



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:39 AM GMT

PDB ID : 3ML6
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.
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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

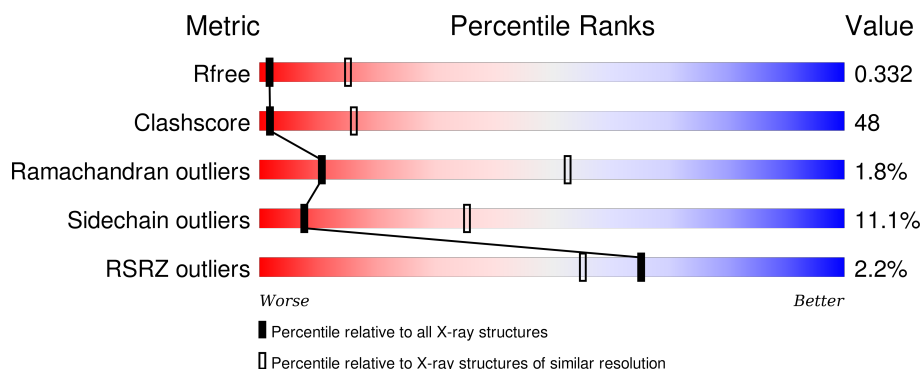
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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.

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	<div><div></div><div>3%</div><div>36%</div><div>46%</div><div>6%</div><div>12%</div></div>

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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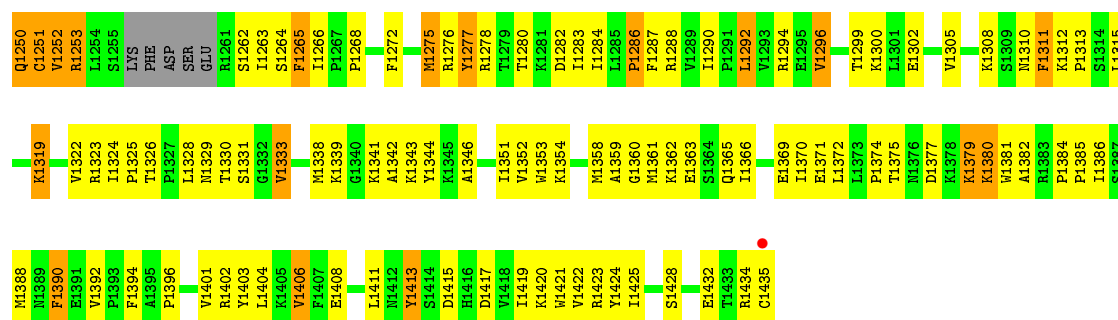
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Chain	Residue	Modelled	Actual	Comment	Reference
E	415	GLY	-	EXPRESSION TAG	UNP Q60838
E	416	ALA	-	EXPRESSION TAG	UNP Q60838
E	1147	GLY	-	LINKER	UNP P84092
E	1148	PRO	-	LINKER	UNP P84092
E	1149	ARG	-	LINKER	UNP P84092
E	1150	PRO	-	LINKER	UNP P84092
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

