wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 11:49 PM EDT

PDB ID	:	5OWV
Title	:	An oligomerised bacterial dynamin pair provides a mechanism for the long-range sensing and tethering of membranes
Authors	:	Liu, J.W.; Noel, J.K.; Low, H.H.
Deposited on	:	2017-09-04
Resolution	:	3.72 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 (1)) were used in the production of this report:

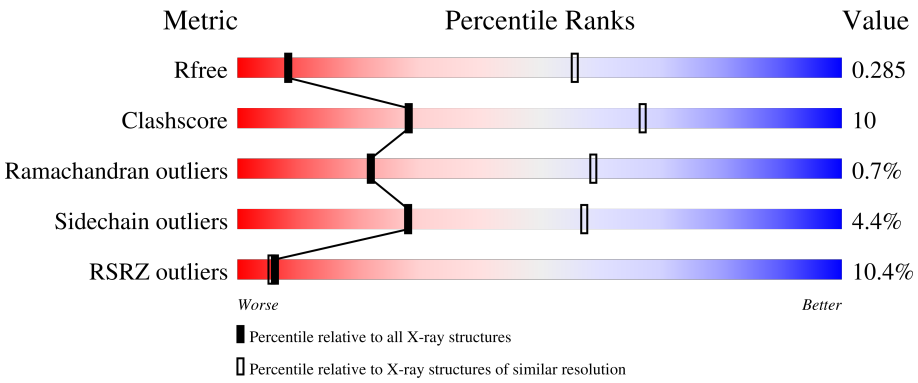
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.72 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	1089 (3.90-3.54)
Clashscore	141614	1012 (3.88-3.56)
Ramachandran outliers	138981	1114 (3.90-3.54)
Sidechain outliers	138945	1110 (3.90-3.54)
RSRZ outliers	127900	1020 (3.90-3.54)

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	732	10% 77% 18% • 5%
1	B	732	9% 65% 14% • 20%
2	C	614	10% 74% 21% • •
2	D	614	9% 68% 25% • •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 19375 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 GTP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	699	5021	3179	858	970	14	0	0	0
1	B	587	4436	2828	739	855	14	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	729	LYS	-	expression tag	UNP A0A1D9BJX7
A	730	LEU	-	expression tag	UNP A0A1D9BJX7
A	731	HIS	-	expression tag	UNP A0A1D9BJX7
A	732	HIS	-	expression tag	UNP A0A1D9BJX7
B	729	LYS	-	expression tag	UNP A0A1D9BJX7
B	730	LEU	-	expression tag	UNP A0A1D9BJX7
B	731	HIS	-	expression tag	UNP A0A1D9BJX7
B	732	HIS	-	expression tag	UNP A0A1D9BJX7

- Molecule 2 is a protein called GTP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	598	4959	3206	799	943	11	0	0	0
2	D	598	4959	3206	799	943	11	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP A0A1D9BKH6
C	-1	SER	-	expression tag	UNP A0A1D9BKH6
C	0	HIS	-	expression tag	UNP A0A1D9BKH6
C	610	HIS	-	expression tag	UNP A0A1D9BKH6

