wwPDB X-ray Structure Validation Summary Report (i)

Aug 30, 2023 – 02:00 AM EDT

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

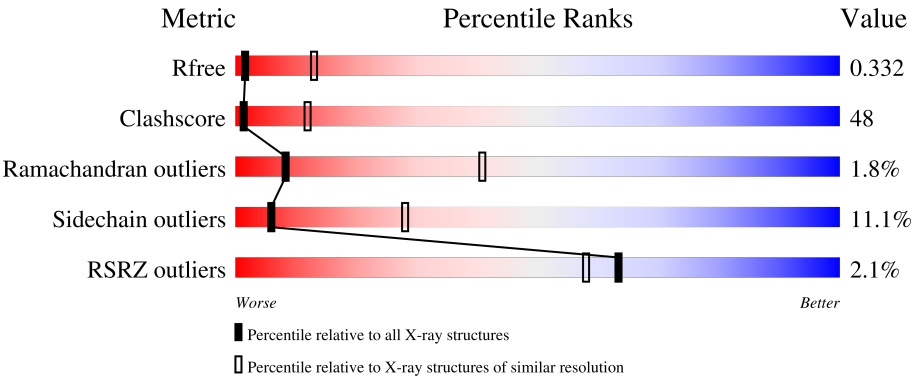
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.50 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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (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 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 <=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	36% 45% 10% 9%
1	B	385	2% 34% 46% 9% 12%
1	C	385	2% 33% 51% 6% 9%
1	D	385	% 30% 49% 8% 13%
1	E	385	3% 32% 50% 6% 12%

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Mol	Chain	Length	Quality of chain
1	F	385	3% 36% 46% 6% 12%

2 Entry composition (i)

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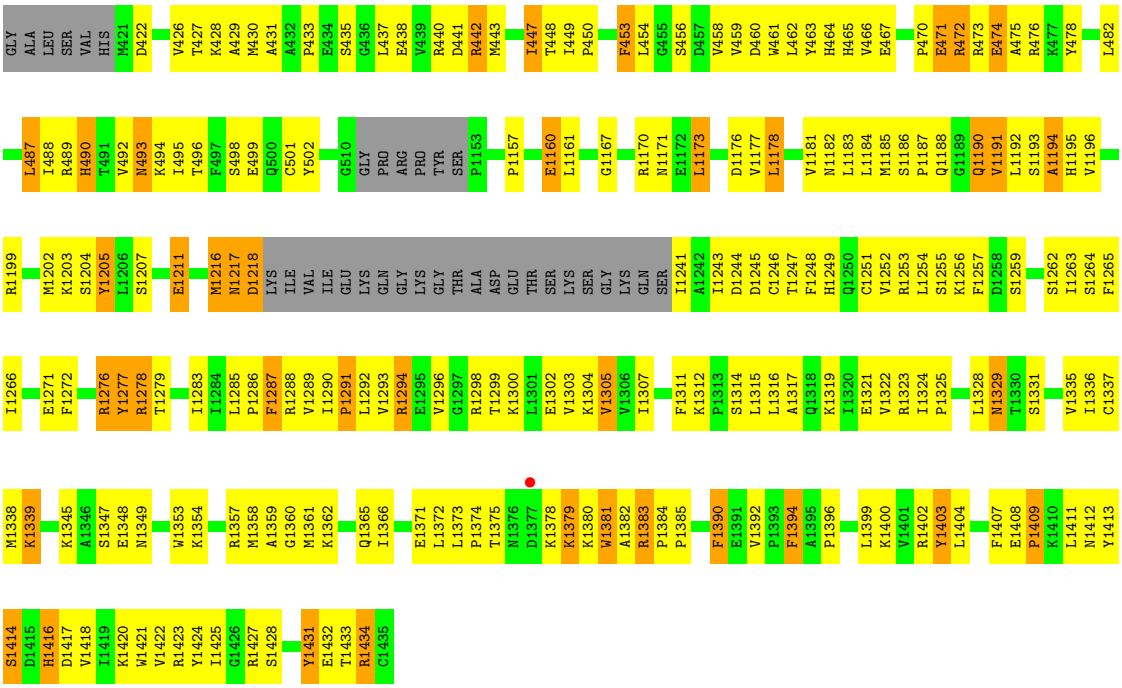
Chain	Residue	Modelled	Actual	Comment	Reference
F	1162	GLU	-	linker	UNP P84092
F	1163	PHE	-	linker	UNP P84092
F	1164	GLY	-	linker	UNP P84092
F	1165	GLY	-	linker	UNP P84092
F	1166	SER	-	linker	UNP P84092
F	1167	GLY	-	linker	UNP P84092
F	1168	GLY	-	linker	UNP P84092
F	1169	SER	-	linker	UNP P84092

