



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 07:45 PM UTC

PDB ID : 3ML6 / pdb\_00003ml6  
Title : a complex between Dishevelled2 and clathrin adaptor AP-2  
Authors : Yu, A.; Xing, Y.; Harrison, S.C.; Kirchhausen, T.L.  
Deposited on : 2010-04-16  
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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>.

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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) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

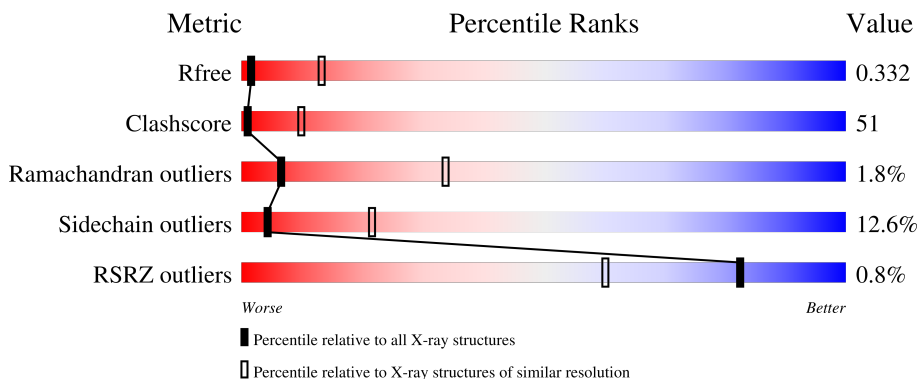
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
$R_{free}$	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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  $\geq 3$ , 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	385	
1	B	385	
1	C	385	
1	D	385	
1	E	385	

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Mol	Chain	Length	Quality of chain
1	F	385	 <p>A horizontal bar chart showing the quality of chain. The bar is divided into four segments: green (33%), yellow (48%), orange (8%), and grey (12%). A small red square is at the beginning of the bar, and a '%' symbol is above it.</p>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16319 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 Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	S	0	0	0
			2787	1790	480	498	19			
1	B	339	Total	C	N	O	S	0	0	0
			2695	1732	466	478	19			
1	C	350	Total	C	N	O	S	0	0	0
			2780	1785	479	497	19			
1	D	336	Total	C	N	O	S	0	0	0
			2668	1716	460	473	19			
1	E	338	Total	C	N	O	S	0	0	0
			2686	1725	463	479	19			
1	F	340	Total	C	N	O	S	0	0	0
			2703	1736	467	481	19			

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	415	GLY	-	expression tag	UNP Q60838
A	416	ALA	-	expression tag	UNP Q60838
A	1147	GLY	-	linker	UNP P84092
A	1148	PRO	-	linker	UNP P84092
A	1149	ARG	-	linker	UNP P84092
A	1150	PRO	-	linker	UNP P84092
A	1151	TYR	-	linker	UNP P84092
A	1152	SER	-	linker	UNP P84092
A	1153	PRO	-	linker	UNP P84092
A	1154	GLN	-	linker	UNP P84092
A	1155	PRO	-	linker	UNP P84092
A	1156	PRO	-	linker	UNP P84092
A	1157	PRO	-	linker	UNP P84092
A	1158	TYR	-	linker	UNP P84092
A	1159	HIS	-	linker	UNP P84092
A	1160	GLU	-	linker	UNP P84092