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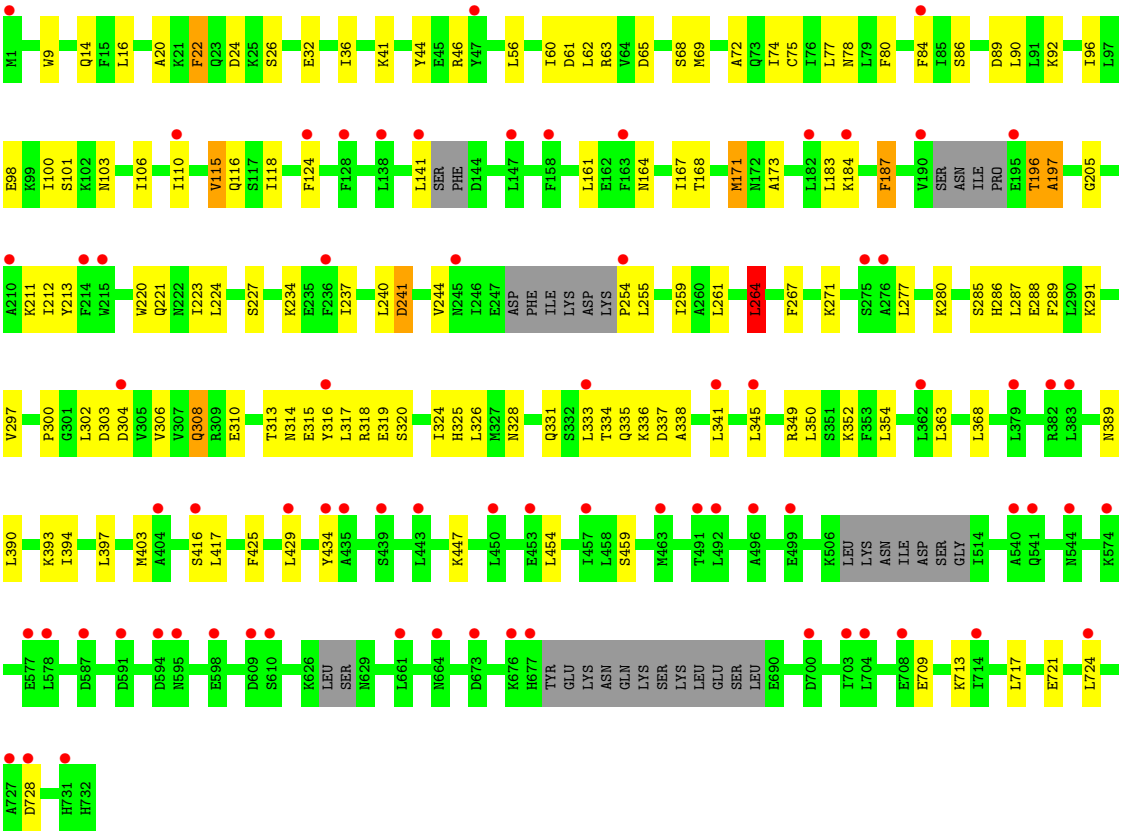
Chain	Residue	Modelled	Actual	Comment	Reference
C	611	HIS	-	expression tag	UNP A0A1D9BKH6
D	-2	GLY	-	expression tag	UNP A0A1D9BKH6
D	-1	SER	-	expression tag	UNP A0A1D9BKH6
D	0	HIS	-	expression tag	UNP A0A1D9BKH6
D	610	HIS	-	expression tag	UNP A0A1D9BKH6
D	611	HIS	-	expression tag	UNP A0A1D9BKH6

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.