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.

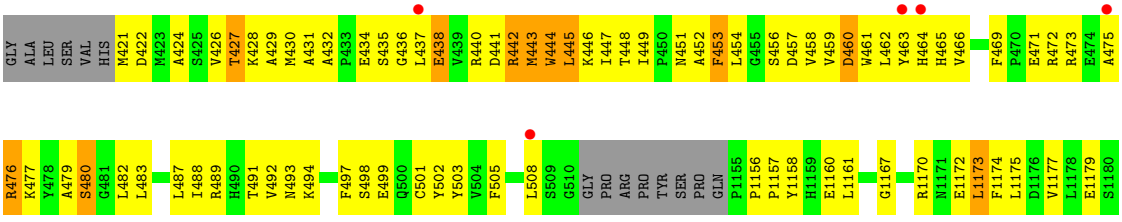
• Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu

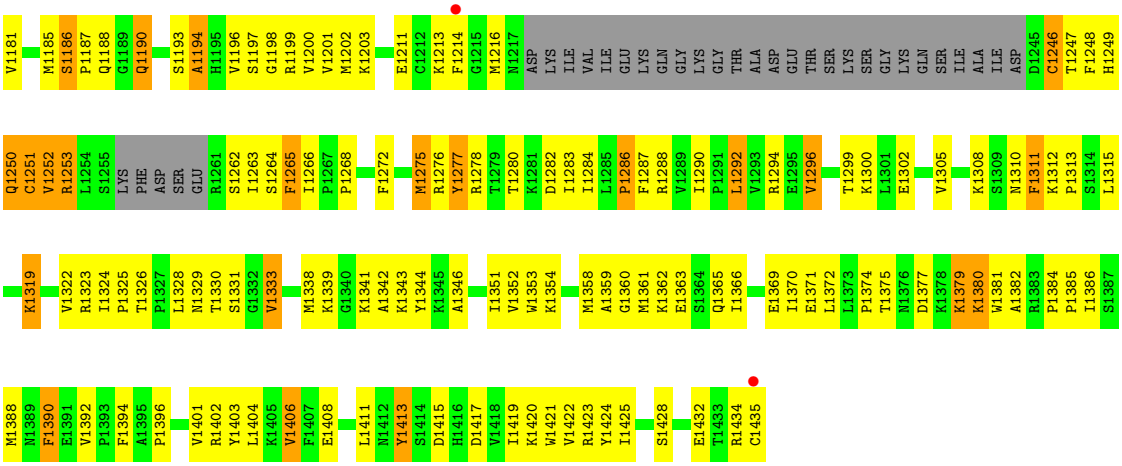
Chain A:



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

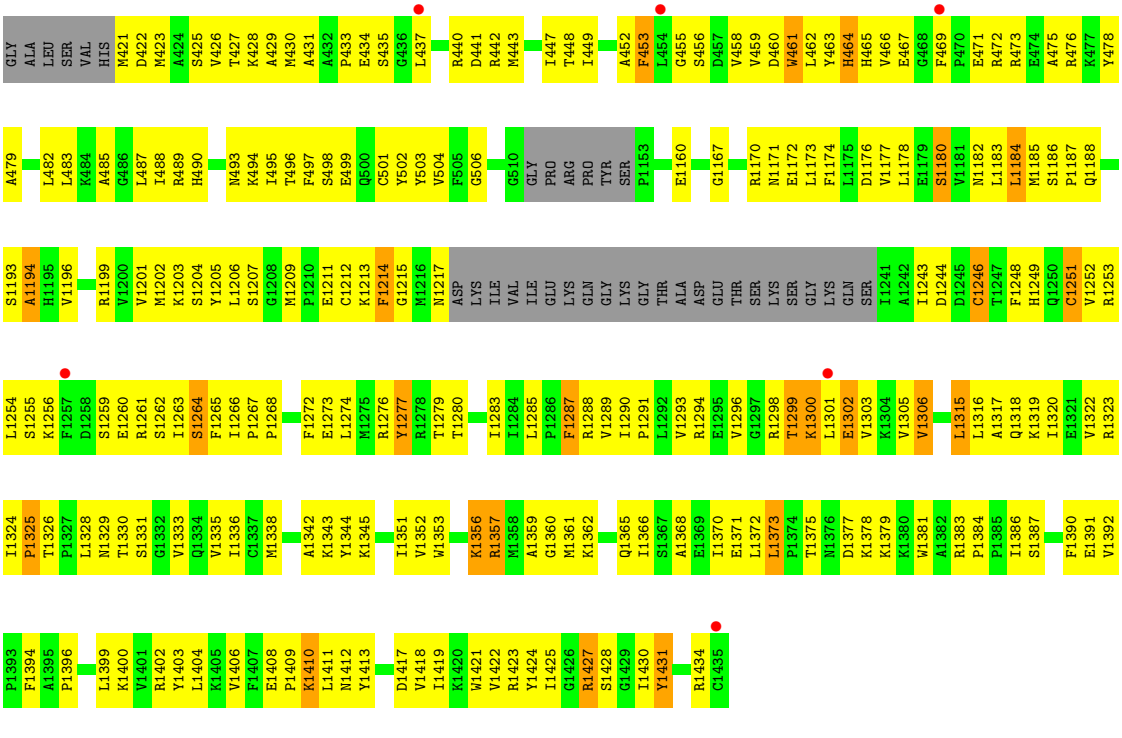
Chain B:





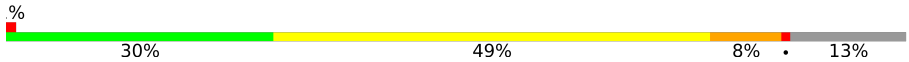
• Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu

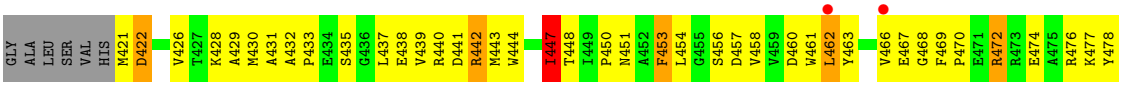
Chain C:

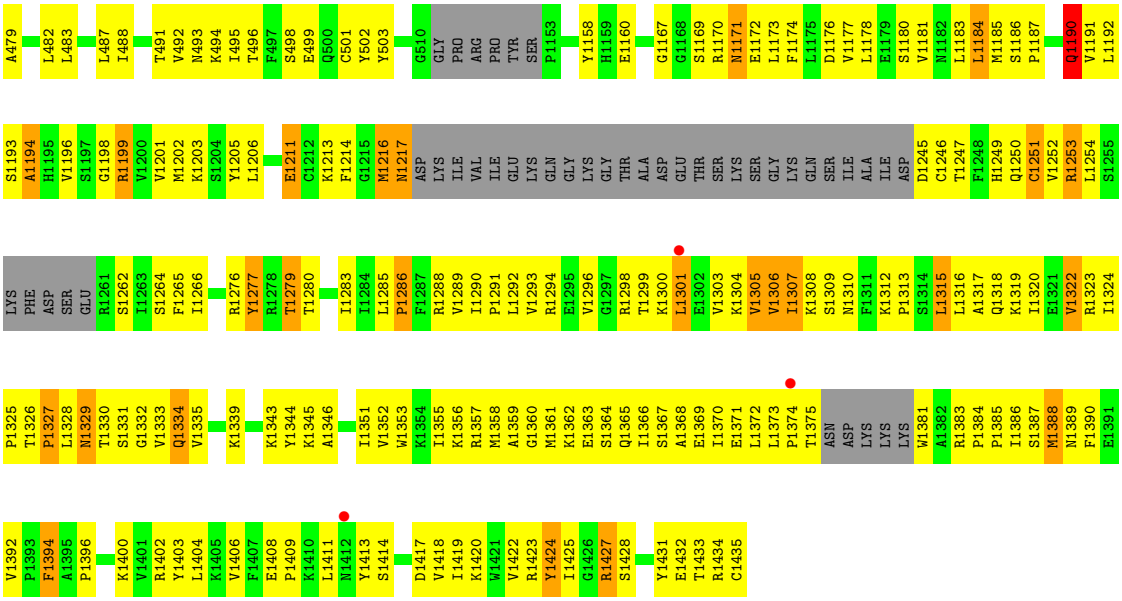


• Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu

Chain D:

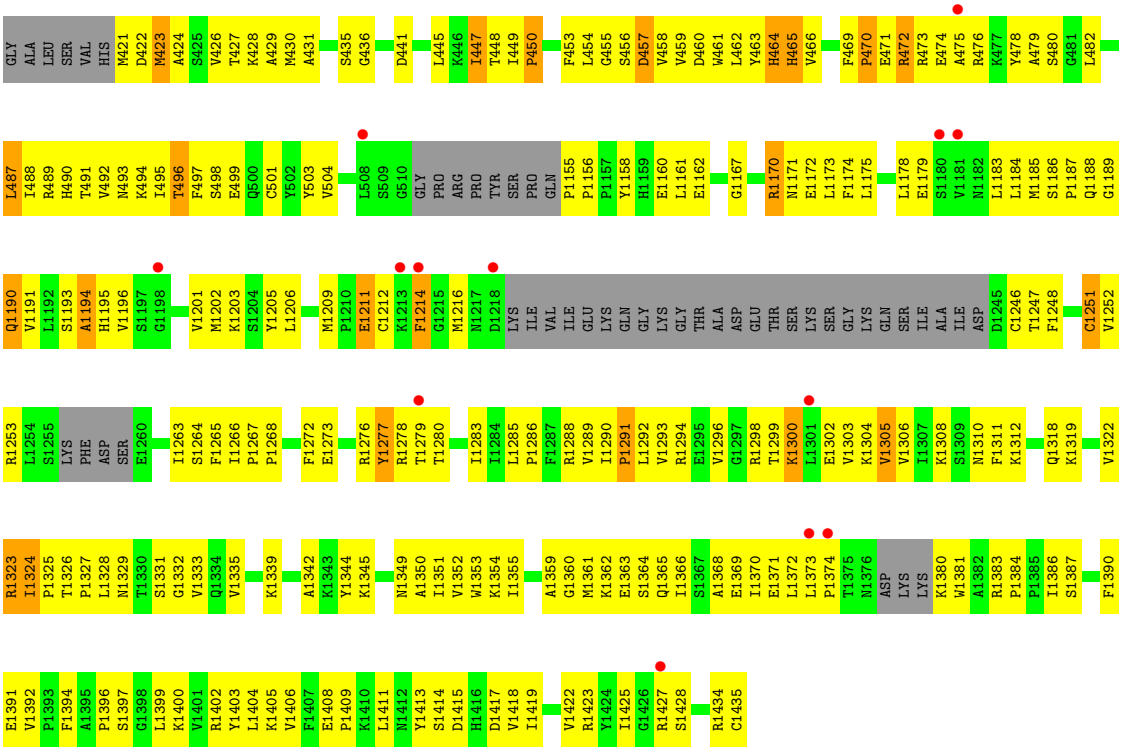






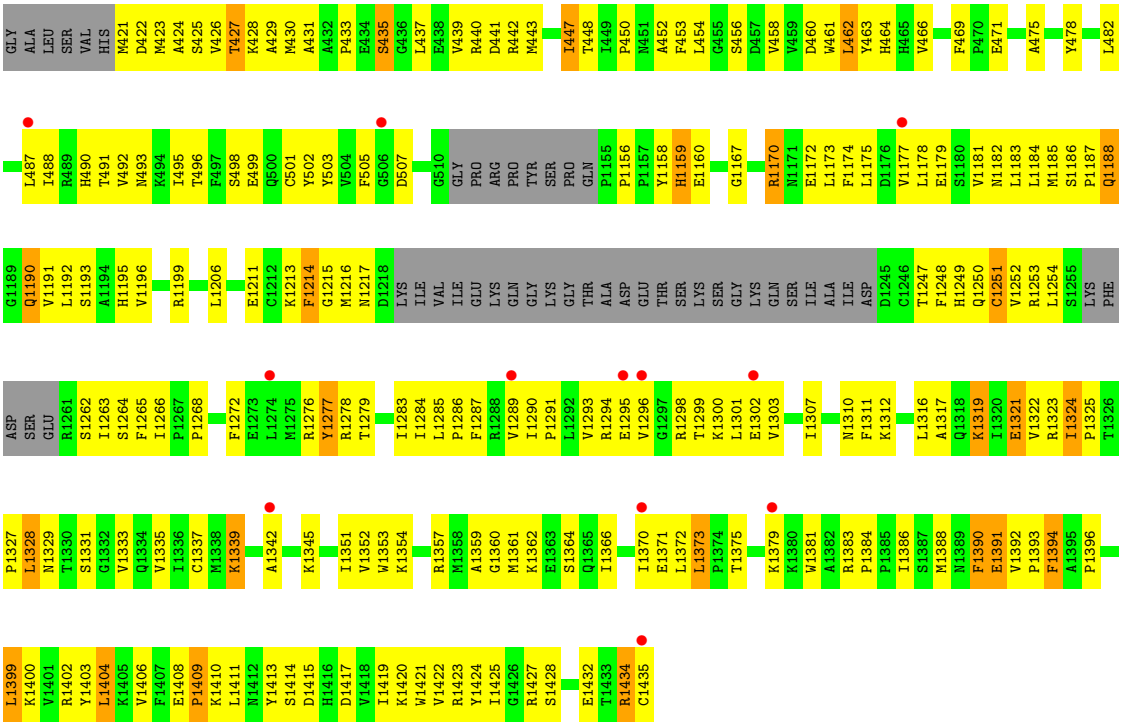
• Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu

Chain E:



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

Chain F:


GLY ALA LEU SER VAL HIS M421 D422 M423 A424 S425 V426 T427 K428 A429 M430 A431 A432 P433 E434 S435 G436 L437 E438 V439 R440 D441 R442 M443 I447 T448 I449 P450 N451 A452 F453 L454 G455 S456 D457 V458 V459 D460 W461 L462 Y463 H464 H465 V466 F469 P470 E471 A475 Y478 L482
L487 I488 R489 H490 T491 V492 N493 K494 I495 T496 F497 S498 E499 Q500 C501 Y502 Y503 V504 F505 C506 D507 C510 GLY PRO ARG PRO TYR SER PRO GLN P1155 P1156 P1157 Y1158 H1159 E1160 G1167 R1170 N1171 E1172 L1173 F1174 L1175 D1176 V1177 L1178 E1179 S1180 V1181 N1182 L1183 L1184 M1185 S1186 P1187 Q1188
G1189 Q1190 V1191 L1192 S1193 A1194 H1195 V1196 R1199 L1206 E1211 C1212 K1213 F1214 G1215 M1216 N1217 D1218 LYS ILE VAL ILE GLU LYS GLN GLY LYS GLY THR ALA ASP GLU THR SER LYS SER GLY LYS GLN SER ILE ALA ILE ASP D1245 C1246 T1247 F1248 H1249 Q1250 C1251 V1252 R1253 L1254 S1255 LYS PHE
ASP SER GLU R1261 S1262 I1263 S1264 F1265 I1266 P1267 P1268 F1272 E1273 L1274 M1275 R1276 Y1277 R1278 T1279 I1283 I1284 L1285 P1286 F1287 R1288 V1289 I1290 P1291 L1292 V1293 R1294 E1295 V1296 G1297 R1298 T1299 K1300 L1301 E1302 V1303 I1307 N1310 F1311 K1312 L1316 A1317 Q1318 K1319 I1320 E1321 V1322 R1323 I1324 P1325 T1326
P1327 L1328 N1329 T1330 S1331 G1332 V1333 Q1334 V1335 I1336 C1337 M1338 K1339 A1342 K1345 I1351 V1352 W1353 K1354 R1357 M1358 A1359 G1360 M1361 K1362 E1363 S1364 Q1365 I1366 I1370 E1371 L1372 L1373 P1374 T1375 K1379 K1380 W1381 A1382 R1383 P1384 P1385 I1386 S1387 M1388 N1389 F1390 E1391 V1392 P1393 F1394 A1395 P1396
L1399 K1400 Y1401 R1402 Y1403 L1404 K1405 V1406 F1407 E1408 P1409 K1410 L1411 N1412 Y1413 S1414 D1415 H1416 D1417 V1418 I1419 K1420 W1421 V1422 R1423 Y1424 I1425 G1426 R1427 S1428 E1432 T1433 R1434 C1435

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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%)	wwPDB-VP
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
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[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	0.53	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(^{o})	Ideal(^{o})
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%)	7 39
1	B	331/385 (86%)	284 (86%)	40 (12%)	7 (2%)	7 38
1	C	344/385 (89%)	288 (84%)	52 (15%)	4 (1%)	13 50
1	D	326/385 (85%)	279 (86%)	41 (13%)	6 (2%)	8 41
1	E	328/385 (85%)	282 (86%)	39 (12%)	7 (2%)	7 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	332/385 (86%)	289 (87%)	38 (11%)	5 (2%)	10 45
All	All	2006/2310 (87%)	1716 (86%)	254 (13%)	36 (2%)	8 41

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%)	262 (85%)	46 (15%)	3 17
1	B	298/337 (88%)	260 (87%)	38 (13%)	4 22
1	C	307/337 (91%)	275 (90%)	32 (10%)	7 31
1	D	295/337 (88%)	258 (88%)	37 (12%)	4 23
1	E	297/337 (88%)	276 (93%)	21 (7%)	14 46
1	F	299/337 (89%)	272 (91%)	27 (9%)	9 37
All	All	1804/2022 (89%)	1603 (89%)	201 (11%)	6 28

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

Mol	Chain	Res	Type
1	C	1431	TYR
1	D	1334	GLN
1	F	1404	LEU
1	D	453	PHE
1	D	1247	THR

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

Mol	Chain	Res	Type
1	F	464	HIS
1	F	1318	GLN
1	F	1159	HIS
1	F	1195	HIS
1	C	451	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 monosaccharides 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

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	351/385 (91%)	0.18	1 (0%)	94	91	91, 112, 131, 141	0
1	B	339/385 (88%)	0.20	7 (2%)	63	58	103, 117, 134, 145	0
1	C	350/385 (90%)	0.25	6 (1%)	70	64	99, 119, 132, 147	0
1	D	336/385 (87%)	0.20	5 (1%)	73	68	97, 117, 129, 136	0
1	E	338/385 (87%)	0.37	13 (3%)	40	36	98, 118, 132, 141	0
1	F	340/385 (88%)	0.32	12 (3%)	44	39	100, 120, 133, 140	0
All	All	2054/2310 (88%)	0.25	44 (2%)	63	58	91, 117, 132, 147	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1181	VAL	3.7
1	F	1296	VAL	3.5
1	F	487	LEU	3.4
1	C	1435	CYS	3.3
1	B	463	TYR	3.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.