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1161	LEU	-	linker	UNP P84092
A	1162	GLU	-	linker	UNP P84092
A	1163	PHE	-	linker	UNP P84092
A	1164	GLY	-	linker	UNP P84092
A	1165	GLY	-	linker	UNP P84092
A	1166	SER	-	linker	UNP P84092
A	1167	GLY	-	linker	UNP P84092
A	1168	GLY	-	linker	UNP P84092
A	1169	SER	-	linker	UNP P84092
B	415	GLY	-	expression tag	UNP Q60838
B	416	ALA	-	expression tag	UNP Q60838
B	1147	GLY	-	linker	UNP P84092
B	1148	PRO	-	linker	UNP P84092
B	1149	ARG	-	linker	UNP P84092
B	1150	PRO	-	linker	UNP P84092
B	1151	TYR	-	linker	UNP P84092
B	1152	SER	-	linker	UNP P84092
B	1153	PRO	-	linker	UNP P84092
B	1154	GLN	-	linker	UNP P84092
B	1155	PRO	-	linker	UNP P84092
B	1156	PRO	-	linker	UNP P84092
B	1157	PRO	-	linker	UNP P84092
B	1158	TYR	-	linker	UNP P84092
B	1159	HIS	-	linker	UNP P84092
B	1160	GLU	-	linker	UNP P84092
B	1161	LEU	-	linker	UNP P84092
B	1162	GLU	-	linker	UNP P84092
B	1163	PHE	-	linker	UNP P84092
B	1164	GLY	-	linker	UNP P84092
B	1165	GLY	-	linker	UNP P84092
B	1166	SER	-	linker	UNP P84092
B	1167	GLY	-	linker	UNP P84092
B	1168	GLY	-	linker	UNP P84092
B	1169	SER	-	linker	UNP P84092
C	415	GLY	-	expression tag	UNP Q60838
C	416	ALA	-	expression tag	UNP Q60838
C	1147	GLY	-	linker	UNP P84092
C	1148	PRO	-	linker	UNP P84092
C	1149	ARG	-	linker	UNP P84092
C	1150	PRO	-	linker	UNP P84092
C	1151	TYR	-	linker	UNP P84092
C	1152	SER	-	linker	UNP P84092

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1153	PRO	-	linker	UNP P84092
C	1154	GLN	-	linker	UNP P84092
C	1155	PRO	-	linker	UNP P84092
C	1156	PRO	-	linker	UNP P84092
C	1157	PRO	-	linker	UNP P84092
C	1158	TYR	-	linker	UNP P84092
C	1159	HIS	-	linker	UNP P84092
C	1160	GLU	-	linker	UNP P84092
C	1161	LEU	-	linker	UNP P84092
C	1162	GLU	-	linker	UNP P84092
C	1163	PHE	-	linker	UNP P84092
C	1164	GLY	-	linker	UNP P84092
C	1165	GLY	-	linker	UNP P84092
C	1166	SER	-	linker	UNP P84092
C	1167	GLY	-	linker	UNP P84092
C	1168	GLY	-	linker	UNP P84092
C	1169	SER	-	linker	UNP P84092
D	415	GLY	-	expression tag	UNP Q60838
D	416	ALA	-	expression tag	UNP Q60838
D	1147	GLY	-	linker	UNP P84092
D	1148	PRO	-	linker	UNP P84092
D	1149	ARG	-	linker	UNP P84092
D	1150	PRO	-	linker	UNP P84092
D	1151	TYR	-	linker	UNP P84092
D	1152	SER	-	linker	UNP P84092
D	1153	PRO	-	linker	UNP P84092
D	1154	GLN	-	linker	UNP P84092
D	1155	PRO	-	linker	UNP P84092
D	1156	PRO	-	linker	UNP P84092
D	1157	PRO	-	linker	UNP P84092
D	1158	TYR	-	linker	UNP P84092
D	1159	HIS	-	linker	UNP P84092
D	1160	GLU	-	linker	UNP P84092
D	1161	LEU	-	linker	UNP P84092
D	1162	GLU	-	linker	UNP P84092
D	1163	PHE	-	linker	UNP P84092
D	1164	GLY	-	linker	UNP P84092
D	1165	GLY	-	linker	UNP P84092
D	1166	SER	-	linker	UNP P84092
D	1167	GLY	-	linker	UNP P84092
D	1168	GLY	-	linker	UNP P84092
D	1169	SER	-	linker	UNP P84092