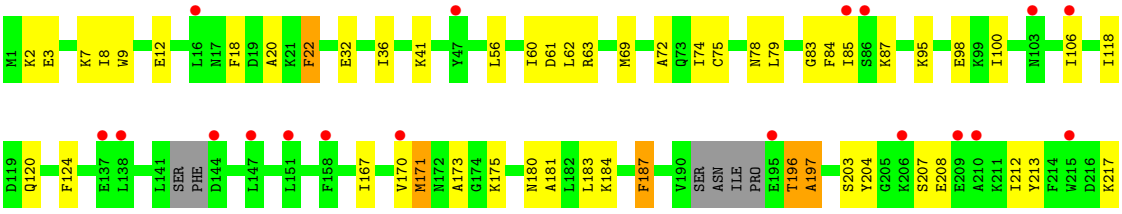
• Molecule 1: GTP-binding protein

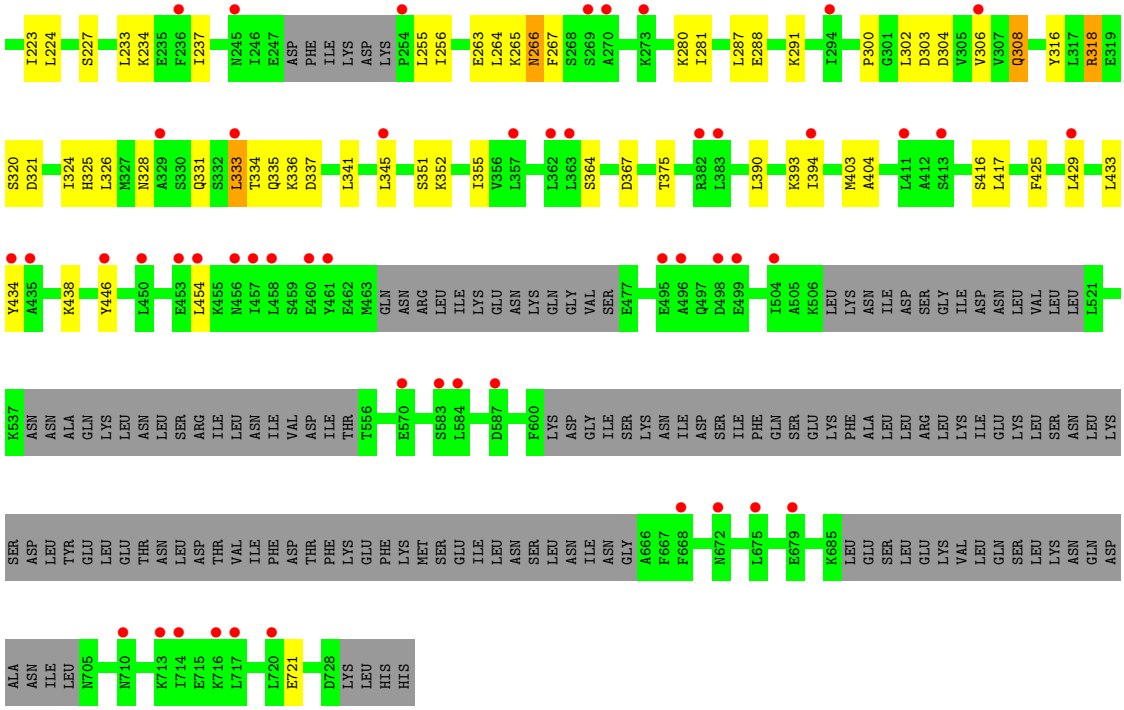
Chain A: 10% 77% 18% • 5%



• Molecule 1: GTP-binding protein

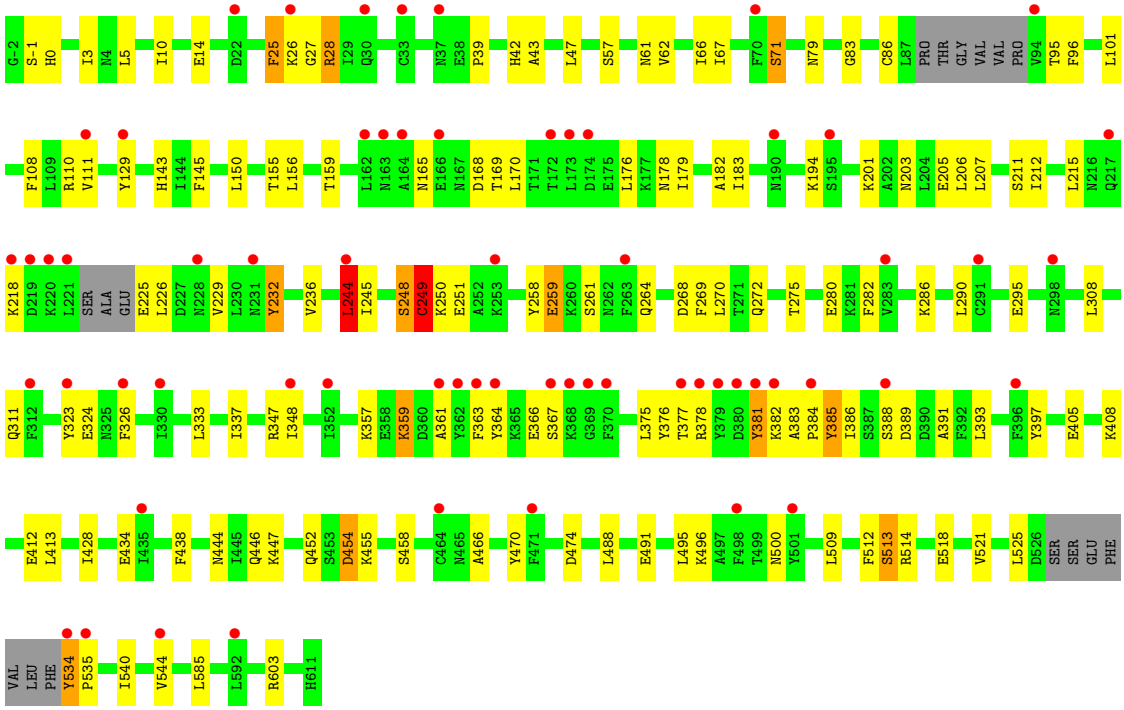
Chain B: 9% 65% 14% • 20%





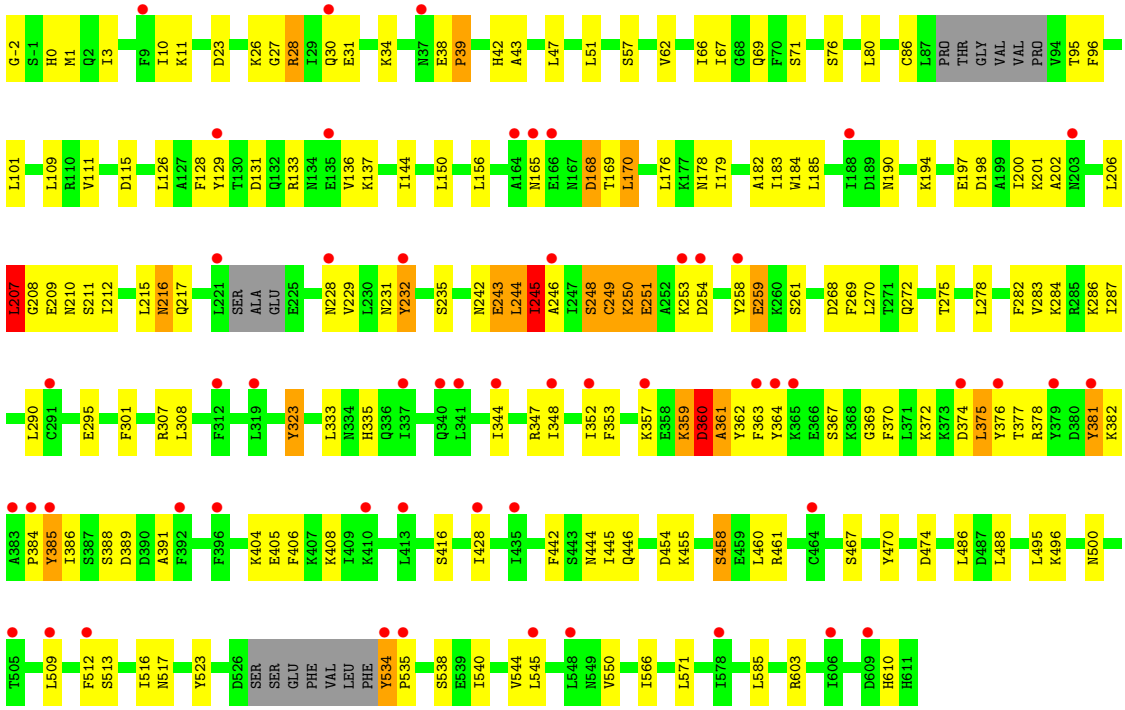
- Molecule 2: GTP-binding protein

Chain C:



- Molecule 2: GTP-binding protein

Chain D:


G-2
S-1
H0
M1
Q2
I3
F9
I10
K11
D23
K26
G27
R28
I29
Q30
E31
K34
N37
E38
P39
H42
A43
L47
L51
S57
V62
I66
I67
G68
Q69
F70
S71
S76
L80
C86
L87
PRO
THR
GLY
VAL
VAL
PRO
V94
T95
F96
L101
L109
R110
V111
D115
L126
A127
F128
Y129
T130
D131
Q132
R133
N134
E135
V136
K137
I144
L150
L156
A164
N165
E166
N167
D168
T169
L170
L176
K177
N178
I179
A182
I183
W184
L185
I188
D189
N190
K194
E197
D198
A199
I200
K201
A202
N203
L206
L207
G208
E209
N210
S211
I212
L215
N216
Q217
L221
SER
ALA
GLU
E225
N228
V229
L230
N231
Y232
S235
N242
E243
L244
I245
A246
I247
S248
C249
K250
E251
A252
K253
D254
Y258
E259
K260
S261
D268
F269
L270
T271
Q272
T275
L278
F282
V283
K284
R285
K286
I287
L290
C291
E295
F301
R307
L308
F312
L319
Y323
L333
N334
H335
Q336
I337
Q340
L341
I344
R347
I348
I352
F353
K357
E358
K359
D360
A361
Y362
F363
Y364
K365
E366
S367
K368
G369
F370
L371
K372
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T377
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K382
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I386
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D390
A391
F392
F396
K404
E405
F406
K407
K408
I409
K410
L413
S416
I428
I435
F442
S443
N444
I445
Q446
D454
K455
S458
E459
L460
R461
C464
S467
Y470
D474
L486
D487
L488
L495
K496
N500
T505
L509
F512
S513
I516
N517
Y523
D526
SER
SER
GLU
PHE
VAL
LEU
PHE
Y534
P535
S538
E539
I540
V544
L545
L548
N549
V550
I566
L571
I578
L585
R603
I606
D609
H610
H611

