



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 12:25 PM 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 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/ValidationPDFNotes.html>

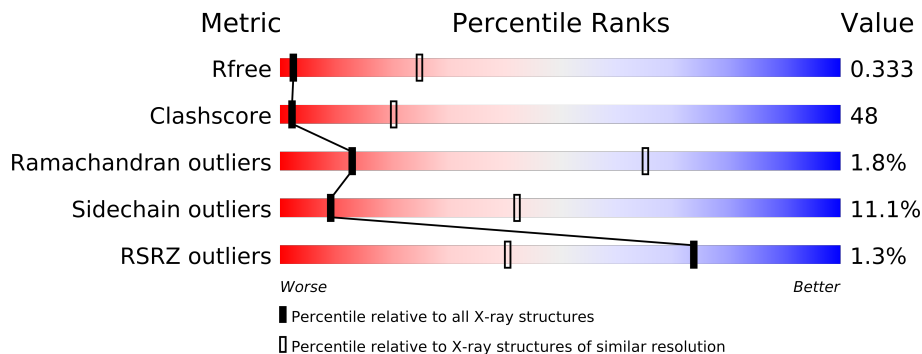
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
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 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}	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)

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.

Mol	Chain	Length	Quality of chain
1	A	385	
1	B	385	
1	C	385	
1	D	385	
1	E	385	
1	F	385	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16319 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 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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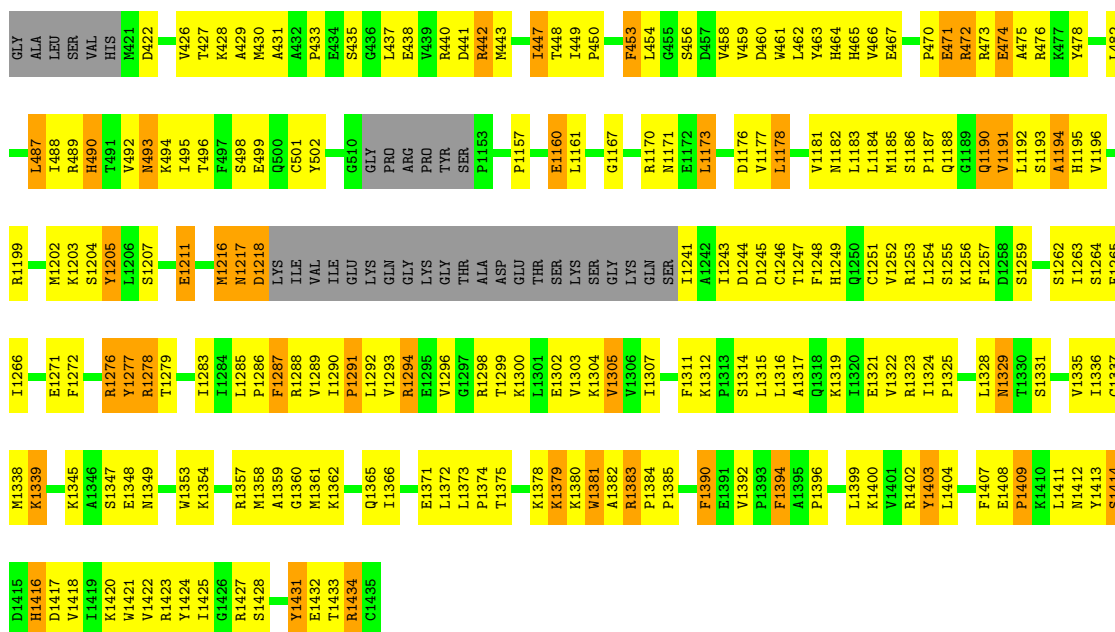
Chain	Residue	Modelled	Actual	Comment	Reference
F	1162	GLU	-	LINKER	UNP P84092
F	1163	PHE	-	LINKER	UNP P84092
F	1164	GLY	-	LINKER	UNP P84092
F	1165	GLY	-	LINKER	UNP P84092
F	1166	SER	-	LINKER	UNP P84092
F	1167	GLY	-	LINKER	UNP P84092
F	1168	GLY	-	LINKER	UNP P84092
F	1169	SER	-	LINKER	UNP P84092

3 Residue-property plots

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.