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Chain	Residue	Modelled	Actual	Comment	Reference
E	415	GLY	-	expression tag	UNP Q60838
E	416	ALA	-	expression tag	UNP Q60838
E	1147	GLY	-	linker	UNP P84092
E	1148	PRO	-	linker	UNP P84092
E	1149	ARG	-	linker	UNP P84092
E	1150	PRO	-	linker	UNP P84092
E	1151	TYR	-	linker	UNP P84092
E	1152	SER	-	linker	UNP P84092
E	1153	PRO	-	linker	UNP P84092
E	1154	GLN	-	linker	UNP P84092
E	1155	PRO	-	linker	UNP P84092
E	1156	PRO	-	linker	UNP P84092
E	1157	PRO	-	linker	UNP P84092
E	1158	TYR	-	linker	UNP P84092
E	1159	HIS	-	linker	UNP P84092
E	1160	GLU	-	linker	UNP P84092
E	1161	LEU	-	linker	UNP P84092
E	1162	GLU	-	linker	UNP P84092
E	1163	PHE	-	linker	UNP P84092
E	1164	GLY	-	linker	UNP P84092
E	1165	GLY	-	linker	UNP P84092
E	1166	SER	-	linker	UNP P84092
E	1167	GLY	-	linker	UNP P84092
E	1168	GLY	-	linker	UNP P84092
E	1169	SER	-	linker	UNP P84092
F	415	GLY	-	expression tag	UNP Q60838
F	416	ALA	-	expression tag	UNP Q60838
F	1147	GLY	-	linker	UNP P84092
F	1148	PRO	-	linker	UNP P84092
F	1149	ARG	-	linker	UNP P84092
F	1150	PRO	-	linker	UNP P84092
F	1151	TYR	-	linker	UNP P84092
F	1152	SER	-	linker	UNP P84092
F	1153	PRO	-	linker	UNP P84092
F	1154	GLN	-	linker	UNP P84092
F	1155	PRO	-	linker	UNP P84092
F	1156	PRO	-	linker	UNP P84092
F	1157	PRO	-	linker	UNP P84092
F	1158	TYR	-	linker	UNP P84092
F	1159	HIS	-	linker	UNP P84092
F	1160	GLU	-	linker	UNP P84092
F	1161	LEU	-	linker	UNP P84092