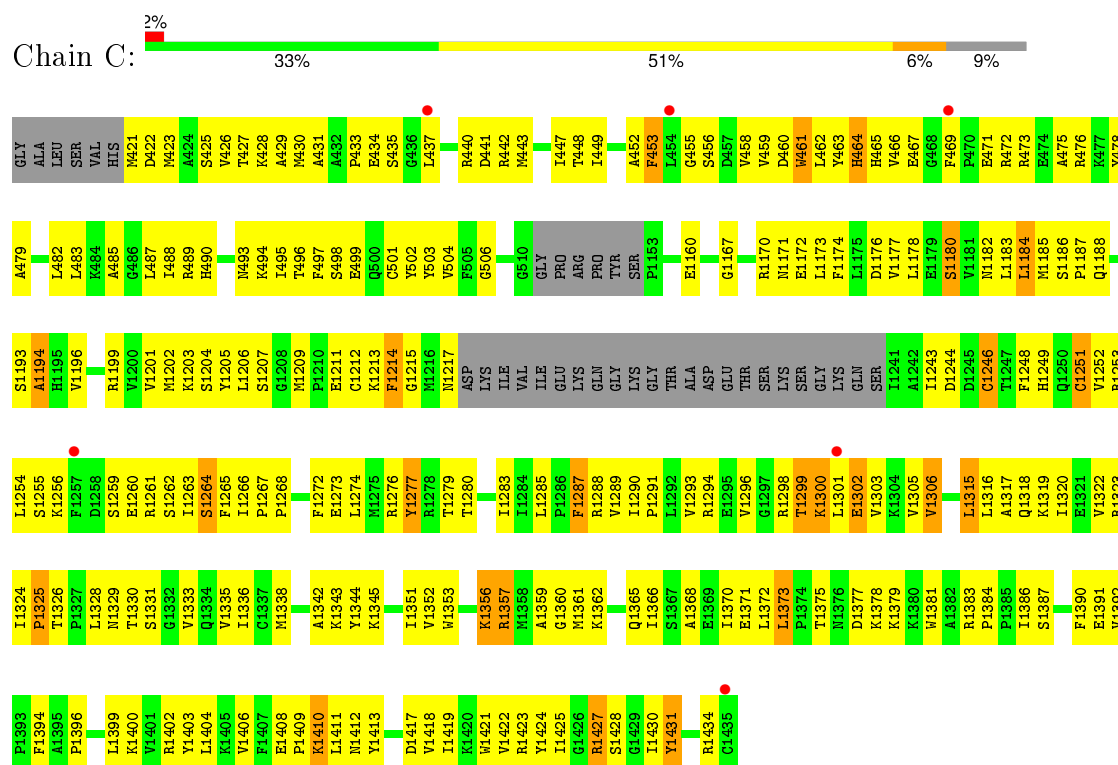
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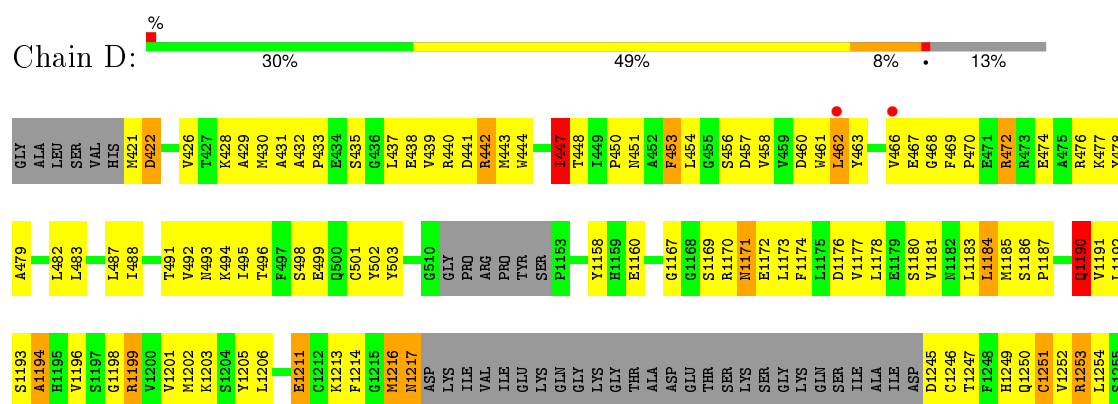
Chain	Residue	Modelled	Actual	Comment	Reference
F	1162	GLU	-	LINKER	UNP P84092
F	1163	PHE	-	LINKER	UNP P84092
F	1164	GLY	-	LINKER	UNP P84092
F	1165	GLY	-	LINKER	UNP P84092
F	1166	SER	-	LINKER	UNP P84092
F	1167	GLY	-	LINKER	UNP P84092
F	1168	GLY	-	LINKER	UNP P84092
F	1169	SER	-	LINKER	UNP P84092