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	112.59Å 226.06Å 317.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	106.13 – 3.72 106.13 – 3.72	Depositor EDS
% Data completeness (in resolution range)	99.5 (106.13-3.72) 99.5 (106.13-3.72)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 3.67Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.259 , 0.286 0.258 , 0.285	Depositor DCC
R_{free} test set	4195 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	147.9	Xtriage
Anisotropy	0.583	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 202.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	19375	wwPDB-VP
Average B, all atoms (Å^2)	212.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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 (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	0.26	0/5069	0.47	1/6846 (0.0%)
1	B	0.26	0/4480	0.46	0/6024
2	C	0.29	0/5044	0.53	2/6771 (0.0%)
2	D	0.29	0/5044	0.55	1/6771 (0.0%)
All	All	0.27	0/19637	0.51	4/26412 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
2	C	0	6
2	D	0	5
All	All	0	18

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	207	LEU	CA-CB-CG	8.76	135.44	115.30
2	C	244	LEU	CA-CB-CG	-6.75	99.78	115.30
1	A	264	LEU	CB-CG-CD2	-5.71	101.29	111.00
2	C	5	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	A	196	THR	Peptide
1	A	255	LEU	Peptide
1	B	196	THR	Peptide
1	B	84	PHE	Peptide

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	5021	0	4509	86	0
1	B	4436	0	4219	73	0
2	C	4959	0	5000	103	0
2	D	4959	0	5000	134	0
All	All	19375	0	18728	375	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 10.

The worst 5 of 375 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)
2:C:364:TYR:CE1	2:D:364:TYR:CE2	2.00	1.46
2:C:364:TYR:CE1	2:D:364:TYR:CD2	2.22	1.26
2:C:364:TYR:HE1	2:D:364:TYR:CD2	1.59	1.14
1:B:263:GLU:OE2	1:B:265:LYS:NZ	1.92	1.00
2:D:202:ALA:HB3	2:D:207:LEU:HD22	1.50	0.94

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	685/732 (94%)	627 (92%)	54 (8%)	4 (1%)	25	61
1	B	569/732 (78%)	514 (90%)	53 (9%)	2 (0%)	34	69
2	C	590/614 (96%)	526 (89%)	59 (10%)	5 (1%)	19	56
2	D	590/614 (96%)	533 (90%)	50 (8%)	7 (1%)	13	48
All	All	2434/2692 (90%)	2200 (90%)	216 (9%)	18 (1%)	22	59

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	245	ILE
2	D	245	ILE
2	D	360	ASP
2	D	361	ALA
1	A	319	GLU

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	448/683 (66%)	434 (97%)	14 (3%)	40	65
1	B	440/683 (64%)	429 (98%)	11 (2%)	47	70
2	C	555/569 (98%)	529 (95%)	26 (5%)	26	56
2	D	555/569 (98%)	519 (94%)	36 (6%)	17	48
All	All	1998/2504 (80%)	1911 (96%)	87 (4%)	28	57

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	168	ASP
2	D	323	TYR
2	D	185	LEU

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Mol	Chain	Res	Type
2	D	245	ILE
2	D	370	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	ASN
2	C	311	GLN
2	D	69	GLN
2	D	216	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 (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	699/732 (95%)	0.57	74 (10%)	6	5	101, 234, 464, 550	0
1	B	587/732 (80%)	0.67	68 (11%)	4	4	100, 213, 427, 486	0
2	C	598/614 (97%)	0.76	63 (10%)	6	5	101, 165, 310, 428	0
2	D	598/614 (97%)	0.72	54 (9%)	9	7	101, 170, 307, 448	0
All	All	2482/2692 (92%)	0.67	259 (10%)	6	5	100, 191, 424, 550	0

The worst 5 of 259 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	221	LEU	9.7
2	C	368	LYS	7.4
2	C	367	SER	7.2
2	C	377	THR	6.6
1	A	591	ASP	6.4

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 monosaccharides 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.