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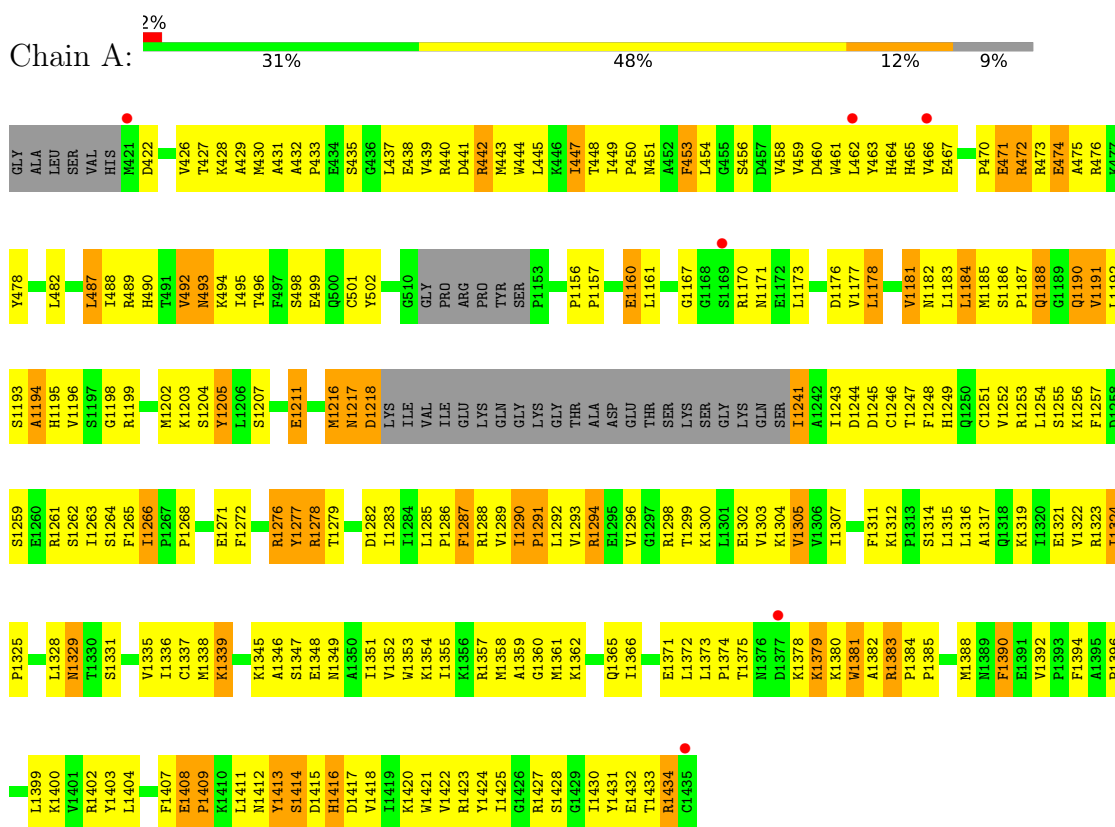
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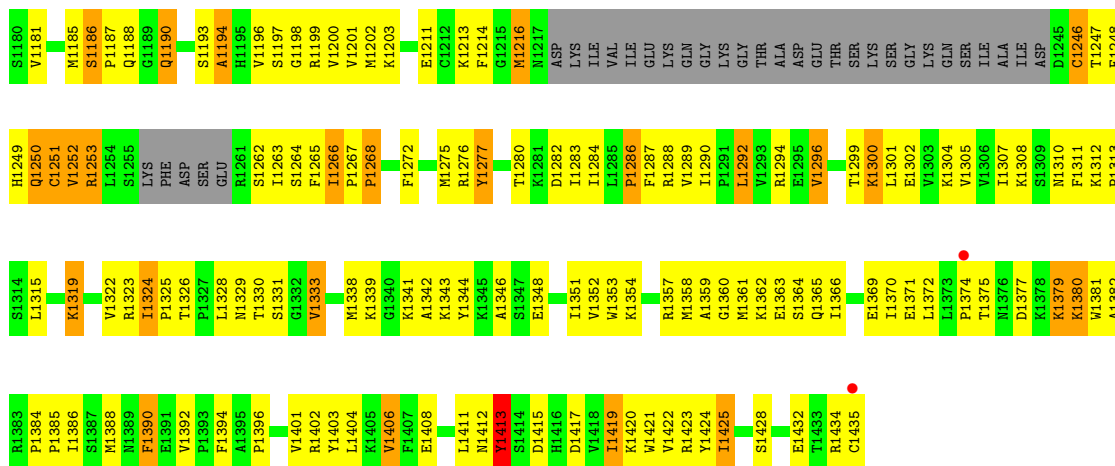
Chain	Residue	Modelled	Actual	Comment	Reference
F	1162	GLU	-	linker	UNP P84092
F	1163	PHE	-	linker	UNP P84092
F	1164	GLY	-	linker	UNP P84092
F	1165	GLY	-	linker	UNP P84092
F	1166	SER	-	linker	UNP P84092
F	1167	GLY	-	linker	UNP P84092
F	1168	GLY	-	linker	UNP P84092
F	1169	SER	-	linker	UNP P84092