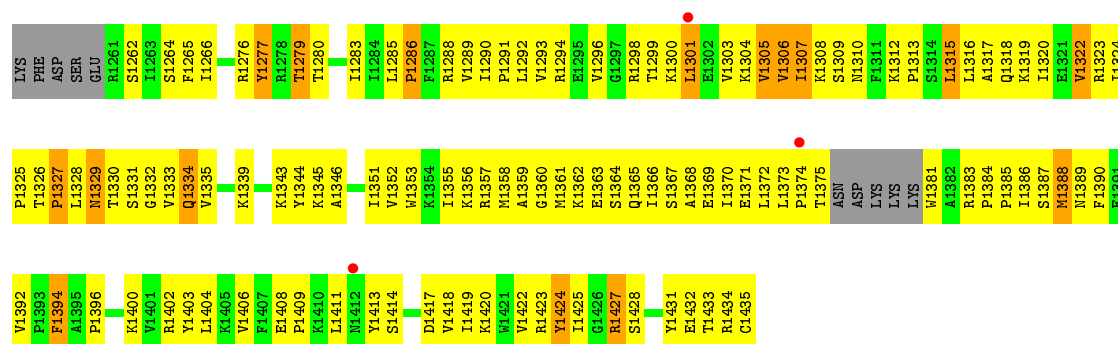


- Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu

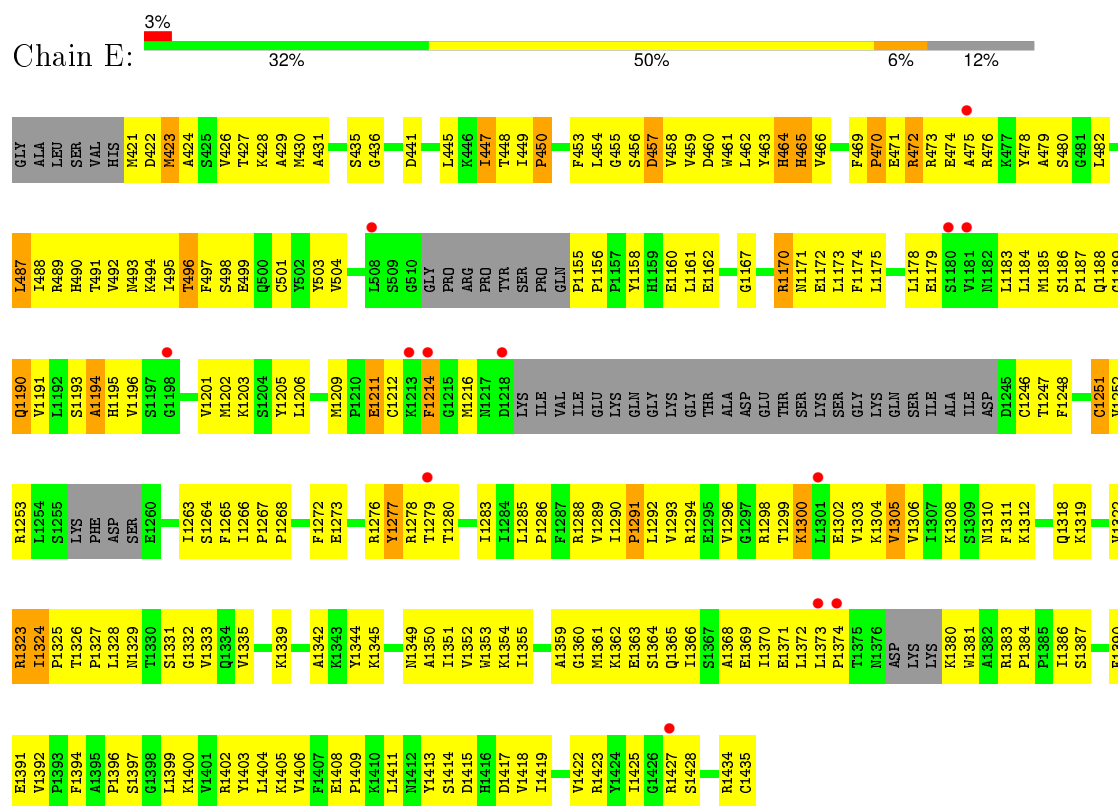


- Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu

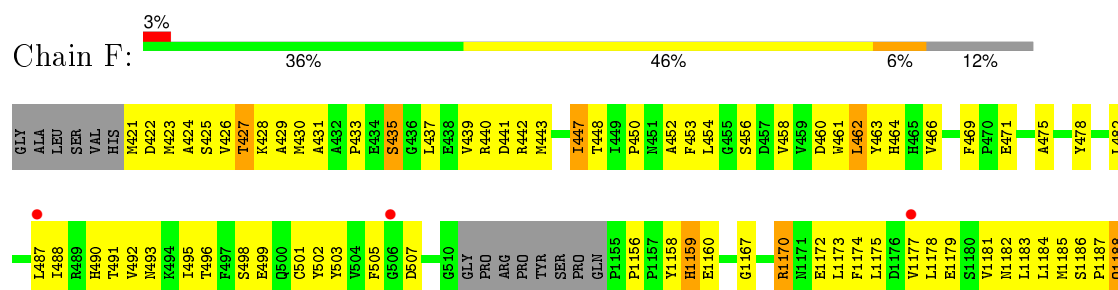




- Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu



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



L1399	L1327	ASP	G1189
K1400	L1328	SER	Q1190
V1401	M1329	GLU	V1191
R1402	T1330	R1261	L1192
Y1403	S1331	S1262	S1193
L1404	G1332	I1263	A1194
V1405	V1333	T1264	H1195
V1406	Q1334	F1265	V1196
F1407	V1335	I1266	
E1408	I1336	P1267	R1199
P1409	C1337	P1268	
K1410	M1338		L1206
L1411	K1339	F1272	
H1412	A1342	E1273	E1211
Y1413		L1274	G1212
S1414	K1345	M1275	K1213
D1415		R1276	F1214
H1416		Y1277	G1215
D1417	I1351	R1278	M1216
V1418	V1352	T1279	M1217
I1419	W1353		D1218
K1420	K1354	I1283	LYS
V1422	R1357	I1284	ILE
R1423	M1358	L1285	VAL
Y1424	A1359	P1286	ILE
I1425	G1360	F1287	GLU
G1426	M1361	R1288	LYS
R1427	K1362	V1289	GLN
S1428	E1363	I1290	GLY
	S1364	P1291	LYS
	I1365	I1292	GLY
	I1366	V1293	THR
E1432		A1294	ALA
T1433		E1295	ASP
R1434		V1296	GLU
C1435	I1370	G1297	THR
	E1371	R1298	SER
	L1372	T1299	LYS
	L1373	K1300	SER
	P1374	L1301	GLY
	T1375	E1302	LYS
		V1303	GLN
	K1379		SER
	K1380		ILE
	M1381	I1307	ALA
	A1382		ILE
	R1383	M1310	ASP
	P1384	F1311	D1245
	P1385	K1312	C1246
	I1386		T1247
	S1387	L1316	F1248
	M1388	A1317	H1249
	M1389	Q1318	Q1250
	F1390	K1319	C1251
	E1391	I1320	V1252
	V1392	E1321	R1253
	P1393	V1322	L1254
	F1394	A1323	S1255
	A1395	I1324	LYS
	P1396	P1325	PHE
		T1326	

