



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 11:19 pm BST

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](mailto: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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

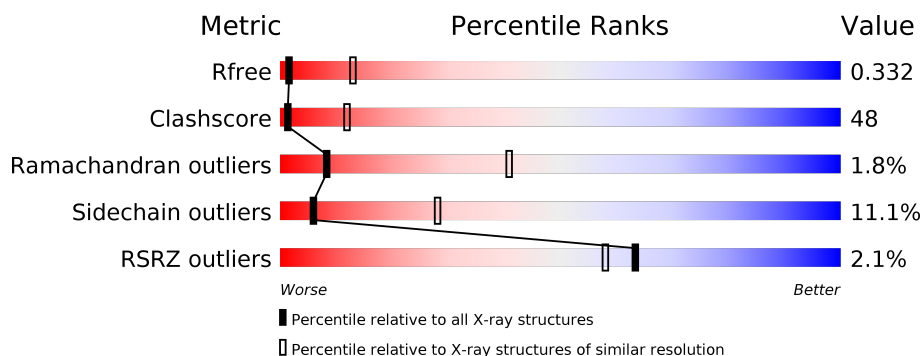
# 1 Overall quality at a glance

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))
$R_{free}$	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 on 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	<div> <div>36%</div> <div>45%</div> <div>10%</div> <div>9%</div> </div>
1	B	385	<div>2%</div> <div>34%</div> <div>46%</div> <div>9%</div> <div>12%</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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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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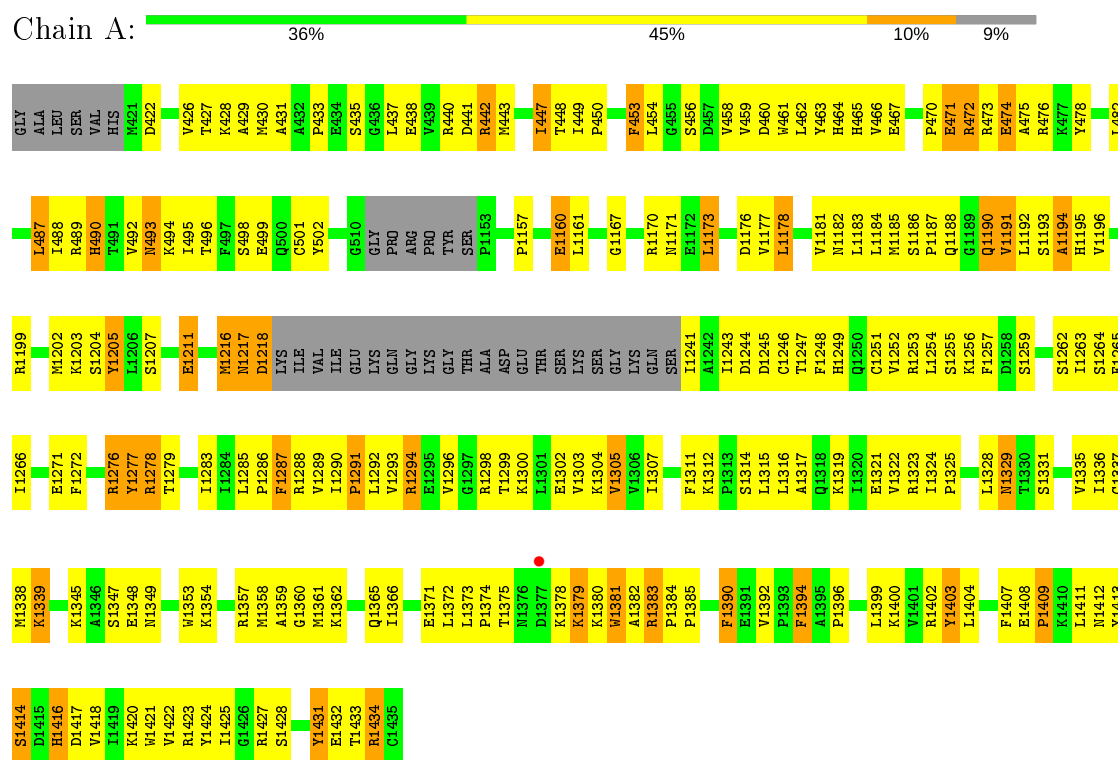
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Chain	Residue	Modelled	Actual	Comment	Reference
F	1162	GLU	-	LINKER	UNP P84092
F	1163	PHE	-	LINKER	UNP P84092
F	1164	GLY	-	LINKER	UNP P84092
F	1165	GLY	-	LINKER	UNP P84092
F	1166	SER	-	LINKER	UNP P84092
F	1167	GLY	-	LINKER	UNP P84092
F	1168	GLY	-	LINKER	UNP P84092
F	1169	SER	-	LINKER	UNP P84092

