	393	THR
1	A	477	GLU
1	A	602	LEU
1	A	647	ARG
2	B	9	LYS
2	B	26	LEU
2	B	38	GLU
2	B	41	LEU
2	B	65	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	ASN
1	A	165	GLN
1	A	220	ASN

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Mol	Chain	Res	Type
1	A	223	HIS
1	A	224	HIS
1	A	261	ASN
1	A	280	GLN
1	A	287	ASN
1	A	302	GLN
1	A	364	GLN
1	A	395	GLN
1	A	516	ASN
1	A	548	GLN
1	A	578	HIS
1	A	611	GLN
1	A	623	GLN
2	B	17	GLN
2	B	51	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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.