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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) 98.1 (49.07-3.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 3.48Å)	Xtriage
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%)	DCC
Wilson B-factor (Å ²)	107.5	Xtriage
Anisotropy	0.646	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 51407 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	16319	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.53	0/2851	0.67	0/3845
1	B	0.50	0/2756	0.66	0/3714
1	C	0.50	0/2844	0.69	2/3835 (0.1%)
1	D	0.53	1/2729 (0.0%)	0.69	2/3680 (0.1%)
1	E	0.52	0/2746	0.68	1/3701 (0.0%)
1	F	0.50	0/2764	0.67	1/3725 (0.0%)
All	All	0.51	1/16690 (0.0%)	0.68	6/22500 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	421	MET	CG-SD	5.74	1.96	1.81

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1184	LEU	CA-CB-CG	8.40	134.62	115.30
1	C	1373	LEU	CA-CB-CG	-6.66	99.99	115.30
1	F	1373	LEU	CA-CB-CG	5.83	128.72	115.30
1	C	461	TRP	O-C-N	-5.75	113.50	122.70
1	E	1170	ARG	CA-C-O	-5.20	109.17	120.10

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	2787	0	2835	277	0
1	B	2695	0	2751	260	0
1	C	2780	0	2826	279	0
1	D	2668	0	2716	272	0
1	E	2686	0	2730	264	0
1	F	2703	0	2755	278	0
All	All	16319	0	16613	1588	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 48.

The worst 5 of 1588 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%)	9	51
1	B	331/385 (86%)	284 (86%)	40 (12%)	7 (2%)	9	50
1	C	344/385 (89%)	288 (84%)	52 (15%)	4 (1%)	16	61
1	D	326/385 (85%)	279 (86%)	41 (13%)	6 (2%)	11	53
1	E	328/385 (85%)	282 (86%)	39 (12%)	7 (2%)	9	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	332/385 (86%)	289 (87%)	38 (11%)	5 (2%)	13	56
All	All	2006/2310 (87%)	1716 (86%)	254 (13%)	36 (2%)	11	53

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 ⓘ

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%)	262 (85%)	46 (15%)	4	22
1	B	298/337 (88%)	260 (87%)	38 (13%)	5	28
1	C	307/337 (91%)	275 (90%)	32 (10%)	9	39
1	D	295/337 (88%)	258 (88%)	37 (12%)	6	29
1	E	297/337 (88%)	276 (93%)	21 (7%)	18	58
1	F	299/337 (89%)	272 (91%)	27 (9%)	12	46
All	All	1804/2022 (89%)	1603 (89%)	201 (11%)	8	35

5 of 201 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1180	SER
1	C	1410	LYS
1	F	1216	MET
1	C	1207	SER
1	C	1300	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1318	GLN
1	D	1318	GLN
1	F	1250	GLN
1	D	451	ASN
1	D	465	HIS

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](#)

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, 95th 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	351/385 (91%)	0.21	1 (0%) 94 91	91, 112, 131, 141	0
1	B	339/385 (88%)	0.23	7 (2%) 67 58	103, 117, 134, 145	0
1	C	350/385 (90%)	0.27	6 (1%) 73 64	99, 119, 132, 147	0
1	D	336/385 (87%)	0.22	5 (1%) 76 67	97, 117, 129, 136	0
1	E	338/385 (87%)	0.40	13 (3%) 44 36	98, 118, 132, 141	0
1	F	340/385 (88%)	0.34	13 (3%) 44 36	100, 120, 133, 140	0
All	All	2054/2310 (88%)	0.28	45 (2%) 65 55	91, 117, 132, 147	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1181	VAL	3.7
1	C	1435	CYS	3.6
1	F	1296	VAL	3.5
1	B	1435	CYS	3.4
1	F	487	LEU	3.4

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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.