### 3 Residue-property plots [i](#)

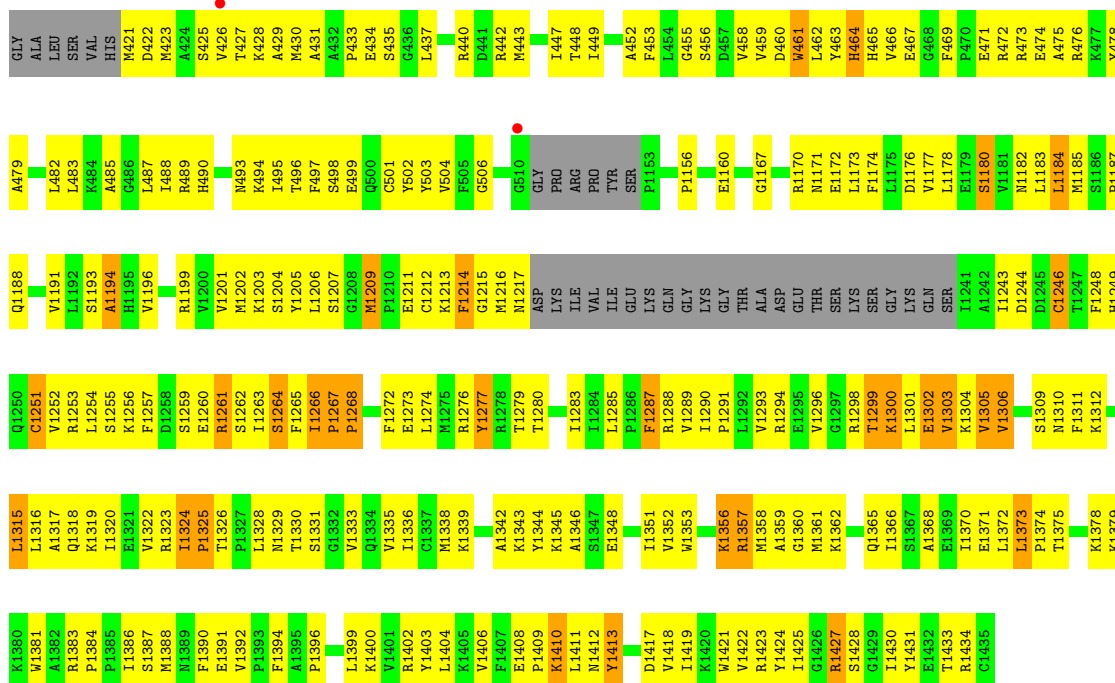
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu