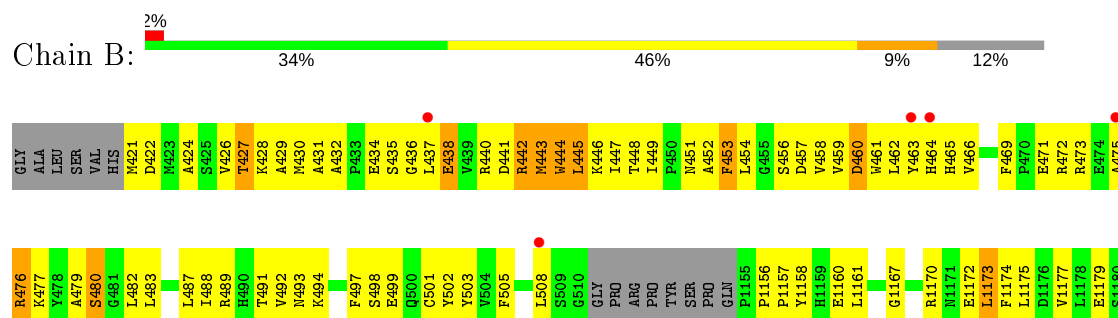
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

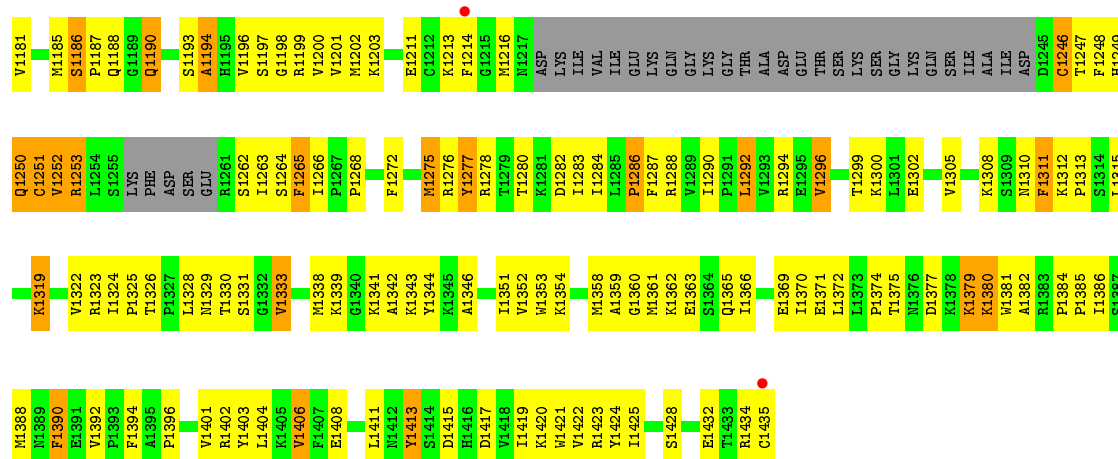
- Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu