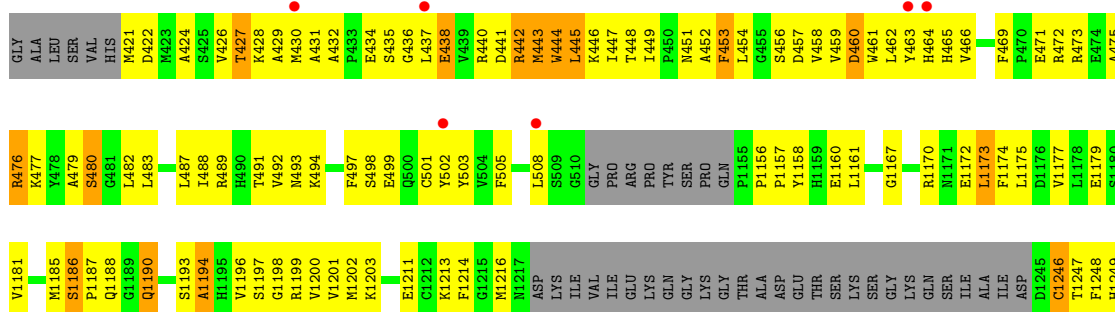
- Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu

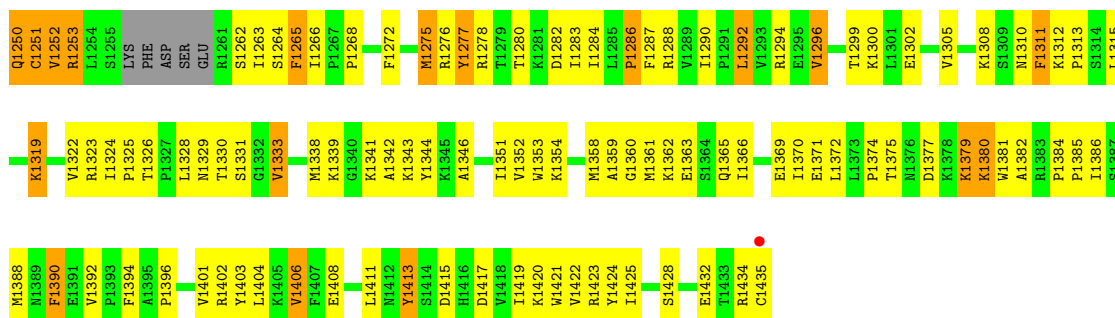
Chain A: 



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

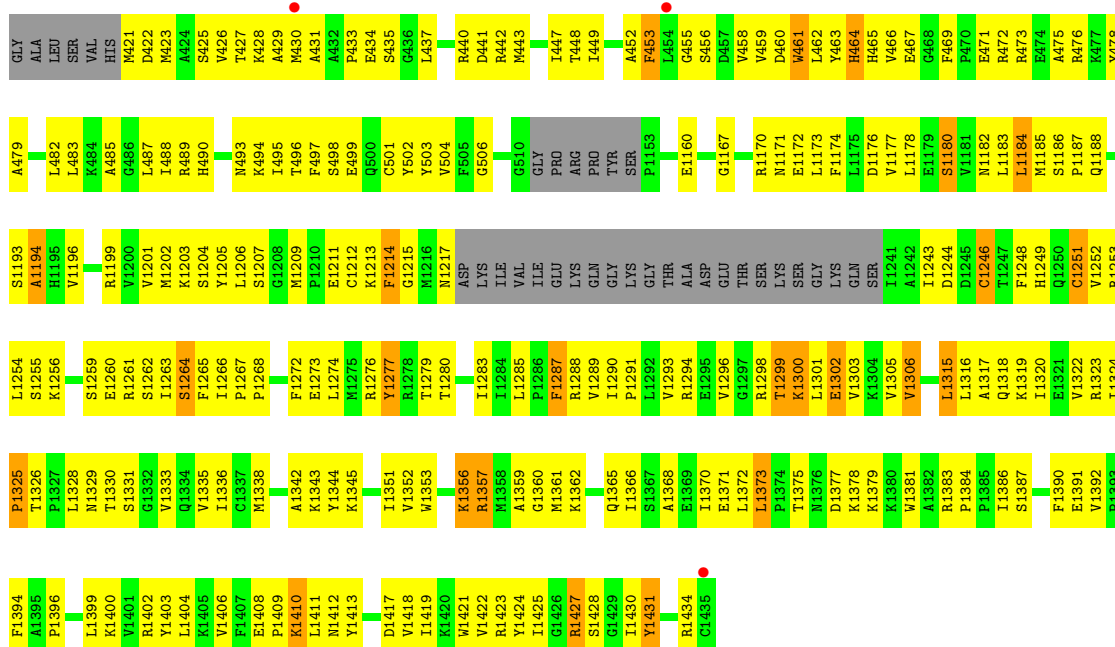
Chain B: 