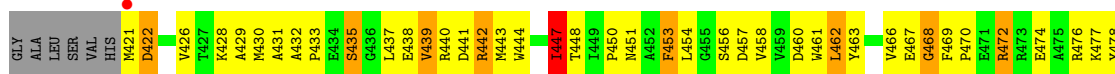


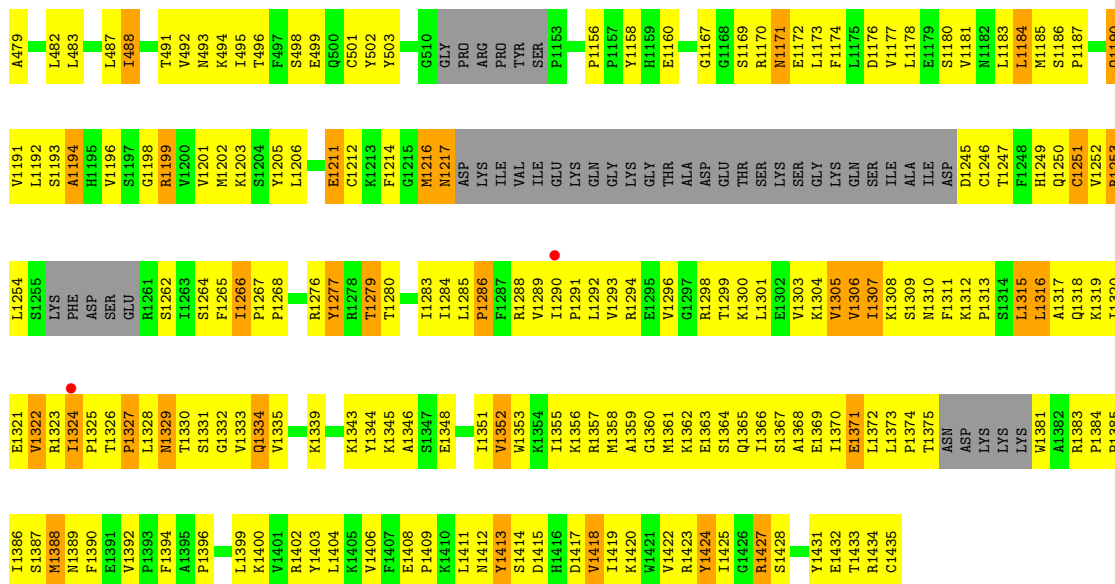


- Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu



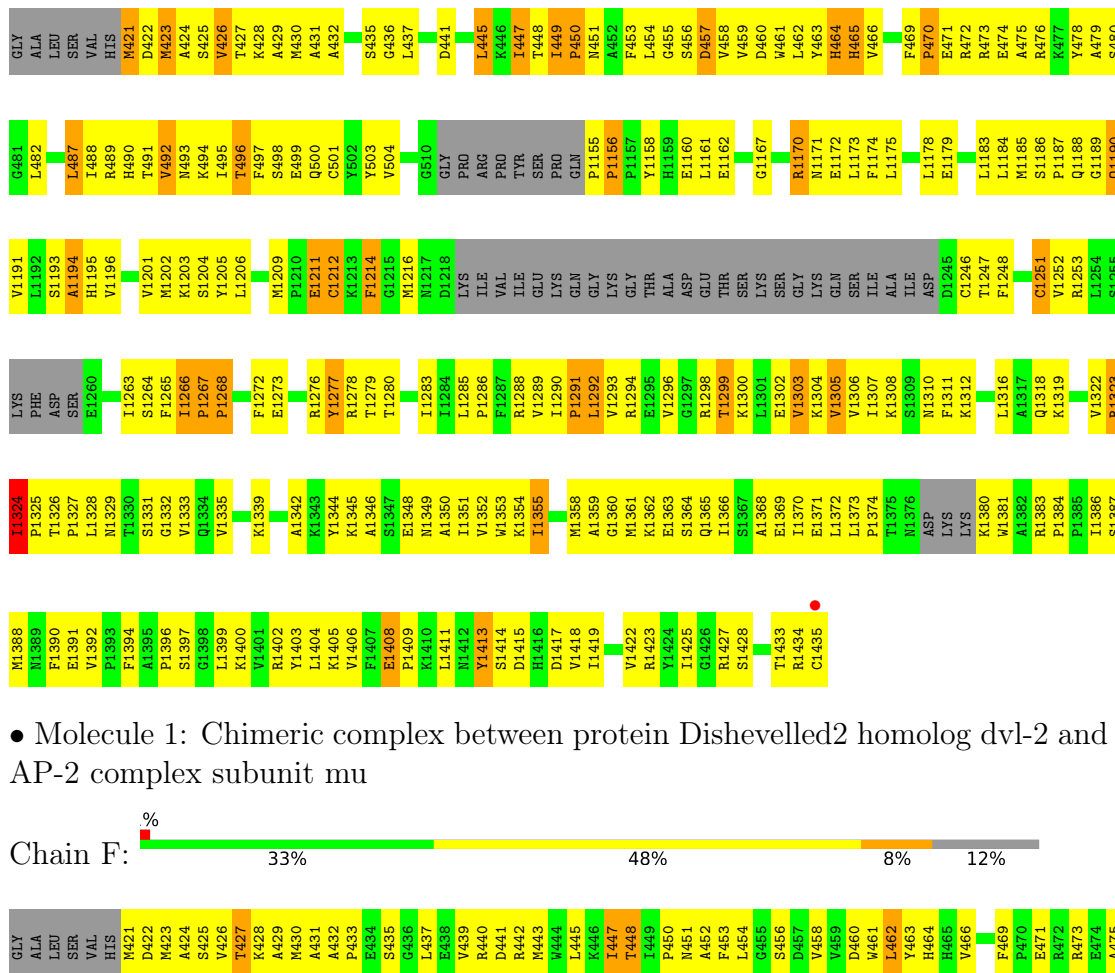
- Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu





- Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu

Chain E: 29% 50% 9% 12%



- Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu

Chain F: 33% 48% 8% 12%

V1392	L1389	L1322	C1251	M1185	Y478
P1393	K1400	R1323	V1252	S1186	L482
F1394	V1401	P1324	R1253	P1187	L487
A1395	R1402	L1325	L1254	Q1188	I488
P1396	Y1403	T1326	S1255	G1189	R489
	L1404	L1327	LYS	Q1190	H490
	K1405	L1328	PHE	V1191	T491
	V1406	M1329	ASP	L1192	V492
	F1407	T1330	SER	S1193	R493
	E1408	G1331	GLU	A1194	K494
	P1409	G1332	R1261	H1195	L495
	K1410	V1333	S1262	V1196	F497
	M1411	Q1334	I1263	S1197	E498
	M1412	V1335	S1264	G1198	E499
	Y1413	K1339	F1265	R1199	O500
	S1414	P1409	I1266	V1200	C501
	D1415	A1342	P1267	V1201	Y502
	H1416	K1345	P1268	L1206	Y503
	D1417	A1346	F1272	E1211	F504
	V1418	A1347	R1276	C1212	F505
	I1419	E1347	Y1277	K1213	G506
	K1420	E1348	R1278	F1214	B507
	W1421	E1349	T1279	G1215	
	V1422	I1351		M1216	
	R1423	V1352		N1217	
	Y1424	W1353		D1218	
	I1425	K1354		LYS	
	G1426	K1355		GLY	
	R1427	K1356		PRO	
	S1428	M1357		PRO	
		A1358		ARG	
		G1359		TYR	
		M1361		GLU	
		K1362		LYS	
		E1363		GLN	
		S1364		LYS	
		G1365		P1155	
		I1366		P1156	
		I1370		P1157	
		E1371		ALA	
		L1372		Y1158	
		L1373		H1159	
		P1374		E1160	
		T1375			
		K1379		G1167	
		K1380		R1170	
		W1381		G1171	
		A1382		LYS	
		R1383		E1172	
		P1384		L1173	
		P1385		F1174	
		P1386		L1175	
		I1387		D1176	
		S1387		V1177	
		M1388		L1178	
		F1389		E1179	
		E1391		S1180	
				C1245	
				T1247	
				F1248	
				H1249	
				L1183	
				L1184	

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	292.37Å 98.14Å 171.32Å 90.00° 121.97° 90.00°	Depositor
Resolution (Å)	49.07 – 3.50 49.07 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.07-3.50) 98.3 (49.07-3.50)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 3.48Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.308 , 0.335 0.308 , 0.332	Depositor DCC
$R_{free}$ test set	2576 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	107.5	Xtrriage
Anisotropy	0.646	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 85.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	16319	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	117.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

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	0.64	0/2851	1.02	13/3845 (0.3%)
1	B	0.58	0/2756	1.01	15/3714 (0.4%)
1	C	0.59	1/2844 (0.0%)	1.02	14/3835 (0.4%)
1	D	0.59	1/2729 (0.0%)	1.01	12/3680 (0.3%)
1	E	0.61	1/2746 (0.0%)	1.02	14/3701 (0.4%)
1	F	0.58	0/2764	0.98	10/3725 (0.3%)
All	All	0.60	3/16690 (0.0%)	1.01	78/22500 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1170	ARG	C-O	-7.73	1.14	1.23
1	C	461	TRP	C-N	-6.28	1.26	1.33
1	D	421	MET	CG-SD	6.13	1.96	1.80