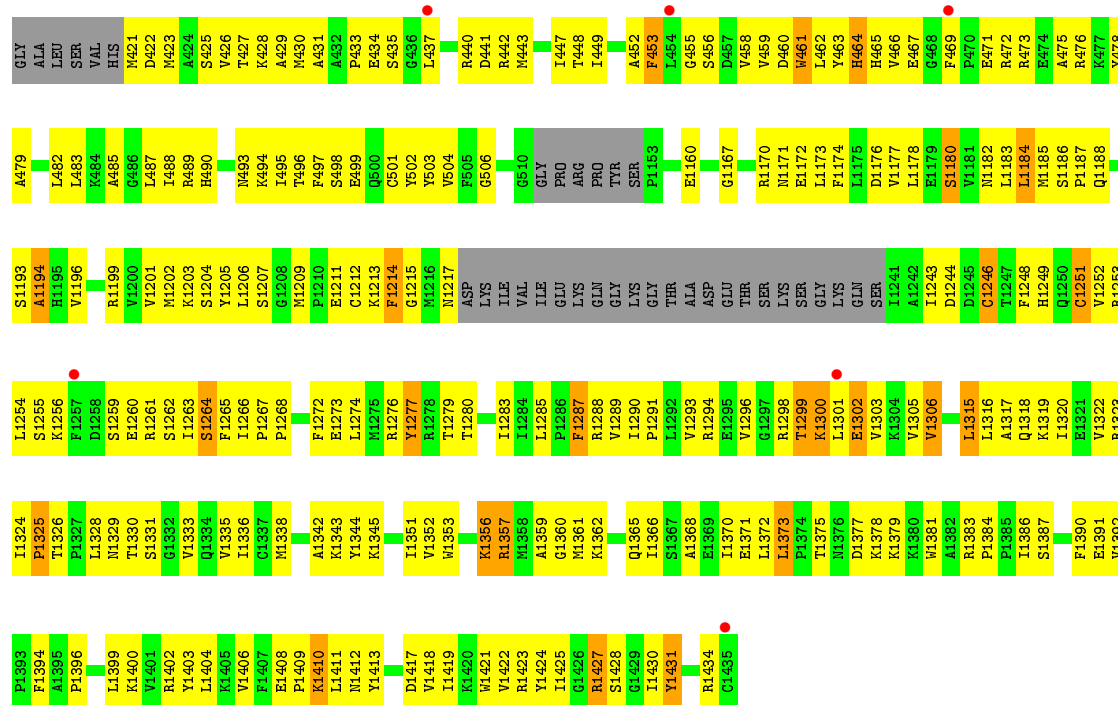
- Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu



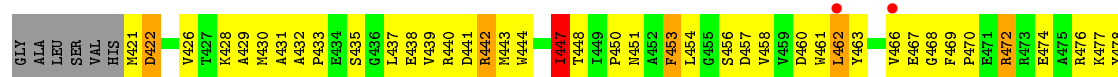




- Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu



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





L1399	L1327	ASP	G1189	L487	GLY
K1400	L1328	SER	Q1190	L488	ALA
V1401	L1329	GLU	V1191	R489	LEU
R1402	T1330	R1261	L1192	R490	SER
Y1403	S1331	I1263	S1193	T491	VAL
L1404	G1332	I1263	A1194	V492	HIS
K1405	V1333	S1264	H1195	R493	
V1406	Q1334	F1265	V1196	K494	M421
F1407	I1336	I1266		T495	D422
E1408	C1337	P1267	R1199	T496	M423
P1409	M1338	P1268	L1206	F497	A424
K1410	K1339	F1272	E1211	S498	S425
L1411	A1342	E1273	G1212	E499	V426
M1412	K1345	M1274	C1213	Q500	T427
Y1413		M1275	K1213	C501	K428
S1414		R1276	G1215	Y502	A429
D1415		Y1277	M1216	F503	M430
H1416		R1278	M1217	F504	A431
D1417		T1279	D1218	G506	A432
V1418		I1283	LYS	D507	R433
I1419		I1284	ILE	G510	E434
K1420		L1285	VAL	GLY	S435
W1421		L1286	ILE	PRO	G436
V1422		P1287	GLU	ARG	L437
R1423		R1288	LYS	PRO	E438
Y1424		G1289	GLN	THR	V439
I1425		M1290	GLY	TYR	R440
G1426		P1291	LYS	SER	D441
R1427		L1292	GLY	PRO	R442
S1428		V1293	THR	GLN	M443
		R1294	ALA	P1185	
E1432		E1295	ASP	P1186	T448
T1433		V1296	GLU	P1187	I449
R1434		G1297	THR	Y1158	N451
C1435		R1298	SER	H1159	A452
		L1372	LYS	E1160	F453
		L1373	SER		L454
		P1374	SER		G455
		T1375	GLY		S456
		K1379	LYS		D457
		K1380	GLN		V458
		W1381	SER		V459
		A1382	ILE		N1171
		R1383	ALA		E1172
		P1384	ILE		L1173
		P1385	ASP		F1174
		I1386	D1245		L1175
		S1387	G1246		Y463
		M1388	T1247		H464
		M1389	F1248		H465
		F1390	F1249		V466
		E1391	H1249		
		V1392	Q1250		F469
		P1393	V1181		P470
		F1394	C1251		E471
		A1395	V1252		
		P1396	L1183		A475
			R1253		
			L1254		
			S1255		
			LYS		Y478
			PHE		L482
					Q1188

## 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) 98.1 (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)	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 <sup>2</sup> )	107.5	Xtriage
Anisotropy	0.646	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 69.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	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 <sup>2</sup> )	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.*

<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	0.53	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 [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	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 ⓘ

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	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, 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%)	0.18	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 [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.