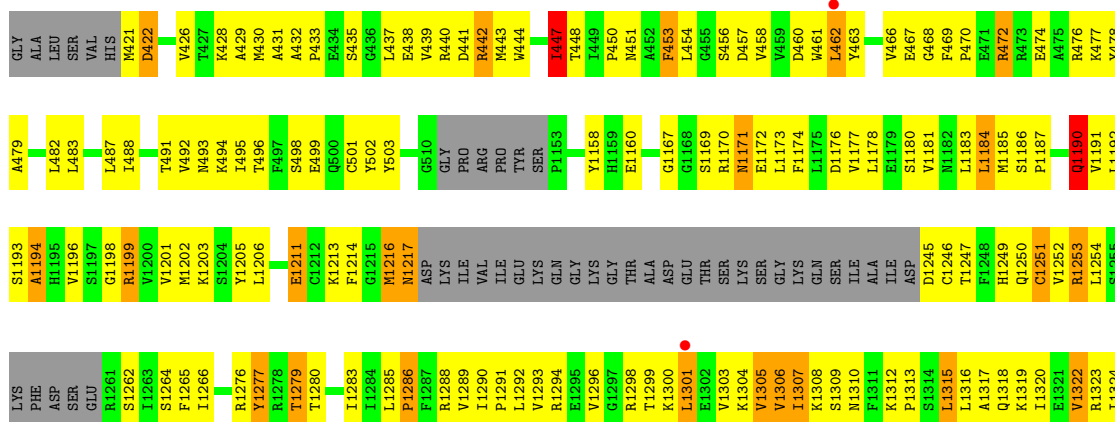
• Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu

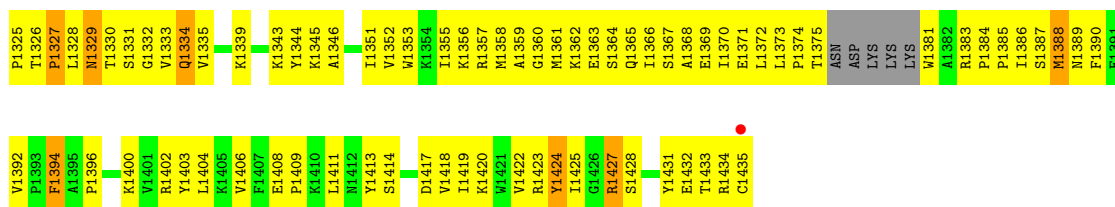
Chain C:



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

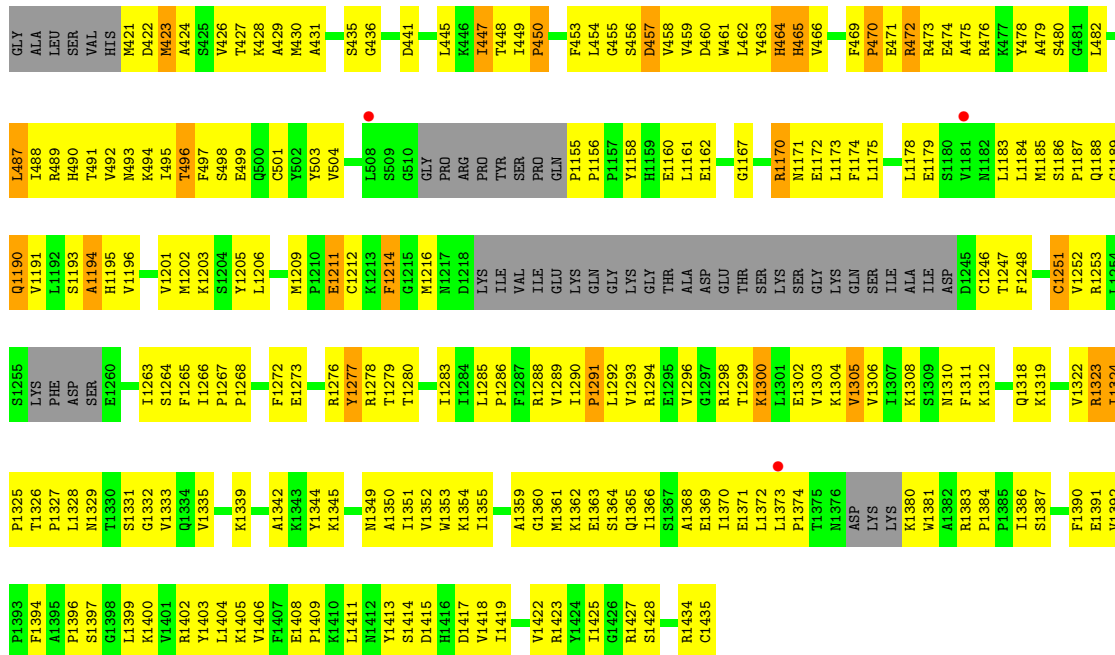
Chain D:





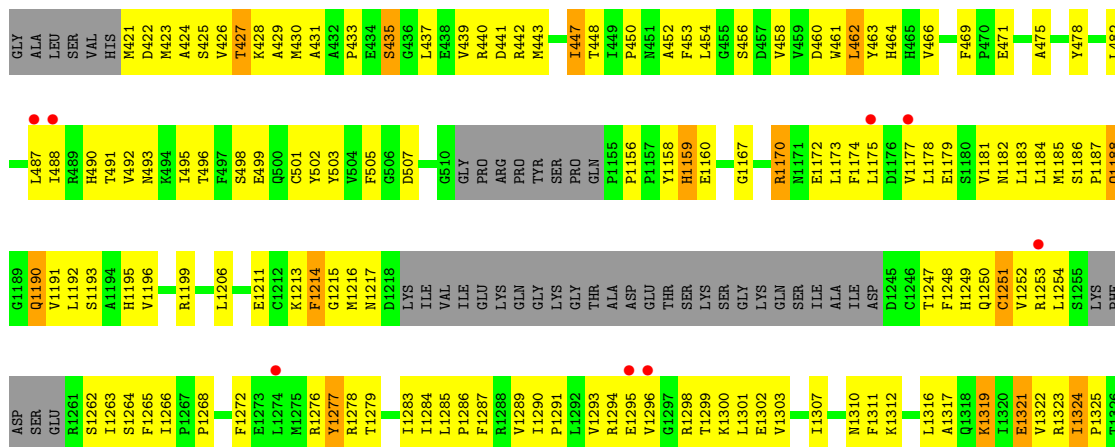
• Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu

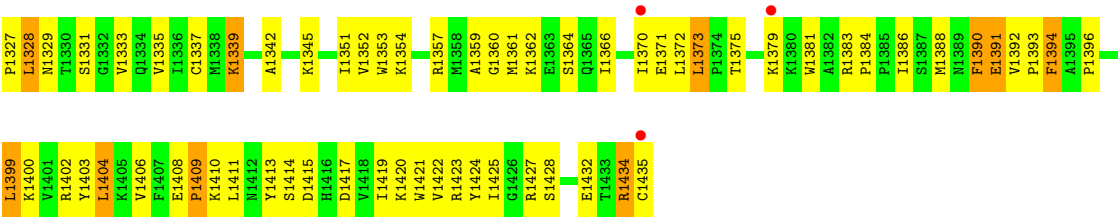
Chain E:



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

Chain F:





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 , 0.333	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 , 66.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.

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 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	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

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 48.

The worst 5 of 1588 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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	345/385 (90%)	294 (85%)	44 (13%)	7 (2%)	11	63
1	B	331/385 (86%)	284 (86%)	40 (12%)	7 (2%)	11	62
1	C	344/385 (89%)	288 (84%)	52 (15%)	4 (1%)	19	75
1	D	326/385 (85%)	279 (86%)	41 (13%)	6 (2%)	13	65
1	E	328/385 (85%)	282 (86%)	39 (12%)	7 (2%)	11	62
1	F	332/385 (86%)	289 (87%)	38 (11%)	5 (2%)	15	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2006/2310 (87%)	1716 (86%)	254 (13%)	36 (2%)	13	65

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	26
1	B	298/337 (88%)	260 (87%)	38 (13%)	6	33
1	C	307/337 (91%)	275 (90%)	32 (10%)	10	47
1	D	295/337 (88%)	258 (88%)	37 (12%)	7	35
1	E	297/337 (88%)	276 (93%)	21 (7%)	21	67
1	F	299/337 (89%)	272 (91%)	27 (9%)	14	55
All	All	1804/2022 (89%)	1603 (89%)	201 (11%)	9	42

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 ⓘ

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 ⓘ

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%)	0.32	0	100	100	91, 112, 131, 141	0
1	B	339/385 (88%)	0.36	7 (2%)	60	29	103, 117, 134, 145	0
1	C	350/385 (90%)	0.35	3 (0%)	81	51	99, 119, 132, 147	0
1	D	336/385 (87%)	0.32	3 (0%)	81	51	97, 117, 129, 136	0
1	E	338/385 (87%)	0.40	3 (0%)	81	51	98, 118, 132, 141	0
1	F	340/385 (88%)	0.42	11 (3%)	45	21	100, 120, 133, 140	0
All	All	2054/2310 (88%)	0.36	27 (1%)	74	40	91, 117, 132, 147	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1435	CYS	3.6
1	B	1435	CYS	3.1
1	F	487	LEU	3.0
1	F	1435	CYS	3.0
1	B	430	MET	2.8

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 carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.