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	E	1170	ARG	CA-C-O	-10.70	109.17	121.16
1	A	1381	TRP	N-CA-C	9.49	122.57	108.14
1	E	1408	GLU	CA-C-O	8.58	130.36	119.54
1	B	1155	PRO	CA-C-N	8.20	128.82	120.38
1	B	1155	PRO	C-N-CA	8.20	128.82	120.38

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	2787	0	2835	290	0
1	B	2695	0	2751	279	0
1	C	2780	0	2826	298	0
1	D	2668	0	2716	283	0
1	E	2686	0	2730	280	0
1	F	2703	0	2755	292	0
All	All	16319	0	16613	1679	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 51.

The worst 5 of 1679 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:1244:ASP:OD1	1:A:1279:THR:HA	1.24	1.37
1:C:462:LEU:O	1:C:466:VAL:HB	1.22	1.28
1:C:458:VAL:O	1:C:462:LEU:HG	1.28	1.24
1:C:462:LEU:O	1:C:466:VAL:CB	1.94	1.15
1:A:462:LEU:O	1:A:466:VAL:HB	1.43	1.14

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	345/385 (90%)	294 (85%)	44 (13%)	7 (2%)	6	32
1	B	331/385 (86%)	284 (86%)	40 (12%)	7 (2%)	5	31
1	C	344/385 (89%)	288 (84%)	52 (15%)	4 (1%)	10	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	326/385 (85%)	279 (86%)	41 (13%)	6 (2%)	6	34
1	E	328/385 (85%)	282 (86%)	39 (12%)	7 (2%)	5	31
1	F	332/385 (86%)	289 (87%)	38 (11%)	5 (2%)	8	37
All	All	2006/2310 (87%)	1716 (86%)	254 (13%)	36 (2%)	6	34

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1251	CYS
1	B	493	ASN
1	B	1379	LYS
1	C	493	ASN
1	E	493	ASN

### 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	308/337 (91%)	257 (83%)	51 (17%)	2	13
1	B	298/337 (88%)	260 (87%)	38 (13%)	4	21
1	C	307/337 (91%)	272 (89%)	35 (11%)	5	24
1	D	295/337 (88%)	253 (86%)	42 (14%)	3	18
1	E	297/337 (88%)	267 (90%)	30 (10%)	7	28
1	F	299/337 (89%)	268 (90%)	31 (10%)	7	27
All	All	1804/2022 (89%)	1577 (87%)	227 (13%)	4	21

5 of 227 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1328	LEU
1	F	1391	GLU
1	D	1277	TYR
1	F	1339	LYS

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Mol	Chain	Res	Type
1	F	448	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	1195	HIS
1	F	1190	GLN
1	E	1318	GLN
1	F	464	HIS
1	F	1217	ASN

### 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 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	351/385 (91%)	0.28	6 (1%) 69 43	91, 112, 131, 141	0
1	B	339/385 (88%)	0.19	2 (0%) 85 65	103, 117, 134, 145	0
1	C	350/385 (90%)	0.12	2 (0%) 85 65	99, 119, 132, 147	0
1	D	336/385 (87%)	0.31	3 (0%) 81 58	97, 117, 129, 136	0
1	E	338/385 (87%)	0.16	1 (0%) 90 76	98, 118, 132, 141	0
1	F	340/385 (88%)	0.12	3 (0%) 81 58	100, 120, 133, 140	0
All	All	2054/2310 (88%)	0.20	17 (0%) 82 60	91, 117, 132, 147	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	1261	ARG	3.6
1	B	1435	CYS	3.5
1	D	421	MET	2.9
1	B	1374	PRO	2.9
1	F	1435	CYS	2.7

### 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 oligosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.